A MORE TIMELY PROCESS FOR IDENTIFYING AND ANALYZING TRENDS OF EMERGING NOVEL PSYCHOACTIVE SUBSTANCES IN THE UNITED STATES

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ABSTRACT

Novel psychoactive substances (NPS) are synthetic drugs that pose serious public health and safety concerns as their ingestion by recreational drug users continues to cause adverse events and death. A multitude of NPS have been implicated in forensic investigations in the United States, but the identification of these emerging substances is challenging and complex, requiring advanced analytical capabilities and novel analysis workflows. The most common and effective manner for identifying NPS is by the use of mass spectrometry, while the true utility of this technology lies within non-targeted acquisition techniques.

This research sought to utilize novel drug screening technologies and customized methodologies to characterize current NPS use in high risk populations through the analysis of biological sample extracts discarded from a partnering forensic toxicology reference laboratory. Specifically, NPS detection, identification, and characterization were the primary foci to produce increased awareness and education on a national level. To accomplish these goals, two novel workflows were developed: sample mining and data mining.

A liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) assay was developed, validated, and implemented for forensic toxicology analytical testing. A SCIEX TripleTOF™ 5600+ QTOF-MS with SWATH® acquisition coupled to a Shimadzu Nexera XR UHPLC was used. Resulting data were compared against an extensive in-house library database containing more than 800 analytes. The

LC-QTOF-MS assay was applied to the re-analysis of biological sample extracts to discover emergent NPS, their metabolites, and trends in use patterns.

In total, 3,543 biological sample extracts were analyzed during this research and 21 emerging NPS were detected, some for the first time, through sample mining. Among these emerging substances were the NPS opioids: isopropyl-U-47700, 3,4-methylenedioxy-U-47700, and fluorofuranylfentanyl; the NPS opioid precursors: *N*-methyl norfentanyl and benzylfuranylfentanyl; the NPS hallucinogens: 2F-deschloroketamine, methoxy-PCP, and hydroxy-PCP; the NPS stimulants: 3,4-methylenedioxy-alpha-PHP, eutylone, and *N*-ethyl hexedrone; and the NPS benzodiazepine: flualprazolam.

With respect to trends, NPS opioid positivity declined over time during this research; however, fentanyl positivity was persistent. Heroin and 3,4-methylenedioxymethamphetamine (MDMA) positivity appeared to decline slightly, but further temporal evaluation is necessary. NPS were less likely to be found in combination with other NPS; only one NPS substance was found in 82.5% of NPS-positive samples. Fentanyl poly-drug use was common, including concurrent or proximate use with traditional opioids (42.8%), NPS opioids (27.3%), cocaine (26.4%), methamphetamine (13.1%), NPS stimulants (4.2%), and other substances.

The evaluation of *in vitro* metabolism for five emerging NPS detected for the first time during this research (3,4-methylenedioxy-U-47700, *ortho*-fluorofuranylfentanyl, 2F-deschloroketamine, eutylone, and *N*-ethyl hexedrone) resulted in the characterization of major metabolic pathways and the identification of metabolites presence *in vivo* by data mining of extract datafiles. These major metabolites provide utility for forensic

laboratories to prolong detection windows for NPS. The primary metabolite identified for 3,4-methylenedioxy-U-47700 was *N*-demethyl-3,4-methylenedioxy-U-47700; the primary metabolite identified for *ortho*-fluorofuranylfentanyl was fluoro-4-ANPP; the primary metabolite identified for 2F-deschloroketamine was 2F-deschloro-norketamine; and the primary metabolites identified for eutylone and *N*-ethyl hexedrone were products of hydrogenation to the beta-ketone.

As shown through this research, NPS continue to appear in forensic toxicology casework and novel assays for their detection and characterization are critical to remaining at the forefront of emerging drug trends and recreational drug use. LC-QTOF-MS was a vital piece of the analytical puzzle for discovering and characterizing emerging NPS and their metabolites. Analytical chemists must continue research involving NPS to broaden our understanding of synthetic drugs and their public health and safety impacts.

ACKNOWLEDGMENTS

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CHAPTER 1

INTRODUCTION

Analytical chemistry is a widely diverse field that houses several chemistry-related professions and applications. These fields are often linked by the techniques and instrumentation utilized to answer complex scientific questions. This applies directly to the field to toxicology and its sub-field forensic toxicology. Toxicology is the study of toxins and their interactions on living organisms, overlapping areas of chemistry, pharmacology, biology, and medicine.[1] Toxins can be everyday compounds or chemicals that humans and animal encounter, but also include xenobiotics, or foreign substances. Drugs, whether therapeutic, abused, or newly synthetized, are classical toxins that fall under the study of toxicology. Drugs of abuse and emerging drug threats more specifically fall under the field of forensic toxicology, as these substances are often linked to crimes or aspects of the law.

Drug-related crimes and fatalities continue to occur in the United States, manifesting in forensic toxicology casework. There are three basic areas of forensic toxicology: post-mortem (or medicolegal death investigation), human performance (or drug-impaired performance, including driving), and drug monitoring (including workplace drug testing).[1,2] While the most commonly encountered areas of forensic toxicology involve drug impairment or workplace drug screening, the third area involving post-mortem investigations can often be the most intricate and multifaceted. Post-mortem forensic toxicology investigations rely heavily on analytical chemistry to determine

toxins, or drugs, present at the time of death. Typical analytical chemistry workflows in modern forensic toxicology use chromatography as a means of separation and mass spectrometry as a means of drug detection.

Through the modernization of technology and science, mass spectrometry has emerged as a vital tool for the characterization of organic compounds (e.g. drugs). Mass spectrometry has become the gold standard in forensic toxicology, and it has high usefulness in determining presence of drugs in biological samples with increased specificity and sensitivity over other analytical techniques. Mass spectrometry does possess limitations with respect to drug identifications, but these limitations can often be remedied or offset during analysis.

As with the modernization of analytical chemistry, there has been an advancement in the complexity of abused drugs. Traditional drugs of abuse, such as heroin, cocaine, and methamphetamine, have remained chemically unchanged over the years, but adaptations of these chemical compounds have emerged. Newly emerging drugs of abuse are classified as "novel (or new) psychoactive substances" (NPS). These substances are chemical modifications to previously characterized drug structures or are newly synthesized drug species designed to act on the same endogenous receptor systems as traditional drugs of abuse. The term "psychoactive" was originally used to denote this activation of endogenous receptor systems, but the current use of the term NPS can include inactive emerging drug species due to limited information regarding psycho-activity and human toxicity.

1.1 Novel Psychoactive Substances (NPS)

Known commonly as synthetic drugs, designer drugs, research chemicals, club drugs, or legal highs, NPS provide special challenges to analytical chemists, forensic toxicologists, drug chemists, and public health and law enforcement agencies. The term designer drug was originally used to characterize heroin-like derivatives, such as fentanyl, but gained circulation with the increased popularity of ecstasy.[3] Since that time in the early 1980s, hundreds of NPS have been synthesized and introduced into drug markets nationally and internationally.[4,5] Synthesis of NPS has been facilitated by pharmaceutical companies researching new drugs for therapeutic value, but these drugs have been pirated from medical journals, scientific literature, or patent filings to be clandestinely manufactured for illicit use.[6] Often the motivation in producing these novel substances is in an attempt to circumvent drug laws or government scheduling.[7] While there is a growing body of literature on NPS, the ever-changing markets and continual introduction of novel compounds makes the need for research focused on rapid identification of novel substances using emerging analytical technologies a critical task.

NPS have been legally defined by the Council of the European Union (EU) as "a new narcotic or psychotropic drug, in pure form or in a preparation, that is not scheduled under the Single Convention on Narcotic Drugs of 1961 or the Convention on Psychotropic Substances of 1971, but which may pose a public health threat comparable to that posed by substances listed in those conventions."[8] However, the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA), an agency under the EU, has made it explicit in its operating guidelines of the European Early Warning System

(EWS) that the term ‘new’ or ‘novel’ does not refer to newly invented, but rather newly misused substances.[9]

There are several classes and subclasses of drugs considered to be NPS, most commonly defined by structure, function, and pharmacological effects. Common classes include stimulants, opioids, benzodiazepines, cannabinoids, and hallucinogens,[10] with distinction from common drugs of abuse by the terms novel (e.g. novel opioids), synthetic (e.g. synthetic stimulants, synthetic cannabinoids), and/or designer (e.g. designer benzodiazepines). Classification as an NPS typically constitutes chemical modifications of previously developed and identified NPS or drugs of abuse.[11] These chemical modifications are preformed to alter pharmacological activity and desired effects.[11] Additionally, chemical modifications to manufacture NPS are derived to produce “legal highs” and circumvent legislation.[12,13]

Recent literature searches or discussions within forensic science, public health, and/or public safety communities will bring to light the recent expansion of interest and challenges regarding identification of NPS, but this only makes up a fraction of the overarching problem. Research on NPS continues to increase with publications on toxicological determination,[14–20] metabolite identification,[21–25] pharmacological characterizations,[26–29] and adverse event reporting.[10,30,31] While this research is imperative to forensic science and forensic toxicology, it does not address the challenges scientists routinely face in terms of timely identification of emerging NPS and inclusion of these emerging drugs into analytical scope(s) of testing. In addition, many forensic

results and findings are often unpublished or published after great lengths in time compared to the date of NPS emergence or period of prevalence.

1.2 Drug Testing for Novel Psychoactive Substances

There are several analytical methods utilized for NPS identification. Gas chromatography mass spectrometry (GC-MS) is the historically prevalent and currently most widely available analytical platform for identification, based on laboratory surveys.[32] GC-MS is a useful screening tool, as non-targeted methods align with mass spectrometer scanning acquisition and well-developed library databases for searching.[33] Liquid chromatography tandem mass spectrometry (LC-MS/MS) is more commonly used for quantitation and confirmation of NPS, as LC-MS/MS methods are specifically targeted, lacking well defined non-targeted capabilities.[34] Liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) is a state-of-the-art analytical platform that utilizes high resolution mass acquisition capability with well-developed and defined screening techniques.[35] LC-QTOF-MS high resolution mass acquisition allows for more specific correlation between data acquired and sample chemistry, adding increased identification power when interrogating known or unknown substances. The main advantage to high resolution mass acquisition is the capability of identifying unknown compounds through accurate mass formula elucidation.[35] By recording the accurate mass of all compounds during analysis, molecular formulae can be determined and, with additional acquisition of accurate mass fragment ions, information about structure can be determined. Depending on the LC-QTOF-MS platform, high

resolution accurate mass library database searching can be performed, at the time of processing (real-time) or any time thereafter (retrospectively). This research specifically focused on exploiting the utility of LC-QTOF-MS.

Following acquisition via LC-QTOF-MS, data processing can be performed in two ways: targeted and non-targeted.[36,37] Targeted data processing utilizes a mass list and/or library database for positive analyte identification based on predetermined criteria. These criteria often include mass error, retention time error, isotope difference/score, and library score. In order for a substance to be positively identified in a sample, it must be incorporated into the processing database(s) and meet all processing criteria, otherwise no identification is made. Targeted data processing is frequently used in routine laboratory testing, as it provides a quick and relatively comprehensive analysis of the data acquired. Non-targeted data processing is often much more ambiguous and variable from laboratory to laboratory and analyst to analyst, largely due to software design and capabilities. Non-targeted data processing is more time and labor intensive, but useful for NPS and drugs of abuse screening.[38–40]

Drug testing by LC-QTOF-MS is a relatively new approach to broad-based drug screening in forensic toxicology laboratories; however, it has proven to be a successful technique for the identification of drugs of abuse[41–43] and NPS.[38–40] Analysis via LC-QTOF-MS can utilize non-targeted data acquisition modes that allow for acquisition of data pertaining to all compounds or analytes within a chromatographic run, regardless of method parameters.[44–46] In this case, non-targeted mass acquisition is designed with parameters favorable to several, if not all, drug categories or classes within a scope of

analysis. Sample separation is often performed using generic gradient conditions, allowing the method to be amenable to differing drug chemistries (e.g. polar vs. non-polar species). Mass spectrometer sample introduction coupled with liquid chromatography is most commonly achieved using positive electrospray ionization, a technique amenable to an array of small molecules (e.g. drugs of abuse, pharmaceutical compounds, NPS, etc.).[47] Mass spectrometer acquisition can be designed to acquire all ions in a scanning cycle, with staggered acquisition of fragment ions for increased specificity (e.g. SWATH® acquisition).[44–46]

1.3 Research Overview

1.3.1 Hypotheses

The scope of this research was to utilize drug screening technologies and methodologies to characterize current NPS use in high risk populations using biological sample extracts discarded from a partnering forensic toxicology reference laboratory. It was proposed that under this model, NPS detection, identification, and characterization could be performed and disseminated within a short time frame for increased awareness and education on the national level. It was hypothesized that from a pharmacoepidemiological point of view, emerging NPS would be identified and classified more closely in time to emergence using a newly developed approach. Furthermore, using the developed model, it was hypothesized that it would be possible to identify candidate NPS metabolites in cases where the parent drug was identified.

1.3.2 Purpose, Goals, and Objectives

The purpose of this research was to demonstrate that LC-QTOF-MS is an accurate and reliable method for identifying NPS and drugs of abuse, and that certain populations are a rich source for identifying emerging substances. This research specifically focused on the monitoring and emergence of NPS through five objectives:

1. Development and validation of an LC-QTOF-MS method for the detection of NPS.
2. Generation and optimization of in-house databases for identification and verification of the most current NPS with continual updates based on recent literature, online forums, newly available certified reference materials, and other emerging NPS identifications.
3. Analysis and rigorous processing and reprocessing of datafiles from authentic forensic casework samples where NPS use is suspected to enhance identification of emerging NPS, including known and currently unknown substances.
4. Data compilation and characterization of NPS emergence and prevalence with timely dissemination of results to law enforcement, emergency medicine, and laboratory personnel, using existing state and national early warning systems.
5. Metabolic profile determination of emerging NPS to discover metabolic species indicative of NPS use, prolonging detection windows and providing insight into potentially active and/or interacting biological transformation products.

Based on these five objectives, the completion of this research was designed to address a large area of need in the forensic science community and beyond: timely, accurate, and precise NPS identifications and trend analyses.

CHAPTER 2

REVIEW OF LITERATURE

2.1 Novel Psychoactive Substances in the United States

The recent emergence and proliferation of NPS in the United States began around 2008 with the discovery of synthetic cannabinoids in seized botanical materials.[48] Although this time point is generally recognized among the forensic science community as the beginning of the current wave of NPS, the introduction of synthetically modified drugs truly dates back to the 1970s and 1980s when synthetic drugs such as 3,4-methylenedioxymethamphetamine (MDMA) and alpha-methylfentanyl became popular or were implicated in drug user deaths, respectively.[49,50] Based on the current definition of NPS, these synthetic drugs, modified based on the structure and activity of methamphetamine (stimulant) and fentanyl (opioid), would meet the criteria for classification as current NPS; however, more historical substances like these are often considered traditional drugs of abuse at this point.

Throughout this chapter, the terms "synthetic" and "NPS" will be used universally and interchangeably to denote specific sub-classifications of NPS. These terms were primarily chosen for consistency and clarity purposes. Each term will be used based on the context of the content, as well as in accordance with industry standards. One may note that the terms "designer" and "novel" are equivalent to the terms "synthetic" and "NPS" used herein. In addition, it is important to note that several of these classes are inherently "synthetic" and, therefore, the term is used only to describe drugs that can be

classified as NPS. In all remaining chapters, the adjective "NPS" will be used universally to denote specific sub-classification of NPS (e.g. NPS stimulants, NPS opioids, etc.).

The first expansion of NPS within the United States began with the initial identifications of the first synthetic cannabinoids, specifically HU-210 and JWH-018 (Figures 1 and 2).[51–61] These synthetic drugs are named after their creators (e.g. Hebrew University and John W. Hoffman) and numbered based on their timepoint in synthetic discovery. When discovered in illicit drug supplies in 2008, this led scientists to believe their identity had be pirated from the patent literature by clandestine chemists, a phenomenon that has plagued the NPS landscape ever since. Subsequently, the turnover of synthetic cannabinoids by year is apparent in data publish by the Drug Enforcement Administration (DEA),[51–61] as scientists now classify these waves of new synthetic cannabinoids as "generations." Since 2008, the structural diversity of synthetic cannabinoids has grown, but simple classifications are still possible due to noticeable head, core, and tail regions, as these features are inherent to activity and efficacy.[62]

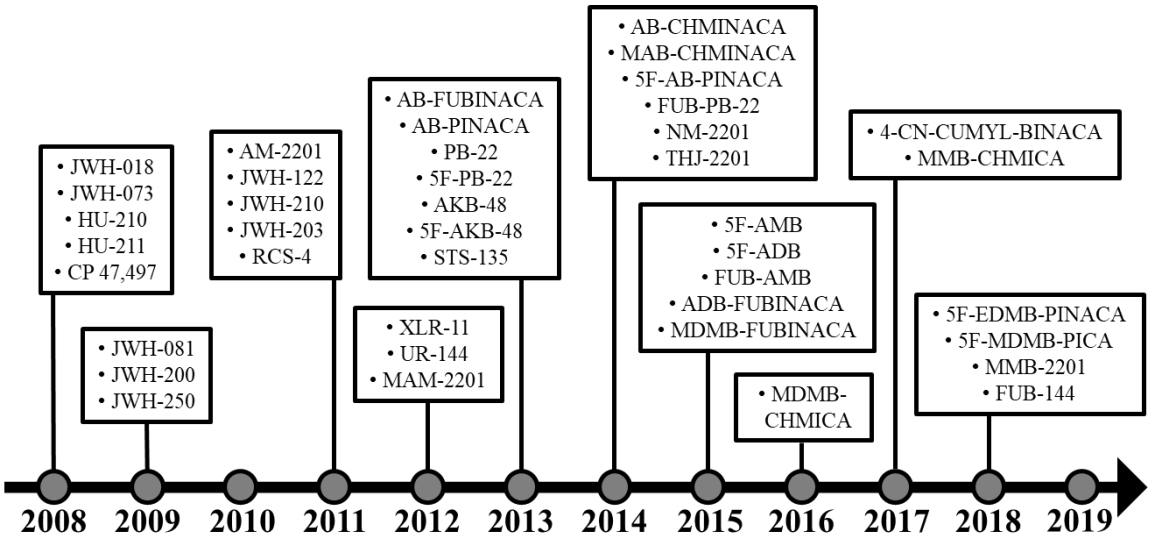


Figure 1: Emergence of synthetic cannabinoids in the United States

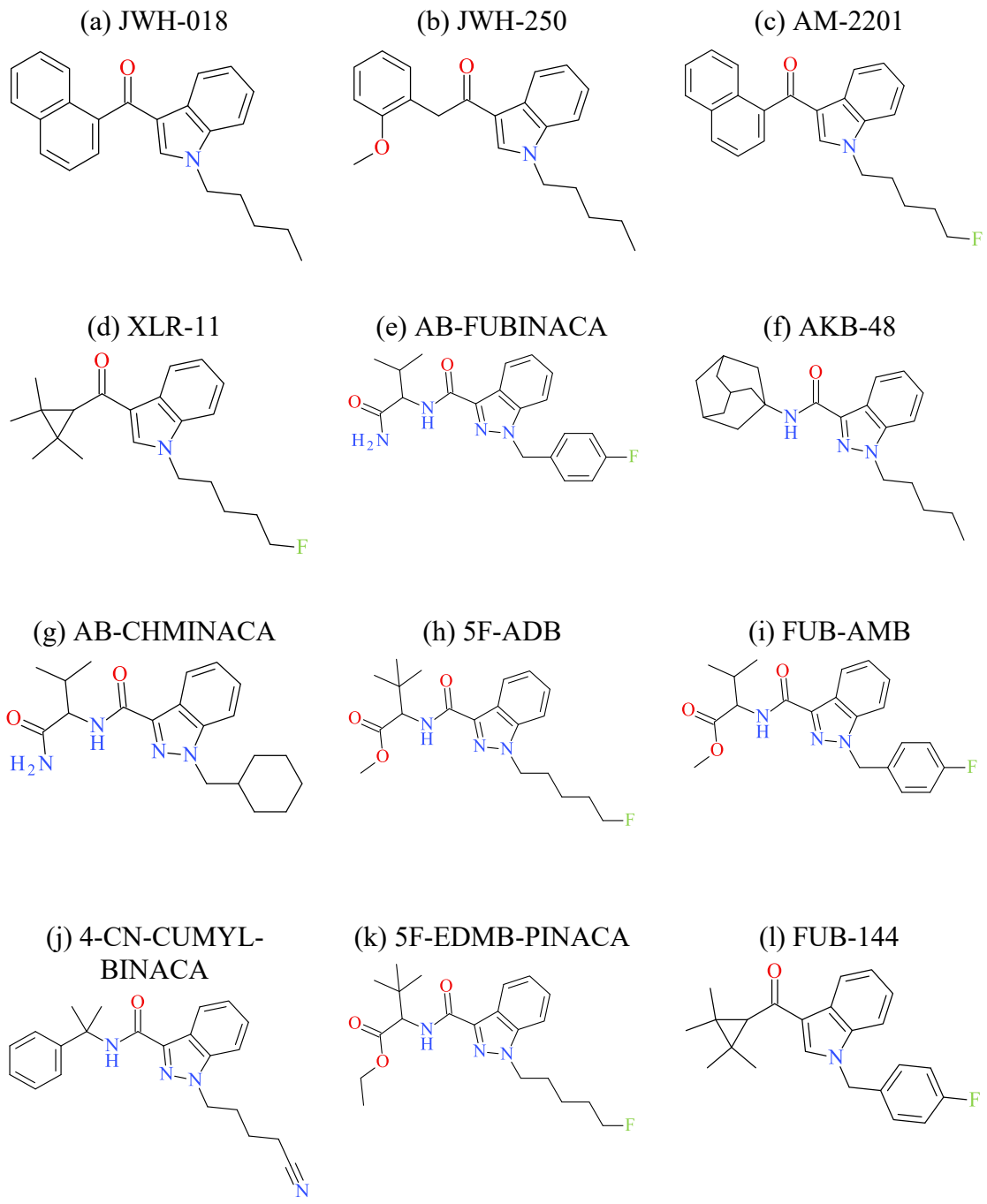


Figure 2: Structures of commonly encountered synthetic cannabinoids

The next class of NPS to emerge within the Unites States were the synthetic hallucinogens, as classified by the DEA (Figure 3).[51–61] Beginning in 2009, a series of drugs named with the term "2C" emerged and proliferated among club and dance scenes.[63] These substances were derived from the structure of phenethylamine, closely resembling the structures of amphetamine and methamphetamine (two commonly abused phenethylamines). The naming "2C" comes from the two carbon spacing between the aromatic group and the amine. Several iterations of the 2C series have emerged since this time in 2009, in addition to other series (e.g. "NBOMe" and "NBOH") containing new function groups (Figure 4). The "NBOMe" and "NBOH" names are derived from the addition to the amine (N) of a benzene ring (B), oxygen (O), and methyl (Me) or hydrogen (H). The synthetic hallucinogen class encompasses other substances and has expanded since 2009, including other synthetic substances modified based on the structures of lysergic acid diethylamide (LSD), psilocin (4-HO-DMT), etc. Reports of synthetic hallucinogen adverse events and death are infrequent due to limited use compared to other classes but are documented in the literature nonetheless.[10,64–67]

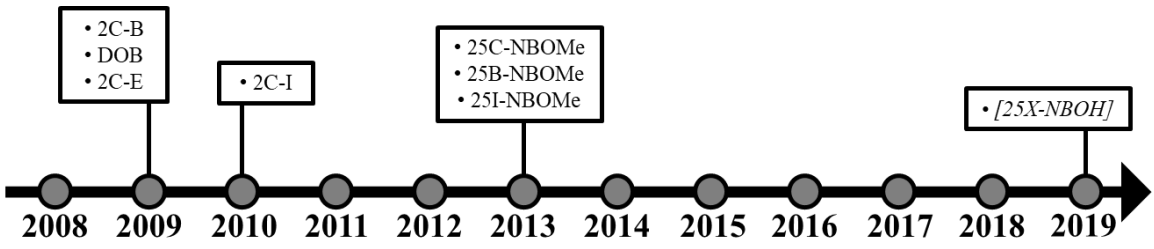


Figure 3: Emergence of synthetic hallucinogens in the United States

(m) 2C-I (n) DOB (o) 25C-NBOMe

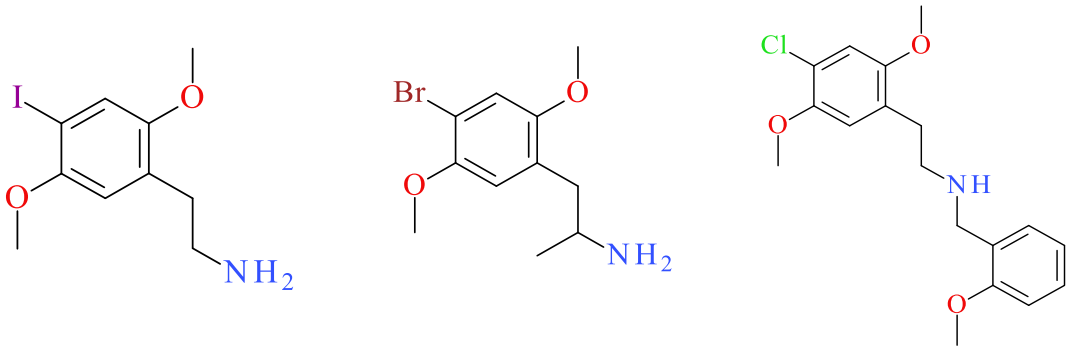


Figure 4: Structures of commonly encountered synthetic hallucinogens

Following the synthetic hallucinogens, the synthetic stimulants began to emerge in 2010 (Figure 5).[51–61] Synthetic stimulants are derived from several traditional stimulant backbones, but the first emergent compounds were related to the plant alkaloid cathinone.[68] Synthetic cathinones, a sub-classification of synthetic stimulants, are also classified as phenethylamines, but contain a *beta* positioned ketone.[69] Since 2010, a vast variety of synthetic stimulants have emerged, the majority of which retain the phenethylamine backbone (Figure 6). Like synthetic hallucinogens, synthetic stimulants have become popular among club and dance cultures, despite the fact that their use has been linked to an increasing number of adverse events and death.[10,29,70–73]

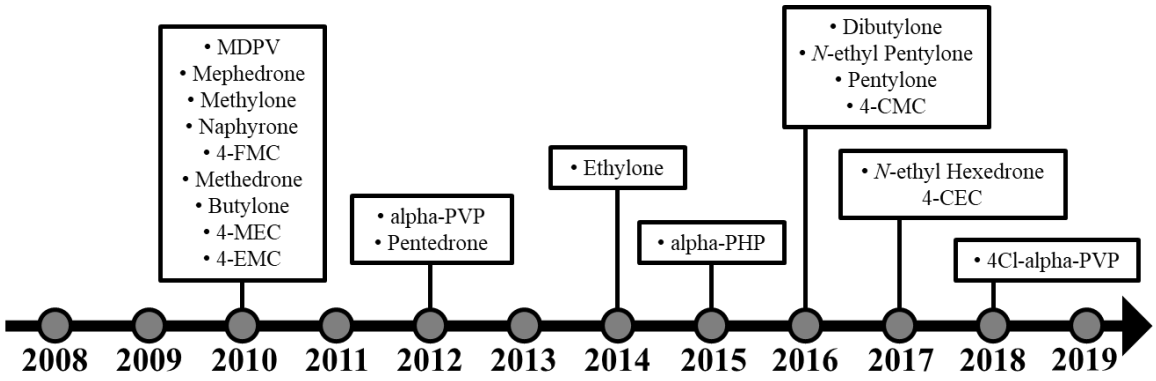


Figure 5: Emergence of synthetic simulants in the United States

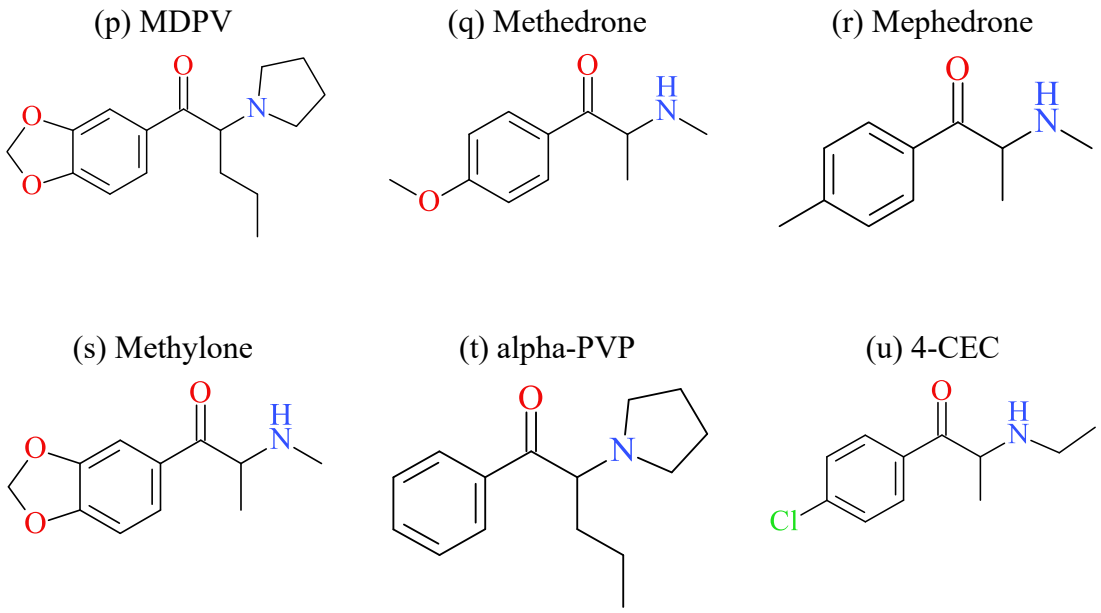


Figure 6: Structures of commonly encountered synthetic stimulants

Fast forward to 2015 and the emergence and proliferation of synthetic opioids becomes apparent (Figure 7).[51–61] Synthetic opioids have received the most attention over recent years due to the large number of increasing deaths,[10,74–76] but it is interesting to note that this NPS class lagged far behind others. The emergence of synthetic opioids is

directly related to the illicit manufacture and modification of fentanyl. While fentanyl is a prescribed and administered analgesic in the United States,[77] its use in inherent form or analogue form has changed the nature of heroin and illicit opioid drug markets. Following 2015, a large number of fentanyl analogues appeared on illicit drug markets with rapid rates of turnover possibly due to national and international control.[51–61] While fentanyl analogues comprise the overwhelming majority of synthetic opioids, different sub-classifications exist, including the U-series (e.g. U-47700, U-49900, etc.) and others (e.g. AH-7921, MT-45, etc.) (Figure 8). As with the synthetic cannabinoids, synthetic opioids have been pirated from the patent literature, arising from publication drafted by prominent pharmaceutical companies (e.g. Janssen, Upjohn, Allen and Hanburys, etc.).[24,78]

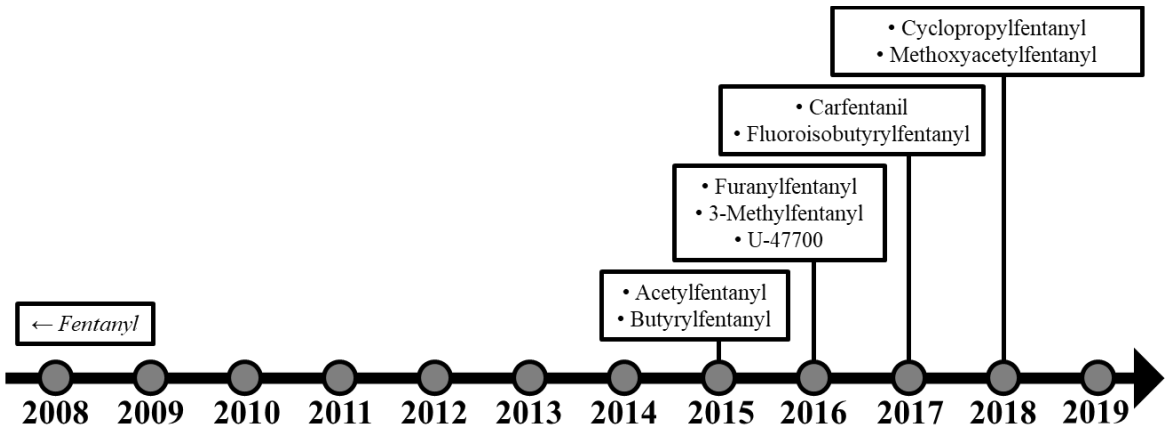
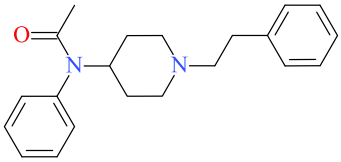
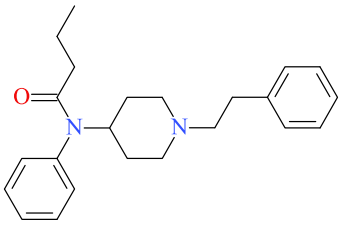


Figure 7: Emergence of synthetic opioids in the United States

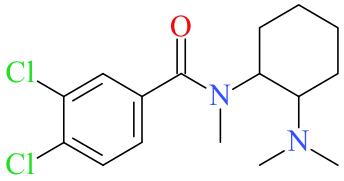
(v) Acetylfentanyl



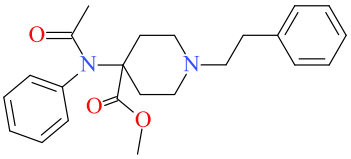
(w) Butyrylfentanyl



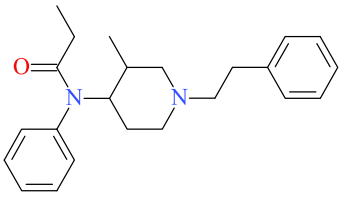
(x) U-47700



(y) Carfentanil



(z) 3-Methylfentanyl



(aa) Cyclopropylfentanyl

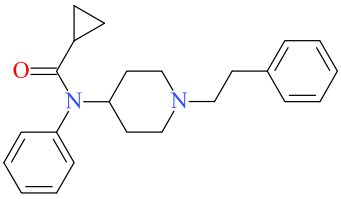


Figure 8: Structures of commonly encountered synthetic opioids

The final class of NPS that appears with frequency in the United States is the synthetic benzodiazepines (Figure 9).[51–61] Unlike the previously mentioned NPS sub-classifications, the synthetic benzodiazepines are often difficult to characterize and describe due to historical use as medications and/or current international use as medications.[10,25,79–83] In addition, novel use and/or abuse can trigger classification as a synthetic benzodiazepine, often blurring these lines. Synthetic benzodiazepines are modified based on the typical "benzodiazepine" core structure, consisting of a fused ring system of benzene and diazepine with an additional benzene substituent (Figure 10). The first appearance of synthetic benzodiazepines not used medicinally in the United States occurred around 2013 (Figure 9), although again this date is subjective.

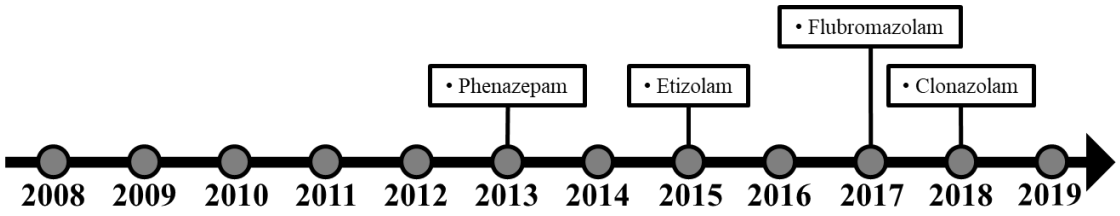


Figure 9: Emergence of synthetic benzodiazepines in the United States

(bb) Phenazepam (cc) Etizolam (dd) Flubromazolam (ee) Clonazolam

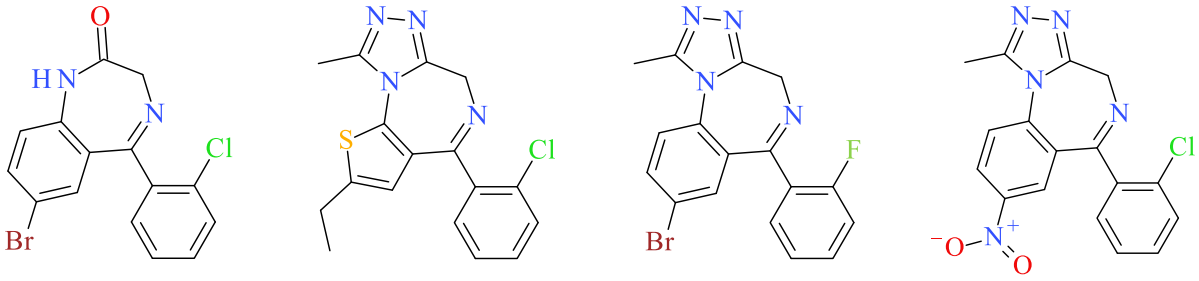


Figure 10: Structures of commonly encountered synthetic benzodiazepines

2.2 Early Warning Systems (EWS)

EWS are avenues for dissemination of information in a timely manner. These systems can be complex and intricate or simple and straightforward, depending on the information being relayed. EWS have been used among other fields, notably with respect to physical or natural disasters, but their traction among scientists has gained interest with advancements in technology (e.g. internet, email). As previously described with the rate at which NPS appear and turnover, paired with their public health and public safety impacts, EWS are now being employed widely among national and international agencies.

Programs that allow laboratories, law enforcement, and emergency medical services to rapidly identify and share data on emerging NPS associated with deaths and adverse events have been shown to be a key contributor to public safety and security. The EMCDDA is a drug monitoring organization founded to provide drug-related information to European public health agencies based on drug trends and drug use statistics.[84] The EMCDDA operates an EWS to share information about NPS,[9] and through this system has identified the emergence of more than 600 NPS, beginning with 13 in 2005, 7 in 2006, 15 in 2007, 13 in 2008, 24 in 2009, 41 in 2010, 48 in 2011, 74 in 2012, 81 in 2013, 101 in 2014, 98 in 2015, 66 in 2016, and 51 in 2017,[4] with several new compounds yet to be reported in 2018 and 2019. In their European Drug Reports, the EMCDDA recognizes the use of illicit substances, including NPS, to be a "global burden of disease." While these reports focus on trends and developments in Europe, the same concerns apply to the United States and its ongoing crisis of drug use and abuse, specifically the "opioid epidemic." These findings in Europe often presage the appearance of the drugs in the United States and other parts of the world.

Currently in the United States, there is no equivalent centralized process for the collection, analysis, and dissemination of data on the identity and prevalence of emerging NPS and their contribution to fatalities and other adverse events, with associated emergency response or deaths in police custody. Drug monitoring initiatives (DMI) have been developed and adopted to track seizures of solid drug materials and prescription drugs; most notably the National Forensic Laboratory Information System (NFLIS) organized by the DEA[85] and other DMI state programs in New Jersey,[86] Maryland,[87] and

New Hampshire.[88] The Centers for Disease Control and Prevention (CDC) have developed a drug monitoring program, but this program currently focuses on prescription medication and clinical aspects.[89] On an ad hoc basis, the CDC tracks localized adverse events and intoxications associated with NPS substances, but the data collected is often based on single incidents with voluntary reporting and focuses more heavily on opioids than NPS as a whole.

Organizations in the United States have developed EWS as a response to the explosion of NPS in drug markets and the onset of the opioid epidemic. NPS Discovery[90] has developed a system for early identification of NPS and timely dissemination of analytical data, drug information, and case information (when available) to appropriate stake holders. The National Drug Early Warning System (NDEWS)[91] also provides an avenue for NPS dissemination, and shares data amongst a wider variety of public health professionals. However, there are no systems in place in the United States to track, coordinate, and provide timely reporting on toxicologically confirmed NPS intoxications.[92]

Internationally, EMCDDA operates an EWS[93] based on emerging NPS identified within the EU and develops detailed reported based on current knowledge of the new substance, including pharmacology and toxicity data, when available; and the United Nations Office on Drugs and Crime (UNDOC) operates an Early Warning Advisory (EWA)[94] where registered users can track NPS identifications and trends from a large number of participating countries (including the United States).

2.3 Mass Spectrometry

Toxicological analyses rely heavily on analytical chemistry methodologies and techniques for the accurate identification and characterization of small molecules (e.g. drugs). Mass spectrometry has greatly advanced toxicological fields by providing more selective and sensitive detection methods, but detection is deeply rooted in an understanding of acquisition modes and data processing strategies. When analyzing biological specimens for the presence of therapeutic, abused, and emerging drugs, the analyst can only discover and identify those drugs detected by the mass spectrometer (or other detection technique) and/or those drugs incorporated into the data processing methods. While this premise may seem rudimentary, it governs routine instrumental analyses and analytical capabilities.

Recent trends with respect to drugs of abuse and NPS, as previously stated, have demonstrated the emergence of up to or exceeding 100 new drugs identified per year,[95] with rates of turnover per drug class a the month timescale. This explosion of new substances is almost impossible for small analytical laboratories to keep up with, compounded by issues involving availability of standard reference material and identity of isobaric analytes.[77,96,97] Large laboratories equipped with state-of-the-art instrumentation often have the capabilities and capacity to tackle emerging drug problems but can lack the expertise or tools for quick and accurate identifications. It is important to note that characterization of emerging substances is significant, as many of these substances can be implicated in or contributors to death. Therefore, a well-developed and comprehensive strategy for the novel characterization of emerging drugs

would greatly benefit analytical laboratories for detection during toxicologically relevant investigation, as well as to reference manufacturer organic chemists for the swift development of standards needed for confirmation and quantitative analyses.

Mass spectrometry (MS), often coupled with liquid chromatography (LC) or gas chromatography (GC), provides the optimal balance between amount of sample needed for analysis, sensitivity of the assay, total analysis time, and chemical information gathered.[98–101] Unlike traditional molecular probing techniques, such as nuclear magnetic resonance (NMR) or infrared spectroscopy (IR), mass spectral analysis can be conducted on complex mixtures and on the sub-nanogram to picogram scale, if not lower.[102] This feeds from the increased sensitivity of mass spectrometers, but this feature if more complex and related to advancements in technology.[103] The total analysis time of a mass spectrometry-based method is variable, but probative screening method can range from 3-10 minutes in length,[104–107] paired with autosampler capabilities that allow for automated and sequenced workflows. The chemical information obtained by a mass spectrometer is variable based on the analyzer in use, but typical data obtained can lead to the identity of chemical formula and basic structural features.[101,108,109] These aspects are key to characterizing emerging or unknown substances.

While it is easy to claim the acquisition of important chemical information by a mass spectrometer, a deeper understanding regarding acquisitions modes and mass analyzers is necessary. Acquisition modes are directly related to mass analyzers and their pairing or use in tandem. For example, quadrupole mass analyzers allow for unit mass filtering and result in the acquisition of nominal mass data.[110] This acquired data can not

directly be used for the accurate determination of chemical formulae but can be used in the determination of rough elemental composition.[110] Ion trap mass analyzers follow similarly to quadrupoles.[110] Time-of-flight and Orbitrap mass analyzers allow for accurate mass identifications, which can subsequently be used for more precise formulae elucidations.[110,111] Other mass analyzers (e.g. magnetic sector) are available for analyses, but their use in current small molecule drug discovery is less common. Pairing of these mass analyzers in tandem, linearly or non-linearly, adds increased analytical capabilities.[112] For example, a quadrupole mass analyzer (and collision cell) placed before an Orbitrap mass analyzer can allow for acquisition of accurate mass fragment ions, an additional tool useful for the elucidation of structural features.

Common commercially available configurations in tandem include quadrupole and time-of-flight mass analyzers (QTOF) or quadrupole and Orbitrap mass analyzers (Q-Orbitrap). For the purposes of this literature search, QTOF and Q-Orbitrap configurations were not be juxtaposed, but rather considered equal for their similar abilities to filter ions and acquire accurate mass measurements. In the analysis of small molecules, the resolution differentiation between time-of-flight and Orbitrap mass analyzers is often unnecessary, although valuable nonetheless. Pairing of a quadrupole ahead of a high resolution mass analyzer allows for ion filtering prior to accurate mass analysis, which leads to options for the isolation of specific ions for independent or clustered acquisition. This isolation directly correlates to the data acquired and the potential results that can be concluded. There is a current balance between acquisition of

all pertinent mass information and acquisition of highly specific mass information, both of which have utility in the drug discovery realm.

Three of the most common acquisition modes for analysis using quadrupole and high resolution mass analyzers are MS^2 (high resolution), MS^e, and MS/MS^{ALL}.[44–46] All three modes acquire accurate mass data for precursor (TOF MS) and product (MSMS) ions (or fragment ions). MS^2 operates the quadrupole as a tradition nominal mass filter resulting in product ion formation from a single precursor ion.[45,46] This results in increased specificity for precursor-product ion linkage. MS^e operates the quadrupole simply as an ion guide resulting in product ion formation for all precursor masses entering the mass spectrometer at the same time point.[45] This results in decreased specificity for precursor-product ion linkage due to uncertainty among analytes fragmenting together but provided benefits during broad screening. MS/MS^{ALL} utilizes the quadrupole as a windowed or segmented mass filter resulting in product ion formation from a specific range of precursor ions.[44–46] This results in intermediate specificity in comparison to MS^2 and MS^e for precursor-product ion linkage with similar benefit for broad screening like MS^e. Choosing the appropriate acquisition mode is critical to understanding the conclusions a chemist can draw from results and the certainty in acquisition of information for probative purposes.

This leads to understanding of data processing strategies, which can be divided into at least three categories: targeted, non-targeted, and manual.[36,37] Targeted and non-targeted data processing, by definition, require a software package or program that allows for automated or streamlined analysis of the data. These strategies also require some level

of input or scope for extraction of results. For example, targeted data processing often requires a list of known substances, including criteria such as mass, formula, and retention time; while non-targeted data processing often require restraints around mass, elemental composition, retention time, etc. Contrarily, manual data processing requires no input of criteria or restraints and is often developed and simulated by the analyst based on visual aspects of the data (e.g. chromatographic peak, large mass, etc.). Positive identification of an analyte after manual data processing includes meeting minimum criteria, as with all data processing (e.g. ppm error, retention time error). A combination of these data processing strategies provides the most comprehensive outlook of the results, but time and computing capabilities become the limiting factors for effective analysis.

Mass spectrometry is an extremely useful tool for the identification of known and unknown compounds due to highly reproduceable and predictable fragmentation patterns.[113,114] Production of stabile ions, such as the acylium and tropylium ions, greatly influence this reproducibility.[115] This is further assisted using electrospray ionization, as this ionization technique provides an increased level of reproducibility over harsher ionization techniques.[116] Several studies have demonstrated the similarities in MS fragmentation between similar compounds, including analogues, homologues, and isobaric species,[117–119] but there is no current research into the collective use of this information for characterization and discovery purposes.

2.3.1 SWATH® Acquisition

SWATH® Acquisition (or simply SWATH®) is a comprehensive data independent acquisition (DIA) process available from SCIEX (Framingham, MA, USA), an instrument manufacturer of high resolution accurate mass spectrometers.[44–46,107,120] SWATH® Acquisition utilizes the acquisition mode MS/MS^{ALL} and is therefore often referred to as "MS/MS^{ALL} with SWATH® Acquisition." When introduced, SWATH® was a groundbreaking feature only available through SCIEX on their platforms due to advanced electronics and ability for their systems to cycle through acquisition parameters. SWATH® was initially developed as an advantageous approach to quantitation in proteomics,[121–124] but quickly found lateral uses among other scientific fields using SCIEX instrumentation. To this day, SWATH® remains a novel approach to drug detection and drug discovery, although other instrument manufacturers have developed similar mass acquisition modes applying MS/MS^{ALL}.

Inherently, SWATH® is a proprietary non-targeted data acquisition mode available on SCIEX high resolution quadrupole time-of-flight mass spectrometers, including instruments in the TripleTOF® and X500 series.[125] By definition, non-targeted acquisition modes allow for collection of data regardless of analytes within a given sample and regardless of knowledge about sample history or contents. This differs from targeted acquisition modes which rely sole on set parameters to detect certain masses (e.g. triple quadrupole mass spectrometry from confirmation), analytes at specific retention times (e.g. dynamic multiple reaction monitoring), etc. Non-targeted acquisition workflows are extremely important for unknown sample screening, as they allow for a

broad scan of possible substances present; whereas, contrarily, targeted acquisition often only allows for single or subset detections. Non-target mass acquisition does have intrinsic limitations (e.g. limit of detection, mass range, etc.), but, in theory, this process allows for collection of all masses within a set runtime given that a molecule enters the mass spectrometer, has properties amenable for ionization, and reaches the detector with a mass to charge ratio within the set parameters.

During acquisition, SWATH® allows for the complete collection of accurate mass data, specifically comprehensive mass measurements for product ions. While precursor ions are acquired during "SWATH® Acquisition experiments", SWATH® is the terminology used to describe the process by which precursor ions are isolated. For the first experiment, precursor ions are acquired via standard TOF MS scan, meaning all ions travel through the quadrupole and collision cell, both acting as "ion guides" rather than mass filters and fragmentors, and end up being filtered in the time-of-flight analyzer for accurate mass measurement (Figure 11).

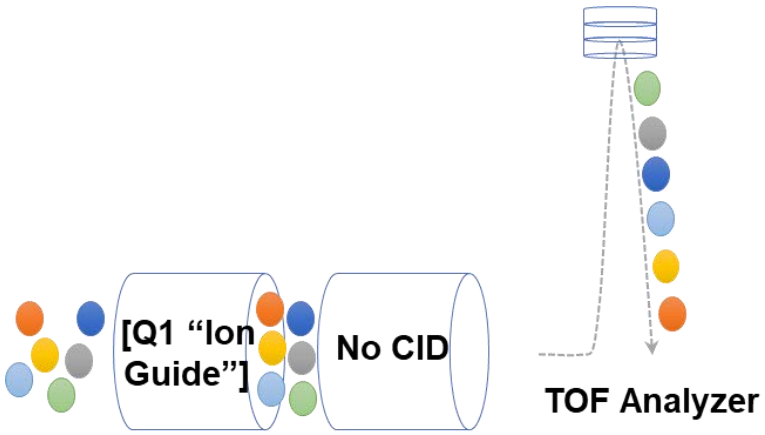


Figure 11: Precursor ion acquisition (TOF MS scan)

For the next experiments (MSMS), product ions are filtered by the quadrupole on a cycling basis (i.e. SWATH®) and fragmented in the collision cell before separation in the time-of-flight analyzer for accurate mass measurement. This quadrupole filtration occurs in mass increments known as Q1 isolation windows (or SWATH® windows). These windows can be customized based on assay need during development (e.g. variable Q1 isolation windows vs. fixed Q1 isolation windows) but are generally 10-30 Da in width for small molecule applications. These windows are designed to span the entirety of the mass range set in the method (e.g. 100-500 Da) and overlap by at least 1 Da to ensure there are no gaps in precursor ion isolation. For example, a SWATH® method could be developed where Q1 isolation occurred from 100 to 150 Da, then 149 to 200 Da, then 199 to 250 Da, and so on. Depictions of this isolation are shown in Figures 12-14.

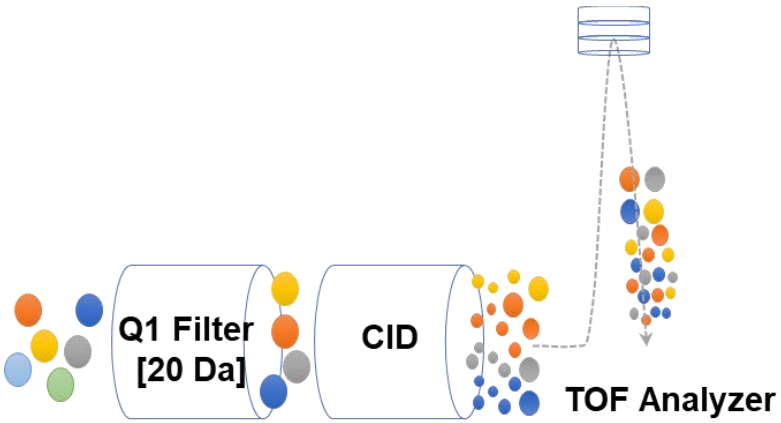


Figure 12: Product ion acquisition (SWATH®)

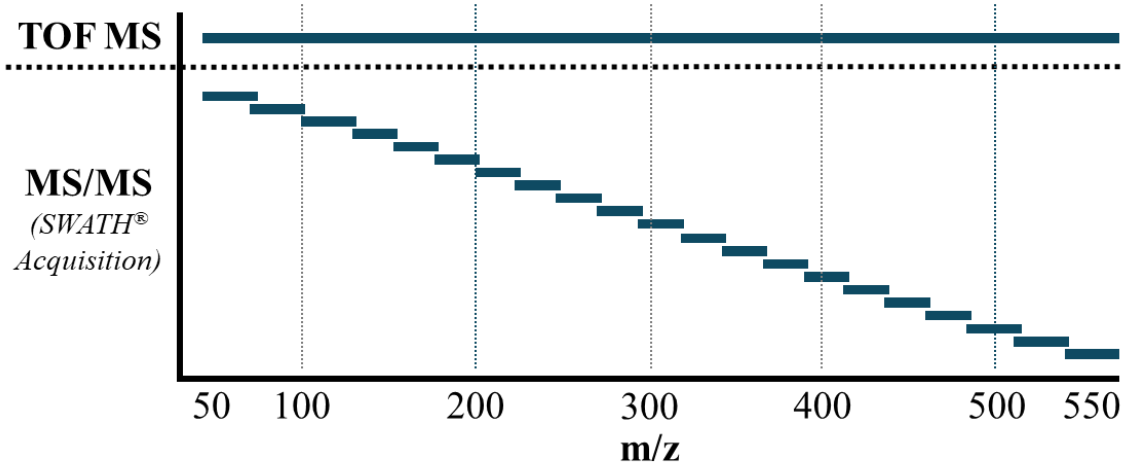


Figure 13: Fixed SWATH® Q1 isolation windows

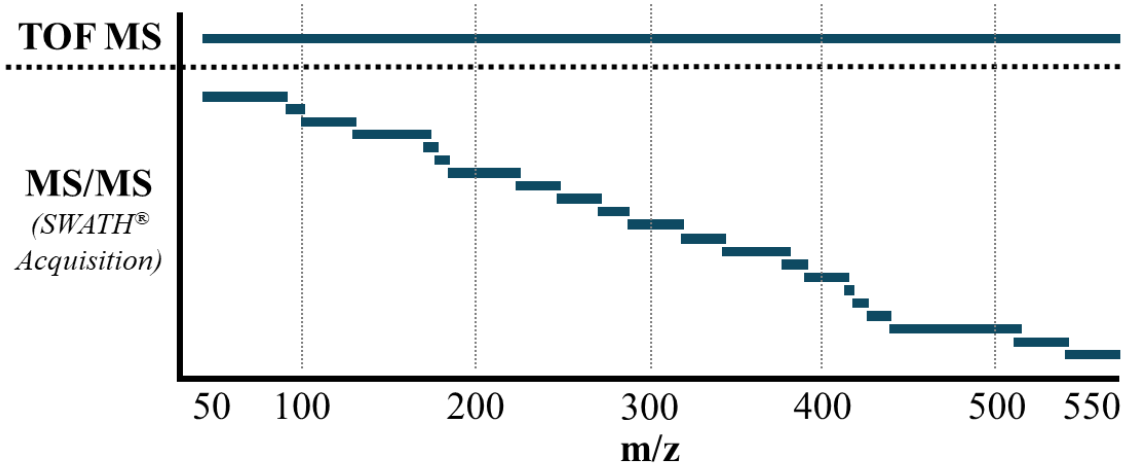


Figure 14: Variable SWATH® Q1 isolation windows

The isolated precursor ions are then fragmented in the collision cell before time-of-flight separation and ultimate detection. A variety of collision cell settings can be used with a SWATH® Acquisition method, but a typical non-target acquisition mode will utilize an approach called a collision energy spread (or rolling collision energy). A

collision energy spread allows for a focal collision energy to be set, as well as a range around the focal point. For example, a collision energy of 35 eV with a spread of ±15 eV would result in cycling energies from 20 to 50 eV. This approach is advantageous for non-targeted screening workflows because it allows for production of a landscape of fragment ions which can then be used for library searching or structural elucidation.

Based on these features, SWATH® Acquisition allows for real-time sample mining and retrospective data mining, as described further in Chapter 3.

CHAPTER 3

SAMPLE MINING VS. DATA MINING

3.1 Introduction

Outside of the complex engineering and technology needed for development and implementation of highly intricate instrumentation, the most challenging aspect of analysis for analytical chemists is formulating raw data into digestible results. With respect to LC-QTOF-MS data acquisition and processing, this relates to the translation of high resolution mass spectrometry (HRMS) data to reviewable criteria or results that can then be stored or culminated in a database (e.g. Excel® spreadsheet) for additional computational analysis. During a single non-targeted LC-QTOF-MS acquisition, thousands to hundreds of thousands of data points are collected. Without a streamlined approach and criteria for determination of positive identifications (paired with software processing capabilities), an analyst can not formulate conclusions in a timely and accurate manner.

The focus of this research was to correlate data features acquired (e.g. mass, retention time, fragmentation pattern, etc.) with those of known analytes. This was conducted through data processing using complex scientific software; however, an approach to data processing first needed to be developed and evaluated to determine its feasibility and accuracy. The complexity of the data acquired during this research was high and the goal was to focus on emerging NPS and their metabolites (if present), as well as traditional drugs of abuse, therapeutic drugs, cutting agents, etc.

3.2 Creating New Workflows

During this research, two workflows for the real-time and retrospective identifications of emerging or previously characterized NPS were developed (Figure 15).

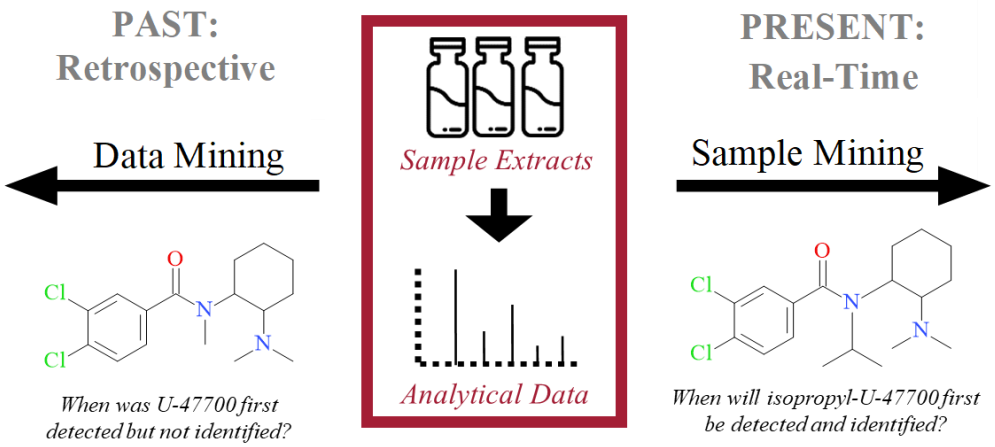


Figure 15: Sample mining vs. data mining

Real-time identifications were made during first-pass data processing against an extensive library database, occurring on average within days to a week of sample reciept and acquisition. This immediate process has been defined as “sample mining.” Sample mining, by this definition, can be applied to sample extracts, biological specimens, datafiles, etc., but has been specifically coined to define the process of identifying NPS through real-time re-analysis of sample extracts. Different from traditional drug testing, sample mining is not a targeted analysis approach, but rather employs non-targeted acquisition for the discovery of substances not within a static, defined scope of testing. In this sense, the purpose of sample mining is contrary to that of drug testing and focuses on drugs not typically seen within the larger, predictable drug using population. The term

"mining" was selected for this type of approach due to the needed analytical expertise and data processing required to discover new substances within a data-rich sample set. Sample mining was conducted on a daily to weekly basis during this research.

On the contrary, data mining is a term used among various applications, including the natural sciences, that refers to retrospective or historical data processing or manipulation strategies. This approach can be applied to large datasets or single datafiles, providing insight into past identifications, trends, correlations, etc. Data mining was defined as the process of identifying NPS in datafiles from sample extracts that were analyzed months to a year before the time of data processing. A recent publication within the forensic community illustrates the value of data mining,[126] but no other literature exists on the true extent and value of data mining within the forensic toxicology community. Data mining was typically conducted using a subset of the database following the addition of standards to the library, occurring monthly or as necessary.

An additional aspect of data mining included a strategy used for *in vivo* characterization of metabolites within datafiles. During this research, metabolism studies were conducted *in vitro* (e.g. microsome incubation) for comparison *in vivo* (e.g. sample extracts from human biological specimens). Metabolites identified *in vitro* were mined in all historical data to determine their prevalence in the subset or population. This process is described at length in Chapter 6.

3.3 Data Processing

Combined targeted and non-targeted data processing strategies were developed and used for real-time and retrospective data processing using PeakView® (Version 1.2) and MasterView™ (Version 1.1) software available from SCIEX. Targeted data processing was defined by use of an extensive in-house library database and mass list, while non-targeted data processing was defined by use of peak finding strategies, emerging drug intelligence, and/or analyst manual review of the data.

Following a statistical comparison of targeted data processing criteria across several analytes and batches of data, the final criteria for targeted data processing was defined. The four main criteria included mass error (ppm error), retention time error, isotope difference, and library score. All criteria were evaluated numerically and weighted (within the software) based on importance for positive analyte identification.

Mass error (also known as ppm error) is a measurement between theoretical exact mass and experimental (or acquired) accurate mass. The resulting value is multiplied by 1,000,000 to give a nominal value that can be used for comparison. Equation 1 shows the calculation used to determine mass error. It is generally accepted that this mass error should be less than 5-10 ppm. Figure 16 shows passing and failing representations of mass error.

$$Mass\ error\ (ppm\ error) = \frac{(Accurate\ mass - Exact\ mass)}{Exact\ mass} \times 10^6$$

Equation 1: Mass error calculation

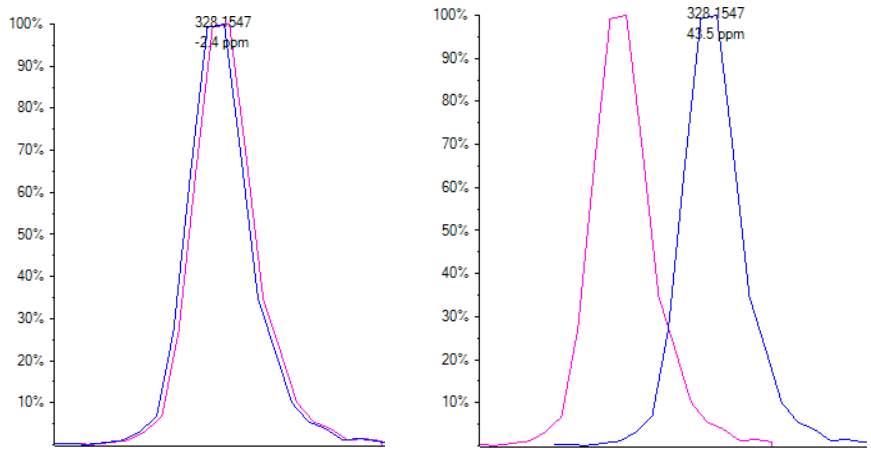


Figure 16: Mass error representation of accurate mass (blue) and exact mass (pink): passing (left) and failing (right) results

Retention time error (or retention time difference) is a measurement between the library retention time of standard reference material and an experimental retention time of an analyte in a sample of interest. The resulting value can be expressed as a measure of time (e.g. minutes) or as a percent. Equation 2 shows the calculation used to determine retention time error. There is no standard criterion for retention time error; rather, this is a result of method parameters and performance (e.g. run time, chromatographic separation, reproducibility, robustness, etc.) and analytical validation results. Figure 17 shows passing and failing representations of retention time error.

$$Retention\ time\ (Rt)\ error\ (difference) = Rt_{measured} - Rt_{actual}$$

Equation 2: Retention time error calculation

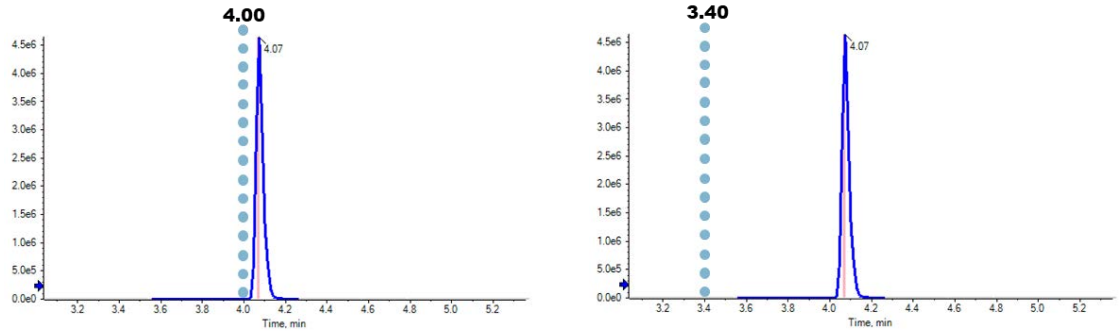


Figure 17: Retention time error representation of acquired chromatographic data (blue line) and standard retention time (pink dots): passing (left) and failing (right) results

Isotope difference is a measurement between the theoretical isotopic distribution of a given formula and that of the acquired analyte in a sample. The measurement considers both the spacing of isotopic contributions and their intensity. For example, if a formula includes chlorine, the isotope difference would measure how close the M+2 contribution is to the theoretical exact mass of that isotope and how intense the M+2 contribution is in relation to the isotopic abundance in nature (i.e. $^{37}Cl \sim 33\%$). The resulting value is expressed as a percent. Like retention time error, there is no standard criterion for isotope difference; rather, this is a result of method parameters and performance and analytical validation results. Figure 18 shows passing and failing representations of isotope difference.

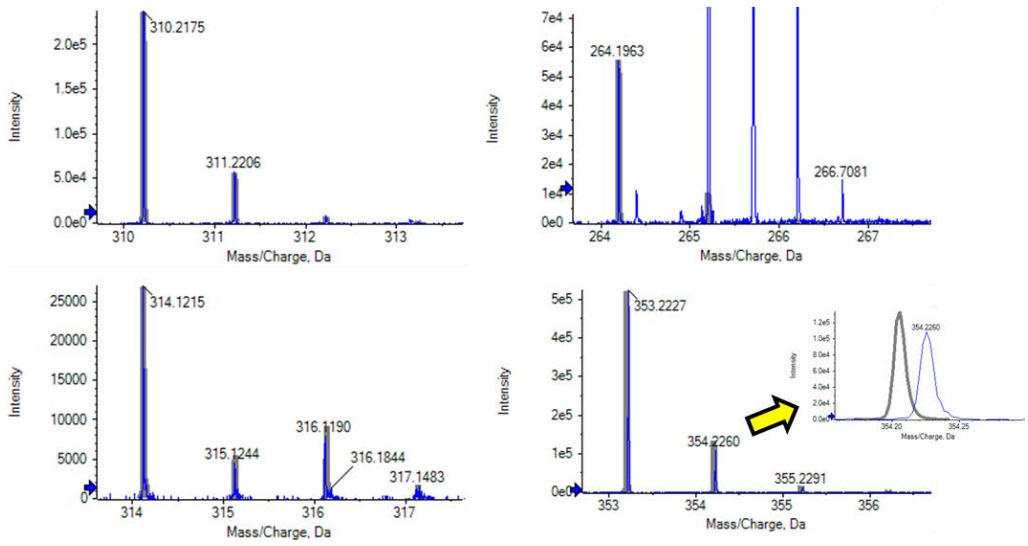


Figure 18: Isotope difference representation of acquired accurate mass distribution (blue) and exact mass distribution (pink): passing (left) and failing (right) results

Library score is a measurement between library reference mass spectral fragmentation data and experimental fragmentation of an analyte in a sample of interest. Similar to isotope difference, this value is calculated based on presence of masses, their spacing, and their intensity, in relation to those in the library. The resulting value is expressed as a score, which is a number calculated out of 100. Figure 19 shows passing and failing representations of library score.

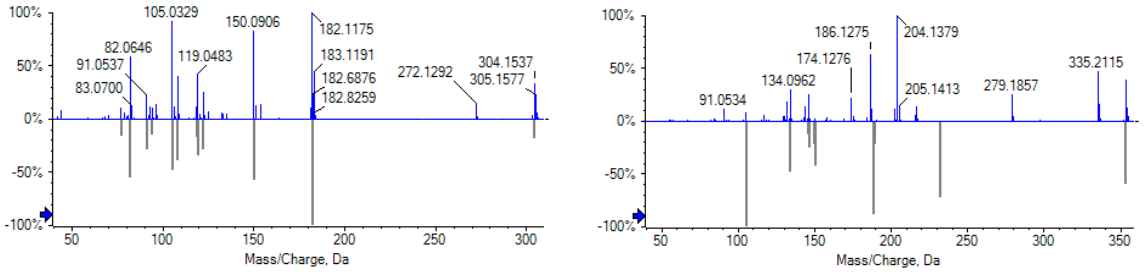


Figure 19: Library score representation of acquired mass spectral data (blue, top) and library database (pink, bottom): passing (left) and failing (right) results

Passing criteria (Figure 20) were defined as ppm error less than 10, retention time error less than 0.35 mins, isotope difference less than 50%, and library score greater than 50. The SCIEX green, yellow, and red "traffic light" categorizing scheme was used for isolation of positive findings from negative findings and the previously mentioned criteria correlate to a yellow coloring for all categories. Category weighting within the software was set as follows: ppm error 30%, retention time error 30%, isotope difference 10%, library score 30%; but it is important to note that the combined score calculated based on these numbers was determined to be unsuitable for positive analyte identification due to variability and inconsistency.

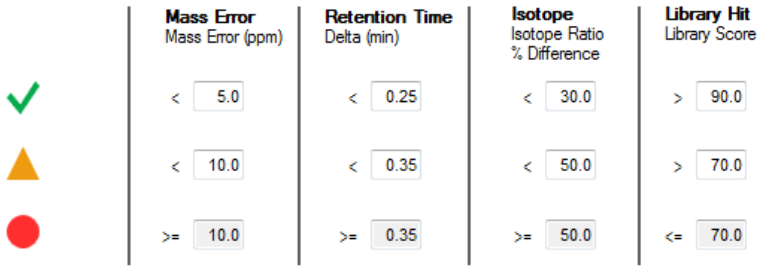


Figure 20: Criteria for positive identification

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Two additional numerical criteria were used for identification: minimum intensity (>800 counts) and signal-to-noise (S/N) ratio (>10). Other criteria evaluated by the analyst included acceptable chromatographic and mass spectral peak shape, acceptable library spectrum, and acceptable control comparison. The control comparison allowed for comparison of chromatographic intensity of an extracted ion chromatogram against a blank or control, which assisted in identifying a peak to be more intense than the "control." This allowed for the differentiation of contamination and/or interferences.

Criteria used for non-targeted data processing differed from that of targeted data processing due to unavailability of standard reference material for retention time and library spectral comparison; therefore, only mass error and isotope distribution were used for positive analyte identification. The retention time and library spectrum of the analyte in question were evaluated by the analyst in comparison to chemically related compounds or parent drug species, but the same numerical comparisons were not able to be calculated. If an emerging NPS was identified using a non-targeted approach, a standard was purchased for analytical comparison and confirmation of the substance.

3.4 Examples of Data Processing

3.4.1 Targeted Data Processing

As previously stated, data processing was conducted using MasterView™ (Version 1.1, SCIEX) software within PeakView® (Version 1.2, SCIEX) software. PeakView® allows for manual data processing, a time consuming process. Contrarily, MasterView™ provided the ability to automatically pull out and analyze specific data

within an acquired datafile based on preprogrammed information. This information was constructed by the analyst and consisted of an extracted ion chromatogram (XIC) list, a library file, and process criteria (Figure 20).

The XIC list was developed in-house based on the acquisition and analysis of standard reference materials. This list consists of analyte name, analyte formula, desired adduct (e.g. H+), retention time, and accurate mass fragment ions (n=5). The analyte formula and desired adduct are then used to calculate the exact mass of the analyte. An example of the XIC list is shown in Figure 21. In this display, the white cells correlate to analyst input information, whereas the gray cells populate with calculated data analysis features once this list is applied to an acquired sample (extraction, or exact, mass is already shown; the data does not need to be processed to determine this value).

#	✓	Mass ✓	RT ✓	Isotope ✓	Library ✓	Formula ✓	Name	Formula	Mass (Da)	Adduct	Extraction Mass (Da)	Expected RT (min)	Fragment Mass (Da)	Found At Mass (Da)	Error (ppm)	Isotope Ratio Difference (%)	Found At RT (min)	RT Delta (min)	Library Hit
2635	✓						para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35							
2636	✓						para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	355.2168						
2637	✓						para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	188.1432						
2638	✓						para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	105.0701						
2639	✓						para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	234.128						
2640	✓						para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	150.0706						

Figure 21: Display of XIC list for *para*-fluorofentanyl

Figure 21 shows six lines for the analyte within the database, one spot with no number entered in the "Fragment Mass (Da)" column and five subsequent spots with five different fragment ions. This setup was designed specifically to allow for processing of TOF MS and MSMS data, from both chromatographic and mass spectral perspectives. Similar to multiple reaction monitoring (MRM) where precursor-product ion transitions are monitor with extracted ion chromatograms, this setup allows for high resolution

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precursor-product ion transition monitoring (similar to MRM^{HR}). This will be explained further below.

The second aspect needed for data processing is a library file. Similar to the XIC list, the library database was generated in-house based on the acquisition and analysis of standard reference materials. Each analyte has a separate entry in the library file, consisting of the analyte name, analyte formula, and MSMS fragment spectrum (Figure 22). The library file and all of its entries are stored separately from MasterView™ and PeakView® in a program called LibraryView™ (Version 1.0, SCIEX). During data processing, MasterView™ compared MSMS spectra from an acquired sample with those in LibraryView™, as the two software applications are paired and work together during data processing.

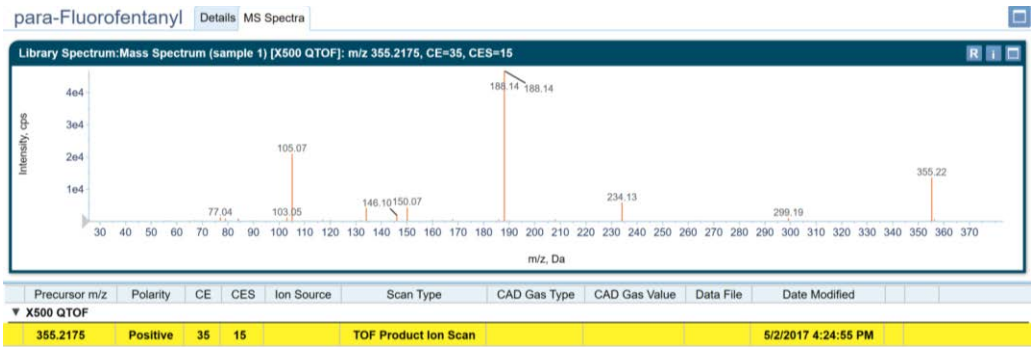

Figure 22: View of library entry for *para*-fluorofentanyl

Following sample acquisition, datafiles were imported into MasterView™ for processing against the defined XIC list and library file. Due to the size of the datafiles and the processing capabilities of MasterView™ and the computer, typically no more

than 50-100 datafiles were imported at the same time. As the library database increased past 700 analytes (>4,200 lines in the XIC list), the time to process increased; processing time for 100 datafiles was roughly 2-3 hours. During this time, MasterView™ was searching for every analyte (exact mass and fragment masses) in the XIC list, determining whether the data acquired matched the information that was input. If correct masses were identified, features of the data were calculated (as explained above). These calculated values were then flagged using the predefined identification criteria and sorted into "positive" results. The positives results were reviewed to determine what analytes were truly present within the datafiles.

An exemplar datafile positive for drugs of abuse and NPS was used to display how processed data viewing is conducted. Figure 23 shows the overall view of MasterView™. The top left windowpane correlates to the extracted ion chromatogram of the analyte selected in this sample. The top right windowpane correlates to the extracted ion chromatogram of the analyte (same exact mass) within a selected control sample (a blank). The middle left windowpane displays all of the samples processed (in this case, only two samples). The middle right windowpane displays the positive XIC list results filtered by the identification criteria. The bottom left windowpane shows the TOF MS spectrum and the bottom right windowpane shows the MSMS fragment ion spectrum. All windowpanes are viewed and reviewed by the analyst during data processing.

Figure 23: Analyst view within MasterView™ for data processing

Figure 24 shows the entire resulting XIC list after data processing and positive filtering (see Figure 20). The light green correlates to analyst input information whereas the dark green correlates to software calculated values. To the right of this figure, green check marks and yellow triangles can be seen; no red circles appear because these correlate to data that fail criteria and have been filtered out.

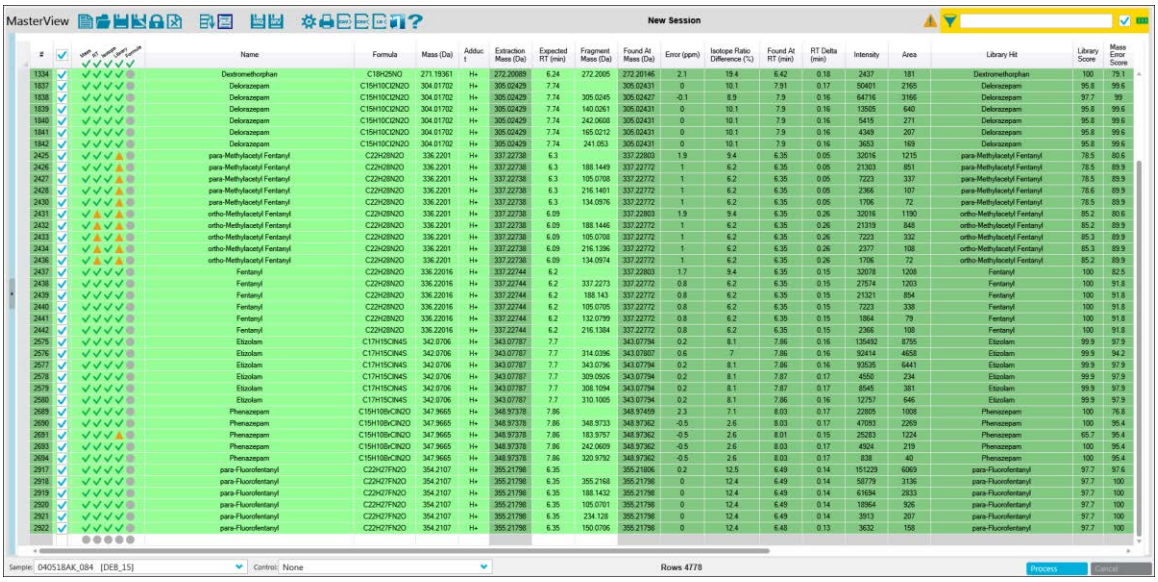

Figure 24: Example of processed data results

Furthermore, Figure 25 shows a zoomed in version for only *para*-fluorofentanyl. The top of this figure shows the analyst input information (light green) and the bottom shows the processing results (dark green), the important pieces of information. Following the columns across for the top row (dark blue), one can see the ppp error (0.2), isotope different (12.5%), retention time delta (0.14 mins), area (6069), and library match (*para*-fluorofentanyl) and score (97.7). All of these criteria are reviewed for positive identification and, in this case, are acceptable.

#	Mass	RT	Isotope	Library	Formula	Name	Formula	Mass (Da)	Adduct	Extraction Mass (Da)	Expected RT (min)	Fragment Mass (Da)
2917	✓	✓	✓	✓	✓	**para-Fluorofentanyl**	**C22H27FN2O**	**354.2107**	**H+**	**355.21798**	**6.35**	
2918	✓	✓	✓	✓	●	para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	355.2168
2919	✓	✓	✓	✓	●	para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	188.1432
2920	✓	✓	✓	✓	●	para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	105.0701
2921	✓	✓	✓	✓	●	para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	234.128
2922	✓	✓	✓	✓	●	para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.21798	6.35	150.0706

#	Mass	RT	Isotope	Library	Formula	Name	Found At Mass (Da)	Error (ppm)	Isotope Ratio Difference (%)	Found At RT (min)	RT Delta (min)	Intensity	Area	Library Hit	Library Score
2917	✓	✓	✓	✓	✓	**para-Fluorofentanyl**	**355.21806**	**0.2**	**12.5**	**6.49**	**0.14**	**151229**	**6069**	**para-Fluorofentanyl**	**97.7**
2918	✓	✓	✓	✓	●	para-Fluorofentanyl	355.21798	0	12.4	6.49	0.14	58779	3136	para-Fluorofentanyl	97.7
2919	✓	✓	✓	✓	●	para-Fluorofentanyl	355.21798	0	12.4	6.49	0.14	61694	2833	para-Fluorofentanyl	97.7
2920	✓	✓	✓	✓	●	para-Fluorofentanyl	355.21798	0	12.4	6.49	0.14	18964	926	para-Fluorofentanyl	97.7
2921	✓	✓	✓	✓	●	para-Fluorofentanyl	355.21798	0	12.4	6.49	0.14	3913	207	para-Fluorofentanyl	97.7
2922	✓	✓	✓	✓	●	para-Fluorofentanyl	355.21798	0	12.4	6.48	0.13	3632	158	para-Fluorofentanyl	97.7

Figure 25: Processed data features for *para*-fluorofentanyl

When the top line for *para*-fluorofentanyl is selected (dark blue), this allows for the other windowpanes to populate with graphs/figures. The next important aspect of data to review is chromatography. Figure 26 shows the chromatography for this selection. When reviewing the data, extracted ion chromatograms from the sample and from the control appear, using the same exact mass for extraction. This allows for the analyst to review the chromatography of the sample, but also to differentiate background or noise from positive analytes, as well as to identify possible contamination. In this example, it is clear that the contribution in the sample is not present in the control (i.e. no peak), and that the identification meets criteria for peak shape and intensity.

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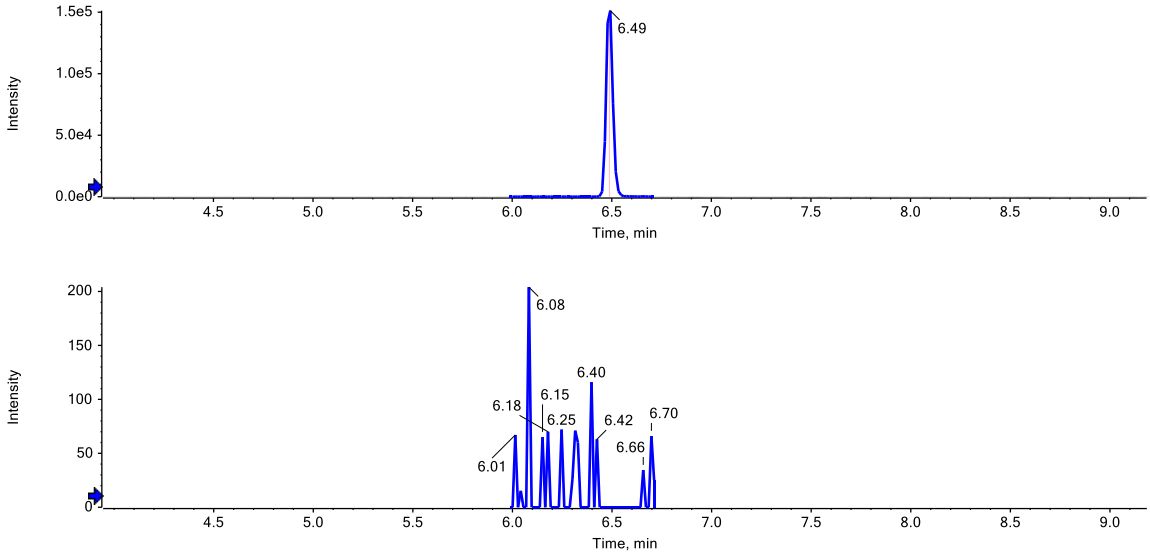

Figure 26: Extracted ion chromatogram for *para*-fluorofentanyl in the sample (top) and the control (bottom)

Continuing with evaluation of the chromatography, the analyst can then select all lines (up to n=6) for a specific analyte in the XIC list, which intern overlays all of the extracted ion chromatograms (Figure 27). This view of the ion profiles provides more information as to where the fragment ions could be coming from. For example, all fragment (product) ions of the same precursor ion should have the same ion profile. This gives the analyst increased confidence with respect to identification of the analyte.

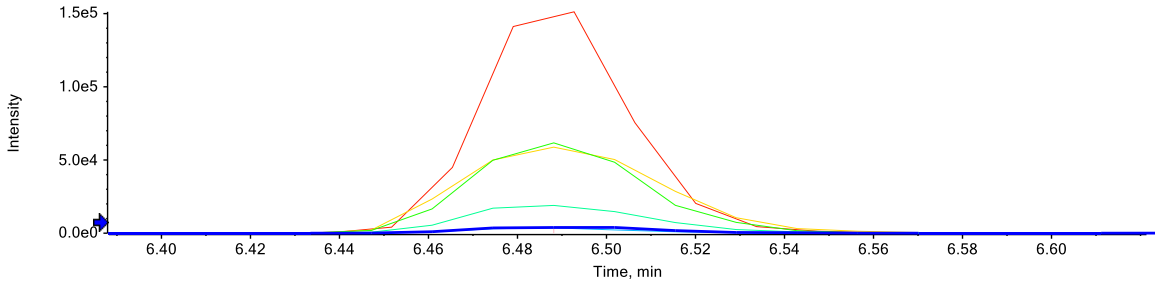

Figure 27: Overlaid extracted ion chromatogram for *para*-fluorofentanyl

The final two aspects of the data to review include the mass spectral figures, arguably the most important aspects to review. The TOF MS data (Figure 28) shows different information about the precursor ion. Similar to chromatography, the analyst reviews the peak shape of the TOF MS data, as this will reveal the cleanliness of the datafile and the possibility of co-eluting ions (seen as peaks offset to those expected). MasterView™ displays a theoretical (or expected) ion trace in this figure (pink) to which the analyst can visually compare. Specifically, the analyst can review the M+2 ion to determine presence or absence of halogens, consistent with or inconsistent with the formula in the XIC list.

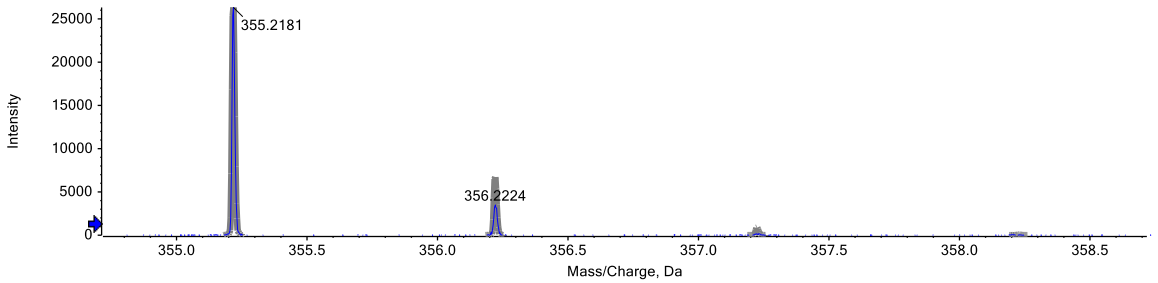

Figure 28: TOF MS data for *para*-fluorofentanyl

The MSMS (fragment) data is the most specific and definitive aspect of data available for review, as shown in Figure 29. This shows the acquired MSMS spectrum on the top and a mirrored spectrum on the bottom that is pulled from the library file. Presence of additional major fragments in the MSMS spectrum could lead the analyst to believe that the identification is inaccurate but could also lead to the identification of a new drug or analogue.

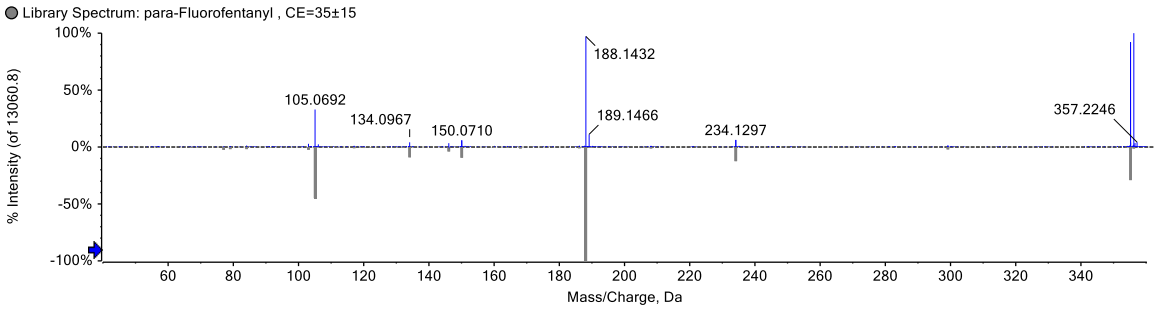

Figure 29: MSMS data for *para*-fluorofentanyl

This process continues repeatedly for all positive hits in the XIC list. Following full review, this exemplar sample would be considered positive for *para*-fluorofentanyl, as well as delorazepam, fentanyl, etizolam, and phenazepam.

3.4.2 Manual Data Processing

For manual data processing, PeakView® can be used to evaluate similar data to that above; however, the calculations are not made automatically. Figure 30 shows the total ion chromatogram for the same sample as above. This shows the complexity of a blood extract and leads to the difficulty of conducting manual data processing. It would

be extremely time consuming to evaluate every peak to determine if it is a drug, a matrix component, or something else.

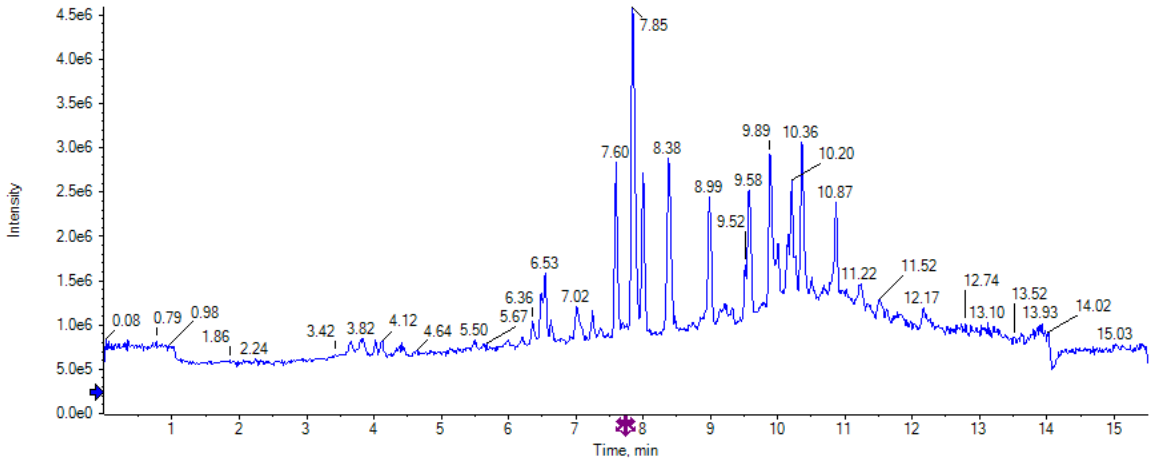

Figure 30: Total ion chromatogram for sample extract

Clicking through the peaks, the analyst will reveal the TOF MS and MSMS spectra. From there, the analyst can manually calculate ppm error or manually compare to known library fragment spectra. While the largest peaks in the chromatogram may seem like a good place to start, its often the smaller peaks that can be more valuable. In this sample (Figure 30), the largest peak (7.85 mins) correlates to an internal standard (etizolam-D3), with minor contribution from etizolam (Figure 31).

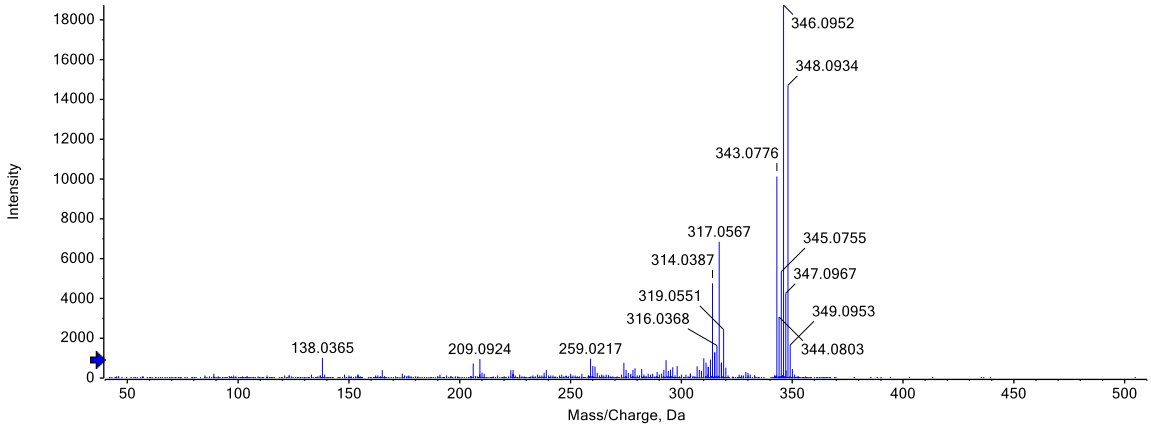

Figure 31: TOF MS data from etizolam (343) and etizolam-D3 (346)

para-Fluorofentanyl in this sample gives rise to a small peak at 6.35 mins. This appears next to a larger peak at 6.43 mins and could be missed if the analyst is not evaluating all peaks present. Figure 32 shows the TOF MS and MSMS data from this peak, matching the data presented above. This demonstrates the difficulty associated with manual data processing; however, this is further complicated when an analyte is not visible in the total ion chromatogram because its intensity does not outmatch that of the background ions.

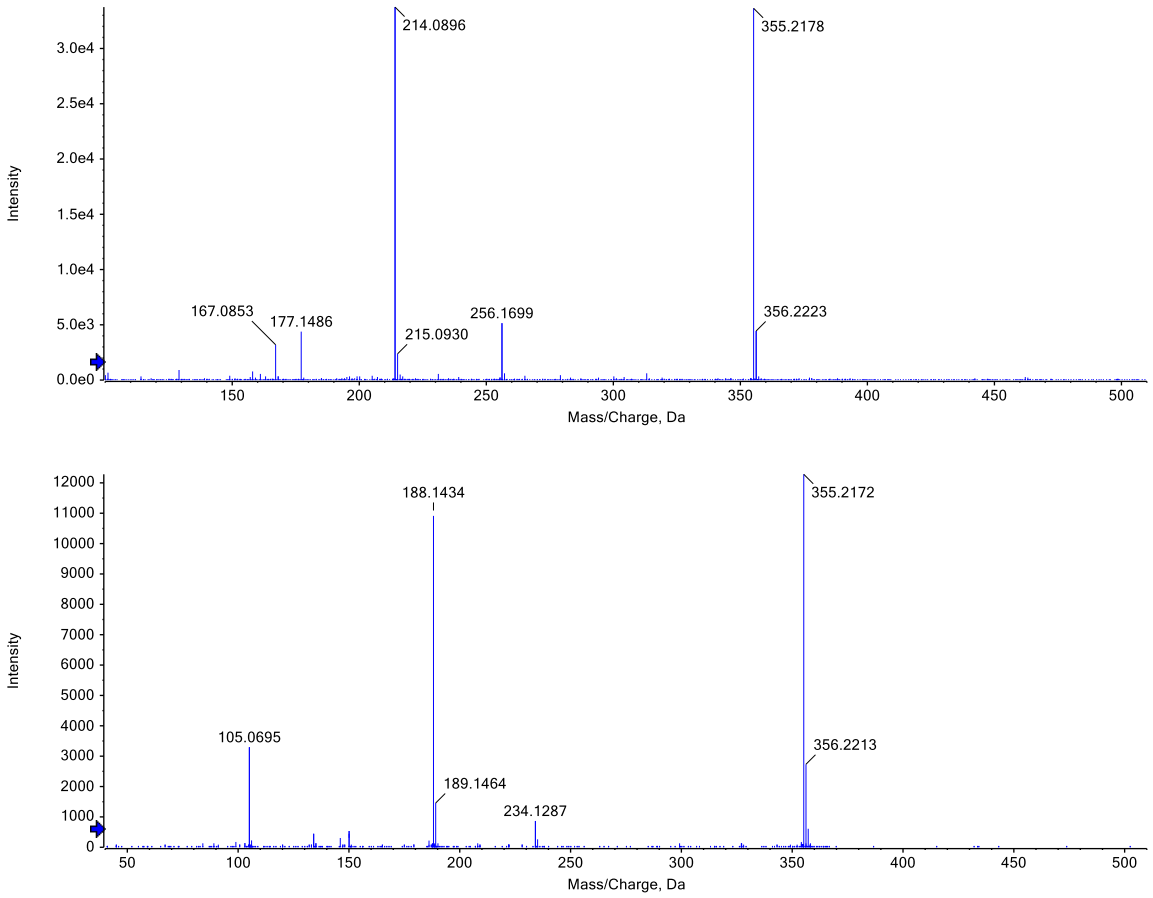

Figure 32: TOF MS (top) and MSMS (bottom) data for *para*-fluorofentanyl

CHAPTER 4

DRUG DISCOVERY

4.1 Introduction

Detailed narrative about the emergence and discovery of NPS has been discussed in Chapters 1 and 2. In short, the discovery of emerging NPS can be difficult due to several factors, including inadequacy of instrumentation, inability to process acquired data, and uncertainly of identifications without standard reference materials. The first part of this research objective was to develop an assay capable of discovering new drugs in biological extracts and then to validate the assay for qualitative use. Based on knowledge of analytical instrumentation and acquisition modes, LC-QTOF-MS was selected as the appropriate analytical platform. This allowed for the execution of a non-target acquisition mode, which in turn allowed for comprehensive acquisition about drugs present in a given sample. Contrary to standard drug testing methodologies, this approach also provided flexibility in terms of new drugs appearing in samples, as method parameters would not need to be changed or adjusted with the emergence of a new substances.

The second part of this research objective was to develop a workflow that would allow for comprehensive data processing. Using LC-QTOF-MS, the acquired datafiles are very large and contain complex information. There is no use to acquiring the data without a proper approach to evaluating it. Therefore, an approach to remain ahead of emerging NPS trends and identifications was developed. This approach focused primarily

on targeted data processing strategies supported by the acquisition of standard reference materials, which were purchased based on intelligence streams.

Based on these considerations, a novel approach to identify and characterize emerging NPS in a timely manner proximate to their first appearance in toxicological casework was developed. Analysis was performed by LC-QTOF-MS on sample extracts acquired from a large independent forensic toxicology laboratory, followed by subsequent processing of datafiles generated. Sample extract is defined herein as the resulting product following extraction (e.g. liquid-liquid, solid phase), often consisting of varying volumes of reconstitution solvent or mobile phase in autosampler vials depending on assay procedure. All results were compiled to track and monitor NPS emergence and prevalence for dissemination to relevant communities. All NPS were identified on a rolling basis as samples were analyzed, processed, and reviewed; and in addition, datafiles were reintegrated as the library database was expanded to include additional NPS.

4.2 Materials

LCMS grade purity solvents (water, methanol, and acetonitrile) were purchased from Honeywell (Morris Plains, NJ, USA) and used for this research. Formic acid ampules (1 mL) were purchased from Thermo Fisher Scientific (Waltham, MA, USA). APCI positive calibration solution was purchased from SCIEX (Framingham, MA, USA).

Standard reference materials were primarily purchased from Cayman Chemical (Ann Arbor, MI, USA) as solid powders and prepared in-house at 1 mg/mL in methanol, or purchased from Cerilliant Corporation (Round Rock, TX, USA) at 1 mg/mL or 100 g/mL. In addition to individually purchased drug standards, four standard mixes were obtained from NMS Labs (Willow Grove, PA, USA) for use in library development and validation. These mixes contained 259 drug species, consisting of abused drugs, therapeutic drugs, emerging drugs, cutting agents or adulterants, and metabolites.

More than 50 NPS standards were purchased during this research including *N*-methyl norfentanyl, 3,4-methylenedioxy-U-47700, isopropyl-U-47700, alpha-PHP, *N*-ethyl hexedrone, *ortho*-fluorofuranylfentanyl, phenylfentanyl, 2F-descloroketamine, 3,4-methylenedioxy-alpha-PHP, eutylone, *N*-ethyl hexylone, *N*-ethyl deschloroketamine, flualprazolam, 3-methoxy-PCP, and 3-hydroxy-PCP. Additional standard materials were acquired during this research from other collaborations with NMS Labs in which the powder material chemical composition was confirmed via GC-MS, LC-QTOF-MS, and NMR analyses. These materials were considered to be standard-quality and were therefore added to the library database. Benzylfuranylfentanyl is an example of a compound in this category.

4.3 Biological Samples

Discarded sample vial extracts were acquired from NMS Labs, a large clinical and forensic toxicology laboratory. These sample extracts contained the extracted and reconstituted product following sample preparation techniques applied to biological

specimens (see below). The sample extracts correlated primarily to blood specimens, but also included urine, serum/plasma, and tissues matrices, all received from a variety of case circumstances, including human performance, clinical, and postmortem investigations. When received at the laboratory, sample extracts were stored in the refrigerator (4 °C) prior to login and analysis.

Due to limited resources for extract analysis compared to sample volume at NMS Labs (i.e. all samples NMS Labs tests could not be re-tested), select sample extracts were designated from testing procedures directed specifically for NPS, including primarily assays for the detection of NPS opioids, NPS stimulants, and NPS benzodiazepines. Assays for the detection of synthetic cannabinoids were not included in this research; although the methodology was capable of detecting synthetic cannabinoids. Less commonly, extracts from assays for common drugs of abuse were also collected, but these extracts comprised a very minor portion of the overall dataset. Literature reports regarding detection of NPS in toxicological casework show that NPS are commonly detected in combination with other NPS,[10] so it was determined that this dataset was the most valuable and appropriate for inclusion in this research.

4.3.1 Human Subjects Research

Prior to inclusion in this research, sample extracts were de-identified. No personally identifiable information was shared or received. This research was determined to be exempt from Institutional Review Board approval due to lack of human subject involvement.

4.3.2 NPS Opioids Sample Preparation

Blood samples were aliquoted (0.5 mL) and fortified with internal standard (25 µL of 0.06 ng/µL). Acetonitrile (1 mL) was then added for protein precipitation, followed by centrifugation at 3,600 rpm for 10 minutes. The supernatant was transferred to a clean test tube and 1 mL of phosphate buffer (0.1 M, pH 6) was added. Samples were extracted via solid phase extraction using Agilent Plexa PCX (3.0 mL, 60 mg) cartridges. To condition the cartridges, 2 mL of methanol was added. To equilibrate the cartridges, 2 mL deionized water was added. Samples were then transferred to the cartridges and allowed to pass through. The cartridges were rinsed using 2 mL hydrochloric acid (0.1 N) and 2 mL of methanol. Samples were eluted from the cartridges using 2 mL ammonium hydroxide in acetonitrile (5:95, v:v). The eluent was evaporated to dryness at 55 °C for 10 minutes. Samples were reconstituted in 1 mL of 0.1% formic acid in deionized water and methanol (80:20, v:v).

4.3.3 NPS Stimulants Sample Preparation

Blood samples were aliquoted (0.5 mL) and fortified with internal standard (25 µL of 2 ng/µL). Acetonitrile (1 mL) was then added for protein precipitation, followed by centrifugation at 3,600 rpm for 10 minutes. The supernatant was transferred to a clean test tube and 1 mL of phosphate buffer (0.1 M, pH 6) was added. Samples were extracted via solid phase extraction using Agilent Plexa PCX 3 (3.0 mL, 30 mg) cartridges. To condition the cartridges, 2 mL of acetonitrile was added. To equilibrate the cartridges, 2 mL deionized water was added. Samples were then transferred to the cartridges and

allowed to pass through. The cartridges were rinsed using 2 mL hydrochloric acid (0.1 N) and 2 mL of acetonitrile. Samples were eluted from the cartridges using 2 mL of water, acetonitrile, and ammonium hydroxide (55:40:5, v:v:v). The eluent was diluted 1:1 with 100 µL of elution solvent and transferred for analysis.

4.3.4 NPS Benzodiazepines Sample Preparation

Blood samples were aliquoted (0.5 mL) and fortified with internal standard (25 µL of 4 ng/µL). Samples were extracted via liquid-liquid extraction using 0.5 mL sodium carbonate (pH 9.0) and 3 mL methyl tert-butyl ether and 1-chlorobutane (60:40, v:v). Samples were capped and rotated for 15 minutes, followed by centrifugation at 3,600 rpm for 10 minutes. The supernatant was removed by freezing the aqueous layer, transferred to a clean test tube, and evaporated to dryness at 40 °C for 15 minutes. Samples were reconstituted in 200 µL of 0.1% formic acid in deionized water and methanol (50:50, v:v).

4.4 Method Parameters

The purpose of this research was to employ a comprehensive, all-inclusive method. A generic assay was developed with long enough run time to create the possibility of adequate separation of analytes, but not too long of a method that would be unbearable in terms of total batch run time. Therefore, it was determined that the use of a generic gradient over 15 minutes was ideal. No further development was considered with

respect to isobaric species or co-eluting analytes; mass separation was determined to be the more ideal separation and speciation method.

Following receipt from NMS Labs, sample extracts were re-analyzed via LC-QTOF-MS. Testing was performed within 2 weeks of receipt of sample extracts, dependent on the number of extracts submitted and instrument capacity or availability. Positive and negative control samples were analyzed following every batch of 20 extracts to monitor instrument performance. LC-QTOF-MS analysis was performed using a SCIEX TripleTOF™ 5600+ (Ontario, Canada) coupled with a Shimadzu Nexera XR ultra high performance liquid chromatograph (Kyoto, Japan).

The injection volume of the assay was 10 µL. Chromatographic separation was achieved using a standard reverse phase gradient from 95% A, 5% B to 5% A, 95% B (Figure 33). Ammonium formate (10mM, pH 3 with formic acid) was used as the aqueous mobile phase, while 0.1% formic acid in methanol/acetonitrile (50:50) was used as the organic mobile phase. A Phenomenex® Kinetex C18 analytical column (50mm x 3.0mm, 2.6µm) was used for analyte separation. The flow rate of the assay was 0.4 mL/min. The column temperature was 30 °C and the autosampler temperature was 15 °C. The resulting LC method had a total run time of 15.5 minutes.

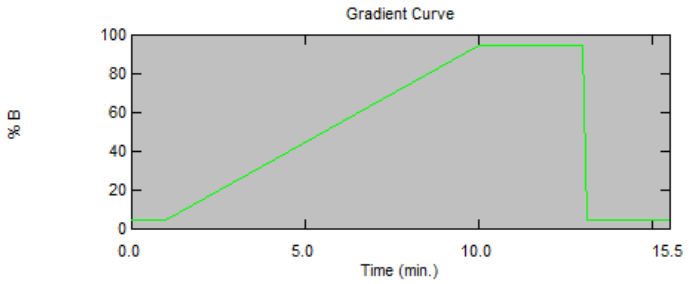

Figure 33: Liquid chromatography reverse-phase gradient

A comprehensive mass acquisition method was developed using SWATH® acquisition. Ionization of analytes was achieved using a DuoSpray™ ion source operating in positive electrospray ionization (ESI+) mode. Source gas parameters were set as follows: ion source gas one 50 psi, ion source gas two 50 psi, and curtain gas 30 psi. The source temperature was set to 600 °C. The IonSpray Voltage Floating (ISVF) was set to 2,500 V.

Precursor ion acquisition was achieved using a TOF MS scan from 100-510 Da. The accumulation time for precursor ions was 0.05 seconds. Product ion acquisition was achieved using SWATH® acquisition. Precursor ions were isolated by the quadrupole (Q1) using a windowed approach (Table 1) where only a range of precursor ions passed through Q1 at a specific time. The mass/charge ratio widths of these windows were variable (6-34 Da) and selected based on the number of analytes clustered around specific masses, overlapping with the windows before and after. These custom designed windows spanned the precursor ion acquisition range (100-510 Da). Following this Q1 windowed isolation, fragmentation occurred using a collision energy spread of 35±15eV. This approach allows for a more complete range of fragment ions produced spanning the mass

range and allows for library database comparisons (i.e. library searching). Fragment ions were acquired from 40-510 Da. The accumulation time for product ions was 0.025 seconds. The total mass acquisition cycle time was 0.77 seconds.

Table 1: Overlapping SWATH® acquisition windows for developed method

Window	Start Mass	End Mass
1	110	130
2	129	160
3	159	170
4	169	180
5	179	190
6	189	196
7	195	210
8	209	230
9	229	240
10	239	255
11	254	264
12	263	272
13	271	283
14	282	288
15	287	301
16	300	311
17	310	318
18	317	329
19	328	342
20	341	358
21	357	376
22	375	386
23	385	402
24	401	417
25	416	450
26	449	479
27	478	510

4.5 Library Database

One main objective of this research was to develop and maintain an extensive and expansive library database. This would allow for the most timely and accurate identifications of emerging NPS. The library database was updated on a rolling basis throughout the course of this research to include new substances for which standard reference materials became available. Typically, the library database was updated on a monthly basis. This update included analysis of standard refence material (1 ng/uL), addition of compound information to the XIC list, and addition of the standard MSMS spectrum to the library file in LibraryView™.

The entire library database can be found in Appendix A in both alphabetical and XIC list formats. In total, the library database contained 796 compounds. Broken down by type (including parent compounds and metabolites), there were 67 drugs of abuse (e.g. cocaine, methamphetamine, heroin), 175 pharmaceutical analytes (e.g. acetaminophen, diphenhydramine, naloxone, trazodone), seven compounds classified as "incidental" (e.g. caffeine, nicotine, quinine), six internal standards, and 541 NPS. Among the NPS, there were 13 NPS benzodiazepines, 54 NPS hallucinogens/dissociatives, 120 NPS opioids, 87 NPS stimulants, two NPS alkaloids (e.g. mitragynine), and three "other" NPS (e.g. UF-17). The largest category of NPS in the library database was synthetic cannabinoids (n=262). This class was not the focus of this study due to chemistry for extraction protocols and were added to the library database as benefit from a separate study; however, these compounds were searched for in the datafiles acquired as part of this research.

4.6 Method Validation

4.6.1 Validation Overview

The described LC-QTOF-MS method was validated for 259 analytes. Method performance was evaluated based on the validation guidelines set forth by the Scientific Working Group for Forensic Toxicology (SWGTOX).[127] Validation experiments were designed to evaluate qualitative identifications and involved precision/accuracy, sensitivity, specificity, carryover, and processed sample stability. The purpose of this validation was to demonstrate the method was suitable of its intended use: qualitative broad-based analyte identification.

4.6.2 Validation Experiments

This evaluation was conducted using four performance mixes containing a wide variety of drugs (n=259), including therapeutic substances, common drugs of abuse, NPS, and metabolites. Each mix was spiked into matrix (e.g. blood), extracted, and analyzed in triplicate over three days, for a total of nine replicates. Analyte specific concentrations in each mix ranged from sub-therapeutic to therapeutic and toxic levels, based on confirmatory capabilities and pharmacological properties. For processed sample stability, a subset of 37 analytes was evaluated using the same criteria as for precision, as well as monitoring peak area ratios over time in reference to the initial analysis. Carryover was evaluated via analysis of blank samples after increased concentration of each analyte.

4.6.3 Validation Results

Overall, all validation data meet acceptability criteria. Data were evaluated within-run (n=3) and between-run (n=9). Criteria evaluated included mass error (ppm error <10), retention time error (RT error <0.35), isotope difference (<50%), and library score (>50). Average peak area is shown for reference. All analytes not detected (ND) during validation experiments were reanalyzed at higher concentration and respective analytical issues were noted for the final method. Accuracy (Table 2), precision (Tables 3 and 4), and processed sample stability (Table 5) results are shown below.

Table 2: Validation data – accuracy

Name	Formula	[M+H]+	Ppm Error	RT Error	Isotope Difference	Library Score	Peak Area	LOD (ng/mL)
10-Hydroxycarbazepine	C15H14N2O2	255.1128	-1.00E-05	0.02	8.9	99	28770	10
1-Hydroxymidazolam	C18H13ClFN3O	342.0804	6.00E-05	0.08	12.4	98	<800	10
25B-NBOMe	C18H22BrNO3	380.0856	-1.00E-04	0.02	12.6	99	<800	1
25C-NBOMe	C18H22ClNO3	336.1361	-1.00E-04	0.02	11.1	100	<800	1
25H-NBOMe	C18H23NO3	302.175	8.00E-05	0.02	8.3	100	<800	1
25I-NBOMe	C18H22INO3	428.0717	2.00E-05	0.02	7.3	99	<800	1
2C-B	C10H14BrNO2	260.0281	2.00E-05	0.02	24.5	92	<800	10
2C-B-FLY	C12H14BrNO2	284.0281	2.00E-05	0.02	15.4	100	<800	10
2C-C	C10H14ClNO2	216.0786	ND	ND	ND	ND	ND	(10)
2C-E	C12H19NO2	210.1489	-2.00E-04	0.02	11.3	90	<800	10
2C-H	C10H15NO2	182.1176	-6.00E-04	0.02	6.7	100	<800	10
2C-I	C10H14INO2	308.0142	8.00E-06	0.02	6.9	99	<800	10
2C-N	C10H14N2O4	227.1026	-4.00E-05	0.03	4.5	94	<800	10
2C-P	C13H21NO2	224.1645	-4.00E-05	0.02	7.9	95	<800	10
2C-T-2	C12H19NO2S	242.1029	ND	ND	ND	ND	ND	(10)
2C-T-7	C13H21NO2S	256.1336	1.00E-03	0.02	17.3	96	<800	10
3,4-DMMC	C12H17NO	192.1383	-3.00E-04	0.02	32.9	100	<800	10
4-MEC	C12H17NO	192.1383	-2.00E-04	0.02	24.1	100	<800	10
5-MeO-DALT	C17H22N2O	271.1805	-5.00E-05	0.01	10.1	98	2156	10
5-MeO-DiPT	C17H26N2O	275.2118	6.00E-05	0.02	8.2	99	2030	10
5-MeO-DMT	C13H18N2O	219.1492	3.00E-05	0.01	8.4	88	1704	10

6-Monoacetylmorphine	C19H21NO4	328.1543	4.00E-05	0.01	8.4	100	1009	2
7-Amino Clonazepam	C15H12ClN3O	286.0742	1.00E-05	0.08	13.1	99	1408	10
7-Amino Flunitrazepam	C16H14FN3O	284.1194	1.00E-04	0.06	9	98	2033	5
7-Hydroxymitragynine	C23H30N2O5	415.2227	ND	ND	ND	ND	ND	(10)
Acetaminophen	C8H9NO2	152.0706	5.00E-05	0.06	6.6	100	70887	100
Acetylfentanyl	C21H26N2O	323.2118	4.00E-05	0.01	7.9	100	<800	0.5
Alfentanil	C21H32N6O3	417.2609	-6.00E-06	0.02	12.7	100	4689	10
Alpha-Hydroxyalprazolam	C17H13ClN4O	325.0851	ND	ND	ND	ND	ND	(20)
Alpha-PVP	C15H21NO	232.1696	-2.00E-05	0.02	8.9	99	6349	2
Alprazolam	C17H13ClN4	309.0902	1.00E-04	0.01	15.7	99	2640	10
Amitriptyline	C20H23N	278.1903	3.00E-04	0.02	11.4	100	41885	50
Amoxapine	C17H16ClN3O	314.1055	3.00E-04	0.02	17.3	100	10236	50
Amphetamine	C9H13N	136.1121	-2.00E-04	0.02	3.1	99	<800	10
AMT	C11H14N2	175.123	-2.00E-04	0.02	5.2	98	<800	10
Aripiprazole	C23H27Cl2N3O2	448.1553	2.00E-05	0.02	15.2	100	3758	50
Atomoxetine	C17H21NO	256.1696	2.00E-04	0.01	10.2	99	47073	10
Atropine	C17H23NO3	290.1751	4.00E-05	0.02	10.5	100	5712	10
BDB	C11H15NO2	194.1176	-2.00E-04	0.03	7	100	866	10
Benzocaine	C9H11NO2	166.0863	-2.00E-04	0.02	6.4	100	2948	25
Benzoylecgonine	C16H19NO4	290.1387	3.00E-04	0.02	7.9	99	<800	100
Benztropine	C21H25NO	308.2009	1.00E-04	0.02	11.4	97	14971	10
Bromo-Dragon FLY	C13H12BrNO2	294.0124	-4.00E-05	0.02	13.8	98	<800	10
Brompheniramine	C16H19BrN2	319.0804	2.00E-04	0.05	10.7	100	2188	10
Bufotenine	C12H16N2O	205.1335	6.00E-05	0.05	7.1	99	<800	10
Buphedrone	C11H15NO	178.1226	-1.00E-04	0.01	5.4	98	<800	100
Bupivacaine	C18H28N2O	289.2274	2.00E-04	0.02	7.2	100	184302	1
Buprenorphine	C29H41NO4	468.3108	-1.00E-04	0.03	15.1	100	<800	1
Bupropion	C13H18ClNO	240.115	ND	ND	ND	ND	ND	(25)
Buspirone	C21H31N5O2	386.2551	4.00E-05	0.02	8.7	100	4249	10
Butorphanol	C21H29NO2	328.2271	4.00E-05	0.02	6.8	100	<800	2
Butylone	C12H15NO3	222.1125	-5.00E-05	0.02	8.6	89	3829	10
BZP	C11H16N2	177.1386	-9.00E-05	0.03	5.2	99	1459	10
Caffeine	C8H10N4O2	195.0877	1.00E-05	0.02	6.3	99	34251	5
Carbamazepine	C15H12N2O	237.1022	2.00E-04	0.01	6.9	100	90138	2
Carbamazepine-10,11-Epoxide	C15H12N2O2	253.0972	9.00E-05	0.23	9.9	98	2243	500
Carisoprodol	C12H24N2O4	261.1809	1.00E-04	0.01	8.5	100	13800	10
Cathinone	C9H11NO	150.0913	ND	ND	ND	ND	ND	(10)
Cephaeline	C28H38N2O4	467.2904	-7.00E-05	0.01	8.1	100	<800	5
Chlordiazepoxide	C16H14ClN3O	300.0898	2.00E-04	0.09	16.3	90	17456	5

Chlorpheniramine	C16H19ClN2	275.131	5.00E-06	0.05	14.4	100	3105	10
Chlorpromazine	C17H19ClN2S	319.103	3.00E-04	0.02	15.3	89	14946	20
Citalopram / Escitalopram	C20H21FN2O	325.1711	2.00E-04	0.02	5.6	100	77498	5
Clobazam	C16H13ClN2O2	301.0738	2.00E-04	0.01	18.5	100	12354	5
Clomipramine	C19H23ClN2	315.1623	2.00E-04	0.01	11.5	99	44329	5
Clonazepam	C15H10ClN3O3	316.0484	-7.00E-06	0.01	11.5	98	<800	10
Clonidine	C9H9Cl2N3	230.0246	-2.00E-05	0.02	14.7	100	1239	5
Clozapine	C18H19ClN4	327.1371	3.00E-04	0.06	16.7	100	28647	5
Cocaethylene	C18H23NO4	318.17	3.00E-04	0.01	10.2	100	25873	1
Cocaine	C17H21NO4	304.1543	2.00E-04	0.02	10.8	100	16658	1
Codeine	C18H21NO3	300.1594	6.00E-05	0.02	10.4	100	3236	10
Cotinine	C10H12N2O	177.1022	4.00E-05	0.03	7.4	98	50205	20
Cyclobenzaprine	C20H21N	276.1747	3.00E-04	0.02	9.2	98	22997	2
DBZP	C18H22N2	267.1856	7.00E-05	0.06	11.5	100	9424	1
Desalkylflurazepam	C15H10ClFN2O	289.0539	4.00E-05	0.01	10.8	99	<800	10
Desipramine	C18H22N2	267.1856	1.00E-04	0.01	8.3	100	44579	1
Desmethylclomipramine	C18H21ClN2	301.1393	2.00E-03	0.01	13.7	96	35893	2
Desmethyldoxepin	C18H19NO	266.1539	7.00E-05	0.02	9.2	92	7280	5
Desmethylsertraline	C16H15Cl2N	292.0654	-3.00E-04	0.02	26.6	100	<800	20
DET	C14H20N2	217.1699	-3.00E-05	0.02	8.6	98	2775	10
Dextro / Levo Methorphan	C18H25NO	272.2009	1.00E-04	0.02	8.3	100	164946	1
Dextrorphan / Levorphanol	C17H23NO	258.1852	2.00E-04	0.02	6.4	100	83228	1
Diacetylmorphine	C21H23NO5	370.1649	-7.00E-05	0.01	9.9	99	<800	10
Diazepam	C16H13ClN2O	285.0789	1.00E-04	0.01	16.1	99	12480	1
Dicyclomine	C19H35NO2	310.2741	1.00E-04	0.01	6.7	100	116691	1
Didesmethylsibutramine	C15H22ClN	252.1514	-5.00E-05	0.02	9.6	99	<800	10
Dihydrocodeine / Hydrocodol	C18H23NO3	302.1751	9.00E-05	0.02	10.2	99	4365	5
Diltiazem	C22H26N2O4S	415.1686	8.00E-05	0.02	7.7	100	73190	2
Diphenhydramine	C17H21NO	256.1696	6.00E-05	0.01	10.4	99	1946	25
DMA	C11H17N	164.1434	-1.00E-04	0.02	8.4	98	5949	10
DMAA (Isomer 1)	C7H17N	116.1434	-3.00E-05	0.03	3.8	100	<800	50
DMT	C12H16N2	189.1386	-2.00E-04	0.02	5.8	99	1227	10
DOB	C11H16BrNO2	274.0437	1.00E-05	0.02	6	94	897	10
DOM	C12H19NO2	210.1489	-8.00E-05	0.02	8.8	98	4179	10
Donepezil	C24H29NO3	380.222	2.00E-04	0.01	13	100	6867	10
Doxepin	C19H21NO	280.1696	2.00E-04	0.01	8.8	86	33133	1
Doxylamine	C17H22N2O	271.1805	1.00E-04	0.12	8	100	18534	2
Duloxetine	C18H19NOS	298.126	5.00E-06	0.02	8.2	100	<800	100
EDDP	C20H23N	278.1903	2.00E-04	0.01	9.8	99	75574	1

Emetine	C29H40N2O4	481.3061	-3.00E-06	0.01	6.5	100	<800	5
Ephedrine / Pseudoephedrine	C10H15NO	166.1226	2.00E-05	0.03	7.4	100	14641	25
Estazolam	C16H11ClN4	295.0745	5.00E-05	0.01	19.9	100	<800	10
Eszopiclone / Zopiclone	C17H17ClN6O3	389.1123	4.00E-05	0.02	8.4	100	<800	10
Ethylone	C12H15NO3	222.1125	-1.00E-04	0.01	5.9	92	911	10
Etodolac	C17H21NO3	288.1594	ND	ND	ND	ND	ND	(50000)
Fentanyl	C22H28N2O	337.2274	-1.00E-05	0.02	8.7	100	<800	1
Flecainide	C17H20F6N2O3	415.1451	2.00E-04	0.02	10.8	100	148993	2
Flunitrazepam	C16H12FN3O3	314.0936	6.00E-05	0.01	14.5	94	<800	5
Fluoxetine	C17H18F3NO	310.1413	3.00E-04	0.02	6.1	100	35380	5
Fluphenazine	C22H26F3N3OS	438.1822	1.00E-04	0.02	12.6	100	1457	5
Flurazepam	C21H23ClFN3O	388.1587	1.00E-04	0.02	17	95	6791	5
Fluvoxamine	C15H21F3N2O2	319.1628	3.00E-04	0.02	9.1	96	36338	10
Glimepiride	C24H34N4O5S	491.2323	-1.00E-04	0.01	22	100	<800	100
Glipizide	C21H27N5O4S	446.1857	ND	ND	ND	ND	ND	(100)
Glutethimide	C13H15NO2	218.1176	-1.00E-04	0.01	6.7	99	822	2500
Guaifenesin	C10H14O4	199.0965	1.00E-04	0.01	6.5	94	27105	100
Haloperidol	C21H23ClFNO2	376.1474	2.00E-04	0.01	15.1	100	3156	10
Hydrocodone	C18H21NO3	300.1594	4.00E-05	0.02	9.4	98	1465	10
Hydromorphone	C17H19NO3	286.1438	-4.00E-05	0.04	5.4	100	<800	2
Hydroxybupropion	C13H18ClNO2	256.1099	1.00E-04	0.02	14.6	99	21654	100
Hydroxyethylflurazepam	C17H14ClFN2O2	333.0801	1.00E-04	0.01	10.1	92	1325	10
Hydroxytriazolam	C17H12Cl2N4O	359.0461	6.00E-05	0.01	10.4	100	<800	5
Hydroxyzine	C21H27ClN2O2	375.1834	4.00E-05	0.02	15.4	100	21450	2
Iloperidone	C24H27FN2O4	427.2028	1.00E-04	0.02	14	100	7589	10
Imipramine	C19H24N2	281.2012	3.00E-04	0.01	8.6	100	54998	2
Indomethacin	C19H16ClNO4	358.0841	8.00E-05	0.01	12	98	<800	5000
Ketamine	C13H16ClNO	238.0993	3.00E-06	0.02	16.7	100	6375	10
Ketoprofen	C16H14O3	255.1016	1.00E-04	0.01	6.3	100	57205	5000
Lacosamide	C13H18N2O3	251.139	-8.00E-05	0.01	5.3	100	<800	1000
Lamotrigine	C9H7N5Cl2	256.0151	0.00E+00	0.02	17.1	96	21099	10
Levamisole	C11H12N2S	205.0794	3.00E-05	0.03	8.3	100	138992	1
Levetiracetam	C8H14N2O2	171.1128	-8.00E-05	0.03	5.2	100	2575	1000
Lidocaine	C14H22N2O	235.1805	6.00E-05	0.01	8.7	100	422206	1
Lorazepam	C15H10Cl2N2O2	321.0192	7.00E-05	0.01	23.2	100	<800	5
Loxapine	C18H18ClN3O	328.1211	2.00E-04	0.02	15	95	23806	5
LSD	C20H25N3O	324.207	2.00E-05	0.02	22.5	96	<800	2
Maprotiline	C20H23N	278.1903	3.00E-04	0.01	11.3	99	42844	5
MBDB	C12H17NO2	208.1332	-7.00E-06	0.01	8	97	7063	10

MBZP	C12H18N2	191.1543	-2.00E-04	0.14	8	99	2127	10
mCPP	C10H13ClN2	197.084	-8.00E-06	0.02	16.1	100	14770	5
MDA	C10H13NO2	180.1019	-3.00E-04	0.02	5.8	100	<800	10
MDEA	C12H17NO2	208.1332	-3.00E-05	0.01	8.8	100	7696	5
MDMA	C11H15NO2	194.1176	-9.00E-05	0.02	7.5	100	4454	5
MDPV	C16H21NO3	276.1594	2.00E-04	0.02	10.3	100	11952	1
MEGX	C12H18N2O	207.1492	4.00E-05	0.02	9.2	100	176153	2
Memantine	C12H21N	180.1747	-1.00E-04	0.02	8.8	98	3209	10
Meperidine	C15H21NO2	248.1645	-4.00E-07	0.01	9.8	100	71577	10
Mephedrone	C11H15NO	178.1226	-6.00E-05	0.02	8	93	4069	10
Mepivacaine	C15H22N2O	247.1805	1.00E-04	0.02	8.8	100	376919	10
Meprobamate	C9H18N2O4	219.1339	4.00E-05	0.02	6.3	100	9157	100
Mescaline	C11H17NO3	212.1281	-9.00E-05	0.01	10	96	<800	10
Mesoridazine	C21H26N2OS2	387.1559	2.00E-04	0.01	12	100	17990	10
Metaxalone	C12H15NO3	222.1125	9.00E-05	0.01	8.2	99	23584	2
Methadone	C21H27NO	310.2165	1.00E-04	0.01	8.4	98	77929	2
Methamphetamine	C10H15N	150.1277	-1.00E-04	0.02	6.7	99	3370	5
Methaqualone	C16H14N2O	251.1179	1.00E-04	0.01	6	100	918038	1
Methcathinone	C10H13NO	164.107	-9.00E-05	0.02	6.5	92	2539	5
Methedrone	C11H15NO2	194.1176	2.00E-05	0.01	7	91	4940	5
Methocarbamol	C11H15NO5	242.1023	6.00E-05	0.02	5.2	99	78241	50
Methoxetamine	C15H21NO2	248.1645	2.00E-05	0.02	8.6	99	<800	2
Methylone	C11H13NO3	208.0968	1.00E-05	0.02	7.8	99	3916	5
Methylphenidate	C14H19NO2	234.1489	6.00E-05	0.01	7.3	100	5204	5
Metoclopramide	C14H22ClN3O2	300.1473	2.00E-04	0.02	14.4	99	5815	5
Mexiletine	C11H17NO	180.1383	-4.00E-06	0.02	7.1	97	53829	25
Midazolam	C18H13ClFN3	326.0855	6.00E-05	0.04	11.3	98	1907	5
Mirtazapine	C17H19N3	266.1652	1.00E-04	0.06	9.2	100	19379	5
Mitragynine	C23H30N2O4	399.2278	8.00E-05	0.02	12.9	98	1782	10
Morphine	C17H19NO3	286.1438	-2.00E-05	0.03	4.3	99	<800	10
Nalbuphine	C21H27NO4	358.2013	7.00E-05	0.01	12.3	98	2634	2
Naloxone	C19H21NO4	328.1543	ND	ND	ND	ND	ND	(1)
Naltrexone	C20H23NO4	342.17	ND	ND	ND	ND	ND	(1)
Naphyrone	C19H23NO	282.1852	7.00E-05	0.02	10.4	100	11182	5
Naproxen	C14H14O3	231.1016	1.00E-04	0.01	6.5	88	<800	50000
Nicotine	C10H14N2	163.123	ND	ND	ND	ND	ND	(100)
Nifedipine	C17H18N2O6	347.1238	1.00E-05	0.01	8.5	96	956	10
Norbuprenorphine	C25H35NO4	414.2639	1.00E-04	0.01	28.7	100	<800	2
Norclozapine	C17H17ClN4	313.1215	3.00E-04	0.08	14.1	100	8018	25

Nordiazepam	C15H11ClON2	271.0633	1.00E-04	0.02	11	98	801	20
Norfentanyl	C14H20N2O	233.1648	3.00E-05	0.02	3.7	100	<800	1
Norflunitrazepam	C15H10FN3O3	300.0779	-6.00E-06	0.01	4	100	<800	20
Norfluoxetine	C16H16F3NO	296.1257	1.00E-04	0.02	7.2	99	1961	100
Norketamine	C12H14ClNO	224.0837	-5.00E-05	0.01	14.3	98	1645	20
Normeperidine	C14H19NO2	234.1489	1.00E-04	0.01	8.1	100	50922	5
Norpropoxyphene	C21H27NO2	326.2115	7.00E-05	0.01	10.2	99	11713	25
Norpseudoephedrine	C9H13NO	152.107	-1.00E-04	0.03	5.4	100	1802	250
Nortriptyline	C19H21N	264.1747	2.00E-04	0.02	10.3	100	31512	2
O-Desmethyltramadol	C15H23NO2	250.1802	4.00E-05	0.02	8.9	100	21037	1
O-Desmethylvenlafaxine	C16H25NO2	264.1958	1.00E-04	0.02	7.7	94	41531	2
Orphenadrine	C18H23NO	270.1852	1.00E-04	0.01	8.1	99	2029	50
Oxazepam	C15H11ClN2O2	287.0582	ND	ND	ND	ND	ND	(20)
Oxycodone	C18H21NO4	316.1543	4.00E-06	0.02	9.9	100	<800	10
Oxymorphone	C17H19NO4	302.1387	-1.00E-05	0.04	7.3	100	<800	2
Papaverine	C20H21NO4	340.4243	-8.00E-02	0.02	7.2	98	383003	2
Paroxetine	C19H20FNO3	330.15	3.00E-04	0.01	11.5	98	7375	20
Pentazocine	C19H27NO	286.2165	2.00E-04	0.02	5.9	100	82994	10
Pentedrone	C12H17NO	192.1383	ND	ND	ND	ND	ND	(2)
Pentylone	C13H17NO3	236.1281	-8.00E-05	0.02	7.7	96	2414	10
Perphenazine	C21H26ClN3OS	404.1558	-2.00E-05	0.03	8.8	100	<800	5
Phenazepam	C15H10BrClN2O	348.9738	2.00E-05	0.01	16.9	99	<800	10
Phencyclidine (PCP)	C17H25N	244.206	1.00E-04	0.02	11.5	100	5876	2
Phendimetrazine	C12H17NO	192.1383	-7.00E-05	0.02	7.1	93	2163	10
Pheniramine	C16H20N2	241.1699	-1.00E-05	0.1	6.3	99	2029	10
Phenmetrazine	C11H15NO	178.1226	-5.00E-05	0.02	8.4	99	6150	10
Phensuximide	C11H11NO2	190.0863	-4.00E-05	0.02	5	99	889	2000
Phentermine	C10H15N	150.1277	-2.00E-05	0.02	5.6	99	2209	25
Phenyltoloxamine	C17H21NO	256.1696	2.00E-04	0.01	8.1	99	55497	5
Phenytoin	C15H12N2O2	253.0972	-6.00E-05	0.01	5.7	100	<800	1000
PMA	C10H15NO	166.1226	-2.00E-04	0.02	4.1	98	<800	10
Primidone	C12H14N2O2	219.1128	1.00E-04	0.02	13	96	13023	250
Procainamide	C13H21N3O	236.1757	6.00E-05	0.07	7.5	100	657580	5
Prochlorperazine	C20H24ClN3S	374.1452	5.00E-05	0.03	17.8	99	2533	10
Promazine	C17H20N2S	285.142	7.00E-05	0.01	6.5	88	42615	5
Promethazine	C17H20N2S	285.142	4.00E-05	0	11.4	86	2466	5
Propoxyphene	C22H29NO2	340.2271	2.00E-04	0.01	8.6	100	65555	25
Protriptyline	C19H21N	264.1747	1.00E-04	0.01	10.6	98	20282	2
Psilocin	C12H16N2O	205.1335	-4.00E-05	0.09	5	80	<800	10

Pyrilamine	C17H23N3O	286.1914	9.00E-05	0.07	9.7	100	39360	5
Pyrovalerone	C16H23NO	246.1852	5.00E-05	0.02	8.9	100	6569	5
Quetiapine	C21H25N3O2S	384.174	2.00E-04	0.03	9.8	100	70926	50
Quinidine	C20H24N2O2	325.1911	-5.00E-05	0.11	8.6	99	340559	1
Quinine	C20H24N2O2	325.1911	2.00E-04	0.09	4.1	99	415220	1
Ramelteon	C16H21NO2	260.1645	-3.00E-05	0.01	9	99	<800	1
Risperidone	C23H27FN4O2	411.2191	1.00E-04	0.04	9.1	100	896	5
Salvinorin B	C21H26O7	391.1751	ND	ND	ND	ND	ND	(10)
Scopolamine	C17H21NO4	304.1543	6.00E-05	0.02	9.1	99	4063	10
Sertraline	C17H17Cl2N	306.0811	-3.00E-05	0.02	17.2	100	1623	10
Sibutramine	C17H26ClN	280.1827	7.00E-05	0.02	28.4	97	1642	10
Sildenafil	C22H30N6O4S	475.2122	3.00E-05	0.02	11.5	100	2649	25
Strychnine	C21H22N2O2	335.1754	2.00E-04	0.02	7.9	100	44764	1
Sufentanil	C22H30N2O2S	387.2101	-5.00E-05	0.02	7.8	99	<800	1
Tadalafil	C22H19N3O4	390.1448	ND	ND	ND	ND	ND	(50)
Tapentadol	C14H23NO	222.1852	1.00E-04	0.01	9.5	100	8632	1
Temazepam	C16H13ClN2O2	301.0738	3.00E-04	0.01	16.9	100	5821	10
Tetrahydrozoline	C13H16N2	201.1386	-2.00E-04	0.02	4.3	100	<800	1
TFMPP	C11H13F3N2	231.1104	1.00E-04	0.02	8.4	99	5260	5
Theophylline	C7H8N4O2	181.072	-1.00E-04	0.03	3.3	99	<800	8000
Thioridazine	C21H26N2S2	371.161	3.00E-04	0.01	12.2	99	12686	1
Ticlopidine	C14H14ClNS	264.0608	2.00E-04	0.04	15.7	100	37438	10
Topiramate	C12H21NO8S	340.1061	4.00E-05	0.01	2.5	74	<800	500
Tramadol	C16H25NO2	264.1958	2.00E-04	0.02	9.1	100	45502	0.5
Tranylcypromine	C9H11N	134.0964	-9.00E-06	0.11	4.5	100	<800	10
Trazodone	C19H22ClN5O	372.1586	1.00E-04	0.02	13.7	100	59326	1
Triazolam	C17H12Cl2N4	343.0512	5.00E-05	0.01	14.5	100	1394	5
Trifluoperazine	C21H24F3N3S	408.1716	3.00E-06	0.02	10.9	100	847	5
Trihexyphenidyl	C20H31NO	302.2478	1.00E-04	0.02	10.3	100	2745	5
Trimipramine	C20H26N2	295.2169	3.00E-04	0.01	9.3	99	44462	5
Triprolidine	C19H22N2	279.1856	3.00E-05	0.04	10.9	100	8058	1
Vardenafil	C23H32N6O4S	489.2279	1.00E-04	0.04	12.7	100	5353	25
Venlafaxine	C17H27NO2	278.2115	3.00E-04	0.02	11.3	100	58576	1
Verapamil	C27H38N2O4	455.2904	2.00E-04	0.02	10.6	100	18121	2
Voriconazole	C16H14F3N5O	350.1223	1.00E-04	0.02	6.7	100	134832	10
Warfarin	C19H16O4	309.1121	1.00E-04	0	11.6	98	2356	250
Xylazine	C12H16N2S	221.1107	-7.00E-06	0.02	7.4	100	2787	5
Yohimbine	C21H26N2O3	355.2016	8.00E-05	0.02	9.7	100	<800	10
Zaleplon	C17H15N5O	306.1349	9.00E-05	0.02	9	98	1290	10

Ziprasidone	C21H21ClN4OS	413.1197	2.00E-04	0.02	15.9	100	<800	10
Zolpidem	C19H21N3O	308.1757	1.00E-04	0.02	11.8	100	11119	10
Zonisamide	C8H8N2O3S	213.0328	8.00E-05	0.02	3.9	91	<800	250

Key: ND – Not detected, (#) – Indicates the concentration at which a compound was not detected during initial validation

Table 3: Validation data – precision (within run, n=3, %CV)

Name	Measured Mass			Isotope Difference			Retention Time			Peak Area		
	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3
10-Hydroxycarbazepine	5.7E-05	9.2E-05	4.8E-05	27.2	31.6	36.2	0.2	0.0	0.0	7.2	4.5	8.4
1-Hydroxymidazolam	8.6E-05	2.1E-04	1.9E-04	4.1	50.0	20.9	0.2	0.0	0.0	14.8	14.7	8.6
25B-NBOMe	4.9E-05	1.2E-04	4.6E-05	38.7	32.6	41.3	0.1	0.1	0.1	16.2	13.1	11.4
25C-NBOMe	1.5E-04	1.8E-04	6.4E-05	15.1	22.3	17.0	0.0	0.1	0.0	6.7	19.8	17.1
25H-NBOMe	8.3E-05	1.3E-04	1.2E-04	61.3	9.2	31.7	0.0	0.0	0.1	3.0	13.6	9.4
25I-NBOMe	9.0E-05	1.6E-04	1.1E-04	26.9	64.4	54.8	0.1	0.1	0.1	5.6	12.4	18.5
2C-B	-	1.7E-04	2.0E-04	-	6.1	56.9	-	0.0	0.0	-	4.6	5.1
2C-E	-	4.6E-04	3.0E-04	-	63.6	24.6	-	0.1	0.0	-	61.2	27.8
2C-I	5.7E-05	1.9E-04	3.9E-04	48.0	101.9	24.6	0.0	0.1	0.1	17.5	46.5	22.0
2C-N	1.5E-04	8.5E-05	7.1E-05	113.6	29.5	19.6	0.1	0.1	0.1	8.0	7.8	10.6
2C-P	2.5E-05	1.7E-04	1.9E-04	36.7	19.7	61.7	0.1	0.1	0.1	26.7	71.3	34.2
3,4-DMMC	1.5E-04	8.1E-05	1.7E-04	2.2	20.3	20.0	0.1	0.0	0.2	19.2	20.2	12.9
4-MEC	2.6E-04	2.0E-04	2.1E-04	23.5	47.1	62.0	0.0	0.1	0.0	19.7	7.5	6.7
5-MeO-DALT	6.3E-05	1.7E-04	2.5E-04	82.1	53.5	50.4	0.0	0.1	0.2	40.4	12.1	10.7
5-MeO-DiPT	1.0E-04	8.2E-05	4.4E-05	32.8	54.7	3.3	0.1	0.1	0.0	67.7	13.5	43.2
6-Monoacetylmorphine	1.2E-04	5.8E-05	1.4E-04	8.8	6.6	54.9	0.1	0.1	0.1	11.3	7.6	17.6
7-Amino Clonazepam	8.8E-05	2.3E-05	4.7E-05	31.0	9.7	30.1	0.1	0.0	0.1	7.8	7.4	8.0
7-Amino Flunitrazepam	3.2E-05	9.4E-05	4.1E-05	8.0	26.8	15.6	0.1	0.1	0.1	21.3	7.2	8.3
Acetaminophen	8.7E-05	2.3E-05	3.2E-05	4.6	3.9	6.6	0.2	0.4	0.5	6.4	11.4	4.1
Acetylfentanyl	1.6E-04	2.4E-04	4.0E-05	86.5	36.4	53.2	0.1	0.1	0.0	11.2	13.0	10.1
Alfentanil	1.3E-04	8.4E-05	1.3E-04	18.7	60.2	17.1	0.1	0.0	0.0	11.8	6.5	4.0
Alpha-PVP	9.7E-05	1.1E-04	4.8E-05	61.3	20.8	20.5	0.0	0.1	0.1	12.3	17.0	13.3
Alprazolam	3.2E-05	1.8E-04	7.4E-05	2.4	17.3	23.4	0.0	0.1	0.1	8.7	10.7	5.4
Amitriptyline	7.5E-05	2.0E-04	6.5E-05	15.6	24.3	3.5	0.1	0.1	0.1	10.5	6.7	2.5
Amoxapine	1.4E-04	1.3E-05	2.0E-04	4.6	13.7	17.2	0.1	0.1	0.1	7.6	9.3	12.4
Amphetamine	3.8E-04	5.4E-04	1.2E-04	103.8	0.0	77.1	0.3	0.3	0.0	16.8	13.8	5.7
AMT	7.2E-05	4.2E-04	9.7E-05	37.6	10.5	72.4	0.1	0.1	0.1	26.8	13.4	11.1
Aripiprazole	8.0E-05	2.0E-04	2.6E-04	17.5	48.2	21.2	0.1	0.1	0.0	6.8	13.4	7.9
Atomoxetine	5.3E-05	9.9E-05	1.5E-04	32.3	14.1	10.3	0.1	0.1	0.1	8.3	4.5	9.0
Atropine	1.2E-04	2.0E-04	1.4E-05	17.0	10.9	13.0	0.0	0.1	0.0	6.7	12.4	15.2

BDB	8.6E-05	7.1E-05	9.4E-05	87.0	61.0	110.2	0.1	0.1	0.1	7.6	13.2	6.0
Benzocaine	1.0E-04	1.7E-04	2.0E-04	12.4	2.6	12.9	0.2	0.0	0.0	18.5	19.2	20.7
Benzoylecgonine	1.0E-04	6.1E-04	-	116.9	81.6	-	0.0	0.2	-	22.5	19.6	-
Benztropine	6.9E-05	1.6E-04	2.4E-04	12.9	40.2	26.4	0.0	0.1	0.1	21.4	15.6	19.6
Bromo-Dragon FLY	1.3E-04	1.1E-04	1.7E-04	51.8	67.4	38.6	0.2	0.1	0.1	2.8	13.3	12.8
Brompheniramine	1.6E-05	6.4E-05	1.3E-04	13.9	18.6	11.7	0.1	0.0	0.0	25.3	3.0	14.1
Bufotenine	1.8E-04	1.5E-04	1.2E-04	26.3	47.8	47.0	0.0	0.8	0.3	25.0	4.9	26.4
Buphedrone	5.2E-05	1.8E-04	1.2E-04	23.7	64.4	64.6	0.0	0.0	0.1	10.1	16.5	12.6
Bupivacaine	1.2E-04	7.0E-05	1.7E-04	53.5	48.3	23.0	0.2	0.0	0.0	4.0	11.6	4.7
Buprenorphine	3.0E-04	-	5.6E-04	48.8	-	79.2	0.2	-	0.1	3.8	-	11.6
Buspirone	9.7E-05	4.1E-05	2.6E-04	15.8	58.8	9.9	0.1	0.1	0.1	6.8	11.4	2.9
Butorphanol	2.5E-05	1.2E-05	1.5E-04	47.3	43.9	45.7	0.0	0.1	0.1	9.2	9.0	6.6
Butylone	2.2E-05	1.4E-04	6.6E-05	5.1	3.4	7.5	0.0	0.1	0.0	6.8	9.5	10.7
BZP	9.6E-05	6.2E-05	8.8E-05	13.8	27.7	49.0	0.5	0.7	0.0	3.7	19.0	9.3
Caffeine	1.2E-04	1.1E-04	7.6E-05	8.9	13.6	67.2	0.1	0.1	0.1	2.0	17.7	14.3
Carbamazepine	8.7E-05	6.0E-05	9.6E-05	37.9	56.1	65.3	0.0	0.0	0.0	7.9	7.5	3.0
Carbamazepine-10, 11 Epoxide	4.9E-05	2.2E-04	4.8E-05	2.1	14.4	2.4	0.1	0.0	0.1	10.0	8.6	3.4
Carisoprodol	3.3E-05	1.7E-04	2.4E-04	2.5	7.8	9.8	0.0	0.1	0.1	4.3	3.9	1.7
Cephaeline	1.2E-04	1.5E-04	1.4E-04	19.9	49.6	44.0	0.1	0.1	0.1	15.4	6.6	10.5
Chlordiazepoxide	3.1E-05	5.5E-05	1.2E-04	12.7	18.9	5.0	0.1	0.1	0.0	2.0	1.7	10.5
Chlorpheniramine	3.7E-05	3.2E-05	8.3E-05	11.0	29.3	6.9	0.1	0.1	0.0	17.8	10.9	13.0
Chlorpromazine	1.1E-04	1.3E-04	1.5E-04	22.1	29.6	2.7	0.1	0.1	0.1	12.3	12.6	3.2
Citalopram / Escitalopram	1.7E-05	2.0E-04	2.4E-04	42.6	18.4	51.2	0.1	0.0	0.0	8.2	15.1	5.5
Clobazam	1.3E-04	9.6E-05	3.0E-05	37.4	14.7	0.3	0.0	0.1	0.0	16.0	14.2	4.3
Clomipramine	2.1E-04	1.7E-04	1.7E-04	16.5	19.9	21.1	0.1	0.1	0.0	8.5	12.2	6.3
Clonazepam	1.1E-04	1.3E-04	2.4E-04	64.6	72.6	68.8	0.1	0.1	0.0	13.8	20.0	5.0
Clonidine	1.5E-05	2.3E-05	3.1E-05	44.9	2.6	36.2	0.3	0.2	0.2	13.0	14.2	11.0
Clozapine	6.3E-05	1.7E-04	2.4E-04	12.8	11.0	9.6	0.2	0.1	0.0	9.4	12.7	13.0
Cocaethylene	1.5E-04	2.0E-05	1.4E-04	3.2	21.7	12.3	0.1	0.1	0.0	5.5	10.5	1.9
Cocaine	8.7E-05	2.2E-04	1.3E-04	27.5	11.8	5.9	0.1	0.0	0.0	3.1	7.7	11.0
Codeine	8.7E-05	8.4E-06	6.0E-05	3.2	22.1	33.0	0.3	0.0	0.2	13.5	9.2	12.6
Cotinine	1.0E-04	9.4E-05	8.8E-05	3.8	3.3	6.3	0.5	0.5	1.5	9.0	5.8	4.1
Cyclobenzaprine	2.0E-04	1.1E-04	1.9E-04	58.8	67.4	18.8	0.1	0.1	0.0	12.4	10.5	3.8
DBZP	7.9E-05	1.3E-04	6.4E-05	13.3	13.7	14.7	0.0	0.1	0.0	13.2	17.0	14.5
Desalkylflurazepam	1.9E-05	1.4E-04	2.5E-04	27.3	15.1	33.8	0.0	0.1	0.0	13.5	10.8	5.4
Desipramine	6.4E-05	2.3E-04	5.8E-05	5.8	41.6	59.9	0.1	0.1	0.0	4.8	14.5	0.9
Desmethylclomipramine	3.8E-05	1.5E-04	1.7E-04	16.2	16.7	28.8	0.1	0.1	0.0	11.8	9.4	3.6
Desmethyldoxepin	1.6E-04	8.5E-05	9.2E-05	42.1	6.6	18.8	0.1	0.1	0.0	10.2	13.2	4.5
DET	2.4E-04	3.5E-05	8.3E-05	20.9	28.3	19.7	0.0	0.1	0.0	27.5	34.1	29.9

Dextro / Levo Methorphan	1.3E-04	1.1E-04	4.6E-04	23.9	51.7	11.3	0.1	0.1	0.0	11.3	8.5	6.0
Dextrorphan / Levorphanol	5.1E-05	1.5E-04	1.0E-04	15.8	67.4	23.8	0.1	0.0	0.0	6.4	11.6	8.9
Diazepam	4.7E-05	2.4E-04	2.0E-04	4.4	11.0	10.7	0.1	0.1	0.1	9.1	8.0	5.7
Dicyclomine	2.0E-04	3.2E-04	1.1E-04	56.0	63.7	50.7	0.1	0.0	0.0	5.3	7.7	6.3
Didesmethylsibutramine	1.2E-04	6.6E-05	6.6E-05	48.0	36.6	15.1	0.1	0.0	0.0	9.2	9.6	4.8
Dihydrocodeine / Hydrocodol	4.0E-05	3.6E-05	1.2E-04	3.5	15.7	21.6	0.2	0.3	0.2	11.8	9.1	7.1
Diltiazem	2.7E-04	7.5E-05	1.2E-04	26.0	64.2	17.0	0.1	0.0	0.1	9.6	11.1	6.9
Diphenhydramine	6.0E-05	7.3E-05	5.7E-05	19.9	16.9	13.1	0.1	0.1	0.0	16.8	4.7	23.2
DMA (Dimethylamphetamine)	1.1E-04	1.1E-04	1.1E-04	4.6	8.6	3.3	0.1	0.0	0.1	7.2	12.4	11.5
DMAA	1.9E-04	2.2E-04	1.3E-04	56.1	29.2	20.8	0.4	0.6	0.4	47.5	47.0	47.0
DMT	7.3E-05	2.3E-04	1.2E-04	37.2	45.5	31.0	0.1	0.1	0.0	19.4	35.0	23.6
DOB	6.2E-05	1.3E-04	1.5E-05	65.5	48.2	40.8	0.1	0.0	0.1	5.4	16.0	16.0
DOM	1.0E-04	2.2E-04	4.1E-05	6.9	4.8	11.1	0.0	0.0	0.0	7.3	13.7	14.4
Donepezil	4.2E-05	2.8E-04	8.3E-05	2.6	57.0	6.7	0.1	0.1	0.1	10.8	4.6	11.0
Doxepin	1.5E-04	1.5E-04	8.3E-05	56.3	14.9	37.6	0.1	0.0	0.0	7.2	1.2	5.0
Doxylamine	9.3E-05	1.7E-04	1.3E-04	69.5	31.6	17.6	0.0	0.3	0.1	9.9	11.7	3.9
Duloxetine	9.6E-05	1.4E-04	1.4E-04	52.2	12.8	46.6	0.1	0.1	0.1	27.2	25.6	26.9
EDDP	1.9E-04	1.1E-04	1.1E-04	6.8	29.0	7.6	0.1	0.1	0.0	5.6	6.6	13.6
Emetine	7.1E-05	9.0E-05	1.4E-04	12.0	80.0	24.7	0.1	0.1	0.1	11.0	13.4	3.8
Ephedrine / Pseudoephedrine	9.3E-05	7.0E-06	1.0E-04	11.5	3.3	3.8	0.2	0.3	0.0	4.5	7.7	6.1
Estazolam	2.3E-04	7.7E-05	8.6E-05	49.5	38.3	70.6	0.1	0.1	0.1	28.1	5.7	1.7
Eszopiclone / Zopiclone	3.4E-05	1.7E-04	1.3E-04	70.3	86.7	61.2	0.1	0.0	0.0	5.1	9.4	1.9
Ethylone	9.0E-05	2.2E-04	4.3E-05	20.3	36.6	8.8	0.0	0.2	0.0	7.8	10.7	13.5
Fentanyl	1.8E-04	1.7E-04	4.1E-04	39.9	14.3	55.4	0.1	0.1	0.1	7.3	17.0	4.4
Flecainide	7.8E-05	1.6E-04	1.5E-04	15.4	19.2	8.8	0.2	0.0	0.0	3.1	16.8	3.0
Flunitrazepam	9.3E-05	1.2E-04	7.0E-05	26.2	111.7	87.5	0.1	0.1	0.1	11.1	10.7	6.2
Fluoxetine	1.6E-04	1.7E-04	1.2E-04	61.6	63.4	23.6	0.1	0.1	0.0	1.6	11.5	5.2
Fluphenazine	3.1E-04	9.7E-05	5.0E-05	14.4	17.2	15.8	0.0	0.1	0.0	2.1	18.7	12.6
Flurazepam	1.3E-04	1.9E-04	4.1E-04	6.3	20.3	5.3	0.1	0.1	0.1	16.7	26.6	9.4
Fluvoxamine	5.5E-05	1.7E-04	1.2E-04	16.4	19.3	6.8	0.1	0.1	0.0	10.5	10.0	5.9
Glimepiride	1.3E-04	3.6E-04	-	86.5	9.6	-	0.2	0.1	-	11.7	35.7	-
Glutethimide	2.3E-05	1.4E-04	1.1E-04	12.4	33.4	23.5	0.1	0.1	0.1	7.9	6.9	3.9
Guaifenesin	7.0E-05	1.0E-04	1.2E-04	24.8	18.0	5.9	0.1	0.0	0.1	6.8	1.8	8.4
Haloperidol	9.5E-05	1.6E-04	5.0E-05	15.9	24.2	19.2	0.1	0.1	0.0	3.8	3.0	9.1
Hydrocodone	5.7E-05	1.3E-04	2.0E-05	44.1	24.9	1.9	0.3	0.1	0.0	6.3	20.2	10.9
Hydromorphone	1.2E-04	9.3E-05	5.7E-05	54.7	15.1	25.3	0.2	0.4	0.0	17.5	4.7	13.8
Hydroxybupropion	1.2E-04	1.9E-04	3.3E-05	50.3	11.2	14.1	0.1	0.1	0.1	4.4	4.8	6.0
Hydroxyethylflurazepam	1.3E-04	1.4E-04	1.1E-04	17.3	55.1	49.0	0.1	0.1	0.1	2.0	8.5	10.6
Hydroxytriazolam	2.1E-04	5.8E-05	2.3E-04	72.5	78.4	88.8	0.1	0.1	0.0	10.2	16.5	20.8

Hydroxyzine	1.0E-04	3.6E-05	1.7E-04	13.4	0.8	10.3	0.1	0.0	0.1	11.2	16.6	10.4
Iloperidone	3.5E-05	1.5E-04	2.1E-05	14.5	42.6	17.1	0.1	0.0	0.0	10.5	6.1	7.6
Imipramine	3.3E-05	2.6E-04	2.6E-04	9.0	58.2	8.3	0.2	0.1	0.0	1.7	8.1	3.4
Indomethacin	1.3E-04	1.8E-04	1.5E-04	34.5	11.1	60.8	0.0	0.1	0.1	1.4	4.4	5.6
Ketamine	1.0E-04	6.4E-05	8.7E-05	8.9	8.2	2.1	0.0	0.0	0.1	7.4	10.1	9.7
Ketoprofen	1.5E-04	1.1E-04	7.2E-05	28.5	101.7	10.7	0.0	0.1	0.1	14.4	15.8	8.1
Lacosamide	4.8E-05	5.8E-05	1.4E-04	63.4	69.3	42.2	0.1	0.0	0.0	18.1	8.1	4.8
Lamotrigine	1.3E-04	2.0E-04	2.4E-04	54.4	6.4	51.4	0.2	0.0	0.1	3.0	1.2	7.8
Levamisole	6.5E-05	8.8E-05	1.2E-04	5.2	19.9	16.2	0.2	0.0	0.0	10.1	6.2	11.8
Levetiracetam	3.1E-05	7.5E-05	1.1E-04	26.4	17.2	27.6	0.2	0.2	0.4	13.2	5.7	8.5
Lidocaine	2.4E-05	1.2E-04	9.2E-05	1.2	13.2	13.3	0.2	0.1	0.1	5.3	9.3	5.6
Loxapine	1.4E-04	1.0E-04	1.7E-04	14.0	4.6	5.7	0.1	0.1	0.1	7.8	5.4	8.5
LSD	2.7E-04	2.2E-04	4.2E-05	11.5	28.7	80.0	0.0	0.3	0.2	13.2	39.8	12.0
Maprotiline	9.5E-05	1.5E-04	1.9E-04	15.0	5.3	11.6	0.1	0.0	0.0	5.8	8.3	4.2
MBDB	6.0E-05	1.0E-04	5.8E-05	20.8	9.2	8.7	0.0	0.1	0.0	7.4	7.0	13.3
MBZP	1.0E-04	1.2E-04	1.3E-04	14.8	5.7	5.5	0.4	0.2	0.2	12.6	15.7	20.2
mCPP	4.3E-05	2.9E-05	2.3E-04	12.8	1.7	2.2	0.2	0.0	0.0	4.3	1.7	9.6
MDA	3.2E-05	9.8E-05	1.2E-04	18.2	97.6	20.8	0.3	0.2	0.2	3.0	10.7	3.3
MDEA	4.1E-05	1.3E-04	5.7E-05	9.5	8.2	1.2	0.1	0.1	0.0	7.3	9.5	9.8
MDMA	7.0E-05	1.1E-04	1.2E-04	13.9	17.6	7.7	0.2	0.1	0.0	7.9	11.7	10.2
MDPV	8.2E-05	2.5E-04	7.1E-05	6.3	19.1	9.9	0.1	0.1	0.0	7.4	7.7	14.9
Memantine	1.5E-04	7.6E-05	1.8E-04	2.6	7.5	8.2	0.2	0.1	0.1	9.4	8.6	11.9
Meperidine	4.1E-05	1.3E-04	5.6E-05	20.7	24.6	8.0	0.2	0.0	0.1	7.4	17.2	7.0
Mephedrone	5.9E-05	7.5E-05	2.0E-04	10.1	4.9	14.8	0.1	0.0	0.1	11.9	13.9	5.6
Mepivacaine	3.2E-05	6.8E-05	8.1E-05	62.5	45.9	21.0	0.1	0.0	0.1	1.3	3.0	5.9
Meprobamate	1.4E-04	1.5E-04	5.6E-05	13.6	15.4	11.7	0.1	0.1	0.0	7.9	9.1	4.2
Mescaline	7.8E-05	1.2E-04	9.2E-05	78.9	59.0	57.0	0.2	0.3	0.2	35.9	5.6	15.8
Mesoridazine	5.8E-05	3.1E-05	1.9E-04	20.9	25.3	12.3	0.1	0.1	0.0	3.3	18.2	24.3
Metaxalone	2.5E-04	1.1E-04	1.3E-04	15.3	15.6	6.6	0.1	0.1	0.0	11.2	7.9	4.3
Methadone	9.1E-05	2.1E-04	2.2E-04	61.0	20.7	65.5	0.1	0.1	0.0	7.9	7.3	4.9
Methamphetamine	4.5E-05	1.3E-04	9.9E-05	8.9	16.0	12.4	0.2	0.2	0.2	8.7	12.1	13.6
Methaqualone	1.0E-04	1.7E-04	7.4E-05	70.9	17.2	6.8	0.1	0.1	0.0	1.7	3.6	0.8
Methcathinone	1.3E-05	3.0E-05	5.3E-05	33.5	5.1	9.8	0.0	0.2	0.2	2.2	10.5	8.5
Methedrone	2.4E-04	7.6E-05	2.3E-04	28.2	6.3	13.1	0.0	0.0	0.1	10.5	5.9	12.9
Methocarbamol	4.1E-05	1.2E-04	4.9E-05	75.0	9.4	68.1	0.1	0.1	0.1	1.1	3.8	13.0
Methoxetamine	1.3E-04	4.7E-05	1.0E-04	54.8	51.7	130.3	0.1	0.1	0.1	0.1	2.3	7.2
Methylone	3.4E-05	2.0E-05	6.9E-05	22.8	5.3	3.0	0.0	0.3	0.0	14.7	9.6	6.9
Methylphenidate	7.3E-05	2.0E-04	1.5E-04	30.0	57.4	6.3	0.1	0.1	0.0	18.0	15.8	5.7
Metoclopramide	2.4E-05	9.5E-05	1.6E-04	11.1	10.6	57.4	0.1	0.1	0.1	12.0	17.8	4.4

Mexiletine	1.9E-05	1.9E-04	1.0E-04	7.7	51.3	6.0	0.2	0.1	0.0	1.6	0.5	9.0
Midazolam	4.0E-05	1.4E-04	3.2E-05	34.6	21.2	22.0	0.2	0.0	0.0	13.0	10.5	9.1
Mirtazapine	1.7E-04	1.4E-04	1.3E-04	52.9	11.0	14.0	0.2	0.0	0.1	9.4	13.0	7.5
Mitragynine	3.6E-05	6.3E-06	2.6E-04	13.8	13.6	7.2	0.1	0.0	0.1	43.3	35.6	61.6
Monoethylglycinexylidide (MEGX)	2.4E-05	8.9E-05	1.8E-04	3.5	16.4	0.6	0.3	0.2	0.2	1.9	6.4	4.0
Morphine	7.9E-05	7.3E-06	5.0E-05	52.2	41.0	72.7	0.0	0.4	0.7	9.2	15.6	4.5
Nalbuphine	7.7E-05	1.7E-04	2.0E-04	8.8	10.4	10.2	0.1	0.0	0.1	18.1	10.1	12.7
Naphyrone	1.2E-04	7.4E-05	2.5E-04	31.7	24.6	12.8	0.1	0.1	0.1	6.4	15.1	15.8
Naproxen	1.2E-04	1.0E-04	1.0E-04	41.0	62.1	10.0	0.1	0.1	0.1	9.3	11.2	13.6
Nifedipine	1.1E-04	2.1E-04	1.2E-04	16.9	11.4	30.8	0.2	0.0	0.1	15.7	11.9	13.4
Norclozapine	6.3E-05	1.5E-04	9.0E-05	7.1	2.8	12.1	0.0	0.1	0.0	11.4	3.6	3.8
Nordiazepam	1.8E-04	2.4E-05	1.4E-04	50.9	17.5	47.9	0.1	0.1	0.1	5.5	8.4	13.8
Norflunitrazepam	5.7E-04	-	3.1E-04	68.1	-	38.7	0.0	-	0.1	12.5	-	17.5
Norfluoxetine	1.0E-04	1.7E-04	1.0E-04	85.8	18.3	74.4	0.1	0.1	0.1	9.0	8.2	8.8
Norketamine	5.8E-05	6.6E-05	8.9E-05	12.6	8.8	7.1	0.1	0.1	0.1	5.4	17.6	11.6
Normeperidine	9.5E-05	2.4E-04	8.8E-05	15.9	8.6	5.5	0.1	0.0	0.0	5.9	9.0	4.6
Norpropoxyphene	1.1E-04	5.8E-05	5.3E-05	10.1	27.2	38.5	0.2	0.1	0.0	16.5	10.2	10.9
Norpseudoephedrine / Phenylpropanolamine	5.0E-05	1.3E-04	2.9E-05	29.7	19.5	21.7	0.2	0.3	0.2	9.4	9.4	6.9
Nortriptyline	4.0E-05	1.1E-04	2.4E-04	61.3	3.5	6.2	0.1	0.1	0.0	5.2	3.7	5.1
O-Desmethyltramadol	1.3E-05	1.1E-04	6.8E-05	7.0	7.0	5.3	0.1	0.1	0.1	1.3	11.9	8.1
O-Desmethylvenlafaxine	1.0E-04	1.3E-04	2.3E-04	5.2	31.8	24.6	0.2	0.1	0.1	2.9	8.0	4.5
Orphenadrine	8.5E-05	3.6E-05	1.8E-04	31.9	44.7	21.1	0.1	0.1	0.1	25.9	18.0	21.5
Oxycodone	6.4E-05	1.8E-04	4.1E-04	80.3	87.7	13.5	0.0	0.3	0.2	6.7	11.1	12.4
Oxymorphone	4.8E-05	5.2E-05	4.4E-05	49.3	38.3	18.4	0.3	0.0	0.8	10.8	12.5	3.5
Papaverine	1.6E-04	2.0E-04	1.6E-04	67.2	68.5	29.4	0.1	0.1	0.0	2.5	3.3	6.1
Paroxetine	1.7E-04	2.4E-05	6.1E-05	6.5	12.8	10.4	0.0	0.1	0.0	9.4	12.0	2.6
Pentazocine	2.4E-05	1.5E-04	4.5E-05	91.8	29.3	69.7	0.1	0.0	0.0	4.3	3.5	2.7
Pentylone	1.3E-04	9.7E-05	4.2E-05	9.4	31.2	22.8	0.0	0.1	0.0	2.1	8.4	12.0
Perphenazine	8.7E-05	1.3E-04	5.2E-06	55.5	44.0	51.4	0.1	0.1	0.0	24.6	44.2	22.2
Phenazepam	1.1E-04	1.5E-04	1.8E-04	43.9	58.4	91.3	0.1	0.1	0.1	1.4	19.9	15.6
Phencyclidine (PCP)	1.3E-04	1.3E-04	9.0E-05	13.7	12.2	13.0	0.1	0.1	0.1	9.9	12.2	5.5
Phendimetrazine	2.5E-04	9.2E-05	3.1E-04	18.2	39.6	8.6	0.2	0.0	0.0	4.2	14.4	16.4
Pheniramine	9.8E-05	3.7E-04	1.2E-04	82.2	68.6	36.2	0.2	0.1	0.1	13.1	4.9	4.4
Phenmetrazine	6.0E-05	2.1E-05	4.7E-05	9.3	9.6	4.3	0.3	0.0	0.0	12.0	10.9	11.6
Phensuximide	5.3E-05	5.5E-05	1.4E-04	94.2	20.9	20.8	0.1	0.1	0.1	11.2	11.0	4.2
Phentermine	1.0E-04	5.4E-05	2.7E-04	73.1	12.8	14.1	0.1	0.1	0.1	13.4	5.0	4.9
Phenyltoloxamine	4.6E-05	1.6E-04	4.1E-05	32.3	29.6	20.9	0.1	0.0	0.1	3.0	2.4	6.2
Phenytoin	1.8E-04	1.5E-04	3.2E-05	79.6	84.1	42.5	0.1	0.1	0.0	13.1	22.3	10.3
PMA (para-Methoxyamphetamine)	1.6E-04	2.0E-04	1.7E-04	10.7	61.8	69.1	0.1	0.1	0.1	2.6	6.6	8.1

Primidone	1.1E-04	3.0E-05	1.1E-04	45.9	82.9	47.3	0.1	0.1	0.1	5.4	2.6	1.8
Procainamide	7.5E-05	5.7E-05	6.4E-05	84.3	17.1	10.3	0.3	0.6	0.0	4.4	3.6	3.7
Prochlorperazine	5.1E-05	1.4E-04	7.9E-05	14.3	10.4	21.1	0.1	0.0	0.0	34.2	19.4	5.3
Promazine	8.4E-05	1.5E-04	4.8E-05	22.8	27.7	24.5	0.2	0.0	0.0	22.4	32.6	10.0
Promethazine	8.4E-05	2.1E-04	2.4E-04	18.3	27.1	4.4	0.1	0.1	0.0	7.5	19.1	4.6
Propoxyphene	2.2E-05	1.8E-04	1.2E-04	60.7	61.3	44.9	0.0	0.1	0.0	7.7	20.3	0.1
Protriptyline	7.0E-05	4.7E-05	1.8E-04	3.3	30.6	40.7	0.1	0.1	0.0	7.7	13.5	4.3
Psilocin	6.7E-05	1.1E-04	4.1E-05	62.6	16.1	53.1	0.2	0.2	0.3	11.4	13.3	32.2
Pyrilamine	3.2E-05	1.0E-04	4.1E-04	19.5	2.0	8.6	0.2	0.0	0.1	16.2	22.3	2.1
Pyrovalerone	8.7E-05	7.9E-05	1.4E-04	77.5	8.6	13.0	0.1	0.1	0.1	10.6	13.4	14.5
Quetiapine	1.6E-04	9.9E-05	1.5E-04	2.4	31.0	25.2	0.1	0.1	0.1	6.3	9.2	4.9
Quinidine	5.4E-05	4.7E-05	4.2E-05	45.2	57.5	74.9	0.2	0.0	0.1	5.4	3.5	2.8
Quinine	5.4E-05	6.0E-05	1.1E-05	66.0	69.5	27.2	0.1	0.1	0.1	8.2	11.7	3.2
Ramelteon	2.4E-04	7.8E-05	2.0E-05	131.8	71.1	92.8	0.2	0.1	0.0	24.8	33.8	24.7
Risperidone	7.1E-05	1.8E-04	1.7E-04	54.0	31.3	83.6	0.2	0.2	0.1	11.1	1.5	12.8
Scopolamine	9.6E-05	8.0E-05	1.3E-04	17.3	69.0	7.9	0.0	0.0	0.0	3.7	15.5	11.0
Sertraline	2.0E-04	2.1E-04	1.1E-04	21.2	12.0	24.1	0.1	0.1	0.0	4.1	12.0	7.4
Sibutramine	1.6E-05	7.5E-05	2.5E-05	28.2	45.0	0.0	0.1	0.1	0.1	18.5	14.1	8.2
Sildenafil	2.2E-04	1.1E-05	4.4E-05	18.5	18.0	29.0	0.1	0.1	0.0	13.0	20.4	3.3
Strychnine	7.9E-05	1.1E-04	1.0E-04	10.0	38.6	27.8	0.0	0.1	0.1	3.7	8.4	15.1
Sufentanil	1.2E-04	6.8E-05	2.5E-04	28.4	19.0	13.6	0.1	0.1	0.1	8.0	11.1	13.5
Tapentadol	1.1E-04	1.4E-04	5.4E-05	19.0	2.6	14.4	0.1	0.1	0.0	8.6	9.6	6.0
Temazepam	1.6E-04	6.5E-05	4.3E-05	9.6	1.1	10.7	0.1	0.1	0.1	7.9	8.3	5.3
Tetrahydrozoline	1.6E-04	1.2E-04	1.0E-04	98.4	22.3	14.0	0.1	0.0	0.1	11.5	14.1	10.5
TFMPP	1.4E-04	1.3E-04	2.9E-05	13.1	18.2	6.0	0.0	0.1	0.1	5.1	15.1	11.7
Theophylline	5.1E-05	8.4E-05	1.7E-04	33.3	30.2	70.9	0.3	0.2	0.0	10.4	9.3	18.9
Thioridazine	7.3E-05	1.5E-04	1.9E-04	19.1	9.4	45.5	0.0	0.1	0.0	31.7	24.2	14.0
Ticlopidine	1.1E-04	2.4E-04	7.0E-05	7.9	18.0	14.7	0.1	0.0	0.0	9.1	9.1	5.2
Tramadol	9.3E-05	4.5E-05	1.3E-04	31.7	3.9	2.7	0.1	0.0	0.0	5.8	6.7	7.5
Tranylcypromine	7.4E-05	1.3E-04	9.5E-05	69.0	40.7	41.4	0.1	0.0	0.0	4.1	3.1	6.8
Trazodone	5.5E-05	4.3E-05	2.0E-04	27.0	4.0	22.9	0.1	0.0	0.1	8.9	9.0	7.0
Triazolam	3.1E-05	1.4E-04	5.3E-05	1.5	9.0	22.3	0.1	0.1	0.1	7.5	9.3	17.6
Trifluoperazine	2.5E-04	1.1E-04	4.7E-05	12.5	18.9	30.9	0.0	0.1	0.1	26.2	48.9	9.2
Trihexyphenidyl	3.1E-05	7.8E-05	1.0E-04	17.0	34.3	23.2	0.1	0.1	0.1	7.2	6.5	20.2
Trimipramine	9.1E-05	2.6E-04	2.1E-04	60.5	11.1	20.7	0.1	0.0	0.0	4.1	7.1	9.7
Triprolidine	4.6E-05	9.8E-05	1.9E-04	6.7	9.6	68.1	0.2	0.1	0.0	16.9	24.6	2.5
Vardenafil	1.5E-04	1.2E-04	2.0E-04	37.8	36.4	35.1	0.1	0.1	0.0	12.4	17.7	5.4
Venlafaxine	4.8E-05	1.1E-04	1.8E-04	19.8	11.2	15.2	0.1	0.1	0.1	8.4	3.3	4.7
Verapamil	4.3E-05	2.6E-04	2.1E-04	50.3	7.1	32.9	0.2	0.0	0.0	7.7	15.9	2.4

Voriconazole	1.1E-04	1.6E-04	1.2E-04	88.1	65.3	66.7	0.2	0.1	0.1	4.3	20.6	6.4
Warfarin	6.7E-05	1.8E-04	3.5E-05	11.5	4.6	12.0	0.0	0.1	0.0	24.4	7.4	8.7
Xylazine	5.5E-05	3.5E-05	1.4E-04	12.2	21.5	15.2	0.1	0.0	0.0	20.6	8.0	7.6
Yohimbine	2.3E-04	1.9E-04	2.1E-04	28.6	5.5	26.1	0.2	0.1	0.1	15.6	8.1	8.1
Zaleplon	2.1E-04	4.6E-05	1.9E-04	23.2	42.2	16.0	0.1	0.1	0.1	5.2	3.2	2.1
Ziprasidone	2.3E-04	1.4E-05	2.6E-04	46.1	18.3	17.8	0.1	0.1	0.1	18.9	1.7	9.9
Zolpidem	7.7E-05	8.6E-05	1.3E-04	44.6	12.4	13.6	0.1	0.0	0.0	8.4	6.4	3.2
Zonisamide	1.0E-04	5.4E-06	1.6E-04	17.5	29.0	27.3	0.1	0.1	0.0	18.7	7.8	15.4

Table 4: Validation data – precision (between run, n=9, %CV)

Name	Measured Mass	Isotope Difference	Retention Time	Peak Area
10-Hydroxycarbazepine	7.6E-05	28.2	0.3	16.0
1-Hydroxymidazolam	1.6E-04	33.4	1.2	26.8
25B-NBOMe	2.3E-04	73.4	0.3	37.7
25C-NBOMe	1.7E-04	18.1	0.3	29.9
25H-NBOMe	1.6E-04	40.6	0.3	25.0
25I-NBOMe	2.6E-04	44.0	0.2	33.7
2C-B	2.8E-04	38.8	0.3	15.1
2C-E	3.6E-04	66.3	0.3	59.3
2C-I	3.0E-04	69.8	0.4	36.4
2C-N	9.6E-05	53.4	0.5	31.0
2C-P	1.5E-04	55.8	0.3	84.6
3,4-DMMC	2.1E-04	30.4	0.4	35.0
4-MEC	1.9E-04	63.5	0.4	39.6
5-MeO-DALT	2.0E-04	60.7	0.3	38.7
5-MeO-DiPT	8.0E-05	58.2	0.4	86.7
6-Monoacetylmorphine	1.0E-04	42.5	0.5	21.8
7-Amino Clonazepam	7.5E-05	26.7	1.7	46.5
7-Amino Flunitrazepam	7.7E-05	18.9	1.2	32.7
Acetaminophen	5.5E-05	5.8	2.4	8.5
Acetylfentanyl	2.2E-04	59.1	0.3	24.3
Alfentanil	1.4E-04	32.7	0.3	11.8
Alpha-PVP	8.1E-05	34.5	0.4	34.8
Alprazolam	1.1E-04	15.1	0.2	44.1
Amitriptyline	1.7E-04	15.6	0.2	11.9
Amoxapine	1.5E-04	11.7	0.3	16.9
Amphetamine	3.9E-04	105.7	0.7	18.1
AMT	3.3E-04	44.0	0.6	29.5

Aripiprazole	2.1E-04	28.3	0.2	16.3
Atomoxetine	1.7E-04	19.5	0.2	9.2
Atropine	1.2E-04	14.3	0.5	16.6
BDB	8.1E-05	77.1	0.5	17.4
Benzocaine	1.7E-04	9.6	0.4	31.6
Benzoylecgonine	4.0E-04	71.2	0.4	23.7
Benztropine	1.7E-04	25.4	0.2	34.8
Bromo-Dragon FLY	1.2E-04	53.2	0.3	27.2
Brompheniramine	1.6E-04	18.7	0.7	35.6
Bufotenine	1.4E-04	39.9	2.3	24.4
Buphedrone	1.4E-04	81.5	0.4	34.9
Bupivacaine	1.1E-04	47.5	0.3	10.9
Buprenorphine	4.3E-04	61.6	0.1	21.5
Buspirone	1.6E-04	36.1	0.3	20.7
Butorphanol	1.1E-04	40.0	0.3	24.6
Butylone	8.1E-05	12.2	0.5	17.8
BZP	8.5E-05	34.8	11.1	26.8
Caffeine	1.3E-04	32.5	0.6	15.0
Carbamazepine	8.0E-05	49.7	0.2	10.0
Carbamazepine-10, 11 Epoxide	1.3E-04	9.7	0.3	28.6
Carisoprodol	1.5E-04	9.2	0.2	15.4
Cephaeline	1.6E-04	57.8	0.4	20.8
Chlordiazepoxide	1.5E-04	17.2	1.5	19.5
Chlorpheniramine	5.1E-05	16.5	0.9	39.8
Chlorpromazine	1.3E-04	24.3	0.2	11.2
Citalopram / Escitalopram	1.7E-04	37.5	0.3	13.1
Clobazam	1.4E-04	27.9	0.2	16.4
Clomipramine	1.8E-04	24.8	0.2	8.9
Clonazepam	1.7E-04	69.9	0.2	24.7
Clonidine	2.8E-05	38.2	0.7	16.2
Clozapine	1.6E-04	13.3	1.0	20.1
Cocaethylene	1.1E-04	20.1	0.2	8.5
Cocaine	1.5E-04	16.7	0.3	20.5
Codeine	5.4E-05	23.3	0.7	25.8
Cotinine	9.7E-05	8.9	4.1	44.9
Cyclobenzaprine	1.7E-04	46.7	0.2	14.9
DBZP	1.3E-04	13.2	1.1	23.1
Desalkylflurazepam	1.6E-04	33.6	0.2	33.6
Desipramine	1.3E-04	36.2	0.2	8.0

Desmethylclomipramine	1.2E-04	22.0	0.2	14.3
Desmethyldoxepin	1.2E-04	24.4	0.2	19.0
DET	1.4E-04	23.2	0.4	41.4
Dextro / Levo Methorphan	2.6E-04	44.0	0.3	15.6
Dextrorphan / Levorphanol	1.0E-04	35.8	0.5	15.3
Diazepam	1.7E-04	15.3	0.2	11.8
Dicyclomine	2.1E-04	54.0	0.1	19.5
Didesmethylsibutramine	1.2E-04	35.0	0.2	22.5
Dihydrocodeine / Hydrocodol	7.3E-05	14.5	0.6	9.0
Diltiazem	1.7E-04	36.1	0.2	10.6
Diphenhydramine	5.6E-05	16.8	0.2	28.2
DMA (Dimethylamphetamine)	1.2E-04	8.5	0.5	14.5
DMAA	2.0E-04	40.0	0.7	47.2
DMT	1.4E-04	43.7	0.6	33.0
DOB	8.7E-05	45.9	0.4	26.0
DOM	1.4E-04	10.0	0.4	18.7
Donepezil	2.0E-04	32.6	0.2	15.3
Doxepin	1.4E-04	38.8	0.2	8.2
Doxylamine	1.6E-04	48.1	3.0	52.9
Duloxetine	1.2E-04	45.0	0.2	39.3
EDDP	1.4E-04	27.2	0.2	8.1
Emetine	1.1E-04	49.2	0.3	26.1
Ephedrine / Pseudoephedrine	9.2E-05	9.7	0.8	18.0
Estazolam	1.4E-04	71.1	0.3	32.6
Eszopiclone / Zopiclone	1.3E-04	68.4	0.4	29.9
Ethylone	1.3E-04	26.4	0.5	23.2
Fentanyl	2.7E-04	42.3	0.3	34.2
Flecainide	1.4E-04	17.1	0.3	15.2
Flunitrazepam	1.7E-04	96.8	0.2	24.8
Fluoxetine	1.8E-04	56.3	0.2	7.3
Fluphenazine	1.7E-04	15.0	0.2	20.0
Flurazepam	3.2E-04	9.3	0.3	18.5
Fluvoxamine	1.1E-04	17.4	0.2	9.4
Glimepiride	2.2E-04	58.4	0.2	21.6
Glutethimide	9.8E-05	23.0	0.3	19.8
Guaifenesin	9.6E-05	18.6	0.3	11.2
Haloperidol	2.0E-04	18.4	0.2	18.5
Hydrocodone	9.4E-05	41.2	0.5	18.2
Hydromorphone	1.0E-04	41.4	2.1	20.9

Hydroxybupropion	1.5E-04	30.2	0.4	58.5
Hydroxyethylflurazepam	1.1E-04	37.1	0.2	18.8
Hydroxytriazolam	2.5E-04	85.3	0.1	26.0
Hydroxyzine	1.1E-04	13.7	0.2	14.9
Iloperidone	1.9E-04	30.7	0.2	15.4
Imipramine	1.9E-04	37.0	0.2	7.4
Indomethacin	1.7E-04	40.5	0.1	11.6
Ketamine	7.8E-05	10.9	0.5	14.7
Ketoprofen	1.1E-04	52.5	0.1	19.5
Lacosamide	1.0E-04	56.0	0.4	16.0
Lamotrigine	2.0E-04	36.8	0.5	65.9
Levamisole	9.6E-05	16.7	0.8	9.8
Levetiracetam	6.8E-05	25.6	1.0	21.1
Lidocaine	1.2E-04	18.6	0.4	6.8
Loxapine	1.8E-04	20.6	0.3	12.3
LSD	1.6E-04	58.3	0.4	24.3
Maprotiline	2.0E-04	13.0	0.2	11.2
MBDB	8.2E-05	13.5	0.5	16.5
MBZP	1.2E-04	10.0	5.1	24.6
mCPP	1.4E-04	10.7	0.5	16.5
MDA	1.4E-04	74.0	0.6	9.5
MDEA	7.4E-05	14.5	0.5	14.2
MDMA	9.9E-05	15.8	0.5	10.8
MDPV	1.5E-04	11.8	0.3	15.0
Memantine	1.3E-04	10.8	0.4	17.3
Meperidine	8.7E-05	17.4	0.3	29.9
Mephedrone	1.3E-04	14.5	0.5	13.4
Mepivacaine	5.9E-05	42.8	0.4	7.8
Meprobamate	1.1E-04	15.0	0.3	17.2
Mescaline	1.3E-04	59.8	0.5	27.1
Mesoridazine	1.3E-04	18.6	0.1	32.5
Metaxalone	1.7E-04	15.6	0.2	14.2
Methadone	1.6E-04	47.6	0.2	13.9
Methamphetamine	1.2E-04	13.2	0.6	16.5
Methaqualone	1.2E-04	33.9	0.2	5.7
Methcathinone	3.7E-05	21.9	0.7	7.7
Methedrone	1.8E-04	24.5	0.5	13.2
Methocarbamol	1.2E-04	52.2	0.4	11.6
Methoxetamine	7.8E-05	144.8	0.4	36.9

Methylone	7.8E-05	16.9	0.7	13.6
Methylphenidate	1.4E-04	41.5	0.3	84.9
Metoclopramide	1.0E-04	29.1	0.5	34.1
Mexiletine	1.3E-04	25.2	0.5	15.4
Midazolam	1.2E-04	37.3	0.6	31.0
Mirtazapine	1.3E-04	28.5	1.2	25.4
Mitragynine	1.8E-04	18.9	0.3	55.3
Monoethylglycinexylidide (MEGX)	1.1E-04	10.8	0.6	10.6
Morphine	5.4E-05	56.7	2.1	18.6
Nalbuphine	1.9E-04	11.5	0.4	16.6
Naphyrone	1.6E-04	21.0	0.3	22.0
Naproxen	1.0E-04	36.2	0.2	10.1
Nifedipine	1.5E-04	19.6	0.2	23.6
Norclozapine	1.5E-04	11.9	1.4	23.2
Nordiazepam	1.2E-04	44.3	0.4	38.8
Norflunitrazepam	3.4E-04	41.6	0.1	27.8
Norfluoxetine	1.1E-04	56.2	0.2	14.3
Norketamine	7.9E-05	16.3	0.5	25.5
Normeperidine	1.4E-04	11.7	0.3	6.4
Norpropoxyphene	7.5E-05	27.5	0.2	17.1
Norpseudoephedrine / Phenylpropanolamine	1.2E-04	23.4	1.7	20.2
Nortriptyline	1.4E-04	31.8	0.1	6.1
O-Desmethyltramadol	8.0E-05	17.8	0.6	12.4
O-Desmethylvenlafaxine	1.5E-04	20.4	0.5	11.3
Orphenadrine	1.1E-04	33.8	0.2	40.7
Oxycodone	2.4E-04	77.2	0.5	30.9
Oxymorphone	6.1E-05	33.7	2.1	13.8
Papaverine	1.6E-04	75.1	0.3	5.0
Paroxetine	2.2E-04	13.2	0.2	8.1
Pentazocine	8.9E-05	78.7	0.3	12.1
Pentylone	1.1E-04	22.5	0.4	24.8
Perphenazine	1.1E-04	44.1	0.3	28.4
Phenazepam	1.5E-04	57.1	0.1	19.7
Phencyclidine (PCP)	1.1E-04	13.0	0.2	14.2
Phendimetrazine	2.6E-04	24.6	0.6	21.5
Pheniramine	2.1E-04	60.0	2.5	29.2
Phenmetrazine	7.3E-05	12.1	0.6	14.4
Phensuximide	8.8E-05	51.3	0.3	19.5
Phentermine	1.8E-04	36.2	0.4	18.7

Phenyltoloxamine	9.7E-05	30.9	0.2	12.5
Phenytoin	1.3E-04	61.0	0.2	21.1
PMA (para-Methoxyamphetamine)	2.1E-04	49.5	0.5	14.8
Primidone	1.1E-04	65.2	0.4	9.6
Procainamide	6.1E-05	41.3	3.0	12.8
Prochlorperazine	9.1E-05	14.1	0.3	29.7
Promazine	1.0E-04	26.5	0.2	21.0
Promethazine	1.8E-04	19.4	0.2	17.4
Propoxyphene	1.9E-04	49.9	0.1	14.3
Protriptyline	1.0E-04	26.0	0.2	10.1
Psilocin	7.6E-05	45.9	1.2	48.8
Pyrilamine	2.1E-04	11.7	1.2	23.4
Pyrovalerone	9.7E-05	38.9	0.4	27.9
Quetiapine	1.5E-04	34.5	0.5	7.9
Quinidine	5.3E-05	71.8	2.3	10.4
Quinine	1.0E-04	80.4	2.1	8.9
Ramelteon	1.4E-04	94.1	0.2	26.4
Risperidone	1.4E-04	50.5	0.6	20.4
Scopolamine	1.6E-04	33.6	0.6	13.6
Sertraline	1.9E-04	27.0	0.2	20.5
Sibutramine	7.6E-05	28.9	0.2	33.7
Sildenafil	1.6E-04	21.2	0.4	25.7
Strychnine	1.1E-04	34.5	0.4	10.3
Sufentanil	1.8E-04	22.0	0.2	18.9
Tapentadol	9.1E-05	16.9	0.4	57.3
Temazepam	1.2E-04	10.7	0.2	18.2
Tetrahydrozoline	1.2E-04	58.0	0.5	27.4
TFMPP	9.6E-05	17.1	0.4	14.6
Theophylline	1.8E-04	57.8	0.9	22.8
Thioridazine	1.3E-04	24.5	0.1	35.1
Ticlopidine	1.4E-04	15.3	0.6	7.3
Tramadol	1.1E-04	16.5	0.4	15.7
Tranylcypromine	9.5E-05	49.3	1.9	22.7
Trazodone	1.2E-04	18.7	0.3	17.8
Triazolam	1.3E-04	32.4	0.1	47.8
Trifluoperazine	1.8E-04	27.3	0.2	43.4
Trihexyphenidyl	7.7E-05	29.9	0.2	19.6
Trimipramine	1.8E-04	35.9	0.1	21.3
Triprolidine	1.1E-04	32.1	0.7	25.4

Vardenafil	1.6E-04	42.2	0.6	40.7
Venlafaxine	1.3E-04	14.2	0.3	6.7
Verapamil	1.9E-04	31.8	0.3	17.6
Voriconazole	1.5E-04	64.2	0.3	21.0
Warfarin	1.4E-04	9.0	0.1	16.2
Xylazine	8.1E-05	18.8	0.4	20.3
Yohimbine	2.0E-04	28.0	0.4	15.5
Zaleplon	1.7E-04	26.5	0.2	9.5
Ziprasidone	1.9E-04	26.8	0.3	30.2
Zolpidem	1.2E-04	30.4	0.4	11.5
Zonisamide	9.8E-05	23.0	0.5	22.8

Table 5: Validation data – processed sample stability

Name	Day 0, Avg. Response	Day 4, Avg. Response	% Difference	Stable?
25H-NBOMe	52806	461	-18	Yes
25I-NBOMe	1293	271	-11.3	Yes
6-MAM	1411	909	-35.6	No
Alpha-PVP	1828	966	-47.2	No
Amphetamine	1622	146	-24.8	Yes
Butylone	60187	2925	-22.4	Yes
Carisoprodol	8342	6770	-18.8	Yes
Cocaethylene	19963	16286	-18.4	Yes
Cocaine	10796	8344	-22.7	Yes
Codeine	3057	2451	-19.8	Yes
Dextromethorphan	48289	39734	-17.7	Yes
Diazepam	10728	8953	-16.5	Yes
Dihydrocodeine	4679	3178	-32.1	No
DOM	529	2783	-16.2	Yes
EDDP	60187	49324	-18	Yes
Ephedrine	6832	2875	-57.9	No
Fentanyl	239	197	-17.4	Yes
Fluphenazine	1293	1798	39.1	Yes
Ketamine	2993	2385	-20.3	Yes
Levamisole	118809	97755	-17.7	Yes
MBZP	845583	1608	-17.8	Yes
MDEA	1622	1177	-27.4	Yes
MDMA	3212	2564	-20.2	Yes
MDPV	5392	4593	-14.8	Yes

Methamphetamine	1739	1326	-23.7	Yes
Methaqualone	845583	742288	-12.2	Yes
Methylone	3459	2613	-24.4	Yes
Midazolam	1859	1866	0.4	Yes
Nordiazepam	529	164	-69	No
Papaverine	408836	339139	-17	Yes
PCP	1411	1983	-18.2	Yes
Pentazocine	69147	57457	-16.9	Yes
Pentylone	19963	1093	-22.6	Yes
Quetiapine	52806	44836	-15.1	Yes
Strychnine	38782	33268	-14.2	Yes
Tramadol	408836	28664	-17.1	Yes
Trazodone	17352	12233	-29.5	Yes
Zolpidem	9085	7684	-15.4	Yes

Increased variability in isotope difference and peak area measurements were determined to be acceptable; larger significance was placed on the compounds being identified rather than significance in fluctuation of peak area, etc. Over the course of this validation, it was determined that some analytes within the predefined mixes were at lower concentration than their limits of detection; therefore, their identification was not evaluated using these calculations (e.g. naloxone 1 ng/mL, naltrexone 1 ng/mL, oxazepam 20 ng/mL).

Subsequently, analytes that did not meet criteria during validation within the prepared mixes were evaluated separately to determine if detection issues were due to interferences, bulk stability, and/or instrument sensitivity. All available analytes were positively and accurately identified upon further analysis. During validation experiments, it was discovered that analytical detection of some analytes was hindered by background or noise in the extracted ion chromatogram channels or TOF MS scans, and therefore the concentration of those analytes would have to be increased for detection (e.g. nicotine,

2C-C). Additionally, an unusual issue was discovered where lidocaine interfered with the M+2 isotope of closely eluting norfentanyl resulting in failed criteria. This was determined to only be an intermittent problem due to chromatographic behavior and only an issue when lidocaine was present at significantly higher concentrations than norfentanyl (e.g. 200 vs. 2 ng/mL, respectively).

For the analytes evaluated during processed sample stability, 33 (86.8%) of the analytes were determined to be stable for at least 96 hours, while nordiazepam, 6-MAM, alpha-PVP, dihydrocodeine, and ephedrine were determined to be "unstable" after this period of time (losing more than 30% of initial peak area), but all were still identified. During evaluation of carryover, the only analyte that was determined to produce carryover at the evaluated elevated concentrations was quinine/quinidine (200 ng/mL). The needle wash incorporated in the LC method used a mixture of isopropanol, acetonitrile, and methanol (60:20:20), which was determined to be valuable for eliminating carryover.

Overall, the validation passed and the LC-QTOF-MS method was determined to be acceptable for its intended use, generating accurate and reliable data.

4.7 NPS Results and Discussion

Over the course of this research, 3,543 sample extracts were re-analyzed using the previously described LC-QTOF-MS workflow. Comprehensive targeted data processing resulted in the identification of a wide-variety of NPS across several categories including commonly encountered NPS incorporated into initial testing procedures, NPS previously

identified in seized drug casework but not in toxicological casework, and NPS identified here for the first time (based on national and international reporting and dissemination). Identified NPS were categorized as NPS opioids, NPS opioid precursors, NPS hallucinogens, NPS stimulants, and NPS benzodiazepines.

Table 6 details the newly discovered NPS detected in forensic toxicology casework, many of which were identified here for the first time.

Table 6: NPS identified during drug discovery

NPS Name	NPS Category	Method of Identification	Date of First Identification	Date of Analysis	Number of Identifications
N-methyl Norfentanyl	OP	SM	4/23/2018	4/10/2018	10
3,4-Methylenedioxy-U-47700	O	SM	5/16/2018	5/7/2018	12
Isopropyl-U-47700	O	SM	5/16/2018	5/14/2018	5
Alpha-PHP	S	SM	5/16/2018	5/14/2018	13
N-ethyl Hexedrone	S	SM	6/7/2018	3/14/2018	5
Benzylfuranylfentanyl	OP	SM	7/20/2018	7/20/2018	5
Phenylfentanyl	O	SM	8/6/2018	8/1/2018	5
2F-Deschloroketamine	H	SM	8/30/2018	8/29/2018	2
3,4-Methylenedioxy-alpha-PHP	S	SM	8/31/2018	8/29/2018	5
Eutylone	S	SM	8/31/2018	8/29/2018	7
N-ethyl Hexylone	S	SM	10/22/2018	10/19/2018	1
N-ethyl Deschloroketamine	H	SM	12/20/2018	12/14/2018	1
Fluorofuranylfentanyl	O	SM	1/18/2019	1/17/2019	2
Fluoro-4-ANPP	OP	SM	1/18/2019	1/17/2019	2
Fluoroethamphetamine	S	SM	2/15/2019	2/15/2019	2
3/4-OH-PCP	H	SM	2/15/2019	2/15/2019	2
Flualprazolam	B	DM	4/22/2019	4/5/2018	3
Fluorofentanyl	O	DM	4/22/2019	4/5/2018	2
4Cl-alpha-PVP	S	DM	4/22/2019	4/5/2018	2
4F-alpha-PHP	S	DM	4/23/2019	5/31/2018	1
Benzylone	S	SM	6/20/2019	6/19/2019	1

Key: SM – Sample mining, DM – Data mining, OP – Opioid Precursor, O – Opioid, S – Stimulant, H – Hallucinogen, B – Benzodiazepine

4.7.1 NPS Opioids

Isopropyl-U-47700 (Figure 34) was identified for the first time in forensic casework during this research on May 16, 2018. The analyte identified in this sample had an accurate mass of 357.1500 Da (Figure 35). The exact mass of isopropyl-U-47700 ($C_{18}H_{26}Cl_2N_2O$) is 357.1495 Da, resulting in a sample ppm error of 1.4. The retention time of this analyte was 7.22 minutes (isopropyl-U-47700 retention time: 7.09 minutes), resulting in a retention time difference of +0.13 minutes. The isotope difference was calculated to be 20.9%. The library comparison (Figure 36) resulted in a library score of 87.3 in comparison to data acquired using standard reference material for isopropyl-U-47700 (Note: the "missing" fragment ions are due to a split between SWATH® windows from the chlorine contribution at M+2). A combined MSMS spectrum is shown in Figure 37. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be isopropyl-U-47700.

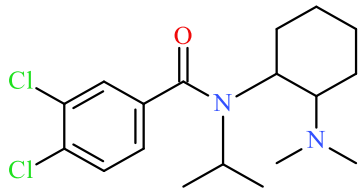

Figure 34: Structure of isopropyl-U-47700

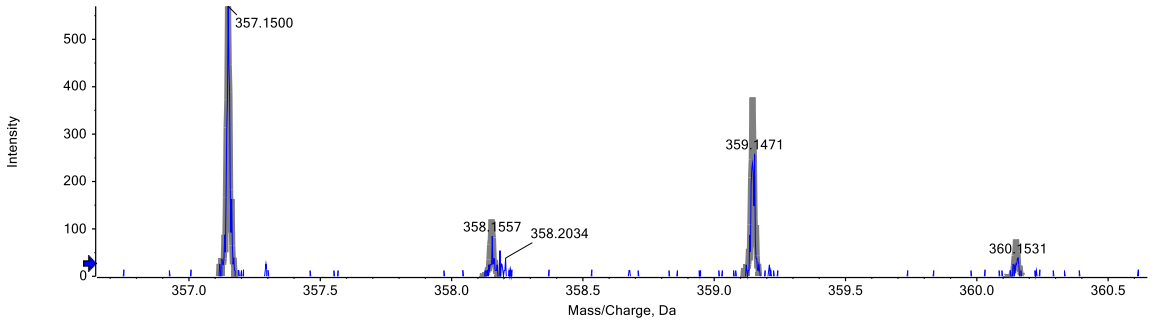

Figure 35: TOF MS data for the analyte identified as isopropyl-U-47700

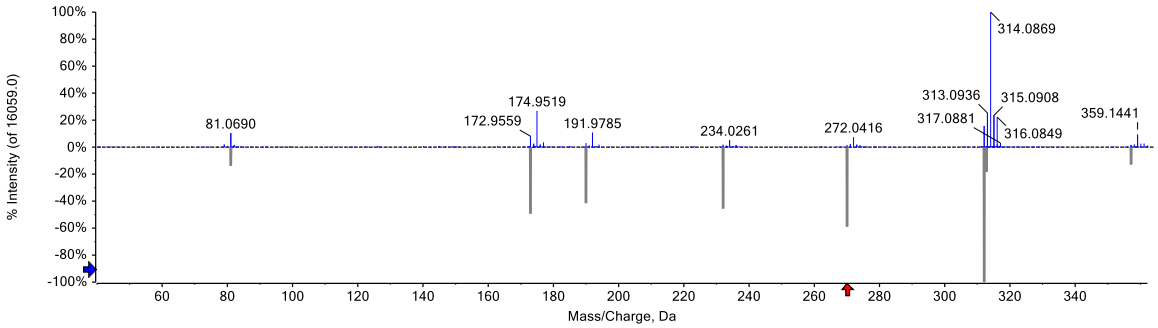

Figure 36: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for isopropyl-U-47700

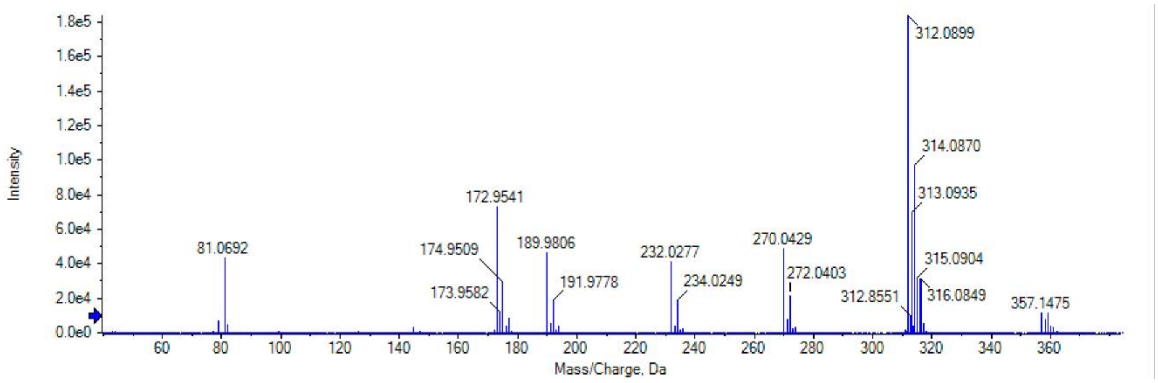

Figure 37: Combined SWATH® fragment (MSMS) data from isopropyl-U-47700

Isopropyl-U-47700, or 3,4-dichloro-N-[2-(dimethylamino)cyclohexyl]-N-isopropyl-benzamide, is a U-47700 analogue, replacing the methyl group on the amide bridge with an isopropyl group. U-47700 was developed and patented by the Upjohn Company in the 1970s where one can also find reference to this isopropyl- analogue.[128] Other than this patent, no literature is available regarding isopropyl-U-47700; therefore, its activity and adverse effects are suspected to be similar to that of U-47700. Real-time sample mining allowed for identification of this novel opioid in four additional specimens. Isopropyl-U-47700 was identified in an extract initially designated for designer opioid confirmation and found in conjunction with methoxyacetylfentanyl (a designer opioid incorporated into the initial scope of testing).

3,4-Methylenedioxy-U-47700 (Figure 38) was identified for the first time in forensic casework during this research on May 16, 2018. The analyte identified in this sample had an accurate mass of 305.1857 Da (Figure 39). The exact mass of 3,4-methylenedioxy-U-47700 ($C_{17}H_{24}N_2O_3$) is 305.1860 Da, resulting in a sample ppm error of -0.9. The retention time of this analyte was 4.94 minutes (3,4-methylenedioxy-U-47700 retention time: 4.90 minutes), resulting in a retention time difference of +0.04 minutes. The isotope difference was calculated to be 14.8%. The library comparison (Figure 40) resulted in a library score of 100 in comparison to data acquired using standard reference material for 3,4-methylenedioxy-U-47700. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be 3,4-methylenedioxy-U-47700.

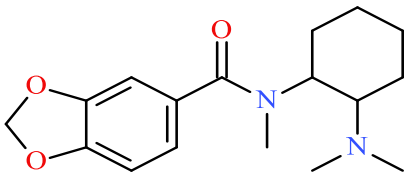

Figure 38: Structure of 3,4-methylenedioxy-U-47700

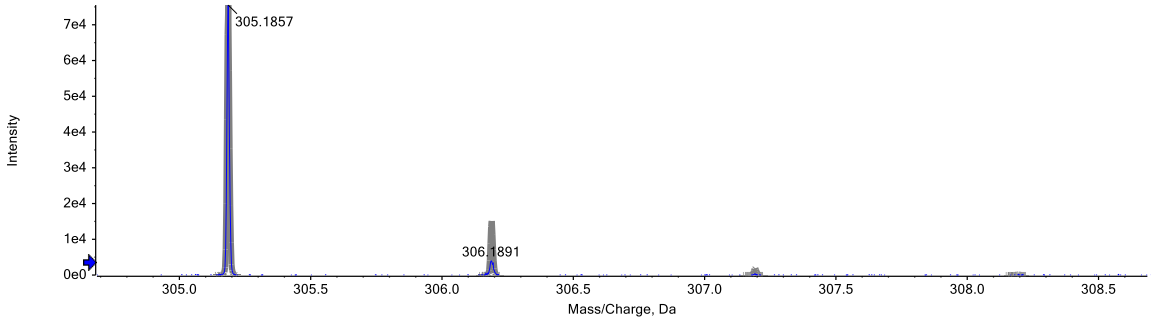

Figure 39: TOF MS data for the analyte identified as 3,4-methylenedioxy-U-47700

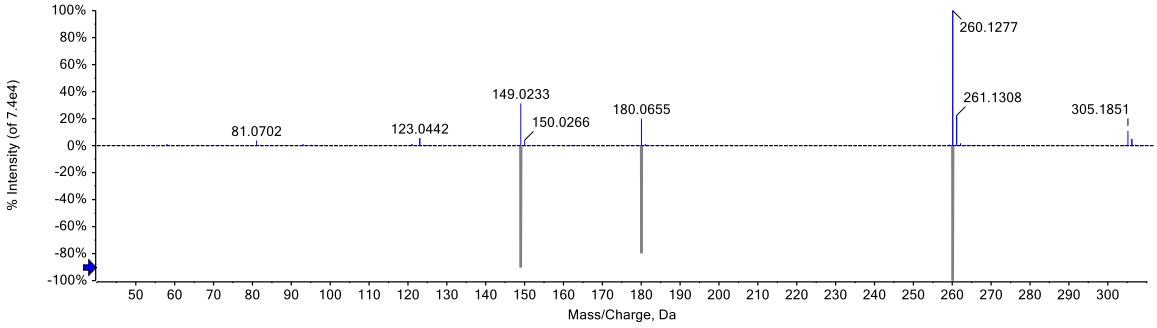

Figure 40: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for 3,4-methylenedioxy-U-47700

3,4-Methylenedioxy-U-47700, or N-[2-(dimethylamino)cyclohexyl]-N-methyl-1,3-benzodioxole-5-carboxamide, is a U-47700 analogue, replacing the dichlorinated portion of the benzamide with a methylenedioxy group. No literature or parent information is available for 3,4-methylenedioxy-U-47700. Retrospective data mining allowed for identification of this novel opioid in eight additional specimens dating back to March 1, 2018. 3,4-Methylenedioxy-U-47700 was identified in an extract initially designated for designer opioid confirmation and found in conjunction with fentanyl, methoxyacetylfentanyl, and cyclopropylfentanyl (designer opioids incorporated into the initial scope of testing).

Both of these U-series analogues (isopropyl-U-47700 and 3,4-methylenedioxy-U-47700) are categorized as non-fentanyl novel synthetic opioids. Their emergence and identification during this research is timely to legislation in the United States regarding the scheduling of fentanyl related substances in February 2018.[129] It is believed that the presence of U-series analogues in forensic casework may continue to increase due to illegality of fentanyl and its analogues. Laboratory personnel and analytical chemists should be aware of these analytes as they are suspected be toxicologically relevant. Due to current lack of testing and knowledge about these novel U-series analogues, the combined threat to public health and public safety is likely not well documented and/or understood.

Fluorofuranylfentanyl (Figure 41) was identified for the first time in forensic casework during this research on January 18, 2019. The analyte identified in this sample had an accurate mass of 393.1973 Da (Figure 42). The exact mass of

fluorofuranylfentanyl ($C_{24}H_{25}FN_2O_2$) is 393.1973 Da, resulting in a sample ppm error of -0.1. The retention time of this analyte was 6.31 minutes (*ortho*-fluorofuranylfentanyl retention time: 6.43 minutes), resulting in a retention time difference of -0.12 minutes. Due to *para*- and *meta*- substituted isobars, identification of the analyte in this case as *ortho*- was not possible. The isotope difference was calculated to be 1.3%. The library comparison (Figure 43) resulted in a library score of 100 in comparison to data acquired using standard reference material for *ortho*-fluorofuranylfentanyl. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be fluorofuranylfentanyl.

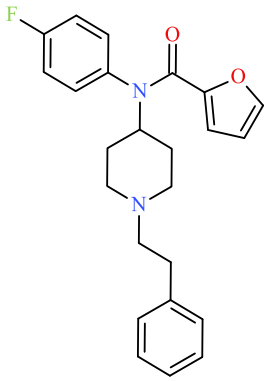

Figure 41: Structure of *para*-fluorofuranylfentanyl

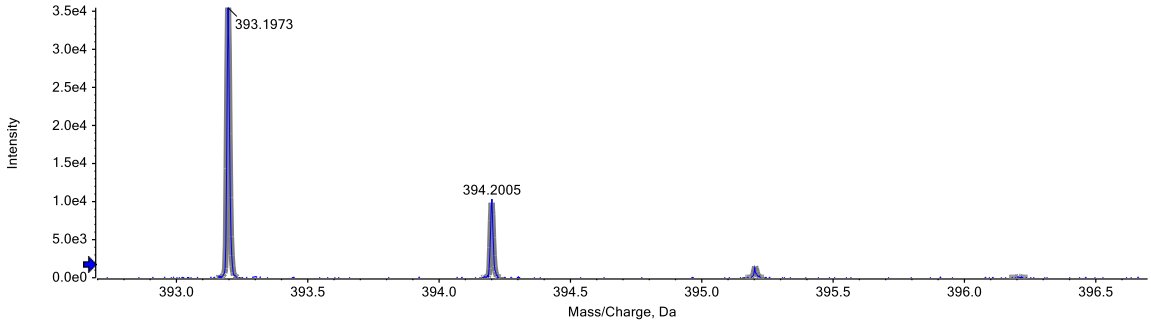

Figure 42: TOF MS data for the analyte identified as fluorofuranylfentanyl

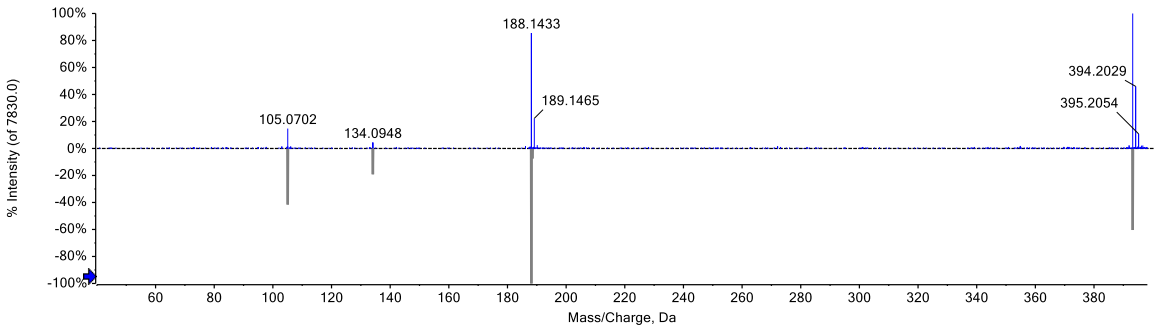

Figure 43: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for fluorofuranylfentanyl

Fluorofuranylfentanyl, or N-(4-fluorophenyl)-N-[1-(2-phenylethyl)-4-piperidyl]furan-2-carboxamide, is a fentanyl analogue, substituting a furan ring onto the propanamide portion of the fentanyl scaffold, as well as a fluorine onto the aniline ring. The position of the fluorine could not be confirmed using this assay, so the *para*- position is used for demonstration. No peer-reviewed literature was discovered regarding fluorofuranylfentanyl, although it is hypothesized to be an active novel opioid based on previously identified fentanyl analogues. Real-time sample mining allowed for identification of this novel opioid in one additional specimen. Fluorofuranylfentanyl was

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identified in conjunction with fluoro-4-ANPP, a suspected metabolite and/or precursor; although its presence is likely due in large part to metabolism based on the previously published metabolism of furanylfentanyl (see Chapter 6 for more details).[130]

Phenylfentanyl (Figure 44) was identified for the first time in forensic casework during this research on August 6, 2018. The analyte identified in this sample had an accurate mass of 385.2275 Da (Figure 45). The exact mass of phenylfentanyl ($C_{26}H_{28}N_2O$) is 385.2275 Da, resulting in a sample ppm error of 0.1. The retention time of this analyte was 6.79 minutes (phenylfentanyl retention time: 6.78 minutes), resulting in a retention time difference of +0.01 minutes. The isotope difference was calculated to be 19.3%. The library comparison (Figure 46) resulted in a library score of 96.5 in comparison to data acquired using standard reference material for phenylfentanyl. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be phenylfentanyl.

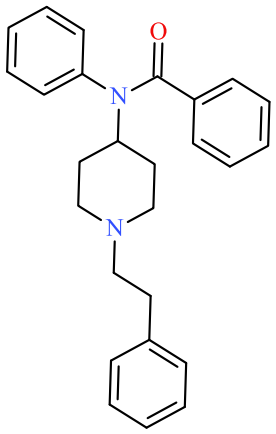

Figure 44: Structure of phenylfentanyl

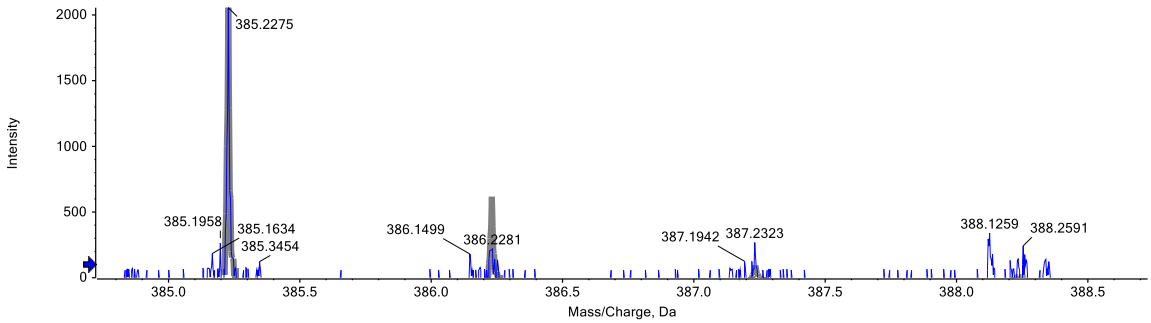

Figure 45: TOF MS data for the analyte identified as phenylfentanyl

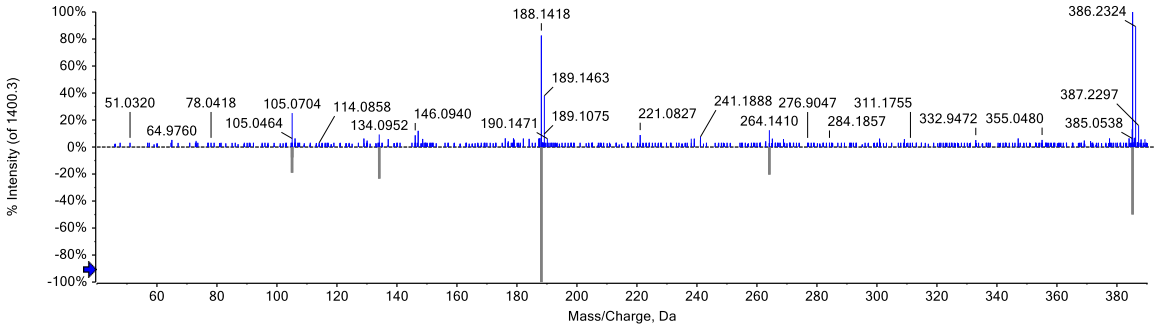

Figure 46: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for phenylfentanyl

Phenylfentanyl, or N-phenyl-N-[1-(2-phenylethyl)-4-piperidyl]benzamide, is a fentanyl analogue, substituting a phenyl ring onto the propanamide portion of the fentanyl scaffold. No peer-reviewed literature was discovered regarding phenylfentanyl, although it is hypothesized to be an active novel opioid based on previously identified fentanyl analogues. Real-time sample mining allowed for identification of this novel opioid in four additional specimens. Phenylfentanyl was identified in an extract initially designated for designer opioid confirmation and found in conjunction with methoxyacetylfentanyl and cyclopropylfentanyl.

4.7.2 NPS Opioid Precursors

N-Methyl norfentanyl (Figure 47) was identified for the first time in forensic toxicology casework during this research on April 23, 2018. The analyte identified in this sample had an accurate mass of 247.1807 Da (Figure 48). The exact mass of *N*-methyl norfentanyl ($C_{15}H_{22}N_2O$) is 247.1805 Da, resulting in a sample ppm error of 0.9. The retention time of this analyte was 4.81 minutes (*N*-methyl norfentanyl retention time: 4.66 minutes), resulting in a retention time difference of +0.15 minutes. The isotope difference was calculated to be 10.6%. The library comparison (Figure 49) resulted in a library score of 99.8 in comparison to data acquired using standard reference material for *N*-methyl norfentanyl. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be *N*-methyl norfentanyl.

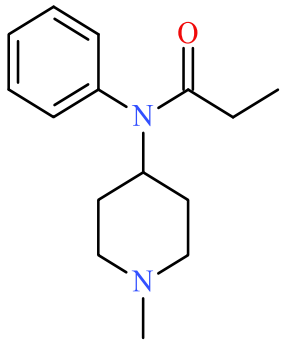

Figure 47: Structure of *N*-methyl norfentanyl

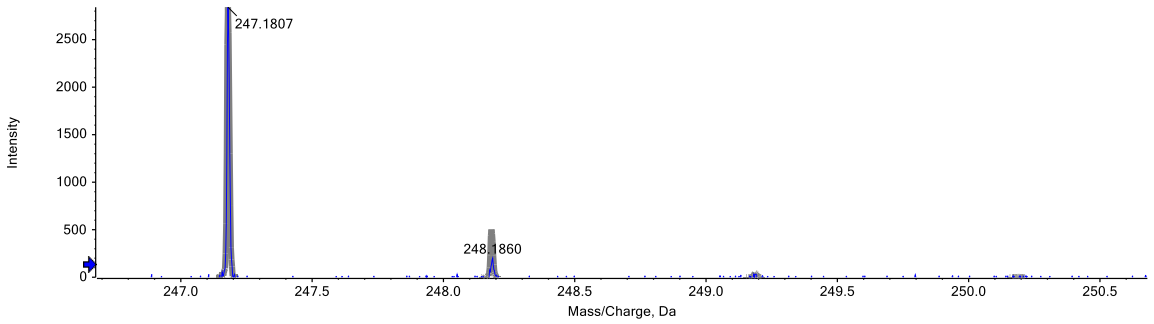

Figure 48: TOF MS data for the analyte identified as *N*-methyl norfentanyl

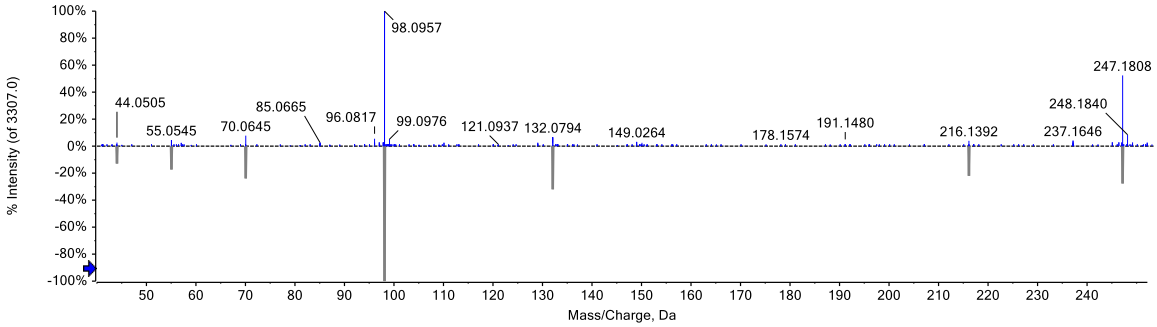

Figure 49: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for *N*-methyl norfentanyl

N-Methyl norfentanyl, or N-(1-methyl-4-piperidyl)-N-phenyl-propanamide, is a suspected fentanyl and/or fentanyl analogue precursor. *N*-Methyl norfentanyl was first identified in seized drug casework in April of 2018.[131] Determination of opioid activity alongside fentanyl and its metabolites revealed *N*-methyl norfentanyl to be inactive.[132] It is hypothesized that *N*-methyl norfentanyl can be clandestinely converted to fentanyl, or one of its phenethyl-variant analogues, using a similar approach to Paul Janssen's synthesis of fentanyl from benzylfentanyl.[133] Retrospective data mining allowed for identification of this fentanyl related precursor in seven additional specimens dating back

to February 7, 2018. It is important to note that all specimens positive for *N*-methyl norfentanyl were positive for fentanyl and not a fentanyl analogue.

Benzylfuranylfentanyl (Figure 50) was identified for the first time in forensic toxicology casework during this research on July 20, 2018. The analyte identified in this sample had an accurate mass of 361.1909 Da (Figure 51). The exact mass of benzylfuranylfentanyl ($C_{23}H_{24}N_2O_2$) is 361.1911 Da, resulting in a sample ppm error of -0.3. The retention time of this analyte was 6.11 minutes (benzylfuranylfentanyl retention time: 6.13 minutes), resulting in a retention time difference of -0.02 minutes. The isotope difference was calculated to be 4.3%. The library comparison (Figure 52) resulted in a library score of 100 in comparison to data acquired using standard reference material for benzylfuranylfentanyl. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be benzylfuranylfentanyl.

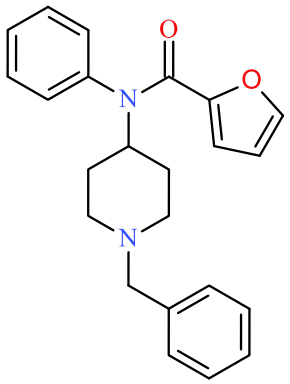

Figure 50: Structure of benzylfuranylfentanyl

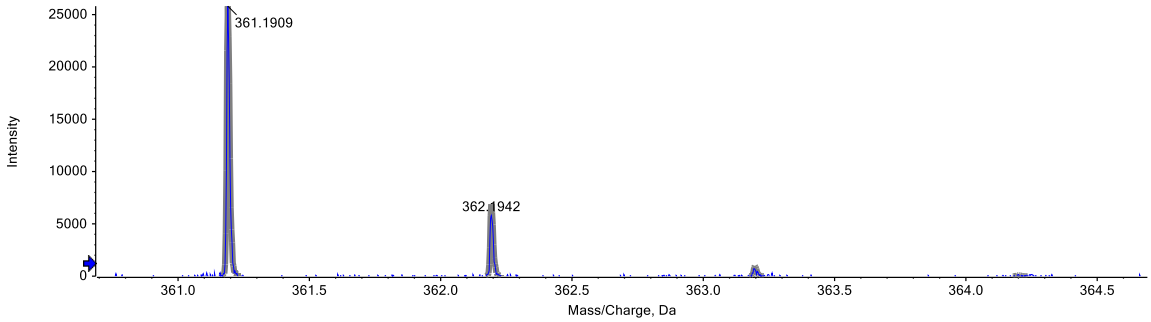

Figure 51: TOF MS data for the analyte identified as benzylfuranylfentanyl

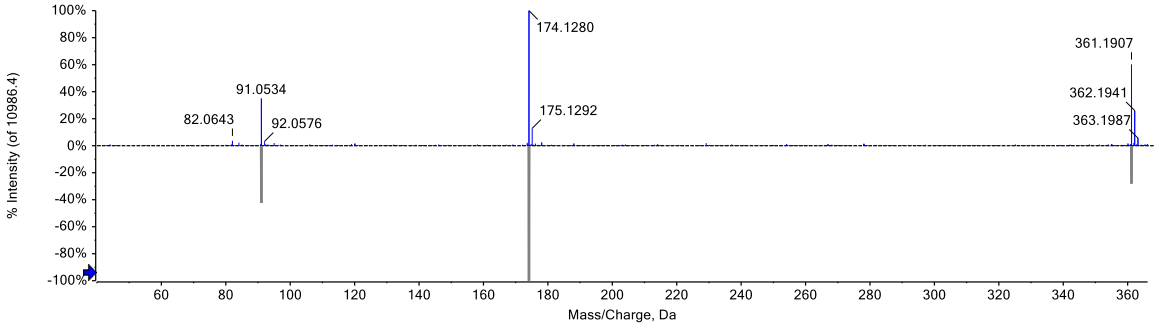

Figure 52: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for benzylfuranylfentanyl

Benzylfuranylfentanyl, or N-(1-benzyl-4-piperidyl)-N-phenyl-furan-2-carboxamide, is a suspected furanylfentanyl and/or fentanyl analogue precursor, and was first identified in seized drug casework in April of 2018.[134] No literature is available regarding activity, although it is hypothesized that benzylfuranylfentanyl is inactive based on the inactivity of benzylfentanyl.[135,136] Real-time sample mining allowed for identification of this fentanyl related precursor in four additional specimens. Furanylfentanyl was not identified with benzylfuranylfentanyl in any of the positive

extracts. Additionally, processing for other theorized furanyl-variant fentanyl analogues (Figure 53) was also negative.

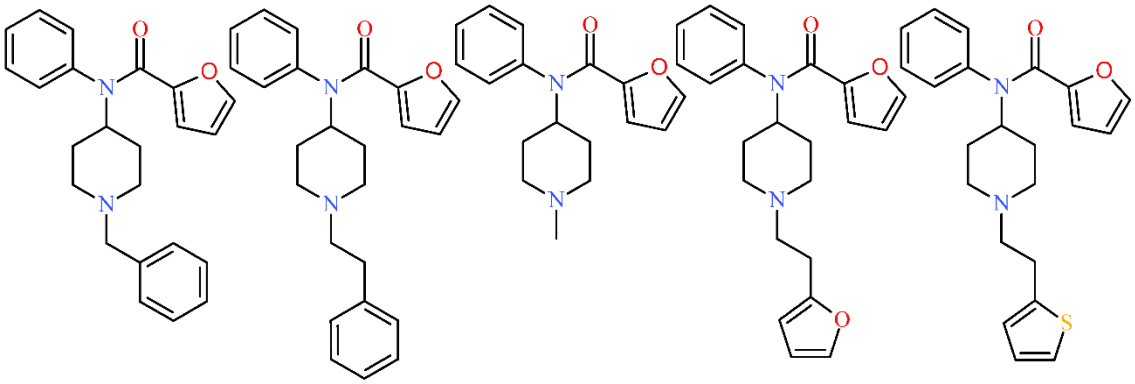

Figure 53: Benzylfuranylfentanyl and suspected furanyl-variant fentanyl analogues

Despropionyl-*ortho*-methylfentanyl and despropionyl-3-methylfentanyl (Figure 54) were identified in forensic toxicology casework on January 18, 2019. The analytes identified in this sample had accurate masses of 295.2167 Da (Figure 55) and 295.2169 Da (Figure 56), respectively. The exact mass of despropionyl-*ortho*-methylfentanyl and despropionyl-3-methylfentanyl ($C_{20}H_{26}N_2$) is 295.2169 Da, resulting in sample ppm errors of -0.3 and 0.1, respectively. The retention times of these analytes were 6.75 and 6.80 minutes (despropionyl-*ortho*-methylfentanyl retention time: 6.73 minutes, and despropionyl-3-methylfentanyl retention time: 6.76 minutes), resulting in a retention time differences of +0.03 minutes and +0.04 minutes, respectively. The isotope differences were calculated to be 1.9% and 4.7%, respectively. The library comparisons (Figure 57 and Figure 58) resulted in library scores of 100 in comparison to data acquired using standard reference material for despropionyl-*ortho*-methylfentanyl and despropionyl-3-

methylfentanyl. The analytes in these samples met all criteria set forth for positive identification and were therefore determined to be despropionyl-*ortho*-methylfentanyl and despropionyl-3-methylfentanyl; however, the exact positioning of the methyl-group was not confirmed (i.e. *ortho*- vs. *para*-, 3- vs. 2-).

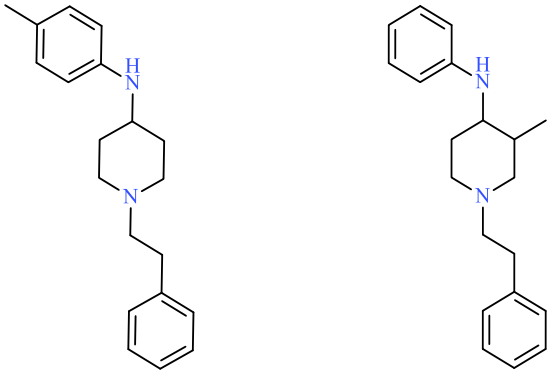

Figure 54: Structure of despropionyl-*ortho*-methylfentanyl (left) and despropionyl-3-methylfentanyl (right)

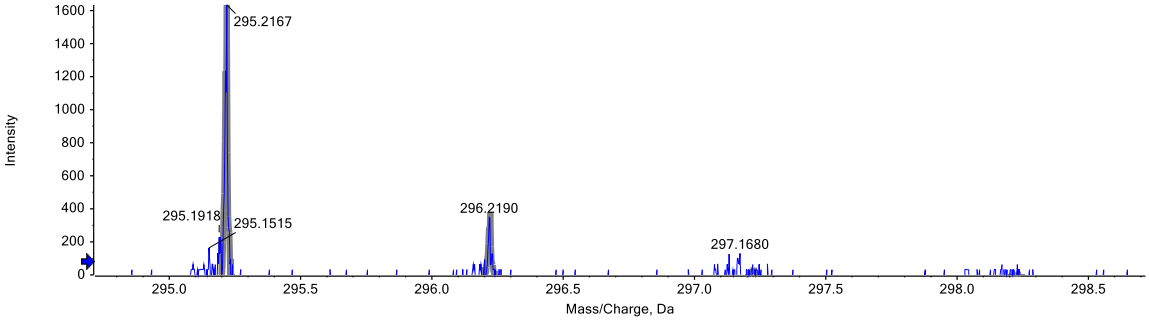

Figure 55: TOF MS data for the analyte identified as despropionyl-*ortho*-methylfentanyl

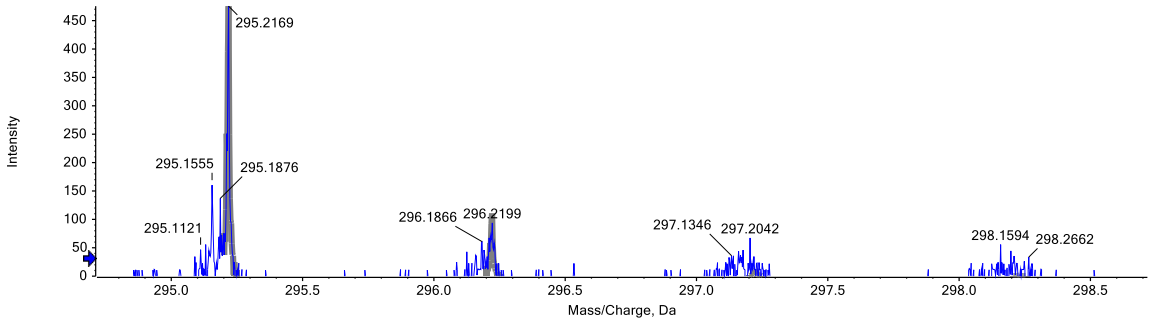

Figure 56: TOF MS data for the analyte identified as despropionyl-3-methylfentanyl

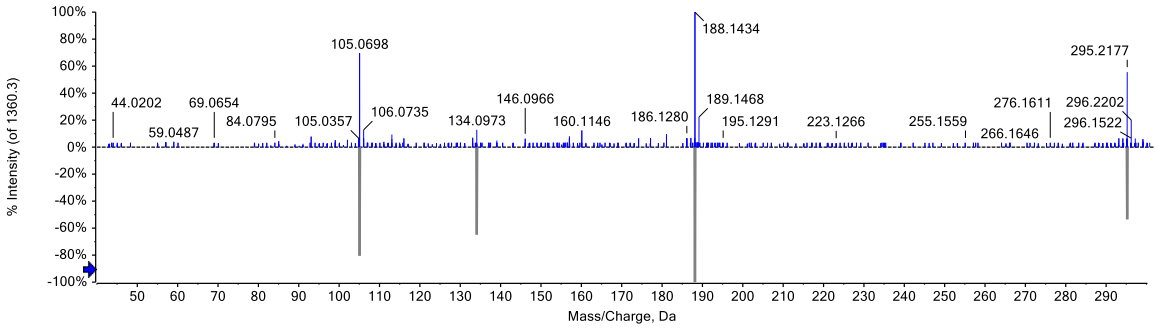

Figure 57: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for despropionyl-*ortho*-methylfentanyl

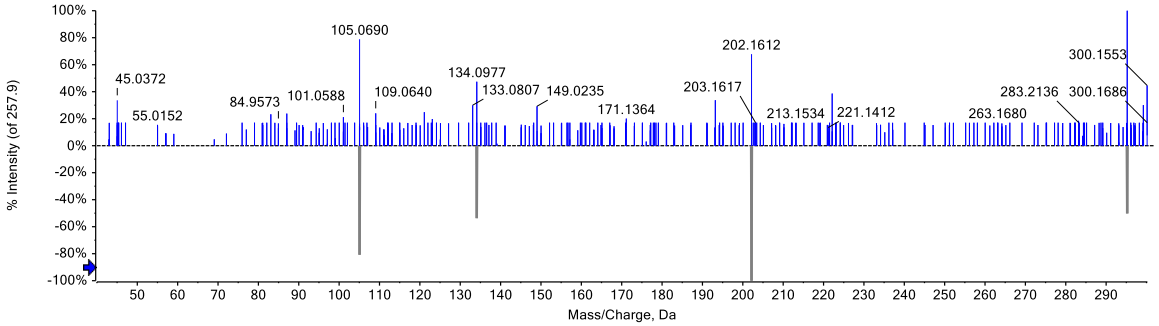

Figure 58: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for despropionyl-3-methylfentanyl

Both despropionyl-*ortho*-methylfentanyl and despropionyl-3-methylfentanyl are suspected precursors in the synthesis of fentanyl analogues and were identified in seized drug casework in March of 2018. Based on the inactivity of despropionyl-fentanyl (or 4-ANPP), it is suspected that these compounds are pharmacologically inactive. Their presence in biological specimens could be toxicologically relevant though.

Fentanyl precursors, or any NPS precursors, identified in forensic casework can provide pieces to the NPS discovery puzzle not attainable through other means, including the identification of clandestine synthesis routes and timely discovery of structurally similar emerging novel drugs. The presence of these precursors in forensic casework is commonly in conjunction with fentanyl or one of its analogues, although increasingly these substances are being detected without a theorized desired active product (e.g. benzylfuranylfentnayl positive but furanylfentanyl negative). Positivity for a precursor can allow an analyst to further investigate a sample in question to determine if a new analogue is present. Although many of these precursors are inactive, or hypothesized to be inactive, and their presence in seized drugs or biological specimens could be imperative to identification of the causative agent.

4.7.3 NPS Hallucinogens

2F-Deschloroketamine (Figure 59) was identified for the first time in forensic toxicology casework during this research on August 30, 2018. The analyte identified in this sample had an accurate mass of 222.1290 Da (Figure 60). The exact mass of 2F-deschloroketamine ($C_{13}H_{16}FNO$) is 222.1289 Da, resulting in a sample ppm error of 0.7.

The retention time of this analyte was 4.32 minutes (2F-deschloroketamine retention time: 4.21 minutes), resulting in a retention time difference of +0.11 minutes. The isotope difference was calculated to be 2.4%. The library comparison (Figure 61) resulted in a library score of 100 in comparison to data acquired using standard reference material for 2F-deschloroketamine. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be 2F-deschloroketamine.

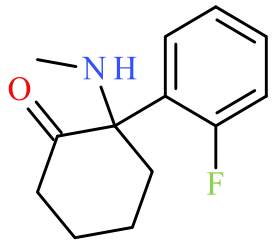

Figure 59: Structure of 2F-deschloroketamine

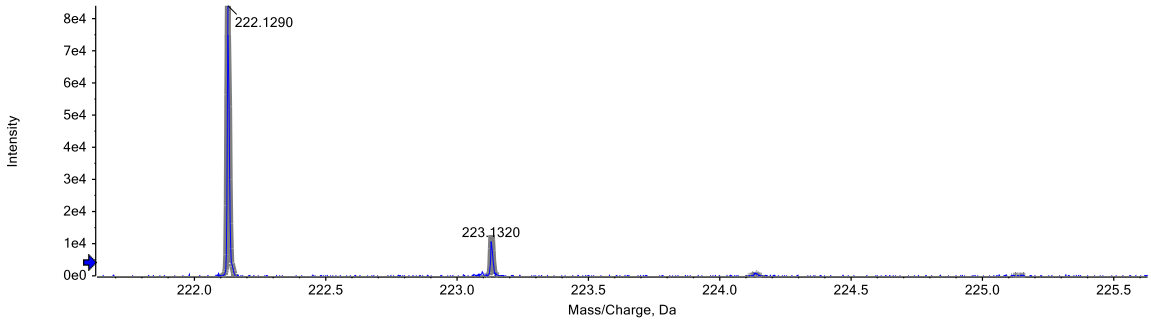

Figure 60: TOF MS data for the analyte identified as 2F-deschloroketamine

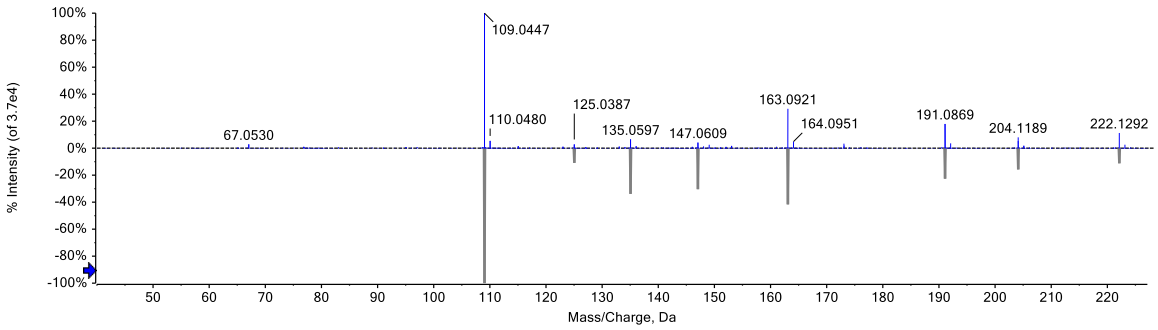

Figure 61: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for 2F-deschloroketamine

2F-Deschloroketamine (2F-DCK), or 2-(2-fluorophenyl)-2-(methylamino)cyclohexanone, is a ketamine analogue. No information regarding activity or toxicity is available. It is hypothesized that 2F-deschloroketamine is active, based on the pharmacological properties and effects of ketamine,[137,138] but this compound has not been studied. Non-targeted data processing of this sample resulted in the identification of 2F-deschloro-norketamine based on the well described metabolism of ketamine.[139] While this finding is not overwhelmingly significant, it demonstrates the utility of the workflows generated and allows for secondary research of metabolism without re-preparation of sample or re-analysis extract (see Chapter 6). 2F-Deschloroketamine was identified in extracts initially designated for designer benzodiazepine and designer opioid confirmation, and found in conjunction with etizolam and fentanyl, respectively (analytes incorporated into the initial scope of testing). 2F-Deschloroketamine was also found in combination with methoxy-PCP.

N-Ethyl deschloroketamine (Figure 62) was identified in forensic toxicology casework during this research on December 20, 2018; although its first detection in

forensic toxicology casework dates back to June 2018.[140] The analyte identified in this sample had an accurate mass of 218.1541 Da (Figure 63). The exact mass of *N*-ethyl deschloroketamine ($C_{14}H_{19}NO$) is 218.1539 Da, resulting in a sample ppm error of 0.6. The retention time of this analyte was 4.54 minutes (*N*-ethyl deschloroketamine retention time: 4.50 minutes), resulting in a retention time difference of +0.04 minutes. The isotope difference was calculated to be 2.4%. The library comparison (Figure 64) resulted in a library score of 93.2 in comparison to data acquired using standard reference material for *N*-ethyl deschloroketamine. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be *N*-ethyl deschloroketamine.

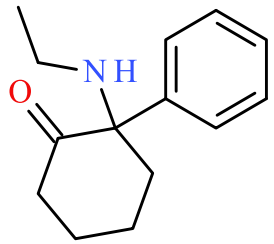

Figure 62: Structure of *N*-ethyl deschloroketamine

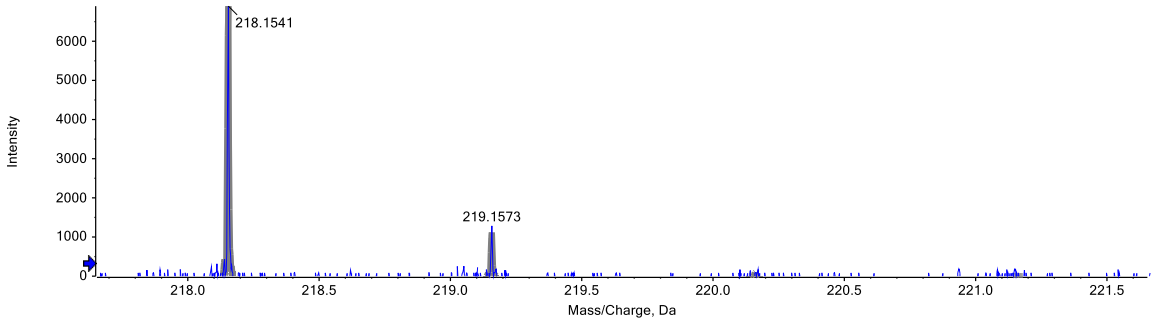

Figure 63: TOF MS data for the analyte identified as *N*-ethyl deschloroketamine

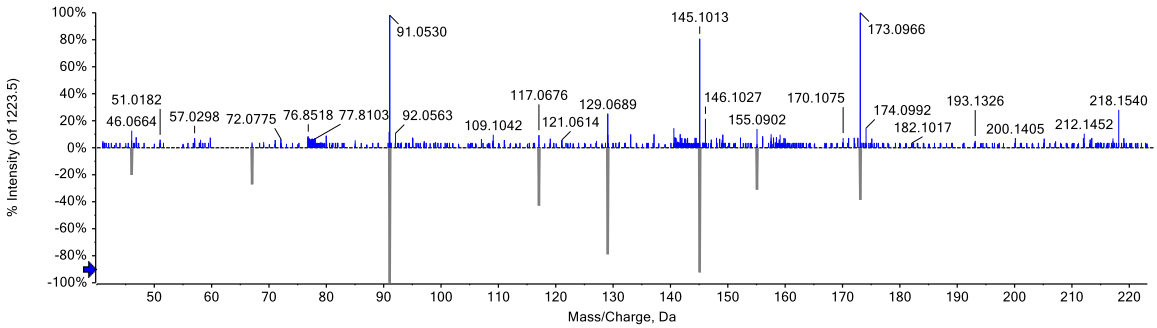

Figure 64: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for *N*-ethyl deschloroketamine

N-Ethyl deschloroketamine (O-PCE), or 2-(ethylamino)-2-phenyl-cyclohexanone, is a ketamine analogue, but no information regarding activity or toxicity is available. Like 2F-deschloroketamine, it is hypothesized that *N*-ethyl deschloroketamine is active based on the pharmacological properties of ketamine, and this NPS has been implicated in a death.[141] *N*-Ethyl deschloroketamine was only identified once during this research. *N*-Ethyl deschloroketamine was identified in an extract initially designated for designer opioid confirmation and found in conjunction with fluoroisobutyrylfentanyl (FIBF) (a designer opioid incorporated into the initial scope of testing).

Hydroxy-PCP (Figure 65), or 2-[1-(1-piperidyl)cyclohexyl]phenol, was identified in two sample extracts during this research, in combination with methoxy-PCP (Figure 65), or 1-[1-(2-methoxyphenyl)cyclohexyl]piperidine. The analyte (hydroxy-PCP) identified in this sample had an accurate mass of 260.2010 Da (Figure 66). The exact mass of hydroxy-PCP ($C_{17}H_{25}NO$) is 260.2009 Da, resulting in a sample ppm error of 0.4. The retention time of this analyte was 5.11 minutes (3-hydroxy-PCP retention time:

5.25 minutes), resulting in a retention time difference of -0.14 minutes. The isotope difference was calculated to be 7.2%. The library comparison (Figure 67) resulted in a library score of 100 in comparison to data acquired using standard reference material for hydroxy-PCP. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be hydroxy-PCP. Distinction between 3-hydroxy-PCP and 4-hydroxy-PCP (as well as 3-methoxy-PCP and 4-methoxy-PCP) was not possible during this research due to close elution of the isobars and identical mass spectral data.

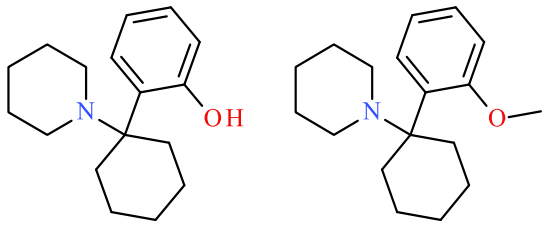

Figure 65: Structure of 3-hydroxy-PCP (left) and 3-methoxy-PCP (right)

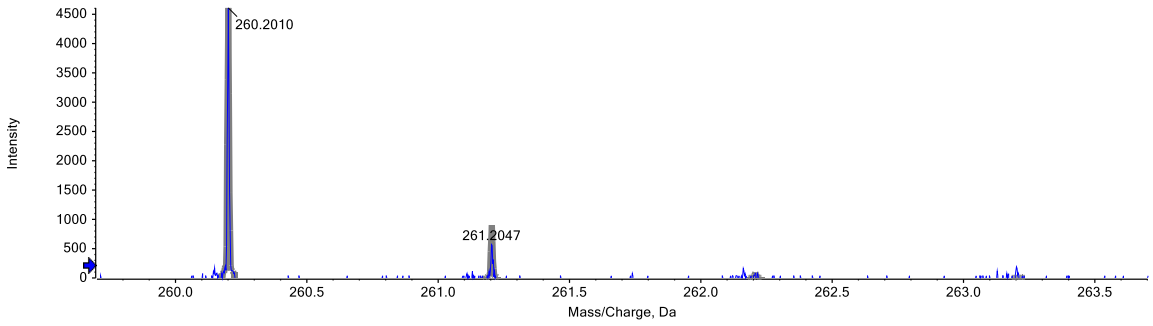

Figure 66: TOF MS data for the analyte identified as hydroxy-PCP

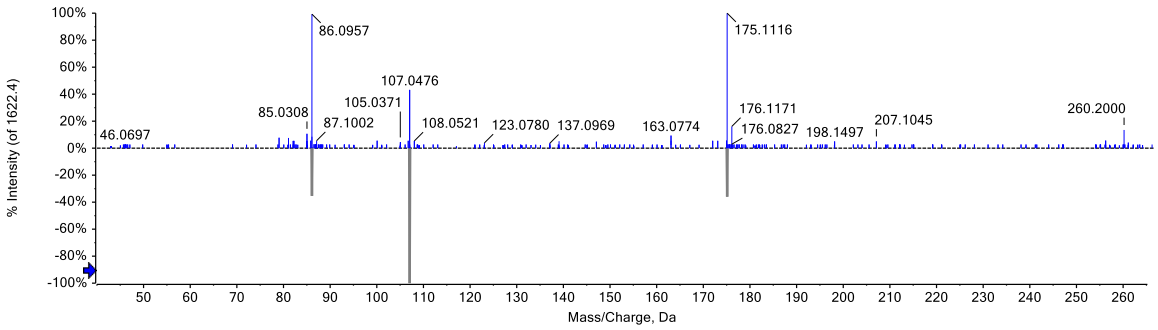

Figure 67: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for hydroxy-PCP

Hydroxy-PCP and methoxy-PCP are classified as phencyclidine (PCP) analogues and have been reported as NPS on their own. Although no literature is available regarding their potency, hydroxy-PCP and methoxy-PCP are suspected to be active drugs. While this finding is not inherently tied to an emerging drug identification, it demonstrates the utility of the data acquired using non-targeted mass acquisition techniques, allowing for the research of metabolism without the need for additional analysis and/or re-analysis. Further research is needed to confirm the biological conversion of methoxy-PCP to hydroxy-PCP, a phenomenon that could have toxic effects if both compounds are active.

4.7.4 NPS Stimulants

Eutylone (bk-EBDB) (Figure 68) was identified for the first time in forensic toxicology casework during this research on August 31, 2018. This finding marks the first time eutylone has been identified as the lone novel stimulant, as it was previously identified in conjunction with *N*-ethyl pentylone and determined to be a synthesis

byproduct rather than active ingredient.[142] The analyte identified in this sample had an accurate mass of 236.1283 Da (Figure 69). The exact mass of eutylone ($C_{13}H_{17}NO_3$) is 236.1281 Da, resulting in a sample ppm error of 0.8. The retention time of this analyte was 4.66 minutes (eutylone retention time: 4.46 minutes), resulting in a retention time difference of +0.2 minutes. The isotope difference was calculated to be 3.7%. The library comparison (Figure 70) resulted in a library score of 100 in comparison to data acquired using standard reference material for eutylone. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be eutylone.

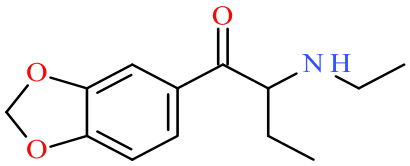

Figure 68: Structure of eutylone

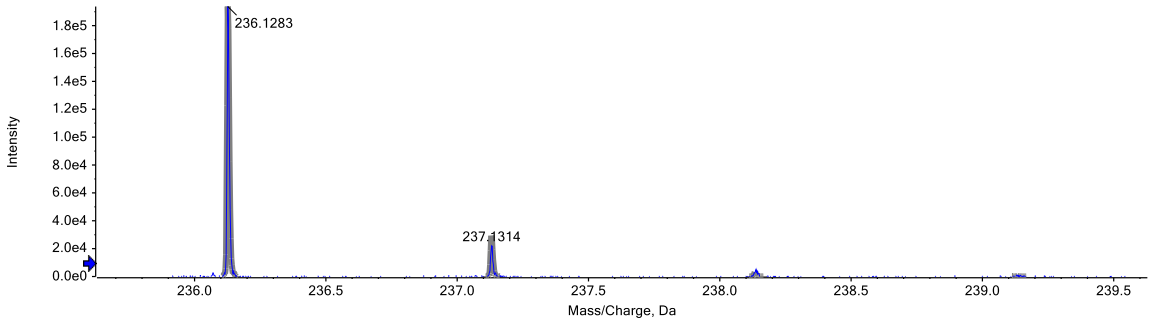

Figure 69: TOF MS data for the analyte identified as eutylone

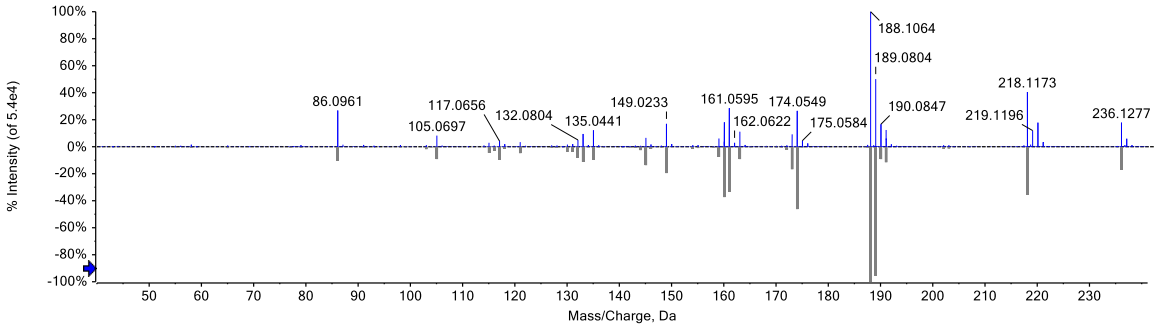

Figure 70: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for eutylone

Eutylone, or 1-(1,3-benzodioxol-5-yl)-2-(ethylamino)butan-1-one, is a synthetic cathinone and analogue of methylone and other *beta*-keto methylenedioxyamphetamines. Eutylone is described in patent literature dating back to 1964,[143] but its presence in seized drug casework only dates back to 2014 in Poland.[144] No information regarding activity or toxicity is currently available. Eutylone was identified in an extract initially designated for designer opioid confirmation and found in conjunction with FIBF.

Alpha-PHP (Figure 71) was identified during this research on May 16, 2018. The analyte identified in this sample had an accurate mass of 246.1863 Da (Figure 72). The exact mass of alpha-PHP ($C_{16}H_{23}NO$) is 246.1852 Da, resulting in a sample ppm error of 4.4. The retention time of this analyte was 5.98 minutes (alpha-PHP retention time: 5.88 minutes), resulting in a retention time difference of +0.1 minutes. The isotope difference was calculated to be 8.2%. The library comparison (Figure 73) resulted in a library score of 80 in comparison to data acquired using standard reference material for alpha-PHP. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be alpha-PHP. Since the time of first identification, an isobaric

analyte to alpha-PHP has emerged: alpha-PiHP. It was determined that the two can not be distinguished by this research, so further characterization might be necessary.

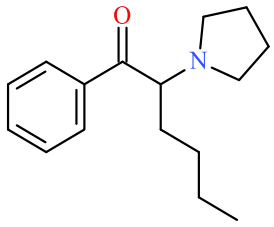

Figure 71: Structure of alpha-PHP

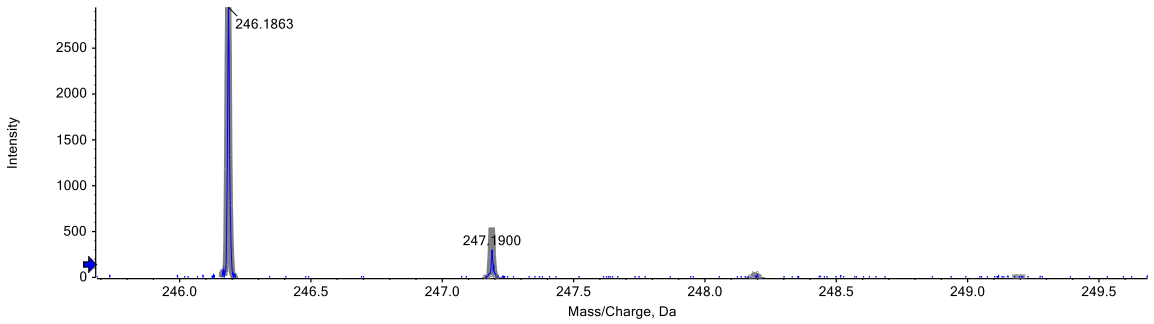

Figure 72: TOF MS data for the analyte identified as alpha-PHP

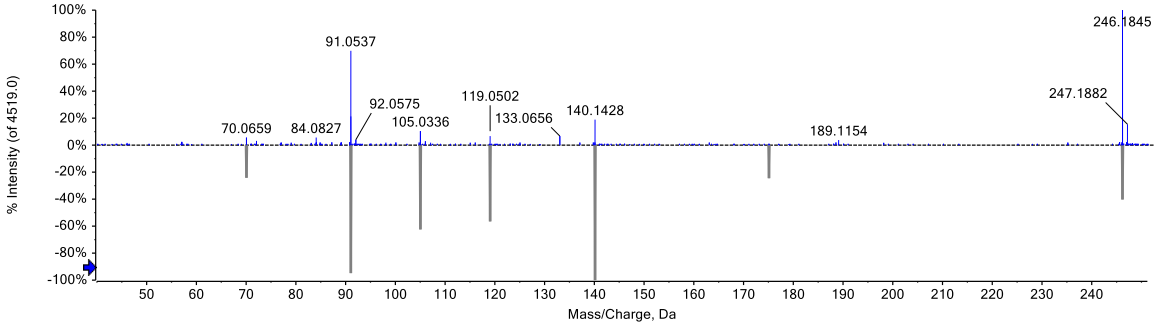

Figure 73: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for alpha-PHP

3,4-Methylenedioxy-alpha-PHP (Figure 74) was identified during this research on August 31, 2018. The analyte identified in this sample had an accurate mass of 290.1749 Da (Figure 75). The exact mass of 3,4-methylenedioxy-alpha-PHP ($C_{17}H_{23}NO_3$) is 290.1751 Da, resulting in a sample ppm error of -0.5. The retention time of this analyte was 6.11 minutes (3,4-methylenedioxy-alpha-PHP retention time: 6.01 minutes), resulting in a retention time difference of +0.1 minutes. The isotope difference was calculated to be 2.6%. The library comparison (Figure 76) resulted in a library score of 97.8 in comparison to data acquired using standard reference material for 3,4-methylenedioxy-alpha-PHP. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be 3,4-methylenedioxy-alpha-PHP.

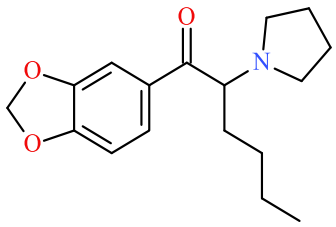

Figure 74: Structure of 3,4-methylenedioxy-alpha-PHP

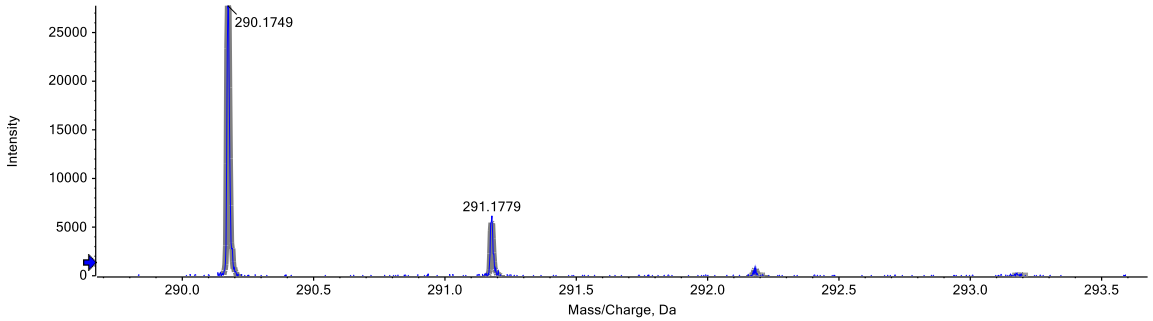

Figure 75: TOF MS data for the analyte identified as 3,4-methylenedioxy-alpha-PHP

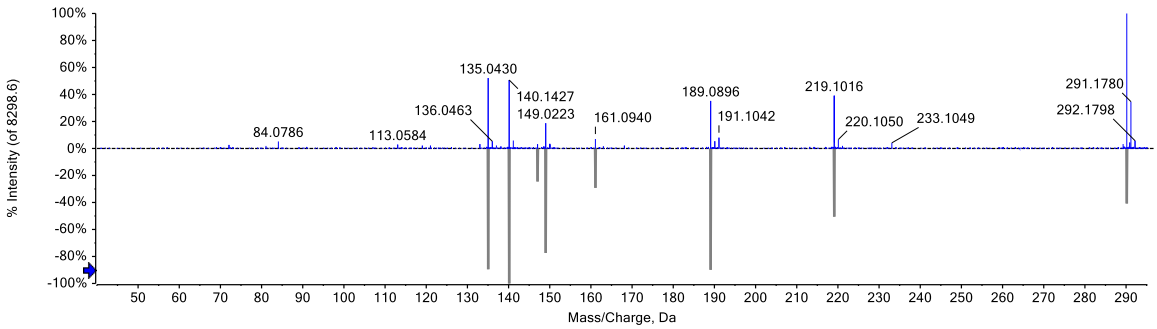

Figure 76: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for 3,4-methylenedioxy-alpha-PHP

Alpha-PHP and 3,4-methylenedioxy-alpha-PHP (MDPHP) are synthetic stimulants and analogues of pyrovalerone and alpha-PVP. PHP stands for pyrrolidinohexiophenone. Alpha-PHP and MDPHP have been identified in other toxicology specimens, as their presence was implicated in a death in 2018.[145] Both alpha-PHP and MDPHP were found in conjunction with designer opioids, including FIBF.

N-Ethyl hexedrone (Figure 77) was identified for the first time in forensic toxicology casework during this research on June 7, 2018. The analyte identified in this sample had an accurate mass of 220.1689 Da (Figure 78). The exact mass of *N*-ethyl

hexedrone ($C_{14}H_{21}NO$) is 220.1696 Da, resulting in a sample ppm error of -2.9. The retention time of this analyte was 5.92 minutes (*N*-ethyl hexedrone retention time: 5.81 minutes), resulting in a retention time difference of +0.11 minutes. The isotope difference was calculated to be 11.0%. The library comparison (Figure 79) resulted in a library score of 85.6 in comparison to data acquired using standard reference material for *N*-ethyl hexedrone. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be *N*-ethyl hexedrone.

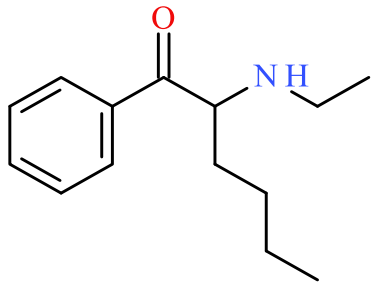

Figure 77: Structure of *N*-ethyl hexedrone

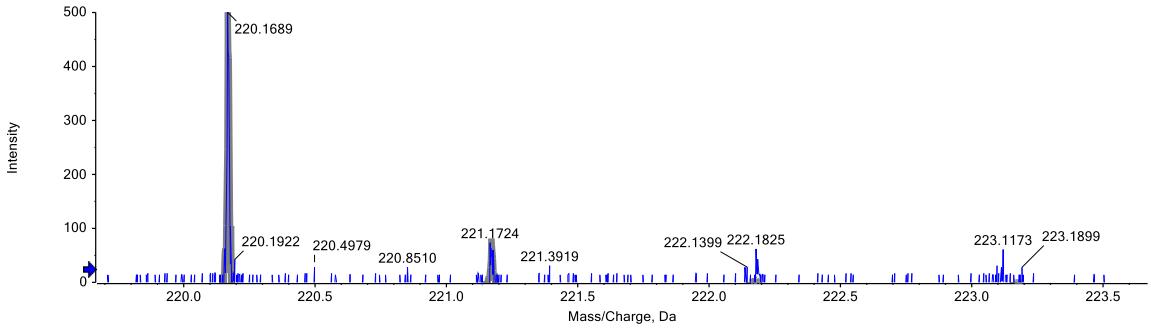

Figure 78: TOF MS data for the analyte identified as *N*-ethyl hexedrone

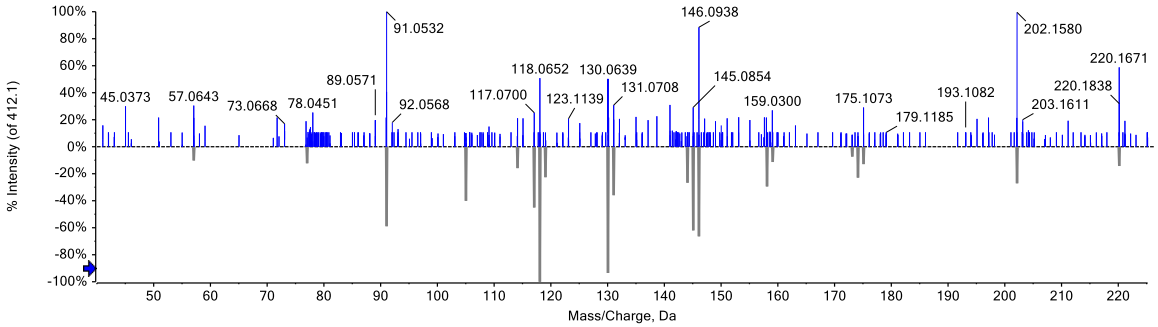

Figure 79: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for *N*-ethyl hexedrone

N-Ethyl hexedrone (hexen, NEH), or 2-(ethylamino)-1-phenyl-hexan-1-one, is a synthetic cathinone and analogue of other *beta*-keto amphetamines. *N*-Ethyl hexedrone is active and highly potent, as described in the literature;[146] although no case reports involving fatalities have been published. *N*-Ethyl hexedrone was identified in extracts initially designated for designer benzodiazepine and designer opioid confirmation, and found in conjunction with diclazepam, etizolam, fentanyl, and FIBF (all analytes incorporated into the initial scope of testing). *N*-Ethyl hexedrone was also found in combination with 4Cl-alpha-PVP, another emergent NPS stimulant.

N-Ethyl hexylone (Figure 80) was first identified in seized drug casework in April of 2018,[147] and subsequently identified in forensic toxicology casework during this research on October 22, 2018. The analyte identified in this sample had an accurate mass of 264.1596 Da (Figure 81). The exact mass of *N*-ethyl hexylone ($C_{15}H_{21}NO_3$) is 264.1594 Da, resulting in a sample ppm error of 0.5. The retention time of this analyte was 5.91 minutes (*N*-ethyl hexylone retention time: 5.96 minutes), resulting in a retention time difference of -0.05 minutes. The isotope difference was calculated to be 13.3%. The

library comparison (Figure 82) resulted in a library score of 100 in comparison to data acquired using standard reference material for *N*-ethyl hexylone. The analyte in the sample met all criteria set forth for positive identification and was therefore determined to be *N*-ethyl hexylone.

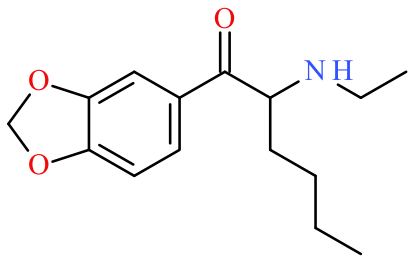

Figure 80: Structure of *N*-ethyl hexylone

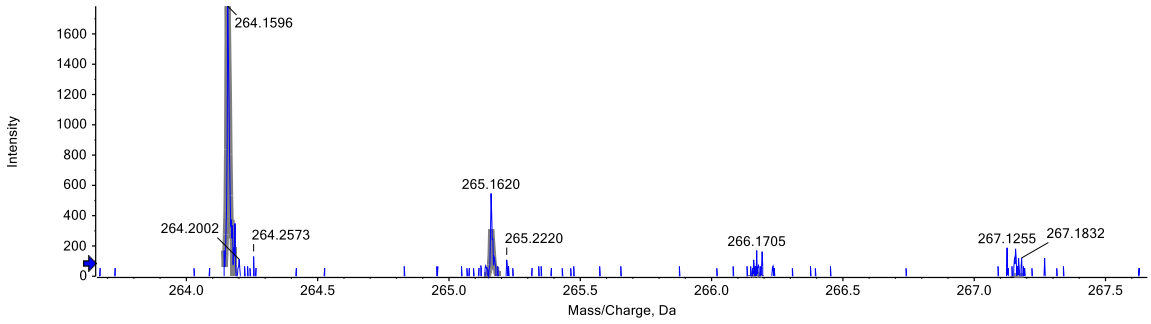

Figure 81: TOF MS data for the analyte identified as *N*-ethyl hexylone

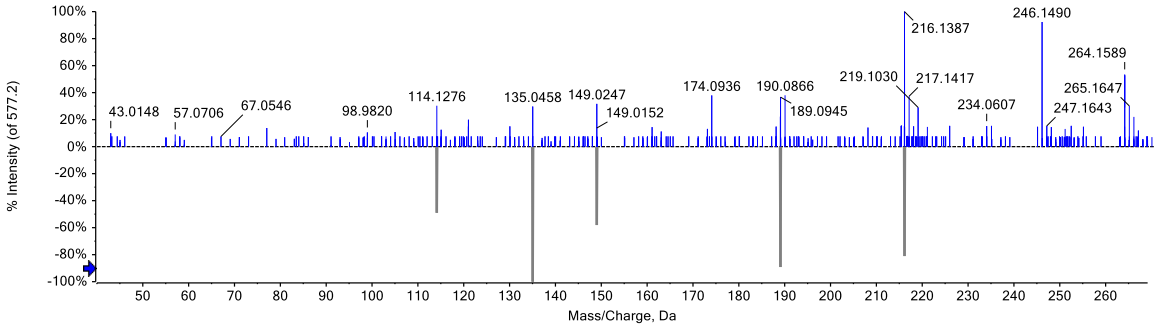

Figure 82: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for *N*-ethyl hexylone

N-Ethyl hexylone, or 1-(1,3-benzodioxol-5-yl)-2-(ethylamino)hexan-1-one, is a synthetic cathinone and analogue of methylone and other *beta*-keto methylenedioxyamphetamines (e.g. eutylone). Like other novel stimulants in this class, the synthesis of *N*-ethyl hexylone has been described in patent literature,[143] but there is no information regarding its activity or toxicity.

4.7.5 NPS Benzodiazepines

Flualprazolam (Figure 83) was first identified during this research on April 22, 2019. The analyte identified in this sample had an accurate mass of 327.0800 Da (Figure 84). The exact mass of flualprazolam ($C_{17}H_{12}ClFN_4$) is 327.0807 Da, resulting in a sample ppm error of -2.1. The retention time of this analyte was 7.30 minutes (flualprazolam retention time: 7.29 minutes), resulting in a retention time difference of +0.01 minutes. The isotope difference was calculated to be 18.5%. The library comparison (Figure 85) resulted in a library score of 98.7 in comparison to data acquired using standard reference material for flualprazolam. The analyte in the sample met all

criteria set forth for positive identification and was therefore determined to be flualprazolam.

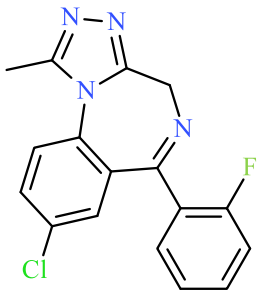

Figure 83: Structure of flualprazolam

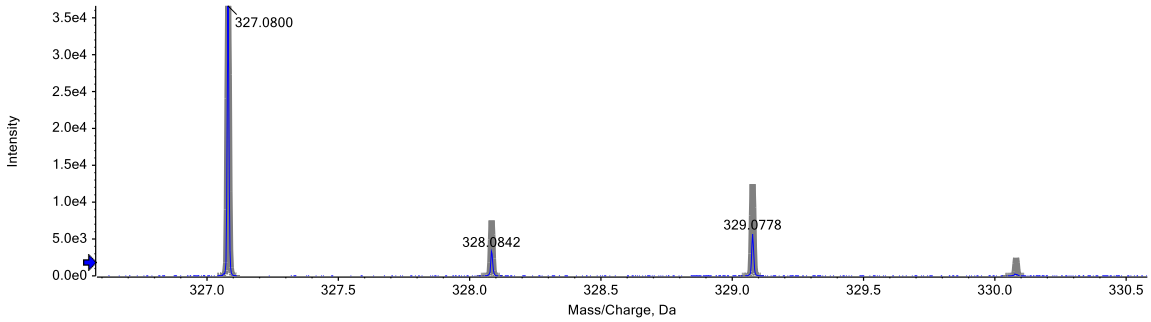

Figure 84: TOF MS data for the analyte identified as flualprazolam

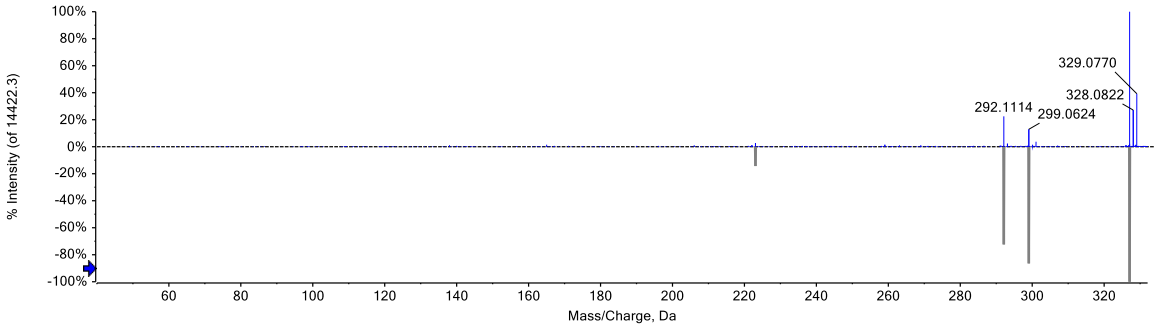

Figure 85: Fragment (MSMS) data from sample (top) and standard reference materials (bottom) for flualprazolam

Flualprazolam, or 8-chloro-6-(2-fluorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine, is a synthetic benzodiazepine and analogue of alprazolam. The synthesis and activity of flualprazolam have been described in the patent literature,[148] but there is no information regarding its toxicity in humans. Flualprazolam was first been reported in seized drug material in December of 2017 by a government agency.

CHAPTER 5

TRENDS

5.1 Introduction

The main driving force behind identification of emergent NPS during this research was the hypothesis that NPS were being used in combination or close temporal proximity with other NPS and/or drugs of abuse. This hypothesis was proven true based on the results outlined in Chapter 4; however, emergent NPS results do not provide answers to the extent of poly-drug use or specific aspects of poly-drug use. Further investigation was necessary to determine how often NPS are found in combination with other NPS, and what specific analyte combinations were prevalent in this subset of a forensic population.

Several studies have outlined the extent of poly-drug use among users of traditional or legacy drugs of abuse (e.g. cocaine, methamphetamine, MDMA, etc.).[149–151] These studies have used differing modes of data collection and interpretation, including drug user surveys, evaluation of seized drug materials, and comparison of toxicological findings. However, these studies each lack aspects critical to determining the true extent of poly-drug use. While drug user surveys provide a look into the habits and behaviors of these individuals, they lack the necessary analytical testing required for accurate data collection and formulation of conclusions. For example, a drug user may say they are using heroin, but without differentiation that the opioid powder is heroin vs. fentanyl one can not accurately assess the drug(s) used. Evaluation of seized drug materials allow for

determination of drug combinations at bulk (or dealer) and street drug (or user) levels, but these results can not account for concurrent drug use or drug use proximate in time (e.g. cyclic depressant and stimulant use). Comparison of toxicological findings provides the best insight into concurrent or near-concurrent drug use, specifically with evaluation of blood results. There are limitations with respect to toxicological findings though, specifically when comparing results from targeted or limited testing procedures. For example, if a blood sample is subjected to analysis for fentanyl only or cocaine only, testing can not determine whether the user was using both an opioid and a stimulant. In many cases, this is common among forensic toxicological analyses, where samples are tested only for specific drugs or drug classes based on findings from autopsy, scene, etc. (there is also a monetary aspect). When considering samples that are screened using broad-based methodologies, these testing results are often lacking as well if a laboratory is not frequently updating the scope of testing to include emerging drugs. Contrary to all of these shortcomings, the non-targeted LC-QTOF-MS methodology developed herein provides the most comprehensive picture to accurately evaluate poly-drug use. To our knowledge, our approach is the only testing procedure that is comprehensively acquiring this data from biological samples in a single analysis.

Determination of poly-drug use is of high importance due to drug-drug interactions and the potential to create morbidity and mortality among drug users. This information is not only important among the forensic toxicology community (for laboratory practice and implementation purposes), but also among public health, public

safety, law enforcement, medicolegal death investigation, emergency medicine, and others.

Since the majority of biological sample extracts received and analyzed during this research were from testing procedures for the evaluation of opioids, the generated dataset provided a unique opportunity to study fentanyl poly-drug use in addition to poly-NPS use. For the purposes of this portion of the research, trends in analytical findings among fentanyl users were first studies, as this was the largest positive subset of data within the population. Fentanyl can be considered an NPS for its novel use among recreation drug users, but its identity was kept separate during classification. Secondarily, trends in analytical findings among NPS users were evaluated.

The opioid epidemic continues to contribute to morbidity and mortality in the United States, growing and evolving since the increase in prevalence of fentanyl in the heroin supply beginning around 2014. Following the identification of mixtures of fentanyl and heroin in seized material, laboratories began identifying new variants of fentanyl, often referred to as analogues or derivatives. The number of new fentanyl analogues in the drug supply increased and diversified until the temporary federal "core structure" scheduling of fentanyl related substances by the Drug Enforcement Administration in February 2018. Now, post fentanyl analogue scheduling, the illicit synthetic opioid market has transitioned back to primarily fentanyl, but with evidence of poly-drug use. Based on this observation, this research sought to document patterns of poly-drug use in forensic toxicology casework to determine what substances were most frequently found in conjunction with fentanyl.

Likewise, what could be considered an NPS epidemic continues to contribute to morbidity and mortality in the United States, growing and evolving since the increase in prevalence of synthetic cannabinoids around 2008. While synthetic cannabinoids were not included in the focus of this research, a multitude of NPS have been discovered since this time. Different waves of NPS can be seen over time, as outlined in Chapter 2, including the explosion of fentanyl analogues prior to individual and core structure scheduling actions. Before the shift in the illicit synthetic opioid market back to fentanyl, the year or so leading up to this transition saw an increase in the use of fluoroisobutyrylfentanyl, the most commonly detected fentanyl analogue among this subset of data. As with fentanyl, this research sought to document patterns of poly-NPS use in forensic toxicology casework to determine what NPS were most frequently found in conjunction with other NPS.

5.2 Methods

As described in Chapter 4, analytical testing was performed via LC-QTOF-MS using a SCIEX TripleTOF™ 5600+ (Ontario, Canada) and Shimadzu Nexera XR UHPLC (Kyoto, Japan). This represents a non-targeted drug testing approach that differs from traditional forensic toxicology testing protocols. Discarded sample vial extracts, primarily collected from testing procedures for the directed analysis of synthetic opioids, were acquired from a large forensic toxicology laboratory (NMS Labs, Willow Grove, PA, USA). All sample extracts were deidentified prior to inclusion in this research. In total, 3,543 sample extracts were analyzed and processed against an extensive, and

continuously updated, in-house library database containing more than 750 drugs, including fentanyl, fentanyl metabolites, fentanyl analogues, other synthetic opioids and drugs of abuse, as well as an extensive number of NPS.

The results from comprehensive data processing included the identification of a wide-variety of substances covering all classes and included parent drugs (e.g. fentanyl), metabolites (e.g. norfentanyl), and synthesis precursors (e.g. 4-ANPP) or byproducts (e.g. acetylfentanyl). For a more accurate determination of drug use, individual identifications were categorized under explicit parent drug groups prior to complex data analysis to determine positivity and combinations (Table 7). For example, results of fentanyl, norfentanyl, and/or beta-hydroxyfentanyl were all categorized as "fentanyl positive"; 4-ANPP and acetylfentanyl were not considered for inclusion based on undistinguishable source. Drug classes evaluated included stimulants (e.g. cocaine, methamphetamine, MDMA), opiates/opioids (e.g. heroin, tramadol, buprenorphine), hallucinogens (e.g. ketamine, phencyclidine), and benzodiazepines (e.g. diazepam, alprazolam), as well as these same classes for NPS (Table 8).

Table 7: Drug, metabolite, and precursor re-classification

Drug Class	Reported Drug Name	Results from LC-QTOF-MS Analysis
Opioid	Fentanyl	Fentanyl, Norfentanyl, and/or beta-Hydroxyfentanyl (excluded: 4-ANPP, Acetylfentanyl)
Opioid	Mitragynine	Mitragynine and/or 7-Hydroxymitragynine
Opiate/ Opioid	Heroin	Diacetylmorphine (Heroin), 6-Monoacetylmorphine (6-MAM), Morphine, Acetylcodeine, Codeine, and/or Norcodeine (excluded: Codeine and/or Norcodeine positives only)
Opioid	Prescription	Oxycodone, Noroxycodone, Oxymorphone, Hydrocodone, Hydromorphone, and Dihydrocodeine
Opioid	Tramadol	Tramadol and/or O-Desmethyltramadol

Opioid	Buprenorphine	Buprenorphine and/or Norbuprenorphine
Opioid	Methadone	Methadone, EDDP, and/or EMDP
Stimulant	Cocaine	Cocaine, Benzoylecgonine (BZE), Norcocaine, and/or Cocaethylene
Stimulant	Methamphetamine	Methamphetamine and/or Amphetamine
Stimulant	MDMA ["Ecstasy"]	MDMA, MDA, and/or MDEA
Stimulant	Other	Methylphenidate
Hallucinogen	Ketamine	Ketamine and/or Norketamine
Hallucinogen	Other	Phencyclidine (PCP), LSD, Psilocin, Mescaline, Bufotenine, *N*,*N*-Dimethyltryptamine (DMT), Salvinorin A
Benzodiazepine	Midazolam	Midazolam and/or 1-Hydroxymidazolam
Benzodiazepine	Clonazepam	Clonazepam and/or 7-Aminoclonazepam
Benzodiazepine	Alprazolam	Alprazolam and/or Alpha-Hydroxyalprazolam
Benzodiazepine	Lorazepam	Lorazepam and/or Delorazepam
Benzodiazepine	Diazepam	Diazepam, Nordiazepam, Oxazepam, and/or Temazepam

Table 8: NPS classification (in alphabetical order)

NPS Class	NPS Category	Results from LC-QTOF-MS Analysis
Opioid	Fentanyl Analogue	3-Methylfentanyl, Acrylfentanyl, Butyrylfentanyl, Carfentanil, Cyclopropylfentanyl, Fluorofentanyl, Fluoroisobutyrylfentanyl, Furanylfentanyl, Methoxyacetylfentanyl, Fluorofuranylfentanyl, Phenylfentanyl, Tetrahydrofuranylfentanyl, Valerylfentanyl (excluded: Acetylfentanyl, Sufentanil)
Opioid	Fentanyl Analogue Precursor	Benzyl Fentanyl, Benzyl Furanylfentanyl, Despropionyl 3-Methylfentanyl, Despropionyl Fluorofentanyl (F-4-ANPP), Despropionyl *ortho*-Methylfentanyl, *N*-methyl Norfentanyl, Benzyl Fluorocyclopropylfentanyl
Opioid	Non-Fentanyl Opioids [NFO]	AH-7921, Isopropyl-U-47700, 3,4-Methylenedioxy-U-47700, *N*,*N*-Didesmethyl-U-47700, *N*-Desmethyl-U-47700, U-47700, U-48800
Stimulant	Pyrrolidine Cathinones	4-Cl-Alpha-PVP, 4F-Alpha-PHP, Alpha-PBP, Alpha-PHP, Alpha-PVP, 3,4-Methylenedioxy-Alpha-PHP (MDPHP), Pyrovalerone
Stimulant	Methylenedioxy Cathinones	Benzylone, Butylone, Dibutylone, Ethylone, Eutylone, Methylone, *N*-Ethyl Hexylone, *N*-Ethyl Pentylone, Pentylone
Stimulant	Other Cathinones	Methcathinone, *N*-Ethyl Hexedrone (Hexen), 4Cl-Isopropylcathinone
Stimulant	Phenethylamines	Fluoroamphetamine (FA), Fluoroethamphetamine (FEA),

		Fluoromethamphetamine (FMA), Methoxyamphetamine (PMA), Methoxymethamphetamine (PMMA)
Stimulant	Other	MBZP
Hallucinogen	Ketamine Analogue	2F-Deschloroketamine, Deschloroketamine, N-ethyl Deschloroketamine
Hallucinogen	PCP Analogue	3/4-MeO-PCP, 3/4-OH-PCP
Hallucinogen	Other	4-HO-DiPT, *N*-Methyltryptamine
Benzodiazepine	Other	Bromazepam, Clonazolam, Diclazepam, Etizolam, Flualprazolam, Flubromazolam, Flubromazepam, Phenazepam, Pyrazolam

5.3 Results and Discussion

5.3.1 Identifications and Overall Trends

In total, 3,543 extracts were acquired between Q1 2018 and Q2 2019, accounting for 16,219 individual results (e.g. parent drug, metabolite, precursor, etc.). To evaluate identifications over time (i.e. temporal trends), the total number of identifications for each drug was tallied and normalized using the total number of extracts analyzed in each specific quarter. This was required to evaluate trends due to the large discrepancy in number of samples analyzed per quarter (e.g. Q2 2018 = 1,490 vs. Q2 2019 = 107).

Fentanyl was the most frequently identified analyte during this research (n=1,268). The positivity of fentanyl and related species is shown in Table 9. Overall fentanyl positivity was stable throughout the course of this research, with the exception of a spike in positivity in Q4 2019. The positivity of 4-ANPP decreased from Q1 2018 to Q2 2019, but this can not be linked to a certain cause due to indistinguishable source. Possible reasons for this decrease in positivity could be better clandestine synthesis of fentanyl or the disappearance of analogues that metabolize to 4-ANPP.

Table 9: Positivity of fentanyl, its metabolites and precursor

Analyte	2018				2019		Overall
	Q1	Q2	Q3	Q4	Q1	Q2	
4-ANPP	91	158	89	25	9	3	**375**
	14.8%	*10.8%*	*12.0%*	*5.3%*	*6.1%*	*2.8%*	***10.6%***
Acetylfentanyl	25	64	44	13	7	4	**157**
	4.1%	*4.4%*	*6.0%*	*2.7%*	*4.7%*	*3.7%*	***4.4%***
beta-Hydroxyfentanyl	7	23	43	4	1	1	**79**
	1.1%	*1.6%*	*5.8%*	*0.8%*	*0.7%*	*0.9%*	***2.2%***
Fentanyl	153	576	329	116	55	39	**1,268**
	24.8%	*39.5%*	*44.5%*	*24.5%*	*37.2%*	*36.4%*	***35.8%***
Norfentanyl	29	132	177	36	5	5	**384**
	4.7%	*9.0%*	*24.0%*	*7.6%*	*3.4%*	*4.7%*	***10.8%***

Several individual temporal trends among NPS can be ascertained based on identifications and positivity shown in Table 10. The most notable trend was a decrease in positivity of all fentanyl analogues and NPS opioids leading up to Q2 2019. The highest positivities for 3-methylfentanyl, acrylfentanyl, carfentanil, cyclopropylfentanyl, furanylfentanyl, methoxyacetylfentanyl, and U-47700 were observed in Q1 2018, with dramatic declines over time. Peak positivity of fluoroisobutyrylfentanyl was observed in Q2 2018, followed by an eventual decline in 2019. While other NPS opioid positivity was decreasing towards the end of 2018, a spike in valerylfentanyl positivity was observed; however, positivity of valerylfentanyl later declined. In terms of NPS stimulants, the positivity of *N*-ethyl pentylone remained steady in 2018 and 2019, with the exception of Q2 2018, while the positivity of eutylone increased in Q1 2019.

Table 10: Positivity of NPS

Analyte	2018				2019		Overall
	Q1	Q2	Q3	Q4	Q1	Q2	
2F-Deschloroketamine	0	0	2	0	0	0	**2**
	0.0%	*0.0%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
3-Methylfentanyl	24	7	2	1	1	0	**35**
	3.9%	*0.5%*	*0.3%*	*0.2%*	*0.7%*	*0.0%*	***1.0%***
3/4-OH-PCP	0	0	0	0	2	0	**2**
	0.0%	*0.0%*	*0.0%*	*0.0%*	*1.4%*	*0.0%*	***0.1%***
3,4-Methylenedioxy-alpha-PHP	0	3	2	0	0	0	**5**
	0.0%	*0.2%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
3,4-Methylenedioxy-U-47700	3	9	0	0	0	0	**12**
	0.5%	*0.6%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.3%***
4-Cl-Alpha-PVP	0	1	0	1	0	0	**2**
	0.0%	*0.1%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
4Cl-Isopropylcathinone	0	0	1	0	0	0	**1**
	0.0%	*0.0%*	*0.1%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
4F-Alpha-PHP	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
4-HO-DiPT	0	1	0	1	0	0	**2**
	0.0%	*0.1%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
3/4-MeO-PCP	13	6	3	0	3	0	**25**
	2.1%	*0.4%*	*0.4%*	*0.0%*	*2.0%*	*0.0%*	***0.7%***
Acrylfentanyl	14	2	0	0	0	0	**16**
	2.3%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.5%***
AH-7921	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Alpha-PBP	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Alpha-PHP	2	8	1	1	0	2	**14**
	0.3%	*0.5%*	*0.1%*	*0.2%*	*0.0%*	*1.9%*	***0.4%***
Alpha-PVP	4	2	0	0	0	0	**6**
	0.6%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.2%***
Benzyl Fentanyl	6	5	0	0	0	0	**11**
	1.0%	*0.3%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.3%***
Benzyl Fluoro-cyclopropylfentanyl	0	0	0	0	2	0	**2**
	0.0%	*0.0%*	*0.0%*	*0.0%*	*1.4%*	*0.0%*	***0.1%***
Benzyl Furanylfentanyl	0	0	5	0	1	0	**6**
	0.0%	*0.0%*	*0.7%*	*0.0%*	*0.7%*	*0.0%*	***0.2%***

Benzylone	0	0	0	0	0	1	**1**
	0.0%	*0.0%*	*0.0%*	*0.0%*	*0.0%*	*0.9%*	***0.03%***
Bromazepam	2	1	3	4	3	0	**13**
	0.3%	*0.1%*	*0.4%*	*0.8%*	*2.0%*	*0.0%*	***0.4%***
Butylone	1	3	3	1	2	0	**10**
	0.2%	*0.2%*	*0.4%*	*0.2%*	*1.4%*	*0.0%*	***0.3%***
Butyrylfentanyl	1	4	3	1	0	0	**9**
	0.2%	*0.3%*	*0.4%*	*0.2%*	*0.0%*	*0.0%*	***0.3%***
Carfentanil	30	16	2	0	0	0	**48**
	4.9%	*1.1%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***1.4%***
Clonazolam	0	9	1	1	0	0	**11**
	0.0%	*0.6%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.3%***
Cyclopropylfentanyl	118	132	50	6	2	1	**309**
	19.2%	*9.0%*	*6.8%*	*1.3%*	*1.4%*	*0.9%*	***8.7%***
Deschloroketamine	2	2	0	0	0	0	**4**
	0.3%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Despropionyl 3-Methylfentanyl	2	0	0	0	0	0	**2**
	0.3%	*0.0%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Despropionyl Fluorofentanyl (F-4-ANPP)	0	1	0	0	3	1	**5**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*2.0%*	*0.9%*	***0.1%***
Despropionyl *ortho*-Methylfentanyl	2	0	0	0	0	0	**2**
	0.3%	*0.0%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Dibutylone	1	4	6	2	0	0	**13**
	0.2%	*0.3%*	*0.8%*	*0.4%*	*0.0%*	*0.0%*	***0.4%***
Diclazepam	3	5	3	5	2	1	**19**
	0.5%	*0.3%*	*0.4%*	*1.1%*	*1.4%*	*0.9%*	***0.5%***
Ethylone	0	0	0	1	0	0	**1**
	0.0%	*0.0%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.03%***
Etizolam	8	34	18	9	16	7	**92**
	1.3%	*2.3%*	*2.4%*	*1.9%*	*10.8%*	*6.5%*	***2.6%***
Eutylone	0	0	1	1	6	2	**10**
	0.0%	*0.0%*	*0.1%*	*0.2%*	*4.1%*	*1.9%*	***0.3%***
Flualprazolam	0	1	0	0	0	2	**3**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*1.9%*	***0.1%***
Flubromazolam	6	27	2	3	4	1	**43**
	1.0%	*1.8%*	*0.3%*	*0.6%*	*2.7%*	*0.9%*	***1.2%***
Flubromazepam	1	4	1	1	0	0	**7**
	0.2%	*0.3%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.2%***
Fluoroamphetamine	0	1	0	0	2	0	**3**

(Fluoroamphetamine)	*0.0%*	*0.1%*	*0.0%*	*0.0%*	*1.4%*	*0.0%*	***0.1%***
Fluoroethamphetamine	0	0	0	0	2	0	**2**
	0.0%	*0.0%*	*0.0%*	*0.0%*	*1.4%*	*0.0%*	***0.1%***
Fluorofentanyl	0	2	0	0	0	0	**2**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Fluorofuranylfentanyl	0	0	0	0	3	0	**3**
	0.0%	*0.0%*	*0.0%*	*0.0%*	*2.0%*	*0.0%*	***0.1%***
Fluoroisobutyrylfentanyl	43	264	86	27	4	6	**430**
	7.0%	*18.1%*	*11.6%*	*5.7%*	*2.7%*	*5.6%*	***12.1%***
Fluoromethamphetamine	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Furanylfentanyl	21	31	7	3	2	0	**64**
	3.4%	*2.1%*	*0.9%*	*0.6%*	*1.4%*	*0.0%*	***1.8%***
Isopropyl-U-47700	0	5	0	0	0	0	**5**
	0.0%	*0.3%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
MBZP	0	1	1	0	0	0	**2**
	0.0%	*0.1%*	*0.1%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Methcathinone	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Methoxyacetylfentanyl	97	109	25	10	2	2	**245**
	15.7%	*7.5%*	*3.4%*	*2.1%*	*1.4%*	*1.9%*	***6.9%***
Methoxyamphetamine (PMA)	0	2	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Methoxymethamphetamine (PMMA)	0	2	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Methylone	1	4	0	2	0	0	**7**
	0.2%	*0.3%*	*0.0%*	*0.4%*	*0.0%*	*0.0%*	***0.2%***
N,N-Didesmethyl-U-47700	5	10	3	1	0	0	**19**
	0.8%	*0.7%*	*0.4%*	*0.2%*	*0.0%*	*0.0%*	***0.5%***
N-Desmethyl-U-47700	18	23	5	3	0	0	**49**
	2.9%	*1.6%*	*0.7%*	*0.6%*	*0.0%*	*0.0%*	***1.4%***
N-Ethyl Deschloroketamine	0	0	0	1	0	0	**1**
	0.0%	*0.0%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.03%***
N-Ethyl Hexedrone (Hexen)	1	2	1	1	0	0	**5**
	0.2%	*0.1%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
N-Ethyl Hexylone	0	0	0	1	0	0	**1**
	0.0%	*0.0%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.03%***
N-Ethyl Pentylone	13	34	30	27	10	0	**114**
	2.1%	*2.3%*	*4.1%*	*5.7%*	*6.8%*	*0.0%*	***3.2%***

N-Methyl Norfentanyl	1	7	4	1	2	0	**15**
	0.2%	*0.5%*	*0.5%*	*0.2%*	*1.4%*	*0.0%*	***0.4%***
N-Methyltryptamine	0	0	1	0	0	0	**1**
	0.0%	*0.0%*	*0.1%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Norcarfentanil	0	2	0	0	0	0	**2**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Pentylone	1	2	0	2	0	0	**5**
	0.2%	*0.1%*	*0.0%*	*0.4%*	*0.0%*	*0.0%*	***0.1%***
Phenazepam	0	3	0	1	0	0	**4**
	0.0%	*0.2%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
Phenylfentanyl	0	0	5	0	0	0	**5**
	0.0%	*0.0%*	*0.7%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Pyrazolam	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Pyrovalerone	1	0	0	0	0	0	**1**
	0.2%	*0.0%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Sufentanil	18	0	0	0	0	0	**18**
	2.9%	*0.0%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.5%***
Tetrahydrofuranylfentanyl (THFF)	0	2	0	0	0	0	**2**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
U-47700	26	40	9	5	0	0	**80**
	4.2%	*2.7%*	*1.2%*	*1.1%*	*0.0%*	*0.0%*	***2.3%***
U-48800	3	15	0	1	0	0	**19**
	0.5%	*1.0%*	*0.0%*	*0.2%*	*0.0%*	*0.0%*	***0.5%***
Valerylfentanyl	0	0	1	7	1	1	**10**
	0.0%	*0.0%*	*0.1%*	*1.5%*	*0.7%*	*0.9%*	***0.3%***

Overall, there was little to no change in temporal trends for the majority of legacy drugs of abuse, as shown in Table 11. However, there appears to be a decline in heroin (e.g. diacetylmorphine, 6-MAM, morphine) positivity in 2019, possibly accounting for the transition of the opioid drug market from heroin to fentanyl. Mitragynine and tramadol positivity were observed to be constant, suggesting opioid users are not largely exploring these drugs as alternatives. Cocaine and methamphetamine positivity were stable; MDMA positivity appears to decline from 2018 to 2019.

Table 11: Positivity of drugs of abuse

Analyte	2018				2019		Overall
	Q1	Q2	Q3	Q4	Q1	Q2	
1-Hydroxymidazolam	0	4	4	1	1	0	**10**
	0.0%	*0.3%*	*0.5%*	*0.2%*	*0.7%*	*0.0%*	***0.3%***
6-Monoacetylmorphine (6-MAM)	16	50	69	17	6	1	**159**
	2.6%	*3.4%*	*9.3%*	*3.6%*	*4.1%*	*0.9%*	***4.5%***
7-Aminoclonazepam	2	19	6	13	1	0	**41**
	0.3%	*1.3%*	*0.8%*	*2.7%*	*0.7%*	*0.0%*	***1.2%***
7-Hydroxymitragynine	6	3	10	10	2	1	**32**
	1.0%	*0.2%*	*1.4%*	*2.1%*	*1.4%*	*0.9%*	***0.9%***
Acetylcodeine	0	5	23	3	0	1	**32**
	0.0%	*0.3%*	*3.1%*	*0.6%*	*0.0%*	*0.9%*	***0.9%***
Alpha-Hydroxyalprazolam	1	0	0	0	0	0	**1**
	0.2%	*0.0%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Alprazolam	58	166	68	35	9	0	**336**
	9.4%	*11.4%*	*9.2%*	*7.4%*	*6.1%*	*0.0%*	***9.5%***
Amphetamine	25	86	42	36	9	0	**198**
	4.1%	*5.9%*	*5.7%*	*7.6%*	*6.1%*	*0.0%*	***5.6%***
Benzoylecgonine (BZE)	105	287	173	44	18	16	**643**
	17.0%	*19.7%*	*23.4%*	*9.3%*	*12.2%*	*15.0%*	***18.1%***
Bufotenine	3	1	4	6	0	0	**14**
	0.5%	*0.1%*	*0.5%*	*1.3%*	*0.0%*	*0.0%*	***0.4%***
Buprenorphine	2	5	20	18	1	0	**46**
	0.3%	*0.3%*	*2.7%*	*3.8%*	*0.7%*	*0.0%*	***1.3%***
Clonazepam	1	1	2	0	0	0	**4**
	0.2%	*0.1%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Cocaethylene	37	86	49	21	10	8	**211**
	6.0%	*5.9%*	*6.6%*	*4.4%*	*6.8%*	*7.5%*	***6.0%***
Cocaine	111	282	159	41	22	18	**633**
	18.0%	*19.3%*	*21.5%*	*8.7%*	*14.9%*	*16.8%*	***17.9%***
Codeine	21	99	115	27	10	4	**276**
	3.4%	*6.8%*	*15.6%*	*5.7%*	*6.8%*	*3.7%*	***7.8%***
Delorazepam	3	9	2	4	5	1	**24**
	0.5%	*0.6%*	*0.3%*	*0.8%*	*3.4%*	*0.9%*	***0.7%***
Diacetylmorphine (Heroin)	2	3	12	2	0	0	**19**
	0.3%	*0.2%*	*1.6%*	*0.4%*	*0.0%*	*0.0%*	***0.5%***
Diazepam	50	60	20	10	4	1	**145**
	8.1%	*4.1%*	*2.7%*	*2.1%*	*2.7%*	*0.9%*	***4.1%***

Dihydrocodeine	6	17	19	21	1	0	**64**
	1.0%	*1.2%*	*2.6%*	*4.4%*	*0.7%*	*0.0%*	***1.8%***
DMT	1	0	2	0	0	0	**3**
	0.2%	*0.0%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
EDDP	17	70	81	16	4	5	**193**
	2.8%	*4.8%*	*11.0%*	*3.4%*	*2.7%*	*4.7%*	***5.4%***
EMDP	1	5	8	4	0	0	**18**
	0.2%	*0.3%*	*1.1%*	*0.8%*	*0.0%*	*0.0%*	***0.5%***
Hydrocodone	12	34	27	19	3	0	**95**
	1.9%	*2.3%*	*3.7%*	*4.0%*	*2.0%*	*0.0%*	***2.7%***
Hydromorphone	2	7	17	16	0	0	**42**
	0.3%	*0.5%*	*2.3%*	*3.4%*	*0.0%*	*0.0%*	***1.2%***
Ketamine	7	12	14	2	0	0	**35**
	1.1%	*0.8%*	*1.9%*	*0.4%*	*0.0%*	*0.0%*	***1.0%***
Lorazepam	2	3	0	0	2	0	**7**
	0.3%	*0.2%*	*0.0%*	*0.0%*	*1.4%*	*0.0%*	***0.2%***
LSD	2	1	2	0	0	0	**5**
	0.3%	*0.1%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
MDA	11	22	7	6	0	0	**46**
	1.8%	*1.5%*	*0.9%*	*1.3%*	*0.0%*	*0.0%*	***1.3%***
MDEA	2	3	0	0	0	0	**5**
	0.3%	*0.2%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
MDMA	19	32	14	6	0	0	**71**
	3.1%	*2.2%*	*1.9%*	*1.3%*	*0.0%*	*0.0%*	***2.0%***
Mescaline	0	0	2	0	0	0	**2**
	0.0%	*0.0%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Methadone	22	67	79	18	5	7	**198**
	3.6%	*4.6%*	*10.7%*	*3.8%*	*3.4%*	*6.5%*	***5.6%***
Methamphetamine	69	199	88	54	26	10	**446**
	11.2%	*13.6%*	*11.9%*	*11.4%*	*17.6%*	*9.3%*	***12.6%***
Methylphenidate	6	9	3	0	1	0	**19**
	1.0%	*0.6%*	*0.4%*	*0.0%*	*0.7%*	*0.0%*	***0.5%***
Midazolam	5	16	7	4	1	1	**34**
	0.8%	*1.1%*	*0.9%*	*0.8%*	*0.7%*	*0.9%*	***1.0%***
Mitragynine	37	46	24	17	7	2	**133**
	6.0%	*3.2%*	*3.2%*	*3.6%*	*4.7%*	*1.9%*	***3.8%***
Morphine	54	191	223	65	19	6	**558**
	8.8%	*13.1%*	*30.2%*	*13.7%*	*12.8%*	*5.6%*	***15.7%***
Norbuprenorphine	2	9	35	20	1	0	**67**

(Norbuprenorphine)	*0.3%*	*0.6%*	*4.7%*	*4.2%*	*0.7%*	*0.0%*	***1.9%***
Norcocaine	27	78	79	9	6	3	**202**
	4.4%	*5.3%*	*10.7%*	*1.9%*	*4.1%*	*2.8%*	***5.7%***
Norcodeine	3	14	44	6	1	0	**68**
	0.5%	*1.0%*	*6.0%*	*1.3%*	*0.7%*	*0.0%*	***1.9%***
Nordiazepam	20	55	17	9	3	0	**104**
	3.2%	*3.8%*	*2.3%*	*1.9%*	*2.0%*	*0.0%*	***2.9%***
Norketamine	4	10	5	3	0	0	**22**
	0.6%	*0.7%*	*0.7%*	*0.6%*	*0.0%*	*0.0%*	***0.6%***
Noroxycodone	12	49	33	26	6	2	**128**
	1.9%	*3.4%*	*4.5%*	*5.5%*	*4.1%*	*1.9%*	***3.6%***
O-Desmethyltramadol	22	23	29	7	6	1	**88**
	3.6%	*1.6%*	*3.9%*	*1.5%*	*4.1%*	*0.9%*	***2.5%***
Oxazepam	1	1	1	1	0	0	**4**
	0.2%	*0.1%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
Oxycodone	19	73	42	28	6	3	**171**
	3.1%	*5.0%*	*5.7%*	*5.9%*	*4.1%*	*2.8%*	***4.8%***
Oxymorphone	2	1	2	4	0	0	**9**
	0.3%	*0.1%*	*0.3%*	*0.8%*	*0.0%*	*0.0%*	***0.3%***
Phencyclidine (PCP)	1	8	9	4	1	0	**23**
	0.2%	*0.5%*	*1.2%*	*0.8%*	*0.7%*	*0.0%*	***0.6%***
Psilocin	3	1	3	0	0	0	**7**
	0.5%	*0.1%*	*0.4%*	*0.0%*	*0.0%*	*0.0%*	***0.2%***
Salvinorin A	0	0	1	0	0	0	**1**
	0.0%	*0.0%*	*0.1%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Temazepam	2	5	1	2	0	0	**10**
	0.3%	*0.3%*	*0.1%*	*0.4%*	*0.0%*	*0.0%*	***0.3%***
Tramadol	31	69	78	21	14	4	**217**
	5.0%	*4.7%*	*10.6%*	*4.4%*	*9.5%*	*3.7%*	***6.1%***

Additional substances were detected during analytical testing, including therapeutic drugs, cutting agents, and other substances. Identifications and positivity for notable analytes are shown in Table 12. No noticeable temporal trends were observed among this group of substances. As expected, naloxone positivity was generally constant. Of important note, cannabinoid metabolites and synthetic cannabinoids identified have

been placed in this category; their identify was not included with NPS or drugs of abuse due to mismatch in chemistry of extraction protocols and detection limits (e.g. these were not readily detected among the extracts).

Table 12: Positivity of other notable analytes

Analyte	2018				2019		Overall
	Q1	Q2	Q3	Q4	Q1	Q2	
Bupivacaine	0	3	0	2	0	0	**5**
	0.0%	*0.2%*	*0.0%*	*0.4%*	*0.0%*	*0.0%*	***0.1%***
10-Hydroxycarbazepine	0	3	1	4	0	0	**8**
	0.0%	*0.2%*	*0.1%*	*0.8%*	*0.0%*	*0.0%*	***0.2%***
5F-ADB	0	0	2	0	0	0	**2**
	0.0%	*0.0%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
5F-ADB Metabolite	0	0	1	0	0	0	**1**
	0.0%	*0.0%*	*0.1%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
AM-3102	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Amitriptyline	22	37	14	9	3	3	**88**
	3.6%	*2.5%*	*1.9%*	*1.9%*	*2.0%*	*2.8%*	***2.5%***
Aripiprazole	11	10	11	2	0	1	**35**
	1.8%	*0.7%*	*1.5%*	*0.4%*	*0.0%*	*0.9%*	***1.0%***
Atropine	15	17	23	4	0	1	**60**
	2.4%	*1.2%*	*3.1%*	*0.8%*	*0.0%*	*0.9%*	***1.7%***
Benztropine	2	16	11	2	0	0	**31**
	0.3%	*1.1%*	*1.5%*	*0.4%*	*0.0%*	*0.0%*	***0.9%***
Bupropion	13	45	22	46	5	4	**135**
	2.1%	*3.1%*	*3.0%*	*9.7%*	*3.4%*	*3.7%*	***3.8%***
Buspirone	3	4	3	8	0	0	**18**
	0.5%	*0.3%*	*0.4%*	*1.7%*	*0.0%*	*0.0%*	***0.5%***
Carbamazepine	1	3	3	4	0	1	**12**
	0.2%	*0.2%*	*0.4%*	*0.8%*	*0.0%*	*0.9%*	***0.3%***
Carboxy-THC	1	5	5	6	1	0	**18**
	0.2%	*0.3%*	*0.7%*	*1.3%*	*0.7%*	*0.0%*	***0.5%***
Carisoprodol	1	2	1	0	0	0	**4**
	0.2%	*0.1%*	*0.1%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Chlordiazepoxide	3	5	2	1	0	0	**11**

(Chlordiazepoxide)	*0.5%*	*0.3%*	*0.3%*	*0.2%*	*0.0%*	*0.0%*	***0.3%***
Chlorpheniramine	7	11	5	7	1	0	**31**
	1.1%	*0.8%*	*0.7%*	*1.5%*	*0.7%*	*0.0%*	***0.9%***
Citalopram	29	79	30	27	5	9	**179**
	4.7%	*5.4%*	*4.1%*	*5.7%*	*3.4%*	*8.4%*	***5.1%***
Clonidine	2	10	9	9	1	0	**31**
	0.3%	*0.7%*	*1.2%*	*1.9%*	*0.7%*	*0.0%*	***0.9%***
Clozapine	2	12	7	2	1	2	**26**
	0.3%	*0.8%*	*0.9%*	*0.4%*	*0.7%*	*1.9%*	***0.7%***
Cyclobenzaprine	34	44	34	19	5	6	**142**
	5.5%	*3.0%*	*4.6%*	*4.0%*	*3.4%*	*5.6%*	***4.0%***
Desmethyldoxepin	5	10	5	7	4	1	**32**
	0.8%	*0.7%*	*0.7%*	*1.5%*	*2.7%*	*0.9%*	***0.9%***
Desmethylsertraline	7	16	3	7	1	0	**34**
	1.1%	*1.1%*	*0.4%*	*1.5%*	*0.7%*	*0.0%*	***1.0%***
Dicyclomine	6	4	2	2	1	0	**15**
	1.0%	*0.3%*	*0.3%*	*0.4%*	*0.7%*	*0.0%*	***0.4%***
Diltiazem	2	7	2	15	0	0	**26**
	0.3%	*0.5%*	*0.3%*	*3.2%*	*0.0%*	*0.0%*	***0.7%***
Diphenhydramine	49	144	155	56	17	7	**428**
	8.0%	*9.9%*	*21.0%*	*11.8%*	*11.5%*	*6.5%*	***12.1%***
Doxepin	5	10	3	7	4	1	**30**
	0.8%	*0.7%*	*0.4%*	*1.5%*	*2.7%*	*0.9%*	***0.8%***
Doxylamine	15	23	12	13	6	2	**71**
	2.4%	*1.6%*	*1.6%*	*2.7%*	*4.1%*	*1.9%*	***2.0%***
Duloxetine	1	12	12	11	0	0	**36**
	0.2%	*0.8%*	*1.6%*	*2.3%*	*0.0%*	*0.0%*	***1.0%***
Fluoxetine	6	32	20	24	6	7	**95**
	1.0%	*2.2%*	*2.7%*	*5.1%*	*4.1%*	*6.5%*	***2.7%***
Fluvoxamine	0	3	1	1	0	0	**5**
	0.0%	*0.2%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
Gabapentin	26	68	60	43	6	5	**208**
	4.2%	*4.7%*	*8.1%*	*9.1%*	*4.1%*	*4.7%*	***5.9%***
Haloperidol	17	11	8	2	1	0	**39**
	2.8%	*0.8%*	*1.1%*	*0.4%*	*0.7%*	*0.0%*	***1.1%***
Hydroxybupropion	30	64	25	30	7	3	**159**
	4.9%	*4.4%*	*3.4%*	*6.3%*	*4.7%*	*2.8%*	***4.5%***
Hydroxyzine	19	71	40	22	9	5	**166**
	3.1%	*4.9%*	*5.4%*	*4.7%*	*6.1%*	*4.7%*	***4.7%***

Lacosamide	0	2	0	0	1	0	**3**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.7%*	*0.0%*	***0.1%***
Lamotrigine	12	19	16	11	2	1	**61**
	1.9%	*1.3%*	*2.2%*	*2.3%*	*1.4%*	*0.9%*	***1.7%***
Levamisole	64	181	103	36	21	10	**415**
	10.4%	*12.4%*	*13.9%*	*7.6%*	*14.2%*	*9.3%*	***11.7%***
Levetiracetam	2	0	3	0	0	1	**6**
	0.3%	*0.0%*	*0.4%*	*0.0%*	*0.0%*	*0.9%*	***0.2%***
Lidocaine	36	106	71	35	13	3	**264**
	5.8%	*7.3%*	*9.6%*	*7.4%*	*8.8%*	*2.8%*	***7.5%***
Loperamide	2	16	10	8	2	0	**38**
	0.3%	*1.1%*	*1.4%*	*1.7%*	*1.4%*	*0.0%*	***1.1%***
mCPP	22	35	29	16	1	2	**105**
	3.6%	*2.4%*	*3.9%*	*3.4%*	*0.7%*	*1.9%*	***3.0%***
Mepivacaine	0	0	2	1	2	0	**5**
	0.0%	*0.0%*	*0.3%*	*0.2%*	*1.4%*	*0.0%*	***0.1%***
Meprobamate	1	1	2	0	0	0	**4**
	0.2%	*0.1%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.1%***
Metoclopramide	0	2	4	1	0	0	**7**
	0.0%	*0.1%*	*0.5%*	*0.2%*	*0.0%*	*0.0%*	***0.2%***
Mirtazapine	4	34	22	12	5	4	**81**
	0.6%	*2.3%*	*3.0%*	*2.5%*	*3.4%*	*3.7%*	***2.3%***
Modafinil	1	0	0	0	1	0	**2**
	0.2%	*0.0%*	*0.0%*	*0.0%*	*0.7%*	*0.0%*	***0.1%***
Monoethylglycinexylidide (MEGX)	8	40	38	17	2	0	**105**
	1.3%	*2.7%*	*5.1%*	*3.6%*	*1.4%*	*0.0%*	***3.0%***
Nalbuphine	0	0	0	4	1	0	**5**
	0.0%	*0.0%*	*0.0%*	*0.8%*	*0.7%*	*0.0%*	***0.1%***
Naloxone	72	156	92	44	18	3	**385**
	11.7%	*10.7%*	*12.4%*	*9.3%*	*12.2%*	*2.8%*	***10.9%***
Naproxen	0	0	1	7	0	0	**8**
	0.0%	*0.0%*	*0.1%*	*1.5%*	*0.0%*	*0.0%*	***0.2%***
N-desmethyl Loperamide	0	17	16	15	3	0	**51**
	0.0%	*1.2%*	*2.2%*	*3.2%*	*2.0%*	*0.0%*	***1.4%***
Norclozapine	2	12	7	2	1	2	**26**
	0.3%	*0.8%*	*0.9%*	*0.4%*	*0.7%*	*1.9%*	***0.7%***
Norfluoxetine	2	22	15	19	7	2	**67**
	0.3%	*1.5%*	*2.0%*	*4.0%*	*4.7%*	*1.9%*	***1.9%***
Nortriptyline	23	41	16	16	4	3	**103**

(Nortriptyline)	*3.7%*	*2.8%*	*2.2%*	*3.4%*	*2.7%*	*2.8%*	***2.9%***
Noscapine	17	54	42	8	4	1	**126**
	2.8%	*3.7%*	*5.7%*	*1.7%*	*2.7%*	*0.9%*	***3.6%***
O-Desmethylvenlafaxine	8	43	12	11	5	1	**80**
	1.3%	*2.9%*	*1.6%*	*2.3%*	*3.4%*	*0.9%*	***2.3%***
Olanzapine	4	15	3	4	1	0	**27**
	0.6%	*1.0%*	*0.4%*	*0.8%*	*0.7%*	*0.0%*	***0.8%***
Orphenadrine	1	3	2	0	0	0	**6**
	0.2%	*0.2%*	*0.3%*	*0.0%*	*0.0%*	*0.0%*	***0.2%***
Papaverine	5	11	11	6	0	0	**33**
	0.8%	*0.8%*	*1.5%*	*1.3%*	*0.0%*	*0.0%*	***0.9%***
Paroxetine	1	19	9	6	0	0	**35**
	0.2%	*1.3%*	*1.2%*	*1.3%*	*0.0%*	*0.0%*	***1.0%***
Phenacetin	0	2	3	2	2	0	**9**
	0.0%	*0.1%*	*0.4%*	*0.4%*	*1.4%*	*0.0%*	***0.3%***
Phenytoin	0	0	1	0	1	0	**2**
	0.0%	*0.0%*	*0.1%*	*0.0%*	*0.7%*	*0.0%*	***0.1%***
Pramiracetam	0	1	0	0	1	0	**2**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.7%*	*0.0%*	***0.1%***
Promethazine	7	16	9	4	4	0	**40**
	1.1%	*1.1%*	*1.2%*	*0.8%*	*2.7%*	*0.0%*	***1.1%***
Quetiapine	29	91	47	34	17	3	**221**
	4.7%	*6.2%*	*6.4%*	*7.2%*	*11.5%*	*2.8%*	***6.2%***
Quinine	134	423	284	76	42	26	**985**
	21.8%	*29.0%*	*38.4%*	*16.1%*	*28.4%*	*24.3%*	***27.8%***
Risperidone	1	3	4	1	0	0	**9**
	0.2%	*0.2%*	*0.5%*	*0.2%*	*0.0%*	*0.0%*	***0.3%***
Sertraline	18	40	32	22	7	3	**122**
	2.9%	*2.7%*	*4.3%*	*4.7%*	*4.7%*	*2.8%*	***3.4%***
Sildenafil	1	2	1	1	0	0	**5**
	0.2%	*0.1%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
Tadalafil	0	3	1	1	0	0	**5**
	0.0%	*0.2%*	*0.1%*	*0.2%*	*0.0%*	*0.0%*	***0.1%***
Tapentadol	0	1	1	1	1	0	**4**
	0.0%	*0.1%*	*0.1%*	*0.2%*	*0.7%*	*0.0%*	***0.1%***
Tetrahydrozoline	0	0	2	5	0	0	**7**
	0.0%	*0.0%*	*0.3%*	*1.1%*	*0.0%*	*0.0%*	***0.2%***
Thebaine	1	2	1	2	1	0	**7**
	0.2%	*0.1%*	*0.1%*	*0.4%*	*0.7%*	*0.0%*	***0.2%***

Tianeptine	0	0	0	0	1	1	**2**
	0.0%	*0.0%*	*0.0%*	*0.0%*	*0.7%*	*0.9%*	***0.1%***
Topiramate	0	0	0	4	0	0	**4**
	0.0%	*0.0%*	*0.0%*	*0.8%*	*0.0%*	*0.0%*	***0.1%***
Trazodone	26	87	49	22	3	3	**190**
	4.2%	*6.0%*	*6.6%*	*4.7%*	*2.0%*	*2.8%*	***5.4%***
UR-144	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Venlafaxine	10	44	13	22	3	1	**93**
	1.6%	*3.0%*	*1.8%*	*4.7%*	*2.0%*	*0.9%*	***2.6%***
Verapamil	3	0	1	0	0	1	**5**
	0.5%	*0.0%*	*0.1%*	*0.0%*	*0.0%*	*0.9%*	***0.1%***
Warfarin	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
XLR-11	0	1	0	0	0	0	**1**
	0.0%	*0.1%*	*0.0%*	*0.0%*	*0.0%*	*0.0%*	***0.03%***
Xylazine	4	21	26	5	3	4	**63**
	0.6%	*1.4%*	*3.5%*	*1.1%*	*2.0%*	*3.7%*	***1.8%***
Yohimbine	2	2	3	3	0	0	**10**
	0.3%	*0.1%*	*0.4%*	*0.6%*	*0.0%*	*0.0%*	***0.3%***
Ziprasidone	1	5	1	0	2	1	**10**
	0.2%	*0.3%*	*0.1%*	*0.0%*	*1.4%*	*0.9%*	***0.3%***
Zolpidem	5	8	7	5	2	1	**28**
	0.8%	*0.5%*	*0.9%*	*1.1%*	*1.4%*	*0.9%*	***0.8%***
Zopiclone	0	1	1	2	0	0	**4**
	0.0%	*0.1%*	*0.1%*	*0.4%*	*0.0%*	*0.0%*	***0.1%***

5.3.2 Fentanyl with Drugs of Abuse or NPS

Overall, 1,301 (36.7%) sample extracts were deemed fentanyl positive (using Table 7). The majority (79.8%) of fentanyl positivity was accompanied by poly-drug use, including the presence of one or more drug(s) of abuse and/or NPS (Table 13). Fentanyl was found in combination with as many as seven drugs and/or NPS (excluding therapeutics, adulterants, etc.).

Table 13: Fentanyl poly-drug use

Fentanyl Poly-Drug Use*	# Positives	% [n=1,301]
Fentanyl + No Other Drug	263	20.2
Fentanyl + One Drug	429	33.0
Fentanyl + Two Drugs	317	24.4
Fentanyl + Three Drugs	163	12.5
Fentanyl + Four Drugs	86	6.6
Fentanyl + Five Drugs	31	2.4
Fentanyl + Six Drugs	6	0.5
Fentanyl + Seven Drugs	6	0.5

**Including Drugs of Abuse and NPS*

Poly-drug use of fentanyl with specific drugs of abuse and classes of NPS is shown in Table 14. With respect to drugs of abuse, fentanyl was most commonly found in combination with stimulants (46.0%) and other opiates/opioids (42.8%). Fentanyl was more commonly found in combination with cocaine (26.4%) than methamphetamine (13.1%). Fentanyl combinations with opioids included heroin (28.3%), tramadol (11.1%), and methadone (9.4%). With respect to NPS, fentanyl was most commonly found in combination with NPS opioids (27.3%) and more rarely found in combination with NPS stimulants (4.2%), NPS benzodiazepines (3.9%), and NPS hallucinogen (1.3%).

Table 14: Fentanyl combinations with other drugs of abuse and/or NPS

Overall Fentanyl Positivity	**# Positives**	**% [n=3,543]**
Total Samples Analyzed	3,543	-
Total Fentanyl Positives	1,301	36.7
Combination by Drugs of Abuse Class	**# Positives**	**% [n=1,301]**
Fentanyl + Traditional Opiate(s)/Opioid(s)	**557**	**42.8**
Fentanyl + Heroin	368	28.3
Fentanyl + Tramadol	144	11.1
Fentanyl + Methadone	122	9.4
Fentanyl + Prescription Opioids	117	9.0
Fentanyl + Mitragynine	41	3.2
Fentanyl + Buprenorphine	38	2.9
Fentanyl + Traditional Stimulant(s)	**598**	**46.0**
Fentanyl + Cocaine	344	26.4
Fentanyl + Methamphetamine	170	13.1
Fentanyl + Cocaine + Methamphetamine	58	4.5
Fentanyl + Other Traditional Stimulant(s) [e.g. MDMA]	26	2.0
Fentanyl + Traditional Hallucinogen(s)	**31**	**2.4**
Fentanyl + Ketamine	13	1.0
Fentanyl + Traditional Benzodiazepine(s)	**249**	**19.1**
Combination by NPS Class	**# Positives**	**% [n=1,301]**
Fentanyl + NPS Opioid(s)	**355**	**27.3**
Fentanyl + Fentanyl Analogue	323	24.8
Fentanyl + Non-Fentanyl Opioid (e.g. U-47700)	26	2.0
Fentanyl + Fentanyl Precursor (Other than 4-ANPP)	25	1.9
Fentanyl + NPS Stimulant(s)	**55**	**4.2**
Fentanyl + Methylenedioxy Cathinones	35	2.7
Fentanyl + Pyrrolidine Cathinones	15	1.2
Fentanyl + Other Cathinones	7	0.5
Fentanyl + Phenethylamines	3	0.2
Fentanyl + NPS Hallucinogen(s)	**17**	**1.3**
Fentanyl + PCP Derivatives	16	1.2
Fentanyl + Ketamine Derivatives	1	0.1
Fentanyl + NPS Benzodiazepine(s)	**51**	**3.9**
Combination by Combined NPS/Drug Category	**# Positives**	**% [n=1,301]**
Fentanyl + Any Opiate(s)/Opioid(s)	771	59.3
Fentanyl + Any Stimulant(s)	625	48.0
Fentanyl + Any Hallucinogen(s)	48	3.7
Fentanyl + Any Benzodiazepine(s)	277	21.3

Tables 15-17 show fentanyl combinations with respect to specific NPS. Fentanyl was commonly found in combination with fentanyl analogues, including fluoroisobutyrylfentanyl (n=179), cyclopropylfentanyl (n=70), and methoxyacetylfentanyl (n=48); the three most commonly encountered fentanyl analogues during this time period. With respect to NPS stimulants and hallucinogens, fentanyl was most commonly found in combination with 3/4-MeO-PCP (n=16) and alpha-PHP (n=10). With respect to NPS benzodiazepines fentanyl was most commonly found in combination with etizolam (n=36).

Table 15: Fentanyl poly-drug use with specific NPS opioids

Fentanyl + NPS Opioid	**# Positives**
Fluoroisobutyrylfentanyl	179
Cyclopropylfentanyl	70
Methoxyacetylfentanyl	48
U-47700	18
Valerylfentanyl	10
N-Methyl Norfentanyl	10
3-Methylfentanyl	9
N-Desmethyl-U-47700	9
Carfentanil	8
Furanylfentanyl	8
Benzyl Fentanyl	8
Benzyl Furanylfentanyl	5
U-48800	5
Butyrylfentanyl	4
N,N-Didesmethyl-U-47700	4
Fluorofentanyl	2
Norcarfentanil	2
Phenylfentanyl	2
Despropionyl *ortho*-Fluorofentanyl	2
Isopropyl-U-47700	2
3,4-Methylenedioxy-U-47700	2

Table 16: Fentanyl poly-drug use with specific NPS stimulants and hallucinogens

Fentanyl + NPS Stimulant/Hallucinogen	# Positives
N-Ethyl Pentylone	33
3/4-MeO-PCP	16
Alpha-PHP	10
N-Ethyl Hexedrone (Hexen)	5
Dibutylone	4
Butylone	3
Pentylone	2
2F-Deschloroketamine	1
4Cl-Alpha-PVP	1
4F-Alpha-PHP	1
Alpha-PBP	1
Alpha-PVP	1
3,4-Methylenedioxy-alpha-PHP	1
Eutylone	1
Methylone	1
Methoxyamphetamine (PMA)	1
Methoxymethamphetamine (PMMA)	1
Methcathinone	1
4Cl-Isopropylcathinone	1
MBZP	1

Table 17: Fentanyl poly-drug use by specific NPS benzodiazepines

Fentanyl + NPS Benzodiazepine	# Positives
Etizolam	36
Diclazepam	8
Flubromazolam	7
Flubromazepam	2
Phenazepam	2
Flualprazolam	1

5.3.3 NPS with Drugs of Abuse or other NPS

Overall, 1,433 (40.4%) sample extracts were deemed NPS positive (using Table 8). The majority (68.0%) of NPS positivity was accompanied by poly-drug use, including the presence of one or more drug(s) of abuse (Table 18); however, the majority (82.5%) of NPS positivity was not accompanied by poly-NPS use (Table 19). NPS were found in combination with as many as nine drugs of abuse (n=1) (excluding therapeutics, adulterants, etc.) and as many as six other NPS.

Table 18: NPS poly-drug use with drugs of abuse

NPS Poly-Drug	**# Positives**	**% [n=1,433]**
NPS + No Drugs of Abuse	459	32.0
NPS + One Drug	441	30.8
NPS + Two Drugs	288	20.1
NPS + Three Drugs	165	11.5
NPS + Four Drugs	46	3.2
NPS + Five Drugs	23	1.6
NPS + Six Drugs	6	0.4
NPS + Seven or More Drugs	5	0.3

Table 19: NPS poly-drug use with other NPS

Poly-NPS Use with NPS	**# Positives**	**% [n=1,433]**
One NPS Substance	1182	82.5
Two NPS Substances	167	11.7
Three NPS Substances	40	2.8
Four NPS Substances	21	1.5
Five NPS Substances	11	0.8
Six NPS Substances	12	0.8

Poly-NPS use is broken down by class in Table 20. NPS opioids were the most commonly detected class, followed by NPS benzodiazepines and NPS stimulants. NPS opioids were most commonly found in combination with other NPS opioids (n=167, 14.9%). NPS stimulants were most commonly found in combination with NPS opioids (n=40, 22.9%). NPS hallucinogens were most commonly found in combination with NPS opioids (n=13, 38.2%). NPS benzodiazepines were most commonly found in combination with NPS opioids (n=14, 7.8%). Among all classes, NPS hallucinogens were the most likely (50%) to be found in combination with another NPS.

Table 20: NPS combinations with other NPS

Overall NPS Positivity	**# Positives**	**% [n=3,543]**
Total Samples Analyzed	3,543	-
Total NPS Positives	1,433	40.4
NPS Positivity by Class	**# Positives**	**% [n=1,433]**
NPS Opioid(s)	1,121	78.2
NPS Stimulant(s)	175	12.2
NPS Hallucinogen(s)	34	2.4
NPS Benzodiazepine(s)	180	12.6
NPS Opioid Combinations	**# Positives**	**% [n=1,121]**
NPS Opioid(s) + NPS Opioid(s)	167	14.9
NPS Opioid(s) + NPS Stimulant(s)	40	3.6
NPS Opioid(s) + NPS Hallucinogen(s)	13	1.2
NPS Opioid(s) + NPS Benzodiazepine(s)	14	1.2
NPS Opioid(s) + Any NPS	**218**	**19.4**
NPS Stimulant Combinations	**# Positives**	**% [n=175]**
NPS Stimulant(s) + NPS Opioid(s)	40	22.9
NPS Stimulant(s) + NPS Stimulant(s)	28	16.0
NPS Stimulant(s) + NPS Hallucinogen(s)	4	2.3
NPS Stimulant(s) + NPS Benzodiazepine(s)	6	3.4
NPS Stimulant(s) + Any NPS	**66**	**37.7**

NPS Hallucinogen Combinations	# Positives	% [n=34]
NPS Hallucinogen(s) + NPS Opioid(s)	13	38.2
NPS Hallucinogen(s) + NPS Stimulant(s)	4	11.8
NPS Hallucinogen(s) + NPS Hallucinogen(s)	3	8.8
NPS Hallucinogen(s) + NPS Benzodiazepine(s)	3	8.8
NPS Hallucinogen(s) + Any NPS	**17**	**50.0**
NPS Benzodiazepine Combinations	**# Positives**	**% [n=180]**
NPS Benzodiazepine(s) + NPS Opioid(s)	14	7.8
NPS Benzodiazepine(s) + NPS Stimulant(s)	6	3.3
NPS Benzodiazepine(s) + NPS Hallucinogen(s)	3	1.7
NPS Benzodiazepine(s) + NPS Benzodiazepine(s)	11	6.1
NPS Benzodiazepine(s) + Any NPS	**27**	**15.0**

The three most commonly encountered NPS were among the opioid class: fluoroisobutyrylfentanyl (n=430), cyclopropylfentanyl (n=309), and methoxyacetylfentanyl (n=245). The fourth most commonly encountered NPS was *N*-ethyl pentylone (n=114), a stimulant. Further down the list, the most commonly encountered NPS benzodiazepine was etizolam (n=92) and the most commonly encountered NPS hallucinogen was 3/4-MeO-PCP (n=25). These six NPS were further investigated to determine how often they were found with other specific NPS.

Fluoroisobutyrylfentanyl was encountered with 19 other NPS (Table 21), most frequently acetylfentanyl (n=30) likely arising from fentanyl positivity. Unsurprisingly, fluoroisobutyrylfentanyl was found in combination with cyclopropylfentanyl (n=13), methoxyacetylfentanyl (n=12), and other NPS opioids. With respect to NPS stimulants, fluoroisobutyrylfentanyl was encountered with alpha-PHP (n=9), *N*-ethyl pentylone (n=3), eutylone (n=3), and *N*-ethyl hexedrone (n=3). Fluoroisobutyrylfentanyl was infrequently found in combination with NPS benzodiazepines and NPS hallucinogens.

Table 21: Fluoroisobutyrylfentanyl in combination with other NPS

Fluoroisobutyrylfentanyl + NPS	# Positives	% [n=430]
Acetylfentanyl	30	7.0%
Methoxyacetylfentanyl	13	3.0%
Cyclopropylfentanyl	12	2.8%
Alpha-PHP	9	2.1%
N-Ethyl Pentylone	9	2.1%
Furanylfentanyl	5	1.2%
U-47700	5	1.2%
Eutylone	3	0.7%
N-Ethyl Hexedrone	3	0.7%
Etizolam	3	0.7%
Despropionyl *ortho*-Fluorofentanyl	2	0.5%
N-Methyl Norfentanyl	1	0.2%
U-48800	1	0.2%
Alpha-PVP	1	0.2%
Deschloroketamine	1	0.2%
N-Ethyl Deschloroketamine	1	0.2%
3/4-MeO-PCP	1	0.2%

Fluoroisobutyrylfentanyl was encountered with 18 drugs of abuse (Table 22), primarily opioids and stimulants. Most frequently, fluoroisobutyrylfentanyl was found in combination with cocaine (n=117), followed by heroin (n=92) and methamphetamine (n=64). With respect to other opioids, fluoroisobutyrylfentanyl was found with methadone (n=27), oxycodone (n=21), tramadol (n=19), and mitragynine (n=10).

Table 22: Fluoroisobutyrylfentanyl in combination with drugs of abuse

Fluoroisobutyrylfentanyl + Drug of Abuse	# Positives	% [n=430]
Cocaine	117	27.2%
Heroin	92	21.4%
Alprazolam	65	15.1%

Methamphetamine	64	14.9%
Methadone	27	6.3%
Diazepam	22	5.1%
Oxycodone	21	4.9%
Tramadol	19	4.4%
Mitragynine	10	2.3%
Phencyclidine (PCP)	5	1.2%
Hydrocodone	4	0.9%
Midazolam	4	0.9%
Dihydrocodeine	2	0.5%
Methylphenidate	2	0.5%
Ketamine	2	0.5%
Oxymorphone	1	0.2%
Hydromorphone	1	0.2%
Buprenorphine	1	0.2%

Cyclopropylfentanyl was encountered with 24 other NPS (Table 23), most frequently methoxyacetylfentanyl (n=29). These two NPS were prevalent in the drug supply at the same time. Unsurprisingly, cyclopropylfentanyl was found in combination with other NPS opioids as well, including U-47700 (n=14), U-48800 (n=12), fluoroisobutyrylfentanyl (n=12), and acetylfentanyl (n=10). With respect to NPS stimulants, cyclopropylfentanyl was encountered with *N*-ethyl pentylone (n=5) and alpha-PVP (n=3), less frequently than in combination with fluoroisobutyrylfentanyl. Cyclopropylfentanyl was infrequently found in combination with NPS benzodiazepines and NPS hallucinogens; however, it was found in combination with 3/4-MeO-PCP on four occasions.

Table 23: Cyclopropylfentanyl in combination with other NPS

Cyclopropylfentanyl + NPS	# Positives	% [n=309]
Methoxyacetylfentanyl	29	9.4%
U-47700	14	4.5%
Fluoroisobutyrylfentanyl	12	3.9%
U-48800	12	3.9%
Acetylfentanyl	10	3.2%
Phenylfentanyl	5	1.6%
N-methyl Norfentanyl	5	1.6%
N-Ethyl Pentylone	5	1.6%
Benzyl Fentanyl	4	1.3%
3/4-MeO-PCP	4	1.3%
Benzyl Furanylfentanyl	3	1.0%
Alpha-PVP	3	1.0%
Carfentanil	2	0.6%
Despropionyl *ortho*-methyl Fentanyl	2	0.6%
Furanylfentanyl	1	0.3%
Benzyl *para*-Fluorocyclopropylfentanyl	1	0.3%
Butylone	1	0.3%
Dibutylone	1	0.3%
MBZP	1	0.3%
Deschloroketamine	1	0.3%
Diclazepam	1	0.3%
Etizolam	1	0.3%

Cyclopropylfentanyl was encountered with 20 drugs of abuse (Table 24), primarily opioids and stimulants. Most frequently, cyclopropylfentanyl was found in combination with cocaine (n=80), followed by heroin (n=51) and methamphetamine (n=33). With respect to other opioids, cyclopropylfentanyl was found with methadone (n=17), oxycodone (n=14), tramadol (n=13), and mitragynine (n=12).

Table 24: Cyclopropylfentanyl in combination with drugs of abuse

Cyclopropylfentanyl + Drug of Abuse	# Positives	% [n=309]
Cocaine	80	25.9%
Heroin	51	16.5%
Methamphetamine	33	10.7%
Alprazolam	26	8.4%
Diazepam	20	6.5%
Methadone	17	5.5%
Oxycodone	14	4.5%
Tramadol	13	4.2%
Mitragynine	12	3.9%
Hydrocodone	8	2.6%
MDMA	7	2.3%
Methylphenidate	6	1.9%
Ketamine	6	1.9%
Midazolam	6	1.9%
Dihydrocodeine	4	1.3%
Buprenorphine	2	0.6%
Oxymorphone	1	0.3%
Clonazepam	1	0.3%
Lorazepam	1	0.3%

Methoxyacetylfentanyl was encountered with 22 other NPS (Table 25), most frequently cyclopropylfentanyl (n=29). Unsurprisingly, methoxyacetylfentanyl was found in combination with other NPS opioids as well, including U-47700 (n=20), fluoroisobutyrylfentanyl (n=13), and acetylfentanyl (n=7). Methoxyacetylfentanyl was also found in combination with 3,4-methylenedioxy-U-47700 (n=11) and isopropyl-U-47700 (n=5), emergent NPS opioids, possibly demonstrating the combination of these NPS opioids in the drug supply. Methoxyacetylfentanyl was less frequently found in combination with NPS stimulants, NPS benzodiazepines, and NPS hallucinogens.

Table 25: Methoxyacetylfentanyl in combination with other NPS

Methoxyacetylfentanyl + NPS	# Positives	% [n=245]
Cyclopropylfentanyl	29	11.8%
U-47700	20	8.2%
Fluoroisobutyrylfentanyl	13	5.3%
3,4-Methylenedioxy-U-47700	11	4.5%
Acetylfentanyl	7	2.9%
3/4-MeO-PCP	6	2.4%
Isopropyl-U-47700	5	2.0%
Furanylfentanyl	3	1.2%
Phenylfentanyl	3	1.2%
N-Ethyl Pentylone	3	1.2%
N-Methyl Norfentanyl	2	0.8%
U-48800	2	0.8%
Alpha-PVP	2	0.8%
Dibutylone	2	0.8%
Benzyl Fentanyl	1	0.4%
Benzyl Furanylfentanyl	1	0.4%
Benzyl *para*-Fluorocyclopropylfentanyl	1	0.4%
3,4-Methylenedioxy-alpha-PHP	1	0.4%
MBZP	1	0.4%
Diclazepam	1	0.4%

Methoxyacetylfentanyl was encountered with 16 drugs of abuse (Table 26), primarily opioids and stimulants. Most frequently, methoxyacetylfentanyl was found in combination with cocaine (n=48), followed by methamphetamine (n=35) and heroin (n=32). With respect to other opioids, methoxyacetylfentanyl was found with oxycodone (n=14), tramadol (n=14), mitragynine (n=12), and methadone (n=11).

Table 26: Methoxyacetylfentanyl in combination with drugs of abuse

Methoxyacetylfentanyl + Drug of Abuse	# Positives	% [n=245]
Cocaine	48	19.6%
Methamphetamine	35	14.3%
Heroin	32	13.1%
Alprazolam	23	9.4%
Oxycodone	14	5.7%
Tramadol	14	5.7%
Mitragynine	12	4.9%
Methadone	11	4.5%
Hydrocodone	8	3.3%
MDMA	6	2.4%
Diazepam	6	2.4%
Dihydrocodeine	2	0.8%
Hydromorphone	1	0.4%
Methylphenidate	1	0.4%
Clonazepam	1	0.4%

N-Ethyl pentylone was encountered with 18 other NPS (Table 27), most frequently fluoroisobutyryllfentanyl (n=9). Unsurprisingly, *N*-ethyl pentylone was found in combination with other NPS simulants of the 3,4-methylenedioxy-cathinone class, including butylone (n=6), eutylone (n=6), dibutylone (n=5), and pentylone (n=3). *N*-Ethyl pentylone was less frequently found in combination with NPS benzodiazepines and NPS hallucinogens.

Table 27: *N*-Ethyl pentylone in combination with other NPS

N-Ethyl Pentylone + NPS	# Positives	% [n=114]
Fluoroisobutyrylfentanyl	9	7.9%
Butylone	6	5.3%
Eutylone	6	5.3%
Cyclopropylfentanyl	5	4.4%

Dibutylone	5	4.4%
Methoxyacetylfentanyl	3	2.6%
Pentylone	3	2.6%
Alpha-PHP	2	1.8%
3/4-MeO-PCP	2	1.8%
3-Methylfentanyl	1	0.9%
Acetylfentanyl	1	0.9%
Benzyl Fentanyl	1	0.9%
N-Methyl Norfentanyl	1	0.9%
3,4-Methylenedioxy-alpha-PHP	1	0.9%
N-Ethyl Hexylone	1	0.9%
Clonazolam	1	0.9%
Etizolam	1	0.9%

N-Ethyl pentylone was encountered with 14 drugs of abuse (Table 28), primarily opioids and stimulants. Most frequently, *N*-ethyl pentylone was found in combination with cocaine (n=19), followed by heroin (n=11) and methamphetamine (n=10). With respect to other opioids, *N*-ethyl pentylone was found with tramadol (n=6), oxycodone (n=5), and methadone (n=3); *N*-ethyl pentylone was not found in combination with mitragynine.

Table 28: *N*-Ethyl pentylone in combination with drugs of abuse

***N*-Ethyl Pentylone + Drug of Abuse**	**# Positives**	**% [n=114]**
Cocaine	19	16.7%
Heroin	11	9.6%
Methamphetamine	10	8.8%
Tramadol	6	5.3%
Oxycodone	5	4.4%
Alprazolam	5	4.4%
Methadone	3	2.6%
Diazepam	3	2.6%
Hydrocodone	2	1.8%

MDMA	2	1.8%
Phencyclidine (PCP)	2	1.8%
Dihydrocodeine	1	0.9%
Buprenorphine	1	0.9%

Etizolam was encountered with 17 other NPS (Table 29) but, contrarily to those reported above, less frequently. Etizolam was found in combination with other NPS benzodiazepines, including diclazepam (n=5) and phenazepam (n=2). Etizolam was found in combination with NPS opioids, including acetylfentanyl (n=4), fluoroisobutyrylfentanyl (n=3), fluorofentanyl (n=2), and U-47700 (n=2). Etizolam was infrequently found with NPS stimulants and NPS hallucinogens.

Table 29: Etizolam in combination with other NPS

Etizolam + NPS	**# Positives**	**% [n=92]**
Diclazepam	5	5.4%
Acetylfentanyl	4	4.3%
Fluoroisobutyrylfentanyl	3	3.3%
Fluorofentanyl	2	2.2%
U-47700	2	2.2%
3/4-MeO-PCP	2	2.2%
Phenazepam	2	2.2%
Cyclopropylfentanyl	1	1.1%
4-Cl-Alpha-PVP	1	1.1%
Benzylone	1	1.1%
N-Ethyl Pentylone	1	1.1%
Fluoroamphetamine	1	1.1%
Fluoromethamphetamine	1	1.1%
N-Ethyl Hexedrone	1	1.1%
2F-Deschloroketamine	1	1.1%

Etizolam was encountered with 17 drugs of abuse (Table 30) and, contrarily to those reported above, was frequently found in combination with alprazolam (n=15). Surprisingly, etizolam was found in combination with mitragynine (n=14) with the second highest frequency, possibly providing insight into drug use preferences of Kratom users. Etizolam was found in combination with cocaine (n=13), methamphetamine (n=11), and, much less frequently, heroin (n=3).

Table 30: Etizolam in combination with drugs of abuse

Etizolam + Drug of Abuse	# Positives	% [n=92]
Alprazolam	15	16.3%
Mitragynine	14	15.2%
Cocaine	13	14.1%
Methamphetamine	11	12.0%
Tramadol	9	9.8%
Methadone	8	8.7%
Diazepam	6	6.5%
Clonazepam	4	4.3%
Heroin	3	3.3%
Hydrocodone	3	3.3%
Oxycodone	2	2.2%
MDMA	1	1.1%
Methylphenidate	1	1.1%
Ketamine	1	1.1%
Midazolam	1	1.1%
Lorazepam	1	1.1%

3/4-MeO-PCP was encountered with 14 other NPS (Table 31), most commonly NPS opioids. 3/4-MeO-PCP was frequently found in combination with methoxyacetylfentanyl (n=6), cyclopropylfentanyl (n=4), and acetylfentanyl (n=2). 3/4-MeO-PCP was found in combination with NPS stimulants, including butylone (n=3), *N*-

ethyl pentylone (n=3), fluoroamphetamine (n=2), and fluoroethamphetamine (n=2). Interestingly, 3/4-MeO-PCP was very infrequently found with other NPS hallucinogens.

Table 31: 3/4-MeO-PCP in combination with other NPS

3/4-MeO-PCP + NPS	# Positives	% [n=25]
Methoxyacetylfentanyl	6	24.0%
Cyclopropylfentanyl	4	16.0%
Butylone	3	12.0%
Acetylfentanyl	2	8.0%
N-Ethyl Pentylone	2	8.0%
Fluoroamphetamine	2	8.0%
Fluoroethamphetamine	2	8.0%
3/4-OH-PCP	2	8.0%
Etizolam	2	8.0%
Fluoroisobutyrylfentanyl	1	4.0%
Dibutylone	1	4.0%
2F-Deschloroketamine	1	4.0%
Diclazepam	1	4.0%
Flubromazolam	1	4.0%

3/4-MeO-PCP was encountered with 10 drugs of abuse (Table 32), primarily opioids and stimulants. Most frequently, 3/4-MeO-PCP was found in combination with cocaine (n=8), followed by alprazolam (n=5) and oxycodone (n=2).

Table 32: 3/4-MeO-PCP in combination with drugs of abuse

3/4-MeO-PCP + Drug of Abuse	# Positives	% [n=25]
Cocaine	8	32.0%
Alprazolam	4	16.0%
Oxycodone	2	8.0%
Tramadol	2	8.0%
Mitragynine	1	4.0%

Heroin	1	4.0%
Clonazepam	1	4.0%
Lorazepam	1	4.0%
Diazepam	1	4.0%

5.4 Conclusions

Providing comprehensive data regarding patterns and practice of combined or concurrent drug use greatly impacts scientific and medical communities, allowing for greater understanding of poly-drug and/or poly-NPS use. This, in turn, can have an impact on policies relating to death investigation and forensic toxicology testing practices, as well as public health and public safety preparedness and response. Comprehensive toxicological testing, as described during this research, is imperative in determining and evaluating the true extent of poly-drug use. A complete cross-comparison of drug results from this research shows that poly-drug use among fentanyl users and poly-drug use among NPS users is common.

Temporal trend analysis of the data generated during this research shows the decline of NPS opioids (e.g. fentanyl analogues) and the persistence of fentanyl through 2019, as well as a slight decline in heroin positivity. Low positivity for all other NPS make it difficult to truly determine temporal trends over this time period. Positivity for the majority of drugs of abuse was stable (e.g. cocaine, methamphetamine); however, the positivity of MDMA appears to be slightly declining.

The results generated for fentanyl poly-drug use demonstrate the great extent to which fentanyl users are using other substances, either concurrently with or in proximity to their fentanyl use. Combined fentanyl and stimulant use neared 50% of the sample set,

a drug use phenomenon that should be carefully monitored over the coming months and years. Fentanyl was commonly encountered with NPS opioids; however, that trend was decreasing toward the end of 2018 and into 2019.

Analysis of poly-NPS use revealed low incidence of combined NPS use, but analysis of poly-drug use among NPS users revealed high incidence of combined NPS use with drugs of abuse. NPS opioids and stimulants were commonly found with the most common drugs of abuse: cocaine, heroin, and methamphetamine. While the positivity for combined NPS use is low, there remains value in monitoring specific NPS combinations for the purposes of adverse event tracking and determination of drug trafficking.

Any poly-drug use is significant from analytical chemistry, forensic toxicology, and public health perspectives, as combined drug use creates drug-drug interactions and more complex adverse effect profiles, in addition to complicating testing protocols and analysis assays. To better understand poly-drug use, laboratories should consider developing all-inclusive, non-targeted assays for more comprehensive determination of all substances onboard at the time of impairment or death.

CHAPTER 6

METABOLISM

6.1 Introduction

As NPS emerge within recreational drug supplies, it is rare that pharmacological studies have been performed to evaluate biological processes such as absorption, distribution, metabolism, and excretion (ADME).[152] When available, this could mean that an NPS was pirated from pharmaceutical patent literature, for which a pharmaceutical company may have studied the biological fate of the drug under research purposes. This is more common for NPS opioids and synthetic cannabinoids due to more extensive research into these classes for therapeutic purposes or value.[10]

During this research, the metabolic fate of emergent NPS was studied in order to characterize the biotransformation products (i.e. metabolites) produced *in vitro* with subsequent confirmation *in vivo*. *In vitro* metabolism studies have been well described in the literature and typically consist of experiments using hepatocytes, S9 fraction, and/or microsomes, all of which can be derived from human liver.[153,154] Hepatocytes are liver cells and, for use in research, result from the homogenization of the liver. Hepatocytes are the closest *in vitro* replication of liver function (i.e. metabolism) but can be the most difficult to handle and store within a standard laboratory setting. Preparation of hepatocytes by centrifugation to remove nuclei, cellular debris, lysosomes, and mitochondria results in a supernatant called S9, consisting of both microsomal and cytosolic fractions. Further preparation by centrifugation at higher force allows for

separation of microsome from cytosol, and the microsomes can be isolated and suspended in buffer for laboratory use. By result, microsomes, often referred to as human liver microsomes (HLM), are the least representative of the true liver and are often considered "super pools" of metabolic activity. However, due to their viability and ease of use in the laboratory, HLMs were used during this research to study *in vitro* metabolism.

HLMs can be advantageous for research purposes, but *in vitro* microsomal results should be interpreted with caution due to their distinction from true *in vivo* liver function. This is generally accepted among those conducting metabolism studies and can ascertained based on published literature pairing HLM studies with either hepatocyte studies and/or *in vivo* studies.[24,155,156] *In vivo* studies of emerging NPS often arise based on recreational drug use as the result of hospitalization or death, for which biological samples have been collected. *In vivo* studies involving the dosing of NPS to human are rarely conducted due to unknown toxicity and adverse event profiles (e.g. death); however, there is literature of *in vivo* NPS benzodiazepine studies following self-administration, as these compounds are usually seen as being safe (or safer) for human consumption.[79,157] During this research, metabolites generated *in vitro* were confirmed *in vivo* through the analysis of biological sample extracts from forensic investigations.

This process of identifying *in vitro* metabolites *in vivo* is considered data mining, as discussed in Chapter 3. Following full characterization *in vitro*, the formula (converted to exact mass), retention time, and MSMS fragment spectrum for each metabolite were used to create an XIC list for data mining of all datafiles acquired.

The purpose of conducting metabolism studies during this research was to assist laboratory scientists, analytical chemists, and toxicologists involved with method development, identifications, and/or interpretation of NPS results. One major goal of studying NPS metabolism is to prolong windows of detection. Metabolites of drugs are often detectable in biological samples (e.g. urine) after parent compounds are eliminated or transformed. Therefore, if metabolites of NPS are incorporated into testing methods, NPS can be detected for longer periods of time after use by monitoring the metabolites. Classical examples are the prolonged detection of morphine after heroin (diacetylmorphine) use and prolonged detection of THC-COOH after THC use, specifically in urine specimens. Furthermore, many NPS are metabolized into biologically active metabolites, which could be other NPS (e.g. methylated analogues) and/or could create increased potency or adverse events due to combined drug effects or toxicity. For example, dibutylone (an *N,N*-dimethyl NPS stimulant) is metabolized to butylone (the *N*-methyl variant), an active NPS in its own right.[158]

6.2 Methods

Metabolic profile determinations of emerging NPS were conducted using *in vitro* and *in vivo* models. *In vitro* incubation was performed using pooled HLMs with added standard reference material: 3,4-methylenedioxy-U-47700, *ortho*-fluorofuranylfentanyl, 2F-deschloroketamine, eutylone, or *N*-ethyl hexedrone. *In vivo* verification of *in vitro* generated metabolites was conducted by reprocessing of biological sample extracts.

6.2.1 Materials and Reagents

Drug standards (3,4-methylenedioxy-U-47700, *ortho*-fluorofuranylfentanyl, 2F-deschloroketamine, eutylone, and *N*-ethyl hexedrone) were purchased from Cayman Chemical (Ann Arbor, MI, USA) and prepared at 1 mg/mL. Diazepam (1 mg/mL) was purchased from Cerilliant (Round Rock, TX, USA) and used as an incubation control. This control was used to monitor microsomal activity through formation of nordiazepam, temazepam, and oxazepam.

Pooled HLMs were purchase from ThermoFisher Scientific (Waltham, MA, USA) correlating to 50 donors and pooled at 20 mg/mL. HLMs were stored in-house at -80 °C prior to use to preserve viability.

Phosphate buffer (100 mM, pH 7.4, with 10mM $MgCl_2$) was prepared in-house by combining 1.7 g sodium phosphate dibasic (anhydrous), 12.15 g sodium phosphate monobasic (monohydrate), and 2.033 g magnesium chloride hexahydrate in 1 L of LCMS grade water. The solution was adjusted to pH 7.4 with sodium hydroxide.

A solution of nicotinamide adenine dinucleotide phosphate (NADPH) (Cayman Chemical) was prepared at 10 mM by dissolving 16.7 mg NADPH sodium salt in 2 mL of LCMS grade water.

6.2.2 Sample Preparation and Incubation

Drug standard (50 µL) was added to clean test tubes and dried to completion at 35 °C. The drug standard was subsequently reconstituted with 50 µL of phosphate buffer and acetonitrile (50:50, v:v). This mixture was added to clean test tubes with

combinations of phosphate buffer, HLMs, and/or NADPH according to Table 33. The sample prepared with only drug standard and buffer was used to make sure no metabolism or breakdown activity was occurring during the incubation, as well as to serve as a source of a reference mass spectrum to create a data processing profile (explained in detail below). The sample prepared with HLMs and no NADPH, a co-factor needed for metabolic activity, was used at the metabolism control, again to monitor possible breakdown products, but also to compare other species generated in the samples to rule out as metabolic products. Each sample containing drug, HLMs, and NADPH was prepared in duplicate to monitor metabolic variation and for additional confirmation of possible metabolites identified. The overall sample preparation and incubation process was performed over three days, for a total of six replicates.

Table 33: Metabolism experiments sample preparation

Sample ID	Phosphate Buffer (µL)	Drug (µL)	NADPH (µL)	HLM (µL)
Standard	595	5	0	0
Control	570	5	0	25
Reaction Mixture	520	5	50	25
Reaction Mixture	520	5	50	25

Prepared samples were then placed in a water bath (37 °C) with slight shaking for incubation and metabolite generation for a 2-hour period of time. All specimens within a single batch were incubated together, under identical conditions. Following incubation, acetonitrile (500 µL) was added to all samples to stop the metabolic reactions. Samples were then transferred to microcentrifuge tubes and centrifuged (10,000 rpm). The

supernatant was transferred to a new test tube and the samples were partially dried at 35 °C for 20 minutes to remove the majority of the organic solvent in the samples (acetonitrile). The supernatant was transferred to a Costar® Spin-X® (Corning Inc., Corning, NY, USA) microcentrifuge tube with a microfilter to remove any remaining cellular material or debris that could be detrimental to the analytical platform and samples were again centrifuged. The resulting sample was transferred to an autosampler vial for analysis by LC-QTOF-MS.

6.2.3 LC-QTOF-MS Analysis

Data was acquired using a SCIEX TripleTOF® 5600+ QTOF (Ontario, Canada) coupled with a Shimadzu Nexera XR UHPLC (Kyoto, Japan). Ammonium formate (10mM, pH 3) and methanol/acetonitrile (50:50) were used as mobile phase in a linear gradient (95:5 to 5:95) with a flow rate of 0.4 mL/min. A Phenomenex® Kinetex C18 analytical column (50mm x 3.0mm, 2.6µm) was used to achieve chromatographic separation of the metabolites. The total analysis run time was 15.5 minutes. This is the same LC method mentioned above (Chapter 4), as using the same LC method allows for retention time comparison *in vitro* vs. *in vivo*.

Mass acquisition for these microsomal samples was performed using a data dependent acquisition mode (information dependent acquisition: IDA), different from the acquisition mode described in Chapter 4 (DIA: SWATH®). Positive electrospray ionization was utilized for ionization. Precursor ions were acquired by a TOF MS scan ranging from 100-1000 Da. Precursor ions were subsequently filtered in the quadrupole

(Q1) using traditional unit mass isolation. Following this filtration, precursor ions were fragmented in the collision cell using a collision energy spread of 35±15eV. This collision energy spread allowed for acquisition of a comprehensive range of fragment ions, both in low and high mass ranges. IDA was used for acquisition of the microsomal samples due to the higher level of certainty gained by isolating just one mass in Q1 and fragmenting just that one mass. Therefore, the resulting fragment ions can be more specifically assigned back to the precursor ion, providing necessary certainty when characterizing unknown compound (e.g. metabolites in this case). In addition, the metabolite software used during this research was only able to process IDA-acquired datafiles. Therefore, acquisition of microsomal samples by IDA was necessary.

6.2.4 Software and Data Processing

Datafiles were processed using MetabolitePilot™ (SCIEX, Version, 1.5), MasterView™ (SCIEX, Version 1.1), PeakView® (SCIEX, Version 2.2). Potential metabolites were identified based on precursor and product ions, and their potential structures were elucidated. These metabolites were then verified in authentic human toxicological specimens (previously described), which had previously tested positive for a respective NPS.

MetabolitePilot™ was used to identify metabolites produced during the microsomal incubations. MetabolitePilot™ is preprogrammed with a list of commonly encountered biotransformations and utilizes these biotransformations alongside predictable isotope patterns, precursor ion intensities, mass defect, and the ability to

identify characteristic product ions and neutral losses in order to pull TOF MS and MSMS data of interest out for review and interpretation by the analyst. For the purposes of this research, all data files for a specific analyte of interest (e.g. *ortho*-fluorofuranylfentanyl, eutylone, etc.) were processed using identical and consistent software parameters, with comparison against a within-batch incubation control. The sample prepared as the "drug standard" with only drug standard and phosphate buffer was used to create a parent "library" entry. The software was then able to identify the appropriate isotope pattern and exact mass, as well as to generate a library spectrum for which the parent in each metabolism sample could be compared for increased certainty in identification.

Using the tools within the MetabolitePilot™ software, metabolite results were manually "reviewed" and "interpreted." In-house analyst review criteria were established following initial software use, which consisted of sorting the generated list of results by percent peak area and combined score, to effectively prioritize the data reviewed rather than review hundreds of "potential" metabolites, many of which were often determined to be not feasible. For review, the percent peak area needed to be greater than 0.1% and the combined score needed to be greater than 70. This combined score was calculated by summing up the processing values for mass defect, isotope pattern, MS/MS spectra, and mass accuracy, and creating a percentage. Additional data reviewed consisted of retention time and TOF MS data to determine consistency with or against the chromatographic elution in relation to the parent and the formula generated against the viability of biotransformation.

MasterView™ was used for qualitative "confirmation" of the proposed metabolites in the authentic human specimens (biological sample extracts) analyzed. During review of the data using MetabolitePilot™, an XIC list was generated to compile the proposed metabolite name, formula, and retention time. All extracts were processed against this generated XIC list. Positive analyte identification was based on pre-established criteria (mass error <10 ppm, retention time error <0.35 minutes, isotope difference <50%, library score >50, signal-to-noise ratio >10, and peak intensity >800 counts), the same criteria used above in Chapter 4.

6.3 Results and Discussion

6.3.1 3,4-Methylenedioxy-U-47700

3,4-Methylenedioxy-U-47700 ($C_{17}H_{24}N_2O_3$) exhibited a protonated ion of 305.1860 Da at 4.81 minutes (Figure 86), with prominent fragment ions of 305.1850, 260.1273, 180.0647, 149.0222, 123.0433, 81.0695, and 58.0285 Da (Figure 87). For characterization and structural elucidation of metabolites, fragment ions 260.1273, 180.0647, and 149.0222 Da were used for diagnostic purposes. The 260.1273 Da fragment ion is produced by cleavage of the tertiary amine attached to the cyclohexyl ring (Figure 88). Change (or no change) to this fragment ion would signify biotransformation on the structure external to the amine (or on the amine). The 180.0647 Da fragment ion is produced by cleavage between the amide and the cyclohexyl ring (Figure 89). Change (or no change) to this fragment ion would signify biotransformation on the 3,4-methylenedioxy-*N*-methyl-benzamide (or to the *N,N*-dimethylamino-cyclohexyl). The

149.0222 Da fragment ion is produced by cleavage between the carbon and nitrogen of the amide (Figure 90). Change (or no change) to this fragment ion would signify biotransformation similar to that of the 180.0647 Da fragment ion but would allow for differentiation of change to the alkyl on the amide nitrogen.

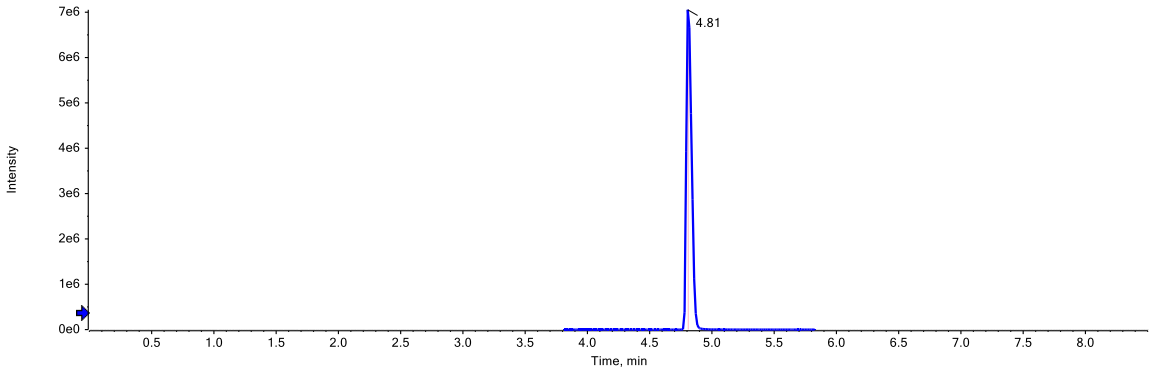

Figure 86: Extracted ion chromatogram of 3,4-methylenedioxy-U-47700

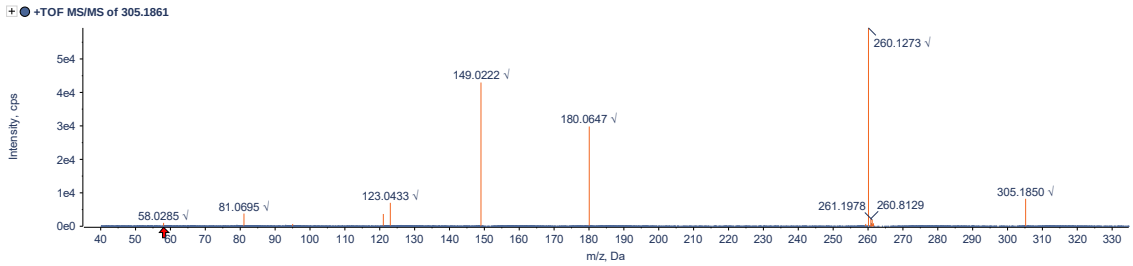

Figure 87: Fragment ion spectrum of 3,4-methylenedioxy-U-47700

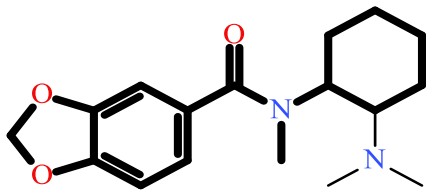

Figure 88: 3,4-Methylenedioxy-U-47700 260.1273 Da fragment ion (bold)

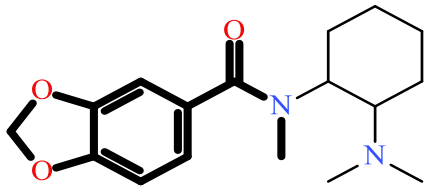

Figure 89: 3,4-Methylenedioxy-U-47700 180.0647 Da fragment ion (bold)

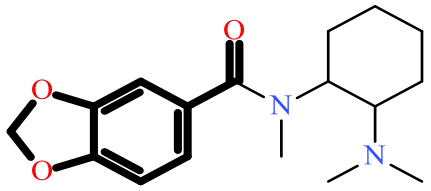

Figure 90: 3,4-Methylenedioxy-U-47700 149.0222 Da fragment ion (bold)

Nine metabolites of 3,4-methylenedioxy-U-47700 were identified *in vitro* following LC-QTOF-MS analysis of the six HLM samples (Figure 91). Corresponding mass, formula, retention time, and fragment data can be found in Table 34.

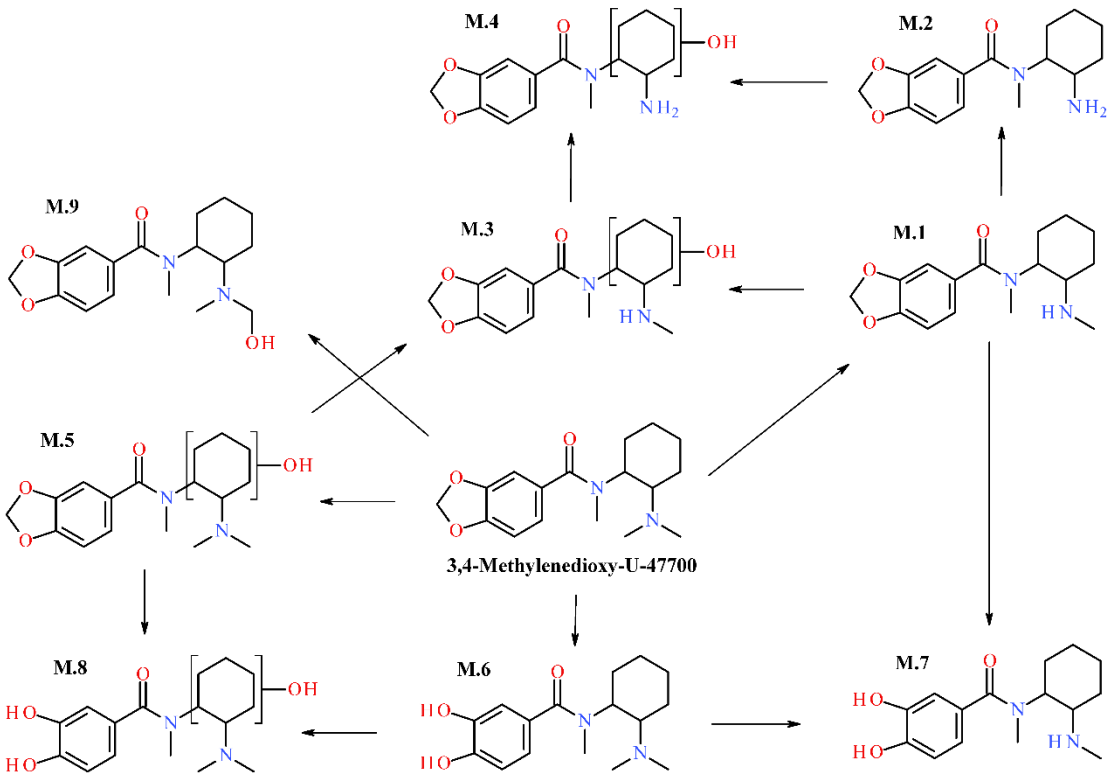

Figure 91: Metabolism scheme of 3,4-methylenedioxy-U-47700

Table 34: Metabolites of 3,4-methylenedioxy-U-47700 generated *in vitro*

ID	Biotransformation	RT (min)	Formula	$[M+H]^+$	Error (ppm)	Product Ions
P.0	3,4-Methylenedioxy-U-47700	4.82	$C_{17}H_{24}N_2O_3$	305.1860	-0.1	260.1273 180.0647 149.0222
M.1	*N*-Demethylation	4.84	$C_{16}H_{22}N_2O_3$	291.1703	0.0	260.1277 180.0650 149.0224
M.2	*N,N*-Didemethylation	4.81	$C_{15}H_{20}N_2O_3$	277.1548	0.3	260.1287 246.1120 180.0694 149.0231
M.3	*N*-Demethylation + Hydroxylation* (Cyclohexyl)	5.26	$C_{16}H_{22}N_2O_4$	307.1653	0.0	260.1280 180.0649 149.0232
M.4	*N,N*-Didemethylation + Hydroxylation* (Cyclohexyl)	5.32	$C_{15}H_{20}N_2O_4$	293.1494	-0.6	260.1279 180.0679 149.0231

M.5	Hydroxylation* (Cyclohexyl)	3.83	$C_{17}H_{24}N_2O_4$	321.1808	-0.2	276.1229 180.0656 149.0232
M.6	Demethylenation	3.65	$C_{16}H_{24}N_2O_3$	293.1860	0.0	248.1272 168.0652 137.0230
M.7	Demethylenation + *N*-Demethylation	3.71	$C_{15}H_{22}N_2O_3$	279.1703	-0.2	248.1278 168.0655 137.0230
M.8	Demethylenation + Hydroxylation* (Cyclohexyl)	3.79	$C_{16}H_{24}N_2O_4$	309.1809	0.0	248.1286 168.0657 137.0229
M.9	Hydroxylation (*N*-Methyl)	4.97	$C_{17}H_{24}N_2O_4$	321.1809	0.1	260.1279 180.0657 149.0230

**Multiple peaks identified due to multiple points of hydroxylation. Earliest in retention time reported.*

3,4-Methylenedioxy-U-47700 was found to undergo *N*-demethylation of the amine to produce M.1 (Figure 91). This metabolite exhibited a protonated ion of 291.1703 Da ($C_{16}H_{22}N_2O_3$) at 4.84 minutes, accounting for the loss of one methyl group (Δ -CH_2). 3,4-Methylenedioxy-U-47700 M.1 exhibited fragment ions of 260.1277, 180.0650, and 149.0224 Da (Figure 92), the same fragment ions as parent 3,4-methylenedioxy-U-47700. This information verifies the *N*-demethylation on the amine vs. the amide.

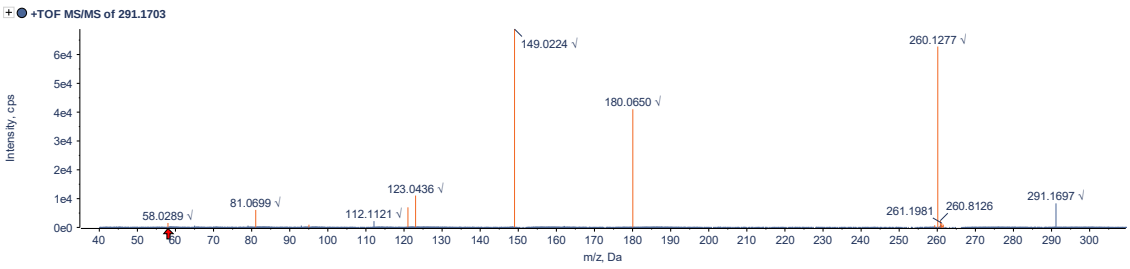

Figure 92: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.1

3,4-Methylenedioxy-U-47700 was further found to undergo *N*-demethylation for a second time to produce M.2 (Figure 91), an *N,N*-didesmethyl metabolite. This metabolite exhibited a protonated ion of 277.1548 Da ($C_{15}H_{20}N_2O_3$) at 4.81 minutes, accounting for the loss of two methyl groups (Δ -C_2H_4). 3,4-Methylenedioxy-U-47700 M.2 exhibited fragment ions of 260.1287, 180.0694, and 149.0231Da (Figure 93), the same fragment ions as parent 3,4-methylenedioxy-U-47700. This information verifies the *N,N*-didemethylation on the amine vs. demethylation to the amide.

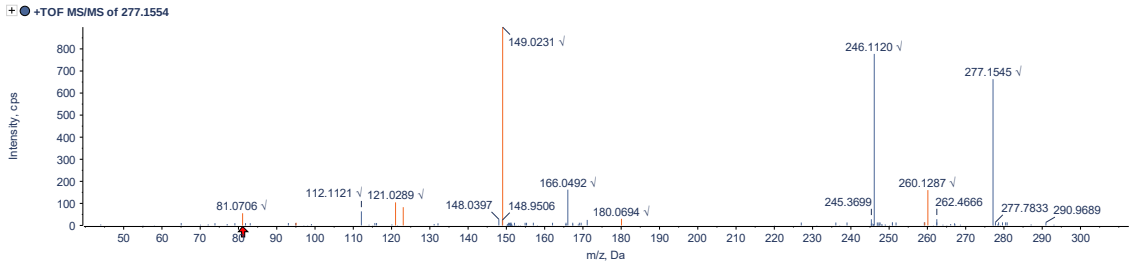

Figure 93: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.2

Combined *N*-demethylation and hydroxylation of 3,4-Methylenedioxy-U-47700 resulted in the identification of M.3 (Figure 91), and further *N*-demethylation resulted in the identification of M.4 (Figure 91). These metabolites exhibited protonated ions of 307.1653 Da ($C_{16}H_{22}N_2O_4$) at 5.26 minutes and 293.1494 Da ($C_{15}H_{20}N_2O_4$) at 5.32 minutes, accounting for the loss of one methyl group and addition of one oxygen (Δ -CH_2 +O) or the loss of two methyl groups and addition of one oxygen (Δ -C_2H_4 +O), respectively. 3,4-Methylenedioxy-U-47700 M.3 and M.4 exhibited fragment ions of 260.1280, 180.0649, and 149.0232 Da (Figure 94) and 260.1279, 180.0679, and

149.0231 Da (Figure 95), respectively. These fragment ions are the same as parent 3,4-methylenedioxy-U-47700 and seem to indicate hydroxylation external to the cyclohexyl ring; however, 3,4-Methylenedioxy-U-47700 M.3 and M.4. exhibited several peaks associated with their exact masses, demonstrating the multiple sites of hydroxylation around the cyclohexyl ring (Figures 96 and 97). In addition, the 260.1280 Da fragment ion can still be formed with this structure if the hydroxy group is fragmented off.

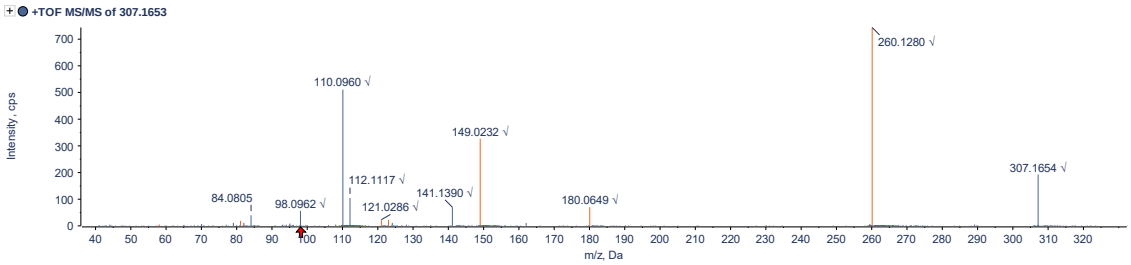

Figure 94: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.3

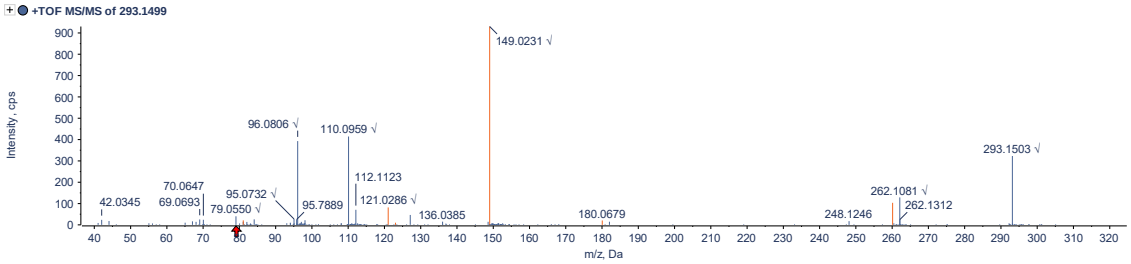

Figure 95: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.4

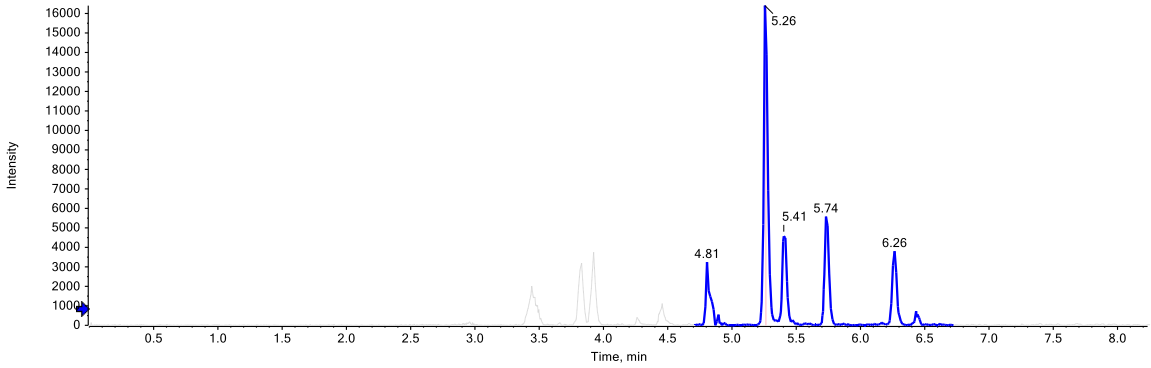

Figure 96: Extracted ion chromatogram of 3,4-methylenedioxy-U-47700 M.3

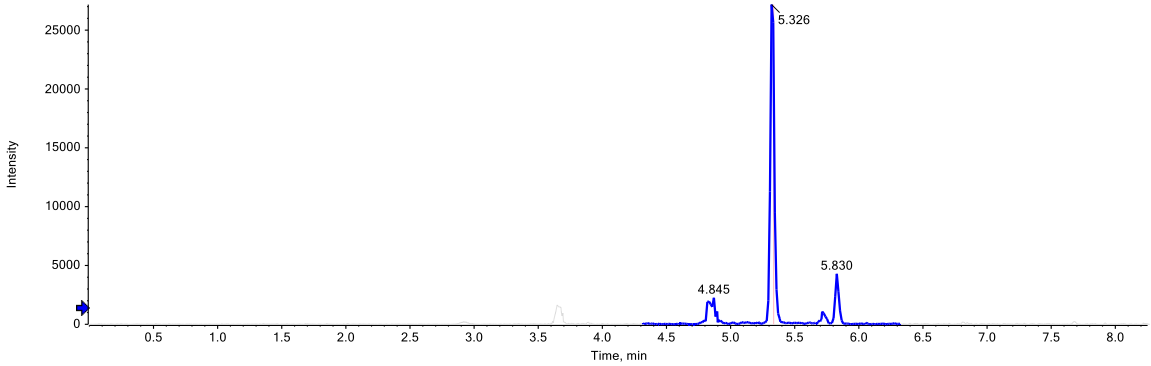

Figure 97: Extracted ion chromatogram of 3,4-methylenedioxy-U-47700 M.4

3,4-Methylenedioxy-U-47700 was found to undergo hydroxylation on the cyclohexyl ring to produce M.5 (Figure 91). This metabolite exhibited a protonated ion of 321.1808 Da ($C_{17}H_{24}N_2O_4$) at 3.83 minutes, accounting for the addition of one oxygen (Δ +O). 3,4-Methylenedioxy-U-47700 M.5 exhibited fragment ions of 276.1229, 180.0656, 149.0232 Da (Figure 98). Ions 180.0656 and 149.0232 Da are the same fragment ions as parent 3,4-methylenedioxy-U-47700, but ion 276.1229 Da is increased 16 mass units due to the oxygen added during hydroxylation. This information verifies the hydroxylation on

the cyclohexyl ring. Due to four possible points of hydroxylation around the cyclohexyl ring, multiple chromatographic peaks were identified for this metabolite (Figure 99); however, this analysis could not differentiate the specific sites of metabolism.

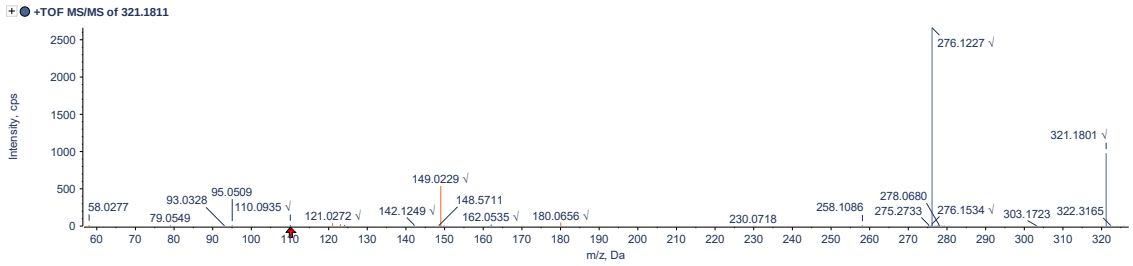

Figure 98: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.5

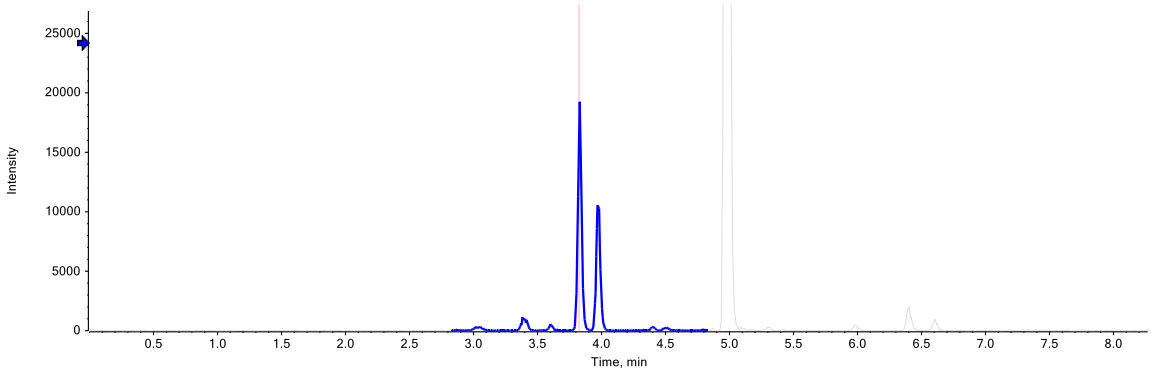

Figure 99: Extracted ion chromatogram of 3,4-methylenedioxy-U-47700 M.4

Due to the presence of the 3,4-methylenedioxy group, 3,4-methylenedioxy-U-47700 was found to undergo demethylenation to produce M.6 (Figure 91). This metabolite exhibited a protonated ion of 293.1860 Da ($C_{16}H_{24}N_2O_3$) at 3.65 minutes, accounting for the loss of one carbon (Δ -C). 3,4-Methylenedioxy-U-47700 M.6 exhibited fragment ions of 248.1272, 168.0652, 137.0230 Da (Figure 100). All three

fragments are 12 mass units less that the fragment ions of parent 3,4-methylenedioxy-U-47700, accounting for the loss of the carbon linker in the 3,4-methylenedioxy group.

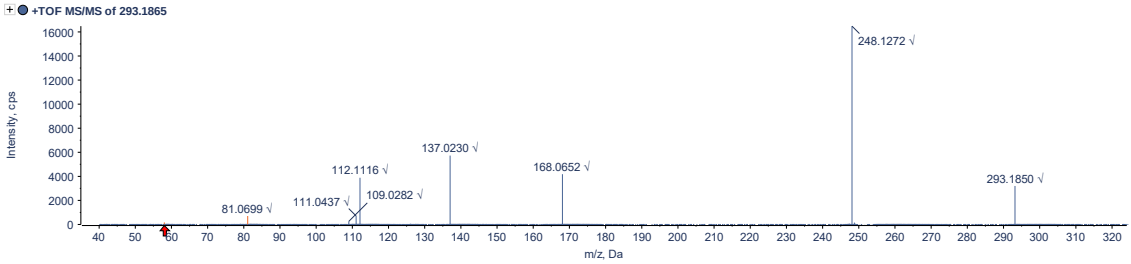

Figure 100: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.6

Biotransformations in addition to demethylenation produced M.7 and M.8 (Figure 91), specifically N-demethylation and hydroxylation, respectively. These metabolites exhibited protonated ions of 279.1703 Da ($C_{15}H_{22}N_2O_3$) at 3.71 minutes and 309.1809 Da ($C_{16}H_{24}N_2O_4$) at 3.79 minutes, accounting for the loss of one carbon and the loss of one methyl group (Δ -C_3H_4) or the loss of one carbon and addition of one oxygen (Δ -C +O), respectively. Both metabolites produced similar fragment ion spectra: 3,4-methylenedioxy-U-47700 M.7 exhibited fragment ions of 248.1278, 168.0655, and 137.0230 Da (Figure 101) and 3,4-methylenedioxy-U-47700 M.8 exhibited fragment ions of 248.1286, 168.0657, and 137.0229 Da (Figure 102). These fragment ions, as with M.6, result from the loss of the carbon linker in the 3,4-methylenedioxy group.

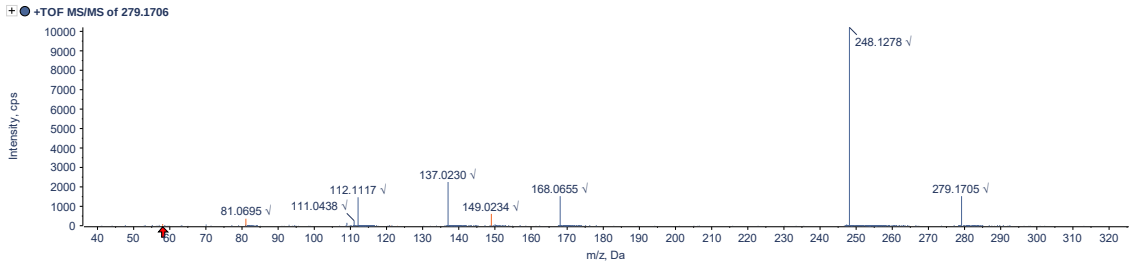

Figure 101: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.7

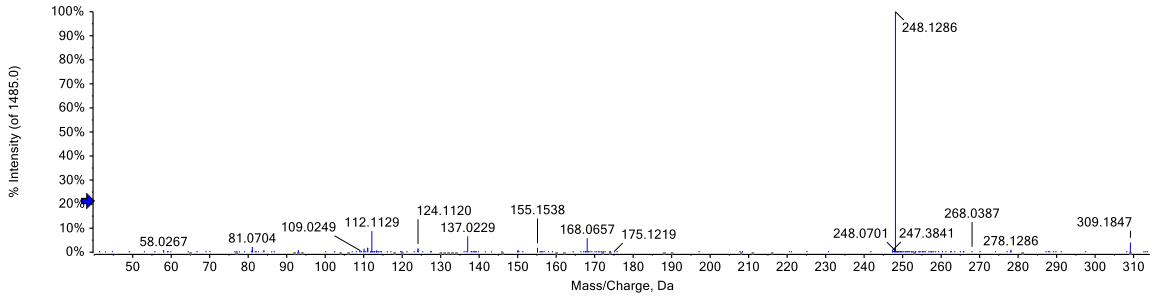

Figure 102: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.8

The last metabolite of 3,4-methylenedioxy-U-47700 identified was the result of hydroxylation to a methyl group attached to the amine M.9 (Figure 91). This metabolite exhibited a protonated ion of 321.1809 Da ($C_{17}H_{24}N_2O_4$) at 4.97 minutes, accounting for the addition of one oxygen (Δ +O). 3,4-Methylenedioxy-U-47700 M.9 exhibited fragment ions of 260.1279, 180.0657, and 149.0230 Da (Figure 103). Since these are the same fragment ions as parent 3,4-methylenedioxy-U-47700 and there is only one chromatographic peak (Figure 104), the site of hydroxylation was attributed to one of the methyl groups attached to the amine.

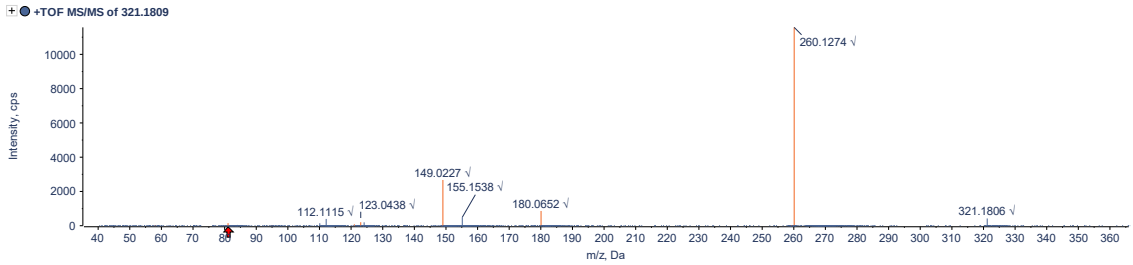

Figure 103: Fragment ion spectrum of 3,4-methylenedioxy-U-47700 M.9

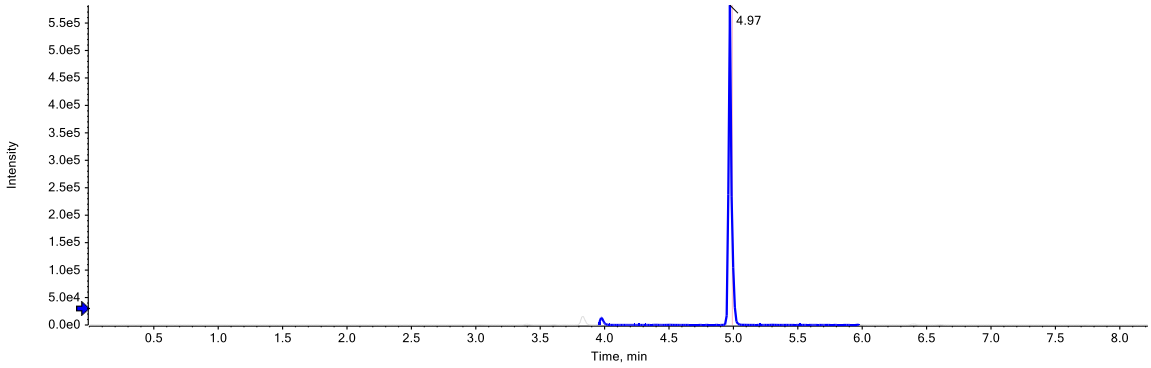

Figure 104: Extracted ion chromatogram of 3,4-methylenedioxy-U-47700 M.9

Following characterization of 3,4-methylenedioxy-U-47700 metabolism *in vitro*, the nine metabolites identified were screened for *in vivo* (i.e. data mining) using biological sample extracts positive for parent 3,4-methylenedioxy-U-47700. In total, the datafiles from ten extracts were determined suitable to processing of metabolites. Table 35 shows the results of parent compound and metabolites identified. Of the nine metabolites, only three were found *in vivo*; although this is not uncommon, as all metabolites identified *in vitro* may not manifest in authentic human specimens. *N*-desmethyl-3,4-methylenedioxy-U-47700 (M.1) was found to be the most prominent metabolite.

Table 35: Metabolites of 3,4-methylenedioxy-U-47700 observed *in vivo*

Sample	3,4-Methylenedioxy-U-47700	M.1 *N*-Demethylation	M.4 *N,N*-Didemethylation + Hydroxylation	M.7 Demethylenation + *N*-Demethylation
1	RT: 4.88 Area: 1,615 *Parent Ratio: 100%*	RT: 4.89 Area: 1,033 *Parent Ratio: 64.0%*	ND	ND
2	RT: 4.86 Area: 16,687 *Parent Ratio: 100%*	RT: 4.87 Area: 8,586 *Parent Ratio: 51.5%*	ND	RT: 4.86 Area: 477 *Parent Ratio: 2.7%*
3	RT: 4.86 Area: 1,142 *Parent Ratio: 100%*	RT: 4.87 Area: 884 *Parent Ratio: 77.4%*	ND	ND
4	RT: 4.94 Area: 34,413 *Parent Ratio: 100%*	RT: 4.95 Area: 7,607 *Parent Ratio: 22.1%*	RT: 3.73 Area: 40 *Parent Ratio: 0.1%*	RT: 4.94 Area: 131 *Parent Ratio: 0.4%*
5	RT: 4.99 Area: 2,567 *Parent Ratio: 100%*	RT: 5.00 Area: 684 *Parent Ratio: 26.6%*	ND	ND
6	RT: 4.99 Area: 11,017 *Parent Ratio: 100%*	RT: 5.00 Area: 144 *Parent Ratio: 1.3%*	ND	ND
7	RT: 4.95 Area: 5,559 *Parent Ratio: 100%*	RT: 4.96 Area: 396 *Parent Ratio: 7.1%*	ND	ND
8	RT: 4.82 Area: 73,077 *Parent Ratio: 100%*	RT: 4.82 Area: 4,379 *Parent Ratio: 6.0%*	ND	ND
9	RT: 4.83 Area: 45,708 *Parent Ratio: 100%*	RT: 4.83 Area: 3,771 *Parent Ratio: 8.3%*	ND	ND
10	RT: 4.98 Area: 3,487 *Parent Ratio: 100%*	RT: 4.99 Area: 3,942 *Parent Ratio: 113%*	ND	ND

Key: RT – retention time (in minutes), ND – None detected,
Parent Ratio = (Parent area / Metabolite area) x 100

Reference material was not available for any metabolites of 3,4-methylenedioxy-U-47700; therefore, exact structure in all cases can not be analytically confirmed by the described methods alone. Further research is needed to confirm the proposed structures. Nonetheless, three metabolites were found in human specimens.

Similar biotransformations to those reported herein for 3,4-methylenedioxy-U-47700 have been reported elsewhere for U-47700 and U-49900,[78] including dealkylated and hydroxylated metabolites. The prominent metabolites of U-47700 and U-49900 were *N*-dealkylated species, in agreement with the prominent findings of *N*-desmethyl-3,4-methylenedioxy-U-47700 (M.1) herein.

6.3.2 ortho-Fluorofuranylfentanyl

ortho-Fluorofuranylfentanyl ($C_{24}H_{25}FN_2O_2$) exhibited a protonated ion of 393.1973 Da at 6.41 minutes (Figure 105), with prominent fragment ions of 272.1080, 244.0767, 228.1020, 206.0610, 188.1422, 146.0960, 134.0960, 105.0691, 95.0127, and 84.0805 Da (Figure 106). For characterization and structural elucidation of metabolites, fragment ions 272.1080, 206.0610, 188.1422, 105.0691, 95.0127, and 84.0805 Da were used for diagnostic purposes. The 272.1080 Da fragment ion is produced by cleavage of the nitrogen in the piperidine ring and the phenethyl group (Figure 107). Change (or no change) to this fragment ion would signify biotransformation external to the phenethyl group. The 206.0610 Da fragment ion is produced by cleavage between the tertiary amine and the piperidine ring (Figure 108). Change (or no change) to this fragment ion would signify biotransformation to the aniline and furfural, external to the phenethyl piperidine region. The 188.1422 and 105.0691 Da fragment ions are produced by cleavage of the phenethyl and phenethyl piperidine groups, respectively (Figure 109). The 95.0127 and 84.0805 Da fragment ions are produced by the fragmentation off all substituents off the of the furan and piperidine rings respectively. Change to the 188.1422/105.0691 Da

fragment ions would signify biotransformation on the phenethyl group, while change to the 84.0805 Da fragment ion would signify biotransformation on the piperidine ring.

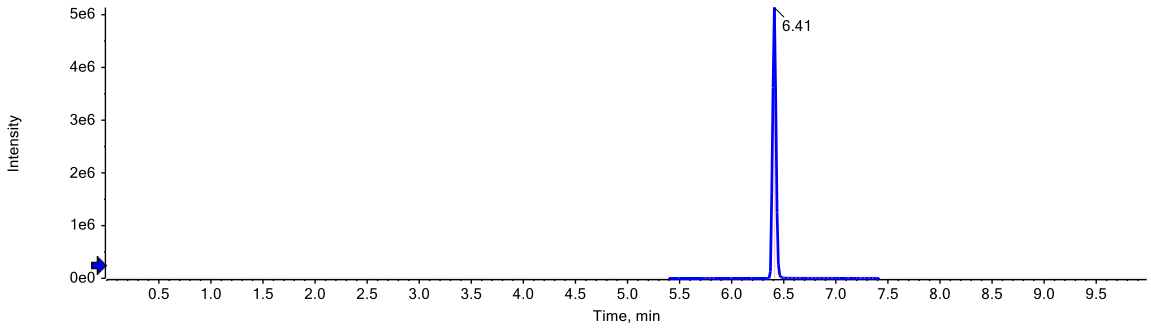

Figure 105: Extracted ion chromatogram of *ortho*-fluorofuranylfentanyl

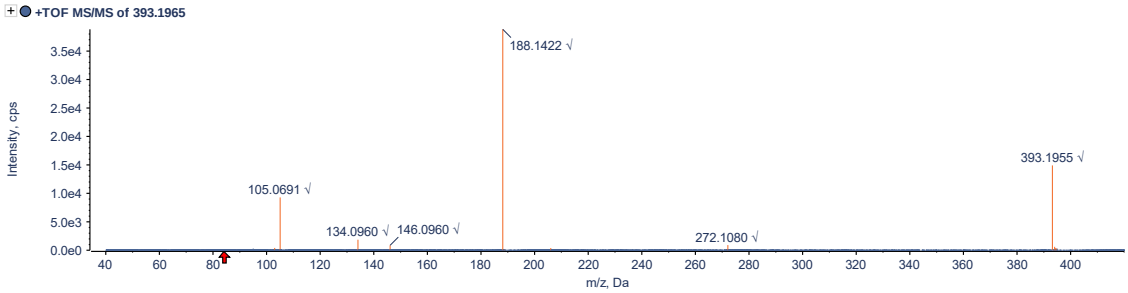

Figure 106: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl

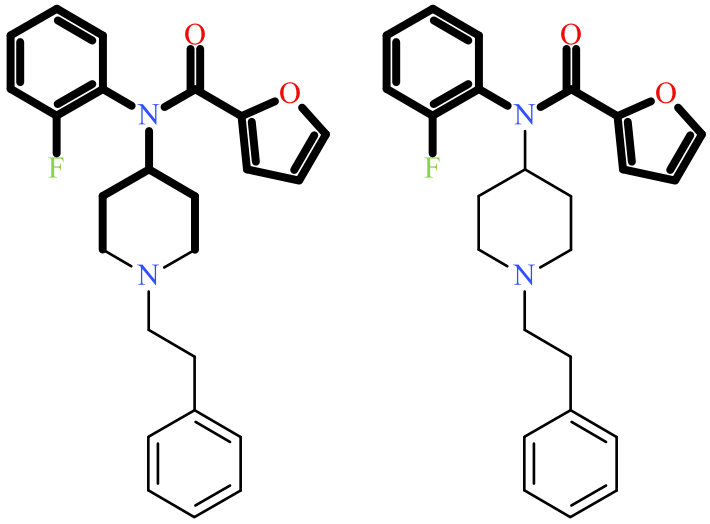

Figure 107: *ortho*-Fluorofuranylfentanyl 272.1080 (left) and 206.0610 (right) Da fragment ions (bold)

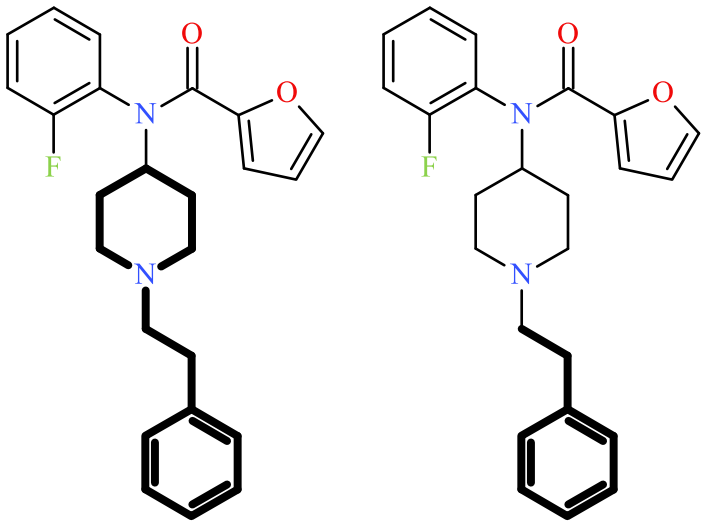

Figure 108: *ortho*-Fluorofuranylfentanyl 188.1422 (left) and 105.0691 (right) Da fragment ions (bold)

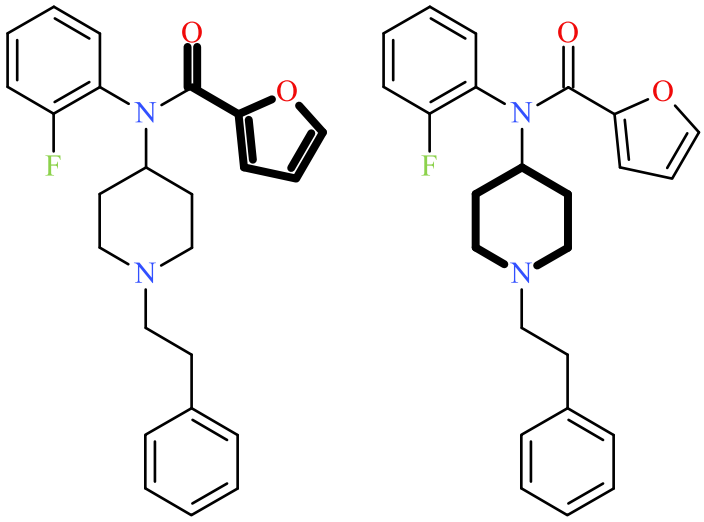

Figure 109: *ortho*-Fluorofuranylfentanyl 95.0127 (left) and 84.0805 (right) Da fragment ions (bold)

Nine metabolites of *ortho*-fluorofuranylfentanyl were identified *in vitro* following LC-QTOF-MS analysis of the six HLM samples (Figure 110). Corresponding mass, formula, retention time, and fragment data can be found in Table 36.

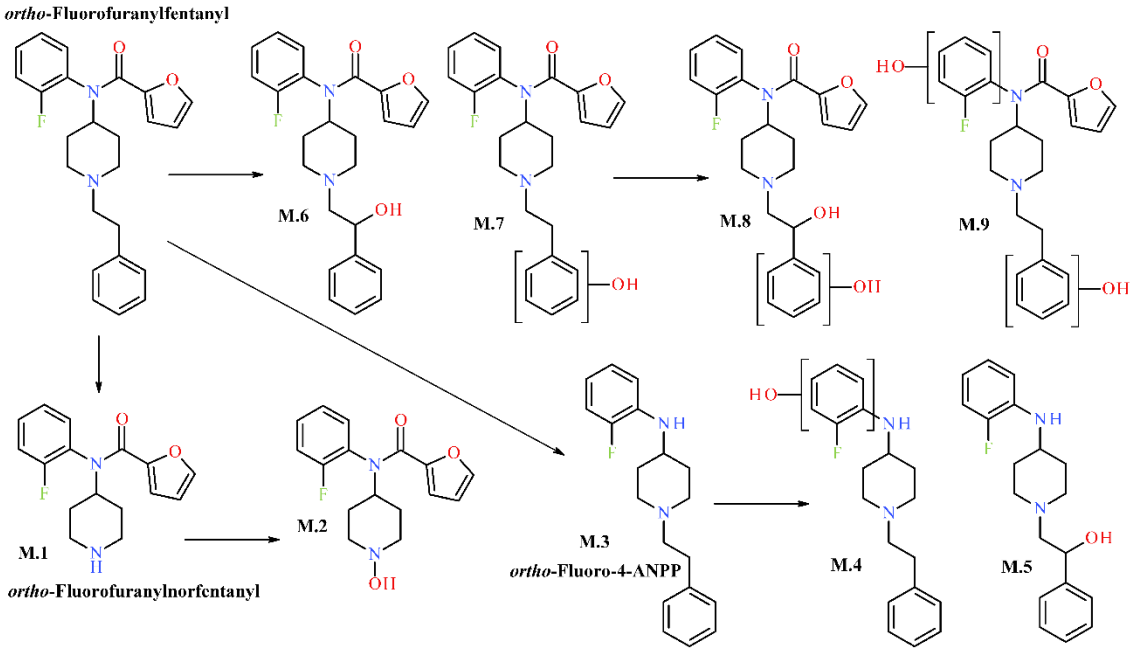

Figure 110: Metabolism scheme of *ortho*-fluorofuranylfentanyl

Table 36: Metabolites of *ortho*-fluorofuranylfentanyl generated *in vitro*

ID	Biotransformation	RT (min)	Formula	$[M+H]^+$	Error (ppm)	Product Ions
P.0	*ortho*-Fluorofuranylfentanyl	6.41	$C_{24}H_{25}FN_2O_2$	393.1973	-0.1	272.1080 206.0610 188.1422 105.0691 95.0127 84.0805
M.1	*N*-Dealkylation [*ortho*-Fluorofuranyl-Norfentanyl]	4.92	$C_{16}H_{17}FN_2O_2$	289.1347	0.1	206.0612 95.0128 84.0805
M.2	*N*-Dealkylation + Hydroxylation (Amine)	5.38	$C_{16}H_{17}FN_2O_3$	305.1297	0.4	206.0614 95.0137 82.0649
M.3	Loss of C5H2O2 [*ortho*-Fluoro-4-ANPP]	6.45	$C_{19}H_{23}FN_2$	299.1918	-0.1	188.1247 105.0693 84.0815
M.4	Loss of C5H2O2 + Hydroxylation (Aniline)	5.23	$C_{19}H_{23}FN_2O$	315.1867	0.1	188.1433 105.0698 84.0811
M.5	Loss of C5H2O2 + Hydroxylation (Ethyl)	6.04	$C_{19}H_{23}FN_2O$	315.1867	0.1	204.1384 105.0696 84.0801

M.6	Hydroxylation (Ethyl)	6.06	$C_{24}H_{25}FN_2O_3$	409.1922	0.1	272.1085 204.1381 95.0126 84.0812
M.7	Hydroxylation (Phenyl)	5.82	$C_{24}H_{25}FN_2O_3$	409.1923	0.2	272.1098 204.1386 121.0645 95.0110 84.0810
M.8	Di-Hydroxylation (Phenyl and Ethyl)	5.58	$C_{24}H_{25}FN_2O_4$	425.1870	-0.3	220.1332 137.0595 95.0121 84.0816
M.9	Di-Hydroxylation (Phenyl and Aniline)	5.99	$C_{24}H_{25}FN_2O_4$	425.1872	0.1	305.1292 121.0644 95.0129

ortho-Fluorofuranylfentanyl was found to undergo *N*-dealkylation to M.1 (Figure 110), or *ortho*-fluorofuranyl-norfentanyl. This metabolite exhibited a protonated ion of 289.1347 Da ($C_{16}H_{17}FN_2O_2$) at 4.92 minutes, accounting for the loss of the phenethyl group (Δ -C_8H_8). *ortho*-Fluorofuranyl-norfentanyl (M.1) exhibited fragment ions of 206.0612, 95.0128, and 84.0805 Da (Figure 111). While these are the same fragment ions as parent *ortho*-fluorofuranylfentanyl, the absence of 188 and 105 fragment ions demonstrates the removal of the phenethyl group.

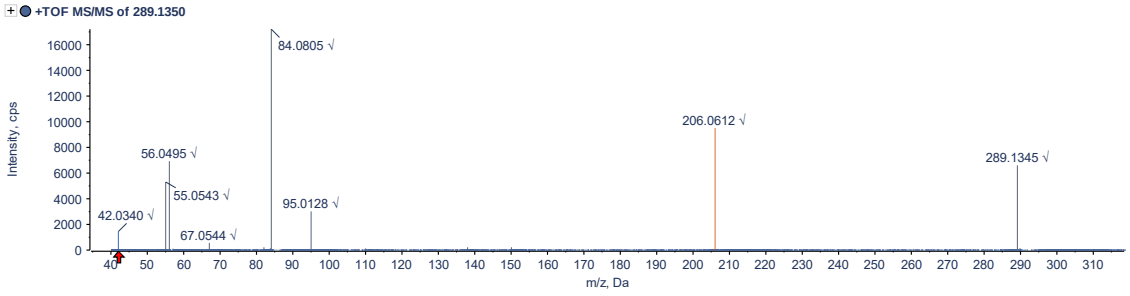

Figure 111: Fragment ion spectrum of *ortho*-fluorofuranyl-norfentanyl (M.1)

ortho-Fluorofuranyl-norfentanyl (M.1) was found to further metabolize via hydroxylation to produce M.2 (Figure 110). This metabolite exhibited a protonated ion of 305.1297 Da ($C_{16}H_{17}FN_2O_3$) at 5.38 minutes, accounting for the loss of the phenethyl group and addition of one oxygen (Δ -C_8H_8 +O vs. parent). *ortho*-Fluorofuranylfentanyl M.2 exhibited fragment ions of 206.0614, 95.0137, and 82.0649 Da (Figure 112), the same fragment ions as *ortho*-fluorofuranyl-norfentanyl (M.1), leading to the point of hydroxylation likely being on the amine of the piperidine ring.

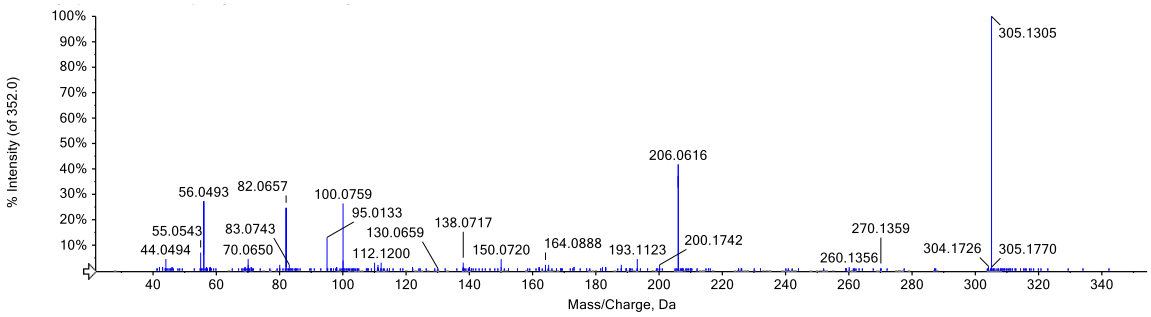

Figure 112: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.2

A prominent metabolite of *ortho*-fluorofuranylfentanyl was produced by removal of the furfural group (i.e. loss of C5H2O2) to produce M.3 (Figure 110), or *ortho*-fluoro-4-ANPP. This metabolite exhibited a protonated ion of 299.1918 Da ($C_{19}H_{23}FN_2$) at 6.45 minutes (Δ -$C_5H_2O_2$). *ortho*-Fluoro-4-ANPP (M.3) exhibited fragment ions of 188.1247, 105.0693, and 84.0815 Da (Figure 113), the same fragments as the parent compound but notifiable missing the 206 fragment ion. Of important note, this biotransformation product was produced during the HLM incubation experiments; this precursor was absent in the standard for *ortho*-fluorofuranylfentanyl.

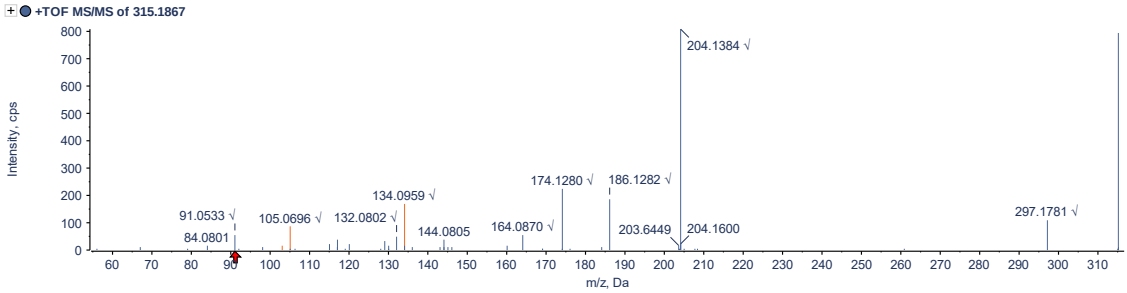

Figure 113: Fragment ion spectrum of *ortho*-fluoro-4-ANPP (M.3)

ortho-Fluoro-4-ANPP (M.3) was found to further metabolize via hydroxylation to produce M.4 and M.5 (Figure 110). These metabolites exhibited protonated ions of 315.1867 Da ($C_{19}H_{23}FN_2O$) at 5.23 and 6.04 minutes, respectively, accounting for the loss of the furfural group and addition of one oxygen (Δ $-C_5H_2O_2$ +O vs. parent). *ortho*-Fluorofuranylfentanyl M.4 exhibited fragment ions of 188.1433, 105.0698, and 84.0811 Da (Figure 114), the same fragment ions of *ortho*-fluoro-4-ANPP (M.3), leading to the point of hydroxylation likely being on the aniline ring.

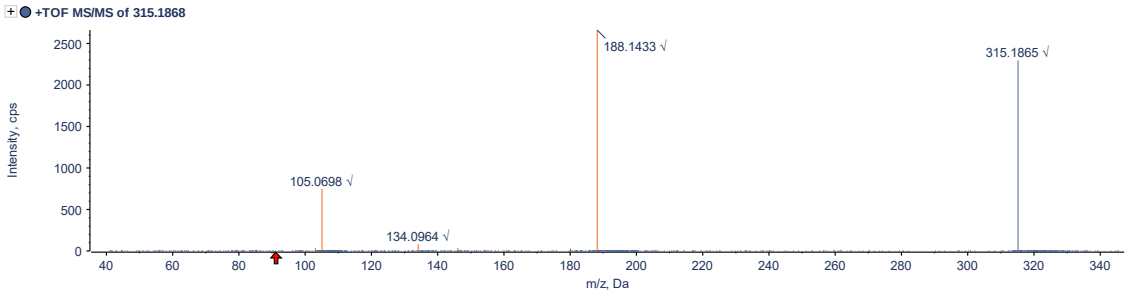

Figure 114: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.4

ortho-Fluorofuranylfentanyl M.5 exhibited fragment ions of 204.1384, 105.0696, and 84.0801 Da (Figure 115). The 204 fragment ion points to hydroxylation on the phenethyl group, while the 105 fragment ion (the same fragment ion as *ortho*-fluoro-4-ANPP, M.3) points towards hydroxylation on the ethyl bridge. If hydroxylation occurred on the phenyl ring, the 105 fragment ion would likely have increased to a 121 fragment ion.

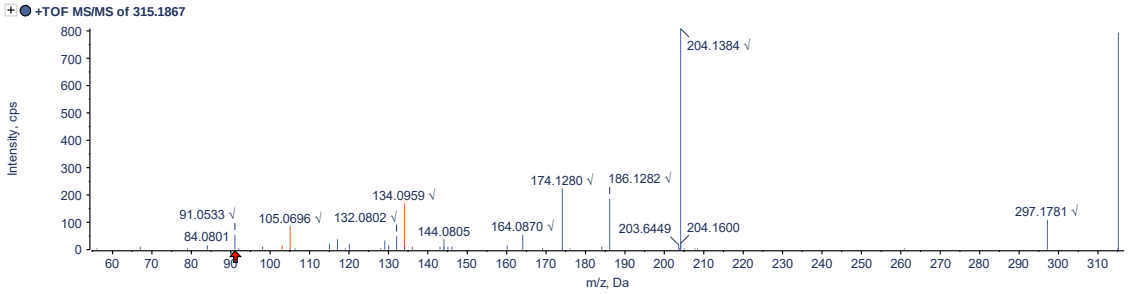

Figure 115: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.5

ortho-Fluorofuranylfentanyl was found to undergo extensive hydroxylation, producing mono-hydroxylated metabolites M.6 and M.7, as well as di-hydroxylated metabolites M.8 and M.9 (Figure 110). The mono-hydroxylated metabolites exhibited protonated ions of 409.1922 and 409.1923 Da ($C_{24}H_{25}FN_2O_3$) at 6.06 and 5.82 minutes, respectively, accounting for the addition of one oxygen (Δ +O). *ortho*-Fluorofuranylfentanyl M.5 exhibited fragment ions of 272.1085, 204.1381, 95.0126, and 84.0812 Da (Figure 116), while *ortho*-fluorofuranylfentanyl M.6 exhibited fragment ions of 272.1098, 204.1386, 121.0645, 95.0110, and 84.0810 Da (Figure 117). Similar to above, the presence of the 204 fragment ions points towards hydroxylation on the

phenethyl group, while presence of a 121 or 105 fragment ion differentiated the position to be on the phenyl ring or ethyl bridge, respectively.

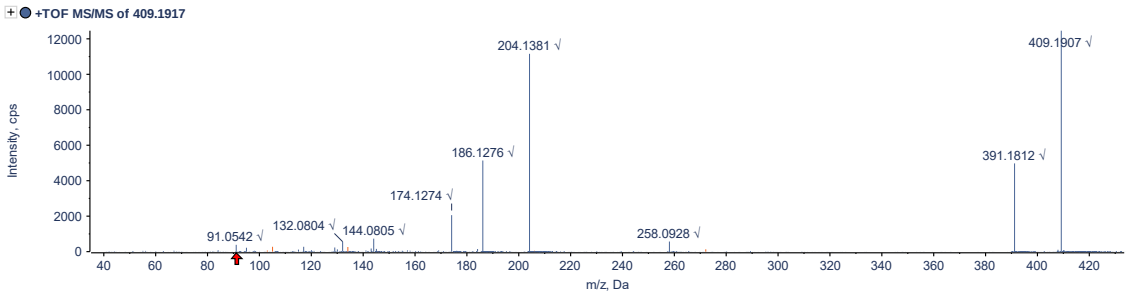

Figure 116: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.6

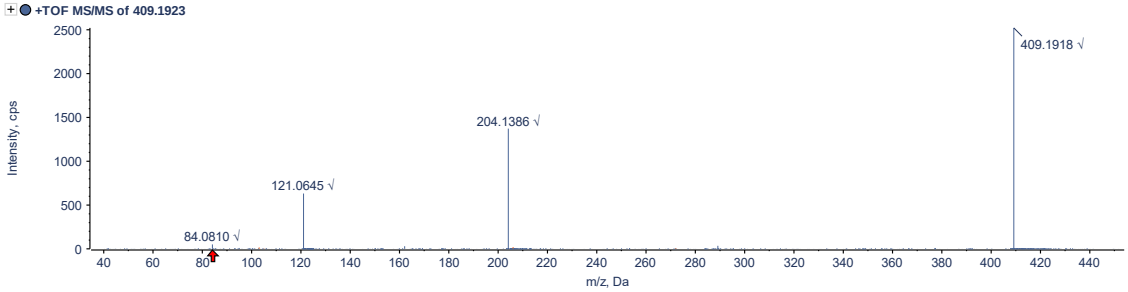

Figure 117: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.7

The di-hydroxylated metabolites exhibited protonated ions of 425.1870 and 425.1872 Da ($C_{24}H_{25}FN_2O_4$) at 5.58 and 5.99 minutes, respectively, accounting for the addition of two oxygens ($\Delta +O_2$). *ortho*-Fluorofuranylfentanyl M.8 exhibited fragment ions of 220.1332, 137.0595, 95.0121, and 84.0816 Da (Figure 118). The presence of the 220 and 137 fragment ions point to both sites of hydrolyzation occurring on the phenethyl group, likely one at the beta-position of the ethyl bridge and one on the phenyl ring. *ortho*-Fluorofuranylfentanyl M.9 exhibited fragment ions of 305.1292, 121.0644, and

95.0129 Da (Figure 119). The presence of the 121 fragment ions pointed to one site of hydrolyzation occurring on the phenyl ring, while the 305 fragment ion pointed to one site of hydrolyzation occurring on the aniline ring.

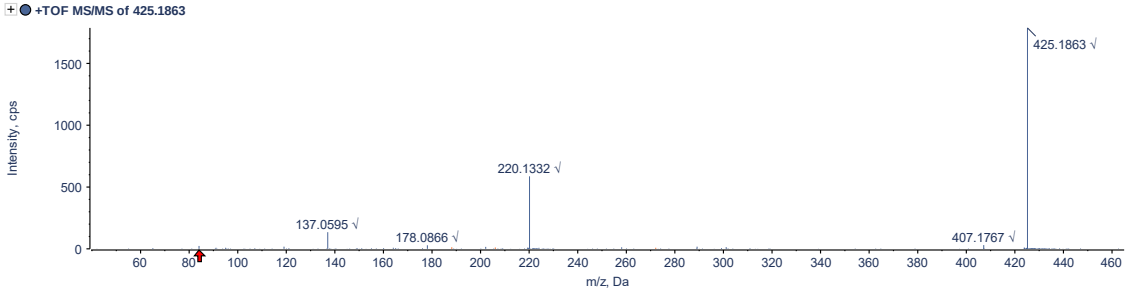

Figure 118: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.8

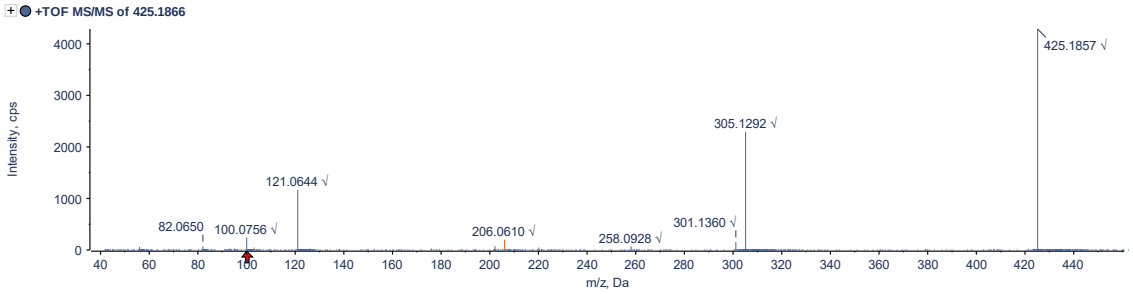

Figure 119: Fragment ion spectrum of *ortho*-fluorofuranylfentanyl M.9

Following characterization of *ortho*-fluorofuranylfentanyl metabolism *in vitro*, the nine metabolites identified were screened for *in vivo* (i.e. data mining) using biological sample extracts positive for parent *ortho*-fluorofuranylfentanyl. In total, the datafiles from three extracts were determined suitable to processing of metabolites. Table 37 shows the results of parent compound and metabolites identified. Of the nine metabolites,

only one was found *in vivo*; although this is not uncommon, as all metabolites identified *in vitro* may not manifest in authentic human specimens.

Table 37: Metabolites of fluorofuranylfentanyl observed *in vivo*

Sample	Fluorofuranylfentanyl	M.3 Fluoro-4-ANPP
1	RT: 6.31 Area: 7,910 *Parent Ratio: 100%*	RT: 6.17 Area: 3,887 *Parent Ratio: 49.8%*
2	RT: 6.47 Area: 1,428 *Parent Ratio: 100%*	RT: 6.33 Area: 2,049 *Parent Ratio: 143%*
3	RT: 6.38 Area: 1,774 *Parent Ratio: 100%*	RT: 6.24 Area: 581 *Parent Ratio: 32.8%*

Key: RT – retention time (in minutes), ND – None detected,
Parent Ratio = (Parent area / Metabolite area) x 100

Fluoro-4-ANPP, the only metabolite identified in the biological extracts, can manifest in biological samples for different reasons. Fluoro-4-ANPP can be used as a synthetic precursor in the production of fluorofuranylfentanyl; therefore, if this material is not used to completion during reaction, it can remain in drug samples that are ingested. From this research, *ortho*-fluoro-4-ANPP was determined to be a metabolite of *ortho*-fluorofuranylfentanyl. The source of fluoro-4-ANPP in the biological extracts can not be determined based on the analyses performed; its presence is hypothesized to be the combination of both scenarios.

Of important note, the position of the fluorine on *ortho*-fluorofuranylfentanyl was known for the *in vitro* metabolism studies due to the reference material purchased. The LC-QTOF-MS method was not capable of determining this position during analysis of

biological extracts; therefore, fluorofuranylfentanyl and fluoro-4-ANPP are reported with these samples without designation for the position.

A unique opportunity presented itself during this research to further study the metabolism of fluorofuranylfentanyl in blood samples from a medical examiner's office in Florida. Following our identification of fluorofuranylfentanyl in January 2019, this emerging NPS opioid proliferated in several states, including Florida, causing many deaths. In collaboration with the Pinellas County Forensic Laboratory, twenty-nine peripheral blood samples from medicolegal death investigations were submitted for analysis of metabolites. The blood samples were prepared via liquid-liquid extract and analyzed by LC-QTOF-MS, as described in Chapter 4. Parent fluorofuranylfentanyl and its metabolites were screening for in the same manner as the biological sample extract. Table 38 details these results.

Table 38: Metabolites of fluorofuranylfentanyl observed *in vivo* – blood specimens

Sample	Fluorofuranyl-fentanyl	M.1 Fluorofuranyl-Norfentanyl	M.3 Fluoro-4-ANPP	M.5 *beta*-OH-Fluoro-4-ANPP
1	Area: 954 *% Parent: 100%*	ND	Area: 342 *% Parent: 35.8%*	ND
2	Area: 1,398 *% Parent: 100%*	ND	Area: 1,483 *% Parent: 106%*	ND
3	Area: 1,564 *% Parent: 100%*	ND	Area: 1,758 *% Parent: 112%*	ND
4	Area: 637 *% Parent: 100%*	ND	Area: 5,070 *% Parent: 796%*	+ *% Parent: N/A*
5	Area: 13,953 *% Parent: 100%*	ND	Area: 3,782 *% Parent: 27.1%*	ND
6	Area: 1,691 *% Parent: 100%*	ND	Area: 2,859 *% Parent: 169%*	+ *% Parent: N/A*
7	Area: 625 *% Parent: 100%*	ND	Area: 369 *% Parent: 59.0%*	ND
8	Area: 17,928 *% Parent: 100%*	+ *% Parent: N/A*	Area: 11,171 *% Parent: 62.3%*	+ *% Parent: N/A*
9	Area: 977 *% Parent: 100%*	ND	Area: 1,650 *% Parent: 169%*	+ *% Parent: N/A*

10	Area: 8,436 *% Parent: 100%*	ND	Area: 29,027 *% Parent: 344%*	Area: 963 *% Parent: 11.4%*
11	Area: 8,686 *% Parent: 100%*	ND	Area: 1,108 *% Parent: 12.8%*	ND
12	Area: 2,309 *% Parent: 100%*	ND	Area: 5,420 *% Parent: 235%*	ND
13	Area: 863 *% Parent: 100%*	ND	Area: 3,228 *% Parent: 374%*	+ *% Parent: N/A*
14	Area: 15,990 *% Parent: 100%*	ND	Area: 1,019 *% Parent: 6.4%*	ND
15	Area: 886 *% Parent: 100%*	ND	Area: 727 *% Parent: 82.1%*	ND
16	Area: 1,125 *% Parent: 100%*	ND	Area: 3,938 *% Parent: 350%*	Area: 100 *% Parent: 8.9%*
17	Area: 15,667 *% Parent: 100%*	+ *% Parent: N/A*	Area: 10,407 *% Parent: 66.4%*	ND
18	Area: 2,643 *% Parent: 100%*	ND	Area: 3,690 *% Parent: 140%*	ND
19	Area: 633 *% Parent: 100%*	ND	Area: 111 *% Parent: 17.5%*	ND
20	Area: 6,449 *% Parent: 100%*	ND	Area: 14,007 *% Parent: 217%*	ND
21	Area: 1,690 *% Parent: 100%*	ND	Area: 2,243 *% Parent: 133%*	Area: 111 *% Parent: 6.5%*
22	Area: 4,293 *% Parent: 100%*	ND	Area: 2,554 *% Parent: 59.5%*	ND
23	Area: 23,543 *% Parent: 100%*	ND	Area: 12,764 *% Parent: 54.2%*	+ *% Parent: N/A*
24	Area: 12,062 *% Parent: 100%*	ND	Area: 4,356 *% Parent: 36.1%*	ND
25	Area: 4,447 *% Parent: 100%*	ND	Area: 2,073 *% Parent: 46.6%*	ND
26	+ *% Parent: N/A*	ND	+ *% Parent: N/A*	ND
27	Area: 1,061 *% Parent: 100%*	ND	Area: 11,376 *% Parent: 1,072%*	Area: 1,242 *% Parent: 117%*
28	Area: 1,931 *% Parent: 100%*	ND	Area: 102 *% Parent: 5.3%*	ND
29	Area: 10,852 *% Parent: 100%*	ND	Area: 11,182 *% Parent: 103%*	ND

Key: RT – retention time (in minutes), ND – None detected, N/A – Not available, % Parent = (Parent area / Metabolite area) x 100

Two additional metabolites of fluorofuranylfentanyl were identified in these peripheral blood samples: fluorofuranyl-norfentanyl (M.1) and *beta*-OH-fluoro-4-ANPP (M.5). Fluorofuranyl-norfentanyl (M.1) was only identified in two blood specimens;

however, it is hypothesized that this would be the major metabolite in urine specimens. While *beta*-OH-fluoro-4-ANPP (M.5) was identified in ten blood specimens, its presence is linked to fluoro-4-ANPP and therefore from an indistinguishable source (i.e. metabolite of precursor fluoro-4-ANPP or metabolite of fluorofuranylfentanyl through fluoro-4-ANPP).

Reference materials for all other metabolites of fluorofuranylfentanyl were not available; therefore, exact structure in all cases can not be analytically confirmed by the described methods alone. Further research is needed to confirm the proposed structures.

Similar biotransformations to those reported herein for fluorofuranylfentanyl have been reported elsewhere for furanylfentanyl[130] and tetrahydrofuranylfentanyl.[159] Similarly, both furanyl analogues of fentanyl readily metabolized to 4-ANPP. The prominent metabolites for both analogues were 4-ANPP (which causes the same issues and questions mentioned here) and furanyl-norfentanyl or tetrahydrofuranyl-norfentanyl.

6.3.3 2F-Deschloroketamine

2F-Deschloroketamine exhibited a protonated ion of 222.1290 Da at 4.18 minutes (Figure 120), with prominent fragment ions of 204.1178, 191.0861, 173.0758, 163.0908, 147.0599, 135.0598, 125.0393, 115.0537, 109.0436, and 67.0540 Da (Figure 121). For characterization and structural elucidation of metabolites, fragment ions 191.0861, 163.0908, and 109.0436 Da were used for diagnostic purposes. The 191.0861 Da fragment ion is produced by cleavage of the methyl amine group (Figure 122). Change (or no change) to this fragment ion would signify biotransformation external to the amine

(or on the amine). The 163.0908 Da fragment ion is produced by cleavage of the methyl amine group and the carbonyl out of the cyclohexyl ring (Figure 123). Change (or no change) to this fragment ion would also signify biotransformation external to the amine (or on the amine). The 109.0436 Da fragment ions is produced by cleavage of the fluoro phenyl ring (Figure 124). Change (or no change) to this fragment ion would signify biotransformation on the fluoro phenyl ring (or external to it).

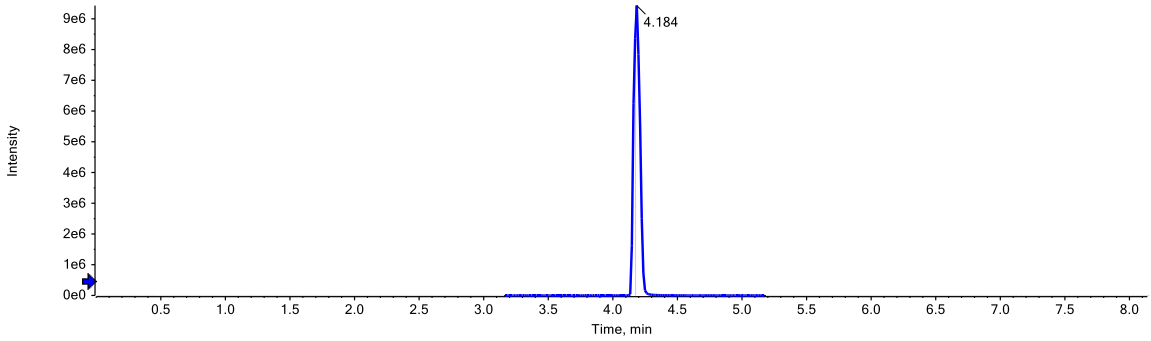

Figure 120: Extracted ion chromatogram of 2F-deschloroketamine

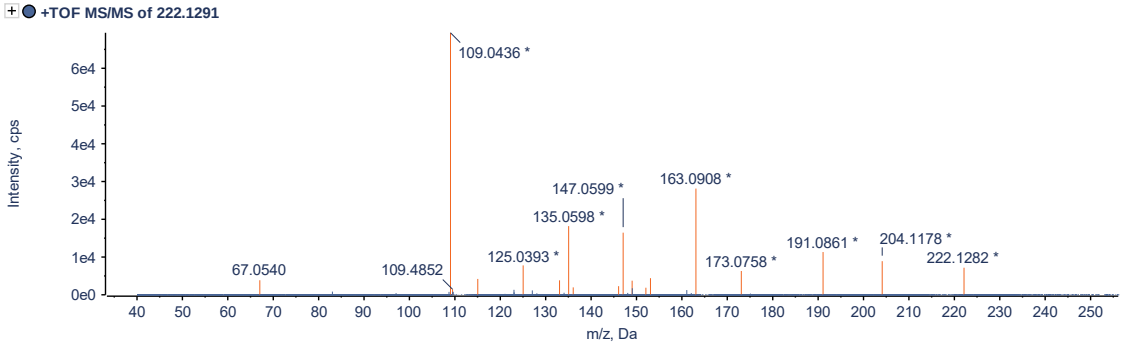

Figure 121: Fragment ion spectrum of 2F-deschloroketamine

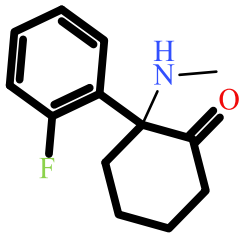

Figure 122: 2F-Deschloroketamine 191.0861 Da fragment ion (bold)

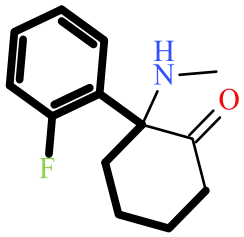

Figure 123: 2F-Deschloroketamine 163.0908 Da fragment ion (bold)

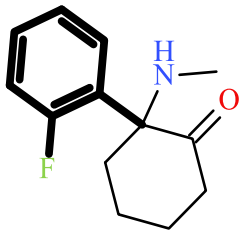

Figure 124: 2F-Deschloroketamine 109.0436 Da fragment ion (bold)

Nine metabolites of 2F-deschloroketamine were identified *in vitro* following LC-QTOF-MS analysis of the six HLM samples (Figure 125). Corresponding mass, formula, retention time, and fragment data can be found in Table 39.

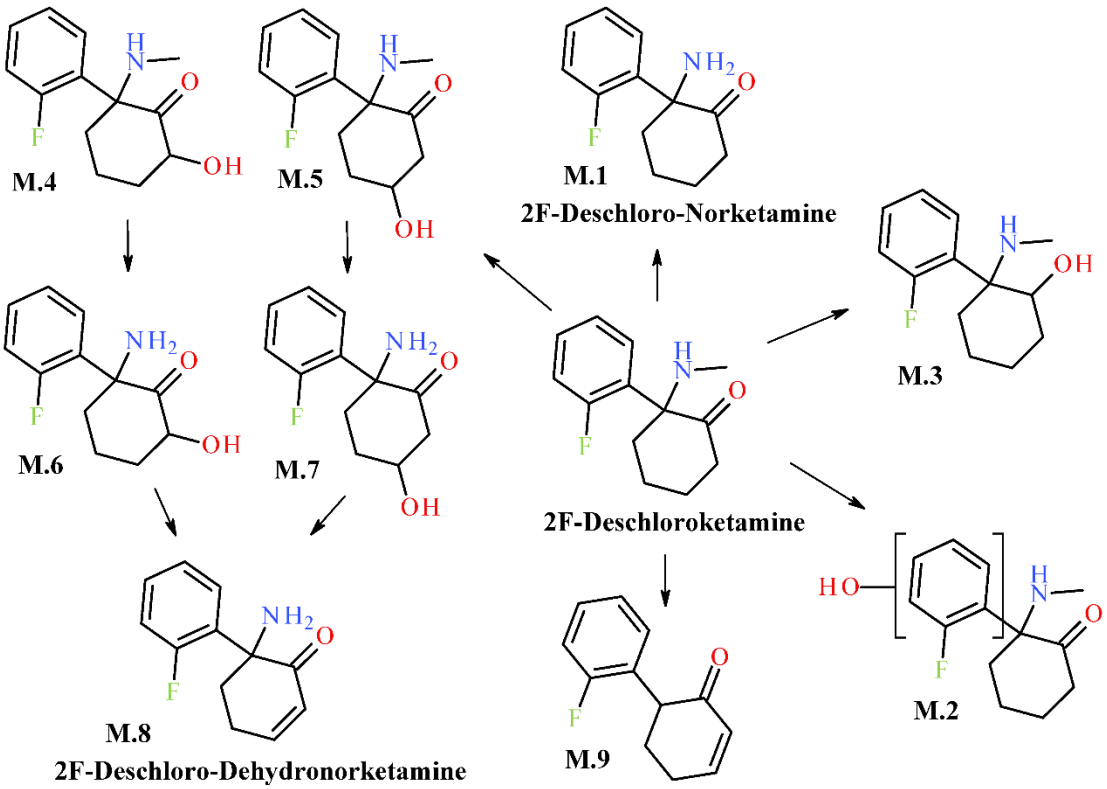

Figure 125: Metabolism scheme of 2F-deschloroketamine

Table 39: Metabolites of 2F-deschloroketamine generated *in vitro*

ID	Biotransformation	RT (min)	Formula	$[M+H]^+$	Error (ppm)	Product Ions
P.0	2F-Deschloroketamine	4.17	$C_{13}H_{16}FNO$	222.1290	0.5	191.0861 163.0908 109.0436
M.1	*N*-Demethylation [2F-Deschloro-Norketamine]	4.02	$C_{12}H_{14}FNO$	208.1132	0.1	191.0862 163.0910 109.0437
M.2	Hydroxylation (Fluorophenyl)	3.94	$C_{13}H_{16}FNO_2$	238.1239	0.5	207.0817 179.0867 125.0396
M.3	Hydrogenation	4.11	$C_{13}H_{18}FNO$	224.1444	-0.5	193.1023 175.0913 109.0444
M.4	Hydroxylation (6 Position, Cyclohexanone)	2.55	$C_{13}H_{16}FNO_2$	238.1239	0.3	179.0866 109.0446
M.5	Hydroxylation (5 Position, Cyclohexanone)	3.14	$C_{13}H_{16}FNO_2$	238.1238	-0.1	207.0818 161.0758 109.0445

M.6	*N*-Demethylation + Hydroxylation (6 Position, Cyclohexanone)	2.06	$C_{12}H_{14}FNO_2$	244.1081	-0.2	179.0868 109.0446
M.7	*N*-Demethylation + Hydroxylation (5 Position, Cyclohexanone)	2.90	$C_{12}H_{14}FNO_2$	224.1082	0.4	207.0817 161.0761 109.0449
M.8	*N*-Demethylation + Dehydrogenation [2F-Deschloro-Dehydronorketamine]	3.50	$C_{12}H_{12}FNO$	206.0976	0.0	189.0709 109.0444
M.9	Loss of CH_3N, Dehydrogenation	4.01	$C_{12}H_{11}FO$	191.0868	0.6	163.0914 109.0442

2F-Deschloroketamine was found to undergo *N*-demethylation of the amine to produce M.1 (Figure 125), or 2F-deschloro-norketamine. This metabolite exhibited a protonated ion of 208.1132 Da ($C_{12}H_{14}FNO$) at 4.02 minutes, accounting for the loss of one methyl group (Δ -CH_2). 2F-Deschloro-norketamine (M.1) exhibited fragment ions of 191.0862, 163.0910, and 109.0437 Da (Figure 126), the same fragment ions as parent 2F-deschloroketamine. This information verifies the *N*-demethylation on the amine vs. the amide.

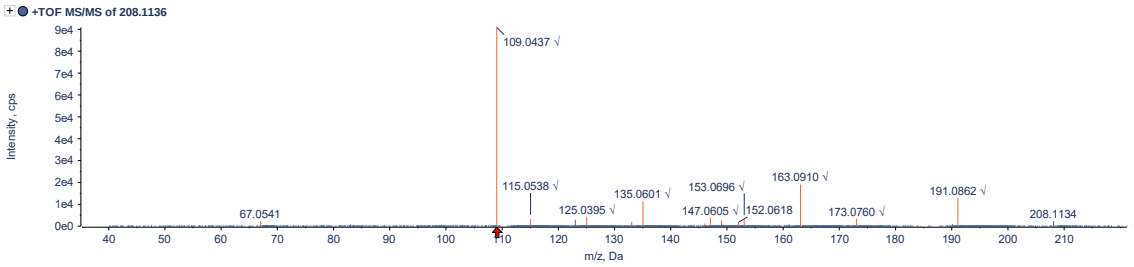

Figure 126: Fragment ion spectrum of 2F-deschloro-norketamine (M.1)

2F-Deschloroketamine was found to undergo hydroxylation of the fluoro phenyl to produce M.2 (Figure 125). This metabolite exhibited a protonated ion of 238.1239 Da

($C_{13}H_{16}FNO_2$) at 3.94 minutes, accounting for the addition of one oxygen (Δ +O). 2F-Deschloroketamine M.2 exhibited fragment ions of 207.0817, 179.0867, and 125.0396 Da (Figure 127). All three fragments are 16 mass units larger than the fragments of parent 2F-deschloroketamine. This information verifies the point of hydroxylation on the fluoro phenyl ring. The exact position can not be determined though the analyses performed. An extracted ion chromatogram shows multiple peaks for this metabolite (Figure 128).

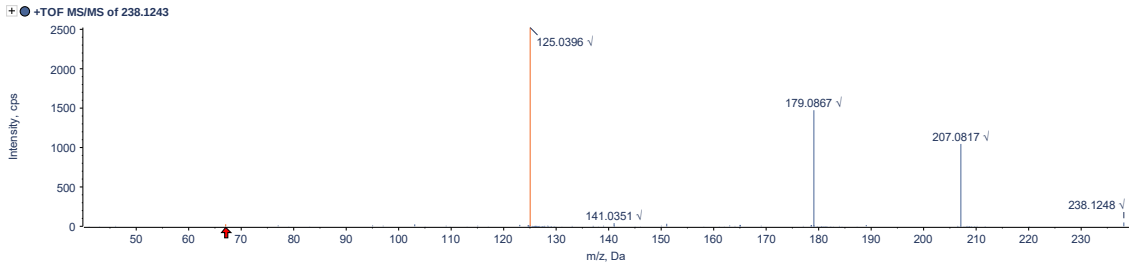

Figure 127: Fragment ion spectrum of 2F-deschloroketamine M.2

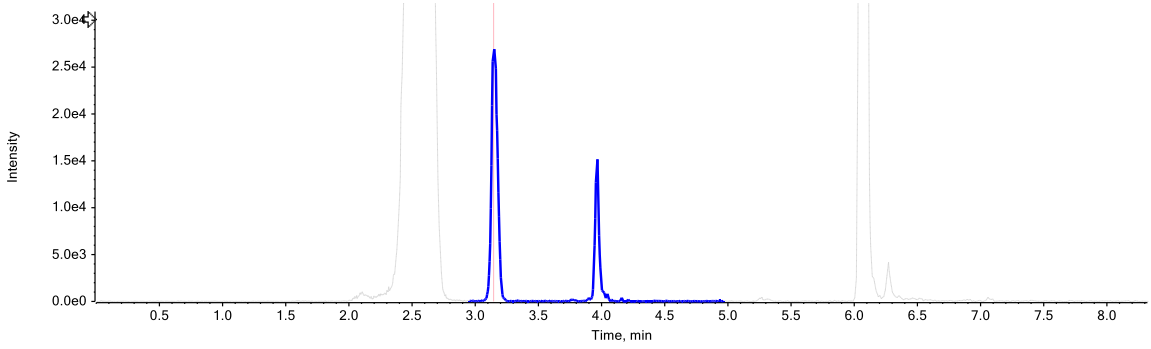

Figure 128: Extracted ion chromatogram of 2F-deschloroketamine M.2

2F-Deschloroketamine was found to undergo hydrogenation, or reduction of the ketone to an alcohol, to produce M.3 (Figure 125). This metabolite exhibited a protonated

ion of 224.1444 Da ($C_{13}H_{18}FNO$) at 4.11 minutes, accounting for the addition of two hydrogens ($\Delta +H_2$). 2F-Deschloroketamine M.3 exhibited fragment ions of 193.1023, 175.0913, and 109.0444 Da (Figure 129). These fragments differ from parent 2F-deschloroketamine, specifically the increase from the 191 fragment ion to 193 demonstrates the biotransformation of the ketone. Of important note, this mass does account for a metabolite and not the M+2 isotopic contribution of the parent compounds; the ion profile of this metabolite and the parent compound were distinct.

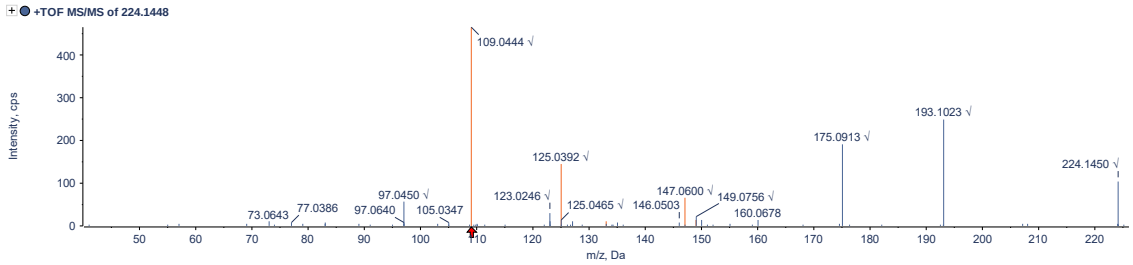

Figure 129: Fragment ion spectrum of 2F-deschloroketamine M.3

Additional hydroxylation of 2F-deschloroketamine produced M.4 at the 6-position and M.5 at the 5- position of the cyclohexyl ring (Figure 125). These metabolites exhibited protonated ions of 238.1239 and 238.1238 Da ($C_{13}H_{16}FNO_2$) at 2.55 and 3.14 minutes (Figure 130), respectively, accounting for the addition of one oxygen ($\Delta +O$). 2F-Deschloroketamine M.4 exhibited fragment ions of 179.0866 and 109.0446 (Figure 131), and 2F-deschloroketamine M.5 exhibited fragment ions of 207.0818, 179.0867, and 109.0445 (Figure 132). Increase of the 163 fragment ion to 179 and no change for the 109 fragment ion lead to positioning of these hydroxyl groups on the cyclohexyl ring. M.4

was hypothesized to be distinguishable as the 6- position due to the more abundant 179.0866 Da fragment ion and less abundant 161.0758 Da fragment ion (Figure 133); and, contrarily, M.5 was hypothesized to be the 5- position.

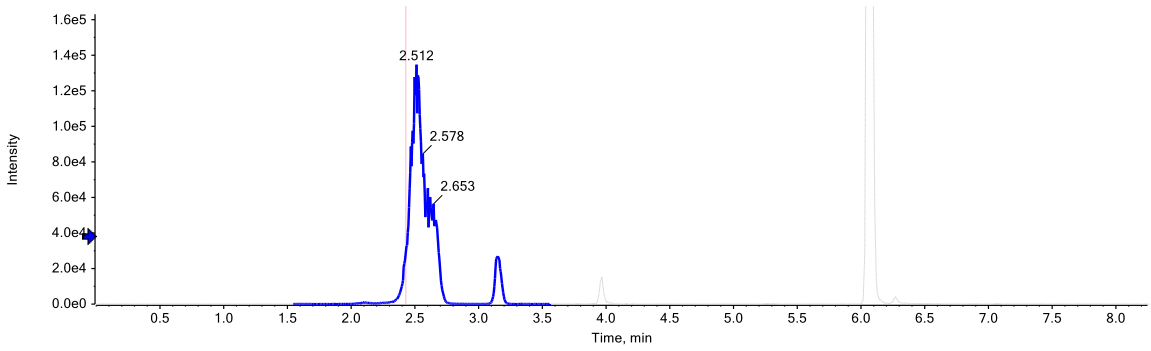

Figure 130: Extracted ion chromatogram of 2F-deschloroketamine M.4 and M.5

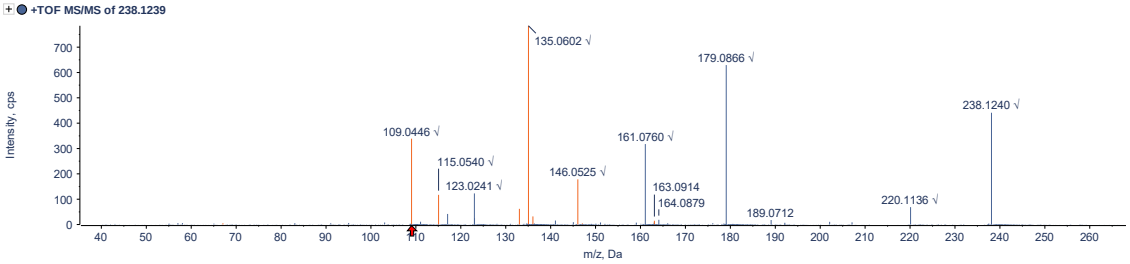

Figure 131: Fragment ion spectrum of 2F-deschloroketamine M.4

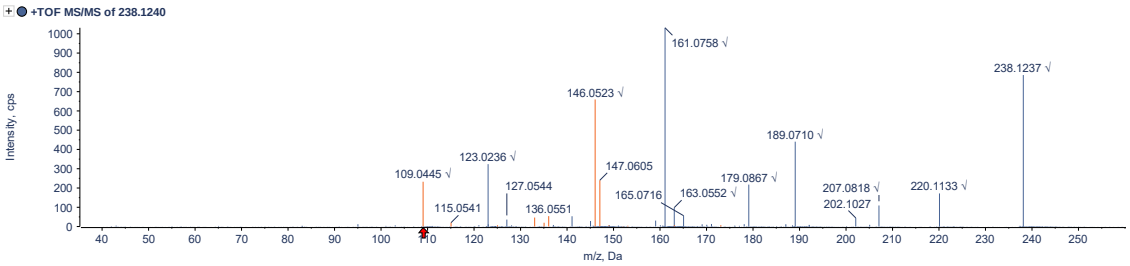

Figure 132: Fragment ion spectrum of 2F-deschloroketamine M.5

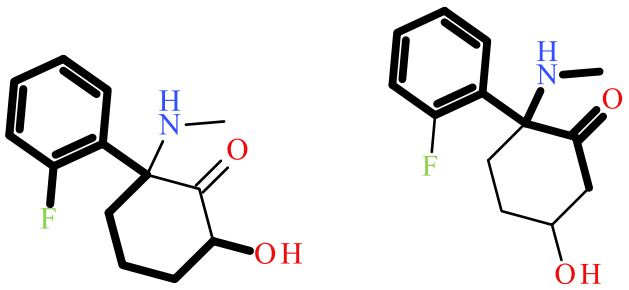

Figure 133: 2F-Deschloroketamine M.4 179.0866 Da (left) and M.5 161.0758 Da (right) fragment ions (bold)

2F-Deschloroketamine M.4 and M.5 were then found to undergo *N*-demethylation to produce M.6 and M.7 (Figure 125). These metabolites exhibited protonated ions of 244.1081 and 244.1082 Da ($C_{12}H_{14}FNO_2$) at 2.06 and 2.90 minutes (Figure 134), respectively, accounting for the addition of one oxygen and loss of one methyl group (Δ -CH_2 +O vs. parent). 2F-Deschloroketamine M.6 exhibited fragment ions of 179.0868 and 109.0446 (Figure 135), and 2F-deschloroketamine M.7 exhibited fragment ions of 207.0817, 179.0871, and 109.0449 (Figure 136). As with that above, M.6 was hypothesized to be distinguishable as the 6- position due to the more abundant 179.0868 Da fragment ion and less abundant 161.0761 Da fragment ion; and, contrarily, M.7 was hypothesized to be the 5- position.

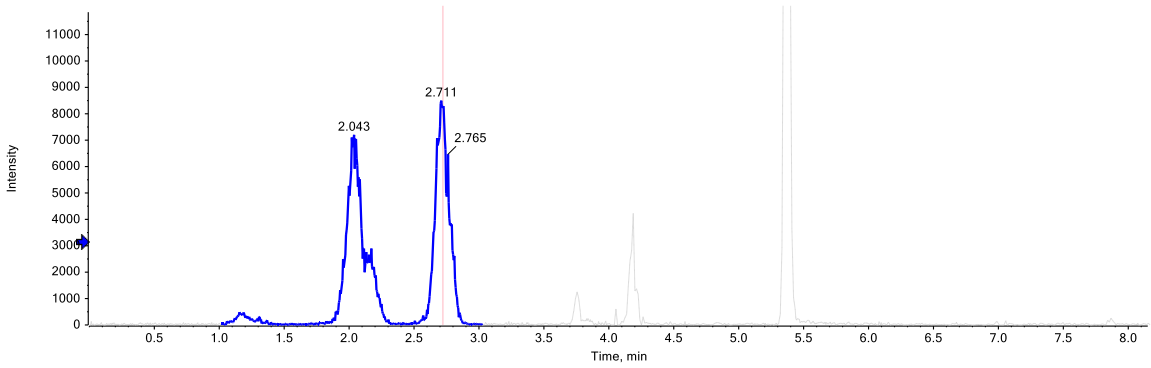

Figure 134: Extracted ion chromatogram of 2F-deschloroketamine M.6 and M.7

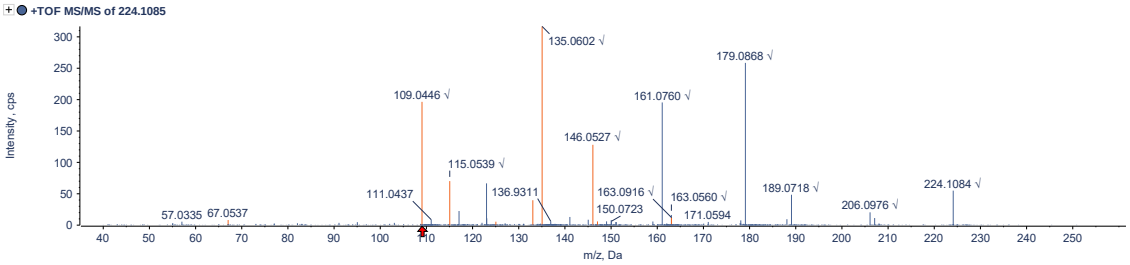

Figure 135: Fragment ion spectrum of 2F-deschloroketamine M.6

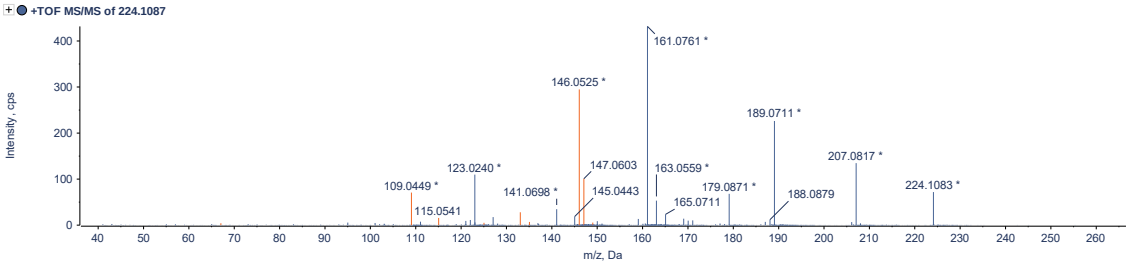

Figure 136: Fragment ion spectrum of 2F-deschloroketamine M.7

Stemming from 2F-deschloroketamine M.6 and M.7, biotransformation of 2F-deschloroketamine ultimately lead to combined *N*-demethylation and hydrogenation to produce M.8 (Figure 125), or 2F-deschloro-dehydronorketamine. This metabolite

exhibited a protonate ions of 206.0976 Da ($C_{12}H_{12}FNO$) at 3.50 minutes, accounting for the loss of one methyl group and two hydrogens (Δ -CH_4). 2F-Deschloro-dehydronorketamine (M.8) exhibited fragment ions of 189.0709 and 109.0444 (Figure 137), pointing to loss of the methyl on the amine, loss of two mass units to the cyclohexyl ring , and no change to the fluoro phenyl ring.

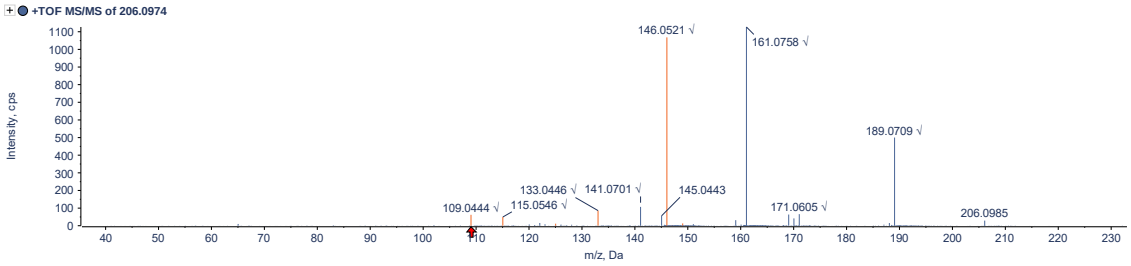

Figure 137: Fragment ion spectrum of 2F-deschloro-dehydronorketamine (M.8)

The final metabolite of 2F-deschloroketamine identified involved the loss of the secondary amine to produce M.9 (Figure 125). This metabolite exhibited a protonated ion of 191.0868 Da ($C_{12}H_{11}FO$) at 4.01 minutes, accounting for the loss of the amine and methyl group, as well as two hydrogens (Δ -CH_5N). 2F-Deschloroketamine M.9 exhibited fragment ions of 163.0914 and 109.0442 Da (Figure 138), the same fragment ions as 2F-deschloroketamine. The location of the double bond is unknown for this metabolite but hypothesized to be the same position as 2F-deschloro-dehydronorketamine (M.8).

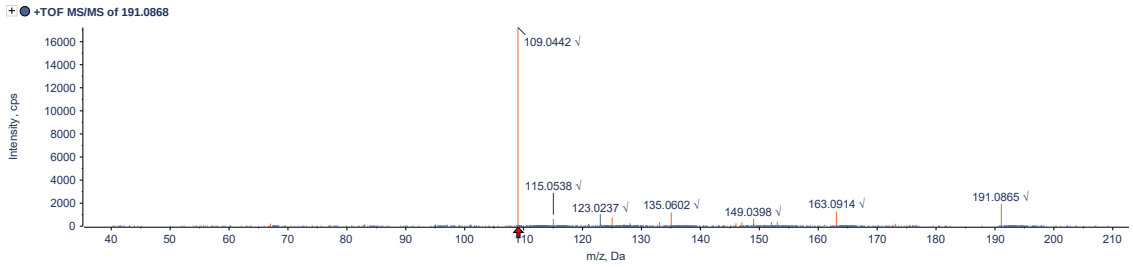

Figure 138: Fragment ion spectrum of 2F-deschloroketamine M.9

Following characterization of 2F-deschloroketamine metabolism *in vitro*, the nine metabolites identified were screened for *in vivo* (i.e. data mining) using biological sample extracts positive for parent 2F-deschloroketamine. In total, the datafiles from two extracts were processed for metabolites. Table 40 shows the results of parent compound and metabolites identified. Of the nine metabolites, only two were found *in vivo*; although this is not uncommon, as all metabolites identified *in vitro* may not manifest in authentic human specimens. 2F-Deschloro-norketamine (M.1) and 2F-deschloroketamine M.3 (hydrogenation) were the two metabolites identified.

Table 40: Metabolites of 2F-deschloroketamine observed *in vivo*

Sample	2F-Deschloroketamine	M.1 2F-Deschloro-Norketamine	M.3 Hydrogenation
1	RT: 4.31 Area: 405 *Parent Ratio: 100%*	ND	ND
2	RT: 4.32 Area: 31,124 *Parent Ratio: 100%*	RT: 4.16 Area: 3,310 *Parent Ratio: 10.6%*	RT: 4.25 Area: 5,869 *Parent Ratio: 18.9%*

Key: RT - retention time (in minutes), ND - None detected
Parent Ratio = (Parent area / Metabolite area) x 100

Reference material for 2F-deschloro-norketamine was available and purchased for comparison during this research, resulting in M.1 confirmation as 2F-deschloro-norketamine. Reference materials for all other metabolites identified were not available; therefore, exact structure in all cases can not be analytically confirmed by the described methods alone. Further research is needed to confirm the proposed structures. Nonetheless, two metabolites were found in human specimens.

The metabolism of ketamine has been well studied and documented.[139] The biotransformations of 2F-deschloroketamine characterized during this research are consistent with the metabolism of ketamine and transformation to norketamine and dehydronorketamine, specifically. Further analysis should be conducted on human urine specimens from individuals who ingested 2F-deschloroketamine to more accurately determine the most prominent metabolite(s); it is hypothesized that this metabolite will be 2F-deschloro-norketamine.

6.3.4 Eutylone

Eutylone exhibited a protonated ion of 236.1281 Da at 4.51 minutes (Figure 139), with prominent fragment ions of 218.1171, 189.0777, 188.1058, 174.0540, 161.0581, 149.0231, 135.0440, 105.0695, and 86.0962 Da (Figure 140). For characterization and structural elucidation of metabolites, fragment ions 188.1058, 149.0231, and 86.0962 Da were used for diagnostic purposes. The 188.1058 Da fragment ion is produced by cleavage of the 3,4-methylenedioxy group (Figure 141). Change (or no change) to this fragment ion would signify biotransformation external to (or within) this ringed feature.

The 149.0231 Da fragment ion is produced by cleavage adjacent to the *beta*-ketone (Figure 142). Change (or no change) to this fragment ion would signify biotransformation to the 3,4-methylenedioxy-benzyl group (or to the alkyl backbone or secondary amine). The 86.0962 Da fragment ion produced is the other half of the molecule from the 149.0231 Da fragment ion (Figure 143). Change (or no change) to this fragment ion would signify biotransformation similar to above.

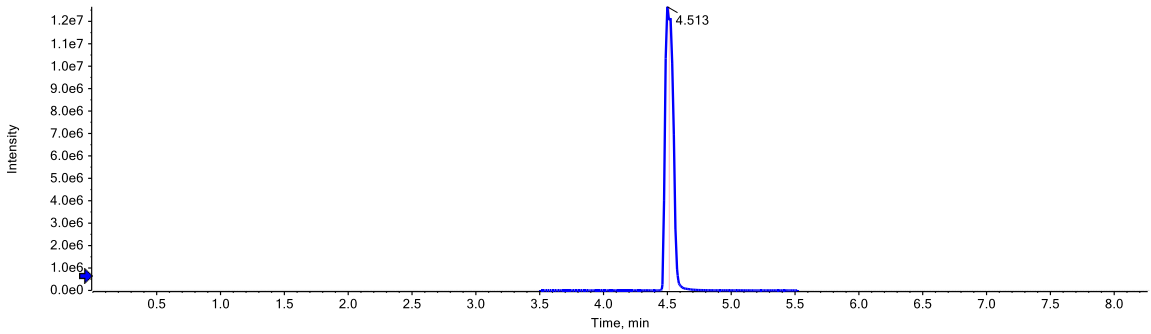

Figure 139: Extracted ion chromatogram of eutylone

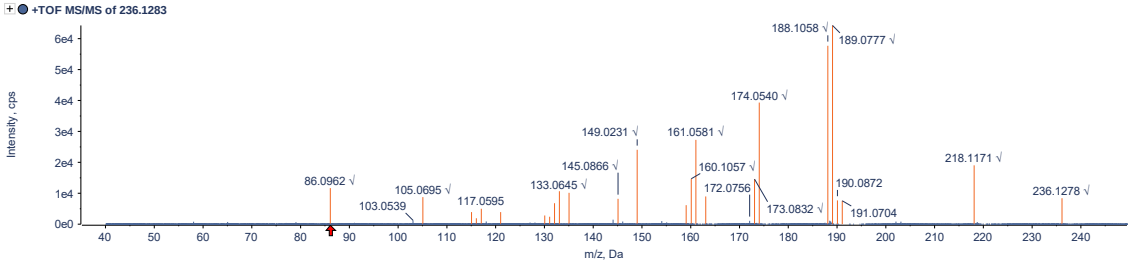

Figure 140: Fragment ion spectrum of eutylone

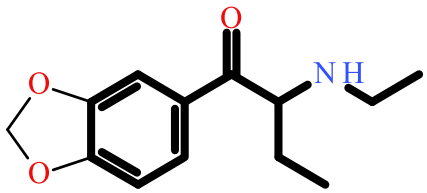

Figure 141: Eutylone 188.1058 Da fragment ions (bold)

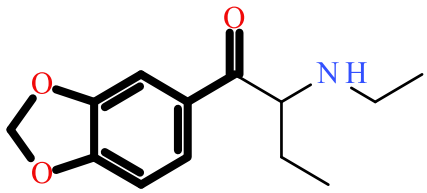

Figure 142: Eutylone 149.0231 Da fragment ion (bold)

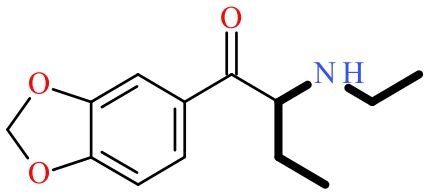

Figure 143: Eutylone 86.0962 Da fragment ion (bold)

Three metabolites of eutylone were identified *in vitro* following LC-QTOF-MS analysis of the six HLM samples (Figure 144). Corresponding mass, formula, retention time, and fragment data can be found in Table 41.

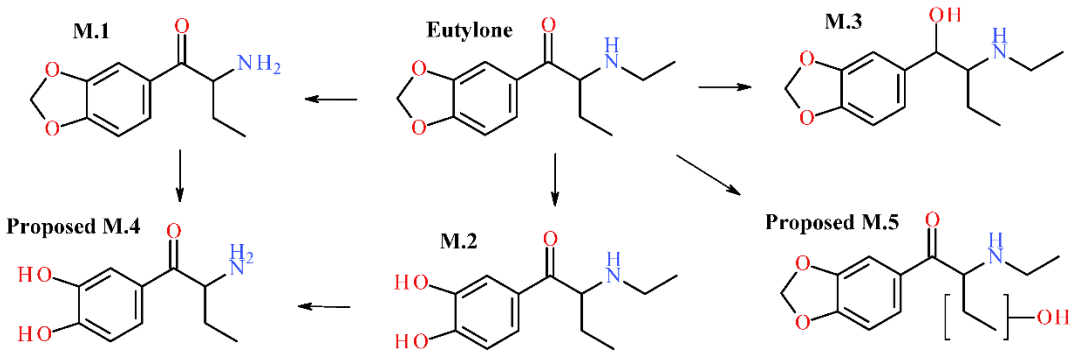

Figure 144: Metabolism scheme of eutylone

Table 41: Metabolites of eutylone generated *in vitro*

ID	Biotransformation	RT (min)	Formula	$[M+H]^+$	Error (ppm)	Product Ions
P.0	Eutylone	4.51	$C_{13}H_{17}NO_3$	236.1281	-0.1	188.1058 149.0231 86.0962
M.1	*N*-Deethylation	4.08	$C_{11}H_{13}NO_3$	208.0969	0.4	160.0756 149.0231 58.0651
M.2	Demethylenation	2.96	$C_{12}H_{17}NO_3$	224.1281	0.0	188.1069 137.0235 86.0699
M.3	Hydrogenation	4.34	$C_{13}H_{19}NO_3$	238.1438	0.1	220.1337 191.0939 135.0444

Eutylone was found to undergo *N*-deethylation of the amine to produce M.1 (Figure 144). This metabolite exhibited a protonated ion of 208.0969 Da ($C_{13}H_{17}NO_3$) at 4.08 minutes, accounting for the loss of the ethyl group (Δ -C_2H_4). Eutylone M.1 exhibited fragment ions of 160.0756, 149.0231, and 58.0651 Da (Figure 145). The 160 and 58 Da fragment ions are both 28 mass units smaller than the fragments of parent eutylone. This information verifies *N*-deethylation of the amine.

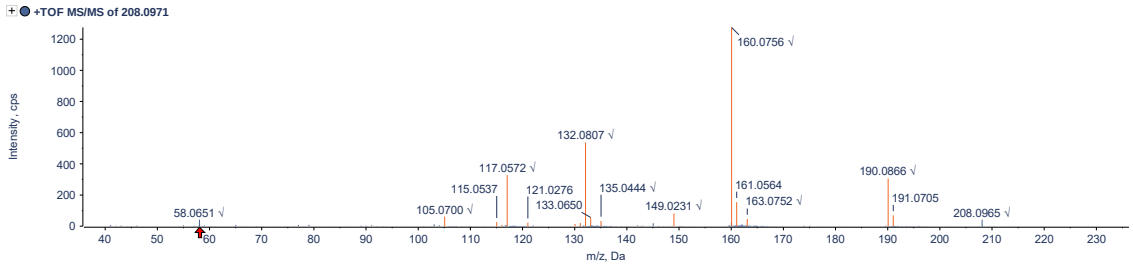

Figure 145: Fragment ion spectrum of eutylone M.1

Eutylone was found to undergo demethylenation to produce M.2 (Figure 144). This metabolite exhibited a protonated ion of 224.12811 Da ($C_{12}H_{17}NO_3$) at 2.96 minutes, accounting for the loss of one carbon (Δ -C). Eutylone M.2 exhibited fragment ions of 188.1069, 137.0235, and 86.0699 Da (Figure 146). The 137 Da fragment ion is 12 mass units smaller than the 149 fragment ion of parent eutylone. This information verifies the biotransformation as demethylenation.

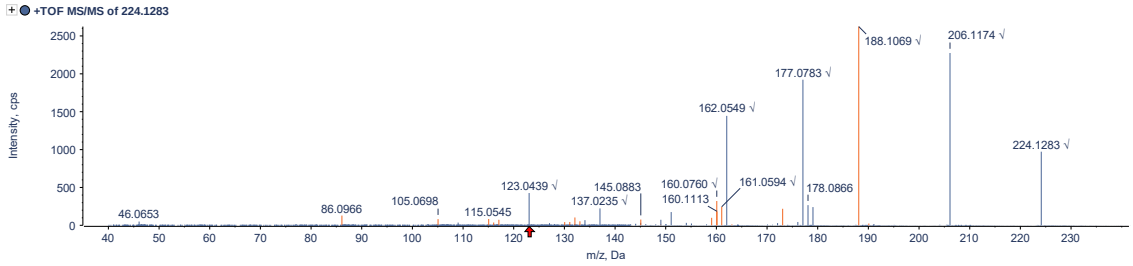

Figure 146: Fragment ion spectrum of eutylone M.2

Eutylone was found to undergo hydrogenation, reduction of the ketone to an alcohol, to produce M.3 (Figure 144). This metabolite exhibited a protonated ion of 238.1438 Da ($C_{13}H_{19}NO_3$) at 4.34 minutes, accounting for the addition of two hydrogens

(Δ +H_2). Eutylone M.3 exhibited fragment ions of 220.1337, 191.0939, and 135.0444 Da (Figure 147), all different from the parent eutylone, which is consistent with the proposed biotransformation.

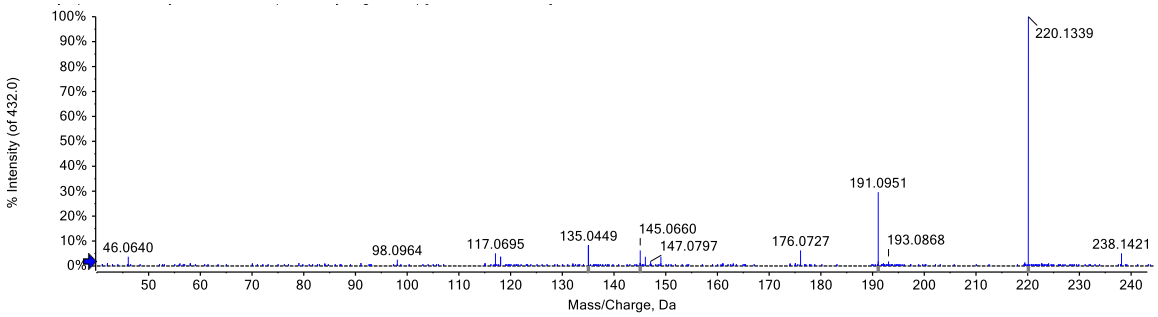

Figure 147: Fragment ion spectrum of eutylone M.3

Since only three metabolites of eutylone were identified using MetabolitePilot™, proposed metabolites from a combination of the previously described biotransformations, or other expected metabolites, were formulated and searched for in the datafiles. The first metabolite included *N*-deethylation and demethylenation of eutylone to produce proposed M.4 (Figure 144) with the formula $C_{10}H_{13}NO_3$. It was expected that this metabolite would have fragment ions of 160, 137, and 58. The second metabolite included hydroxylation eutylone on the alkyl backbone to produce proposed M.5 (Figure 144) with the formula $C_{13}H_{17}NO_4$. It was expected that this metabolite would have fragment ions of 204, 149, and 102. Neither of these metabolites were identified in HLM samples or extracts positive for eutylone; however, they should be considered when testing human urine samples in the future.

Following characterization of eutylone metabolism *in vitro*, the three metabolites identified (and two proposed) were screened for *in vivo* (i.e. data mining) using biological sample extracts positive for parent eutylone. In total, the datafiles from nine extracts were determined suitable to processing of metabolites. Table 42 shows the results of parent compound and metabolites identified. Of the five total metabolites, only the three found *in vitro* were also found *in vivo*. Eutylone M.3 (hydrogenation) appears to be the most prominent metabolite and an appropriate biomarker for monitoring eutylone ingestion.

Table 42: Metabolites of eutylone observed *in vivo*

Sample	Eutylone	M.1 *N*-Deethylation	M.2 Demethylenation	M.3 Hydrogenation
1	RT: 4.66 Area: 118,714 *Parent Ratio: 100%*	RT: 4.20 Area: 1,057 *Parent Ratio: 0.9%*	RT: 3.01 Area: 482 *Parent Ratio: 0.4%*	RT: 4.47 Area: 2,640 *Parent Ratio: 2.2%*
2	RT: 4.58 Area: 15,079 *Parent Ratio: 100%*	RT: 4.10 Area: 121 *Parent Ratio: 0.8%*	ND	ND
3	RT: 4.52 Area: 331,382 *Parent Ratio: 100%*	ND	ND	RT: 4.33 Area: 1,868 *Parent Ratio: 0.6%*
4	RT: 4.54 Area: 6,833 *Parent Ratio: 100%*	ND	ND	ND
5	RT: 4.53 Area: 6,349 *Parent Ratio: 100%*	RT: 4.09 Area: 79 *Parent Ratio: 1.2%*	ND	ND
6	RT: 4.34 Area: 7,647 *Parent Ratio: 100%*	ND	ND	ND
7	RT: 4.36 Area: 6,878 *Parent Ratio: 100%*	ND	ND	ND
8	RT: 4.39 Area: 1,537 *Parent Ratio: 100%*	ND	ND	ND
9	RT: 4.53 Area: 1,150 *Parent Ratio: 100%*	ND	ND	ND

Key: RT - retention time (in minutes), ND - None detected
Parent Ratio = (Parent area / Metabolite area) x 100

Reference material was not available for any metabolites of eutylone; therefore, exact structure in all cases can not be analytically confirmed by the described methods alone. Further research is needed to confirm the proposed structures. Nonetheless, all three metabolites were found in human specimens.

Similar biotransformations to those reported herein for eutylone have been reported elsewhere for butylone,[160] dibutylone,[158] and *N*-ethyl pentylone.[142] Most notably, these publications show dealkylated and hydrogenated metabolites. For all, the most prominent metabolite was the dealkylated metabolite, but the hydrogenated metabolite was abundantly identified. Importantly for the metabolism of eutylone, eutylone M.1 is a common, isobaric metabolite with *N*-desmethyl butylone and *N,N*-didesmethyl dibutylone. This means that the identification of this metabolite alone would not allow for determination of parent drug ingested. The hydrogenated metabolite of all three analytes though is unique and therefore serves as a more appropriate biomarker.

6.3.5 N-Ethyl Hexedrone

N-Ethyl hexedrone exhibited a protonated ion of 220.1696 Da at 5.78 minutes (Figure 148), with prominent fragment ions 202.1580, 174.1270, 158.0958, 146.0652, 130.0639, 118.0639, 105.0329, and 91.0532 Da (Figure 149). For characterization and structural elucidation of metabolites, fragment ions 174.1270, 146.0652, and 105.0329 Da were used for diagnostic purposes. The 174.1270 Da fragment ion is produced by cleavage of the *beta*-ketone and ethyl group on the amine (Figure 150). Change (or no

change) to this fragment ion would signify biotransformation on the phenyl ring or alkyl backbone (or to the *beta*-ketone or on the *N*-ethyl group). The 146.0652 Da fragment ion is produced by cleavage of the *beta*-ketone and alkyl backbone (Figure 151). Change (or no change) to this fragment ion would signify biotransformation to the phenyl ring or *N*-ethyl group (or to the *beta*-ketone or on the alkyl backbone). The 105.0329 Da fragment ion produced is by cleavage adjacent to the *beta*-ketone (Figure 152). Change (or no change) to this fragment ion would signify biotransformation to the phenyl ring or *beta*-ketone (or external to this region of the molecule). The 91.0532 Da fragment was further used for differentiation of biotransformation on the phenyl ring vs. to the *beta*-ketone.

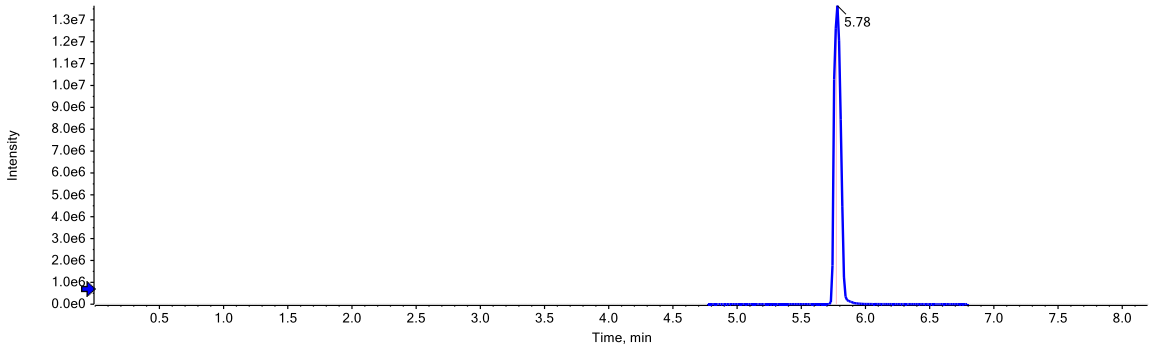

Figure 148: Extracted ion chromatogram of *N*-ethyl hexedrone

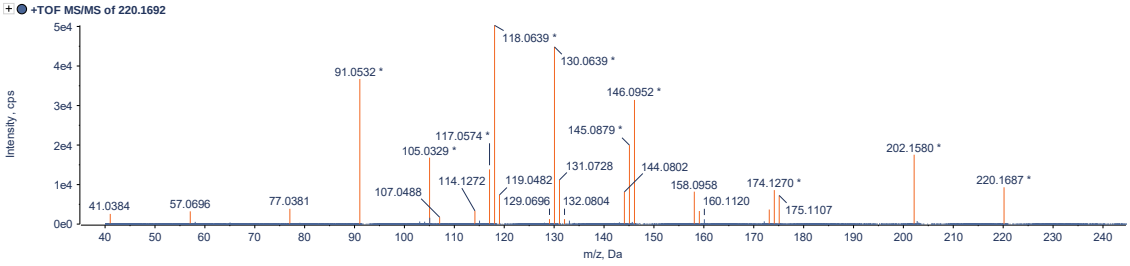

Figure 149: Fragment ion spectrum of *N*-ethyl hexedrone

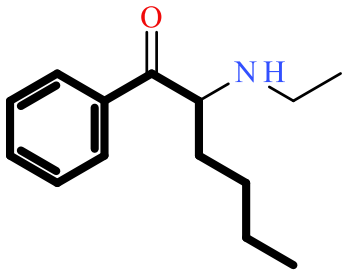

Figure 150: *N*-Ethyl hexedrone 174.1270 Da fragment ion (bold)

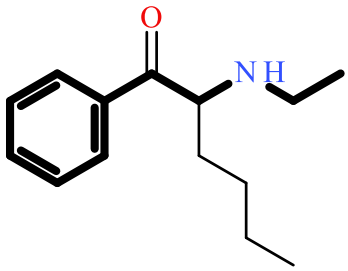

Figure 151: *N*-Ethyl hexedrone 146.0652 Da fragment ion (bold)

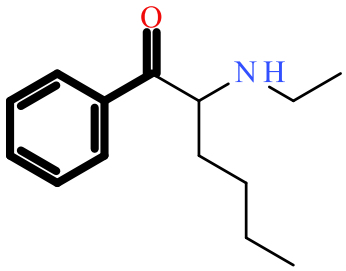

Figure 152: *N*-Ethyl hexedrone 105.0329 Da fragment ion (bold)

Five metabolites of eutylone were identified *in vitro* following LC-QTOF-MS analysis of the six HLM samples (Figure 153). Corresponding mass, formula, retention time, and fragment data can be found in Table 43.

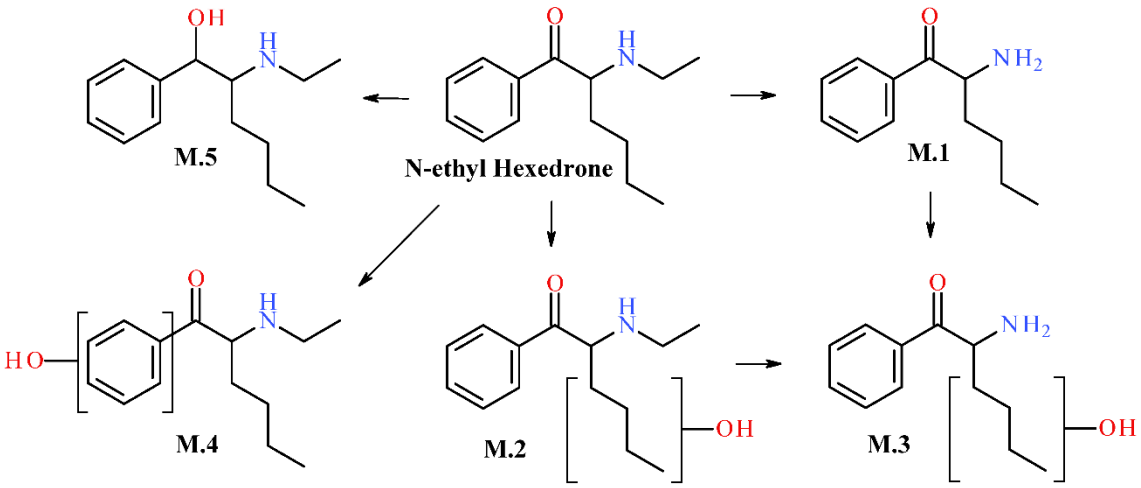

Figure 153: Metabolism scheme of *N*-ethyl hexedrone

Table 43: Metabolites of *N*-ethyl hexedrone generated *in vitro*

ID	Biotransformation	RT (min)	Formula	$[M+H]^+$	Error (ppm)	Product Ions
P.0	*N*-ethyl Hexedrone	5.78	$C_{14}H_{21}NO$	220.1696	0.0	174.1270 146.0652 105.0329
M.1	*N*-Deethylation	5.51	$C_{12}H_{17}NO$	192.1383	-0.1	174.1270 105.0333
M.2	Hydroxylation* (Alkyl)	4.12	$C_{14}H_{21}NO_2$	236.1645	-0.1	200.1433 158.0959 117.0692 105.0333
M.3	*N*-Deethylation + Hydroxylation (Alkyl)	3.72	$C_{12}H_{17}NO_2$	208.1332	0	190.1223 117.0691 105.0328
M.4	Hydroxylation* (Benzyl)	5.04	$C_{14}H_{21}NO_2$	236.1643	-0.8	191.1057 161.0830 121.0287
M.5	Hydrogenation	5.98	$C_{14}H_{23}NO$	222.1853	0.2	204.1741 91.0539

**Multiple peaks identified due to multiple points of hydroxylation. Earliest in retention time reported.*

N-Ethyl hexedrone was found to undergo *N*-deethylation of the amine to produce M.1 (Figure 153). This metabolite exhibited a protonated ion of 192.1383 Da ($C_{13}H_{17}NO_3$) at 5.51 minutes, accounting for the loss of the ethyl group (Δ -C_2H_4). *N*-Ethyl hexedrone M.1 exhibited fragment ions of 174.1270 and 105.0333 Da (Figure 154), the same as parent *N*-ethyl hexedrone, verifying *N*-deethylation on the amine.

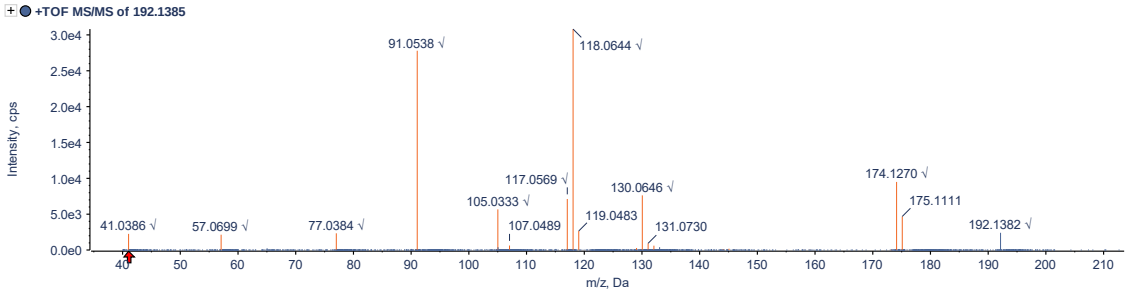

Figure 154: Fragment ion spectrum of *N*-ethyl hexedrone M.1

N-Ethyl hexedrone was found to undergo hydroxylation on the alkyl backbone to produce M.2 (Figure 153). This metabolite exhibited a protonated ion of 236.1645 Da ($C_{14}H_{21}NO_2$) at 4.12 minutes, accounting for the addition of one oxygen (Δ +O). *N*-Ethyl hexedrone M.2 exhibited fragment ions of 200.1433, 158.0959, 117.0692, and 105.0333 Da (Figure 155). The 200 Da fragment ion is 16 mass units larger than the 174 fragment ion of parent *N*-ethyl hexedrone; the 105 fragment ion remains unchanged. This information verifies the biotransformation as hydroxylation on the alkyl backbone; however, the analysis performed could not differentiate the exact site of hydroxylation on the six carbon backbone.

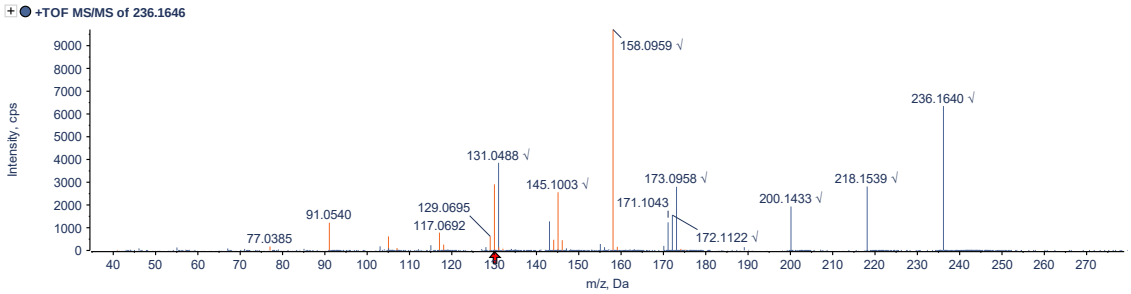

Figure 155: Fragment ion spectrum of *N*-ethyl hexedrone M.2

Combining M.1 and M.2, *N*-ethyl hexedrone was found to undergo *N*-deethylation and hydroxylation to produce M.3 (Figure 153). This metabolite exhibited a protonated ion of 208.1332 Da ($C_{12}H_{17}NO_2$) at 3.72 minutes, accounting for the loss of an ethyl and the addition of one oxygen (Δ -C_2H_4 +O). *N*-Ethyl hexedrone M.3 exhibited fragment ions of 190.1223, 117.0691, and 105.0328 Da (Figure 156). Most notably, the 105 fragmentation remained unchanged, demonstrating the hydroxylation occurred on the alkyl backbone.

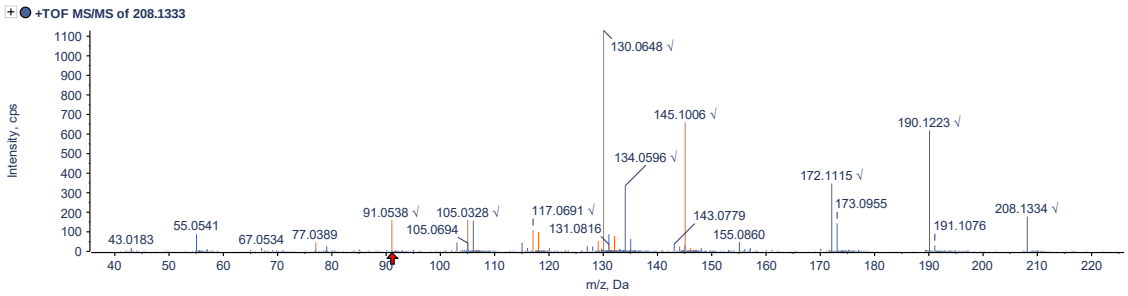

Figure 156: Fragment ion spectrum of *N*-ethyl hexedrone M.3

Additional hydroxylated metabolites of *N*-ethyl hexedrone was identified during evaluation of incubation extracts, occurring on the phenyl ring to produce M.4 (Figure 153); the sites of metabolism could not be distinguished. This metabolite exhibited a protonated ion of 236.1643 Da ($C_{14}H_{21}NO_2$) at 5.04 minutes, accounting for the addition of one oxygen (Δ +O). *N*-Ethyl hexedrone M.4 exhibited fragment ions of 191.1057, 161.0830, and 121.0287 Da (Figure 157); the 121 Da fragment ion is 16 mass units larger than the 105 fragment ion of parent *N*-ethyl hexedrone. This information verifies the biotransformation as hydroxylation on the phenyl ring. Including those of *N*-ethyl hexedrone M.2, several hydroxylated species were found during this research (Figure 158), and the only differentiation available was that of biotransformation on the alkyl backbone vs. phenyl ring.

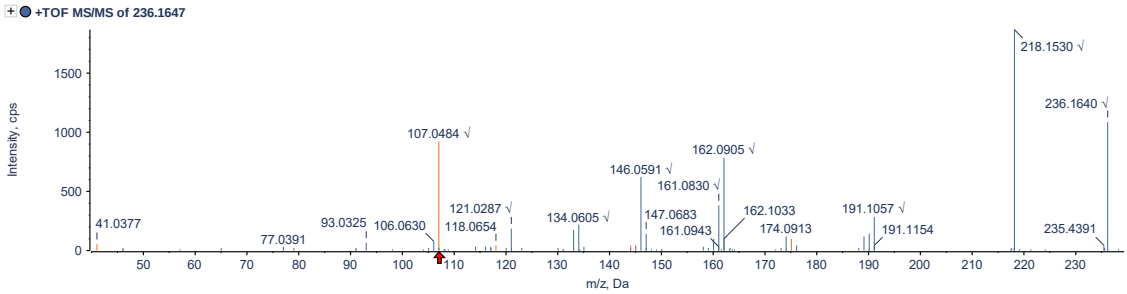

Figure 157: Fragment ion spectrum of *N*-ethyl hexedrone M.4

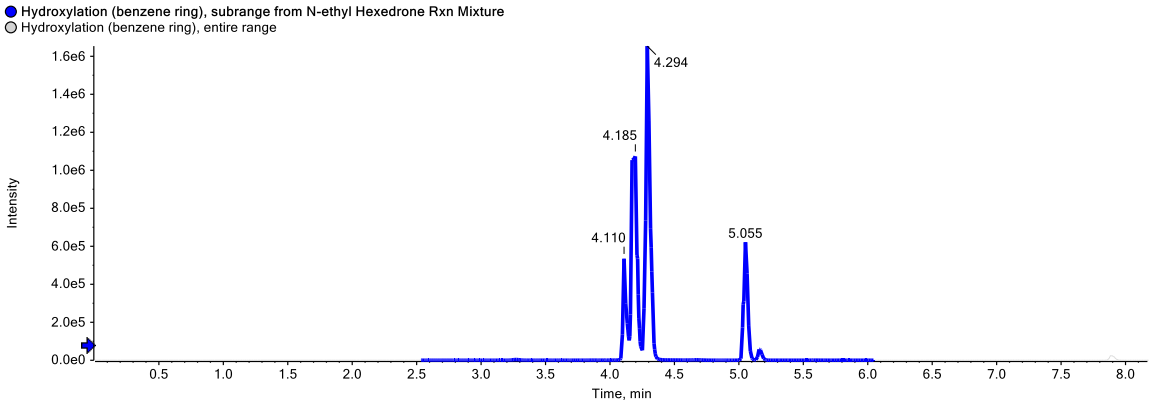

Figure 158: Extracted ion chromatogram of *N*-ethyl hexedrone M.2/M.4

The final metabolite of *N*-ethyl hexedrone involved hydrogenation, or reduction of the ketone to an alcohol, to produce M.5 (Figure 153). This metabolite exhibited a protonated ion of 222.1853 Da ($C_{14}H_{23}NO$) at 4.34 minutes, accounting for the addition of two hydrogens (Δ +H_2). *N*-Ethyl hexedrone M.5 exhibited fragment ions of 204.1741 and 91.0539 Da (Figure 159). The 204 fragment ion accounts for the loss of water, or fragmentation of the hydroxyl group. Arguably, this was the most unique metabolite of *N*-ethyl hexedrone identified, similar in scenario to that of eutylone.

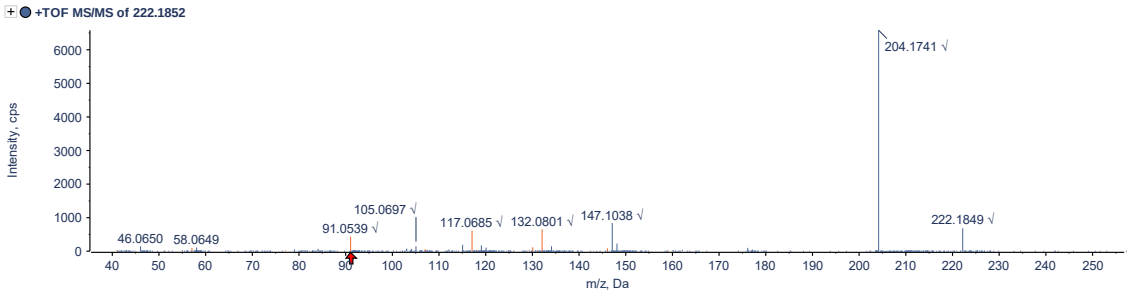

Figure 159: Fragment ion spectrum of *N*-ethyl hexedrone M.5

Following characterization of *N*-ethyl hexedrone metabolism *in vitro*, the five metabolites identified were screened for *in vivo* (i.e. data mining) using biological sample extracts positive for parent *N*-ethyl hexedrone. In total, the datafiles from three extracts were determined suitable to processing of metabolites. Table 44 shows the results of parent compound and metabolites identified. Of the five metabolites, only one was found *in vivo*, in only one sample. While, *N*-ethyl hexedrone M.5 (hydrogenation) appears to be the most prominent metabolite and an appropriate biomarker for monitoring *N*-ethyl hexedrone ingestion, further analysis of additional human samples should be conducted.

Table 44: Metabolites of *N*-ethyl hexedrone observed *in vivo*

Sample	*N*-ethyl Hexedrone	M.5 Hydrogenation
1	RT: 5.80 Area: 2,547 *Parent Ratio: 100%*	ND
2	RT: 5.92 Area: 4,030 *Parent Ratio: 100%*	ND
3	RT: 5.82 Area: 1,498 *Parent Ratio: 100%*	RT: 6.02 Area: 1,190 *Parent Ratio: 79.4%*

Key: RT - retention time (in minutes), ND - None detected, Parent Ratio = (Parent area / Metabolite area) x 100

Reference material was not available for any metabolites of *N*-ethyl hexedrone; therefore, exact structure in all cases can not be analytical confirmed by the described methods alone. Further research is needed to confirm the proposed structures. Nonetheless, all three metabolites were found in human specimens.

6.3.5 Additional Data Mining for Metabolites

Data mining was conducted using MasterView™ on datafiles from all 3,543 extracts for all metabolites identified during HLM incubations. This included datafiles that were not positive for a parent NPS compound in the library database. Positive identifications were filtered using the same criteria as presented above in Chapter 4. All results were manually reviewed by the analysts to determine accuracy of reported metabolites, with specific emphasis the criteria for peak area and peak shape. Overall, only one additional metabolite other than those reported above were detected; however, an interesting phenomenon were discovered. Low positivity was not unexpected, as the majority of extracts correlate to blood specimens (rather than urine specimens which would be more likely to produce metabolites in the absence of parent compounds).

The hydrogenated metabolite of *N*-ethyl hexedrone (M.5) was detected in an extract without the presence of *N*-ethyl hexedrone. This is of great interest due to the uniqueness of this metabolite in relation to *N*-ethyl hexedrone (i.e. this metabolite likely does not come from another NPS). The data for this identification is shown in Figures 160-162. The accurate mass of the metabolite was 222.1853 Da, with a resulting ppm error of 0.4 ($C_{14}H_{23}NO$; exact mass: 222.1852). The retention time of the metabolite was 6.07, with a resulting retention time difference of 0.09 mins (expected retention time: 5.98 mins). The fragment spectrum (Figure 162) matched that acquired during the HLM study (Figure 159), with prominent fragments of 204.1752 and 91.0523 Da (expected fragments: 204.1741 and 91.0539 Da). The peak area of this identification was 5,869. As previously mentioned, *N*-ethyl hexedrone was not present in this sample (Figure 163).

Other positives findings included fentanyl, flubromazelam, delorazepam, xylazine and lidocaine; no other substance was hypothesized to produce this metabolite.

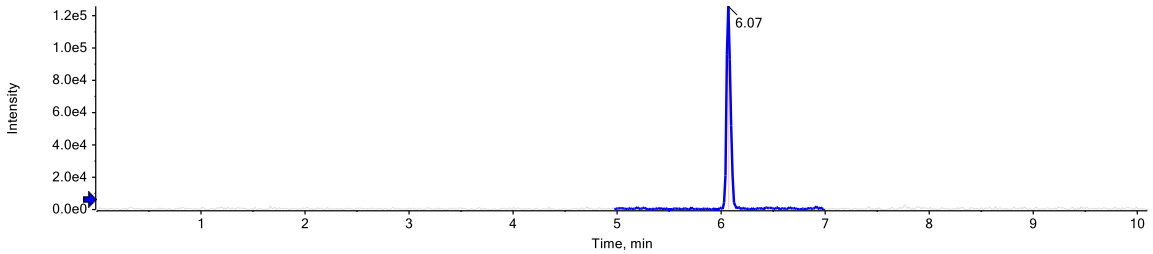

Figure 160: Chromatogram of *N*-ethyl hexedrone M.5 in sample extract

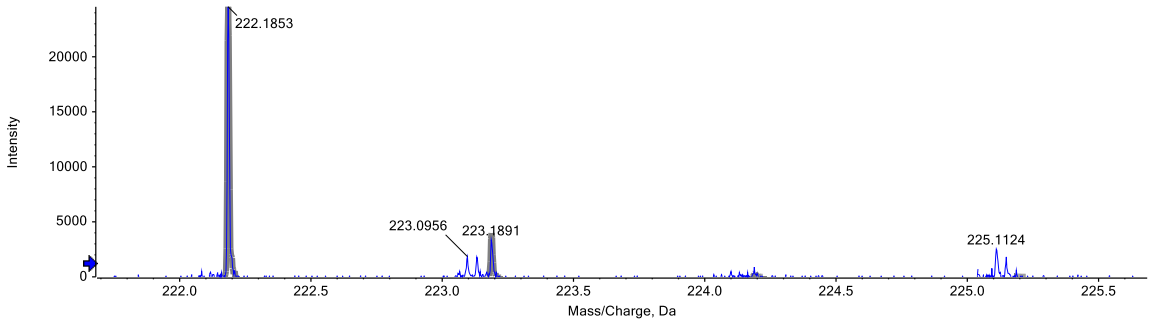

Figure 161: TOF MS spectrum of *N*-ethyl hexedrone M.5 in sample extract

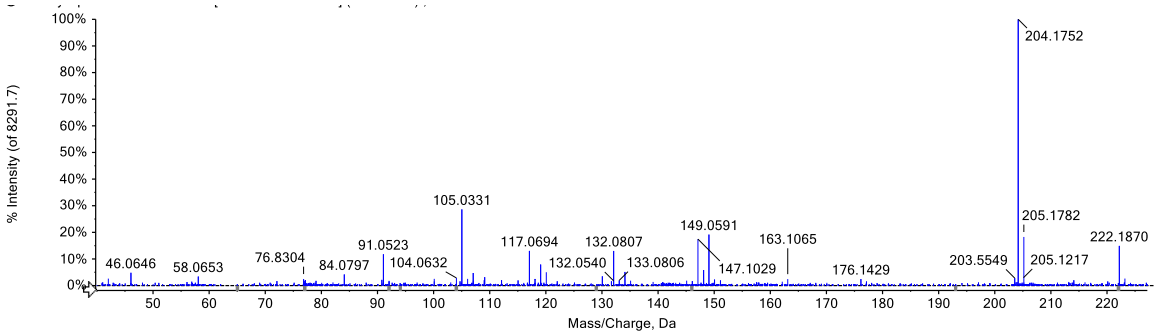

Figure 162: MSMS fragment spectrum of *N*-ethyl hexedrone M.5 in sample extract

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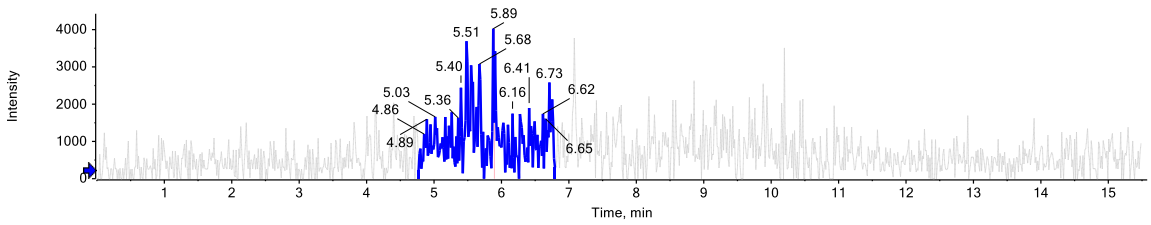

Figure 163: Chromatogram of *N*-ethyl hexedrone in sample extract

One unexpected finding during this data mining was the indistinguishable nature of eutylone M.3 (hydrogenation) and a similar hydrogenated metabolite of dibutylone. This metabolite was found in combination with dibutylone. Dibutylone (*N,N*-dimethyl) is a positional isomer of eutylone (*N*-ethyl), but their MSMS fragment spectra are distinguishable. Figure 164 shows the structure of both parent compounds and metabolites. Figure 165 shows the MSMS fragment spectrum of dibutylone in comparison to eutylone. Figure 166 shows the MSMS fragment spectrum of the dibutylone metabolite; the dibutylone metabolite spectrum is identical to that presented above from eutylone M.3 (Figure 147). This finding is significant due to the inability to determine the parent compounds (eutylone vs. dibutylone) based on MSMS spectra of the metabolite alone. Similarly, retention time is not a distinguishing feature (4.34 mins for eutylone M.3 vs. 4.22 for the dibutylone metabolite). Incorporation of other metabolites would need to be used to determine ingestion of eutylone vs. ingestion of dibutylone, in the absence of the parent compound.

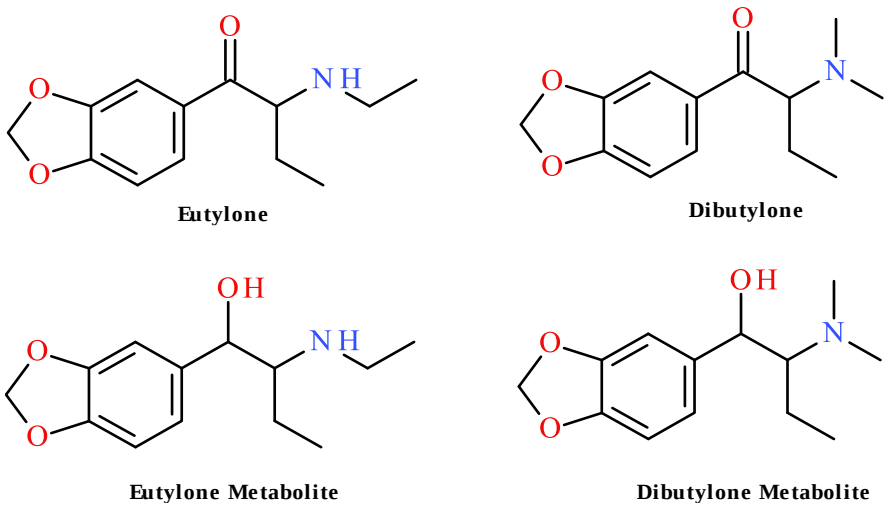

Figure 164: Structures of eutylone, dibutylone, and their hydrogenated metabolites

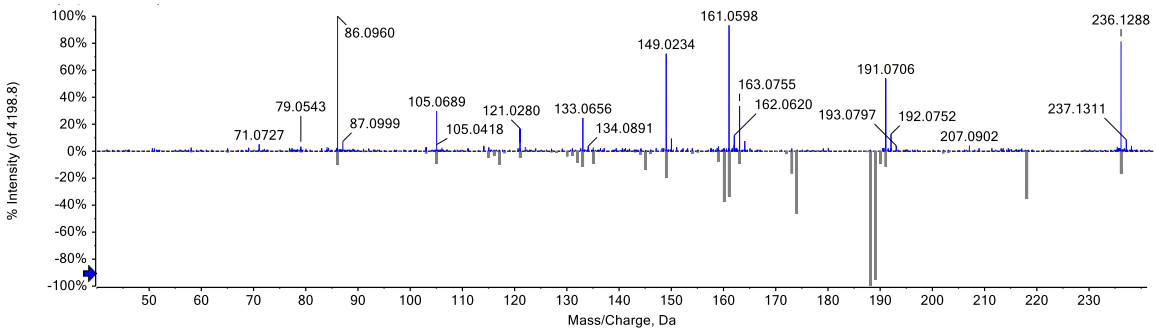

Figure 165: MSMS fragment spectrum of dibutylone in the extract (top) and the library spectrum for eutylone (bottom)

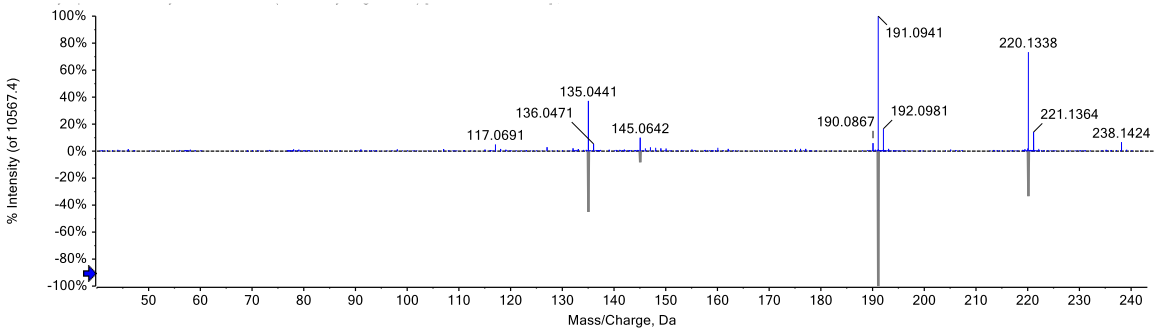

Figure 166: MSMS fragment spectrum of dibutylone hydrogenated metabolite in the extract (top) and the library spectrum for this metabolite (bottom)

6.4 Conclusion

Based on the results presented above, the developed workflow for characterization of metabolites *in vitro* and identification of metabolites *in vivo* proved to be a valuable approach, specifically in terms of conducting timely experiments and reporting. Characterization of metabolites *in vitro* resulted in the discovery of several more metabolites than those identified *in vivo*, in almost all cases, demonstrating the need for testing of human biological specimens collected after toxicologically confirmed cases of ingestion. All metabolites identified *in vitro* may not be identified *in vivo* (especially when using microsomes) or be useful for testing *in vivo* (i.e. uniqueness to parent). At least one unique metabolite, meaning those that are the results of distinguishable source, was identified for all five NPS studied; however, a unique metabolite was not always the most prominent metabolite. In the future, laboratories should consider this approach for rapid analysis of emergent NPS to discover metabolites or important biomarkers of recent drug use.

CHAPTER 7

CONCLUSIONS

The primary objective of this research was to develop a more timely process for individual identification and trend analysis of emerging NPS in the United States through analysis of authentic human biological specimens. NPS represent one of the most challenging classes of abused drugs due to their evolving and ever-changing nature. Despite the fact that NPS continue to be implicated in a large number of deaths nationally (e.g. opioid epidemic), NPS continue to emerge on a cycling basis, often creating increased threats to public health and public safety due to higher potency and toxicity. This dissertation focused on multiple aspects related to the identification of NPS and characterization of the current states of synthetic drug use and markets. First, a novel approach to drug detection was created using sample mining and data mining. A novel LC-QTOF-MS assay was developed and validated for the purposes of broad-based drug detection. Second, this assay was applied to the analysis of sample extracts from a large forensic toxicology laboratory. This collaboration proved highly successful, as several emerging NPS were discovered. Third, the compilation of drug testing results was evaluated to determine trends among NPS users. This established a basis for confirming increased rates of poly-drug use. Fourth, *in vitro* and *in vivo* metabolite generation and identification studies were conducted to advance the knowledge of NPS biotransformation, using five newly identified NPS and a data mining workflow.

7.1 Utility of LC-QTOF-MS in Forensic Toxicology

This research demonstrates the overall effectiveness of LC-QTOF-MS for application in forensic toxicology, specifically relating to emerging drug discovery, comprehensive drug detection, and metabolite characterization. Non-targeted data acquisition proved useful for the detection and identification of NPS, allowing for a dynamic workflow and assay that could be utilized as new and emerging drugs became present in illicit drug supplies.

SWATH® acquisition allowed for complete and comprehensive acquisition of fragment ion data that was critical for the overall determination of positive findings during data processing. Acquisition of fragmentation data using LC-QTOF-MS (vs. LC-TOF-MS) proved valuable for the differentiation of some isobaric species and distinction from complex biological matrices. However, some isobaric, structurally similar analytes (e.g. fentanyl and its analogues) could not be distinguished by fragmentation pattern, as these compounds produced similar or identical spectra due to reproducibility of stable fragment ions.

The developed workflows to conduct sample mining and data mining were highly successful for the real-time identification of emerging drug threats (e.g. NPS) and the retrospective determinations of first appearance, as well as retrospective characterization of metabolites present. Sample mining was largely more successful due to up-to-date drug intelligence and monitoring, paired with the ability to rapidly update the library database of the LC-QTOF-MS workflow, another great advantage to this assay.

While the sophisticated acquisition of immense data using LC-QTOF-MS was important, it should be noted that sample mining and data mining can be conducted using other analytical platforms. For example, a non-HRMS techniques such as GC-MS can be utilized for sample mining and data mining, by definition. However, the user may need access to applicable software applications (e.g. Automated Mass Spectral Deconvolution and Identification Software [AMDIS] from NIST) to assist with data processing. The acquisition of accurate mass data is not a limiting factor for these two processes; although its use certainly dictates the results one can conclude.

The HRMS data acquired via LC-QTOF-MS allowed for formula generation and structural elucidation, key aspects of data analysis and review that are not available from other HRMS platforms. Acquisition of accurate mass allowed for determination of chemical formula for comparative purposes during sample mining and drug discovery, as well as for formulative purposed during metabolite discovery. Acquisition of accurate mass fragment data allowed for the elucidation of structure, or at least structural features. This permits LC-QTOF-MS to be a far superior technique for analytical chemistry and forensic toxicology workflows in this arena, paired with sensitivity, compared to NMR and/or IR spectroscopy.

7.2 Emerging NPS Prevalence in the United States

NPS continue to emerge on illicit drug markets, as shown through their detection in biological specimens from toxicological investigations herein. Based on the results of this research, biological extracts for sample mining and archived datafiles for data mining

proved to be rich datasets for the identification and discovery of emerging NPS. NPS discovered during this research were frequently found in conjunction with other NPS and/or drugs of abuse, a phenomenon hypothesized based on recent literature reports.

The majority of emerging NPS discovered for the first time using the described methodology were of the NPS opioid and NPS stimulant classes. This is consistent with national and global trend data associated with NPS use (excluding synthetic cannabinoids). This expansion in the number of novel opioids detected in populations in the United States is not surprising based on the current opioid epidemic. Contrarily, the number of NPS opioid precursors detected was surprising, especially those detected in the absence of theorized active parent compounds (e.g. benzylfuranylfentanyl positive in the absence of furanylfentanyl). The presence of NPS opioid precursors is suspected to be linked to NPS opioid synthesis, but no data or studies have confirmed this theory. Regardless of the user or dealer intent, it is clear that NPS opioid precursors are relevant to toxicological analyses, especially in the absence of human toxicity data.

In total, 21 emergent NPS were discovered using the LC-QTOF-MS assay through sample mining and data mining between Q1 2018 and Q2 2019. Most notably, analogues of U-47700 were discovered here for the first time in forensic toxicology casework, specifically 3,4-methylenedioxy-U-47700 and isopropyl-U-47700. This occurred shortly after the scheduling of fentanyl related substances by the DEA, and this rise (and subsequent fall) in non-fentanyl related opioids was apparent through this research. Another NPS opioids, fluorofuranylfentanyl, was also discovered here for the first time in forensic toxicology casework and reported to the scientific community. This

was followed by its rapid proliferation in the opioid drug supply, causing several deaths in Florida, Ohio, and other states. In addition to NPS opioids, the NPS stimulant eutylone was discovered in forensic toxicology casework here for the first time. Eutylone was previously characterized in seized drug materials; however, its detection during this research marked the beginning of its proliferation and distribution in the stimulant drug supply (e.g. Ecstasy).

Forensic laboratories not currently utilizing updated broad-based screening methodologies or retrospective data analysis workflows should be aware that NPS in toxicological specimens could go undetected, including those found concurrently with other NPS. Additionally, forensic laboratories should consider employing sample mining and data mining approaches using a variety of available analytical platforms.

7.3 NPS Trends in the United States

NPS trend analyses are of timely importance due to the short life span of these synthetic drugs in comparison to traditional drugs of abuse. It is not uncommon for a specific NPS to be present in the drug supply for only a few months to a year (e.g. fluorofuranylfentanyl). It is imperative that timely trend analyses are conducted on NPS to ensure the window of use is not missed when developing and validating new analytical methods. Additionally, this leads to a need for up-to-date scopes of toxicology testing, which can only be as good as drug surveillance and intelligence allow.

During this research, NPS opioids (e.g. fentanyl analogues) declined in positivity over time (Q1 2018 to Q2 2019), a temporal change that has also been document among

other fields of study. Contrarily, fentanyl positivity was persistent through 2019. Fentanyl currently dominates opioid drug supplies and there is no evidence that this will change in the near future. Temporal trend analyses showed the slight decline for legacy drugs of abuse, heroin and MDMA, as the drug markets for these analytes shift to fentanyl and methamphetamine, respectively.

The use of forensic toxicology sample extracts proved to be a reliable means for determination of poly-drug use. Fentanyl poly-drug use was common, whereas poly-NPS use was less common. Concurrent or combined fentanyl and stimulant use neared 50%, a drug use phenomenon that should be carefully monitored as drug deaths from cocaine and methamphetamine continue to increase causing public health concern. Fentanyl was commonly encountered with NPS opioids during this research, but likely declining among current positivity. NPS were commonly found with the most common drugs of abuse: cocaine, heroin, and methamphetamine.

Poly-drug use is significant from analytical chemistry, forensic toxicology, and public health perspectives, as combined drug use creates drug-drug interactions and more complex adverse effect profiles, in addition to complicating testing protocols, analysis workflows, and analytical assays. To better understand and document poly-drug use, laboratories should consider developing all-inclusive, non-targeted assays for more comprehensive determination of all substances onboard at the time of impairment or death.

7.4 Metabolism of NPS

Five emergent NPS were selected during this research to evaluate in terms of metabolism in order to characterize biotransformation products that would be useful for future forensic toxicology analytical testing. The NPS selected were 3,4-methylenedioxy-U-47700, *ortho*-fluorofuranylfentanyl, 2F-deschloroketamine, eutylone, and *N*-ethyl hexedrone. No previously literature reports were available for the metabolism of these compounds. A wide variety of chemistries and molecular structures were selected for diversity.

Nine metabolites of 3,4-methylenedioxy-U-47700 were identified *in vitro* while only three metabolites were identified *in vivo*. It was determined that *N*-demethyl-3,4-methylenedioxy-U-47700 (M.1) was the most appropriate biomarker for monitoring its use. This metabolite is considered unique to this NPS opioid and follows similar metabolism pathways previous published (i.e. U-47700).

Nine metabolites of *ortho*-fluorofuranylfentanyl were identified *in vitro* while only one metabolite was identified *in vivo*. This metabolite was fluoro-4-ANPP; however, the usefulness of this analyte as a biomarker is low due to its use suspected use a synthesis precursor. Additional blood specimens from overdose deaths were analyzed for fluorofuranylfentanyl metabolites, but these samples also did not result in a large number of abundant metabolites identified. The most unique metabolite of fluorofuranylfentanyl was determined to be fluorofuranyl-norfentanyl (M.1). Future studies should be conducted to determine its viability as a biomarker in urine specimens.

Nine metabolites of 2F-deschloroketamine were identified *in vitro* while only two metabolites were identified *in vivo*. It was determined that 2F-deschloro-norketamine (M.1) was the most appropriate biomarker for monitoring its use. This metabolite is considered unique to this NPS hallucinogen and follows similar metabolism pathways previous published (i.e. ketamine).

Only three metabolites of eutylone were identified *in vitro* and all three were also identified *in vivo*. It was determined that hydrogenation of eutylone to produce M.3 was the most appropriate biomarker for monitoring its use. This metabolite is considered unique to this NPS stimulant; however, issues with its distinction from the hydrogenated metabolite of dibutylone arose. It is suggested that multiple metabolites are consider when monitoring the use of these NPS stimulants.

Five metabolites of *N*-ethyl hexedrone were identified *in vitro* while only one metabolite was identified *in vivo*. This metabolite was determined to be unique to *N*-ethyl hexedrone and is a hydrogenation product (M.5). *N*-ethyl hexedrone M.5 was discovered in an extract negative for *N*-ethyl hexedrone, further contributing to the conclusion that this is an appropriate biomarker. Additionally, this finding demonstrates the true value of comprehensive data mining for these metabolites identified *in vitro*.

These unique metabolites of emergent NPS should be considered for inclusion in scopes of testing to prolong detection windows of these substances and to more accurately characterize specific NPS use. A rapid approach was developed to studying metabolism and it should be considered when emergent NPS are discovered with increasing prevalence in seized drug and/or toxicology casework.

7.5 Research Limitations and Knowledge Gaps

One major limitation to this research was the inability to distinguish some isobaric species, an issue which was known at the onset of study design and could not be universally overcome. For example, the LC-QTOF-MS could not distinguish *ortho*- vs. *meta*- vs. *para*-fluorofuranylfentanyl. It was determined that isobaric confirmation was not necessary for this study, and rather the overall identification of an emergent NPS was more valuable. However, future targeted studies should evaluate the extent of isobaric emergent NPS.

A knowledge gap still exists relating to the identification of NPS opioid precursors. Some of these precursors were detected with a synthesis product (e.g. *N*-methyl norfentanyl and fentanyl), but some precursors were not (e.g. benzylfuranylfentanyl). Further research into these substances is warranted from several angles. First, research should be conducted to determine the feasibility of converting these NPS fentanyl precursor into fentanyl analogues, with focus on methods that could be conducted clandestinely. Second, comprehensive characterization of possible fentanyl analogues that could be created from the precursors should be conducted. Third, the effects and toxicity of precursors should be evaluated. While it is known that some NPS opioid precursors are not opioid receptor agonists, their effects on other receptor systems and the body should be considered as they continue to appear in toxicology casework.

Another limitation to this study was the inability to correlate analytical findings with demographic information and/or case histories. This was largely due to IRB and human subject restriction, but also was impacted by the large volume of samples. Future

importance could be placed on retrospective collection of demographic information. This would allow for geographical trends to be evaluated, including possible connections or correlations with drug trafficking.

7.6 Future Directions

The developed approach herein for sample mining and data mining could be applied to other professions and fields of study. While these workflows were developed to complement drug testing methodologies, the approach could easily fit into current clinical testing protocols that are currently being employed in hospitals and emergency departments. In addition, sample mining could be conducted among environmental testing fields. For example, there is increased awareness about opioids in water supplies and this type of approach could benefit environmental testing programs. The pharmaceutical industry could also benefit from sample mining and data mining, especially in the area of counterfeit determination and analysis.

Additional data processing strategies could be developed for more timely and accurate identifications. This could lead to a more time efficient process that would allow for quick reporting and increased sample analysis. In addition, an approach to prophetic data processing could be beneficial. For example, one could develop an approach that screens based on different chemical properties (e.g. fragment ions instead of precursor ions) rather than intact molecule behavior.

One of the limitations to the metabolism studies conducted was the inability to test authentic human urine specimens. Future studies could include this analysis, as well

as a more quantitative approach to accurately determining major and minor metabolites. In addition, future research could focus on determination of metabolite activity. This information would greatly assist in the understanding of toxicity profiles and adverse events reported.

An interesting area of future work could include a deeper look into drug combinations, with respect to demographic information, as mentioned above. Combinations of NPS have been found to be more specific than typical abused drug combinations. NPS combination can be rare as seen in the data collected as part of this research. Further evaluation of drug combination could be explored, both for adverse event tracking and the possibility of determining patterns of drug trafficking.

7.7 Finis

As NPS continue to appear in forensic toxicology casework, novel assays for their detection and characterization will be critical to analytical chemistry efforts involved in developing and maintaining testing methodologies. Without state-of-the-art instrumentation and processing workflows, the identification of NPS will be hindered. The landscape of NPS positivity appears to be changing, as it has since NPS were first identified in the United States around 2008. Timely and accurate understanding of the NPS landscape and illicit drug markets is critical, but this is not possible without appropriate assays for drug discovery and scientists with expertise to review and interpret results and data. As the "opioid-epidemic" moves towards a "poly-drug epidemic," non-targeted data acquisition, possibly using LC-QTOF-MS, will become more of a necessity,

as its use in aiding the discovery of emergent NPS has been impactful. Analytical chemists must continue research involving identification, characterization, and proliferation of NPS to broaden the understanding of these synthetic drugs and their public health and safety impacts from objective and scientific perspectives.

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APPENDIX A

LC-QTOF-MS LIBRARY DATABASE

Table A1: Categorized library database (alphabetical order)

Name	Formula	[M+H]+	Type	Subtype 1	Subtype 2	Subtype 3	SWATH® Window
1-(4-methylbenzyl) piperazine	C12H18N2	191.1543	NPS	Stimulant	Piperazine	Parent	6
10-Hydroxycarbazepine	C15H14N2O2	255.1128	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Metabolite	11
1-Hydroxymidazolam	C18H13ClFN3O	342.0804	Pharmaceutical	Benzodiazepine	-	Metabolite	20
1P-LSD	C23H29N3O2	380.2333	NPS	Hallucinogen	Other	Parent	22
2',5'-Dimethoxyfentanyl	C24H32N2O3	397.2486	NPS	Opioid	Fentalog	Parent	23
25B-NBOMe	C18H22BrNO3	380.0856	NPS	Hallucinogen	Phenethylamine	Parent	22
25C-NBOH	C17H20ClNO3	322.1205	NPS	Hallucinogen	Other	Parent	18
25C-NBOMe	C18H22ClNO3	336.1361	NPS	Hallucinogen	Phenethylamine	Parent	19
25D-NBOMe	C19H25NO3	316.1907	NPS	Hallucinogen	Phenethylamine	Parent	17
25E-NBOH	C19H25NO3	316.1907	NPS	Hallucinogen	Phenethylamine	Parent	17
25E-NBOMe	C20H27NO3	330.2064	NPS	Hallucinogen	Phenethylamine	Parent	19
25H-NBOMe	C18H23NO3	302.1750	NPS	Hallucinogen	Phenethylamine	Parent	16
25I-NBOMe	C18H22INO3	428.0717	NPS	Hallucinogen	Phenethylamine	Parent	25
25N-NBOMe	C18H22N2O5	347.1602	NPS	Hallucinogen	Phenethylamine	Parent	20
25T2-NBOMe	C19H25NO3S	348.1628	NPS	Hallucinogen	Phenethylamine	Parent	20
25T4-NBOMe	C21H29NO3S	376.1941	NPS	Hallucinogen	Phenethylamine	Parent	22
25T7-NBOMe	C21H29NO3S	376.1941	NPS	Hallucinogen	Phenethylamine	Parent	22
2C-B	C10H14BrNO2	260.0281	NPS	Hallucinogen	Phenethylamine	Parent	11
2C-B-FLY	C12H14BrNO2	284.0281	NPS	Hallucinogen	Phenethylamine	Parent	14
2C-C	C10H14ClNO2	216.0786	NPS	Hallucinogen	Phenethylamine	Parent	8
2C-D	C11H17NO2	196.1332	NPS	Hallucinogen	Phenethylamine	Parent	7
2-CDMC	C11H14ClNO	212.0837	NPS	Stimulant	Cathinone	Parent	8
2C-E	C12H19NO2	210.1489	NPS	Hallucinogen	Phenethylamine	Parent	8
2C-G	C12H19NO2	210.1489	NPS	Hallucinogen	Phenethylamine	Parent	8
2C-H	C10H15NO2	182.1176	NPS	Hallucinogen	Phenethylamine	Parent	5
2C-I	C10H14INO2	308.0142	NPS	Hallucinogen	Phenethylamine	Parent	16
2C-N	C10H14N2O4	227.1026	NPS	Hallucinogen	Phenethylamine	Parent	8
2C-P	C13H21NO2	224.1645	NPS	Hallucinogen	Phenethylamine	Parent	8
2C-T-2	C12H19NO2S	242.1029	NPS	Hallucinogen	Phenethylamine	Parent	10
2C-T-7	C13H21NO2S	256.1336	NPS	Hallucinogen	Phenethylamine	Parent	11
2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	154.1027	NPS	Stimulant	Phenethylamine	Parent	2
2F-Deschloroketamine	C13H16FNO	222.1289	NPS	Dissociative	Other	Parent	8
2'-Fluorofentanyl	C22H27FN2O	355.2180	NPS	Opioid	Fentalog	Parent	20
2-methyl AP-237	C18H26N2O	287.2118	NPS	Opioid	Other	Parent	14
2-MMA/3-MMA (Methoxymethamphetamine)	C11H17NO	180.1383	NPS	Stimulant	Phenethylamine	Parent	5
3,4-Dimethyl Alpha-PVP	C17H25NO	260.2009	NPS	Stimulant	Cathinone	Parent	11
3,4-DMMC	C12H17NO	192.1383	NPS	Stimulant	Cathinone	Parent	6
3-CAF	C24H15FN2O2	383.1190	NPS	Synthetic Cannabinoid	Other	Parent	22
3-CDMC	C11H14ClNO	212.0837	NPS	Stimulant	Cathinone	Parent	8
3-FMA/4-FMA (Fluoromethamphetamine)	C10H14FN	168.1183	NPS	Stimulant	Phenethylamine	Parent	3
3-FMC/4-FMC (Fluoromethcathinone, Flephedrone)	C10H12FNO	182.0976	NPS	Stimulant	Cathinone	Parent	5
3F-MT-45	C24H31FN2	367.2544	NPS	Opioid	Other	Parent	21
3-MeO-PCE	C15H23NO	234.1852	NPS	Hallucinogen	Other	Parent	9
3-Methylbutyrylfentanyl	C24H32N2O	365.2587	NPS	Opioid	Fentalog	Parent	21
3-Methylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
3-OH-PCP	C17H25NO	260.2009	NPS	Hallucinogen	Other	Parent	11
4-ANBP	C18H22N2	267.1856	NPS	Opioid	Fentalog	Precursor	12
4-ANPP	C19H24N2	281.2012	NPS	Opioid	Fentalog	Precursor	13
4-Bromomethcathinone	C10H12BrNO	242.0175	NPS	Stimulant	Cathinone	Parent	10
4-CDMC	C11H14ClNO	212.0837	NPS	Stimulant	Cathinone	Parent	8
4Cl-alpha-PVP	C15H20ClNO	266.1306	NPS	Stimulant	Cathinone	Parent	12
4Cl-Isopropylcathinone	C12H16ClNO	226.0993	NPS	Stimulant	Cathinone	Parent	8

4-cyano CUMYL-BUT7AICA	C22H24N4O	361.2023	NPS	Synthetic Cannabinoid	Other	Parent	21
4-cyano CUMYL-BUTINACA	C22H24N4O	361.2023	NPS	Synthetic Cannabinoid	Other	Parent	21
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	366.1812	NPS	Synthetic Cannabinoid	Other	Metabolite	21
4-EEC (Ethylethcathinone)	C13H19NO	206.1539	NPS	Stimulant	Cathinone	Parent	7
4-Ethyl-n,n-DMC (4-ethyl-n,n-dimethylcathinone)	C13H19NO	206.1539	NPS	Stimulant	Cathinone	Parent	7
4F-alpha-PHP	C16H22FNO	264.1758	NPS	Stimulant	Cathinone	Parent	12
4F-alpha-PVP	C15H20FNO	250.1602	NPS	Stimulant	Cathinone	Parent	10
4F-CUMYL-5F-PINACA	C22H25F2N3O	386.2039	NPS	Synthetic Cannabinoid	Other	Parent	23
4F-MDMB-BINACA	C19H26FN3O3	364.2031	NPS	Synthetic Cannabinoid	Other	Parent	21
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	350.1875	NPS	Synthetic Cannabinoid	Other	Metabolite	20
4-HO-DiPT	C16H24N2O	261.1961	NPS	Hallucinogen	Tryptamine	Parent	11
4-HO-MET	C18H23NO2	219.1492	NPS	Hallucinogen	Tryptamine	Parent	8
4-MDEC	C14H21NO	220.1696	NPS	Stimulant	Cathinone	Parent	8
4-MEC	C12H17NO	192.1383	NPS	Stimulant	Cathinone	Parent	6
4-MeO-PCP	C18H27NO	274.2165	NPS	Hallucinogen	Other	Parent	13
4-MeOPP	C11H16N2O	193.1335	NPS	Stimulant	Piperazine	Parent	6
4-Methoxybutyrylfentanyl	C24H32N2O2	381.2172	NPS	Opioid	Fentalog	Parent	22
4'-Methylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
4'-Methyl Hexedrone	C14H21NO	220.1696	NPS	Stimulant	Cathinone	Parent	8
4-Methylaminorex	C10H12N2O	177.1022	Drug of Abuse	Stimulant	Other	Parent	4
4OH-MDMB-BINACA	C19H27N3O4	362.2074	NPS	Synthetic Cannabinoid	Other	Metabolite	21
4-Phenylfentanyl	C28H32N2O	413.2587	NPS	Opioid	Fentalog	Parent	24
4-Phenyl-U-51754	C23H30N2O	351.2430	NPS	Opioid	Utopioid	Parent	20
5-APB/6-APB	C11H13NO	176.1070	NPS	Stimulant	Phenethylamine	Parent	4
5Br-AKB-48	C23H30BrN3O	444.1645	NPS	Synthetic Cannabinoid	Other	Parent	25
5Br-THJ-018	C23H21BrN2O	421.0910	NPS	Synthetic Cannabinoid	Other	Parent	25
5Cl-AB-PINACA	C18H25ClN4O2	365.1739	NPS	Synthetic Cannabinoid	Other	Parent	21
5Cl-AKB-48	C23H30ClN3O	400.2150	NPS	Synthetic Cannabinoid	Other	Parent	23
5Cl-THJ-018	C23H21ClN2O	377.1415	NPS	Synthetic Cannabinoid	Other	Parent	22
5F JWH-018 Adamantyl Analogue	C24H30FNO	368.2384	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-7-QUPAIC	C22H20FN3O2	378.1612	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-AB-FUPPYCA	C20H26F2N4O2	393.2097	NPS	Synthetic Cannabinoid	Other	Parent	23
5F-ABICA	C19H26FN3O2	348.2082	NPS	Synthetic Cannabinoid	Other	Parent	20
5F-ADB	C20H28FN3O3	378.2188	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	364.2031	NPS	Synthetic Cannabinoid	Other	Metabolite	21
5F-ADBICA	C20H28FN3O2	362.2238	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-ADB-PINACA	C19H27FN4O2	363.2191	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-AEB	C20H28FN3O3	378.2188	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-AKB48 (5F-APINACA)	C23H30FN3O	384.2446	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-AMB	C19H26FN3O3	364.2031	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	350.1875	NPS	Synthetic Cannabinoid	Other	Metabolite	20
5F-APINAC	C23H29FN2O2	385.2286	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-BEPIRAPIM	C25H30FN3O	408.2446	NPS	Synthetic Cannabinoid	Other	Parent	24
5F-CUMYL-P7AICA	C22H26FN3O	368.2132	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-CUMYL-PeGACLONE	C25H27FN2O	391.2180	NPS	Synthetic Cannabinoid	Other	Parent	23

5F-CUMYL-PICA	C23H27FN2O	367.2180	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-CUMYL-PINACA	C22H26FN3O	368.2133	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-EDMB-PINACA	C21H30FN3O3	392.2344	NPS	Synthetic Cannabinoid	Other	Parent	23
5F-AB-PINACA	C18H25FN4O2	349.2034	NPS	Synthetic Cannabinoid	Other	Parent	20
5F-CYPPICA	C18H23FN2O	303.1867	NPS	Synthetic Cannabinoid	Other	Parent	16
5F-PY-PICA	C18H23FN2O	303.1867	NPS	Synthetic Cannabinoid	Other	Parent	16
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	311.1554	NPS	Synthetic Cannabinoid	Other	Parent	16
5F-MDMB-PICA	C21H29FN2O3	377.2235	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	363.2079	NPS	Synthetic Cannabinoid	Other	Metabolite	21
5F-MN-18	C23H22FN3O	376.1820	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-MPP-PICA	C24H27FN2O3	411.2079	NPS	Synthetic Cannabinoid	Other	Parent	24
5F-NNEI	C24H23FN2O	375.1867	NPS	Synthetic Cannabinoid	Other	Parent	21
5F-NPB-22	C22H20FN3O2	378.1612	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	251.1190	NPS	Synthetic Cannabinoid	Other	Metabolite	10
5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	377.1660	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-PB-22 3-Carboxyindole	C14H16FNO2	250.1238	NPS	Synthetic Cannabinoid	Other	Metabolite	10
5F-PCN	C23H22FN3O	376.1820	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-PY-PINACA	C17H22FN3O	304.1820	NPS	Synthetic Cannabinoid	Other	Parent	16
5F-SDB-005	C23H21FN2O2	377.1660	NPS	Synthetic Cannabinoid	Other	Parent	22
5F-SDB-006	C21H23FN2O	339.1867	NPS	Synthetic Cannabinoid	Other	Parent	19
5F-THJ	C22H21FN4O	377.1772	NPS	Synthetic Cannabinoid	Other	Parent	22
5-IT	C11H14N2	175.1230	NPS	Stimulant	Phenethylamine	Parent	4
5-MeO-Amt (5-Methoxy-alpha-methyltryptamine)	C12H16N2O	205.1335	NPS	Hallucinogen	Tryptamine	Parent	7
5-MeO-DALT	C17H22N2O	271.1805	NPS	Hallucinogen	Tryptamine	Parent	12
5-MeO-DiPT	C17H26N2O	275.2118	NPS	Hallucinogen	Tryptamine	Parent	13
5-MeO-DMT	C13H18N2O	219.1492	NPS	Hallucinogen	Tryptamine	Parent	8
6-Methoxy Methylone	C12H15NO4	238.1074	NPS	Stimulant	Cathinone	Parent	9
6-Monoacetylmorphine	C19H21NO4	328.1543	Drug of Abuse	Opiate	Other	Metabolite	18
7-Amino Clonazepam	C15H12ClN3O	286.0742	Drug of Abuse	Benzodiazepine	Other	Metabolite	14
7-Amino Flunitrazepam	C16H14FN3O	284.1194	Pharmaceutical	Benzodiazepine	Other	Metabolite	14
7-Hydroxymitragynine	C23H30N2O5	415.2227	NPS	Alkaloid	Natural	Metabolite	24
A-796,260	C22H30N2O2	355.2380	NPS	Synthetic Cannabinoid	Other	Parent	20
A-834,735	C22H29NO2	340.2271	NPS	Synthetic Cannabinoid	Other	Parent	19
A-836339	C16H26N2O2S	311.1788	NPS	Synthetic Cannabinoid	Other	Parent	17
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	350.2478	NPS	Synthetic Cannabinoid	Other	Parent	20
AB-005	C23H32N2O	353.2587	NPS	Synthetic Cannabinoid	Other	Parent	20
AB-BICA	C21H23N3O2	350.1863	NPS	Synthetic Cannabinoid	Other	Parent	20
AB-CHFUPYCA	C22H29FN4O2	401.2347	NPS	Synthetic Cannabinoid	Other	Parent	24
AB-CHMICA	C21H29N3O2	356.2333	NPS	Synthetic Cannabinoid	Other	Parent	20
AB-CHMINACA	C20H28N4O2	357.2285	NPS	Synthetic Cannabinoid	Other	Parent	20
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	357.2285	NPS	Synthetic Cannabinoid	Other	Parent	20
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	358.2125	NPS	Synthetic Cannabinoid	Other	Metabolite	21

AB-FUBICA	C21H22FN3O2	368.1769	NPS	Synthetic Cannabinoid	Other	Parent	21
AB-FUBINACA	C20H21FN4O2	369.1721	NPS	Synthetic Cannabinoid	Other	Parent	21
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	399.1463	NPS	Synthetic Cannabinoid	Other	Metabolite	23
AB-PINACA	C18H26N4O2	331.2129	NPS	Synthetic Cannabinoid	Other	Parent	19
AB-PINACA N-Pentanoic Acid	C18H24N4O4	361.1870	NPS	Synthetic Cannabinoid	Other	Metabolite	21
Acetaminophen	C8H9NO2	152.0706	Pharmaceutical	Analgesic	Other	Parent	2
Acetylfentanyl	C21H26N2O	323.2118	NPS	Opioid	Fentalog	Parent	18
Acetylfentanyl 4-Methylphenethyl Analogue	C22H28N2O	337.2274	NPS	Opioid	Fentalog	Parent	19
Acetylcodeine	C20H23NO4	342.1700	Drug of Abuse	Opiate	Other	Parent	20
ACHMINACA	C25H33N3O	392.2696	NPS	Synthetic Cannabinoid	Other	Parent	23
Acrylfentanyl	C22H26N2O	335.2118	NPS	Opioid	Fentalog	Parent	19
ADB-BICA	C22H25N3O2	364.2020	NPS	Synthetic Cannabinoid	Other	Parent	21
ADB-BINACA	C21H24N4O2	365.1972	NPS	Synthetic Cannabinoid	Other	Parent	21
ADB-FUBICA	C22H24FN3O2	382.1925	NPS	Synthetic Cannabinoid	Other	Parent	22
ADB-FUBINACA	C21H23FN4O2	383.1878	NPS	Synthetic Cannabinoid	Other	Parent	22
ADB-FUPYCA	C21H28F2N4O2	407.2253	NPS	Synthetic Cannabinoid	Other	Parent	24
ADBICA	C20H29N3O2	344.2333	NPS	Synthetic Cannabinoid	Other	Parent	20
ADBICA N-Pentanoic Acid	C20H27N3O4	374.2074	NPS	Synthetic Cannabinoid	Other	Metabolite	21
ADB-PINACA	C19H28N4O2	345.2285	NPS	Synthetic Cannabinoid	Other	Parent	20
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	375.2027	NPS	Synthetic Cannabinoid	Other	Metabolite	21
AH-7921	C16H22Cl2N2O	329.1182	NPS	Opioid	Other	Parent	19
AKB-48 (APINACA)	C23H31N3O	366.2540	NPS	Synthetic Cannabinoid	Other	Parent	21
AKB-48 N-Pentanoic Acid	C23H29N3O3	396.2282	NPS	Synthetic Cannabinoid	Other	Metabolite	23
ALD-52	C22H27N3O2	366.2176	NPS	Hallucinogen	Other	Parent	21
Alfentanil	C21H32N6O3	417.2609	Pharmaceutical	Opioid	Fentalog	Parent	25
AL-LAD	C22H27N3O	350.2227	NPS	Hallucinogen	Other	Parent	20
Allylescaline	C13H19NO3	238.1438	NPS	Hallucinogen	Other	Parent	9
Alpha-Hydroxyalprazolam	C17H13ClN4O	325.0851	Drug of Abuse	Benzodiazepine	Other	Metabolite	18
alpha'-Methylbutyrylfentanyl	C24H32N2O	365.2587	NPS	Opioid	Fentalog	Parent	21
Alpha-PBP	C14H19NO	218.1539	NPS	Stimulant	Cathinone	Parent	8
Alpha-PHP	C16H23NO	246.1852	NPS	Stimulant	Cathinone	Parent	10
Alpha-PHpP (PV8)	C17H25NO	260.2009	NPS	Stimulant	Cathinone	Parent	11
Alpha-PiHP	C16H23NO	246.1852	NPS	Stimulant	Cathinone	Parent	10
Alpha-PPP	C13H17NO	204.1383	NPS	Stimulant	Cathinone	Parent	7
Alpha-PVP	C15H21NO	232.1696	NPS	Stimulant	Cathinone	Parent	9
Alpha-PVT	C13H19NOS	238.1260	NPS	Stimulant	Cathinone	Parent	9
Alprazolam	C17H13ClN4	309.0902	Drug of Abuse	Benzodiazepine	Other	Parent	16
Alprazolam-D5	C17H8[2H]5ClN4	314.1215	ISTD	Benzodiazepine	Other	Parent	17
AM-1220	C26H26N2O	383.2118	NPS	Synthetic Cannabinoid	Other	Parent	22
AM-1235	C24H21FN2O3	405.1609	NPS	Synthetic Cannabinoid	Other	Parent	24
AM-1241	C22H22IN3O3	504.0779	NPS	Synthetic Cannabinoid	Other	Parent	27
AM-1248	C26H34N2O	391.2744	NPS	Synthetic Cannabinoid	Other	Parent	23
AM-2201	C24H22FNO	360.1758	NPS	Synthetic Cannabinoid	Other	Parent	21
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	376.1820	NPS	Synthetic Cannabinoid	Other	Parent	22
AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	361.1711	NPS	Synthetic Cannabinoid	Other	Parent	21
AM-2232	C24H20N2O	353.1648	NPS	Synthetic Cannabinoid	Other	Parent	20
AM-2233	C22H23IN2O	459.0928	NPS	Synthetic Cannabinoid	Other	Parent	26

AM-3102	C21H41NO2	340.3210	NPS	Synthetic Cannabinoid	Other	Parent	19
AM-630	C23H25IN2O3	505.0983	NPS	Synthetic Cannabinoid	Other	Parent	27
AM-679	C20H20INO	418.0662	NPS	Synthetic Cannabinoid	Other	Parent	25
AM-694	C20H19FINO	436.0568	NPS	Synthetic Cannabinoid	Other	Parent	25
AMB	C19H27N3O3	346.2125	NPS	Synthetic Cannabinoid	Other	Parent	20
a-Methylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
a-Methylacetylfentanyl	C22H28N2O	337.2274	NPS	Opioid	Fentalog	Parent	19
Amitriptyline	C20H23N	278.1903	Pharmaceutical	Antidepressant	Other	Parent	13
Amoxapine	C17H16ClN3O	314.1055	Pharmaceutical	Antidepressant	Other	Parent	17
Amphetamine	C9H13N	136.1121	Drug of Abuse	Stimulant	Phenethylamine	Parent	2
AMT	C11H14N2	175.1230	NPS	Hallucinogen	Tryptamine	Parent	4
Aniracetam	C12H13NO3	220.0968	Pharmaceutical	Nootropic	Other	Parent	8
APICA	C24H32N2O	365.2587	NPS	Synthetic Cannabinoid	Other	Parent	21
APINAC (AKB57)	C23H30N2O2	367.2380	NPS	Synthetic Cannabinoid	Other	Parent	21
APP-BINACA	C21H24N4O2	365.1972	NPS	Synthetic Cannabinoid	Other	Parent	21
APP-CHMINACA	C24H28N4O2	405.2285	NPS	Synthetic Cannabinoid	Other	Parent	24
APP-FUBINACA	C24H21FN4O2	417.1721	NPS	Synthetic Cannabinoid	Other	Parent	25
APP-PICA	C23H27N3O2	378.2176	NPS	Synthetic Cannabinoid	Other	Parent	22
Aripiprazole	C23H27Cl2N3O2	448.1553	Pharmaceutical	Antipsychotic	Other	Parent	25
ATHPINACA	C24H31N3O2	394.2489	NPS	Synthetic Cannabinoid	Other	Parent	23
Atomoxetine	C17H21NO	256.1696	Pharmaceutical	Antidepressant	Other	Parent	11
Atropine	C17H23NO3	290.1751	Pharmaceutical	Anticholinergic	Other	Parent	15
Azidoindolene 1 (1)	C21H28FN3O2	374.2238	NPS	Synthetic Cannabinoid	Other	Parent	21
Azidoindolene 1 (2)	C21H28FN3O2	374.2238	NPS	Synthetic Cannabinoid	Other	Parent	21
BB-22 (QUCHIC)	C25H24N2O2	385.1911	NPS	Synthetic Cannabinoid	Other	Parent	22
BB-22 3-Carboxyindole	C16H19NO2	258.1489	NPS	Synthetic Cannabinoid	Other	Metabolite	11
BBOP	C13H9NO2	212.0706	ISTD	Other	Other	Parent	8
BDB	C11H15NO2	194.1176	NPS	Stimulant	Phenethylamine	Parent	6
Benzocaine	C9H11NO2	166.0863	Pharmaceutical	Anesthetic	Cutting Agent	Parent	3
Benzodioxolefentanyl	C27H28N2O3	429.2172	NPS	Opioid	Fentalog	Parent	25
Benzoylecgonine	C16H19NO4	290.1387	Drug of Abuse	Stimulant	Other	Metabolite	15
Benztropine	C21H25NO	308.2009	Pharmaceutical	Anticholinergic	Other	Parent	16
Benzylcarfentanil	C23H28N2O3	381.2172	NPS	Opioid	Fentalog	Precursor	22
Benzylfentanyl	C21H26N2O	323.2118	NPS	Opioid	Fentalog	Precursor	18
Benzylfuranylfentanyl	C23H24N2O2	361.1911	NPS	Opioid	Fentalog	Precursor	21
Benzylphenylfentanyl	C25H26N2O	371.2118	NPS	Opioid	Fentalog	Precursor	21
Benzylone	C17H17NO3	284.1281	NPS	Stimulant	Cathinone	Parent	14
beta-Hydroxyfentanyl	C22H28N2O2	353.2224	Drug of Abuse	Opioid	Fentalog	Metabolite	20
bk-EABDI	C15H21NO	232.1696	NPS	Stimulant	Cathinone	Parent	9
b-Methylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
b'-Phenylfentanyl	C28H32N2O	413.2587	NPS	Opioid	Fentalog	Parent	24
Bromadol	C22H28BrNO	402.1427	NPS	Opioid	Other	Parent	24
Bromazepam	C14H10BrN3O	316.0080	NPS	Benzodiazepine	Other	Parent	17
Bromo-Dragon FLY	C13H12BrNO2	294.0124	NPS	Hallucinogen	Phenethylamine	Parent	15
Brompheniramine	C16H19BrN2	319.0804	Pharmaceutical	Antihistamine	Other	Parent	18
Bufotenine	C12H16N2O	205.1335	Drug of Abuse	Hallucinogen	Tryptamine	Parent	7
Buphedrone	C11H15NO	178.1226	NPS	Stimulant	Cathinone	Parent	4
Bupivacaine	C18H28N2O	289.2274	Pharmaceutical	Anesthetic	Other	Parent	15
Buprenorphine	C29H41NO4	468.3108	Pharmaceutical	Opioid	Other	Metabolite	26
Bupropion	C13H18ClNO	240.1150	Pharmaceutical	Antidepressant	Other	Parent	10
Buspirone	C21H31N5O2	386.2551	Pharmaceutical	Anxiolytic	Other	Parent	23
Butorphanol	C21H29NO2	328.2271	Pharmaceutical	Opioid	Other	Parent	18
Butrylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
Butylone	C12H15NO3	222.1125	NPS	Stimulant	Cathinone	Parent	8
BZP	C11H16N2	177.1386	NPS	Stimulant	Piperazine	Parent	4
Caccure 907	C15H21NO2S	280.1366	NPS	Stimulant	Cathinone	Parent	13
Caffeine	C8H10N4O2	195.0877	Incidental	Stimulant	Other	Parent	6
Cannabidiol (CBD)	C21H30O2	315.2319	Drug of Abuse	Cannabinoid	Other	Parent	17
Cannabinol (CBN)	C21H26O2	311.2006	Drug of Abuse	Cannabinoid	Other	Parent	17

Carbamazepine	C15H12N2O	237.1022	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Metabolite	9
Carbamazepine-10, 11 Epoxide	C15H12N2O2	253.0972	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Metabolite	10
Carboxy-THC	C21H28O4	345.2060	Drug of Abuse	Cannabinoid	Other	Metabolite	20
Carfentanil	C24H30N2O3	395.2329	NPS	Opioid	Fentalog	Parent	23
Carisoprodol	C12H24N2O4	261.1809	Pharmaceutical	Muscle Relaxant	Other	Parent	11
Cathinone	C9H11NO	150.0913	NPS	Stimulant	Cathinone	Parent	2
CB-13	C26H24O2	369.1849	NPS	Synthetic Cannabinoid	Other	Parent	21
CB-25	C25H41NO3	404.3159	NPS	Synthetic Cannabinoid	Other	Parent	24
CB-52	C26H43NO3	418.3316	NPS	Synthetic Cannabinoid	Other	Parent	25
CB-86	C26H43NO3	418.3316	NPS	Synthetic Cannabinoid	Other	Parent	25
CBL-018	C24H23NO2	358.1802	NPS	Synthetic Cannabinoid	Other	Parent	21
Cephaeline	C28H38N2O4	467.2904	Pharmaceutical	Alkaloid	Other	Parent	26
Chlordiazepoxide	C16H14ClN3O	300.0898	Pharmaceutical	Benzodiazepine	Other	Parent	15
Chlorpheniramine	C16H19ClN2	275.1310	Pharmaceutical	Antihistamine	Other	Parent	13
Chlorpromazine	C17H19ClN2S	319.1030	Pharmaceutical	Antipsychotic	Other	Parent	18
Citalopram / Escitalopram	C20H21FN2O	325.1711	Pharmaceutical	Antidepressant	Other	Parent	18
Clobazam	C16H13ClN2O2	301.0738	Pharmaceutical	Benzodiazepine	Other	Parent	16
Clomipramine	C19H23ClN2	315.1623	Pharmaceutical	Antidepressant	Other	Parent	17
Clonazelam	C17H12ClN5O2	354.0752	NPS	Benzodiazepine	Other	Parent	20
Clonazepam	C15H10ClN3O3	316.0484	Drug of Abuse	Benzodiazepine	Other	Parent	17
Clonidine	C9H9Cl2N3	230.0246	Pharmaceutical	Antihypertensive	Other	Parent	9
Clozapine	C18H19ClN4	327.1371	Pharmaceutical	Antipsychotic	Other	Parent	18
Cocaethylene	C18H23NO4	318.1700	Drug of Abuse	Stimulant	Other	Metabolite	18
Cocaine	C17H21NO4	304.1543	Drug of Abuse	Stimulant	Other	Parent	16
Codeine	C18H21NO3	300.1594	Drug of Abuse	Opiate	Other	Parent	15
Cotinine	C10H12N2O	177.1022	Incidental	Stimulant	Other	Metabolite	4
CP-55,940	C24H40O3	377.3050	NPS	Synthetic Cannabinoid	Other	Parent	22
Crotonylfentanyl	C23H28N2O	349.2274	NPS	Opioid	Fentalog	Parent	20
CUMYL-PeGACLONE	C25H28N2O	373.2274	NPS	Synthetic Cannabinoid	Other	Parent	21
CUMYL-PICA	C23H28N2O	349.2274	NPS	Synthetic Cannabinoid	Other	Parent	20
CUMYL-THPINACA	C23H27N3O2	378.2176	NPS	Synthetic Cannabinoid	Other	Parent	22
Cyclobenzaprine	C20H21N	276.1747	Pharmaceutical	Muscle Relaxant	Other	Parent	13
Cyclobutylfentanyl	C24H30N2O	363.2431	NPS	Opioid	Fentalog	Parent	21
Cyclohexylfentanyl	C26H34N2O	391.2744	NPS	Opioid	Fentalog	Parent	23
Cyclopentylfentanyl	C25H32N2O	377.2587	NPS	Opioid	Fentalog	Parent	22
Cyclopropylfentanyl	C23H28N2O	349.2274	NPS	Opioid	Fentalog	Parent	20
DBZP	C18H22N2	267.1856	NPS	Stimulant	Piperazine	Parent	12
Delorazepam	C15H10Cl2N2O	305.0243	NPS	Benzodiazepine	Other	Parent	16
Desalkylflurazepam	C15H10ClFN2O	289.0539	Pharmaceutical	Benzodiazepine	Other	Metabolite	15
Deschloroketamine	C13H17NO	204.1383	NPS	Dissociative	Other	Parent	7
Deschloronorketamine	C12H15NO	190.1226	NPS	Dissociative	Other	Metabolite	5
Desipramine	C18H22N2	267.1856	Pharmaceutical	Antidepressant	Other	Parent	12
Desmethylclomipramine	C18H21ClN2	301.1393	Pharmaceutical	Antidepressant	Other	Metabolite	16
Desmethyldoxepin	C18H19NO	266.1539	Pharmaceutical	Antidepressant	Other	Metabolite	12
Desmethylsertraline	C16H15Cl2N	292.0654	Pharmaceutical	Antidepressant	Other	Metabolite	15
Desomorphine	C17H21NO2	272.1645	Drug of Abuse	Opioid	Other	Parent	13
Despropionyl 2'-Fluoro-ortho-Fluorofentanyl	C19H22F2N2	317.1824	NPS	Opioid	Fentalog	Precursor	18
Despropionyl 3-Methylfentanyl	C20H26N2	295.2169	NPS	Opioid	Fentalog	Precursor	15
Despropionyl ortho-Fluorofentanyl	C19H23FN2	299.1918	NPS	Opioid	Fentalog	Precursor	15
Despropionyl ortho-Methylfentanyl	C20H26N2	295.2169	NPS	Opioid	Fentalog	Precursor	15
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	217.1699	NPS	Hallucinogen	Tryptamine	Parent	8
Dextro / Levo Methorphan	C18H25NO	272.2009	Pharmaceutical	Antitussive	Other	Parent	13
Dextrorphan / Levorphanol	C17H23NO	258.1852	Pharmaceutical	Antitussive	Cutting Agent	Metabolite	11
Diacetylmorphine	C21H23NO5	370.1649	Drug of Abuse	Opiate	Other	Parent	21
Diazepam	C16H13ClN2O	285.0789	Drug of Abuse	Benzodiazepine	Other	Parent	14
Dibutylone (bk-DMBDB)	C13H17NO3	236.1281	NPS	Stimulant	Cathinone	Parent	9
Dichloroethcathinone (DCEC)	C11H13Cl2NO	246.0447	NPS	Stimulant	Cathinone	Parent	10
Diclazepam	C16H12Cl2N2O	319.0399	NPS	Benzodiazepine	Other	Parent	18
Dicyclomine	C19H35NO2	310.2741	Pharmaceutical	Anticholinergic	Other	Parent	16
Didesmethylsibutramine	C15H22ClN	252.1514	Pharmaceutical	Stimulant	Phenethylamine	Metabolite	10

Diethylone	C14H19NO3	250.1438	NPS	Stimulant	Cathinone	Parent	10
Diethylpentylone	C16H23NO3	278.1751	NPS	Stimulant	Cathinone	Parent	13
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	387.2243	NPS	Opioid	Fentalog	Parent	23
Difluorofentanyl	C22H26F2N2O	373.2086	NPS	Opioid	Fentalog	Parent	21
Dihydrocodeine / Hydrocodol	C18H23NO3	302.1751	Drug of Abuse	Opioid	Other	Parent	16
Diltiazem	C22H26N2O4S	415.1686	Pharmaceutical	Cardiovascular	Other	Parent	24
Dimethocaine	C16H26N2O2	279.2067	Pharmaceutical	Anesthetic	Other	Parent	13
Dimethylone	C12H15NO3	222.1125	NPS	Stimulant	Cathinone	Parent	8
Dimethylpentylone	C14H19NO3	250.1438	NPS	Stimulant	Cathinone	Parent	10
Diphenhydramine	C17H21NO	256.1696	Pharmaceutical	Antihistamine	Cutting Agent	Parent	11
DMA (Dimethylamphetamine)	C11H17N	164.1434	Drug of Abuse	Stimulant	Phenethylamine	Parent	3
DMAA 1 (Methylhexanamine)	C7H17N	116.1434	Drug of Abuse	Stimulant	Other	Parent	1
DMAA 2 (Methylhexanamine)	C7H17N	116.1434	Drug of Abuse	Stimulant	Other	Parent	1
DMT	C12H16N2	189.1386	NPS	Hallucinogen	Tryptamine	Parent	5
DOB	C11H16BrNO2	274.0437	NPS	Hallucinogen	Phenethylamine	Parent	13
DOC (4-Chloro-2,5-dimethoxyamphetamine)	C11H16ClNO2	230.0942	NPS	Hallucinogen	Phenethylamine	Parent	9
DOM	C12H19NO2	210.1489	NPS	Hallucinogen	Phenethylamine	Parent	8
Donepezil	C24H29NO3	380.2220	Pharmaceutical	Other	Other	Parent	22
Doxepin	C19H21NO	280.1696	Pharmaceutical	Antidepressant	Other	Parent	13
Doxylamine	C17H22N2O	271.1805	Pharmaceutical	Antidepressant	Other	Parent	12
Duloxetine	C18H19NOS	298.1260	Pharmaceutical	Antidepressant	Other	Parent	15
EAM-2201	C26H26FNO	388.2071	NPS	Synthetic Cannabinoid	Other	Parent	23
EDDP	C20H23N	278.1903	Drug of Abuse	Opioid	Other	Metabolite	13
EG018	C28H25NO	392.2009	NPS	Synthetic Cannabinoid	Other	Parent	23
EG-2201	C28H24FNO	410.1915	NPS	Synthetic Cannabinoid	Other	Parent	24
EMB-FUBINACA	C22H24FN3O3	398.1875	NPS	Synthetic Cannabinoid	Other	Parent	23
EMDP	C19H21N	264.1747	Drug of Abuse	Opioid	Other	Metabolite	12
Emetine	C29H40N2O4	481.3061	Pharmaceutical	Other	Other	Parent	27
Ephedrine / Pseudoephedrine	C10H15NO	166.1226	Incidental	Antihistamine, Decongestant	Other	Parent	3
Estazolam	C16H11ClN4	295.0745	Pharmaceutical	Benzodiazepine	Other	Parent	15
Eszopiclone / Zopiclone	C17H17ClN6O3	389.1123	Pharmaceutical	Hypnotic, Sedative	Other	Parent	23
Etaqualone	C17H16N2O	265.1335	Pharmaceutical	Hypnotic, Sedative	Other	Parent	12
Ethacathinone (ETH-CAT)	C11H15NO	178.1226	NPS	Stimulant	Cathinone	Parent	4
ETH-LAD	C21H27N3O	338.2227	NPS	Hallucinogen	Other	Parent	19
Ethoxyacetylfentanyl	C23H30N2O2	367.2380	NPS	Opioid	Fentalog	Parent	21
Ethylenedioxy-U-47700	C18H26N2O3	319.2016	NPS	Opioid	Utopioid	Parent	18
Ethylenedioxy-U-51754	C19H28N2O3	333.2176	NPS	Opioid	Utopioid	Parent	19
Ethylindolefentanyl	C24H29N3O	376.2383	NPS	Opioid	Fentalog	Parent	22
Ethylmorphine	C19H23NO3	314.1751	Drug of Abuse	Opioid	Other	Parent	17
Ethylone	C12H15NO3	222.1125	NPS	Stimulant	Cathinone	Parent	8
Ethylphenidate (EPH)	C15H21NO2	248.1645	NPS	Stimulant	Other	Parent	10
Eticyclidine (PCE)	C14H21N	204.1747	NPS	Hallucinogen	Other	Parent	7
Etilamfetamine (N-Ethylamphetamine)	C11H17N	164.1434	Drug of Abuse	Stimulant	Phenethylamine	Parent	3
Etizolam	C17H15ClN4S	343.0779	NPS	Benzodiazepine	Other	Parent	20
Etodolac	C17H21NO3	288.1594	Pharmaceutical	NSAID	Other	Parent	15
Eutylone (bk-EBDB)	C13H17NO3	236.1281	NPS	Stimulant	Cathinone	Parent	9
F-2201	C24H21F2NO	378.1664	NPS	Synthetic Cannabinoid	Other	Parent	22
FAB-144	C20H27FN2O	331.2180	NPS	Synthetic Cannabinoid	Other	Parent	19
FDU-NNEI	C26H19FN2O	395.1554	NPS	Synthetic Cannabinoid	Other	Parent	23
FDU-PB-22	C26H18FNO2	396.1394	NPS	Synthetic Cannabinoid	Other	Parent	23
Fenfluramine	C12H16F3N	232.1308	Pharmaceutical	Antiobesity	Other	Parent	9
Fentanyl	C22H28N2O	337.2274	Drug of Abuse	Opioid	Fentalog	Parent	19
Fentanyl Methyl Carbamate	C21H26N2O2	339.2067	NPS	Opioid	Fentalog	Parent	19
Flecainide	C17H20F6N2O3	415.1451	Pharmaceutical	Antiarrhythmic	Other	Parent	24
Flualprazolam	C17H12ClFN4	327.0807	NPS	Benzodiazepine	Other	Parent	18
Flubromazelam	C17H12BrFN4	371.0302	NPS	Benzodiazepine	Other	Parent	21
Flubromazepam	C15H10BrFN2O	333.0033	NPS	Benzodiazepine	Other	Parent	19
Flunitrazepam	C16H12FN3O3	314.0936	Pharmaceutical	Benzodiazepine	Other	Parent	17
Fluoroethamphetamine	C11H16FN	182.1340	NPS	Stimulant	Phenethylamine	Parent	5
Fluoroisobutyrylfentanyl	C23H29FN2O	369.2337	NPS	Opioid	Fentalog	Parent	21
Fluoro-JWH-019	C25H24FNO	374.1915	NPS	Synthetic Cannabinoid	Other	Parent	21
Fluoxetine	C17H18F3NO	310.1413	Pharmaceutical	Antidepressant	Other	Parent	16

Fluphenazine	C22H26F3N3OS	438.1822	Pharmaceutical	Antipsychotic	Other	Parent	25
Flurazepam	C21H23ClFN3O	388.1587	Pharmaceutical	Benzodiazepine	Other	Parent	23
Flutoprazepam	C19H16ClFN2O	343.1008	NPS	Benzodiazepine	Other	Parent	20
Fluvoxamine	C15H21F3N2O2	319.1628	Pharmaceutical	Anxiolytic	Other	Parent	18
FUB-144	C23H24FNO	350.1915	NPS	Synthetic Cannabinoid	Other	Parent	20
FUB-AKB-48	C25H26FN3O	404.2133	NPS	Synthetic Cannabinoid	Other	Parent	24
FUBIMINA N-pentanoic acid	C23H20N2O3	373.1547	NPS	Synthetic Cannabinoid	Other	Metabolite	21
FUB-JWH-018	C26H18FNO	380.1445	NPS	Synthetic Cannabinoid	Other	Parent	22
FUB-NPB-22	C24H16FN3O2	398.1299	NPS	Synthetic Cannabinoid	Other	Parent	23
FUB-PB-22	C25H17FN2O2	397.1347	NPS	Synthetic Cannabinoid	Other	Parent	23
FUB-PB-22 3-Carboxyindole	C16H12FNO2	270.0925	NPS	Synthetic Cannabinoid	Other	Metabolite	12
Furanylfentanyl	C24H26N2O2	375.2067	NPS	Opioid	Fentalog	Parent	21
Furanyl UF-17	C19H24N2O2	313.1911	NPS	Other	Other	Parent	17
Furanylethylfentanyl	C20H26N2O2	327.2067	NPS	Opioid	Fentalog	Parent	18
Gabapentin	C9H17NO2	172.1332	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Parent	4
Glimepiride	C24H34N4O5S	491.2323	Pharmaceutical	Other	Other	Parent	27
Glipizide	C21H27N5O4S	446.1857	Pharmaceutical	Hypoglycemic Agent	Other	Parent	25
Glutethimide	C13H15NO2	218.1176	Pharmaceutical	Hypnotic, Sedative	Other	Parent	8
Guaifenesin	C10H14O4	199.0965	Pharmaceutical	Expectorant	Other	Parent	7
Haloperidol	C21H23ClFNO2	376.1474	Pharmaceutical	Antipsychotic	Other	Parent	22
Hexanoylfentanyl	C25H34N2O	379.2744	NPS	Opioid	Fentalog	Parent	22
Hexedrone	C13H19NO	206.1539	NPS	Stimulant	Cathinone	Parent	7
HU-210/HU-211	C25H38O3	387.2894	NPS	Synthetic Cannabinoid	Other	Parent	23
HU-308	C27H42O3	415.3207	NPS	Synthetic Cannabinoid	Other	Parent	24
HU-331	C21H28O3	329.2111	NPS	Synthetic Cannabinoid	Other	Parent	19
Hydrocodone	C18H21NO3	300.1594	Drug of Abuse	Opioid	Other	Parent	15
Hydromorphone	C17H19NO3	286.1438	Drug of Abuse	Opioid	Other	Parent	14
Hydroxybupropion	C13H18ClNO2	256.1099	Pharmaceutical	Antidepressant	Other	Metabolite	11
Hydroxyethylflurazepam	C17H14ClFN2O2	333.0801	Pharmaceutical	Benzodiazepine	Other	Metabolite	19
Hydroxy-THC	C21H30O3	331.2268	Drug of Abuse	Cannabinoid	Other	Metabolite	19
Hydroxytriazolam	C17H12Cl2N4O	359.0461	Pharmaceutical	Benzodiazepine	Other	Metabolite	21
Hydroxyzine	C21H27ClN2O2	375.1834	Pharmaceutical	Antihistamine, Anxiolytic	Other	Parent	21
Iloperidone	C24H27FN2O4	427.2028	Pharmaceutical	Antipsychotic	Other	Parent	25
Imipramine	C19H24N2	281.2012	Pharmaceutical	Antidepressant	Other	Parent	13
IMMA (BML-190)	C23H23ClN2O4	427.1419	NPS	Synthetic Cannabinoid	Other	Parent	25
Indomethacin	C19H16ClNO4	358.0841	Pharmaceutical	NSAID	Other	Parent	21
Isobutyl-PINAC	C17H24N2O2	289.1911	NPS	Synthetic Cannabinoid	Other	Parent	15
Isobutyrylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
Isopropylphenidate	C16H23NO2	262.1802	NPS	Stimulant	Other	Parent	11
Isopropyl-U-47700	C18H26Cl2N2O	357.1495	NPS	Opioid	Utopioid	Parent	20
JWH-007	C25H25NO	356.2009	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-011	C27H29NO	384.2322	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-015	C23H21NO	328.1696	NPS	Synthetic Cannabinoid	Other	Parent	18
JWH-016	C24H23NO	342.1852	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-018	C24H23NO	342.1852	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-018 6-Methoxyindole Analogue	C25H25NO2	372.1958	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	358.1914	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-018 Benzimidazole Analogue	C23H22N2O	343.1805	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	342.1852	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	356.1645	NPS	Synthetic Cannabinoid	Other	Parent	20

JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	420.0958	NPS	Synthetic Cannabinoid	Other	Parent	25
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	376.1463	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-018 N-Pentanoic Acid	C24H21NO3	372.1594	NPS	Synthetic Cannabinoid	Other	Metabolite	21
JWH-019	C25H25NO	356.2009	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-020	C26H27NO	370.2165	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-022	C24H21NO	340.1696	NPS	Synthetic Cannabinoid	Other	Parent	19
JWH-030	C20H21NO	292.1696	NPS	Synthetic Cannabinoid	Other	Parent	15
JWH-031	C21H23NO	306.1852	NPS	Synthetic Cannabinoid	Other	Parent	16
JWH-071	C21H17NO	300.1383	NPS	Synthetic Cannabinoid	Other	Parent	15
JWH-072	C22H19NO	314.1539	NPS	Synthetic Cannabinoid	Other	Parent	17
JWH-073	C23H21NO	328.1696	NPS	Synthetic Cannabinoid	Other	Parent	18
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	342.1852	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-073 6-Methoxyindole Analogue	C24H23NO2	358.1802	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-080	C24H23NO2	358.1802	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-081	C25H25NO2	372.1958	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	398.2115	NPS	Synthetic Cannabinoid	Other	Parent	23
JWH-098	C26H27NO2	386.2115	NPS	Synthetic Cannabinoid	Other	Parent	23
JWH-116	C26H27NO	370.2165	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-122	C25H25NO	356.2009	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	354.1852	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-133	C22H32O	313.2526	NPS	Synthetic Cannabinoid	Other	Parent	17
JWH-145	C26H25NO	368.2009	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-146	C28H29NO	396.2322	NPS	Synthetic Cannabinoid	Other	Parent	23
JWH-147	C27H27NO	382.2165	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-149	C26H27NO	370.2165	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-167	C21H23NO	306.1852	NPS	Synthetic Cannabinoid	Other	Parent	16
JWH-175	C24H25N	328.2060	NPS	Synthetic Cannabinoid	Other	Parent	18
JWH-176	C25H24	325.1951	NPS	Synthetic Cannabinoid	Other	Parent	18
JWH-180	C25H25NO	356.2009	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-182	C27H29NO	384.2322	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-193	C26H26N2O2	399.2067	NPS	Synthetic Cannabinoid	Other	Parent	23
JWH-198	C26H26N2O3	415.2016	NPS	Synthetic Cannabinoid	Other	Parent	24
JWH-200	C25H24N2O2	385.1911	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-200 Analogue	C22H30N2O2	355.2380	NPS	Synthetic Cannabinoid	Other	Parent	20
JWH-201	C22H25NO2	336.1958	NPS	Synthetic Cannabinoid	Other	Parent	19
JWH-203	C21H22ClNO	340.1475	NPS	Synthetic Cannabinoid	Other	Parent	19
JWH-210	C26H27NO	370.2165	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-213	C27H29NO	384.2322	NPS	Synthetic Cannabinoid	Other	Parent	22

JWH-249	C21H22BrNO	384.0958	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-250	C22H25NO2	336.1958	NPS	Synthetic Cannabinoid	Other	Parent	19
JWH-251	C22H25NO	320.2009	NPS	Synthetic Cannabinoid	Other	Parent	18
JWH-302	C22H25NO2	336.1958	NPS	Synthetic Cannabinoid	Other	Parent	19
JWH-307	C26H24FNO	386.1915	NPS	Synthetic Cannabinoid	Other	Parent	23
JWH-309	C30H27NO	418.2165	NPS	Synthetic Cannabinoid	Other	Parent	25
JWH-368	C26H24FNO	386.1915	NPS	Synthetic Cannabinoid	Other	Parent	23
JWH-369	C26H24ClNO	402.1619	NPS	Synthetic Cannabinoid	Other	Parent	24
JWH-370	C27H27NO	382.2165	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-387	C24H22BrNO	420.0958	NPS	Synthetic Cannabinoid	Other	Parent	25
JWH-398	C24H22ClNO	376.1463	NPS	Synthetic Cannabinoid	Other	Parent	22
JWH-412	C24H22FNO	360.1758	NPS	Synthetic Cannabinoid	Other	Parent	21
JWH-424	C24H22BrNO	420.0958	NPS	Synthetic Cannabinoid	Other	Parent	25
Ketamine	C13H16ClNO	238.0993	Drug of Abuse	Hallucinogen	Other	Parent	9
Ketoprofen	C16H14O3	255.1016	Pharmaceutical	NSAID	Other	Parent	11
KM 233	C25H30O2	363.2319	NPS	Synthetic Cannabinoid	Other	Parent	21
Lacosamide	C13H18N2O3	251.1390	Pharmaceutical	Anticonvulsant	Other	Parent	10
Lamotrigine	C9H7N5Cl2	256.0151	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Parent	11
Levamisole	C11H12N2S	205.0794	Pharmaceutical	Antihelmintic	Cutting Agent	Parent	7
Levetiracetam	C8H14N2O2	171.1128	Pharmaceutical	Antiepileptic	Other	Parent	4
Lidocaine	C14H22N2O	235.1805	Pharmaceutical	Antiarrhythmic	Cutting Agent	Parent	9
Lisdexamphetamine	C15H25N3O	264.2070	Pharmaceutical	Stimulant	Phenethylamine	Parent	12
Loperamide	C29H33ClN2O2	477.2303	Pharmaceutical	Antidiarrheal	Other	Parent	26
Lorazepam	C15H10Cl2N2O2	321.0192	Drug of Abuse	Benzodiazepine	Other	Parent	18
Loxapine	C18H18ClN3O	328.1211	Pharmaceutical	Benzodiazepine	Other	Parent	18
LSD	C20H25N3O	324.2070	Drug of Abuse	Hallucinogen	Other	Parent	18
M-144	C22H30FNO	344.2384	NPS	Synthetic Cannabinoid	Other	Parent	20
MAB-CHMINACA	C21H30N4O2	371.2442	NPS	Synthetic Cannabinoid	Other	Parent	21
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	372.2282	NPS	Synthetic Cannabinoid	Other	Metabolite	21
MA-CHMINACA	C21H29N3O3	372.2282	NPS	Synthetic Cannabinoid	Other	Parent	21
MAM-2201	C25H24FNO	374.1915	NPS	Synthetic Cannabinoid	Other	Parent	21
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	390.1619	NPS	Synthetic Cannabinoid	Other	Parent	23
Maprotiline	C20H23N	278.1903	Pharmaceutical	Antidepressant	Other	Parent	13
MBDB	C12H17NO2	208.1332	NPS	Stimulant	Phenethylamine	Parent	7
MBZP	C12H18N2	191.1543	NPS	Stimulant	Piperazine	Parent	6
MCHB-1	C28H37N3O2	448.2959	NPS	Synthetic Cannabinoid	Other	Parent	25
mCPP	C10H13ClN2	197.0840	Pharmaceutical	Antidepressant	Other	Metabolite	7
MDA	C10H13NO2	180.1019	Drug of Abuse	Stimulant	Phenethylamine	Parent	5
MDA 19	C21H23N3O2	350.1863	NPS	Synthetic Cannabinoid	Other	Parent	20
MDA 77	C21H23N3O3	366.1812	NPS	Synthetic Cannabinoid	Other	Parent	21
MDAI (5,6-Methylenedioxy-2-aminoindane)	C10H11NO2	178.0863	NPS	Stimulant	Other	Parent	4
MDEA	C12H17NO2	208.1332	Drug of Abuse	Stimulant	Phenethylamine	Parent	7
MDMA	C11H15NO2	194.1176	Drug of Abuse	Stimulant	Phenethylamine	Parent	6
MDMA-D5	C11H10[2H]5NO2	199.1489	ISTD	Stimulant	Phenethylamine	Parent	7
MDMB-4en-PINACA	C20H27N3O3	358.2125	NPS	Synthetic Cannabinoid	Other	Parent	21
MDMB-CHMCZCA	C27H34N2O3	435.2642	NPS	Synthetic Cannabinoid	Other	Parent	25
MDMB-CHMICA	C23H32N2O3	385.2486	NPS	Synthetic Cannabinoid	Other	Parent	22

MDMB-CHMINACA	C22H31N3O3	386.2438	NPS	Synthetic Cannabinoid	Other	Parent	23
MDMB-FUBICA	C23H25FN2O3	397.1922	NPS	Synthetic Cannabinoid	Other	Parent	23
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	383.1766	NPS	Synthetic Cannabinoid	Other	Metabolite	22
MDMB-FUBINACA	C22H24FN3O3	398.1875	NPS	Synthetic Cannabinoid	Other	Parent	23
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	384.1718	NPS	Synthetic Cannabinoid	Other	Metabolite	22
MDPBP	C15H19NO3	262.1438	NPS	Stimulant	Cathinone	Parent	11
MDPPP	C14H17NO3	248.1281	NPS	Stimulant	Cathinone	Parent	10
MDPV	C16H21NO3	276.1594	NPS	Stimulant	Cathinone	Parent	13
Mebroqualone	C15H11BrN2O	315.0128	NPS	Other	Other	Parent	17
Medazepam	C16H15ClN2	271.0997	Pharmaceutical	Benzodiazepine	Other	Parent	12
Memantine	C12H21N	180.1747	Pharmaceutical	Other	Other	Parent	5
MeO-MDA	C11H15NO3	210.1125	NPS	Stimulant	Phenethylamine	Parent	8
Meperidine	C15H21NO2	248.1645	Pharmaceutical	Analgesic, Anesthetic	Other	Parent	10
Mephedrone	C11H15NO	178.1226	NPS	Stimulant	Cathinone	Parent	4
Mepirapim	C19H27N3O	314.2227	NPS	Synthetic Cannabinoid	Other	Parent	17
Mepivacaine	C15H22N2O	247.1805	Pharmaceutical	Analgesic	Other	Parent	10
MePPP	C14H19NO	218.1539	NPS	Stimulant	Cathinone	Parent	8
Meprobamate	C9H18N2O4	219.1339	Pharmaceutical	Muscle Relaxant	Other	Parent	8
Mescaline	C11H17NO3	212.1281	Drug of Abuse	Hallucinogen	Phenethylamine	Parent	8
Mesoridazine	C21H26N2OS2	387.1559	Pharmaceutical	Other	Other	Parent	23
Metaxalone	C12H15NO3	222.1125	Pharmaceutical	Muscle Relaxant	Other	Parent	8
Methacrylfentanyl	C23H28N2O	349.2274	NPS	Opioid	Fentalog	Parent	20
Methadone	C21H27NO	310.2165	Drug of Abuse	Opioid	Other	Parent	16
Methamphetamine	C10H15N	150.1277	Drug of Abuse	Stimulant	Phenethylamine	Parent	2
Methaqualone	C16H14N2O	251.1179	Pharmaceutical	Hypnotic, Sedative	Other	Parent	10
Methcathinone	C10H13NO	164.1070	NPS	Stimulant	Cathinone	Parent	3
Methedrone	C11H15NO2	194.1176	NPS	Stimulant	Cathinone	Parent	6
Methiopropamine	C8H13NS	156.0842	Drug of Abuse	Stimulant	Other	Parent	2
Methocarbamol	C11H15NO5	242.1023	Pharmaceutical	Muscle Relaxant	Other	Parent	10
Methohexital	C14H18N2O3	263.1390	Pharmaceutical	Anaesthetics	Other	Parent	11
Methoxetamine	C15H21NO2	248.1645	NPS	Dissociative	Other	Parent	10
Methoxyacetylfentanyl	C22H28N2O2	353.2224	NPS	Opioid	Fentalog	Parent	20
Methylenedioxy-alpha-PHP	C17H23NO3	290.1751	NPS	Stimulant	Cathinone	Parent	15
Methylenedioxy-U-47700	C17H24N2O3	305.1860	NPS	Opioid	Utopioid	Parent	16
Methylone	C11H13NO3	208.0968	NPS	Stimulant	Cathinone	Parent	7
Methylone-D3	C11H10[2H]3NO3	211.1157	ISTD	Stimulant	Cathinone	Parent	8
Methylphenidate	C14H19NO2	234.1489	Pharmaceutical	Stimulant	Other	Parent	9
Metoclopramide	C14H22ClN3O2	300.1473	Pharmaceutical	Antiemetic	Other	Parent	15
Mexiletine	C11H17NO	180.1383	Pharmaceutical	Antiarrhythmic	Other	Parent	5
MFUBINAC	C16H13FN2O2	285.1034	NPS	Synthetic Cannabinoid	Other	Parent	14
Midazolam	C18H13ClFN3	326.0855	Pharmaceutical	Benzodiazepine	Other	Parent	18
Mirtazapine	C17H19N3	266.1652	Pharmaceutical	Antidepressant	Other	Parent	12
Mitragynine	C23H30N2O4	399.2278	NPS	Alkaloid	Natural	Parent	23
MMB-018	C20H28N2O3	345.2173	NPS	Synthetic Cannabinoid	Other	Parent	20
MMB-022	C20H26N2O3	343.2016	NPS	Synthetic Cannabinoid	Other	Parent	20
MMB-2201	C20H27FN2O3	363.2079	NPS	Synthetic Cannabinoid	Other	Parent	21
MMB-CHMICA	C22H30N2O3	371.2329	NPS	Synthetic Cannabinoid	Other	Parent	21
MMB-FUBICA	C22H23FN2O3	383.1766	NPS	Synthetic Cannabinoid	Other	Parent	22
MMB-FUBINACA	C21H22FN3O3	384.1718	NPS	Synthetic Cannabinoid	Other	Parent	22
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	370.1562	NPS	Synthetic Cannabinoid	Other	Metabolite	21
MN-18	C23H23N3O	358.1914	NPS	Synthetic Cannabinoid	Other	Parent	21
MN-25	C26H37N3O3	440.2912	NPS	Synthetic Cannabinoid	Other	Parent	25
MN-25 2-Methyl Derivative	C27H39N3O3	454.3064	NPS	Synthetic Cannabinoid	Other	Parent	26
MO-CHMINACA	C22H30N2O4	387.2278	NPS	Synthetic Cannabinoid	Other	Parent	23
Modafinil	C15H15NO2S	274.0896	Pharmaceutical	Antipsychotic	Other	Parent	13

Monoethylglycinexylidide (MEGX)	C12H18N2O	207.1492	Pharmaceutical	Antiarrhythmic	Cutting Agent	Metabolite	7
MOPPP	C14H19NO2	234.1489	NPS	Stimulant	Cathinone	Parent	9
Morphine	C17H19NO3	286.1438	Drug of Abuse	Opiate	Other	Parent	14
Morphine-D3	C17H16[2H]3NO3	289.1626	ISTD	Opiate	Other	Parent	15
MPBP	C15H21NO	232.1695	NPS	Stimulant	Cathinone	Parent	9
MPHP	C17H25NO	260.2009	NPS	Stimulant	Cathinone	Parent	11
MT-45	C24H32N2	349.2638	NPS	Opioid	Other	Parent	20
N,N-Didesmethyl U-47700	C14H18Cl2N2O	301.0869	Drug of Abuse	Opioid	Utopioid	Metabolite	16
N-Acetyl 25I-NBOMe	C20H24INO4	470.0823	NPS	Hallucinogen	Phenethylamine	Parent	26
Nalbuphine	C21H27NO4	358.2013	Pharmaceutical	Opioid	Other	Parent	21
Naloxone	C19H21NO4	328.1543	Pharmaceutical	Antagonist - Opioid	Other	Parent	18
Naltrexone	C20H23NO4	342.1700	Pharmaceutical	Antagonist - Opioid	Other	Parent	20
Naphyrone	C19H23NO	282.1852	NPS	Stimulant	Cathinone	Parent	13
Naproxen	C14H14O3	231.1016	Pharmaceutical	NSAID	Other	Parent	9
N-Benzyl-3,4-DMA	C18H23NO2	286.1802	NPS	Stimulant	Phenethylamine	Parent	14
N-Butyl Hexedrone	C16H25NO	248.2009	NPS	Stimulant	Cathinone	Parent	10
N-Butyl Pentylone	C16H23NO3	278.1751	NPS	Stimulant	Cathinone	Parent	13
N-Desmethyl Loperamide	C28H31ClN2O2	463.2148	Pharmaceutical	Antidiarrheal	Other	Metabolite	26
N-Desmethyl U-47700	C15H20Cl2N2O	315.1026	NPS	Opioid	Utopioid	Metabolite	17
N-Ethyl Deschloroketamine	C14H19NO	218.1539	NPS	Dissociative	Other	Parent	8
N-Ethyl Hexedrone (Hexen)	C14H21NO	220.1696	NPS	Stimulant	Cathinone	Parent	8
N-Ethyl Hexylone	C15H21NO3	264.1594	NPS	Stimulant	Cathinone	Parent	12
N-Ethyl Pentylone	C14H19NO3	250.1438	NPS	Stimulant	Cathinone	Parent	10
N-Ethyl Phenethylamine	C10H15N	150.1277	NPS	Stimulant	Phenethylamine	Parent	2
N-Ethylbuphedrone (NEB)	C12H17NO	192.1383	NPS	Stimulant	Cathinone	Parent	6
Nicotine	C10H14N2	163.1230	Incidental	Stimulant	Other	Parent	3
Nifedipine	C17H18N2O6	347.1238	Drug of Abuse	Antihypertensive	Other	Parent	20
Nimetazepam	C16H13N3O3	296.1029	Pharmaceutical	Benzodiazepine	Other	Parent	15
Nitrazolam	C17H13N5O2	320.1142	NPS	Benzodiazepine	Other	Parent	18
NM-2201	C24H22FNO2	376.1707	NPS	Synthetic Cannabinoid	Other	Parent	22
N-methyl Carfentanyl	C17H24N2O3	305.1860	NPS	Opioid	Fentalog	Precursor	16
N-methyl Cyclopropylnorfentanyl	C16H22N2O	259.1805	NPS	Opioid	Fentalog	Precursor	11
N-methyl Norfentanyl	C15H22N2O	247.1805	NPS	Opioid	Fentalog	Precursor	10
N-Methyl U-47931E	C16H23BrN2O	339.1067	NPS	Opioid	Utopioid	Parent	19
N-Methyltryptamine (NMT)	C11H14N2	175.1230	NPS	Hallucinogen	Tryptamine	Parent	4
NNEI	C24H24N2O	357.1961	NPS	Synthetic Cannabinoid	Other	Parent	20
Norbuprenorphine	C25H35NO4	414.2639	Pharmaceutical	Opioid	Other	Metabolite	24
Norcarfentanil	C16H22N2O3	291.1703	NPS	Opioid	Fentalog	Metabolite	15
Norclozapine	C17H17ClN4	313.1215	Pharmaceutical	Antipsychotic	Other	Metabolite	17
Norcocaine	C16H19NO4	290.1387	Drug of Abuse	Stimulant	Other	Metabolite	15
Norcodeine	C17H19NO3	286.1438	Drug of Abuse	Opiate	Other	Parent	14
Nordiazepam	C15H11ClON2	271.0633	Drug of Abuse	Benzodiazepine	Other	Metabolite	12
Norfentanyl	C14H20N2O	233.1648	Drug of Abuse	Opioid	Fentalog	Metabolite	9
Norflunitrazepam	C15H10FN3O3	300.0779	Pharmaceutical	Benzodiazepine	Other	Metabolite	15
Norfluoxetine	C16H16F3NO	296.1257	Pharmaceutical	Antidepressant	Other	Metabolite	15
Norfuranylfentanyl	C16H18N2O2	271.1441	NPS	Opioid	Fentalog	Metabolite	12
Norketamine	C12H14ClNO	224.0837	Drug of Abuse	Hallucinogen	Other	Metabolite	8
Normeperidine	C14H19NO2	234.1489	Pharmaceutical	Analgesic, Anesthetic	Other	Metabolite	9
Noroxycodone	C17H19NO4	302.1387	Drug of Abuse	Opioid	Other	Metabolite	16
Norpropoxyphene	C21H27NO2	326.2115	Pharmaceutical	Analgesic	Other	Metabolite	18
Norpseudoephedrine / Phenylpropanolamine	C9H13NO	152.1070	Incidental	Antihistamine, Decongestant	Other	Parent	2
Nortriptyline	C19H21N	264.1747	Pharmaceutical	Antidepressant	Other	Metabolite	12
Noscapine	C22H23NO7	414.1547	Drug of Abuse	Opiate	Alkaloid	Parent	24
NPB-22	C22H21N3O2	360.1707	NPS	Synthetic Cannabinoid	Other	Parent	21
NPP	C13H17NO	204.1383	NPS	Opioid	Fentalog	Precursor	7
N-Propyl Pentedrone	C14H21NO	220.1696	NPS	Stimulant	Cathinone	Parent	8
N-Propylamphetamine	C12H19N	178.1590	ISTD	Stimulant	Phenethylamine	Parent	4
Ocfentanil	C22H27FN2O2	371.2129	NPS	Opioid	Fentalog	Parent	21
O-Desmethyltramadol	C15H23NO2	250.1802	Drug of Abuse	Opioid	Other	Metabolite	10
O-Desmethylvenlafaxine	C16H25NO2	264.1958	Pharmaceutical	Antidepressant	Other	Metabolite	12
Olanzapine	C17H20N4S	313.1482	Pharmaceutical	Antipsychotic	Other	Parent	17
Oliceridine	C22H30N2O2S	387.2101	Pharmaceutical	Opioid	Other	Parent	23
ORG 28611	C23H33N3O2	384.2646	NPS	Synthetic Cannabinoid	Other	Parent	22
Orphenadrine	C18H23NO	270.1852	Pharmaceutical	Antihistamine	Other	Parent	12

ortho-Fluorofuranylfentanyl	C24H25FN2O2	393.1973	NPS	Opioid	Fentalog	Parent	23
ortho-Isopropylfuranylfentanyl	C27H32N2O2	417.2537	NPS	Opioid	Fentalog	Parent	25
ortho-Methoxyfuranylfentanyl	C25H28N2O3	405.2173	NPS	Opioid	Fentalog	Parent	24
ortho-Methylacrylfentanyl	C23H28N2O	349.2274	NPS	Opioid	Fentalog	Parent	20
ortho-Methylfuranylfentanyl	C25H28N2O2	389.2224	NPS	Opioid	Fentalog	Parent	23
ortho-Methylmethoxyfentanyl	C23H30N2O2	367.2380	NPS	Opioid	Fentalog	Parent	21
ortho-Methylacetylfentanyl	C22H28N2O	337.2274	NPS	Opioid	Fentalog	Parent	19
Oxazepam	C15H11ClN2O2	287.0582	Drug of Abuse	Benzodiazepine	Other	Metabolite	14
Oxycodone	C18H21NO4	316.1543	Drug of Abuse	Opioid	Other	Parent	17
Oxymorphone	C17H19NO4	302.1387	Drug of Abuse	Opioid	Other	Parent	16
Papaverine	C20H21NO4	340.1543	Drug of Abuse	Opiate	Alkaloid	Parent	19
para-Chloroacrylfentanyl	C22H25ClN2O	369.1728	NPS	Opioid	Fentalog	Parent	21
para-Chlorocyclopentylfentanyl	C25H31ClN2O	411.2198	NPS	Opioid	Fentalog	Parent	24
para-Chlorocyclopropylfentanyl	C23H27ClN2O	383.1885	NPS	Opioid	Fentalog	Parent	22
para-Chlorofuranylfentanyl	C24H25ClN2O2	409.1677	NPS	Opioid	Fentalog	Parent	24
para-Chlorovalerylfentanyl	C24H31ClN2O	399.2198	NPS	Opioid	Fentalog	Parent	23
para-Chloroisobutyrylfentanyl	C23H29ClN2O	385.2041	NPS	Opioid	Fentalog	Parent	22
Para-Fluoro-4-ANBP	C18H21FN2	285.1762	NPS	Opioid	Fentalog	Precursor	14
para-Fluoroacetylfentanyl	C21H25FN2O	341.2024	NPS	Opioid	Fentalog	Parent	20
para-Fluorocyclopropylfentanyl	C23H27FN2O	367.2180	NPS	Opioid	Fentalog	Parent	21
para-Fluorovalerylfentanyl	C24H31FN2O	383.2493	NPS	Opioid	Fentalog	Parent	22
para-Fluoroacrylfentanyl	C22H25FN2O	353.2024	NPS	Opioid	Fentalog	Parent	20
para-Fluorobutyrylfentanyl	C23H29FN2O	369.2337	NPS	Opioid	Fentalog	Parent	21
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	353.2024	NPS	Opioid	Fentalog	Precursor	20
para-Fluorofentanyl	C22H27FN2O	355.2180	NPS	Opioid	Fentalog	Parent	20
para-Methoxyacrylfentanyl	C23H28N2O2	365.2224	NPS	Opioid	Fentalog	Parent	21
para-Methoxyfentanyl	C23H30N2O2	367.2380	NPS	Opioid	Fentalog	Parent	21
para-Methoxymethoxyacetylfentanyl	C23H30N2O3	383.2329	NPS	Opioid	Fentalog	Parent	22
para-Methoxyacetylfentanyl	C22H28N2O2	353.2224	NPS	Opioid	Fentalog	Parent	20
para-Methylacrylfentanyl	C23H28N2O	349.2274	NPS	Opioid	Fentalog	Parent	20
para-Methylcyclopropylfentanyl	C24H30N2O	363.2431	NPS	Opioid	Fentalog	Parent	21
para-Methylfentanyl	C23H30N2O	351.2430	NPS	Opioid	Fentalog	Parent	20
para-Methylisobutyrylfentanyl	C24H32N2O	365.2587	NPS	Opioid	Fentalog	Parent	21
para-Methyltetrahydrofuranylfentanyl	C25H32N2O2	393.2537	NPS	Opioid	Fentalog	Parent	23
para-Methylacetylfentanyl	C22H28N2O	337.2274	NPS	Opioid	Fentalog	Parent	19
Paroxetine	C19H20FNO3	330.1500	Pharmaceutical	Antidepressant	Other	Parent	19
PB-22	C23H22N2O2	359.1754	NPS	Synthetic Cannabinoid	Other	Parent	21
PB-22 3-Carboxyindole	C14H17NO2	232.1332	NPS	Synthetic Cannabinoid	Other	Metabolite	9
Pentazocine	C19H27NO	286.2165	Pharmaceutical	Opioid	Other	Parent	14
Pentedrone	C12H17NO	192.1383	NPS	Stimulant	Cathinone	Parent	6
Pentylone	C13H17NO3	236.1281	NPS	Stimulant	Cathinone	Parent	9
Perphenazine	C21H26ClN3OS	404.1558	Pharmaceutical	Antipsychotic	Other	Parent	24
PF-03550096	C19H28N4O4	377.2183	NPS	Synthetic Cannabinoid	Other	Parent	22
Phenacetin	C10H13NO2	180.1019	Pharmaceutical	Analgesic	Cutting Agent	Parent	5
Phenazepam	C15H10BrClN2O	348.9738	NPS	Benzodiazepine	Other	Parent	20
Phenazolam	C17H12BrClN4	387.0007	NPS	Benzodiazepine	Other	Parent	23
Phencyclidine (PCP)	C17H25N	244.2060	Drug of Abuse	Hallucinogen	Other	Parent	10
Phendimetrazine	C12H17NO	192.1383	Pharmaceutical	Stimulant	Other	Parent	6
Phenibut	C10H13NO2	180.1019	Pharmaceutical	Depressant	Other	Parent	5
Pheniramine	C16H20N2	241.1699	Pharmaceutical	Antihistamine	Other	Parent	10
Phenmetrazine	C11H15NO	178.1226	Pharmaceutical	Stimulant	Other	Parent	4
Phenpromethamine	C10H15N	150.1277	Drug of Abuse	Stimulant	Phenethylamine	Parent	2
Phensuximide	C11H11NO2	190.0863	Pharmaceutical	Anticonvulsant	Other	Parent	5
Phentermine	C10H15N	150.1277	Drug of Abuse	Stimulant	Phenethylamine	Parent	2
Phenylfentanyl	C26H28N2O	385.2274	NPS	Opioid	Fentalog	Parent	22
Phenylacetylfentanyl	C27H30N2O	399.2431	NPS	Opioid	Fentalog	Parent	23
Phenyltoloxamine	C17H21NO	256.1696	Pharmaceutical	Antihistamine	Other	Parent	11
Phenytoin	C15H12N2O2	253.0972	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Parent	10
Pivaloylfentanyl	C24H32N2O	365.2587	NPS	Opioid	Fentalog	Parent	21
PMA (para-Methoxyamphetamine)	C10H15NO	166.1226	NPS	Stimulant	Phenethylamine	Parent	3
PMMA (para-Methoxymethamphetamine)	C11H17NO	180.1383	NPS	Stimulant	Phenethylamine	Parent	5
Pramiracetam	C14H27N3O2	270.2176	Pharmaceutical	Nootropic	Other	Parent	12
Pravadoline (WIN-48,098)	C23H26N2O3	379.2016	NPS	Synthetic Cannabinoid	Other	Parent	22

Primidone	C12H14N2O2	219.1128	Pharmaceutical	Anticonvulsant	Other	Parent	8
Procainamide	C13H21N3O	236.1757	Pharmaceutical	Antiarrhythmic	Other	Parent	9
Prochlorperazine	C20H24ClN3S	374.1452	Pharmaceutical	Antipsychotic	Other	Parent	21
Promazine	C17H20N2S	285.1420	Pharmaceutical	Antipsychotic	Other	Parent	14
Promethazine	C17H20N2S	285.1420	Pharmaceutical	Antihistamine	Other	Parent	14
Propoxyphene	C22H29NO2	340.2271	Pharmaceutical	Analgesic	Other	Parent	19
Propylone	C13H17NO3	236.1281	NPS	Stimulant	Cathinone	Parent	9
Propyl-U-47700	C18H26Cl2N2O	357.1495	NPS	Opioid	Utopioid	Parent	20
Protriptyline	C19H21N	264.1747	Pharmaceutical	Antidepressant	Other	Parent	12
PSB-SB1202	C23H26O4	367.1904	NPS	Synthetic Cannabinoid	Other	Parent	21
Psilocin	C12H16N2O	205.1335	Drug of Abuse	Hallucinogen	Tryptamine	Parent	7
Psilocybin	C12H17N2O4P	285.0999	Drug of Abuse	Hallucinogen	Tryptamine	Parent	14
PTI-1	C21H29N3S	356.2155	NPS	Synthetic Cannabinoid	Other	Parent	20
PTI-2	C23H33N3OS	400.2417	NPS	Synthetic Cannabinoid	Other	Parent	23
PX1	C23H26FN3O2	396.2082	NPS	Synthetic Cannabinoid	Other	Parent	23
PX2	C22H25FN4O2	397.2034	NPS	Synthetic Cannabinoid	Other	Parent	23
Pyrazolam	C16H12BrN5	354.0348	NPS	Benzodiazepine	Other	Parent	20
Pyrilamine	C17H23N3O	286.1914	Pharmaceutical	Antihistamine	Other	Parent	14
Pyrovalerone	C16H23NO	246.1852	NPS	Stimulant	Cathinone	Parent	10
Quetiapine	C21H25N3O2S	384.1740	Pharmaceutical	Antipsychotic	Other	Parent	22
Quinidine	C20H24N2O2	325.1911	Pharmaceutical	Antiarrhythmic	Other	Parent	18
Quinine	C20H24N2O2	325.1911	Incidental	Antimalarial	Cutting Agent	Parent	18
Ramelteon	C16H21NO2	260.1645	Pharmaceutical	Sleep Agent	Other	Parent	11
RCS-4	C21H23NO2	322.1802	NPS	Synthetic Cannabinoid	Other	Parent	18
RCS-4 C4 Homolog	C20H21NO2	308.1645	NPS	Synthetic Cannabinoid	Other	Parent	16
RCS-8	C25H29NO2	376.2271	NPS	Synthetic Cannabinoid	Other	Parent	22
Remifentanyl Acid	C18H26N2O5	363.1914	Pharmaceutical	Opioid	Fentalog	Metabolite	21
Risperidone	C23H27FN4O2	411.2191	Pharmaceutical	Antipsychotic	Other	Parent	24
Rolicyclidine	C16H23N	230.1903	NPS	Dissociative	Other	Parent	9
Ropivacaine	C17H26N2O	275.2118	Pharmaceutical	Anesthetic	Other	Parent	13
Salvinorin A	C23H28O8	433.1857	Drug of Abuse	Hallucinogen	Natural	Parent	25
Salvinorin B	C21H26O7	391.1751	Drug of Abuse	Hallucinogen	Natural	Parent	23
SBD-006	C21H24N2O	321.1961	NPS	Synthetic Cannabinoid	Other	Parent	18
Scopolamine	C17H21NO4	304.1543	Pharmaceutical	Anesthetic	Other	Parent	16
SDB-005	C23H22N2O2	359.1754	NPS	Synthetic Cannabinoid	Other	Parent	21
SDB-006 N-Phenyl Analogue	C20H22N2O	307.1805	NPS	Synthetic Cannabinoid	Other	Parent	16
Senecioylfentanyl	C24H30N2O	363.2431	NPS	Opioid	Fentalog	Parent	21
SER-601	C28H38N2O2	435.3006	NPS	Synthetic Cannabinoid	Other	Parent	25
Sertraline	C17H17Cl2N	306.0811	Pharmaceutical	Antidepressant	Other	Parent	16
Sibutramine	C17H26ClN	280.1827	Pharmaceutical	Stimulant	Phenethylamine	Parent	13
Sildenafil	C22H30N6O4S	475.2122	Pharmaceutical	Erectile Dysfunction	Other	Parent	26
ß-Hydroxythiofentanyl	C20H26N2O2S	359.1788	NPS	Opioid	Fentalog	Parent	21
Strychnine	C21H22N2O2	335.1754	Incidental	Pesticide	Other	Parent	19
STS-135	C24H31FN2O	383.2493	NPS	Synthetic Cannabinoid	Other	Parent	22
Sufentanil	C22H30N2O2S	387.2101	Pharmaceutical	Opioid	Fentalog	Parent	23
Tadalafil	C22H19N3O4	390.1448	Pharmaceutical	Erectile Dysfunction	Other	Parent	23
Tapentadol	C14H23NO	222.1852	Pharmaceutical	Opioid	Other	Parent	8
Temazepam	C16H13ClN2O2	301.0738	Drug of Abuse	Benzodiazepine	Other	Metabolite	16
Tertylone	C14H19NO3	250.1438	NPS	Stimulant	Cathinone	Parent	10
Tetrahydrofuranylfentanyl	C24H30N2O2	379.2380	NPS	Opioid	Fentalog	Parent	22
Tetrahydrothiophenefentanyl	C24H30N2OS	395.2152	NPS	Opioid	Fentalog	Parent	23
Tetrahydrozoline	C13H16N2	201.1386	Pharmaceutical	Vasoconstrictor	Other	Parent	7
Tetramethylcyclopropylfentanyl	C27H36N2O	405.2900	NPS	Opioid	Fentalog	Parent	24
TFMPP	C11H13F3N2	231.1104	NPS	Stimulant	Piperazine	Parent	9
THC	C21H30O2	315.2319	Drug of Abuse	Cannabinoid	Other	Parent	17
THCA	C22H30O4	359.2217	NPS	Synthetic Cannabinoid	Other	Parent	21
Thebaine	C19H21NO3	312.1594	Pharmaceutical	Opioid	Other	Parent	17
Theophylline	C7H8N4O2	181.0720	Pharmaceutical	Bronchodilator	Other	Parent	5
Thienylfentanyl	C19H24N2OS	329.1682	NPS	Opioid	Fentalog	Parent	19

Thiofentanyl	C20H26N2OS	343.1838	NPS	Opioid	Fentalog	Parent	20
Thiophenefentanyl	C24H26N2OS	391.1839	NPS	Opioid	Fentalog	Parent	23
Thioridazine	C21H26N2S2	371.1610	Pharmaceutical	Antipsychotic	Other	Parent	21
THJ	C22H22N4O	359.1866	NPS	Synthetic Cannabinoid	Other	Parent	21
THJ-018	C23H22N2O	343.1805	NPS	Synthetic Cannabinoid	Other	Parent	20
THJ-2201	C23H21FN2O	361.1711	NPS	Synthetic Cannabinoid	Other	Parent	21
Tianeptine	C21H25ClN2O4S	437.1296	Pharmaceutical	Antidepressant	Other	Parent	25
Ticlopidine	C14H14ClNS	264.0608	Pharmaceutical	Other	Other	Parent	12
Topiramate	C12H21NO8S	340.1061	Pharmaceutical	Anticonvulsant, Antiepileptic	Other	Parent	19
Tramadol	C16H25NO2	264.1958	Drug of Abuse	Opioid	Other	Parent	12
Tranylcypromine	C9H11N	134.0964	Pharmaceutical	Antidepressant	Other	Parent	2
Trazodone	C19H22ClN5O	372.1586	Pharmaceutical	Antidepressant	Other	Parent	21
Triazolam	C17H12Cl2N4	343.0512	Pharmaceutical	Benzodiazepine	Other	Parent	20
Trifluoperazine	C21H24F3N3S	408.1716	NPS	Synthetic Cannabinoid	Other	Parent	24
Trihexyphenidyl	C20H31NO	302.2478	Pharmaceutical	Antimuscarinic	Other	Parent	16
Trimipramine	C20H26N2	295.2169	Pharmaceutical	Antidepressant	Other	Parent	15
Triprolidine	C19H22N2	279.1856	Pharmaceutical	Antihistamine	Other	Parent	13
U-47700	C16H22Cl2N2O	329.1182	NPS	Opioid	Utopioid	Parent	19
U-47931E	C15H21BrN2O	325.0910	NPS	Opioid	Utopioid	Parent	18
U-48520	C16H23ClN2O	295.1572	NPS	Opioid	Utopioid	Parent	15
U-48800	C17H24Cl2N2O	343.1338	NPS	Opioid	Utopioid	Parent	20
U-49900	C18H26N2OCl2	357.1495	NPS	Opioid	Utopioid	Parent	20
U-50488	C19H26Cl2N2O	369.1495	NPS	Opioid	Utopioid	Parent	21
U-51754	C17H24Cl2N2O	343.1338	NPS	Opioid	Utopioid	Parent	20
U-62066	C22H30Cl2N2O2	425.1757	NPS	Opioid	Utopioid	Parent	25
U-69593	C22H32N2O2	357.2537	NPS	Opioid	Utopioid	Parent	20
UF-17	C17H26N2O	275.2118	NPS	Other	Other	Parent	13
UR-144	C21H29NO	312.2322	NPS	Synthetic Cannabinoid	Other	Parent	17
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	390.1427	NPS	Synthetic Cannabinoid	Other	Parent	23
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	346.1932	NPS	Synthetic Cannabinoid	Other	Parent	20
UR-144 N-Heptyl Analogue	C23H33NO	340.2635	NPS	Synthetic Cannabinoid	Other	Parent	19
UR-144 N-Pentanoic Acid	C21H27NO3	342.2064	NPS	Synthetic Cannabinoid	Other	Metabolite	20
URB-447	C25H21ClN2O	401.1415	NPS	Synthetic Cannabinoid	Other	Parent	24
Urea Fentanyl	C22H29N3O	352.2383	NPS	Opioid	Fentalog	Parent	20
Valerylfentanyl	C24H32N2O	365.2587	NPS	Opioid	Fentalog	Parent	21
Vardenafil	C23H32N6O4S	489.2279	Pharmaceutical	Erectile Dysfunction	Other	Parent	27
Venlafaxine	C17H27NO2	278.2115	Pharmaceutical	Antidepressant	Other	Parent	13
Verapamil	C27H38N2O4	455.2904	Pharmaceutical	Other	Other	Parent	26
Voriconazole	C16H14F3N5O	350.1223	Pharmaceutical	Antifungal	Other	Parent	20
W15	C19H21ClN2O2S	377.1085	NPS	Opioid	Other	Parent	22
W18	C19H20ClN3O4S	422.0935	NPS	Opioid	Other	Parent	25
Warfarin	C19H16O4	309.1121	Pharmaceutical	Anticoagulant	Other	Parent	16
WIN 55,212-3	C27H26N2O3	427.2016	NPS	Synthetic Cannabinoid	Other	Parent	25
WIN-54,461	C23H25BrN2O3	457.1121	NPS	Synthetic Cannabinoid	Other	Parent	26
XLR-11	C21H28FNO	330.2228	NPS	Synthetic Cannabinoid	Other	Parent	19
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	310.2165	NPS	Synthetic Cannabinoid	Other	Parent	16
XLR-12	C20H24F3NO	352.1883	NPS	Synthetic Cannabinoid	Other	Parent	20
Xylazine	C12H16N2S	221.1107	Pharmaceutical	Analgesic, Muscle Relaxant	Cutting Agent	Parent	8
Yohimbine	C21H26N2O3	355.2016	Pharmaceutical	Erectile Dysfunction	Natural	Parent	20
Zaleplon	C17H15N5O	306.1349	Pharmaceutical	Hypnotic, Sedative	Other	Parent	16
Ziprasidone	C21H21ClN4OS	413.1197	Pharmaceutical	Antipsychotic	Other	Parent	24
Zolpidem	C19H21N3O	308.1757	Pharmaceutical	Hypnotic, Sedative	Other	Parent	16
Zonisamide	C8H8N2O3S	213.0328	Pharmaceutical	Antiepileptic	Other	Parent	8

Table A2: Library database in XIC list format (mass order)

Name	Formula	Mass (Da)	Adduct	Extraction Mass (Da)	Expected RT (min)	Fragment Mass (Da)
Methylhexanamine (DMAA 1)	C7H17N	115.1361	H+	116.1434	4.03	
Methylhexanamine (DMAA 1)	C7H17N	115.1361	H+	116.1434	4.03	57.0725
Methylhexanamine (DMAA 1)	C7H17N	115.1361	H+	116.1434	4.03	41.0426
Methylhexanamine (DMAA 1)	C7H17N	115.1361	H+	116.1434	4.03	43.0581
Methylhexanamine (DMAA 1)	C7H17N	115.1361	H+	116.1434	4.03	55.0569
Methylhexanamine (DMAA 1)	C7H17N	115.1361	H+	116.1434	4.03	116.1438
Methylhexanamine (DMAA 2)	C7H17N	115.1361	H+	116.1434	4.11	
Methylhexanamine (DMAA 2)	C7H17N	115.1361	H+	116.1434	4.11	57.0725
Methylhexanamine (DMAA 2)	C7H17N	115.1361	H+	116.1434	4.11	41.0426
Methylhexanamine (DMAA 2)	C7H17N	115.1361	H+	116.1434	4.11	43.0581
Methylhexanamine (DMAA 2)	C7H17N	115.1361	H+	116.1434	4.11	55.0569
Methylhexanamine (DMAA 2)	C7H17N	115.1361	H+	116.1434	4.11	116.1438
Tranylcypromine	C9H11N	133.0891	H+	134.0964	5.45	
Tranylcypromine	C9H11N	133.0891	H+	134.0964	5.45	77.0406
Tranylcypromine	C9H11N	133.0891	H+	134.0964	5.45	105.071
Tranylcypromine	C9H11N	133.0891	H+	134.0964	5.45	134.0974
Tranylcypromine	C9H11N	133.0891	H+	134.0964	5.45	103.0552
Tranylcypromine	C9H11N	133.0891	H+	134.0964	5.45	79.0566
Amphetamine	C9H13N	135.1048	H+	136.1121	3.56	
Amphetamine	C9H13N	135.1048	H+	136.1121	3.56	91.0554
Amphetamine	C9H13N	135.1048	H+	136.1121	3.56	65.0407
Amphetamine	C9H13N	135.1048	H+	136.1121	3.56	136.0211
Amphetamine	C9H13N	135.1048	H+	136.1121	3.56	119.0859
Amphetamine	C9H13N	135.1048	H+	136.1121	3.56	109.0099
Cathinone	C9H11NO	149.0841	H+	150.0913	2.8	
Cathinone	C9H11NO	149.0841	H+	150.0913	2.8	117.0573
Cathinone	C9H11NO	149.0841	H+	150.0913	2.8	132.0808
Cathinone	C9H11NO	149.0841	H+	150.0913	2.8	105.07
Cathinone	C9H11NO	149.0841	H+	150.0913	2.8	77.0397
Cathinone	C9H11NO	149.0841	H+	150.0913	2.8	79.0553
Methamphetamine	C10H15N	149.1204	H+	150.1277	3.82	
Methamphetamine	C10H15N	149.1204	H+	150.1277	3.82	91.0551
Methamphetamine	C10H15N	149.1204	H+	150.1277	3.82	65.0406
Methamphetamine	C10H15N	149.1204	H+	150.1277	3.82	119.0856
Methamphetamine	C10H15N	149.1204	H+	150.1277	3.82	150.1273
Methamphetamine	C10H15N	149.1204	H+	150.1277	3.82	103.0545
Phentermine	C10H15N	149.1204	H+	150.1277	4.17	
Phentermine	C10H15N	149.1204	H+	150.1277	4.17	91.0051
Phentermine	C10H15N	149.1204	H+	150.1277	4.17	133.1013
Phentermine	C10H15N	149.1204	H+	150.1277	4.17	105.07
Phentermine	C10H15N	149.1204	H+	150.1277	4.17	65.0404
Phentermine	C10H15N	149.1204	H+	150.1277	4.17	55.0564
N-ethyl Phenethylamine	C10H15N	149.1205	H+	150.1277	3.51	
N-ethyl Phenethylamine	C10H15N	149.1205	H+	150.1277	3.51	105.0692
N-ethyl Phenethylamine	C10H15N	149.1205	H+	150.1277	3.51	103.0533
N-ethyl Phenethylamine	C10H15N	149.1205	H+	150.1277	3.51	79.0536
N-ethyl Phenethylamine	C10H15N	149.1205	H+	150.1277	3.51	77.0381
N-ethyl Phenethylamine	C10H15N	149.1205	H+	150.1277	3.51	150.1271
Phenpromethamine	C10H15N	149.1205	H+	150.1277	3.76	
Phenpromethamine	C10H15N	149.1205	H+	150.1277	3.76	91.0537
Phenpromethamine	C10H15N	149.1205	H+	150.1277	3.76	119.0852
Phenpromethamine	C10H15N	149.1205	H+	150.1277	3.76	65.0384
Phenpromethamine	C10H15N	149.1205	H+	150.1277	3.76	150.1276
Phenpromethamine	C10H15N	149.1205	H+	150.1277	3.76	41.0385
Acetaminophen (Paracetamol)	C8H9NO2	151.0633	H+	152.0706	2.44	
Acetaminophen (Paracetamol)	C8H9NO2	151.0633	H+	152.0706	2.44	110.0605
Acetaminophen (Paracetamol)	C8H9NO2	151.0633	H+	152.0706	2.44	65.0408
Acetaminophen (Paracetamol)	C8H9NO2	151.0633	H+	152.0706	2.44	152.0705
Acetaminophen (Paracetamol)	C8H9NO2	151.0633	H+	152.0706	2.44	93.0346
Acetaminophen (Paracetamol)	C8H9NO2	151.0633	H+	152.0706	2.44	92.0505
Norpseudoephedrine/Phenylpropanolamine	C9H13NO	151.0997	H+	152.1070	2.31	
Norpseudoephedrine/Phenylpropanolamine	C9H13NO	151.0997	H+	152.1070	2.31	115.0547
Norpseudoephedrine/Phenylpropanolamine	C9H13NO	151.0997	H+	152.1070	2.31	117.0704
Norpseudoephedrine/Phenylpropanolamine	C9H13NO	151.0997	H+	152.1070	2.31	134.0969
Norpseudoephedrine/Phenylpropanolamine	C9H13NO	151.0997	H+	152.1070	2.31	91.0554
Norpseudoephedrine/Phenylpropanolamine	C9H13NO	151.0997	H+	152.1070	2.31	118.0652
2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	153.0954	H+	154.1027	3.74	
2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	153.0954	H+	154.1027	3.74	109.0446

2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	153.0954	H+	154.1027	3.74	83.0299
2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	153.0954	H+	154.1027	3.74	137.0759
2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	153.0954	H+	154.1027	3.74	89.0393
2-FA/3-FA/4-FA (Fluoroamphetamine)	C9H12FN	153.0954	H+	154.1027	3.74	57.0157
Methiopropamine	C8H13NS	155.0769	H+	156.0841	3.14	
Methiopropamine	C8H13NS	155.0769	H+	156.0841	3.14	97.0109
Methiopropamine	C8H13NS	155.0769	H+	156.0841	3.14	125.0418
Methiopropamine	C8H13NS	155.0769	H+	156.0841	3.14	58.0675
Methiopropamine	C8H13NS	155.0769	H+	156.0841	3.14	91.055
Methiopropamine	C8H13NS	155.0769	H+	156.0841	3.14	53.0413
Nicotine	C10H14N2	162.1157	H+	163.1230	1.1	
Nicotine	C10H14N2	162.1157	H+	163.1230	1.1	130.0656
Nicotine	C10H14N2	162.1157	H+	163.1230	1.1	117.0579
Nicotine	C10H14N2	162.1157	H+	163.1230	1.1	132.0811
Nicotine	C10H14N2	162.1157	H+	163.1230	1.1	163.1237
Nicotine	C10H14N2	162.1157	H+	163.1230	1.1	77.0397
Methcathinone	C10H13NO	163.0997	H+	164.1070	3.15	
Methcathinone	C10H13NO	163.0997	H+	164.1070	3.15	131.0727
Methcathinone	C10H13NO	163.0997	H+	164.1070	3.15	130.0649
Methcathinone	C10H13NO	163.0997	H+	164.1070	3.15	146.0963
Methcathinone	C10H13NO	163.0997	H+	164.1070	3.15	105.0704
Methcathinone	C10H13NO	163.0997	H+	164.1070	3.15	103.0549
DMA (Dimethylamphetamine)	C11H17N	163.1361	H+	164.1434	3.94	
DMA (Dimethylamphetamine)	C11H17N	163.1361	H+	164.1434	3.94	91.0552
DMA (Dimethylamphetamine)	C11H17N	163.1361	H+	164.1434	3.94	164.143
DMA (Dimethylamphetamine)	C11H17N	163.1361	H+	164.1434	3.94	119.0858
DMA (Dimethylamphetamine)	C11H17N	163.1361	H+	164.1434	3.94	65.0407
DMA (Dimethylamphetamine)	C11H17N	163.1361	H+	164.1434	3.94	46.0687
Etilamfetamine (N-Ethylamphetamine)	C11H17N	163.1361	H+	164.1434	4.19	
Etilamfetamine (N-Ethylamphetamine)	C11H17N	163.1361	H+	164.1434	4.19	91.0548
Etilamfetamine (N-Ethylamphetamine)	C11H17N	163.1361	H+	164.1434	4.19	164.1433
Etilamfetamine (N-Ethylamphetamine)	C11H17N	163.1361	H+	164.1434	4.19	119.0856
Etilamfetamine (N-Ethylamphetamine)	C11H17N	163.1361	H+	164.1434	4.19	65.0404
Etilamfetamine (N-Ethylamphetamine)	C11H17N	163.1361	H+	164.1434	4.19	46.0684
Benzocaine	C9H11NO2	165.0790	H+	166.0863	6.06	
Benzocaine	C9H11NO2	165.0790	H+	166.0863	6.06	120.0448
Benzocaine	C9H11NO2	165.0790	H+	166.0863	6.06	138.0552
Benzocaine	C9H11NO2	165.0790	H+	166.0863	6.06	94.0661
Benzocaine	C9H11NO2	165.0790	H+	166.0863	6.06	77.04
Benzocaine	C9H11NO2	165.0790	H+	166.0863	6.06	92.0504
Ephedrine/Pseudoephedrine	C10H15NO	165.1154	H+	166.1226	3.21	
Ephedrine/Pseudoephedrine	C10H15NO	165.1154	H+	166.1226	3.21	115.0545
Ephedrine/Pseudoephedrine	C10H15NO	165.1154	H+	166.1226	3.21	133.0886
Ephedrine/Pseudoephedrine	C10H15NO	165.1154	H+	166.1226	3.21	148.112
Ephedrine/Pseudoephedrine	C10H15NO	165.1154	H+	166.1226	3.21	117.0697
Ephedrine/Pseudoephedrine	C10H15NO	165.1154	H+	166.1226	3.21	132.081
PMA (para-methoxyamphetamine)	C10H15NO	165.1154	H+	166.1226	3.99	
PMA (para-methoxyamphetamine)	C10H15NO	165.1154	H+	166.1226	3.99	121.065
PMA (para-methoxyamphetamine)	C10H15NO	165.1154	H+	166.1226	3.99	149.096
PMA (para-methoxyamphetamine)	C10H15NO	165.1154	H+	166.1226	3.99	91.0551
PMA (para-methoxyamphetamine)	C10H15NO	165.1154	H+	166.1226	3.99	77.0396
PMA (para-methoxyamphetamine)	C10H15NO	165.1154	H+	166.1226	3.99	78.0472
3-FMA/4-FMA	C10H14FN	167.1110	H+	168.1183	4.06	
3-FMA/4-FMA	C10H14FN	167.1110	H+	168.1183	4.06	109.0447
3-FMA/4-FMA	C10H14FN	167.1110	H+	168.1183	4.06	168.1183
3-FMA/4-FMA	C10H14FN	167.1110	H+	168.1183	4.06	137.0761
3-FMA/4-FMA	C10H14FN	167.1110	H+	168.1183	4.06	83.0303
3-FMA/4-FMA	C10H14FN	167.1110	H+	168.1183	4.06	108.7171
Levetiracetam	C8H14N2O2	170.1055	H+	171.1128	3.11	
Levetiracetam	C8H14N2O2	170.1055	H+	171.1128	3.11	126.0915
Levetiracetam	C8H14N2O2	170.1055	H+	171.1128	3.11	69.0355
Levetiracetam	C8H14N2O2	170.1055	H+	171.1128	3.11	98.0972
Levetiracetam	C8H14N2O2	170.1055	H+	171.1128	3.11	154.0863
Levetiracetam	C8H14N2O2	170.1055	H+	171.1128	3.11	41.0432
Gabapentin	C9H17NO2	171.1259	H+	172.1332	3.38	
Gabapentin	C9H17NO2	171.1259	H+	172.1332	3.38	154.1228
Gabapentin	C9H17NO2	171.1259	H+	172.1332	3.38	137.0963
Gabapentin	C9H17NO2	171.1259	H+	172.1332	3.38	95.0865
Gabapentin	C9H17NO2	171.1259	H+	172.1332	3.38	55.0208
Gabapentin	C9H17NO2	171.1259	H+	172.1332	3.38	67.0563
5-IT	C11H14N2	174.1157	H+	175.1230	3.77	
5-IT	C11H14N2	174.1157	H+	175.1230	3.77	130.0648
5-IT	C11H14N2	174.1157	H+	175.1230	3.77	117.0573
5-IT	C11H14N2	174.1157	H+	175.1230	3.77	158.0962

5-IT	C11H14N2	174.1157	H+	175.1230	3.77	143.0728
5-IT	C11H14N2	174.1157	H+	175.1230	3.77	103.0545
AMT (alpha-Methyltryptamine)	C11H14N2	174.1157	H+	175.1230	4.21	
AMT (alpha-Methyltryptamine)	C11H14N2	174.1157	H+	175.1230	4.21	143.0729
AMT (alpha-Methyltryptamine)	C11H14N2	174.1157	H+	175.1230	4.21	130.0654
AMT (alpha-Methyltryptamine)	C11H14N2	174.1157	H+	175.1230	4.21	158.0964
AMT (alpha-Methyltryptamine)	C11H14N2	174.1157	H+	175.1230	4.21	117.0577
AMT (alpha-Methyltryptamine)	C11H14N2	174.1157	H+	175.1230	4.21	115.0545
N-methyltryptamine (NMT)	C11H14N2	174.1157	H+	175.1230	3.8	
N-methyltryptamine (NMT)	C11H14N2	174.1157	H+	175.1230	3.8	144.0804
N-methyltryptamine (NMT)	C11H14N2	174.1157	H+	175.1230	3.8	143.0729
N-methyltryptamine (NMT)	C11H14N2	174.1157	H+	175.1230	3.8	132.0811
N-methyltryptamine (NMT)	C11H14N2	174.1157	H+	175.1230	3.8	115.0545
N-methyltryptamine (NMT)	C11H14N2	174.1157	H+	175.1230	3.8	117.0652
5-APB/6-APB	C11H13NO	175.0997	H+	176.1070	4.62	
5-APB/6-APB	C11H13NO	175.0997	H+	176.1070	4.62	131.0494
5-APB/6-APB	C11H13NO	175.0997	H+	176.1070	4.62	91.055
5-APB/6-APB	C11H13NO	175.0997	H+	176.1070	4.62	159.0805
5-APB/6-APB	C11H13NO	175.0997	H+	176.1070	4.62	116.0625
5-APB/6-APB	C11H13NO	175.0997	H+	176.1070	4.62	115.0547
4-Methylaminorex	C10H12N2O	176.0950	H+	177.1022	4.2	
4-Methylaminorex	C10H12N2O	176.0950	H+	177.1022	4.2	117.0701
4-Methylaminorex	C10H12N2O	176.0950	H+	177.1022	4.2	115.0545
4-Methylaminorex	C10H12N2O	176.0950	H+	177.1022	4.2	134.0965
4-Methylaminorex	C10H12N2O	176.0950	H+	177.1022	4.2	91.0553
4-Methylaminorex	C10H12N2O	176.0950	H+	177.1022	4.2	119.0731
Cotinine	C10H12N2O	176.0950	H+	177.1022	1.07	
Cotinine	C10H12N2O	176.0950	H+	177.1022	1.07	80.0507
Cotinine	C10H12N2O	176.0950	H+	177.1022	1.07	177.1018
Cotinine	C10H12N2O	176.0950	H+	177.1022	1.07	98.0608
Cotinine	C10H12N2O	176.0950	H+	177.1022	1.07	146.0598
Cotinine	C10H12N2O	176.0950	H+	177.1022	1.07	118.0651
BZP (Benzylpiperazine)	C11H16N2	176.1313	H+	177.1386	1.46	
BZP (Benzylpiperazine)	C11H16N2	176.1313	H+	177.1386	1.46	91.055
BZP (Benzylpiperazine)	C11H16N2	176.1313	H+	177.1386	1.46	177.1385
BZP (Benzylpiperazine)	C11H16N2	176.1313	H+	177.1386	1.46	65.0407
BZP (Benzylpiperazine)	C11H16N2	176.1313	H+	177.1386	1.46	85.0772
BZP (Benzylpiperazine)	C11H16N2	176.1313	H+	177.1386	1.46	56.0522
MDAI	C10H11NO2	177.0790	H+	178.0863	3.34	
MDAI	C10H11NO2	177.0790	H+	178.0863	3.34	103.0544
MDAI	C10H11NO2	177.0790	H+	178.0863	3.34	131.049
MDAI	C10H11NO2	177.0790	H+	178.0863	3.34	161.0596
MDAI	C10H11NO2	177.0790	H+	178.0863	3.34	178.0858
MDAI	C10H11NO2	177.0790	H+	178.0863	3.34	102.0467
Buphedrone	C11H15NO	177.1154	H+	178.1226	3.95	
Buphedrone	C11H15NO	177.1154	H+	178.1226	3.95	131.0726
Buphedrone	C11H15NO	177.1154	H+	178.1226	3.95	130.0646
Buphedrone	C11H15NO	177.1154	H+	178.1226	3.95	91.055
Buphedrone	C11H15NO	177.1154	H+	178.1226	3.95	132.0807
Buphedrone	C11H15NO	177.1154	H+	178.1226	3.95	160.1117
Ethacathinone (ETH-CAT)	C11H15NO	177.1154	H+	178.1226	3.54	
Ethacathinone (ETH-CAT)	C11H15NO	177.1154	H+	178.1226	3.54	130.0649
Ethacathinone (ETH-CAT)	C11H15NO	177.1154	H+	178.1226	3.54	131.0729
Ethacathinone (ETH-CAT)	C11H15NO	177.1154	H+	178.1226	3.54	132.0806
Ethacathinone (ETH-CAT)	C11H15NO	177.1154	H+	178.1226	3.54	117.0581
Ethacathinone (ETH-CAT)	C11H15NO	177.1154	H+	178.1226	3.54	105.0702
Mephedrone	C11H15NO	177.1154	H+	178.1226	4.27	
Mephedrone	C11H15NO	177.1154	H+	178.1226	4.27	145.0878
Mephedrone	C11H15NO	177.1154	H+	178.1226	4.27	144.08
Mephedrone	C11H15NO	177.1154	H+	178.1226	4.27	160.1114
Mephedrone	C11H15NO	177.1154	H+	178.1226	4.27	119.0854
Mephedrone	C11H15NO	177.1154	H+	178.1226	4.27	130.065
Phenmetrazine	C11H15NO	177.1154	H+	178.1226	3.74	
Phenmetrazine	C11H15NO	177.1154	H+	178.1226	3.74	115.0544
Phenmetrazine	C11H15NO	177.1154	H+	178.1226	3.74	117.0692
Phenmetrazine	C11H15NO	177.1154	H+	178.1226	3.74	178.1224
Phenmetrazine	C11H15NO	177.1154	H+	178.1226	3.74	91.0552
Phenmetrazine	C11H15NO	177.1154	H+	178.1226	3.74	134.0966
N-Propylamphetamine	C12H19N	177.1518	H+	178.1590	4.97	
N-Propylamphetamine	C12H19N	177.1518	H+	178.1590	4.97	91.0537
N-Propylamphetamine	C12H19N	177.1518	H+	178.1590	4.97	119.0851
N-Propylamphetamine	C12H19N	177.1518	H+	178.1590	4.97	178.159
N-Propylamphetamine	C12H19N	177.1518	H+	178.1590	4.97	65.0384
N-Propylamphetamine	C12H19N	177.1518	H+	178.1590	4.97	60.0809

Phenacetin	C10H13NO2	179.0946	H+	180.1019	5.72	
Phenacetin	C10H13NO2	179.0946	H+	180.1019	5.72	110.0604
Phenacetin	C10H13NO2	179.0946	H+	180.1019	5.72	138.0913
Phenacetin	C10H13NO2	179.0946	H+	180.1019	5.72	180.102
Phenacetin	C10H13NO2	179.0946	H+	180.1019	5.72	152.0705
Phenacetin	C10H13NO2	179.0946	H+	180.1019	5.72	109.0525
MDA (3,4-Methylenedioxyamphetamine)	C10H13NO2	179.0946	H+	180.1019	3.83	
MDA (3,4-Methylenedioxyamphetamine)	C10H13NO2	179.0946	H+	180.1019	3.83	105.0701
MDA (3,4-Methylenedioxyamphetamine)	C10H13NO2	179.0946	H+	180.1019	3.83	135.0439
MDA (3,4-Methylenedioxyamphetamine)	C10H13NO2	179.0946	H+	180.1019	3.83	163.0751
MDA (3,4-Methylenedioxyamphetamine)	C10H13NO2	179.0946	H+	180.1019	3.83	133.0649
MDA (3,4-Methylenedioxyamphetamine)	C10H13NO2	179.0946	H+	180.1019	3.83	103.0548
Phenibut	C10H13NO2	179.0946	H+	180.1019	2.03	
Phenibut	C10H13NO2	179.0946	H+	180.1019	2.03	117.0703
Phenibut	C10H13NO2	179.0946	H+	180.1019	2.03	115.0546
Phenibut	C10H13NO2	179.0946	H+	180.1019	2.03	145.065
Phenibut	C10H13NO2	179.0946	H+	180.1019	2.03	127.0541
Phenibut	C10H13NO2	179.0946	H+	180.1019	2.03	180.1016
2-MMA/3-MMA	C11H17NO	179.1310	H+	180.1383	4.53	
2-MMA/3-MMA	C11H17NO	179.1310	H+	180.1383	4.53	121.0647
2-MMA/3-MMA	C11H17NO	179.1310	H+	180.1383	4.53	91.0552
2-MMA/3-MMA	C11H17NO	179.1310	H+	180.1383	4.53	149.096
2-MMA/3-MMA	C11H17NO	179.1310	H+	180.1383	4.53	93.0709
2-MMA/3-MMA	C11H17NO	179.1310	H+	180.1383	4.53	180.1386
Mexiletine	C11H17NO	179.1310	H+	180.1383	5.25	
Mexiletine	C11H17NO	179.1310	H+	180.1383	5.25	58.0672
Mexiletine	C11H17NO	179.1310	H+	180.1383	5.25	105.0702
Mexiletine	C11H17NO	179.1310	H+	180.1383	5.25	121.0648
Mexiletine	C11H17NO	179.1310	H+	180.1383	5.25	103.0546
Mexiletine	C11H17NO	179.1310	H+	180.1383	5.25	79.0554
PMMA	C11H17NO	179.1310	H+	180.1383	4.15	
PMMA	C11H17NO	179.1310	H+	180.1383	4.15	121.0647
PMMA	C11H17NO	179.1310	H+	180.1383	4.15	91.0552
PMMA	C11H17NO	179.1310	H+	180.1383	4.15	149.096
PMMA	C11H17NO	179.1310	H+	180.1383	4.15	93.071
PMMA	C11H17NO	179.1310	H+	180.1383	4.15	180.1389
Memantine	C12H21N	179.1674	H+	180.1747	5.97	
Memantine	C12H21N	179.1674	H+	180.1747	5.97	163.1478
Memantine	C12H21N	179.1674	H+	180.1747	5.97	107.0857
Memantine	C12H21N	179.1674	H+	180.1747	5.97	91.055
Memantine	C12H21N	179.1674	H+	180.1747	5.97	180.1738
Memantine	C12H21N	179.1674	H+	180.1747	5.97	135.1161
Theophylline	C7H8N4O2	180.0647	H+	181.0720	3.32	
Theophylline	C7H8N4O2	180.0647	H+	181.0720	3.32	124.0504
Theophylline	C7H8N4O2	180.0647	H+	181.0720	3.32	181.0717
Theophylline	C7H8N4O2	180.0647	H+	181.0720	3.32	96.0565
Theophylline	C7H8N4O2	180.0647	H+	181.0720	3.32	69.0466
Theophylline	C7H8N4O2	180.0647	H+	181.0720	3.32	42.0381
3-FMC/4-FMC	C10H12FNO	181.0903	H+	182.0976	3.43	
3-FMC/4-FMC	C10H12FNO	181.0903	H+	182.0976	3.43	149.0624
3-FMC/4-FMC	C10H12FNO	181.0903	H+	182.0976	3.43	148.0548
3-FMC/4-FMC	C10H12FNO	181.0903	H+	182.0976	3.43	164.0861
3-FMC/4-FMC	C10H12FNO	181.0903	H+	182.0976	3.43	123.0599
3-FMC/4-FMC	C10H12FNO	181.0903	H+	182.0976	3.43	103.0544
2C-H (3,4-Dimethoxyphenethylamine)	C10H15NO2	181.1103	H+	182.1176	4.16	
2C-H (3,4-Dimethoxyphenethylamine)	C10H15NO2	181.1103	H+	182.1176	4.16	150.0676
2C-H (3,4-Dimethoxyphenethylamine)	C10H15NO2	181.1103	H+	182.1176	4.16	135.0442
2C-H (3,4-Dimethoxyphenethylamine)	C10H15NO2	181.1103	H+	182.1176	4.16	165.091
2C-H (3,4-Dimethoxyphenethylamine)	C10H15NO2	181.1103	H+	182.1176	4.16	105.0704
2C-H (3,4-Dimethoxyphenethylamine)	C10H15NO2	181.1103	H+	182.1176	4.16	103.0546
Fluoroethamphetamine	C11H16FN	181.1267	H+	182.1340	4.5	
Fluoroethamphetamine	C11H16FN	181.1267	H+	182.1340	4.5	109.0442
Fluoroethamphetamine	C11H16FN	181.1267	H+	182.1340	4.5	182.1337
Fluoroethamphetamine	C11H16FN	181.1267	H+	182.1340	4.5	137.0754
Fluoroethamphetamine	C11H16FN	181.1267	H+	182.1340	4.5	83.0286
Fluoroethamphetamine	C11H16FN	181.1267	H+	182.1340	4.5	46.0647
DMT (N,N-Dimethyltryptamine)	C12H16N2	188.1313	H+	189.1386	3.89	
DMT (N,N-Dimethyltryptamine)	C12H16N2	188.1313	H+	189.1386	3.89	144.0811
DMT (N,N-Dimethyltryptamine)	C12H16N2	188.1313	H+	189.1386	3.89	58.0678
DMT (N,N-Dimethyltryptamine)	C12H16N2	188.1313	H+	189.1386	3.89	143.0734
DMT (N,N-Dimethyltryptamine)	C12H16N2	188.1313	H+	189.1386	3.89	117.0694
DMT (N,N-Dimethyltryptamine)	C12H16N2	188.1313	H+	189.1386	3.89	115.0545
Phensuximide	C11H11NO2	189.0790	H+	190.0863	5.63	
Phensuximide	C11H11NO2	189.0790	H+	190.0863	5.63	150.0705

Phensuximide	C11H11NO2	189.0790	H+	190.0863	5.63	58.0313
Phensuximide	C11H11NO2	189.0790	H+	190.0863	5.63	131.0493
Phensuximide	C11H11NO2	189.0790	H+	190.0863	5.63	190.0867
Phensuximide	C11H11NO2	189.0790	H+	190.0863	5.63	120.0811
Deschloronorketamine	C12H15NO	189.1154	H+	190.1226	4.09	
Deschloronorketamine	C12H15NO	189.1154	H+	190.1226	4.09	91.0531
Deschloronorketamine	C12H15NO	189.1154	H+	190.1226	4.09	145.0995
Deschloronorketamine	C12H15NO	189.1154	H+	190.1226	4.09	173.0948
Deschloronorketamine	C12H15NO	189.1154	H+	190.1226	4.09	129.0691
Deschloronorketamine	C12H15NO	189.1154	H+	190.1226	4.09	117.069
1-(4-methylbenzyl) piperazine	C12H18N2	190.1470	H+	191.1543	3.04	
1-(4-methylbenzyl) piperazine	C12H18N2	190.1470	H+	191.1543	3.04	105.0697
1-(4-methylbenzyl) piperazine	C12H18N2	190.1470	H+	191.1543	3.04	191.1514
1-(4-methylbenzyl) piperazine	C12H18N2	190.1470	H+	191.1543	3.04	103.0545
1-(4-methylbenzyl) piperazine	C12H18N2	190.1470	H+	191.1543	3.04	79.0554
1-(4-methylbenzyl) piperazine	C12H18N2	190.1470	H+	191.1543	3.04	77.0399
MBZP (Methylbenzylpiperazine)	C12H18N2	190.1470	H+	191.1543	3.04	
MBZP (Methylbenzylpiperazine)	C12H18N2	190.1470	H+	191.1543	3.04	105.0705
MBZP (Methylbenzylpiperazine)	C12H18N2	190.1470	H+	191.1543	3.04	191.1538
MBZP (Methylbenzylpiperazine)	C12H18N2	190.1470	H+	191.1543	3.04	103.0545
MBZP (Methylbenzylpiperazine)	C12H18N2	190.1470	H+	191.1543	3.04	79.0557
MBZP (Methylbenzylpiperazine)	C12H18N2	190.1470	H+	191.1543	3.04	77.0398
3,4-DMMC (3,4-dimethylmethcathinone)	C12H17NO	191.1310	H+	192.1383	5.09	
3,4-DMMC (3,4-dimethylmethcathinone)	C12H17NO	191.1310	H+	192.1383	5.09	159.1035
3,4-DMMC (3,4-dimethylmethcathinone)	C12H17NO	191.1310	H+	192.1383	5.09	158.0957
3,4-DMMC (3,4-dimethylmethcathinone)	C12H17NO	191.1310	H+	192.1383	5.09	144.0801
3,4-DMMC (3,4-dimethylmethcathinone)	C12H17NO	191.1310	H+	192.1383	5.09	174.1272
3,4-DMMC (3,4-dimethylmethcathinone)	C12H17NO	191.1310	H+	192.1383	5.09	133.101
4-MEC (4-methylethcathinone)	C12H17NO	191.1310	H+	192.1383	4.59	
4-MEC (4-methylethcathinone)	C12H17NO	191.1310	H+	192.1383	4.59	144.0804
4-MEC (4-methylethcathinone)	C12H17NO	191.1310	H+	192.1383	4.59	145.088
4-MEC (4-methylethcathinone)	C12H17NO	191.1310	H+	192.1383	4.59	131.0739
4-MEC (4-methylethcathinone)	C12H17NO	191.1310	H+	192.1383	4.59	119.0856
4-MEC (4-methylethcathinone)	C12H17NO	191.1310	H+	192.1383	4.59	146.0959
N-Ethylbuphedrone (NEB)	C12H17NO	191.1310	H+	192.1383	4.22	
N-Ethylbuphedrone (NEB)	C12H17NO	191.1310	H+	192.1383	4.22	130.0646
N-Ethylbuphedrone (NEB)	C12H17NO	191.1310	H+	192.1383	4.22	91.0549
N-Ethylbuphedrone (NEB)	C12H17NO	191.1310	H+	192.1383	4.22	145.0883
N-Ethylbuphedrone (NEB)	C12H17NO	191.1310	H+	192.1383	4.22	174.1275
N-Ethylbuphedrone (NEB)	C12H17NO	191.1310	H+	192.1383	4.22	146.0959
Pentedrone	C12H17NO	191.1310	H+	192.1383	4.76	
Pentedrone	C12H17NO	191.1310	H+	192.1383	4.76	131.0724
Pentedrone	C12H17NO	191.1310	H+	192.1383	4.76	132.0802
Pentedrone	C12H17NO	191.1310	H+	192.1383	4.76	91.0547
Pentedrone	C12H17NO	191.1310	H+	192.1383	4.76	144.0801
Pentedrone	C12H17NO	191.1310	H+	192.1383	4.76	130.0647
Phendimetrazine	C12H17NO	191.1310	H+	192.1383	3.73	
Phendimetrazine	C12H17NO	191.1310	H+	192.1383	3.73	192.1384
Phendimetrazine	C12H17NO	191.1310	H+	192.1383	3.73	146.0963
Phendimetrazine	C12H17NO	191.1310	H+	192.1383	3.73	148.1119
Phendimetrazine	C12H17NO	191.1310	H+	192.1383	3.73	115.0542
Phendimetrazine	C12H17NO	191.1310	H+	192.1383	3.73	17.0699
4-MeOPP	C11H16N2O	192.1263	H+	193.1335	3.69	
4-MeOPP	C11H16N2O	192.1263	H+	193.1335	3.69	150.0914
4-MeOPP	C11H16N2O	192.1263	H+	193.1335	3.69	133.0525
4-MeOPP	C11H16N2O	192.1263	H+	193.1335	3.69	119.0728
4-MeOPP	C11H16N2O	192.1263	H+	193.1335	3.69	193.1339
4-MeOPP	C11H16N2O	192.1263	H+	193.1335	3.69	176.1074
BDB (1,3-benzodioxolylbutanamine)	C11H15NO2	193.1103	H+	194.1176	4.51	
BDB (1,3-benzodioxolylbutanamine)	C11H15NO2	193.1103	H+	194.1176	4.51	135.0434
BDB (1,3-benzodioxolylbutanamine)	C11H15NO2	193.1103	H+	194.1176	4.51	177.0908
BDB (1,3-benzodioxolylbutanamine)	C11H15NO2	193.1103	H+	194.1176	4.51	147.0801
BDB (1,3-benzodioxolylbutanamine)	C11H15NO2	193.1103	H+	194.1176	4.51	119.0854
BDB (1,3-benzodioxolylbutanamine)	C11H15NO2	193.1103	H+	194.1176	4.51	105.0339
MDMA (3,4-Methylenedioxymethamphetamine)	C11H15NO2	193.1103	H+	194.1176	4.01	
MDMA (3,4-Methylenedioxymethamphetamine)	C11H15NO2	193.1103	H+	194.1176	4.01	135.0436
MDMA (3,4-Methylenedioxymethamphetamine)	C11H15NO2	193.1103	H+	194.1176	4.01	105.0699
MDMA (3,4-Methylenedioxymethamphetamine)	C11H15NO2	193.1103	H+	194.1176	4.01	133.0645
MDMA (3,4-Methylenedioxymethamphetamine)	C11H15NO2	193.1103	H+	194.1176	4.01	163.0749

MDMA (3,4-Methylenedioxymethamphetamine)	C11H15NO2	193.1103	H+	194.1176	4.01	103.0546
Methedrone (4-MMC)	C11H15NO2	193.1103	H+	194.1176	3.91	
Methedrone (4-MMC)	C11H15NO2	193.1103	H+	194.1176	3.91	161.0829
Methedrone (4-MMC)	C11H15NO2	193.1103	H+	194.1176	3.91	146.0595
Methedrone (4-MMC)	C11H15NO2	193.1103	H+	194.1176	3.91	145.0881
Methedrone (4-MMC)	C11H15NO2	193.1103	H+	194.1176	3.91	176.1063
Methedrone (4-MMC)	C11H15NO2	193.1103	H+	194.1176	3.91	135.0803
Caffeine	C8H10N4O2	194.0804	H+	195.0877	3.92	
Caffeine	C8H10N4O2	194.0804	H+	195.0877	3.92	138.0659
Caffeine	C8H10N4O2	194.0804	H+	195.0877	3.92	110.0717
Caffeine	C8H10N4O2	194.0804	H+	195.0877	3.92	195.0872
Caffeine	C8H10N4O2	194.0804	H+	195.0877	3.92	123.043
Caffeine	C8H10N4O2	194.0804	H+	195.0877	3.92	83.0617
2C-D	C11H17NO2	195.1259	H+	196.1332	5.12	
2C-D	C11H17NO2	195.1259	H+	196.1332	5.12	164.0829
2C-D	C11H17NO2	195.1259	H+	196.1332	5.12	149.06
2C-D	C11H17NO2	195.1259	H+	196.1332	5.12	179.1065
2C-D	C11H17NO2	195.1259	H+	196.1332	5.12	91.0551
2C-D	C11H17NO2	195.1259	H+	196.1332	5.12	117.0702
mCPP (meta-Chlorophenylpiperazine)	C10H13ClN2	196.0767	H+	197.0840	5	
mCPP (meta-Chlorophenylpiperazine)	C10H13ClN2	196.0767	H+	197.0840	5	154.0419
mCPP (meta-Chlorophenylpiperazine)	C10H13ClN2	196.0767	H+	197.0840	5	119.0732
mCPP (meta-Chlorophenylpiperazine)	C10H13ClN2	196.0767	H+	197.0840	5	118.0655
mCPP (meta-Chlorophenylpiperazine)	C10H13ClN2	196.0767	H+	197.0840	5	197.084
mCPP (meta-Chlorophenylpiperazine)	C10H13ClN2	196.0767	H+	197.0840	5	195.0683
Guaifenesin	C10H14O4	198.0892	H+	199.0965	4.85	
Guaifenesin	C10H14O4	198.0892	H+	199.0965	4.85	122.0358
Guaifenesin	C10H14O4	198.0892	H+	199.0965	4.85	110.0364
Guaifenesin	C10H14O4	198.0892	H+	199.0965	4.85	121.0284
Guaifenesin	C10H14O4	198.0892	H+	199.0965	4.85	125.0597
Guaifenesin	C10H14O4	198.0892	H+	199.0965	4.85	93.0341
MDMA-D5	C11H10[2H]5NO2	198.1417	H+	199.1489	3.98	
MDMA-D5	C11H10[2H]5NO2	198.1417	H+	199.1489	3.98	165.0882
MDMA-D5	C11H10[2H]5NO2	198.1417	H+	199.1489	3.98	107.083
MDMA-D5	C11H10[2H]5NO2	198.1417	H+	199.1489	3.98	136.0505
MDMA-D5	C11H10[2H]5NO2	198.1417	H+	199.1489	3.98	135.077
MDMA-D5	C11H10[2H]5NO2	198.1417	H+	199.1489	3.98	199.1502
Tetrahydrozoline	C13H16N2	200.1313	H+	201.1386	4.23	
Tetrahydrozoline	C13H16N2	200.1313	H+	201.1386	4.23	201.1382
Tetrahydrozoline	C13H16N2	200.1313	H+	201.1386	4.23	131.0851
Tetrahydrozoline	C13H16N2	200.1313	H+	201.1386	4.23	91.0548
Tetrahydrozoline	C13H16N2	200.1313	H+	201.1386	4.23	71.0616
Tetrahydrozoline	C13H16N2	200.1313	H+	201.1386	4.23	173.1077
Alpha-PPP	C13H17NO	203.1310	H+	204.1382	3.82	
Alpha-PPP	C13H17NO	203.1310	H+	204.1382	3.82	105.0697
Alpha-PPP	C13H17NO	203.1310	H+	204.1382	3.82	98.0967
Alpha-PPP	C13H17NO	203.1310	H+	204.1382	3.82	204.1379
Alpha-PPP	C13H17NO	203.1310	H+	204.1382	3.82	133.0645
Alpha-PPP	C13H17NO	203.1310	H+	204.1382	3.82	103.0546
NPP	C13H17NO	203.1310	H+	204.1383	3.28	
NPP	C13H17NO	203.1310	H+	204.1383	3.28	105.0703
NPP	C13H17NO	203.1310	H+	204.1383	3.28	204.1392
NPP	C13H17NO	203.1310	H+	204.1383	3.28	103.0545
NPP	C13H17NO	203.1310	H+	204.1383	3.28	79.0547
NPP	C13H17NO	203.1310	H+	204.1383	3.28	134.0967
Deschloroketamine	C13H17NO	203.1310	H+	204.1383	4.29	
Deschloroketamine	C13H17NO	203.1310	H+	204.1383	4.29	145.1008
Deschloroketamine	C13H17NO	203.1310	H+	204.1383	4.29	129.07
Deschloroketamine	C13H17NO	203.1310	H+	204.1383	4.29	91.0541
Deschloroketamine	C13H17NO	203.1310	H+	204.1383	4.29	173.0961
Deschloroketamine	C13H17NO	203.1310	H+	204.1383	4.29	117.0699
Eticyclidine (PCE)	C14H21N	203.1674	H+	204.1747	5.71	
Eticyclidine (PCE)	C14H21N	203.1674	H+	204.1747	5.71	91.0544
Eticyclidine (PCE)	C14H21N	203.1674	H+	204.1747	5.71	159.1169
Eticyclidine (PCE)	C14H21N	203.1674	H+	204.1747	5.71	117.0695
Eticyclidine (PCE)	C14H21N	203.1674	H+	204.1747	5.71	81.0699
Eticyclidine (PCE)	C14H21N	203.1674	H+	204.1747	5.71	46.0653
Levamisole	C11H12N2S	204.0721	H+	205.0794	3.53	
Levamisole	C11H12N2S	204.0721	H+	205.0794	3.53	178.0684
Levamisole	C11H12N2S	204.0721	H+	205.0794	3.53	205.0795
Levamisole	C11H12N2S	204.0721	H+	205.0794	3.53	123.0267
Levamisole	C11H12N2S	204.0721	H+	205.0794	3.53	129.0704
Levamisole	C11H12N2S	204.0721	H+	205.0794	3.53	118.0657

5-MeO-Amt	C12H16N2O	204.1263	H+	205.1335	4.29	
5-MeO-Amt	C12H16N2O	204.1263	H+	205.1335	4.29	147.0676
5-MeO-Amt	C12H16N2O	204.1263	H+	205.1335	4.29	173.0833
5-MeO-Amt	C12H16N2O	204.1263	H+	205.1335	4.29	188.1068
5-MeO-Amt	C12H16N2O	204.1263	H+	205.1335	4.29	132.0444
5-MeO-Amt	C12H16N2O	204.1263	H+	205.1335	4.29	130.0652
Bufotenine	C12H16N2O	204.1263	H+	205.1335	1.94	
Bufotenine	C12H16N2O	204.1263	H+	205.1335	1.94	160.0756
Bufotenine	C12H16N2O	204.1263	H+	205.1335	1.94	58.068
Bufotenine	C12H16N2O	204.1263	H+	205.1335	1.94	115.0547
Bufotenine	C12H16N2O	204.1263	H+	205.1335	1.94	132.081
Bufotenine	C12H16N2O	204.1263	H+	205.1335	1.94	117.0577
Psilocin	C12H16N2O	204.1263	H+	205.1335	3	
Psilocin	C12H16N2O	204.1263	H+	205.1335	3	160.0755
Psilocin	C12H16N2O	204.1263	H+	205.1335	3	58.0675
Psilocin	C12H16N2O	204.1263	H+	205.1335	3	115.0543
Psilocin	C12H16N2O	204.1263	H+	205.1335	3	87.0453
Psilocin	C12H16N2O	204.1263	H+	205.1335	3	149.0226
4-EEC (Ethylethcathinone)	C13H19NO	205.1467	H+	206.1539	5.44	
4-EEC (Ethylethcathinone)	C13H19NO	205.1467	H+	206.1539	5.44	144.08
4-EEC (Ethylethcathinone)	C13H19NO	205.1467	H+	206.1539	5.44	159.1035
4-EEC (Ethylethcathinone)	C13H19NO	205.1467	H+	206.1539	5.44	188.1427
4-EEC (Ethylethcathinone)	C13H19NO	205.1467	H+	206.1539	5.44	160.1116
4-EEC (Ethylethcathinone)	C13H19NO	205.1467	H+	206.1539	5.44	158.0959
4-ethyl-n,n-DMC	C13H19NO	205.1467	H+	206.1539	5.28	
4-ethyl-n,n-DMC	C13H19NO	205.1467	H+	206.1539	5.28	105.0706
4-ethyl-n,n-DMC	C13H19NO	205.1467	H+	206.1539	5.28	72.0828
4-ethyl-n,n-DMC	C13H19NO	205.1467	H+	206.1539	5.28	133.0995
4-ethyl-n,n-DMC	C13H19NO	205.1467	H+	206.1539	5.28	161.0965
4-ethyl-n,n-DMC	C13H19NO	205.1467	H+	206.1539	5.28	206.1545
Hexedrone	C13H19NO	205.1467	H+	206.1539	5.63	
Hexedrone	C13H19NO	205.1467	H+	206.1539	5.63	132.0808
Hexedrone	C13H19NO	205.1467	H+	206.1539	5.63	144.0806
Hexedrone	C13H19NO	205.1467	H+	206.1539	5.63	177.0576
Hexedrone	C13H19NO	205.1467	H+	206.1539	5.63	188.1434
Hexedrone	C13H19NO	205.1467	H+	206.1539	5.63	206.1538
Monoethylglycinexylidide (MEGX)	C12H18N2O	206.1419	H+	207.1492	3.76	
Monoethylglycinexylidide (MEGX)	C12H18N2O	206.1419	H+	207.1492	3.76	58.0674
Monoethylglycinexylidide (MEGX)	C12H18N2O	206.1419	H+	207.1492	3.76	207.1496
Monoethylglycinexylidide (MEGX)	C12H18N2O	206.1419	H+	207.1492	3.76	122.0966
Monoethylglycinexylidide (MEGX)	C12H18N2O	206.1419	H+	207.1492	3.76	150.0912
Monoethylglycinexylidide (MEGX)	C12H18N2O	206.1419	H+	207.1492	3.76	107.0732
Methylone (MDMC, bk-MDMA)	C11H13NO3	207.0895	H+	208.0968	3.52	
Methylone (MDMC, bk-MDMA)	C11H13NO3	207.0895	H+	208.0968	3.52	160.0756
Methylone (MDMC, bk-MDMA)	C11H13NO3	207.0895	H+	208.0968	3.52	132.0808
Methylone (MDMC, bk-MDMA)	C11H13NO3	207.0895	H+	208.0968	3.52	190.0861
Methylone (MDMC, bk-MDMA)	C11H13NO3	207.0895	H+	208.0968	3.52	117.0574
Methylone (MDMC, bk-MDMA)	C11H13NO3	207.0895	H+	208.0968	3.52	208.0867
MBDB	C12H17NO2	207.1259	H+	208.1332	4.65	
MBDB	C12H17NO2	207.1259	H+	208.1332	4.65	135.0438
MBDB	C12H17NO2	207.1259	H+	208.1332	4.65	208.1334
MBDB	C12H17NO2	207.1259	H+	208.1332	4.65	177.0909
MBDB	C12H17NO2	207.1259	H+	208.1332	4.65	147.0803
MBDB	C12H17NO2	207.1259	H+	208.1332	4.65	119.0858
MDEA (3,4-Methylenedioxyethylamphetamine)	C12H17NO2	207.1259	H+	208.1332	4.34	
MDEA (3,4-Methylenedioxyethylamphetamine)	C12H17NO2	207.1259	H+	208.1332	4.34	135.0443
MDEA (3,4-Methylenedioxyethylamphetamine)	C12H17NO2	207.1259	H+	208.1332	4.34	105.0706
MDEA (3,4-Methylenedioxyethylamphetamine)	C12H17NO2	207.1259	H+	208.1332	4.34	163.0756
MDEA (3,4-Methylenedioxyethylamphetamine)	C12H17NO2	207.1259	H+	208.1332	4.34	133.0651
MDEA (3,4-Methylenedioxyethylamphetamine)	C12H17NO2	207.1259	H+	208.1332	4.34	103.0547
MeO-MDA	C11H15NO3	209.1052	H+	210.1125	4.31	
MeO-MDA	C11H15NO3	209.1052	H+	210.1125	4.31	165.054
MeO-MDA	C11H15NO3	209.1052	H+	210.1125	4.31	135.0796
MeO-MDA	C11H15NO3	209.1052	H+	210.1125	4.31	107.0485
MeO-MDA	C11H15NO3	209.1052	H+	210.1125	4.31	193.0857
MeO-MDA	C11H15NO3	209.1052	H+	210.1125	4.31	152.0462
2C-E	C12H19NO2	209.1416	H+	210.1489	5.9	
2C-E	C12H19NO2	209.1416	H+	210.1489	5.9	178.0983

2C-E	C12H19NO2	209.1416	H+	210.1489	5.9	193.1218
2C-E	C12H19NO2	209.1416	H+	210.1489	5.9	163.0754
2C-E	C12H19NO2	209.1416	H+	210.1489	5.9	135.0799
2C-E	C12H19NO2	209.1416	H+	210.1489	5.9	105.0702
2C-G	C12H19NO2	209.1416	H+	210.1489	5.66	
2C-G	C12H19NO2	209.1416	H+	210.1489	5.66	178.0988
2C-G	C12H19NO2	209.1416	H+	210.1489	5.66	163.0755
2C-G	C12H19NO2	209.1416	H+	210.1489	5.66	193.1226
2C-G	C12H19NO2	209.1416	H+	210.1489	5.66	148.0887
2C-G	C12H19NO2	209.1416	H+	210.1489	5.66	135.0808
DOM	C12H19NO2	209.1416	H+	210.1489	5.48	
DOM	C12H19NO2	209.1416	H+	210.1489	5.48	163.0744
DOM	C12H19NO2	209.1416	H+	210.1489	5.48	135.0797
DOM	C12H19NO2	209.1416	H+	210.1489	5.48	178.0981
DOM	C12H19NO2	209.1416	H+	210.1489	5.48	165.0903
DOM	C12H19NO2	209.1416	H+	210.1489	5.48	193.1214
Methylone-D3	C11H10[2H]3NO3	210.1084	H+	211.1157	3.5	
Methylone-D3	C11H10[2H]3NO3	210.1084	H+	211.1157	3.5	163.0946
Methylone-D3	C11H10[2H]3NO3	210.1084	H+	211.1157	3.5	135.0097
Methylone-D3	C11H10[2H]3NO3	210.1084	H+	211.1157	3.5	193.1053
Methylone-D3	C11H10[2H]3NO3	210.1084	H+	211.1157	3.5	211.1156
Methylone-D3	C11H10[2H]3NO3	210.1084	H+	211.1157	3.5	117.0576
BBOP	C13H9NO2	211.0633	H+	212.0706	7.27	
BBOP	C13H9NO2	211.0633	H+	212.0706	7.27	212.0699
BBOP	C13H9NO2	211.0633	H+	212.0706	7.27	194.0597
BBOP	C13H9NO2	211.0633	H+	212.0706	7.27	166.0646
BBOP	C13H9NO2	211.0633	H+	212.0706	7.27	156.0803
BBOP	C13H9NO2	211.0633	H+	212.0706	7.27	139.0536
2-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.01	
2-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.01	139.0279
2-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.01	103.053
2-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.01	72.0802
2-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.01	212.0831
2-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.01	167.0249
3-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.49	
3-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.49	139.0279
3-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.49	103.053
3-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.49	72.0802
3-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.49	212.0831
3-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.49	167.0249
4-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.59	
4-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.59	139.0279
4-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.59	103.053
4-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.59	72.0802
4-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.59	212.0831
4-CDMC	C11H14ClNO	211.0764	H+	212.0837	4.59	167.0249
Mescaline	C11H17NO3	211.1208	H+	212.1281	3.77	
Mescaline	C11H17NO3	211.1208	H+	212.1281	3.77	165.0542
Mescaline	C11H17NO3	211.1208	H+	212.1281	3.77	180.0774
Mescaline	C11H17NO3	211.1208	H+	212.1281	3.77	195.101
Mescaline	C11H17NO3	211.1208	H+	212.1281	3.77	164.0828
Mescaline	C11H17NO3	211.1208	H+	212.1281	3.77	149.0594
Zonisamide	C8H8N2O3S	212.0256	H+	213.0328	4.59	
Zonisamide	C8H8N2O3S	212.0256	H+	213.0328	4.59	132.0445
Zonisamide	C8H8N2O3S	212.0256	H+	213.0328	4.59	77.0399
Zonisamide	C8H8N2O3S	212.0256	H+	213.0328	4.59	104.0496
Zonisamide	C8H8N2O3S	212.0256	H+	213.0328	4.59	102.0344
Zonisamide	C8H8N2O3S	212.0256	H+	213.0328	4.59	213.0334
2C-C	C10H14ClNO2	215.0713	H+	216.0786	5.14	
2C-C	C10H14ClNO2	215.0713	H+	216.0786	5.14	184.0287
2C-C	C10H14ClNO2	215.0713	H+	216.0786	5.14	199.052
2C-C	C10H14ClNO2	215.0713	H+	216.0786	5.14	169.0054
2C-C	C10H14ClNO2	215.0713	H+	216.0786	5.14	77.0403
2C-C	C10H14ClNO2	215.0713	H+	216.0786	5.14	149.0615
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	216.1626	H+	217.1699	4.7	
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	216.1626	H+	217.1699	4.7	144.0809
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	216.1626	H+	217.1699	4.7	86.0977
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	216.1626	H+	217.1699	4.7	143.0729
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	216.1626	H+	217.1699	4.7	117.0695
DET (N,N-Diethyltryptamine, T-9)	C14H20N2	216.1626	H+	217.1699	4.7	115.0546
Glutethimide	C13H15NO2	217.1103	H+	218.1176	6.82	
Glutethimide	C13H15NO2	217.1103	H+	218.1176	6.82	131.0858
Glutethimide	C13H15NO2	217.1103	H+	218.1176	6.82	91.0553
Glutethimide	C13H15NO2	217.1103	H+	218.1176	6.82	218.1176

Glutethimide	C13H15NO2	217.1103	H+	218.1176	6.82	190.122
Glutethimide	C13H15NO2	217.1103	H+	218.1176	6.82	173.0974
MePPP	C14H19NO	217.1467	H+	218.1539	4.79	
MePPP	C14H19NO	217.1467	H+	218.1539	4.79	119.085
MePPP	C14H19NO	217.1467	H+	218.1539	4.79	98.0967
MePPP	C14H19NO	217.1467	H+	218.1539	4.79	147.0799
MePPP	C14H19NO	217.1467	H+	218.1539	4.79	218.1538
MePPP	C14H19NO	217.1467	H+	218.1539	4.79	117.0698
N-ethyl Deschloroketamine	C14H19NO	217.1467	H+	218.1539	4.5	
N-ethyl Deschloroketamine	C14H19NO	217.1467	H+	218.1539	4.5	145.101
N-ethyl Deschloroketamine	C14H19NO	217.1467	H+	218.1539	4.5	91.0543
N-ethyl Deschloroketamine	C14H19NO	217.1467	H+	218.1539	4.5	129.07
N-ethyl Deschloroketamine	C14H19NO	217.1467	H+	218.1539	4.5	173.0965
N-ethyl Deschloroketamine	C14H19NO	217.1467	H+	218.1539	4.5	117.0699
Alpha-PBP	C14H19NO	217.1467	H+	218.1539	4.33	
Alpha-PBP	C14H19NO	217.1467	H+	218.1539	4.33	91.0551
Alpha-PBP	C14H19NO	217.1467	H+	218.1539	4.33	112.1123
Alpha-PBP	C14H19NO	217.1467	H+	218.1539	4.33	218.1538
Alpha-PBP	C14H19NO	217.1467	H+	218.1539	4.33	147.0804
Alpha-PBP	C14H19NO	217.1467	H+	218.1539	4.33	105.034
Primidone	C12H14N2O2	218.1055	H+	219.1128	4.75	
Primidone	C12H14N2O2	218.1055	H+	219.1128	4.75	91.055
Primidone	C12H14N2O2	218.1055	H+	219.1128	4.75	117.0701
Primidone	C12H14N2O2	218.1055	H+	219.1128	4.75	162.0913
Primidone	C12H14N2O2	218.1055	H+	219.1128	4.75	119.0858
Primidone	C12H14N2O2	218.1055	H+	219.1128	4.75	106.0657
Meprobamate	C9H18N2O4	218.1267	H+	219.1339	5.66	
Meprobamate	C9H18N2O4	218.1267	H+	219.1339	5.66	55.0569
Meprobamate	C9H18N2O4	218.1267	H+	219.1339	5.66	91.102
Meprobamate	C9H18N2O4	218.1267	H+	219.1339	5.66	158.1177
Meprobamate	C9H18N2O4	218.1267	H+	219.1339	5.66	69.0717
Meprobamate	C9H18N2O4	218.1267	H+	219.1339	5.66	62.0258
4-HO-MET	C18H23NO2	218.1419	H+	219.1492	3.51	
4-HO-MET	C18H23NO2	218.1419	H+	219.1492	3.51	160.0753
4-HO-MET	C18H23NO2	218.1419	H+	219.1492	3.51	72.0806
4-HO-MET	C18H23NO2	218.1419	H+	219.1492	3.51	115.0539
4-HO-MET	C18H23NO2	218.1419	H+	219.1492	3.51	219.1492
4-HO-MET	C18H23NO2	218.1419	H+	219.1492	3.51	132.0808
5-MeO-DMT	C13H18N2O	218.1419	H+	219.1492	4.08	
5-MeO-DMT	C13H18N2O	218.1419	H+	219.1492	4.08	174.0913
5-MeO-DMT	C13H18N2O	218.1419	H+	219.1492	4.08	58.0677
5-MeO-DMT	C13H18N2O	218.1419	H+	219.1492	4.08	159.0676
5-MeO-DMT	C13H18N2O	218.1419	H+	219.1492	4.08	131.0727
5-MeO-DMT	C13H18N2O	218.1419	H+	219.1492	4.08	130.065
Aniracetam	C12H13NO3	219.0895	H+	220.0968	5.81	
Aniracetam	C12H13NO3	219.0895	H+	220.0968	5.81	135.0441
Aniracetam	C12H13NO3	219.0895	H+	220.0968	5.81	107.0498
Aniracetam	C12H13NO3	219.0895	H+	220.0968	5.81	77.0402
Aniracetam	C12H13NO3	219.0895	H+	220.0968	5.81	92.0269
Aniracetam	C12H13NO3	219.0895	H+	220.0968	5.81	220.0969
N-Ethyl Hexedrone (Hexen)	C14H21NO	219.1623	H+	220.1696	5.81	
N-Ethyl Hexedrone (Hexen)	C14H21NO	219.1623	H+	220.1696	5.81	118.0651
N-Ethyl Hexedrone (Hexen)	C14H21NO	219.1623	H+	220.1696	5.81	130.0651
N-Ethyl Hexedrone (Hexen)	C14H21NO	219.1623	H+	220.1696	5.81	146.0962
N-Ethyl Hexedrone (Hexen)	C14H21NO	219.1623	H+	220.1696	5.81	202.1592
N-Ethyl Hexedrone (Hexen)	C14H21NO	219.1623	H+	220.1696	5.81	220.1698
4'-Methyl Hexedrone	C14H21NO	219.1623	H+	220.1696	6.32	
4'-Methyl Hexedrone	C14H21NO	219.1623	H+	220.1696	6.32	105.0701
4'-Methyl Hexedrone	C14H21NO	219.1623	H+	220.1696	6.32	145.0878
4'-Methyl Hexedrone	C14H21NO	219.1623	H+	220.1696	6.32	131.0726
4'-Methyl Hexedrone	C14H21NO	219.1623	H+	220.1696	6.32	158.0959
4'-Methyl Hexedrone	C14H21NO	219.1623	H+	220.1696	6.32	202.1588
4-MDEC	C14H21NO	219.1623	H+	220.1696	5.04	
4-MDEC	C14H21NO	219.1623	H+	220.1696	5.04	119.048
4-MDEC	C14H21NO	219.1623	H+	220.1696	5.04	100.1112
4-MDEC	C14H21NO	219.1623	H+	220.1696	5.04	147.0795
4-MDEC	C14H21NO	219.1623	H+	220.1696	5.04	220.1689
4-MDEC	C14H21NO	219.1623	H+	220.1696	5.04	117.069
N-propyl Pentedrone	C14H21NO	219.1623	H+	220.1696	5.57	
N-propyl Pentedrone	C14H21NO	219.1623	H+	220.1696	5.57	118.0639
N-propyl Pentedrone	C14H21NO	219.1623	H+	220.1696	5.57	130.0638
N-propyl Pentedrone	C14H21NO	219.1623	H+	220.1696	5.57	160.1109
N-propyl Pentedrone	C14H21NO	219.1623	H+	220.1696	5.57	105.0325
N-propyl Pentedrone	C14H21NO	219.1623	H+	220.1696	5.57	91.0537

Xylazine	C12H16N2S	220.1034	H+	221.1107	4.79	
Xylazine	C12H16N2S	220.1034	H+	221.1107	4.79	221.1108
Xylazine	C12H16N2S	220.1034	H+	221.1107	4.79	164.0527
Xylazine	C12H16N2S	220.1034	H+	221.1107	4.79	90.0378
Xylazine	C12H16N2S	220.1034	H+	221.1107	4.79	147.0912
Xylazine	C12H16N2S	220.1034	H+	221.1107	4.79	120.081
Butylone (bk-MBDB)	C12H15NO3	221.1052	H+	222.1125	4.2	
Butylone (bk-MBDB)	C12H15NO3	221.1052	H+	222.1125	4.2	174.0898
Butylone (bk-MBDB)	C12H15NO3	221.1052	H+	222.1125	4.2	175.0622
Butylone (bk-MBDB)	C12H15NO3	221.1052	H+	222.1125	4.2	146.095
Butylone (bk-MBDB)	C12H15NO3	221.1052	H+	222.1125	4.2	131.0727
Butylone (bk-MBDB)	C12H15NO3	221.1052	H+	222.1125	4.2	204.1014
Dimethylone	C12H15NO3	221.1052	H+	222.1125	3.68	
Dimethylone	C12H15NO3	221.1052	H+	222.1125	3.68	147.0441
Dimethylone	C12H15NO3	221.1052	H+	222.1125	3.68	72.0826
Dimethylone	C12H15NO3	221.1052	H+	222.1125	3.68	222.1127
Dimethylone	C12H15NO3	221.1052	H+	222.1125	3.68	149.0596
Dimethylone	C12H15NO3	221.1052	H+	222.1125	3.68	119.0494
Ethylone (MDEC, bk-MDEA)	C12H15NO3	221.1052	H+	222.1125	3.87	
Ethylone (MDEC, bk-MDEA)	C12H15NO3	221.1052	H+	222.1125	3.87	174.0893
Ethylone (MDEC, bk-MDEA)	C12H15NO3	221.1052	H+	222.1125	3.87	175.0622
Ethylone (MDEC, bk-MDEA)	C12H15NO3	221.1052	H+	222.1125	3.87	146.0932
Ethylone (MDEC, bk-MDEA)	C12H15NO3	221.1052	H+	222.1125	3.87	204.1012
Ethylone (MDEC, bk-MDEA)	C12H15NO3	221.1052	H+	222.1125	3.87	222.112
Metaxalone	C12H15NO3	221.1052	H+	222.1125	7.08	
Metaxalone	C12H15NO3	221.1052	H+	222.1125	7.08	105.0705
Metaxalone	C12H15NO3	221.1052	H+	222.1125	7.08	161.0962
Metaxalone	C12H15NO3	221.1052	H+	222.1125	7.08	133.1011
Metaxalone	C12H15NO3	221.1052	H+	222.1125	7.08	146.0726
Metaxalone	C12H15NO3	221.1052	H+	222.1125	7.08	135.0806
2F-Deschloroketamine	C13H16FNO	221.1216	H+	222.1289	4.21	
2F-Deschloroketamine	C13H16FNO	221.1216	H+	222.1289	4.21	109.0446
2F-Deschloroketamine	C13H16FNO	221.1216	H+	222.1289	4.21	163.0917
2F-Deschloroketamine	C13H16FNO	221.1216	H+	222.1289	4.21	191.087
2F-Deschloroketamine	C13H16FNO	221.1216	H+	222.1289	4.21	147.0606
2F-Deschloroketamine	C13H16FNO	221.1216	H+	222.1289	4.21	222.1293
Tapentadol	C14H23NO	221.1780	H+	222.1852	5.16	
Tapentadol	C14H23NO	221.1780	H+	222.1852	5.16	107.0497
Tapentadol	C14H23NO	221.1780	H+	222.1852	5.16	121.0653
Tapentadol	C14H23NO	221.1780	H+	222.1852	5.16	222.1854
Tapentadol	C14H23NO	221.1780	H+	222.1852	5.16	135.0805
Tapentadol	C14H23NO	221.1780	H+	222.1852	5.16	77.0401
Norketamine	C12H14ClNO	223.0764	H+	224.0837	4.45	
Norketamine	C12H14ClNO	223.0764	H+	224.0837	4.45	125.0154
Norketamine	C12H14ClNO	223.0764	H+	224.0837	4.45	207.057
Norketamine	C12H14ClNO	223.0764	H+	224.0837	4.45	179.0618
Norketamine	C12H14ClNO	223.0764	H+	224.0837	4.45	163.0304
Norketamine	C12H14ClNO	223.0764	H+	224.0837	4.45	224.0831
2C-P	C13H21NO2	223.1572	H+	224.1645	6.57	
2C-P	C13H21NO2	223.1572	H+	224.1645	6.57	207.1374
2C-P	C13H21NO2	223.1572	H+	224.1645	6.57	192.1144
2C-P	C13H21NO2	223.1572	H+	224.1645	6.57	163.0751
2C-P	C13H21NO2	223.1572	H+	224.1645	6.57	135.0802
2C-P	C13H21NO2	223.1572	H+	224.1645	6.57	105.0702
4Cl-Isopropylcathinone	C12H16ClNO	225.0920	H+	226.0993	5.3	
4Cl-Isopropylcathinone	C12H16ClNO	225.0920	H+	226.0993	5.3	131.072
4Cl-Isopropylcathinone	C12H16ClNO	225.0920	H+	226.0993	5.3	166.041
4Cl-Isopropylcathinone	C12H16ClNO	225.0920	H+	226.0993	5.3	139.0294
4Cl-Isopropylcathinone	C12H16ClNO	225.0920	H+	226.0993	5.3	103.0534
4Cl-Isopropylcathinone	C12H16ClNO	225.0920	H+	226.0993	5.3	208.0883
2C-N	C10H14N2O4	226.0954	H+	227.1026	4.37	
2C-N	C10H14N2O4	226.0954	H+	227.1026	4.37	210.076
2C-N	C10H14N2O4	226.0954	H+	227.1026	4.37	151.075
2C-N	C10H14N2O4	226.0954	H+	227.1026	4.37	195.0524
2C-N	C10H14N2O4	226.0954	H+	227.1026	4.37	165.0543
2C-N	C10H14N2O4	226.0954	H+	227.1026	4.37	121.0645
Clonidine	C9H9Cl2N3	229.0174	H+	230.0246	3.4	
Clonidine	C9H9Cl2N3	229.0174	H+	230.0246	3.4	230.0245
Clonidine	C9H9Cl2N3	229.0174	H+	230.0246	3.4	44.0529
Clonidine	C9H9Cl2N3	229.0174	H+	230.0246	3.4	212.9978
Clonidine	C9H9Cl2N3	229.0174	H+	230.0246	3.4	194.0472
Clonidine	C9H9Cl2N3	229.0174	H+	230.0246	3.4	186.9812
DOC	C11H16ClNO2	229.0870	H+	230.0942	5.46	
DOC	C11H16ClNO2	229.0870	H+	230.0942	5.46	185.0359

DOC	C11H16ClNO2	229.0870	H+	230.0942	5.46	155.0254
DOC	C11H16ClNO2	229.0870	H+	230.0942	5.46	213.0673
DOC	C11H16ClNO2	229.0870	H+	230.0942	5.46	198.044
DOC	C11H16ClNO2	229.0870	H+	230.0942	5.46	183.0206
Rolicyclidine	C16H23N	229.1831	H+	230.1903	5.8	
Rolicyclidine	C16H23N	229.1831	H+	230.1903	5.8	72.08
Rolicyclidine	C16H23N	229.1831	H+	230.1903	5.8	91.0534
Rolicyclidine	C16H23N	229.1831	H+	230.1903	5.8	159.1159
Rolicyclidine	C16H23N	229.1831	H+	230.1903	5.8	117.0693
Rolicyclidine	C16H23N	229.1831	H+	230.1903	5.8	81.0695
Naproxen	C14H14O3	230.0943	H+	231.1016	7.79	
Naproxen	C14H14O3	230.0943	H+	231.1016	7.79	185.0959
Naproxen	C14H14O3	230.0943	H+	231.1016	7.79	170.0724
Naproxen	C14H14O3	230.0943	H+	231.1016	7.79	153.0699
Naproxen	C14H14O3	230.0943	H+	231.1016	7.79	154.0778
Naproxen	C14H14O3	230.0943	H+	231.1016	7.79	169.065
TFMPP	C11H13F3N2	230.1031	H+	231.1104	5.67	
TFMPP	C11H13F3N2	230.1031	H+	231.1104	5.67	188.0691
TFMPP	C11H13F3N2	230.1031	H+	231.1104	5.67	231.111
TFMPP	C11H13F3N2	230.1031	H+	231.1104	5.67	141.0007
TFMPP	C11H13F3N2	230.1031	H+	231.1104	5.67	77.0401
TFMPP	C11H13F3N2	230.1031	H+	231.1104	5.67	158.0274
Fenfluramine	C12H16F3N	231.1235	H+	232.1308	5.86	
Fenfluramine	C12H16F3N	231.1235	H+	232.1308	5.86	159.0415
Fenfluramine	C12H16F3N	231.1235	H+	232.1308	5.86	232.1308
Fenfluramine	C12H16F3N	231.1235	H+	232.1308	5.86	187.0729
Fenfluramine	C12H16F3N	231.1235	H+	232.1308	5.86	109.0451
Fenfluramine	C12H16F3N	231.1235	H+	232.1308	5.86	139.0356
PB-22 3-Carboxyindole	C14H17NO2	231.1259	H+	232.1332	8.82	
PB-22 3-Carboxyindole	C14H17NO2	231.1259	H+	232.1332	8.82	118.065
PB-22 3-Carboxyindole	C14H17NO2	231.1259	H+	232.1332	8.82	132.081
PB-22 3-Carboxyindole	C14H17NO2	231.1259	H+	232.1332	8.82	188.1435
PB-22 3-Carboxyindole	C14H17NO2	231.1259	H+	232.1332	8.82	232.1336
PB-22 3-Carboxyindole	C14H17NO2	231.1259	H+	232.1332	8.82	214.1224
MPBP	C15H21NO	231.1623	H+	232.1695	5.26	
MPBP	C15H21NO	231.1623	H+	232.1695	5.26	105.07
MPBP	C15H21NO	231.1623	H+	232.1695	5.26	112.1121
MPBP	C15H21NO	231.1623	H+	232.1695	5.26	119.0491
MPBP	C15H21NO	231.1623	H+	232.1695	5.26	161.0955
MPBP	C15H21NO	231.1623	H+	232.1695	5.26	232.1695
bk-EABDI	C15H21NO	231.1623	H+	232.1696	6.17	
bk-EABDI	C15H21NO	231.1623	H+	232.1696	6.17	185.1192
bk-EABDI	C15H21NO	231.1623	H+	232.1696	6.17	214.1585
bk-EABDI	C15H21NO	231.1623	H+	232.1696	6.17	170.0961
bk-EABDI	C15H21NO	231.1623	H+	232.1696	6.17	131.0847
bk-EABDI	C15H21NO	231.1623	H+	232.1696	6.17	232.1688
Alpha-PVP	C15H21NO	231.1623	H+	232.1696	5.1	
Alpha-PVP	C15H21NO	231.1623	H+	232.1696	5.1	232.1703
Alpha-PVP	C15H21NO	231.1623	H+	232.1696	5.1	91.0556
Alpha-PVP	C15H21NO	231.1623	H+	232.1696	5.1	126.1281
Alpha-PVP	C15H21NO	231.1623	H+	232.1696	5.1	105.0344
Alpha-PVP	C15H21NO	231.1623	H+	232.1696	5.1	161.0958
Norfentanyl	C14H20N2O	232.1576	H+	233.1648	4.63	
Norfentanyl	C14H20N2O	232.1576	H+	233.1648	4.63	84.0816
Norfentanyl	C14H20N2O	232.1576	H+	233.1648	4.63	233.1645
Norfentanyl	C14H20N2O	232.1576	H+	233.1648	4.63	56.0521
Norfentanyl	C14H20N2O	232.1576	H+	233.1648	4.63	55.057
Norfentanyl	C14H20N2O	232.1576	H+	233.1648	4.63	150.0911
Methylphenidate	C14H19NO2	233.1416	H+	234.1489	5.05	
Methylphenidate	C14H19NO2	233.1416	H+	234.1489	5.05	84.0822
Methylphenidate	C14H19NO2	233.1416	H+	234.1489	5.05	234.1495
Methylphenidate	C14H19NO2	233.1416	H+	234.1489	5.05	56.0521
Methylphenidate	C14H19NO2	233.1416	H+	234.1489	5.05	217.1084
Methylphenidate	C14H19NO2	233.1416	H+	234.1489	5.05	174.1277
MOPPP	C14H19NO2	233.1416	H+	234.1489	4.43	
MOPPP	C14H19NO2	233.1416	H+	234.1489	4.43	135.0798
MOPPP	C14H19NO2	233.1416	H+	234.1489	4.43	98.0965
MOPPP	C14H19NO2	233.1416	H+	234.1489	4.43	234.1486
MOPPP	C14H19NO2	233.1416	H+	234.1489	4.43	163.0749
MOPPP	C14H19NO2	233.1416	H+	234.1489	4.43	105.07
Normeperidine	C14H19NO2	233.1416	H+	234.1489	5.4	
Normeperidine	C14H19NO2	233.1416	H+	234.1489	5.4	160.1121
Normeperidine	C14H19NO2	233.1416	H+	234.1489	5.4	234.1492
Normeperidine	C14H19NO2	233.1416	H+	234.1489	5.4	56.0522

Normeperidine	C14H19NO2	233.1416	H+	234.1489	5.4	42.0381
Normeperidine	C14H19NO2	233.1416	H+	234.1489	5.4	188.1071
3-MeO-PCE	C15H23NO	233.1780	H+	234.1852	6	
3-MeO-PCE	C15H23NO	233.1780	H+	234.1852	6	121.0642
3-MeO-PCE	C15H23NO	233.1780	H+	234.1852	6	189.1272
3-MeO-PCE	C15H23NO	233.1780	H+	234.1852	6	91.0536
3-MeO-PCE	C15H23NO	233.1780	H+	234.1852	6	81.0691
3-MeO-PCE	C15H23NO	233.1780	H+	234.1852	6	46.0645
Lidocaine	C14H22N2O	234.1732	H+	235.1805	4.28	
Lidocaine	C14H22N2O	234.1732	H+	235.1805	4.28	86.0973
Lidocaine	C14H22N2O	234.1732	H+	235.1805	4.28	58.0675
Lidocaine	C14H22N2O	234.1732	H+	235.1805	4.28	235.1801
Lidocaine	C14H22N2O	234.1732	H+	235.1805	4.28	134.0962
Lidocaine	C14H22N2O	234.1732	H+	235.1805	4.28	-
Propylone	C13H17NO3	235.1208	H+	236.1281	4.55	
Propylone	C13H17NO3	235.1208	H+	236.1281	4.55	188.1078
Propylone	C13H17NO3	235.1208	H+	236.1281	4.55	175.0632
Propylone	C13H17NO3	235.1208	H+	236.1281	4.55	146.0605
Propylone	C13H17NO3	235.1208	H+	236.1281	4.55	160.1112
Propylone	C13H17NO3	235.1208	H+	236.1281	4.55	218.1187
Dibutylone (bk-DMBDB)	C13H17NO3	235.1208	H+	236.1281	4.31	
Dibutylone (bk-DMBDB)	C13H17NO3	235.1208	H+	236.1281	4.31	149.023
Dibutylone (bk-DMBDB)	C13H17NO3	235.1208	H+	236.1281	4.31	161.0593
Dibutylone (bk-DMBDB)	C13H17NO3	235.1208	H+	236.1281	4.31	236.1283
Dibutylone (bk-DMBDB)	C13H17NO3	235.1208	H+	236.1281	4.31	191.077
Dibutylone (bk-DMBDB)	C13H17NO3	235.1208	H+	236.1281	4.31	163.0751
Eutylone (bk-EBDB)	C13H17NO3	235.1208	H+	236.1281	4.46	
Eutylone (bk-EBDB)	C13H17NO3	235.1208	H+	236.1281	4.46	188.106
Eutylone (bk-EBDB)	C13H17NO3	235.1208	H+	236.1281	4.46	189.078
Eutylone (bk-EBDB)	C13H17NO3	235.1208	H+	236.1281	4.46	174.0544
Eutylone (bk-EBDB)	C13H17NO3	235.1208	H+	236.1281	4.46	218.1171
Eutylone (bk-EBDB)	C13H17NO3	235.1208	H+	236.1281	4.46	236.1286
Pentylone (bk-MBDP)	C13H17NO3	235.1208	H+	236.1281	4.98	
Pentylone (bk-MBDP)	C13H17NO3	235.1208	H+	236.1281	4.98	188.107
Pentylone (bk-MBDP)	C13H17NO3	235.1208	H+	236.1281	4.98	175.0654
Pentylone (bk-MBDP)	C13H17NO3	235.1208	H+	236.1281	4.98	218.118
Pentylone (bk-MBDP)	C13H17NO3	235.1208	H+	236.1281	4.98	236.1277
Pentylone (bk-MBDP)	C13H17NO3	235.1208	H+	236.1281	4.98	205.0866
Procainamide	C13H21N3O	235.1685	H+	236.1757	1.97	
Procainamide	C13H21N3O	235.1685	H+	236.1757	1.97	163.0862
Procainamide	C13H21N3O	235.1685	H+	236.1757	1.97	120.0443
Procainamide	C13H21N3O	235.1685	H+	236.1757	1.97	236.1757
Procainamide	C13H21N3O	235.1685	H+	236.1757	1.97	100.1127
Procainamide	C13H21N3O	235.1685	H+	236.1757	1.97	92.0506
Carbamazepine	C15H12N2O	236.0950	H+	237.1022	6.76	
Carbamazepine	C15H12N2O	236.0950	H+	237.1022	6.76	194.0956
Carbamazepine	C15H12N2O	236.0950	H+	237.1022	6.76	192.08
Carbamazepine	C15H12N2O	236.0950	H+	237.1022	6.76	193.0879
Carbamazepine	C15H12N2O	236.0950	H+	237.1022	6.76	237.1018
Carbamazepine	C15H12N2O	236.0950	H+	237.1022	6.76	179.0721
Ketamine	C13H16ClNO	237.0920	H+	238.0993	4.54	
Ketamine	C13H16ClNO	237.0920	H+	238.0993	4.54	125.0155
Ketamine	C13H16ClNO	237.0920	H+	238.0993	4.54	179.0621
Ketamine	C13H16ClNO	237.0920	H+	238.0993	4.54	238.0999
Ketamine	C13H16ClNO	237.0920	H+	238.0993	4.54	220.0892
Ketamine	C13H16ClNO	237.0920	H+	238.0993	4.54	207.0571
6-Methoxy Methylone	C12H15NO4	237.1001	H+	238.1074	4.23	
6-Methoxy Methylone	C12H15NO4	237.1001	H+	238.1074	4.23	190.0868
6-Methoxy Methylone	C12H15NO4	237.1001	H+	238.1074	4.23	189.0791
6-Methoxy Methylone	C12H15NO4	237.1001	H+	238.1074	4.23	162.092
6-Methoxy Methylone	C12H15NO4	237.1001	H+	238.1074	4.23	147.0681
6-Methoxy Methylone	C12H15NO4	237.1001	H+	238.1074	4.23	58.0656
Alpha-PVT	C13H19NOS	237.1187	H+	238.1260	4.59	
Alpha-PVT	C13H19NOS	237.1187	H+	238.1260	4.59	126.1274
Alpha-PVT	C13H19NOS	237.1187	H+	238.1260	4.59	238.126
Alpha-PVT	C13H19NOS	237.1187	H+	238.1260	4.59	167.0523
Alpha-PVT	C13H19NOS	237.1187	H+	238.1260	4.59	110.99
Alpha-PVT	C13H19NOS	237.1187	H+	238.1260	4.59	97.011
Allylesclaine	C13H19NO3	237.1365	H+	238.1438	4.98	
Allylesclaine	C13H19NO3	237.1365	H+	238.1438	4.98	165.0547
Allylesclaine	C13H19NO3	237.1365	H+	238.1438	4.98	221.1174
Allylesclaine	C13H19NO3	237.1365	H+	238.1438	4.98	180.078
Allylesclaine	C13H19NO3	237.1365	H+	238.1438	4.98	133.0286
Allylesclaine	C13H19NO3	237.1365	H+	238.1438	4.98	129.0699

Bupropion	C13H18ClNO	239.1077	H+	240.1150	5.63	
Bupropion	C13H18ClNO	239.1077	H+	240.1150	5.63	131.0724
Bupropion	C13H18ClNO	239.1077	H+	240.1150	5.63	166.0414
Bupropion	C13H18ClNO	239.1077	H+	240.1150	5.63	184.052
Bupropion	C13H18ClNO	239.1077	H+	240.1150	5.63	167.0252
Bupropion	C13H18ClNO	239.1077	H+	240.1150	5.63	139.0304
Pheniramine	C16H20N2	240.1626	H+	241.1699	4.44	
Pheniramine	C16H20N2	240.1626	H+	241.1699	4.44	196.1122
Pheniramine	C16H20N2	240.1626	H+	241.1699	4.44	168.0803
Pheniramine	C16H20N2	240.1626	H+	241.1699	4.44	167.0735
Pheniramine	C16H20N2	240.1626	H+	241.1699	4.44	118.065
Pheniramine	C16H20N2	240.1626	H+	241.1699	4.44	91.0557
4-Bromomethcathinone	C10H12BrNO	241.0102	H+	242.0175	4.81	
4-Bromomethcathinone	C10H12BrNO	241.0102	H+	242.0175	4.81	145.088
4-Bromomethcathinone	C10H12BrNO	241.0102	H+	242.0175	4.81	144.0805
4-Bromomethcathinone	C10H12BrNO	241.0102	H+	242.0175	4.81	132.057
4-Bromomethcathinone	C10H12BrNO	241.0102	H+	242.0175	4.81	242.0175
4-Bromomethcathinone	C10H12BrNO	241.0102	H+	242.0175	4.81	224.007
Methocarbamol	C11H15NO5	241.0950	H+	242.1023	5.18	
Methocarbamol	C11H15NO5	241.0950	H+	242.1023	5.18	118.0498
Methocarbamol	C11H15NO5	241.0950	H+	242.1023	5.18	122.0363
Methocarbamol	C11H15NO5	241.0950	H+	242.1023	5.18	57.0359
Methocarbamol	C11H15NO5	241.0950	H+	242.1023	5.18	62.0257
Methocarbamol	C11H15NO5	241.0950	H+	242.1023	5.18	125.0598
2C-T-2	C12H19NO2S	241.1137	H+	242.1209	5.71	
2C-T-2	C12H19NO2S	241.1137	H+	242.1209	5.71	225.0945
2C-T-2	C12H19NO2S	241.1137	H+	242.1209	5.71	210.0709
2C-T-2	C12H19NO2S	241.1137	H+	242.1209	5.71	134.0725
2C-T-2	C12H19NO2S	241.1137	H+	242.1209	5.71	164.0833
2C-T-2	C12H19NO2S	241.1137	H+	242.1209	5.71	195.0478
PCP (Phencyclidine)	C17H25N	243.1987	H+	244.2060	5.93	
PCP (Phencyclidine)	C17H25N	243.1987	H+	244.2060	5.93	91.0552
PCP (Phencyclidine)	C17H25N	243.1987	H+	244.2060	5.93	86.0975
PCP (Phencyclidine)	C17H25N	243.1987	H+	244.2060	5.93	159.117
PCP (Phencyclidine)	C17H25N	243.1987	H+	244.2060	5.93	81.0708
PCP (Phencyclidine)	C17H25N	243.1987	H+	244.2060	5.93	117.0699
Dichloroethcathinone (DCEC)	C11H13Cl2NO	245.0374	H+	246.0447	5.83	
Dichloroethcathinone (DCEC)	C11H13Cl2NO	245.0374	H+	246.0447	5.83	193.0641
Dichloroethcathinone (DCEC)	C11H13Cl2NO	245.0374	H+	246.0447	5.83	178.0404
Dichloroethcathinone (DCEC)	C11H13Cl2NO	245.0374	H+	246.0447	5.83	165.0329
Dichloroethcathinone (DCEC)	C11H13Cl2NO	245.0374	H+	246.0447	5.83	228.0329
Dichloroethcathinone (DCEC)	C11H13Cl2NO	245.0374	H+	246.0447	5.83	246.0434
Alpha-PHP	C16H23NO	245.1780	H+	246.1852	5.88	
Alpha-PHP	C16H23NO	245.1780	H+	246.1852	5.88	140.143
Alpha-PHP	C16H23NO	245.1780	H+	246.1852	5.88	105.0332
Alpha-PHP	C16H23NO	245.1780	H+	246.1852	5.88	91.054
Alpha-PHP	C16H23NO	245.1780	H+	246.1852	5.88	246.1859
Alpha-PHP	C16H23NO	245.1780	H+	246.1852	5.88	175.1119
Alpha-PiHP	C16H23NO	245.1780	H+	246.1852	5.8	
Alpha-PiHP	C16H23NO	245.1780	H+	246.1852	5.8	140.1422
Alpha-PiHP	C16H23NO	245.1780	H+	246.1852	5.8	105.0324
Alpha-PiHP	C16H23NO	245.1780	H+	246.1852	5.8	91.0533
Alpha-PiHP	C16H23NO	245.1780	H+	246.1852	5.8	119.048
Alpha-PiHP	C16H23NO	245.1780	H+	246.1852	5.8	189.1143
Pyrovalerone	C16H23NO	245.1780	H+	246.1852	5.86	
Pyrovalerone	C16H23NO	245.1780	H+	246.1852	5.86	105.0706
Pyrovalerone	C16H23NO	245.1780	H+	246.1852	5.86	246.1857
Pyrovalerone	C16H23NO	245.1780	H+	246.1852	5.86	175.1121
Pyrovalerone	C16H23NO	245.1780	H+	246.1852	5.86	126.1281
Pyrovalerone	C16H23NO	245.1780	H+	246.1852	5.86	119.0496
N-methyl Norfentanyl	C15H22N2O	246.1732	H+	247.1805	4.66	
N-methyl Norfentanyl	C15H22N2O	246.1732	H+	247.1805	4.66	98.0699
N-methyl Norfentanyl	C15H22N2O	246.1732	H+	247.1805	4.66	247.1812
N-methyl Norfentanyl	C15H22N2O	246.1732	H+	247.1805	4.66	216.1387
N-methyl Norfentanyl	C15H22N2O	246.1732	H+	247.1805	4.66	132.0809
N-methyl Norfentanyl	C15H22N2O	246.1732	H+	247.1805	4.66	70.0656
Mepivacaine	C15H22N2O	246.1732	H+	247.1805	4.41	
Mepivacaine	C15H22N2O	246.1732	H+	247.1805	4.41	98.0968
Mepivacaine	C15H22N2O	246.1732	H+	247.1805	4.41	247.1807
Mepivacaine	C15H22N2O	246.1732	H+	247.1805	4.41	70.0668
Mepivacaine	C15H22N2O	246.1732	H+	247.1805	4.41	150.0913
Mepivacaine	C15H22N2O	246.1732	H+	247.1805	4.41	42.0381
MDPPP	C14H17NO3	247.1208	H+	248.1281	4.09	
MDPPP	C14H17NO3	247.1208	H+	248.1281	4.09	147.0433

MDPPP	C14H17NO3	247.1208	H+	248.1281	4.09	98.0966
MDPPP	C14H17NO3	247.1208	H+	248.1281	4.09	248.1277
MDPPP	C14H17NO3	247.1208	H+	248.1281	4.09	149.059
MDPPP	C14H17NO3	247.1208	H+	248.1281	4.09	177.0542
Ethylphenidate (EPH)	C15H21NO2	247.1572	H+	248.1645	5.61	
Ethylphenidate (EPH)	C15H21NO2	247.1572	H+	248.1645	5.61	84.0818
Ethylphenidate (EPH)	C15H21NO2	247.1572	H+	248.1645	5.61	248.1646
Ethylphenidate (EPH)	C15H21NO2	247.1572	H+	248.1645	5.61	56.0522
Ethylphenidate (EPH)	C15H21NO2	247.1572	H+	248.1645	5.61	174.1279
Ethylphenidate (EPH)	C15H21NO2	247.1572	H+	248.1645	5.61	129.077
Meperidine	C15H21NO2	247.1572	H+	248.1645	5.37	
Meperidine	C15H21NO2	247.1572	H+	248.1645	5.37	174.1273
Meperidine	C15H21NO2	247.1572	H+	248.1645	5.37	220.1329
Meperidine	C15H21NO2	247.1572	H+	248.1645	5.37	248.1644
Meperidine	C15H21NO2	247.1572	H+	248.1645	5.37	70.0668
Meperidine	C15H21NO2	247.1572	H+	248.1645	5.37	131.0856
Methoxetamine	C15H21NO2	247.1572	H+	248.1645	4.97	
Methoxetamine	C15H21NO2	247.1572	H+	248.1645	4.97	121.0653
Methoxetamine	C15H21NO2	247.1572	H+	248.1645	4.97	203.1068
Methoxetamine	C15H21NO2	247.1572	H+	248.1645	4.97	175.1116
Methoxetamine	C15H21NO2	247.1572	H+	248.1645	4.97	248.1658
Methoxetamine	C15H21NO2	247.1572	H+	248.1645	4.97	185.0961
N-butyl Hexedrone	C16H25NO	247.1936	H+	248.2009	6.62	
N-butyl Hexedrone	C16H25NO	247.1936	H+	248.2009	6.62	118.0647
N-butyl Hexedrone	C16H25NO	247.1936	H+	248.2009	6.62	91.0541
N-butyl Hexedrone	C16H25NO	247.1936	H+	248.2009	6.62	132.0806
N-butyl Hexedrone	C16H25NO	247.1936	H+	248.2009	6.62	174.1273
N-butyl Hexedrone	C16H25NO	247.1936	H+	248.2009	6.62	230.1896
5F-PB-22 3-Carboxyindole	C14H16FNO2	249.1165	H+	250.1238	7.89	
5F-PB-22 3-Carboxyindole	C14H16FNO2	249.1165	H+	250.1238	7.89	118.0643
5F-PB-22 3-Carboxyindole	C14H16FNO2	249.1165	H+	250.1238	7.89	206.1334
5F-PB-22 3-Carboxyindole	C14H16FNO2	249.1165	H+	250.1238	7.89	250.1233
5F-PB-22 3-Carboxyindole	C14H16FNO2	249.1165	H+	250.1238	7.89	132.08
5F-PB-22 3-Carboxyindole	C14H16FNO2	249.1165	H+	250.1238	7.89	130.0647
N-Ethyl Pentylone	C14H19NO3	249.1365	H+	250.1438	5.26	
N-Ethyl Pentylone	C14H19NO3	249.1365	H+	250.1438	5.26	202.1213
N-Ethyl Pentylone	C14H19NO3	249.1365	H+	250.1438	5.26	189.0775
N-Ethyl Pentylone	C14H19NO3	249.1365	H+	250.1438	5.26	135.0435
N-Ethyl Pentylone	C14H19NO3	249.1365	H+	250.1438	5.26	149.0227
N-Ethyl Pentylone	C14H19NO3	249.1365	H+	250.1438	5.26	250.1434
Dimethylpentylone	C14H19NO3	249.1365	H+	250.1438	5.13	
Dimethylpentylone	C14H19NO3	249.1365	H+	250.1438	5.13	135.0441
Dimethylpentylone	C14H19NO3	249.1365	H+	250.1438	5.13	100.112
Dimethylpentylone	C14H19NO3	249.1365	H+	250.1438	5.13	149.0234
Dimethylpentylone	C14H19NO3	249.1365	H+	250.1438	5.13	175.0756
Dimethylpentylone	C14H19NO3	249.1365	H+	250.1438	5.13	205.0863
Diethylone	C14H19NO3	249.1365	H+	250.1438	4.29	
Diethylone	C14H19NO3	249.1365	H+	250.1438	4.29	147.0449
Diethylone	C14H19NO3	249.1365	H+	250.1438	4.29	149.0603
Diethylone	C14H19NO3	249.1365	H+	250.1438	4.29	119.0498
Diethylone	C14H19NO3	249.1365	H+	250.1438	4.29	100.1127
Diethylone	C14H19NO3	249.1365	H+	250.1438	4.29	177.0559
Tertylone	C14H19NO3	249.1365	H+	250.1438	4.94	
Tertylone	C14H19NO3	249.1365	H+	250.1438	4.94	146.0609
Tertylone	C14H19NO3	249.1365	H+	250.1438	4.94	118.0653
Tertylone	C14H19NO3	249.1365	H+	250.1438	4.94	176.0715
Tertylone	C14H19NO3	249.1365	H+	250.1438	4.94	194.0822
Tertylone	C14H19NO3	249.1365	H+	250.1438	4.94	250.1452
4F-alpha-PVP	C15H20FNO	249.1529	H+	250.1602	5.37	
4F-alpha-PVP	C15H20FNO	249.1529	H+	250.1602	5.37	109.0445
4F-alpha-PVP	C15H20FNO	249.1529	H+	250.1602	5.37	126.1278
4F-alpha-PVP	C15H20FNO	249.1529	H+	250.1602	5.37	179.0868
4F-alpha-PVP	C15H20FNO	249.1529	H+	250.1602	5.37	250.16
4F-alpha-PVP	C15H20FNO	249.1529	H+	250.1602	5.37	123.0243
O-Desmethyltramadol	C15H23NO2	249.1729	H+	250.1802	3.93	
O-Desmethyltramadol	C15H23NO2	249.1729	H+	250.1802	3.93	58.0678
O-Desmethyltramadol	C15H23NO2	249.1729	H+	250.1802	3.93	250.1806
O-Desmethyltramadol	C15H23NO2	249.1729	H+	250.1802	3.93	42.038
O-Desmethyltramadol	C15H23NO2	249.1729	H+	250.1802	3.93	232.1694
O-Desmethyltramadol	C15H23NO2	249.1729	H+	250.1802	3.93	145.0651
Methaqualone	C16H14N2O	250.1106	H+	251.1179	7.14	
Methaqualone	C16H14N2O	250.1106	H+	251.1179	7.14	132.0809
Methaqualone	C16H14N2O	250.1106	H+	251.1179	7.14	251.1187
Methaqualone	C16H14N2O	250.1106	H+	251.1179	7.14	117.0577

Methaqualone	C16H14N2O	250.1106	H+	251.1179	7.14	120.0451
Methaqualone	C16H14N2O	250.1106	H+	251.1179	7.14	144.0449
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	250.1118	H+	251.1190	7.4	
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	250.1118	H+	251.1190	7.4	233.108
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	250.1118	H+	251.1190	7.4	145.0394
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	250.1118	H+	251.1190	7.4	213.1019
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	250.1118	H+	251.1190	7.4	177.0454
5F-NPB-22 3-Carboxyindazole	C13H15FN2O2	250.1118	H+	251.1190	7.4	149.0236
Lacosamide	C13H18N2O3	250.1317	H+	251.1390	4.84	
Lacosamide	C13H18N2O3	250.1317	H+	251.1390	4.84	91.0556
Lacosamide	C13H18N2O3	250.1317	H+	251.1390	4.84	74.0621
Lacosamide	C13H18N2O3	250.1317	H+	251.1390	4.84	116.0716
Lacosamide	C13H18N2O3	250.1317	H+	251.1390	4.84	108.0816
Lacosamide	C13H18N2O3	250.1317	H+	251.1390	4.84	149.0228
Didesmethylsibutramine	C15H22ClN	251.1441	H+	252.1514	7.53	
Didesmethylsibutramine	C15H22ClN	251.1441	H+	252.1514	7.53	125.0149
Didesmethylsibutramine	C15H22ClN	251.1441	H+	252.1514	7.53	139.0309
Didesmethylsibutramine	C15H22ClN	251.1441	H+	252.1514	7.53	153.0466
Didesmethylsibutramine	C15H22ClN	251.1441	H+	252.1514	7.53	103.0547
Didesmethylsibutramine	C15H22ClN	251.1441	H+	252.1514	7.53	151.0312
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	H+	253.0972	5.94	
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	H+	253.0972	5.94	180.0802
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	H+	253.0972	5.94	182.0956
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	H+	253.0972	5.94	210.0908
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	H+	253.0972	5.94	236.0702
Carbamazepine 10,11-epoxide	C15H12N2O2	252.0899	H+	253.0972	5.94	167.0725
Phenytoin	C15H12N2O2	252.0899	H+	253.0972	6.71	
Phenytoin	C15H12N2O2	252.0899	H+	253.0972	6.71	182.0964
Phenytoin	C15H12N2O2	252.0899	H+	253.0972	6.71	104.05
Phenytoin	C15H12N2O2	252.0899	H+	253.0972	6.71	253.0974
Phenytoin	C15H12N2O2	252.0899	H+	253.0972	6.71	225.1026
Phenytoin	C15H12N2O2	252.0899	H+	253.0972	6.71	132.0443
Ketoprofen	C16H14O3	254.0943	H+	255.1016	7.71	
Ketoprofen	C16H14O3	254.0943	H+	255.1016	7.71	105.0338
Ketoprofen	C16H14O3	254.0943	H+	255.1016	7.71	209.0956
Ketoprofen	C16H14O3	254.0943	H+	255.1016	7.71	255.1016
Ketoprofen	C16H14O3	254.0943	H+	255.1016	7.71	194.0724
Ketoprofen	C16H14O3	254.0943	H+	255.1016	7.71	177.0548
10-Hydroxycarbazepine	C15H14N2O2	254.1055	H+	255.1128	5.62	
10-Hydroxycarbazepine	C15H14N2O2	254.1055	H+	255.1128	5.62	194.0958
10-Hydroxycarbazepine	C15H14N2O2	254.1055	H+	255.1128	5.62	192.08
10-Hydroxycarbazepine	C15H14N2O2	254.1055	H+	255.1128	5.62	193.088
10-Hydroxycarbazepine	C15H14N2O2	254.1055	H+	255.1128	5.62	237.1017
10-Hydroxycarbazepine	C15H14N2O2	254.1055	H+	255.1128	5.62	179.0722
Lamotrigine	C9H7Cl2N5	255.0079	H+	256.0151	4.92	
Lamotrigine	C9H7Cl2N5	255.0079	H+	256.0151	4.92	256.0154
Lamotrigine	C9H7Cl2N5	255.0079	H+	256.0151	4.92	210.983
Lamotrigine	C9H7Cl2N5	255.0079	H+	256.0151	4.92	166.0294
Lamotrigine	C9H7Cl2N5	255.0079	H+	256.0151	4.92	158.9767
Lamotrigine	C9H7Cl2N5	255.0079	H+	256.0151	4.92	186.9829
Hydroxybupropion	C13H18ClNO2	255.1026	H+	256.1099	5.07	
Hydroxybupropion	C13H18ClNO2	255.1026	H+	256.1099	5.07	238.0989
Hydroxybupropion	C13H18ClNO2	255.1026	H+	256.1099	5.07	139.0308
Hydroxybupropion	C13H18ClNO2	255.1026	H+	256.1099	5.07	131.073
Hydroxybupropion	C13H18ClNO2	255.1026	H+	256.1099	5.07	167.0481
Hydroxybupropion	C13H18ClNO2	255.1026	H+	256.1099	5.07	166.0418
2C-T-7 (2,5-dimethoxy-4-n-propylthiophenethylamine)	C13H21NO2S	255.1293	H+	256.1366	6.4	
2C-T-7 (2,5-dimethoxy-4-n-propylthiophenethylamine)	C13H21NO2S	255.1293	H+	256.1366	6.4	239.1105
2C-T-7 (2,5-dimethoxy-4-n-propylthiophenethylamine)	C13H21NO2S	255.1293	H+	256.1366	6.4	197.063
2C-T-7 (2,5-dimethoxy-4-n-propylthiophenethylamine)	C13H21NO2S	255.1293	H+	256.1366	6.4	224.0866
2C-T-7 (2,5-dimethoxy-4-n-propylthiophenethylamine)	C13H21NO2S	255.1293	H+	256.1366	6.4	182.0392
2C-T-7 (2,5-dimethoxy-4-n-propylthiophenethylamine)	C13H21NO2S	255.1293	H+	256.1366	6.4	167.0162
Atomoxetine	C17H21NO	255.1623	H+	256.1696	6.84	
Atomoxetine	C17H21NO	255.1623	H+	256.1696	6.84	44.0533
Atomoxetine	C17H21NO	255.1623	H+	256.1696	6.84	256.1694
Atomoxetine	C17H21NO	255.1623	H+	256.1696	6.84	117.0702
Atomoxetine	C17H21NO	255.1623	H+	256.1696	6.84	148.1116
Atomoxetine	C17H21NO	255.1623	H+	256.1696	6.84	163.075

Diphenhydramine	C17H21NO	255.1623	H+	256.1696	6.33	
Diphenhydramine	C17H21NO	255.1623	H+	256.1696	6.33	167.0849
Diphenhydramine	C17H21NO	255.1623	H+	256.1696	6.33	165.0694
Diphenhydramine	C17H21NO	255.1623	H+	256.1696	6.33	152.0616
Diphenhydramine	C17H21NO	255.1623	H+	256.1696	6.33	166.0774
Diphenhydramine	C17H21NO	255.1623	H+	256.1696	6.33	151.054
Phenyltoloxamine	C17H21NO	255.1623	H+	256.1696	6.67	
Phenyltoloxamine	C17H21NO	255.1623	H+	256.1696	6.67	72.0826
Phenyltoloxamine	C17H21NO	255.1623	H+	256.1696	6.67	256.1698
Phenyltoloxamine	C17H21NO	255.1623	H+	256.1696	6.67	70.0672
Phenyltoloxamine	C17H21NO	255.1623	H+	256.1696	6.67	44.0537
Phenyltoloxamine	C17H21NO	255.1623	H+	256.1696	6.67	133.0652
BB-22 3-Carboxyindole	C16H19NO2	257.1416	H+	258.1489	9.33	
BB-22 3-Carboxyindole	C16H19NO2	257.1416	H+	258.1489	9.33	118.0646
BB-22 3-Carboxyindole	C16H19NO2	257.1416	H+	258.1489	9.33	258.148
BB-22 3-Carboxyindole	C16H19NO2	257.1416	H+	258.1489	9.33	214.1585
BB-22 3-Carboxyindole	C16H19NO2	257.1416	H+	258.1489	9.33	176.0702
BB-22 3-Carboxyindole	C16H19NO2	257.1416	H+	258.1489	9.33	132.0804
Dextrorphan/Levorphanol	C17H23NO	257.1780	H+	258.1852	4.86	
Dextrorphan/Levorphanol	C17H23NO	257.1780	H+	258.1852	4.86	258.1852
Dextrorphan/Levorphanol	C17H23NO	257.1780	H+	258.1852	4.86	199.1114
Dextrorphan/Levorphanol	C17H23NO	257.1780	H+	258.1852	4.86	201.1272
Dextrorphan/Levorphanol	C17H23NO	257.1780	H+	258.1852	4.86	157.0646
Dextrorphan/Levorphanol	C17H23NO	257.1780	H+	258.1852	4.86	133.0648
N-methyl Cyclopropyl Norfentanyl	C16H22N2O	258.1732	H+	259.1805	5	
N-methyl Cyclopropyl Norfentanyl	C16H22N2O	258.1732	H+	259.1805	5	98.0962
N-methyl Cyclopropyl Norfentanyl	C16H22N2O	258.1732	H+	259.1805	5	259.1811
N-methyl Cyclopropyl Norfentanyl	C16H22N2O	258.1732	H+	259.1805	5	228.1386
N-methyl Cyclopropyl Norfentanyl	C16H22N2O	258.1732	H+	259.1805	5	191.1546
N-methyl Cyclopropyl Norfentanyl	C16H22N2O	258.1732	H+	259.1805	5	132.0807
2C-B	C10H14BrNO2	259.0208	H+	260.0281	5.36	
2C-B	C10H14BrNO2	259.0208	H+	260.0281	5.36	227.9777
2C-B	C10H14BrNO2	259.0208	H+	260.0281	5.36	243.0018
2C-B	C10H14BrNO2	259.0208	H+	260.0281	5.36	212.9543
2C-B	C10H14BrNO2	259.0208	H+	260.0281	5.36	164.0825
2C-B	C10H14BrNO2	259.0208	H+	260.0281	5.36	134.073
Ramelteon	C16H21NO2	259.1572	H+	260.1645	7.35	
Ramelteon	C16H21NO2	259.1572	H+	260.1645	7.35	159.0805
Ramelteon	C16H21NO2	259.1572	H+	260.1645	7.35	204.1386
Ramelteon	C16H21NO2	259.1572	H+	260.1645	7.35	187.1111
Ramelteon	C16H21NO2	259.1572	H+	260.1645	7.35	260.1645
Ramelteon	C16H21NO2	259.1572	H+	260.1645	7.35	133.0663
Alpha-PHpP (PV8)	C17H25NO	259.1936	H+	260.2008	6.50	
Alpha-PHpP (PV8)	C17H25NO	259.1936	H+	260.2008	6.50	154.1585
Alpha-PHpP (PV8)	C17H25NO	259.1936	H+	260.2008	6.50	260.2011
Alpha-PHpP (PV8)	C17H25NO	259.1936	H+	260.2008	6.50	189.1229
Alpha-PHpP (PV8)	C17H25NO	259.1936	H+	260.2008	6.50	119.0492
Alpha-PHpP (PV8)	C17H25NO	259.1936	H+	260.2008	6.50	105.0338
MPHP	C17H25NO	259.1936	H+	260.2008	6.47	
MPHP	C17H25NO	259.1936	H+	260.2008	6.47	105.0701
MPHP	C17H25NO	259.1936	H+	260.2008	6.47	140.1431
MPHP	C17H25NO	259.1936	H+	260.2008	6.47	119.0491
MPHP	C17H25NO	259.1936	H+	260.2008	6.47	189.1271
MPHP	C17H25NO	259.1936	H+	260.2008	6.47	260.2014
3,4-Dimethyl Alpha-PVP	C17H25NO	259.1936	H+	260.2013	6.53	
3,4-Dimethyl Alpha-PVP	C17H25NO	259.1936	H+	260.2013	6.53	133.0647
3,4-Dimethyl Alpha-PVP	C17H25NO	259.1936	H+	260.2013	6.53	126.1276
3,4-Dimethyl Alpha-PVP	C17H25NO	259.1936	H+	260.2013	6.53	119.0855
3,4-Dimethyl Alpha-PVP	C17H25NO	259.1936	H+	260.2013	6.53	260.2028
3,4-Dimethyl Alpha-PVP	C17H25NO	259.1936	H+	260.2013	6.53	189.1283
3-OH-PCP	C17H25NO	259.1936	H+	260.2009	5.25	
3-OH-PCP	C17H25NO	259.1936	H+	260.2009	5.25	107.0492
3-OH-PCP	C17H25NO	259.1936	H+	260.2009	5.25	86.0968
3-OH-PCP	C17H25NO	259.1936	H+	260.2009	5.25	175.1117
3-OH-PCP	C17H25NO	259.1936	H+	260.2009	5.25	81.0705
3-OH-PCP	C17H25NO	259.1936	H+	260.2009	5.25	260.2011
Carisoprodol	C12H24N2O4	260.1736	H+	261.1809	7.2	
Carisoprodol	C12H24N2O4	260.1736	H+	261.1809	7.2	62.026
Carisoprodol	C12H24N2O4	260.1736	H+	261.1809	7.2	55.0571
Carisoprodol	C12H24N2O4	260.1736	H+	261.1809	7.2	97.1021
Carisoprodol	C12H24N2O4	260.1736	H+	261.1809	7.2	200.1649
Carisoprodol	C12H24N2O4	260.1736	H+	261.1809	7.2	176.1284
4-HO-DiPT	C16H24N2O	260.1889	H+	261.1961	4.68	
4-HO-DiPT	C16H24N2O	260.1889	H+	261.1961	4.68	160.0764

4-HO-DiPT	C16H24N2O	260.1889	H+	261.1961	4.68	114.1287
4-HO-DiPT	C16H24N2O	260.1889	H+	261.1961	4.68	115.055
4-HO-DiPT	C16H24N2O	260.1889	H+	261.1961	4.68	261.1976
4-HO-DiPT	C16H24N2O	260.1889	H+	261.1961	4.68	132.0812
MDPBP	C15H19NO3	261.1365	H+	262.1438	4.58	
MDPBP	C15H19NO3	261.1365	H+	262.1438	4.58	161.059
MDPBP	C15H19NO3	261.1365	H+	262.1438	4.58	121.1121
MDPBP	C15H19NO3	261.1365	H+	262.1438	4.58	262.1434
MDPBP	C15H19NO3	261.1365	H+	262.1438	4.58	191.0697
MDPBP	C15H19NO3	261.1365	H+	262.1438	4.58	163.075
Isopropylphenidate	C16H23NO2	261.1729	H+	262.1802	6.22	
Isopropylphenidate	C16H23NO2	261.1729	H+	262.1802	6.22	220.1342
Isopropylphenidate	C16H23NO2	261.1729	H+	262.1802	6.22	174.1284
Isopropylphenidate	C16H23NO2	261.1729	H+	262.1802	6.22	84.0815
Isopropylphenidate	C16H23NO2	261.1729	H+	262.1802	6.22	262.1813
Isopropylphenidate	C16H23NO2	261.1729	H+	262.1802	6.22	56.0502
Methohexital	C14H18N2O3	262.1317	H+	263.1390	7.66	
Methohexital	C14H18N2O3	262.1317	H+	263.1390	7.66	221.0905
Methohexital	C14H18N2O3	262.1317	H+	263.1390	7.66	178.0833
Methohexital	C14H18N2O3	262.1317	H+	263.1390	7.66	109.1014
Methohexital	C14H18N2O3	262.1317	H+	263.1390	7.66	183.0779
Methohexital	C14H18N2O3	262.1317	H+	263.1390	7.66	263.1392
Ticlopidine	C14H14ClNS	263.0535	H+	264.0608	5.42	
Ticlopidine	C14H14ClNS	263.0535	H+	264.0608	5.42	125.0152
Ticlopidine	C14H14ClNS	263.0535	H+	264.0608	5.42	154.0415
Ticlopidine	C14H14ClNS	263.0535	H+	264.0608	5.42	264.061
Ticlopidine	C14H14ClNS	263.0535	H+	264.0608	5.42	99
Ticlopidine	C14H14ClNS	263.0535	H+	264.0608	5.42	89.0396
N-ethyl Hexylone	C15H21NO3	263.1521	H+	264.1594	5.96	
N-ethyl Hexylone	C15H21NO3	263.1521	H+	264.1594	5.96	216.1371
N-ethyl Hexylone	C15H21NO3	263.1521	H+	264.1594	5.96	189.0797
N-ethyl Hexylone	C15H21NO3	263.1521	H+	264.1594	5.96	135.0427
N-ethyl Hexylone	C15H21NO3	263.1521	H+	264.1594	5.96	149.0226
N-ethyl Hexylone	C15H21NO3	263.1521	H+	264.1594	5.96	114.1271
EMDP	C19H21N	263.1674	H+	264.1747	7.38	
EMDP	C19H21N	263.1674	H+	264.1747	7.38	235.1348
EMDP	C19H21N	263.1674	H+	264.1747	7.38	220.1112
EMDP	C19H21N	263.1674	H+	264.1747	7.38	264.1743
EMDP	C19H21N	263.1674	H+	264.1747	7.38	234.127
EMDP	C19H21N	263.1674	H+	264.1747	7.38	219.1045
Nortriptyline	C19H21N	263.1674	H+	264.1747	7.2	
Nortriptyline	C19H21N	263.1674	H+	264.1747	7.2	117.07
Nortriptyline	C19H21N	263.1674	H+	264.1747	7.2	105.0703
Nortriptyline	C19H21N	263.1674	H+	264.1747	7.2	191.0855
Nortriptyline	C19H21N	263.1674	H+	264.1747	7.2	91.055
Nortriptyline	C19H21N	263.1674	H+	264.1747	7.2	233.1326
Protriptyline	C19H21N	263.1674	H+	264.1747	7.04	
Protriptyline	C19H21N	263.1674	H+	264.1747	7.04	191.0848
Protriptyline	C19H21N	263.1674	H+	264.1747	7.04	155.0851
Protriptyline	C19H21N	263.1674	H+	264.1747	7.04	264.1741
Protriptyline	C19H21N	263.1674	H+	264.1747	7.04	233.1321
Protriptyline	C19H21N	263.1674	H+	264.1747	7.04	177.0698
4F-alpha-PHP	C16H22FNO	263.1685	H+	264.1758	6.06	
4F-alpha-PHP	C16H22FNO	263.1685	H+	264.1758	6.06	140.1432
4F-alpha-PHP	C16H22FNO	263.1685	H+	264.1758	6.06	109.0445
4F-alpha-PHP	C16H22FNO	263.1685	H+	264.1758	6.06	123.0244
4F-alpha-PHP	C16H22FNO	263.1685	H+	264.1758	6.06	264.1775
4F-alpha-PHP	C16H22FNO	263.1685	H+	264.1758	6.06	193.1029
O-Desmethylvenlafaxine	C16H25NO2	263.1885	H+	264.1958	4.61	
O-Desmethylvenlafaxine	C16H25NO2	263.1885	H+	264.1958	4.61	58.0673
O-Desmethylvenlafaxine	C16H25NO2	263.1885	H+	264.1958	4.61	107.0495
O-Desmethylvenlafaxine	C16H25NO2	263.1885	H+	264.1958	4.61	264.1958
O-Desmethylvenlafaxine	C16H25NO2	263.1885	H+	264.1958	4.61	246.1851
O-Desmethylvenlafaxine	C16H25NO2	263.1885	H+	264.1958	4.61	201.127
Tramadol	C16H25NO2	263.1885	H+	264.1958	4.94	
Tramadol	C16H25NO2	263.1885	H+	264.1958	4.94	58.0677
Tramadol	C16H25NO2	263.1885	H+	264.1958	4.94	264.1957
Tramadol	C16H25NO2	263.1885	H+	264.1958	4.94	42.0382
Tramadol	C16H25NO2	263.1885	H+	264.1958	4.94	246.1851
Tramadol	C16H25NO2	263.1885	H+	264.1958	4.94	121.0647
Lisdexamphetamine	C15H25N3O	263.1998	H+	264.2070	3.22	
Lisdexamphetamine	C15H25N3O	263.1998	H+	264.2070	3.22	84.082
Lisdexamphetamine	C15H25N3O	263.1998	H+	264.2070	3.22	264.2077
Lisdexamphetamine	C15H25N3O	263.1998	H+	264.2070	3.22	247.1809

Lisdexamphetamine	C15H25N3O	263.1998	H+	264.2070	3.22	136.1121
Lisdexamphetamine	C15H25N3O	263.1998	H+	264.2070	3.22	129.1022
Etaqualone	C17H16N2O	264.1263	H+	265.1335	7.73	
Etaqualone	C17H16N2O	264.1263	H+	265.1335	7.73	265.1343
Etaqualone	C17H16N2O	264.1263	H+	265.1335	7.73	146.0958
Etaqualone	C17H16N2O	264.1263	H+	265.1335	7.73	235.0876
Etaqualone	C17H16N2O	264.1263	H+	265.1335	7.73	161.0713
Etaqualone	C17H16N2O	264.1263	H+	265.1335	7.73	131.0732
4-Cl-alpha-PVP	C15H20ClNO	265.1233	H+	266.1306	6.15	
4-Cl-alpha-PVP	C15H20ClNO	265.1233	H+	266.1306	6.15	125.0152
4-Cl-alpha-PVP	C15H20ClNO	265.1233	H+	266.1306	6.15	138.9942
4-Cl-alpha-PVP	C15H20ClNO	265.1233	H+	266.1306	6.15	195.0564
4-Cl-alpha-PVP	C15H20ClNO	265.1233	H+	266.1306	6.15	266.1307
4-Cl-alpha-PVP	C15H20ClNO	265.1233	H+	266.1306	6.15	223.0754
Desmethyldoxepin	C18H19NO	265.1467	H+	266.1539	6.52	
Desmethyldoxepin	C18H19NO	265.1467	H+	266.1539	6.52	107.0497
Desmethyldoxepin	C18H19NO	265.1467	H+	266.1539	6.52	266.154
Desmethyldoxepin	C18H19NO	265.1467	H+	266.1539	6.52	235.1119
Desmethyldoxepin	C18H19NO	265.1467	H+	266.1539	6.52	220.0882
Desmethyldoxepin	C18H19NO	265.1467	H+	266.1539	6.52	202.0776
Mirtazapine	C17H19N3	265.1579	H+	266.1652	5.08	
Mirtazapine	C17H19N3	265.1579	H+	266.1652	5.08	195.0911
Mirtazapine	C17H19N3	265.1579	H+	266.1652	5.08	266.165
Mirtazapine	C17H19N3	265.1579	H+	266.1652	5.08	72.0822
Mirtazapine	C17H19N3	265.1579	H+	266.1652	5.08	209.1072
Mirtazapine	C17H19N3	265.1579	H+	266.1652	5.08	194.0837
DBZP (Dibenzylpiperazine)	C18H22N2	266.1783	H+	267.1856	5.54	
DBZP (Dibenzylpiperazine)	C18H22N2	266.1783	H+	267.1856	5.54	91.0551
DBZP (Dibenzylpiperazine)	C18H22N2	266.1783	H+	267.1856	5.54	267.1855
DBZP (Dibenzylpiperazine)	C18H22N2	266.1783	H+	267.1856	5.54	175.123
DBZP (Dibenzylpiperazine)	C18H22N2	266.1783	H+	267.1856	5.54	134.0964
DBZP (Dibenzylpiperazine)	C18H22N2	266.1783	H+	267.1856	5.54	120.0807
Desipramine	C18H22N2	266.1783	H+	267.1856	7.04	
Desipramine	C18H22N2	266.1783	H+	267.1856	7.04	72.0827
Desipramine	C18H22N2	266.1783	H+	267.1856	7.04	208.1125
Desipramine	C18H22N2	266.1783	H+	267.1856	7.04	193.089
Desipramine	C18H22N2	266.1783	H+	267.1856	7.04	44.0537
Desipramine	C18H22N2	266.1783	H+	267.1856	7.04	267.1864
4-ANBP	C18H22N2	266.1783	H+	267.1856	5.78	
4-ANBP	C18H22N2	266.1783	H+	267.1856	5.78	147.1278
4-ANBP	C18H22N2	266.1783	H+	267.1856	5.78	91.0542
4-ANBP	C18H22N2	266.1783	H+	267.1856	5.78	267.1857
4-ANBP	C18H22N2	266.1783	H+	267.1856	5.78	120.0807
4-ANBP	C18H22N2	266.1783	H+	267.1856	5.78	84.0808
FUB-PB-22 3-Carboxyindole	C16H12FNO2	269.0852	H+	270.0925	8.2	
FUB-PB-22 3-Carboxyindole	C16H12FNO2	269.0852	H+	270.0925	8.2	109.0445
FUB-PB-22 3-Carboxyindole	C16H12FNO2	269.0852	H+	270.0925	8.2	270.0905
FUB-PB-22 3-Carboxyindole	C16H12FNO2	269.0852	H+	270.0925	8.2	226.1058
FUB-PB-22 3-Carboxyindole	C16H12FNO2	269.0852	H+	270.0925	8.2	174.0542
FUB-PB-22 3-Carboxyindole	C16H12FNO2	269.0852	H+	270.0925	8.2	83.0289
Orphenadrine	C18H23NO	269.1780	H+	270.1852	6.8	
Orphenadrine	C18H23NO	269.1780	H+	270.1852	6.8	181.1006
Orphenadrine	C18H23NO	269.1780	H+	270.1852	6.8	166.0771
Orphenadrine	C18H23NO	269.1780	H+	270.1852	6.8	165.0695
Orphenadrine	C18H23NO	269.1780	H+	270.1852	6.8	179.0854
Orphenadrine	C18H23NO	269.1780	H+	270.1852	6.8	153.0699
Pramiracetam	C14H27N3O2	269.2103	H+	270.2176	2.44	
Pramiracetam	C14H27N3O2	269.2103	H+	270.2176	2.44	169.097
Pramiracetam	C14H27N3O2	269.2103	H+	270.2176	2.44	98.0608
Pramiracetam	C14H27N3O2	269.2103	H+	270.2176	2.44	270.2179
Pramiracetam	C14H27N3O2	269.2103	H+	270.2176	2.44	228.1708
Pramiracetam	C14H27N3O2	269.2103	H+	270.2176	2.44	128.1436
Nordiazepam	C15H11ClN2O	270.0560	H+	271.0633	7.68	
Nordiazepam	C15H11ClN2O	270.0560	H+	271.0633	7.68	271.0629
Nordiazepam	C15H11ClN2O	270.0560	H+	271.0633	7.68	140.026
Nordiazepam	C15H11ClN2O	270.0560	H+	271.0633	7.68	208.099
Nordiazepam	C15H11ClN2O	270.0560	H+	271.0633	7.68	165.0211
Nordiazepam	C15H11ClN2O	270.0560	H+	271.0633	7.68	243.0677
Medazepam	C16H15ClN2	270.0924	H+	271.0997	6.4	
Medazepam	C16H15ClN2	270.0924	H+	271.0997	6.4	271.0998
Medazepam	C16H15ClN2	270.0924	H+	271.0997	6.4	207.1039
Medazepam	C16H15ClN2	270.0924	H+	271.0997	6.4	242.0732
Medazepam	C16H15ClN2	270.0924	H+	271.0997	6.4	180.0448
Medazepam	C16H15ClN2	270.0924	H+	271.0997	6.4	91.055

Norfuranylfentanyl	C16H18N2O2	270.1368	H+	271.1441	4.81	
Norfuranylfentanyl	C16H18N2O2	270.1368	H+	271.1441	4.81	84.0807
Norfuranylfentanyl	C16H18N2O2	270.1368	H+	271.1441	4.81	188.0706
Norfuranylfentanyl	C16H18N2O2	270.1368	H+	271.1441	4.81	56.0494
Norfuranylfentanyl	C16H18N2O2	270.1368	H+	271.1441	4.81	95.0127
Norfuranylfentanyl	C16H18N2O2	270.1368	H+	271.1441	4.81	271.0441
5-MeO-DALT	C17H22N2O	270.1732	H+	271.1805	5.4	
5-MeO-DALT	C17H22N2O	270.1732	H+	271.1805	5.4	174.0915
5-MeO-DALT	C17H22N2O	270.1732	H+	271.1805	5.4	110.097
5-MeO-DALT	C17H22N2O	270.1732	H+	271.1805	5.4	159.068
5-MeO-DALT	C17H22N2O	270.1732	H+	271.1805	5.4	143.0726
5-MeO-DALT	C17H22N2O	270.1732	H+	271.1805	5.4	131.0726
Doxylamine	C17H22N2O	270.1732	H+	271.1805	4.41	
Doxylamine	C17H22N2O	270.1732	H+	271.1805	4.41	182.096
Doxylamine	C17H22N2O	270.1732	H+	271.1805	4.41	167.0723
Doxylamine	C17H22N2O	270.1732	H+	271.1805	4.41	271.1806
Doxylamine	C17H22N2O	270.1732	H+	271.1805	4.41	90.0924
Doxylamine	C17H22N2O	270.1732	H+	271.1805	4.41	166.065
Desomorphine	C17H21NO2	271.1572	H+	272.1645	3.86	
Desomorphine	C17H21NO2	271.1572	H+	272.1645	3.86	272.1645
Desomorphine	C17H21NO2	271.1572	H+	272.1645	3.86	215.1067
Desomorphine	C17H21NO2	271.1572	H+	272.1645	3.86	195.0805
Desomorphine	C17H21NO2	271.1572	H+	272.1645	3.86	167.0854
Desomorphine	C17H21NO2	271.1572	H+	272.1645	3.86	197.0961
Dextromethorphan	C18H25NO	271.1936	H+	272.2009	6.24	
Dextromethorphan	C18H25NO	271.1936	H+	272.2009	6.24	272.2005
Dextromethorphan	C18H25NO	271.1936	H+	272.2009	6.24	215.1423
Dextromethorphan	C18H25NO	271.1936	H+	272.2009	6.24	213.127
Dextromethorphan	C18H25NO	271.1936	H+	272.2009	6.24	147.0801
Dextromethorphan	C18H25NO	271.1936	H+	272.2009	6.24	171.0799
DOB	C11H16BrNO2	273.0364	H+	274.0437	5.66	
DOB	C11H16BrNO2	273.0364	H+	274.0437	5.66	228.9853
DOB	C11H16BrNO2	273.0364	H+	274.0437	5.66	178.0986
DOB	C11H16BrNO2	273.0364	H+	274.0437	5.66	257.0164
DOB	C11H16BrNO2	273.0364	H+	274.0437	5.66	241.9936
DOB	C11H16BrNO2	273.0364	H+	274.0437	5.66	226.97
Modafinil	C15H15NO2S	273.0824	H+	274.0896	6.4	
Modafinil	C15H15NO2S	273.0824	H+	274.0896	6.4	167.0858
Modafinil	C15H15NO2S	273.0824	H+	274.0896	6.4	165.07
Modafinil	C15H15NO2S	273.0824	H+	274.0896	6.4	152.0622
Modafinil	C15H15NO2S	273.0824	H+	274.0896	6.4	151.0546
Modafinil	C15H15NO2S	273.0824	H+	274.0896	6.4	128.0632
4-MeO-PCP	C18H27NO	273.2093	H+	274.2165	6.25	
4-MeO-PCP	C18H27NO	273.2093	H+	274.2165	6.25	189.1286
4-MeO-PCP	C18H27NO	273.2093	H+	274.2165	6.25	121.066
4-MeO-PCP	C18H27NO	273.2093	H+	274.2165	6.25	147.0807
4-MeO-PCP	C18H27NO	273.2093	H+	274.2165	6.25	86.0984
4-MeO-PCP	C18H27NO	273.2093	H+	274.2165	6.25	81.072
Chlorpheniramine	C16H19ClN2	274.1237	H+	275.1310	5.81	
Chlorpheniramine	C16H19ClN2	274.1237	H+	275.1310	5.81	230.0728
Chlorpheniramine	C16H19ClN2	274.1237	H+	275.1310	5.81	167.0729
Chlorpheniramine	C16H19ClN2	274.1237	H+	275.1310	5.81	202.042
Chlorpheniramine	C16H19ClN2	274.1237	H+	275.1310	5.81	201.0342
Chlorpheniramine	C16H19ClN2	274.1237	H+	275.1310	5.81	180.0806
UF-17	C17H26N2O	274.2045	H+	275.2118	5.59	
UF-17	C17H26N2O	274.2045	H+	275.2118	5.59	174.1268
UF-17	C17H26N2O	274.2045	H+	275.2118	5.59	230.1526
UF-17	C17H26N2O	274.2045	H+	275.2118	5.59	150.0906
UF-17	C17H26N2O	274.2045	H+	275.2118	5.59	275.2105
UF-17	C17H26N2O	274.2045	H+	275.2118	5.59	81.0696
5-MeO-DiPT	C17H26N2O	274.2045	H+	275.2118	5.34	
5-MeO-DiPT	C17H26N2O	274.2045	H+	275.2118	5.34	174.0917
5-MeO-DiPT	C17H26N2O	274.2045	H+	275.2118	5.34	114.1283
5-MeO-DiPT	C17H26N2O	274.2045	H+	275.2118	5.34	159.0682
5-MeO-DiPT	C17H26N2O	274.2045	H+	275.2118	5.34	275.2124
5-MeO-DiPT	C17H26N2O	274.2045	H+	275.2118	5.34	143.0731
Ropivacaine	C17H26N2O	274.2045	H+	275.2118	5.25	
Ropivacaine	C17H26N2O	274.2045	H+	275.2118	5.25	126.1278
Ropivacaine	C17H26N2O	274.2045	H+	275.2118	5.25	275.2121
Ropivacaine	C17H26N2O	274.2045	H+	275.2118	5.25	84.0821
Ropivacaine	C17H26N2O	274.2045	H+	275.2118	5.25	98.0974
Ropivacaine	C17H26N2O	274.2045	H+	275.2118	5.25	150.0914
MDPV	C16H21NO3	275.1521	H+	276.1594	5.29	
MDPV	C16H21NO3	275.1521	H+	276.1594	5.29	276.1601

MDPV	C16H21NO3	275.1521	H+	276.1594	5.29	126.128
MDPV	C16H21NO3	275.1521	H+	276.1594	5.29	135.0442
MDPV	C16H21NO3	275.1521	H+	276.1594	5.29	175.0755
MDPV	C16H21NO3	275.1521	H+	276.1594	5.29	149.0233
Cyclobenzaprine	C20H21N	275.1674	H+	276.1747	7.02	
Cyclobenzaprine	C20H21N	275.1674	H+	276.1747	7.02	216.0934
Cyclobenzaprine	C20H21N	275.1674	H+	276.1747	7.02	215.0856
Cyclobenzaprine	C20H21N	275.1674	H+	276.1747	7.02	279.175
Cyclobenzaprine	C20H21N	275.1674	H+	276.1747	7.02	231.1171
Cyclobenzaprine	C20H21N	275.1674	H+	276.1747	7.02	205.1016
N-butyl Pentylone	C16H23NO3	277.1678	H+	278.1751	6.2	
N-butyl Pentylone	C16H23NO3	277.1678	H+	278.1751	6.2	230.1528
N-butyl Pentylone	C16H23NO3	277.1678	H+	278.1751	6.2	188.105
N-butyl Pentylone	C16H23NO3	277.1678	H+	278.1751	6.2	135.0433
N-butyl Pentylone	C16H23NO3	277.1678	H+	278.1751	6.2	260.1641
N-butyl Pentylone	C16H23NO3	277.1678	H+	278.1751	6.2	217.1092
Diethylpentylone	C16H23NO3	277.1678	H+	278.1751	5.51	
Diethylpentylone	C16H23NO3	277.1678	H+	278.1751	5.51	175.0759
Diethylpentylone	C16H23NO3	277.1678	H+	278.1751	5.51	149.0238
Diethylpentylone	C16H23NO3	277.1678	H+	278.1751	5.51	135.0441
Diethylpentylone	C16H23NO3	277.1678	H+	278.1751	5.51	128.1434
Diethylpentylone	C16H23NO3	277.1678	H+	278.1751	5.51	205.0869
Amitriptyline	C20H23N	277.1830	H+	278.1903	7.21	
Amitriptyline	C20H23N	277.1830	H+	278.1903	7.21	117.0695
Amitriptyline	C20H23N	277.1830	H+	278.1903	7.21	191.0847
Amitriptyline	C20H23N	277.1830	H+	278.1903	7.21	105.0698
Amitriptyline	C20H23N	277.1830	H+	278.1903	7.21	233.132
Amitriptyline	C20H23N	277.1830	H+	278.1903	7.21	218.1086
EDDP	C20H23N	277.1830	H+	278.1903	6.54	
EDDP	C20H23N	277.1830	H+	278.1903	6.54	278.1898
EDDP	C20H23N	277.1830	H+	278.1903	6.54	249.1503
EDDP	C20H23N	277.1830	H+	278.1903	6.54	234.1269
EDDP	C20H23N	277.1830	H+	278.1903	6.54	186.1271
EDDP	C20H23N	277.1830	H+	278.1903	6.54	219.1038
Maprotiline	C20H23N	277.1830	H+	278.1903	7.16	
Maprotiline	C20H23N	277.1830	H+	278.1903	7.16	219.1165
Maprotiline	C20H23N	277.1830	H+	278.1903	7.16	250.1588
Maprotiline	C20H23N	277.1830	H+	278.1903	7.16	117.0701
Maprotiline	C20H23N	277.1830	H+	278.1903	7.16	191.0852
Maprotiline	C20H23N	277.1830	H+	278.1903	7.16	278.1902
Venlafaxine	C17H27NO2	277.2042	H+	278.2115	5.78	
Venlafaxine	C17H27NO2	277.2042	H+	278.2115	5.78	58.0674
Venlafaxine	C17H27NO2	277.2042	H+	278.2115	5.78	121.0651
Venlafaxine	C17H27NO2	277.2042	H+	278.2115	5.78	147.0805
Venlafaxine	C17H27NO2	277.2042	H+	278.2115	5.78	260.2013
Venlafaxine	C17H27NO2	277.2042	H+	278.2115	5.78	278.2117
Triprolidine	C19H22N2	278.1783	H+	279.1856	6.11	
Triprolidine	C19H22N2	278.1783	H+	279.1856	6.11	208.1119
Triprolidine	C19H22N2	278.1783	H+	279.1856	6.11	193.0887
Triprolidine	C19H22N2	278.1783	H+	279.1856	6.11	149.0234
Triprolidine	C19H22N2	278.1783	H+	279.1856	6.11	192.0809
Triprolidine	C19H22N2	278.1783	H+	279.1856	6.11	207.1044
Dimethocaine	C16H26N2O2	278.1994	H+	279.2067	4.66	
Dimethocaine	C16H26N2O2	278.1994	H+	279.2067	4.66	120.0442
Dimethocaine	C16H26N2O2	278.1994	H+	279.2067	4.66	142.1586
Dimethocaine	C16H26N2O2	278.1994	H+	279.2067	4.66	279.207
Dimethocaine	C16H26N2O2	278.1994	H+	279.2067	4.66	206.1179
Dimethocaine	C16H26N2O2	278.1994	H+	279.2067	4.66	160.1697
Caccure 907	C15H21NO2S	279.1293	H+	280.1366	7.06	
Caccure 907	C15H21NO2S	279.1293	H+	280.1366	7.06	165.0728
Caccure 907	C15H21NO2S	279.1293	H+	280.1366	7.06	128.1063
Caccure 907	C15H21NO2S	279.1293	H+	280.1366	7.06	146.072
Caccure 907	C15H21NO2S	279.1293	H+	280.1366	7.06	117.0692
Caccure 907	C15H21NO2S	279.1293	H+	280.1366	7.06	88.076
Doxepin	C19H21NO	279.1623	H+	280.1696	6.52	
Doxepin	C19H21NO	279.1623	H+	280.1696	6.52	107.0496
Doxepin	C19H21NO	279.1623	H+	280.1696	6.52	280.1696
Doxepin	C19H21NO	279.1623	H+	280.1696	6.52	235.112
Doxepin	C19H21NO	279.1623	H+	280.1696	6.52	117.0702
Doxepin	C19H21NO	279.1623	H+	280.1696	6.52	141.07
Sibutramine	C17H26ClN	279.1754	H+	280.1827	7.49	
Sibutramine	C17H26ClN	279.1754	H+	280.1827	7.49	125.0149
Sibutramine	C17H26ClN	279.1754	H+	280.1827	7.49	139.0301
Sibutramine	C17H26ClN	279.1754	H+	280.1827	7.49	153.0461

Sibutramine	C17H26ClN	279.1754	H+	280.1827	7.49	151.0306
Sibutramine	C17H26ClN	279.1754	H+	280.1827	7.49	179.062
Imipramine	C19H24N2	280.1939	H+	281.2012	7.32	
Imipramine	C19H24N2	280.1939	H+	281.2012	7.32	86.0976
Imipramine	C19H24N2	280.1939	H+	281.2012	7.32	208.1124
Imipramine	C19H24N2	280.1939	H+	281.2012	7.32	44.0537
Imipramine	C19H24N2	280.1939	H+	281.2012	7.32	193.0887
Imipramine	C19H24N2	280.1939	H+	281.2012	7.32	281.202
4-ANPP	C19H24N2	280.1940	H+	281.2012	6.12	
4-ANPP	C19H24N2	280.1940	H+	281.2012	6.12	188.143
4-ANPP	C19H24N2	280.1940	H+	281.2012	6.12	105.0703
4-ANPP	C19H24N2	280.1940	H+	281.2012	6.12	281.2005
4-ANPP	C19H24N2	280.1940	H+	281.2012	6.12	134.0958
4-ANPP	C19H24N2	280.1940	H+	281.2012	6.12	146.0957
Naphyrone	C19H23NO	281.1780	H+	282.1852	6.7	
Naphyrone	C19H23NO	281.1780	H+	282.1852	6.7	141.07
Naphyrone	C19H23NO	281.1780	H+	282.1852	6.7	282.1859
Naphyrone	C19H23NO	281.1780	H+	282.1852	6.7	211.1122
Naphyrone	C19H23NO	281.1780	H+	282.1852	6.7	155.0494
Naphyrone	C19H23NO	281.1780	H+	282.1852	6.7	126.128
2C-B-FLY	C12H14BrNO2	283.0208	H+	284.0281	5.5	
2C-B-FLY	C12H14BrNO2	283.0208	H+	284.0281	5.5	267.0021
2C-B-FLY	C12H14BrNO2	283.0208	H+	284.0281	5.5	188.0831
2C-B-FLY	C12H14BrNO2	283.0208	H+	284.0281	5.5	173.0597
2C-B-FLY	C12H14BrNO2	283.0208	H+	284.0281	5.5	145.0644
2C-B-FLY	C12H14BrNO2	283.0208	H+	284.0281	5.5	159.0441
7-Aminoflunitrazepam	C16H14FN3O	283.1121	H+	284.1194	5.3	
7-Aminoflunitrazepam	C16H14FN3O	283.1121	H+	284.1194	5.3	284.1199
7-Aminoflunitrazepam	C16H14FN3O	283.1121	H+	284.1194	5.3	135.0918
7-Aminoflunitrazepam	C16H14FN3O	283.1121	H+	284.1194	5.3	227.0982
7-Aminoflunitrazepam	C16H14FN3O	283.1121	H+	284.1194	5.3	256.1249
7-Aminoflunitrazepam	C16H14FN3O	283.1121	H+	284.1194	5.3	226.0905
Benzylone	C17H17NO3	283.1208	H+	284.1281	5.71	
Benzylone	C17H17NO3	283.1208	H+	284.1281	5.71	91.0546
Benzylone	C17H17NO3	283.1208	H+	284.1281	5.71	266.1182
Benzylone	C17H17NO3	283.1208	H+	284.1281	5.71	236.1071
Benzylone	C17H17NO3	283.1208	H+	284.1281	5.71	146.0598
Benzylone	C17H17NO3	283.1208	H+	284.1281	5.71	284.1292
Diazepam	C16H13ClN2O	284.0716	H+	285.0789	8.12	
Diazepam	C16H13ClN2O	284.0716	H+	285.0789	8.12	285.079
Diazepam	C16H13ClN2O	284.0716	H+	285.0789	8.12	257.0844
Diazepam	C16H13ClN2O	284.0716	H+	285.0789	8.12	228.0576
Diazepam	C16H13ClN2O	284.0716	H+	285.0789	8.12	222.1151
Diazepam	C16H13ClN2O	284.0716	H+	285.0789	8.12	193.0885
Psilocybin	C12H17N2O4P	284.0926	H+	285.0999	1.13	
Psilocybin	C12H17N2O4P	284.0926	H+	285.0999	1.13	285.1007
Psilocybin	C12H17N2O4P	284.0926	H+	285.0999	1.13	240.0421
Psilocybin	C12H17N2O4P	284.0926	H+	285.0999	1.13	205.1332
Psilocybin	C12H17N2O4P	284.0926	H+	285.0999	1.13	58.0675
Psilocybin	C12H17N2O4P	284.0926	H+	285.0999	1.13	160.0755
MFUBINAC	C16H13FN2O2	284.0961	H+	285.1034	8.67	
MFUBINAC	C16H13FN2O2	284.0961	H+	285.1034	8.67	109.0444
MFUBINAC	C16H13FN2O2	284.0961	H+	285.1034	8.67	253.0765
MFUBINAC	C16H13FN2O2	284.0961	H+	285.1034	8.67	225.0816
MFUBINAC	C16H13FN2O2	284.0961	H+	285.1034	8.67	83.0289
MFUBINAC	C16H13FN2O2	284.0961	H+	285.1034	8.67	285.102
Promazine	C17H20N2S	284.1347	H+	285.1420	6.89	
Promazine	C17H20N2S	284.1347	H+	285.1420	6.89	86.0978
Promazine	C17H20N2S	284.1347	H+	285.1420	6.89	212.0531
Promazine	C17H20N2S	284.1347	H+	285.1420	6.89	58.0678
Promazine	C17H20N2S	284.1347	H+	285.1420	6.89	285.1425
Promazine	C17H20N2S	284.1347	H+	285.1420	6.89	240.0849
Promethazine	C17H20N2S	284.1347	H+	285.1420	6.78	
Promethazine	C17H20N2S	284.1347	H+	285.1420	6.78	198.0368
Promethazine	C17H20N2S	284.1347	H+	285.1420	6.78	86.0975
Promethazine	C17H20N2S	284.1347	H+	285.1420	6.78	240.0841
Promethazine	C17H20N2S	284.1347	H+	285.1420	6.78	285.142
Promethazine	C17H20N2S	284.1347	H+	285.1420	6.78	225.0609
Para-Fluoro 4-ANBP	C18H21FN2	284.1689	H+	285.1762	5.92	
Para-Fluoro 4-ANBP	C18H21FN2	284.1689	H+	285.1762	5.92	174.1267
Para-Fluoro 4-ANBP	C18H21FN2	284.1689	H+	285.1762	5.92	91.0535
Para-Fluoro 4-ANBP	C18H21FN2	284.1689	H+	285.1762	5.92	285.1748
Para-Fluoro 4-ANBP	C18H21FN2	284.1689	H+	285.1762	5.92	84.0805
Para-Fluoro 4-ANBP	C18H21FN2	284.1689	H+	285.1762	5.92	138.0717

7-Aminoclonazepam	C15H12ClN3O	285.0669	H+	286.0742	4.74	
7-Aminoclonazepam	C15H12ClN3O	285.0669	H+	286.0742	4.74	286.0745
7-Aminoclonazepam	C15H12ClN3O	285.0669	H+	286.0742	4.74	250.098
7-Aminoclonazepam	C15H12ClN3O	285.0669	H+	286.0742	4.74	222.1028
7-Aminoclonazepam	C15H12ClN3O	285.0669	H+	286.0742	4.74	121.0763
7-Aminoclonazepam	C15H12ClN3O	285.0669	H+	286.0742	4.74	195.0916
Hydromorphone	C17H19NO3	285.1365	H+	286.1438	2.61	
Hydromorphone	C17H19NO3	285.1365	H+	286.1438	2.61	286.1443
Hydromorphone	C17H19NO3	285.1365	H+	286.1438	2.61	185.0597
Hydromorphone	C17H19NO3	285.1365	H+	286.1438	2.61	157.0646
Hydromorphone	C17H19NO3	285.1365	H+	286.1438	2.61	227.0702
Hydromorphone	C17H19NO3	285.1365	H+	286.1438	2.61	199.075
Morphine	C17H19NO3	285.1365	H+	286.1438	1.57	
Morphine	C17H19NO3	285.1365	H+	286.1438	1.57	286.1438
Morphine	C17H19NO3	285.1365	H+	286.1438	1.57	201.0909
Morphine	C17H19NO3	285.1365	H+	286.1438	1.57	229.086
Morphine	C17H19NO3	285.1365	H+	286.1438	1.57	211.0754
Morphine	C17H19NO3	285.1365	H+	286.1438	1.57	185.0597
Norcodeine	C17H19NO3	285.1365	H+	286.1438	3.39	
Norcodeine	C17H19NO3	285.1365	H+	286.1438	3.39	286.1442
Norcodeine	C17H19NO3	285.1365	H+	286.1438	3.39	268.1339
Norcodeine	C17H19NO3	285.1365	H+	286.1438	3.39	243.1018
Norcodeine	C17H19NO3	285.1365	H+	286.1438	3.39	225.0913
Norcodeine	C17H19NO3	285.1365	H+	286.1438	3.39	215.1066
N-benzyl-3,4-DMA	C18H23NO2	285.1729	H+	286.1802	5.63	
N-benzyl-3,4-DMA	C18H23NO2	285.1729	H+	286.1802	5.63	151.0743
N-benzyl-3,4-DMA	C18H23NO2	285.1729	H+	286.1802	5.63	179.1055
N-benzyl-3,4-DMA	C18H23NO2	285.1729	H+	286.1802	5.63	286.1789
N-benzyl-3,4-DMA	C18H23NO2	285.1729	H+	286.1802	5.63	164.0827
N-benzyl-3,4-DMA	C18H23NO2	285.1729	H+	286.1802	5.63	136.0512
Pyrilamine	C17H23N3O	285.1841	H+	286.1914	5.69	
Pyrilamine	C17H23N3O	285.1841	H+	286.1914	5.69	121.0649
Pyrilamine	C17H23N3O	285.1841	H+	286.1914	5.69	241.1336
Pyrilamine	C17H23N3O	285.1841	H+	286.1914	5.69	286.192
Pyrilamine	C17H23N3O	285.1841	H+	286.1914	5.69	77.0401
Pyrilamine	C17H23N3O	285.1841	H+	286.1914	5.69	91.0552
Pentazocine	C19H27NO	285.2093	H+	286.2165	5.78	
Pentazocine	C19H27NO	285.2093	H+	286.2165	5.78	218.1531
Pentazocine	C19H27NO	285.2093	H+	286.2165	5.78	286.2165
Pentazocine	C19H27NO	285.2093	H+	286.2165	5.78	175.1113
Pentazocine	C19H27NO	285.2093	H+	286.2165	5.78	69.0714
Pentazocine	C19H27NO	285.2093	H+	286.2165	5.78	173.0657
Oxazepam	C15H11ClN2O2	286.0509	H+	287.0582	7.18	
Oxazepam	C15H11ClN2O2	286.0509	H+	287.0582	7.18	241.0527
Oxazepam	C15H11ClN2O2	286.0509	H+	287.0582	7.18	269.0476
Oxazepam	C15H11ClN2O2	286.0509	H+	287.0582	7.18	287.0584
Oxazepam	C15H11ClN2O2	286.0509	H+	287.0582	7.18	231.0684
Oxazepam	C15H11ClN2O2	286.0509	H+	287.0582	7.18	104.0499
2-methyl AP-237	C18H26N2O	286.2045	H+	287.2118	5.61	
2-methyl AP-237	C18H26N2O	286.2045	H+	287.2118	5.61	117.069
2-methyl AP-237	C18H26N2O	286.2045	H+	287.2118	5.61	115.0534
2-methyl AP-237	C18H26N2O	286.2045	H+	287.2118	5.61	91.054
2-methyl AP-237	C18H26N2O	286.2045	H+	287.2118	5.61	169.133
2-methyl AP-237	C18H26N2O	286.2045	H+	287.2118	5.61	287.2117
Etodolac	C17H21NO3	287.1521	H+	288.1594	8.67	
Etodolac	C17H21NO3	287.1521	H+	288.1594	8.67	172.1119
Etodolac	C17H21NO3	287.1521	H+	288.1594	8.67	144.0799
Etodolac	C17H21NO3	287.1521	H+	288.1594	8.67	143.0725
Etodolac	C17H21NO3	287.1521	H+	288.1594	8.67	210.1271
Etodolac	C17H21NO3	287.1521	H+	288.1594	8.67	224.1425
Desalkylflurazepam	C15H10ClFN2O	288.0466	H+	289.0538	7.5	
Desalkylflurazepam	C15H10ClFN2O	288.0466	H+	289.0538	7.5	289.0536
Desalkylflurazepam	C15H10ClFN2O	288.0466	H+	289.0538	7.5	140.0252
Desalkylflurazepam	C15H10ClFN2O	288.0466	H+	289.0538	7.5	226.0896
Desalkylflurazepam	C15H10ClFN2O	288.0466	H+	289.0538	7.5	261.0569
Desalkylflurazepam	C15H10ClFN2O	288.0466	H+	289.0538	7.5	214.0407
Morphine-D3	C17H16[2H]3NO3	288.1553	H+	289.1626	1.52	
Morphine-D3	C17H16[2H]3NO3	288.1553	H+	289.1626	1.52	289.163
Morphine-D3	C17H16[2H]3NO3	288.1553	H+	289.1626	1.52	201.0907
Morphine-D3	C17H16[2H]3NO3	288.1553	H+	289.1626	1.52	229.0857
Morphine-D3	C17H16[2H]3NO3	288.1553	H+	289.1626	1.52	165.0691
Morphine-D3	C17H16[2H]3NO3	288.1553	H+	289.1626	1.52	271.1515
Isobutyl-PINAC	C17H24N2O2	288.1838	H+	289.1911	10.5	
Isobutyl-PINAC	C17H24N2O2	288.1838	H+	289.1911	10.5	215.1173

Isobutyl-PINAC	C17H24N2O2	288.1838	H+	289.1911	10.5	145.0385
Isobutyl-PINAC	C17H24N2O2	288.1838	H+	289.1911	10.5	233.1278
Isobutyl-PINAC	C17H24N2O2	288.1838	H+	289.1911	10.5	117.0438
Isobutyl-PINAC	C17H24N2O2	288.1838	H+	289.1911	10.5	57.0701
Bupivacaine	C18H28N2O	288.2202	H+	289.2274	5.86	
Bupivacaine	C18H28N2O	288.2202	H+	289.2274	5.86	140.1432
Bupivacaine	C18H28N2O	288.2202	H+	289.2274	5.86	289.2274
Bupivacaine	C18H28N2O	288.2202	H+	289.2274	5.86	98.0969
Bupivacaine	C18H28N2O	288.2202	H+	289.2274	5.86	84.0819
Bupivacaine	C18H28N2O	288.2202	H+	289.2274	5.86	150.091
Benzoylecgonine	C16H19NO4	289.1314	H+	290.1387	4.49	
Benzoylecgonine	C16H19NO4	289.1314	H+	290.1387	4.49	168.1016
Benzoylecgonine	C16H19NO4	289.1314	H+	290.1387	4.49	290.1389
Benzoylecgonine	C16H19NO4	289.1314	H+	290.1387	4.49	105.034
Benzoylecgonine	C16H19NO4	289.1314	H+	290.1387	4.49	272.1289
Benzoylecgonine	C16H19NO4	289.1314	H+	290.1387	4.49	150.0915
Norcocaine	C16H19NO4	289.1314	H+	290.1387	5.41	
Norcocaine	C16H19NO4	289.1314	H+	290.1387	5.41	136.0754
Norcocaine	C16H19NO4	289.1314	H+	290.1387	5.41	168.1017
Norcocaine	C16H19NO4	289.1314	H+	290.1387	5.41	290.1388
Norcocaine	C16H19NO4	289.1314	H+	290.1387	5.41	108.0813
Norcocaine	C16H19NO4	289.1314	H+	290.1387	5.41	105.0341
Methylenedioxy-alpha-PHP	C17H23NO3	289.1678	H+	290.1751	6.01	
Methylenedioxy-alpha-PHP	C17H23NO3	289.1678	H+	290.1751	6.01	189.0911
Methylenedioxy-alpha-PHP	C17H23NO3	289.1678	H+	290.1751	6.01	149.0233
Methylenedioxy-alpha-PHP	C17H23NO3	289.1678	H+	290.1751	6.01	140.1434
Methylenedioxy-alpha-PHP	C17H23NO3	289.1678	H+	290.1751	6.01	135.0438
Methylenedioxy-alpha-PHP	C17H23NO3	289.1678	H+	290.1751	6.01	219.1021
Atropine	C17H23NO3	289.1678	H+	290.1751	4.45	
Atropine	C17H23NO3	289.1678	H+	290.1751	4.45	290.1753
Atropine	C17H23NO3	289.1678	H+	290.1751	4.45	124.1125
Atropine	C17H23NO3	289.1678	H+	290.1751	4.45	168.1021
Atropine	C17H23NO3	289.1678	H+	290.1751	4.45	93.0708
Atropine	C17H23NO3	289.1678	H+	290.1751	4.45	105.034
Norcarfentanil	C16H22N2O3	290.1630	H+	291.1703	5.08	
Norcarfentanil	C16H22N2O3	290.1630	H+	291.1703	5.08	146.0961
Norcarfentanil	C16H22N2O3	290.1630	H+	291.1703	5.08	113.0593
Norcarfentanil	C16H22N2O3	290.1630	H+	291.1703	5.08	231.1494
Norcarfentanil	C16H22N2O3	290.1630	H+	291.1703	5.08	175.1228
Norcarfentanil	C16H22N2O3	290.1630	H+	291.1703	5.08	142.0858
Desmethylsertraline	C16H15Cl2N	291.0582	H+	292.0654	7.59	
Desmethylsertraline	C16H15Cl2N	291.0582	H+	292.0654	7.59	158.9764
Desmethylsertraline	C16H15Cl2N	291.0582	H+	292.0654	7.59	275.0365
Desmethylsertraline	C16H15Cl2N	291.0582	H+	292.0654	7.59	129.0697
Desmethylsertraline	C16H15Cl2N	291.0582	H+	292.0654	7.59	91.0542
Desmethylsertraline	C16H15Cl2N	291.0582	H+	292.0654	7.59	122.9964
JWH-030	C20H21NO	291.1623	H+	292.1696	9.83	
JWH-030	C20H21NO	291.1623	H+	292.1696	9.83	155.0496
JWH-030	C20H21NO	291.1623	H+	292.1696	9.83	127.0541
JWH-030	C20H21NO	291.1623	H+	292.1696	9.83	164.1078
JWH-030	C20H21NO	291.1623	H+	292.1696	9.83	292.1716
JWH-030	C20H21NO	291.1623	H+	292.1696	9.83	94.029
Bromo-DragonFLY	C13H12BrNO2	293.0051	H+	294.0124	6.5	
Bromo-DragonFLY	C13H12BrNO2	293.0051	H+	294.0124	6.5	198.0669
Bromo-DragonFLY	C13H12BrNO2	293.0051	H+	294.0124	6.5	248.9539
Bromo-DragonFLY	C13H12BrNO2	293.0051	H+	294.0124	6.5	276.9855
Bromo-DragonFLY	C13H12BrNO2	293.0051	H+	294.0124	6.5	171.0437
Bromo-DragonFLY	C13H12BrNO2	293.0051	H+	294.0124	6.5	169.0646
Estazolam	C16H11ClN4	294.0672	H+	295.0745	7.19	
Estazolam	C16H11ClN4	294.0672	H+	295.0745	7.19	267.0568
Estazolam	C16H11ClN4	294.0672	H+	295.0745	7.19	295.0759
Estazolam	C16H11ClN4	294.0672	H+	295.0745	7.19	205.0768
Estazolam	C16H11ClN4	294.0672	H+	295.0745	7.19	241.0526
Estazolam	C16H11ClN4	294.0672	H+	295.0745	7.19	240.045
U-48520	C16H23ClN2O	294.1499	H+	295.1572	5.53	
U-48520	C16H23ClN2O	294.1499	H+	295.1572	5.53	250.0982
U-48520	C16H23ClN2O	294.1499	H+	295.1572	5.53	138.9939
U-48520	C16H23ClN2O	294.1499	H+	295.1572	5.53	170.0364
U-48520	C16H23ClN2O	294.1499	H+	295.1572	5.53	81.0701
U-48520	C16H23ClN2O	294.1499	H+	295.1572	5.53	295.1565
Trimipramine	C20H26N2	294.2096	H+	295.2169	7.31	
Trimipramine	C20H26N2	294.2096	H+	295.2169	7.31	100.1124
Trimipramine	C20H26N2	294.2096	H+	295.2169	7.31	58.0674
Trimipramine	C20H26N2	294.2096	H+	295.2169	7.31	295.2172

Trimipramine	C20H26N2	294.2096	H+	295.2169	7.31	208.1123
Trimipramine	C20H26N2	294.2096	H+	295.2169	7.31	250.1594
Despropionyl ortho-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.72	
Despropionyl ortho-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.72	188.1435
Despropionyl ortho-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.72	105.0695
Despropionyl ortho-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.72	295.2174
Despropionyl ortho-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.72	134.0961
Despropionyl ortho-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.72	146.0699
Despropionyl 3-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.76	
Despropionyl 3-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.76	202.1595
Despropionyl 3-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.76	105.0694
Despropionyl 3-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.76	134.0963
Despropionyl 3-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.76	295.2174
Despropionyl 3-Methylfentanyl	C20H26N2	294.2096	H+	295.2169	6.76	69.0699
Nimetazepam	C16H13N3O3	295.0957	H+	296.1029	7.36	
Nimetazepam	C16H13N3O3	295.0957	H+	296.1029	7.36	250.1093
Nimetazepam	C16H13N3O3	295.0957	H+	296.1029	7.36	296.1028
Nimetazepam	C16H13N3O3	295.0957	H+	296.1029	7.36	268.1082
Nimetazepam	C16H13N3O3	295.0957	H+	296.1029	7.36	222.1135
Nimetazepam	C16H13N3O3	295.0957	H+	296.1029	7.36	221.1068
Norfluoxetine	C16H16F3NO	295.1184	H+	296.1257	7.36	
Norfluoxetine	C16H16F3NO	295.1184	H+	296.1257	7.36	134.0956
Norfluoxetine	C16H16F3NO	295.1184	H+	296.1257	7.36	149.0228
Norfluoxetine	C16H16F3NO	295.1184	H+	296.1257	7.36	105.07
Norfluoxetine	C16H16F3NO	295.1184	H+	296.1257	7.36	59.0506
Norfluoxetine	C16H16F3NO	295.1184	H+	296.1257	7.36	57.0724
Duloxetine	C18H19NOS	297.1187	H+	298.1260	7.13	
Duloxetine	C18H19NOS	297.1187	H+	298.1260	7.13	44.0535
Duloxetine	C18H19NOS	297.1187	H+	298.1260	7.13	124.0343
Duloxetine	C18H19NOS	297.1187	H+	298.1260	7.13	298.1263
Duloxetine	C18H19NOS	297.1187	H+	298.1260	7.13	267.0841
Duloxetine	C18H19NOS	297.1187	H+	298.1260	7.13	239.0533
Despropionyl ortho-Fluorofentanyl	C19H23FN2	298.1845	H+	299.1918	6.46	
Despropionyl ortho-Fluorofentanyl	C19H23FN2	298.1845	H+	299.1918	6.46	188.1432
Despropionyl ortho-Fluorofentanyl	C19H23FN2	298.1845	H+	299.1918	6.46	105.0692
Despropionyl ortho-Fluorofentanyl	C19H23FN2	298.1845	H+	299.1918	6.46	299.1919
Despropionyl ortho-Fluorofentanyl	C19H23FN2	298.1845	H+	299.1918	6.46	134.0692
Despropionyl ortho-Fluorofentanyl	C19H23FN2	298.1845	H+	299.1918	6.46	146.0957
Norflunitrazepam	C15H10FN3O3	299.0706	H+	300.0779	6.85	
Norflunitrazepam	C15H10FN3O3	299.0706	H+	300.0779	6.85	300.0787
Norflunitrazepam	C15H10FN3O3	299.0706	H+	300.0779	6.85	254.0856
Norflunitrazepam	C15H10FN3O3	299.0706	H+	300.0779	6.85	225.0816
Norflunitrazepam	C15H10FN3O3	299.0706	H+	300.0779	6.85	198.0707
Norflunitrazepam	C15H10FN3O3	299.0706	H+	300.0779	6.85	253.0772
Chlordiazepoxide	C16H14ClN3O	299.0825	H+	300.0898	6.06	
Chlordiazepoxide	C16H14ClN3O	299.0825	H+	300.0898	6.06	282.0786
Chlordiazepoxide	C16H14ClN3O	299.0825	H+	300.0898	6.06	227.0494
Chlordiazepoxide	C16H14ClN3O	299.0825	H+	300.0898	6.06	283.0864
Chlordiazepoxide	C16H14ClN3O	299.0825	H+	300.0898	6.06	300.0898
Chlordiazepoxide	C16H14ClN3O	299.0825	H+	300.0898	6.06	247.1103
JWH-071	C21H17NO	299.1310	H+	300.1383	9.33	
JWH-071	C21H17NO	299.1310	H+	300.1383	9.33	155.0494
JWH-071	C21H17NO	299.1310	H+	300.1383	9.33	172.0759
JWH-071	C21H17NO	299.1310	H+	300.1383	9.33	127.054
JWH-071	C21H17NO	299.1310	H+	300.1383	9.33	300.1396
JWH-071	C21H17NO	299.1310	H+	300.1383	9.33	144.0449
Metoclopramide	C14H22ClN3O2	299.1401	H+	300.1473	4.67	
Metoclopramide	C14H22ClN3O2	299.1401	H+	300.1473	4.67	227.058
Metoclopramide	C14H22ClN3O2	299.1401	H+	300.1473	4.67	184.016
Metoclopramide	C14H22ClN3O2	299.1401	H+	300.1473	4.67	300.1476
Metoclopramide	C14H22ClN3O2	299.1401	H+	300.1473	4.67	212.0348
Metoclopramide	C14H22ClN3O2	299.1401	H+	300.1473	4.67	183.0321
Codeine	C18H21NO3	299.1521	H+	300.1594	3.48	
Codeine	C18H21NO3	299.1521	H+	300.1594	3.48	300.1594
Codeine	C18H21NO3	299.1521	H+	300.1594	3.48	215.1069
Codeine	C18H21NO3	299.1521	H+	300.1594	3.48	243.1022
Codeine	C18H21NO3	299.1521	H+	300.1594	3.48	225.0913
Codeine	C18H21NO3	299.1521	H+	300.1594	3.48	199.0758
Hydrocodone	C18H21NO3	299.1521	H+	300.1594	3.92	
Hydrocodone	C18H21NO3	299.1521	H+	300.1594	3.92	300.159
Hydrocodone	C18H21NO3	299.1521	H+	300.1594	3.92	199.0744
Hydrocodone	C18H21NO3	299.1521	H+	300.1594	3.92	241.0683
Hydrocodone	C18H21NO3	299.1521	H+	300.1594	3.92	171.0798
Hydrocodone	C18H21NO3	299.1521	H+	300.1594	3.92	243.1015

Clobazam	C16H13ClN2O2	300.0666	H+	301.0738	7.55	
Clobazam	C16H13ClN2O2	300.0666	H+	301.0738	7.55	259.0634
Clobazam	C16H13ClN2O2	300.0666	H+	301.0738	7.55	301.0741
Clobazam	C16H13ClN2O2	300.0666	H+	301.0738	7.55	224.0947
Clobazam	C16H13ClN2O2	300.0666	H+	301.0738	7.55	153.0212
Clobazam	C16H13ClN2O2	300.0666	H+	301.0738	7.55	105.0339
Temazepam	C16H13ClN2O2	300.0666	H+	301.0738	7.6	
Temazepam	C16H13ClN2O2	300.0666	H+	301.0738	7.6	255.0679
Temazepam	C16H13ClN2O2	300.0666	H+	301.0738	7.6	301.0741
Temazepam	C16H13ClN2O2	300.0666	H+	301.0738	7.6	283.0635
Temazepam	C16H13ClN2O2	300.0666	H+	301.0738	7.6	228.0571
Temazepam	C16H13ClN2O2	300.0666	H+	301.0738	7.6	193.0887
N,N-Didesmethyl U-47700	C14H18Cl2N2O	300.0796	H+	301.0869	6.17	
N,N-Didesmethyl U-47700	C14H18Cl2N2O	300.0796	H+	301.0869	6.17	172.9551
N,N-Didesmethyl U-47700	C14H18Cl2N2O	300.0796	H+	301.0869	6.17	189.981
N,N-Didesmethyl U-47700	C14H18Cl2N2O	300.0796	H+	301.0869	6.17	203.9969
N,N-Didesmethyl U-47700	C14H18Cl2N2O	300.0796	H+	301.0869	6.17	270.0441
N,N-Didesmethyl U-47700	C14H18Cl2N2O	300.0796	H+	301.0869	6.17	284.0593
Desmethylclomipramine	C18H21ClN2	300.1393	H+	301.1466	7.67	
Desmethylclomipramine	C18H21ClN2	300.1393	H+	301.1466	7.67	72.0823
Desmethylclomipramine	C18H21ClN2	300.1393	H+	301.1466	7.67	242.0732
Desmethylclomipramine	C18H21ClN2	300.1393	H+	301.1466	7.67	301.1465
Desmethylclomipramine	C18H21ClN2	300.1393	H+	301.1466	7.67	270.1047
Desmethylclomipramine	C18H21ClN2	300.1393	H+	301.1466	7.67	227.0498
Noroxycodone	C17H19NO4	301.1314	H+	302.1387	3.72	
Noroxycodone	C17H19NO4	301.1314	H+	302.1387	3.72	284.1275
Noroxycodone	C17H19NO4	301.1314	H+	302.1387	3.72	227.0938
Noroxycodone	C17H19NO4	301.1314	H+	302.1387	3.72	187.0749
Noroxycodone	C17H19NO4	301.1314	H+	302.1387	3.72	302.1384
Noroxycodone	C17H19NO4	301.1314	H+	302.1387	3.72	229.0858
Oxymorphone	C17H19NO4	301.1314	H+	302.1387	1.98	
Oxymorphone	C17H19NO4	301.1314	H+	302.1387	1.98	284.128
Oxymorphone	C17H19NO4	301.1314	H+	302.1387	1.98	302.1388
Oxymorphone	C17H19NO4	301.1314	H+	302.1387	1.98	227.0937
Oxymorphone	C17H19NO4	301.1314	H+	302.1387	1.98	242.1175
Oxymorphone	C17H19NO4	301.1314	H+	302.1387	1.98	198.091
25H-NBOMe	C18H23NO3	301.1678	H+	302.1751	6.45	
25H-NBOMe	C18H23NO3	301.1678	H+	302.1751	6.45	121.0653
25H-NBOMe	C18H23NO3	301.1678	H+	302.1751	6.45	302.1766
25H-NBOMe	C18H23NO3	301.1678	H+	302.1751	6.45	91.0556
25H-NBOMe	C18H23NO3	301.1678	H+	302.1751	6.45	93.0714
25H-NBOMe	C18H23NO3	301.1678	H+	302.1751	6.45	285.1455
Dihydrocodeine/Hydrocodol	C18H23NO3	301.1678	H+	302.1751	3.39	
Dihydrocodeine/Hydrocodol	C18H23NO3	301.1678	H+	302.1751	3.39	302.1751
Dihydrocodeine/Hydrocodol	C18H23NO3	301.1678	H+	302.1751	3.39	199.075
Dihydrocodeine/Hydrocodol	C18H23NO3	301.1678	H+	302.1751	3.39	201.0906
Dihydrocodeine/Hydrocodol	C18H23NO3	301.1678	H+	302.1751	3.39	245.1171
Dihydrocodeine/Hydrocodol	C18H23NO3	301.1678	H+	302.1751	3.39	277.1061
Trihexyphenidyl	C20H31NO	301.2406	H+	302.2478	7.05	
Trihexyphenidyl	C20H31NO	301.2406	H+	302.2478	7.05	98.0972
Trihexyphenidyl	C20H31NO	301.2406	H+	302.2478	7.05	302.2485
Trihexyphenidyl	C20H31NO	301.2406	H+	302.2478	7.05	284.2375
Trihexyphenidyl	C20H31NO	301.2406	H+	302.2478	7.05	267.1966
Trihexyphenidyl	C20H31NO	301.2406	H+	302.2478	7.05	117.0707
5-fluoro CYPPICA	C18H23FN2O	302.1794	H+	303.1867	8.42	
5-fluoro CYPPICA	C18H23FN2O	302.1794	H+	303.1867	8.42	232.1136
5-fluoro CYPPICA	C18H23FN2O	302.1794	H+	303.1867	8.42	206.134
5-fluoro CYPPICA	C18H23FN2O	302.1794	H+	303.1867	8.42	144.0437
5-fluoro CYPPICA	C18H23FN2O	302.1794	H+	303.1867	8.42	132.0805
5-fluoro CYPPICA	C18H23FN2O	302.1794	H+	303.1867	8.42	303.188
5-fluoro PY-PICA	C18H23FN2O	302.1794	H+	303.1867	8.32	
5-fluoro PY-PICA	C18H23FN2O	302.1794	H+	303.1867	8.32	232.1132
5-fluoro PY-PICA	C18H23FN2O	302.1794	H+	303.1867	8.32	98.0592
5-fluoro PY-PICA	C18H23FN2O	302.1794	H+	303.1867	8.32	144.0436
5-fluoro PY-PICA	C18H23FN2O	302.1794	H+	303.1867	8.32	303.1876
5-fluoro PY-PICA	C18H23FN2O	302.1794	H+	303.1867	8.32	55.0536
Cocaine	C17H21NO4	303.1471	H+	304.1543	5.24	
Cocaine	C17H21NO4	303.1471	H+	304.1543	5.24	182.1175
Cocaine	C17H21NO4	303.1471	H+	304.1543	5.24	304.1548
Cocaine	C17H21NO4	303.1471	H+	304.1543	5.24	82.0665
Cocaine	C17H21NO4	303.1471	H+	304.1543	5.24	105.0339
Cocaine	C17H21NO4	303.1471	H+	304.1543	5.24	150.0912
Scopolamine	C17H21NO4	303.1471	H+	304.1543	3.76	
Scopolamine	C17H21NO4	303.1471	H+	304.1543	3.76	138.0916

Scopolamine	C17H21NO4	303.1471	H+	304.1543	3.76	304.1554
Scopolamine	C17H21NO4	303.1471	H+	304.1543	3.76	156.1021
Scopolamine	C17H21NO4	303.1471	H+	304.1543	3.76	111.1173
Scopolamine	C17H21NO4	303.1471	H+	304.1543	3.76	121.065
5F-PY-PINACA	C17H22FN3O	303.1747	H+	304.1820	8.66	
5F-PY-PINACA	C17H22FN3O	303.1747	H+	304.1820	8.66	233.1086
5F-PY-PINACA	C17H22FN3O	303.1747	H+	304.1820	8.66	213.1018
5F-PY-PINACA	C17H22FN3O	303.1747	H+	304.1820	8.66	145.039
5F-PY-PINACA	C17H22FN3O	303.1747	H+	304.1820	8.66	177.0453
5F-PY-PINACA	C17H22FN3O	303.1747	H+	304.1820	8.66	304.1822
Delorazepam	C15H10Cl2N2O	304.0170	H+	305.0243	7.74	
Delorazepam	C15H10Cl2N2O	304.0170	H+	305.0243	7.74	305.0245
Delorazepam	C15H10Cl2N2O	304.0170	H+	305.0243	7.74	140.0261
Delorazepam	C15H10Cl2N2O	304.0170	H+	305.0243	7.74	242.0608
Delorazepam	C15H10Cl2N2O	304.0170	H+	305.0243	7.74	165.0212
Delorazepam	C15H10Cl2N2O	304.0170	H+	305.0243	7.74	241.053
N-methyl Carfentanyl	C17H24N2O3	304.1787	H+	305.1860	5.02	
N-methyl Carfentanyl	C17H24N2O3	304.1787	H+	305.1860	5.02	146.0969
N-methyl Carfentanyl	C17H24N2O3	304.1787	H+	305.1860	5.02	189.1394
N-methyl Carfentanyl	C17H24N2O3	304.1787	H+	305.1860	5.02	113.0599
N-methyl Carfentanyl	C17H24N2O3	304.1787	H+	305.1860	5.02	158.097
N-methyl Carfentanyl	C17H24N2O3	304.1787	H+	305.1860	5.02	202.1235
Methylenedioxy-U-47700	C17H24N2O3	304.1787	H+	305.1860	4.90	
Methylenedioxy-U-47700	C17H24N2O3	304.1787	H+	305.1860	4.90	260.1291
Methylenedioxy-U-47700	C17H24N2O3	304.1787	H+	305.1860	4.90	149.0236
Methylenedioxy-U-47700	C17H24N2O3	304.1787	H+	305.1860	4.90	180.0658
Methylenedioxy-U-47700	C17H24N2O3	304.1787	H+	305.1860	4.90	123.0442
Methylenedioxy-U-47700	C17H24N2O3	304.1787	H+	305.1860	4.90	305.1866
Sertraline	C17H17Cl2N	305.0738	H+	306.0811	7.59	
Sertraline	C17H17Cl2N	305.0738	H+	306.0811	7.59	158.9757
Sertraline	C17H17Cl2N	305.0738	H+	306.0811	7.59	275.0389
Sertraline	C17H17Cl2N	305.0738	H+	306.0811	7.59	129.0695
Sertraline	C17H17Cl2N	305.0738	H+	306.0811	7.59	240.0694
Sertraline	C17H17Cl2N	305.0738	H+	306.0811	7.59	205.1004
Zaleplon	C17H15N5O	305.1277	H+	306.1349	6.7	
Zaleplon	C17H15N5O	305.1277	H+	306.1349	6.7	306.1353
Zaleplon	C17H15N5O	305.1277	H+	306.1349	6.7	236.0933
Zaleplon	C17H15N5O	305.1277	H+	306.1349	6.7	264.1249
Zaleplon	C17H15N5O	305.1277	H+	306.1349	6.7	260.0936
Zaleplon	C17H15N5O	305.1277	H+	306.1349	6.7	219.0665
JWH-031	C21H23NO	305.1780	H+	306.1861	10.22	
JWH-031	C21H23NO	305.1780	H+	306.1861	10.22	155.0495
JWH-031	C21H23NO	305.1780	H+	306.1861	10.22	127.0542
JWH-031	C21H23NO	305.1780	H+	306.1861	10.22	306.1859
JWH-031	C21H23NO	305.1780	H+	306.1861	10.22	178.1233
JWH-031	C21H23NO	305.1780	H+	306.1861	10.22	94.0297
JWH-167	C21H23NO	305.1780	H+	306.1852	9.95	
JWH-167	C21H23NO	305.1780	H+	306.1852	9.95	214.1226
JWH-167	C21H23NO	305.1780	H+	306.1852	9.95	188.1436
JWH-167	C21H23NO	305.1780	H+	306.1852	9.95	144.044
JWH-167	C21H23NO	305.1780	H+	306.1852	9.95	91.0541
JWH-167	C21H23NO	305.1780	H+	306.1852	9.95	306.1862
SDB-006 N-Phenyl Analogue	C20H22N2O	306.1732	H+	307.1805	9.63	
SDB-006 N-Phenyl Analogue	C20H22N2O	306.1732	H+	307.1805	9.63	214.1232
SDB-006 N-Phenyl Analogue	C20H22N2O	306.1732	H+	307.1805	9.63	188.144
SDB-006 N-Phenyl Analogue	C20H22N2O	306.1732	H+	307.1805	9.63	144.0443
SDB-006 N-Phenyl Analogue	C20H22N2O	306.1732	H+	307.1805	9.63	132.0807
SDB-006 N-Phenyl Analogue	C20H22N2O	306.1732	H+	307.1805	9.63	307.1818
2C-I	C10H14INO2	307.0069	H+	308.0142	5.73	
2C-I	C10H14INO2	307.0069	H+	308.0142	5.73	290.9884
2C-I	C10H14INO2	307.0069	H+	308.0142	5.73	275.965
2C-I	C10H14INO2	307.0069	H+	308.0142	5.73	260.9415
2C-I	C10H14INO2	307.0069	H+	308.0142	5.73	164.0835
2C-I	C10H14INO2	307.0069	H+	308.0142	5.73	149.0593
RCS-4 C4 Homolog	C20H21NO2	307.1572	H+	308.1645	9.57	
RCS-4 C4 Homolog	C20H21NO2	307.1572	H+	308.1645	9.57	135.044
RCS-4 C4 Homolog	C20H21NO2	307.1572	H+	308.1645	9.57	200.108
RCS-4 C4 Homolog	C20H21NO2	307.1572	H+	308.1645	9.57	107.0489
RCS-4 C4 Homolog	C20H21NO2	307.1572	H+	308.1645	9.57	308.1664
RCS-4 C4 Homolog	C20H21NO2	307.1572	H+	308.1645	9.57	77.0384
Zolpidem	C19H21N3O	307.1685	H+	308.1757	5.52	
Zolpidem	C19H21N3O	307.1685	H+	308.1757	5.52	308.175
Zolpidem	C19H21N3O	307.1685	H+	308.1757	5.52	235.1225
Zolpidem	C19H21N3O	307.1685	H+	308.1757	5.52	236.1304

Zolpidem	C19H21N3O	307.1685	H+	308.1757	5.52	263.1176
Zolpidem	C19H21N3O	307.1685	H+	308.1757	5.52	248.0931
Benzatropine	C21H25NO	307.1936	H+	308.2009	7.21	
Benzatropine	C21H25NO	307.1936	H+	308.2009	7.21	308.2009
Benzatropine	C21H25NO	307.1936	H+	308.2009	7.21	167.0852
Benzatropine	C21H25NO	307.1936	H+	308.2009	7.21	165.0701
Benzatropine	C21H25NO	307.1936	H+	308.2009	7.21	152.0621
Benzatropine	C21H25NO	307.1936	H+	308.2009	7.21	142.1231
Alprazolam	C17H13ClN4	308.0829	H+	309.0902	7.45	
Alprazolam	C17H13ClN4	308.0829	H+	309.0902	7.45	309.0905
Alprazolam	C17H13ClN4	308.0829	H+	309.0902	7.45	281.0723
Alprazolam	C17H13ClN4	308.0829	H+	309.0902	7.45	274.1215
Alprazolam	C17H13ClN4	308.0829	H+	309.0902	7.45	205.0766
Alprazolam	C17H13ClN4	308.0829	H+	309.0902	7.45	241.0534
Warfarin	C19H16O4	308.1049	H+	309.1121	8.12	
Warfarin	C19H16O4	308.1049	H+	309.1121	8.12	163.0389
Warfarin	C19H16O4	308.1049	H+	309.1121	8.12	251.0705
Warfarin	C19H16O4	308.1049	H+	309.1121	8.12	173.0235
Warfarin	C19H16O4	308.1049	H+	309.1121	8.12	147.0807
Warfarin	C19H16O4	308.1049	H+	309.1121	8.12	121.0288
Fluoxetine	C17H18NOF3	309.1340	H+	310.1413	7.4	
Fluoxetine	C17H18NOF3	309.1340	H+	310.1413	7.4	44.0534
Fluoxetine	C17H18NOF3	309.1340	H+	310.1413	7.4	310.1413
Fluoxetine	C17H18NOF3	309.1340	H+	310.1413	7.4	282.0757
Fluoxetine	C17H18NOF3	309.1340	H+	310.1413	7.4	148.1122
Fluoxetine	C17H18NOF3	309.1340	H+	310.1413	7.4	275.1261
Methadone	C21H27NO	309.2093	H+	310.2165	7.25	
Methadone	C21H27NO	309.2093	H+	310.2165	7.25	105.0335
Methadone	C21H27NO	309.2093	H+	310.2165	7.25	265.1583
Methadone	C21H27NO	309.2093	H+	310.2165	7.25	219.1166
Methadone	C21H27NO	309.2093	H+	310.2165	7.25	223.1116
Methadone	C21H27NO	309.2093	H+	310.2165	7.25	310.2162
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	309.2093	H+	310.2165	10.50	
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	309.2093	H+	310.2165	10.50	125.0956
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	309.2093	H+	310.2165	10.50	212.1067
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	309.2093	H+	310.2165	10.50	310.2167
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	309.2093	H+	310.2165	10.50	292.2062
XLR-11 N-(4-Pentenyl) Analogue	C21H27NO	309.2093	H+	310.2165	10.50	277.1827
Dicyclomine (Dicycloverine)	C19H35NO2	309.2668	H+	310.2741	8.24	
Dicyclomine (Dicycloverine)	C19H35NO2	309.2668	H+	310.2741	8.24	109.1012
Dicyclomine (Dicycloverine)	C19H35NO2	309.2668	H+	310.2741	8.24	165.1633
Dicyclomine (Dicycloverine)	C19H35NO2	309.2668	H+	310.2741	8.24	237.1843
Dicyclomine (Dicycloverine)	C19H35NO2	309.2668	H+	310.2741	8.24	310.2739
Dicyclomine (Dicycloverine)	C19H35NO2	309.2668	H+	310.2741	8.24	155.1063
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	310.1481	H+	311.1554	8.20	
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	310.1481	H+	311.1554	8.20	291.1501
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	310.1481	H+	311.1554	8.20	235.0872
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	310.1481	H+	311.1554	8.20	223.0871
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	310.1481	H+	311.1554	8.20	144.0443
5-Fluoropentyl-3-pyridinoylindole	C19H19FN2O	310.1481	H+	311.1554	8.20	311.1561
A-836339	C16H26N2O2S	310.1715	H+	311.1788	8.52	
A-836339	C16H26N2O2S	310.1715	H+	311.1788	8.52	187.0899
A-836339	C16H26N2O2S	310.1715	H+	311.1788	8.52	125.0953
A-836339	C16H26N2O2S	310.1715	H+	311.1788	8.52	155.0635
A-836339	C16H26N2O2S	310.1715	H+	311.1788	8.52	129.0476
A-836339	C16H26N2O2S	310.1715	H+	311.1788	8.52	311.1795
Cannabinol (CBN)	C21H26O2	310.1933	H+	311.2006	10.71	
Cannabinol (CBN)	C21H26O2	310.1933	H+	311.2006	10.71	223.1112
Cannabinol (CBN)	C21H26O2	310.1933	H+	311.2006	10.71	311.2009
Cannabinol (CBN)	C21H26O2	310.1933	H+	311.2006	10.71	293.1906
Cannabinol (CBN)	C21H26O2	310.1933	H+	311.2006	10.71	241.1224
Cannabinol (CBN)	C21H26O2	310.1933	H+	311.2006	10.71	208.0881
Thebaine	C19H21NO3	311.1521	H+	312.1594	5.02	
Thebaine	C19H21NO3	311.1521	H+	312.1594	5.02	58.0676
Thebaine	C19H21NO3	311.1521	H+	312.1594	5.02	251.0706
Thebaine	C19H21NO3	311.1521	H+	312.1594	5.02	312.1598
Thebaine	C19H21NO3	311.1521	H+	312.1594	5.02	266.0943
Thebaine	C19H21NO3	311.1521	H+	312.1594	5.02	249.0913
UR-144	C21H29NO	311.2249	H+	312.2322	10.7	
UR-144	C21H29NO	311.2249	H+	312.2322	10.7	125.0963
UR-144	C21H29NO	311.2249	H+	312.2322	10.7	312.2303
UR-144	C21H29NO	311.2249	H+	312.2322	10.7	214.1227
UR-144	C21H29NO	311.2249	H+	312.2322	10.7	294.2179
UR-144	C21H29NO	311.2249	H+	312.2322	10.7	279.199

Norclozapine	C17H17ClN4	312.1142	H+	313.1215	6.1	
Norclozapine	C17H17ClN4	312.1142	H+	313.1215	6.1	270.0794
Norclozapine	C17H17ClN4	312.1142	H+	313.1215	6.1	313.1216
Norclozapine	C17H17ClN4	312.1142	H+	313.1215	6.1	192.0681
Norclozapine	C17H17ClN4	312.1142	H+	313.1215	6.1	227.0371
Norclozapine	C17H17ClN4	312.1142	H+	313.1215	6.1	296.0957
Olanzapine	C17H20N4S	312.1409	H+	313.1481	3.9	
Olanzapine	C17H20N4S	312.1409	H+	313.1481	3.9	256.0897
Olanzapine	C17H20N4S	312.1409	H+	313.1481	3.9	313.1481
Olanzapine	C17H20N4S	312.1409	H+	313.1481	3.9	282.1059
Olanzapine	C17H20N4S	312.1409	H+	313.1481	3.9	213.0479
Olanzapine	C17H20N4S	312.1409	H+	313.1481	3.9	198.0243
Furanyl UF-17	C19H24N2O2	312.1838	H+	313.1911	5.73	
Furanyl UF-17	C19H24N2O2	312.1838	H+	313.1911	5.73	188.0683
Furanyl UF-17	C19H24N2O2	312.1838	H+	313.1911	5.73	268.1317
Furanyl UF-17	C19H24N2O2	312.1838	H+	313.1911	5.73	95.0122
Furanyl UF-17	C19H24N2O2	312.1838	H+	313.1911	5.73	313.1888
Furanyl UF-17	C19H24N2O2	312.1838	H+	313.1911	5.73	172.1116
JWH-133	C22H32O	312.2453	H+	313.2526	12.33	
JWH-133	C22H32O	312.2453	H+	313.2526	12.33	85.1024
JWH-133	C22H32O	312.2453	H+	313.2526	12.33	91.0552
JWH-133	C22H32O	312.2453	H+	313.2526	12.33	229.1587
JWH-133	C22H32O	312.2453	H+	313.2526	12.33	173.0961
JWH-133	C22H32O	312.2453	H+	313.2526	12.33	149.0232
Flunitrazepam	C16H12FN3O3	313.0863	H+	314.0935	7.28	
Flunitrazepam	C16H12FN3O3	313.0863	H+	314.0935	7.28	268.1002
Flunitrazepam	C16H12FN3O3	313.0863	H+	314.0935	7.28	314.0935
Flunitrazepam	C16H12FN3O3	313.0863	H+	314.0935	7.28	239.0976
Flunitrazepam	C16H12FN3O3	313.0863	H+	314.0935	7.28	240.1046
Flunitrazepam	C16H12FN3O3	313.0863	H+	314.0935	7.28	286.0991
Amoxapine	C17H16ClN3O	313.0982	H+	314.1055	6.81	
Amoxapine	C17H16ClN3O	313.0982	H+	314.1055	6.81	271.0633
Amoxapine	C17H16ClN3O	313.0982	H+	314.1055	6.81	314.1057
Amoxapine	C17H16ClN3O	313.0982	H+	314.1055	6.81	297.0796
Amoxapine	C17H16ClN3O	313.0982	H+	314.1055	6.81	245.0478
Amoxapine	C17H16ClN3O	313.0982	H+	314.1055	6.81	228.0211
Alprazolam-D5	C17H8[2H]5ClN4	313.1143	H+	314.1215	7.41	
Alprazolam-D5	C17H8[2H]5ClN4	313.1143	H+	314.1215	7.41	314.1221
Alprazolam-D5	C17H8[2H]5ClN4	313.1143	H+	314.1215	7.41	286.1038
Alprazolam-D5	C17H8[2H]5ClN4	313.1143	H+	314.1215	7.41	279.1537
Alprazolam-D5	C17H8[2H]5ClN4	313.1143	H+	314.1215	7.41	260.0974
Alprazolam-D5	C17H8[2H]5ClN4	313.1143	H+	314.1215	7.41	245.0801
JWH-072	C22H19NO	313.1467	H+	314.1539	9.59	
JWH-072	C22H19NO	313.1467	H+	314.1539	9.59	155.0487
JWH-072	C22H19NO	313.1467	H+	314.1539	9.59	186.0914
JWH-072	C22H19NO	313.1467	H+	314.1539	9.59	127.0541
JWH-072	C22H19NO	313.1467	H+	314.1539	9.59	314.1542
JWH-072	C22H19NO	313.1467	H+	314.1539	9.59	144.0446
Ethylmorphine	C19H23NO3	313.1678	H+	314.1751	4.2	
Ethylmorphine	C19H23NO3	313.1678	H+	314.1751	4.2	314.1751
Ethylmorphine	C19H23NO3	313.1678	H+	314.1751	4.2	256.0897
Ethylmorphine	C19H23NO3	313.1678	H+	314.1751	4.2	313.1481
Ethylmorphine	C19H23NO3	313.1678	H+	314.1751	4.2	282.1059
Ethylmorphine	C19H23NO3	313.1678	H+	314.1751	4.2	239.1071
Mepirapim	C19H27N3O	313.2154	H+	314.2227	6.84	
Mepirapim	C19H27N3O	313.2154	H+	314.2227	6.84	217.1227
Mepirapim	C19H27N3O	313.2154	H+	314.2227	6.84	144.0437
Mepirapim	C19H27N3O	313.2154	H+	314.2227	6.84	314.223
Mepirapim	C19H27N3O	313.2154	H+	314.2227	6.84	116.049
Mepirapim	C19H27N3O	313.2154	H+	314.2227	6.84	158.0598
Mebroqualone	C15H11BrN2O	314.0055	H+	315.0128	7.48	
Mebroqualone	C15H11BrN2O	314.0055	H+	315.0128	7.48	315.0117
Mebroqualone	C15H11BrN2O	314.0055	H+	315.0128	7.48	195.9746
Mebroqualone	C15H11BrN2O	314.0055	H+	315.0128	7.48	154.9477
Mebroqualone	C15H11BrN2O	314.0055	H+	315.0128	7.48	144.044
Mebroqualone	C15H11BrN2O	314.0055	H+	315.0128	7.48	120.0437
N-Desmethyl U-47700	C15H20Cl2N2O	314.0953	H+	315.1026	6.19	
N-Desmethyl U-47700	C15H20Cl2N2O	314.0953	H+	315.1026	6.19	172.9555
N-Desmethyl U-47700	C15H20Cl2N2O	314.0953	H+	315.1026	6.19	284.0614
N-Desmethyl U-47700	C15H20Cl2N2O	314.0953	H+	315.1026	6.19	203.9976
N-Desmethyl U-47700	C15H20Cl2N2O	314.0953	H+	315.1026	6.19	144.9593
N-Desmethyl U-47700	C15H20Cl2N2O	314.0953	H+	315.1026	6.19	81.0712
Clomipramine	C19H23ClN2	314.1550	H+	315.1623	7.66	
Clomipramine	C19H23ClN2	314.1550	H+	315.1623	7.66	86.0972

Clomipramine	C19H23ClN2	314.1550	H+	315.1623	7.66	58.0674
Clomipramine	C19H23ClN2	314.1550	H+	315.1623	7.66	315.1623
Clomipramine	C19H23ClN2	314.1550	H+	315.1623	7.66	242.0732
Clomipramine	C19H23ClN2	314.1550	H+	315.1623	7.66	270.1046
Cannabidiol (CBD)	C21H30O2	314.2246	H+	315.2319	10.18	
Cannabidiol (CBD)	C21H30O2	314.2246	H+	315.2319	10.18	193.1225
Cannabidiol (CBD)	C21H30O2	314.2246	H+	315.2319	10.18	315.2324
Cannabidiol (CBD)	C21H30O2	314.2246	H+	315.2319	10.18	259.1695
Cannabidiol (CBD)	C21H30O2	314.2246	H+	315.2319	10.18	123.0442
Cannabidiol (CBD)	C21H30O2	314.2246	H+	315.2319	10.18	135.1168
THC	C21H30O2	314.2246	H+	315.2319	10.92	
THC	C21H30O2	314.2246	H+	315.2319	10.92	193.1228
THC	C21H30O2	314.2246	H+	315.2319	10.92	315.2325
THC	C21H30O2	314.2246	H+	315.2319	10.92	259.1701
THC	C21H30O2	314.2246	H+	315.2319	10.92	123.0446
THC	C21H30O2	314.2246	H+	315.2319	10.92	135.1174
Bromazepam	C14H10BrN3O	315.0007	H+	316.0080	6.45	
Bromazepam	C14H10BrN3O	315.0007	H+	316.0080	6.45	316.008
Bromazepam	C14H10BrN3O	315.0007	H+	316.0080	6.45	182.0833
Bromazepam	C14H10BrN3O	315.0007	H+	316.0080	6.45	209.095
Bromazepam	C14H10BrN3O	315.0007	H+	316.0080	6.45	288.0118
Bromazepam	C14H10BrN3O	315.0007	H+	316.0080	6.45	261.0014
Clonazepam	C15H10ClN3O3	315.0411	H+	316.0483	7.11	
Clonazepam	C15H10ClN3O3	315.0411	H+	316.0483	7.11	316.048
Clonazepam	C15H10ClN3O3	315.0411	H+	316.0483	7.11	270.0551
Clonazepam	C15H10ClN3O3	315.0411	H+	316.0483	7.11	214.0418
Clonazepam	C15H10ClN3O3	315.0411	H+	316.0483	7.11	241.0514
Clonazepam	C15H10ClN3O3	315.0411	H+	316.0483	7.11	207.0903
Oxycodone	C18H21NO4	315.1471	H+	316.1543	3.73	
Oxycodone	C18H21NO4	315.1471	H+	316.1543	3.73	298.145
Oxycodone	C18H21NO4	315.1471	H+	316.1543	3.73	316.1553
Oxycodone	C18H21NO4	315.1471	H+	316.1543	3.73	256.1334
Oxycodone	C18H21NO4	315.1471	H+	316.1543	3.73	241.1096
Oxycodone	C18H21NO4	315.1471	H+	316.1543	3.73	187.076
25E-NBOH	C19H25NO3	315.1834	H+	316.1907	7.3	
25E-NBOH	C19H25NO3	315.1834	H+	316.1907	7.3	193.1218
25E-NBOH	C19H25NO3	315.1834	H+	316.1907	7.3	178.0982
25E-NBOH	C19H25NO3	315.1834	H+	316.1907	7.3	107.0484
25E-NBOH	C19H25NO3	315.1834	H+	316.1907	7.3	316.1903
25E-NBOH	C19H25NO3	315.1834	H+	316.1907	7.3	210.1485
25D-NBOMe	C19H25NO3	315.1834	H+	316.1907	7.04	
25D-NBOMe	C19H25NO3	315.1834	H+	316.1907	7.04	121.0647
25D-NBOMe	C19H25NO3	315.1834	H+	316.1907	7.04	316.191
25D-NBOMe	C19H25NO3	315.1834	H+	316.1907	7.04	179.1067
25D-NBOMe	C19H25NO3	315.1834	H+	316.1907	7.04	164.0832
25D-NBOMe	C19H25NO3	315.1834	H+	316.1907	7.04	91.0551
Despropionyl 2'-Fluoro ortho-Fluorofentanyl	C19H22F2N2	316.1751	H+	317.1824	6.58	
Despropionyl 2'-Fluoro ortho-Fluorofentanyl	C19H22F2N2	316.1751	H+	317.1824	6.58	206.1343
Despropionyl 2'-Fluoro ortho-Fluorofentanyl	C19H22F2N2	316.1751	H+	317.1824	6.58	123.0597
Despropionyl 2'-Fluoro ortho-Fluorofentanyl	C19H22F2N2	316.1751	H+	317.1824	6.58	317.1826
Despropionyl 2'-Fluoro ortho-Fluorofentanyl	C19H22F2N2	316.1751	H+	317.1824	6.58	152.0867
Despropionyl 2'-Fluoro ortho-Fluorofentanyl	C19H22F2N2	316.1751	H+	317.1824	6.58	103.0539
Cocaethylene	C18H23NO4	317.1627	H+	318.1700	5.75	
Cocaethylene	C18H23NO4	317.1627	H+	318.1700	5.75	196.1327
Cocaethylene	C18H23NO4	317.1627	H+	318.1700	5.75	318.1695
Cocaethylene	C18H23NO4	317.1627	H+	318.1700	5.75	82.0664
Cocaethylene	C18H23NO4	317.1627	H+	318.1700	5.75	150.0912
Cocaethylene	C18H23NO4	317.1627	H+	318.1700	5.75	105.0338
Diclazepam	C16H12Cl2N2O	318.0327	H+	319.0399	8.21	
Diclazepam	C16H12Cl2N2O	318.0327	H+	319.0399	8.21	319.039
Diclazepam	C16H12Cl2N2O	318.0327	H+	319.0399	8.21	227.0487
Diclazepam	C16H12Cl2N2O	318.0327	H+	319.0399	8.21	154.041
Diclazepam	C16H12Cl2N2O	318.0327	H+	319.0399	8.21	291.0442
Diclazepam	C16H12Cl2N2O	318.0327	H+	319.0399	8.21	256.0757
Brompheniramine	C16H19BrN2	318.0732	H+	319.0804	6.02	
Brompheniramine	C16H19BrN2	318.0732	H+	319.0804	6.02	274.0224
Brompheniramine	C16H19BrN2	318.0732	H+	319.0804	6.02	167.0726
Brompheniramine	C16H19BrN2	318.0732	H+	319.0804	6.02	319.0808

Brompheniramine	C16H19BrN2	318.0732	H+	319.0804	6.02	245.9912
Brompheniramine	C16H19BrN2	318.0732	H+	319.0804	6.02	244.9836
Chlorpromazine	C17H19ClN2S	318.0957	H+	319.1030	7.54	
Chlorpromazine	C17H19ClN2S	318.0957	H+	319.1030	7.54	86.0973
Chlorpromazine	C17H19ClN2S	318.0957	H+	319.1030	7.54	319.1028
Chlorpromazine	C17H19ClN2S	318.0957	H+	319.1030	7.54	58.0674
Chlorpromazine	C17H19ClN2S	318.0957	H+	319.1030	7.54	246.0138
Chlorpromazine	C17H19ClN2S	318.0957	H+	319.1030	7.54	239.0762
Fluvoxamine	C15H21F3N2O2	318.1555	H+	319.1628	7.25	
Fluvoxamine	C15H21F3N2O2	318.1555	H+	319.1628	7.25	71.0506
Fluvoxamine	C15H21F3N2O2	318.1555	H+	319.1628	7.25	200.0681
Fluvoxamine	C15H21F3N2O2	318.1555	H+	319.1628	7.25	228.0996
Fluvoxamine	C15H21F3N2O2	318.1555	H+	319.1628	7.25	226.0641
Fluvoxamine	C15H21F3N2O2	318.1555	H+	319.1628	7.25	45.0371
Ethylenedioxy-U-47700	C18H26N2O3	318.1943	H+	319.2016	5	
Ethylenedioxy-U-47700	C18H26N2O3	318.1943	H+	319.2016	5	274.1439
Ethylenedioxy-U-47700	C18H26N2O3	318.1943	H+	319.2016	5	163.0387
Ethylenedioxy-U-47700	C18H26N2O3	318.1943	H+	319.2016	5	194.081
Ethylenedioxy-U-47700	C18H26N2O3	318.1943	H+	319.2016	5	137.0594
Ethylenedioxy-U-47700	C18H26N2O3	318.1943	H+	319.2016	5	319.2023
Nitrazolam	C17H13N5O2	319.1069	H+	320.1142	6.53	
Nitrazolam	C17H13N5O2	319.1069	H+	320.1142	6.53	292.0962
Nitrazolam	C17H13N5O2	319.1069	H+	320.1142	6.53	274.1218
Nitrazolam	C17H13N5O2	319.1069	H+	320.1142	6.53	320.1154
Nitrazolam	C17H13N5O2	319.1069	H+	320.1142	6.53	246.1035
Nitrazolam	C17H13N5O2	319.1069	H+	320.1142	6.53	198.0904
JWH-251	C22H25NO	319.1936	H+	320.2009	10.14	
JWH-251	C22H25NO	319.1936	H+	320.2009	10.14	214.1219
JWH-251	C22H25NO	319.1936	H+	320.2009	10.14	105.0697
JWH-251	C22H25NO	319.1936	H+	320.2009	10.14	320.2007
JWH-251	C22H25NO	319.1936	H+	320.2009	10.14	144.044
JWH-251	C22H25NO	319.1936	H+	320.2009	10.14	119.0492
Lorazepam	C15H10Cl2N2O2	320.0119	H+	321.0192	7.28	
Lorazepam	C15H10Cl2N2O2	320.0119	H+	321.0192	7.28	275.0133
Lorazepam	C15H10Cl2N2O2	320.0119	H+	321.0192	7.28	312.0196
Lorazepam	C15H10Cl2N2O2	320.0119	H+	321.0192	7.28	303.0092
Lorazepam	C15H10Cl2N2O2	320.0119	H+	321.0192	7.28	229.0526
Lorazepam	C15H10Cl2N2O2	320.0119	H+	321.0192	7.28	163.0058
SBD-006	C21H24N2O	320.1889	H+	321.1961	9.53	
SBD-006	C21H24N2O	320.1889	H+	321.1961	9.53	214.123
SBD-006	C21H24N2O	320.1889	H+	321.1961	9.53	188.1438
SBD-006	C21H24N2O	320.1889	H+	321.1961	9.53	132.0808
SBD-006	C21H24N2O	320.1889	H+	321.1961	9.53	91.0542
SBD-006	C21H24N2O	320.1889	H+	321.1961	9.53	321.1974
25C-NBOH	C17H20ClNO3	321.1132	H+	322.1205	6.57	
25C-NBOH	C17H20ClNO3	321.1132	H+	322.1205	6.57	199.0517
25C-NBOH	C17H20ClNO3	321.1132	H+	322.1205	6.57	107.0476
25C-NBOH	C17H20ClNO3	321.1132	H+	322.1205	6.57	184.0279
25C-NBOH	C17H20ClNO3	321.1132	H+	322.1205	6.57	216.0783
25C-NBOH	C17H20ClNO3	321.1132	H+	322.1205	6.57	322.1208
RCS-4	C21H23NO2	321.1729	H+	322.1802	9.98	
RCS-4	C21H23NO2	321.1729	H+	322.1802	9.98	135.0437
RCS-4	C21H23NO2	321.1729	H+	322.1802	9.98	322.1809
RCS-4	C21H23NO2	321.1729	H+	322.1802	9.98	214.1227
RCS-4	C21H23NO2	321.1729	H+	322.1802	9.98	144.0438
RCS-4	C21H23NO2	321.1729	H+	322.1802	9.98	107.0487
Benzyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	6.02	
Benzyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	6.02	174.1285
Benzyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	6.02	91.0546
Benzyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	6.02	323.2139
Benzyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	6.02	216.1396
Benzyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	6.02	132.0811
Acetyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	5.69	
Acetyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	5.69	188.1433
Acetyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	5.69	323.2106
Acetyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	5.69	105.0699
Acetyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	5.69	202.126
Acetyl Fentanyl	C21H26N2O	322.2045	H+	323.2118	5.69	134.0962
LSD (Lysergide)	C20H25N3O	323.1998	H+	324.2070	5.62	
LSD (Lysergide)	C20H25N3O	323.1998	H+	324.2070	5.62	223.1221
LSD (Lysergide)	C20H25N3O	323.1998	H+	324.2070	5.62	324.2067
LSD (Lysergide)	C20H25N3O	323.1998	H+	324.2070	5.62	281.1646
LSD (Lysergide)	C20H25N3O	323.1998	H+	324.2070	5.62	208.0881
LSD (Lysergide)	C20H25N3O	323.1998	H+	324.2070	5.62	197.1067

Alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	H+	325.0851	7.11	
Alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	H+	325.0851	7.11	325.0853
Alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	H+	325.0851	7.11	297.0674
Alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	H+	325.0851	7.11	279.0676
Alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	H+	325.0851	7.11	216.0807
Alpha-Hydroxyalprazolam	C17H13ClN4O	324.0778	H+	325.0851	7.11	307.0725
U-47931E	C15H21BrN2O	324.0837	H+	325.0910	5.82	
U-47931E	C15H21BrN2O	324.0837	H+	325.0910	5.82	199.9717
U-47931E	C15H21BrN2O	324.0837	H+	325.0910	5.82	182.9453
U-47931E	C15H21BrN2O	324.0837	H+	325.0910	5.82	280.0351
U-47931E	C15H21BrN2O	324.0837	H+	325.0910	5.82	154.9499
U-47931E	C15H21BrN2O	324.0837	H+	325.0910	5.82	126.1288
Citalopram / Escitalopram	C20H21FN2O	324.1638	H+	325.1711	6.45	
Citalopram / Escitalopram	C20H21FN2O	324.1638	H+	325.1711	6.45	109.0447
Citalopram / Escitalopram	C20H21FN2O	324.1638	H+	325.1711	6.45	262.1024
Citalopram / Escitalopram	C20H21FN2O	324.1638	H+	325.1711	6.45	325.1711
Citalopram / Escitalopram	C20H21FN2O	324.1638	H+	325.1711	6.45	234.0714
Citalopram / Escitalopram	C20H21FN2O	324.1638	H+	325.1711	6.45	116.0497
Quinidine	C20H24N2O2	324.1838	H+	325.1911	4.87	
Quinidine	C20H24N2O2	324.1838	H+	325.1911	4.87	325.1904
Quinidine	C20H24N2O2	324.1838	H+	325.1911	4.87	307.1796
Quinidine	C20H24N2O2	324.1838	H+	325.1911	4.87	253.133
Quinidine	C20H24N2O2	324.1838	H+	325.1911	4.87	184.075
Quinidine	C20H24N2O2	324.1838	H+	325.1911	4.87	160.0751
Quinine	C20H24N2O2	324.1838	H+	325.1911	5.01	
Quinine	C20H24N2O2	324.1838	H+	325.1911	5.01	325.1906
Quinine	C20H24N2O2	324.1838	H+	325.1911	5.01	307.1796
Quinine	C20H24N2O2	324.1838	H+	325.1911	5.01	253.1329
Quinine	C20H24N2O2	324.1838	H+	325.1911	5.01	184.075
Quinine	C20H24N2O2	324.1838	H+	325.1911	5.01	160.075
JWH-176	C25H24	324.1878	H+	325.1951	12.32	
JWH-176	C25H24	324.1878	H+	325.1951	12.32	255.1166
JWH-176	C25H24	324.1878	H+	325.1951	12.32	141.0692
JWH-176	C25H24	324.1878	H+	325.1951	12.32	325.1923
JWH-176	C25H24	324.1878	H+	325.1951	12.32	240.0933
JWH-176	C25H24	324.1878	H+	325.1951	12.32	117.0689
Midazolam	C18H13ClFN3	325.0782	H+	326.0855	6.37	
Midazolam	C18H13ClFN3	325.0782	H+	326.0855	6.37	326.0853
Midazolam	C18H13ClFN3	325.0782	H+	326.0855	6.37	291.1166
Midazolam	C18H13ClFN3	325.0782	H+	326.0855	6.37	244.032
Midazolam	C18H13ClFN3	325.0782	H+	326.0855	6.37	249.0818
Midazolam	C18H13ClFN3	325.0782	H+	326.0855	6.37	290.1089
Norpropoxyphene	C21H27NO2	325.2042	H+	326.2115	7.11	
Norpropoxyphene	C21H27NO2	325.2042	H+	326.2115	7.11	44.0535
Norpropoxyphene	C21H27NO2	325.2042	H+	326.2115	7.11	143.0859
Norpropoxyphene	C21H27NO2	325.2042	H+	326.2115	7.11	252.1751
Norpropoxyphene	C21H27NO2	325.2042	H+	326.2115	7.11	326.0885
Norpropoxyphene	C21H27NO2	325.2042	H+	326.2115	7.11	298.07
Flualprazolam	C17H12ClFN4	326.0735	H+	327.0807	7.29	
Flualprazolam	C17H12ClFN4	326.0735	H+	327.0807	7.29	299.0616
Flualprazolam	C17H12ClFN4	326.0735	H+	327.0807	7.29	292.1111
Flualprazolam	C17H12ClFN4	326.0735	H+	327.0807	7.29	327.08
Flualprazolam	C17H12ClFN4	326.0735	H+	327.0807	7.29	223.0674
Flualprazolam	C17H12ClFN4	326.0735	H+	327.0807	7.29	165.0202
Clozapine	C18H19ClN4	326.1298	H+	327.1371	6.29	
Clozapine	C18H19ClN4	326.1298	H+	327.1371	6.29	270.0789
Clozapine	C18H19ClN4	326.1298	H+	327.1371	6.29	327.1371
Clozapine	C18H19ClN4	326.1298	H+	327.1371	6.29	296.0955
Clozapine	C18H19ClN4	326.1298	H+	327.1371	6.29	227.0373
Clozapine	C18H19ClN4	326.1298	H+	327.1371	6.29	192.0682
Furanylethylfentanyl	C20H26N2O2	326.1994	H+	327.2067	5.75	
Furanylethylfentanyl	C20H26N2O2	326.1994	H+	327.2067	5.75	178.1214
Furanylethylfentanyl	C20H26N2O2	326.1994	H+	327.2067	5.75	146.0953
Furanylethylfentanyl	C20H26N2O2	326.1994	H+	327.2067	5.75	189.137
Furanylethylfentanyl	C20H26N2O2	326.1994	H+	327.2067	5.75	202.1211
Furanylethylfentanyl	C20H26N2O2	326.1994	H+	327.2067	5.75	245.1632
Loxapine	C18H18ClN3O	327.1138	H+	328.1211	6.82	
Loxapine	C18H18ClN3O	327.1138	H+	328.1211	6.82	271.063
Loxapine	C18H18ClN3O	327.1138	H+	328.1211	6.82	328.1213
Loxapine	C18H18ClN3O	327.1138	H+	328.1211	6.82	297.0797
Loxapine	C18H18ClN3O	327.1138	H+	328.1211	6.82	228.0215
Loxapine	C18H18ClN3O	327.1138	H+	328.1211	6.82	193.0522
6-Monoacetylmorphine	C19H21NO4	327.1471	H+	328.1543	3.91	
6-Monoacetylmorphine	C19H21NO4	327.1471	H+	328.1543	3.91	328.155

6-Monoacetylmorphine	C19H21NO4	327.1471	H+	328.1543	3.91	211.0753
6-Monoacetylmorphine	C19H21NO4	327.1471	H+	328.1543	3.91	165.0697
6-Monoacetylmorphine	C19H21NO4	327.1471	H+	328.1543	3.91	193.0645
6-Monoacetylmorphine	C19H21NO4	327.1471	H+	328.1543	3.91	268.1331
Naloxone	C19H21NO4	327.1471	H+	328.1543	3.47	
Naloxone	C19H21NO4	327.1471	H+	328.1543	3.47	310.144
Naloxone	C19H21NO4	327.1471	H+	328.1543	3.47	328.1546
Naloxone	C19H21NO4	327.1471	H+	328.1543	3.47	268.1331
Naloxone	C19H21NO4	327.1471	H+	328.1543	3.47	253.11
Naloxone	C19H21NO4	327.1471	H+	328.1543	3.47	212.0709
JWH-015	C23H21NO	327.1623	H+	328.1696	9.74	
JWH-015	C23H21NO	327.1623	H+	328.1696	9.74	155.0487
JWH-015	C23H21NO	327.1623	H+	328.1696	9.74	200.1065
JWH-015	C23H21NO	327.1623	H+	328.1696	9.74	127.0539
JWH-015	C23H21NO	327.1623	H+	328.1696	9.74	328.1698
JWH-015	C23H21NO	327.1623	H+	328.1696	9.74	158.0598
JWH-073	C23H21NO	327.1623	H+	328.1696	10	
JWH-073	C23H21NO	327.1623	H+	328.1696	10	155.0489
JWH-073	C23H21NO	327.1623	H+	328.1696	10	200.1067
JWH-073	C23H21NO	327.1623	H+	328.1696	10	127.0539
JWH-073	C23H21NO	327.1623	H+	328.1696	10	328.1701
JWH-073	C23H21NO	327.1623	H+	328.1696	10	144.0443
JWH-175	C24H25N	327.1987	H+	328.2060	11.34	
JWH-175	C24H25N	327.1987	H+	328.2060	11.34	141.0695
JWH-175	C24H25N	327.1987	H+	328.2060	11.34	328.2065
JWH-175	C24H25N	327.1987	H+	328.2060	11.34	115.0545
JWH-175	C24H25N	327.1987	H+	328.2060	11.34	200.1431
JWH-175	C24H25N	327.1987	H+	328.2060	11.34	186.1268
Butorphanol	C21H29NO2	327.2198	H+	328.2271	5.65	
Butorphanol	C21H29NO2	327.2198	H+	328.2271	5.65	328.2277
Butorphanol	C21H29NO2	327.2198	H+	328.2271	5.65	310.2172
Butorphanol	C21H29NO2	327.2198	H+	328.2271	5.65	282.1863
Butorphanol	C21H29NO2	327.2198	H+	328.2271	5.65	242.1548
Butorphanol	C21H29NO2	327.2198	H+	328.2271	5.65	185.0955
AH-7921	C16H22Cl2N2O	328.1109	H+	329.1182	6.45	
AH-7921	C16H22Cl2N2O	328.1109	H+	329.1182	6.45	172.9551
AH-7921	C16H22Cl2N2O	328.1109	H+	329.1182	6.45	284.0604
AH-7921	C16H22Cl2N2O	328.1109	H+	329.1182	6.45	329.1181
AH-7921	C16H22Cl2N2O	328.1109	H+	329.1182	6.45	189.982
AH-7921	C16H22Cl2N2O	328.1109	H+	329.1182	6.45	201.9824
U-47700	C16H22Cl2N2O	328.1109	H+	329.1182	6.21	
U-47700	C16H22Cl2N2O	328.1109	H+	329.1182	6.21	284.0597
U-47700	C16H22Cl2N2O	328.1109	H+	329.1182	6.21	172.9549
U-47700	C16H22Cl2N2O	328.1109	H+	329.1182	6.21	203.997
U-47700	C16H22Cl2N2O	328.1109	H+	329.1182	6.21	329.1176
U-47700	C16H22Cl2N2O	328.1109	H+	329.1182	6.21	144.9604
Thienyl Fentanyl	C19H24N2OS	328.1609	H+	329.1682	5.75	
Thienyl Fentanyl	C19H24N2OS	328.1609	H+	329.1682	5.75	97.0111
Thienyl Fentanyl	C19H24N2OS	328.1609	H+	329.1682	5.75	180.0825
Thienyl Fentanyl	C19H24N2OS	328.1609	H+	329.1682	5.75	329.1657
Thienyl Fentanyl	C19H24N2OS	328.1609	H+	329.1682	5.75	82.0653
Thienyl Fentanyl	C19H24N2OS	328.1609	H+	329.1682	5.75	273.1405
HU-331	C21H28O3	328.2038	H+	329.2111	10.82	
HU-331	C21H28O3	328.2038	H+	329.2111	10.82	329.2115
HU-331	C21H28O3	328.2038	H+	329.2111	10.82	287.1642
HU-331	C21H28O3	328.2038	H+	329.2111	10.82	286.1564
HU-331	C21H28O3	328.2038	H+	329.2111	10.82	229.0855
HU-331	C21H28O3	328.2038	H+	329.2111	10.82	259.1691
Paroxetine	C19H20FNO3	329.1427	H+	330.1500	6.96	
Paroxetine	C19H20FNO3	329.1427	H+	330.1500	6.96	330.1499
Paroxetine	C19H20FNO3	329.1427	H+	330.1500	6.96	192.1179
Paroxetine	C19H20FNO3	329.1427	H+	330.1500	6.96	70.0667
Paroxetine	C19H20FNO3	329.1427	H+	330.1500	6.96	44.0533
Paroxetine	C19H20FNO3	329.1427	H+	330.1500	6.96	151.0382
25E-NBOMe	C20H27NO3	329.1991	H+	330.2064	7.58	
25E-NBOMe	C20H27NO3	329.1991	H+	330.2064	7.58	121.0647
25E-NBOMe	C20H27NO3	329.1991	H+	330.2064	7.58	330.2065
25E-NBOMe	C20H27NO3	329.1991	H+	330.2064	7.58	193.1223
25E-NBOMe	C20H27NO3	329.1991	H+	330.2064	7.58	91.0552
25E-NBOMe	C20H27NO3	329.1991	H+	330.2064	7.58	93.0707
XLR-11	C21H28FNO	329.2155	H+	330.2228	10.02	
XLR-11	C21H28FNO	329.2155	H+	330.2228	10.02	125.0964
XLR-11	C21H28FNO	329.2155	H+	330.2228	10.02	330.2216
XLR-11	C21H28FNO	329.2155	H+	330.2228	10.02	232.1137

XLR-11	C21H28FNO	329.2155	H+	330.2228	10.02	312.2126
XLR-11	C21H28FNO	329.2155	H+	330.2228	10.02	297.1895
AB-PINACA	C18H26N4O2	330.2056	H+	331.2129	8.8	
AB-PINACA	C18H26N4O2	330.2056	H+	331.2129	8.8	215.1172
AB-PINACA	C18H26N4O2	330.2056	H+	331.2129	8.8	286.191
AB-PINACA	C18H26N4O2	330.2056	H+	331.2129	8.8	145.0392
AB-PINACA	C18H26N4O2	330.2056	H+	331.2129	8.8	314.1864
AB-PINACA	C18H26N4O2	330.2056	H+	331.2129	8.8	331.2125
FAB-144	C20H27FN2O	330.2107	H+	331.2180	10.65	
FAB-144	C20H27FN2O	330.2107	H+	331.2180	10.65	233.1092
FAB-144	C20H27FN2O	330.2107	H+	331.2180	10.65	213.1025
FAB-144	C20H27FN2O	330.2107	H+	331.2180	10.65	177.0462
FAB-144	C20H27FN2O	330.2107	H+	331.2180	10.65	145.0398
FAB-144	C20H27FN2O	330.2107	H+	331.2180	10.65	313.2084
Hydroxy-THC	C21H30O3	330.2195	H+	331.2268	9.86	
Hydroxy-THC	C21H30O3	330.2195	H+	331.2268	9.86	313.2161
Hydroxy-THC	C21H30O3	330.2195	H+	331.2268	9.86	331.2269
Hydroxy-THC	C21H30O3	330.2195	H+	331.2268	9.86	201.0909
Hydroxy-THC	C21H30O3	330.2195	H+	331.2268	9.86	193.1221
Hydroxy-THC	C21H30O3	330.2195	H+	331.2268	9.86	295.206
Flubromazepam	C15H10BrFN2O	331.9961	H+	333.0033	7.65	
Flubromazepam	C15H10BrFN2O	331.9961	H+	333.0033	7.65	333.0027
Flubromazepam	C15H10BrFN2O	331.9961	H+	333.0033	7.65	226.0898
Flubromazepam	C15H10BrFN2O	331.9961	H+	333.0033	7.65	183.9751
Flubromazepam	C15H10BrFN2O	331.9961	H+	333.0033	7.65	305.0084
Flubromazepam	C15H10BrFN2O	331.9961	H+	333.0033	7.65	257.991
Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	H+	333.0801	7.31	
Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	H+	333.0801	7.31	333.0802
Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	H+	333.0801	7.31	109.0452
Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	H+	333.0801	7.31	305.0861
Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	H+	333.0801	7.31	315.0704
Hydroxyethylflurazepam	C17H14ClFN2O2	332.0728	H+	333.0801	7.31	211.0792
Ethylenedioxy-U-51754	C19H28N2O3	332.2100	H+	333.2173	5.31	
Ethylenedioxy-U-51754	C19H28N2O3	332.2100	H+	333.2173	5.31	288.1597
Ethylenedioxy-U-51754	C19H28N2O3	332.2100	H+	333.2173	5.31	208.0968
Ethylenedioxy-U-51754	C19H28N2O3	332.2100	H+	333.2173	5.31	112.1118
Ethylenedioxy-U-51754	C19H28N2O3	332.2100	H+	333.2173	5.31	149.0595
Ethylenedioxy-U-51754	C19H28N2O3	332.2100	H+	333.2173	5.31	333.2174
Strychnine	C21H22N2O2	334.1681	H+	335.1754	4.34	
Strychnine	C21H22N2O2	334.1681	H+	335.1754	4.34	335.1757
Strychnine	C21H22N2O2	334.1681	H+	335.1754	4.34	184.076
Strychnine	C21H22N2O2	334.1681	H+	335.1754	4.34	364.1031
Strychnine	C21H22N2O2	334.1681	H+	335.1754	4.34	307.1453
Strychnine	C21H22N2O2	334.1681	H+	335.1754	4.34	222.0919
Acrylfentantyl	C22H26N2O	334.2045	H+	335.2118	6.17	
Acrylfentantyl	C22H26N2O	334.2045	H+	335.2118	6.17	188.1425
Acrylfentantyl	C22H26N2O	334.2045	H+	335.2118	6.17	105.0701
Acrylfentantyl	C22H26N2O	334.2045	H+	335.2118	6.17	335.2099
Acrylfentantyl	C22H26N2O	334.2045	H+	335.2118	6.17	214.1214
Acrylfentantyl	C22H26N2O	334.2045	H+	335.2118	6.17	134.0959
25C-NBOMe	C18H22ClNO3	335.1288	H+	336.1361	7	
25C-NBOMe	C18H22ClNO3	335.1288	H+	336.1361	7	121.0648
25C-NBOMe	C18H22ClNO3	335.1288	H+	336.1361	7	336.1372
25C-NBOMe	C18H22ClNO3	335.1288	H+	336.1361	7	91.0551
25C-NBOMe	C18H22ClNO3	335.1288	H+	336.1361	7	93.0702
25C-NBOMe	C18H22ClNO3	335.1288	H+	336.1361	7	155.0704
JWH-201	C22H25NO2	335.1885	H+	336.1958	9.89	
JWH-201	C22H25NO2	335.1885	H+	336.1958	9.89	121.0641
JWH-201	C22H25NO2	335.1885	H+	336.1958	9.89	135.0436
JWH-201	C22H25NO2	335.1885	H+	336.1958	9.89	149.0595
JWH-201	C22H25NO2	335.1885	H+	336.1958	9.89	214.1229
JWH-201	C22H25NO2	335.1885	H+	336.1958	9.89	336.1963
JWH-302	C22H25NO2	335.1885	H+	336.1958	9.92	
JWH-302	C22H25NO2	335.1885	H+	336.1958	9.92	214.1235
JWH-302	C22H25NO2	335.1885	H+	336.1958	9.92	121.0643
JWH-302	C22H25NO2	335.1885	H+	336.1958	9.92	188.1443
JWH-302	C22H25NO2	335.1885	H+	336.1958	9.92	144.0444
JWH-302	C22H25NO2	335.1885	H+	336.1958	9.92	336.1988
JWH-250	C22H25NO2	335.1885	H+	336.1958	9.93	
JWH-250	C22H25NO2	335.1885	H+	336.1958	9.93	121.0648
JWH-250	C22H25NO2	335.1885	H+	336.1958	9.93	200.1431
JWH-250	C22H25NO2	335.1885	H+	336.1958	9.93	336.1957
JWH-250	C22H25NO2	335.1885	H+	336.1958	9.93	303.1622
JWH-250	C22H25NO2	335.1885	H+	336.1958	9.93	214.1226

a-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	5.95	
a-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	5.95	202.1565
a-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	5.95	119.0848
a-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	5.95	337.2262
a-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	5.95	91.0545
a-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	5.95	219.148
Acetyl Fentanyl 4-Methylphenethyl Analog	C22H28N2O	336.2201	H+	337.2274	6.30	
Acetyl Fentanyl 4-Methylphenethyl Analog	C22H28N2O	336.2201	H+	337.2274	6.30	202.155
Acetyl Fentanyl 4-Methylphenethyl Analog	C22H28N2O	336.2201	H+	337.2274	6.30	119.0841
Acetyl Fentanyl 4-Methylphenethyl Analog	C22H28N2O	336.2201	H+	337.2274	6.30	337.2222
Acetyl Fentanyl 4-Methylphenethyl Analog	C22H28N2O	336.2201	H+	337.2274	6.30	160.1096
Acetyl Fentanyl 4-Methylphenethyl Analog	C22H28N2O	336.2201	H+	337.2274	6.30	132.079
para-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.30	
para-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.30	188.1449
para-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.30	105.0708
para-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.30	216.1401
para-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.30	146.0975
para-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.30	134.0976
ortho-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.09	
ortho-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.09	188.1446
ortho-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.09	105.0708
ortho-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.09	216.1396
ortho-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.09	146.0974
ortho-Methylacetyl Fentanyl	C22H28N2O	336.2201	H+	337.2274	6.09	134.0974
Fentanyl	C22H28N2O	336.2202	H+	337.2274	6.2	
Fentanyl	C22H28N2O	336.2202	H+	337.2274	6.2	337.2273
Fentanyl	C22H28N2O	336.2202	H+	337.2274	6.2	188.143
Fentanyl	C22H28N2O	336.2202	H+	337.2274	6.2	105.0705
Fentanyl	C22H28N2O	336.2202	H+	337.2274	6.2	132.0799
Fentanyl	C22H28N2O	336.2202	H+	337.2274	6.2	216.1384
ETH-LAD	C21H27N3O	337.2154	H+	338.2227	5.81	
ETH-LAD	C21H27N3O	337.2154	H+	338.2227	5.81	237.1383
ETH-LAD	C21H27N3O	337.2154	H+	338.2227	5.81	338.2227
ETH-LAD	C21H27N3O	337.2154	H+	338.2227	5.81	309.1833
ETH-LAD	C21H27N3O	337.2154	H+	338.2227	5.81	281.1643
ETH-LAD	C21H27N3O	337.2154	H+	338.2227	5.81	265.1337
N-methyl U-47931E	C16H23BrN2O	338.0994	H+	339.1067	5.71	
N-methyl U-47931E	C16H23BrN2O	338.0994	H+	339.1067	5.71	294.0475
N-methyl U-47931E	C16H23BrN2O	338.0994	H+	339.1067	5.71	182.9433
N-methyl U-47931E	C16H23BrN2O	338.0994	H+	339.1067	5.71	213.9858
N-methyl U-47931E	C16H23BrN2O	338.0994	H+	339.1067	5.71	339.1054
N-methyl U-47931E	C16H23BrN2O	338.0994	H+	339.1067	5.71	154.948
5F-SDB-006	C21H23FN2O	338.1794	H+	339.1867	8.84	
5F-SDB-006	C21H23FN2O	338.1794	H+	339.1867	8.84	232.1135
5F-SDB-006	C21H23FN2O	338.1794	H+	339.1867	8.84	206.1342
5F-SDB-006	C21H23FN2O	338.1794	H+	339.1867	8.84	339.1878
5F-SDB-006	C21H23FN2O	338.1794	H+	339.1867	8.84	144.0439
5F-SDB-006	C21H23FN2O	338.1794	H+	339.1867	8.84	132.0808
Fentanyl Methyl Carbamate	C21H26N2O2	338.1994	H+	339.2067	6.05	
Fentanyl Methyl Carbamate	C21H26N2O2	338.1994	H+	339.2067	6.05	188.1434
Fentanyl Methyl Carbamate	C21H26N2O2	338.1994	H+	339.2067	6.05	105.0698
Fentanyl Methyl Carbamate	C21H26N2O2	338.1994	H+	339.2067	6.05	339.2065
Fentanyl Methyl Carbamate	C21H26N2O2	338.1994	H+	339.2067	6.05	134.0964
Fentanyl Methyl Carbamate	C21H26N2O2	338.1994	H+	339.2067	6.05	146.0961
Topiramate	C12H21NO8S	339.0988	H+	340.1061	6.04	
Topiramate	C12H21NO8S	339.0988	H+	340.1061	6.04	340.1544
Topiramate	C12H21NO8S	339.0988	H+	340.1061	6.04	184.0966
Topiramate	C12H21NO8S	339.0988	H+	340.1061	6.04	127.0389
Topiramate	C12H21NO8S	339.0988	H+	340.1061	6.04	59.0511
Topiramate	C12H21NO8S	339.0988	H+	340.1061	6.04	324.1235
JWH-203	C21H22ClNO	339.1390	H+	340.1463	10.27	
JWH-203	C21H22ClNO	339.1390	H+	340.1463	10.27	125.0148
JWH-203	C21H22ClNO	339.1390	H+	340.1463	10.27	340.1468
JWH-203	C21H22ClNO	339.1390	H+	340.1463	10.27	214.1233
JWH-203	C21H22ClNO	339.1390	H+	340.1463	10.27	188.1436
JWH-203	C21H22ClNO	339.1390	H+	340.1463	10.27	144.0445
Papaverine	C20H21NO4	339.1471	H+	340.1543	5.6	
Papaverine	C20H21NO4	339.1471	H+	340.1543	5.6	340.1544
Papaverine	C20H21NO4	339.1471	H+	340.1543	5.6	202.0855
Papaverine	C20H21NO4	339.1471	H+	340.1543	5.6	324.1226
Papaverine	C20H21NO4	339.1471	H+	340.1543	5.6	296.128
Papaverine	C20H21NO4	339.1471	H+	340.1543	5.6	171.0674
JWH-022	C24H21NO	339.1623	H+	340.1696	10.12	
JWH-022	C24H21NO	339.1623	H+	340.1696	10.12	155.0491

JWH-022	C24H21NO	339.1623	H+	340.1696	10.12	340.17
JWH-022	C24H21NO	339.1623	H+	340.1696	10.12	212.1073
JWH-022	C24H21NO	339.1623	H+	340.1696	10.12	127.0538
JWH-022	C24H21NO	339.1623	H+	340.1696	10.12	144.0442
A-834,735	C22H29NO2	339.2198	H+	340.2271	9.61	
A-834,735	C22H29NO2	339.2198	H+	340.2271	9.61	125.0955
A-834,735	C22H29NO2	339.2198	H+	340.2271	9.61	340.2269
A-834,735	C22H29NO2	339.2198	H+	340.2271	9.61	242.1177
A-834,735	C22H29NO2	339.2198	H+	340.2271	9.61	322.1271
A-834,735	C22H29NO2	339.2198	H+	340.2271	9.61	307.1936
Propoxyphene	C22H29NO2	339.2198	H+	340.2271	7.13	
Propoxyphene	C22H29NO2	339.2198	H+	340.2271	7.13	58.0677
Propoxyphene	C22H29NO2	339.2198	H+	340.2271	7.13	143.0856
Propoxyphene	C22H29NO2	339.2198	H+	340.2271	7.13	266.1905
Propoxyphene	C22H29NO2	339.2198	H+	340.2271	7.13	91.0552
Propoxyphene	C22H29NO2	339.2198	H+	340.2271	7.13	128.0622
UR-144 N-Heptyl Analogue	C23H33NO	339.2562	H+	340.2635	11.35	
UR-144 N-Heptyl Analogue	C23H33NO	339.2562	H+	340.2635	11.35	125.0957
UR-144 N-Heptyl Analogue	C23H33NO	339.2562	H+	340.2635	11.35	242.1451
UR-144 N-Heptyl Analogue	C23H33NO	339.2562	H+	340.2635	11.35	340.2638
UR-144 N-Heptyl Analogue	C23H33NO	339.2562	H+	340.2635	11.35	322.2534
UR-144 N-Heptyl Analogue	C23H33NO	339.2562	H+	340.2635	11.35	307.2304
AM-3102	C21H41NO2	339.3137	H+	340.3210	11.42	
AM-3102	C21H41NO2	339.3137	H+	340.3210	11.42	76.0754
AM-3102	C21H41NO2	339.3137	H+	340.3210	11.42	340.3223
AM-3102	C21H41NO2	339.3137	H+	340.3210	11.42	323.2963
AM-3102	C21H41NO2	339.3137	H+	340.3210	11.42	58.065
AM-3102	C21H41NO2	339.3137	H+	340.3210	11.42	135.1166
para-Fluoro Acetylfentanyl	C21H25FN2O	340.1951	H+	341.2024	5.89	
para-Fluoro Acetylfentanyl	C21H25FN2O	340.1951	H+	341.2024	5.89	188.1431
para-Fluoro Acetylfentanyl	C21H25FN2O	340.1951	H+	341.2024	5.89	105.0692
para-Fluoro Acetylfentanyl	C21H25FN2O	340.1951	H+	341.2024	5.89	341.2024
para-Fluoro Acetylfentanyl	C21H25FN2O	340.1951	H+	341.2024	5.89	220.1133
para-Fluoro Acetylfentanyl	C21H25FN2O	340.1951	H+	341.2024	5.89	150.0711
1-Hydroxymidazolam	C18H13ClFN3O	341.0731	H+	342.0804	6.61	
1-Hydroxymidazolam	C18H13ClFN3O	341.0731	H+	342.0804	6.61	324.07
1-Hydroxymidazolam	C18H13ClFN3O	341.0731	H+	342.0804	6.61	342.0806
1-Hydroxymidazolam	C18H13ClFN3O	341.0731	H+	342.0804	6.61	203.037
1-Hydroxymidazolam	C18H13ClFN3O	341.0731	H+	342.0804	6.61	168.0677
1-Hydroxymidazolam	C18H13ClFN3O	341.0731	H+	342.0804	6.61	297.058
Acetylcodeine	C20H23NO4	341.1627	H+	342.1700	5.14	
Acetylcodeine	C20H23NO4	341.1627	H+	342.1700	5.14	342.1694
Acetylcodeine	C20H23NO4	341.1627	H+	342.1700	5.14	225.0903
Acetylcodeine	C20H23NO4	341.1627	H+	342.1700	5.14	282.1488
Acetylcodeine	C20H23NO4	341.1627	H+	342.1700	5.14	197.0953
Acetylcodeine	C20H23NO4	341.1627	H+	342.1700	5.14	165.0693
Naltrexone	C20H23NO4	341.1627	H+	342.1700	3.8	
Naltrexone	C20H23NO4	341.1627	H+	342.1700	3.8	121.0648
Naltrexone	C20H23NO4	341.1627	H+	342.1700	3.8	200.1432
Naltrexone	C20H23NO4	341.1627	H+	342.1700	3.8	336.1957
Naltrexone	C20H23NO4	341.1627	H+	342.1700	3.8	303.1622
Naltrexone	C20H23NO4	341.1627	H+	342.1700	3.8	214.1226
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	341.1780	H+	342.1852	10.17	
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	341.1780	H+	342.1852	10.17	155.0487
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	341.1780	H+	342.1852	10.17	144.0441
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	341.1780	H+	342.1852	10.17	272.1079
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	341.1780	H+	342.1852	10.17	127.0538
JWH-018 N-(1,1-Dimethylpropyl) Isomer	C24H23NO	341.1780	H+	342.1852	10.17	342.1858
JWH-018	C24H23NO	341.1780	H+	342.1852	10.35	
JWH-018	C24H23NO	341.1780	H+	342.1852	10.35	155.0484
JWH-018	C24H23NO	341.1780	H+	342.1852	10.35	342.1849
JWH-018	C24H23NO	341.1780	H+	342.1852	10.35	214.1218
JWH-018	C24H23NO	341.1780	H+	342.1852	10.35	127.0536
JWH-018	C24H23NO	341.1780	H+	342.1852	10.35	144.0439
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	341.1780	H+	342.1852	10.18	
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	341.1780	H+	342.1852	10.18	169.065
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	341.1780	H+	342.1852	10.18	200.1073
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	341.1780	H+	342.1852	10.18	141.0699
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	341.1780	H+	342.1852	10.18	115.0451
JWH-073 2-Methylnaphthyl Analogue	C24H23NO	341.1780	H+	342.1852	10.18	342.1862
JWH-016	C24H23NO	341.1780	H+	342.1852	10.24	
JWH-016	C24H23NO	341.1780	H+	342.1852	10.24	155.0495
JWH-016	C24H23NO	341.1780	H+	342.1852	10.24	342.1868
JWH-016	C24H23NO	341.1780	H+	342.1852	10.24	214.1235

JWH-016	C24H23NO	341.1780	H+	342.1852	10.24	127.0542
JWH-016	C24H23NO	341.1780	H+	342.1852	10.24	158.0607
UR-144 N-Pentanoic Acid	C21H27NO3	341.1991	H+	342.2064	9.27	
UR-144 N-Pentanoic Acid	C21H27NO3	341.1991	H+	342.2064	9.27	125.095
UR-144 N-Pentanoic Acid	C21H27NO3	341.1991	H+	342.2064	9.27	342.2037
UR-144 N-Pentanoic Acid	C21H27NO3	341.1991	H+	342.2064	9.27	244.0957
UR-144 N-Pentanoic Acid	C21H27NO3	341.1991	H+	342.2064	9.27	144.0434
UR-144 N-Pentanoic Acid	C21H27NO3	341.1991	H+	342.2064	9.27	324.1948
Triazolam	C17H12Cl2N4	342.0439	H+	343.0512	7.47	
Triazolam	C17H12Cl2N4	342.0439	H+	343.0512	7.47	343.0511
Triazolam	C17H12Cl2N4	342.0439	H+	343.0512	7.47	308.0822
Triazolam	C17H12Cl2N4	342.0439	H+	343.0512	7.47	315.0327
Triazolam	C17H12Cl2N4	342.0439	H+	343.0512	7.47	239.038
Triazolam	C17H12Cl2N4	342.0439	H+	343.0512	7.47	279.0692
Etizolam	C17H15ClN4S	342.0706	H+	343.0779	7.7	
Etizolam	C17H15ClN4S	342.0706	H+	343.0779	7.7	314.0396
Etizolam	C17H15ClN4S	342.0706	H+	343.0779	7.7	343.0796
Etizolam	C17H15ClN4S	342.0706	H+	343.0779	7.7	309.0926
Etizolam	C17H15ClN4S	342.0706	H+	343.0779	7.7	308.1094
Etizolam	C17H15ClN4S	342.0706	H+	343.0779	7.7	310.1005
Flutoprazepam	C19H16ClFN2O	342.0935	H+	343.1008	9.04	
Flutoprazepam	C19H16ClFN2O	342.0935	H+	343.1008	9.04	289.0525
Flutoprazepam	C19H16ClFN2O	342.0935	H+	343.1008	9.04	343.0993
Flutoprazepam	C19H16ClFN2O	342.0935	H+	343.1008	9.04	140.0255
Flutoprazepam	C19H16ClFN2O	342.0935	H+	343.1008	9.04	226.0893
Flutoprazepam	C19H16ClFN2O	342.0935	H+	343.1008	9.04	261.0583
U-51754	C17H24Cl2N2O	342.1265	H+	343.1338	6.82	
U-51754	C17H24Cl2N2O	342.1265	H+	343.1338	6.82	298.0737
U-51754	C17H24Cl2N2O	342.1265	H+	343.1338	6.82	218.0113
U-51754	C17H24Cl2N2O	342.1265	H+	343.1338	6.82	112.1114
U-51754	C17H24Cl2N2O	342.1265	H+	343.1338	6.82	158.9747
U-51754	C17H24Cl2N2O	342.1265	H+	343.1338	6.82	343.1304
U-48800	C17H24Cl2N2O	342.1266	H+	343.1339	6.71	
U-48800	C17H24Cl2N2O	342.1266	H+	343.1339	6.71	298.0775
U-48800	C17H24Cl2N2O	342.1266	H+	343.1339	6.71	218.0144
U-48800	C17H24Cl2N2O	342.1266	H+	343.1339	6.71	112.1124
U-48800	C17H24Cl2N2O	342.1266	H+	343.1339	6.71	158.9761
U-48800	C17H24Cl2N2O	342.1266	H+	343.1339	6.71	81.0705
THJ-018	C23H22N2O	342.1732	H+	343.1805	10.72	
THJ-018	C23H22N2O	342.1732	H+	343.1805	10.72	215.1198
THJ-018	C23H22N2O	342.1732	H+	343.1805	10.72	145.0407
THJ-018	C23H22N2O	342.1732	H+	343.1805	10.72	343.1842
THJ-018	C23H22N2O	342.1732	H+	343.1805	10.72	117.0451
THJ-018	C23H22N2O	342.1732	H+	343.1805	10.72	155.0496
JWH-018 Benzimidazole Analogue	C23H22N2O	342.1732	H+	343.1805	10.55	
JWH-018 Benzimidazole Analogue	C23H22N2O	342.1732	H+	343.1805	10.55	215.1186
JWH-018 Benzimidazole Analogue	C23H22N2O	342.1732	H+	343.1805	10.55	155.0495
JWH-018 Benzimidazole Analogue	C23H22N2O	342.1732	H+	343.1805	10.55	273.1032
JWH-018 Benzimidazole Analogue	C23H22N2O	342.1732	H+	343.1805	10.55	145.04
JWH-018 Benzimidazole Analogue	C23H22N2O	342.1732	H+	343.1805	10.55	343.1819
Thiofentanyl	C20H26N2OS	342.1765	H+	343.1838	6.02	
Thiofentanyl	C20H26N2OS	342.1765	H+	343.1838	6.02	194.0984
Thiofentanyl	C20H26N2OS	342.1765	H+	343.1838	6.02	111.0258
Thiofentanyl	C20H26N2OS	342.1765	H+	343.1838	6.02	146.0954
Thiofentanyl	C20H26N2OS	342.1765	H+	343.1838	6.02	343.1819
Thiofentanyl	C20H26N2OS	342.1765	H+	343.1838	6.02	245.1633
MMB-022	C20H26N2O3	342.1943	H+	343.2016	9.25	
MMB-022	C20H26N2O3	342.1943	H+	343.2016	9.25	212.1074
MMB-022	C20H26N2O3	342.1943	H+	343.2016	9.25	158.0597
MMB-022	C20H26N2O3	342.1943	H+	343.2016	9.25	144.0438
MMB-022	C20H26N2O3	342.1943	H+	343.2016	9.25	103.065
MMB-022	C20H26N2O3	342.1943	H+	343.2016	9.25	116.0495
ADBICA	C20H29N3O2	343.2260	H+	344.2333	9.05	
ADBICA	C20H29N3O2	343.2260	H+	344.2333	9.05	214.1219
ADBICA	C20H29N3O2	343.2260	H+	344.2333	9.05	327.2061
ADBICA	C20H29N3O2	343.2260	H+	344.2333	9.05	144.044
ADBICA	C20H29N3O2	343.2260	H+	344.2333	9.05	299.2119
ADBICA	C20H29N3O2	343.2260	H+	344.2333	9.05	158.0602
M-144	C22H30FNO	343.2311	H+	344.2384	10.61	
M-144	C22H30FNO	343.2311	H+	344.2384	10.61	246.1286
M-144	C22H30FNO	343.2311	H+	344.2384	10.61	125.0954
M-144	C22H30FNO	343.2311	H+	344.2384	10.61	344.2386
M-144	C22H30FNO	343.2311	H+	344.2384	10.61	326.228
M-144	C22H30FNO	343.2311	H+	344.2384	10.61	158.0595

Carboxy-THC	C21H28O4	344.1988	H+	345.2060	10.05	
Carboxy-THC	C21H28O4	344.1988	H+	345.2060	10.05	327.1966
Carboxy-THC	C21H28O4	344.1988	H+	345.2060	10.05	299.2013
Carboxy-THC	C21H28O4	344.1988	H+	345.2060	10.05	345.207
Carboxy-THC	C21H28O4	344.1988	H+	345.2060	10.05	193.1226
Carboxy-THC	C21H28O4	344.1988	H+	345.2060	10.05	119.0857
MMB-018	C20H28N2O3	344.2100	H+	345.2173	9.58	
MMB-018	C20H28N2O3	344.2100	H+	345.2173	9.58	214.1231
MMB-018	C20H28N2O3	344.2100	H+	345.2173	9.58	144.044
MMB-018	C20H28N2O3	344.2100	H+	345.2173	9.58	116.0492
MMB-018	C20H28N2O3	344.2100	H+	345.2173	9.58	345.2181
MMB-018	C20H28N2O3	344.2100	H+	345.2173	9.58	158.0601
ADB-PINACA	C19H28N4O2	344.2212	H+	345.2285	9.26	
ADB-PINACA	C19H28N4O2	344.2212	H+	345.2285	9.26	215.1171
ADB-PINACA	C19H28N4O2	344.2212	H+	345.2285	9.26	300.2067
ADB-PINACA	C19H28N4O2	344.2212	H+	345.2285	9.26	145.0389
ADB-PINACA	C19H28N4O2	344.2212	H+	345.2285	9.26	328.202
ADB-PINACA	C19H28N4O2	344.2212	H+	345.2285	9.26	232.1441
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	345.1859	H+	346.1932	10.46	
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	345.1859	H+	346.1932	10.46	125.0966
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	345.1859	H+	346.1932	10.46	248.0849
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	345.1859	H+	346.1932	10.46	346.1949
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	345.1859	H+	346.1932	10.46	328.1846
UR-144 N-(5-Chloropentyl) Analogue	C21H28ClNO	345.1859	H+	346.1932	10.46	313.1613
AMB	C19H27N3O3	345.2052	H+	346.2125	10.02	
AMB	C19H27N3O3	345.2052	H+	346.2125	10.02	215.1183
AMB	C19H27N3O3	345.2052	H+	346.2125	10.02	145.0393
AMB	C19H27N3O3	345.2052	H+	346.2125	10.02	286.1919
AMB	C19H27N3O3	345.2052	H+	346.2125	10.02	346.2123
AMB	C19H27N3O3	345.2052	H+	346.2125	10.02	314.187
Nifedipine	C17H18N2O6	346.1165	H+	347.1238	7.64	
Nifedipine	C17H18N2O6	346.1165	H+	347.1238	7.64	254.1044
Nifedipine	C17H18N2O6	346.1165	H+	347.1238	7.64	195.0906
Nifedipine	C17H18N2O6	346.1165	H+	347.1238	7.64	239.0816
Nifedipine	C17H18N2O6	346.1165	H+	347.1238	7.64	211.0857
Nifedipine	C17H18N2O6	346.1165	H+	347.1238	7.64	194.0823
25N-NBOMe	C18H22N2O5	346.1529	H+	347.1601	6.45	
25N-NBOMe	C18H22N2O5	346.1529	H+	347.1601	6.45	121.0646
25N-NBOMe	C18H22N2O5	346.1529	H+	347.1601	6.45	347.1604
25N-NBOMe	C18H22N2O5	346.1529	H+	347.1601	6.45	91.0552
25N-NBOMe	C18H22N2O5	346.1529	H+	347.1601	6.45	93.0708
25N-NBOMe	C18H22N2O5	346.1529	H+	347.1601	6.45	301.1669
25T2-NBOMe	C19H25NO3S	347.1555	H+	348.1628	6.91	
25T2-NBOMe	C19H25NO3S	347.1555	H+	348.1628	6.91	121.0645
25T2-NBOMe	C19H25NO3S	347.1555	H+	348.1628	6.91	211.0784
25T2-NBOMe	C19H25NO3S	347.1555	H+	348.1628	6.91	91.055
25T2-NBOMe	C19H25NO3S	347.1555	H+	348.1628	6.91	348.1627
25T2-NBOMe	C19H25NO3S	347.1555	H+	348.1628	6.91	331.1367
5F-ABICA	C19H26FN3O2	347.2009	H+	348.2082	7.89	
5F-ABICA	C19H26FN3O2	347.2009	H+	348.2082	7.89	232.1138
5F-ABICA	C19H26FN3O2	347.2009	H+	348.2082	7.89	144.0442
5F-ABICA	C19H26FN3O2	347.2009	H+	348.2082	7.89	331.1822
5F-ABICA	C19H26FN3O2	347.2009	H+	348.2082	7.89	116.049
5F-ABICA	C19H26FN3O2	347.2009	H+	348.2082	7.89	348.2085
Phenazepam	C15H10BrClN2O	347.9665	H+	348.9738	7.86	
Phenazepam	C15H10BrClN2O	347.9665	H+	348.9738	7.86	348.9733
Phenazepam	C15H10BrClN2O	347.9665	H+	348.9738	7.86	183.9757
Phenazepam	C15H10BrClN2O	347.9665	H+	348.9738	7.86	206.0841
Phenazepam	C15H10BrClN2O	347.9665	H+	348.9738	7.86	242.0609
Phenazepam	C15H10BrClN2O	347.9665	H+	348.9738	7.86	320.9792
5-fluoro AB-PINACA	C18H25FN4O2	348.1962	H+	349.2034	8.03	
5-fluoro AB-PINACA	C18H25FN4O2	348.1962	H+	349.2034	8.03	233.1091
5-fluoro AB-PINACA	C18H25FN4O2	348.1962	H+	349.2034	8.03	304.1832
5-fluoro AB-PINACA	C18H25FN4O2	348.1962	H+	349.2034	8.03	213.1025
5-fluoro AB-PINACA	C18H25FN4O2	348.1962	H+	349.2034	8.03	177.0462
5-fluoro AB-PINACA	C18H25FN4O2	348.1962	H+	349.2034	8.03	332.178
CUMYL-PICA	C23H28N2O	348.2202	H+	349.2274	9.99	
CUMYL-PICA	C23H28N2O	348.2202	H+	349.2274	9.99	119.0848
CUMYL-PICA	C23H28N2O	348.2202	H+	349.2274	9.99	188.143
CUMYL-PICA	C23H28N2O	348.2202	H+	349.2274	9.99	231.1501
CUMYL-PICA	C23H28N2O	348.2202	H+	349.2274	9.99	214.1226
CUMYL-PICA	C23H28N2O	348.2202	H+	349.2274	9.99	132.0803
Methacrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.34	
Methacrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.34	188.1433

Methacrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.34	105.0692
Methacrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.34	349.2279
Methacrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.34	134.096
Methacrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.34	228.1389
para-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.69	
para-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.69	188.1437
para-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.69	105.0698
para-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.69	349.2282
para-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.69	228.1386
para-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.69	146.0965
ortho-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.51	
ortho-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.51	188.1436
ortho-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.51	349.2282
ortho-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.51	105.0699
ortho-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.51	228.1387
ortho-Methyl Acrylfentanyl	C23H28N2O	348.2202	H+	349.2274	6.51	146.0965
Cyclopropyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.48	
Cyclopropyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.48	188.144
Cyclopropyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.48	349.2273
Cyclopropyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.48	228.1377
Cyclopropyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.48	281.2014
Cyclopropyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.48	105.071
Crotonyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.52	
Crotonyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.52	188.1438
Crotonyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.52	105.0695
Crotonyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.52	228.1381
Crotonyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.52	349.2275
Crotonyl Fentanyl	C23H28N2O	348.2202	H+	349.2274	6.52	134.0961
MT-45	C24H32N2	348.2566	H+	349.2638	7.40	
MT-45	C24H32N2	348.2566	H+	349.2638	7.40	181.1008
MT-45	C24H32N2	348.2566	H+	349.2638	7.40	169.1692
MT-45	C24H32N2	348.2566	H+	349.2638	7.40	166.0771
MT-45	C24H32N2	348.2566	H+	349.2638	7.40	349.2643
MT-45	C24H32N2	348.2566	H+	349.2638	7.40	179.0852
Voriconazole	C16H14F3N5O	349.1150	H+	350.1223	7.36	
Voriconazole	C16H14F3N5O	349.1150	H+	350.1223	7.36	281.0892
Voriconazole	C16H14F3N5O	349.1150	H+	350.1223	7.36	224.0622
Voriconazole	C16H14F3N5O	349.1150	H+	350.1223	7.36	127.0626
Voriconazole	C16H14F3N5O	349.1150	H+	350.1223	7.36	155.0299
Voriconazole	C16H14F3N5O	349.1150	H+	350.1223	7.36	263.0791
MDA 19	C21H23N3O2	349.1790	H+	350.1863	10.56	
MDA 19	C21H23N3O2	349.1790	H+	350.1863	10.56	105.0321
MDA 19	C21H23N3O2	349.1790	H+	350.1863	10.56	77.0377
MDA 19	C21H23N3O2	349.1790	H+	350.1863	10.56	321.1732
MDA 19	C21H23N3O2	349.1790	H+	350.1863	10.56	51.0224
MDA 19	C21H23N3O2	349.1790	H+	350.1863	10.56	145.0374
AB-BICA	C21H23N3O2	349.1790	H+	350.1863	8.09	
AB-BICA	C21H23N3O2	349.1790	H+	350.1863	8.09	234.0921
AB-BICA	C21H23N3O2	349.1790	H+	350.1863	8.09	91.0543
AB-BICA	C21H23N3O2	349.1790	H+	350.1863	8.09	333.1606
AB-BICA	C21H23N3O2	349.1790	H+	350.1863	8.09	305.1838
AB-BICA	C21H23N3O2	349.1790	H+	350.1863	8.09	350.1865
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	233.1074
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	304.1808
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	213.1014
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	350.1859
5F-AMB 3-Methylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	145.0388
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	219.0919
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	304.1811
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	145.0385
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	350.186
4F-MDMB-BINACA 3,3-Dimethylbutanoic Acid	C18H24FN3O3	349.1802	H+	350.1875	8.58	177.0452
FUB-144	C23H24FNO	349.1842	H+	350.1915	10.29	
FUB-144	C23H24FNO	349.1842	H+	350.1915	10.29	125.0964
FUB-144	C23H24FNO	349.1842	H+	350.1915	10.29	109.0449
FUB-144	C23H24FNO	349.1842	H+	350.1915	10.29	350.1934

FUB-144	C23H24FNO	349.1842	H+	350.1915	10.29	252.0836
FUB-144	C23H24FNO	349.1842	H+	350.1915	10.29	332.1826
AL-LAD	C22H27N3O	349.2154	H+	350.2227	6.00	
AL-LAD	C22H27N3O	349.2154	H+	350.2227	6.00	309.1837
AL-LAD	C22H27N3O	349.2154	H+	350.2227	6.00	208.0976
AL-LAD	C22H27N3O	349.2154	H+	350.2227	6.00	281.1648
AL-LAD	C22H27N3O	349.2154	H+	350.2227	6.00	350.2237
AL-LAD	C22H27N3O	349.2154	H+	350.2227	6.00	182.0835
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	349.2406	H+	350.2478	11.18	
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	349.2406	H+	350.2478	11.18	135.1166
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	349.2406	H+	350.2478	11.18	350.2486
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	349.2406	H+	350.2478	11.18	107.0856
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	349.2406	H+	350.2478	11.18	93.0702
AB-001 (JWH-018 Adamantyl Analogue)	C24H31NO	349.2406	H+	350.2478	11.18	79.0545
a-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.36	
a-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.36	202.1582
a-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.36	351.2408
a-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.36	119.085
a-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.36	91.049
a-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.36	216.137
para-Methyl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.80	
para-Methyl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.80	188.1423
para-Methyl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.80	105.0697
para-Methyl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.80	351.2409
para-Methyl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.80	230.1522
para-Methyl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.80	146.0952
b-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.58	
b-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.58	202.1571
b-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.58	351.2394
b-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.58	119.0844
b-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.58	91.054
b-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.58	216.1391
Isobutyryl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.66	
Isobutyryl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.66	188.1423
Isobutyryl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.66	351.2405
Isobutyryl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.66	105.0695
Isobutyryl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.66	230.1522
Isobutyryl Fentanyl	C23H30N2O	350.2358	H+	351.2431	6.66	281.9997
3-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2430	6.49	
3-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2430	6.49	202.1586
3-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2430	6.49	351.2432
3-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2430	6.49	105.07
3-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2430	6.49	134.09629
3-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2430	6.49	230.1538
Butryl Fentanyl	C23H30N2O	350.2358	H+	351.2430	6.67	
Butryl Fentanyl	C23H30N2O	350.2358	H+	351.2430	6.67	188.1431
Butryl Fentanyl	C23H30N2O	350.2358	H+	351.2430	6.67	351.2436
Butryl Fentanyl	C23H30N2O	350.2358	H+	351.2430	6.67	105.0702
Butryl Fentanyl	C23H30N2O	350.2358	H+	351.2430	6.67	230.1539
Butryl Fentanyl	C23H30N2O	350.2358	H+	351.2430	6.67	281.2019
4-Phenyl-U-51754	C23H30N2O	350.2358	H+	351.2431	7.28	
4-Phenyl-U-51754	C23H30N2O	350.2358	H+	351.2431	7.28	306.1849
4-Phenyl-U-51754	C23H30N2O	350.2358	H+	351.2431	7.28	226.122
4-Phenyl-U-51754	C23H30N2O	350.2358	H+	351.2431	7.28	112.1114
4-Phenyl-U-51754	C23H30N2O	350.2358	H+	351.2431	7.28	167.0849
4-Phenyl-U-51754	C23H30N2O	350.2358	H+	351.2431	7.28	351.2425
4'-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.75	
4'-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.75	202.1587
4'-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.75	119.085
4'-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.75	351.2424
4'-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.75	216.1382
4'-Methyl fentanyl	C23H30N2O	350.2358	H+	351.2431	6.75	160.1121
XLR-12	C20H24F3NO	351.1810	H+	352.1883	10.21	
XLR-12	C20H24F3NO	351.1810	H+	352.1883	10.21	254.0793
XLR-12	C20H24F3NO	351.1810	H+	352.1883	10.21	125.096
XLR-12	C20H24F3NO	351.1810	H+	352.1883	10.21	352.1889
XLR-12	C20H24F3NO	351.1810	H+	352.1883	10.21	319.1552
XLR-12	C20H24F3NO	351.1810	H+	352.1883	10.21	334.1785
Urea Fentanyl	C22H29N3O	351.2311	H+	352.2383	6.39	
Urea Fentanyl	C22H29N3O	351.2311	H+	352.2383	6.39	188.1437
Urea Fentanyl	C22H29N3O	351.2311	H+	352.2383	6.39	105.07
Urea Fentanyl	C22H29N3O	351.2311	H+	352.2383	6.39	352.2387
Urea Fentanyl	C22H29N3O	351.2311	H+	352.2383	6.39	134.0968
Urea Fentanyl	C22H29N3O	351.2311	H+	352.2383	6.39	231.1495

AM-2232	C24H20N2O	352.1576	H+	353.1648	8.92	
AM-2232	C24H20N2O	352.1576	H+	353.1648	8.92	155.0489
AM-2232	C24H20N2O	352.1576	H+	353.1648	8.92	225.1028
AM-2232	C24H20N2O	352.1576	H+	353.1648	8.92	127.0539
AM-2232	C24H20N2O	352.1576	H+	353.1648	8.92	353.1664
AM-2232	C24H20N2O	352.1576	H+	353.1648	8.92	144.0445
para-Fluoroacryl Fentanyl	C22H25FN2O	352.1950	H+	353.2023	6.28	
para-Fluoroacryl Fentanyl	C22H25FN2O	352.1950	H+	353.2023	6.28	188.1424
para-Fluoroacryl Fentanyl	C22H25FN2O	352.1950	H+	353.2023	6.28	105.07
para-Fluoroacryl Fentanyl	C22H25FN2O	352.1950	H+	353.2023	6.28	353.201
para-Fluoroacryl Fentanyl	C22H25FN2O	352.1950	H+	353.2023	6.28	232.1124
para-Fluoroacryl Fentanyl	C22H25FN2O	352.1950	H+	353.2023	6.28	150.0705
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	352.1951	H+	353.2024	6.33	
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	352.1951	H+	353.2024	6.33	174.128
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	352.1951	H+	353.2024	6.33	91.0543
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	352.1951	H+	353.2024	6.33	353.2024
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	352.1951	H+	353.2024	6.33	285.1766
para-Fluorocyclopropylbenzylfentanyl	C22H25FN2O	352.1951	H+	353.2024	6.33	246.1293
Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.66	
Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.66	188.1425
Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.66	105.0701
Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.66	353.2198
Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.66	232.1323
Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.66	146.0956
beta-Hydroxy Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.91	
beta-Hydroxy Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.91	204.1386
beta-Hydroxy Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.91	186.1277
beta-Hydroxy Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.91	279.1852
beta-Hydroxy Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.91	134.0966
beta-Hydroxy Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.91	335.2119
para-Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.98	
para-Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.98	188.1447
para-Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.98	105.0704
para-Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.98	232.1344
para-Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.98	162.092
para-Methoxyacetyl Fentanyl	C22H28N2O2	352.2151	H+	353.2224	5.98	353.2241
AB-005	C23H32N2O	352.2515	H+	353.2587	7.76	
AB-005	C23H32N2O	352.2515	H+	353.2587	7.76	125.0963
AB-005	C23H32N2O	352.2515	H+	353.2587	7.76	112.1122
AB-005	C23H32N2O	352.2515	H+	353.2587	7.76	98.0966
AB-005	C23H32N2O	352.2515	H+	353.2587	7.76	256.1705
AB-005	C23H32N2O	352.2515	H+	353.2587	7.76	353.2605
Pyrazolam	C16H12BrN5	353.0276	H+	354.0348	6.18	
Pyrazolam	C16H12BrN5	353.0276	H+	354.0348	6.18	354.0328
Pyrazolam	C16H12BrN5	353.0276	H+	354.0348	6.18	326.0212
Pyrazolam	C16H12BrN5	353.0276	H+	354.0348	6.18	285.0002
Pyrazolam	C16H12BrN5	353.0276	H+	354.0348	6.18	206.082
Pyrazolam	C16H12BrN5	353.0276	H+	354.0348	6.18	167.0719
Clonazelam	C17H12ClN5O2	353.0680	H+	354.0752	6.94	
Clonazelam	C17H12ClN5O2	353.0680	H+	354.0752	6.94	354.0761
Clonazelam	C17H12ClN5O2	353.0680	H+	354.0752	6.94	308.0827
Clonazelam	C17H12ClN5O2	353.0680	H+	354.0752	6.94	326.0575
Clonazelam	C17H12ClN5O2	353.0680	H+	354.0752	6.94	280.0647
Clonazelam	C17H12ClN5O2	353.0680	H+	354.0752	6.94	273.1142
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	353.1780	H+	354.1852	10.41	
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	353.1780	H+	354.1852	10.41	169.0647
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	353.1780	H+	354.1852	10.41	212.1075
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	353.1780	H+	354.1852	10.41	141.0699
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	353.1780	H+	354.1852	10.41	354.1859
JWH-122 N-(4-Pentenyl) Analogue	C25H23NO	353.1780	H+	354.1852	10.41	115.054
Yohimbine	C21H26N2O3	354.1943	H+	355.2016	5.32	
Yohimbine	C21H26N2O3	354.1943	H+	355.2016	5.32	355.2013
Yohimbine	C21H26N2O3	354.1943	H+	355.2016	5.32	144.0807
Yohimbine	C21H26N2O3	354.1943	H+	355.2016	5.32	212.1277
Yohimbine	C21H26N2O3	354.1943	H+	355.2016	5.32	338.175
Yohimbine	C21H26N2O3	354.1943	H+	355.2016	5.32	326.1749
para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.35	
para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.35	355.2168
para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.35	188.1432
para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.35	105.0701
para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.35	234.128
para-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.35	150.0706
2'-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.34	
2'-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.34	206.1338

2'-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.34	123.0598
2'-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.34	355.2179
2'-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.34	216.1383
2'-Fluorofentanyl	C22H27FN2O	354.2107	H+	355.2180	6.34	152.0866
A-796,260	C22H30N2O2	354.2307	H+	355.2380	7.82	
A-796,260	C22H30N2O2	354.2307	H+	355.2380	7.82	125.0959
A-796,260	C22H30N2O2	354.2307	H+	355.2380	7.82	114.0915
A-796,260	C22H30N2O2	354.2307	H+	355.2380	7.82	355.2385
A-796,260	C22H30N2O2	354.2307	H+	355.2380	7.82	268.1706
A-796,260	C22H30N2O2	354.2307	H+	355.2380	7.82	257.1297
JWH-200 Analogue	C22H30N2O2	354.2307	H+	355.2380	7.82	
JWH-200 Analogue	C22H30N2O2	354.2307	H+	355.2380	7.82	125.0961
JWH-200 Analogue	C22H30N2O2	354.2307	H+	355.2380	7.82	114.0913
JWH-200 Analogue	C22H30N2O2	354.2307	H+	355.2380	7.82	355.2381
JWH-200 Analogue	C22H30N2O2	354.2307	H+	355.2380	7.82	97.1014
JWH-200 Analogue	C22H30N2O2	354.2307	H+	355.2380	7.82	231.1495
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	355.1572	H+	356.1645	9.12	
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	355.1572	H+	356.1645	9.12	155.049
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	355.1572	H+	356.1645	9.12	127.0539
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	355.1572	H+	356.1645	9.12	356.1656
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	355.1572	H+	356.1645	9.12	284.108
JWH-018 N-(4,5-Epoxypentyl) Analogue	C24H21NO2	355.1572	H+	356.1645	9.12	228.1027
JWH-180	C25H25NO	355.1936	H+	356.2009	10.63	
JWH-180	C25H25NO	355.1936	H+	356.2009	10.63	197.0964
JWH-180	C25H25NO	355.1936	H+	356.2009	10.63	186.0915
JWH-180	C25H25NO	355.1936	H+	356.2009	10.63	356.2018
JWH-180	C25H25NO	355.1936	H+	356.2009	10.63	141.0698
JWH-180	C25H25NO	355.1936	H+	356.2009	10.63	144.0441
JWH-007	C25H25NO	355.1936	H+	356.2009	10.47	
JWH-007	C25H25NO	355.1936	H+	356.2009	10.47	155.049
JWH-007	C25H25NO	355.1936	H+	356.2009	10.47	356.2016
JWH-007	C25H25NO	355.1936	H+	356.2009	10.47	228.1386
JWH-007	C25H25NO	355.1936	H+	356.2009	10.47	127.0543
JWH-007	C25H25NO	355.1936	H+	356.2009	10.47	158.0603
JWH-019	C25H25NO	355.1936	H+	356.2009	10.66	
JWH-019	C25H25NO	355.1936	H+	356.2009	10.66	155.0487
JWH-019	C25H25NO	355.1936	H+	356.2009	10.66	356.2017
JWH-019	C25H25NO	355.1936	H+	356.2009	10.66	228.1384
JWH-019	C25H25NO	355.1936	H+	356.2009	10.66	127.054
JWH-019	C25H25NO	355.1936	H+	356.2009	10.66	144.0445
JWH-122	C25H25NO	355.1936	H+	356.2009	10.62	
JWH-122	C25H25NO	355.1936	H+	356.2009	10.62	169.0644
JWH-122	C25H25NO	355.1936	H+	356.2009	10.62	214.122
JWH-122	C25H25NO	355.1936	H+	356.2009	10.62	356.2012
JWH-122	C25H25NO	355.1936	H+	356.2009	10.62	141.0696
JWH-122	C25H25NO	355.1936	H+	356.2009	10.62	144.0444
PTI-1	C21H29N3S	355.2082	H+	356.2155	8.57	
PTI-1	C21H29N3S	355.2082	H+	356.2155	8.57	283.1273
PTI-1	C21H29N3S	355.2082	H+	356.2155	8.57	356.216
PTI-1	C21H29N3S	355.2082	H+	356.2155	8.57	227.0646
PTI-1	C21H29N3S	355.2082	H+	356.2155	8.57	213.0485
PTI-1	C21H29N3S	355.2082	H+	356.2155	8.57	156.0689
AB-CHMICA	C21H29N3O2	355.2260	H+	356.2333	9.18	
AB-CHMICA	C21H29N3O2	355.2260	H+	356.2333	9.18	240.1384
AB-CHMICA	C21H29N3O2	355.2260	H+	356.2333	9.18	144.0437
AB-CHMICA	C21H29N3O2	355.2260	H+	356.2333	9.18	339.2066
AB-CHMICA	C21H29N3O2	355.2260	H+	356.2333	9.18	116.0487
AB-CHMICA	C21H29N3O2	355.2260	H+	356.2333	9.18	356.2329
U-49900	C18H26N2OCl2	356.1422	H+	357.1495	6.50	
U-49900	C18H26N2OCl2	356.1422	H+	357.1495	6.50	357.1491
U-49900	C18H26N2OCl2	356.1422	H+	357.1495	6.50	284.061
U-49900	C18H26N2OCl2	356.1422	H+	357.1495	6.50	203.9977
U-49900	C18H26N2OCl2	356.1422	H+	357.1495	6.50	172.9557
U-49900	C18H26N2OCl2	356.1422	H+	357.1495	6.50	144.9605
Isopropyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.09	
Isopropyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.09	312.0926
Isopropyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.09	270.0456
Isopropyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.09	232.0297
Isopropyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.09	189.9824
Isopropyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.09	172.9557
Propyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.25	
Propyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.25	312.0912
Propyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.25	232.0282
Propyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.25	172.9551

Propyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.25	357.1492
Propyl-U-47700	C18H26Cl2N2O	356.1422	H+	357.1495	7.25	189.9823
NNEI	C24H24N2O	356.1889	H+	357.1961	9.92	
NNEI	C24H24N2O	356.1889	H+	357.1961	9.92	214.1231
NNEI	C24H24N2O	356.1889	H+	357.1961	9.92	144.0443
NNEI	C24H24N2O	356.1889	H+	357.1961	9.92	357.197
NNEI	C24H24N2O	356.1889	H+	357.1961	9.92	188.1439
NNEI	C24H24N2O	356.1889	H+	357.1961	9.92	116.0494
AB-CHMINACA	C20H28N4O2	356.2212	H+	357.2285	9.39	
AB-CHMINACA	C20H28N4O2	356.2212	H+	357.2285	9.39	241.1347
AB-CHMINACA	C20H28N4O2	356.2212	H+	357.2285	9.39	312.208
AB-CHMINACA	C20H28N4O2	356.2212	H+	357.2285	9.39	145.0399
AB-CHMINACA	C20H28N4O2	356.2212	H+	357.2285	9.39	340.2027
AB-CHMINACA	C20H28N4O2	356.2212	H+	357.2285	9.39	357.2294
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	356.2212	H+	357.2285	8.58	
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	356.2212	H+	357.2285	8.58	216.1131
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	356.2212	H+	357.2285	8.58	145.0392
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	356.2212	H+	357.2285	8.58	357.229
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	356.2212	H+	357.2285	8.58	312.2076
AB-CHMINACA 2'-Indazole Isomer	C20H28N4O2	356.2212	H+	357.2285	8.58	241.1342
U-69593	C22H32N2O2	356.2464	H+	357.2537	5.62	
U-69593	C22H32N2O2	356.2464	H+	357.2537	5.62	286.181
U-69593	C22H32N2O2	356.2464	H+	357.2537	5.62	168.1385
U-69593	C22H32N2O2	356.2464	H+	357.2537	5.62	137.0961
U-69593	C22H32N2O2	356.2464	H+	357.2537	5.62	91.0544
U-69593	C22H32N2O2	356.2464	H+	357.2537	5.62	357.2541
Indomethacin	C19H16ClNO4	357.0768	H+	358.0841	8.89	
Indomethacin	C19H16ClNO4	357.0768	H+	358.0841	8.89	138.9948
Indomethacin	C19H16ClNO4	357.0768	H+	358.0841	8.89	110.9999
Indomethacin	C19H16ClNO4	357.0768	H+	358.0841	8.89	174.0916
Indomethacin	C19H16ClNO4	357.0768	H+	358.0841	8.89	358.0849
Indomethacin	C19H16ClNO4	357.0768	H+	358.0841	8.89	340.2339
JWH-080	C24H23NO2	357.1729	H+	358.1802	10.28	
JWH-080	C24H23NO2	357.1729	H+	358.1802	10.28	185.0602
JWH-080	C24H23NO2	357.1729	H+	358.1802	10.28	200.1073
JWH-080	C24H23NO2	357.1729	H+	358.1802	10.28	358.1818
JWH-080	C24H23NO2	357.1729	H+	358.1802	10.28	157.065
JWH-080	C24H23NO2	357.1729	H+	358.1802	10.28	144.0447
JWH-073 6-Methoxyindole Analogue	C24H23NO2	357.1729	H+	358.1802	10.07	
JWH-073 6-Methoxyindole Analogue	C24H23NO2	357.1729	H+	358.1802	10.07	155.0482
JWH-073 6-Methoxyindole Analogue	C24H23NO2	357.1729	H+	358.1802	10.07	127.0529
JWH-073 6-Methoxyindole Analogue	C24H23NO2	357.1729	H+	358.1802	10.07	358.1796
JWH-073 6-Methoxyindole Analogue	C24H23NO2	357.1729	H+	358.1802	10.07	230.1172
JWH-073 6-Methoxyindole Analogue	C24H23NO2	357.1729	H+	358.1802	10.07	174.0545
CBL-018	C24H23NO2	357.1729	H+	358.1802	10.92	
CBL-018	C24H23NO2	357.1729	H+	358.1802	10.92	214.1228
CBL-018	C24H23NO2	357.1729	H+	358.1802	10.92	144.0432
CBL-018	C24H23NO2	357.1729	H+	358.1802	10.92	116.0486
CBL-018	C24H23NO2	357.1729	H+	358.1802	10.92	158.0586
CBL-018	C24H23NO2	357.1729	H+	358.1802	10.92	43.0536
MN-18	C23H23N3O	357.1841	H+	358.1914	10.72	
MN-18	C23H23N3O	357.1841	H+	358.1914	10.72	215.1185
MN-18	C23H23N3O	357.1841	H+	358.1914	10.72	145.0398
MN-18	C23H23N3O	357.1841	H+	358.1914	10.72	358.1941
MN-18	C23H23N3O	357.1841	H+	358.1914	10.72	170.0673
MN-18	C23H23N3O	357.1841	H+	358.1914	10.72	117.0451
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	357.1841	H+	358.1914	10.83	
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	357.1841	H+	358.1914	10.83	214.1231
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	357.1841	H+	358.1914	10.83	144.044
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	357.1841	H+	358.1914	10.83	358.192
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	357.1841	H+	358.1914	10.83	116.0496
JWH-018 8-Quinolinyl Carboxamide	C23H23N3O	357.1841	H+	358.1914	10.83	171.0556
Nalbuphine	C21H27NO4	357.1940	H+	358.2013	4.28	
Nalbuphine	C21H27NO4	357.1940	H+	358.2013	4.28	340.1912
Nalbuphine	C21H27NO4	357.1940	H+	358.2013	4.28	358.2017
Nalbuphine	C21H27NO4	357.1940	H+	358.2013	4.28	296.1648
Nalbuphine	C21H27NO4	357.1940	H+	358.2013	4.28	272.1286
Nalbuphine	C21H27NO4	357.1940	H+	358.2013	4.28	254.1172
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	357.2052	H+	358.2125	9.84	
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	357.2052	H+	358.2125	9.84	241.1324
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	357.2052	H+	358.2125	9.84	145.0382
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	357.2052	H+	358.2125	9.84	312.2056
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	357.2052	H+	358.2125	9.84	358.2108
AB-CHMINACA 3-Methylbutanoic Acid	C20H27N3O3	357.2052	H+	358.2125	9.84	340.2018

MDMB-4en-PINACA	C20H27N3O3	357.2052	H+	358.2125	10.04	
MDMB-4en-PINACA	C20H27N3O3	357.2052	H+	358.2125	10.04	213.1015
MDMB-4en-PINACA	C20H27N3O3	357.2052	H+	358.2125	10.04	298.1904
MDMB-4en-PINACA	C20H27N3O3	357.2052	H+	358.2125	10.04	145.0389
MDMB-4en-PINACA	C20H27N3O3	357.2052	H+	358.2125	10.04	358.2109
MDMB-4en-PINACA	C20H27N3O3	357.2052	H+	358.2125	10.04	230.1287
Hydroxytriazolam	C17H12Cl2N4O	358.0388	H+	359.0461	7.02	
Hydroxytriazolam	C17H12Cl2N4O	358.0388	H+	359.0461	7.02	359.0465
Hydroxytriazolam	C17H12Cl2N4O	358.0388	H+	359.0461	7.02	331.0278
Hydroxytriazolam	C17H12Cl2N4O	358.0388	H+	359.0461	7.02	176.0274
Hydroxytriazolam	C17H12Cl2N4O	358.0388	H+	359.0461	7.02	341.0371
Hydroxytriazolam	C17H12Cl2N4O	358.0388	H+	359.0461	7.02	313.0305
SDB-005	C23H22N2O2	358.1681	H+	359.1754	10.74	
SDB-005	C23H22N2O2	358.1681	H+	359.1754	10.74	215.1182
SDB-005	C23H22N2O2	358.1681	H+	359.1754	10.74	145.0394
SDB-005	C23H22N2O2	358.1681	H+	359.1754	10.74	117.0447
SDB-005	C23H22N2O2	358.1681	H+	359.1754	10.74	43.0542
SDB-005	C23H22N2O2	358.1681	H+	359.1754	10.74	359.1767
PB-22	C23H22N2O2	358.1681	H+	359.1754	10.12	
PB-22	C23H22N2O2	358.1681	H+	359.1754	10.12	214.1223
PB-22	C23H22N2O2	358.1681	H+	359.1754	10.12	144.0433
PB-22	C23H22N2O2	358.1681	H+	359.1754	10.12	359.175
PB-22	C23H22N2O2	358.1681	H+	359.1754	10.12	158.0598
PB-22	C23H22N2O2	358.1681	H+	359.1754	10.12	116.0485
b-Hydroxythiofentanyl	C20H26N2O2S	358.1715	H+	359.1788	5.66	
b-Hydroxythiofentanyl	C20H26N2O2S	358.1715	H+	359.1788	5.66	192.0826
b-Hydroxythiofentanyl	C20H26N2O2S	358.1715	H+	359.1788	5.66	146.0953
b-Hydroxythiofentanyl	C20H26N2O2S	358.1715	H+	359.1788	5.66	341.1661
b-Hydroxythiofentanyl	C20H26N2O2S	358.1715	H+	359.1788	5.66	285.1399
b-Hydroxythiofentanyl	C20H26N2O2S	358.1715	H+	359.1788	5.66	359.1767
THJ	C22H22N4O	358.1794	H+	359.1866	11.09	
THJ	C22H22N4O	358.1794	H+	359.1866	11.09	215.1184
THJ	C22H22N4O	358.1794	H+	359.1866	11.09	145.0395
THJ	C22H22N4O	358.1794	H+	359.1866	11.09	341.1764
THJ	C22H22N4O	358.1794	H+	359.1866	11.09	359.1875
THJ	C22H22N4O	358.1794	H+	359.1866	11.09	117.0445
THCA	C22H30O4	358.2144	H+	359.2217	11.13	
THCA	C22H30O4	358.2144	H+	359.2217	11.13	359.2225
THCA	C22H30O4	358.2144	H+	359.2217	11.13	316.1672
THCA	C22H30O4	358.2144	H+	359.2217	11.13	259.0966
THCA	C22H30O4	358.2144	H+	359.2217	11.13	317.1756
THCA	C22H30O4	358.2144	H+	359.2217	11.13	285.1489
NPB-22	C22H21N3O2	359.1634	H+	360.1707	9.83	
NPB-22	C22H21N3O2	359.1634	H+	360.1707	9.83	215.1189
NPB-22	C22H21N3O2	359.1634	H+	360.1707	9.83	145.0396
NPB-22	C22H21N3O2	359.1634	H+	360.1707	9.83	360.1714
NPB-22	C22H21N3O2	359.1634	H+	360.1707	9.83	117.0449
NPB-22	C22H21N3O2	359.1634	H+	360.1707	9.83	43.0544
JWH-412	C24H22FNO	359.1685	H+	360.1758	10.64	
JWH-412	C24H22FNO	359.1685	H+	360.1758	10.64	173.0404
JWH-412	C24H22FNO	359.1685	H+	360.1758	10.64	360.1789
JWH-412	C24H22FNO	359.1685	H+	360.1758	10.64	214.1242
JWH-412	C24H22FNO	359.1685	H+	360.1758	10.64	145.0453
JWH-412	C24H22FNO	359.1685	H+	360.1758	10.64	125.0387
AM-2201	C24H22FNO	359.1685	H+	360.1758	9.62	
AM-2201	C24H22FNO	359.1685	H+	360.1758	9.62	155.0494
AM-2201	C24H22FNO	359.1685	H+	360.1758	9.62	360.1767
AM-2201	C24H22FNO	359.1685	H+	360.1758	9.62	232.114
AM-2201	C24H22FNO	359.1685	H+	360.1758	9.62	127.0544
AM-2201	C24H22FNO	359.1685	H+	360.1758	9.62	163.0751
THJ-2201	C23H21FN2O	360.1638	H+	361.1711	10.05	
THJ-2201	C23H21FN2O	360.1638	H+	361.1711	10.05	233.108
THJ-2201	C23H21FN2O	360.1638	H+	361.1711	10.05	213.1015
THJ-2201	C23H21FN2O	360.1638	H+	361.1711	10.05	177.0455
THJ-2201	C23H21FN2O	360.1638	H+	361.1711	10.05	145.0388
THJ-2201	C23H21FN2O	360.1638	H+	361.1711	10.05	361.1698
AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	360.1638	H+	361.1711	9.80	
AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	360.1638	H+	361.1711	9.80	233.1097
AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	360.1638	H+	361.1711	9.80	177.0465
AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	360.1638	H+	361.1711	9.80	155.0497

AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	360.1638	H+	361.1711	9.80	273.1039
AM-2201 Benzimidazole Analogue (FUBIMINA)	C23H21FN2O	360.1638	H+	361.1711	9.80	361.1734
AB-PINACA N-Pentanoic Acid	C18H24N4O4	360.1798	H+	361.1870	6.79	
AB-PINACA N-Pentanoic Acid	C18H24N4O4	360.1798	H+	361.1870	6.79	245.0916
AB-PINACA N-Pentanoic Acid	C18H24N4O4	360.1798	H+	361.1870	6.79	217.0964
AB-PINACA N-Pentanoic Acid	C18H24N4O4	360.1798	H+	361.1870	6.79	298.1541
AB-PINACA N-Pentanoic Acid	C18H24N4O4	360.1798	H+	361.1870	6.79	227.0807
AB-PINACA N-Pentanoic Acid	C18H24N4O4	360.1798	H+	361.1870	6.79	316.1646
Benzyl Furanylfentanyl	C23H24N2O2	360.1838	H+	361.1911	6.13	
Benzyl Furanylfentanyl	C23H24N2O2	360.1838	H+	361.1911	6.13	174.1272
Benzyl Furanylfentanyl	C23H24N2O2	360.1838	H+	361.1911	6.13	91.0539
Benzyl Furanylfentanyl	C23H24N2O2	360.1838	H+	361.1911	6.13	361.1905
Benzyl Furanylfentanyl	C23H24N2O2	360.1838	H+	361.1911	6.13	254.1181
Benzyl Furanylfentanyl	C23H24N2O2	360.1838	H+	361.1911	6.13	132.0802
4-cyano CUMYL-BUTINACA	C22H24N4O	360.1950	H+	361.2023	8.91	
4-cyano CUMYL-BUTINACA	C22H24N4O	360.1950	H+	361.2023	8.91	226.0987
4-cyano CUMYL-BUTINACA	C22H24N4O	360.1950	H+	361.2023	8.91	119.0856
4-cyano CUMYL-BUTINACA	C22H24N4O	360.1950	H+	361.2023	8.91	145.04
4-cyano CUMYL-BUTINACA	C22H24N4O	360.1950	H+	361.2023	8.91	361.2028
4-cyano CUMYL-BUTINACA	C22H24N4O	360.1950	H+	361.2023	8.91	91.0545
4-cyano CUMYL-BUT7AICA	C22H24N4O	360.1950	H+	361.2023	8.05	
4-cyano CUMYL-BUT7AICA	C22H24N4O	360.1950	H+	361.2023	8.05	226.0964
4-cyano CUMYL-BUT7AICA	C22H24N4O	360.1950	H+	361.2023	8.05	200.1172
4-cyano CUMYL-BUT7AICA	C22H24N4O	360.1950	H+	361.2023	8.05	119.0838
4-cyano CUMYL-BUT7AICA	C22H24N4O	360.1950	H+	361.2023	8.05	243.1232
4-cyano CUMYL-BUT7AICA	C22H24N4O	360.1950	H+	361.2023	8.05	361.2007
4OH-MDMB-BINACA	C19H27N3O4	361.2002	H+	362.2074	8.29	
4OH-MDMB-BINACA	C19H27N3O4	361.2002	H+	362.2074	8.29	217.0955
4OH-MDMB-BINACA	C19H27N3O4	361.2002	H+	362.2074	8.29	302.1841
4OH-MDMB-BINACA	C19H27N3O4	361.2002	H+	362.2074	8.29	145.0388
4OH-MDMB-BINACA	C19H27N3O4	361.2002	H+	362.2074	8.29	199.0853
4OH-MDMB-BINACA	C19H27N3O4	361.2002	H+	362.2074	8.29	175.0492
5F-ADBICA	C20H28FN3O2	361.2166	H+	362.2238	8.25	
5F-ADBICA	C20H28FN3O2	361.2166	H+	362.2238	8.25	232.1128
5F-ADBICA	C20H28FN3O2	361.2166	H+	362.2238	8.25	345.1972
5F-ADBICA	C20H28FN3O2	361.2166	H+	362.2238	8.25	144.0442
5F-ADBICA	C20H28FN3O2	361.2166	H+	362.2238	8.25	317.2026
5F-ADBICA	C20H28FN3O2	361.2166	H+	362.2238	8.25	116.0495
Remifentanyl Acid	C23H29ClN2O	362.1841	H+	363.1914	5.21	
Remifentanyl Acid	C23H29ClN2O	362.1841	H+	363.1914	5.21	146.0961
Remifentanyl Acid	C23H29ClN2O	362.1841	H+	363.1914	5.21	113.0599
Remifentanyl Acid	C23H29ClN2O	362.1841	H+	363.1914	5.21	214.1068
Remifentanyl Acid	C23H29ClN2O	362.1841	H+	363.1914	5.21	247.1434
Remifentanyl Acid	C23H29ClN2O	362.1841	H+	363.1914	5.21	259.1799
MMB-2201	C20H27FN2O3	362.2006	H+	363.2079	8.88	
MMB-2201	C20H27FN2O3	362.2006	H+	363.2079	8.88	232.1142
MMB-2201	C20H27FN2O3	362.2006	H+	363.2079	8.88	144.0436
MMB-2201	C20H27FN2O3	362.2006	H+	363.2079	8.88	116.0492
MMB-2201	C20H27FN2O3	362.2006	H+	363.2079	8.88	363.2096
MMB-2201	C20H27FN2O3	362.2006	H+	363.2079	8.88	212.1078
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	362.2006	H+	363.2079	8.74	
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	362.2006	H+	363.2079	8.74	232.1119
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	362.2006	H+	363.2079	8.74	144.0436
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	362.2006	H+	363.2079	8.74	363.2066
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	362.2006	H+	363.2079	8.74	116.0489
5F-MDMB-PICA 3,3-Dimethylbutanoic Acid	C20H27FN2O3	362.2006	H+	363.2079	8.74	212.1055
5F-ADB-PINACA	C19H27FN4O2	362.2118	H+	363.2191	8.41	
5F-ADB-PINACA	C19H27FN4O2	362.2118	H+	363.2191	8.41	233.108
5F-ADB-PINACA	C19H27FN4O2	362.2118	H+	363.2191	8.41	318.1974
5F-ADB-PINACA	C19H27FN4O2	362.2118	H+	363.2191	8.41	213.1017
5F-ADB-PINACA	C19H27FN4O2	362.2118	H+	363.2191	8.41	346.192
5F-ADB-PINACA	C19H27FN4O2	362.2118	H+	363.2191	8.41	177.0457
KM 233	C25H30O2	362.2246	H+	363.2319	10.92	
KM 233	C25H30O2	362.2246	H+	363.2319	10.92	119.0852
KM 233	C25H30O2	362.2246	H+	363.2319	10.92	363.2331
KM 233	C25H30O2	362.2246	H+	363.2319	10.92	91.054

KM 233	C25H30O2	362.2246	H+	363.2319	10.92	285.1868
KM 233	C25H30O2	362.2246	H+	363.2319	10.92	245.1546
para-Methyl Cyclopropylfentanyl	C24H30N2O	362.2358	H+	363.2431	7.01	
para-Methyl Cyclopropylfentanyl	C24H30N2O	362.2358	H+	363.2431	7.01	188.1424
para-Methyl Cyclopropylfentanyl	C24H30N2O	362.2358	H+	363.2431	7.01	105.0687
para-Methyl Cyclopropylfentanyl	C24H30N2O	362.2358	H+	363.2431	7.01	363.2412
para-Methyl Cyclopropylfentanyl	C24H30N2O	362.2358	H+	363.2431	7.01	242.1528
para-Methyl Cyclopropylfentanyl	C24H30N2O	362.2358	H+	363.2431	7.01	146.0955
Cyclobutylfentanyl	C24H30N2O	362.2358	H+	363.2431	6.95	
Cyclobutylfentanyl	C24H30N2O	362.2358	H+	363.2431	6.95	188.143
Cyclobutylfentanyl	C24H30N2O	362.2358	H+	363.2431	6.95	105.0694
Cyclobutylfentanyl	C24H30N2O	362.2358	H+	363.2431	6.95	363.2426
Cyclobutylfentanyl	C24H30N2O	362.2358	H+	363.2431	6.95	242.1538
Cyclobutylfentanyl	C24H30N2O	362.2358	H+	363.2431	6.95	281.2018
Senecioyl Fentanyl	C24H30N2O	362.2358	H+	363.2431	6.88	
Senecioyl Fentanyl	C24H30N2O	362.2358	H+	363.2431	6.88	188.1431
Senecioyl Fentanyl	C24H30N2O	362.2358	H+	363.2431	6.88	83.049
Senecioyl Fentanyl	C24H30N2O	362.2358	H+	363.2431	6.88	281.2012
Senecioyl Fentanyl	C24H30N2O	362.2358	H+	363.2431	6.88	105.0697
Senecioyl Fentanyl	C24H30N2O	362.2358	H+	363.2431	6.88	363.2421
ADB-BICA	C22H25N3O2	363.1947	H+	364.2020	8.54	
ADB-BICA	C22H25N3O2	363.1947	H+	364.2020	8.54	234.0928
ADB-BICA	C22H25N3O2	363.1947	H+	364.2020	8.54	347.1775
ADB-BICA	C22H25N3O2	363.1947	H+	364.2020	8.54	91.0546
ADB-BICA	C22H25N3O2	363.1947	H+	364.2020	8.54	319.1824
ADB-BICA	C22H25N3O2	363.1947	H+	364.2020	8.54	206.098
5F-AMB	C19H26FN3O3	363.1958	H+	364.2031	9.23	
5F-AMB	C19H26FN3O3	363.1958	H+	364.2031	9.23	233.1095
5F-AMB	C19H26FN3O3	363.1958	H+	364.2031	9.23	213.1029
5F-AMB	C19H26FN3O3	363.1958	H+	364.2031	9.23	304.1831
5F-AMB	C19H26FN3O3	363.1958	H+	364.2031	9.23	177.0463
5F-AMB	C19H26FN3O3	363.1958	H+	364.2031	9.23	145.0398
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	363.1958	H+	364.2031	9	
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	363.1958	H+	364.2031	9	233.1072
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	363.1958	H+	364.2031	9	318.1962
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	363.1958	H+	364.2031	9	213.1013
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	363.1958	H+	364.2031	9	364.2013
5F-ADB 3,3-Dimethylbutanoic Acid	C19H26FN3O3	363.1958	H+	364.2031	9	145.0387
4F-MDMB-BINACA	C19H26FN3O3	363.1958	H+	364.2031	9.37	
4F-MDMB-BINACA	C19H26FN3O3	363.1958	H+	364.2031	9.37	219.0934
4F-MDMB-BINACA	C19H26FN3O3	363.1958	H+	364.2031	9.37	304.1824
4F-MDMB-BINACA	C19H26FN3O3	363.1958	H+	364.2031	9.37	145.0393
4F-MDMB-BINACA	C19H26FN3O3	363.1958	H+	364.2031	9.37	364.2037
4F-MDMB-BINACA	C19H26FN3O3	363.1958	H+	364.2031	9.37	236.1199
5Cl-AB-PINACA	C18H25ClN4O2	364.1666	H+	365.1739	8.58	
5Cl-AB-PINACA	C18H25ClN4O2	364.1666	H+	365.1739	8.58	249.0796
5Cl-AB-PINACA	C18H25ClN4O2	364.1666	H+	365.1739	8.58	320.1534
5Cl-AB-PINACA	C18H25ClN4O2	364.1666	H+	365.1739	8.58	213.103
5Cl-AB-PINACA	C18H25ClN4O2	364.1666	H+	365.1739	8.58	145.04
5Cl-AB-PINACA	C18H25ClN4O2	364.1666	H+	365.1739	8.58	348.1481
ADB-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.71	
ADB-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.71	235.0869
ADB-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.71	320.1758
ADB-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.71	348.1701
ADB-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.71	252.1131
ADB-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.71	91.0544
APP-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.75	
APP-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.75	201.1019
APP-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.75	320.1758
APP-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.75	145.039
APP-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.75	348.1706
APP-BINACA	C21H24N4O2	364.1899	H+	365.1972	8.75	365.1982
para-Methoxy Acrylfentanyl	C23H28N2O2	364.2151	H+	365.2224	6.34	
para-Methoxy Acrylfentanyl	C23H28N2O2	364.2151	H+	365.2224	6.34	188.1436
para-Methoxy Acrylfentanyl	C23H28N2O2	364.2151	H+	365.2224	6.34	105.0697
para-Methoxy Acrylfentanyl	C23H28N2O2	364.2151	H+	365.2224	6.34	244.1339
para-Methoxy Acrylfentanyl	C23H28N2O2	364.2151	H+	365.2224	6.34	162.0912
para-Methoxy Acrylfentanyl	C23H28N2O2	364.2151	H+	365.2224	6.34	365.2233
APICA	C24H32N2O	364.2515	H+	365.2587	10.83	
APICA	C24H32N2O	364.2515	H+	365.2587	10.83	135.1161
APICA	C24H32N2O	364.2515	H+	365.2587	10.83	365.2586
APICA	C24H32N2O	364.2515	H+	365.2587	10.83	214.1226
APICA	C24H32N2O	364.2515	H+	365.2587	10.83	188.1431
APICA	C24H32N2O	364.2515	H+	365.2587	10.83	107.085

alpha'-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.11	
alpha'-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.11	188.1429
alpha'-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.11	365.2574
alpha'-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.11	244.169
alpha'-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.11	105.0695
alpha'-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.11	281.201
3-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.07	
3-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.07	202.1585
3-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.07	365.258
3-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.07	244.1694
3-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.07	105.0691
3-Methyl Butyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.07	134.0958
para-Methyl Isobutyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.2	
para-Methyl Isobutyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.2	188.1428
para-Methyl Isobutyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.2	105.069
para-Methyl Isobutyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.2	365.2574
para-Methyl Isobutyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.2	244.1688
para-Methyl Isobutyrylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.2	295.2174
Pivaloylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.23	
Pivaloylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.23	188.1425
Pivaloylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.23	105.0689
Pivaloylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.23	365.2576
Pivaloylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.23	57.0695
Pivaloylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.23	244.1697
Valerylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.17	
Valerylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.17	188.1432
Valerylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.17	365.2574
Valerylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.17	244.1688
Valerylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.17	105.0701
Valerylfentanyl	C24H32N2O	364.2515	H+	365.2587	7.17	281.201
MDA 77	C21H23N3O3	365.1739	H+	366.1812	10.30	
MDA 77	C21H23N3O3	365.1739	H+	366.1812	10.30	105.0334
MDA 77	C21H23N3O3	365.1739	H+	366.1812	10.30	366.1825
MDA 77	C21H23N3O3	365.1739	H+	366.1812	10.30	77.0389
MDA 77	C21H23N3O3	365.1739	H+	366.1812	10.30	337.1694
MDA 77	C21H23N3O3	365.1739	H+	366.1812	10.30	175.0504
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	365.1739	H+	366.1812	8.43	
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	365.1739	H+	366.1812	8.43	231.0758
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	365.1739	H+	366.1812	8.43	213.0653
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	365.1739	H+	366.1812	8.43	119.0852
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	365.1739	H+	366.1812	8.43	248.1024
4-cyano CUMYL-BUTINACA N-Butanoic Acid	C21H23N3O3	365.1739	H+	366.1812	8.43	145.0393
ALD-52	C22H27N3O2	365.2103	H+	366.2176	5.97	
ALD-52	C22H27N3O2	365.2103	H+	366.2176	5.97	265.1337
ALD-52	C22H27N3O2	365.2103	H+	366.2176	5.97	232.1751
ALD-52	C22H27N3O2	365.2103	H+	366.2176	5.97	366.2168
ALD-52	C22H27N3O2	365.2103	H+	366.2176	5.97	239.1176
ALD-52	C22H27N3O2	365.2103	H+	366.2176	5.97	223.1227
AKB-48 (APINACA)	C23H31N3O	365.2467	H+	366.2540	11.3	
AKB-48 (APINACA)	C23H31N3O	365.2467	H+	366.2540	11.3	135.1162
AKB-48 (APINACA)	C23H31N3O	365.2467	H+	366.2540	11.3	366.2541
AKB-48 (APINACA)	C23H31N3O	365.2467	H+	366.2540	11.3	107.0854
AKB-48 (APINACA)	C23H31N3O	365.2467	H+	366.2540	11.3	215.1179
AKB-48 (APINACA)	C23H31N3O	365.2467	H+	366.2540	11.3	93.0705
PSB-SB1202	C23H26O4	366.1831	H+	367.1904	11.03	
PSB-SB1202	C23H26O4	366.1831	H+	367.1904	11.03	259.1341
PSB-SB1202	C23H26O4	366.1831	H+	367.1904	11.03	121.0647
PSB-SB1202	C23H26O4	366.1831	H+	367.1904	11.03	367.1918
PSB-SB1202	C23H26O4	366.1831	H+	367.1904	11.03	203.0711
PSB-SB1202	C23H26O4	366.1831	H+	367.1904	11.03	91.0546
5F-CUMYL-PICA	C23H27FN2O	366.2107	H+	367.2180	9.37	
5F-CUMYL-PICA	C23H27FN2O	366.2107	H+	367.2180	9.37	249.142
5F-CUMYL-PICA	C23H27FN2O	366.2107	H+	367.2180	9.37	206.1354
5F-CUMYL-PICA	C23H27FN2O	366.2107	H+	367.2180	9.37	119.0862
5F-CUMYL-PICA	C23H27FN2O	366.2107	H+	367.2180	9.37	232.1449
5F-CUMYL-PICA	C23H27FN2O	366.2107	H+	367.2180	9.37	367.2209
para-Fluoro Cyclopropylfentanyl	C23H27FN2O	366.2107	H+	367.2180	6.6	
para-Fluoro Cyclopropylfentanyl	C23H27FN2O	366.2107	H+	367.2180	6.6	188.1428

para-Fluoro Cyclopropylfentanyl	C23H27FN2O	366.2107	H+	367.2180	6.6	105.0692
para-Fluoro Cyclopropylfentanyl	C23H27FN2O	366.2107	H+	367.2180	6.6	367.2167
para-Fluoro Cyclopropylfentanyl	C23H27FN2O	366.2107	H+	367.2180	6.6	246.1285
para-Fluoro Cyclopropylfentanyl	C23H27FN2O	366.2107	H+	367.2180	6.6	150.0709
APINAC (AKB57)	C23H30N2O2	366.2307	H+	367.2380	11.53	
APINAC (AKB57)	C23H30N2O2	366.2307	H+	367.2380	11.53	135.1161
APINAC (AKB57)	C23H30N2O2	366.2307	H+	367.2380	11.53	367.238
APINAC (AKB57)	C23H30N2O2	366.2307	H+	367.2380	11.53	107.0852
APINAC (AKB57)	C23H30N2O2	366.2307	H+	367.2380	11.53	93.0689
APINAC (AKB57)	C23H30N2O2	366.2307	H+	367.2380	11.53	79.054
ortho-Methyl Methoxyfentanyl	C23H30N2O2	366.2307	H+	367.2380	5.99	
ortho-Methyl Methoxyfentanyl	C23H30N2O2	366.2307	H+	367.2380	5.99	188.1441
ortho-Methyl Methoxyfentanyl	C23H30N2O2	366.2307	H+	367.2380	5.99	105.0701
ortho-Methyl Methoxyfentanyl	C23H30N2O2	366.2307	H+	367.2380	5.99	367.2392
ortho-Methyl Methoxyfentanyl	C23H30N2O2	366.2307	H+	367.2380	5.99	246.1503
ortho-Methyl Methoxyfentanyl	C23H30N2O2	366.2307	H+	367.2380	5.99	146.0971
Ethoxyacetyl Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.05	
Ethoxyacetyl Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.05	188.1435
Ethoxyacetyl Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.05	105.0694
Ethoxyacetyl Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.05	367.238
Ethoxyacetyl Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.05	246.1491
Ethoxyacetyl Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.05	146.0958
para-Methoxy Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.45	
para-Methoxy Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.45	188.1434
para-Methoxy Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.45	105.0694
para-Methoxy Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.45	367.2384
para-Methoxy Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.45	246.1494
para-Methoxy Fentanyl	C23H30N2O2	366.2307	H+	367.2380	6.45	162.0911
3F-MT-45	C24H31FN2	366.2471	H+	367.2544	7.6	
3F-MT-45	C24H31FN2	366.2471	H+	367.2544	7.6	199.091
3F-MT-45	C24H31FN2	366.2471	H+	367.2544	7.6	169.1696
3F-MT-45	C24H31FN2	366.2471	H+	367.2544	7.6	179.0853
3F-MT-45	C24H31FN2	366.2471	H+	367.2544	7.6	367.2532
3F-MT-45	C24H31FN2	366.2471	H+	367.2544	7.6	121.0445
AB-FUBICA	C21H22FN3O2	367.1696	H+	368.1769	8.16	
AB-FUBICA	C21H22FN3O2	367.1696	H+	368.1769	8.16	252.0819
AB-FUBICA	C21H22FN3O2	367.1696	H+	368.1769	8.16	109.0439
AB-FUBICA	C21H22FN3O2	367.1696	H+	368.1769	8.16	351.1497
AB-FUBICA	C21H22FN3O2	367.1696	H+	368.1769	8.16	323.1549
AB-FUBICA	C21H22FN3O2	367.1696	H+	368.1769	8.16	368.1754
JWH-145	C26H25NO	367.1936	H+	368.2009	10.79	
JWH-145	C26H25NO	367.1936	H+	368.2009	10.79	155.0495
JWH-145	C26H25NO	367.1936	H+	368.2009	10.79	127.0542
JWH-145	C26H25NO	367.1936	H+	368.2009	10.79	368.2021
JWH-145	C26H25NO	367.1936	H+	368.2009	10.79	240.1382
JWH-145	C26H25NO	367.1936	H+	368.2009	10.79	101.037
5F-CUMYL-PINACA	C22H26FN3O	367.2060	H+	368.2133	9.73	
5F-CUMYL-PINACA	C22H26FN3O	367.2060	H+	368.2133	9.73	233.109
5F-CUMYL-PINACA	C22H26FN3O	367.2060	H+	368.2133	9.73	119.0853
5F-CUMYL-PINACA	C22H26FN3O	367.2060	H+	368.2133	9.73	213.1022
5F-CUMYL-PINACA	C22H26FN3O	367.2060	H+	368.2133	9.73	145.0395
5F-CUMYL-PINACA	C22H26FN3O	367.2060	H+	368.2133	9.73	177.0462
5F-CUMYL-P7AICA	C22H26FN3O	367.2060	H+	368.2133	8.81	
5F-CUMYL-P7AICA	C22H26FN3O	367.2060	H+	368.2133	8.81	250.1357
5F-CUMYL-P7AICA	C22H26FN3O	367.2060	H+	368.2133	8.81	233.1086
5F-CUMYL-P7AICA	C22H26FN3O	367.2060	H+	368.2133	8.81	207.1301
5F-CUMYL-P7AICA	C22H26FN3O	367.2060	H+	368.2133	8.81	119.0837
5F-CUMYL-P7AICA	C22H26FN3O	367.2060	H+	368.2133	8.81	368.214
5F JWH-018 Adamantyl Analogue	C24H30FNO	367.2311	H+	368.2384	10.55	
5F JWH-018 Adamantyl Analogue	C24H30FNO	367.2311	H+	368.2384	10.55	135.1164
5F JWH-018 Adamantyl Analogue	C24H30FNO	367.2311	H+	368.2384	10.55	368.2391
5F JWH-018 Adamantyl Analogue	C24H30FNO	367.2311	H+	368.2384	10.55	107.0849
5F JWH-018 Adamantyl Analogue	C24H30FNO	367.2311	H+	368.2384	10.55	93.0696
5F JWH-018 Adamantyl Analogue	C24H30FNO	367.2311	H+	368.2384	10.55	79.0544
U-50488	C19H26Cl2N2O	368.1422	H+	369.1495	6.91	
U-50488	C19H26Cl2N2O	368.1422	H+	369.1495	6.91	298.0747
U-50488	C19H26Cl2N2O	368.1422	H+	369.1495	6.91	218.0121
U-50488	C19H26Cl2N2O	368.1422	H+	369.1495	6.91	122.1118
U-50488	C19H26Cl2N2O	368.1422	H+	369.1495	6.91	369.1476
U-50488	C19H26Cl2N2O	368.1422	H+	369.1495	6.91	158.9753
AB-FUBINACA	C20H21FN4O2	368.1649	H+	369.1721	8.31	
AB-FUBINACA	C20H21FN4O2	368.1649	H+	369.1721	8.31	253.0777
AB-FUBINACA	C20H21FN4O2	368.1649	H+	369.1721	8.31	109.0443
AB-FUBINACA	C20H21FN4O2	368.1649	H+	369.1721	8.31	324.1513

AB-FUBINACA	C20H21FN4O2	368.1649	H+	369.1721	8.31	352.1457
AB-FUBINACA	C20H21FN4O2	368.1649	H+	369.1721	8.31	369.1725
para-Chloro Acrylfentanyl	C22H25ClN2O	368.1655	H+	369.1728	6.78	
para-Chloro Acrylfentanyl	C22H25ClN2O	368.1655	H+	369.1728	6.78	188.1429
para-Chloro Acrylfentanyl	C22H25ClN2O	368.1655	H+	369.1728	6.78	105.0694
para-Chloro Acrylfentanyl	C22H25ClN2O	368.1655	H+	369.1728	6.78	369.1721
para-Chloro Acrylfentanyl	C22H25ClN2O	368.1655	H+	369.1728	6.78	248.0838
para-Chloro Acrylfentanyl	C22H25ClN2O	368.1655	H+	369.1728	6.78	134.0963
CB-13	C26H24O2	368.1776	H+	369.1849	11.45	
CB-13	C26H24O2	368.1776	H+	369.1849	11.45	155.0487
CB-13	C26H24O2	368.1776	H+	369.1849	11.45	171.0434
CB-13	C26H24O2	368.1776	H+	369.1849	11.45	369.1852
CB-13	C26H24O2	368.1776	H+	369.1849	11.45	299.1068
CB-13	C26H24O2	368.1776	H+	369.1849	11.45	127.0538
para-Fluorobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.81	
para-Fluorobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.81	188.1426
para-Fluorobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.81	105.0699
para-Fluorobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.81	369.2318
para-Fluorobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.81	248.1433
para-Fluorobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.81	150.0707
Fluoroisobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.88	
Fluoroisobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.88	188.1431
Fluoroisobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.88	105.0702
Fluoroisobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.88	369.2331
Fluoroisobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.88	248.1443
Fluoroisobutyryl Fentanyl	C23H29FN2O	368.2264	H+	369.2337	6.88	150.0711
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	369.1489	H+	370.1562	8.81	
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	369.1489	H+	370.1562	8.81	253.0768
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	369.1489	H+	370.1562	8.81	109.0444
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	369.1489	H+	370.1562	8.81	324.1497
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	369.1489	H+	370.1562	8.81	370.1549
MMB-FUBINACA 3-Methylbutanoic Acid	C20H20FN3O3	369.1489	H+	370.1562	8.81	352.1453
Diacetylmorphine (Heroin)	C21H23NO5	369.1576	H+	370.1649	5.14	
Diacetylmorphine (Heroin)	C21H23NO5	369.1576	H+	370.1649	5.14	370.1639
Diacetylmorphine (Heroin)	C21H23NO5	369.1576	H+	370.1649	5.14	328.1541
Diacetylmorphine (Heroin)	C21H23NO5	369.1576	H+	370.1649	5.14	268.1329
Diacetylmorphine (Heroin)	C21H23NO5	369.1576	H+	370.1649	5.14	211.0751
Diacetylmorphine (Heroin)	C21H23NO5	369.1576	H+	370.1649	5.14	310.144
JWH-116	C26H27NO	369.2093	H+	370.2165	10.84	
JWH-116	C26H27NO	369.2093	H+	370.2165	10.84	155.0494
JWH-116	C26H27NO	369.2093	H+	370.2165	10.84	370.2186
JWH-116	C26H27NO	369.2093	H+	370.2165	10.84	242.1549
JWH-116	C26H27NO	369.2093	H+	370.2165	10.84	127.0451
JWH-116	C26H27NO	369.2093	H+	370.2165	10.84	172.0763
JWH-149	C26H27NO	369.2093	H+	370.2165	10.82	
JWH-149	C26H27NO	369.2093	H+	370.2165	10.82	169.0651
JWH-149	C26H27NO	369.2093	H+	370.2165	10.82	288.1387
JWH-149	C26H27NO	369.2093	H+	370.2165	10.82	370.2181
JWH-149	C26H27NO	369.2093	H+	370.2165	10.82	141.07
JWH-149	C26H27NO	369.2093	H+	370.2165	10.82	158.0604
JWH-020	C26H27NO	369.2093	H+	370.2165	10.96	
JWH-020	C26H27NO	369.2093	H+	370.2165	10.96	155.0488
JWH-020	C26H27NO	369.2093	H+	370.2165	10.96	370.2167
JWH-020	C26H27NO	369.2093	H+	370.2165	10.96	242.1541
JWH-020	C26H27NO	369.2093	H+	370.2165	10.96	127.0541
JWH-020	C26H27NO	369.2093	H+	370.2165	10.96	144.0446
JWH-210	C26H27NO	369.2093	H+	370.2165	10.85	
JWH-210	C26H27NO	369.2093	H+	370.2165	10.85	183.0797
JWH-210	C26H27NO	369.2093	H+	370.2165	10.85	214.1219
JWH-210	C26H27NO	369.2093	H+	370.2165	10.85	370.2172
JWH-210	C26H27NO	369.2093	H+	370.2165	10.85	155.085
JWH-210	C26H27NO	369.2093	H+	370.2165	10.85	144.0441
Flubromazelam	C17H12BrFN4	370.0229	H+	371.0302	7.39	
Flubromazelam	C17H12BrFN4	370.0229	H+	371.0302	7.39	371.031
Flubromazelam	C17H12BrFN4	370.0229	H+	371.0302	7.39	292.1127
Flubromazelam	C17H12BrFN4	370.0229	H+	371.0302	7.39	343.0125
Flubromazelam	C17H12BrFN4	370.0229	H+	371.0302	7.39	237.0955
Flubromazelam	C17H12BrFN4	370.0229	H+	371.0302	7.39	223.07031
Thioridazine	C21H26N2S2	370.1537	H+	371.1610	7.98	
Thioridazine	C21H26N2S2	370.1537	H+	371.1610	7.98	126.1279
Thioridazine	C21H26N2S2	370.1537	H+	371.1610	7.98	371.1607
Thioridazine	C21H26N2S2	370.1537	H+	371.1610	7.98	98.0971
Thioridazine	C21H26N2S2	370.1537	H+	371.1610	7.98	266.99
Thioridazine	C21H26N2S2	370.1537	H+	371.1610	7.98	355.0698

Benzyl Phenylfentanyl	C25H26N2O	370.2045	H+	371.2118	6.56	
Benzyl Phenylfentanyl	C25H26N2O	370.2045	H+	371.2118	6.56	174.1281
Benzyl Phenylfentanyl	C25H26N2O	370.2045	H+	371.2118	6.56	105.0337
Benzyl Phenylfentanyl	C25H26N2O	370.2045	H+	371.2118	6.56	91.0546
Benzyl Phenylfentanyl	C25H26N2O	370.2045	H+	371.2118	6.56	371.2124
Benzyl Phenylfentanyl	C25H26N2O	370.2045	H+	371.2118	6.56	267.001
Ocfentanil	C22H27FN2O2	370.2056	H+	371.2129	5.74	
Ocfentanil	C22H27FN2O2	370.2056	H+	371.2129	5.74	188.1427
Ocfentanil	C22H27FN2O2	370.2056	H+	371.2129	5.74	105.07
Ocfentanil	C22H27FN2O2	370.2056	H+	371.2129	5.74	371.2108
Ocfentanil	C22H27FN2O2	370.2056	H+	371.2129	5.74	250.1227
Ocfentanil	C22H27FN2O2	370.2056	H+	371.2129	5.74	146.0958
MMB-CHMICA	C22H30N2O3	370.2256	H+	371.2329	9.96	
MMB-CHMICA	C22H30N2O3	370.2256	H+	371.2329	9.96	240.1391
MMB-CHMICA	C22H30N2O3	370.2256	H+	371.2329	9.96	144.044
MMB-CHMICA	C22H30N2O3	370.2256	H+	371.2329	9.96	371.2331
MMB-CHMICA	C22H30N2O3	370.2256	H+	371.2329	9.96	116.0486
MMB-CHMICA	C22H30N2O3	370.2256	H+	371.2329	9.96	97.1019
MAB-CHMINACA	C21H30N4O2	370.2369	H+	371.2442	9.79	
MAB-CHMINACA	C21H30N4O2	370.2369	H+	371.2442	9.79	241.134
MAB-CHMINACA	C21H30N4O2	370.2369	H+	371.2442	9.79	326.2235
MAB-CHMINACA	C21H30N4O2	370.2369	H+	371.2442	9.79	354.2179
MAB-CHMINACA	C21H30N4O2	370.2369	H+	371.2442	9.79	145.0391
MAB-CHMINACA	C21H30N4O2	370.2369	H+	371.2442	9.79	371.2451
Trazodone	C19H22ClN5O	371.1513	H+	372.1586	5.87	
Trazodone	C19H22ClN5O	371.1513	H+	372.1586	5.87	176.081
Trazodone	C19H22ClN5O	371.1513	H+	372.1586	5.87	372.1574
Trazodone	C19H22ClN5O	371.1513	H+	372.1586	5.87	148.0508
Trazodone	C19H22ClN5O	371.1513	H+	372.1586	5.87	356.0701
Trazodone	C19H22ClN5O	371.1513	H+	372.1586	5.87	267.9992
JWH-018 N-Pentanoic Acid	C24H21NO3	371.1521	H+	372.1594	8.76	
JWH-018 N-Pentanoic Acid	C24H21NO3	371.1521	H+	372.1594	8.76	155.0482
JWH-018 N-Pentanoic Acid	C24H21NO3	371.1521	H+	372.1594	8.76	372.1574
JWH-018 N-Pentanoic Acid	C24H21NO3	371.1521	H+	372.1594	8.76	127.0531
JWH-018 N-Pentanoic Acid	C24H21NO3	371.1521	H+	372.1594	8.76	244.0967
JWH-018 N-Pentanoic Acid	C24H21NO3	371.1521	H+	372.1594	8.76	144.0435
JWH-018 6-Methoxyindole Analogue	C25H25NO2	371.1885	H+	372.1958	10.39	
JWH-018 6-Methoxyindole Analogue	C25H25NO2	371.1885	H+	372.1958	10.39	155.049
JWH-018 6-Methoxyindole Analogue	C25H25NO2	371.1885	H+	372.1958	10.39	127.0541
JWH-018 6-Methoxyindole Analogue	C25H25NO2	371.1885	H+	372.1958	10.39	372.1967
JWH-018 6-Methoxyindole Analogue	C25H25NO2	371.1885	H+	372.1958	10.39	244.1341
JWH-018 6-Methoxyindole Analogue	C25H25NO2	371.1885	H+	372.1958	10.39	174.0551
JWH-081	C25H25NO2	371.1885	H+	372.1958	10.49	
JWH-081	C25H25NO2	371.1885	H+	372.1958	10.49	185.0596
JWH-081	C25H25NO2	371.1885	H+	372.1958	10.49	214.1224
JWH-081	C25H25NO2	371.1885	H+	372.1958	10.49	372.1963
JWH-081	C25H25NO2	371.1885	H+	372.1958	10.49	157.0648
JWH-081	C25H25NO2	371.1885	H+	372.1958	10.49	144.0445
MA-CHMINACA	C21H29N3O3	371.2209	H+	372.2282	10.41	
MA-CHMINACA	C21H29N3O3	371.2209	H+	372.2282	10.41	241.1341
MA-CHMINACA	C21H29N3O3	371.2209	H+	372.2282	10.41	145.0392
MA-CHMINACA	C21H29N3O3	371.2209	H+	372.2282	10.41	312.2079
MA-CHMINACA	C21H29N3O3	371.2209	H+	372.2282	10.41	340.2031
MA-CHMINACA	C21H29N3O3	371.2209	H+	372.2282	10.41	372.2289
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	371.2209	H+	372.2282	10.19	
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	371.2209	H+	372.2282	10.19	241.1332
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	371.2209	H+	372.2282	10.19	372.2279
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	371.2209	H+	372.2282	10.19	326.2224
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	371.2209	H+	372.2282	10.19	145.0391
MAB-CHMINACA 3,3-Dimethylbutanoic Acid	C21H29N3O3	371.2209	H+	372.2282	10.19	354.2145
FUBIMINA N-pentanoic acid	C23H20N2O3	372.1474	H+	373.1547	8.67	
FUBIMINA N-pentanoic acid	C23H20N2O3	372.1474	H+	373.1547	8.67	273.1024
FUBIMINA N-pentanoic acid	C23H20N2O3	372.1474	H+	373.1547	8.67	201.1024
FUBIMINA N-pentanoic acid	C23H20N2O3	372.1474	H+	373.1547	8.67	155.0489
FUBIMINA N-pentanoic acid	C23H20N2O3	372.1474	H+	373.1547	8.67	145.0395
FUBIMINA N-pentanoic acid	C23H20N2O3	372.1474	H+	373.1547	8.67	373.1549
Difluorofentanyl	C22H26F2N2O	372.2013	H+	373.2086	6.52	
Difluorofentanyl	C22H26F2N2O	372.2013	H+	373.2086	6.52	206.1326

Difluorofentanyl	C22H26F2N2O	372.2013	H+	373.2086	6.52	123.0594
Difluorofentanyl	C22H26F2N2O	372.2013	H+	373.2086	6.52	373.2068
Difluorofentanyl	C22H26F2N2O	372.2013	H+	373.2086	6.52	234.1282
Difluorofentanyl	C22H26F2N2O	372.2013	H+	373.2086	6.52	152.0862
CUMYL-PeGACLONE	C25H28N2O	372.2202	H+	373.2274	10.2	
CUMYL-PeGACLONE	C25H28N2O	372.2202	H+	373.2274	10.2	255.1492
CUMYL-PeGACLONE	C25H28N2O	372.2202	H+	373.2274	10.2	119.0847
CUMYL-PeGACLONE	C25H28N2O	372.2202	H+	373.2274	10.2	327.1383
CUMYL-PeGACLONE	C25H28N2O	372.2202	H+	373.2274	10.2	185.0701
CUMYL-PeGACLONE	C25H28N2O	372.2202	H+	373.2274	10.2	167.0595
Prochlorperazine	C20H24ClN3S	373.1379	H+	374.1452	7.95	
Prochlorperazine	C20H24ClN3S	373.1379	H+	374.1452	7.95	141.1387
Prochlorperazine	C20H24ClN3S	373.1379	H+	374.1452	7.95	374.145
Prochlorperazine	C20H24ClN3S	373.1379	H+	374.1452	7.95	113.1077
Prochlorperazine	C20H24ClN3S	373.1379	H+	374.1452	7.95	70.0668
Prochlorperazine	C20H24ClN3S	373.1379	H+	374.1452	7.95	246.0138
Fluoro-JWH-019	C25H24FNO	373.1842	H+	374.1915	10.32	
Fluoro-JWH-019	C25H24FNO	373.1842	H+	374.1915	10.32	155.0493
Fluoro-JWH-019	C25H24FNO	373.1842	H+	374.1915	10.32	246.1294
Fluoro-JWH-019	C25H24FNO	373.1842	H+	374.1915	10.32	374.1924
Fluoro-JWH-019	C25H24FNO	373.1842	H+	374.1915	10.32	127.0541
Fluoro-JWH-019	C25H24FNO	373.1842	H+	374.1915	10.32	144.0449
MAM-2201	C25H24FNO	373.1842	H+	374.1915	9.91	
MAM-2201	C25H24FNO	373.1842	H+	374.1915	9.91	169.0639
MAM-2201	C25H24FNO	373.1842	H+	374.1915	9.91	232.1122
MAM-2201	C25H24FNO	373.1842	H+	374.1915	9.91	374.1913
MAM-2201	C25H24FNO	373.1842	H+	374.1915	9.91	141.0691
MAM-2201	C25H24FNO	373.1842	H+	374.1915	9.91	144.0439
ADBICA N-Pentanoic Acid	C20H27N3O4	373.2002	H+	374.2074	7.23	
ADBICA N-Pentanoic Acid	C20H27N3O4	373.2002	H+	374.2074	7.23	244.0949
ADBICA N-Pentanoic Acid	C20H27N3O4	373.2002	H+	374.2074	7.23	357.1777
ADBICA N-Pentanoic Acid	C20H27N3O4	373.2002	H+	374.2074	7.23	144.0431
ADBICA N-Pentanoic Acid	C20H27N3O4	373.2002	H+	374.2074	7.23	374.2042
ADBICA N-Pentanoic Acid	C20H27N3O4	373.2002	H+	374.2074	7.23	329.1844
Azidoindolene 1 (1)	C21H28FN3O2	373.2166	H+	374.2238	9.47	
Azidoindolene 1 (1)	C21H28FN3O2	373.2166	H+	374.2238	9.47	125.0955
Azidoindolene 1 (1)	C21H28FN3O2	373.2166	H+	374.2238	9.47	97.1007
Azidoindolene 1 (1)	C21H28FN3O2	373.2166	H+	374.2238	9.47	374.2243
Azidoindolene 1 (1)	C21H28FN3O2	373.2166	H+	374.2238	9.47	69.0691
Azidoindolene 1 (1)	C21H28FN3O2	373.2166	H+	374.2238	9.47	55.0534
Azidoindolene 1 (2)	C21H28FN3O2	373.2166	H+	374.2238	10.47	
Azidoindolene 1 (2)	C21H28FN3O2	373.2166	H+	374.2238	10.47	125.0955
Azidoindolene 1 (2)	C21H28FN3O2	373.2166	H+	374.2238	10.47	97.1007
Azidoindolene 1 (2)	C21H28FN3O2	373.2166	H+	374.2238	10.47	374.2243
Azidoindolene 1 (2)	C21H28FN3O2	373.2166	H+	374.2238	10.47	69.0691
Azidoindolene 1 (2)	C21H28FN3O2	373.2166	H+	374.2238	10.47	55.0534
Hydroxyzine	C21H27ClN2O2	374.1761	H+	375.1834	7.15	
Hydroxyzine	C21H27ClN2O2	374.1761	H+	375.1834	7.15	201.0458
Hydroxyzine	C21H27ClN2O2	374.1761	H+	375.1834	7.15	166.0771
Hydroxyzine	C21H27ClN2O2	374.1761	H+	375.1834	7.15	165.0697
Hydroxyzine	C21H27ClN2O2	374.1761	H+	375.1834	7.15	375.1828
Hydroxyzine	C21H27ClN2O2	374.1761	H+	375.1834	7.15	173.128
5F-NNEI	C24H23FN2O	374.1794	H+	375.1867	9.27	
5F-NNEI	C24H23FN2O	374.1794	H+	375.1867	9.27	232.1136
5F-NNEI	C24H23FN2O	374.1794	H+	375.1867	9.27	375.1879
5F-NNEI	C24H23FN2O	374.1794	H+	375.1867	9.27	144.0438
5F-NNEI	C24H23FN2O	374.1794	H+	375.1867	9.27	206.1337
5F-NNEI	C24H23FN2O	374.1794	H+	375.1867	9.27	116.0496
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	374.1954	H+	375.2027	7.31	
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	374.1954	H+	375.2027	7.31	245.09
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	374.1954	H+	375.2027	7.31	217.0953
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	374.1954	H+	375.2027	7.31	330.1783
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	374.1954	H+	375.2027	7.31	227.0797
ADB-PINACA N-Pentanoic Acid	C19H26N4O4	374.1954	H+	375.2027	7.31	358.1729
Furanyl Fentanyl	C24H26N2O2	374.1994	H+	375.2067	6.30	
Furanyl Fentanyl	C24H26N2O2	374.1994	H+	375.2067	6.30	188.1432
Furanyl Fentanyl	C24H26N2O2	374.1994	H+	375.2067	6.30	375.2071
Furanyl Fentanyl	C24H26N2O2	374.1994	H+	375.2067	6.30	105.0702
Furanyl Fentanyl	C24H26N2O2	374.1994	H+	375.2067	6.30	134.0965
Furanyl Fentanyl	C24H26N2O2	374.1994	H+	375.2067	6.30	254.118
JWH-398	C24H22ClNO	375.1390	H+	376.1463	10.94	
JWH-398	C24H22ClNO	375.1390	H+	376.1463	10.94	189.0099
JWH-398	C24H22ClNO	375.1390	H+	376.1463	10.94	376.1466
JWH-398	C24H22ClNO	375.1390	H+	376.1463	10.94	161.0148

JWH-398	C24H22ClNO	375.1390	H+	376.1463	10.94	214.1231
JWH-398	C24H22ClNO	375.1390	H+	376.1463	10.94	126.0462
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	375.1390	H+	376.1463	10.09	
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	375.1390	H+	376.1463	10.09	155.049
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	375.1390	H+	376.1463	10.09	376.1464
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	375.1390	H+	376.1463	10.09	248.084
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	375.1390	H+	376.1463	10.09	127.0537
JWH-018 N-(5-Chloropentyl) Analogue	C24H22ClNO	375.1390	H+	376.1463	10.09	144.0443
Haloperidol	C21H23ClFNO2	375.1401	H+	376.1474	6.65	
Haloperidol	C21H23ClFNO2	375.1401	H+	376.1474	6.65	165.071
Haloperidol	C21H23ClFNO2	375.1401	H+	376.1474	6.65	376.1477
Haloperidol	C21H23ClFNO2	375.1401	H+	376.1474	6.65	123.0243
Haloperidol	C21H23ClFNO2	375.1401	H+	376.1474	6.65	358.1376
Haloperidol	C21H23ClFNO2	375.1401	H+	376.1474	6.65	206.0977
NM-2201	C24H22FNO2	375.1635	H+	376.1707	10.19	
NM-2201	C24H22FNO2	375.1635	H+	376.1707	10.19	232.1126
NM-2201	C24H22FNO2	375.1635	H+	376.1707	10.19	144.0439
NM-2201	C24H22FNO2	375.1635	H+	376.1707	10.19	116.0495
NM-2201	C24H22FNO2	375.1635	H+	376.1707	10.19	212.1067
NM-2201	C24H22FNO2	375.1635	H+	376.1707	10.19	69.0721
5F-MN-18	C23H22FN3O	375.1747	H+	376.1820	9.99	
5F-MN-18	C23H22FN3O	375.1747	H+	376.1820	9.99	233.1091
5F-MN-18	C23H22FN3O	375.1747	H+	376.1820	9.99	213.1024
5F-MN-18	C23H22FN3O	375.1747	H+	376.1820	9.99	145.0395
5F-MN-18	C23H22FN3O	375.1747	H+	376.1820	9.99	177.0461
5F-MN-18	C23H22FN3O	375.1747	H+	376.1820	9.99	376.1822
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	375.1747	H+	376.1820	10.16	
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	375.1747	H+	376.1820	10.16	232.1135
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	375.1747	H+	376.1820	10.16	144.0438
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	375.1747	H+	376.1820	10.16	376.182
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	375.1747	H+	376.1820	10.16	116.049
AM-2201 8-Quinolinyl Carboxamide	C23H22FN3O	375.1747	H+	376.1820	10.16	171.0551
5F-PCN	C23H22FN3O	375.1747	H+	376.1820	6.80	
5F-PCN	C23H22FN3O	375.1747	H+	376.1820	6.80	376.1812
5F-PCN	C23H22FN3O	375.1747	H+	376.1820	6.80	356.1749
5F-PCN	C23H22FN3O	375.1747	H+	376.1820	6.80	288.1128
5F-PCN	C23H22FN3O	375.1747	H+	376.1820	6.80	233.1082
5F-PCN	C23H22FN3O	375.1747	H+	376.1820	6.80	145.0393
25T4-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.73	
25T4-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.73	121.0645
25T4-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.73	376.1941
25T4-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.73	239.1101
25T4-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.73	197.063
25T4-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.73	91.055
25T7-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.85	
25T7-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.85	121.0647
25T7-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.85	376.1943
25T7-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.85	239.1103
25T7-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.85	91.0552
25T7-NBOMe	C21H29NO3S	375.1868	H+	376.1941	7.85	359.1683
RCS-8	C25H29NO2	375.2198	H+	376.2271	10.68	
RCS-8	C25H29NO2	375.2198	H+	376.2271	10.68	121.0644
RCS-8	C25H29NO2	375.2198	H+	376.2271	10.68	376.2268
RCS-8	C25H29NO2	375.2198	H+	376.2271	10.68	343.1934
RCS-8	C25H29NO2	375.2198	H+	376.2271	10.68	354.154
RCS-8	C25H29NO2	375.2198	H+	376.2271	10.68	240.1746
Ethylindole Fentanyl	C24H29N3O	375.2311	H+	376.2383	6.53	
Ethylindole Fentanyl	C24H29N3O	375.2311	H+	376.2383	6.53	144.0804
Ethylindole Fentanyl	C24H29N3O	375.2311	H+	376.2383	6.53	189.1382
Ethylindole Fentanyl	C24H29N3O	375.2311	H+	376.2383	6.53	245.1643
Ethylindole Fentanyl	C24H29N3O	375.2311	H+	376.2383	6.53	376.2368
Ethylindole Fentanyl	C24H29N3O	375.2311	H+	376.2383	6.53	233.1645
W15	C19H21ClN2O2S	376.1012	H+	377.1085	9.03	
W15	C19H21ClN2O2S	376.1012	H+	377.1085	9.03	105.0699
W15	C19H21ClN2O2S	376.1012	H+	377.1085	9.03	377.1088
W15	C19H21ClN2O2S	376.1012	H+	377.1085	9.03	273.0461
W15	C19H21ClN2O2S	376.1012	H+	377.1085	9.03	174.9611
W15	C19H21ClN2O2S	376.1012	H+	377.1085	9.03	110.9995
5Cl-THJ-018	C23H21ClN2O	376.1342	H+	377.1415	10.39	
5Cl-THJ-018	C23H21ClN2O	376.1342	H+	377.1415	10.39	249.0799
5Cl-THJ-018	C23H21ClN2O	376.1342	H+	377.1415	10.39	213.103
5Cl-THJ-018	C23H21ClN2O	376.1342	H+	377.1415	10.39	145.0398
5Cl-THJ-018	C23H21ClN2O	376.1342	H+	377.1415	10.39	377.1426
5Cl-THJ-018	C23H21ClN2O	376.1342	H+	377.1415	10.39	193.0171

5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	376.1587	H+	377.1660	9.41	
5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	376.1587	H+	377.1660	9.41	232.1143
5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	376.1587	H+	377.1660	9.41	144.0441
5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	376.1587	H+	377.1660	9.41	116.0491
5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	376.1587	H+	377.1660	9.41	377.1668
5F-PB-22 (5-fluoro QUPIC)	C23H21FN2O2	376.1587	H+	377.1660	9.41	158.06
5F-SDB-005	C23H21FN2O2	376.1587	H+	377.1660	10.12	
5F-SDB-005	C23H21FN2O2	376.1587	H+	377.1660	10.12	233.1088
5F-SDB-005	C23H21FN2O2	376.1587	H+	377.1660	10.12	213.1023
5F-SDB-005	C23H21FN2O2	376.1587	H+	377.1660	10.12	177.0457
5F-SDB-005	C23H21FN2O2	376.1587	H+	377.1660	10.12	145.0392
5F-SDB-005	C23H21FN2O2	376.1587	H+	377.1660	10.12	69.07
5F-THJ	C22H21FN4O	376.1699	H+	377.1772	10.40	
5F-THJ	C22H21FN4O	376.1699	H+	377.1772	10.40	233.1091
5F-THJ	C22H21FN4O	376.1699	H+	377.1772	10.40	213.1025
5F-THJ	C22H21FN4O	376.1699	H+	377.1772	10.40	359.1672
5F-THJ	C22H21FN4O	376.1699	H+	377.1772	10.40	377.1785
5F-THJ	C22H21FN4O	376.1699	H+	377.1772	10.40	145.0397
PF-03550096	C19H28N4O4	376.2111	H+	377.2183	7.63	
PF-03550096	C19H28N4O4	376.2111	H+	377.2183	7.63	203.1176
PF-03550096	C19H28N4O4	376.2111	H+	377.2183	7.63	147.0548
PF-03550096	C19H28N4O4	376.2111	H+	377.2183	7.63	314.1868
PF-03550096	C19H28N4O4	376.2111	H+	377.2183	7.63	332.1971
PF-03550096	C19H28N4O4	376.2111	H+	377.2183	7.63	246.124
5F-MDMB-PICA	C21H29FN2O3	376.2162	H+	377.2235	9.33	
5F-MDMB-PICA	C21H29FN2O3	376.2162	H+	377.2235	9.33	232.1152
5F-MDMB-PICA	C21H29FN2O3	376.2162	H+	377.2235	9.33	144.0452
5F-MDMB-PICA	C21H29FN2O3	376.2162	H+	377.2235	9.33	116.0502
5F-MDMB-PICA	C21H29FN2O3	376.2162	H+	377.2235	9.33	377.225
5F-MDMB-PICA	C21H29FN2O3	376.2162	H+	377.2235	9.33	158.0608
Cyclopentyl Fentanyl	C25H32N2O	376.2514	H+	377.2587	7.30	
Cyclopentyl Fentanyl	C25H32N2O	376.2514	H+	377.2587	7.30	188.1423
Cyclopentyl Fentanyl	C25H32N2O	376.2514	H+	377.2587	7.30	377.2566
Cyclopentyl Fentanyl	C25H32N2O	376.2514	H+	377.2587	7.30	281.2
Cyclopentyl Fentanyl	C25H32N2O	376.2514	H+	377.2587	7.30	256.1684
Cyclopentyl Fentanyl	C25H32N2O	376.2514	H+	377.2587	7.30	105.0698
CP-55,940	C24H40O3	376.2978	H+	377.3050	9.85	
CP-55,940	C24H40O3	376.2978	H+	377.3050	9.85	233.1902
CP-55,940	C24H40O3	376.2978	H+	377.3050	9.85	215.1437
CP-55,940	C24H40O3	376.2978	H+	377.3050	9.85	121.1007
CP-55,940	C24H40O3	376.2978	H+	377.3050	9.85	139.1119
CP-55,940	C24H40O3	376.2978	H+	377.3050	9.85	377.1748
5F-NPB-22	C22H20FN3O2	377.1540	H+	378.1612	9.17	
5F-NPB-22	C22H20FN3O2	377.1540	H+	378.1612	9.17	233.1084
5F-NPB-22	C22H20FN3O2	377.1540	H+	378.1612	9.17	213.1017
5F-NPB-22	C22H20FN3O2	377.1540	H+	378.1612	9.17	177.0452
5F-NPB-22	C22H20FN3O2	377.1540	H+	378.1612	9.17	145.0387
5F-NPB-22	C22H20FN3O2	377.1540	H+	378.1612	9.17	378.1615
5F-7-QUPAIC	C22H20FN3O2	377.1540	H+	378.1612	8.93	
5F-7-QUPAIC	C22H20FN3O2	377.1540	H+	378.1612	8.93	233.1079
5F-7-QUPAIC	C22H20FN3O2	377.1540	H+	378.1612	8.93	145.0385
5F-7-QUPAIC	C22H20FN3O2	377.1540	H+	378.1612	8.93	378.16
5F-7-QUPAIC	C22H20FN3O2	377.1540	H+	378.1612	8.93	117.044
5F-7-QUPAIC	C22H20FN3O2	377.1540	H+	378.1612	8.93	358.1559
F-2201	C24H21F2NO	377.1591	H+	378.1664	9.95	
F-2201	C24H21F2NO	377.1591	H+	378.1664	9.95	173.0395
F-2201	C24H21F2NO	377.1591	H+	378.1664	9.95	378.167
F-2201	C24H21F2NO	377.1591	H+	378.1664	9.95	232.1133
F-2201	C24H21F2NO	377.1591	H+	378.1664	9.95	145.0441
F-2201	C24H21F2NO	377.1591	H+	378.1664	9.95	125.0382
CUMYL-THPINACA	C23H27N3O2	377.2103	H+	378.2176	9.19	
CUMYL-THPINACA	C23H27N3O2	377.2103	H+	378.2176	9.19	243.114
CUMYL-THPINACA	C23H27N3O2	377.2103	H+	378.2176	9.19	119.0855
CUMYL-THPINACA	C23H27N3O2	377.2103	H+	378.2176	9.19	233.1175
CUMYL-THPINACA	C23H27N3O2	377.2103	H+	378.2176	9.19	260.1409
CUMYL-THPINACA	C23H27N3O2	377.2103	H+	378.2176	9.19	378.172
APP-PICA	C23H27N3O2	377.2103	H+	378.2176	9.05	
APP-PICA	C23H27N3O2	377.2103	H+	378.2176	9.05	214.1233
APP-PICA	C23H27N3O2	377.2103	H+	378.2176	9.05	144.0444
APP-PICA	C23H27N3O2	377.2103	H+	378.2176	9.05	361.1917
APP-PICA	C23H27N3O2	377.2103	H+	378.2176	9.05	378.2184
APP-PICA	C23H27N3O2	377.2103	H+	378.2176	9.05	116.0491
5F-ADB	C20H28FN3O3	377.2115	H+	378.2188	9.62	
5F-ADB	C20H28FN3O3	377.2115	H+	378.2188	9.62	233.1091

5F-ADB	C20H28FN3O3	377.2115	H+	378.2188	9.62	318.1982
5F-ADB	C20H28FN3O3	377.2115	H+	378.2188	9.62	213.1023
5F-ADB	C20H28FN3O3	377.2115	H+	378.2188	9.62	177.046
5F-ADB	C20H28FN3O3	377.2115	H+	378.2188	9.62	145.0395
5F-AEB	C20H28FN3O3	377.2115	H+	378.2188	9.6	
5F-AEB	C20H28FN3O3	377.2115	H+	378.2188	9.6	233.1087
5F-AEB	C20H28FN3O3	377.2115	H+	378.2188	9.6	213.1018
5F-AEB	C20H28FN3O3	377.2115	H+	378.2188	9.6	304.1825
5F-AEB	C20H28FN3O3	377.2115	H+	378.2188	9.6	145.0391
5F-AEB	C20H28FN3O3	377.2115	H+	378.2188	9.6	177.0457
Pravadoline (WIN-48,098)	C23H26N2O3	378.1943	H+	379.2016	6.78	
Pravadoline (WIN-48,098)	C23H26N2O3	378.1943	H+	379.2016	6.78	135.0437
Pravadoline (WIN-48,098)	C23H26N2O3	378.1943	H+	379.2016	6.78	114.0916
Pravadoline (WIN-48,098)	C23H26N2O3	378.1943	H+	379.2016	6.78	379.2017
Pravadoline (WIN-48,098)	C23H26N2O3	378.1943	H+	379.2016	6.78	107.0496
Pravadoline (WIN-48,098)	C23H26N2O3	378.1943	H+	379.2016	6.78	134.6365
Tetrahydrofuran Fentanyl	C24H30N2O2	378.2307	H+	379.2380	5.90	
Tetrahydrofuran Fentanyl	C24H30N2O2	378.2307	H+	379.2380	5.90	379.2369
Tetrahydrofuran Fentanyl	C24H30N2O2	378.2307	H+	379.2380	5.90	188.1431
Tetrahydrofuran Fentanyl	C24H30N2O2	378.2307	H+	379.2380	5.90	134.0962
Tetrahydrofuran Fentanyl	C24H30N2O2	378.2307	H+	379.2380	5.90	105.0702
Tetrahydrofuran Fentanyl	C24H30N2O2	378.2307	H+	379.2380	5.90	285.149
Hexanoyl Fentanyl	C25H34N2O	378.2671	H+	379.2744	7.75	
Hexanoyl Fentanyl	C25H34N2O	378.2671	H+	379.2744	7.75	188.1432
Hexanoyl Fentanyl	C25H34N2O	378.2671	H+	379.2744	7.75	379.2734
Hexanoyl Fentanyl	C25H34N2O	378.2671	H+	379.2744	7.75	105.0693
Hexanoyl Fentanyl	C25H34N2O	378.2671	H+	379.2744	7.75	258.1855
Hexanoyl Fentanyl	C25H34N2O	378.2671	H+	379.2744	7.75	134.096
25B-NBOMe	C18H22BrNO3	379.0783	H+	380.0856	7.14	
25B-NBOMe	C18H22BrNO3	379.0783	H+	380.0856	7.14	121.0651
25B-NBOMe	C18H22BrNO3	379.0783	H+	380.0856	7.14	380.0859
25B-NBOMe	C18H22BrNO3	379.0783	H+	380.0856	7.14	91.0555
25B-NBOMe	C18H22BrNO3	379.0783	H+	380.0856	7.14	93.0709
25B-NBOMe	C18H22BrNO3	379.0783	H+	380.0856	7.14	243.0013
FUB-JWH-018	C26H18FNO	379.1372	H+	380.1445	9.91	
FUB-JWH-018	C26H18FNO	379.1372	H+	380.1445	9.91	155.0497
FUB-JWH-018	C26H18FNO	379.1372	H+	380.1445	9.91	127.0547
FUB-JWH-018	C26H18FNO	379.1372	H+	380.1445	9.91	109.045
FUB-JWH-018	C26H18FNO	379.1372	H+	380.1445	9.91	252.0836
FUB-JWH-018	C26H18FNO	379.1372	H+	380.1445	9.91	380.1458
Donepezil	C24H29NO3	379.2147	H+	380.2220	6.13	
Donepezil	C24H29NO3	379.2147	H+	380.2220	6.13	380.2221
Donepezil	C24H29NO3	379.2147	H+	380.2220	6.13	91.0552
Donepezil	C24H29NO3	379.2147	H+	380.2220	6.13	326.2124
Donepezil	C24H29NO3	379.2147	H+	380.2220	6.13	288.1598
Donepezil	C24H29NO3	379.2147	H+	380.2220	6.13	273.1488
1P-LSD	C23H29N3O2	379.2260	H+	380.2333	6.49	
1P-LSD	C23H29N3O2	379.2260	H+	380.2333	6.49	279.1487
1P-LSD	C23H29N3O2	379.2260	H+	380.2333	6.49	380.2313
1P-LSD	C23H29N3O2	379.2260	H+	380.2333	6.49	337.1898
1P-LSD	C23H29N3O2	379.2260	H+	380.2333	6.49	253.1326
1P-LSD	C23H29N3O2	379.2260	H+	380.2333	6.49	223.1223
Benzyl Carfentanil	C23H28N2O3	380.2099	H+	381.2172	6.34	
Benzyl Carfentanil	C23H28N2O3	380.2099	H+	381.2172	6.34	321.1944
Benzyl Carfentanil	C23H28N2O3	380.2099	H+	381.2172	6.34	654.1684
Benzyl Carfentanil	C23H28N2O3	380.2099	H+	381.2172	6.34	232.1316
Benzyl Carfentanil	C23H28N2O3	380.2099	H+	381.2172	6.34	202.1211
Benzyl Carfentanil	C23H28N2O3	380.2099	H+	381.2172	6.34	146.0953
4-Methoxybutyryl Fentanyl	C24H32N2O2	380.2463	H+	381.2536	6.87	
4-Methoxybutyryl Fentanyl	C24H32N2O2	380.2463	H+	381.2536	6.87	242.2829
4-Methoxybutyryl Fentanyl	C24H32N2O2	380.2463	H+	381.2536	6.87	142.1581
4-Methoxybutyryl Fentanyl	C24H32N2O2	380.2463	H+	381.2536	6.87	186.22
4-Methoxybutyryl Fentanyl	C24H32N2O2	380.2463	H+	381.2536	6.87	100.1115
4-Methoxybutyryl Fentanyl	C24H32N2O2	380.2463	H+	381.2536	6.87	130.1564
ADB-FUBICA	C22H24FN3O2	381.1853	H+	382.1925	8.64	
ADB-FUBICA	C22H24FN3O2	381.1853	H+	382.1925	8.64	252.0805
ADB-FUBICA	C22H24FN3O2	381.1853	H+	382.1925	8.64	109.0436
ADB-FUBICA	C22H24FN3O2	381.1853	H+	382.1925	8.64	365.1637
ADB-FUBICA	C22H24FN3O2	381.1853	H+	382.1925	8.64	337.1693
ADB-FUBICA	C22H24FN3O2	381.1853	H+	382.1925	8.64	382.1908
JWH-147	C27H27NO	381.2093	H+	382.2165	10.97	
JWH-147	C27H27NO	381.2093	H+	382.2165	10.97	155.0494
JWH-147	C27H27NO	381.2093	H+	382.2165	10.97	127.0541
JWH-147	C27H27NO	381.2093	H+	382.2165	10.97	382.2185

JWH-147	C27H27NO	381.2093	H+	382.2165	10.97	254.1558
JWH-147	C27H27NO	381.2093	H+	382.2165	10.97	126.0469
JWH-370	C27H27NO	381.2093	H+	382.2165	9.92	
JWH-370	C27H27NO	381.2093	H+	382.2165	9.92	155.0492
JWH-370	C27H27NO	381.2093	H+	382.2165	9.92	127.0541
JWH-370	C27H27NO	381.2093	H+	382.2165	9.92	382.2179
JWH-370	C27H27NO	381.2093	H+	382.2165	9.92	254.1543
JWH-370	C27H27NO	381.2093	H+	382.2165	9.92	184.076
3-CAF	C24H15FN2O2	382.1118	H+	383.1190	10.45	
3-CAF	C24H15FN2O2	382.1118	H+	383.1190	10.45	239.0622
3-CAF	C24H15FN2O2	382.1118	H+	383.1190	10.45	211.0668
3-CAF	C24H15FN2O2	382.1118	H+	383.1190	10.45	191.0605
3-CAF	C24H15FN2O2	382.1118	H+	383.1190	10.45	184.0559
3-CAF	C24H15FN2O2	382.1118	H+	383.1190	10.45	383.1203
MMB-FUBICA	C22H23FN2O3	382.1693	H+	383.1766	9.07	
MMB-FUBICA	C22H23FN2O3	382.1693	H+	383.1766	9.07	252.0825
MMB-FUBICA	C22H23FN2O3	382.1693	H+	383.1766	9.07	109.0444
MMB-FUBICA	C22H23FN2O3	382.1693	H+	383.1766	9.07	383.1772
MMB-FUBICA	C22H23FN2O3	382.1693	H+	383.1766	9.07	224.0879
MMB-FUBICA	C22H23FN2O3	382.1693	H+	383.1766	9.07	351.1497
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	382.1693	H+	383.1766	8.94	
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	382.1693	H+	383.1766	8.94	252.0812
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	382.1693	H+	383.1766	8.94	109.0446
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	382.1693	H+	383.1766	8.94	383.177
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	382.1693	H+	383.1766	8.94	365.1629
MDMB-FUBICA 3,3-Dimethylbutanoic Acid	C22H23FN2O3	382.1693	H+	383.1766	8.94	224.0885
ADB-FUBINACA	C21H23FN4O2	382.1805	H+	383.1878	8.65	
ADB-FUBINACA	C21H23FN4O2	382.1805	H+	383.1878	8.65	253.0776
ADB-FUBINACA	C21H23FN4O2	382.1805	H+	383.1878	8.65	338.1668
ADB-FUBINACA	C21H23FN4O2	382.1805	H+	383.1878	8.65	109.0453
ADB-FUBINACA	C21H23FN4O2	382.1805	H+	383.1878	8.65	366.1612
ADB-FUBINACA	C21H23FN4O2	382.1805	H+	383.1878	8.65	270.1054
para-Chloro Cyclopropylfentanyl	C23H27ClN2O	382.1812	H+	383.1885	7.07	
para-Chloro Cyclopropylfentanyl	C23H27ClN2O	382.1812	H+	383.1885	7.07	188.1434
para-Chloro Cyclopropylfentanyl	C23H27ClN2O	382.1812	H+	383.1885	7.07	383.1879
para-Chloro Cyclopropylfentanyl	C23H27ClN2O	382.1812	H+	383.1885	7.07	105.0697
para-Chloro Cyclopropylfentanyl	C23H27ClN2O	382.1812	H+	383.1885	7.07	262.0994
para-Chloro Cyclopropylfentanyl	C23H27ClN2O	382.1812	H+	383.1885	7.07	69.0337
AM-1220	C26H26N2O	382.2045	H+	383.2118	7.16	
AM-1220	C26H26N2O	382.2045	H+	383.2118	7.16	112.1122
AM-1220	C26H26N2O	382.2045	H+	383.2118	7.16	155.0491
AM-1220	C26H26N2O	382.2045	H+	383.2118	7.16	98.0972
AM-1220	C26H26N2O	382.2045	H+	383.2118	7.16	383.2115
AM-1220	C26H26N2O	382.2045	H+	383.2118	7.16	286.1228
para-Methoxy Methoxyacetylfentanyl	C23H30N2O3	382.2256	H+	383.2329	5.86	
para-Methoxy Methoxyacetylfentanyl	C23H30N2O3	382.2256	H+	383.2329	5.86	188.1429
para-Methoxy Methoxyacetylfentanyl	C23H30N2O3	382.2256	H+	383.2329	5.86	105.0694
para-Methoxy Methoxyacetylfentanyl	C23H30N2O3	382.2256	H+	383.2329	5.86	383.2319
para-Methoxy Methoxyacetylfentanyl	C23H30N2O3	382.2256	H+	383.2329	5.86	262.1448
para-Methoxy Methoxyacetylfentanyl	C23H30N2O3	382.2256	H+	383.2329	5.86	134.0959
STS-135	C24H31FN2O	382.2420	H+	383.2493	10.25	
STS-135	C24H31FN2O	382.2420	H+	383.2493	10.25	135.1166
STS-135	C24H31FN2O	382.2420	H+	383.2493	10.25	232.1138
STS-135	C24H31FN2O	382.2420	H+	383.2493	10.25	383.2498
STS-135	C24H31FN2O	382.2420	H+	383.2493	10.25	206.1339
STS-135	C24H31FN2O	382.2420	H+	383.2493	10.25	107.0855
para-Fluoro Valerylfentanyl	C24H31FN2O	382.2420	H+	383.2493	7.38	
para-Fluoro Valerylfentanyl	C24H31FN2O	382.2420	H+	383.2493	7.38	188.1429
para-Fluoro Valerylfentanyl	C24H31FN2O	382.2420	H+	383.2493	7.38	105.0692
para-Fluoro Valerylfentanyl	C24H31FN2O	382.2420	H+	383.2493	7.38	383.2484
para-Fluoro Valerylfentanyl	C24H31FN2O	382.2420	H+	383.2493	7.38	262.1597
para-Fluoro Valerylfentanyl	C24H31FN2O	382.2420	H+	383.2493	7.38	299.192
JWH-249	C21H22BrNO	383.0885	H+	384.0958	10.35	
JWH-249	C21H22BrNO	383.0885	H+	384.0958	10.35	168.9645
JWH-249	C21H22BrNO	383.0885	H+	384.0958	10.35	214.1234
JWH-249	C21H22BrNO	383.0885	H+	384.0958	10.35	188.1442
JWH-249	C21H22BrNO	383.0885	H+	384.0958	10.35	384.0966
JWH-249	C21H22BrNO	383.0885	H+	384.0958	10.35	144.0447

MMB-FUBINACA	C21H22FN3O3	383.1645	H+	384.1718	9.42	
MMB-FUBINACA	C21H22FN3O3	383.1645	H+	384.1718	9.42	253.078
MMB-FUBINACA	C21H22FN3O3	383.1645	H+	384.1718	9.42	109.0443
MMB-FUBINACA	C21H22FN3O3	383.1645	H+	384.1718	9.42	324.1517
MMB-FUBINACA	C21H22FN3O3	383.1645	H+	384.1718	9.42	384.1737
MMB-FUBINACA	C21H22FN3O3	383.1645	H+	384.1718	9.42	352.1472
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	383.1645	H+	384.1718	9.19	
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	383.1645	H+	384.1718	9.19	253.0755
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	383.1645	H+	384.1718	9.19	338.1637
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	383.1645	H+	384.1718	9.19	109.0437
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	383.1645	H+	384.1718	9.19	384.169
MDMB-FUBINACA 3,3-Dimethylbutanoic Acid	C21H22FN3O3	383.1645	H+	384.1718	9.19	270.104
Quetiapine	C21H25N3O2S	383.1667	H+	384.1740	6.43	
Quetiapine	C21H25N3O2S	383.1667	H+	384.1740	6.43	253.0795
Quetiapine	C21H25N3O2S	383.1667	H+	384.1740	6.43	279.0954
Quetiapine	C21H25N3O2S	383.1667	H+	384.1740	6.43	384.1744
Quetiapine	C21H25N3O2S	383.1667	H+	384.1740	6.43	221.1075
Quetiapine	C21H25N3O2S	383.1667	H+	384.1740	6.43	210.0376
JWH-182	C27H29NO	383.2249	H+	384.2322	11.18	
JWH-182	C27H29NO	383.2249	H+	384.2322	11.18	197.0695
JWH-182	C27H29NO	383.2249	H+	384.2322	11.18	214.123
JWH-182	C27H29NO	383.2249	H+	384.2322	11.18	384.2337
JWH-182	C27H29NO	383.2249	H+	384.2322	11.18	141.0698
JWH-182	C27H29NO	383.2249	H+	384.2322	11.18	169.1011
JWH-213	C27H29NO	383.2249	H+	384.2322	11.05	
JWH-213	C27H29NO	383.2249	H+	384.2322	11.05	183.08
JWH-213	C27H29NO	383.2249	H+	384.2322	11.05	228.138
JWH-213	C27H29NO	383.2249	H+	384.2322	11.05	384.232
JWH-213	C27H29NO	383.2249	H+	384.2322	11.05	155.085
JWH-213	C27H29NO	383.2249	H+	384.2322	11.05	115.0532
JWH-011	C27H29NO	383.2249	H+	384.2322	10.97	
JWH-011	C27H29NO	383.2249	H+	384.2322	10.97	155.0487
JWH-011	C27H29NO	383.2249	H+	384.2322	10.97	384.2326
JWH-011	C27H29NO	383.2249	H+	384.2322	10.97	127.0535
JWH-011	C27H29NO	383.2249	H+	384.2322	10.97	286.1233
JWH-011	C27H29NO	383.2249	H+	384.2322	10.97	256.1703
5F-AKB48 (5F-APINACA)	C23H30FN3O	383.2373	H+	384.2446	10.56	
5F-AKB48 (5F-APINACA)	C23H30FN3O	383.2373	H+	384.2446	10.56	135.1168
5F-AKB48 (5F-APINACA)	C23H30FN3O	383.2373	H+	384.2446	10.56	384.2449
5F-AKB48 (5F-APINACA)	C23H30FN3O	383.2373	H+	384.2446	10.56	107.0861
5F-AKB48 (5F-APINACA)	C23H30FN3O	383.2373	H+	384.2446	10.56	93.071
5F-AKB48 (5F-APINACA)	C23H30FN3O	383.2373	H+	384.2446	10.56	79.0559
ORG 28611	C23H33N3O2	383.2573	H+	384.2646	7.73	
ORG 28611	C23H33N3O2	383.2573	H+	384.2646	7.73	270.1502
ORG 28611	C23H33N3O2	383.2573	H+	384.2646	7.73	174.0558
ORG 28611	C23H33N3O2	383.2573	H+	384.2646	7.73	384.2644
ORG 28611	C23H33N3O2	383.2573	H+	384.2646	7.73	159.0323
ORG 28611	C23H33N3O2	383.2573	H+	384.2646	7.73	97.1023
BB-22 (QUCHIC)	C25H24N2O2	384.1838	H+	385.1911	10.32	
BB-22 (QUCHIC)	C25H24N2O2	384.1838	H+	385.1911	10.32	240.138
BB-22 (QUCHIC)	C25H24N2O2	384.1838	H+	385.1911	10.32	144.0438
BB-22 (QUCHIC)	C25H24N2O2	384.1838	H+	385.1911	10.32	385.1914
BB-22 (QUCHIC)	C25H24N2O2	384.1838	H+	385.1911	10.32	158.0597
BB-22 (QUCHIC)	C25H24N2O2	384.1838	H+	385.1911	10.32	116.0491
JWH-200	C25H24N2O2	384.1838	H+	385.1911	7.42	
JWH-200	C25H24N2O2	384.1838	H+	385.1911	7.42	155.0487
JWH-200	C25H24N2O2	384.1838	H+	385.1911	7.42	114.0916
JWH-200	C25H24N2O2	384.1838	H+	385.1911	7.42	385.1914
JWH-200	C25H24N2O2	384.1838	H+	385.1911	7.42	127.0542
JWH-200	C25H24N2O2	384.1838	H+	385.1911	7.42	70.0669
para-Chlorobutyryl Fentanyl	C23H29ClN2O	384.1968	H+	385.2041	7.28	
para-Chlorobutyryl Fentanyl	C23H29ClN2O	384.1968	H+	385.2041	7.28	188.1417
para-Chlorobutyryl Fentanyl	C23H29ClN2O	384.1968	H+	385.2041	7.28	105.0692
para-Chlorobutyryl Fentanyl	C23H29ClN2O	384.1968	H+	385.2041	7.28	385.1999
para-Chlorobutyryl Fentanyl	C23H29ClN2O	384.1968	H+	385.2041	7.28	264.1124
para-Chlorobutyryl Fentanyl	C23H29ClN2O	384.1968	H+	385.2041	7.28	134.0952
Phenyl Fentanyl	C26H28N2O	384.2202	H+	385.2274	6.78	
Phenyl Fentanyl	C26H28N2O	384.2202	H+	385.2274	6.78	188.1446

Phenyl Fentanyl	C26H28N2O	384.2202	H+	385.2274	6.78	264.1402
Phenyl Fentanyl	C26H28N2O	384.2202	H+	385.2274	6.78	146.0971
Phenyl Fentanyl	C26H28N2O	384.2202	H+	385.2274	6.78	134.0971
Phenyl Fentanyl	C26H28N2O	384.2202	H+	385.2274	6.78	105.0342
5F-APINAC	C23H29FN2O2	384.2213	H+	385.2286	10.97	
5F-APINAC	C23H29FN2O2	384.2213	H+	385.2286	10.97	135.1159
5F-APINAC	C23H29FN2O2	384.2213	H+	385.2286	10.97	385.229
5F-APINAC	C23H29FN2O2	384.2213	H+	385.2286	10.97	107.085
5F-APINAC	C23H29FN2O2	384.2213	H+	385.2286	10.97	93.0686
5F-APINAC	C23H29FN2O2	384.2213	H+	385.2286	10.97	79.0531
MDMB-CHMICA	C23H32N2O3	384.2413	H+	385.2486	10.33	
MDMB-CHMICA	C23H32N2O3	384.2413	H+	385.2486	10.33	240.1394
MDMB-CHMICA	C23H32N2O3	384.2413	H+	385.2486	10.33	144.0446
MDMB-CHMICA	C23H32N2O3	384.2413	H+	385.2486	10.33	385.2487
MDMB-CHMICA	C23H32N2O3	384.2413	H+	385.2486	10.33	116.0503
MDMB-CHMICA	C23H32N2O3	384.2413	H+	385.2486	10.33	97.1017
JWH-307	C26H24FNO	385.1842	H+	386.1915	10.61	
JWH-307	C26H24FNO	385.1842	H+	386.1915	10.61	155.0485
JWH-307	C26H24FNO	385.1842	H+	386.1915	10.61	127.054
JWH-307	C26H24FNO	385.1842	H+	386.1915	10.61	386.1904
JWH-307	C26H24FNO	385.1842	H+	386.1915	10.61	369.1246
JWH-307	C26H24FNO	385.1842	H+	386.1915	10.61	258.1292
JWH-368	C26H24FNO	385.1842	H+	386.1915	10.80	
JWH-368	C26H24FNO	385.1842	H+	386.1915	10.80	155.0486
JWH-368	C26H24FNO	385.1842	H+	386.1915	10.80	127.0534
JWH-368	C26H24FNO	385.1842	H+	386.1915	10.80	386.192
JWH-368	C26H24FNO	385.1842	H+	386.1915	10.80	258.1297
JWH-368	C26H24FNO	385.1842	H+	386.1915	10.80	188.0505
4F-CUMYL-5F-PINACA	C22H25F2N3O	385.1966	H+	386.2039	9.37	
4F-CUMYL-5F-PINACA	C22H25F2N3O	385.1966	H+	386.2039	9.37	233.1094
4F-CUMYL-5F-PINACA	C22H25F2N3O	385.1966	H+	386.2039	9.37	137.0759
4F-CUMYL-5F-PINACA	C22H25F2N3O	385.1966	H+	386.2039	9.37	213.1023
4F-CUMYL-5F-PINACA	C22H25F2N3O	385.1966	H+	386.2039	9.37	250.1358
4F-CUMYL-5F-PINACA	C22H25F2N3O	385.1966	H+	386.2039	9.37	177.0456
JWH-098	C26H27NO2	385.2042	H+	386.2115	10.6	
JWH-098	C26H27NO2	385.2042	H+	386.2115	10.6	185.0588
JWH-098	C26H27NO2	385.2042	H+	386.2115	10.6	386.2107
JWH-098	C26H27NO2	385.2042	H+	386.2115	10.6	228.138
JWH-098	C26H27NO2	385.2042	H+	386.2115	10.6	157.0643
JWH-098	C26H27NO2	385.2042	H+	386.2115	10.6	158.0597
MDMB-CHMINACA	C22H31N3O3	385.2365	H+	386.2438	10.61	
MDMB-CHMINACA	C22H31N3O3	385.2365	H+	386.2438	10.61	241.1319
MDMB-CHMINACA	C22H31N3O3	385.2365	H+	386.2438	10.61	326.2207
MDMB-CHMINACA	C22H31N3O3	385.2365	H+	386.2438	10.61	145.0382
MDMB-CHMINACA	C22H31N3O3	385.2365	H+	386.2438	10.61	386.2414
MDMB-CHMINACA	C22H31N3O3	385.2365	H+	386.2438	10.61	354.2157
Buspirone	C21H31N5O2	385.2478	H+	386.2551	5.88	
Buspirone	C21H31N5O2	385.2478	H+	386.2551	5.88	386.2541
Buspirone	C21H31N5O2	385.2478	H+	386.2551	5.88	122.0715
Buspirone	C21H31N5O2	385.2478	H+	386.2551	5.88	265.191
Buspirone	C21H31N5O2	385.2478	H+	386.2551	5.88	222.1485
Buspirone	C21H31N5O2	385.2478	H+	386.2551	5.88	150.1023
Phenazolam	C17H12BrClN4	385.9934	H+	387.0007	7.62	
Phenazolam	C17H12BrClN4	385.9934	H+	387.0007	7.62	386.9999
Phenazolam	C17H12BrClN4	385.9934	H+	387.0007	7.62	308.0822
Phenazolam	C17H12BrClN4	385.9934	H+	387.0007	7.62	358.9817
Phenazolam	C17H12BrClN4	385.9934	H+	387.0007	7.62	388.9974
Phenazolam	C17H12BrClN4	385.9934	H+	387.0007	7.62	360.9793
Mesoridazine	C21H26N2OS2	386.1487	H+	387.1559	6.45	
Mesoridazine	C21H26N2OS2	386.1487	H+	387.1559	6.45	126.1275
Mesoridazine	C21H26N2OS2	386.1487	H+	387.1559	6.45	98.0968
Mesoridazine	C21H26N2OS2	386.1487	H+	387.1559	6.45	387.1561
Mesoridazine	C21H26N2OS2	386.1487	H+	387.1559	6.45	372.1325
Mesoridazine	C21H26N2OS2	386.1487	H+	387.1559	6.45	274.0362
Oliceridine	C22H30N2O2S	386.2028	H+	387.2101	6.49	
Oliceridine	C22H30N2O2S	386.2028	H+	387.2101	6.49	244.1701
Oliceridine	C22H30N2O2S	386.2028	H+	387.2101	6.49	127.0211
Oliceridine	C22H30N2O2S	386.2028	H+	387.2101	6.49	387.2098
Oliceridine	C22H30N2O2S	386.2028	H+	387.2101	6.49	99.2062
Oliceridine	C22H30N2O2S	386.2028	H+	387.2101	6.49	58.995
Sufentanil	C22H30N2O2S	386.2028	H+	387.2101	6.89	
Sufentanil	C22H30N2O2S	386.2028	H+	387.2101	6.89	238.1256
Sufentanil	C22H30N2O2S	386.2028	H+	387.2101	6.89	387.21
Sufentanil	C22H30N2O2S	386.2028	H+	387.2101	6.89	355.1834

Sufentanil	C22H30N2O2S	386.2028	H+	387.2101	6.89	111.026
Sufentanil	C22H30N2O2S	386.2028	H+	387.2101	6.89	140.1068
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	386.2170	H+	387.2243	6.84	
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	386.2170	H+	387.2243	6.84	220.1491
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	386.2170	H+	387.2243	6.84	387.2235
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	386.2170	H+	387.2243	6.84	123.06
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	386.2170	H+	387.2243	6.84	248.1447
Difluoro-cis-3-Methylfentanyl	C23H28F2N2O	386.2170	H+	387.2243	6.84	152.0868
MO-CHMINACA	C22H30N2O4	386.2206	H+	387.2278	10.76	
MO-CHMINACA	C22H30N2O4	386.2206	H+	387.2278	10.76	241.1333
MO-CHMINACA	C22H30N2O4	386.2206	H+	387.2278	10.76	145.0381
MO-CHMINACA	C22H30N2O4	386.2206	H+	387.2278	10.76	387.2304
MO-CHMINACA	C22H30N2O4	386.2206	H+	387.2278	10.76	327.2269
MO-CHMINACA	C22H30N2O4	386.2206	H+	387.2278	10.76	259.1443
HU-210/HU-211	C25H38O3	386.2821	H+	387.2894	10.95	
HU-210/HU-211	C25H38O3	386.2821	H+	387.2894	10.95	243.1374
HU-210/HU-211	C25H38O3	386.2821	H+	387.2894	10.95	201.0905
HU-210/HU-211	C25H38O3	386.2821	H+	387.2894	10.95	71.0867
HU-210/HU-211	C25H38O3	386.2821	H+	387.2894	10.95	387.2895
HU-210/HU-211	C25H38O3	386.2821	H+	387.2894	10.95	369.2793
Flurazepam	C21H23ClFN3O	387.1514	H+	388.1586	6.41	
Flurazepam	C21H23ClFN3O	387.1514	H+	388.1586	6.41	315.0686
Flurazepam	C21H23ClFN3O	387.1514	H+	388.1586	6.41	388.1579
Flurazepam	C21H23ClFN3O	387.1514	H+	388.1586	6.41	355.0694
Flurazepam	C21H23ClFN3O	387.1514	H+	388.1586	6.41	317.085
Flurazepam	C21H23ClFN3O	387.1514	H+	388.1586	6.41	266.9986
EAM-2201	C26H26FNO	387.1998	H+	388.2071	10.18	
EAM-2201	C26H26FNO	387.1998	H+	388.2071	10.18	183.0795
EAM-2201	C26H26FNO	387.1998	H+	388.2071	10.18	232.1122
EAM-2201	C26H26FNO	387.1998	H+	388.2071	10.18	388.2065
EAM-2201	C26H26FNO	387.1998	H+	388.2071	10.18	155.0847
EAM-2201	C26H26FNO	387.1998	H+	388.2071	10.18	144.044
Eszopiclone / Zopiclone	C17H17ClN6O3	388.1051	H+	389.1123	4.93	
Eszopiclone / Zopiclone	C17H17ClN6O3	388.1051	H+	389.1123	4.93	245.0226
Eszopiclone / Zopiclone	C17H17ClN6O3	388.1051	H+	389.1123	4.93	217.0277
Eszopiclone / Zopiclone	C17H17ClN6O3	388.1051	H+	389.1123	4.93	356.0709
Eszopiclone / Zopiclone	C17H17ClN6O3	388.1051	H+	389.1123	4.93	345.1227
Eszopiclone / Zopiclone	C17H17ClN6O3	388.1051	H+	389.1123	4.93	267.999
ortho-Methyl Furanylfentanyl	C25H28N2O2	388.2151	H+	389.2224	6.66	
ortho-Methyl Furanylfentanyl	C25H28N2O2	388.2151	H+	389.2224	6.66	188.1433
ortho-Methyl Furanylfentanyl	C25H28N2O2	388.2151	H+	389.2224	6.66	105.0692
ortho-Methyl Furanylfentanyl	C25H28N2O2	388.2151	H+	389.2224	6.66	389.2222
ortho-Methyl Furanylfentanyl	C25H28N2O2	388.2151	H+	389.2224	6.66	268.1335
ortho-Methyl Furanylfentanyl	C25H28N2O2	388.2151	H+	389.2224	6.66	146.0962
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	389.1354	H+	390.1427	10.58	
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	389.1354	H+	390.1427	10.58	125.0962
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	389.1354	H+	390.1427	10.58	292.0345
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	389.1354	H+	390.1427	10.58	390.1436
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	389.1354	H+	390.1427	10.58	372.1327
UR-144 N-(5-Bromopentyl) Analogue	C21H28BrNO	389.1354	H+	390.1427	10.58	357.1104
Tadalafil	C22H19N3O4	389.1376	H+	390.1448	7.39	
Tadalafil	C22H19N3O4	389.1376	H+	390.1448	7.39	121.0651
Tadalafil	C22H19N3O4	389.1376	H+	390.1448	7.39	268.1077
Tadalafil	C22H19N3O4	389.1376	H+	390.1448	7.39	390.1446
Tadalafil	C22H19N3O4	389.1376	H+	390.1448	7.39	380.0859
Tadalafil	C22H19N3O4	389.1376	H+	390.1448	7.39	262.0857
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	389.1546	H+	390.1619	10.35	
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	389.1546	H+	390.1619	10.35	169.0646
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	389.1546	H+	390.1619	10.35	248.084
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	389.1546	H+	390.1619	10.35	390.1619
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	389.1546	H+	390.1619	10.35	141.0692
MAM-2201 N-(5-Chloropentyl) Analogue	C25H24ClNO	389.1546	H+	390.1619	10.35	115.0539
Salvinorin B	C21H26O7	390.1679	H+	391.1751	6.81	
Salvinorin B	C21H26O7	390.1679	H+	391.1751	6.81	149.0227
Salvinorin B	C21H26O7	390.1679	H+	391.1751	6.81	258.0668
Salvinorin B	C21H26O7	390.1679	H+	391.1751	6.81	251.1277
Salvinorin B	C21H26O7	390.1679	H+	391.1751	6.81	167.0336
Salvinorin B	C21H26O7	390.1679	H+	391.1751	6.81	145.1043
Thiophene Fentanyl	C24H26N2OS	390.1766	H+	391.1839	6.84	
Thiophene Fentanyl	C24H26N2OS	390.1766	H+	391.1839	6.84	188.1442
Thiophene Fentanyl	C24H26N2OS	390.1766	H+	391.1839	6.84	105.0699
Thiophene Fentanyl	C24H26N2OS	390.1766	H+	391.1839	6.84	270.0955
Thiophene Fentanyl	C24H26N2OS	390.1766	H+	391.1839	6.84	391.185
Thiophene Fentanyl	C24H26N2OS	390.1766	H+	391.1839	6.84	110.9899

5F-CUMYL-PeGACLONE	C25H27FN2O	390.2107	H+	391.2180	9.43	
5F-CUMYL-PeGACLONE	C25H27FN2O	390.2107	H+	391.2180	9.43	273.1403
5F-CUMYL-PeGACLONE	C25H27FN2O	390.2107	H+	391.2180	9.43	119.0853
5F-CUMYL-PeGACLONE	C25H27FN2O	390.2107	H+	391.2180	9.43	253.1339
5F-CUMYL-PeGACLONE	C25H27FN2O	390.2107	H+	391.2180	9.43	185.0709
5F-CUMYL-PeGACLONE	C25H27FN2O	390.2107	H+	391.2180	9.43	91.0547
Cyclohexyl Fentanyl	C26H34N2O	390.2671	H+	391.2744	7.63	
Cyclohexyl Fentanyl	C26H34N2O	390.2671	H+	391.2744	7.63	188.1437
Cyclohexyl Fentanyl	C26H34N2O	390.2671	H+	391.2744	7.63	105.0695
Cyclohexyl Fentanyl	C26H34N2O	390.2671	H+	391.2744	7.63	281.2017
Cyclohexyl Fentanyl	C26H34N2O	390.2671	H+	391.2744	7.63	270.1853
Cyclohexyl Fentanyl	C26H34N2O	390.2671	H+	391.2744	7.63	391.275
AM-1248	C26H34N2O	390.2671	H+	391.2744	8.13	
AM-1248	C26H34N2O	390.2671	H+	391.2744	8.13	135.1165
AM-1248	C26H34N2O	390.2671	H+	391.2744	8.13	391.2739
AM-1248	C26H34N2O	390.2671	H+	391.2744	8.13	112.1123
AM-1248	C26H34N2O	390.2671	H+	391.2744	8.13	98.0972
AM-1248	C26H34N2O	390.2671	H+	391.2744	8.13	294.186
EG018	C28H25NO	391.1936	H+	392.2009	11.30	
EG018	C28H25NO	391.1936	H+	392.2009	11.30	155.0483
EG018	C28H25NO	391.1936	H+	392.2009	11.30	392.1996
EG018	C28H25NO	391.1936	H+	392.2009	11.30	246.1379
EG018	C28H25NO	391.1936	H+	392.2009	11.30	127.0538
EG018	C28H25NO	391.1936	H+	392.2009	11.30	179.0725
5F-EDMB-PINACA	C21H30FN3O3	391.2271	H+	392.2344	9.92	
5F-EDMB-PINACA	C21H30FN3O3	391.2271	H+	392.2344	9.92	233.1089
5F-EDMB-PINACA	C21H30FN3O3	391.2271	H+	392.2344	9.92	318.1982
5F-EDMB-PINACA	C21H30FN3O3	391.2271	H+	392.2344	9.92	213.1018
5F-EDMB-PINACA	C21H30FN3O3	391.2271	H+	392.2344	9.92	145.0391
5F-EDMB-PINACA	C21H30FN3O3	391.2271	H+	392.2344	9.92	392.2347
ACHMINACA	C25H33N3O	391.2624	H+	392.2696	11.84	
ACHMINACA	C25H33N3O	391.2624	H+	392.2696	11.84	135.1166
ACHMINACA	C25H33N3O	391.2624	H+	392.2696	11.84	392.2695
ACHMINACA	C25H33N3O	391.2624	H+	392.2696	11.84	107.0855
ACHMINACA	C25H33N3O	391.2624	H+	392.2696	11.84	149.0231
ACHMINACA	C25H33N3O	391.2624	H+	392.2696	11.84	241.1347
ortho-Fluoro Furanylfentanyl	C24H25FN2O2	392.1900	H+	393.1973	6.43	
ortho-Fluoro Furanylfentanyl	C24H25FN2O2	392.1900	H+	393.1973	6.43	188.1439
ortho-Fluoro Furanylfentanyl	C24H25FN2O2	392.1900	H+	393.1973	6.43	105.0698
ortho-Fluoro Furanylfentanyl	C24H25FN2O2	392.1900	H+	393.1973	6.43	393.1973
ortho-Fluoro Furanylfentanyl	C24H25FN2O2	392.1900	H+	393.1973	6.43	272.1093
ortho-Fluoro Furanylfentanyl	C24H25FN2O2	392.1900	H+	393.1973	6.43	146.0962
5F-AB-FUPPYCA	C20H26F2N4O2	392.2024	H+	393.2097	8.7	
5F-AB-FUPPYCA	C20H26F2N4O2	392.2024	H+	393.2097	8.7	348.1901
5F-AB-FUPPYCA	C20H26F2N4O2	392.2024	H+	393.2097	8.7	260.121
5F-AB-FUPPYCA	C20H26F2N4O2	392.2024	H+	393.2097	8.7	189.0468
5F-AB-FUPPYCA	C20H26F2N4O2	392.2024	H+	393.2097	8.7	277.1168
5F-AB-FUPPYCA	C20H26F2N4O2	392.2024	H+	393.2097	8.7	393.2122
para-Methyl Tetrahydrofuranylfentanyl	C25H32N2O2	392.2464	H+	393.2537	6.49	
para-Methyl Tetrahydrofuranylfentanyl	C25H32N2O2	392.2464	H+	393.2537	6.49	188.1432
para-Methyl Tetrahydrofuranylfentanyl	C25H32N2O2	392.2464	H+	393.2537	6.49	105.0694
para-Methyl Tetrahydrofuranylfentanyl	C25H32N2O2	392.2464	H+	393.2537	6.49	393.2528
para-Methyl Tetrahydrofuranylfentanyl	C25H32N2O2	392.2464	H+	393.2537	6.49	146.0965
para-Methyl Tetrahydrofuranylfentanyl	C25H32N2O2	392.2464	H+	393.2537	6.49	134.0961
ATHPINACA	C24H31N3O2	393.2416	H+	394.2489	10.3	
ATHPINACA	C24H31N3O2	393.2416	H+	394.2489	10.3	135.1167
ATHPINACA	C24H31N3O2	393.2416	H+	394.2489	10.3	107.0854
ATHPINACA	C24H31N3O2	393.2416	H+	394.2489	10.3	394.2482
ATHPINACA	C24H31N3O2	393.2416	H+	394.2489	10.3	93.0703
ATHPINACA	C24H31N3O2	393.2416	H+	394.2489	10.3	258.1245
FDU-NNEI	C26H19FN2O	394.1481	H+	395.1554	9.44	
FDU-NNEI	C26H19FN2O	394.1481	H+	395.1554	9.44	252.0827
FDU-NNEI	C26H19FN2O	394.1481	H+	395.1554	9.44	109.0443
FDU-NNEI	C26H19FN2O	394.1481	H+	395.1554	9.44	395.1562
FDU-NNEI	C26H19FN2O	394.1481	H+	395.1554	9.44	226.1034
FDU-NNEI	C26H19FN2O	394.1481	H+	395.1554	9.44	224.0879
Tetrahydrothiophene Fentanyl	C24H30N2OS	394.2079	H+	395.2152	6.72	
Tetrahydrothiophene Fentanyl	C24H30N2OS	394.2079	H+	395.2152	6.72	188.1414
Tetrahydrothiophene Fentanyl	C24H30N2OS	394.2079	H+	395.2152	6.72	105.0685
Tetrahydrothiophene Fentanyl	C24H30N2OS	394.2079	H+	395.2152	6.72	395.2106
Tetrahydrothiophene Fentanyl	C24H30N2OS	394.2079	H+	395.2152	6.72	274.1242
Tetrahydrothiophene Fentanyl	C24H30N2OS	394.2079	H+	395.2152	6.72	134.0954
Carfentanil	C24H30N2O3	394.2256	H+	395.2329	6.54	
Carfentanil	C24H30N2O3	394.2256	H+	395.2329	6.54	335.2116

Carfentanil	C24H30N2O3	394.2256	H+	395.2329	6.54	246.1485
Carfentanil	C24H30N2O3	394.2256	H+	395.2329	6.54	113.0599
Carfentanil	C24H30N2O3	394.2256	H+	395.2329	6.54	279.1851
Carfentanil	C24H30N2O3	394.2256	H+	395.2329	6.54	395.2323
FDU-PB-22	C26H18FNO2	395.1322	H+	396.1394	10.44	
FDU-PB-22	C26H18FNO2	395.1322	H+	396.1394	10.44	252.0827
FDU-PB-22	C26H18FNO2	395.1322	H+	396.1394	10.44	109.0445
FDU-PB-22	C26H18FNO2	395.1322	H+	396.1394	10.44	224.088
FDU-PB-22	C26H18FNO2	395.1322	H+	396.1394	10.44	83.0293
FDU-PB-22	C26H18FNO2	395.1322	H+	396.1394	10.44	396.1442
PX1	C23H26FN3O2	395.2009	H+	396.2082	8.23	
PX1	C23H26FN3O2	395.2009	H+	396.2082	8.23	232.1123
PX1	C23H26FN3O2	395.2009	H+	396.2082	8.23	379.1807
PX1	C23H26FN3O2	395.2009	H+	396.2082	8.23	144.0435
PX1	C23H26FN3O2	395.2009	H+	396.2082	8.23	396.2089
PX1	C23H26FN3O2	395.2009	H+	396.2082	8.23	116.0491
AKB-48 N-Pentanoic Acid	C23H29N3O3	395.2209	H+	396.2282	9.74	
AKB-48 N-Pentanoic Acid	C23H29N3O3	395.2209	H+	396.2282	9.74	135.1161
AKB-48 N-Pentanoic Acid	C23H29N3O3	395.2209	H+	396.2282	9.74	396.2269
AKB-48 N-Pentanoic Acid	C23H29N3O3	395.2209	H+	396.2282	9.74	107.0861
AKB-48 N-Pentanoic Acid	C23H29N3O3	395.2209	H+	396.2282	9.74	378.2174
AKB-48 N-Pentanoic Acid	C23H29N3O3	395.2209	H+	396.2282	9.74	244.1053
JWH-146	C28H29NO	395.2249	H+	396.2322	11.32	
JWH-146	C28H29NO	395.2249	H+	396.2322	11.32	155.0486
JWH-146	C28H29NO	395.2249	H+	396.2322	11.32	127.053
JWH-146	C28H29NO	395.2249	H+	396.2322	11.32	396.2324
JWH-146	C28H29NO	395.2249	H+	396.2322	11.32	268.1702
JWH-146	C28H29NO	395.2249	H+	396.2322	11.32	170.0598
FUB-PB-22	C25H17FN2O2	396.1274	H+	397.1347	9.57	
FUB-PB-22	C25H17FN2O2	396.1274	H+	397.1347	9.57	252.0826
FUB-PB-22	C25H17FN2O2	396.1274	H+	397.1347	9.57	109.0446
FUB-PB-22	C25H17FN2O2	396.1274	H+	397.1347	9.57	397.134
FUB-PB-22	C25H17FN2O2	396.1274	H+	397.1347	9.57	224.0878
FUB-PB-22	C25H17FN2O2	396.1274	H+	397.1347	9.57	83.0293
MDMB-FUBICA	C23H25FN2O3	396.1849	H+	397.1922	9.46	
MDMB-FUBICA	C23H25FN2O3	396.1849	H+	397.1922	9.46	252.0831
MDMB-FUBICA	C23H25FN2O3	396.1849	H+	397.1922	9.46	109.0447
MDMB-FUBICA	C23H25FN2O3	396.1849	H+	397.1922	9.46	397.1933
MDMB-FUBICA	C23H25FN2O3	396.1849	H+	397.1922	9.46	224.0875
MDMB-FUBICA	C23H25FN2O3	396.1849	H+	397.1922	9.46	365.1664
PX2	C22H25FN4O2	396.1962	H+	397.2034	8.46	
PX2	C22H25FN4O2	396.1962	H+	397.2034	8.46	233.1093
PX2	C22H25FN4O2	396.1962	H+	397.2034	8.46	352.1827
PX2	C22H25FN4O2	396.1962	H+	397.2034	8.46	213.1028
PX2	C22H25FN4O2	396.1962	H+	397.2034	8.46	177.0461
PX2	C22H25FN4O2	396.1962	H+	397.2034	8.46	145.0395
2',5'-Dimethoxyfentanyl	C24H32N2O3	396.2413	H+	397.2486	6.03	
2',5'-Dimethoxyfentanyl	C24H32N2O3	396.2413	H+	397.2486	6.03	165.0906
2',5'-Dimethoxyfentanyl	C24H32N2O3	396.2413	H+	397.2486	6.03	248.1646
2',5'-Dimethoxyfentanyl	C24H32N2O3	396.2413	H+	397.2486	6.03	397.2477
2',5'-Dimethoxyfentanyl	C24H32N2O3	396.2413	H+	397.2486	6.03	150.0676
2',5'-Dimethoxyfentanyl	C24H32N2O3	396.2413	H+	397.2486	6.03	206.1179
FUB-NPB-22	C24H16FN3O2	397.1227	H+	398.1299	9.38	
FUB-NPB-22	C24H16FN3O2	397.1227	H+	398.1299	9.38	253.0777
FUB-NPB-22	C24H16FN3O2	397.1227	H+	398.1299	9.38	109.0444
FUB-NPB-22	C24H16FN3O2	397.1227	H+	398.1299	9.38	398.1301
FUB-NPB-22	C24H16FN3O2	397.1227	H+	398.1299	9.38	225.0825
FUB-NPB-22	C24H16FN3O2	397.1227	H+	398.1299	9.38	253.6441
MDMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.66	
MDMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.66	253.0755
MDMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.66	338.1641
MDMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.66	109.0442
MDMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.66	398.1848
MDMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.66	366.1592
EMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.77	
EMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.77	253.0778
EMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.77	109.0444
EMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.77	324.1517
EMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.77	398.1881
EMB-FUBINACA	C22H24FN3O3	397.1802	H+	398.1875	9.77	352.1493
JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	397.2042	H+	398.2115	10.94	
JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	397.2042	H+	398.2115	10.94	185.0598
JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	397.2042	H+	398.2115	10.94	240.1389
JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	397.2042	H+	398.2115	10.94	398.2126

JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	397.2042	H+	398.2115	10.94	157.0645
JWH-081 N-(Cyclohexylmethyl) Analogue	C27H27NO2	397.2042	H+	398.2115	10.94	144.0443
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	398.1390	H+	399.1463	7.55	
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	398.1390	H+	399.1463	7.55	253.0762
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	398.1390	H+	399.1463	7.55	354.123
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	398.1390	H+	399.1463	7.55	109.044
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	398.1390	H+	399.1463	7.55	382.1177
AB-FUBINACA Oxobutanoic Acid	C20H19FN4O4	398.1390	H+	399.1463	7.55	310.1339
JWH-193	C26H26N2O2	398.1994	H+	399.2067	7.95	
JWH-193	C26H26N2O2	398.1994	H+	399.2067	7.95	169.065
JWH-193	C26H26N2O2	398.1994	H+	399.2067	7.95	114.0914
JWH-193	C26H26N2O2	398.1994	H+	399.2067	7.95	399.2077
JWH-193	C26H26N2O2	398.1994	H+	399.2067	7.95	141.07
JWH-193	C26H26N2O2	398.1994	H+	399.2067	7.95	312.1384
para-Chloro Valerylfentanyl	C24H31ClN2O	398.2125	H+	399.2198	7.83	
para-Chloro Valerylfentanyl	C24H31ClN2O	398.2125	H+	399.2198	7.83	188.1431
para-Chloro Valerylfentanyl	C24H31ClN2O	398.2125	H+	399.2198	7.83	105.069
para-Chloro Valerylfentanyl	C24H31ClN2O	398.2125	H+	399.2198	7.83	399.2185
para-Chloro Valerylfentanyl	C24H31ClN2O	398.2125	H+	399.2198	7.83	315.1624
para-Chloro Valerylfentanyl	C24H31ClN2O	398.2125	H+	399.2198	7.83	278.1304
Mitragynine	C23H30N2O4	398.2206	H+	399.2278	6.49	
Mitragynine	C23H30N2O4	398.2206	H+	399.2278	6.49	399.2285
Mitragynine	C23H30N2O4	398.2206	H+	399.2278	6.49	174.0912
Mitragynine	C23H30N2O4	398.2206	H+	399.2278	6.49	226.1437
Mitragynine	C23H30N2O4	398.2206	H+	399.2278	6.49	238.1439
Mitragynine	C23H30N2O4	398.2206	H+	399.2278	6.49	367.2024
Phenylacetyl Fentanyl	C27H30N2O	398.2358	H+	399.2431	7.3	
Phenylacetyl Fentanyl	C27H30N2O	398.2358	H+	399.2431	7.3	188.1433
Phenylacetyl Fentanyl	C27H30N2O	398.2358	H+	399.2431	7.3	105.0693
Phenylacetyl Fentanyl	C27H30N2O	398.2358	H+	399.2431	7.3	399.2421
Phenylacetyl Fentanyl	C27H30N2O	398.2358	H+	399.2431	7.3	278.1544
Phenylacetyl Fentanyl	C27H30N2O	398.2358	H+	399.2431	7.3	146.0959
5Cl-AKB-48	C23H30ClN3O	399.2077	H+	400.2150	11	
5Cl-AKB-48	C23H30ClN3O	399.2077	H+	400.2150	11	135.1159
5Cl-AKB-48	C23H30ClN3O	399.2077	H+	400.2150	11	400.2149
5Cl-AKB-48	C23H30ClN3O	399.2077	H+	400.2150	11	107.0849
5Cl-AKB-48	C23H30ClN3O	399.2077	H+	400.2150	11	93.0693
5Cl-AKB-48	C23H30ClN3O	399.2077	H+	400.2150	11	79.0539
PTI-2	C23H33N3OS	399.2344	H+	400.2417	8.8	
PTI-2	C23H33N3OS	399.2344	H+	400.2417	8.8	283.1271
PTI-2	C23H33N3OS	399.2344	H+	400.2417	8.8	400.2416
PTI-2	C23H33N3OS	399.2344	H+	400.2417	8.8	213.0482
PTI-2	C23H33N3OS	399.2344	H+	400.2417	8.8	227.0645
PTI-2	C23H33N3OS	399.2344	H+	400.2417	8.8	186.0374
URB-447	C25H21ClN2O	400.1342	H+	401.1415	9.68	
URB-447	C25H21ClN2O	400.1342	H+	401.1415	9.68	105.0332
URB-447	C25H21ClN2O	400.1342	H+	401.1415	9.68	401.1422
URB-447	C25H21ClN2O	400.1342	H+	401.1415	9.68	296.1084
URB-447	C25H21ClN2O	400.1342	H+	401.1415	9.68	276.1254
URB-447	C25H21ClN2O	400.1342	H+	401.1415	9.68	171.0917
AB-CHFUPYCA	C22H29FN4O2	400.2275	H+	401.2347	9.56	
AB-CHFUPYCA	C22H29FN4O2	400.2275	H+	401.2347	9.56	285.1406
AB-CHFUPYCA	C22H29FN4O2	400.2275	H+	401.2347	9.56	356.2144
AB-CHFUPYCA	C22H29FN4O2	400.2275	H+	401.2347	9.56	189.0462
AB-CHFUPYCA	C22H29FN4O2	400.2275	H+	401.2347	9.56	384.2087
AB-CHFUPYCA	C22H29FN4O2	400.2275	H+	401.2347	9.56	401.2345
Bromadol	C22H28BrNO	401.1354	H+	402.1427	6.37	
Bromadol	C22H28BrNO	401.1354	H+	402.1427	6.37	339.0738
Bromadol	C22H28BrNO	401.1354	H+	402.1427	6.37	143.0855
Bromadol	C22H28BrNO	401.1354	H+	402.1427	6.37	46.0651
Bromadol	C22H28BrNO	401.1354	H+	402.1427	6.37	168.9648
Bromadol	C22H28BrNO	401.1354	H+	402.1427	6.37	220.9963
JWH-369	C26H24ClNO	401.1546	H+	402.1619	10.92	
JWH-369	C26H24ClNO	401.1546	H+	402.1619	10.92	155.0498
JWH-369	C26H24ClNO	401.1546	H+	402.1619	10.92	127.0546
JWH-369	C26H24ClNO	401.1546	H+	402.1619	10.92	402.1643
JWH-369	C26H24ClNO	401.1546	H+	402.1619	10.92	274.0995
JWH-369	C26H24ClNO	401.1546	H+	402.1619	10.92	204.0229
Perphenazine	C21H26ClN3OS	403.1485	H+	404.1558	7.74	
Perphenazine	C21H26ClN3OS	403.1485	H+	404.1558	7.74	404.1572
Perphenazine	C21H26ClN3OS	403.1485	H+	404.1558	7.74	171.1492
Perphenazine	C21H26ClN3OS	403.1485	H+	404.1558	7.74	143.1178
Perphenazine	C21H26ClN3OS	403.1485	H+	404.1558	7.74	246.0155
Perphenazine	C21H26ClN3OS	403.1485	H+	404.1558	7.74	100.0748

FUB-AKB-48	C25H26FN3O	403.2060	H+	404.2133	10.81	
FUB-AKB-48	C25H26FN3O	403.2060	H+	404.2133	10.81	135.1164
FUB-AKB-48	C25H26FN3O	403.2060	H+	404.2133	10.81	107.0846
FUB-AKB-48	C25H26FN3O	403.2060	H+	404.2133	10.81	404.2139
FUB-AKB-48	C25H26FN3O	403.2060	H+	404.2133	10.81	93.0695
FUB-AKB-48	C25H26FN3O	403.2060	H+	404.2133	10.81	79.0539
CB-25	C25H41NO3	403.3086	H+	404.3159	10.57	
CB-25	C25H41NO3	403.3086	H+	404.3159	10.57	58.0673
CB-25	C25H41NO3	403.3086	H+	404.3159	10.57	181.1219
CB-25	C25H41NO3	403.3086	H+	404.3159	10.57	404.3155
CB-25	C25H41NO3	403.3086	H+	404.3159	10.57	347.2582
CB-25	C25H41NO3	403.3086	H+	404.3159	10.57	387.2899
AM-1235	C24H21FN2O3	404.1536	H+	405.1609	9.97	
AM-1235	C24H21FN2O3	404.1536	H+	405.1609	9.97	277.0985
AM-1235	C24H21FN2O3	404.1536	H+	405.1609	9.97	155.049
AM-1235	C24H21FN2O3	404.1536	H+	405.1609	9.97	405.1612
AM-1235	C24H21FN2O3	404.1536	H+	405.1609	9.97	127.0539
AM-1235	C24H21FN2O3	404.1536	H+	405.1609	9.97	189.0297
ortho-Methoxy Furanylfentanyl	C25H28N2O3	404.2100	H+	405.2173	6.49	
ortho-Methoxy Furanylfentanyl	C25H28N2O3	404.2100	H+	405.2173	6.49	188.1438
ortho-Methoxy Furanylfentanyl	C25H28N2O3	404.2100	H+	405.2173	6.49	105.0696
ortho-Methoxy Furanylfentanyl	C25H28N2O3	404.2100	H+	405.2173	6.49	405.2176
ortho-Methoxy Furanylfentanyl	C25H28N2O3	404.2100	H+	405.2173	6.49	284.1289
ortho-Methoxy Furanylfentanyl	C25H28N2O3	404.2100	H+	405.2173	6.49	134.0965
APP-CHMINACA	C24H28N4O2	404.2212	H+	405.2285	9.53	
APP-CHMINACA	C24H28N4O2	404.2212	H+	405.2285	9.53	241.1328
APP-CHMINACA	C24H28N4O2	404.2212	H+	405.2285	9.53	360.2063
APP-CHMINACA	C24H28N4O2	404.2212	H+	405.2285	9.53	388.2012
APP-CHMINACA	C24H28N4O2	404.2212	H+	405.2285	9.53	145.0389
APP-CHMINACA	C24H28N4O2	404.2212	H+	405.2285	9.53	405.2284
Tetramethylcyclopropyl Fentanyl	C27H36N2O	404.2828	H+	405.2900	8.21	
Tetramethylcyclopropyl Fentanyl	C27H36N2O	404.2828	H+	405.2900	8.21	125.0966
Tetramethylcyclopropyl Fentanyl	C27H36N2O	404.2828	H+	405.2900	8.21	281.202
Tetramethylcyclopropyl Fentanyl	C27H36N2O	404.2828	H+	405.2900	8.21	188.1441
Tetramethylcyclopropyl Fentanyl	C27H36N2O	404.2828	H+	405.2900	8.21	97.1017
Tetramethylcyclopropyl Fentanyl	C27H36N2O	404.2828	H+	405.2900	8.21	105.0704
ADB-FUPYCA	C21H28F2N4O2	406.2180	H+	407.2253	9.1	
ADB-FUPYCA	C21H28F2N4O2	406.2180	H+	407.2253	9.1	362.2035
ADB-FUPYCA	C21H28F2N4O2	406.2180	H+	407.2253	9.1	407.2249
ADB-FUPYCA	C21H28F2N4O2	406.2180	H+	407.2253	9.1	274.1351
ADB-FUPYCA	C21H28F2N4O2	406.2180	H+	407.2253	9.1	206.0723
ADB-FUPYCA	C21H28F2N4O2	406.2180	H+	407.2253	9.1	189.0454
Trifluoperazine	C21H24F3N3S	407.1643	H+	408.1716	8.27	
Trifluoperazine	C21H24F3N3S	407.1643	H+	408.1716	8.27	408.1717
Trifluoperazine	C21H24F3N3S	407.1643	H+	408.1716	8.27	141.1387
Trifluoperazine	C21H24F3N3S	407.1643	H+	408.1716	8.27	113.1075
Trifluoperazine	C21H24F3N3S	407.1643	H+	408.1716	8.27	280.0399
Trifluoperazine	C21H24F3N3S	407.1643	H+	408.1716	8.27	70.0669
5F-BEPIRAPIM	C25H30FN3O	407.2373	H+	408.2446	7.15	
5F-BEPIRAPIM	C25H30FN3O	407.2373	H+	408.2446	7.15	232.1141
5F-BEPIRAPIM	C25H30FN3O	407.2373	H+	408.2446	7.15	144.0443
5F-BEPIRAPIM	C25H30FN3O	407.2373	H+	408.2446	7.15	408.2448
5F-BEPIRAPIM	C25H30FN3O	407.2373	H+	408.2446	7.15	116.0493
5F-BEPIRAPIM	C25H30FN3O	407.2373	H+	408.2446	7.15	212.1079
para-Chloro Furanylfentanyl	C24H25ClN2O2	408.1605	H+	409.1677	6.92	
para-Chloro Furanylfentanyl	C24H25ClN2O2	408.1605	H+	409.1677	6.92	188.1444
para-Chloro Furanylfentanyl	C24H25ClN2O2	408.1605	H+	409.1677	6.92	105.07
para-Chloro Furanylfentanyl	C24H25ClN2O2	408.1605	H+	409.1677	6.92	409.1696
para-Chloro Furanylfentanyl	C24H25ClN2O2	408.1605	H+	409.1677	6.92	146.0971
para-Chloro Furanylfentanyl	C24H25ClN2O2	408.1605	H+	409.1677	6.92	136.0969
EG-2201	C28H24FNO	409.1842	H+	410.1915	10.74	
EG-2201	C28H24FNO	409.1842	H+	410.1915	10.74	155.0493
EG-2201	C28H24FNO	409.1842	H+	410.1915	10.74	410.1933
EG-2201	C28H24FNO	409.1842	H+	410.1915	10.74	282.1303
EG-2201	C28H24FNO	409.1842	H+	410.1915	10.74	127.0541
EG-2201	C28H24FNO	409.1842	H+	410.1915	10.74	179.0736
5F-MPP-PICA	C24H27FN2O3	410.2006	H+	411.2079	9.16	
5F-MPP-PICA	C24H27FN2O3	410.2006	H+	411.2079	9.16	232.1143
5F-MPP-PICA	C24H27FN2O3	410.2006	H+	411.2079	9.16	144.0441
5F-MPP-PICA	C24H27FN2O3	410.2006	H+	411.2079	9.16	411.2075
5F-MPP-PICA	C24H27FN2O3	410.2006	H+	411.2079	9.16	116.0498
5F-MPP-PICA	C24H27FN2O3	410.2006	H+	411.2079	9.16	212.1072
Risperidone	C23H27FN4O2	410.2118	H+	411.2191	5.78	
Risperidone	C23H27FN4O2	410.2118	H+	411.2191	5.78	191.1179

Risperidone	C23H27FN4O2	410.2118	H+	411.2191	5.78	411.2196
Risperidone	C23H27FN4O2	410.2118	H+	411.2191	5.78	110.0606
Risperidone	C23H27FN4O2	410.2118	H+	411.2191	5.78	190.5367
Risperidone	C23H27FN4O2	410.2118	H+	411.2191	5.78	163.1215
para-Chloro Cyclopentylfentanyl	C25H31ClN2O	410.2125	H+	411.2198	7.91	
para-Chloro Cyclopentylfentanyl	C25H31ClN2O	410.2125	H+	411.2198	7.91	188.143
para-Chloro Cyclopentylfentanyl	C25H31ClN2O	410.2125	H+	411.2198	7.91	411.2186
para-Chloro Cyclopentylfentanyl	C25H31ClN2O	410.2125	H+	411.2198	7.91	105.0693
para-Chloro Cyclopentylfentanyl	C25H31ClN2O	410.2125	H+	411.2198	7.91	69.0695
para-Chloro Cyclopentylfentanyl	C25H31ClN2O	410.2125	H+	411.2198	7.91	315.1614
Ziprasidone	C21H21ClN4OS	412.1125	H+	413.1197	6.32	
Ziprasidone	C21H21ClN4OS	412.1125	H+	413.1197	6.32	413.1204
Ziprasidone	C21H21ClN4OS	412.1125	H+	413.1197	6.32	194.0366
Ziprasidone	C21H21ClN4OS	412.1125	H+	413.1197	6.32	177.0481
Ziprasidone	C21H21ClN4OS	412.1125	H+	413.1197	6.32	159.0676
Ziprasidone	C21H21ClN4OS	412.1125	H+	413.1197	6.32	166.0423
b'-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.6	
b'-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.6	188.1433
b'-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.6	105.0698
b'-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.6	413.2579
b'-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.6	292.1698
b'-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.6	281.2019
4-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.55	
4-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.55	264.1753
4-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.55	134.0964
4-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.55	413.2584
4-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.55	105.07
4-Phenyl Fentanyl	C28H32N2O	412.2515	H+	413.2587	7.55	174.1279
Noscapine	C22H23NO7	413.1475	H+	414.1547	5.66	
Noscapine	C22H23NO7	413.1475	H+	414.1547	5.66	220.0964
Noscapine	C22H23NO7	413.1475	H+	414.1547	5.66	353.1016
Noscapine	C22H23NO7	413.1475	H+	414.1547	5.66	414.1544
Noscapine	C22H23NO7	413.1475	H+	414.1547	5.66	365.1025
Noscapine	C22H23NO7	413.1475	H+	414.1547	5.66	323.0912
Norbuprenorphine	C25H35NO4	413.2566	H+	414.2639	5.81	
Norbuprenorphine	C25H35NO4	413.2566	H+	414.2639	5.81	414.2656
Norbuprenorphine	C25H35NO4	413.2566	H+	414.2639	5.81	396.2582
Norbuprenorphine	C25H35NO4	413.2566	H+	414.2639	5.81	340.1884
Norbuprenorphine	C25H35NO4	413.2566	H+	414.2639	5.81	297.1556
Norbuprenorphine	C25H35NO4	413.2566	H+	414.2639	5.81	193.123
Flecainide	C17H20F6N2O3	414.1378	H+	415.1451	6.49	
Flecainide	C17H20F6N2O3	414.1378	H+	415.1451	6.49	398.117
Flecainide	C17H20F6N2O3	414.1378	H+	415.1451	6.49	415.1435
Flecainide	C17H20F6N2O3	414.1378	H+	415.1451	6.49	301.0284
Flecainide	C17H20F6N2O3	414.1378	H+	415.1451	6.49	98.0969
Flecainide	C17H20F6N2O3	414.1378	H+	415.1451	6.49	232.0964
Diltiazem	C22H26N2O4S	414.1613	H+	415.1686	6.68	
Diltiazem	C22H26N2O4S	414.1613	H+	415.1686	6.68	178.0315
Diltiazem	C22H26N2O4S	414.1613	H+	415.1686	6.68	415.1682
Diltiazem	C22H26N2O4S	414.1613	H+	415.1686	6.68	310.0901
Diltiazem	C22H26N2O4S	414.1613	H+	415.1686	6.68	150.0369
Diltiazem	C22H26N2O4S	414.1613	H+	415.1686	6.68	370.111
JWH-198	C26H26N2O3	414.1943	H+	415.2016	7.81	
JWH-198	C26H26N2O3	414.1943	H+	415.2016	7.81	185.0594
JWH-198	C26H26N2O3	414.1943	H+	415.2016	7.81	114.0908
JWH-198	C26H26N2O3	414.1943	H+	415.2016	7.81	415.2015
JWH-198	C26H26N2O3	414.1943	H+	415.2016	7.81	157.0647
JWH-198	C26H26N2O3	414.1943	H+	415.2016	7.81	142.0414
7-Hydroxymitragynine	C23H30N2O5	414.2155	H+	415.2227	5.29	
7-Hydroxymitragynine	C23H30N2O5	414.2155	H+	415.2227	5.29	415.2241
7-Hydroxymitragynine	C23H30N2O5	414.2155	H+	415.2227	5.29	190.0867
7-Hydroxymitragynine	C23H30N2O5	414.2155	H+	415.2227	5.29	397.2124
7-Hydroxymitragynine	C23H30N2O5	414.2155	H+	415.2227	5.29	238.1435
7-Hydroxymitragynine	C23H30N2O5	414.2155	H+	415.2227	5.29	240.1588
HU-308	C27H42O3	414.3134	H+	415.3207	11.93	
HU-308	C27H42O3	414.3134	H+	415.3207	11.93	415.3201
HU-308	C27H42O3	414.3134	H+	415.3207	11.93	215.1054
HU-308	C27H42O3	414.3134	H+	415.3207	11.93	151.0742
HU-308	C27H42O3	414.3134	H+	415.3207	11.93	229.1219
HU-308	C27H42O3	414.3134	H+	415.3207	11.93	271.1693
APP-FUBINACA	C24H21FN4O2	416.1649	H+	417.1721	8.68	
APP-FUBINACA	C24H21FN4O2	416.1649	H+	417.1721	8.68	253.0771
APP-FUBINACA	C24H21FN4O2	416.1649	H+	417.1721	8.68	372.1505
APP-FUBINACA	C24H21FN4O2	416.1649	H+	417.1721	8.68	109.0441

APP-FUBINACA	C24H21FN4O2	416.1649	H+	417.1721	8.68	400.1447
APP-FUBINACA	C24H21FN4O2	416.1649	H+	417.1721	8.68	417.1715
ortho-Isopropyl Furanylfentanyl	C27H32N2O2	416.2464	H+	417.2537	7.38	
ortho-Isopropyl Furanylfentanyl	C27H32N2O2	416.2464	H+	417.2537	7.38	188.1441
ortho-Isopropyl Furanylfentanyl	C27H32N2O2	416.2464	H+	417.2537	7.38	105.07
ortho-Isopropyl Furanylfentanyl	C27H32N2O2	416.2464	H+	417.2537	7.38	417.2542
ortho-Isopropyl Furanylfentanyl	C27H32N2O2	416.2464	H+	417.2537	7.38	296.1656
ortho-Isopropyl Furanylfentanyl	C27H32N2O2	416.2464	H+	417.2537	7.38	146.00968
Alfentanil	C21H32N6O3	416.2536	H+	417.2609	6.23	
Alfentanil	C21H32N6O3	416.2536	H+	417.2609	6.23	268.1771
Alfentanil	C21H32N6O3	416.2536	H+	417.2609	6.23	197.1286
Alfentanil	C21H32N6O3	416.2536	H+	417.2609	6.23	417.2609
Alfentanil	C21H32N6O3	416.2536	H+	417.2609	6.23	385.2353
Alfentanil	C21H32N6O3	416.2536	H+	417.2609	6.23	314.187
AM-679	C20H20INO	417.0590	H+	418.0662	9.96	
AM-679	C20H20INO	417.0590	H+	418.0662	9.96	230.9294
AM-679	C20H20INO	417.0590	H+	418.0662	9.96	418.0658
AM-679	C20H20INO	417.0590	H+	418.0662	9.96	291.1619
AM-679	C20H20INO	417.0590	H+	418.0662	9.96	202.9344
AM-679	C20H20INO	417.0590	H+	418.0662	9.96	234.0916
JWH-309	C30H27NO	417.2093	H+	418.2165	11.24	
JWH-309	C30H27NO	417.2093	H+	418.2165	11.24	155.0492
JWH-309	C30H27NO	417.2093	H+	418.2165	11.24	127.054
JWH-309	C30H27NO	417.2093	H+	418.2165	11.24	418.2169
JWH-309	C30H27NO	417.2093	H+	418.2165	11.24	290.1547
JWH-309	C30H27NO	417.2093	H+	418.2165	11.24	220.0767
CB-86	C26H43NO3	417.3243	H+	418.3316	10.78	
CB-86	C26H43NO3	417.3243	H+	418.3316	10.78	58.065
CB-86	C26H43NO3	417.3243	H+	418.3316	10.78	418.3332
CB-86	C26H43NO3	417.3243	H+	418.3316	10.78	361.2755
CB-86	C26H43NO3	417.3243	H+	418.3316	10.78	292.1918
CB-86	C26H43NO3	417.3243	H+	418.3316	10.78	125.096
CB-52	C26H43NO3	417.3243	H+	418.3316	10.89	
CB-52	C26H43NO3	417.3243	H+	418.3316	10.89	58.067
CB-52	C26H43NO3	417.3243	H+	418.3316	10.89	418.3315
CB-52	C26H43NO3	417.3243	H+	418.3316	10.89	361.2739
CB-52	C26H43NO3	417.3243	H+	418.3316	10.89	291.1957
CB-52	C26H43NO3	417.3243	H+	418.3316	10.89	125.0592
JWH-387	C24H22BrNO	419.0885	H+	420.0958	11.02	
JWH-387	C24H22BrNO	419.0885	H+	420.0958	11.02	232.959
JWH-387	C24H22BrNO	419.0885	H+	420.0958	11.02	420.0951
JWH-387	C24H22BrNO	419.0885	H+	420.0958	11.02	214.1223
JWH-387	C24H22BrNO	419.0885	H+	420.0958	11.02	204.964
JWH-387	C24H22BrNO	419.0885	H+	420.0958	11.02	144.0431
JWH-424	C24H22BrNO	419.0885	H+	420.0958	10.33	
JWH-424	C24H22BrNO	419.0885	H+	420.0958	10.33	232.9597
JWH-424	C24H22BrNO	419.0885	H+	420.0958	10.33	420.0945
JWH-424	C24H22BrNO	419.0885	H+	420.0958	10.33	324.1748
JWH-424	C24H22BrNO	419.0885	H+	420.0958	10.33	284.1074
JWH-424	C24H22BrNO	419.0885	H+	420.0958	10.33	204.9651
JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	419.0885	H+	420.0958	10.21	
JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	419.0885	H+	420.0958	10.21	155.0491
JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	419.0885	H+	420.0958	10.21	420.0957
JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	419.0885	H+	420.0958	10.21	292.0334
JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	419.0885	H+	420.0958	10.21	127.0537
JWH-018 N-(5-Bromopentyl) Analogue	C24H22BrNO	419.0885	H+	420.0958	10.21	144.043
5Br-THJ-018	C23H21BrN2O	420.0837	H+	421.0910	10.51	
5Br-THJ-018	C23H21BrN2O	420.0837	H+	421.0910	10.51	293.0289
5Br-THJ-018	C23H21BrN2O	420.0837	H+	421.0910	10.51	213.1022
5Br-THJ-018	C23H21BrN2O	420.0837	H+	421.0910	10.51	421.0914
5Br-THJ-018	C23H21BrN2O	420.0837	H+	421.0910	10.51	145.0391
5Br-THJ-018	C23H21BrN2O	420.0837	H+	421.0910	10.51	236.9655
W18	C19H20ClN3O4S	421.0863	H+	422.0935	8.75	
W18	C19H20ClN3O4S	421.0863	H+	422.0935	8.75	273.0453
W18	C19H20ClN3O4S	421.0863	H+	422.0935	8.75	422.0928
W18	C19H20ClN3O4S	421.0863	H+	422.0935	8.75	174.9607
W18	C19H20ClN3O4S	421.0863	H+	422.0935	8.75	110.9993
W18	C19H20ClN3O4S	421.0863	H+	422.0935	8.75	150.0544
U-62066	C22H30Cl2N2O2	424.1684	H+	425.1757	6.95	
U-62066	C22H30Cl2N2O2	424.1684	H+	425.1757	6.95	354.1009
U-62066	C22H30Cl2N2O2	424.1684	H+	425.1757	6.95	168.1386
U-62066	C22H30Cl2N2O2	424.1684	H+	425.1757	6.95	137.0961
U-62066	C22H30Cl2N2O2	424.1684	H+	425.1757	6.95	425.1736
U-62066	C22H30Cl2N2O2	424.1684	H+	425.1757	6.95	218.0135

IMMA (BML-190)	C23H23ClN2O4	426.1346	H+	427.1419	8.92	
IMMA (BML-190)	C23H23ClN2O4	426.1346	H+	427.1419	8.92	138.9946
IMMA (BML-190)	C23H23ClN2O4	426.1346	H+	427.1419	8.92	312.0799
IMMA (BML-190)	C23H23ClN2O4	426.1346	H+	427.1419	8.92	427.1435
IMMA (BML-190)	C23H23ClN2O4	426.1346	H+	427.1419	8.92	110.9995
IMMA (BML-190)	C23H23ClN2O4	426.1346	H+	427.1419	8.92	88.0761
WIN 55,212-3	C27H26N2O3	426.1943	H+	427.2016	9.17	
WIN 55,212-3	C27H26N2O3	426.1943	H+	427.2016	9.17	155.0489
WIN 55,212-3	C27H26N2O3	426.1943	H+	427.2016	9.17	427.2024
WIN 55,212-3	C27H26N2O3	426.1943	H+	427.2016	9.17	127.0542
WIN 55,212-3	C27H26N2O3	426.1943	H+	427.2016	9.17	100.0765
WIN 55,212-3	C27H26N2O3	426.1943	H+	427.2016	9.17	340.1356
Iloperidone	C24H27FN2O4	426.1955	H+	427.2028	6.61	
Iloperidone	C24H27FN2O4	426.1955	H+	427.2028	6.61	427.2028
Iloperidone	C24H27FN2O4	426.1955	H+	427.2028	6.61	261.1402
Iloperidone	C24H27FN2O4	426.1955	H+	427.2028	6.61	233.1084
Iloperidone	C24H27FN2O4	426.1955	H+	427.2028	6.61	190.0663
Iloperidone	C24H27FN2O4	426.1955	H+	427.2028	6.61	124.112
25I-NBOMe	C18H22INO3	427.0644	H+	428.0717	7.39	
25I-NBOMe	C18H22INO3	427.0644	H+	428.0717	7.39	121.0648
25I-NBOMe	C18H22INO3	427.0644	H+	428.0717	7.39	428.072
25I-NBOMe	C18H22INO3	427.0644	H+	428.0717	7.39	91.0552
25I-NBOMe	C18H22INO3	427.0644	H+	428.0717	7.39	93.0704
25I-NBOMe	C18H22INO3	427.0644	H+	428.0717	7.39	272.1414
Benzodioxole Fentanyl	C27H28N2O3	428.2099	H+	429.2172	6.80	
Benzodioxole Fentanyl	C27H28N2O3	428.2099	H+	429.2172	6.80	188.142
Benzodioxole Fentanyl	C27H28N2O3	428.2099	H+	429.2172	6.80	149.0225
Benzodioxole Fentanyl	C27H28N2O3	428.2099	H+	429.2172	6.80	429.2129
Benzodioxole Fentanyl	C27H28N2O3	428.2099	H+	429.2172	6.80	105.0698
Benzodioxole Fentanyl	C27H28N2O3	428.2099	H+	429.2172	6.80	308.1259
Salvinorin A	C23H28O8	432.1784	H+	433.1857	7.98	
Salvinorin A	C23H28O8	432.1784	H+	433.1857	7.98	373.1651
Salvinorin A	C23H28O8	432.1784	H+	433.1857	7.98	295.1334
Salvinorin A	C23H28O8	432.1784	H+	433.1857	7.98	313.1438
Salvinorin A	C23H28O8	432.1784	H+	433.1857	7.98	323.1285
Salvinorin A	C23H28O8	432.1784	H+	433.1857	7.98	355.1548
MDMB-CHMCZCA	C27H34N2O3	434.2569	H+	435.2642	10.93	
MDMB-CHMCZCA	C27H34N2O3	434.2569	H+	435.2642	10.93	290.156
MDMB-CHMCZCA	C27H34N2O3	434.2569	H+	435.2642	10.93	194.0614
MDMB-CHMCZCA	C27H34N2O3	434.2569	H+	435.2642	10.93	179.0742
MDMB-CHMCZCA	C27H34N2O3	434.2569	H+	435.2642	10.93	435.2659
MDMB-CHMCZCA	C27H34N2O3	434.2569	H+	435.2642	10.93	166.0656
SER-601	C28H38N2O2	434.2933	H+	435.3006	11.58	
SER-601	C28H38N2O2	434.2933	H+	435.3006	11.58	135.1163
SER-601	C28H38N2O2	434.2933	H+	435.3006	11.58	284.1652
SER-601	C28H38N2O2	434.2933	H+	435.3006	11.58	435.3015
SER-601	C28H38N2O2	434.2933	H+	435.3006	11.58	417.2908
SER-601	C28H38N2O2	434.2933	H+	435.3006	11.58	107.0847
AM-694	C20H19FINO	435.0495	H+	436.0568	9.23	
AM-694	C20H19FINO	435.0495	H+	436.0568	9.23	230.9291
AM-694	C20H19FINO	435.0495	H+	436.0568	9.23	436.0561
AM-694	C20H19FINO	435.0495	H+	436.0568	9.23	309.1522
AM-694	C20H19FINO	435.0495	H+	436.0568	9.23	202.9342
AM-694	C20H19FINO	435.0495	H+	436.0568	9.23	234.091
Tianeptine	C21H25ClN2O4S	436.1224	H+	437.1296	6.67	
Tianeptine	C21H25ClN2O4S	436.1224	H+	437.1296	6.67	292.0191
Tianeptine	C21H25ClN2O4S	436.1224	H+	437.1296	6.67	228.0567
Tianeptine	C21H25ClN2O4S	436.1224	H+	437.1296	6.67	437.1282
Tianeptine	C21H25ClN2O4S	436.1224	H+	437.1296	6.67	246.0125
Tianeptine	C21H25ClN2O4S	436.1224	H+	437.1296	6.67	193.0881
Fluphenazine	C22H26F3N3OS	437.1749	H+	438.1821	8.08	
Fluphenazine	C22H26F3N3OS	437.1749	H+	438.1821	8.08	438.1825
Fluphenazine	C22H26F3N3OS	437.1749	H+	438.1821	8.08	171.1492
Fluphenazine	C22H26F3N3OS	437.1749	H+	438.1821	8.08	143.1179
Fluphenazine	C22H26F3N3OS	437.1749	H+	438.1821	8.08	280.0401
Fluphenazine	C22H26F3N3OS	437.1749	H+	438.1821	8.08	398.1693
MN-25	C26H37N3O3	439.2835	H+	440.2908	8.44	
MN-25	C26H37N3O3	439.2835	H+	440.2908	8.44	261.1608
MN-25	C26H37N3O3	439.2835	H+	440.2908	8.44	353.2239
MN-25	C26H37N3O3	439.2835	H+	440.2908	8.44	114.0914
MN-25	C26H37N3O3	439.2835	H+	440.2908	8.44	440.2925
MN-25	C26H37N3O3	439.2835	H+	440.2908	8.44	287.1406
5Br-AKB-48	C23H30BrN3O	443.1572	H+	444.1645	11.19	
5Br-AKB-48	C23H30BrN3O	443.1572	H+	444.1645	11.19	135.1163

5Br-AKB-48	C23H30BrN3O	443.1572	H+	444.1645	11.19	444.1658
5Br-AKB-48	C23H30BrN3O	443.1572	H+	444.1645	11.19	107.085
5Br-AKB-48	C23H30BrN3O	443.1572	H+	444.1645	11.19	310.0569
5Br-AKB-48	C23H30BrN3O	443.1572	H+	444.1645	11.19	213.1044
Glipizide	C21H27N5O4S	445.1784	H+	446.1857	7.52	
Glipizide	C21H27N5O4S	445.1784	H+	446.1857	7.52	321.1018
Glipizide	C21H27N5O4S	445.1784	H+	446.1857	7.52	286.0649
Glipizide	C21H27N5O4S	445.1784	H+	446.1857	7.52	167.106
Glipizide	C21H27N5O4S	445.1784	H+	446.1857	7.52	304.076
Glipizide	C21H27N5O4S	445.1784	H+	446.1857	7.52	347.0815
Aripiprazole	C23H27Cl2N3O2	447.1480	H+	448.1553	7.22	
Aripiprazole	C23H27Cl2N3O2	447.1480	H+	448.1553	7.22	448.1553
Aripiprazole	C23H27Cl2N3O2	447.1480	H+	448.1553	7.22	285.0927
Aripiprazole	C23H27Cl2N3O2	447.1480	H+	448.1553	7.22	176.071
Aripiprazole	C23H27Cl2N3O2	447.1480	H+	448.1553	7.22	218.1181
Aripiprazole	C23H27Cl2N3O2	447.1480	H+	448.1553	7.22	98.0973
MCHB-1	C28H37N3O2	447.2886	H+	448.2959	9.8	
MCHB-1	C28H37N3O2	447.2886	H+	448.2959	9.8	448.2968
MCHB-1	C28H37N3O2	447.2886	H+	448.2959	9.8	352.2026
MCHB-1	C28H37N3O2	447.2886	H+	448.2959	9.8	279.1137
MCHB-1	C28H37N3O2	447.2886	H+	448.2959	9.8	230.1295
MCHB-1	C28H37N3O2	447.2886	H+	448.2959	9.8	159.0562
MN-25 2-Methyl Derivative	C27H39N3O3	453.2991	H+	454.3064	8.76	
MN-25 2-Methyl Derivative	C27H39N3O3	453.2991	H+	454.3064	8.76	114.0908
MN-25 2-Methyl Derivative	C27H39N3O3	453.2991	H+	454.3064	8.76	275.1752
MN-25 2-Methyl Derivative	C27H39N3O3	453.2991	H+	454.3064	8.76	454.3054
MN-25 2-Methyl Derivative	C27H39N3O3	453.2991	H+	454.3064	8.76	190.1228
MN-25 2-Methyl Derivative	C27H39N3O3	453.2991	H+	454.3064	8.76	137.1322
Verapamil	C27H38N2O4	454.2832	H+	455.2904	7.02	
Verapamil	C27H38N2O4	454.2832	H+	455.2904	7.02	165.0905
Verapamil	C27H38N2O4	454.2832	H+	455.2904	7.02	455.2889
Verapamil	C27H38N2O4	454.2832	H+	455.2904	7.02	303.2066
Verapamil	C27H38N2O4	454.2832	H+	455.2904	7.02	150.0673
Verapamil	C27H38N2O4	454.2832	H+	455.2904	7.02	260.1645
WIN-54,461	C23H25BrN2O3	456.1049	H+	457.1121	8.13	
WIN-54,461	C23H25BrN2O3	456.1049	H+	457.1121	8.13	135.0433
WIN-54,461	C23H25BrN2O3	456.1049	H+	457.1121	8.13	114.0908
WIN-54,461	C23H25BrN2O3	456.1049	H+	457.1121	8.13	457.1125
WIN-54,461	C23H25BrN2O3	456.1049	H+	457.1121	8.13	107.0482
WIN-54,461	C23H25BrN2O3	456.1049	H+	457.1121	8.13	70.0649
AM-2233	C22H23IN2O	458.0855	H+	459.0928	6.73	
AM-2233	C22H23IN2O	458.0855	H+	459.0928	6.73	112.1118
AM-2233	C22H23IN2O	458.0855	H+	459.0928	6.73	98.0966
AM-2233	C22H23IN2O	458.0855	H+	459.0928	6.73	459.0926
AM-2233	C22H23IN2O	458.0855	H+	459.0928	6.73	362.0036
AM-2233	C22H23IN2O	458.0855	H+	459.0928	6.73	230.9295
N-desmethyl Loperamide	C28H31ClN2O2	462.2074	H+	463.2147	7.43	
N-desmethyl Loperamide	C28H31ClN2O2	462.2074	H+	463.2147	7.43	252.139
N-desmethyl Loperamide	C28H31ClN2O2	462.2074	H+	463.2147	7.43	196.1122
N-desmethyl Loperamide	C28H31ClN2O2	462.2074	H+	463.2147	7.43	463.2143
N-desmethyl Loperamide	C28H31ClN2O2	462.2074	H+	463.2147	7.43	117.0699
N-desmethyl Loperamide	C28H31ClN2O2	462.2074	H+	463.2147	7.43	224.1062
Cephaeline	C28H38N2O4	466.2832	H+	467.2904	3.97	
Cephaeline	C28H38N2O4	466.2832	H+	467.2904	3.97	467.2907
Cephaeline	C28H38N2O4	466.2832	H+	467.2904	3.97	450.2643
Cephaeline	C28H38N2O4	466.2832	H+	467.2904	3.97	246.1494
Cephaeline	C28H38N2O4	466.2832	H+	467.2904	3.97	422.2329
Cephaeline	C28H38N2O4	466.2832	H+	467.2904	3.97	274.1805
Buprenorphine	C29H41NO4	467.3036	H+	468.3108	6.55	
Buprenorphine	C29H41NO4	467.3036	H+	468.3108	6.55	468.312
Buprenorphine	C29H41NO4	467.3036	H+	468.3108	6.55	414.2655
Buprenorphine	C29H41NO4	467.3036	H+	468.3108	6.55	396.2196
Buprenorphine	C29H41NO4	467.3036	H+	468.3108	6.55	187.0763
Buprenorphine	C29H41NO4	467.3036	H+	468.3108	6.55	115.0743
N-acetyl 25I-NBOMe	C20H24INO4	469.0750	H+	470.0823	9.63	
N-acetyl 25I-NBOMe	C20H24INO4	469.0750	H+	470.0823	9.63	121.0645
N-acetyl 25I-NBOMe	C20H24INO4	469.0750	H+	470.0823	9.63	470.082
N-acetyl 25I-NBOMe	C20H24INO4	469.0750	H+	470.0823	9.63	362.0253
N-acetyl 25I-NBOMe	C20H24INO4	469.0750	H+	470.0823	9.63	343.1781
N-acetyl 25I-NBOMe	C20H24INO4	469.0750	H+	470.0823	9.63	284.1411
Sildenafil	C22H30N6O4S	474.2049	H+	475.2122	6.69	
Sildenafil	C22H30N6O4S	474.2049	H+	475.2122	6.69	475.2113
Sildenafil	C22H30N6O4S	474.2049	H+	475.2122	6.69	10.1
Sildenafil	C22H30N6O4S	474.2049	H+	475.2122	6.69	58.0675

Sildenafil	C22H30N6O4S	474.2049	H+	475.2122	6.69	311.1505
Sildenafil	C22H30N6O4S	474.2049	H+	475.2122	6.69	283.1192
Loperamide	C29H33ClN2O2	476.2231	H+	477.2303	7.91	
Loperamide	C29H33ClN2O2	476.2231	H+	477.2303	7.91	266.1553
Loperamide	C29H33ClN2O2	476.2231	H+	477.2303	7.91	210.1278
Loperamide	C29H33ClN2O2	476.2231	H+	477.2303	7.91	477.231
Loperamide	C29H33ClN2O2	476.2231	H+	477.2303	7.91	238.1235
Loperamide	C29H33ClN2O2	476.2231	H+	477.2303	7.91	432.1745
Emetine	C29H40N2O4	480.2988	H+	481.3061	4.5	
Emetine	C29H40N2O4	480.2988	H+	481.3061	4.5	481.3081
Emetine	C29H40N2O4	480.2988	H+	481.3061	4.5	464.2829
Emetine	C29H40N2O4	480.2988	H+	481.3061	4.5	274.1799
Emetine	C29H40N2O4	480.2988	H+	481.3061	4.5	246.1495
Emetine	C29H40N2O4	480.2988	H+	481.3061	4.5	436.252
Vardenafil	C23H32N6O4S	488.2206	H+	489.2279	6.55	
Vardenafil	C23H32N6O4S	488.2206	H+	489.2279	6.55	489.2262
Vardenafil	C23H32N6O4S	488.2206	H+	489.2279	6.55	151.0866
Vardenafil	C23H32N6O4S	488.2206	H+	489.2279	6.55	312.1581
Vardenafil	C23H32N6O4S	488.2206	H+	489.2279	6.55	377.1266
Vardenafil	C23H32N6O4S	488.2206	H+	489.2279	6.55	376.107
Glimepiride	C24H34N4O5S	490.2250	H+	491.2323	9.06	
Glimepiride	C24H34N4O5S	490.2250	H+	491.2323	9.06	126.0915
Glimepiride	C24H34N4O5S	490.2250	H+	491.2323	9.06	352.1324
Glimepiride	C24H34N4O5S	490.2250	H+	491.2323	9.06	335.1061
Glimepiride	C24H34N4O5S	490.2250	H+	491.2323	9.06	181.0967
Glimepiride	C24H34N4O5S	490.2250	H+	491.2323	9.06	167.0157
AM-1241	C22H22IN3O3	503.0706	H+	504.0779	7.09	
AM-1241	C22H22IN3O3	503.0706	H+	504.0779	7.09	98.0969
AM-1241	C22H22IN3O3	503.0706	H+	504.0779	7.09	504.0769
AM-1241	C22H22IN3O3	503.0706	H+	504.0779	7.09	112.1124
AM-1241	C22H22IN3O3	503.0706	H+	504.0779	7.09	406.9889
AM-1241	C22H22IN3O3	503.0706	H+	504.0779	7.09	275.9153
AM-630	C23H25IN2O3	504.0910	H+	505.0983	8.41	
AM-630	C23H25IN2O3	504.0910	H+	505.0983	8.41	135.0439
AM-630	C23H25IN2O3	504.0910	H+	505.0983	8.41	114.0915
AM-630	C23H25IN2O3	504.0910	H+	505.0983	8.41	505.0986
AM-630	C23H25IN2O3	504.0910	H+	505.0983	8.41	107.0491
AM-630	C23H25IN2O3	504.0910	H+	505.0983	8.41	100.0756