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Abstract

The emergence of designer drugs as abused substances has seen a dramatic increase over the past few years. Forensic laboratories are faced with a challenge in identifying these compounds because reference standards for many of the compounds do not exist. In addition, some current cheminformatic databases are static and updated periodically, thereby requiring users to re-download or purchase an upgrade to access the additional spectra. ForensicDB addresses this need by providing the forensic community with a peer-reviewed, Web-accessible, continuously updated database of multiple spectral methods that is provided at no cost to the user.

The goal of this project was to expand ForensicDB capacity for user traffic and database queries, increase participation of associate curators to manage the review of records, and further develop software automation to improve management of submitted records. Inclusion of nuclear magnetic resonance data in the database was originally proposed, but with the increased presence of designer drugs, it became evident that the focus should be on the inclusion of more relevant compounds and spectral data to assist the forensic practitioner.

The project resulted in an increase in database traffic and community submissions to ForensicDB, as well as an increase in volunteers willing to review spectral data. This project also resulted in the development of a Web-portal for user submissions that is in its final stages of testing.

Executive Summary

Research Purpose

Forensic laboratories are faced with a challenge when attempting to identify an unknown compound in a sample substance. A useful tool to aid in identification is a cheminformatic database populated with reference spectra. Although many laboratories create internal databases of these spectra, such databases are generally small, contain limited records, and are not useful to the broader forensics community.

Widely available spectral and cheminformatic databases are provided through both private and commercial organizations. One of the most popular private databases is the American Academy of Forensic Sciences (AAFS) mass spectrometry database (<http://www.ualberta.ca/~gjones/mslib.htm>). Although commercial databases contain more compounds, they can be expensive to access and often require proprietary software that is designed to be installed on a single computer. In addition, many commercial databases are static, and for those that are updated periodically, users must download the updates to a local computer. If updates are not downloaded regularly, users may not have the most reliable data and may not realize that they are using outdated information. This is a significant problem in a time when new designer drugs are being discovered at a rapid rate.

In the past year, the rise in prevalence of the synthetic cannabinoid, or “Spice,” materials and other “legal high” compounds (i.e., legal products that have a similar structure and produce similar pharmacological effects as their illegal counterparts) has challenged the laboratory system’s ability to reliably handle and identify these compounds. Although approximately 20 primary compounds have been seen in available materials, the series of cannabimimetic compounds includes hundreds if not thousands of potential compounds. This is further complicated with inclusion of the synthetic cathinone analogs, tryptamines, and, potentially, cocaine analogs, all compounds that are challenging to regulate. In addition, clandestine chemists rapidly move from one compound to another as they are regulated, thereby creating an ongoing identification challenge. This challenge is evident from monitoring the clandestine laboratory investigating chemists’ mailing list (CLIC List) and the “unknowns” forum on Forendex, where users are reaching out to the community for assistance in determining unknowns by uploading PDF files of their spectra and asking if other professionals recognize a compound.

ForensicDB (www.forensicDB.org), the cheminformatic database developed at RTI International (RTI) as part of this collaborative agreement, is designed to help users objectively determine their unknown compound by performing a spectral similarity search between their raw data and the spectra of reference standards in the database. Because most of the currently available spectral databases are static or may only be updated on an annual basis, there is a need in the community for assistance to laboratory personnel attempting to identify unknowns. ForensicDB addresses this need by providing the forensics community with a free, Web-accessible, centrally curated database that is updated continuously.

Research Design and Methods

The Project as Originally Proposed

Created under a previous National Institutes of Justice (NIJ) cooperative agreement (2008-DN-BX-K180), ForensicDB was originally intended to be a spectral database for only Direct

online database training sessions to educate users on the searching and navigating of ForensicDB. This will also remain an outlet for RTI to communicate with the community about changes that may be necessary to facilitate the use and acceptance of ForensicDB.

We plan to expand database content by focusing on the growing number of community submissions by requesting spectra from participants in online forums and discussions, as well as by promoting ForensicDB at conferences in the form of scientific presentations and at booths where users can be given a live demonstration of the database. In addition to individual data submissions, RTI will continue to reach out to the community to incorporate large spectral libraries from collaborations with manufacturers of reference material. RTI staff will also monitor current literature, such as the *Microgram Journal* for sources of spectra of unusual substances.

The current bottle neck of ForensicDB is the review process. Although we have gained more reviewers, we are still in need of volunteers to help with the review process. More reviewers would help with the current backlog of data, which would result in more data being publically available in a timely manner. This would be an advantage to the public and increase the usefulness of ForensicDB.

Several facilities are independently working on database efforts. There is significant overlap of the same compounds, from the same institution, and same source material in each of these databases. There exists a need to unify these efforts in order to consolidate data and make it easily accessible. RTI has initiated communications between the most prominent of these database efforts—ForensicDB, Forendex, and SWGDRUG—as well as several other organizations to discuss the best strategy moving forward to make reliable reference spectra widely available to the forensics community.

As RTI is now the holder of the Forensic Technology Center of Excellence funded by NIH, maintaining and expanding this technology assistance to the community appears to be a viable option for maintaining ForensicDB and its availability. Also, this appears to be a viable option for addressing the critical needs of the community for more accessible information and facilitating cooperation between all of the library and standard efforts currently available. RTI and its partners are actively pursuing the concepts to be able to serve the practitioner community.

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6. Dissemination of Research Findings

The development of ForensicDB has been presented as platform presentations at several national and international forensic science conferences; at an ACD/Labs software user group meeting; and at multiple professional meetings (**Table 6-1**). The database was also mentioned in several workshops and presentations at conferences (Table 6-1). ForensicDB has been referenced in several journal articles (Cox et al., 2012; Grabenauer et al., 2012; Wiley et al., 2011) and has been highlighted in interviews for an editorial in *Scientific Computing World* for their August/September issue examining cheminformatics in forensics.

Table 6-1. Presentations at Scientific Meetings

| Location and Date of Presentation | Title |
|---|---|
| Society of Forensic Toxicologists, 2010; Richmond, VA | <i>Development of a Web-accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories</i> |
| Canadian Society of Forensic Science, 2010; Toronto, Canada | <i>Overview of a Public Web-accessible Cheminformatics Database for Shared Utilization by Forensic Laboratories</i> |
| American Academy of Forensic Sciences, 2011; Chicago, IL | <i>Development of a Web-accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories</i> |
| ACD/Labs North American Users' Meeting, 2011; Princeton, NJ | <i>Development of a Web-accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories</i> |
| Society of Forensic Toxicologists/ The International Association of Forensic Toxicologists, 2011; San Francisco, CA | <i>Status Update for ForensicDB: A Web-accessible Spectral Database for Shared Utilization by Forensic Laboratories</i> |
| Society of Forensic Toxicologists/ The International Association of Forensic Toxicologists, 2011; San Francisco, CA | <i>Advanced LC-MS Approaches for the Detection of Synthetic Cannabinoids in Unknown Samples*</i> |
| Southwestern Association of Toxicologists Meeting, 2012; San Antonio, TX | Invited as a keynote speaker about the ForensicDB effort to the SAT attendance of approximately 60 toxicologists and chemists from the southwestern region. |
| Mid-Atlantic Association of Forensic Scientist Meeting, 2012; Ellicott City, MD | Synthetic Cannabinoids workshop and discussion of the ForensicDB effort to a workshop attendance of approximately 80 predominantly forensic chemists in the mid-Atlantic region. ** |
| Southern Association of Forensic Scientist Meeting, 2012; Pensacola, FL | <i>Future workshop on Emerging Drugs and the Tools and Strategies that Forensic Chemists Can Use to Deal With Them ***</i> |

* Poster presentation that referenced www.forensicdb.org

** ForensicDB discussion during a workshop

*** Invited to discuss ForensicDB at a future workshop

ForensicDB was promoted at several conferences at RTI's exhibit booth and will continue to be part of RTI's exhibit booth at upcoming conferences. **Table 6-2** shows a list of conferences where the database was promoted.

Table 6-2. Conferences where ForensicDB Was Promoted at RTI's Exhibit Booth

| Location and Date of Presentation |
|--|
| American Academy of Forensic Sciences Meeting 2012, Atlanta, GA |
| California Homicide Investigators Association Meeting 2012, Las Vegas, NV |
| North Carolina Division of the International Association for Identification Meeting 2012, Wilmington, NC |
| Technical Working Group Meeting 2012, Washington, DC |
| Indigent Defense Services Meeting 2012, Durham, NC |
| Southwestern Association of Toxicologists Meeting 2012, San Antonio, TX |
| Mid-Atlantic Association of Forensic Scientist Meeting 2012, Ellicott City, MD |
| Midwestern Association of Crime Lab Directors Meeting 2012, Columbus, OH |
| NIJ Conference 2012, Washington, DC |
| International Association of Coroners and Medical Examiners Meeting 2012, Las Vegas, NV |
| Association of Firearm and Toolmark Examiners Meeting 2012, Buffalo, NY |
| NIJ Law Enforcement Technology Conference 2012, Stevensville, MD |
| Association of Forensic DNA Analysts and Administrators Meeting 2012, San Antonio, TX |
| Society of Forensic Toxicologists Meeting 2012, Boston, MA |
| National Association of Prosecutor Coordinators Meeting 2012, Deadwood, SD |
| National District Attorney's Association Meeting 2012, Mystic, CT |
| International Association for Identification Meeting 2012, Phoenix, AZ |
| Midwestern Association of Forensic Scientist Meeting 2012, Milwaukee, WI |
| International Association of Chiefs of Police Meeting 2012, San Diego, CA |
| Southern Association of Forensic Scientist Meeting 2012, Pensacola, FL |
| National Association of Medical Examiners Meeting 2012, Baltimore, MD |
| Southwestern Association of Forensic Scientist Meeting 2012, Scottsdale, AZ |
| Northeastern Association of Forensic Scientist Meeting 2012, Saratoga Springs, NY |