Figure 3 illustrates the methods used in our laboratory for the synthesis of the isomers needed to complete modifications at Regions A, B, and C shown in Figure 1. The starting point in the synthetic pathway is a substituted benzaldehyde or benzoic acid. Many mono-substituted benzaldehydes or benzoic acids are available from commercial sources and all six regioisomeric dimethoxybenzaldehydes are commercially available. The precursor chemicals for all the possible regioisomeric imposter compounds are commercially available. Isomer issues are not quite so central in forensic analysis for those natural product drugs (THC, cocaine, etc.) synthesized by a plant in an enzymatically controlled (isomeric specific) process.

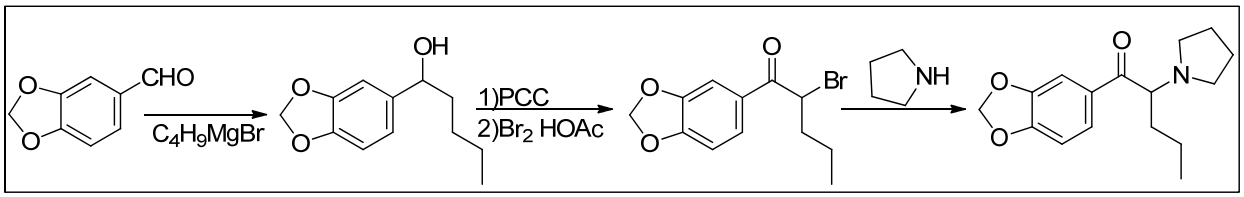

Figure 3. General synthesis for the bath salt aminoketones using the synthesis of MDPV as an example.

The analytical methods have focused on those techniques in routine use in forensic laboratories: GC, GC-MS, IR, GC-IR and related techniques. Additionally some GC-MS/MS product ion studies have been done as well as some preliminary GC-TOF-MS studies. The initial analytical studies consisted of a complete profile on each of the amines and ketone, including GC-MS, IR and GC-IR. The chromatographic elution properties and retention data via capillary GC retention studies have been collected for each compound followed by the chromatographic evaluation of each group of compounds based upon structural types. Spectrophotometric techniques such as infrared spectrophotometry have allowed for the differentiation among some of the aromatic ring substitution patterns and allow for the detection of those isomeric substances containing a carbonyl-group in the side chain. With an ample number of structural types available in this study, the various ring substituents and patterns can be individualized as a result of this work.