FLORIDA INTERNATIONAL UNIVERSITY

Miami, Florida

APPLICATION OF HIGH RESOLUTION MASS SPECTROMETRY FOR THE SCREENING AND CONFIRMATION OF NOVEL PSYCHOACTIVE SUBSTANCES

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Joshua Zolton Seither

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To: Dean Michael R. Heithaus
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This dissertation, written by Joshua Zolton Seither, and entitled Application of High-Resolution Mass Spectrometry for the Screening and Confirmation of Novel Psychoactive Substances, having been approved in respect to style and intellectual content, is referred to you for judgment.

We have read this dissertation and recommend that it be approved.

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Date of Defense: April 25, 2018

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ABSTRACT OF THE DISSERTATION

APPLICATION OF HIGH RESOLUTION MASS SPECTROMETRY FOR THE SCREENING AND CONFIRMATION OF NOVEL PSYCHOACTIVE SUBSTANCES

by

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Florida International University, 2018

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Professor Anthony DeCaprio, Major Professor

There has been an emergence of novel psychoactive substances (NPS) in forensic casework globally. Although the reported prevalence of these compounds has been relatively low in comparison to traditional drugs of abuse, published case studies suggest that some NPS have significant pharmacological effects that may cause severe impairment and/or death. Because of these effects, it is important that toxicology laboratories have the capability of identifying these compounds to complete a comprehensive toxicological analysis for human performance and post-mortem investigations.

Recently, mass spectrometry has gained favor over traditional screening assays such as immunoassays for the identification of NPS in biological specimens. This trend is mainly a result of the fact that mass spectrometry provides the required sensitivity and selectivity for a broader range of analytes. High resolution tandem mass spectrometry has been suggested for analysis of NPS, as this technique further increases selectivity by increasing mass accuracy and providing MS/MS spectral data. The main goal of the present study was to investigate the applicability of using high resolution mass

spectrometry to screen for and confirm a large number of novel psychoactive substances. The present study consisted of three main tasks, which included 1) the creation of a large high resolution MS/MS spectral library and database, 2) the development of a solid phase extraction (SPE) method and acquisition methods, and 3) a collision induced dissociation (CID) study of regioisomeric NPS compounds.

The MS/MS spectral library created contains spectral data for 252 NPS. In addition, 875 NPS entities were included in the compound database. The library and database can be used by toxicology laboratories to aid in the identification of NPS in casework using MS/MS spectral data and full scan MS data, respectively. The analytical method developed used SPE and high resolution mass spectrometry (HRMS). The HRMS method demonstrated limits of detection ranging from 0.5- 5 ng/mL for NPS from various structural drug classes. The CID experiments demonstrated that relative ion abundance alone could be used to differentiate some sets of regioisomers. The present work can aid toxicology laboratories in the identification of NPS and demonstrates the applicability of HRMS for their screening and confirmation.

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LIST OF ABBREVIATIONS, ACRONYMS, AND SYMBOLS

α-PVP	alpha-Pyrrolidinopentiophenone
Δ9-THC	delta-9-tetrahydrocannabinol
2-EEC	2-Ethylethcathinone
2-FA	2-Fluoroamphetamine
2-FEC	2-Fluoroethcathinone
2-FMA	2-Fluoromethamphetamine
2-FMC	2-Fluoromethcathinone
2-MeOMC	2- Methoxymethcathinone
2,3-MDMC	2,3-Methylenedioxymethcathinone
2,3-MDPV	2,3-Methylenedioxy Pyrovalerone
3-EEC	3-Ethylethcathinone
3-FA	3-Fluoroamphetamine
3-FEC	3-Fluoroethcathinone
3-FMA	3-Fluoromethamphetamine
3-FMC	3-Fluoromethcathinone
3-MeOMC	3-Methoxymethcathinone
3-MeO-PCP	3-Methoxy-phenylcyclidine
3-MEC	3-Methylethcathinone
3-MMC	3-Methylmethcathinone
4-EEC	4-Ethylethcathinone
4-FA	4-Fluoroamphetamine
4-FEC	4-Fluoroethcathinone

4-FMA	4-Fluoromethamphetamine
4-FMC	4-Fluoromethcathinone
4-MEC	4-Methylethcathinone
4-MeO-DMT	4-methoxy-N,N-dimethyltryptamine
4-MeOMC	4-Methoxymethcathinone
4-MeO-PCP	4-Methoxy-phenylcyclidine
5-MeO-DMT	5-methoxy-N,N-dimethyltryptamine
ANOVA	Analysis of Variance
APCI	Atmospheric Pressure Chemical Ionization
BZP	1-Benzylpiperazine
CAS	Chemical Abstracts Service
CB_1	Cannabinoid Type 1 Receptor
CB_2	Cannabinoid Type 2 Receptor
CEDIA	Cloned Enzyme Donor Immunoassay
CEF	Compound Exchange Format
CI	Chemical Ionization
CID	Collision Induced Dissociation
CNS	Central Nervous System
DAT	Dopamine Transporter
DART	Direct Analysis in Real Time
DEA	Drug Enforcement Administration
DESI	Desorption Electrospray Ionization
DMT	N,N-Dimethyltryptamine

EI	Electron Ionization
ELISA	Enzyme Linked Immunosorbent Assay
EMCDDA	European Monitoring Centre for Drugs and Drug Addiction
EMIT	Enzyme Multiplied Immunoassay Technique
ESI	Electrospray Ionization
FIA	Flow Injection Analysis
GABA	γ-aminobutyric acid
GC-MS	Gas Chromatography Mass Spectrometry
HEIA	Homogeneous Enzyme Immunoassay
HPLC	High Performance Liquid Chromatography
HRMS	High Resolution Mass Spectrometry
ICR	Ion Cyclotron Resonance
IRD	Infrared Detection
IUPAC	International Union of Pure and Applied Chemistry
KE	Kinetic Energy
KIMS	Kinetic Interaction of Microparticles in Solution
LC-MS	Liquid Chromatography Mass Spectrometry
LLE	Liquid-Liquid Extraction
LSD	Lysergic acid diethylamide
mCPP	1-(3-chlorophenyl)-piperazine
MDMA	3,4-Methylenedioxymethamphetamine
MDPV	3,4-Methylenedioxypyrovalerone
MS	Mass Spectrometry

MS/MS	Tandem Mass Spectrometry
m/z	Mass to Charge Ratio
NDEWS	National Drug Early Warning System
NET	Norepinephrine Transporter
NIST	National Institute of Standards and Technology
NMDA	N-methyl-D-aspartate Receptor
NMR	Nuclear Magnetic Resonance
NPS	Novel Psychoactive Substance
PCDL	Personal Compound Database and Library
PCE	N-ethyl-1-1phenylcyclohexylamine
PCiP	1-Phenyl-N-(propan-2-yl)cyclohexan-1-amine
PCP	Phencyclidine
PCPr	N-Propyl-1-phenylcyclohexylamine
PDA	Photodiode Array
PIKHAL	Phenethylamines I Have Known and Loved
ppm	Parts Per Million
QC	Quality Control
QTOF	Quadrupole Time-of-Flight Mass Spectrometry
QqQ	Triple Quadrupole Mass Spectrometry
SERT	Serotonin transporter
SIM	Selected Ion Monitoring
SPE	Solid Phase Extraction
SWGTOX	Scientific Working Group for Forensic Toxicology

TFMPP	1-(3-trifluoromethylphenyl)-piperazine
TIC	Total Ion Chromatogram
TIHKAL	Tryptamines I Have Known and Loved
TOF	Time of Flight Mass Spectrometry
TSPO	Translocator protein
UNODC	United Nations Office on Drugs and Crime
UPLC	Ultra Performance Liquid Chromatography

1. INTRODUCTION

The identification of psychoactive substances is necessary in forensic toxicological investigations, as questions of impairment or cause of death typically arise. Currently, forensic toxicology laboratories employ methodologies that can readily detect the presence of traditional drugs of abuse in different human matrices. However, over the past decade there has been an emergence, in some cases a reemergence, of compounds known as novel psychoactive substances (NPS). These substances are manufactured and/or used to evade current laws but are intended to provide comparable pharmacological effects as more common illicit drugs of abuse. NPS are diverse and are classified by chemical structure and/or pharmacological effects. Identification of these substances is challenging to forensic toxicology laboratories, as routine screening techniques, such as immunoassays, cannot detect the presence of many of these substances, as traditional immunoassay panels often have low cross reactivity with these compounds. Additional challenges include identifying structurally related substances, including isobars and isomers, varying legality and pharmacological effects, and rapidly changing popularity and use of these substances. In order to identify NPS in routine casework, many forensic toxicology laboratories have turned to mass spectrometry in an attempt to detect and confirm these substances.

The present research was designed to help forensic toxicology laboratories identify NPS by exploring the usefulness of high resolution mass spectrometry (HRMS) in identifying these compounds. In order to accomplish this task, a high resolution MS/MS spectral library was created using NPS standards. A database containing structural and molecular information was created to supplement the spectral library. A sensitive

analytical method was developed that is able to identify NPS from various drug classes in human blood specimens. Also, an investigation into the reproducibility of MS/MS spectral data generated by collision induced dissociation (CID) was performed, to determine if select regioisomeric NPS could be distinguished from each other using CID MS/MS spectral data alone. The work will aid forensic toxicology laboratories in the identification of NPS in routine case work.

2. LITERATURE REVIEW

2.1 Novel Psychoactive Substances Background

Novel psychoactive substances (NPS) are psychotropic compounds that have been manufactured and/or used to evade current drug laws [1]. They are intended to produce pharmacological effects comparable to those of common illicit drugs and are often structurally related to illicit or restricted compounds [2]. NPS are also commonly known as “designer drugs,” “research chemicals,” or “legal highs” [3-4]. NPS have recently experienced an increase in the popularity among drug users [5]. Perceived benefits of NPS use include evading current drug laws or punishments associated with illicit drug use and a belief that these substances are safer than traditional drugs of abuse. In some cases, NPS are easier and less expensive to obtain when compared to traditional drugs of abuse [6-7]. Typically, these substances are produced in China and South East Asia, sold on the internet under various names such as “research chemicals,” “legal highs,” “bath salts,” “plant food,” and generally are labelled “not for human consumption” [8-10].

Many of the NPS have been “rediscovered” from previous scientific research. A prime example of this phenomenon is the synthetic cannabinoid drug class. Many of the synthetic cannabinoids were originally investigated by pharmaceutical companies or research groups in an attempt to learn more about the cannabinoid activity of these compounds, with the hope of identifying drugs for legitimate medicinal use [11]. During these investigations, hundreds of compounds with slight structural modifications were created and documented in the scientific literature [12]. Ultimately, these compounds were determined not to be suitable for human use and further studies were not performed. Around 2006, some of these compounds started to appear in seized drug materials and

later were observed in forensic toxicological investigations [11]. Since then multiple synthetic cannabinoids and/or metabolites have been detected in drug seizure cases and in forensic toxicological case reports [13-16]. Many of these compounds, specifically the JWH series of synthetic cannabinoids, were documented in previous scientific work [12, 17],although there have also been emerging NPS compounds that are novel derivatives previously not reported in literature.

Because the vast majority of NPS have not been evaluated in animal or human pharmacological studies, available health data are limited for most of these compounds [18]. Consequently, there is a risk of unintended pharmacological effects, including severe impairment, toxicity and even death when using these substances [19]. The potential dangers of NPS have been documented by poison control call reports, reported emergency room visits, and forensic toxicology reports involving both antemortem and postmortem cases [20-27].

In response to the proliferation of NPS, many governments and organizations have created programs in an attempt to address this issue. Early drug detection programs, such as Sweden's STRIDA project, the European Union's European Monitoring Centre for Drugs and Drug Addiction (EMCDDA) Early Warning System, the United Nations Office on Drugs and Crime (UNODC) Early Warning Advisory on NPS, and the United States National Institute on Drug Abuse's National Drug Early Warning System (NDEWS) have been created to identify and report on new NPS that have been observed in literature, poison control reports, hospital and forensic cases [7, 28].

In addition, governing bodies have enacted legislation in an attempt to combat the use of these compounds. The United States Drug Enforcement Administration (DEA) has

federally controlled many NPS from various structural and pharmacological classes, including cathinones, phenethylamines, piperazines, synthetic cannabinoids, synthetic opioids, and tryptamines, using either analogue-based or emergency scheduling procedures. Similar efforts have been observed in many other countries [29-30]. As a consequence of this legislation and the reported effects of these substances, a need has been created for forensic and clinical toxicology laboratories to be able to reliably detect these compounds in human specimens.

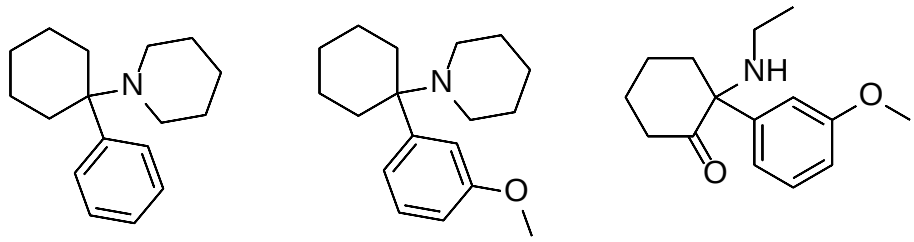
2.2 Novel Psychoactive Substance Classes

Novel psychoactive substances encompass a large, structurally diverse group of compounds. Typically, these substances are classified on the basis of their chemical structure and/or purported pharmacological effects. The NPS classes that have been identified in previous literature include but are not limited to arylcyclohexylamines, benzodiazepines, cathinones, phenethylamines, piperazines, synthetic cannabinoids, synthetic opioids, and tryptamines.

While there has been progress in determining the mechanism of action for NPS substances by assessing receptor binding affinities with *in silico* and *in vitro* models, the mechanism of action is not known for every NPS. In some classes, such as the cathinones, structurally related analogues have varying pharmacological effects. In addition, various analogues in the synthetic cannabinoid class have been reported to have significantly different cannabinoid CB_1 and CB_2 receptor binding affinities, which also results in varying pharmacological effects [31-32]. The elucidation of the mechanism of action is further complicated by the fact that controlled human studies have not been

conducted for these compounds and the fact that psychoactive metabolites may be formed which can prolong or create pharmacological effects.

2.2.1 Arylcyclohexylamines



PCP 3-MeO-PCP Methoxetamine

Figure 1. Selected novel psychoactive substances that are in the arylcyclohexylamines class.

Arylcyclohexylamines are compounds that consist of an aromatic ring, a cyclohexane ring and an amine moiety. They are commonly believed to have phencyclidine (PCP)- or ketamine-like pharmacological activity [33]. Arylcyclohexylamines have been reported to have high affinity for the N-methyl-D-aspartate (NMDA) receptors, where they act as antagonists [33]. Some derivatives were also reported to have noticeable affinities for the serotonin transporter and/or for the sigma receptors [34]. In addition, some derivatives are also thought to act as dopamine reuptake inhibitors [35].

Arylcyclohexylamines are classified as dissociative anesthetics [36]. They are reported to produce anesthesia, agitation, euphoria, insomnia, tachycardia, ataxia and hallucinogenic effects [37]. Acute toxicity of methoxetamine has been documented in three hospital cases, where each patient was described to be in a “dissociative/catatonic” state with acute sympathomimetic toxicity symptoms present. These symptoms included

tachycardia and hypertension [38]. Fatal intoxications have also been reported involving structural analogs of PCP [39].

The first arylcyclohexylamine to be reported in literature was 1-(1-phenycyclohexyl)-amine (PCA) in 1907 [40]. The most well know arylcyclohexylamine, 1-(1-phenylcyclohexyl) piperidine (PCP), was first synthesized in 1956 and human trials for PCP began in 1957 [40]. Phencyclidine, also known as PCP, was used for nearly a decade as an anesthetic before being withdrawn from the market in favor of another arylcyclohexylamine, ketamine, which had fewer documented side effects compared to PCP [40]. Phencyclidine is controlled as a Schedule II drug by the United States DEA [39]. Ketamine is still used today in the medical and veterinary fields. In addition to legitimate medicinal use, illicit ketamine use has been documented, which led this compound to be controlled. It is currently listed as a Schedule III controlled substance by the United States DEA.

Many arylcylcohexylamine substances were synthesized and explored by pharmaceutical companies and research groups for medicinal use. Like other NPS drug classes, some of these derivatives have appeared in the illicit drug market. Examples include N-ethyl-1-1phenylcyclohexylamine (PCE), N-Propyl-1-phenylcyclohexylamine (PCPr), and 1-Phenyl-N-(propan-2-yl)cyclohexan-1-amine (PCiP). They were reported in the illicit drug market beginning in the1960s to the 1990s [33].

More recently, over 25 additional arylcyclohexylamines were identified in the illicit drug market by drug seizures and toxicological investigations. At least a dozen of these compounds were first observed after 2005, suggesting that there is still interest in this drug class among illicit drug manufacturers and users [40]. For example, Backberg

reported that 3-methoxy-phenylcyclidine (3-MeO-PCP) and/or 4-methoxy-phenylcyclidine (4-MeO-PCP) were detected in over 80 patients between July 2013 and March 2015 from emergency rooms and intensive care units in Sweden [41]. In 2016, Fassette and Martinez reported that methoxetamine was identified and confirmed in an impaired driver [42]. In 2017, two fatal polydrug intoxications involving 3-MeO-PCP were reported by Mitchell-Mata, et al. [39].

2.2.2 Benzodiazepines

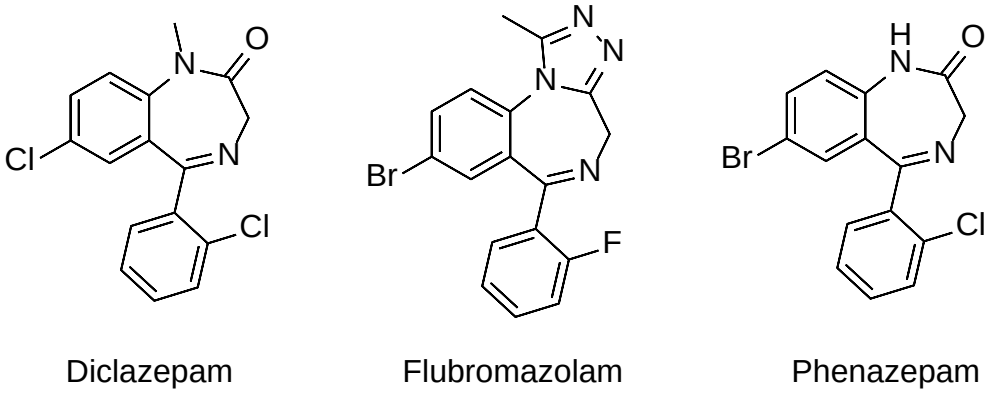


Figure 2. Selected novel psychoactive substances from the benzodiazepine class.

Consistent with benzodiazepines that have medicinal use, designer benzodiazepines have a core structure that consists of a benzene ring fused to a diazepine ring. Typically, this core structure has a second benzyl ring attached to it. Most benzodiazepines bind to γ-aminobutyric acid (GABA) receptors in the human body, where they act as allosteric modulators. The binding of benzodiazepines to the GABA receptor increases the affinity of GABA to the receptor and enhances the effect of the GABA neurotransmitter [43]. It also has been documented that some benzodiazepines, such as 4-chlorodiazepam and diazepam, also bind to the translocator protein (TSPO) [44].

Benzodiazepines are classified as central nervous system depressants. Amnesic, anxiolytic, and sedative effects have been well documented with benzodiazepine use [45]. However, benzodiazepines such as 4-chlorodiazepam that only bind to the TSPO have been shown to create anxiolytic effects without the sedative effect [44]. Duration of action can vary greatly among benzodiazepines. In addition, some benzodiazepines are metabolized into psychoactive metabolites which can further extend the duration of action of the initial benzodiazepine ingestion. Acute intoxications resulting in hospitalization and death have been documented with nonmedical use of benzodiazepines, including designer benzodiazepines [46-47]. Benzodiazepines have also been confirmed in impaired driving cases, as well as in drug-facilitated crime cases [48-50].

The first designer benzodiazepines, phenazepam and nimetazepam, were identified in Europe in 2007 [44]. Since then, many benzodiazepine related compounds have been seen in the illicit drug market. The majority of these compounds are failed pharmaceutical candidates diverted to illicit use, with their synthesis and relative potency well detailed in literature. In contrast, some compounds, such as flubromazolam, appear to be novel and as such have not been described in literature [51-53].

Recently, there has been an increase in the number of different designer benzodiazepines confirmed in forensic toxicological investigations. Hoiseth, et al. reported that clonazolam, diclazepam, flubromazepam, flubromazolam and/or pyrazolam was detected in 77 criminal cases in Norway from July 2013 to May 2016 [54]. In Sweden, between February 2014 and November 2015 there were 191 clinical samples that tested positive with immunoassay screening by CEDIA, but were negative using a

traditional benzodiazepine confirmation assay that included at least one designer benzodiazepine. In the Swedish study, 11 different designer benzodiazepines were reported, with flubromazolam and meclonazepam being the most frequently observed [55].

2.2.3 Cathinones

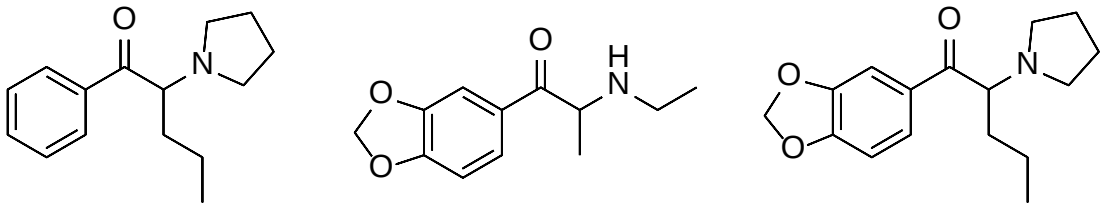


Figure 3 Selected novel psychoactive substances from the cathinone class.

Cathinones are β-keto substituted phenethylamines. They act as modulators of the plasma membrane monoamine transporters, which include the dopamine transporters (DAT), norepinephrine transporters (NET) and the serotonin transporters (SERT) [56-57]. The function of these transporters is to regulate the concentration of the monoamine neurotransmitters by removing them from the synaptic cleft. There is variability among the different cathinone derivatives in terms of their interactions with the different monoamine transporters, which may explain the differences observed in their pharmacological effects [58].

Synthetic cathinones are classified as central nervous system stimulants and have pharmacological effects generally comparable to amphetamine, cocaine, methamphetamine and/or 3,4-methylenedioxymethamphetamine (MDMA) [20, 59-60]. Pharmacological effects that have been documented with synthetic cathinone use include

agitation, blurred vision, dehydration, dysphoria, increased blood pressure, increased body temperature, insomnia, nausea, paranoia, psychosis, sympathomimetic effects, and tachycardia [20, 61-62]. Hospitalization and/or death has also been attributed to the illicit use of cathinones [63-66].

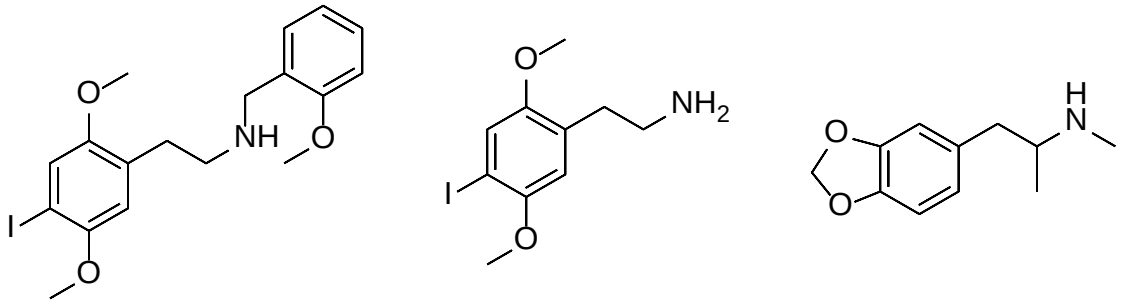
Cathinone is the main psychoactive compound that is found in the fresh leaf of the *Catha edulis* plant, which have been used since the eleventh century for its psychoactive effects [67-68]. In 2010, the first cases of synthetic cathinone use were reported to United States poison control centers. Within the first eight months there were over 1400 cases reported to the poison control center [69]. In 2011, the DEA added the first synthetic cathinones methylone, MDPV, and mephedrone to the Schedule 1 controlled list [70]. Since then, newer synthetic cathinone derivatives, such as ethylone, pentedrone, *alpha*-pyrrolidinopentiophenone (α-PVP), and N-ethylpentylone, have appeared in the illicit drug market [25, 71-72].

In Italy between 2013 and 2015, the most frequently observed synthetic cathinones in seized drug material were 3-methylmethcathinone (3-MMC) with 35 cases, 4-methylethcathinone (4-MEC) with 33 cases, and MDPV with 16 cases [2]. Adamowicz reported that α-PVP was found in 66 cases from Poland between early 2014 and mid-2015 [73].

2.2.4 Phenethylamines

Phenethylamines are compounds that contain a phenyl ring and an amino group that are bonded together by an ethyl alkyl chain. The structural drug class includes both amphetamine and methamphetamine along with many other derivatives. Phenethylamines inhibit the dopamine, the serotonin and/or the norepinephrine transporters, thereby

increasing levels of the corresponding neurotransmitters in the synaptic cleft [8]. Alternatively, a few can act as agonists of the receptors themselves.



25I-NBOMe 2C-I MDMA

Figure 4. Selected novel psychoactive substances from the phenethylamine class.

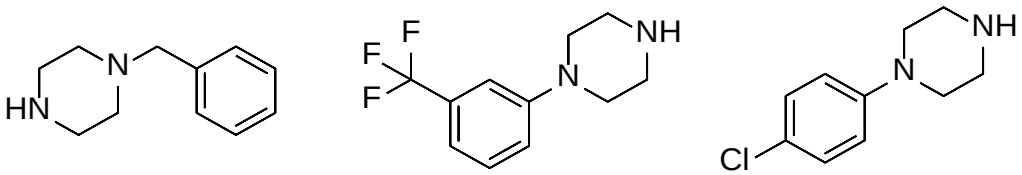
Phenethylamines are in general considered to have CNS stimulant properties [6]. In addition, some substituted phenethylamines, such as compounds from the 2C-X subclasses, have also been reported to induce hallucinogenic effects, as most of these compounds have affinity for the serotonin receptors [74]. Agitation, convulsions, dissociation, euphoria, hallucinations, hyperthermia, kidney failure, liver failure, psychosis and respiratory deficits have been observed with phenethylamine use [74-75]. Hospitalization and death have also been reported with phenethylamine intoxications [24, 76-78].

One of the most well-known phenethylamines is 3,4-methylenedioxymethamphetamine (MDMA). MDMA was first synthesized by a pharmaceutical company in 1912 and began to be seen in the illicit drug market in the 1960s [79]. In the 1970s and 1980s its popularity increased as a recreational drug, prompting eventual control by the United States DEA [80]. In 1991, Dr. Alexander Shulgin, a medicinal chemist who had formerly worked for BioRad Laboratories and

Dow Chemical Co. before becoming an independent consultant, published a book entitled PIKHAL (Phenethylamines I Have Known and Loved) which described the detailed chemical synthesis and human pharmacological effects of 179 phenethylamines [81]. Some of the compounds detailed Shulgin's book have been subsequently identified in forensic toxicological investigations.

Recently, the most commonly identified phenethylamines in forensic casework have been the N-benzyl substituted phenethylamines, which are known as "NBOMe" derivatives. They are considered highly potent hallucinogens due to their increased affinity for the 5-HT_{2A} serotonin receptor and have been sold as alternatives to LSD [77]. The N-benzyl substituted phenethylamines that have been confirmed in biological specimens are 25B-NBOMe and 25I-NBOMe [76, 82]. In addition to toxicological investigations, Kaizaki-Mitsumoto reported that six new phenethylamine compounds, including three NBOMe derivatives, were identified in drug material obtained in Japan in 2015 [83].

2.2.5 Piperazines



Benzylpiperazine TFMPP pCPP

Figure 5. Selected novel psychoactive substances from the piperazine class.

There are two main piperazine structural groups that have been observed in illicit materials, benzylpiperazines and phenylpiperazines [84]. Piperazine derivatives typically contain a substitution on the benzyl ring or the phenyl ring. Pharmacological activity

varies depending on the substitution of the piperazine structure and whether the compound is a benzylpiperazine or a phenylpiperazine. Benzylpiperazines have been found to stimulate dopamine, serotonin, and norepinephrine release and also inhibit the reuptake of these neurotransmitters [85]. While phenylpiperazines act directly on the serotonin transporters, they exhibit little effect on the dopamine and norepinephrine transporters [6].

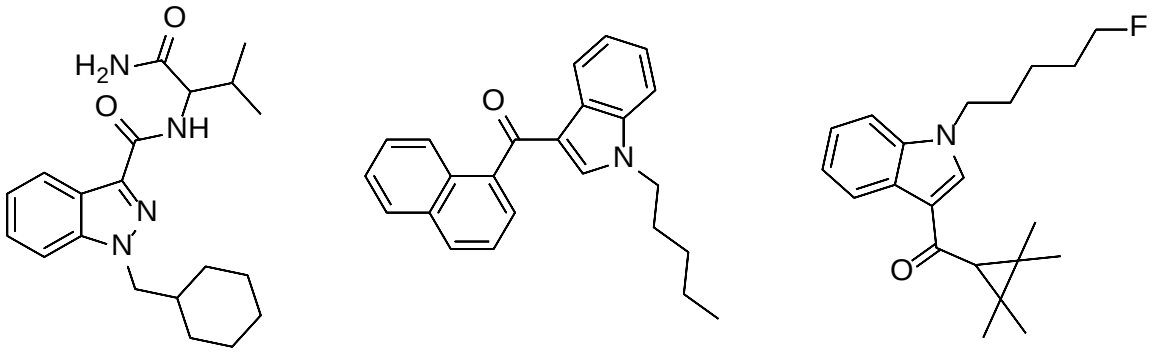
Piperazines have been generally recognized as CNS stimulants with some compounds having hallucinogenic effects [86]. Reported pharmacological effects of piperazine use include agitation, anxiety, hallucinations, hyperthermia, seizures, and tachycardia [85-87]. Piperazines are thought to be less potent then amphetamine, however, intoxications requiring hospitalization or resulting in death have been documented in previous literature [18, 86, 88].

Piperazine was originally synthesized as an anthelminthic in the 1940s, however it was observed to have effects similar to amphetamine. During the 1960s and 1970s, benzylpiperazine derivatives were explored as antidepressants [89]. Piperazine derivatives became popular party drugs in the 1990s [18, 90]. In 2010, Dickson reported the confirmation of the most popular piperazines; 1-benzylpiperazine (BZP), 1-(3-trifluoromethylphenyl)-piperazine (TFMPP), and 1-(3-chlorophenyl)-piperazine (mCPP) in urine specimens [91]. The popularity of piperazines decreased substantially when the cathinone class appeared on the market and gained favor among drug users [19].

2.2.6 Synthetic Cannabinoids

Synthetic cannabinoids are compounds that act on the cannabinoid receptors CB_1 and CB_2 [8]. The synthetic cannabinoids class is a very structurally diverse class with

most of the compounds not structurally related to delta-9-tetrahydrocannabinol (Δ^9-THC), the main psychoactive compound in marijuana [92]. Many classes of synthetic cannabinoids incorporate various chemical skeletons such as indole, indazole, naphthyl, or pyrroles moieties.



AB-CHMINACA JWH-018 XLR-11

Figure 6. Selected novel psychoactive substances from the synthetic cannabinoid class.

Synthetic cannabinoids were originally thought to act like traditional cannabinoids such as Δ^9-THC. However, while this is true for some synthetic cannabinoids, atypical cannabinoid pharmacological effects have been reported with their use [93]. The affinity and agonist activity for the CB_1 and/or CB_2 receptors vary among the different synthetic cannabinoids, which may cause the different observed pharmacological effects [32, 94]. Reported effects include agitation, anxiety, hallucinations, hyperthermia, paranoia, psychosis, renal failure, seizures, tachycardia, and vomiting [95-96]. Hospitalization and death have also been reported with synthetic cannabinoid use [97-99].

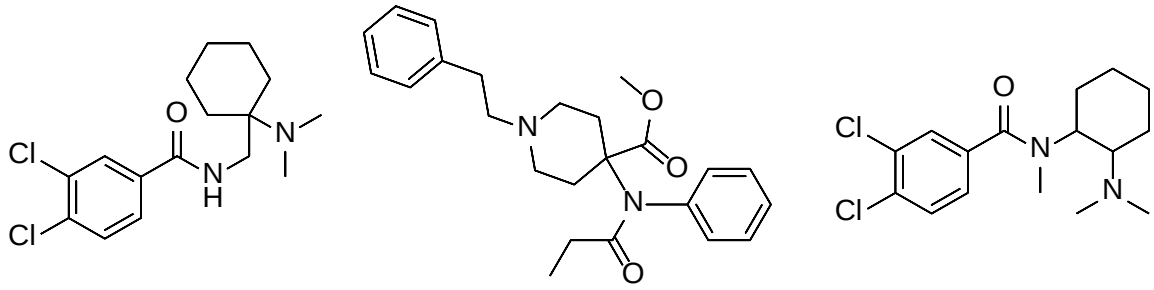
In attempt to find compounds that could create the analgesic and anti-inflammatory effects of Δ^9-THC without the psychoactive side effects, various research groups and pharmaceutical companies created and published synthesis details for

hundreds of CB_1 and CB_2 agonists [12, 18]. Some of these synthetic cannabinoid compounds have been confirmed in herbal products that were sold over the internet and in forensic toxicological specimens [11, 100].

Synthetic cannabinoids were first confirmed in Europe in the mid-2000s and were identified in the United States shortly thereafter [101]. The synthetic cannabinoids JWH-018, JWH-073, CP 47,497 and HU-210 were the first derivatives identified in herbal material [11]. Since then, many more compounds have been seen. Synthetic cannabinoids are considered to have multiple synthetic generations, as newer derivatives rapidly appear on the market after governments ban existing compounds or the popularity of particular synthetic cannabinoids declines [96]. Tynon reported that between March 2015 and December 2015, 537 blood samples contained at least one synthetic cannabinoid. The most commonly identified synthetic cannabinoids in the Tynon report were AB-CHMINACA and ADB-CHMINACA [102]. Previously unreported synthetic cannabinoids continue to be identified in seized drug material to the present [103-104].

2.2.7 Synthetic Opioids

Synthetic opioids are compounds that are agonists or antagonists of the δ, κ, and μ opioid receptors [105]. Synthetic opioids are made with chemical precursors that are readily available and cheaper than the opium extracted from poppy plants, which is needed to produce traditional opiates [106]. There is some structural diversity in this class of NPS, which can be generally classified as fentanyl analogs and non-fentanyl like synthetic opioids. Synthetic opioids have a wide range of potency according to preclinical data [105].



AH-7921 Carfentanil U-47700

Figure 7. Selected novel psychoactive substances from the synthetic opioid class.

Synthetic opioids, like traditional opioids, act as opioid analgesics. Opioids block the transmission of painful stimuli and in some instances produce euphoria [107]. Opioids are typically used therapeutically to manage pain from surgical procedures or from chronic pain. They have also been used as antitussives and for their antidiarrheal properties [107]. In addition, there are opioid antagonists that are used to treat opioid intoxications and withdrawal symptoms. Potency of the different synthetic opioids and their affinity for the different opioid receptors have been cited as the main differences in pharmacological effects [108]. Many synthetic opioid intoxications have resulted in hospitalization and/or death [109-112].

Between 2002 and 2011 it was estimated that 25 million people used prescription opioids for nonmedical use [113]. In 2010 there were 16,751 opioid related deaths in the United States, which prompted local, state and federal governments to create programs to improve opioid prescribing practices and to penalized doctors and clinics for writing unnecessary prescriptions [113]. As prescription opioids became less available, it appears that many users turned to illicit opioids, as evident by the increased use of heroin and other synthetic opioids [114]. Over time, illicit laboratories began to synthesize fentanyl and other synthetic opioids as cheaper alternatives to heroin or other controlled opioids.

Recently, fentanyl and other synthetic opioids have appeared in heroin, drug material sold as heroin, and in counterfeit benzodiazepine or opioid pharmaceuticals [106, 115]. In addition, there are drug users who intentionally seek out new synthetic opioid analogs, behavior which has also been observed with other NPS classes [106]. Acetyl fentanyl may have been the first synthetic opioid that was used as a novel psychoactive substance. Since then, many fentanyl derivatives and other synthetic opioids have appeared in the illicit drug market [105]. Recent literature has reported the confirmation of carfentanil, furanyl fentanyl, and 4-fluoroisobutyryl fentanyl in forensic toxicological investigations [116-118]. Other synthetic opioids that are not structurally related to fentanyl have also been reported. The most common of these non-fentanyl derivatives reported in literature include AH-7921, U-47700 and MT-45 [109, 119].

2.2.8 Tryptamines

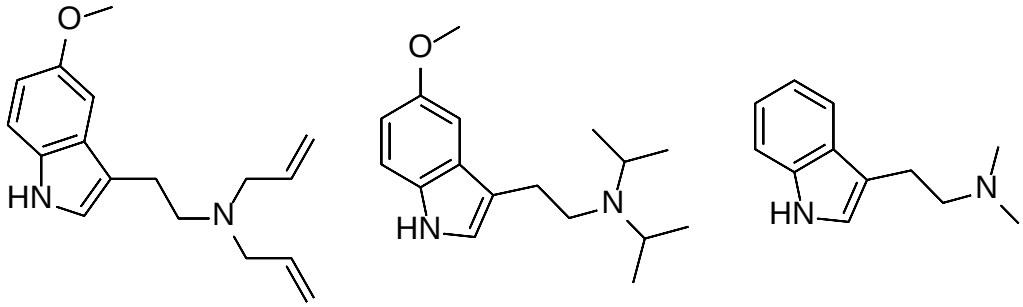


Figure 8. Selected novel psychoactive substances from the tryptamine class.

Tryptamines are compounds that contain an indole moiety with an ethylamine side chain and are structurally related to the neurotransmitter serotonin. Tryptamine modifications include substitutions on the indole ring, alkyl chain, and/or the amino group [120]. Tryptamines primarily act as agonists on the 5-HT_{2A} receptor of the

serotonin receptor family. Sigma-1 receptor activity has also been documented with tryptamine use [121].

In general, tryptamines are considered hallucinogens, with some derivatives having stimulant like activity [120]. They have a relatively short duration of action, however some tryptamines have been reported to have a relatively quick onset of action [122]. Clinical effects observed with tryptamine use include anxiety, diaphoresis, diarrhea, drowsiness, dysphoria, euphoria, hallucination, hypertension, nausea, rhabdomyolysis, tachycardia, and tachypnea [123]. Hospitalization and/or death has been reported with tryptamine intoxications [120, 124].

The compound N,N-dimethyltryptamine (DMT) is found in hundreds of plants around the world and endogenously at low concentrations in humans. The tryptamine DMT has been used for many centuries for religious and spiritual purposes [121]. Other natural tryptamines have been identified in mushrooms (4-phosphoryloxy-N,N-dimethyltryptamine; psilocybin and 4-hydroxy-N,N-dimethyltryptamine; psilocin) and secretions of the desert toad *Bufo alvarius* (5-hydroxy-N,N-dimethyltryptamine; bufotenine) [123].

Arguably the best known tryptamine analog, lysergic acid diethylamide (LSD), was synthesized in 1938 and was eventually banned in 1966 [123]. In 1997, Dr. Alexander Shulgin published a sequel to PIHKAL, entitled “TIHKAL: the continuation”, which detailed the synthesis and provided user information for 55 tryptamine derivatives [125]. Some of the compounds described were subsequently identified in forensic toxicological investigations [124]. However, as evident from recent poison control center reports, self-reported drug use, and prevalence studies, it appears that tryptamines are not

as prevalent as they once were, with only a few cases of tryptamine use recently reported [19-21, 126].

2.3 Identification of Drugs of Abuse and Novel Psychoactive Substances

2.3.1 Routine Forensic Toxicological Analysis

Forensic and clinical toxicology laboratories routinely employ screening and confirmation techniques for detection of drugs in human specimens. Screening techniques in a forensic laboratory typically include targeted immunoassays coupled with an untargeted mass spectrometric analysis. Screening techniques are typically less time consuming and more cost effective than confirmation techniques. Using the results of the screening assays, specimens are typically further analyzed by a more selective confirmation assay utilizing mass spectrometry. A qualitative or quantitative result is generated using the confirmation method.

2.3.2 Immunoassays

Immunoassays have been employed in forensic laboratories as a screening method because minimal sample preparation is needed, lower cost, the time of analysis is typically shorter than those of confirmation methods. Immunoassays are also readily available commercially. Various immunoassay techniques, which include but are not limited to Enzyme Linked Immunosorbent Assay (ELISA), Enzyme Multiplied Immunoassay Technique (EMIT), Kinetic Interaction of Microparticles in Solution (KIMS), Cloned Enzyme Donor Immunoassay (CEDIA) and Homogeneous Enzyme Immunoassay (HEIA), have been used in forensic toxicology laboratories. Immunoassays typically utilize competitive binding of the free target analyte and a modified target analyte in order to detect drugs of abuse in case specimens. The modifications of the

targeted analyte are different among the techniques used but can include labelled target analytes that can be conjugated with enzymes or microparticles. Absorbance at various wavelengths is typically measured to determine if a drug is present in a sample [127].

Immunoassays use antibodies that are targeted for a certain drug or drug class. The specificity varies among antibodies used and the purpose of the assay. Some immunoassay panels are created to target for one specific analyte, while other panels are created to be cross reactive with as many compounds from a drug class as possible. In both types of panels, both endogenous or exogenous compounds may be present that can create false positive or negative results [128]. While immunoassays can be very sensitive, they are not selective enough to confirm the presence of a drug of abuse or NPS in forensic toxicological investigations [129]. A positive result from an immunoassay needs to be confirmed by a more selective methodology. Typically, mass spectrometry is used to confirm drugs of abuse.

Successful identification of NPS using immunoassays varies among individual compounds, the immunoassay technique, and the reagents used [130-133]. For example, the designer benzodiazepine drug class has exhibited the most compounds with significant cross reactivity across multiple immunoassay techniques [43]. However, the majority of NPS have low or no cross reactivity with commonly used immunoassay drug panels [134]. For this reason, many forensic toxicology laboratories are moving towards screening assays that utilize mass spectrometry in an attempt to reliably identify NPS in routine case work.

2.3.3 Sample Preparation

Sample preparation is generally needed before a specimen can be analyzed by a confirmatory assay that utilizes a mass spectrometer. The most common sample preparation techniques utilized in forensic toxicology laboratories are liquid/liquid extraction (LLE) and solid phase extraction (SPE) methodologies. However, “dilute and shoot” and “crash and shoot” sample preparation methods are also gaining favor among laboratories that utilize liquid chromatography mass spectrometers.

LLE methodology isolates the analyte of interest by using two liquids that are immiscible with each other. Typically, these methods consist of an organic solvent and an aqueous solvent. The target analyte will favor one of the solvents because of its relative solubility in each solvent. As most drugs of abuse and NPS are considered weak acids or weak bases, manipulation of the pH can be used to favor one solvent over the other in terms of solubility. The LLE approach also helps remove compounds from the specimen that do not have similar chemical properties of the analytes of interest. The technique enables the use of wash steps, also known as “back extraction,” as solvents that do not contain the target analyte can be discarded and replaced with another solvent to help further remove unwanted compounds. Typically, the organic solvent is the final solvent that contains the target analyte(s). The organic solvent is then dried down under nitrogen before being reconstituted with an appropriate solvent prior to mass spectral analysis [135].

SPE methodology utilizes a cartridge with a sorbent bed mass consisting of silica or a polymeric resin containing certain chemical functional groups. The typical methodology implements a column condition step which is used to prime the extraction

cartridge to ensure that the functional groups of the bed are active. Then the buffered sample is added to the extraction cartridge. Wash solvents are added to the extraction cartridge to remove unnecessary compounds found endogenously or exogenously in the sample such as carbohydrates, lipids, and proteins. The analyte of interest is retained on the extraction cartridge bed mass during the loading and wash steps. The analyte is finally eluted when the proper elution solvent is added to the extraction cartridge. The eluent is then dried down under nitrogen gas before being reconstituted with the appropriate solution before mass spectral analysis [135].

In SPE, analytes are retained on the basis of the chemical properties of the sorbent bed mass and the analyte itself. Typically, ionic bonding and hydrophobic interactions are used to facilitate the retention of the analyte. As in LLE, the pH of the solvents and solubility of the analyte in the various solvents can greatly affect whether or not an analyte or other compounds are retained on the sorbent bed mass [135].

Dilute and shoot methods typically incorporate a hydrolysis step for urine samples before being diluted with a buffer or mobile phase. Crash and shoot methods typically employ an acetonitrile protein precipitation (crash) step for blood samples before being diluted with buffer or mobile phase. With both techniques, the diluted samples are then injected onto the liquid chromatography mass spectrometer (LC-MS) which, unlike the gas chromatography mass spectrometer (GC-MS), is compatible with aqueous samples. While sample preparation is considerably quicker than LLE and SPE methods, “dilute and shoot” and “crash and shoot” methods do not remove as many endogenous and/or exogenous compounds. Not removing these compounds could be a concern during the analysis, as matrix effects are observed more frequently using LC-MS methodology. In

addition, more maintenance may be needed in order to maintain the performance of the LC-MS instrumentation.

All of the extraction techniques mentioned have been described in the literature as methods that can identify NPS in human specimens. Tynon et al. and Knittel et al. both utilized LLE methodologies to identify synthetic cannabinoids in human specimens [102, 136]. Concheiro et al. utilized a SPE method to identify 40 NPS, mainly from the synthetic cathinone and piperazine drug classes [137]. Bell et al. described a "dilute and shoot" method that could detect eight compounds from the synthetic cathinone and piperazine drug classes in urine specimens [138]. Adamowicz et al. described a method that utilized a protein crash before analyzing blood specimens that could detect 143 NPS from the various designer drug classes [9]. Many more analytical methods for the detection of NPS in human specimens have been reported and reviewed in recent literature [139-141].

2.3.4 Instrumental Analysis

2.3.4.1 Gas Chromatography Mass Spectrometry

Gas chromatography mass spectrometry (GC-MS) is a powerful analytical technique for the identification of compounds in forensic toxicology specimens. Gas chromatography mass spectrometry, known as the "gold standard" in forensic toxicology, couples two analytical methodologies which enables it to have high resolving power and high selectivity. The first analytical methodology employed with GC-MS is gas chromatography. Gas chromatography is a technique that is used to separate analytes of interest from other endogenous or exogenous compounds that are present in an extracted forensic toxicology specimen. The separation is accomplished by first injecting a small

amount of an extracted sample into an injection port. The injection port is kept at a high temperature and the liquid sample is then vaporized into gas. The vaporized sample is then carried through an analytical column by a carrier gas typically consisting of helium. The sample then interacts with the analytical column and compounds are retained on the column for different amounts of time due to the affinity of compound with the analytical column itself. Retention times are established for each analyte of interest and are used to aid in the confirmation of a target analyte.

The second analytical technique is mass spectrometry. After compounds and analytes of interest are eluted from the GC analytical column they are introduced to an ionization chamber of the mass spectrometry. Typically, electron ionization (EI) or chemical ionization (CI) are the ionization sources utilized in GC-MS, with the EI method being the most commonly used. In electron ionization, compounds and analytes are bombarded by electrons which create a positively charged molecular ion by removing one of the electrons in the molecule. Most of the time this molecular ion is unstable, which induces fragmentation or rearrangement to form more stable fragment ions. These ions then enter a mass analyzer. Typically, the ionization source is set to 70 eV to ensure reproducibility across different laboratories and manufacturers.

The quadrupole is the most commonly used mass analyzer for GC-MS analyses in forensic toxicology laboratories. A quadrupole consists of four rods that uses the combination of both radio frequency and direct current voltages to filter ions with a certain mass per unit charge (*m/z*) value. Full scan MS and selected ion monitoring (SIM) are the acquisition modes that can be used to acquire MS data using a single quadrupole [142]. In the full scan MS acquisition mode, the instrument quickly cycles through a

defined range of masses at a defined step size in an attempt to collect as much spectral data from a larger range of masses. This acquisition mode is used for screening. The SIM acquisition mode only obtains spectral data on select ions that are predetermined. The instrument spends more cycle time filtering these ions, thus the sensitivity of the GC-MS is increased when utilizing the SIM acquisition mode. The SIM acquisition mode is used for targeted confirmation assays where the targeted analytes are already known.

2.3.4.2 Liquid Chromatography Mass Spectrometry

Liquid chromatography mass spectrometry (LC-MS) is gaining popularity in forensic toxicology laboratories because of the increased selectivity, specificity, and sensitivity [143]. Similar to the GC-MS, two analytical techniques are couple together in LC-MS methodology; a separation technique and an identification technique. However, unlike GC-MS, the sample and mobile phase remain in the liquid phase until they reach the ionization chamber of the mass spectrometer. The sample is injected into the mobile phase and then carried to the analytical column. Separation of analytes of interest and other compounds occurs in the analytical column and the duration of retention depends on the affinity between the stationary phase and the analyte itself. After compounds are eluted from the analytical column, they are then carried to the ionization chamber of the instrument.

The most commonly used ionization source in LC-MS methodology is electrospray ionization (ESI). Electrospray ionization is considered a softer ionization technique which allows the formation and detection of the molecular ion to occur more frequently than harder ionization techniques such as EI. Gas phase ions are created in the electrospray chamber by first nebulizing the liquid stream coming from the LC system.

The liquid mobile phase creates what is called a Taylor cone at the end of the nebulizer. A fine mist of droplets is emitted from the Taylor cone which is then subjected to heated gas which helps rapidly evaporate the solvent [144]. The droplets continue to shrink until they reach the Rayleigh limit, where the surface tension of the droplet can no longer sustain the Coulombic force of repulsion between the ions. At this point a Coulombic explosion occurs and many smaller droplets are created from the larger droplets. This process repeats itself many times until the gas phase ionized analytes are formed [145]. Ions then enter an ion capillary and then analyzed/filtered out by the mass spectrometer.

One major concern with electrospray ionization is that it is susceptible to matrix effects [146]. Matrix effects are defined as differences in analyte response associated with the presence of co-eluting compounds from a sample matrix. An increased analyte response is considered ion enhancement and a decreased analyte response is considered ion suppression [147].

Many types of mass spectrometers have been coupled with liquid chromatography. They include quadrupole, ion trap, and time of flight mass analyzers. Tandem mass spectrometry is frequently used with LC-MS, which increases its sensitivity and selectivity. Many forensic toxicology laboratories currently utilize LC-MS instrumentation.

2.3.4.3 High Resolution Mass Spectrometry

High resolution mass spectrometry (HRMS) is a term given to mass analyzers that can achieve a resolution of 20,000 (full width half maximum) or mass accuracy below 5 ppm [148]. These include time of flight (TOF), ion trap, and ion cyclotron (ICR) mass analyzers. The primary advantage of HRMS when compared to lower resolution mass

spectrometry is that this technique has higher resolving power, which results in increased mass accuracy. As a result of this high resolving power, some compounds that are considered isobaric on low resolution instrumentation can be identified solely on the basis of the accurate mass determined for the molecular ion.

The TOF mass analyzer is able to achieve high resolution by measuring the flight time of an ion through a flight tube and then assigning a mass to charge ratio, *m/z*, using the time of flight. The flight time is directly proportional to the root of the mass to charge ratio of the ion and this calculation is shown below.

$$t_F = \frac{L}{v} \quad \text{(Equation 1)}$$

$$KE = zeV = \frac{1}{2}mv^2 \quad \text{(Equation 2)}$$

$$t_F = L\sqrt{\frac{m}{2zeV}} \quad \text{(Equation 3)}$$

Equation 1 displays the time of flight, t_F, calculation, where the length of the flight tube is represented by *L* and the velocity is represented by *v*. The kinetic energy, KE, equation is shown in equation 2 where the charge, *z*, the electronic charge, *e*, and the voltage difference, *V*, are used. Kinetic energy can also be determined with mass, *m*, and velocity, *v*, which is also shown in equation 2. Equation 3 is created after substituting the velocity in equation 1 with equation 2. When determining mass in the time of flight mass analyzer, the flight tube length is fixed and the kinetic energy is assumed to be equal for all ions entering the flight tube. Therefore, equation 3 shows that the time of flight is directly proportional to the root of the mass to charge ratio of the ion [149]. Reference masses are constantly present during the full scan acquisition and are used to make in-

time x-axis corrections to ensure high mass accuracy. Measurements with mass errors less than 5 ppm are typically observed using the time of flight instrument.

HRMS is gaining popularity in the clinical and forensic toxicology fields, as evident by the increasing number of application papers published [150]. Typically, these applications utilize a full scan acquisition method in a systematic toxicological analysis. There are targeted acquisition methods published as well. The benefits of HRMS for the identification of NPS include the acquisition of full scan data even in targeted acquisition modes. The full scan data collection allows for spectral data to be collected from unknown or untargeted compounds. In addition, the spectral data can be retrospectively analyzed without processing a second aliquot of the sample, which can be useful when a new NPS is identified.

HRMS was shown to perform better as a screening technique for the identification of synthetic cannabinoid substances than immunoassays specifically created for these compounds [151]. The flexibility of HRMS is also an advantage over traditional immunoassays. HRMS allows laboratories to create analytical methods that can detect newer NPS quicker than the time it takes to develop an immunoassay for the same compounds. It is expected that more laboratories will turn to HRMS as the cost of the instrumentation decreases.

2.3.4.4 Collision Induced Dissociation

Collision induced dissociation (CID) is a common dissociation (fragmentation) technique in tandem mass spectrometry. It is used to created product ions that can be used to help identify a compound in a specimen. Collision induced dissociation can occur in space or in time, depending on the mass analyzer used. For CID experiments in space, the

dissociation occurs in a collision cell which is positioned in between two mass analyzers, such as in a triple quadrupole or quadrupole-time of flight instrument. For CID in time, an ion trap is used to isolate a precursor ion before collision energy is applied.

In both techniques, an inert gas such as nitrogen is present in the collision cell and a single or very few collisions occur between the precursor ion and the gas molecules in low energy experiments [152]. CID is typically described in two steps; the activation step which is created from the kinetic energy transfer of the collision and the dissociation step which occurs shortly after [153]. Products ions are formed after the dissociation step.

The product ions formed by the dissociation step are used in various ways depending on the acquisition method of the mass spectrometer. If a targeted acquisition method is employed in the second mass analyzer only specific predetermined product ions are analyzed. This technique is commonly used in tandem mass spectrometers to measure known transitions. This allows for a more sensitive and specific method of identification of known compounds in forensic specimens. If a scan acquisition method is employed after the dissociation, then all product ions generated from the precursor ion can be observed and used for identification. This technique is used to generate MS/MS spectral data.

2.3.4.5 Mass Spectral Libraries

Mass spectral libraries aid in the identification of compounds in forensic toxicological Specimens, as they provide a spectral reference for known standards. Some extensive libraries that contain thousands of compounds have been created using both GC-MS and LC-MS instrumentation [154-155]. Many are commercially available, including a library produced at the National Institute of Standards and Technology (NIST).

In an attempt to ensure reproducible spectra across different instruments and manufacturers, standardized MS conditions have been employed. For example, spectral libraries generated by electron ionization utilize conditions that are standardized at 70 eV. Differences in LC-MS instrumentation has initially limited the generation of universal libraries. In-source fragmentation can vary greatly among different LC-MS manufacturers and techniques. However, it has been observed that when CID is employed, the spectral data are more reproducible than in-source fragmentation across manufacturers [156-157]. The reproducibility of MS/MS spectral data is credited to fewer experimental factors at play compared to in-source fragmentation techniques. The two factors that do need to be standardized in CID are the collision energy and the collision gas pressure [158].

While there have been extensive GC-MS and LC-MS libraries created and used, many do not contain a large representation of NPS. Consequently, there is a need to update or create new libraries to ensure that NPS spectral data are present. In addition, these libraries need to be able to be modified quickly and easily, as new NPS appear on the illicit drug market frequently.

2.4 Regioisomers

Among the various NPS classes, there are many compounds that are structurally related to each other and which include many isomeric compounds. Isomers are compounds that have the same molecular formula. Isomers are divided into two major groups that include constitutional isomers and stereoisomers. Stereoisomers differ in spatial orientation of their atoms, while constitutional isomers, also known as structural isomers, differ in the attachment of the various atoms that compose the molecule.

Regioisomers are a type of constitutional isomers in which a certain atom or substituent varies in the location of the molecule. Typically, these substitutions are observed around an aromatic ring or on an alkyl chain.

Identification of regioisomeric compounds can be challenging for forensic toxicology laboratories, as such labs are often restricted in their choice of analytical methods because of the requirements of the various analytical techniques. For example, the sample purity and the sensitivity needed for an identification of a compound using NMR is not compatible with toxicological samples as these samples are complex with endogenous and exogenous compounds and typically have trace amounts of drugs present. Most toxicology laboratories use mass spectrometry as the analytical technique of choice as this provides the necessary sensitivity and selectivity needed for the proper identification of compounds. Unfortunately, regioisomeric compounds commonly produce very similar if not identical mass spectral data, which can complicate the identification of a specific compound. In order to unequivocally identify a specific regioisomer using mass spectrometry a separation technique, such as gas chromatography or liquid chromatography, is typically employed, where retention times are utilized as an additional parameter in specific compound identification.

Previous work from Kusano et al. described the successfully differentiation of two sets of regioisomeric synthetic cannabinoids, JWH-122 and JWH-201. In this work, many of the regioisomers could be resolved using gas chromatography, with a few co-eluting regioisomers. In order to successfully distinguish the regioisomers from each other, MS/MS data along with the retention time were used [159]. Takeda et al. described the successful separation of regioisomeric synthetic cathinones using a naphthyethyl

analytical column in an LC-MS/MS application where spectral data were identical for all three regioisomers [160]. Differentiation of regioisomeric phenethylamines and synthetic cannabinoids by GC-MS/MS or LC-MS/MS has also been reported [161-164].

2.5 Challenges in Identifying Novel Psychoactive Substances

The identification of NPS in human matrices poses one of the biggest challenges facing forensic toxicology laboratories today. Identification of these compounds is complicated because of to the sheer number of different derivatives, many of which are structurally related. There are hundreds of NPS that have been observed and reported in literature, from drug seizures and toxicological cases, and on drug user forums. In addition, with the observed NPS structural skeletons, there remains the possibility of hundreds of additional derivatives as different substitutions on the skeletons can be made. Also, the possibility of novel or unique skeletons exist, as has been observed in the evolution of new synthetic cannabinoid and synthetic opioid NPS. For example, compounds with skeletons not previously observed were first detected in drugs such as MT-45 and AB-CHMINACA.

Another major challenge is that NPS fall in and out of favor very quickly as a consequence of user reports, legality and availability. Multiple structural generations have been seen in the different NPS classes, specifically in the synthetic cannabinoid class [96]. As new NPS compounds enter the market, a need for new updated methods to ensure detection of these compounds in case samples is created.

In attempting to keep up with the constantly changing drug targets, obtaining drug standards and validating new methods can be very time consuming and can deplete the resources of the forensic laboratory quickly. In addition, identification is sometimes

better with newer instrumentation such as LC-MS/MS, LC-TOF, or LC-ion traps because of the sensitivity and the spectral data collected by these instruments. Many of these compounds are structurally alike and spectral data may look nearly identical when analyzed by GC-MS, which is commonly used in forensic toxicology laboratories. Typically, LC-MS instrumentation is more expensive than GC-MS instrumentation, so cost may create another issue for forensic toxicology laboratories in their detection of NPS.

While there has been an effort to profile the metabolism of some novel psychoactive substances with *in vitro* metabolism studies, there are many NPS with unknown metabolic pathways or major metabolites. The unknown metabolites may be a challenge for some forensic laboratories where only urine specimens are submitted for investigations, particularly for synthetic cannabinoids. Parent compounds from some NPS classes may not be detected in urine and thus the use of a compound may be missed. While parent compounds from other classes, such as synthetic opioids and synthetic cathinones, have been identified in urine specimens, synthetic cannabinoids are typically metabolized into multiple products before being excreted in the urine. In fact, some of the synthetic cannabinoids share common metabolites with other structurally related synthetic cannabinoids. The shared metabolites can prevent the unequivocal determination of the parent NPS used. The lack of available metabolite standards from commercial sources may also hinder the confirmation of NPS use in toxicological case samples, as these standards are needed before identification can be reported in case samples.

To further complicate identification of NPS in toxicological cases, use of such derivatives tends to be somewhat regionalized. Compounds that are found in seized material in Europe and Japan may not be found or not found as quickly in material that was seized in the United States. In addition, many of these compounds are brought into the United States via online purchases from China. Determining which NPS to target in analytical methods can be difficult. Forensic toxicology laboratories should consult with local forensic laboratories who identify compounds in seized drug material. However, ideally an analytical method that is sensitive and non-targeted should be employed for the identification of these compounds for forensic toxicological analyses.

3. DEVELOPMENT OF A COMPOUND DATABASE AND HRMS SPECTRAL LIBRARY

3.1 Abstract

With the recent rise in popularity and use of novel psychoactive substances (NPS), there is a need within the forensic science community to be able to comprehensively screen for the many possible drugs in this class. Traditional drug screening methods, such as immunoassays, are currently unable to detect many of the newer NPS. To detect NPS for screening purposes, liquid chromatography (LC) coupled to high resolution mass spectrometry (HRMS) instrumentation has been suggested. In the present project designed to explore the screening potential of HRMS for these drugs, an LC-QTOF-MS based high resolution MS/MS designer drug spectral library was created with the instrument operated in positive electrospray ionization mode. The library contains data for 252 NPS from different classes including cathinones, piperazines, phenethylamines, tryptamines and synthetic cannabinoids. High resolution MS/MS spectra were collected by flow injection analysis under standardized conditions at three different collision energies (10, 20, and 40 eV) for each compound. In addition to the spectral library, a compound database was created to further enhance the screening potential of the LC-QTOF-MS. This database contains chemical and structural information for 875 potential designer drug compounds and metabolites that can be used to help aid in the identification of unknowns in a full mass scan. To demonstrate the

applicability of the HRMS library, 13 blind spiked serum samples and four authentic drug seizure case samples were analyzed by LC-QTOF-MS. The HRMS library search successfully identified all compounds present in the blind samples except for three synthetic cannabinoid compounds. In addition, results of the QTOF-based seized drug analyses were consistent with the official forensic laboratory results. The combination of a high resolution MS/MS library, compound database, and accurate mass LC-QTOF-MS based analysis represents a useful tool for the identification of NPS in forensic screening applications.

3.2 Introduction

Although the concept of emerging drugs of abuse ("designer drugs" or novel psychoactive substances; NPS) is not new, such compounds have experienced a resurgence in many parts of the world, as evidenced by the emergency scheduling of NPS by the United States Drug Enforcement Administration (DEA), European Union and other countries [1-3]. There have been different motivations for the creation of these designer drug entities. Some were developed by the pharmaceutical industry in drug discovery programs but then diverted to illicit use, while others have been created for the sole purpose of recreational use. Perceived advantages of using NPS include avoiding legal liability, an assumption that they are safe, and a relatively low cost compared to other abused street drugs [4-5]. In addition, NPS have been relatively easy to obtain; a simple online search will lead to multiple websites where designer drugs are for sale [6]. Many such drugs have chemical structural features in common with a scheduled drug of abuse, often representing just a slight modification of the original structure. In any case,

these modified structures are expected (or assumed) to produce pharmacological effects by acting on the same receptors as with typical drugs of abuse.

Information on the pharmacological and toxicological effects of NPS are, for the most part, limited, with most data available from case reports where the actual drug used may not be confirmed and where polydrug use is often the norm [7-8]. The vast majority of these drugs are not tested extensively before being sold and used [9]. Recently, there have been efforts to assess NPS pharmacology with *in silico* and *in vitro* models [10-12]. However, due to the fact that there are new NPS compounds being introduced on a regular basis, it is difficult to keep up with the generation of relevant data. The indiscriminate use of such untested compounds, some of which may have high potency, has led to reported cases of emergency hospitalization and/or death [8, 13-16].

Due to the increase in use and new federal and state legislation banning some NPS, it is important to be able to comprehensively screen for such compounds in clinical and forensic laboratories. While the need to be able to screen for NPS is undisputed, there are limitations that must be overcome in order to develop successful screening approaches. First, most labs do not have methods in place to detect more than a few NPS entities. Traditional drug screening methods such as immunoassays do not detect the majority of NPS, and most compounds do not cross-react with the commercially available immunoassays that screen for traditional drugs of abuse [17-18]. While there are ongoing efforts to create immunoassays for the larger universe of NPS, this process is time consuming and very costly [19-20]. Another major issue is the constantly evolving chemical identities of these compounds due to the rapid replacement of emergency scheduled drugs with new entities designed to avoid legal implications of continued use

of those that are banned. This trend makes it extremely difficult for forensic laboratories to keep up with screening and identification.

In order to overcome these issues, many labs have turned to mass spectrometric screening approaches for NPS. The majority of such methods employ GC-MS or LC-QqQ-MS instrumentation [21-23]. Recently, high resolution mass spectrometry (HRMS) has begun to gain popularity for the comprehensive screening of drugs, including drugs of abuse [24-26]. The HRMS screening approach offers a number of advantages, including high resolution and high mass accuracy, both of which increase the confidence of compound identification and selectivity of the method. A molecular formula can be generated based on the accurate ion mass and isotopic peak pattern [27-28]. In particular, this approach would be expected to be effective in identifying the minor mass differences that are often present in NPS.

Standardized spectral libraries are critical to screening and identification of known and unknown compounds present in a sample [29]. While there are extensive libraries available for GC-MS spectral data, LC-MS and LC-MS/MS spectral data libraries are more limited [30-31]. In addition, these libraries typically have limited novel psychoactive substances. The present study reports the development of a comprehensive compound database for 875 unique chemical entities considered as possible designer drugs, in addition to a full HRMS spectral library for 252 of these compounds. In order to test the preliminary applicability of these tools for unknown drug identification, 13 blind spiked serum samples and four authentic seized drug samples were analyzed.

3.3 Materials and Methods:

3.3.1 Chemicals and materials:

Drug standards were obtained from Cayman Chemical Co. (Ann Arbor, MI) and Cerilliant Corp. (Round Rock, TX) and were provided as neat weighed solids or as standards in solution. Optima grade methanol (ThermoFisher Scientific, Waltham, MA) was used to prepare 1 mg/mL stock solutions from the neat standards. For some compounds, dimethyl sulfoxide (ThermoFisher Scientific) was used due to solubility issues encountered with the use of methanol. Standards provided in solution were used as received. All standards were then diluted to a concentration of 10 μg/mL using methanol. Finally, working solutions were created by diluting the 10 μg/mL standards to a concentration of 1 μg/mL with methanol. Each standard was given an in-house identification number (i.e., FIU-nnnn) which aided in the traceability of the compounds throughout sample preparation and analysis. Solvents used for liquid chromatography included acetonitrile (Optima LC/MS grade) and water (Optima LC/MS grade) from ThermoFisher Scientific. Liquid chromatography additives used included formic acid (Optima LC/MS) and ammonium formate (99%) from ThermoFisher Scientific. Pooled human serum was purchased from BioreclamationIVT (Westbury, NY). Solid phase extraction cartridges (Bond Elut Plexa PCX 30 mg, 3 mL) were purchased from Agilent Technologies (Santa Clara, CA).

3.3.2 Instrumentation and Software:

Analytical instrumentation included an Agilent 1290 Infinity UHPLC system coupled to an Agilent 6530 Accurate-Mass QTOF MS (Agilent Technologies, Santa

Clara, USA). The QTOF-MS was operated in positive-ion electrospray mode with Jet Stream ESI Technology.

Agilent MassHunter LC/MS Acquisition software for the 6200 series TOF/6500 series QTOF (Version B.05.00) and MassHunter Qualitative Analysis software (Version B.05.00) were used to acquire and process the data. MassHunter Personal Computer Database Library (PCDL) Manager software (Version B.04.00, Build 92.0) was used to create the high resolution MS/MS spectral library and the compound database. ChemDraw Pro (Version 12.0.2.1076) was used to create and import the chemical structure of each NPS into the PCDL.

3.3.3 Creation of the comprehensive compound database:

Chemical compounds to be included as potential NPS entities were identified from multiple publicly available sources, including peer reviewed literature research articles and reviews, government publications, commercial standard supplier documentation, and websites including online drug forums. Once a potential NPS was identified, chemical and structural information were verified by attempting to find multiple corroborating sources for each drug. After verification, the structure of each drug was recorded using the ChemDraw software. The chemical structure was then imported into the database as a .mol file using the MassHunter PCDL Manager software. Using the chemical structure, a search was performed using SciFinder to identify chemical information such as CAS Registry Number and IUPAC name. A similar search was done on ChemSpider to obtain a ChemSpider number. For each NPS in the database, information such as compound name, chemical formula, monoisotopic mass,

chemical structure, and IUPAC name were added to the database, in addition to CAS registry number and ChemSpider number if available.

3.3.4 Creation of the HRMS spectral library:

Flow injection analysis (FIA) was employed for acquisition of MS/MS data for all NPS standards. The FIA method employed an injection volume of 1 μL with direct injection from the autosampler into the ion source. The mobile phases consisted of 5 mM ammonium formate and 0.1% formic acid in water (A) and acetonitrile/water (90/10 v/v) with 1.0% formic acid (B), pumped at 0.4 mL/min of 50% B. A positive mode electrospray ionization (ESI) targeted MS/MS method was used to collect the data. The source parameters were: drying gas temperature 325 ^{o}C; drying gas flow 5 L/min; nebulizer 30 psi; sheath gas temperature 375^{o} C; sheath gas flow 12 L/min. Scan source parameters used included: VCap voltage 4000 V; nozzle voltage 0 V; fragmentor 140 V. The quadrupole used a narrow isolation mass window of 1.3 amu.

Three discrete collision cell energy levels were used in the CID; 10, 20, and 40 eV. The MS range was 50-1700 m/z. The MS acquisition rate was 10 spectra/s while the MS/MS acquisition rate was 3 spectra/s. In order for the spectral data to be added to the MS/MS spectral library, a compound had to produce a base peak of at least 1000 counts. If the NPS standard achieved this requirement, then the compound information and fragment ion spectrum from each collision energy was exported to a compound exchange format (.CEF) file and then imported into the PCDL using PCDL Manager software. An arginine standard was run with each batch of standards as a QC check to make sure the instrument was properly tuned and calibrated.

3.3.5 Analysis of blind samples:

Thirteen blind samples were created by spiking up to five different NPS standards per sample into pooled blank human serum. The final concentration of each drug was approximately 1 μg/mL. The spiked serum samples were subjected to solid phase extraction (SPE) utilizing a positive pressure manifold and polymeric mix mode extraction cartridges prior to instrumental analysis. The SPE sample pretreatment consisted of adding 1 mL of a 2% aqueous formic acid solution to 0.5 mL of sample. One mL of methanol was added as a conditioning step prior to adding the pretreated sample to the extraction cartridges. The wash step consisted of adding 1 mL of 2% aqueous formic acid followed by 1 mL of a 50:50 methanol: water solution. The SPE cartridges were then dried down for 5-10 minutes with N_2 at maximum pressure. The elution step consisted of adding 1 mL of a 50:50:2 ethyl acetate:methanol:ammonium hydroxide solution. The samples were acidified with 100 μL of 25 mM HCl. The eluent was dried down under N_2 at room temperature. The samples were reconstituted with 100 μL of HPLC grade water.

The reconstituted samples were then analyzed by LC-QTOF-MS under two different acquisition methods; a full scan MS method and an Auto MS/MS method. Full scan MS method was more sensitive and generated better chromatographic peak shape when compared to Auto MS/MS due to the fact that, in full scan, the quadrupole did not isolate specific ions and therefore the duty cycle was faster. While the Auto MS/MS method was less sensitive, it was needed to provide MS/MS data for compounds with abundances greater than the set acquisition threshold. These MS/MS data were used for subsequent library searches.

The LC gradient used for both acquisition methods employed a flow rate of 0.4 mL/min using an aqueous mobile phase (A) consisting of 5 mM ammonium formate plus 0.1% formic acid in water and an organic mobile phase (B) consisting of acetonitrile/1.0% formic acid in water (90/10 v/v). The gradient was as follows: a hold of 20% B to 1 min, an increase to 70% B at 5 min, an increase to 100% B at 8.75 min, and a hold of 100% B until 13 min. An additional post-run time of 3 min was used to allow for re-equilibration at 20% B. The column used was an Agilent Zorbax Eclipse Plus C18 Rapid Resolution HD (3.0 x 100 mm, 1.8 micron). The column was maintained at a temperature of 40oC. The injection volume was set to 20 µL.

Source parameters for the full scan method were: drying gas temperature 325 ^{o}C; drying gas flow 8 L/min; nebulizer 35 psi; sheath gas temperature 400 ^{o}C; sheath gas flow 12 L/min. Scan source parameters used were: VCap voltage 3500 V; nozzle voltage 0 V; fragmentor 125 V. MS range was 100-1000 m/z and the acquisition rate was 1.5 spectra/s. The Auto MS/MS method used the same source and scan parameters. In addition, the MS mass range was 100-1000 m/z with an MS acquisition rate of 3 spectra/s, while the MS/MS mass range was 50-1000 m/z with an acquisition rate of 3 spectra/s. MS/MS fragmentation was performed at three collision cell energies of 10, 20, and 40 eV. The quadrupole used a narrow isolation width of 1.3 amu. Reference mass correction was enabled, using masses 121.0509 m/z and 922.0098 m/z.

Agilent MassHunter Qualitative software was used to perform library and database searches. This process entailed using the “Find Compounds by Auto MS/MS”, the “Search Accurate Mass Library”, and the “Search Database” commands. The “Find Compounds by Auto MS/MS” command created a list of potential compounds that met

the MS/MS acquisition threshold and MS/MS spectral data was collected. The potential compound list was typically greater than 500 compounds per sample. This compound list was then subjected to an accurate mass library search. Both a forward search (matching peaks in the sample against the library) and reverse search (matching peaks in the library against the sample) were employed. The parameters of this search included precursor ion expansion of ±10 ppm + 2 mDa and product ion expansion of ±20 ppm + 2 mDa. The acceptable mass error window for the product ion is larger than expected when using HRMS. However, this was used to account for the fact that the MS/MS library was not curated, therefore there may have been mass errors in the product ions at the time of spectral collection. The library search parameters used set the minimum forward and reverse score to 70.

Compounds that were identified by the library search were then selected for a database search which compared the mass of a compound in the sample to the molecular formula in the database. The mass tolerance was set to 10 ppm for the database search. Criteria for a positive identification were a "database" score of >70 and a library score of >80. In addition, the mass error had to be <10 ppm and the extracted ion chromatogram was visual inspected to ensure the signal was not due to noise.

3.3.6 Analysis of authentic seized drug case samples:

Methanol extracts of four different seized drug samples were obtained from the Miami-Dade Police Department Forensic Laboratory. Two 10× dilutions of the methanol extract were made with water and were analyzed by LC-QTOF-MS by both MS full scan and Auto MS/MS acquisition methods. The method parameters and data analysis procedures were the same as those previously described for the blind serum samples.

3.4 Results and Discussion:

There are numerous advantages in using high resolution, high mass accuracy MS for screening of clinical and forensic related samples, many of which have been discussed in the literature [27, 32-33]. Arguably, the biggest advantage of using high resolution LC-QTOF-MS instrumentation is that an analyst may potentially identify a compound in a sample based on the accurate mass and isotopic distribution with high confidence. Another major advantage is the extended dynamic range available in newer instruments, which allows for high mass accuracy at both low and high analyte concentrations and which facilitates screening of cases where the concentration of an analyte is unknown. Furthermore, the MS/MS capabilities of the QTOF allow for identification of a compound based on fragmentation patterns, which can be useful to distinguish among structural isomers, i.e., compounds have the same chemical formula and thus the same molecular ion.

Another advantage of using HRMS instrumentation such as LC-QTOF-MS in clinical and forensic laboratories is that the instrument acquires both high resolution full scan MS and MS/MS fragmentation data when a MS/MS acquisition method is selected. This approach allows the investigator to obtain more information about potential unknown compounds that were not subjected to MS/MS, either because they were not specifically targeted (i.e., when using a targeted MS/MS method) or when the abundance of the precursor ion did not meet the threshold required to trigger MS/MS (i.e., in auto MS/MS methods). The supplemental full scan MS data are very beneficial for the analyst, as they allow a retrospective analysis of a sample to be done by simply reprocessing the data file with an alternate compound database. This is a valuable tool in

the case of screening for NPS because as new drugs are created they can be identified in cases that were previously analyzed with an older database without the need of re-extracting the sample.

To further realize the full potential of the LC-QTOF-MS as a screening tool, comprehensive high resolution MS/MS spectral libraries and compound databases are needed. There has been considerable work by various groups directed towards the creation of HRMS libraries containing up to several thousand drugs and toxic compounds [30, 34]. Several recent published reports have used high resolution MS instrumentation for comprehensive screening of licit and illicit drugs [35-38]. For example, using QTOF-MS and both negative and positive ESI, Broecker et al. generated an HRMS library for more than 2,500 drugs and other toxicologically relevant xenobiotics [30]. Fragmentation profiles for each compound determined at three different CID energies were included. The applicability of the method for screening purposes was evaluated with both spiked blood and urine and a set of authentic postmortem specimens. Rosano et al. reported a validated comprehensive screening method for almost 1,000 drugs using UPLC coupled to QTOF-MS based on "MS^E-TOF" analysis [35]. In this approach, CID energies were ramped from 10 to 40 eV to generate qualifier fragment ions specific to each drug entity. The method was further validated by assessment of 300 postmortem specimens and comparison of results to those obtained by single- and triple-quadrupole LC-MS instrumentation.

The results of both of these reports confirm the value of HRMS as a screening tool in forensic toxicology. However, previous work has primarily focused on typical drugs that are seen more routinely in clinical toxicology rather than on NPS. A few

reports on the application of HRMS specifically for NPS analysis are available, primarily using LC-TOF-MS based methods which have only targeted a small number of drugs, typically from a single class of compounds [39-41]. In contrast, comprehensive HRMS based screening and confirmatory methods for NPS are not currently available.

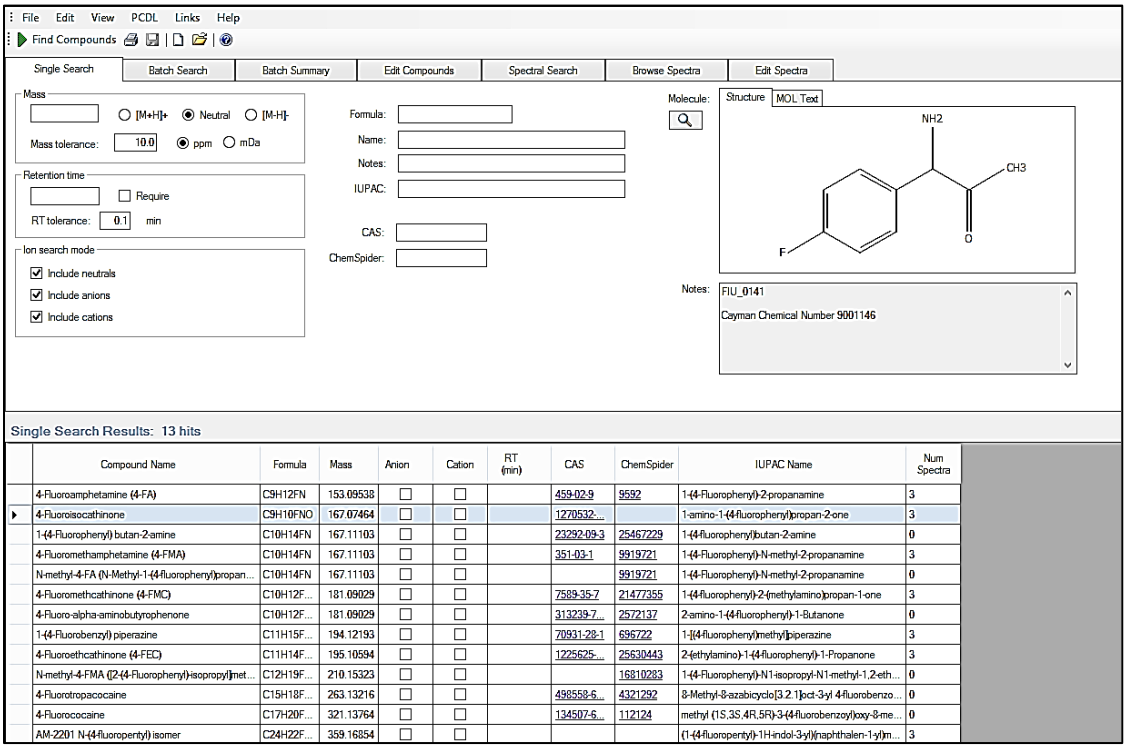
The major goal of the present project was to create a HRMS spectral library for as many NPS standards from the synthetic stimulant, hallucinogen, and cannabinoid classes as were currently available (260 at the time of the study), using an LC-QTOF-MS based approach similar to that reported previously [30]. In addition to the spectral library, a linked "compound database" was created that contains relevant information for 875 current and/or potential NPS entities. For the purposes of the project, the compound database was constructed as a repository containing names, chemical formulae, structures, and neutral masses as minimal information for each drug entry. Such a database was anticipated to be a useful stand-alone tool for identifying NPS in authentic samples following HRMS analysis, based on comparison of the high resolution spectrum of precursor ions with the accurate mass and isotopic ratio patterns of compounds in the database. However, once MS/MS product ion spectra are added to the database, it is more accurately referred to as a "mass spectral library".

3.4.1 Compound database:

In order to include as many NPS as possible in the full compound database, extensive literature and on-line searches were performed. Initially, government reports were reviewed to identify compounds of potential interest. Literature reviews also produced relevant information and additional reports described the presence of designer drugs in authentic cases. Product lists from commercial sources were also of value.

Online websites, such as those based on the books written by Dr. Alexander and Ann Shulgin ("PiHKAL" and "TiHKAL") [42-43] were very useful for selecting compounds for inclusion in the database. Online forums were also important for identifying new NPS entities being discussed by drug users, as were websites of companies selling "research chemicals". Although such sources are not peer reviewed and their reliability may be in question, it was important to include any compounds that may be emerging on the street market.

A total of 875 unique structural entities considered to be potential NPS compounds were identified and added to the compound database (see Appendix 1 for a complete listing). Most of these compounds belong to the cannabinoid, cathinone, tryptamine, piperazine, and phenethylamine structural classes, although compounds from other classes were also represented. Within the cannabinoid class, numerous structural subcategories were also identified. For each drug entity, information such as street or common name, chemical formula, monoisotopic mass, chemical structure, and IUPAC name was added to the database. Additional information, such as CAS registry numbers and ChemSpider numbers, was also added if available. Figure 9 displays a representative screen shot of the compound database generated by the software (i.e., MassHunter PCDL Manager) with details for the compound 4-fluoroisocathinone shown. As can be seen, in addition to the information described above, the entry for each compound also indicates whether HRMS spectral data were successfully acquired (i.e., "Num Spectra" column). The development of the compound database is an ongoing and dynamic process; as new drugs are created and reported for the purpose of circumventing existing legislation, they are added to the resource.



Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Num Spectra
4-Fluoroamphetamine (4-FA)	C9H12FN	153.09538	☐	☐		459-02-9	9592	1-(4-Fluorophenyl)-2-propanamine	3
4-Fluoroisocathinone	C9H10FNO	167.07464	☐	☐		1270532-...		1-amino-1-(4-fluorophenyl)propan-2-one	3
1-(4-Fluorophenyl) butan-2-amine	C10H14FN	167.11103	☐	☐		23292-09-3	25467229	1-(4-fluorophenyl)butan-2-amine	0
4-Fluoromethamphetamine (4-FMA)	C10H14FN	167.11103	☐	☐		351-03-1	9919721	1-(4-Fluorophenyl)-N-methyl-2-propanamine	3
N-methyl-4-FA (N-Methyl-1-(4-fluorophenyl)propan...	C10H14FN	167.11103	☐	☐			9919721	1-(4-Fluorophenyl)-N-methyl-2-propanamine	0
4-Fluoromethcathinone (4-FMC)	C10H12F...	181.09029	☐	☐		7589-35-7	21477355	1-(4-fluorophenyl)-2-(methylamino)propan-1-one	3
4-Fluoro-alpha-aminobutyrophenone	C10H12F...	181.09029	☐	☐		313239-7...	2572137	2-amino-1-(4-fluorophenyl)-1-Butanone	0
1-(4-Fluorobenzyl) piperazine	C11H15F...	194.12193	☐	☐		70931-28-1	696722	1-[(4-fluorophenyl)methyl]piperazine	3
4-Fluoroethcathinone (4-FEC)	C11H14F...	195.10594	☐	☐		1225625-...	25630443	2-(ethylamino)-1-(4-fluorophenyl)-1-Propanone	3
N-methyl-4-FMA ([2-(4-Fluorophenyl)-isopropyl]met...	C12H19F...	210.15323	☐	☐			16810283	1-(4-Fluorophenyl)-N1-isopropyl-N1-methyl-1,2-eth...	0
4-Fluorotropacocaine	C15H18F...	263.13216	☐	☐		498558-6...	4321292	8-Methyl-8-azabicyclo[3.2.1]oct-3-yl 4-fluorobenzo...	0
4-Fluorococaine	C17H20F...	321.13764	☐	☐		134507-6...	112124	methyl (1S,3S,4R,5R)-3-(4-fluorobenzoyl)oxy-8-me...	0
AM-2201 N-(4-fluoropentyl) isomer	C24H22F...	359.16854	☐	☐				(1-(4-fluoropentyl)-1H-indol-3-yl)(naphthalen-1-yl)m...	3

Figure 9. An image of the PCDL software that was utilized to generate the database and the MS/MS spectral library.

3.4.2 Development of the high resolution MS/MS spectral library:

A total of 260 designer drug standards (selected from the 875 entities in the compound database) were commercially available for the creation of a high resolution MS/MS spectral library. For this purpose, each standard was initially analyzed via flow injection by QTOF-MS. A targeted method for each standard was created. Source and acquisition parameters were chosen in order to be comparable to previously created libraries using similar instrumentation. Three predetermined collision cell energies (10, 20, and 40 eV) were used to promote fragmentation of the target ions. In order to qualify for inclusion in the MS/MS library, each designer drug standard had to produce a base

peak of at least 1000 counts, a requirement which ensured that background noise was minimized in the MS/MS spectral data.

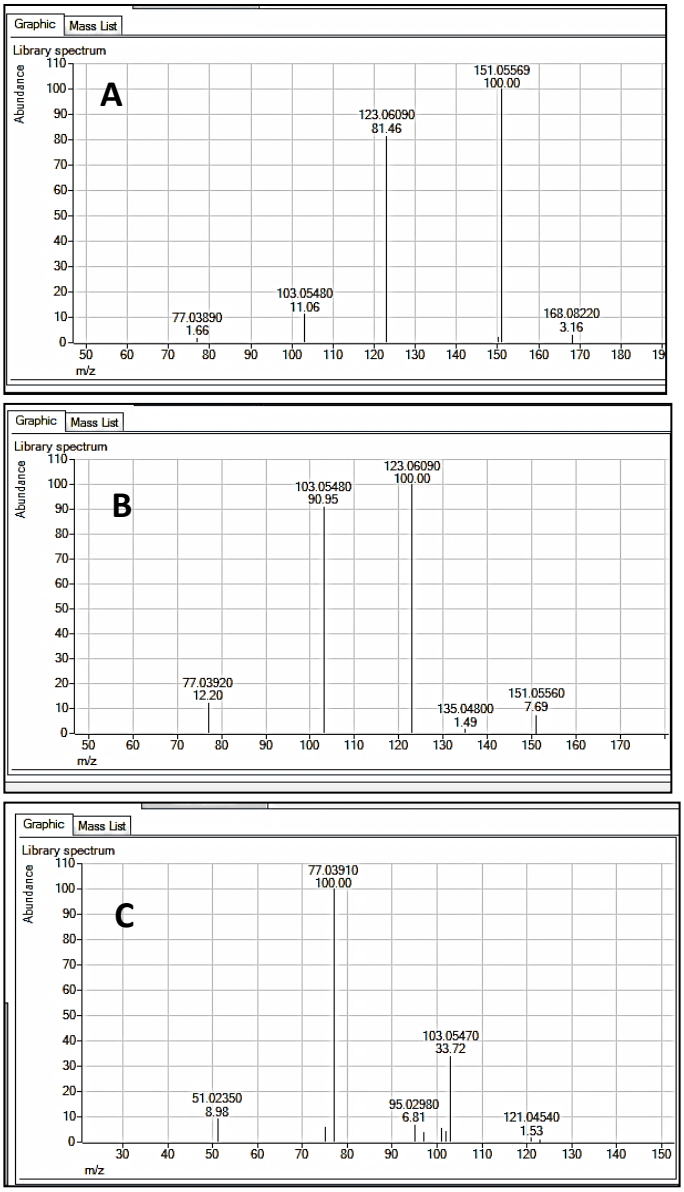


Figure 10. Images of the PDCL software showing the MS/MS spectral data of 4-Fluoroisocathinone. MS/MS spectral data is shown at various collision energy levels: A) 10eV, B) 20 eV, and C) 40 eV.

Structural details of all standards included in the database are shown in Appendix 2, Appendix 3, and Appendix 4. In addition, complete information on relative ion abundances of each ion at each of the three collision energies for all standards are shown

in Appendix 5. Based on the requirement for a 1000-count MS threshold, spectral data for 252 of the 260 available standards were added to the final library (Table 1). All of the compounds that failed to produce the required base peak intensity were synthetic cannabinoids. These included CP-47497, CP-47497 epimer, CP-47497 para-quinone analog, CP-47497 C8-homolog, CP-47497 C8-homolog 3-epimer, CP-55940, CP-55940 5-epimer, and JZL-184. Difficulties with directly analyzing cannabinoids from the CP class using positive ESI have been previously reported in the literature [44]. In an attempt to overcome this limitation, these analytes were analyzed by negative mode ESI. Five out of the eight compounds successfully met the 1000 count base peak requirement. The three compounds that did not meet this requirement in negative ESI-mode were CP-47,497 para-quinone analog, (±) 3-epi-CP-47,497-C8-homolog, and JZL-184. Electrospray ionization may not be suitable and alternative ionization sources may be needed for analysis of these compounds.

Table 1. The amount of NPS by structural class included in the Compound Database and MS/MS Spectral Library

Structural Class	Number in Compound Database	Number in Spectral Library
Stimulants/Hallucinogens		
Arylcyclohexylamine	14	1
Cathinone	131	56
Indane	6	3
Phenethylamine	274	25
Piperazine	25	7
Pyrrolidine	2	2
Tryptamine	75	7
Other	10	3
Cannabinoids		
2-Naphthoylindole	14	14
Adamantoylindole	4	2

Adamantylindazolecarboxamide	3	1
Adamantylindolecarboxamide	2	2
Benzimidazole	4	0
Benzoylindole	18	12
Cyclohexylphenol	11	0[a]
Cyclopropanoylindazole	1	0
Cyclopropanoylindole	18	2
Indazole	33	0
Indole	35	4
Naphthoylindazole	2	0
Naphthoylindole	122	69
Naphthoylpyrrole	9	9
Naphthylmethylindole	1	1
Phenylacetylindole	18	13
Pyrazole	1	0
Other	42	19[b]
Total	875	252

[a]Seven cyclohexylphenol cannabinoid standards were analyzed (see text) but none reached the 1000-count threshold required for inclusion.
[b]One "other cannabinoid" standard in this group (JZL-184) did not reach the 1000-count threshold required for inclusion.

3.4.3 Analysis of blind samples:

To test the applicability of the high resolution MS/MS spectral library for screening and identification, 13 blind human spiked serum samples were prepared and analyzed by the LC-QTOF-MS. A gradient method using a C18 column was developed to provide separation of the various NPS. Two acquisition methods were used; a full scan MS method and an Auto MS/MS method. The full scan method offers higher sensitivity and better TIC peak shape, since it does not collect MS/MS data. In contrast, the Auto MS/MS method offers higher selectivity based on the MS/MS spectral library search of the product ions. Potential compounds of interest were identified using the

Qualitative Analysis Software “Find Compounds by Auto MS/MS”, “Search Library”, and “Search Database” functions. Initially, the Find Compounds by Auto MS/MS function identified over 500 compounds per sample. This list of compounds was then subjected to a library search in which one to seven potential compounds were identified per sample. The library search utilizes MS/MS spectral data to generate a match score. Forward and reverse library scores are provided based on how well the sample spectra matches the library spectra and vice versa. The Search Database command was then used on the compounds identified by the library search. Finally, a database score was generated based on how well the mass matches the formula in the database.

The library and database searches both successfully detected 32 compounds present in the blind spiked samples, with the library match score ranging from 80.43 to 100 and the database match score ranging from 51.17 to 99.65 (Table 2). Based on this identification technique, which used the “Find by Auto MS/MS” results, library scores, and the database score, there were a total of three false negative results, thus demonstrating a true positive rate of 91.4%. The three false negatives came from the synthetic cannabinoid class of NPS, including CB-13, JWH-250, and AM 2233. In addition, there were four false positives using this technique, including ethyl amphetamine in one sample and N,N-dimethylcathinone in three samples. While further investigation is needed, these false positives may have been due to impurities in or degradation of the standard.

LC retention times, which can be added to the database and which are sometimes needed as an additional identification tool, were not utilized here, in order to demonstrate the practicality of this database/library for laboratories that do not have access to

standards for every compound of interest. The combination of database and library match scores generated a very high true positive rate, which suggests that this technique could be useful in presumptively identifying a compound without a drug standard. In contrast, the “Find by Formula” score, which is a popular identification technique using this software, when used alone generated a low true positive rate, suggesting that while it can be useful in preliminary screening for compounds, there should be more caution with presumptively identifying a compound by this approach.

Table 2. Compounds identified in the blind spiked serum samples. Library and database scores are shown as a percentage. Detection of compounds utilizing a 1,000 and a 10,000 peak area filter are designated "+" for positively identifying the compound and "-" for not identifying a compound.

	Drug(s)	Library Score	Database Score	Detected at 1000 TIC	Detected at 10000 TIC		Drug(s)	Library Score	Database Score	Detected at 1000 TIC	Detected at 10000 TIC
Sample 1	AM-1220	99.96	88.82	+	+	**Sample 8**	3,4-Dimethylmethcathinone	99.81	99.31	+	+
							AKB48	96.20	94.45	+	-
Sample 2	methylone	98.23	90.37	+	+		AM2233	-	-	-	-
	2C-D	98.75	90.21	+	+		JWH 200	98.82	85.63	+	+
	CB-13	-	-	-	-		RCS-4	99.67	96.29	+	+
Sample 3	MDPV	95.38	90.88	+	+	**Sample 9**	AM694	99.77	98.22	+	+
	AM2201	100	95.11	+	+		JWH 203	99.18	88.57	+	+
	JWH 081	99.12	88.03	+	+		JWH 398	100	95.11	+	-
	RCS-8	99.35	74.94	+	+		Cannabipiperidiethanone	99.49	97.98	+	+
Sample 4	None	-	-	-	-		Pentylone	96.40	81.39	+	+
Sample 5	2C-I	97.18	77.69	+	+	**Sample 10**	4-MMC	99.50	93.16	+	+
	2C-T-2	98.73	94.31	+	+	**Sample 11**	JWH 018	100	78.17	+	+
	2C-H	98.13	80.84	+	+		Methoxetamine	94.23	86.39	+	+
	JWH 250	-	-	-	-	**Sample 12**	2C-E	98.53	82.38	+	+
Sample 6	2C-T-4	96.41	96.32	+	+		2C-N	81.29	79.65	+	+
	2C-C	99.43	94.9	+	+		2C-P	96.64	79.77	+	+
Sample 7	JWH 018 adamantyl carboxamide	99.78	99.19	+	+		JWH 073	99.34	51.17	+	-
	JWH 019	98.92	98.99	+	+		JWH 122	99.55	60.04	+	+
	JWH 022	97.45	99.65	+	+	**Sample 13**	None	-	-	-	-

3.4.4 Analysis of case samples:

To demonstrate the applicability of the high resolution MS/MS spectral library and compound database to identification of authentic case materials, four seized drug samples were obtained from the Miami-Dade Police Department. The samples were provided as methanol extracts, with no information regarding the identity or concentration of the drugs present. Similar to the blind serum samples described above, the case samples were analyzed by LC-QTOF-MS using two methods; a full scan MS method and an Auto MS/MS method. For these samples, the full scan MS method was used to determine the retention time of candidate unknown compounds in the methanol extract, while the Auto MS/MS method was used to identify such compounds based on a spectral library search. For the latter, analysis was done with the Qualitative Analysis Software using the "Find Compounds by Formula" and "Search by Accurate Mass" algorithms.

Similar to the serum sample study, this process generated multiple hits for potential compounds in the sample based on molecular formulas provided in the database. A library search was then performed on the identified compounds, a process which generated two high quality matches based on accurate mass data, isotopic distribution, and MS/MS fragmentation patterns (Figure 11). The matches for all four samples included methylone and 2,3-methylenedioxymethcathinone (2,3-MDMC), which are structural isomers with the molecular formula $C_{11}H_{13}NO_3$. The correct identity was ultimately made by including LC retention time in the analysis, as shown by the TIC data of standards and case samples (Figure 12). The high MS spectral matches for both

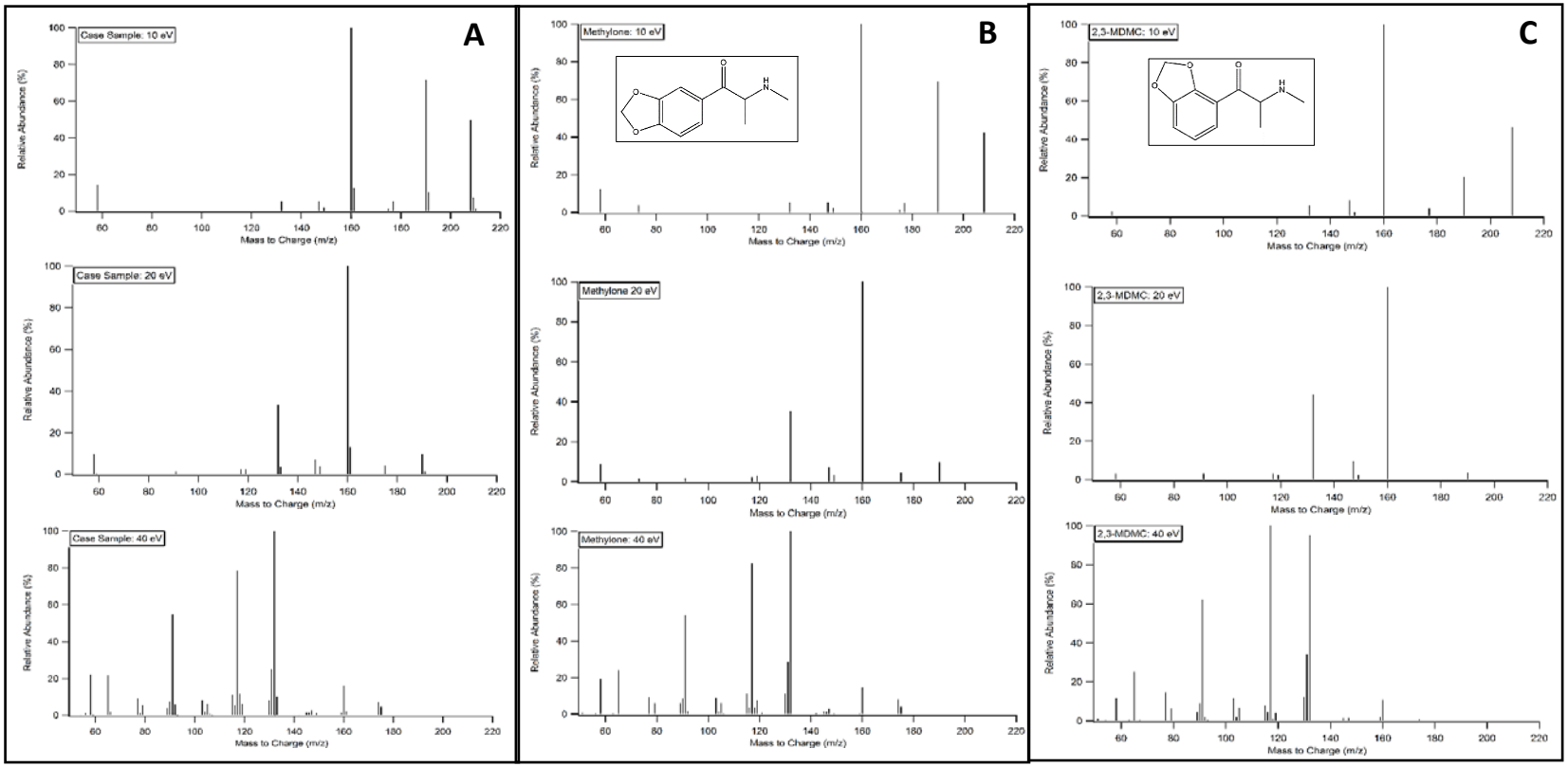


Figure 11. MS/MS spectral data of the case sample (column A), the methylone standard (column B), and the 2,3-MDMC standard (column C) at various collision energies (10, 20, and 40 eV).

compounds in this case sample illustrate the importance of LC separation for the identification of isomeric designer drugs when using LC-QTOF-MS as a screening method. Without separation, methylone and 2,3-MDMC would have been difficult to differentiate based on MS/MS spectral data alone. As a result of these analyses, it was confirmed that all four case samples contained methylone, a finding that was consistent with the official laboratory findings.

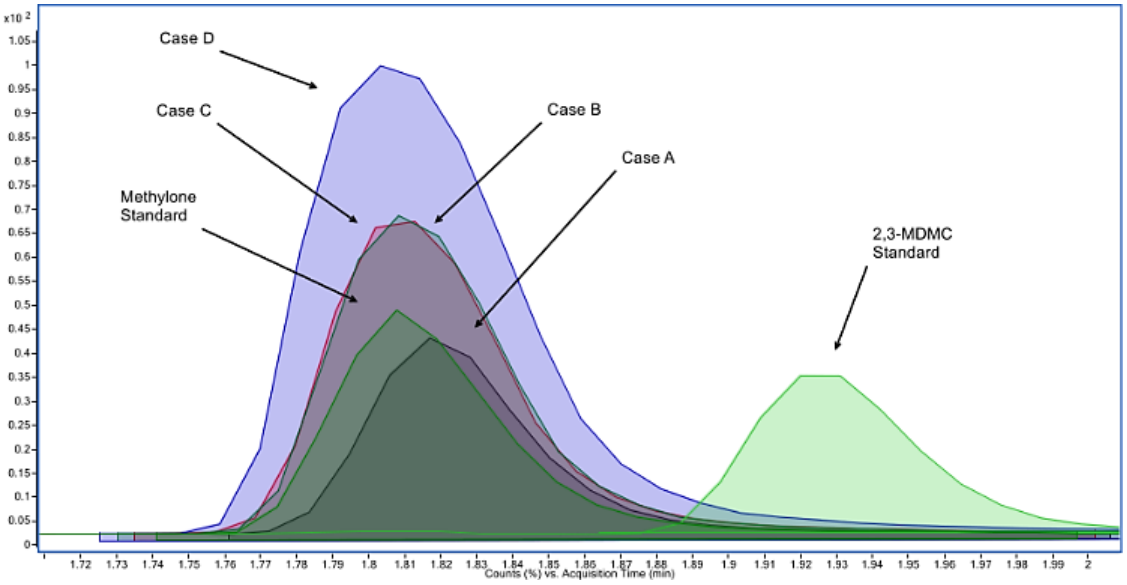


Figure 12. Overlaid extracted ion chromatograms of the 208.0968 m/z ion for Cases A- D, the methylone standard, and the 2,3-MDMC standard.

3.5 Conclusions:

A compound database containing information for 875 NPS was created in order to help confirm the presence of such drugs in forensic related samples. This database includes information such as chemical formula, chemical structure, IUPAC name, CAS/Chemspider numbers, and monoisotopic mass for each compound. A high resolution MS/MS library was also created that contains spectra for 252 compounds from

multiple NPS classes, with the greatest number coming from the synthetic cannabinoid and cathinone classes. Three collision energies (10, 20, and 40 eV) were used for each designer drug standard in order to obtain more information about fragmentation patterns and also to aid in differentiating structurally similar designer drug compounds. Standardized LC retention time data were also added to the library to further facilitate compound identification.

Blind spiked serum specimens, each containing between zero and five NPS, were analyzed by the LC-QTOF-MS method, with successful identification of 32 out of 35 spiked compounds with very high true positive and true negative rates. In addition to the spiked specimens, four drug seizure case samples were analyzed to demonstrate the practical application of the high resolution MS/MS spectral library. Analysis of these samples and comparison to the library produced high match scores for the structural isomers methylone and 2,3-MDMC. By using a gradient LC separation prior to MS analysis, the true match (i.e., methylone) was confirmed. Proving that this library and database can be used to help aid in the identification of novel psychoactive substances in forensic specimens.

There are many potential advantages of using the high mass accuracy and resolution of LC-QTOF-MS for screening of NPS entities, including identification of compounds with high confidence. MS/MS capabilities provide additional confidence when identifying compounds in a forensic sample. Further work is underway to determine the limit of detection, matrix effects, and other formal validation parameters in order to evaluate this technique for practical routine forensic toxicological screening of NPS.

4. COLLISION INDUCED DISSOCIATION STUDIES

4.1 Abstract:

Identification of novel psychoactive substances (NPS) is complicated by the fact that many such compounds are closely related structurally. There are many structural isomers and regioisomers among the various NPS classes that make it challenging to confirm their presence in seized materials or toxicological specimens. Previous literature has suggested that utilizing mass spectrometric methods that employ soft ionization followed by ion dissociation to produce characteristic fragments may be a useful approach to differentiate such regioisomers. Earlier work in this laboratory to develop a high resolution MS/MS spectral library for hundreds of NPS entities indicated that some sets of regioisomers had identical product ions but with different relative abundances. The objective of the present study was to evaluate the relative ion abundances of 15 sets of regioisomers from several NPS classes, with the goal of determining if relative abundance trends of MS/MS spectral data could reliably differentiate such regioisomers. Parameters examined included reproducibility, the effects of relative concentration, and the use of different mobile phases for all 15 sets of regioisomers. Results demonstrated that every set of regioisomers examined had at least one unique or semi-unique ion that could be used to aid in differentiating one or more regioisomers from the other members of the group. In addition, the applicability of the approach to improve NPS regioisomer differentiation was further tested by spiking several sets of compounds into blank human serum, followed by solid phase extraction and LC-MS/MS analysis. These findings indicate that MS/MS data alone can be used to distinguish some sets of NPS regioisomers, without the need for complex separation or analysis approaches.

4.2 Introduction:

Recently there has been an increase in the popularity and use of novel psychoactive substances (NPS) among drug users [2, 5]. Typically, these substances are available online as "research chemicals" or as "legal highs" [4]. They are generally classified by their chemical structure and/or their pharmacodynamic effect [165]. Some of the NPS classes include, but are not limited to, cathinones, phenethylamines, synthetic cannabinoids and tryptamines [2]. As these compounds are psychoactive, there is a need for forensic scientists to be able to identify and confirm these substances in routine casework, as questions of impairment or cause of death often surround these cases.

Identifying and confirming NPS in human matrices has proven to be challenging for a number of reasons. One problem is that NPS often have low cross reactivity in traditional screening assays such as the immunoassay panels that are routinely used in forensic toxicology laboratories [131]. Another challenge is the ever-changing structural nature of such compounds, which necessitates that analytical methodology be routinely expanded or updated to include these new compounds. As governments learn of a new NPS and enact legislation making the possession or distribution of such compounds illegal, new replacement substances rapidly appear. For example, the cathinone methylone was very popular in the United States until it was scheduled by the U.S Drug Enforcement Administration (DEA) and the Chinese government enacted legislation which helped deter production of methylone. After these governmental actions, ethylone started to appear in forensic cases, later followed by the emergence of α-PVP and other derivatives as replacements. As an example of this phenomenon, the number of α-PVP

positive cases in Miami, FL has dropped over the past two years, only to be replaced by N-ethyl pentylone in human performance cases.

Unequivocal identification of NPS in casework is further complicated by the fact that, among the various NPS classes, there are many substances that are structurally related, including isobars, structural isomers, and regioisomers [166-167]. Previous literature has reported the use of a variety of analytical techniques in attempts to distinguish regioisomers in both forensic drug chemistry and toxicology applications. Instrumentation and techniques utilized to identify isomeric NPS include gas chromatography-infrared detection (GC-IRD), gas chromatography mass spectrometry (GC-MS), gas chromatography tandem mass spectrometry (GC-MS/MS), liquid chromatography mass spectrometry (LC-MS), liquid chromatography photodiode array (LC-PDA), liquid chromatography tandem mass spectrometry (LC-MS/MS), and Raman spectroscopy [122, 163, 168-171].

Previous work in this laboratory on the development of a comprehensive, high resolution MS/MS spectral library for NPS that included many regioisomers revealed that that some regioisomers produced identical product ions but with different relative abundances. The present study evaluates the usability of such relative abundance trends for distinguishing regioisomers of NPS. It was hypothesized that if such relative abundance trends are reproducible, MS/MS spectral data of NPS regioisomers alone may be sufficient to distinguish them from each other. This could be useful in cases where NPS regioisomers cannot be fully resolved using chromatographic techniques or in applications where a separation step is not employed, such as in DART or DESI-MS approaches.

4.3 Materials and Methods:

4.3.1 Chemicals and reagents:

Drugs standards were obtained from Cayman Chemical Company (Ann Arbor, MI, USA). Acetonitrile, ammonium formate, formic acid, methanol, and water were obtained from Thermo Fisher Scientific (Waltham, MA, USA). Liquid chromatography solvents and additives were purchased at the HPLC grade or higher. Negative whole blood was collected from a willing volunteer and contained sodium fluoride and potassium oxalate as a preservative.

4.3.2 Instrumentation and Software:

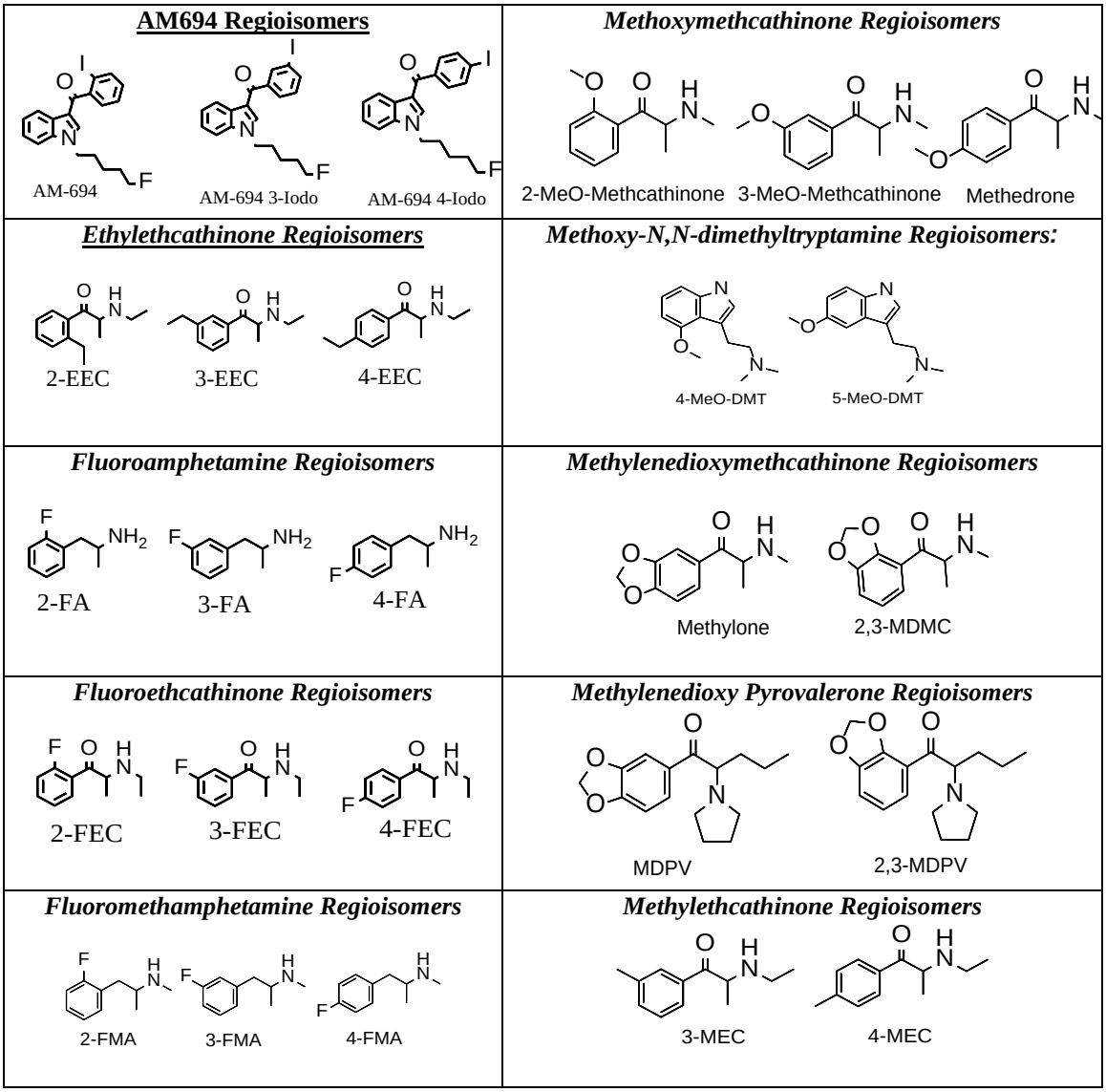
Analytical instrumentation included an Agilent 1290 Infinity UHPLC system coupled to an Agilent 6530 Accurate-Mass QTOF MS (Agilent Technologies, Santa Clara, USA). The QTOF-MS was operated in positive-ion electrospray mode with Jet Stream ESI Technology.

Agilent MassHunter LC/MS Acquisition software for the 6200 series TOF/6500 series QTOF (Version B.05.00) and MassHunter Qualitative Analysis software (Version B.05.00) were used to acquire and process the data. MassHunter Personal Computer Database Library (PCDL) Manager software (Version B.04.00, Build 92.0) was used to create the high resolution MS/MS spectral library and the compound database.

4.3.3 Selection of NPS Isomers:

The approach for the selection of compounds for this study initially involved identifying regioisomeric NPS among the several hundred standards available in the laboratory. These were then grouped based on the shared chemical structure skeleton, and the sets then named based on the compound name without inclusion of the positional

substitution (*e.g.*, JWH 203; fluoroamphetamine). The substitution patterns of the NPS compounds from the cathinone, phenethylamine, and synthetic cannabinoid classes consisted of modifications on the benzoyl or benzyl moieties, while substitution of the tryptamine class consisted of modifications on the indole moiety. Of the 15 selected regioisomers sets, 11 included three regioisomeric compounds in each set, while four had two regioisomeric compounds in the set. The chemical structures of the regioisomers selected for this study are displayed in Figure 13.



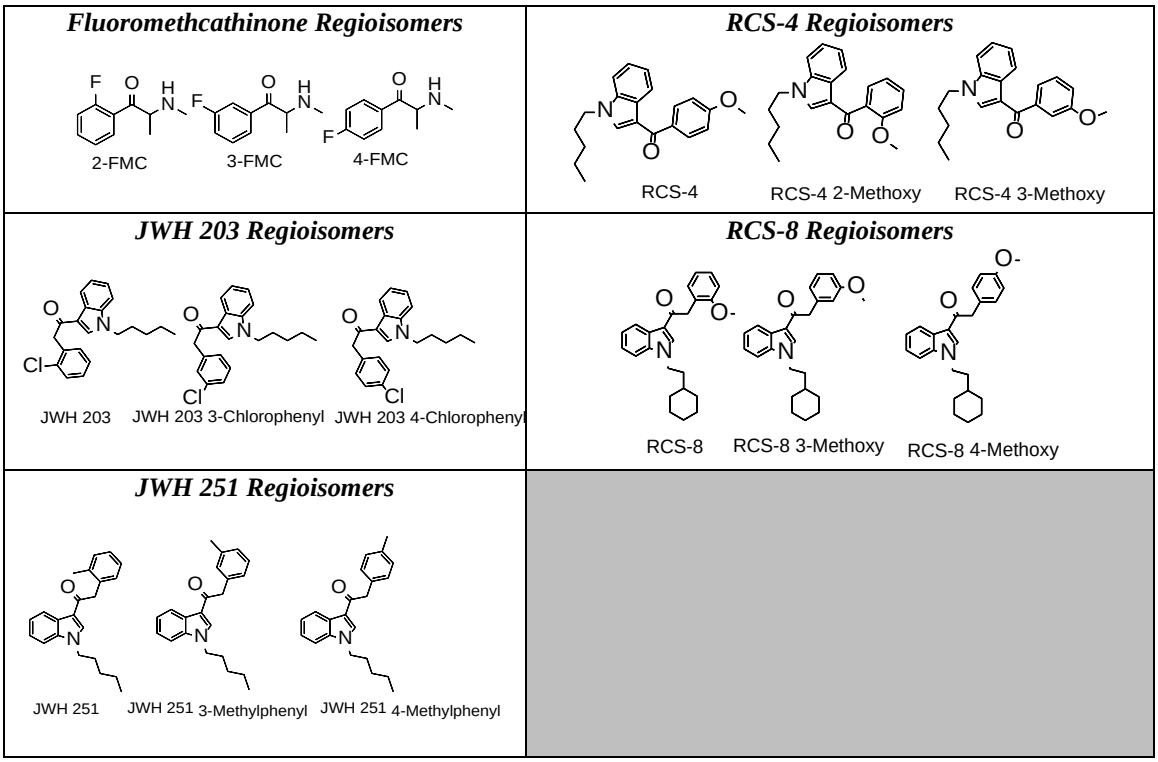


Figure 13. The chemical structures of each of the NPS selected for this study. Regioisomers were grouped and evaluated to determine if MS/MS data alone could be used to distinguish these compounds from each other.

4.3.4 Collision Induced Dissociation Studies:

Commercially available drug standards were each diluted to a concentration of 1,000 ng/mL in HPLC grade methanol. Each diluted standard was injected five times per day on three different days. The method employed an isocratic flow injection analysis (FIA) that used the targeted MS/MS acquisition mode. Mobile phase A consisted of 5 mM ammonium formate with 0.1% formic acid in HPLC grade water. Mobile phase B consisted of 90:10 acetonitrile: water with 0.1% formic acid. The percentage of mobile phase B used in the method was 50%. Injection volume was set to 1 µL. The source parameters were: Gas Temp: 325°C, Gas Flow 5 L/min, Nebulizer 30 psig, Sheath Gas Temp 375°C, Sheath Gas Flow 12 L/min, VCap 4000 V, Nozzle Voltage 0 V, Fragmentor 140 V, Skimmer 65 V. MS/MS Range was 50 - 1700 *m/z*. The MS scan rate

was 10 spectra/s and the MS/MS scan rate was 3 spectra/s. MS/MS was performed at three different collision energies; 10, 20 and 40 eV. The isolation width was set at narrow (1.3 amu). Each analyte had its own method which varied only by the mass that was being targeted.

The "Find Compounds by Targeted MS/MS" algorithm was used to extract the MS/MS data. Any product ion that produced a relative abundance greater than 15% for any set of regioisomers was noted and evaluated to determine the reproducibility of that product ion's relative abundance.

The purpose of this experiment was to identify product ions that had relative abundances that were able to distinguish at least one regioisomers from another and to determine the reproducibility of the relative abundance of these product ions over the course of multiple injections over multiple days. It is important to establish that the relative abundances of the product ions are reproducible before evaluating additional variables such as concentration, mobile phase composition and solid phase. The product ions that were determined to be significantly different and did not have overlapping relative abundance ranges were selected and evaluated in further experiments described below.

4.3.5 CID Concentration Dependence:

Drug standards were diluted to final concentrations of 100 ng/mL and 4,000 ng/mL in methanol. Both concentration levels of each drug standard were injected five times on three different days. The same targeted acquisition, data analysis and statistical analysis methods that were used in the first experiment were used in this experiment as well. The

only difference was that product ions that were identified as significantly different between regioisomers in first experiment were analyzed in this follow up experiment.

The purpose of this experiment was to ensure that varying concentrations would not affect the relative abundance of the selected product ions. Concentrations selected for this experiment represented the concentration in the LC vial of an extracted sample with a low blood concentration and a high blood concentration after a solid phase extraction method. In routine casework, drug concentrations vary among samples so it is necessary to ensure that relative abundance remains consistent with different concentrations of a targeted regioisomer.

4.3.6 CID Mobile Phase Dependence:

Drug standards were diluted to a final concentration of 1,000 ng/mL and injected under four different mobile phase compositions which included: 1) 5 mM ammonium formate in HPLC grade water with 0.1% formic acid, 2) HPLC grade water with 0.1% formic acid, 3) acetonitrile with 0.1% formic acid, and 4) methanol with 0.1% formic acid. Product ions identified in the first experiment as ions of interest were analyzed and compared to determine if the mobile phase affected the relative abundance results of the individual regioisomers.

It has been documented that relative abundances of product ions may vary when analyzed in different mobile phase compositions. In order to determine if there were any differences in the relative abundances, four different mobile phase compositions were selected. Two aqueous and two organic mobile phase compositions. This experiment utilized 100% organic or aqueous compositions to replicate the extremes of a LC gradient where in some methods the mobile phase composition is either 100 % aqueous or 100%

organic. The initial reproducibility experiment was performed with a 50:50 aqueous: organic mobile phase. If relative abundance differences were observed when compared to the original reproducibility experiment they were noted.

4.3.7 Solid Phase Extraction Study:

Four sets of regioisomers were selected and split among three drug mixes. Each drug mix contained only one regioisomer from each set of regioisomers. These drug mixes were used to spike negative whole blood specimens to a final concentration of 100 ng/mL for each regioisomer.

The spiked blood samples were then treated with 1 mL of cold acetonitrile before being centrifuged at 3500 rpm at -10ºC for 10 min. The supernatant was transferred to a test tube and 2 mL of 0.1 M ammonium acetate buffer (pH 4.8) was added and the sample was vortexed. Solid phase extraction (SPE) cartridges (Agilent Bond Elut Plexa) were conditioned by adding 1 mL of methanol followed by addition of 1 mL of ammonium acetate buffer. The samples were then added to the conditioned SPE cartridges. Then, 3 mL of the ammonium acetate buffer was used for the first wash step. The second wash step employed (50:50) deionized water: methanol. Maximum pressure (25 psi) was applied to the SPE cartridges for five min. Two 1 mL aliquots of elution solvent, consisting of acetonitrile with 2% ammonium hydroxide, were added. The eluents were collected in the same tube and dried under N_2 at 35ºC. The sample was reconstituted with 100 µL of mobile phase. Ions of interest, determined from the previous experiments, were analyzed to determine if there was an effect on the relative abundances due to the solid phase extraction method.

The purpose of this experiment was to determine if the relative abundance averages and patterns of product ions of regioisomers were consistent after processing a sample using a solid phase extraction method. This experiment simulated a commonly used extraction technique for blood specimens in forensic toxicology laboratories. This experiment tests the applicability of using the relative abundance to differentiate regioisomers in blood specimens.

4.3.8 Data Analyses:

Initially, MS/MS spectral data was evaluated for every regioisomeric NPS that was selected for this study. The purpose of this evaluation was to identify product ions that had a relative abundance greater than 15% for at least one compound in the set of regioisomers. The mean, range, and standard deviation of the relative abundance were determined for each product ion of interest. In addition, statistical analyses were performed utilizing ANOVA and t-tests to determine if there were significant differences between the average relative abundances of the product ions among the different regioisomers in the specific set.

In regioisomeric sets that contained three compounds, an ANOVA analysis was first performed. If the result of this analysis suggested that there was a significant difference between the average of the relative abundances, then three separate t-tests were performed to determine where the significant difference was in the set of regioisomers. The Bonferroni correction was used in order to reduce the likelihood of generating a type I error when performing multiple t-tests. In addition to establishing whether the averages of the relative abundances were significantly different, the ranges of the relative abundance were also evaluated to see if there was any overlap among regioisomeric

compounds. If such overlap was present among a set of regioisomers, it would make it difficult to distinguish the regioisomers from each other based on relative abundance alone.

For regioisomeric sets that only contained two compounds, the t-test was performed to determine if the average of the relative abundance was significantly different when compared to the other regioisomer in that set. In addition, the ranges of the relative abundance were evaluated to determine if there was any overlap between the two regioisomers.

In order to determine whether or not the relative abundance could be used to differentiate regioisomers form each other, the designations “unique ion” and “semi-unique ion” were used in this study. The “unique ion” designation referred to a product ion that could be used to differentiate all of the regioisomeric compounds from each other in a certain set of regioisomers, based on the relative abundance of that ion. This meant that the average of the relative abundance of the product ion was significantly different and the range of the relative abundance did not overlap with any of the other regioisomeric compounds in that set. The designation “semi-unique” referred to a product ion that could be used to distinguish one regioisomer from another regioisomer but not to distinguish all of the regioisomers from each other. The same criteria as for the “unique ion” designation, which included the average of the relative abundance being significantly different and the range of the relative abundance not overlapping when comparing another regioisomer in the set, were employed for “semi-unique” ions. However, the semi-unique ion designation did not satisfy the criteria for every

regioisomer in the set, and thus could only be used to distinguish one regioisomer from another.

4.4 Results:

4.4.1 Differentiation of Regioisomers:

There was at least one unique or semi-unique ion that could be used to help distinguish a specific regioisomer from another based on the relative abundance alone in every set of regioisomers evaluated. The number of both unique ions and semi-unique ions identified per set of regioisomers ranged from 0 to 7. Figure 14 provides an example of the JWH 203 set of regioisomers. Unique and semi-unique ions are designated on the MS/MS spectra. The sets of regioisomers and the number of unique and semi-unique ions for each regioisomer set are listed in Table 3. Specific data for each regioisomer set are described below.

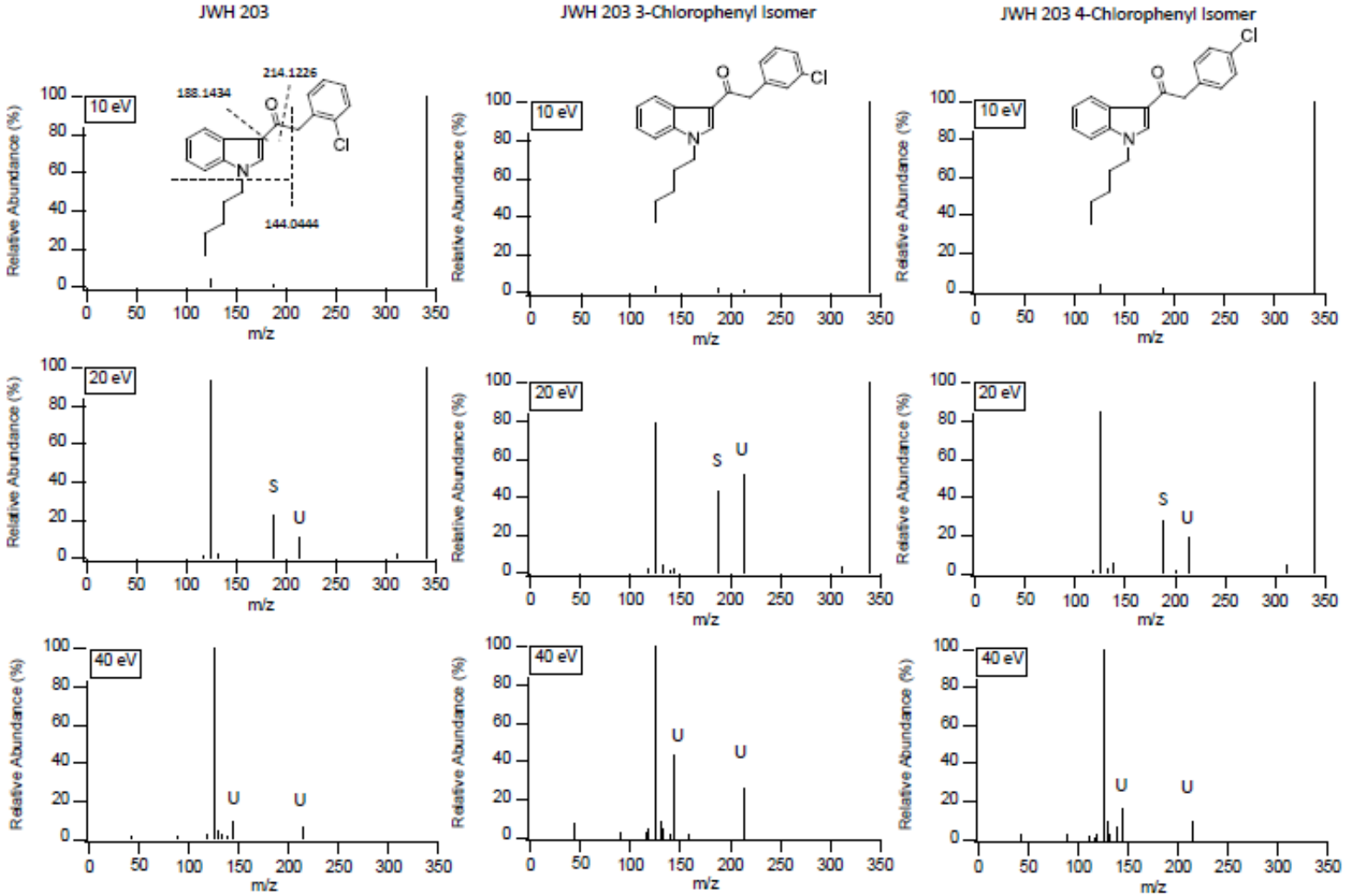


Figure 14. The MS/MS of the JWH 203 regioisomers at various collision energies. Unique ions are designated with a "U" and semi-unique ions are designated with a "S".

Table 3. Ions Present in MS/MS spectral data with a relative abundance greater than 15% for at least one regioisomer. The ions that are bolded and underlined represent unique ions which can be used to distinguish all of theother regioisomers from each other in the set. The ions that are bolded and have an asterisk represent semi-unique ions which can be used to distinguish one regioisomer from another regioisomer but cannot be used to differentiate all of the regioisomers in the set.

Group	Compounds	CE	Ions
AM 694	AM694 AM694 -3 iodo isomer AM 694 4-iodo isomer	10 20 40	436.0568 230.9301, 309.1523, 436.0568 **202.9352***, 230.9301
Ethylethcathinone	2-Ethylethcathinone 3-Ethylethcathinone 4-Ethylethcathinone	10 20 40	159.1043, 160.1121, 188.1434, **206.1539*** 132.0808, 144.0808, 159.1043, 160.1121, **188.1434*** 105.0699, 130.0651, 144.0808
Fluoroamphetamine	2-Fluoroamphetamine 3-Fluoroamphetamine 4-Fluoroamphetamine	10 20 40	109.0448, **137.0761*** 109.0448 83.0292, 109.0448
Fluoroethcathinone	2-Fluoroethcathinone 3-Fluoroethcathinone 4-Fluoroethcathinone	10 20 40	**150.0714***, 178.1027, **196.1132*** 103.0554, **123.0605***, 135.0479, 148.0557, **149.0635***, 150.0714, **163.0792***, **178.1027*** **77.0386***, 95.0292, 103.0554, 108.0370, 109.0448, **115.0554***, **135.0479***, 148.057
Fluoromethamphetamine	2-Fluoromethamphetamine 3-Fluoromethamphetamine 4-Fluoromethamphetamine	10 20 40	109.0448, **137.0761***, **168.1183*** 109.0448 83.0292, 109.0448
Fluoromethcathinone	2-Fluoromethcathinone 3-Fluoromethcathinone 4-Fluoromethcathinone	10 20 40	149.0635, 164.0870, **182.0976*** 123.0605, 148.0557,149.0635, 164.0870 77.0386, 103.0542, 148.0557, 149.0635
JWH 203	JWH 203 JWH 203 3-chlorophenyl JWH 203 4-chlorophenyl	10 20 40	340.1463 125.0153, **188.1434***, **214.1226**, 340.1463 125.0153, **144.0444**, **214.1226**
JWH 251	JWH 251 JWH-251 3-methylphenyl JWH-251 4-methylphenyl	10 20 40	320.2009 105.0699, **188.1434***, **214.1226***, **320.2009*** 43.0542, 105.0699, **144.0444***, **214.1226***
Methoxymethcathinone	2- methoxymethcathinone 3-methoxymethcathinone Methedrone	10 20 40	**161.0835***, 176.1070, **194.1176*** 135.0804, 145.0886, 146.0600, 161.0835, 176.1070 **58.0651**, 77.0386, 79.0542, 91.0542, 103.0542, 105.0699, 117.0573, 118.0651, 132.0808, 144.0808, **146.0600***, **160.0757***
Methoxy-N,N-dimethyltryptamine	4-methoxy DMT 5-methoxy-DMT	10 20 40	58.0651,**174.0913**, **219.1492** 58.0651, **159.0679**, **174.0913** 58.0651, **130.0651**, 131.0730, 143.0730, **159.0679**
Methylenedioxymethcathinone	2,3-MDMC Methylone	10 20	**58.0651**, 160.0757, **190.0863**, 208.0968 **132.0808**, 160.0747

		40	58.0651, 65.0386, 91.0542, **117.0573**, 131.0730, 132.0808
Methylenedioxy Pyrovalerone	2,3-MDPV MDPV	10	276.1594
		20	**126.1277**, **135.0441**, 147.0804, **149.0233**, 175.0754, **205.0858**, **276.1594**
		40	65.0386, 84.0808, 121.0284, **126.1277**, **135.0441**, **149.0233**, 175.0754
Methylethcathinone	3-Methylethcathinone 4-Methylethcathinone	10	145.0886, 146.0964,174.1277, **192.1383**
		20	119.0855, 131.0730, 144.0808, 145.0886, 146.0964, 159.1043, 174.1277
		40	77.0386, 91.0542, 115.0542, 130.0651, 131.0730,144.0808
RCS-4	RCS 4 RCS-4 2-methoxy isomer RCS-4 3-methoxy isomer	10	135.0441, 322.1802
		20	135.0441, **322.1802**
		40	**77.0386***, 92.0257, **107.0491**,**135.0441***, 144.0444
RCS-8	RCS-8 RCS-8 3-methoxy isomer RCS-8 4-methoxy isomer	10	376.2271
		20	**121.0648**, **228.1747**, **254.1539**, 376.2271
		40	69.0699, **91.0542**, 93.0699, 121.0648, 135.0441, **144.0808***, **254.1539**

4.4.1.1 AM694 regioisomer set:

AM694 ((1-(5-fluoropentyl)-1H-indol-3-yl)(2-iodophenyl)methanone), AM694 3-iodo isomer ((1-(5-fluoropentyl)-1H-indol-3-yl)(3-iodophenyl)methanone) and AM 694 4-iodo isomer ((1-(5-fluoropentyl)-1H-indol-3-yl)(3-iodophenyl)methanone) differ based only on the substitution of an iodine atom on the benzoyl group. Three ions of interest were identified in this set of regioisomers; 202.9352 *m/z* ($C_6H_4I^+$) at 40 eV, 230.9301 m/z ($C_7H_4IO^+$) at 20 eV, and 436.0568 *m/z* ($C_{20}H_{20}FINO^+$) at 20 eV.

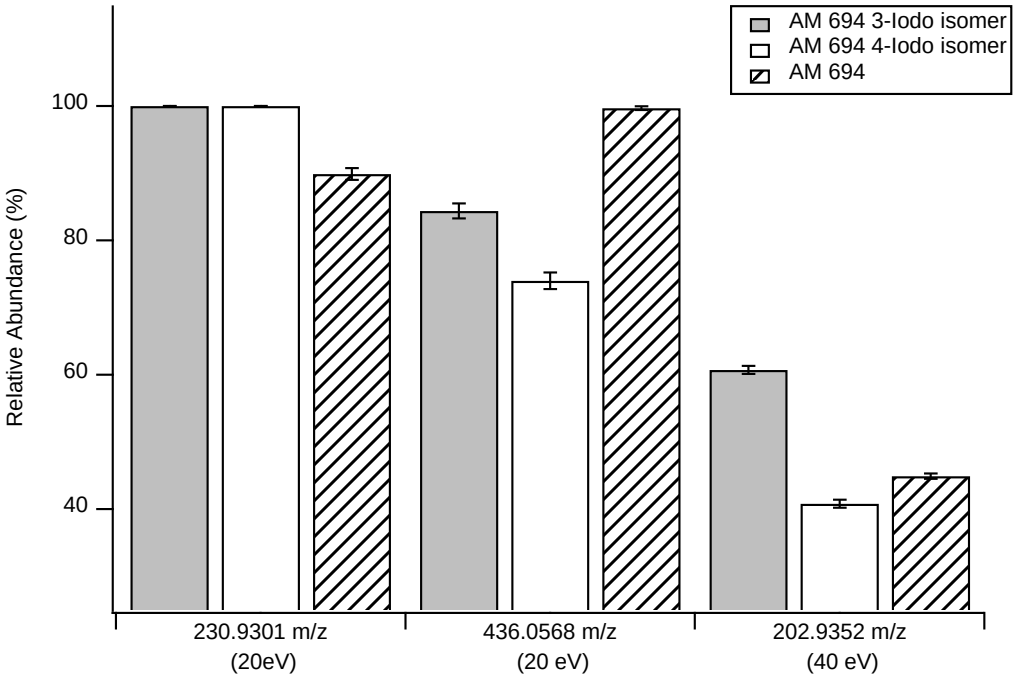


Figure 15. The relative abundance of the ions of interest for the AM 694 set of regioisomers. Error bars represent standard error (SE).

Reproducibility experiments demonstrated that the 202.9352 *m/z* at 40 eV ion could be used to distinguish the 3-iodo isomer from both AM 694 (*i.e.*, the 2-iodo isomer) and the 4-iodo isomers but not AM 694 and the 4-iodo isomer from each other. The *m/z* 436.0568 at 20 eV ion could distinguish AM 694 from both the 3- and 4-iodo isomers.

The *m/z* 436.0568 at 20 eV ion was not reliable as a distinguishing ion in the concentration experiment, as the relative abundance ranges overlapped between the regioisomers in both high and low concentrations. For this set of regioisomers, it was determined that there was one semi-unique ion that could be used to distinguish one regioisomer from the other.

4.4.1.2 Ethylethcathinone regioisomer set:

Three regioisomers, 2-ethylethcathinone (2-EEC; 2-(ethylamino)-1-(2-ethylphenyl)propan-1-one), 3-ethylethcathinone (3-EEC; 2-(ethylamino)-1-(3-ethylphenyl)propan-1-one) and 4-ethylethcathinone (4-EEC; 2-(ethylamino)-1-(4-ethylphenyl)propan-1-one), differ from each other based on the substitution of an ethyl group on the benzoyl group. Two ions of interest were identified; 188.1434 *m/z* ($C_{13}H_{18}N^+$) at 20 eV, and 206.1539 *m/z* ($C_{13}H_{20}NO^+$) at 10 eV.

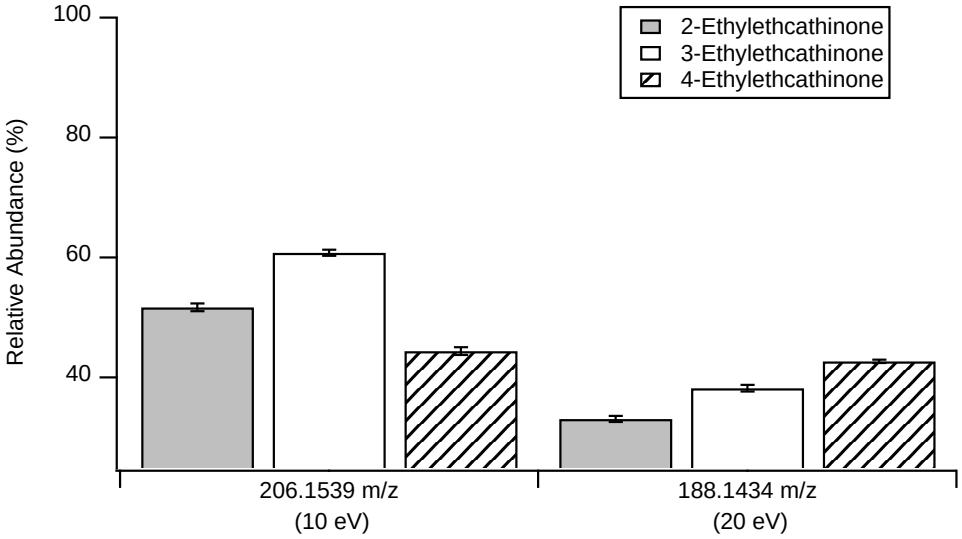


Figure 16. The relative abundance of the ions of interest for the ethylethcathinone set of regioisomers. Error bars represent SE.

The reproducibility experiment demonstrated that the 206.1539 *m/z* at 10 eV ion could differentiate 3-EEC from 4-EEC. The 188.1434 *m/z* at 20 eV ion could distinguish

2-EEC from 4-EEC. The relative abundance trends in the concentration. For this set of regioisomers, it was determined that there were two semi-unique ions that can be used to distinguish one regioisomer from the other two.

4.4.1.3 Fluoroamphetamine regioisomer set:

Three regioisomers, 2-fluoroamphetamine (2-FA; 1-(2-fluorophenyl)propan-2-amine), 3-fluoroamphetamine (3-FA; 1-(3-fluorophenyl)propan-2-amine) and 4-fluoroamphetamine (4-FA; 1-(4-fluorophenyl)propan-2-amine), differ from each other based on the substitution of a fluorine atom on the benzyl group. Three ions of interest were identified in this set of regioisomers; 83.0292 *m/z* ($C_5H_4F^+$) at 40 eV, 109.0448 *m/z* ($C_7H_6F^+$) at 40 eV, and 137.0761 *m/z* ($C_9H_{10}F^+$) at 10 eV.

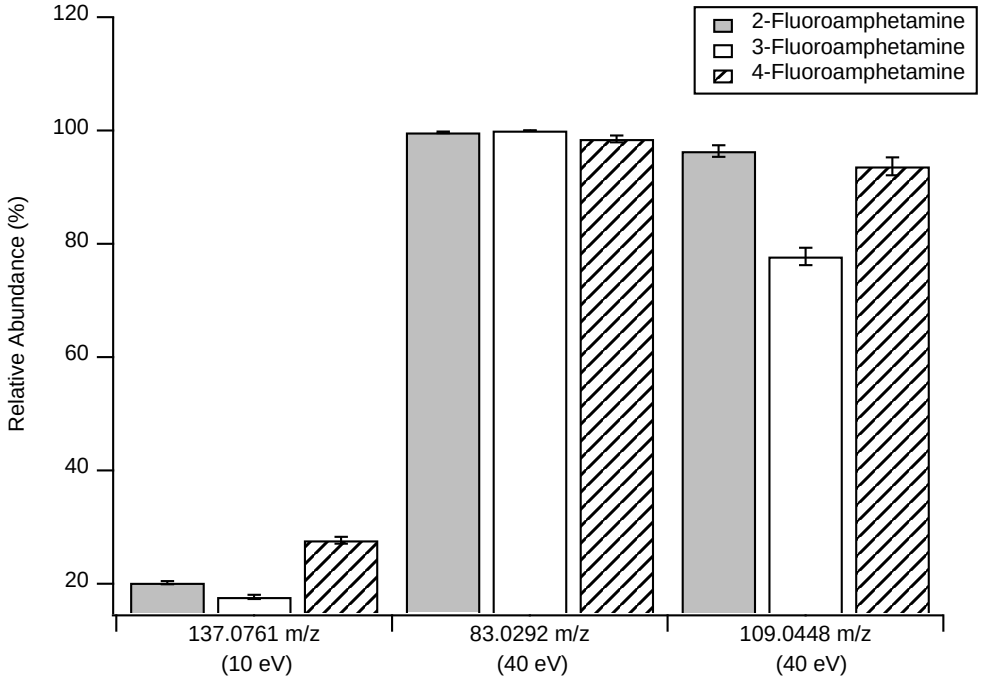


Figure 17. The relative abundance of the ions of interest for the fluoroamphetamine set of regioisomers. Error bars represent SE.

In the reproducibility experiment, it was determined that one ion of interest, 137.0761 *m/z* at 10 eV, could distinguish 4-FA from the 3-FA isomer. However, this ion

could not differentiate the 2-FA and the 3-FA isomers. This trend was also consistent in the concentration experiment. The other ions of interest had overlapping relative abundance ranges, which made them unsuitable for differentiating the regioisomers in this set.

4.4.1.4 Fluoroethcathinone regioisomer set:

Three regioisomers, 2-fluoroethcathinone (2-FEC; 2-(ethylamino)-1-(2-fluorophenyl)propan-1-one), 3-fluoroethcathinone (3-FEC; 2-(ethylamino)-1-(3-fluorophenyl)propan-1-one), and 4-fluoroethcathinone (4-FEC; 2-(ethylamino)-1-(4-fluorophenyl)propan-1-one), differ from each other based on the substitution of a fluorine atom on the benzoyl group. Nine ions of interest were identified; 77.0386 *m/z* ($C_6H_5^+$) at 40 eV, 115.0554 *m/z* ($C_6H_8FO^+$) at 40 eV, 123.0605 *m/z* ($C_8H_8F^+$) at 20 eV, 135.0479 *m/z* ($C_8H_6FN^+$) at 40 eV, 149.0635 *m/z* ($C_9H_8FN^+$) at 20 eV, 150.0714 *m/z* ($C_9H_9FN^+$) at 10eV, 163.0792 *m/z* ($C_{10}H_{10}FN^+$) at 20 eV, 178.1027 *m/z* ($C_{11}H_{13}FN^+$) at 20 eV, and 196.1132 *m/z* ($C_{11}H_{15}FNO^+$) at 10 eV.

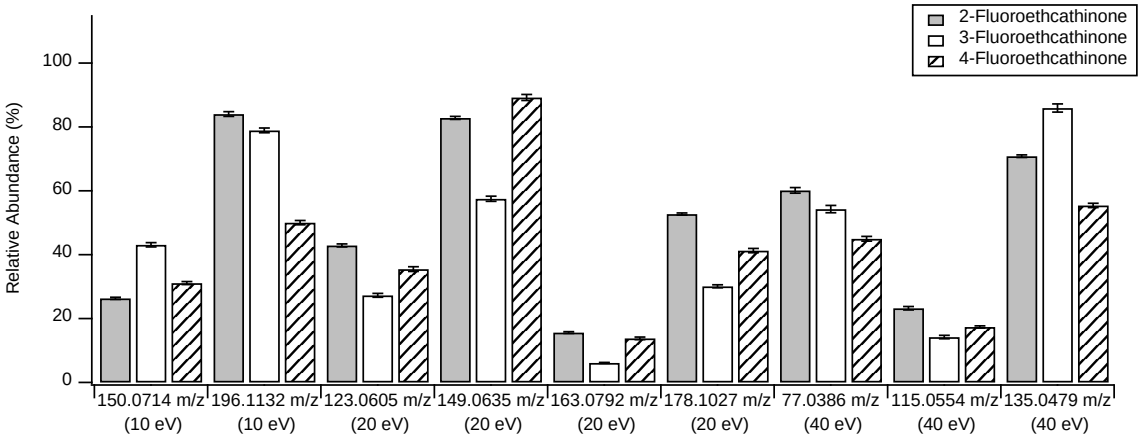


Figure 18. The relative abundance of the ions of interest for the fluoroethcathinone set of regioisomers. Error bars represent SE.

Two ions of interest had relative abundance averages that were significantly different and did not have overlapping ranges for all three regioisomers in the reproducibility experiment. These ions were 178.1027 *m/z* at 20 eV and 135.0479 *m/z* at 40 eV. The 150.0714 *m/z* at 10eV, 149.0635 *m/z* at 20 eV, and 163.0792 *m/z* at 20 eV ions could only distinguish 3-FEC from both 2-FEC and 4-FEC. The 196.1132 *m/z* at 10 eV ion could only distinguish 4-FEC from both 2-FEC and 3-FEC. The 123.0605 *m/z* at 20 eV ion could only distinguish 2-FEC from 3-FEC. The 77.0386 *m/z* at 40 eV ion could only distinguish 2-FEC from 4-FEC. The 115.0554 *m/z* at 40 eV and 150.0714 *m/z* at 10 eV ions could not be used to distinguish any regioisomers from each other, as each had overlapping relative abundance ranges.

In the concentration experiment, the relative abundances were the same for all of the ions except for the 178.1027 *m/z* at 20 eV and 77.0386 *m/z* at 40 eV ions. The relative abundance range of the 178.1027 *m/z* at 20 eV ion overlapped between the 2-FEC and 4-FEC regioisomers in the low concentration experiment, thus rendering this ion only useful for distinguishing 3-FEC from either 2- or 4-EC. The 77.0386 *m/z* at 40 eV ion had overlapping relative abundance ranges for all three regioisomers in the low concentration experiment, making this ion unusable when attempting to resolve regioisomers based off of relative abundance. It was determined that for this set of regioisomers there were no unique ions but there were seven semi-unique ions that could be used to distinguish one regioisomer from the other two regioisomers.

4.4.1.5 Fluoromethamphetamine regioisomer set:

Three regioisomers, 2-fluoromethamphetamine (2-FMA; 1-(2-fluorophenyl)-N-methylpropan-2-amine), 3-fluoromethamphetamine (3-FMA; 1-(3-fluorophenyl)-N-

methylpropan-2-amine) and 4-fluoromethamphetamine (4-FMA; 1-(4-fluorophenyl)-N-methylpropan-2-amine), differ from each other based on the substitution of a fluorine atom on the benzyl group. Three ions of interest were identified; 83.0292 *m/z* ($C_5H_4F^+$) at 40 eV, 137.0761 *m/z* ($C_9H_{10}F^+$) at 10 eV, and 168.1183 *m/z* ($C_{10}H_{15}FN^+$) at 10 eV.

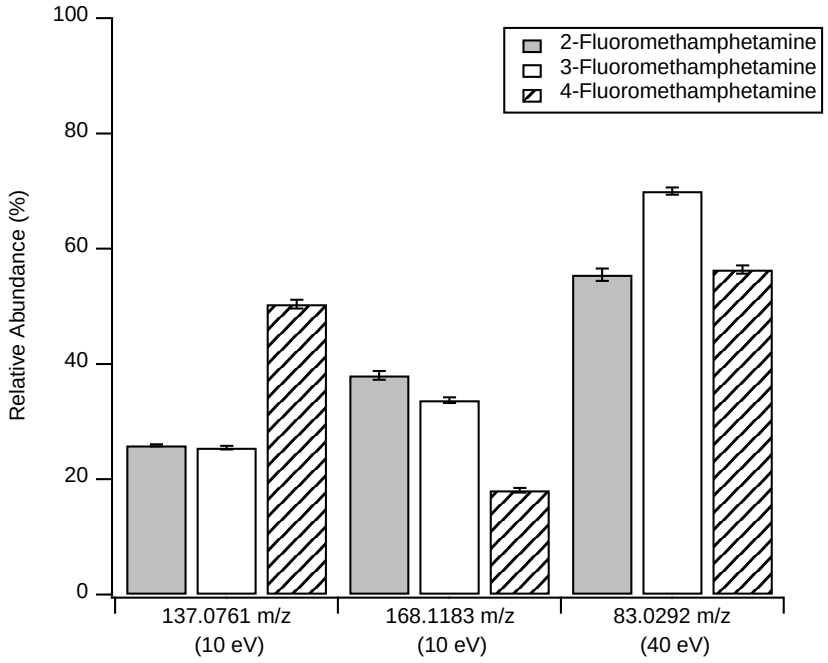


Figure 19. The relative abundance of the ions of interest for the fluoromethamphetamine set of regioisomers. Error bars represent SE.

The reproducibility experiment demonstrated that both the 137.0761 *m/z* at 10 eV and the 168.1183 *m/z* at 10 eV ions could differentiate 4-FMA from both the 2-FMA and 3-FMA isomers. However, these ions were unable to differentiate the 2-FMA and 3-FMA isomers. The 83.0292 *m/z* at 40 eV ion could distinguish 3-FMA from the 4-FMA isomer.

The relative abundance averages in the concentration were higher for the 137.0761 *m/z* at 10 eV and 168.1183 *m/z* at 10 eV ions and were lower for the 83.0292 *m/z* at 40 eV ion when compared to the reproducibility experiment. Besides the overall difference in the relative abundance, the trends remained consistent, with one exception.

The relative abundance range difference for the 83.0292 *m/z* at 40 eV ion in the concentration experiment was 1% between the 3-FMA and 4-FMA isomers; therefore, it may not be a reliable ion to use. There were two ions of interest that were semi-unique and could be used to differentiate one regioisomer from the other two in this set.

4.4.1.6 Fluoromethcathinone regioisomer set:

Three regioisomers, 2-fluoromethcathinone (2-FMC; 1-(2-fluorophenyl)-2-(methylamino)propan-1-one), 3-fluoromethcathinone (3-FMC; 1-(3-fluorophenyl)-2-(methylamino)propan-1-one), and 4-fluoromethcathinone (4-FMC; 1-(4-fluorophenyl)-2-(methylamino)propan-1-one), differ from each other based on the substitution of a fluorine atom on the benzoyl group. Three ions of interest were identified; 103.0542 *m/z* ($C_8H_7^+$) at 40 eV, 123.0605 *m/z* ($C_8H_8F^+$) at 20 eV, and 182.0976 *m/z* ($C_{10}H_{13}FNO^+$) at 10 eV.

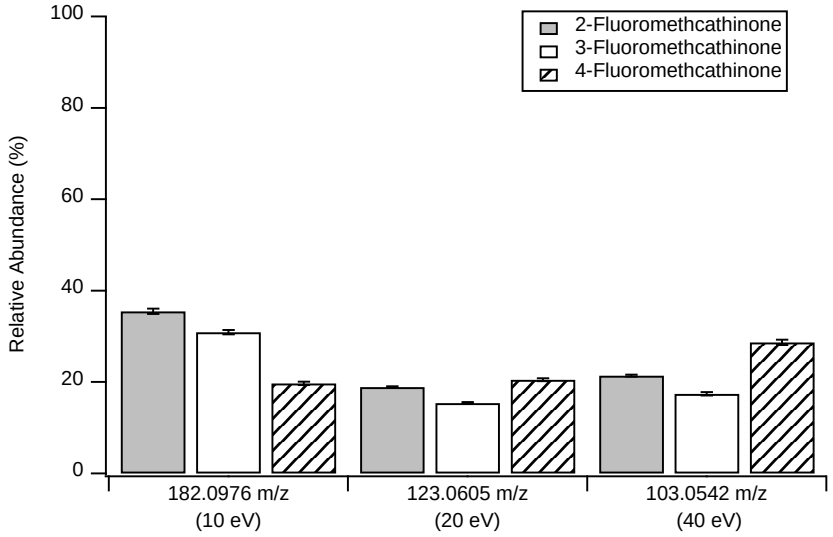


Figure 20. The relative abundance of the ions of interest for the fluoromethcathinone set of regioisomers. Error bars represent SE.

The reproducibility experiment demonstrated that the 182.0976 *m/z* at 10 eV ion could distinguish 4-FMC from 2-FMC and 3-FMC. However, this ion could not

distinguish 2-FMC from 3-FMC. The 103.0542 *m/z* at 40 eV ion could distinguish 3-FMC from both 2-FMC and 4-FMC. However, since the minimum and maximum relative abundances were less than 1% for 2-FMC and 3-FMC, this ion cannot be used to differentiate between these two isomers.

Trends observed in the concentration were consistent with what was observed in the reproducibility experiment. It was determined that one semi-unique ion could be used to differentiate one FMC regioisomer from the other two in the set.

4.4.1.7 JWH 203 regioisomer set:

Three regioisomers, JWH 203 (2-(2-chlorophenyl)-1-(1-pentyl-1H-indol-3-yl)ethan-1-one), JWH 203 3-chlorophenyl isomer (2-(3-chlorophenyl)-1-(1-pentyl-1H-indol-3-yl)ethan-1-one), and JWH 203 4-chlorophenyl isomer (2-(4-chlorophenyl)-1-(1-pentyl-1H-indol-3-yl)ethan-1-one), differ from each other based on the substitution of a chlorine atom on the benzyl group. Four ions of interest were identified; 144.0444 *m/z* ($C_9H_6NO^+$) at 40 eV, 188.1434 *m/z* ($C_{13}H_{18}N^+$) at 20 eV, 214.1226 *m/z* ($C_{14}H_{16}NO^+$) at both 20 eV and 40 eV.

The relative abundance of all four ions of interest were significantly different and did not have overlapping ranges in the reproducibility experiment. While the relative abundance trends in the concentration experiment followed those seen in the reproducibility experiment, the difference in the relative abundance ranges between JWH 203 and the JWH 203 4-chlorophenyl isomer was less than 1% for the 188.1434 *m/z* at 20 eV ion. Due to the difference in ranges being so small, this ion could not distinguish JWH 203 and the JWH 203 4-chlorophenyl isomer. However, the 188.1434 *m/z* at 20 eV ion could distinguish JWH 203 3-chlorophenyl isomer from both JWH 203 and JWH 203

4-chlorophenyl isomer.

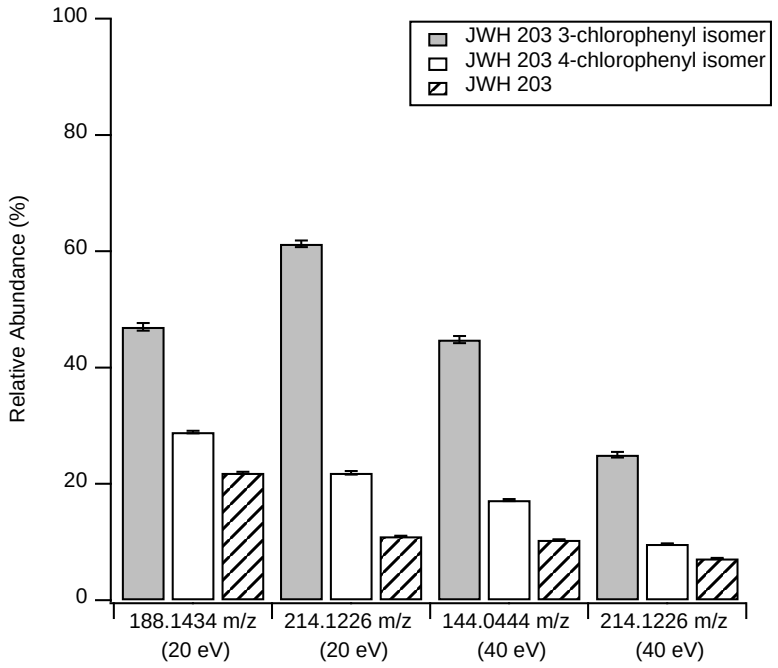


Figure 21. The relative abundance of the ions of interest for the JWH 203 set of regioisomers. Error bars represent SE.

It was determined that three unique ions of interest could be used to distinguish the three JWH 203 regioisomers from each other and one semi-unique ion could be used to distinguish one isomer from the other two regioisomers in this set.

4.4.1.8 JWH 251 regioisomer set:

Three regioisomers, JWH 251 (2-(2-methylphenyl)-1-(1-pentylindol-3-yl)ethenone), JWH-251 3-methylphenyl isomer (2-(3-methylphenyl)-1-(1-pentylindol-3-yl)ethenone), and JWH-251 4-methylphenyl isomer (2-(4-methylphenyl)-1-(1-pentylindol-3-yl)ethenone), differ from each other based on the substitution of a methyl group on the benzyl group. Five ions of interest were identified; 144.0444 *m/z* ($C_9H_6NO^+$) at 40 eV,

188.1434 *m/z* ($C_{13}H_{18}N^+$) at 20 eV, 214.1226 *m/z* ($C_{14}H_{16}NO^+$) at both 20 eV and 40 eV, and 320.2009 *m/z* ($C_{22}H_{26}NO^+$) at 20 eV.

The reproducibility experiment demonstrated that the 214.1226 *m/z* at 40 eV ion could distinguish all three regioisomers from each other. The 188.1434 *m/z* at 20 eV and the 320.2009 *m/z* at 20 eV ions could distinguish JWH 251 3-methylphenyl isomer from both JWH 251 and JWH 251 4-methylphenyl isomer, but could not distinguish JWH 251 and JWH 251 4-methylphenyl isomer from each other. The 214.1226 *m/z* at 20 eV and the 144.0444 *m/z* at 40 eV ions could distinguish JWH 251 4-methylphenyl isomer from JWH 251 and the JWH 251 3-methylphenyl isomer, but could not differentiate JWH 251 and JWH 251 3-methylphenyl isomer from each other.

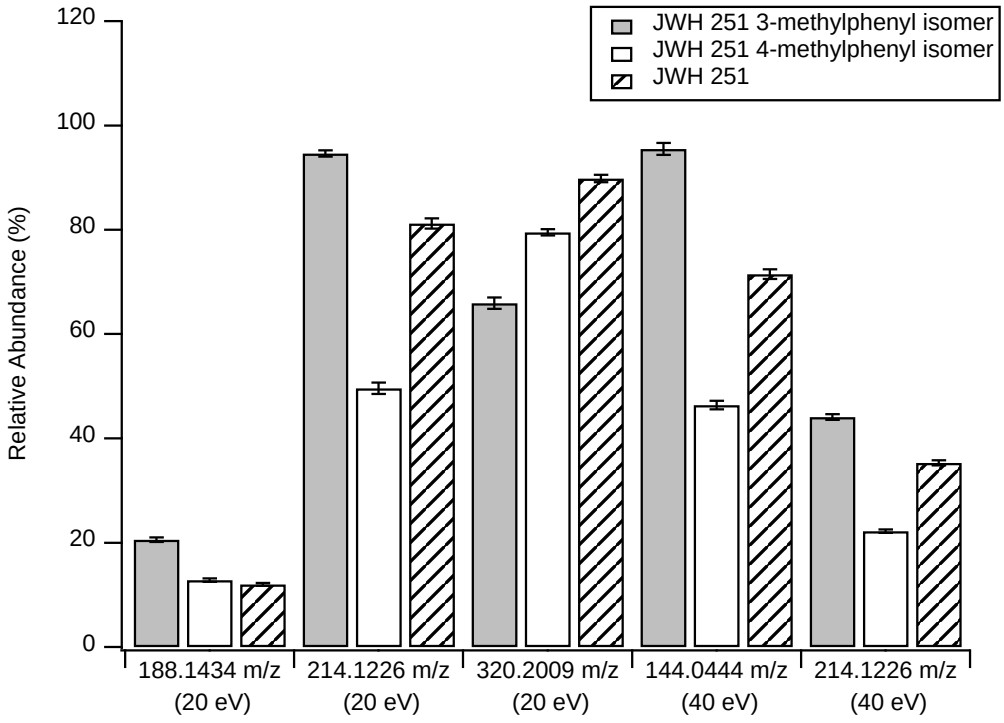


Figure 22. The relative abundance of the ions of interest for the JWH 251 set of regioisomers. Error bars represent SE.

The relative abundance ranges for 214.1226 *m/z* at 40 eV ion overlapped between the JWH 251 and JWH 251 3-methylphenyl isomers in the concentration experiment thus making this ion unreliable for distinguishing these isomers. However, the unique 214.1226 *m/z* at 40 eV ion could be used to distinguish JWH 251 4-methylphenyl isomer from both JWH-251 and JWH 251 3-Methylphenyl isomer.

4.4.1.9 Methoxymethcathinone regioisomer set:

Three regioisomers, 2- methoxymethcathinone (2-MeOMC; 1-(2-methoxyphenyl)-2-(methylamino)propan-1-one), 3-methoxymethcathinone (3-MeOMC; 1-(3-methoxyphenyl)-2-(methylamino)propan-1-one), and 4-methoxymethcathinone (Methedrone; 1-(4-methoxyphenyl)-2-(methylamino)propan-1-one), differ from each other based on the substitution of a methoxy group on the benzoyl group. Five ions of interest were identified; 58.0651 *m/z* ($C_3H_8N^+$) at 40 eV, 146.0600 *m/z* ($C_9H_8NO^+$) at 40 eV, 160.0757 *m/z* ($C_{10}H_{10}NO^+$) at 40 eV, 161.0835 *m/z* ($C_{10}H_{11}NO^+$) at 10 eV, and 194.1176 *m/z* ($C_{11}H_{16}NO_2^+$) at 10 eV.

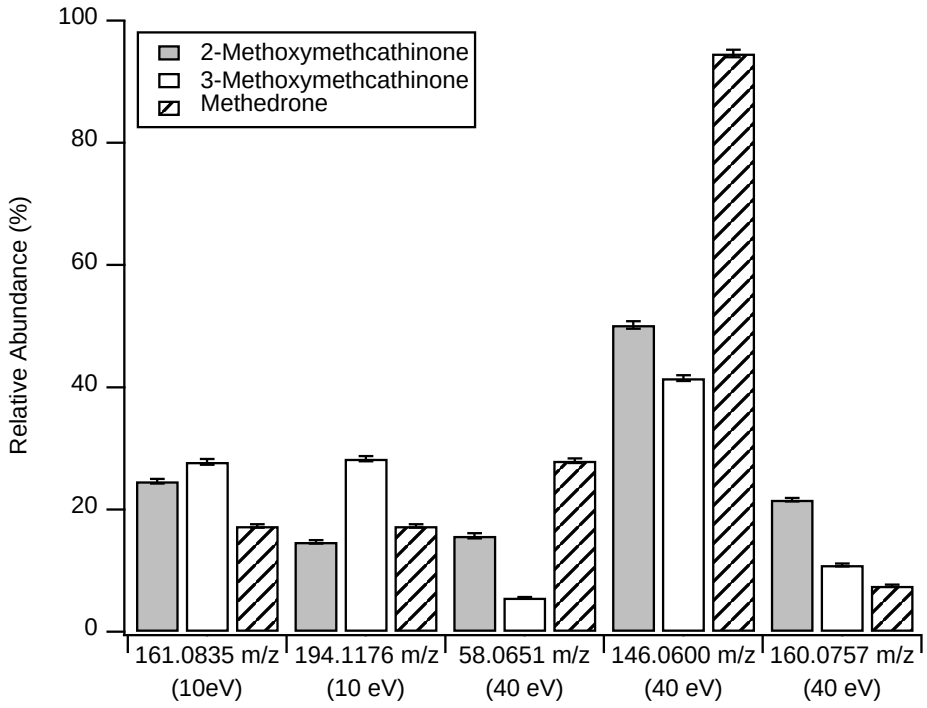


Figure 23. The relative abundance of the ions of interest for the methoxymethcathinone set of regioisomers. Error bars represent SE.

The results of the reproducibility experiment demonstrated that two of the five ions of interest, 58.0651 *m/z* at 40 eV and 146.0600 *m/z* at 40 eV, could distinguish the three regioisomers from each other. The other ions of interest could distinguish one regioisomer from the other two in the set. The 161.0835 *m/z* at 10 eV ion could distinguish Methedrone from both 2-MeOMC and 3-MeOMC. The 194.1176 *m/z* at 10 eV ion was able to distinguish 3-MeOMC from both Methedrone and 2-MeOMC. The 160.0757 *m/z* at 40 eV ion was able to distinguish 2-MeOMC from both Methedrone and 3-MeOMC.

The concentration experiment yielded similar results to the reproducibility study with the exception of the 146.0600 *m/z* at 40 eV ion. The average relative abundance of this ion overlapped between 2-MeOMC and 3-MeOMC thus making it an unreliable ion to differentiate these two regioisomers.

Only one unique ion of interest was able to distinguish all three regioisomers from each other. The other four semi-unique ions of interest were able to distinguish one regioisomer from the other two regioisomers of interest.

4.4.1.10 Methoxy-N,N-dimethyltryptamine regioisomer set:

The two regioisomers, 4-methoxy-N,N-dimethyltryptamine (4-MeO-DMT; 2-(4-methoxy-1H-indol-3-yl)-N,N-dimethylethan-1-amine) and 5-methoxy-N,N-dimethyltryptamine (5-MeO-DMT; 2-(5-methoxy-1H-indol-3-yl)-N,N-dimethylethan-1-amine), differ from each other based on the substitution of a methoxy group on the indole ring. Six ions of interest were identified for these regioisomers; 130.0651 *m/z* ($C_9H_8N^+$) at 40 eV, 159.0679 *m/z* ($C_{10}H_9NO^+$) at both 20 eV and 40 eV, 174.0913 *m/z* ($C_{11}H_{12}NO^+$) at both 10 eV and 20 eV, and 219.1492 *m/z* ($C_{13}H_{19}N_2O^+$) at 10 eV.

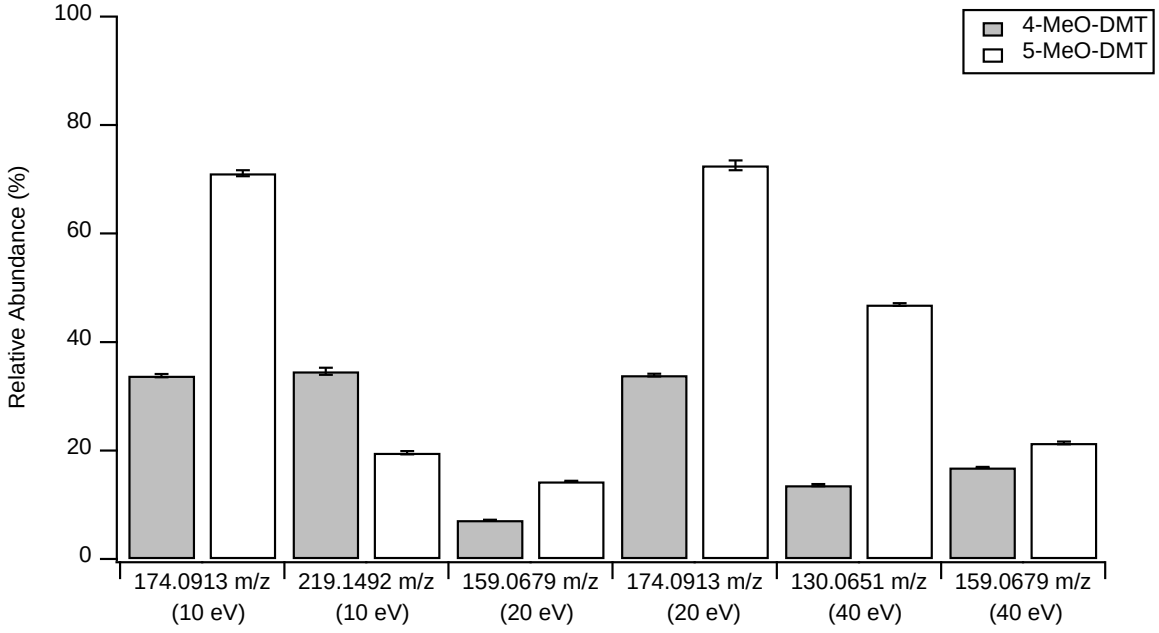


Figure 24. The relative abundance of the ions of interest for the MeO-DMT set of regioisomers. Error bars represent SE.

The relative abundance mean of the ions of interest were all significantly different from each other and there were no overlapping ranges between them. The concentration

experiment experiment generated similar trends between the two regioisomers' ions of interest. The 159.0679 *m/z* at 40 eV ion had ranges that were very close to each other for the two regioisomers. For example, in the reproducibility study, 4-MeO-DMT had a maximum relative abundance of 17.54% and 5-MeO-DMT had a minimum relative of abundance of 17.93%. In an abundance of caution, this product ion was excluded due to these close ranges. After the exclusion of the 159.0679 *m/z* at 40 eV ion, there were five unique ions of interest that could be used to distinguish the two regioisomers from each other.

4.4.1.11 Methylenedioxymethcathinone regioisomer set:

Two regioisomers, 2,3-methylenedioxymethcathinone (2,3-MDMC; 1-(1,3-benzodioxol-4-yl)-2-(methylamino)-1-propanone) and 3,4-methylenedioxymethcathinone (Methylone; 1-(1,3-benzodioxol-5-yl)-2-(methylamino)propan-1-one), differ from each other based on the substitution of a methylenedioxy group on the benzoyl group. Six ions of interest were identified; 58.0651 *m/z* ($C_3H_8N^+$) at 10 eV, 91.0542 *m/z* ($C_7H_7^+$) at 40 eV, 117.0573 *m/z* ($C_8H_7N^+$) at 40 eV, 132.0808 *m/z* ($C_9H_{10}N^+$) at both 20 eV and 40 eV, and 190.0863 *m/z* ($C_{11}H_{12}NO_2^+$) at 10 eV.

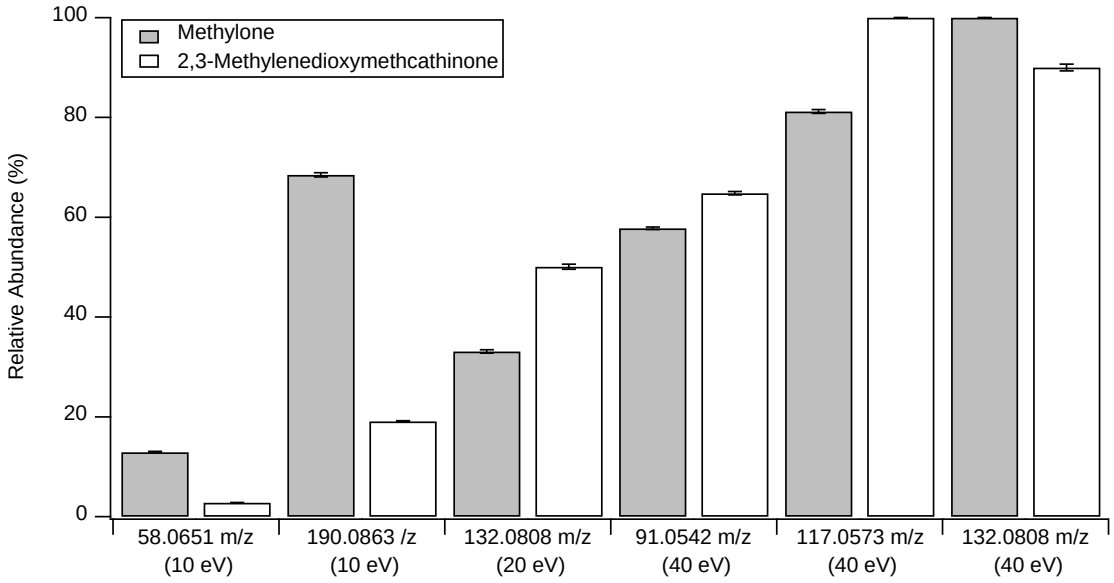


Figure 25. The relative abundance of the ions of interest for the methylenedioxymethcathinone set of regioisomers. Error bars represent SE.

All six ions of interest had relative abundances that were significantly different from each other and did not overlap between the two regioisomers in the reproducibility experiment. In the concentration experiment, the 91.0542 *m/z* at 40 eV ion and the 132.0808 *m/z* at 40 eV ion both had overlapping relative abundance ranges, which eliminated them from being reliable ions to distinguish the two regioisomers from each other. It was determined that four of the six ions of interest were unique ions and could be used to distinguish the two regioisomers from each other.

4.4.1.12 Methylenedioxy Pyrovalerone regioisomer set:

The two regioisomers, 2,3-methylenedioxypyrovalerone (2,3-MDPV; 1-(1,3-benzodioxol-4-yl)-2-pyrrolidin-1-ylpentan-1-one) and methylenedioxypyrovalerone (MDPV; 1-(1,3-benzodioxol-5-yl)-2-pyrrolidin-1-yl-pentan-1-one), differ from each other based on the position of substitution of the methylenedioxy group on the benzoyl group. The ions identified to be of interest were 126.1277 *m/z* ($C_8H_{16}N^+$) at both 20 eV

and 40 eV, 135.0441 *m/z* ($C_8H_7O_2^+$) at both 20 eV and 40 eV, 149.0233 *m/z* ($C_8H_5O_3^+$) at both 20 eV and 40 eV, 205.0858 *m/z* ($C_8H_5O_3^+$) at 20 eV, and 276.1594 *m/z* ($C_{16}H_{22}NO_3^+$) at 20 eV.

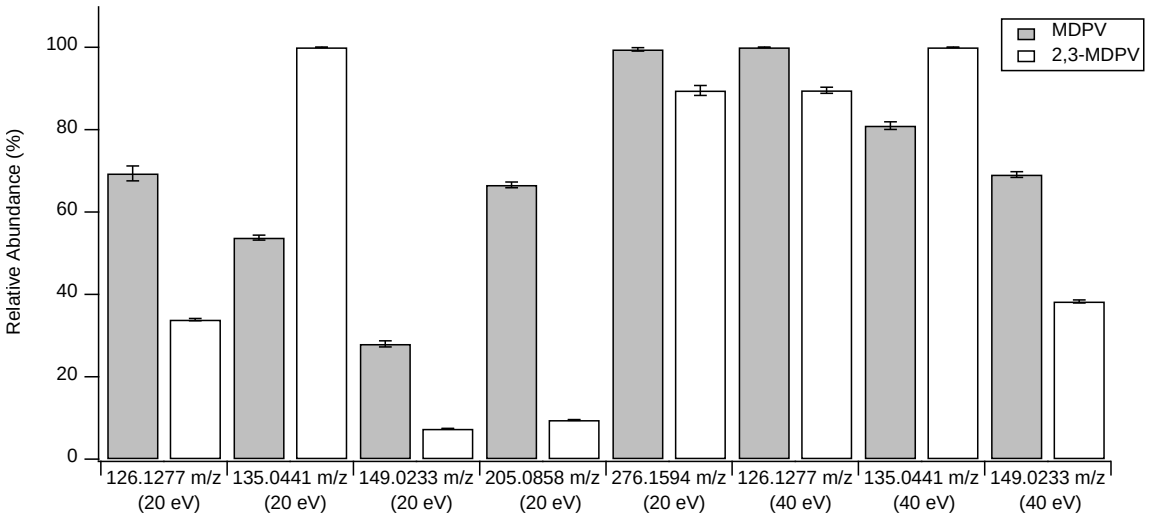


Figure 26. The relative abundance of the ions of interest for the MDPV set of regioisomers. Error bars represent SE.

Reproducibility studies demonstrated that the relative abundances of the seven of the eight ions of interest were significantly different and their ranges did not overlap between the two regioisomers. The only ion that did not satisfy this requirement was the 276.1594 *m/z* ion at 20 eV. For this ion the mean was significantly different but the range overlapped. This ion was therefore not included in the concentration and mobile phase experiments.

For the remaining seven ions of interest, the average relative abundance varied slightly between the high and low concentrations of the same regioisomer. However, the trends between the two regioisomers remained and the two regioisomers could be differentiated based on the relative abundance for each of the seven product ions. This

data suggests that seven unique ions could be used to differentiate these two regioisomers from each other.

4.4.1.13 Methylethcathinone regioisomers set:

Two regioisomers, 3-methylethcathinone (3-MEC; 2-(ethylamino)-1-(3-methylphenyl)propan-1-one) and 4-methylethcathinone (4-MEC; 2-(ethylamino)-1-(4-methylphenyl)propan-1-one), differ from each other based on the substitution of a methyl group on the benzoyl group. Four ions of interest were identified; 91.0542 *m/z* ($C_7H_7^+$) at 40 eV, 119.0855 *m/z* ($C_9H_{11}^+$) at 20 eV, 174.1277 *m/z* ($C_{12}H_{16}N^+$) at 20 eV, 192.1383 *m/z* ($C_{12}H_{18}NO^+$) at 10 eV.

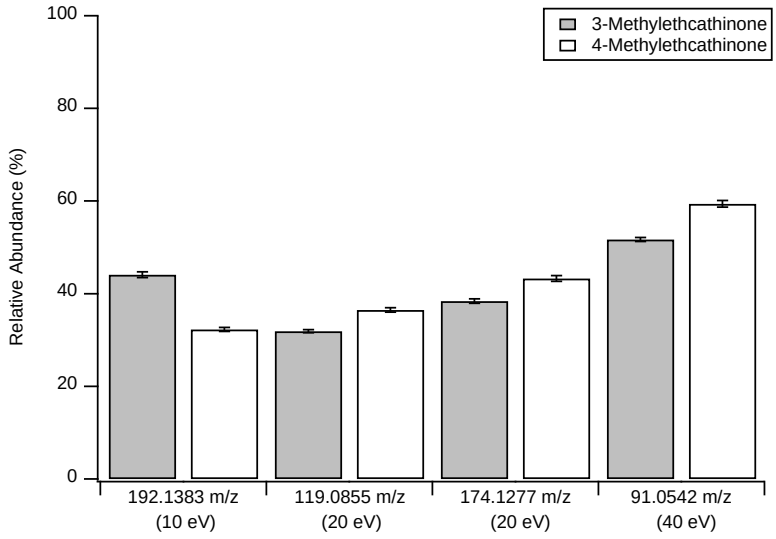


Figure 27. The relative abundance of the ions of interest for the fluoroethcathinone set of regioisomers. Error bars represent SE.

In the reproducibility experiment, only one ion of interest, 192.1383 *m/z* at 10 eV, could distinguish the regioisomers. The other three ions of interest had significant differences between the average relative abundance. However, the range of the relative abundance overlapped between the two regioisomers, rendering these ions not reliable to differentiate the two regioisomers based on relative abundance.

The concentration experiment exhibited similar trends, with the only difference being the higher relative abundance averages for ions 192.1383 *m/z* at 10 eV and 174.1277 *m/z* at 20 eV. The 192.1383 *m/z* at 10 eV ion could still differentiate between the regioisomers. It was determined that one unique ion of interest could be used to differentiate the two regioisomers in this set.

4.4.1.14 RCS 4 regioisomer set:

Three regioisomers, RCS-4 (4-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone , RCS-4 2-methoxy isomer (2-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone and RCS-4 3-methoxy isomer (3-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone, differ from each other based on the substitution of a methoxy group on the benzoyl group. Four ions of interest were identified; 77.0386 *m/z* ($C_6H_5^+$) at 40 eV, 107.0491 *m/z* ($C_7H_7O^+$) at 40 eV, 135.0441 *m/z* ($C_8H_7O_2^+$) at 40 eV, and 322.1802 *m/z* ($C_{21}H_{24}NO_2^+$) at 20 eV.

The reproducibility experiment demonstrated that both the 322.1802 *m/z* at 20 eV and the 107.0491 *m/z* at 40 eV ions could distinguish all three regioisomers. The 77.0386 *m/z* at 40 eV and 107.0491 *m/z* at 40 eV ions could differentiate the RCS-4 3-methoxy isomer from both RCS-4 and the RCS-4 2-methoxy isomer. However, these two ions could not distinguish RCS-4 and the RCS-4 2-methoxy isomers from each other.

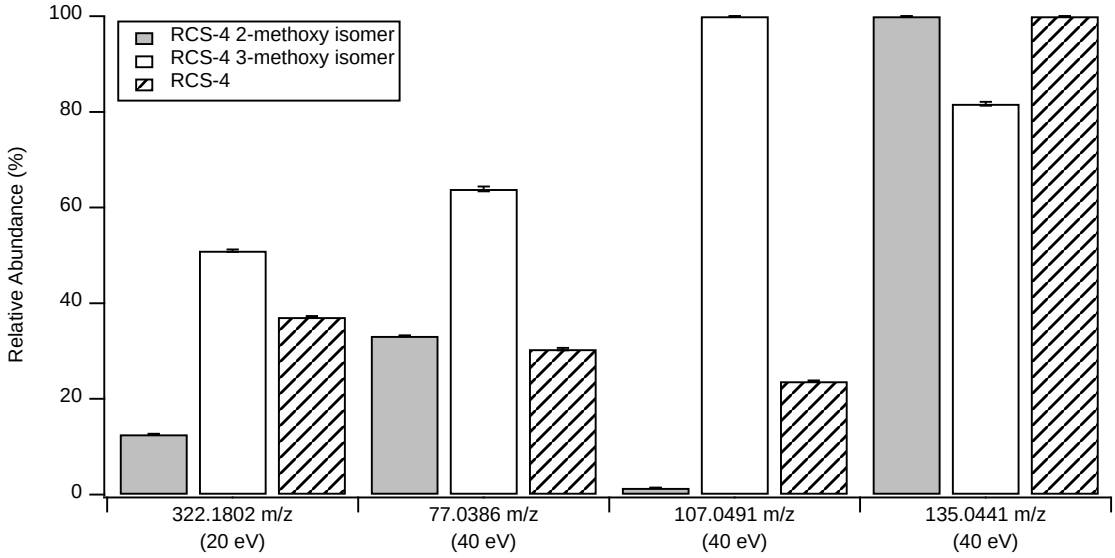


Figure 28. The relative abundance of the ions of interest for the RCS-8 set of regioisomers. Error bars represent SE.

The trends observed in the reproducibility experiment were similar to those observed in the concentration experiment. The only exception was for the 77.0386 *m/z* at 40 eV ion, for which the overlap between RCS-4 and the RCS-4 2-methoxy isomer observed in the reproducibility experiment was not present in the concentration experiment. It was determined that two ions can be used to distinguish all three regioisomers from each other and two ions can be used to distinguish one regioisomer from the other two regioisomers.

4.4.1.15 RCS-8 regioisomer experiment:

Three regioisomers, RCS-8 (1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(2-methoxyphenyl)ethan-1-one), RCS-8 3-methoxy isomer (1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(3-methoxyphenyl)ethan-1-one), and RCS-8 4-methoxy isomer (1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(4-methoxyphenyl)ethan-1-one), differ from each other based on the substitution of a methoxy group on the benzyl group. Six ions of interest were identified; 91.0542 *m/z* ($C_7H_7^+$) at 40 eV, 121.0648 *m/z* ($C_8H_9O^+$) at 20 eV,

144.0444 *m/z* ($C_9H_6NO^+$) at 40 eV, 228.1747 *m/z* ($C_{16}H_{22}N^+$) at 20 eV, and 254.1539 *m/z* ($C_{17}H_{20}NO^+$) at 20 eV and 40 eV.

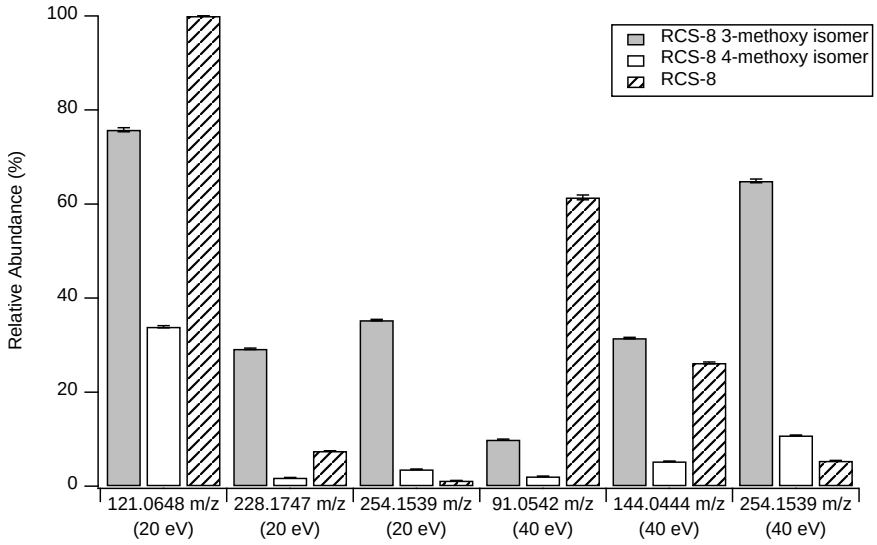


Figure 29. The relative abundance of the ions of interest for the RCS-8 set of regioisomers. Error bars represent SE.

The reproducibility study demonstrated that the relative abundance of all six ions of interest were significantly different from each other and did not have overlapping ranges. In the concentration study, the average relative abundance followed trends observed in the reproducibility study. However, for the 144.0444 *m/z* at 40 eV ion, the range overlapped between RCS-8 and the RCS-8 3-methoxy regioisomer in the low concentration replicates. Due to this overlap, the 144.0444 *m/z* at 40 eV ion could not differentiate RCS-8 from the RCS-8 3-methoxy isomer. However, this semi-unique ion could differentiate the RCS-8 4-methoxy isomer from both RCS-8 and the RCS-8 3-methoxy isomer. The remaining five unique ions of interest could distinguish all three regioisomers from each other.

Four of the ions of interest had relative abundance averages that were consistent with the averages obtained in the reproducibility experiment. The 121.0648 *m/z* at 20 eV ion

had elevated relative abundance averages greater than 5% for both the RCS-8 3-methoxy isomer and the RCS-8 4-methoxy isomer when compared to the reproducibility experiment. The relative abundance average for RCS-8 121.0648 *m/z* at 20 eV ion remained at 100% in every experiment. The 254.1539 *m/z* at 40 eV ion had a slightly different relative abundance average for the RCS-8 3-methoxy isomer. The relative abundance average difference was less than 3% for the other two regioisomers when compared to the reproducibility study.

4.4.2 Mobile Phase Experiment

All of the sets of regioisomers were evaluated under different mobile phase conditions to evaluate how reproducible the relative abundances were using different mobile phase compositions. For this study two aqueous (5 mM AF in HPLC Water with 0.1% FA and HPLC with 0.1% FA) and two organic (Acetonitrile with 0.1% formic acid and methanol with 0.1% formic acid) mobile phase compositions were used. Ten of the fifteen sets of regioisomers had ions with consistent relative abundances among all four mobile phase compositions. The five sets of regioisomers that were not consistent were all from the synthetic cannabinoid NPS class. The number of ions affected by the mobile phase composition varied for each set of regioisomers.

In the AM-694 set of regioisomers, three ions of interest had average relative abundance differences greater than 5%. These differences were observed in the 230.9301 *m/z* at 20 eV ion for the AM-694 3-iodo isomer. The 436.0568 *m/z* at 20 eV ion and the 202.9352 *m/z* at 40 eV ion both had variation in both the AM-694 3-iodo isomer and the AM-694 4-iodo isomer. These differences were observed when comparing the aqueous and the organic mobile phase compositions.

Significant differences were observed in the mobile phase experiment for JWH 203 3-chlorophenyl isomer's relative abundance mean of the four ions of interest when comparing the aqueous and organic mobile phases to each other. Interestingly, this phenomenon was not observed in JWH-203 and the JWH-203 4-chlorophenyl isomer. The organic mobile phase compositions produced similar results to the reproducibility experiment.

In the JWH-251 set of regioisomers four of the five ions of interest had at least one regioisomer with a difference in the average relative abundance greater than 5% observed. The 214.1226 *m/z* at 20 eV ion and the 144.044 *m/z* at 20 eV ion had differences in both the JWH-251 3-methylphenyl isomer and JWH-251 4-methylphenyl isomer. The 320.2009 *m/z* at 20 eV ion had differences observed in the relative abundance of the JWH-251 3-methylphenyl isomer. The 214.1226 *m/z* at 40 eV ion had difference observed in the relative abundance of the JWH-251 4-methylphenyl isomer.

In the RCS-4 set of regioisomers there were four ions of interests that had average relative significant differences among the various mobile phase compositions. Like the JWH 203 set of regioisomers, the RCS-4 3-methoxy isomer was the only isomer to have significant differences among the mobile phase compositions. These differences were not observed in RCS-4 and the RCS-4 methoxy isomer.

In the RCS-8 set of regioisomers, six ions of interest had relative abundance differences greater than 5% when analyzed utilizing the various mobile phase compositions. The 121.0648 *m/z* at 20 eV, 228.1747 *m/z* at 20 eV, and 254.1539 *m/z* at 20 eV ions had differences in the relative abundance of both the RCS-8 3-methoxy isomer and the RCS-8 4-methoxy isomer. All of the RCS-8 regioisomers had different relative

abundances for the 91.0542 *m/z* at 40 eV, 144.0444 *m/z* at 40 eV, and 254.1539 *m/z* at 40 eV ions when comparing the abundances obtained utilizing the various mobile phase compositions.

4.4.3 Solid Phase Extraction Experiment

Four sets of regioisomers were selected for further evaluation. These sets included two cathinone sets (fluoroethcathinone and methoxymethcathinone) and two synthetic cannabinoid sets (JWH-203 and RCS-8). These sets were selected to represent various NPS classes and due to the fact that these sets had many unique and semi-unique ions identified in previous experiments. This experiment was performed to determine if the trends observed in previous experiments are consistent after a solid phase extraction from human blood.

Unless noted in Table 4, all of the ions of interest had relative abundances within 5% of the average relative abundance determined in the reproducibility study. Three sets of regioisomers, fluoroethcathinone, methoxymethcathinone and RCS-8, had at least two ions of interest that had a relative abundance greater than 5%. The difference in relative abundances were not seen in ions from the JWH-203 regioisomer set.

In the fluoroethcathinone regioisomer set, three ions had elevated relative abundances when compared to the previous experiments. However, the trends noted for these three ions remained the same in terms of differentiating regioisomers. The 150.0714 *m/z* at 10eV and 178.1027 *m/z* at 20 eV ions can be used to distinguish 3-FEC from both 2-FEC and 4-FEC. While the 196.1132 *m/z* at 10 eV ion can be used to distinguish 4-FEC from both 2-FEC and 3-FEC.

The methoxymethcathinone regioisomer set had two ions of interested with elevated relative abundances. Similar to the fluoroethcathinone regioisomer set, although the relative abundance was elevated the trends observed in previous experiments were consistent. The 161.0835 *m/z* at 10 eV ion can be used to distinguish methedrone from both 2-MeOMEC and 3-MeOMEC. The 194.1176 *m/z* at 10 eV ion ca be used to distinguish 3-MeOMEC from both 2-MeOMEC and methedrone.

Table 4. All of the ions of interest in the four sets of regioisomers where relative abundances were inconsistent (>5% difference) between the reproducibility experiment and the solid phase extraction experiment for at least one regioisomer in the set. The JWH 203 set of regioisomers was also evaluated during the solid phase extraction experiment. However, there were no inconsistent ions observed with this set of regioisomers.

				Reproducibility		SPE	
Regioisomer Set	**Compound**	**Product Ion**	**CE**	**Average (%)**	**RSD**	**Average (%)**	**RSD**
Fluoroethcathinone	2-Fluoroethcathinone	150.07179	10 eV	26.3	6.1%	35.7	0.1%
	3-Fluoroethcathinone			43.1	6.7%	52.5	1.7%
	4-Fluoroethcathinone			31.1	6.8%	40.9	2.3%
	2-Fluoroethcathinone	196.11391	10 eV	84.0	4.0%	98.7	2.2%
	3-Fluoroethcathinone			78.9	4.1%	100.0	0.0%
	4-Fluoroethcathinone			50.0	6.0%	72.8	0.8%
	2-Fluoroethcathinone	178.1031	20 eV	52.7	3.1%	61.7	6.8%
	3-Fluoroethcathinone			30.1	7.4%	38.8	1.2%
	4-Fluoroethcathinone			41.3	7.0%	53.2	2.2%
Methoxymethcathinone	Methedrone	161.0836	10 eV	17.3	6.3%	24.5	3.5%
	2-Methoxymethcathinone			24.6	5.8%	32.8	2.2%
	3-Methoxymethcathinone			27.8	6.6%	39.2	0.8%
	Methedrone	194.1178	10 eV	17.3	6.6%	26.8	0.9%
	2-Methoxymethcathinone			14.7	7.9%	24.5	2.1%
	3-Methoxymethcathinone			28.3	6.0%	41.9	1.8%
RCS-8	RCS-8 3-methoxy isomer	121.0637	20 eV	75.8	2.5%	95.3	1.1%
	RCS-8 4-methoxy isomer			33.9	3.1%	43.6	2.6%
	RCS-8			100.0	0.0%	100.0	0.0%
	RCS-8 3-methoxy isomer	254.1532	40 eV	64.9	2.7%	57.0	2.4%

	RCS-8 4-methoxy isomer			10.8	3.4%	8.7	3.6%
	RCS-8			5.4	5.5%	4.3	5.4%

The RCS-8 regioisomer set had one ion of interest that had elevated relative abundances and one ion of interest that had lower relative abundances when compared to the reproducibility experiment. The observed trends in differentiating the regioisomers also were consistent with this group. The 121.0637 *m/z* at 20 eV and the 254.1532 *m/z* at 40 eV were both able to successfully differentiate all three regioisomers from each other.

4.5 Discussion:

Mass spectrometry is the preferred way to confirm the presence of these compounds in forensic toxicology specimens as this methodology provides the sensitivity and selectivity needed to detect the presence of small concentrations of drugs in human matrices. Both gas chromatography mass spectrometry (GC-MS) and liquid chromatography mass spectrometry (LC-MS) methodologies have been employed to confirm the presence of novel psychoactive compounds in previous literature. The identification of compounds using these methodologies rely on retention time and fragmentation patterns. It may be difficult to distinguish structurally similar compounds from each other as they may have similar retention times and/or fragment/product ions using these techniques [172]. The compounds that pose the greatest concern are isobars and isomers as they have the same molecular ion or are undistinguishable thus needing retention time and/or fragmentation patterns to resolve these compounds.

This challenge can be observed in both GC-MS and LC-MS methodology. The use of electron ionization in GC-MS can make the identification of novel psychoactive substances more complicated as typically the molecular ion is not present therefore

structurally similar non-isomeric compounds can produce indistinguishable spectral data. The use of “soft” ionization such as CI, ESI, or APCI can help alleviate this issue as a molecular ion is typically generated using these ionizations techniques. The use of “soft” ionization techniques with spectrometers is the preferred way to confirm the presence of these compounds as molecular ion and product ions may be used to distinguish novel psychoactive compounds from each other.

Examples of this include Inoue et al. evaluating both electron ionization and chemical ionization with tandem mass spectrometry in order to differentiate bromo-amphetamine and bromo-methamphetime regioisomers [161]. They concluded that CI-MS/MS provide positional information that can be used to differentiate the various isomers. Similar results were reported by Westphal et al. in their study with fluoroamphetamine regioisomers and Negishi et al with their study of chloroamphetamine regioisomers [162, 173].

In attempt to explore the usability of relative abundance of the ions of interest in differentiating regioisomers from mass spectral data alone, three experiments were performed on all fifteen sets of regioisomers available in the laboratory. These experiments included reproducibility, concentration, and mobile phase experiments. Four out of the fifteen sets of regioisomers were then subjected to a solid phase extraction experiment as well.

These experiments were designed to simulate common situations encountered during a routine forensic toxicological confirmation analysis utilizing mass spectrometry. First it is imperative that the relative abundance of the ions of interest were reproducible while injecting the same concentration multiple times per day over the course of multiple days.

The concentration experiment was performed to ensure that the relative abundances deemed reproducible from the first experiment are consistent over a broad range of concentrations as drug concentrations in authentic forensic specimens are unknown at the time of screening. The mobile phase experiment was used to evaluate if there was any difference in the relative abundance of the ions of interest in the different mobile phase extremes, 100% aqueous and 100% organic. Lastly, the solid phase extraction experiment was to simulate an actual case work up and used to determine if the same trends from the neat injections applied to the extracted samples. The extract was separated by a LC gradient before being analyzed by the LC-QTOF-MS.

In assessing the different product ions of interest, they were sorted in two categories if the ion could be useful in differentiating a regioisomer. The two categories were unique ions and semi-unique ions. Unique ions are able to be used to differentiate all of the regioisomers in the set based off of the relative abundance. Semi-unique ions are able to differentiate one regioisomer from the remaining regioisomers in the set, however the semi-unique ion cannot differentiate all of the regioisomers in the set from each other. The criteria used to establish unique and semi-unique ions was that the relative abundance average of the ion of interest had to be significantly different between regioisomers in the reproducibility experiment and the relative abundance range of the ion of interest could not overlap between the regioisomers.

All fifteen sets of regioisomers had at least one unique or semi-unique ion of interest that could be used to aid in differentiating regioisomers from each other. The sets of regioisomers that had the largest amount of unique ions were the methylenedioxy pyrovalerone group which had seven unique ions, the methoxy-N,-N-dimethyltryptamine

group which had five unique ions and the RCS-8 group which had five unique ions and one semi-unique ion. The substitution of these regioisomers consisted of a methoxy group (RCS-8) or methylenedioxy group on various positions of an aromatic ring.

The sets of regioisomers that yielded the lowest number of useful ions were the AM 694, fluoroamphetamine, and fluoromethcathinone groups. Each set had just one semi-unique ion that could be used to differentiate one regioisomer from the other compounds in the group. These compounds had an iodine atom (AM-694) or a fluorine atom substituted on various positions of an aromatic ring.

In this experiment the groups of regioisomers that generated those most ions of interest were regioisomers that had an electron donating group substituted around the aromatic ring (methoxy or methylenedioxy). While the groups of regioisomers that generated the least amount of useful ions had an electron withdrawing group substituted around an aromatic ring (halogen). While these trends were consistent with the groups with the most and least amount of useful ions, there were exceptions. For example the JWH 203 set of regioisomers, which has a halogen (Chlorine atom) substituted around an aromatic ring, had three unique ions that could distinguish all three regioisomers from each other and had one semi-unique compound. The semi-unique ion could differentiate the JWH 203 3-chlorophenyl isomer (meta-substitution) from both JWH 203 (ortho-substitution) and the JWH 203 4-chlorophenyl isomers (para-substitution). However, it could not be used to distinguish the JWH 203 from the JWH 203 4-chlorophenyl isomer.

The differences in the relative abundance between regioisomers can be attributed to the differences in structures. While collision induced dissociation fragmentation pathways are not completely known. There have been conclusions deduced based on

physical chemistry computational experiments and observations from experiments utilizing the mass spectrometer. These conclusions include that some ions are favored more than others and more likely to be seen in MS/MS spectra based on the differences in protonation site, bond strength, ion formation, ion stability, steric and kinetic factors [174]. In addition protonation site is also important as this will affect the fragmentation patterns observed. It was reported by Wang et. al that various mobile phase compositions affected the relative abundance observed in various small molecules [175]. They proposed that the reason for this was the change of the ratio of the isomeric cations that were formed in the ESI process. The favored protonation site was different depending on the mobile phase composition.

Also of note was the differences observed in the relative abundance of some ions of interest following the SPE extraction method. These differences in relative abundances could be possibly explained by the different mobile phase composition at the time these compounds came off the analytical compound in comparison to the mobile phase composition of the previous experiments. Such that one protonation site if favored more than the other in the different compositions as suggested by a previous study. Another explanation could suggest that matrix effects may affect protonation. Future studies will be needed to evaluate this.

4.6 Conclusions:

The reproducibility of the relative abundance was evaluated by both inter and intraday experiments, a concentration experiment, and a mobile phase experiment for every set of regioisomers. A solid phase experiment was performed on four of the fifteen groups of regioisomers. It was determined that every set of regioisomers in this study had

at least one unique or semi-unique ion that could be used to help aid in differentiating one regioisomer from the other regioisomers in the group. A few groups of regioisomers had different relative abundance patterns when subjected to different mobile phases, which has been observed previously in experiments analyzing different analytes. In addition, the solid phase extraction experiment generated different relative abundance averages for some ions when compared to the previous experiments.

While MS/MS spectral alone may not be able to be used to distinguish every regioisomer from each other, this study demonstrates that evaluating the regioisomers relative abundance from collision induced dissociation spectral data may be a useful tool when differentiating regioisomers for some groups of regioisomers. This potentially could be used when separation techniques are not employed or when regioisomers are not resolved by a separation technique. Exact analytical conditions need to be known and used before employing this strategy as differences may affect the protonation site favorability of the compound and thus generate differences in the relative abundance of the ions of interest.

5. SOLID PHASE EXTRACTION AND LC-QTOF-MS ACQUISITION METHOD

5.1 Abstract

NPS have been detected and reported in many ante-mortem and post-mortem toxicological investigations. Many of the methods used to identify these substances utilize targeted acquisition methods for a specific NPS drug class. The popularity and use of a particular NPS changes quite frequently. As a result, new psychoactive substances are routinely being identified in drug seizure cases and toxicological investigations. Due to this, an untargeted, comprehensive screening method is needed for the identification of these compounds for toxicological investigations.

Utilizing a liquid chromatography quadrupole time of flight mass spectrometry (LC-QTOF-MS), a SPE method and two acquisition methods were developed in order to detect NPS from multiple NPS classes in human blood specimens. Thirty-three NPS representing the arylcyclohexylamine, cathinone, phenethylamine, and synthetic cannabinoid classes were selected to demonstrate the applicability of these newly developed methods. The limits of detection for these compounds were also determined to range from sub ng/mL to the low ng/mL concentration levels in a human blood matrix for both acquisition methods. Matrix effects and recovery yields were evaluated in this study. It was determined that 26 of the 33 substances displayed ion enhancement or ion suppression of less than 25%. Recovery yields ranged from 18% to 91%, with 20 compounds having recovery yields greater than 50%.

The developed methods can be used in toxicological laboratories as untargeted acquisition methods to detect the presence of NPS in human blood specimens. While the full scan acquisition method was shown to be overall more sensitive, the “All Ions”

acquisition method was more selective, as MS/MS product ions are also generated and used to confirm the presence of a particular NPS. As both methods are non-targeted acquisition methods, the capability of reanalyzing the data without re-extracting blood specimens is possible. This is advantageous as this saves laboratories time and also conserves the blood sample which can be limited in some toxicological investigations.

5.2 Introduction

NPS are psychotropic compounds that are created and/or used to evade current drug laws. NPS are also known as designer drugs, research chemicals, and legal highs. NPS have been categorized by classes which are based on the structure of the compound and/or the intended pharmacological effect of the substance. The classes of NPS include but are not limited to: arylcyclohexylamines, benzodiazepines, cathinones, phenethylamines, piperazines, synthetic cannabinoids, synthetic opioids, and tryptamines.

The capability of identifying NPS in human specimens is necessary in order to perform a comprehensive drug analysis in forensic toxicological investigations where questions of impairment or cause of death questions typically arise. This is due to the fact that there have been reports of acute intoxications involving different NPS classes that are associated with impairment, hospitalization, and death [6, 85, 176-177]. While the reported prevalence of NPS has been low in comparison to traditional drugs of abuse, there may be an underreporting of these compounds as some laboratories do not have analytical methods that capable or not sensitive enough to detect them [178].

The toxicology field is aware of the need to be able to detect NPS and laboratories have created analytical methods to confirm and/or quantitate their presence in human specimens [179]. Various sample pretreatment techniques such as liquid/liquid extraction

(LLE), solid phase extraction (SPE), and “dilute and shoot” have been used in these methods prior to instrumental analysis [136, 138, 180-181]. Analytical methods typical utilize mass spectrometry that is coupled with a separation technique, such as gas chromatography or liquid chromatography, as this provides the necessary selectivity and sensitivity required for detecting analytes of interest in forensic toxicological specimens. Various ionization techniques as well as different mass analyzers, including tandem mass spectrometers, have been employed to confirm the presence of NPS as well [140, 159, 166].

Most of the published methods target a small number of NPS and/or only target a specific structural class [179, 182]. However, there have been some methods that are more comprehensive and some untargeted methods have been published [143]. In addition, both data dependent acquisition and data independent acquisition methods have been used in an attempt to screen for compounds of interest in forensic toxicological investigations.

Due to its capabilities, high resolution time of flight mass spectrometry has gained favor in the forensic toxicology field as a way to detect NPS. High resolution ensures high mass accuracy which enables toxicologists to resolve previously isobaric compounds, which can include endogenous and exogenous compounds, based on accurate mass of the ion alone. This creates more confidence in the identification of a compound. The time of flight mass spectrometer also enables the toxicologist to collect data from a large mass range and while maintaining high sensitivity. The full scan data that is collected can be used to identify new NPS that were previously unknown or

untargeted. The full scan data also enables toxicologists to retrospectively analyze case data for the presence of NPS that were unknown at the time of the analysis.

The aim of this work was to create a comprehensive extraction and acquisition method utilizing HRMS that can be used to identify the presence of NPS in human blood specimens. A set of NPS were selected from various classes to demonstrate the applicability of this method for identifying NPS from different NPS. Various method performance parameters such as limit of detection, matrix effects and recovery percentage were determined for the created method.

5.3 Materials and Methods

5.3.1 Chemicals and reagents

Drug standards were obtained from Cayman Chemical Company (Ann Arbor, MI) and Cerilliant Corporation (Round Rock, TX) as neat weighed solids or as standards in solution. Optima grade methanol (ThermoFisher Scientific) was used to prepare 1 mg/mL stock solutions from the neat standards. For some compounds, dimethyl sulfoxide (ThermoFisher Scientific) was used due to solubility issues encountered with the use of methanol. Standards provided in solution were used as received. All standards were then diluted to a concentration of 10 μg/mL using methanol. Finally, working solutions were created by diluting the 10 μg/mL standards to a concentration of 1 μg/mL with methanol. Solvents used for liquid chromatography included acetonitrile (Optima LC/MS grade) and water (Optima LC/MS grade) from ThermoFisher Scientific. Liquid chromatography additives used included formic acid (Optima LC/MS) from Fisher Scientific and ammonium formate (99%) from Acros Organics.

5.3.2 Instrumentation

Analytical instrumentation included an Agilent 1290 Infinity UHPLC system coupled to an Agilent 6530 Accurate-Mass QTOF MS (Agilent Technologies, Santa Clara, USA). The QTOF-MS was operated in positive-ion electrospray mode with a Jet Stream ESI ionization source.

Agilent MassHunter LC/MS Acquisition software for the 6200 series TOF/6500 series QTOF, MassHunter Qualitative Analysis software, and Mass Hunter Quantitative Analysis software were used to acquire and process the data. MassHunter Personal Computer Database Library (PCDL) Manager software was used as this contained a high resolution MS/MS spectral library and compound database for the novel psychoactive substances of interest.

5.3.3 Sample Pretreatment

A 1 mL aliquot of sample was treated with 1 mL of cold acetonitrile. The sample was then centrifuged at 3500 rpm at -10 C for 10 minutes. The supernatant was transfer to a new clean salinized tube before 2 mL of a 0.1 M ammonium acetate buffer (pH =4.8) was added. The sample was then vortexed and then subjected to a solid phase extraction method utilizing a positive pressure solid phase extraction manifold.

The solid phase extraction method consisted of cartridge conditioning steps of 1 mL of methanol followed by 1 mL of 0.1 M ammonium acetate buffer (pH = 4.8). The sample was then loaded onto the extraction cartridge. Wash steps included 3 mL of the ammonium acetate buffer followed by 3 mL of a solution consisting of 50:50 (*v:v*) deionized water: methanol. The extraction cartridge was then dried under nitrogen gas at max pressure for 5 minutes. The elution step consisted of two 1 mL aliquots of

acetonitrile with 2% ammonium hydroxide. The eluent was collected and dried down under nitrogen gas at 35 C. The sample was then reconstituted with 100 µL of the initial mobile phase composition.

5.3.4 Instrumental Analysis

Two different acquisition methods were used to confirm the presence of novel psychoactive substances. The first method employed a full scan MS acquisition method to acquire spectral data. The second method utilized the "All Ions Mode" acquisition technique to acquire spectral data.

The injection volume was set to 10 µL. An inline filter frit and an Agilent Poroshell 120 EC-C18 (2.1 x 100 mm 2.7 Micron) analytical column were used. Mobile phase A consisted of 5 mM ammonium formate in water with 0.1% formic acid. Mobile phase B consisted of 90:10 (acetonitrile: mobile phase A) with 0.1% formic acid. A LC gradient method was used with the initial mobile phase composition of 5% B. Mobile phase B was then increase to 20% by 1.00 minutes, increased to 70% by 5.00 minutes, and further increased to 100% B by 8.75 minutes. This mobile phase composition was held until 13.00 minutes and at 13.01 minutes the mobile phase composition was returned to 5% B. A 3 minute post time was used to re-equilibrate the column in between injections. The column compartment temperature was set to 40 C.

Both methods utilized a Jet Stream Electrospray ionization source operated in positive mode. The source parameters used included: Gas temperature of 325 C, Gas flow of 8 L/min, Nebulizer was set to 35 psig, Sheath Gas Temperature of 400 C, Sheath Gas Flow of 12 L/min, VCap of 3500 V, Nozzle Voltage of 0V, Fragmentor Voltage of 115

V, Skimmer 1 of 65 V. Reference mass were enabled and used both the 121.0509 m/z and 922.0098 m/z ions to perform real time x-axis recalibration.

The full scan acquisition method used a scan rate of 3 spectra/second and the mass range used was from 25 m/z to 1000 m/z. The All Ions acquisition method also used a scan rate of 3 spectra/second. The mass range was from 50 m/z to 1000 m/z. In addition, the All Ions acquisition method utilized three scan segments that were continuously cycled through the entire method. The only difference in these scan segments was the collision energy which was set to 0 eV, 20 eV, and 40 eV respectively.

5.3.5 Data Analysis

The MassHunter quantitative analysis software was used to process the data for both acquisition methods. The full scan method utilized accurate mass and retention time to identify the analytes of interest. The All Ions acquisition also utilized accurate mass and retention time. In addition, the All Ions acquisition method also used two qualifier ions that were previously determined from the creation of a high resolution MS/MS spectral library for identification purposes. Product ion ratios had to agree within 20% of known standards.

5.3.6 Limit of Detection

The limit of detection for the selected NPS was determined by fortifying a negative blood source at the following concentrations: 0.1 ng/mL, 0.5 ng/mL, 1 ng/mL, 5 ng/mL and 10 ng/mL. Concentrations were prepared in triplicate. The positive identification criteria used for the full scan data included a Gaussian peak shape, retention time within 3% of a 100 ng/mL control sample retention time, and a signal to noise ratio greater than 3. The accurate mass tolerance of the extracted ion chromatogram was set to +/- 20 ppm.

The All Ions acquisition method had the same criteria as the full scan acquisition method with an additional requirement of two product ions that had to have qualifier ratios agreeing within +/- 20 % of the qualifier ratio of the 100 ng/mL control. The reported limit of detection was the concentration where all three concentration replicates successfully met the positive identification criteria for the individual analyte.

5.3.7 Matrix Effects and Recovery

Matrix effects and recovery percentage were determined by analyzing and comparing the peak area of three different experiments performed in triplicate. The first experiment involved fortifying a blood sample with the NPS mix to a final concentration of 100 ng/mL and processing the sample through the solid phase extraction method as described earlier. This experiment was considered the pre-extraction addition experiment. The second and third experiments involved fortifying a solution consisting of the initial mobile phase to a concentration of 1,000 ng/mL. This was the concentration, assuming 100% recovery, of the analytes after being processed by the solid phase extraction method and reconstituted with 100 µL of the initial mobile phase composition solution. In experiment 2, a negative blood sample was processed by the solid phase extraction method as described before with the exception of the reconstitution step. An aliquot of 100 µL of the 1,000 ng/mL solution was added to the sample and replaces the reconstitution step. This experiment was considered the post-extraction addition experiment. The third experiment did not utilize the solid phase extraction method. In this experiment the 1,000 ng/mL solution was directly analyzed by the LC-QTOF-MS and was known as the neat experiment.

All three experiments were analyzed by the LC-QTOF-MS utilizing the full scan MS acquisition method. The peak area of the post-extraction addition experiment was compared to the peak area of the neat experiment to determine the matrix effects. The recovery percentage was determined by comparing the peak area of the pre-extraction addition experiment to the post-extraction addition experiment.

5.4 Results and Discussion

A SPE method and two acquisition methods utilizing a LC-QTOF-MS were developed and optimized in order to successfully identify NPS in human blood. Thirty-three NPS were selected to demonstrate the applicability of this method for identifying compounds from different

Substance	Class	$(M+H)^+$	RT (Min.)	Full Scan LOD (ng/mL)	All Ions LOD (ng/mL)	Matrix Effect	Recovery
2C-C	Phenethylamine	216.0786	2.9	0.5	0.5	-8%	28%
2C-D	Phenethylamine	196.1332	2.8	0.5	0.5	-5%	42%
2C-E	Phenethylamine	210.1489	3.3	0.5	1	-12%	44%
2C-H	Phenethylamine	182.1176	2.3	0.5	0.5	-4%	46%
2C-I	Phenethylamine	308.0142	3.2	0.5	0.5	-6%	34%
2C-N	Phenethylamine	227.1027	2.5	0.5	5	-4%	42%
2C-P	Phenethylamine	224.1645	3.7	1	5	-13%	37%
2C-T-2	Phenethylamine	242.1209	3.2	0.5	1	-6%	40%
2C-T-4	Phenethylamine	256.1366	3.5	0.5	0.5	-9%	40%
3,4-Dimethylmethcathinone	Cathinone	192.1383	2.8	0.1	0.5	-4%	91%
4-MMC	Cathinone	178.1226	2.4	0.1	1	-2%	79%
AKB48	Syn. Cannabinoid	366.2540	10.0	5	5	-8%	75%
AM1220	Syn. Cannabinoid	383.2118	4.4	0.5	5	-40%	56%
AM2201	Syn. Cannabinoid	360.1758	7.2	0.1	0.5	-17%	65%
AM2233	Syn. Cannabinoid	459.0928	4.1	0.5	0.5	-62%	50%
AM694	Syn. Cannabinoid	436.0568	6.8	5	1	-75%	19%
Cannabipiperidiethanone	Syn. Cannabinoid	377.2224	4.0	5	5	-55%	33%
CB-13	Syn. Cannabinoid	369.1849	10.4	5	5	-32%	44%
JWH 018	Syn. Cannabinoid	342.1853	8.3	0.5	1	-16%	68%
JWH 018 adamantyl carboxamide	Syn. Cannabinoid	365.2588	8.7	0.5	5	-7%	80%
JWH 019	Syn. Cannabinoid	356.2009	8.8	0.5	1	-6%	84%
JWH 022	Syn. Cannabinoid	340.1696	7.8	0.5	0.5	-10%	77%
JWH 073	Syn. Cannabinoid	328.1696	7.8	0.5	0.5	-14%	76%
JWH 081	Syn. Cannabinoid	372.1958	8.5	0.1	0.5	-9%	73%
JWH 122	Syn. Cannabinoid	356.2009	8.9	0.5	0.5	-19%	89%

JWH 200	Syn. Cannabinoid	385.1911	4.5	0.5	0.5	-44%	57%
JWH 203	Syn. Cannabinoid	340.1463	8.1	1	5	-36%	49%
JWH 250	Syn. Cannabinoid	336.1958	7.6	0.1	5	-11%	81%
JWH 398	Syn. Cannabinoid	376.1463	9.2	0.5	0.5	-13%	73%
MDPV	Cathinone	276.1594	3.0	0.1	0.5	-4%	80%
Methoxetamine	Arylcyclohexylamine	248.1645	2.7	0.1	0.5	-2%	82%
RCS-4	Syn. Cannabinoid	322.1802	7.4	0.5	5	-17%	70%
RCS-8	Syn. Cannabinoid	376.2271	8.8	0.5	5	-10%	81%

Table 5. The limit of detection (Full scan and All Ion Mode), matrix effect, and recovery percentage of the NPS that were used to evaluate the SPE and acquisition methods.

NPS classes. NPS classes present in the selected group of compounds include arylcyclohexylamine, cathinone, phenethylamines, and synthetic cannabinoids. At the time of development, these compounds were among the most popular NPS and/or recently controlled substances by various governments.

The optimization of the SPE method included modifying a generic basic drug extraction. The SPE sorbent bed consisted of a polymeric mixed mode resin that contained as cation exchanger and hydrophobic regions. Initially, eluents from the various solid phase extraction steps were analyzed to determine at which points analytes were being retained or being lost. Various conditioning steps, sample pretreatments, wash steps, and elution solvents were evaluated and optimized. As the solid phase extraction bed utilized two primary retention mechanisms including ionic bonding and hydrophobic interactions, solvents with varying pH levels and polarities were investigated. In addition to the SPE method, the sample pretreatment step was also optimized by evaluating the addition of buffers with different pH levels and an addition of an acetonitrile crash with different acetonitrile and sample ratios.

The analytical method optimization focused on two major areas. The ionization source parameters and the acquisition mode parameters. Electrospray ionization has been known to be an inefficient ionization technique when compare to other techniques like electron impact ionization, therefore it was necessary to find the optimal source conditions that will yield the most amount of protonated adducts for identification as this can affect sensitivity. Various source parameters were evaluated including: nozzle voltage, drying gas flow rate, nebulizer pressure, sheath gas temperature, fragmentor voltage, and capillary voltage.

The acquisition method optimization included evaluating acquisition rates for both the full scan acquisition and All Ions acquisition methods. The Auto MS/MS acquisition technique was initially evaluated in this stage of the work; however, it was determined that it may not be a practical acquisition mode for toxicological investigations. The data mining was very consuming and the analytes of interest have varying ionization efficiencies make it difficult to set the thresholds needed for the acquisition and data analysis methods. The full scan and All Ions acquisition methods were used in further experiments to evaluate performance.

While many targeted methods have been published and are necessary for quantitation purposes, there lies a need to be able to screen compounds that are unknown. Both methods presented here can be used to accomplish this challenge as both of these methods are non-targeted acquisition methods. The full scan acquisition method was typically more sensitive when compared to the All Ions method. However, the All Ions method was more selective as it provided MS/MS product ions that could be used to further confirm the presence of a NPS.

Another advantage of acquiring untargeted data is the capability of retrospective analysis for the detection of newer NPS in previously analyzed samples. Once a new NPS is identified, data files can be reanalyzed to determine if the NPS is present in cases that were analyzed previously. This saves time and also the limited resource of the sample as a re-extraction is not required. In addition, the stability of many NPS in the various matrices have not been completely evaluated. Therefore, a NPS may be missed if a sample is reanalyzed months or years later if the substance in not stable in the collected matrix.

The limit of detection for the selected compounds was evaluated and determined for each acquisition method. The limit of detections ranged from 0.1 ng/mL to 5 ng/mL for the full scan acquisition method and ranged from 0.5 ng/mL to 5 ng/mL for the All Ions acquisition method. With the exception of AM-694, the limits of detection determined for all of the NPS in the full scan MS acquisition method were either equal to or less than the limits of detection determined using the All Ions acquisition method. The sensitivity displayed by the limit of detection in both of these methods is necessary as some NPS have been demonstrated to be very potent and reported in cases with low ng/mL concentration levels.

Matrix effects were evaluated to determine the extent of ion enhancement and/or ion suppression utilizing this methodology. Slight ion suppression (< 25%) was observed for 26 of the 33 compounds. The seven compounds that exhibited major ion suppression came from the synthetic cannabinoid drug class. The ion suppression for these compounds ranged from 32.1% to 75.4%. Future studies are needed to determine if this suppression is reproducible (RSD <15%) in different sources of the blood matrix. If it is determined to be reproducible than it will satisfy ion enhancement and suppression recommendations proposed by SWGTOX.

Recovery was also determined for each NPS. The recovery yield ranged from 18.7% to 91.2%, with twenty of the thirty-three substances having recoveries greater than a 50% recovery yield. Ideally recoveries for each compound would be closer to a 100%. However, as this method was designed to be as comprehensive as possible, compound recovery percentages may be lower than of other methods that target a specific drug class that have similar chemical properties. AM-694 was the compound that had lowest

recovery percentage of 18.7%. However, AM-694 had limits of detection of 5 and 1 ng/mL for the full scan acquisition method and the All Ions method acquisition method respectively which may be sufficient for identifying AM-694 in toxicological investigations.

5.5 Conclusions

The two acquisition methods that were created are able to successfully identify 33 selected NPS at low or sub ng/mL concentration levels in blood specimens. The limit of detection for these compounds ranged between 0.1 ng/mL to 5 ng/mL and 0.5 ng/mL to 5 ng/mL for the full scan acquisition method and the All Ions acquisition method respectively. While the full scan acquisition method is more sensitive, the All Ions mode provided more selectivity by utilizing product ion ratios in order to further confirm the presence of a NPS. Matrix effects were evaluated and 26 out of the 33 compounds did not exhibit significant ion enhancement or ion suppression. Seven synthetic cannabinoids displayed ion suppression greater than 25%. Further studies are needed to determine if this suppression is reproducible in different sources of the blood matrix.

These two methods can be used in forensic or clinical toxicology laboratories as a way to identify NPS in a human blood sample. As these methods are non-targeted, these methods have the potential to identify new NPS that may be present in a sample. This is advantageous as new NPS appear on the market quite frequently. In addition, retrospective data analysis is also possible with these untargeted methods. Retrospective identification of NPS can be performed without re-extracting the samples.

Future work is needed to further explore the capabilities of these two methods. Ideally a larger set of NPS from the various drug classes will be used to further evaluate the capabilities of this method for the identification of NPS in blood specimens.

6. SUMMARY

If recent drug use trends continue, novel psychoactive substances will burden both forensic and clinical toxicology laboratories for years to come. Currently, resources that are needed in order to successfully screen and confirm these compounds may be too great for some laboratories. However, this issue needs to be addressed as many of these substances have been documented to be very potent, causing severe impairment or even death. The capability of identifying these substances in human performance and post mortem cases is necessary in order for a complete comprehensive toxicological investigation. This project's aim was to help aid the toxicology community in achieving that goal by generating a large high resolution MS/MS spectral library and compound database that contained hundreds of NPS and by creating a method that can used to identify NPS from different drug classes. In addition, a collision induced dissociation study was perform to determine if MS/MS spectral data alone could be used to distinguish even the most difficult NPS, regioisomers.

Recently, mass spectrometry has gained favor over traditional screening techniques such as immunoassays for the identification of NPS. This is mainly due to the fact that developing immunoassays to detect NPS is a time- consuming process and NPSusage changes relatively quickly. In addition, mass spectrometry provides an easily amenable identification technique that achieves the selectivity and sensitivity requirements needed to identify NPS in toxicological samples.

Spectral libraries and compound databases are very useful when screening toxicological specimens by mass spectrometry. These resources can help direct investigations when drug standards are not readily available or when it is cost prohibited

to purchase a large amount of NPS standards. When this data is acquired on a high resolution tandem mass spectrometer such as the LC-QTOF, which was used for this project, the selectivity is increased which enables a greater confidence in the identification of a compound based on accurate mass and MS/MS spectral data. The toxicology laboratory can then focus on these identified compounds in an attempt to confirm the presence of a novel psychoactive substance in a specimen. The MS/MS spectral library and compound database created by this work can help forensic toxicology laboratories save time and resources when trying to identify NPS in human specimens.

In addition to spectral libraries and compound databases, sample preparation techniques are necessary in order to analyze toxicological specimens by mass spectrometry. Recently, there have been simpler extraction methods such as “dilute and shoot” and “protein crash” methods described in literature as liquid chromatography mass spectrometers are able to analyze aqueous samples. Unfortunately, there are drawbacks associated with these methods. The major drawback is the matrix effect phenomenon which is frequently observed in electrospray ionization, a common ionization source used in liquid chromatography mass spectrometry. These extraction techniques typically do not remove as many endogenous and exogenous compounds from the specimen as more intensive extraction methods do. This also leads to more instrument maintenance and shorter analytical column life which results in using more of the laboratory’s resources. This research generated a solid phase extraction method that was able to successfully extract compounds from multiple NPS classes with limit of detections ranging from sub to low ng/mL concentrations. This method removed provided a cleaner and more concentrated extract when compared to the simpler extraction methods.

One of the main advantages of using tandem mass spectrometry is the increased selectivity. In targeted acquisition methods, ions of interest are filtered out before being subjected to ion dissociation. LC-QTOF-MS instrumentation, which couples a quadruple mass analyzer to a time of flight mass analyzer was used for this work. In this instrumentation the collision cell is in-line between the two mass analyzers and ions pass through this cell before entering the time of flight mass analyzer. Collision induced dissociation occurs at varying collision energies in the collision cell which results in product ions which can help elucidate the chemical structure of a precursor ion. This increased selectivity is needed as there are many structurally similar compounds in the NPS classes. While some isobars and isomers can be differentiated by retention time or by MS/MS data, there are some regioisomers which may be difficult to resolve by these means. Another part of this work was to evaluate the differences in relative abundance between regioisomers to determine if MS/MS spectral data alone could be used to differentiate the various regioisomers. The results of this study show that relative abundance of selected product ions could be used to help differentiate some regioisomer sets but not all of the regioisomer sets. This suggests that this is very compound specific.

Future work will be needed as newer NPS appear in the drug market. Libraries and databases will need to be expanded to account for these new compounds. In addition extraction and acquisition methods may need to be modified in order to identify newer NPS in human matrices. The LC-QTOF-MS and other high resolution LC-MS instruments should continue to gain favor as a screening technique over immunoassay based approaches for novel psychoactive substances in human matrices due to the various

advantages of using high resolution mass spectrometry which include but not limited to both high sensitivity and high selectivity.

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APPENDICES

Appendix 1. Compounds included in the compound database.

Common/Street Name	Abbreviation	Chemical Name	CAS Number	Molecular Formula	Structural Class
AM-2201 2'-naphthyl isomer		(1-(5-fluoropentyl)-1H-indol-3-yl)(naphthalen-2-yl)methanone		C24H22FNO	2-Naphthoylindole
JWH-018 2'-naphthyl isomer		naphthalen-2-yl-(1-pentylindol-3-yl)methanone	1131605-25-8	C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(1,1-dimethylpropyl) isomer		(1-(2-methylbutan-2-yl)indol-3-yl)-naphthalen-2-ylmethanone	1869951-99-4	C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(1,2-dimethylpropyl) isomer		(1-(3-methylbutan-2-yl)-1H-indol-3-yl)(naphthalen-2-yl)methanone		C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(1-ethylpropyl)		naphthalen-2-yl-(1-pentan-3-ylindol-3-yl)methanone	1869959-37-4	C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(1-methylbutyl) isomer		naphthalen-2-yl(1-(pentan-2-yl)-1H-indol-3-yl)methanone		C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(2,2-dimethylpropyl) isomer		[1-(2,2-dimethylpropyl)indol-3-yl]-naphthalen-2-ylmethanone	1869954-38-0	C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(2-methylbutyl) isomer		1-(2-methylbutyl)-1H-indol-3-yl)(naphthalen-2-yl) methanone		C24H23NO	2-Naphthoylindole
JWH-018 2'-naphthyl-N-(3-methylbutyl) isomer		(1-isopentyl-1H-indol-3-yl)(naphthalen-2-yl)methanone		C24H23NO	2-Naphthoylindole
JWH-073 2'-naphthyl isomer		(1-butylindol-3-yl)-naphthalen-2-ylmethanone		C23H21NO	2-Naphthoylindole
JWH-073 2'-naphthyl-N-(1,1-dimethylethyl) isomer		(1-(tert-butyl)-1H-indol-3-yl)(naphthalen-2-yl)methanone		C23H21NO	2-Naphthoylindole
JWH-073 2'-naphthyl-N-(1-methylpropyl) isomer		(1-butan-2-ylindol-3-yl)-naphthalen-2-ylmethanone		C23H21NO	2-Naphthoylindole
JWH-073 2'-naphthyl-N-(2-methylpropyl) isomer		[1-(2-methylpropyl)indol-3-yl]-naphthalen-2-ylmethanone		C23H21NO	2-Naphthoylindole
JWH-200 2'-naphthyl isomer		[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-2-naphthalenyl-methanone	133438-66-1	C25H24N2O2	2-Naphthoylindole
5-Fluoro JWH 018 adamantyl analog	5F-AB-001	[1-(5-fluoropentyl)-1H-indol-3-yl]tricyclo[3.3.1.13,7]dec-1-yl-methanone	1364933-62-9	C24H30FNO	Adamantoylindole
AM-1248		[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]tricyclo[3.3.1.13,7]dec-1-yl-methanone	335160-66-2	C26H34N2O	Adamantoylindole
AM-1248 azepane isomer		(3,5,7)-adamantan-1-yl(1-(1-methylazepan-3-yl)-1H-indol-3-yl)methanone		C26H34N2O	Adamantoylindole
JWH-018 adamantyl analog		1-adamantyl-(1-pentylindol-3-yl)methanone	1345973-49-0	C24H31NO	Adamantoylindole
AKB48		1-pentyl-N-tricyclo[3.3.1.13,7]dec-1-yl-1H-indazole-3-carboxamide	1345973-53-6	C23H31N3O	Adamantylindazolecarboxamide
AKB48 N-(4-fluorobenzyl) analog	FUB-AKB48	N-((3s,5s,7s)-adamantan-1-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide		C25H26FN3O	Adamantylindazolecarboxamide

AKB48 N-(5-fluoropentyl) analog	5F-AKB48	N-((3s,5s,7s)-adamantan-1-yl)-1-(5-fluoropentyl)-1H-indazole-3-carboxamide	1400742-13-3	C23H30FN3O	Adamantylindazolecarboxamide
JWH-018 adamantyl carboxamide		1-pentyl-N-tricyclo[3.3.1.13,7]dec-1-yl-1H-indole-3-carboxamide	1345973-50-3	C24H32N2O	Adamantylindolecarboxamide
STS-135		1-(5-fluoropentyl)-N-tricyclo[3.3.1.13,7]dec-1-yl-1H-indole-3-carboxamide	1354631-26-7	C25H34FNO	Adamantylindolecarboxamide
3-Hydroxy eticyclidine	3-HO-PCE	3-[1-(ethylamino)cyclohexyl]phenol		C14H21NO	Arylcyclohexylamine
3-Hydroxy phencyclidine	3-HO-PCP	3-[1-(1-piperidinyl)cyclohexyl]phenol	79787-43-2	C17H25NO	Arylcyclohexylamine
3-Methoxy phencyclidine	3-MeO-PCP	1-[1-(3-methoxyphenyl)cyclohexyl]piperidine	72242-03-6	C18H27NO	Arylcyclohexylamine
4-Methoxy phencyclidine	4-MeO-PCP	1-[1-(4-methoxyphenyl)cyclohexyl]piperidine	2201-35-6	C18H27NO	Arylcyclohexylamine
Benocyclidine	BTPC	1-(1-benzo[b]thien-2-ylcyclohexyl)piperidine	112726-66-6	C19H25NS	Arylcyclohexylamine
Eticyclidine	PCE	N-ethyl phenylcyclohexylamine	2201-15-2	C14H21N	Arylcyclohexylamine
Methoxetamine	MXE	2-(3-methoxyphenyl)-2-(N-ethylamino)cyclohexanone	1239908-48-5	C15H21NO2	Arylcyclohexylamine
PCEEA		N-(1-phenylcyclohexyl)-2-ethoxyethanamine		C16H25NO	Arylcyclohexylamine
PCEPA		N-(1-phenylcyclohexyl)-3-ethoxypropanamine		C17H27NO	Arylcyclohexylamine
PCMEA		N-(1-phenylcyclohexyl)-2-methoxyethanamine		C15H23NO	Arylcyclohexylamine
PCMPA		N-(1-phenylcyclohexyl)-3-methoxypropanamine		C16H25NO	Arylcyclohexylamine
Phencyclamine	PCPr	1-phenyl-N-propyl-cyclohexanamine	18949-81-0	C15H23N	Arylcyclohexylamine
Phencyclidine	PCP	1-(1-phenylcyclohexyl)piperidine	77-10-1	C17H25N	Arylcyclohexylamine
Rolicyclidine	PCPy	1-(1-phenylcyclohexyl)pyrrolidine	2201-39-0	C16H23N	Arylcyclohexylamine
AM-2201 benzimidazole analog	FUBIMINA	(1-(5-fluoropentyl)-1H-benzo[d]imidazol-2-yl)(naphthalen-1-yl)methanone	1984789-90-3	C23H21FN2O	Benzimidazole
JWH-018 benzimidazole analog	BIM-018	naphthalen-1-yl(1-pentyl-1H-benzo[d]imidazol-2-yl)methanone		C23H22N2O	Benzimidazole
MCHB-1		1-(cyclohexylmethyl)-2-[(4-ethoxyphenyl)methyl]-N,N-diethyl-1H-benzimidazole-5-carboxamide	1046140-32-2	C28H37N3O2	Benzimidazole
PF-03550096		N-[(1S)-1-(aminocarbonyl)-2,2-dimethylpropyl]-2,3-dihydro-3-(3-hydroxy-3-methylbutyl)-2-oxo-1H-benzimidazole-1-carboxamide	910376-39-5	C19H28N4O4	Benzimidazole
AM-2233		(2-iodophenyl)[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]methanone	444912-75-8	C22H23IN2O	Benzoylindole
AM-630		(6-iodo-2-methyl-1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl)(4-methoxyphenyl)methanone	164178-33-0	C23H25IN2O3	Benzoylindole
AM-679		(2-iodophenyl)(1-pentyl-1H-indol-3-yl)methanone	335160-91-3	C20H20INO	Benzoylindole
AM-694		[1-(5-fluoropentyl)-1H-indol-3-yl](2-iodophenyl)methanone	335161-03-0	C20H19FINO	Benzoylindole
AM-694 3-iodo isomer		(1-(5-fluoropentyl)-1H-indol-3-yl)(3-iodophenyl)methanone	1427325-91-4	C20H19FINO	Benzoylindole

AM-694 4-iodo isomer		(1-(5-fluoropentyl)-1H-indol-3-yl)(4-iodophenyl)methanone	1427325-92-5	C20H19FINO	Benzoylindole
RCS-4		(4-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone	1345966-78-0	C21H23NO2	Benzoylindole
RCS-4 2-methoxy isomer		(2-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone	1345966-76-8	C21H23NO2	Benzoylindole
RCS-4 3-methoxy isomer		(3-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone	1379922-51-6	C21H23NO2	Benzoylindole
RCS-4 M10 metabolite		(1-(5-hydroxypentyl)-1H-indol-3-yl)(4-hydroxyphenyl)methanone		C20H21NO3	Benzoylindole
RCS-4 M11 metabolite		5-(3-(4-hydroxybenzoyl)-1H-indol-1-yl)pentan-2-one		C20H19NO3	Benzoylindole
RCS-4 M9 metabolite		(1-(4-hydroxypentyl)-1H-indol-3-yl)(4-hydroxyphenyl)methanone		C20H21NO3	Benzoylindole
RCS-4 N-(4-hydroxypentyl) metabolite		(1-(4-hydroxypentyl)-1H-indol-3-yl)(4-methoxyphenyl)methanone	1448893-03-5	C21H33NO3	Benzoylindole
RCS-4 N-(5-carboxypentyl) metabolite		5-(3-(4-methoxybenzoyl)-1H-indol-1-yl)pentanoic acid	1427521-39-8	C21H21NO4	Benzoylindole
RCS-4 N-(5-hydroxypentyl) metabolite		(1-(5-hydroxypentyl)-1H-indol-3-yl)(4-methoxyphenyl)methanone	1379604-66-6	C21H23NO3	Benzoylindole
RCS-4-C4 Homolog		(4-methoxyphenyl)(1-butyl-1H-indol-3-yl)methanone	1345966-77-9	C20H21NO2	Benzoylindole
WIN 48,098	Pravadoline	(4-methoxyphenyl)[2-methyl]-1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-methanone	92623-83-1	C23H26N2O3	Benzoylindole
WIN 54,461		[6-bromo-2-methyl-1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl](4-methoxyphenyl)methanone	166599-63-9	C23H25BrN2O3	Benzoylindole
2,3-Dimethylethcathinone	2,3-DMEC	1-(2,3-dimethylphenyl)-2-(ethylamino)-1-propanone		C13H19NO	Cathinone
2,3-Dimethylmethcathinone	2,3-DMMC	1-(2,3-Dimethylphenyl)-2-(methylamino)-1-propanone		C12H17NO	Cathinone
2,3-Ethylone isomer	2,3-bk-MDEA	1-(benzo[d][1,3]dioxol-4-yl)-2-(ethylamino)-1-propanone		C12H15NO3	Cathinone
2,3-Methylenedioxy Pyrovalerone	2,3-MDPV	1-(benzo[d][1,3]dioxol-4-yl)-2-(piperidin-1-yl)pentan-1-one		C16H21NO3	Cathinone
2,3-Methylenedioxymethcathinone	2,3-MDMC	1-(benzo[d][1,3]dioxol-4-yl)-2-(methylamino)propan-1-one		C11H13NO3	Cathinone
2,3-Pentylone isomer		1-(benzo[d][1,3]dioxol-4-yl)-2-(methylamino)pentan-1-one		C13H17NO3	Cathinone
2,4-Dimethylethcathinone	2,4-DMEC	1-(2,4-dimethylphenyl)-2-(ethylamino)-1-propanone		C13H19NO	Cathinone
2,4-Dimethylmethcathinone	2,4-DMMC	1-(2,4-dimethylphenyl)-2-(methylamino)propan-1-one	1081772-06-6	C12H17NO	Cathinone
2-Ethylethcathinone	2-EEC	2-(ethylamino)-1-(2-ethylphenyl)propan-1-one		C13H19NO	Cathinone
2-Ethylmethcathinone	2-EMC	1-(2-ethylphenyl)-2-(methylamino)propan-1-one		C12H17NO	Cathinone
2-Fluoroethcathinone	2-FEC	2-(ethylamino)-1-(2-fluorophenyl)propan-1-one		C11H14FNO	Cathinone
2-Fluoromethcathinone	2-FMC	1-(2-fluorophenyl)-2-(methylamino)propan-1-one	1186137-35-8	C10H12FNO	Cathinone
2-Methoxymethcathinone	2-MeOMC	1-(2-methoxyphenyl)-2-(methylamino)propan-1-one	882302-55-8	C11H15NO2	Cathinone
2-Methylethcathinone	2-MEC	2-(ethylamino)-1-(o-tolyl)propan-1-one		C12H17NO	Cathinone

2-Methylmethcathinone	2-MMC	2-(methylamino)-1-(2-methylphenyl)propan-1-one	1246911-71-6	C11H15NO	Cathinone
2-Methyl-α-Pyrrolidinobutiophenone	2-MePBP	2-(pyrrolidin-1-yl)-1-(o-tolyl)butan-1-one		C15H21NO	Cathinone
2-Methyl-α-Pyrrolidinopropiophenone		2-(pyrrolidin-1-yl)-1-(o-tolyl)propan-1-one		C14H19NO	Cathinone
3,4-Dimethoxymethcathinone		1-(3,4-dimethoxyphenyl)-2-(methylamino)-1-propanone		C12H17NO3	Cathinone
3,4-Dimethoxy-α-Pyrrolidinohexanophenone	3,4-dimethoxy-α-PHP	1-(3,4-dimethoxyphenyl)-2-(pyrrolidin-1-yl)hexan-1-one		C18H27NO3	Cathinone
3,4-Dimethoxy-α-Pyrrolidinopentiophenone	3,4-Dimethoxy-α-PVP	1-(3,4-dimethoxyphenyl)-2-(1-pyrrolidinyl)pentan-1-one	850442-84-1	C17H25NO3	Cathinone
3,4-Dimethylethcathinone	3,4-DMEC	1-(3,4-dimethylphenyl)-2-(ethylamino)propan-1-one	1225811-81-3	C13H19NO	Cathinone
3,4-Dimethylmethcathinone	3,4-DMMC	1-(3,4-dimethylphenyl)-2-(methylamino)propan-1-one	1082110-00-6	C12H17NO	Cathinone
3,4-Ethylenedioxymethcathinone	bk-EDMA, 3,4-EDMC	1-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(methylamino)-1-propanone		C12H15NO3	Cathinone
3,4-Methylenedioxy-5-methylethcathinone		2-(ethylamino)-1-(7-methyl-1,3-benzodioxol-5-yl)-1-propanone		C13H17NO3	Cathinone
3,4-Methylenedioxy-N-benzylcathinone	BMDP	1-(1,3-benzodioxol-5-yl)-2-(phenylamino)propan-1-one	1357477-43-0	C16H15NO3	Cathinone
3,4-Methylenedioxy-PV8		1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1-heptanone		C18H25NO3	Cathinone
3,4-Methylenedioxypyrovalerone	MDPV	1-(1,3-benzodioxol-5-yl)-2-pyrrolidin-1-yl-pentan-1-one	687603-66-3	C16H21NO3	Cathinone
3,4-Methylenedioxy-α-pyrrolidinobutyrophenone	MDPBP	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)butan-1-one	784985-33-7	C15H19NO3	Cathinone
3,4-Methylenedioxy-α-Pyrrolidinohexanophenone	3,4-MDPHP	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1hexanone		C17H23NO3	Cathinone
3,4-Methylenedioxy-α-pyrrolidinopropiophenone	MDPPP	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)propan-1-one	783241-66-7	C14H17NO3	Cathinone
3,4-Tetramethylene-α-Pyrrolidinovalerophenone	TH-PVP	2-(pyrrolidin-1-yl)-1-(5,6,7,8-tetrahydronaphthalen-2-yl)pentan-1-one		C19H27NO	Cathinone
3,4-Trimethylene-α-Ethylaminovalerophenone	bk-IVP	1-(2,3-dihydro-1H-inden-5-yl)-2-(ethylamino)pentan-1-one		C16H23NO	Cathinone
3,4-Trimethylene-α-Pyrrolidinohexanophenone	5-BPDi	1-(2,3-dihydro-1H-inden-5-yl)-2-(pyrrolidin-1-yl)hexan-1-one		C19H27NO	Cathinone
3-Bromomethcathinone	3-BMC	1-(3-bromophenyl)-2-(methylamino)propan-1-one	486459-02-3	C10H12BrNO	Cathinone
3-Chloromethcathinone	3-CMC	1-(3-chlorophenyl)-2-(methylamino)-1-propanone		C10H12ClNO	Cathinone
3-Desoxy-3,4-Methylenedioxy Pyrovalerone	5-DBFPV	1-(2,3-dihydrobenzofuran-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one		C17H23NO2	Cathinone
3-Ethylethcathinone	3-EEC	2-(ethylamino)-1-(3-ethylphenyl)propan-1-one		C13H19NO	Cathinone
3-Ethylmethcathinone	3-EMC	1-(3-ethylphenyl)-2-(methylamino)propan-1-one		C12H17NO	Cathinone
3-Fluoroethcathinone	3-FEC	2-(ethylamino)-1-(3-fluorophenyl)propan-1-one		C11H14FNO	Cathinone
3-Fluoromethcathinone	3-FMC	1-(3-fluorophenyl)-2-(methylamino)propan-1-one	1049677-77-1	C10H12FNO	Cathinone
3-Fluoro-α-Pyrrolidinopropiophenone	3-fluoro-α-PPP	1-(3-fluorophenyl)-2-(1-pyrrolidinyl)-1-propanone		C13H16FNO	Cathinone

3-Methoxymethcathinone	3-MeOMC	1-(3-methoxyphenyl)-2-(methylamino)propan-1-one	882302-56-9	C11H15NO2	Cathinone
3-Methylbuphedrone	3-methyl BP	2-(methylamino)-1-(m-tolyl)butan-1-one		C12H17NO	Cathinone
3-Methylethcathinone	3-MEC	2-(ethylamino)-1-(m-tolyl)propan-1-one		C12H17NO	Cathinone
3-Methylmethcathinone	3-MMC	2-(methylamino)-1-(3-methylphenyl)propan-1-one	1246911-86-3	C11H15NO	Cathinone
3-Methyl-α-Pyrrolidinobutiophenone	3-MePBP	2-(pyrrolidin-1-yl)-1-(m-tolyl)butan-1-one		C15H21NO	Cathinone
4-Bromomethcathinone	4-BMC	1-(4-bromophenyl)-2-(methylamino)propan-1-one	486459-03-4	C10H12BrNO	Cathinone
4-Chloromethcathinone	4-CMC	1-(4-chlorophenyl)-2-(methylamino)-1-propanone		C10H12ClNO	Cathinone
4-Chloro-α-Pyrrolidinopropiophenone	4-chloro PPP	1-(4-chlorophenyl)-2-(1-pyrrolidinyl)-1-propanone		C13H16ClNO	Cathinone
4-Ethylcathinone	4-EC	2-amino-1-(4-ethylphenyl)propan-1-one	805951-15-9	C11H15NO	Cathinone
4-Ethylethcathinone	4-EEC	2-(ethylamino)-1-(4-ethylphenyl)propan-1-one	1225619-32-8	C13H19NO	Cathinone
4-Ethylmethcathinone	4-EMC	1-(4-ethylphenyl)-2-(methylamino)propan-1-one	1225622-14-9	C12H17NO	Cathinone
4-Ethyl-N,N-dimethylcathinone		2-(dimethylamino)-1-(4-ethylphenyl)propan-1-one	1157738-27-6	C13H19NO	Cathinone
4-Fluoro Pentedrone	4-FPD	1-(4-fluorophenyl)-2-(methylamino)pentan-1-one		C12H16FNO	Cathinone
4-Fluoro PV8	4-fluoro α-PHPP	1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)heptan-1-one,		C17H24FNO	Cathinone
4-Fluoro PV8 piperidine analog		1-(4-fluorophenyl)-2-(piperidin-1-yl)heptan-1-one		C18H26FNO	Cathinone
4-Fluoro PV9	para-fluoro-PV9	1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)octan-1-one		C18H26FNO	Cathinone
4-Fluoro-(methylamino)butyrophenone	4-F-MABP, 4-FBP	1-(4-fluorophenyl)-2-(methylamino)butan-1-one	1368599-12-5	C11H14FNO	Cathinone
4-Fluoroethcathinone	4-FEC	2-(ethylamino)-1-(4-fluorophenyl)propan-1-one	1225625-74-0	C11H14FNO	Cathinone
4-Fluoromethcathinone	4-FMC	1-(4-fluorophenyl)-2-(methylamino)propan-1-one	7589-35-7	C10H12FNO	Cathinone
4-Fluoro-N-Isopropyl-Pentedrone	4-fluoro NPP	1-(4-fluorophenyl)-2-(isopropylamino)pentan-1-one		C14H20FNO	Cathinone
4-Fluoro-α-Pyrrolidinobutiophenone	4-fluoro PBP	1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)butan-1-one		C14H18FNO	Cathinone
4-Fluoro-α-Pyrrolidinopentiophenone	4-fluoro-α-PVP	1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-pentanone		C15H20FNO	Cathinone
4-Fluoro-α-Pyrrolidinopropiophenone	4-fluoro-α-PPP	1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-propanone		C13H16FNO	Cathinone
4-Methoxy PV8		1-(4-methoxyphenyl)-2-(pyrrolidin-1-yl)heptan-1-one		C18H27NO2	Cathinone
4-Methoxy PV9		1-(4-methoxyphenyl)-2-(pyrrolidin-1-yl)octan-1-one		C19H29NO2	Cathinone
4-Methoxy-N,N-Dimethylcathinone		2-(dimethylamino)-1-(4-methoxyphenyl)-1-propanone		C12H17NO2	Cathinone
4-Methoxy-α-Pyrrolidinobutiophenone	4-MeOPBP	1-(4-methoxyphenyl)-2-(pyrrolidin-1-yl)butan-1-one		C15H21NO2	Cathinone
4-Methoxy-α-Pyrrolidinopentiophenone	4-MeO-α-PVP	1-(4-methoxyphenyl)-2-(1-pyrrolidinyl)-1-pentanone		C16H23NO2	Cathinone

4-Methoxy-α-pyrrolidinopropiophenone	4-MeO-α-PPP	1-(4-methoxyphenyl)-2-(1-pyrrolidinyl)-1-propanone	478243-09-3	C14H19NO2	Cathinone
4-Methyl Pentedrone	4-MPD	2-(methylamino)-1-(p-tolyl)pentan-1-one		C13H19NO	Cathinone
4-Methylbuphedrone	4-MeBP	2-(methylamino)-1-(4-methylphenyl)butan-1-one	1337016-51-9	C12H17NO	Cathinone
4-Methylethcathinone	4-MEC	2-(ethylamino)-1-(4-methylphenyl)propan-1-one	1225617-18-4	C12H17NO	Cathinone
4-Methylmethcathinone	4-MMC	2-(methylamino)-1-(4-methylphenyl)propan-1-one	1189726-22-4	C11H15NO	Cathinone
4-Methyl-N,N-Dimethylcathinone	4-methyl-N,N-DMC	2-(dimethylamino)-1-(4-methylphenyl)-1-propanone		C12H17NO	Cathinone
4-Methyl-N-Methylbuphedrone		2-(dimethylamino)-1-(p-tolyl)butan-1-one		C13H19NO	Cathinone
4-Methyl-N-methylhexanophenone		2-(methylamino)-1-(p-tolyl)hexan-1-one		C14H21NO	Cathinone
4-Methyl-α-ethylaminobutiophenone		2-(ethylamino)-1-(4-methylphenyl)-1-butanone		C13H19NO	Cathinone
4-Methyl-α-ethylaminopentiophenone		2-(ethylamino)-1-(4-methylphenyl)-1-pentanone		C14H21NO	Cathinone
4-Methyl-α-pyrrolidinobutiophenone	MPBP	1-(4-methylphenyl)-2-(1-pyrrolidinyl)butan-1-one	732180-91-5	C15H21NO	Cathinone
4-Methyl-α-Pyrrolidinobutiophenone		1-(4-methylphenyl)-2-(1-pyrrolidinyl)-1-butanone		C15H21NO	Cathinone
4-Methyl-α-pyrrolidinohexanophenone	4-MePHP	2-(pyrrolidin-1-yl)-1-(p-tolyl)hexan-1-one	34138-58-4	C17H25NO	Cathinone
4-Methyl-α-Pyrrolidinohexanophenone	4-methyl-α-PHP	2-(pyrrolidin-1-yl)-1-(p-tolyl)hexan-1-one		C17H25NO	Cathinone
4-Methyl-α-pyrrolidinopropiophenone	4-MePPP	1-(4-methylphenyl)-2-(1-pyrrolidinyl)propan-1-one	28117-80-8	C14H19NO	Cathinone
4-Methyl-α-Pyrrolidinopropiophenone	4-methyl PPP	2-(pyrrolidin-1-yl)-1-(p-tolyl)propan-1-one		C14H19NO	Cathinone
5-Methoxy Methylone		1-(7-methoxybenzo[d][1,3]dioxol-5-yl)-2-(methylamino)propan-1-one		C12H15NO4	Cathinone
6-Methoxy Methylone		1-(6-methoxybenzo[d][1,3]dioxol-5-yl)-2-(methylamino)propan-1-one		C12H15NO4	Cathinone
7-MAPB		1-(benzofuran-7-yl)-N-methylpropan-2-amine		C12H15NO	Cathinone
Benzedrone	4-MBC	2-(benzylamino)-1-(p-tolyl)propan-1-one	1225617-75-3	C17H19NO	Cathinone
Benzedrone		1-(4-methylphenyl)-2-[(phenylmethyl)amino]-1-propanone		C17H19NO	Cathinone
bk-2C-B		2-amino-1-(4-bromo-2,5-dimethoxyphenyl)-ethanone		C10H12BrNO3	Cathinone
bk-EABDI	bk-IBP	1-(2,3-dihydro-1H-inden-5-yl)-2-(ethylamino)butan-1-one		C15H21NO	Cathinone
Buphedrone	MABP	2-(methylamino)-1-phenylbutan-1-one	408332-79-6	C11H15NO	Cathinone
Butylone	bk-MBDB	1-(1,3-benzodioxol-5-yl)-2-(methylamino)butan-1-one	802575-11-7	C12H15NO3	Cathinone
Cathinone		(2S)-2-amino-1-phenylpropan-1-one	71031-15-7	C9H11NO	Cathinone
Dibutylone	bk-DMBDB	1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)butan-1-one	802286-83-5	C13H17NO3	Cathinone
Dimethylone	bk-MDDMA	1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)propan-1-one	765231-58-1	C12H15NO3	Cathinone

DL-4662		1-(3,4-dimethoxyphenyl)-2-(ethylamino)pentan-1-one		C15H23NO3	Cathinone
Ethcathinone	ETH-CAT	2-ethylamino-1-phenyl-propan-1-one	18259-37-5	C11H15NO	Cathinone
Ethylone	MDEC, bk-MDEA	1-(1,3-benzodioxol-5-yl)-2-(ethylamino)propan-1-one	1112937-64-0	C12H15NO3	Cathinone
Eutylone	bk-EBDB	1-(1,3-benzodioxol-5-yl)-2-(ethylamino)butan-1-one	802855-66-9	C13H17NO3	Cathinone
Methcathinone	M-CAT	2-(methylamino)-1-phenylpropan-1-one	5650-44-2	C10H13NO	Cathinone
Methedrone	PMMC, bk-PMMA	1-(4-methoxyphenyl)-2-(methylamino)propan-1-one	530-54-1	C11H15NO2	Cathinone
Methylbuphedrone	3-MeBP	2-(methylamino)-1-(m-tolyl)butan-1-one		C12H17NO	Cathinone
Methylone	MDMC, bk-MDMA	1-(1,3-benzodioxol-5-yl)-2-(methylamino)propan-1-one	186028-79-5	C11H13NO3	Cathinone
N,N-Diethylcathinone		2-(diethylamino)-1-phenyl-1-propanone	90-84-6	C13H19NO	Cathinone
N,N-Dimethylcathinone		2-(dimethylamino)-1-phenyl-1-propanone	15351-09-4	C11H15NO	Cathinone
N,N-Dimethylpentylone	bk-DMBDP	1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)-1-pentanone		C14H19NO3	Cathinone
N-Acetyl-3,4-Methylenedioxymethcathinone	N-acetyl-3,4-MDMC	N-[2-(1,3-benzodioxol-5-yl)-1-methyl-2-oxoethyl]-N-methyl-acetamide		C13H15NO4	Cathinone
Naphyrone		1-(naphthalen-2-yl)-2-(pyrrolidin-1-yl)pentan-1-one	850352-53-3	C19H23NO	Cathinone
Naphyrone 1-naphthyl isomer		1-(naphthalen-1-yl)-2-(pyrrolidin-1-yl)pentan-1-one	1349245-31-3	C19H23NO	Cathinone
N-Ethylbuphedrone	NEB	2-(ethylamino)-1-phenylbutan-1-one		C12H17NO	Cathinone
N-Ethyl-N-Methylcathinone		2-(ethyl(methyl)amino)-1-phenylpropan-1-one		C12H17NO	Cathinone
N-Ethylpentylone		1-(1,3-benzodioxol-5-yl)-2-(ethylamino)-1-pentanone		C14H19NO3	Cathinone
nor-Mephedrone		2-amino-1-(4-methylphenyl)propan-1-one	31952-47-3	C10H13NO	Cathinone
NRG-3		2-(methylamino)-1-(naphthalen-2-yl)pentan-1-one		C16H19NO	Cathinone
Pentedrone		2-(methylamino)-1-phenyl-pentan-1-one	879722-57-3	C12H17NO	Cathinone
Pentylone	bk-MBDP	1-(1,3-benzodioxol-5-yl)-2-(methylamino)pentan-1-one	698963-77-8	C13H17NO3	Cathinone
PV8		1-phenyl-2-(1-pyrrolidinyl)-1-heptanone		C17H25NO	Cathinone
PV9		1-phenyl-2-(pyrrolidin-1-yl)octan-1-one		C18H27NO	Cathinone
Pyrovalerone		1-(4-methylphenyl)-2-(1-pyrrolidinyl)pentan-1-one	3563-49-3	C16H23NO	Cathinone
α-Dimethylaminopentiophenone		2-(dimethylamino)-1-phenyl-1-pentanone		C13H19NO	Cathinone
α-Ethylaminopentiophenone		2-(ethylamino)-1-phenyl-1-pentanone		C13H19NO	Cathinone
α-Methylaminohexanophenone		2-(methylamino)-1-phenylhexan-1-one		C13H19NO	Cathinone
α-Phthalimidopropiophenone	α-PAPP	2-(1-methyl-2-oxo-2-phenylethyl)-1H-isoindole-1,3(2H)-dione		C17H13NO3	Cathinone

α-Piperidinobutiophenone	α-PipBP	1-phenyl-2-(1-piperidinyl)-1-butanone		C15H21NO	Cathinone
α-Propylaminopentiophenone	N-Propylpentedrone	1-phenyl-2-(propylamino)-1-pentanone		C14H21NO	Cathinone
α-Pyrrolidinobutiophenone	α-PBP	1-phenyl-2-(1-pyrrolidinyl)butan-1-one	13415-82-2	C14H19NO	Cathinone
α-Pyrrolidinopentiophenone	α-PVP	1-phenyl-2-(1-pyrrolidinyl)pentan-1-one	14530-33-7	C15H21NO	Cathinone
α-Pyrrolidinopentiothiophenone	a-PVT	2-(pyrrolidin-1-yl)-1-(thiophen-2-yl)pentan-1-one		C13H19NOS	Cathinone
α-Pyrrolidinopropiophenone	α-PPP	1-phenyl-2-(1-pyrrolidinyl)propan-1-one	19134-50-0	C13H17NO	Cathinone
CP 47,497		2-(3-hydroxycyclohexyl)-5-(2-methyl-2-octanyl)phenol	70434-82-1	C21H34O2	Cyclohexylphenol
CP 47,497 epimer		rel-2[(1S,3S)-3-hydroxycyclohexyl)]-5-(2-methyloctan-2-yl)phenol		C21H34O2	Cyclohexylphenol
CP 47,497-C7-hydroxy metabolite		5-(8-hydroxy-2-methyloctan-2-yl)-2-((1S,3R)-3-hydroxycyclohexyl)phenol	1554485-44-7	C21H34O3	Cyclohexylphenol
CP 47,497-C8-homolog		2-(3-hydroxycyclohexyl)-5-(2-methylnonan-2-yl)phenol	70434-92-3	C22H36O2	Cyclohexylphenol
CP 47,497-C8-homolog 3-epimer		rel-2-[(1S,3S)-3-hydroxycyclohexyl)]-5-(2-methylnonan-2-yl)phenol		C22H36O2	Cyclohexylphenol
CP 47,497-C8-homolog C8-hydroxy metabolite		5-(9-hydroxy-2-methylnonan-2-yl)-2-((1S,3R)-3-hydroxycyclohexyl)phenol	1554485-48-1	C22H36O3	Cyclohexylphenol
CP 47,497-para-quinone analog		3R-hydroxy-4-(2-methyloctan-2-yl)-[1,1S-bi(cyclohexane)]-3,6-diene-2,5-dione		C21H32O3	Cyclohexylphenol
CP 50,556-1		[(6S,6aR,9R,10aR)- 9-hydroxy- 6-methyl- 3-[(2R)-5-phenylpentan- 2-yl]oxy- 5,6,6a,7,8,9,10,10a-octahydrophenanthridin- 1-yl] acetate	71048-87-8	C27H35NO4	Cyclohexylphenol
CP 55,244		(2S,4S,4aS,6R,8aR)-6-(hydroxymethyl)-4-[2-hydroxy-4-(2-methyloctan-2-yl)phenyl]-1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalen-2-ol	79678-32-3	C26H42O3	Cyclohexylphenol
CP 55,940		2-[(1S,2R,5S)-5-hydroxy-2-(3-hydroxypropyl)cyclohexyl]-5-(2-methyl-2-octanyl)phenol	83002-04-4	C24H40O3	Cyclohexylphenol
CP 55,940 5-epimer		rel-2-((1R,2R,5S)-5-hydroxy-2-(3-hydroxypropyl)cyclohexyl)-5-(2-methyloctan-2-yl)phenol		C24H40O3	Cyclohexylphenol
FAB-144		(1-(5-fluoropentyl)-1H-indazol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C20H27FN2O	Cyclopropanoylindazole
A-796,260		[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)methanone	895155-26-7	C22H30N2O2	Cyclopropanoylindole
A-834,735		[1-[(tetrahydro-2H-pyran-4-yl)methyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)methanone	895155-57-4	C22H29NO2	Cyclopropanoylindole
AB-005		[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)-methanone	895155-25-6	C23H32N2O	Cyclopropanoylindole
FUB-144	FUB-UR-144	(1-(4-fluorobenzyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C23H24FNO	Cyclopropanoylindole
MDMB-CHMICA	MMB-CHMINACA	methyl (S)-2-(1-(cyclohexylmethyl)-1H-indole-3-carboxamido)-3,3-dimethylbutanoate		C23H32N2O3	Cyclopropanoylindole
UR-144		(1-pentyl-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone	1199943-44-6	C21H29NO	Cyclopropanoylindole

UR-144 N-(2-chloropentyl) analog		(1-(2-chloropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C21H28ClNO	Cyclopropanoylindole
UR-144 N-(3-chloropentyl) analog		(1-(3-chloropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C21H28ClNO	Cyclopropanoylindole
UR-144 N-(5-bromopentyl) analog		(1-(5-bromopentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C21H28BrNO	Cyclopropanoylindole
UR-144 N-(5-chloropentyl) analog		(1-(5-chloropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone	1445577-42-3	C21H28ClNO	Cyclopropanoylindole
UR-144 N-(5-methylhexyl) analog		(1-(5-methylhexyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C23H33NO	Cyclopropanoylindole
UR-144 N-heptyl analog		(1-heptyl-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C23H33NO	Cyclopropanoylindole
XLR-11		(1-(5-fluoropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone	1364933-54-9	C21H28FNO	Cyclopropanoylindole
XLR-11 N-(2-fluoropentyl) isomer		(1-(2-fluoropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C21H28FNO	Cyclopropanoylindole
XLR-11 N-(3-fluoropentyl) isomer		(1-(3-fluoropentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C21H28FNO	Cyclopropanoylindole
XLR-11 N-(4-hydroxypentyl) metabolite		(1-(5-fluoro-4-hydroxypentyl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C21H28FNO2	Cyclopropanoylindole
XLR11 N-(4-pentenyl) analog		(1-(pent-4-en-1-yl)-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone	1445578-20-0	C21H27NO	Cyclopropanoylindole
XLR12		(2,2,3,3-tetramethylcyclopropyl)[1-(4,4,4-trifluorobutyl)-1H-indol-3-yl]-methanone	895155-78-9	C20H24F3NO	Cyclopropanoylindole
1-Aminoindane		2,3-dihydro-1H-inden-1-amine	34698-41-4	C9H11N	Indane
2-Aminoindane	2-AI	2,3-dihydro-1H-inden-2-amine	2975-41-9	C9H11N	Indane
5-(2-Aminopropyl)-2,3-dihydro-1H-indene	5-APDI	1-(2,3-dihydro-1H-inden-5-yl)propan-2-amine	152624-02-7	C12H17N	Indane
5,6-Methylenedioxy-2-aminoindane	MDAI	6,7-dihydro-5H-cyclopenta[f][1,3]benzodioxol-6-amine	132741-81-2	C10H11NO2	Indane
5-Iodo-2-aminoindane	5-IAI	5-iodo-2,3-dihydro-1H-inden-2-amine	132367-76-1	C9H10IN	Indane
5-Methoxy-6-methyl-2-aminoindane	MMAI	2,3-dihydro-5-methoxy-6-methyl-1H-inden-2-amine	132980-16-6	C11H15NO	Indane
5-Chloro AB-PINACA		N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-chloropentyl)-1H-indazole-3-carboxamide	1801552-02-2	C18H25ClN4O2	Indazole
5-Fluoro ABICA		N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-fluoropentyl)-1H-indole-3-carboxamide	1801338-26-0	C19H26FN3O2	Indazole
5-Fluoro AB-PINACA		N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-fluoropentyl)-1H-indazole-3-carboxamide	1800101-60-3	C18H25FN4O2	Indazole
5-Fluoro ADB	5-fluoro MDMB-PINACA	methyl (R)-2-(1-(5-fluoropentyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate		C20H28FN3O3	Indazole
5-Fluoro ADB-PINACA		N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(5-fluoropentyl)-1H-indazole-3-carboxamide		C19H27FN4O2	Indazole
5-Fluoro AEB	5F-EMB-PINACA	ethyl (1-(5-fluoropentyl)-1H-indazole-3-carbonyl)-L-valinate		C20H28FN3O3	Indazole
5-Fluoro AMB	5-fluoro AMP	N-[[1-(5-fluoropentyl)-1H-indazol-3-yl]carbonyl]-L-valine, methyl ester	1801552-03-3	C19H26FN3O3	Indazole
5-Fluoro CUMYL-PINACA		1-(5-fluoropentyl)-N-(1-methyl-1-phenylethyl)-1H-indazole-3-carboxamide	1400742-16-6	C22H26FN3O	Indazole

5-Fluoro MN-18		1-(5-fluoropentyl)-N-1-naphthalenyl-1H-indazole-3-carboxamide	1445581-91-8	C23H22FN3O	Indazole
5-Fluoro NPB-22		1-(5-fluoropentyl)-8-quinolinyl ester-1H-indazole-3-carboxylic acid	1445579-79-2	C22H20FN3O2	Indazole
5-Fluoro SDB-005		naphthalen-1-yl 1-(5-fluoropentyl)-1H-indazole-3-carboxylate		C23H21FN2O2	Indazole
5-Fluoro THJ		1-(5-fluoropentyl)-N-(quinolin-8-yl)-1H-indazole-3-carboxamide		C22H21FN4O	Indazole
AB-CHMINACA		N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(cyclohexylmethyl)-1H-indazole-3-carboxamide	1185887-21-1	C20H28N4O2	Indazole
AB-FUBINACA		N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxamide	1185282-01-2	C20H21FN4O2	Indazole
AB-PINACA		(S)-N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1H-indazole-3-carboxamide	1445752-09-9	C18H26N4O2	Indazole
ADB-FUBINACA		N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxamide	1445583-51-6	C21H23FN4O2	Indazole
ADB-PINACA		N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-pentyl-1H-indazole-3-carboxamide	1633766-73-0	C19H28N4O2	Indazole
AMB	AMP	methyl (1-pentyl-1H-indazole-3-carbonyl)-L-valinate		C19H27N3O3	Indazole
APP-CHMINACA	PX 3	N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-1-(cyclohexylmethyl)-1H-Indazole-3-carboxamide	1185887-14-2	C24H28N4O2	Indazole
APP-FUBINACA		N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxamide	1185282-03-4	C24H21FN4O2	Indazole
CUMYL-THPINACA		N-(1-methyl-1-phenylethyl)-1-[(tetrahydro-2H-pyran-4-yl)methyl]-1H-indazole-3-carboxamide	1400742-50-8	C23H27N3O2	Indazole
FUB-AMB	AMB-FUBINACA	methyl (1-(4-fluorobenzyl)-1H-indazole-3-carbonyl)-L-valinate		C21H22FN3O3	Indazole
FUB-NPB-22	5-fluoro NIN	quinolin-8-yl 1-(4-fluorobenzyl)-1H-indazole-3-carboxylate		C24H16FN3O2	Indazole
M-144	XLR11 2-methylindole analog	(1-(5-fluoropentyl)-2-methyl-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone		C22H30FNO	Indazole
MAB-CHMINACA	ADB-CHMINACA	N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indazole-3-carboxamide		C21H30N4O2	Indazole
MA-CHMINACA	AMB-CHMINACA	methyl (1-(cyclohexylmethyl)-1H-indazole-3-carbonyl)-L-valinate		C21H29N3O3	Indazole
MDMB-CHMINACA		N-[[1-(cyclohexylmethyl)-1H-indazol-3-yl]carbonyl]-3-methyl-L-valine, methyl ester	1185888-32-7	C22H31N3O3	Indazole
MDMB-FUBINACA	FUB-MDMB	methyl (S)-2-(1-(4-fluorobenzyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate		C22H24FN3O3	Indazole
MN-18		N-1-naphthalenyl-1-pentyl-1H-indazole-3-carboxamide	1391484-80-2	C23H23N3O	Indazole
MO-CHMINACA	MO-AMB	1-methoxy-3,3-dimethyl-1-oxobutan-2-yl 1-(cyclohexylmethyl)-1H-indazole-3-carboxylate		C22H30N2O4	Indazole
NPB-22		1-pentyl-1H-indazole-3-carboxylic acid, 8-quinolinyl ester	1445579-61-2	C22H21N3O2	Indazole
SDB-005		naphthalen-1-yl 1-pentyl-1H-indazole-3-carboxylate		C23H22N2O2	Indazole
THJ		1-pentyl-N-(quinolin-8-yl)-1H-indazole-3-carboxamide		C22H22N4O	Indazole

5-Chloro NNEI	5-chloro MN-24	1-(5-chloropentyl)-N-(naphthalen-1-yl)-1H-indole-3-carboxamide		C24H23ClN2O	Indole
5-Fluoro ADBICA		N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-(5-fluoropentyl)-1H-indole-3-carboxamide	1863065-82-0	C20H28FN3O2	Indole
5-Fluoro CUMYL-PICA		1-(5-fluoropentyl)-N-(1-methyl-1-phenylethyl)-1H-indole-3-carboxamide	1400742-18-8	C23H27FN2O	Indole
5-Fluoro NNEI	5-fluoro MN-24	1-(5-fluoropentyl)-N-(naphthalen-1-yl)-1H-indole-3-carboxamide	1445580-60-8	C24H23FN2O	Indole
5-Fluoro PB-22	5-fluoro QUPIC	1-(5-fluoropentyl)-8-quinolinyl ester-1H-indole-3-carboxylic acid	1400742-41-7	C23H21FN2O2	Indole
5-Fluoro SDB-006		N-benzyl-1-(5-fluoropentyl)-1H-indole-3-carboxamide		C21H23FN2O	Indole
5-Fluoropentyl-3-pyridinoylindole		(1-(5-fluoropentyl)-1H-indol-3-yl)(pyridin-3-yl)methanone		C19H19FN2O	Indole
AB-CHMICA		(S)-N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indole-3-carboxamide		C21H29N3O2	Indole
ADB-CHMICA	MAB-CHMICA	N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indole-3-carboxamide		C22H31N3O2	Indole
ADBICA		N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1H-indole-3-carboxamide	1445583-48-1	C20H29N3O2	Indole
AM-1241		(2-iodo-5-nitrophenyl)(1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl)methanone	444912-48-5	C22H22IN3O3	Indole
AM2201 8-quinolinyl carboxamide		1-(5-fluoropentyl)-N-(quinolin-8-yl)-1H-indole-3-carboxamide		C23H22FN3O	Indole
APP-PICA		(S)-N-(1-amino-1-oxo-3-phenylpropan-2-yl)-1-pentyl-1H-indole-3-carboxamide		C23H27N3O2	Indole
BB-22	QUCHIC	1-(cyclohexylmethyl)-8-quinolinyl ester-1H-indole-3-carboxylic acid	1400742-42-8	C25H24N2O2	Indole
CBL-018		naphthalen-1-yl 1-pentyl-1H-indole-3-carboxylate		C24H23NO2	Indole
CUMYL-PICA		N-(1-methyl-1-phenylethyl)-1-pentyl-1H-indole-3-carboxamide	1400742-32-6	C23H28N2O	Indole
FDU-NNEI		1-(4-fluorobenzyl)-N-(naphthalen-1-yl)-1H-indole-3-carboxamide		C26H19FN2O	Indole
FDU-PB-22		1-[(4-fluorophenyl)methyl]-1H-indole-3-carboxylic acid, 1-naphthalenyl ester	1883284-94-3	C26H18FNO2	Indole
FUB-PB-22		1-[(4-fluorophenyl)methyl]-1H-indole-3-carboxylic acid, 8-quinolinyl ester	1800098-36-5	C25H17FN2O2	Indole
IMMA		1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetic acid	53-86-1	C23H23ClN2O4	Indole
MDA 19		(2Z)-2-(1-hexyl-1,2-dihydro-2-oxo-3H-indol-3-ylidene)hydrazide, benzoic acid	1048973-47-2	C21H23N3O2	Indole
MDA 77		2Z-(1,2-dihydro-6-methoxy-2-oxo-1-pentyl-3H-indol-3-ylidene)hydrazide, benzoic acid	1103774-21-5	C21H23N3O3	Indole
MMB018		methyl (1-pentyl-1H-indole-3-carbonyl)-L-valinate		C20H28N2O3	Indole
MMB2201	AMB-PICA	methyl (1-(5-fluoropentyl)-1H-indole-3-carbonyl)-L-valinate		C20H27FN2O3	Indole
MMB-CHMICA		methyl (1-(cyclohexylmethyl)-1H-indole-3-carbonyl)-L-valinate		C22H30N2O3	Indole

MN-25	UR-12	7-methoxy-1-[2-(4-morpholinyl)ethyl]-N-[(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1H-indole-3-carboxamide	501926-82-5	C26H37N3O3	Indole
MN-25-2-methyl derivative		7-methoxy-2-methyl-1-[2-(4-morpholinyl)ethyl]-N-[(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1H-indole-3-carboxamide	501927-29-3	C27H39N3O3	Indole
NM2201	CBL-2201	naphthalen-1-yl 1-(5-fluoropentyl)-1H-indole-3-carboxylate		C24H22FNO2	Indole
NNEI		N-1-naphthalenyl-1-pentyl-1H-indole-3-carboxamide	1338925-11-3	C24H24N2O	Indole
PB-22 (QUPIC)		1-pentyl-1H-indole-3-carboxylic acid 8-quinolinyl ester	1400742-17-7	C23H22N2O2	Indole
PTI-1		N,N-diethyl-2-(1-pentyl-1H-indol-3-yl-4-thiazolemethanamine		C21H29N3S	Indole
PTI-2		N-(2-methoxyethyl)-N-(1-methylethyl)-2-(1-pentyl-1H-indol-3-yl)-4-thiazolemethanamine		C23H33N3OS	Indole
PX 1	5-fluoro APP-PICA	(S)-N-(1-amino-1-oxo-3-phenylpropan-2-yl)-1-(5-fluoropentyl)-1H-indole-3-carboxamide		C23H26FN3O2	Indole
PX 2	5-fluoro APP-PINACA	(R)-N-(1-amino-1-oxo-3-phenylpropan-2-yl)-1-(5-fluoropentyl)-1H-indazole-3-carboxamide		C22H25FN4O2	Indole
SDB-006 N-phenyl analog		1-pentyl-N-phenyl-1H-indole-3-carboxamide	1430634-87-9	C20H22N2O	Indole
THJ 018	JWH 018 indazole analog	1-naphthalenyl(1-pentyl-1H-indazol-3-yl)-methanone	1364933-55-0	C23H22N2O	Naphthoylindazole
THJ2201		[1-(5-fluoropentyl)-1H-indazol-3-yl]-1-naphthalenyl-methanone	1801552-01-1	C23H21FN2O	Naphthoylindazole
1-Naphthoyl indole		1H-indol-3-yl-1-naphthalenyl-methanone	109555-87-5	C19H13NO	Naphthoylindole
3-CAF		naphthalen-2-yl 1-(2-fluorophenyl)-1H-indazole-3-carboxylate		C24H15FN2O2	Naphthoylindole
AM-1220		[1-[[(2R)-1-methyl-2-piperidyl]methyl]indol-3-yl]-(1-naphthyl)methanone	137642-54-7	C26H26N2O	Naphthoylindole
AM-1235		[1-(5-fluoropentyl)-6-nitro-1H-indol-3-yl]-1-naphthalenyl-methanone	335161-27-8	C24H21FN2O3	Naphthoylindole
AM-2201		[1-(5-fluoropentyl)indol-3-yl]-naphthalen-1-yl-methanone	335161-24-5	C24H22FNO	Naphthoylindole
AM-2201 6-hydroxyindole metabolite		(1-(5-fluoropentyl)-6-hydroxy-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427521-35-4	C24H22FNO2	Naphthoylindole
AM-2201 7-hydroxyindole metabolite		(1-(5-fluoropentyl)-7-hydroxy-1H-indol-3-yl)(naphthalen-1-yl)methanone	1537889-11-4	C24H22FNO2	Naphthoylindole
AM-2201 N-(4-hydroxypentyl) metabolite		(1-(5-fluoro-4-hydroxypentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427521-34-3	C24H22FNO2	Naphthoylindole
AM-2201 N-(2-fluoropentyl) isomer		(1-(2-fluoropentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C24H22FNO	Naphthoylindole
AM-2201 N-(3-fluoropentyl) isomer		(1-(3-fluoropentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C24H22FNO	Naphthoylindole
AM-2201 N-(4-fluoropentyl) isomer		(1-(4-fluoropentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427325-95-8	C24H22FNO	Naphthoylindole
AM-2232		3-(1-naphthalenylcarbonyl)-1H-indole-1-pentanenitrile	335161-19-8	C24H20N2O	Naphthoylindole
Cl2201		(4-chloro-1-naphthalenyl)[1-(5-fluoropentyl)-1H-indol-3-yl]-methanone	1391486-12-6	C24H21ClFNO	Naphthoylindole

EAM-2201		(4-ethyl-1-naphthalenyl)[1-(5-fluoropentyl)-1H-indol-3-yl]methanone	1364933-60-7	C26H26FNO	Naphthoylindole
F2201	5-fluoro JWH 412	(4-fluoro-1-naphthalenyl)[1-(5-fluoropentyl)-1H-indol-3-yl]-methanone	1391485-39-4	C24H21F2NO	Naphthoylindole
FUB-JWH 018		(1-(4-fluorobenzyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C26H18FNO	Naphthoylindole
JWH 081-N-(cyclohexylmethyl) analog		[1-(cyclohexylmethyl)-1H-indol-3-yl](4-methoxy-1-naphthalenyl)-methanone	1373876-34-6	C27H27NO2	Naphthoylindole
JWH-007		(2-methyl-1-pentyl-1H-indol-3-yl)-1-naphthalenyl-methanone	155471-10-6	C25H25NO	Naphthoylindole
JWH-011		[2-methyl-1-(1-methylhexyl)-1H-indol-3-yl]-1-naphthalenyl-methanone	155471-13-9	C27H29NO	Naphthoylindole
JWH-015		(2-methyl-1-propyl-1H-indol-3-yl)-1-naphthalenyl-methanone	155471-08-2	C23H21NO	Naphthoylindole
JWH-016		(1-butyl-2-methyl-1H-indol-3-yl)-1-naphthalenyl-methanone	155471-09-3	C24H23NO	Naphthoylindole
JWH-018		(1-pentyl-1H-indol-3-yl)-1-naphthalenyl-methanone	209414-07-3	C24H23NO	Naphthoylindole
JWH-018 4-hydroxyindole metabolite		(4-hydroxy-1-pentyl-1H-indol-3-yl)(naphthalen-1-yl) methanone	1307803-42-4	C24H23NO2	Naphthoylindole
JWH-018 5-hydroxyindole metabolite		(5-hydroxy-1-pentyl-1H-indol-3-yl)(naphthalen-1-yl) methanone	1307803-43-5	C24H23NO2	Naphthoylindole
JWH-018 6-hydroxyindole metabolite		(6-hydroxy-1-pentyl-1H-indol-3-yl)(naphthalen-1-yl) methanone	1307803-44-6	C24H23NO2	Naphthoylindole
JWH-018 6-methoxyindole analog		(6-methoxy-1-pentyl-1H-indol-3-yl)(naphthalen-1-yl) methanone	1427325-49-2	C25H25NO2	Naphthoylindole
JWH-018 7-hydroxyindole metabolite		(7-hydroxy-1-pentyl-1H-indol-3-yl)naphthalen-1-yl) methanone	1307803-45-7	C24H23NO2	Naphthoylindole
JWH-018 N-(1,1-dimethylpropyl) isomer		naphthalen-1-yl(1-(tert-pentyl)-1H-indol-3-yl)methanone	1358118-35-0	C24H23NO	Naphthoylindole
JWH-018 N-(1,2-dimethylpropyl) isomer		(1-(3-methylbutan-2-yl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427325-40-3	C24H23NO	Naphthoylindole
JWH-018 N-(1-ethylpropyl) isomer		naphthalen-1-yl(1-(pentan-3-yl)-1H-indol-3-yl)methanone		C24H23NO	Naphthoylindole
JWH-018 N-(1-methylbutyl) isomer		naphthalen-1-yl(1-(pentan-2-yl)-1H-indol-3-yl)methanone	1427325-45-8	C24H23NO	Naphthoylindole
JWH-018 N-(2,2-dimethylpropyl) isomer		naphthalen-1-yl(1-neopentyl-1H-indol-3-yl) methanone	1427325-47-0	C24H23NO	Naphthoylindole
JWH-018 N-(2-hydroxypentyl) metabolite		(1-(2-hydroxypentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C24H23NO2	Naphthoylindole
JWH-018 N-(2-methylbutyl) isomer		N-(2-methylbutyl)-3-(1-naphthoyl)indole	1427325-50-5	C24H23NO	Naphthoylindole
JWH-018 N-(3-hydroxypentyl) metabolite		(1-(3-hydroxypentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C24H23NO2	Naphthoylindole
JWH-018 N-(3-methylbutyl) isomer		N-(3-methylbutyl)-3-(1-naphthoyl)indole	1346604-93-0	C24H23NO	Naphthoylindole
JWH-018 N-(4,5-epoxypentyl) analog		naphthalen-1-yl(1-(3-(oxiran-2-yl)propyl)-1H-indol-3-yl)methanone		C24H21NO2	Naphthoylindole
JWH-018 N-(4-hydroxypentyl) metabolite		(1-(4-hydroxypentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1320363-47-0	C24H23NO2	Naphthoylindole
JWH-018 N-(4-oxo-pentyl) metabolite		5-(3-(1-naphthoyl)-1H-indol-1-yl)pentan-2-one		C24H21NO2	Naphthoylindole

JWH-018 N-(5-bromopentyl) analog		(1-(5-bromopentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1445578-62-0	C24H22BrNO	Naphthoylindole
JWH-018 N-(5-chloropentyl) analog		(1-(5-chloropentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1445578-56-2	C24H22ClNO	Naphthoylindole
JWH-018 N-(5-hydroxypentyl) metabolite		(1-(5-hydroxypentyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	335161-21-2	C24H23NO2	Naphthoylindole
JWH-018 N-(5-hydroxypentyl) β-D-glucuronide		(2S,3S,4S,5R)-6-((5-(3-(1-naphthoyl)-1H-indol-1-yl)pentyl)oxy)-3,4,5-trihydroxytetrahydro-2H-pyran-2-carboxylic acid	1307803-55-9	C30H31NO8	Naphthoylindole
JWH-018 N-pentanoic acid metabolite		5-(3-(1-naphthoyl)-1H-indol-1-yl)pentanoic acid	1254475-87-0	C24H21NO3	Naphthoylindole
JWH-018 2-hydroxyindole metabolite		(2-hydroxy-1-pentyl-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427325-32-3	C24H23NO2	Naphthoylindole
JWH-019		(1-hexyl-1H-indol-3-yl)-1-naphthalenyl-methanone	209414-08-4	C25H25NO	Naphthoylindole
JWH-019 5-hydroxyindole metabolite		(1-hexyl-5-hydroxy-1H-indol-3-yl)(naphthalen-1-yl)methanone	1379604-70-2	C25H25NO2	Naphthoylindole
JWH-019 N-(6-hydroxyhexyl) metabolite		(1-(6-hydroxyhexyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1435934-29-4	C25H25NO2	Naphthoylindole
JWH-020		(1-heptyl-1H-indol-3-yl)-1-naphthalenyl-methanone	209414-09-5	C26H27NO	Naphthoylindole
JWH-022		1-naphthalenyl[1-(4-penten-1-yl)-1H-indol-3-yl] methanone	209414-16-4	C24H21NO	Naphthoylindole
JWH-071		(1-ethyl-1H-indol-3-yl)-1-naphthalenyl-methanone	209414-05-1	C21H17NO	Naphthoylindole
JWH-072		1-naphthalenyl(1-propyl-1H-indol-3-yl)methanone	209414-06-2	C22H19NO	Naphthoylindole
JWH-073		(1-butyl-1H-indol-3-yl)-1-naphthalenyl-methanone	208987-48-8	C23H21NO	Naphthoylindole
JWH-073 2-hydroxyindole metabolite		(1-butyl-2-hydroxy-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427325-54-9	C23H21NO2	Naphthoylindole
JWH-073 2-methylnaphthyl analog		(1-butyl-1H-indol-3-yl)(2-methylnaphthalen-1-yl)methanone	1427325-61-8	C24H23NO	Naphthoylindole
JWH-073 4-hydroxyindole metabolite		(1-butyl-4-hydroxy-1H-indol-3-yl)(naphthalen-1-yl)methanone	1307803-46-8	C23H21NO2	Naphthoylindole
JWH-073 4-methylnaphthyl analog		(1-butyl-1H-indol-3-yl)(4-methylnaphthalen-1-yl)methanone	1354631-21-2	C24H23NO	Naphthoylindole
JWH-073 5-hydroxyindole metabolite		(1-butyl-5-hydroxy-1H-indol-3-yl)(naphthalen-1-yl) methanone	1307803-47-9	C23H21NO2	Naphthoylindole
JWH-073 6-hydroxyindole metabolite		(1-butyl-6-hydroxy-1H-indol-3-yl)(naphthalen-1-yl) methanone	1307803-48-0	C23H21NO2	Naphthoylindole
JWH-073 6-methoxyindole analog		(1-butyl-6-methoxy-1H-indol-3-yl)(naphthalen-1-yl)methanone		C24H23NO2	Naphthoylindole
JWH-073 7-hydroxyindole metabolite		(1-butyl-7-hydroxy-1H-indol-3-yl)(naphthalen-1-yl) methanone	1307803-49-1	C23H21NO2	Naphthoylindole
JWH-073 N-(1,1-dimethylethyl) isomer		(1-(tert-butyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C23H21NO	Naphthoylindole
JWH-073 N-(1-methylpropyl) isomer		(1-(sec-butyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C23H21NO	Naphthoylindole
JWH-073 N-(2-methylpropyl) isomer		(1-isobutyl-1H-indol-3-yl)(naphthalen-1-yl)methanone		C23H21NO	Naphthoylindole
JWH-073 N-(3-hydroxybutyl) metabolite		(1-(3-hydroxybutyl)-1H-indol-3-yl)(naphthalen-1-yl) methanone	1320363-48-1	C23H21NO2	Naphthoylindole

JWH-073 N-(4-hydroxybutyl) metabolite		(1-(4-hydroxybutyl)-1H-indol-3-yl)(naphthalen-1-yl) methanone	335161-14-3	C23H21NO2	Naphthoylindole
JWH-073 N-butanoic acid metabolite		4-(3-(1-naphthoyl)-1H-indol-1-yl)butanoic acid	1307803-52-6	C23H19NO3	Naphthoylindole
JWH-080		(1-butyl-1H-indol-3-yl)(4-methoxy-1-naphthalenyl) methanone	210179-44-5	C24H23NO2	Naphthoylindole
JWH-081		(4-methoxy-1-naphthalenyl)(1-pentyl-1H-indol-3-yl) methanone	210179-46-7	C25H25NO2	Naphthoylindole
JWH-081 2-methoxynaphthyl isomer		(2-methoxy-1-naphthalenyl)(1-pentyl-1H-indol-3-yl) methanone	824960-76-1	C25H25NO2	Naphthoylindole
JWH-081 3-methoxynaphthyl isomer		(3-methoxynaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C25H25NO2	Naphthoylindole
JWH-081 5-methoxynaphthyl isomer		(5-methoxynaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1427325-65-2	C25H25NO2	Naphthoylindole
JWH-081 6-methoxynaphthyl isomer		(6-methoxy-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)methanone	824961-41-3	C25H25NO2	Naphthoylindole
JWH-081 7-methoxynaphthyl isomer		(7-methoxy-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)methanone	824961-61-7	C25H25NO2	Naphthoylindole
JWH-081 8-methoxynaphthyl isomer		(8-methoxynaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1349837-48-4	C25H25NO2	Naphthoylindole
JWH-081 N-(5-hydroxypentyl) metabolite		(1-(5-hydroxypentyl)-1H-indol-3-yl)(4-methoxynaphthalen-1-yl)methanone		C25H25NO3	Naphthoylindole
JWH-098		(4-methoxy-1-naphthalenyl)(2-methyl-1-pentyl-1H-indol-3-yl)methanone	316189-74-9	C26H27NO2	Naphthoylindole
JWH-116		(2-ethyl-1-pentyl-1H-indol-3-yl)-1-naphthalenyl-methanone	619294-64-3	C26H27NO	Naphthoylindole
JWH-122		(4-methyl-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)methanone	619294-47-2	C25H25NO	Naphthoylindole
JWH-122 2-methylnaphthyl isomer		(2-methylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1427325-69-6	C25H25NO	Naphthoylindole
JWH-122 3-methylnaphthyl isomer		(3-methylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1391052-25-7	C25H25NO	Naphthoylindole
JWH-122 5-methylnaphthyl isomer		(5-methylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1391052-02-0	C25H25NO	Naphthoylindole
JWH-122 6-methylnaphthyl isomer		(6-methylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1427325-68-5	C25H25NO	Naphthoylindole
JWH-122 7-methylnaphthyl isomer		(7-methyl-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)methanone	824960-56-7	C25H25NO	Naphthoylindole
JWH-122 8-methylnaphthyl isomer		(8-methylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C25H25NO	Naphthoylindole
JWH-122 N-(4-pentenyl) analog		(4-methylnaphthalen-1-yl)(1-(pent-4-en-1-yl)-1H-indol-3-yl)methanone	1445577-68-3	C25H23NO	Naphthoylindole
JWH-122 N-(5-hydroxypentyl) metabolite		(1-(5-hydroxypentyl)-1H-indol-3-yl)(4-methylnaphthalen-1-yl)methanone	1379604-68-8	C24H23NO2	Naphthoylindole
JWH-149		(4-methyl-1-naphthalenyl)(2-methyl-1-pentyl-1H-indol-3-yl)methanone	548461-82-1	C26H27NO	Naphthoylindole
JWH-180		(1-propyl-1H-indol-3-yl)(4-propyl-1-naphthalenyl)methanone	824959-87-7	C25H25NO	Naphthoylindole
JWH-182		(1-pentyl-1H-indol-3-yl)(4-propyl-1-naphthalenyl) methanone	824960-02-3	C27H29NO	Naphthoylindole
JWH-193		(4-methyl-1-naphthalenyl)[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]methanone	133438-58-1	C26H26N2O2	Naphthoylindole

JWH-198		(1-(2-morpholin-4-ylethyl)indol-3-yl)-4-methoxynaphthalen-1-yl-methanone	166599-76-4	C26H26N2O3	Naphthoylindole
JWH-200		[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-1-naphthalenyl-methanone	103610-04-4	C25H24N2O2	Naphthoylindole
JWH-200 4-hydroxyindole metabolite		4-hydroxy[1-[2-(4-morpholinyl)ethyl]-1H-indol-3-yl]-1-naphthalenyl-methanone	1427325-73-2	C25H24N2O3	Naphthoylindole
JWH-200 5-hydroxyindole metabolite		(5-hydroxy-1-(2-morpholinoethyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	133438-72-9	C25H24N2O3	Naphthoylindole
JWH-200 6-hydroxyindole metabolite		(6-hydroxy-1-(2-morpholinoethyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone	1427325-76-5	C25H24N2O3	Naphthoylindole
JWH-200 7-hydroxyindole metabolite		(7-hydroxy-1-(2-morpholinoethyl)-1H-indol-3-yl)(naphthalen-1-yl)methanone		C25H24N2O3	Naphthoylindole
JWH-210		(4-ethyl-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)methanone	824959-81-1	C26H27NO	Naphthoylindole
JWH-210 2-ethylnaphthyl isomer		(2-ethylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1427325-79-8	C26H27NO	Naphthoylindole
JWH-210 3-ethylnaphthyl isomer		(3-ethylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C26H27NO	Naphthoylindole
JWH-210 5-ethylnaphthyl isomer		(5-ethylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C26H27NO	Naphthoylindole
JWH-210 5-hydroxyindole metabolite		(4-ethylnaphthalen-1-yl)(5-hydroxy-1-pentyl-1H-indol-3-yl)methanone	1427325-81-2	C26H27NO2	Naphthoylindole
JWH-210 6-ethylnaphthyl isomer		(6-ethylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C26H27NO	Naphthoylindole
JWH-210 7-ethylnaphthyl isomer		(7-ethyl-1-naphthalenyl)(1-pentyl-1H-indol-3-yl) methanone	824960-64-7	C26H27NO	Naphthoylindole
JWH-210 8-ethylnaphthyl isomer		(8-ethylnaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C26H27NO	Naphthoylindole
JWH-210 N-(4-hydroxypentyl) metabolite		(4-ethylnaphthalen-1-yl)(1-(4-hydroxypentyl)-1H-indol-3-yl)methanone	1427521-37-6	C26H27NO2	Naphthoylindole
JWH-210 N-(5-carboxypentyl) metabolite		5-(3-(4-ethyl-1-naphthoyl)-1H-indol-1-yl)pentanoic acid	1427521-36-5	C26H25NO3	Naphthoylindole
JWH-210 N-(5-hydroxypentyl) metabolite		(4-ethylnaphthalen-1-yl)(1-(5-hydroxypentyl)-1H-indol-3-yl)methanone	1427521-40-1	C26H27NO2	Naphthoylindole
JWH-387		(4-bromo-1-naphthalenyl)(1-pentyl-1H-indol-3-yl) methanone	1366067-59-5	C24H22BrNO	Naphthoylindole
JWH-398		(4-chloronaphthalen-1-yl)(1-pentylindolin-3-yl) methanone	1292765-18-4	C24H22ClNO	Naphthoylindole
JWH-398 2-chloronaphthyl isomer		(2-chloronaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1391054-25-3	C24H22ClNO	Naphthoylindole
JWH-398 3-chloronaphthyl isomer		(3-chloronaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C24H22ClNO	Naphthoylindole
JWH-398 5-chloronaphthyl isomer		(5-chloronaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1427325-89-0	C24H22ClNO	Naphthoylindole
JWH-398 6-chloronaphthyl isomer		(6-chloronaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone		C24H22ClNO	Naphthoylindole
JWH-398 7-chloronaphthyl isomer		(7-chloronaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1391051-95-8	C24H22ClNO	Naphthoylindole
JWH-398 8-chloronaphthyl isomer		(8-chloronaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1366067-88-0	C24H22ClNO	Naphthoylindole
JWH-398 N-(5-hydroxypentyl) metabolite		(4-chloronaphthalen-1-yl)(1-(5-hydroxypentyl)-1H-indol-3-yl)methanone	1379604-69-9	C24H22ClNO2	Naphthoylindole

JWH-412		(4-fluoro-1-naphthalenyl)(1-pentyl-1H-indol-3-yl)methanone	1364933-59-4	C24H22FNO	Naphthoylindole
JWH-424		(8-bromonaphthalen-1-yl)(1-pentyl-1H-indol-3-yl)methanone	1366068-04-3	C24H22BrNO	Naphthoylindole
MAM-2201		[1-(5-fluoropentyl)-1H-indol-3-yl](4-methyl-1-naphthalenyl)methanone	1354631-24-5	C25H24FNO	Naphthoylindole
MAM-2201 N-(3-fluoropentyl) isomer		(1-(3-fluoropentyl)-1H-indol-3-yl)(4-methylnaphthalen-1-yl)methanone		C25H24FNO	Naphthoylindole
MAM-2201 N-(5-chloropentyl) analog		(1-(5-chloropentyl)-1H-indol-3-yl)(4-methylnaphthalen-1-yl)methanone	1445578-25-5	C25H24ClNO	Naphthoylindole
JWH-030		1-naphthalenyl(1-pentyl-1H-pyrrol-3-yl)methanone	162934-73-8	C20H21NO	Naphthoylpyrrole
JWH-031		(1-hexyl-1H-pyrrol-3-yl)-1-naphthalenyl-methanone	162934-74-9	C21H23NO	Naphthoylpyrrole
JWH-145		1-naphthalenyl(1-pentyl-5-phenyl-1H-pyrrol-3-yl) methanone	914458-19-8	C26H25NO	Naphthoylpyrrole
JWH-147		(1-hexyl-5-phenyl-1H-pyrrol-3-yl)-1-naphthalenyl-methanone	914458-20-1	C27H27NO	Naphthoylpyrrole
JWH-307		5-(2-fluorophenic)-1-1pentylpyrro(-3-yl)-naphthalene-1-yl-methanone	914458-26-7	C26H24FNO	Naphthoylpyrrole
JWH-309		1-naphthalenyl[5-(1-naphthalenyl)-1-pentyl-1H-pyrrol-3-yl]methanone	914458-42-7	C30H27NO	Naphthoylpyrrole
JWH-368		[5-(3-fluorophenyl)-1-pentyl-1H-pyrrol-3-yl]-1-naphthalenyl-methanone	914458-31-4	C26H24FNO	Naphthoylpyrrole
JWH-369		[5-(2-chlorophenyl)-1-pentyl-1H-pyrrol-3-yl]-1-naphthalenyl-methanone	914458-27-8	C26H24ClNO	Naphthoylpyrrole
JWH-370		[5-(2-methylphenyl)-1-pentyl-1H-pyrrol-3-yl]-1-naphthalenyl-methanone	914458-22-3	C27H27NO	Naphthoylpyrrole
JWH-175		3-(1-naphthalenylmethyl)-1-pentyl-1H-indole	619294-35-8	C24H25N	Naphthylmethylindole
2-Fluoroisocathinone	2-FIC	1-amino-1-(2-fluorophenyl)propan-2-one		C9H10FNO	Other
2-Thiothinone		2-(methylamino)-1-(2-thienyl)-1-propanone		C8H11NOS	Other
3-Fluorophenmetrazine	3-FPM	2-(3-fluorophenyl)-3-methylmorpholine		C11H14FNO	Other
Isopentedrone		1-(methylamino)-1-phenylpentan-2-one		C12H17NO	Other
MTTA		3,4-dihydro-2-[(methylamino)methyl]-1(2H)-naphthalenone		C12H15NO	Other
4-Quinolone-3-carboxamide		1,4-dihydro-8-methoxy-4-oxo-1-pentyl-N-tricyclo[3.3.1.13,7]dec-1-yl-3-quinolinecarboxamide	1314230-69-7	C26H34N2O3	Other Cannabinoid
5-Fluoro PCN	5-fluoro MN-21	1-(5-fluoropentyl)-N-(naphthalen-1-yl)-1H-pyrrolo[3,2-c]pyridine-3-carboxamide		C23H22FN3O	Other Cannabinoid
AM-1172		4-hydroxy-N-[(5Z,8Z,11Z,14Z)-5,8,11,14-icosatetraen-1-yl]benzamide	251908-92-6	C27H39NO2	Other Cannabinoid
AM-251		1-(2,4-dichlorophenyl)-5-(4-iodophenyl)-4-methyl-N-piperidin-1-yl-pyrazole-3-carboxamide	183232-66-8	C22H21Cl2IN4O	Other Cannabinoid
AM-3102		N-[(1R)-2-hydroxy-1-methylethyl-9Z-octadecenamide	213182-22-0	C21H41NO2	Other Cannabinoid
AM-356		N-(2-hydroxy-1R-methylethyl)-5Z,8Z,11Z,14Z-eicosatetraenamide	157182-49-5	C23H39NO2	Other Cannabinoid

Cannabipiperidiethanone		2-(2-methoxyphenyl)-1-[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]ethanone	1345970-43-5	C24H28N2O2	Other Cannabinoid
CB-13		1-naphthyl[4-(pentyloxy)-1-naphthyl]methanone	432047-72-8	C26H24O2	Other Cannabinoid
CB-25		N-cyclopropyl-11-(3-hydroxy-5-pentylphenoxy)undecanamide	869376-63-6	C25H41NO3	Other Cannabinoid
CB-52		N-cyclopropyl-11-(5-hydroxy-2-pentylphenoxy)undecanamide	869376-90-9	C25H41NO3	Other Cannabinoid
CB-86		N-cyclopropyl-8-[3-(1,1-dimethylheptyl)-5-hydroxyphenoxy]octanamide	1150586-64-3	C26H43NO3	Other Cannabinoid
Dimethylheptylpyran		6,6,9-trimethyl-3-(3-methyl-2-octanyl)-7,8,9,10-tetrahydro-6H-benzo[c]chromen-1-ol	32904-22-6	C25H38O2	Other Cannabinoid
EG 018		naphthalen-1-yl(9-pentyl-9H-carbazol-3-yl)methanone		C28H25NO	Other Cannabinoid
EG 2201		(9-(5-fluoropentyl)-9H-carbazol-3-yl)(naphthalen-1-yl)methanone		C28H24FNO	Other Cannabinoid
HU-210		3-(1,1-dimethylheptyl)-6aR,7,10,10aR-tetrahydro-1-hydroxy-6,6-dimethyl-6H-dibenzo[b,d]pyran-9-methanol	112830-95-2	C25H38O3	Other Cannabinoid
HU-211		3-(1,1-dimethylheptyl)-6aS,7,10,10aS-tetrahydro-1-hydroxy-6,6-dimethyl-6H-dibenzo[b,d]pyran-9-methanol	112924-45-5	C25H38O3	Other Cannabinoid
HU-308		4-[4-(1,1-dimethylheptyl)-2,6-dimethoxyphenyl]-6,6-dimethyl-bicyclo[3.1.1]hept-2-ene-2-methanol	256934-39-1	C27H42O3	Other Cannabinoid
HU-331		3-hydroxy-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-2,5-cyclohexadiene-1,4-dione	137252-25-6	C21H28O3	Other Cannabinoid
JP 104		3-carbamoyl-biphenyl-3-yl-undecynecarbamate	887264-45-1	C25H30N2O3	Other Cannabinoid
JW 618		1,1,1,3,3,3-hexafluoropropan-2-yl-methyl(3-(pyridin-4-yl)benzyl)carbamate		C17H14F6N2O2	Other Cannabinoid
JW 642		1,1,1,3,3,3-hexafluoropropan-2-yl 4-(3-phenoxybenzyl)piperazine-1-carboxylate	1416133-89-5	C21H20F6N2O3	Other Cannabinoid
JWH-133		(6aR,10aR)-3-(1,1-dimethylbutyl)-6a,7,10,10a-tetrahydro -6,6,9-trimethyl-6H-dibenzo[b,d]pyran		C22H32O	Other Cannabinoid
JWH-176		1-([(1e)-3-pentylinden-1-ylidine]methyl)naphthalene	619294-62-1	C25H24	Other Cannabinoid
JZL 184		4-nitrophenyl-4-(dibenzo[d][1,3]dioxol-5-yl(hydroxy)methyl)piperidine-1-carboxylate	1101854-58-3	C27H24N2O9	Other Cannabinoid
JZL 195		4-nitrophenyl 4-(3-phenoxybenzyl)piperazine-1-carboxylate	1210004-12-8	C24H23N3O5	Other Cannabinoid
KML29		1,1,1,3,3,3-hexafluoropropan-2-yl 4-(bis(benzo[d][1,3]dioxol-5-yl)(hydroxy)methyl)piperidine-1-carboxylate	1380424-42-9	C24H21F6NO7	Other Cannabinoid
Nabilone		(6aR,10aR)-1-hydroxy-6,6-dimethyl-3-(2-methyl-2-octanyl)-6,6a,7,8,10,10a-hexahydro-9H-benzo[c]chromen-9-one	56496-90-3	C24H36O3	Other Cannabinoid
O-1125		6-[(6aR,10aR)-1-hydroxy-6,6,9-trimethyl-6a,7,10,10a-tetrahydrobenzo[c]chromen-3-yl]-N,N,6-trimethylheptanamide		C26H39NO3	Other Cannabinoid
O-1238		(6aS)-3-[(2Z)-6-azido-2-hexen-1-yl]-6,6,9-trimethyl-6a,7,10,10a-tetrahydro-6H-benzo[c]chromen-1-ol		C22H29N3O2	Other Cannabinoid

O-1302		N-(piperidinyl)-1-(2,4-dichlorophenyl)-4-methyl-5-(4-pentylphenyl)-1H-pyrazole-3-carboxamide		C27H32Cl2N4O	Other Cannabinoid
O-1602		5-methyl-4-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-1,3-benzenediol	317321-41-8	C17H22O2	Other Cannabinoid
O-1821		5-methyl-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-1,3-benzenediol	35482-50-9	C17H22O2	Other Cannabinoid
O-1918		1,3-dimethoxy-5-methyl-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]benzene	536697-79-7	C19H26O2	Other Cannabinoid
O-806		3-(6-bromohex-2-ynyl)-6,6,9-trimethyl-6a,7,10,10a-tetrahydrobenzo[c]chromen-1-ol		C22H27BrO2	Other Cannabinoid
O-823		7-[(6aR,10aR)-1-hydroxy-6,6,9-trimethyl-6a,7,10,10a-tetrahydrobenzo[c]chromen-3-yl]hept-5-yne-nitrile		C23H27NO2	Other Cannabinoid
SER-601		1,4-dihydro-6-(1-methylethyl)-4-oxo-1-pentyl-N-tricyclo[3.3.1.13,7]dec-1-yl-3-quinolinecarboxamide	1048038-90-9	C28H38N2O2	Other Cannabinoid
URB447		[4-amino-1-[(4-chlorophenyl)methyl]-2-methyl-5-phenyl-1H-pyrrol-3-yl]phenyl-methanone	1132922-57-6	C25H21ClN2O	Other Cannabinoid
URB597		(3-(aminocarbonyl)[1,1-biphenyl]-3-yl)-cyclohexylcarbamate	546141-08-6	C20H22N2O3	Other Cannabinoid
URB602		cyclohexyl biphenyl-3-ylcarbamate	565460-15-3	C19H21NO2	Other Cannabinoid
URB754		6-methyl-2-[(4-methylphenyl)amino]-1-benzoxazin-4-one	86672-58-4	C16H14N2O2	Other Cannabinoid
URB937		3-carbamoyl-6-hydroxy-[1,1-biphenyl]-3-yl cyclohexylcarbamate	1357160-72-5	C20H22N2O4	Other Cannabinoid
WIN 55,212-2		(R)-(+)-[2,3-dihydro-5-methyl-3-(4-morpholinylmethyl)pyrrolo[1,2,3-de]-1,4-benzoxazin-6-yl]-1-napthalenylmethanone	131543-22-1	C27H26N2O3	Other Cannabinoid
4-Fluoroisocathinone		1-amino-1-(4-fluorophenyl)propan-2-one	1270532-42-7	C9H10FNO	Other Stimulant
Desoxypipradrol	2-DPMP	2-benzhydrylpiperidine	519-74-4	C18H21N	Other Stimulant
Ethylphenidate		Ethyl phenyl(2-piperidinyl)acetate	19716-79-1	C15H21NO2	Other Stimulant
MDMA methylene homolog		3-(1,3-benzenodioxol-5-yl)-N,2-dimethylpropan-1-amine		C12H17NO2	Other Stimulant
Tenocyclidine	TCP	1-[1-(2-thienyl)cyclohexyl]piperidine	21500-98-1	C15H23NS	Other Stimulant
3-Methoxy-4-Methylamphetamine	MMA	1-(3-methoxy-4-methylphenyl)propan-2-amine	87179-33-7	C11H17NO	Phenethylamine
1-(4-Fluorophenyl) butan-2-amine		α-ethyl-4-fluoro-benzeneethanamine	23292-09-3	C10H14FN	Phenethylamine
1,4-Dimethoxynaphthyl-2-ethylamine	2C-G-N	2-(1,4-dimethoxynaphthalen-2-yl)ethanamine	207740-21-4	C14H17NO2	Phenethylamine
1,4-Dimethoxynaphthyl-2-isopropylamine	G-N	1-(1,4-dimethoxynaphthalen-2-yl)propan-2-amine		C15H19NO2	Phenethylamine
2-(2,5-Dimethoxy-4-methylphenyl)cyclopropylamine	DMCPA	2-(2,5-dimethoxy-4-methylphenyl)cyclopropanamine	69854-49-5	C12H17NO2	Phenethylamine
2-(3,4-Dimethoxyphenyl)-N-methylethylamine	N-Me-DMPEA	3,4-dimethoxy-N-methyl-benzeneethanamine	3490-06-0	C11H17NO2	Phenethylamine
2,3,4,5-Tetramethoxyamphetamine		2,3,4,5-tetramethoxy-α-methyl-benzeneethanamine	23693-26-7	C13H21NO4	Phenethylamine
2,3,4-Trimethoxyamphetamine	TMA-3	1-(2,3,4-trimethoxyphenyl)-2-propanamine	1082-23-1	C12H19NO3	Phenethylamine

2,3,5-Trimethoxyamphetamine	TMA-4	1-(2,3,5-trimethoxyphenyl)-2-propanamine	23693-14-3	C12H19NO3	Phenethylamine
2,3,6-Trimethoxyamphetamine	TMA-5	1-(2,3,6-trimethoxyphenyl)-2-propanamine	20513-16-0	C12H19NO3	Phenethylamine
2,3-Dimethoxy-4,5-methylenedioxyamphetamine	DMMDA-2	1-(6,7-dimethoxy-1,3-benzodioxol-5-yl)propan-2-amine		C12H17NO4	Phenethylamine
2,3-Methylenedioxyamphetamine	2,3-MDA	1-(1,3-benzodioxol-4-yl)propan-2-amine	23693-17-6	C10H13NO2	Phenethylamine
2,3-Methylenedioxymethylamphetamine	2,3-MDMA	N,α-dimethyl-1,3-benzodioxole-4-ethanamine	168967-99-5	C11H15NO2	Phenethylamine
2,4,5-Triethoxyamphetamine	EEE	2,4,5-triethoxy-α-methyl-benzeneethanamine	23693-42-7	C15H25NO3	Phenethylamine
2,4,5-Trimethoxyamphetamine	TMA-2	1-(2,4,5-trimethoxyphenyl)-2-propanamine	1083-09-6	C12H19NO3	Phenethylamine
2,4,5-Trimethoxyphenethylamine	2C-O	2-(2,4,5-trimethoxyphenyl)ethanamine	15394-83-9	C11H17NO3	Phenethylamine
2,4,6-Trimethoxyamphetamine	TMA-6	1-(2,4,6-trimethoxyphenyl)-2-propanamine	15402-79-6	C12H19NO3	Phenethylamine
2,4-Diethoxy-5-methoxyamphetamine	EEM	1-(2,4-diethoxy-5-methoxyphenyl)propan-2-amine	23693-33-6	C14H23NO3	Phenethylamine
2,4-Dimethoxy-5-ethoxyamphetamine	MME	1-(5-ethoxy-2,4-dimethoxyphenyl)propan-2-amine	23693-32-5	C13H21NO3	Phenethylamine
2,4-Dimethoxyamphetamine	2,4-DMA	1-(2,4-dimethoxyphenyl)propan-2-amine	23690-13-3	C11H17NO2	Phenethylamine
2,5,β-Trimethoxy-4-methylphenethylamine	BOD	2-(2,5-dimethoxy-4-methylphenyl)-2-methoxyethanamine	98537-41-8	C12H19NO3	Phenethylamine
2,5-Bismethylthio-4-methylamphetamine	bis-TOM	1-[4-methyl-2,5-bis(methylsulfanyl)phenyl]propan-2-amine		C12H19NS2	Phenethylamine
2,5-Diethoxy-4-methoxyamphetamine	EME	1-(2,5-diethoxy-4-methoxyphenyl)propan-2-amine	23693-34-7	C14H23NO3	Phenethylamine
2,5-Dimethoxy-3,4-(tetramethylene)amphetamine	G-4	1-(1,4-dimethoxy-5,6,7,8-tetrahydronaphthalen-2-yl)propan-2-amine		C15H23NO2	Phenethylamine
2,5-Dimethoxy-3,4-(tetramethylene)phenethylamine	2C-G-4	2-(1,4-dimethoxy-5,6,7,8-tetrahydronaphthalen-2-yl)ethanamine	952006-59-6	C14H21NO2	Phenethylamine
2,5-Dimethoxy-3,4-(trimethylene)amphetamine	G-3	1-(4,7-dimethoxy-2,3-dihydro-1H-inden-5-yl)propan-2-amine		C14H21NO2	Phenethylamine
2,5-Dimethoxy-3,4-(trimethylene)phenethylamine	2C-G-3	2-(4,7-dimethoxy-2,3-dihydro-1H-inden-5-yl)ethanamine	207740-19-0	C13H19NO2	Phenethylamine
2,5-Dimethoxy-3,4-dimethylphenethylamine	2C-G	2-(2,5-dimethoxy-3,4-dimethylphenyl)ethanamine	207740-18-9	C12H19NO2	Phenethylamine
2,5-Dimethoxy-3,4-methylenedioxyamphetamine	DMMDA	1-(4,7-dimethoxy-1,3-benzodioxol-5-yl)propan-2-amine	15183-13-8	C12H17NO4	Phenethylamine
2,5-Dimethoxy-4-(2-fluoroethyl)amphetamine	DOEF	1-[4-(2-fluoroethyl)-2,5-dimethoxyphenyl]propan-2-amine	121649-01-2	C13H20FNO2	Phenethylamine
2,5-Dimethoxy-4-(2-fluoroethylthio)phenethylamine	2C-T-21	2-(4-[(2-fluoroethyl)sulfanyl]-2,5-dimethoxyphenyl)ethanamine	207740-33-8	C12H18FNO2S	Phenethylamine
2,5-Dimethoxy-4-(2-methoxyethylthio)phenethylamine	2C-T-13	2-(2,5-dimethoxy-4-[(2-methoxyethyl)sulfanyl]phenyl)ethanamine	207740-30-5	C13H21NO3S	Phenethylamine
2,5-Dimethoxy-4-Bromo-N-(2-methoxybenzyl)phenethylamine	25B-NBOMe	4-bromo-2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]benzeneethanamine	1026511-90-9	C18H22BrNO3	Phenethylamine
2,5-Dimethoxy-4-bromophenethylamine	2C-B	2-(4-bromo-2,5-dimethoxyphenyl)ethanamine	66142-81-2	C10H14BrNO2	Phenethylamine
2,5-Dimethoxy-4-chloroamphetamine	DOC	1-(4-chloro-2,5-dimethoxyphenyl)-2-propanamine	123431-31-2	C11H16ClNO2	Phenethylamine

2,5-Dimethoxy-4-Chloro-N-(2-methoxybenzyl)phenethylamine	25C-NBOMe	4-chloro-2,5-dimethoxy-N-[(2-methoxyphenyl)methyl]benzeneethanamine	1227608-02-7	C18H22ClNO3	Phenethylamine
2,5-Dimethoxy-4-chlorophenethylamine	2C-C	4-chloro-2,5-dimethoxy-benzeneethanamine	88441-14-9	C10H14ClNO2	Phenethylamine
2,5-Dimethoxy-4-cyclopropylmethylthiophenethylamine	2C-T-8	2-(4-[(cyclopropylmethyl)sulfanyl]-2,5-dimethoxyphenyl)ethanamine	207740-27-0	C14H21NO2S	Phenethylamine
2,5-Dimethoxy-4-cyclopropylthiophenethylamine	2C-T-15	2-[4-(cyclopropylsulfanyl)-2,5-dimethoxyphenyl]ethanamine	952006-95-0	C13H19NO2S	Phenethylamine
2,5-Dimethoxy-4-ethoxyamphetamine	MEM	1-(4-ethoxy-2,5-dimethoxyphenyl)propan-2-amine	16128-88-4	C13H21NO3	Phenethylamine
2,5-Dimethoxy-4-ethylamphetamine	DOET	2,5-dimethoxy-4-ethylamphetamine	22004-32-6	C13H21NO2	Phenethylamine
2,5-Dimethoxy-4-ethylphenethylamine	2C-E	2-(4-ethyl-2,5-dimethoxyphenyl)ethanamine	71539-34-9	C12H19NO2	Phenethylamine
2,5-Dimethoxy-4-ethylthioamphetamine	ALEPH-2	1-[4-(ethylsulfanyl)-2,5-dimethoxyphenyl]propan-2-amine	185562-00-9	C13H21NO2S	Phenethylamine
2,5-Dimethoxy-4-ethylthio-N-hydroxyphenethylamine	HOT-2	2-[4-(ethylsulfanyl)-2,5-dimethoxyphenyl]-N-hydroxyethanamine	207740-38-3	C12H19NO3S	Phenethylamine
2,5-Dimethoxy-4-ethylthiophenethylamine	2C-T-2	2-(4-ethylsulfanyl-2,5-dimethoxyphenyl)ethanamine	207740-24-7	C12H19NO2S	Phenethylamine
2,5-Dimethoxy-4-fluorophenethylamine	2C-F	2-(4-fluoro-2,5-dimethoxyphenyl)ethanamine	207740-15-6	C10H14FNO2	Phenethylamine
2,5-Dimethoxy-4-iodo-N-(2,3-methylenedioxybenzyl)phenethylamine	25I-NBMD	N-(benzo[d][1,3]dioxol-4-ylmethyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine	919797-25-4	C18H20INO4	Phenethylamine
2,5-Dimethoxy-4-iodo-N-(2-methoxybenzyl)phenethylamine	25I-NBOMe	2-(4-iodo-2,5-dimethoxyphenyl)-N-[(2-methoxyphenyl)methyl]ethanamine	919797-19-6	C18H22INO3	Phenethylamine
2,5-Dimethoxy-4-iodophenethylamine	2C-I	2-(4-iodo-3-methoxyphenyl)-2-methoxyethanamine	64584-32-3	C10H14INO2	Phenethylamine
2,5-Dimethoxy-4-isopropoxyphenethylamine	2C-O-4	2-[2,5-dimethoxy-4-(propan-2-yloxy)phenyl]ethanamine		C13H21NO3	Phenethylamine
2,5-Dimethoxy-4-isopropylthioamphetamine	ALEPH-4	1-[4-(isopropylsulfanyl)-2,5-dimethoxyphenyl]-2-propanamine	123643-26-5	C14H23NO2S	Phenethylamine
2,5-Dimethoxy-4-isopropylthiophenethylamine	2C-T-4	2-[4-(isopropylthio)-2,5-dimethoxyphenyl]ethanamine	207740-25-8	C13H21NO2S	Phenethylamine
2,5-Dimethoxy-4-methylamphetamine	DOM	1-(2,5-dimethoxy-4-methylphenyl)propan-2-amine	18539-33-8	C12H19NO2	Phenethylamine
2,5-Dimethoxy-4-methylphenethylamine	2C-D	2-(2,5-dimethoxy-4-methylphenyl)ethanamine	24333-19-5	C11H17NO2	Phenethylamine
2,5-Dimethoxy-4-methylselenophenethylamine	2C-SE	2-[2,5-dimethoxy-4-(methylselanyl)phenyl]ethanamine		C11H17NO2Se	Phenethylamine
2,5-Dimethoxy-4-methylthioamphetamine	ALEPH, DOT	1-(2,5-dimethoxy-4-methylsulfanylphenyl)propan-2-amine	61638-07-1	C12H19NO2S	Phenethylamine
2,5-Dimethoxy-4-methylthiophenethylamine	2C-T	2,5-dimethoxy-4-(methylthio)-benzeneethanamine	61638-09-3	C11H17NO2S	Phenethylamine
2,5-Dimethoxy-4-n-amylamphetamine	DOAM	1-(2,5-dimethoxy-4-pentylphenyl)propan-2-amine	63779-90-8	C16H27NO2	Phenethylamine
2,5-Dimethoxy-4-n-butylamphetamine	DOBU	1-(4-butyl-2,5-dimethoxyphenyl)propan-2-amine	63779-89-5	C15H25NO2	Phenethylamine
2,5-Dimethoxy-4-nitrophenethylamine	2C-N	2,5-dimethoxy-4-nitro-benzeneethanamine	261789-00-8	C10H14N2O4	Phenethylamine
2,5-Dimethoxy-4-n-propylphenethylamine	2C-P	2-(2,5-dimethoxy-4-propylphenyl)ethanamine	207740-22-5	C13H21NO2	Phenethylamine
2,5-Dimethoxy-4-n-propylthioamphetamine	ALEPH-7	1-[2,5-dimethoxy-4-(propylsulfanyl)phenyl]-2-propanamine	207740-16-7	C14H23NO2S	Phenethylamine

2,5-Dimethoxy-4-n-propylthiophenethylamine	2C-T-7	2-(2,5-dimethoxy-4-propylsulfanylphenyl)ethanamine	207740-26-9	C13H21NO2S	Phenethylamine
2,5-Dimethoxy-4-phenylthioamphetamine	ALEPH-6	1-[2,5-dimethoxy-4-(phenylsulfanyl)phenyl]-2-propanamine	952006-44-9	C17H21NO2S	Phenethylamine
2,5-Dimethoxy-4-propoxyamphetamine	MPM	1-(2,5-dimethoxy-4-propoxyphenyl)propan-2-amine		C14H23NO3	Phenethylamine
2,5-Dimethoxy-4-sec-butylthio-N-hydroxyphenethylamine	HOT-17	2-[4-(butan-2-ylsulfanyl)-2,5-dimethoxyphenyl]-N-hydroxyethanamine	207740-40-7	C14H23NO3S	Phenethylamine
2,5-Dimethoxy-4-sec-butylthiophenethylamine	2C-T-17	2-[4-(butan-2-ylsulfanyl)-2,5-dimethoxyphenyl]ethanamine	207740-32-7	C14H23NO2S	Phenethylamine
2,5-Dimethoxy-4-tert-butylthiophenethylamine	2C-T-9	2-[4-(tert-butylsulfanyl)-2,5-dimethoxyphenyl]ethanamine		C14H23NO2S	Phenethylamine
2,5-Dimethoxyamphetamine	2,5-DMA	1-(2,5-dimethoxyphenyl)propan-2-amine	2801-68-5	C11H17NO2	Phenethylamine
2,5-Dimethoxy-N-(2-methoxybenzyl)-4-methylphenethylamine	25D-NBOMe	2-(2,5-dimethoxy-4-methylphenyl)-N-(2-methoxybenzyl)ethanamine	1354632-02-2	C19H25NO3	Phenethylamine
2,5-Dimethoxy-N-(2-methoxybenzyl)phenethylamine	25H-NBOMe	2,5-dimethoxy-*N*-[(2-methoxyphenyl) methyl]benzeneethanamine	919797-16-3	C18H23NO3	Phenethylamine
2,5-Dimethoxy-N,N-dimethyl-4-iodoamphetamine	IDNNA	1-(4-iodo-2,5-dimethoxyphenyl)-N,N-dimethylpropan-2-amine	67707-78-2	C13H20INO2	Phenethylamine
2,5-Dimethoxy-N-hydroxy-4-n-propylthiophenethylamine	HOT-7	2-[2,5-dimethoxy-4-(propylsulfanyl)phenyl]-N-hydroxyethanamine	207740-39-4	C13H21NO3S	Phenethylamine
2,5-Dimethoxy-N-methylamphetamine	Methyl-DMA	1-(2,5-dimethoxyphenyl)-N-methylpropan-2-amine	54687-43-3	C12H19NO2	Phenethylamine
2,5-Dimethoxyphenethylamine	2C-H	2-(2,5-dimethoxyphenyl)ethanamine	3600-86-0	C10H15NO2	Phenethylamine
2,5-Dimethoxy-β-hydroxy-4-methylphenethylamine	BOHD	2-amino-1-(2,5-dimethoxy-4-methylphenyl)ethanol	29348-16-1	C11H17NO3	Phenethylamine
2,6-Dimethoxy-4-isopropylthiophenethylamine	2C-T-4 (Ψ homologue)	2-[4-(isopropylthio)-2,6-dimethoxyphenyl]ethanamine		C13H21NO2S	Phenethylamine
2,6-Dimethoxy-4-methylamphetamine	DOM (Ψ homologue)	1-(2,6-dimethoxy-4-methylphenyl)propan-2-amine		C12H19NO2	Phenethylamine
2,N-Dimethyl-4,5-methylenedioxyamphetamine	MADAM-6	N-methyl-1-(6-methyl-1,3-benzodioxol-5-yl)propan-2-amine	207740-46-3	C12H17NO2	Phenethylamine
25B-NBF	2C-B-NBF	2-(4-Bromo-2,5-dimethoxyphenyl)-N-(2-fluorobenzyl)ethan-1-amine		C17H19BrFNO2	Phenethylamine
25B-NBOH		2-({[2-(4-Bromo-2,5-dimethoxyphenyl)ethyl]amino}methyl)phenol		C17H20BrNO3	Phenethylamine
25C-NB3OMe	-	2-(4-Chloro-2,5-dimethoxyphenyl)-N-(3-methoxybenzyl)ethan-1-amine		C18H22ClNO3	Phenethylamine
25C-NBF		2-(4-Chloro-2,5-dimethoxyphenyl)-N-(2-fluorobenzyl)ethan-1-amine		C17H19ClFNO2	Phenethylamine
25C-NBOH		2-[[[2-(4-chloro-2,5-dimethoxyphenyl)ethyl]amino]methyl]-phenol		C17H20ClNO3	Phenethylamine
25E-NBOMe		2-(4-ethyl-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethan-1-amine		C20H27NO3	Phenethylamine
25G-NBOMe		2-(2,5-Dimethoxy-3,4-dimethylphenyl)-N-(2-methoxybenzyl)ethan-1-amine		C20H27NO3	Phenethylamine
25H-NBOMe imine analog		(e)-2-(2,5-dimethoxyphenyl)-N-(2-methoxybenzylidene)ethanamine		C18H21NO3	Phenethylamine
25I-NBOH		2-({[2-(4-Iodo-2,5-dimethoxyphenyl)ethyl]amino}methyl)phenol		C17H20INO3	Phenethylamine

25I-NBOMe 3-methoxy isomer		2-(4-iodo-2,5-dimethoxyphenyl)-N-(3-methoxybenzyl)ethan-1-amine		C18H22INO3	Phenethylamine
25I-NBOMe 4-methoxy isomer		2-(4-iodo-2,5-dimethoxyphenyl)-N-(4-methoxybenzyl)ethan-1-amine		C18H22INO3	Phenethylamine
25I-NBOMe imine analog		(e)-2-(4-iodo-2,5-dimethoxyphenyl)-N-(2-methoxybenzylidene)ethanamine		C18H20INO3	Phenethylamine
25iP-NBOMe		2-(4-isopropyl-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethan-1-amine		C21H29NO3	Phenethylamine
25N-NBOMe		2-(2,5-dimethoxy-4-nitrophenyl)-N-(2-methoxybenzyl)ethanamine		C18H22N2O5	Phenethylamine
25T2-NBOMe		2-[4-(Ethylsulfanyl)-2,5-dimethoxyphenyl]-N-(2-methoxybenzyl)ethan-1-amine		C20H27NO3S	Phenethylamine
25T4-NBOMe		2-[2,5-Dimethoxy-4-(propan-2-ylsulfanyl)phenyl]-N-(2-methoxybenzyl)ethan-1-amine		C21H29NO3S	Phenethylamine
25T7-NBOMe		2-[2,5-Dimethoxy-4-(propylsulfanyl)phenyl]-N-(2-methoxybenzyl)ethan-1-amine		C21H29NO3S	Phenethylamine
2-Bromo-4,5-methylenedioxyamphetamine	6-Br-MDA	1-(6-bromo-1,3-benzodioxol-5-yl)propan-2-amine		C10H12BrNO2	Phenethylamine
2C-B-Fly		2-(4-bromo-2,3,6,7-tetrahydrofuro[2,3-f][1]benzofuran-8-yl)ethanamine	178557-21-6	C12H14BrNO2	Phenethylamine
2C-iP		2-[2,5-Dimethoxy-4-(propan-2-yl)phenyl]ethan-1-amine		C13H21NO2	Phenethylamine
2C-TFM		2-[2,5-Dimethoxy-4-(trifluoromethyl)phenyl]ethan-1-amine		C11H14F3NO2	Phenethylamine
2-Ethoxy-4,5-dimethoxyamphetamine	EMM	1-(2-ethoxy-4,5-dimethoxyphenyl)propan-2-amine	23693-30-3	C13H21NO3	Phenethylamine
2-Ethylamino-1-(3,4-methylenedioxyphenyl)butane	EBDB, Ethyl-J	1-(1,3-benzodioxol-5-yl)-N-ethylbutan-2-amine	167394-39-0	C13H19NO2	Phenethylamine
2-Fluoroamphetamine	2-FA	1-(2-fluorophenyl)propan-2-amine	1716-60-5	C9H12FN	Phenethylamine
2-Fluoromethamphetamine	2-FMA	2-fluoro-N,α-dimethyl-benzeneethanamine	1017176-48-5	C10H14FN	Phenethylamine
2-Methoxy-3,4-methylenedioxyamphetamine	MMDA-3a	1-(4-methoxy-1,3-benzodioxol-5-yl)propan-2-amine		C11H15NO3	Phenethylamine
2-Methoxy-4,5-diethoxyamphetamine	MEE	1-(4,5-diethoxy-2-methoxyphenyl)propan-2-amine	23693-35-8	C14H23NO3	Phenethylamine
2-Methoxy-4,5-methylenedioxyamphetamine	MMDA-2	1-(6-methoxy-2H-benzo[d]1,3-dioxolan-5-yl)prop-2-ylamine	23693-18-7	C11H15NO3	Phenethylamine
2-Methoxy-4-methyl-5-methylsulfinylamphetamine	TOMSO	1-[2-methoxy-4-methyl-5-(methylsulfinyl)phenyl]propan-2-amine		C12H19NO2S	Phenethylamine
2-Methoxy-4-methyl-5-methylthioamphetamine	5-TOM	1-[2-methoxy-4-methyl-5-(methylsulfanyl)phenyl]propan-2-amine		C12H19NOS	Phenethylamine
2-Methoxyamphetamine	2-MeO-Amp	1-(2-methoxyphenyl)propan-2-amine	15402-84-3	C10H15NO	Phenethylamine
2-Methoxymethamphetamine	2-MeO-MA	2-methoxy-N,α-dimethyl-benzeneethanamine	93-30-1	C11H17NO	Phenethylamine
2-Methoxy-N-methyl-4,5-methylenedioxyamphetamine	Methyl-MMDA-2	1-(6-methoxy-1,3-benzodioxol-5-yl)-N-methylpropan-2-amine		C12H17NO3	Phenethylamine
2-Methylamino-1-(3,4-methylenedioxyphenyl)butane	MBDB	1-(1,3-benzodioxol-5-yl)-N-methylbutan-2-amine	103818-46-8	C12H17NO2	Phenethylamine
2-Methylamino-1-phenylbutane		α-ethyl-N-methyl-benzeneethanamine		C11H17N	Phenethylamine
2-Methylamphetamine	2-MA	1-(2-methylphenyl)propan-2-amine	5580-32-5	C10H15N	Phenethylamine

2-Methylmethamphetamine	2-MMA	N,α,2-trimethyl-benzeneethanamine	861007-65-0	C11H17N	Phenethylamine
2-Thioisomescaline	2-TIM	2-[3,4-dimethoxy-2-(methylsulfanyl)phenyl]ethanamine		C11H17NO2S	Phenethylamine
2-TOM	2-TOM	1-[5-methoxy-4-methyl-2-(methylsulfanyl)phenyl]propan-2-amine		C12H19NOS	Phenethylamine
3,4,5,β-Tetramethoxyphenethylamine	BOM	2-methoxy-2-(3,4,5-trimethoxyphenyl)ethanamine	98537-40-7	C12H19NO4	Phenethylamine
3,4-Dihydroxymethamphetamine	HHMA	4-[2-(methylamino)propyl]-1,2-benzenediol		C10H15NO2	Phenethylamine
3,4-Dimethoxyamphetamine	3,4-DMA	1-(3,4-dimethoxyphenyl)propan-2-amine	120-26-3	C11H17NO2	Phenethylamine
3,4-Dimethoxymethamphetamine	3,4-DMMA	3,4-dimethoxy-N,α-dimethyl-benzeneethanamine	33236-61-2	C12H19NO2	Phenethylamine
3,4-Dimethoxy-N,N,α-trimethyl-amphetamine		3,4-dimethoxy-N,N,α-trimethyl-benzeneethanamine	58993-77-4	C13H21NO2	Phenethylamine
3,4-Dimethoxyphenethylamine	DMPEA	2-(3,4-dimethoxyphenyl)ethanamine	120-20-7	C10H15NO2	Phenethylamine
3,4-Dimethoxy-β-hydroxyphenethylamine	DME	2-amino-1-(3,4-dimethoxyphenyl)ethanol	6924-15-8	C10H15NO3	Phenethylamine
3,4-Dimethyl-2,5-dimethoxyamphetamine	Ganesha	2-(2,5-dimethoxy-3,4-dimethyl-phenyl)-1-methyl-ethylamine	207740-37-2	C13H21NO2	Phenethylamine
3,4-Ethylenedioxy-N-methylamphetamine	EDMA	1-(2,3-dihydro-1,4-benzodioxin-6-yl)-N-methylpropan-2-amine		C12H17NO2	Phenethylamine
3,4-Methylenedioxy-2-methylthioamphetamine	2T-MMDA-3a	1-[4-(methylsulfanyl)-1,3-benzodioxol-5-yl]propan-2-amine		C11H15NO2S	Phenethylamine
3,4-Methylenedioxyamphetamine	MDA	1-(1,3-benzodioxol-5-yl)propan-2-amine	4764-17-4	C10H13NO2	Phenethylamine
3,4-Methylenedioxy-N-(2-methoxyethyl)amphetamine	MDMEOET	1-(1,3-benzodioxol-5-yl)-N-(2-methoxyethyl)propan-2-amine	74698-44-5	C13H19NO3	Phenethylamine
3,4-Methylenedioxy-N,N-dimethylamphetamine	MDDM	1-(1,3-benzodioxol-5-yl)-N,N-dimethylpropan-2-amine	74698-50-3	C12H17NO2	Phenethylamine
3,4-Methylenedioxy-N-allylamphetamine	MDAL	N-[1-(1,3-benzodioxol-5-yl)propan-2-yl]prop-2-en-1-amine	74698-45-6	C13H17NO2	Phenethylamine
3,4-Methylenedioxy-N-benzylamphetamine	MDBZ	1-(1,3-benzodioxol-5-yl)-N-benzylpropan-2-amine	65033-29-6	C17H19NO2	Phenethylamine
3,4-Methylenedioxy-N-butylamphetamine	MDBU	N-[1-(1,3-benzodioxol-5-yl)propan-2-yl]butan-1-amine	74698-38-7	C14H21NO2	Phenethylamine
3,4-Methylenedioxy-N-cyclopropylmethylamphetamine	MDCPM	1-(1,3-benzodioxol-5-yl)-N-(cyclopropylmethyl)propan-2-amine	22698-08-4	C14H19NO2	Phenethylamine
3,4-Methylenedioxy-N-ethylamphetamine	MDEA	1-(1,3-benzodioxol-5-yl)-N-ethylpropan-2-amine	82801-81-8	C12H17NO2	Phenethylamine
3,4-Methylenedioxy-N-ethyl-α-propylphenethylamine	EBDP, Ethyl-K	1-(1,3-benzodioxol-5-yl)-N-ethylpentan-2-amine	952016-47-6	C14H21NO2	Phenethylamine
3,4-Methylenedioxy-N-hydroxyethylamphetamine	MDHOET	2-([1-(1,3-benzodioxol-5-yl)propan-2-yl]amino)ethanol	74698-43-4	C12H17NO3	Phenethylamine
3,4-Methylenedioxy-N-hydroxy-N-methylamphetamine	MDHMA	1-(1,3-benzodioxol-5-yl)-N-hydroxy-N-methylpropan-2-amine	214414-88-7	C11H15NO3	Phenethylamine
3,4-Methylenedioxy-N-isopropylamphetamine	N-Isopropyl-MDA	1-(1,3-benzodioxol-5-yl)-N-(propan-2-yl)propan-2-amine	74698-37-6	C13H19NO2	Phenethylamine
3,4-Methylenedioxy-N-methylamphetamine	MDMA	1-(1,3-benzodioxol-5-yl)-N-methylpropan-2-amine	42542-10-9	C11H15NO2	Phenethylamine
3,4-Methylenedioxy-N-methylphentermine	MDMP	1-(1,3-benzodioxol-5-yl)-N,2-dimethylpropan-2-amine	81262-69-3	C12H17NO2	Phenethylamine

3,4-Methylenedioxy-N-methyoxyamphetamine	MDMEO	1-(1,3-benzodioxol-5-yl)-N-methoxypropan-2-amine	74698-48-9	C11H15NO3	Phenethylamine
3,4-Methylenedioxy-N-propargylamphetamine	MDPL	N-[1-(1,3-benzodioxol-5-yl)propan-2-yl]prop-2-yn-1-amine	74698-46-7	C13H15NO2	Phenethylamine
3,4-Methylenedioxy-N-propylamphetamine	MDPR	N-[1-(1,3-benzodioxol-5-yl)propan-2-yl]propan-1-amine	74698-36-5	C13H19NO2	Phenethylamine
3,4-Methylenedioxyphenethylamine	MDPEA	2-(1,3-benzodioxol-5-yl)ethanamine	1484-85-1	C9H11NO2	Phenethylamine
3,4-Methylenedioxyphentermine	MDPH	1-(1,3-benzodioxol-5-yl)-2-methylpropan-2-amine	39235-63-7	C11H15NO2	Phenethylamine
3,4-Methylenedioxy-α-propyl-N-methylphenethylamine	MBDP	1-(1,3-benzodioxol-5-yl)-N-methylpentan-2-amine	952016-78-3	C13H19NO2	Phenethylamine
3,4-Methylenedioxy-β-methoxyphenethylamine	BOH	2-(1,3-benzodioxol-5-yl)-2-methoxyethanamine	73304-06-0	C10H13NO3	Phenethylamine
3,4-Norbornyl-2,5-dimethoxyamphetamine	G-5	1-(5,8-dimethoxy-1,2,3,4-tetrahydro-1,4-methanonaphthalen-6-yl)propan-2-amine		C16H23NO2	Phenethylamine
3,4-Norbornyl-2,5-dimethoxyphenethylamine	2C-G-5	2-(5,8-dimethoxy-1,2,3,4-tetrahydro-1,4-methanonaphthalen-6-yl)ethanamine	207740-20-3	C15H21NO2	Phenethylamine
3,5-Dimethoxy-4-ethoxyamphetamine	3C-E	1-(4-ethoxy-3,5-dimethoxyphenyl)propan-2-amine	146849-92-5	C13H21NO3	Phenethylamine
3,5-Dimethoxy-4-n-propoxyamphetamine	3C-P	3,5-dimethoxy-α-methyl-4-propoxy-benzeneethanamine	501700-11-4	C14H23NO3	Phenethylamine
3,5-Methoxy-4-trideutero methoxy phenethylamine	4-D	3,5-Methoxy-4-trideuteromethoxyphenethylamine		C11H14D3NO3	Phenethylamine
30C-NBOMe		2-(4-chloro-2,5-dimethoxyphenyl)-N-(3,4,5-trimethoxybenzyl)ethanamine		C20H26ClNO5	Phenethylamine
3C-B-FLY		8-bromo-2,3,6,7-tetrahydro-a-methyl-benzo[1,2-b:4,5-b]difuran-4-ethanamine	219986-75-1	C13H16BrNO2	Phenethylamine
3-Fluoro-4-methoxyamphetamine		1-(3-fluoro-4-methoxyphenyl)propan-2-amine	863667-46-3	C10H14FNO	Phenethylamine
3-Fluoroamphetamine	3-FA	1-(3-fluorophenyl)-2-propanamine	1626-71-7	C9H12FN	Phenethylamine
3-Fluoromethamphetamine	3-FMA	3-fluoro-N,α-dimethyl-benzeneethanamine	1182818-14-9	C10H14FN	Phenethylamine
3-Methoxy-4,5-ethylenedioxyamphetamine	MEDA	1-(8-methoxy-2,3-dihydro-1,4-benzodioxin-6-yl)propan-2-amine	23693-25-6	C12H17NO3	Phenethylamine
3-Methoxy-4,5-methylenedioxyamphetamine	MMDA	1-(7-methoxy-1,3-benzodioxol-5-yl)propan-2-amine	13674-05-0	C11H15NO3	Phenethylamine
3-Methoxy-4,5-methylenedioxyphenethylamine	MMDPEA	2-(7-methoxy-1,3-benzodioxol-5-yl)ethanamine	23693-38-1	C10H13NO3	Phenethylamine
3-Methoxy-4-allyloxy-phenethylamine	MAPEA	2-[3-Methoxy-4-(prop-2-en-1-yloxy)phenyl]ethanamine		C11H15NO2	Phenethylamine
3-Methoxy-4-ethoxyphenethylamine	MEPEA	2-(4-ethoxy-3-methoxyphenyl)ethanamine	36377-59-0	C11H17NO2	Phenethylamine
3-Methoxyamphetamine		1-(3-methoxyphenyl)propan-2-amine	17862-85-0	C10H15NO	Phenethylamine
3-Methoxymethamphetamine	3-MeO-MA	1-(3-methoxyphenyl)-N-methylpropan-2-amine	124206-66-2	C11H17NO	Phenethylamine
3-Methoxytyramine	3-MT	4-(2-aminoethyl)-2-methoxyphenol		C9H13NO2	Phenethylamine
3-Methyl-4,5-methylenedioxyamphetamine	5-Me-MDA	1-(7-methyl-1,3-benzodioxol-5-yl)-2-propanamine	749191-14-8	C11H15NO2	Phenethylamine
3-Methylamphetamine	3-MA	1-(3-methylphenyl)propan-2-amine	588-06-7	C10H15N	Phenethylamine

3-Methylmethamphetamine	3-MMA	N-methyl-1-(3-methylphenyl)-2-propanamine	861007-68-3	C11H17N	Phenethylamine
3-Thioasymbescaline	3-TASB	2-[4-ethoxy-3-(ethylsulfanyl)-5-methoxyphenyl]ethanamine		C13H21NO2S	Phenethylamine
3-Thioescaline	3-TE	2-[4-ethoxy-3-methoxy-5-(methylsulfanyl)phenyl]ethanamine		C12H19NO2S	Phenethylamine
3-Thioisomescaline	3-TIM	2-[2,4-dimethoxy-3-(methylsulfanyl)phenyl]ethanamine		C11H17NO2S	Phenethylamine
3-Thiomescaline	3-TM	2-[3,4-dimethoxy-5-(methylsulfanyl)phenyl]ethanamine		C11H17NO2S	Phenethylamine
3-Thiometaescaline	3-TME	2-[3-(ethylsulfanyl)-4,5-dimethoxyphenyl]ethanamine		C12H19NO2S	Phenethylamine
3-Thiosymbescaline	3-TSB	2-[3-ethoxy-5-(ethylsulfanyl)-4-methoxyphenyl]ethanamine		C13H21NO2S	Phenethylamine
3-Thiotrescaline	3-T-TRIS	2-[3,4-diethoxy-5-(ethylsulfanyl)phenyl]ethanamine		C14H23NO2S	Phenethylamine
4,5-Dimethoxy-2-methylthioamphetamine	o-DOT	1-[4,5-dimethoxy-2-(methylsulfanyl)phenyl]propan-2-amine		C12H19NO2S	Phenethylamine
4,5-Thiomethyleneoxy-2-methoxyamphetamine	4T-MMDA-2	1-(5-methoxy-1,3-benzoxathiol-6-yl)propan-2-amine		C11H15NO2S	Phenethylamine
4-APB		α-methyl-4-benzofuranethanamine		C11H13NO	Phenethylamine
4-Benzyloxy-3,5-dimethoxyamphetamine	3C-BZ	1-[4-(benzyloxy)-3,5-dimethoxyphenyl]propan-2-amine	147947-26-0	C18H23NO3	Phenethylamine
4-Bromo-2,5-dimethoxy-N-methylamphetamine	Methyl-DOB	1-(4-bromo-2,5-dimethoxyphenyl)-N-methylpropan-2-amine	155638-80-5	C12H18BrNO2	Phenethylamine
4-Bromo-2,5-β-trimethoxyphenethylamine	BOB	2-(4-bromo-2,5-dimethoxyphenyl)-2-methoxyethanamine	98537-42-9	C11H16BrNO3	Phenethylamine
4-Bromo-3,5-dimethoxyamphetamine		1-(4-bromo-3,5-dimethoxyphenyl)propan-2-amine		C11H16BrNO2	Phenethylamine
4-Chlorophenylisobutylamine	4-CAB	1-(4-chlorophenyl)butan-2-amine		C10H14ClN	Phenethylamine
4-Cyclopropylmethoxy-3,5-dimethoxyphenethylamine	CPM	2-[4-(cyclopropylmethoxy)-3,5-dimethoxyphenyl]ethanamine	207740-23-6	C14H21NO3	Phenethylamine
4-Ethyl-2-methoxy-5-methylthioamphetamine	5-TOET	1-[4-ethyl-2-methoxy-5-(methylsulfanyl)phenyl]propan-2-amine		C13H21NOS	Phenethylamine
4-Fluoroamphetamine	4-FA	1-(4-fluorophenyl)-2-propanamine	459-02-9	C9H12FN	Phenethylamine
4-Fluoromethamphetamine	4-FMA	1-(4-fluorophenyl)-N-methyl-2-propanamine	351-03-1	C10H14FN	Phenethylamine
4-Hydroxy-3-methoxyamphetamine	HMA	5-(2-aminopropyl)-2-methoxyphenol		C10H15NO2	Phenethylamine
4-Hydroxy-3-methoxyethylamphetamine	HMEA	4-[2-(ethylamino)propyl]-2-methoxyphenol	69389-97-5	C12H19NO2	Phenethylamine
4-Hydroxy-3-methoxymethamphetamine	HMMA	2-methoxy-5-[2-(methylamino)propyl]phenol		C11H17NO2	Phenethylamine
4-Hydroxyamphetamine	4-HA	4-(2-aminopropyl)phenol	103-86-6	C9H13NO	Phenethylamine
4-Hydroxymethamphetamine	4-HO-MA	4-[2-(methylamino)propyl]phenol	370-14-9	C10H15NO	Phenethylamine
4-Iodo-2,5-dimethoxyamphetamine	DOI	1-(4-iodo-2,5-dimethoxyphenyl)propan-2-amine	64584-34-5	C11H16INO2	Phenethylamine
4-MAPB		1-(benzofuran-4-yl)-N-methylpropan-2-amine		C12H15NO	Phenethylamine

4-Methoxy-2,3-methylenedioxyamphetamine	MMDA-3b	1-(7-methoxy-1,3-benzodioxol-4-yl)propan-2-amine		C11H15NO3	Phenethylamine
4-Methoxyamphetamine	PMA	1-(4-methoxyphenyl)propan-2-amine	64-13-1	C10H15NO	Phenethylamine
4-Methoxyethylamphetamine	PMEA	N-ethyl-1-(4-methoxyphenyl)propan-2-amine	14367-46-5	C12H19NO	Phenethylamine
4-Methoxymethamphetamine	PMMA	1-(4-methoxyphenyl)-N-methylpropan-2-amine	22331-70-0	C11H17NO	Phenethylamine
4-Methoxyphenylethylamine		2-(4-methoxyphenyl)ethylamine	55-81-2	C9H13NO	Phenethylamine
4-Methyl-2,5-dimethoxymethamphetamine	MDOM	1-(2,5-dimethoxy-4-methylphenyl)-N-methylpropan-2-amine	92206-37-6	C13H21NO2	Phenethylamine
4-Methyl-3,5-dimethoxyphenethylamine	DESOXY	2-(3,5-dimethoxy-4-methylphenyl)ethanamine	63037-49-0	C11H17NO2	Phenethylamine
4-Methylamphetamine	4-MA	1-(4-methylphenyl)propan-2-amine	22683-78-9	C10H15N	Phenethylamine
4-Methylmethamphetamine	4-MMA	N-methyl-1-(4-methylphenyl)-2-propanamine	714965-56-7	C11H17N	Phenethylamine
4-Methylthioamphetamine	4-MTA	1-(4-methylsulfanylphenyl)propan-2-amine	14116-06-4	C10H15NS	Phenethylamine
4-Methylthiobutylamphetamine	4-MTBA	4-(2-methyliminohydrazinyl)benzoic acid	40843-84-3	C8H9N3O2	Phenethylamine
4-Methylthiodimethamphetamine	4-MTDMA	N,N-dimethyl-1-(4-methylsulfanylphenyl)propan-2-amine	634607-25-3	C12H19NS	Phenethylamine
4-Methylthioethylamphetamine	4-MTEA	N-ethyl-1-[4-(methylsulfanyl)phenyl]propan-2-amine	634607-27-5	C12H19NS	Phenethylamine
4-Methylthiomethamphetamine	4-MTMA	N-methyl-1-(4-methylsulfanylphenyl)propan-2-amine	547736-90-3	C11H17NS	Phenethylamine
4-Methylthiopropylamphetamine	4-MTPA	α-methyl-4-(methylthio)-N-propyl-benzeneethanamine	634607-29-7	C13H21NS	Phenethylamine
4-Nitro-2,5-dimethoxyamphetamine	DON	1-(2,5-dimethoxy-4-nitrophenyl)propan-2-amine	67460-68-8	C11H16N2O4	Phenethylamine
4-Propyl-2,5-dimethoxyamphetamine	DOPR	1-(2,5-dimethoxy-4-propylphenyl)propan-2-amine	63779-88-4	C14H23NO2	Phenethylamine
4-propynyloxy-3,5-dimethoxyphenethylamine	Propynyl	2-[3,5-dimethoxy-4-(prop-2-yn-1-yloxy)phenyl]ethanamine	952017-05-9	C13H17NO3	Phenethylamine
4-Thioasymbescaline	4-TASB	2-[3-ethoxy-4-(ethylsulfanyl)-5-methoxyphenyl]ethanamine		C13H21NO2S	Phenethylamine
4-Thiobuscaline	TB	2-[4-(butylsulfanyl)-3,5-dimethoxyphenyl]ethanamine		C14H23NO2S	Phenethylamine
4-Thioescaline	4-TE	2-[4-(ethylsulfanyl)-3,5-dimethoxyphenyl]ethanamine		C12H19NO2S	Phenethylamine
4-Thioisomescaline	4-TIM	2-[2,3-dimethoxy-4-(methylsulfanyl)phenyl]ethanamine		C11H17NO2S	Phenethylamine
4-Thiomescaline	4-TM	2-[3,5-dimethoxy-4-(methylsulfanyl)phenyl]ethanamine		C11H17NO2S	Phenethylamine
4-Thiometaescaline	4-TME	2-[3-ethoxy-5-methoxy-4-(methylsulfanyl)phenyl]ethanamine		C12H19NO2S	Phenethylamine
4-Thiosymbescaline	4-TSB	2-[3,5-diethoxy-4-(methylsulfanyl)phenyl]ethanamine		C13H21NO2S	Phenethylamine
4-Thiotrescaline	4-T-TRIS	2-[3,5-diethoxy-4-(ethylsulfanyl)phenyl]ethanamine		C14H23NO2S	Phenethylamine
5-(2-Aminopropyl)-2,3-dihydrobenzofuran	5-APDB	2,3-dihydro-α-methyl-5-benzofuranethanamine	152624-03-8	C11H15NO	Phenethylamine

5-(2-Aminopropyl)benzofuran	5-APB	1-(1-benzofuran-5-yl)-2-propanamine	286834-81-9	C11H13NO	Phenethylamine
5-Bromo-2,4-dimethoxyamphetamine	meta-DOB	1-(5-bromo-2,4-dimethoxyphenyl)propan-2-amine	60917-67-1	C11H16BrNO2	Phenethylamine
5-Ethoxy-2-methoxy-4-methylamphetamine	5-Et-DOM	1-(5-ethoxy-2-methoxy-4-methylphenyl)propan-2-amine		C13H21NO2	Phenethylamine
5-Fluoro-2-methoxyamphetamine		1-(5-fluoro-2-methoxyphenyl)propan-2-amine	863667-45-2	C10H14FNO	Phenethylamine
5-Methylthio-2,4-dimethoxyamphetamine	meta-DOT	1-[2,4-dimethoxy-5-(methylsulfanyl)phenyl]propan-2-amine	79440-52-1	C12H19NO2S	Phenethylamine
5-Thioasymbescaline	5-TASB	2-[3,4-diethoxy-5-(methylsulfanyl)phenyl]ethanamine		C13H21NO2S	Phenethylamine
5-Thiometaescaline	5-TME	2-[3-ethoxy-4-methoxy-5-(methylsulfanyl)phenyl]ethanamine		C12H19NO2S	Phenethylamine
6-(2-Aminopropyl)-2,2-dimethyl-5-methoxy-2,3-dihydrobenzofuran	F-22	1-(5-methoxy-2,2-dimethyl-2,3-dihydro-1-benzofuran-6-yl)propan-2-amine	952016-51-2	C14H21NO2	Phenethylamine
6-(2-Aminopropyl)-2,3-dihydrobenzofuran	6-APDB	1-(2,3-dihydro-1-benzofuran-6-yl)propan-2-amine	152623-93-3	C11H15NO	Phenethylamine
6-(2-Aminopropyl)-5-methoxy-2-methyl-2,3-dihydrobenzofuran	F-2	1-(5-methoxy-2-methyl-2,3-dihydro-1-benzofuran-6-yl)propan-2-amine		C13H19NO2	Phenethylamine
6-(2-Aminopropyl)benzofuran	6-APB	1-(1-benzofuran-6-yl)-2-propanamine	286834-85-3	C11H13NO	Phenethylamine
Allylescaline		2-[4-(allyloxy)-3,5-dimethoxyphenyl]ethanamine		C12H17NO3	Phenethylamine
Amphetamine		1-phenylpropan-2-amine	300-62-9	C9H13N	Phenethylamine
Ariadne	α-Et-DOM	1-(2,5-dimethoxy-4-methylphenyl)butan-2-amine	52842-59-8	C13H21NO2	Phenethylamine
Asymbescaline		2-(3,4-diethoxy-5-methoxyphenyl)ethanamine	63918-08-1	C13H21NO3	Phenethylamine
Benzodioxolylbutanamine	BDB	1-(1,3-benzodioxol-5-yl)butan-2-amine	107447-03-0	C11H15NO2	Phenethylamine
Bromo-DragonFLY		(2R)-1-(8-bromofuro[2,3-f][1]benzofuran-4-yl)-2-propanamine	502759-67-3	C13H12BrNO2	Phenethylamine
Bromo-DragonFLY		8-bromo-α-methyl-benzo[1,2-b:4,5-b]difuran-4-ethanamine		C13H12BrNO2	Phenethylamine
Buscaline		2-(4-butoxy-3,5-dimethoxyphenyl)ethanamine	64778-75-2	C14H23NO3	Phenethylamine
Dimethoxybromoamphetamine	DOB	2,5-dimethoxy-4-bromoamphetamine	64638-07-9	C11H16BrNO2	Phenethylamine
Dimethylamphetamine	N,N-DMA	N,N-dimethyl-1-phenylpropan-2-amine	4075-96-1	C11H17N	Phenethylamine
Dimethylphenethylamine		N,N-dimethyl-2-phenylethanamine	1126-71-2	C10H15N	Phenethylamine
Escaline		3,5-dimethoxy-4-ethoxy-phenethylamine	39201-82-6	C12H19NO3	Phenethylamine
Ethylamphetamine		N-ethyl-1-phenylpropan-2-amine	457-87-4	C11H17N	Phenethylamine
Hordenine		4-(2-dimethylaminoethyl)phenol	539-15-1	C10H15NO	Phenethylamine
Isomescaline		2-(2,3,4-trimethoxyphenyl)ethanamine		C11H17NO3	Phenethylamine
Isoproscaline		2-[3,5-dimethoxy-4-(propan-2-yloxy)phenyl]ethanamine		C13H21NO3	Phenethylamine

Mescaline		2-(3,4,5-trimethoxyphenyl)ethanamine	54-04-6	C11H17NO3	Phenethylamine
Mescaline NBOMe		N-(2-methoxybenzyl)-3,4,5-trimethoxyphenethylamine		C19H25NO4	Phenethylamine
Metaescaline		2-(3-ethoxy-4,5-dimethoxyphenyl)ethanamine		C12H19NO3	Phenethylamine
Metaproscaline		2-(3,4-dimethoxy-5-propoxyphenyl)ethanamine		C13H21NO3	Phenethylamine
Methallylescaline		2-(3,5-dimethoxy-4-[(2-methylprop-2-en-1-yl)oxy]phenyl)ethanamine		C14H21NO3	Phenethylamine
Methamphetamine		(2S)-N-methyl-1-phenylpropan-2-amine	537-46-2	C10H15N	Phenethylamine
Methylthio-ethyl-methoxyamphetamine	2-TOET	1-[4-ethyl-5-methoxy-2-(methylsulfanyl)phenyl]propan-2-amine		C13H21NOS	Phenethylamine
N-(2-Fluorobenzyl)-4-iodo-2,5-dimethoxyphenethylamine	25I-NBF	N-(2-fluorobenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine	919797-21-0	C17H19FINO2	Phenethylamine
N-Acetyl 4,4-methylene dianiline	N-Acetyl-MDA	N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl] acetamide	36209-71-9	C12H15NO3	Phenethylamine
N-Ethyl-4-fluoroamphetamine	N-Ethyl-4-FA	N-ethyl-1-(4-fluorophenyl)-2-propanamine		C11H16FN	Phenethylamine
N-Hydroxy-3,4-methylenedioxyamphetamine	N-HO-MDA	1-(1,3-benzodioxol-5-yl)-N-hydroxypropan-2-amine	74698-47-8	C10H13NO3	Phenethylamine
N-Hydroxy-4-fluoroamphetamine	N-HO-4-FA	4-fluoro-*N*-hydroxy-α-methyl-benzeneethanamine	1112937-74-2	C9H12FNO	Phenethylamine
Phenescaline		2-[3,5-dimethoxy-4-(2-phenylethoxy)phenyl]ethanamine	207740-42-9	C18H23NO3	Phenethylamine
Phenethylamine		2-phenylethanamine	64-04-0	C8H11N	Phenethylamine
Propylamphetamine		N-(1-methyl-2-phenylethyl)propan-1-amine	51799-32-7	C12H19N	Phenethylamine
Proscaline		3,5-dimethoxy-4-n-propoxy-phenethylamine	39201-78-0	C13H21NO3	Phenethylamine
Symbescaline		2-(3,5-diethoxy-4-methoxyphenyl)ethanamine	90109-61-8	C13H21NO3	Phenethylamine
Thioproscaline		2-[3,5-dimethoxy-4-(propylsulfanyl)phenyl]ethanamine	90109-55-0	C13H21NO2S	Phenethylamine
Trescaline		2-(3,4,5-triethoxyphenyl)ethanamine		C14H23NO3	Phenethylamine
Trimethoxyamphetamine	TMA	1-(3,4,5-trimethoxyphenyl)propan-2-amine	1082-88-8	C12H19NO3	Phenethylamine
α-Ethylmescaline		1-(3,4,5-trimethoxyphenyl)butan-2-amine	17097-73-3	C13H21NO3	Phenethylamine
α-Ethyl-N-methylpiperonylamine	M-ALPHA	α-ethyl-N-methyl-1,3-benzodioxole-5-methanamine	127292-43-7	C11H15NO2	Phenethylamine
α-Ethylphenethylamine	AEPEA	1-phenylbutan-2-amine	53309-89-0	C10H15N	Phenethylamine
β-Methylphenethylamine	BMPEA	β-methyl-benzeneethanamine		C9H13N	Phenethylamine
JWH-167		1-(1-pentyl-1H-indol-3-yl)-2-phenyl-ethanone	864445-37-4	C21H23NO	Phenylacetylindole
JWH-201		2-(4-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl) ethanone	864445-47-6	C22H25NO2	Phenylacetylindole
JWH-203		2-(2-chlorophenyl)-1-(1-pentyl-1H-indol-3-yl)ethanone	864445-54-5	C21H22ClNO	Phenylacetylindole

JWH-203 3-chlorophenyl isomer		2-(3-chlorophenyl)-1-(1-pentyl-1H-indol-3-yl)ethanone	864445-56-7	C21H22ClNO	Phenylacetylindole
JWH-203 4-chlorophenyl isomer		2-(4-chlorophenyl)-1-(1-pentyl-1H-indol-3-yl)ethanone	864445-58-9	C21H22ClNO	Phenylacetylindole
JWH-249		2-(2-bromophenyl)-1-(1-pentyl-1H-indol-3-yl) ethanone	864445-60-3	C21H22BrNO	Phenylacetylindole
JWH-250		1-(1-pentyl-1H-indol-3-yl)-2-(2-methoxyphenyl) ethanone	864445-43-2	C22H25NO2	Phenylacetylindole
JWH-250 5-hydroxyindole metabolite		1-(5-hydroxy-1-pentyl-1H-indol-3-yl)-2-(2-methoxyphenyl)ethanone	1379604-67-7	C22H25NO3	Phenylacetylindole
JWH-250 N-(4-hydroxypentyl) metabolite		1-(1-(4-hydroxypentyl)-1H-indol-3-yl)-2-(2-methoxyphenyl)ethanone	1427521-38-7	C22H25NO3	Phenylacetylindole
JWH-250 N-(5-carboxypentyl) metabolite		5-(3-(2-(2-methoxyphenyl)acetyl)-1H-indol-1-yl)pentanoic acid	1379604-65-5	C22H23NO4	Phenylacetylindole
JWH-250 N-(5-hydroxypentyl) metabolite		1-(1-(5-hydroxypentyl)-1H-indol-3-yl)-2-(2-methoxyphenyl)ethanone	1427325-83-4	C22H25NO3	Phenylacetylindole
JWH-251		2-(2-methylphenyl)-1-(1-pentyl-1H-indol-3-yl) methanone	864445-39-6	C22H25NO	Phenylacetylindole
JWH-251 3-methylphenyl isomer		1-(1-pentyl-1H-indol-3-yl)-2-(m-tolyl)ethanone	1427325-88-9	C22H25NO	Phenylacetylindole
JWH-251 4-methylphenyl isomer		2-(4-methylphenyl)-1-(1-pentyl-1H-indol-3-yl) ethanone	864445-41-0	C22H25NO	Phenylacetylindole
JWH-302		2-(3-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl) ethanone	864445-45-4	C22H25NO2	Phenylacetylindole
RCS-8		1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(2-methoxyphenyl)ethanone	1345970-42-4	C25H29NO2	Phenylacetylindole
RCS-8 3-methoxy isomer		1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(3-methoxyphenyl)ethanone	1427326-08-6	C25H29NO2	Phenylacetylindole
RCS-8 4-methoxy isomer		1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(4-methoxyphenyl)ethanone	1427326-10-0	C25H29NO2	Phenylacetylindole
1-(2,3-Dimethylphenyl)piperazine	2,3-XP	1-(2,3-dimethylphenyl)piperazine	1013-22-5	C12H18N2	Piperazine
1-(2,4-Dimethylphenyl)piperazine	2,4-XP	1-(2,4-dimethylphenyl)piperazine	1013-76-9	C12H18N2	Piperazine
1-(2,5-Dimethylphenyl)piperazine	2,5-XP	1-(2,5-dimethylphenyl)piperazine	1013-25-8	C12H18N2	Piperazine
1-(2-Chlorophenyl) piperazine	oCPP	1-(2-chlorophenyl) piperazine	39512-50-0	C10H13ClN2	Piperazine
1-(2-Fluorophenyl)piperazine	2-FPP	1-(2-fluorophenyl)piperazine	1011-15-0	C10H13FN2	Piperazine
1-(2-Methoxyphenyl)piperazine	2-MeOPP	1-(2-methoxyphenyl)piperazine	5464-78-8	C11H16N2O	Piperazine
1-(2-Phenylethyl)piperazine	2-PEP	1-(2-phenylethyl)piperazine	5321-49-3	C12H18N2	Piperazine
1-(3,4-Dimethylphenyl)piperazine	3,4-XP	1-(3,4-dimethylphenyl)piperazine	1014-05-7	C12H18N2	Piperazine
1-(3,4-Methylenedioxybenzyl)piperazine	MDBZP	1-(benzo[1,3]dioxol-5-ylmethyl)piperazine	32231-06-4	C12H16N2O2	Piperazine
1-(3-Fluorophenyl)piperazine	3-FPP	1-(3-fluorophenyl)piperazine	3801-89-6	C10H13FN2	Piperazine
1-(3-Methoxyphenyl)piperazine	3-MeOPP	1-(3-methoxyphenyl)piperazine	16015-71-7	C11H16N2O	Piperazine
1-(3-Thienylmethyl)piperazine	3-TMP	1-(thiophen-3-ylmethyl)piperazine	130288-91-4	C9H14N2S	Piperazine

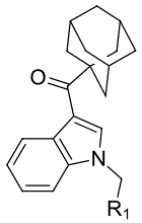
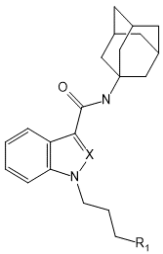
1-(4-Chlorophenyl)piperazine	pCPP	1-(4-chlorophenyl)piperazine	38212-33-8	C10H13ClN2	Piperazine
1-(4-Methoxyphenyl)piperazine	4-MeOPP	1-(4-methoxyphenyl)piperazine	38212-30-5	C11H16N2O	Piperazine
1-[(4-Bromo-2,5-dimethoxybenzyl)-piperazine	2C-B-BZP	1-[(4-bromo-2,5-dimethoxyphenyl)methyl]-piperazine	1094424-37-9	C13H19BrN2O2	Piperazine
1-[4-(Trifluoromethyl)phenyl]piperazine	4-TFMPP	1-[4-(trifluoromethyl)phenyl]piperazine	30459-17-7	C11H13F3N2	Piperazine
1-Benzyl-4-methylpiperazine	MBZP	1-benzyl-4-methylpiperazine	374898-00-7	C12H18N2	Piperazine
3-Methylbenzylpiperazine		1-[(3-methylphenyl)methyl]piperazine	5321-48-2	C12H18N2	Piperazine
3-Trifluoromethylphenylpiperazine	TFMPP	1-[3-(trifluoromethyl)phenyl]piperazine	15532-75-9	C11H13F3N2	Piperazine
4-Fluorobenzylpiperazine	4-FBZP	1-[(4-fluorophenyl)methyl]piperazine	70931-28-1	C11H15FN2	Piperazine
Benzylpiperazine	BZP	1-benzylpiperazine	110475-31-5	C11H16N2	Piperazine
Dibenzylpiperazine	DBZP	1,4-dibenzylpiperazine	1034-11-3	C18H22N2	Piperazine
meta-Chlorophenylpiperazine	mCPP	1-(3-chlorophenyl)piperazine	6640-24-0	C10H13ClN2	Piperazine
para-Fluorophenylpiperazine	4-FPP	1-(4-fluorophenyl)piperazine	2252-63-3	C10H13FN2	Piperazine
Phenylpiperazine		1-phenylpiperazine	92-54-6	C10H14N2	Piperazine
5-Fluoro-3,5-AB-PFUPPYCA	5-fluoro AB-FUPPYCA	(S)-N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl)-3-(4-fluorophenyl)-1H-pyrazole-5-carboxamide		C20H26F2N4O2	Pyrazole
2-Diphenylmethylpyrrolidine	Desoxy-D2PM	2-(diphenylmethyl)-pyrrolidine	383127-45-5	C17H19N	Pyrrolidine
Diphenylprolinol	D2PM	diphenyl-2-pyrrolidinemethanol	112068-01-6	C17H19NO	Pyrrolidine
2,N,N-Trimethyltryptamine	2-Me-DMT	N,N-dimethyl-2-(2-methyl-1H-indol-3-yl)ethanamine	1080-95-1	C13H18N2	Tryptamine
2,α-Dimethyltryptamine	2,α-DMT	1-(2-methyl-1H-indol-3-yl)propan-2-amine	4966-28-3	C12H16N2	Tryptamine
4-Acetoxy-N,N-diethyltryptamine	4-Acetoxy-DET	3-[2-(diethylamino)ethyl]-, 4-acetate1H-indol-4-ol	1135424-15-5	C16H22N2O2	Tryptamine
4-Acetoxy-N,N-diisopropyltryptamine	4-Acetoxy-DiPT	3-[2-(dipropan-2-ylamino)ethyl]-1H-indol-4-yl acetate	936015-60-0	C18H26N2O2	Tryptamine
4-Acetoxy-N,N-dimethyltryptamine	4-Acetoxy-DMT	[3-[2-(dimethylamino)ethyl]-1H-indol-4-yl] acetate	92292-84-7	C14H18N2O2	Tryptamine
4-Acetoxy-N-isopropyl-N-methyltryptamine	4-Acetoxy-MiPT	3-[2-[methyl(1-methylethyl)amino]ethyl]-, 4-1H-indol-4-ol	1024612-25-6	C16H22N2O2	Tryptamine
4-Acetoxy-N-methyl-N-ethyltryptamine	4-Acetoxy-MET	3-(2-[ethyl(methyl)amino]ethyl)-1H-indol-4-yl acetate	1445751-40-5	C15H20N2O2	Tryptamine
4-Hydroxy-N,N-diisopropyltryptamine	4-HO-DiPT	3-(2-[di(propan-2-yl)amino]ethyl)-1H-indol-4-ol	132328-45-1	C16H24N2O	Tryptamine
4-Hydroxy-N-isopropyl-N-methyltryptamine	4-HO-MiPT	3-[2-[methyl(propan-2-yl)amino]ethyl]-1H-indol-4-ol	77872-43-6	C14H20N2O	Tryptamine
4-Hydroxy-N-methyl-N-propyltryptamine	4-HO-MPT	3-(2-[methyl(propyl)amino]ethyl)-1H-indol-4-ol	763035-03-6	C14H20N2O	Tryptamine
4-Hydroxypyrrolidyltryptamine	4-HO-pyr-T	3-[2-(pyrrolidin-1-yl)ethyl]-1H-indol-4-ol	63097-26-7	C14H18N2O	Tryptamine

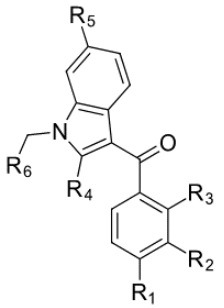
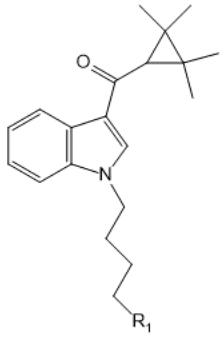
4-Methoxy-N,N-dimethyltryptamine	4-MeO-DMT	2-(4-methoxy-1H-indol-3-yl)-N,N-dimethyl-ethanamine	3965-97-7	C13H18N2O	Tryptamine
5-(2-Aminopropyl)indole	5-API	1-(1H-indol-5-yl)propan-2-amine	3784-30-3	C11H14N2	Tryptamine
5,6-Dimethoxy-N-isopropyl-N-methyltryptamine	5,6-MeO-MiPT	N-[2-(5,6-dimethoxy-1H-indol-3-yl)ethyl]-N-methylpropan-2-amine		C16H24N2O2	Tryptamine
5-Hydroxytryptamine	5-HO-T	3-(2-aminoethyl)-1H-indol-5-ol	50-67-9	C10H12N2O	Tryptamine
5-Methoxy-2,N,N-trimethyltryptamine	5-MeO-TMT	2-(5-methoxy-2-methyl-1H-indol-3-yl)-N,N-dimethylethanamine		C14H20N2O	Tryptamine
5-Methoxy-N,N-dimethyltryptamine	5-MeO-DMT	2-(5-methoxy-1H-indol-3-yl)-N,N-dimethylethanamine	1019-45-0	C13H18N2O	Tryptamine
5-Methoxy-N,N-dipropyltryptamine	5-MeO-DPT	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-N-propyl-propan-1-amine	2427-80-7	C17H26N2O	Tryptamine
5-Methoxy-N,N-tetramethylenetryptamine	5-MeO-pyr-T	5-methoxy-3-[2-(pyrrolidin-1-yl)ethyl]-1H-indole	3949-14-2	C15H20N2O	Tryptamine
5-Methoxy-N-ethyl-N-isopropyltryptamine	5-MeO-EiPT	N-ethyl-N-[2-(5-methoxy-1H-indol-3-yl)ethyl]propan-2-amine	850032-66-5	C16H26N2O	Tryptamine
5-Methoxy-N-methyltryptamine	5-MeO-NMT	2-(5-methoxy-1H-indol-3-yl)-N-methylethanamine	2009-03-2	C12H16N2O	Tryptamine
5-Methoxytryptamine	5-MeO-T	2-(5-methoxy-1H-indol-3-yl)ethanamine	608-07-1	C11H14N2O	Tryptamine
5-Methoxy-α-methyltryptamine	5-MeO-AMT	1-(5-methoxy-1H-indol-3-yl)-2-propanamine	1137-04-8	C12H16N2O	Tryptamine
6-(2-Aminopropyl)indole	6-API	α-methyl-1H-indole-6-ethanamine	21005-63-0	C11H14N2	Tryptamine
6,N,N-Triethyl-6-norlysergamide	ETH-LAD	(8β)-N,N,6-triethyl-9,10-didehydroergoline-8-carboxamide	65527-62-0	C21H27N3O	Tryptamine
6-Allyl-N,N-diethyl-6-norlysergamide	AL-LAD	(8β)-N,N-diethyl-6-(prop-2-en-1-yl)-9,10-didehydroergoline-8-carboxamide	65527-61-9	C22H27N3O	Tryptamine
6-Methoxy-1,2,3,4-tetrahydroharman	6-MeO-THH	2,3,4,9-tetrahydro-6-methoxy-1-methyl-1H-pyrido[3,4-b]indole	1210-56-6	C13H16N2O	Tryptamine
6-Propyl-6-nor-lysergic acid diethylamide	PRO-LAD	(8β)-N,N-diethyl-6-propyl-9,10-didehydroergoline-8-carboxamide	65527-63-1	C22H29N3O	Tryptamine
7-Methoxy-1,2,3,4-tetrahydroharman	7-MeO-THH	2,3,4,9-tetrahydro-7-methoxy-1-methyl-1H-pyrido[3,4-b]indole	17019-01-1	C13H16N2O	Tryptamine
Dimethyltryptamine N-oxide	DMT-N-oxide	[2-(1H-indol-3-yl)ethyl]dimethylamine oxide		C12H16N2O	Tryptamine
Harmine		7-methoxy-1-methyl-9H-β-carboline	442-51-3	C13H12N2O	Tryptamine
H-Hydroxy-a-methyltryptamine	N-OH-AMT	N-hydroxy-α-methyl-1H-indole-3-ethanamine	63-33-2	C11H14N2O	Tryptamine
Ibogaine		12-methoxyibogamine	83-74-9	C20H26N2O	Tryptamine
Methylbutyltryptamine	MBT	N-[2-(1H-indol-3-yl)ethyl]-N-methylbutan-1-amine		C15H22N2	Tryptamine
Methylethyltryptamine	MET	N-ethyl-2-(1H-indol-3-yl)-N-methylethanamine	5599-69-9	C13H18N2	Tryptamine
Methylisopropyltryptamine	MiPT	N-methyl-N-(1-methylethyl)-1H-indole-3-ethanamine	96096-52-5	C14H20N2	Tryptamine
N,N-Diallyl-5-methoxytryptamine	5-MeO-DALT	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-N-prop-2-enylprop-2-en-1-amine	928822-98-4	C17H22N2O	Tryptamine
N,N-Diallyltryptamine	DALT	N-allyl-N-[2-(1H-indol-3-yl)ethyl]-2-propen-1-amine	60676-77-9	C16H20N2	Tryptamine

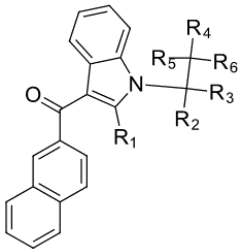
N,N-Dibutyl-4-hydroxytryptamine	4-HO-DBT	3-[2-(dibutylamino)ethyl]-1H-indol-4-ol	63065-89-4	C18H28N2O	Tryptamine
N,N-Dibutyltryptamine	DBT	N-butyl-N-[2-(1H-indol-3-yl)ethyl]butan-1-amine	15741-77-2	C18H28N2	Tryptamine
N,N-Diethyl-2-methyltryptamine	2-Me-DET	N,N-diethyl-2-(2-methyl-1H-indol-3-yl)ethanamine	26628-88-6	C15H22N2	Tryptamine
N,N-Diethyl-4-hydroxytryptamine	4-HO-DET	3-[2-(diethylamino)ethyl]-1H-indol-4-ol	22204-89-3	C14H20N2O	Tryptamine
N,N-Diethyl-4-phosphoryloxytryptamine	4-HO-DET phosphate ester	3-[2-(diethylamino)ethyl]-1H-indol-4-yl dihydrogen phosphate		C14H21N2O4P	Tryptamine
N,N-Diethyl-5-methoxytryptamine	5-MeO-DET	N,N-diethyl-5-methoxy-1H-indole-3-ethanamine	1218-40-2	C15H22N2O	Tryptamine
N,N-Diethyl-d-lysergamide	LSD	(8β)-N,N-diethyl-6-methyl-9,10-didehydroergoline-8-carboxamide	50-37-3	C20H25N3O	Tryptamine
N,N-Diethyltryptamine	DET	N,N-diethyl-2-(1H-indol-3-yl)ethanamine	61-51-8	C14H20N2	Tryptamine
N,N-Diisobutyltryptamine	DiBT	N-[2-(1H-indol-3-yl)ethyl]-N-isobutyl-2-methyl-1-propanamine	15741-78-3	C18H28N2	Tryptamine
N,N-Diisopropyl-4,5-methylenedioxytryptamine	4,5-MDO-DiPT	N-[2-(6H-[1,3]dioxolo[4,5-e]indol-8-yl)ethyl]-N-(propan-2-yl)propan-2-amine		C17H24N2O2	Tryptamine
N,N-Diisopropyl-5,6-methylenedioxytryptamine	5,6-MDO-DiPT	N-[2-(5H-[1,3]dioxolo[4,5-f]indol-7-yl)ethyl]-N-(propan-2-yl)propan-2-amine		C17H24N2O2	Tryptamine
N,N-Diisopropyl-5-methoxytryptamine	5-MeO-DiPT	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-N-propan-2-ylpropan-2-amine	4021-34-5	C17H26N2O	Tryptamine
N,N-Diisopropyltryptamine	DiPT	N-[2-(1H-indol-3-yl)ethyl]-N-isopropyl-2-propanamine	14780-24-6	C16H24N2	Tryptamine
N,N-Dimethyl-4,5-methylenedioxytryptamine	4,5-MDO-DMT	2-(6H-[1,3]dioxolo[4,5-e]indol-8-yl)-N,N-dimethylethanamine		C13H16N2O2	Tryptamine
N,N-Dimethyl-4-hydroxytryptamine	4-HO-DMT	3-[2-(dimethylamino)ethyl]-1H-indol-4-ol	520-53-6	C12H16N2O	Tryptamine
N,N-Dimethyl-5,6-methylenedioxytryptamine	5,6-MDO-DMT	2-(5H-[1,3]dioxolo[4,5-f]indol-7-yl)-N,N-dimethylethanamine		C13H16N2O2	Tryptamine
N,N-Dimethyl-5-hydroxytryptamine	5-HO-DMT	3-[2-(dimethylamino)ethyl]-1H-indol-5-ol	487-93-4	C12H16N2O	Tryptamine
N,N-Dimethyl-5-methylthiotryptamine	5-MeS-DMT	N,N-dimethyl-2-[5-(methylsulfanyl)-1H-indol-3-yl]ethanamine	5102-11-4	C13H18N2S	Tryptamine
N,N-Dimethyltryptamine	DMT	2-(1H-indol-3-yl)-N,N-dimethylethanamine	61-50-7	C12H16N2	Tryptamine
N,N-Dipropyl-4-hydroxytryptamine	4-HO-DPT	3-[2-(dipropylamino)ethyl]-1H-indol-4-ol	63065-88-3	C16H24N2O	Tryptamine
N,N-Dipropyltryptamine	DPT	N-[2-(1H-indol-3-yl)ethyl]-N-propylpropan-1-amine	61-52-9	C16H24N2	Tryptamine
N,N-Tetramethylenetryptamine	Pyr-T	3-[2-(pyrrolidin-1-yl)ethyl]-1H-indole	14008-96-9	C14H18N2	Tryptamine
N-Ethyl-4-hydroxy-N-methyltryptamine	4-HO-MET	3-[2-[ethyl(methyl)amino]ethyl]-1H-indol-4-ol	77872-41-4	C13H18N2O	Tryptamine
N-Ethyl-N-isopropyltryptamine	EiPT	N-ethyl-N-[2-(1H-indol-3-yl)ethyl]propan-2-amine	848130-11-0	C15H22N2	Tryptamine
N-Ethyltryptamine	NET	N-ethyl-2-(1H-indol-3-yl)ethanamine	61-53-0	C12H16N2	Tryptamine
N-Isopropyl-4-methoxy-N-methyltryptamine	4-MeO-MiPT	N-[2-(4-methoxy-1H-indol-3-yl)ethyl]-N-methylpropan-2-amine		C15H22N2O	Tryptamine
N-Isopropyl-5-methoxy-N-methyltryptamine	5-MeO-MiPT	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-N-methylpropan-2-amine	96096-55-8	C15H22N2O	Tryptamine

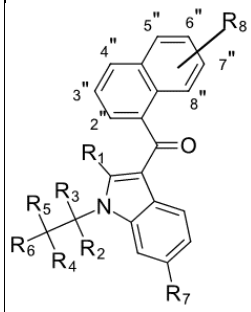
N-Isopropyl-N-methyl-5,6-methylenedioxytryptamine	5,6-MDO-MiPT	N-[2-(5H-[1,3]dioxolo[4,5-f]indol-7-yl)ethyl]-N-methylpropan-2-amine		C15H20N2O2	Tryptamine
N-Isopropyltryptamine	NiPT	N-[2-(1H-indol-3-yl)ethyl]propan-2-amine	14121-10-9	C13H18N2	Tryptamine
N-Methyltryptamine	NMT	2-(1H-indol-3-yl)-N-methylethanamine	61-49-4	C11H14N2	Tryptamine
Psilocybin		3-[2-(dimethylamino)ethyl]-1H-indol-4-yl dihydrogen phosphate	520-52-5	C12H17N2O4P	Tryptamine
Tryptamine		2-(1H-indol-3-yl)ethanamine	61-54-1	C10H12N2	Tryptamine
α,N-Dimethyl-5-methoxytryptamine	α,N,O-TMS	1-(5-methoxy-1H-indol-3-yl)-N-methylpropan-2-amine	4822-13-3	C13H18N2O	Tryptamine
α,N-Dimethyltryptamine	α,N-DMT	1-(1H-indol-3-yl)-N-methylpropan-2-amine		C12H16N2	Tryptamine
α-Ethyl-5-methoxytryptamine	5-MeO-α-ET	α-ethyl-5-methoxy-1H-indole-3-ethanamine	4765-10-0	C13H18N2O	Tryptamine
α-Ethyltryptamine	AET	1-(1H-indol-3-yl)butan-2-amine	2235-90-7	C12H16N2	Tryptamine
α-Methyltryptamine	AMT	1-(1H-indol-3-yl)propan-2-amine	299-26-3	C11H14N2	Tryptamine

Appendix 2. The chemical structures of the synthetic cannabinoids that were added to the MS/MS spectral library.

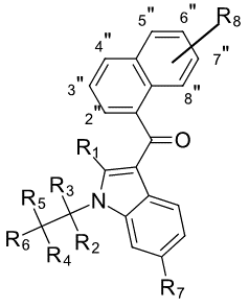
Structural Class	Compound	Substitution								
		R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	X
Adamantoylindoles										
	JWH-018 adamantyl analog	$(CH_2)_3CH_3$	-	-	-	-	-	-	-	-
	AM 1248	N-Methylpiperidine								
Adamantyl indazolecarboxamides and indolecarboxamides										
	AKB48	CH_2CH_3	-	-	-	-	-	-	-	N
	JWH-018 adamantyl carboxamide	CH_2CH_3	-	-	-	-	-	-	-	CH
	STS-135	$(CH_2)_2F$	-	-	-	-	-	-	-	CH
Benzoylindoles										
	AM-2233	H	H	I	H	H	N-Methylpiperidine			
	AM-630	OCH_3	H	H	CH_3	I	CH_2-(morpholine)			
	AM-679	H	H	I	H	H	$(CH_2)_3CH_3$	-	-	-

	AM-694	H	H	I	H	H	$(CH_2)_4F$	-	-	-
	AM-694 3-iodo isomer	H	I	H	H	H	$(CH_2)_4F$	-	-	-
	AM-694 4-iodo isomer	I	H	H	H	H	$(CH_2)_4F$	-	-	-
	RCS-4	OCH_3	H	H	H	H	$(CH_2)_3CH_3$	-	-	-
	RCS-4 2-methoxy isomer	H	H	OCH_3	H	H	$(CH_2)_3CH_3$	-	-	-
	RCS-4 3-methoxy isomer	H	OCH_3	H	H	H	$(CH_2)_3CH_3$	-	-	-
	RCS-4 C_4 homolog	OCH_3	H	H	H	H	$(CH_2)_2CH_3$	-	-	-
	WIN-48,098	OCH_3	H	H	CH_3	H	CH_2-(morpholine)	-	-	-
	WIN-54,461	OCH_3	H	H	CH_3	Br	CH_2-(morpholine)	-	-	-
Cyclopropanoylindoles										
	UR-144	CH_3	-	-	-	-	-	-	-	-
	XLR-11	CH_2F	-	-	-	-	-	-	-	-
Naphthoylindoles (2')										
	AM-2201 2'-naphthyl isomer	H	H	H	$(CH_2)_3F$	H	H			-
	JWH-018 2'-naphthyl-N-(1-ethylpropyl)	H	CH_2CH_3	H	CH_3	H	H			-
	JWH-018 2'-naphthyl isomer	H	H	H	$(CH_2)_2CH_3$	H	H			-
	JWH-018 2'-naphthyl-N-(1,1-	H	CH_3	CH_3	CH_3	H	H			-

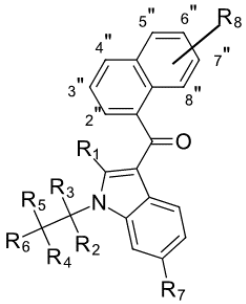
	dimethylpropyl) isomer									
	JWH-018 2'-naphthyl-N-(1,2-dimethylpropyl) isomer	H	CH_3	H	CH_3	CH_3	H			-
	JWH-018 2'-naphthyl-N-(1-methylbutyl) isomer	H	CH_3	H	CH_2CH_3	H	H			-
	JWH-018 2'-naphthyl-N-(2,2-dimethylpropyl) isomer	H	H	H	CH_3	CH_3	CH_3			-
	JWH-018 2'-naphthyl-N-(2-methylbutyl) isomer	H	H	H	CH_2CH_3	CH_3	H			-
	JWH-018 2'-naphthyl-N-(3-methylbutyl) isomer	H	H	H	$CH(CH_3)_2$	H	H			-
	JWH-073 2'-naphthyl isomer	H	H	H	CH_2CH_3	H	H			-
	JWH-073 2'-naphthyl-N-(1,1-dimethylethyl) isomer	H	CH_3	CH_3	H	H	H			-
	JWH-073 2'-naphthyl-N-(1-methylpropyl) isomer	H	CH_3	H	CH_3	H	H			-
	JWH-073 2'-naphthyl-N-(2-methylpropyl) isomer	H	H	H	CH_3	CH_3	H			-
	JWH-200 2'-naphthyl isomer	H	H	H	morpholine	H	H			-
Naphthoylindoles										
	AM-1235	H	H	H	H	H	$(CH_2)_3F$	NO_2	H	-
	AM-2201	H	H	H	H	H	$(CH_2)_3F$	H	H	-
	AM-2201 N-(2-fluoropentyl) isomer	H	H	H	H	F	$(CH_2)_2CH_3$	H	H	-



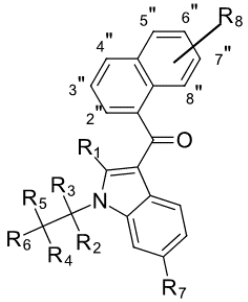
AM-2201 N-(3-fluoropentyl) isomer	H	H	H	H	H	$CHFCH_2CH_3$	H	H	-
AM-2201 N-(4-fluoropentyl) isomer	H	H	H	H	H	CH_2CHFCH_3	H	H	-
AM-2232	H	H	H	H	H	$(CH_2)_2C{\equiv}N$	H	H	-
JWH-007	CH_3	H	H	H	H	$(CH_2)_2CH_3$	H	H	-
JWH-011	CH_3	CH_3	H	H	H	$(CH_2)_3CH_3$	H	H	-
JWH-015	CH_3	H	H	H	H	CH_3	H	H	-
JWH-016	CH_3	H	H	H	H	CH_2CH_3	H	H	-
JWH-018	H	H	H	H	H	$(CH_2)_2CH_3$	H	H	-
JWH-018 6-methoxyindole analog	H	H	H	H	H	$(CH_2)_2CH_3$	OCH_3	H	-
JWH-018 N-(1,1-dimethylpropyl) isomer	H	CH_3	CH_3	H	H	CH_3	H	H	-
JWH-018 N-(1,2-dimethylpropyl) isomer	H	CH_3	H	H	CH_3	CH_3	H	H	-
JWH-018 N-(1-ethylpropyl) isomer	H	CH_2CH_3	H	H	H	CH_3	H	H	-
JWH-018 N-(1-methylbutyl) isomer	H	CH_3	H	H	H	CH_2CH_3	H	H	-
JWH-018 N-(2,2-dimethylpropyl) isomer	H	H	H	CH_3	CH_3	CH_3	H	H	-
JWH-018 N-(2-methylbutyl) isomer	H	H	H	H	CH_3	CH_2CH_3	H	H	-
JWH-018 N-(3-methylbutyl) isomer	H	H	H	H	H	$CH(CH_3)_2$	H	H	-
JWH-018 N-(4,5-epoxypentyl) analog	H	H	H	H	H	CH_2CHCH_2O	H	H	-

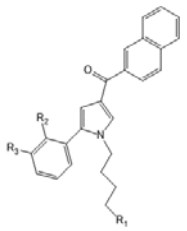
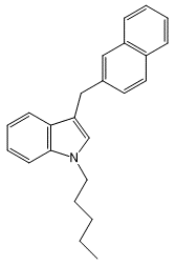
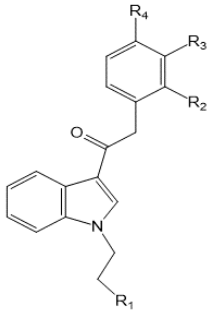


JWH-018 N-(5-bromopentyl) analog	H	H	H	H	H	$(CH_2)_3Br$	H	H	-
JWH-018 N-(5-chloropentyl) analog	H	H	H	H	H	$(CH_2)_3Cl$	H	H	-
JWH-019	H	H	H	H	H	$(CH_2)_3CH_3$	H	H	-
JWH-020	H	H	H	H	H	$(CH_2)_4CH_3$	H	H	-
JWH-022	H	H	H	H	H	$CH_2CH{=}CH_2$	H	H	-
JWH-072	H	H	H	H	H	CH_3	H	H	-
JWH-073	H	H	H	H	H	CH_2CH_3	H	H	-
JWH-073 2-methylnaphthyl analog	H	H	H	H	H	CH_2CH_3	H	CH_3 (C_2")	-
JWH-073 4-methylnaphthyl analog	H	H	H	H	H	CH_2CH_3	H	CH_3 (C_4")	-
JWH-073 N-(1,1-dimethylethyl) isomer	H	CH_3	CH_3	H	H	H	H	H	-
JWH-073 N-(1-methylpropyl) isomer	H	CH_3	H	H	H	CH_3	H	H	-
JWH-073 N-(2-methylpropyl) isomer	H	H	H	H	CH_3	CH_3	H	H	-
JWH-081	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_4")	-
JWH-081 2-methoxynaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_2")	-
JWH-081 3-methoxynaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_3")	-
JWH-081 5-methoxynaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_5")	-
JWH-081 6-methoxynaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_6")	-



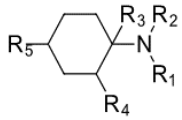
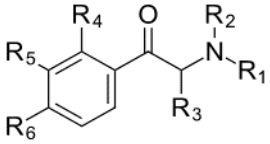
JWH-081 7-methoxynaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_7")	-
JWH-081 8-methoxynaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_8")	-
JWH-098	CH_3	H	H	H	H	$(CH_2)_2CH_3$	H	OCH_3 (C_4")	-
JWH-122	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_4")	-
JWH-122 2-methylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_2")	-
JWH-122 3-methylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_3")	-
JWH-122 5-methylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_5")	-
JWH-122 6-methylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_6")	-
JWH-122 7-methylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_7")	-
JWH-122 8-methylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_3 (C_8")	-
JWH-122 N-(4-pentenyl) analog	H	H	H	H	H	$CH_2CH=CH_2$	H	CH_3 (C_4")	-
JWH-180	H	H	H	H	H	CH_3	H	$(CH_2)_2CH_3$ (C_4")	-
JWH-182	H	H	H	H	H	$(CH_2)_2CH_3$	H	$(CH_2)_2CH_3$ (C_4")	-
JWH-200	H	H	H	H	H	morpholine	H	H	-
JWH-210	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_4")	-
JWH-210 2-ethylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_2")	-

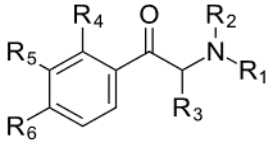
	JWH-210 3-ethylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_3")	-
	JWH-210 5-ethylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_5")	-
	JWH-210 6-ethylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_6")	-
	JWH-210 7-ethylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_7")	-
	JWH-210 8-ethylnaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	CH_2CH_3 (C_8")	-
	JWH-398	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_4")	-
	JWH-398 2-chloronaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_2")	-
	JWH-398 3-chloronaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_3")	-
	JWH-398 5-chloronaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_5")	-
	JWH-398 6-chloronaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_6")	-
	JWH-398 7-chloronaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_7")	-
	JWH-398 8-chloronaphthyl isomer	H	H	H	H	H	$(CH_2)_2CH_3$	H	Cl (C_8")	-
	JWH-424	H	H	H	H	H	$(CH_2)_2CH_3$	H	Br (C_8")	-
	MAM-2201	H	H	H	H	H	$(CH_2)_3F$	H	CH_3 (C_4")	-
Naphthoylpyrroles										
	JWH-145	CH_3	H	H	-	-	-	-	-	-
	JWH-147	CH_2CH_3	H	H	-	-	-	-	-	-

	JWH-307	CH_3	F	H	-	-	-	-	-	-
	JWH-309	CH_3	$CH{=}CHCH{=}CHR_3$ Benzyl	$CH{=}CHCH{=}CHR_2$ Benzyl	-	-	-	-	-	-
	JWH-368	CH_3	H	F	-	-	-	-	-	-
	JWH-369	CH_3	Cl	H	-	-	-	-	-	-
	JWH-370	CH_3	CH_3	H						
Naphthylmethylindole										
	JWH 175	-	-	-	-	-	-	-	-	-
Phenylacetylindoles										
	JWH-201	$(CH_2)_2CH_3$	H	H	OCH_3	-	-	-	-	-
	JWH-203	$(CH_2)_2CH_3$	Cl	H	H	-	-	-	-	-
	JWH-203 3-chlorophenyl isomer	$(CH_2)_2CH_3$	H	Cl	H	-	-	-	-	-
	JWH-203 4-chlorophenyl isomer	$(CH_2)_2CH_3$	H	H	Cl	-	-	-	-	-
	JWH-249	$(CH_2)_2CH_3$	Br	H	H	-	-	-	-	-
	JWH-250	$(CH_2)_2CH_3$	OCH_3	H	H	-	-	-	-	-
	JWH-251	$(CH_2)_2CH_3$	CH_3	H	H	-	-	-	-	-
	JWH-251 3-methylphenyl isomer	$(CH_2)_2CH_3$	H	CH_3	H	-	-	-	-	-
	JWH-251 4-methylphenyl isomer	$(CH_2)_2CH_3$	H	H	CH_3	-	-	-	-	-

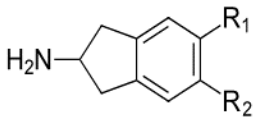
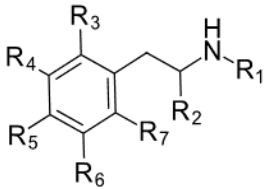
	JWH-302	$(CH_2)_2CH_3$	H	OCH_3	H	-	-	-	-	-
	RCS-8	cyclohexyl	OCH_3	H	H	-	-	-	-	-
	RCS-8 3-methoxy isomer	cyclohexyl	H	OCH_3	H	-	-	-	-	-
	RCS-8 4-methoxy isomer	cyclohexyl	H	H	OCH_3	-	-	-	-	-

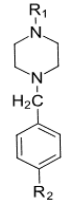
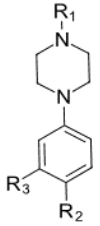
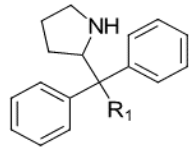
Appendix 3. The chemical structures of the non-synthetic cannabinoids that were added to the MS/MS library.

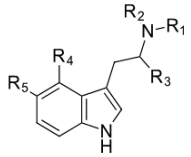
Structural Class	Compound	Substitution						
		R_1	R_2	R_3	R_4	R_5	R_6	R_7
Arylcyclohexylamines								
	Methoxetamine	H	CH_2CH_3	phenyl (3-MeO)	=O	H	-	-
Cathinones								
	2,3-MDMC	CH_3	H	CH_3	OCH_2OR_5	OCH_2OR_4	H	-
	2,3-MDPV	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_2CH_3$	OCH_2OR_5	OCH_2OR_4	H	-
	2,3-Pentylone	CH_3	H	$(CH_2)_2CH_3$	OCH_2OR_5	OCH_2OR_4	H	-
	2-Ethylethcathinone	CH_2CH_3	H	CH_3	CH_2CH_3	H	H	-
	2-Ethylmethcathinone	CH_3	H	CH_3	CH_2CH_3	H	H	-
	2-Fluoroethcathinone	CH_2CH_3	H	CH_3	F	H	H	-
	2-Fluoromethcathinone	CH_3	H	CH_3	F	H	H	-
	2-Methylethcathinone	CH_2CH_3	H	CH_3	CH_3	H	H	-
	2-Methoxymethcathinone	CH_3	H	CH_3	OCH_3	H	H	-
	3,4-Methylenedioxy-α-pyrrolidinobutyrophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_2CH_3	H	OCH_2OR_6	OCH_2OR_5	-
	2-Methylmethcathinone	CH_3	H	CH_3	CH_3	H	H	-
	3-Methyl-α-Pyrrolidinobutiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_2CH_3	H	CH_3	H	-
	3,4-Dimethylmethcathinone	CH_3	H	CH_3	H	CH_3	CH_3	-
	3-Ethylethcathinone	CH_2CH_3	H	CH_3	H	CH_2CH_3	H	-
	3-Ethylmethcathinone	CH_3	H	CH_3	H	CH_2CH_3	H	-
	3-Fluoroethcathinone	CH_2CH_3	H	CH_3	H	F	H	-
	3-Fluoromethcathinone	CH_3	H	CH_3	H	F	H	-
	3-Methylethcathinone	CH_2CH_3	H	CH_3	H	CH_3	H	-
	3-Methoxymethcathinone	CH_3	H	CH_3	H	OCH_3	H	-
	3-Methylmethcathinone	CH_3	H	CH_3	H	CH_3	H	-



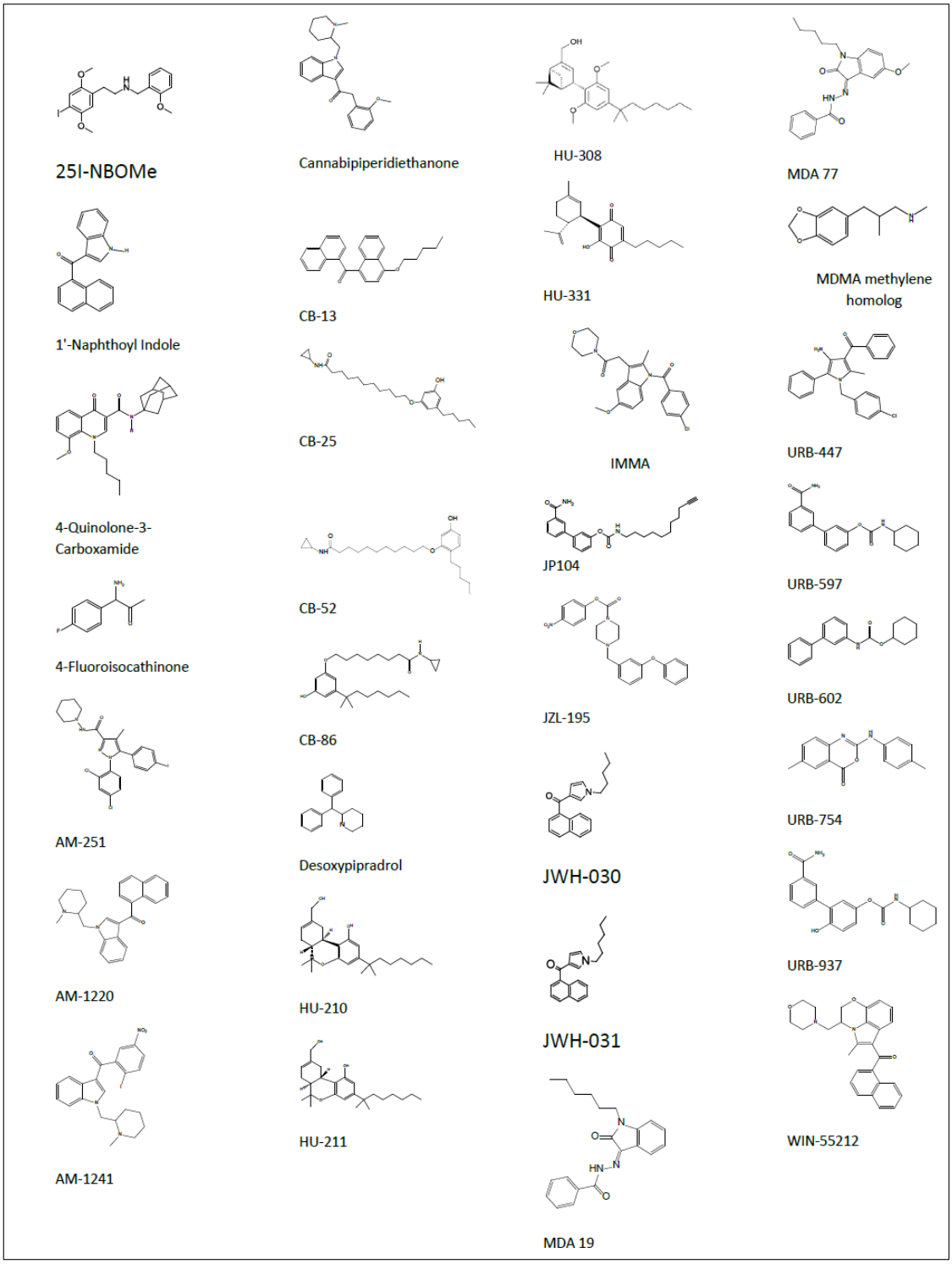
4-Ethylethcathinone	CH_2CH_3	H	CH_3	H	H	CH_2CH_3	-
4-Ethylmethcathinone	CH_3	H	CH_3	H	H	CH_2CH_3	-
4-Ethyl-N,N-dimethylcathinone	CH_3	CH_3	CH_3	H	H	CH_2CH_3	-
4-Fluoroethcathinone	CH_2CH_3	H	CH_3	H	H	F	-
4-Fluoromethcathinone	CH_3	H	CH_3	H	H	F	-
4-Methylethcathinone	CH_2CH_3	H	CH_3	H	H	CH_3	-
4'-Methyl-α-pyrrolidinohexanophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_3CH_3$	H	H	CH_3	-
4'-Methyl-α-pyrrolidinopropiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_3	H	H	CH_3	-
4-Methylmethcathinone	CH_3	H	CH_3	H	H	CH_3	-
Dibutylone	CH_3	CH_3	CH_2CH_3	H	OCH_2OR_6	OCH_2OR_5	-
Eutylone	CH_2CH_3	H	CH_2CH_3	H	OCH_2OR_6	OCH_2OR_5	-
Butylone	CH_3	H	CH_2CH_3	H	OCH_2OR_6	OCH_2OR_5	-
Dimethylone	CH_3	CH_3	CH_3	H	OCH_2OR_6	OCH_2OR_5	-
Cathinone	H	H	CH_3	H	H	H	-
Ethcathinone	CH_2CH_3	H	CH_3	H	H	H	-
Buphedrone	CH_3	H	CH_2CH_3	H	H	H	-
Ethylone	CH_2CH_3	H	CH_3	H	OCH_2OR_6	OCH_2OR_5	-
3,4-Methylenedioxy-α-pyrrolidinobutiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_2CH_3	H	OCH_2OR_6	OCH_2OR_5	-
3,4-Methylenedioxy-α-pyrrolidinopropiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_3	H	OCH_2OR_6	OCH_2OR_5	-
3,4-Methylenedioxypyrovalerone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_2CH_3$	H	OCH_2OR_6	OCH_2OR_5	-
Methcathinone	CH_3	H	CH_3	H	H	H	-
Methedrone	CH_3	H	CH_3	H	H	OCH_3	-
Methylone	CH_3	H	CH_3	H	OCH_2OR_6	OCH_2OR_5	-
4-Methoxy-α-pyrrolidinopropiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_3	H	H	OCH_3	-
4-Methyl-α-pyrrolidinobutiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_2CH_3	H	H	CH_3	-
N,N-Diethylcathinone	CH_2CH_3	CH_2CH_3	CH_3	H	H	H	-
N,N-Dimethylcathinone	CH_3	CH_3	CH_3	H	H	H	-
Naphyrone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_2CH_3$	H	$C_4H_4R_6$	$C_4H_4R_5$	-
Naphyrone 1-naphthyl isomer	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_2CH_3$	$C_4H_4R_5$	$C_4H_4R_4$	H	-
nor-Mephedrone	H	H	CH_3	H	H	CH_3	-

	Pentedrone	CH_3	H	$(CH_2)_2CH_3$	H	H	H	-
	Pentylone	CH_3	H	$(CH_2)_2CH_3$	H	OCH_2OR_6	OCH_2OR_5	-
	Pyrovalerone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_2CH_3$	H	H	CH_3	-
	α-Pyrrolidinobutiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_2CH_3	H	H	H	-
	α-Pyrrolidinopropiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	CH_3	H	H	H	-
	α-Pyrrolidinopentiophenone	$(CH_2)_4R_2$	$(CH_2)_4R_1$	$(CH_2)_2CH_3$	H	H	H	-
Indanes								
	2-Aminoindane	H	H	-	-	-	-	-
	5-IAI	I	H	-	-	-	-	-
	MDAI	OCH_2OR_2	OCH_2OR_1	-	-	-	-	-
Phenethylamines								
	2C-B	H	H	OCH_3	H	Br	OCH_3	H
	2C-C	H	H	OCH_3	H	Cl	OCH_3	H
	2C-D	H	H	OCH_3	H	CH_3	OCH_3	H
	2C-E	H	H	OCH_3	H	CH_2CH_3	OCH_3	H
	2C-H	H	H	OCH_3	H	H	OCH_3	H
	2C-I	H	H	OCH_3	H	I	OCH_3	H
	2C-N	H	H	OCH_3	H	NO_2	OCH_3	H
	2C-P	H	H	OCH_3	H	$(CH_2)_2CH_3$	OCH_3	H
	2C-T-2	H	H	OCH_3	H	SCH_2CH_3	OCH_3	H
	2C-T-4	H	H	OCH_3	H	$SCH(CH_3)_2$	OCH_3	H
	2C-T-7	H	H	OCH_3	H	$S(CH_2)_2CH_3$	OCH_3	H
	2-Fluoroamphetamine	H	CH_3	F	H	H	H	H
	2-Fluoromethamphetamine	CH_3	CH_3	F	H	H	H	H
	3,4-Dimethoxymethamphetamine	CH_3	CH_3	H	OCH_3	OCH_3	H	H
	3-Fluoroamphetamine	H	CH_3	H	F	H	H	H
	3-Fluoromethamphetamine	CH_3	CH_3	H	F	H	H	H
	4-Fluoroamphetamine	H	CH_3	H	H	F	H	H
	4-Fluoromethamphetamine	CH_3	CH_3	H	H	F	H	H
	5-APB	H	CH_3	H	$CH{=}CHOR_5$	$OCH{=}CHR_4$	H	H

	DOB	H	CH_3	OCH_3	H	Br	OCH_3	H
	DOM	H	CH_3	OCH_3	H	CH_3	OCH_3	H
	Ethylamphetamine	CH_2CH_3	CH_3	H	H	H	H	H
	TMA	H	CH_3	H	OCH_3	OCH_3	OCH_3	H
	TMA-2	H	CH_3	OCH_3	H	OCH_3	OCH_3	H
Piperazines (Benzylpiperazines)								
	4-Fluorobenzylpiperazine	H	F	-	-	-	-	-
	Benzylpiperazine	H	H	-	-	-	-	-
	Dibenzylpiperazine	$CH_2C_6H_5$	H	-	-	-	-	-
Piperazines (Phenylpiperazines)								
	para-Fluorophenylpiperazine	H	F	H	-	-	-	-
	meta-Chlorophenylpiperazine	H	H	Cl	-	-	-	-
	Phenylpiperazine	H	H	H	-	-	-	-
	3-Trifluoromethylphenylpiperazine	H	H	CF_3	-	-	-	-
Pyrrolidines								
	Diphenylprolinol	OH	-	-	-	-	-	-
	2-Diphenylmethylpyrrolidine	H	-	-	-	-	-	-
Tryptamines								
	4-Methoxy-N,N-dimethyltryptamine	CH_3	CH_3	H	OCH_3	H	-	-
	N,N-Diallyl-5-methoxytryptamine	$CH_2CH{=}CH_2$	$CH_2CH{=}CH_2$	H	H	OCH_3	-	-

	N,N-Diisopropyl-5-methoxytryptamine	$CH(CH_3)_2$	$CH(CH_3)_2$	H	H	OCH_3	-	-
	5-Methoxy-N,N-dimethyltryptamine	CH_3	CH_3	H	H	OCH_3	-	-
	N-Isopropyl-5-methoxy-N-methyltryptamine	$CH(CH_3)_2$	CH_3	H	H	OCH_3	-	-
	α-Methyltryptamine	H	H	CH_3	H	H	-	-
	N,N-Dimethyltryptamine	CH_3	CH_3	H	H	H	-	-

Appendix 4. The chemical structures of novel psychoactive substances that were added to the MS/MS spectral library that were not included in Appendix 2 and 3.



Appendix 5. The novel psychoactive substances that were added to the library along with the ions that had a relative abundance greater than 10% in the MS/MS spectra at the various collision energies.

Substance	CE	Ion (Relative Abundance %)
1-Naphthoyl Indole	10 eV	272.1062 (100), 155.0489 (19), 144.0441 (11)
	20 eV	155.0488 (100), 144.0443 (55), 272.1067 (14), 127.0542 (12)
	40 eV	127.0539 (100), 144.0441 (30), 116.0494 (18), 155.0488 (12)
2,3-Methylenedioxy Pyrovalerone	10 eV	276.1588 (100)
	20 eV	135.0437 (100), 276.1592 (97), 175.0751 (77), 126.1277 (34)
	40 eV	135.0441 (100), 126.1278 (88), 149.0233 (37), 84.0809 (23), 65.0386 (17), 175.0753 (15), 79.0544 (12), 77.0387 (12), 146.0361 (11)
2,3-Methylenedioxymethcathinone	10 eV	160.0749 (100), 208.0965 (46), 190.0859 (20)
	20 eV	160.0747 (100), 132.0804 (44), 147.0435 (10)
	40 eV	117.057 (100), 132.0804 (95), 91.054 (62), 131.0724 (34), 65.0383 (25), 77.0383 (14), 130.0647 (12), 103.0539 (12), 58.0649 (12), 160.0753 (11)
2,3-Pentylone isomer	10 eV	236.1277 (100), 188.1067 (76), 218.1175 (49), 175.075 (30), 135.0441 (24), 205.0858 (20)
	20 eV	188.1066 (100), 135.0441 (42), 175.0748 (38), 160.1116 (22), 218.1174 (19)
	40 eV	131.0729 (100), 135.0439 (29), 159.0676 (27), 77.0387 (21), 130.0652 (19), 65.0387 (13), 79.0543 (12), 91.0543 (11)
2,4,5-Trimethoxyamphetamine	10 eV	209.116 (100)
	20 eV	194.0932 (100), 209.1168 (91), 181.0854 (78), 179.0698 (45), 178.0982 (35), 151.0747 (31), 121.0643 (11), 177.0903 (10), 162.0671 (10),
	40 eV	91.0539 (100), 151.0745 (77), 123.0436 (65), 103.0538 (52), 121.0641 (52), 179.0695 (48), 107.0489 (46), 77.0382 (43), 136.0513 (39), 105.0694 (37), 79.0539 (36), 135.0794 (28), 131.0485 (27), 78.046 (26), 119.0485 (26), 108.0566 (26), 121.0283 (25), 65.0383 (21), 133.064 (21), 147.0792 (20), 115.0539 (20), 123.0771 (20), 163.0745 (14), 67.054 (13), 147.0434 (13), 149.0589 (13), 95.0488 (12), 110.0359 (12), 117.0691 (11), 93.0695 (11), 137.0591 (11), 135.0436 (11), 93.0332 (10), 80.0616 (10)
2,5-Dimethoxy-4-bromophenethylamine	10 eV	243.0012 (100), 227.9772 (16)
	20 eV	227.9779 (100), 243.001 (69), 164.0819 (30), 134.0721 (18), 212.955 (16), 149.0598 (12),
	40 eV	212.954 (100), 106.0417 (67), 91.0537 (65), 119.0493 (33), 227.9775 (22), 134.0718 (21), 121.0642 (21), 149.0591 (17), 78.0458 (15), 104.061 (13), 184.9602 (12)
2,5-Dimethoxy-4-chlorophenethylamine	10 eV	199.0525 (100), 184.0288 (17)
	20 eV	184.029 (100), 199.0525 (44), 169.0055 (20), 164.0834 (20)
	40 eV	169.0054 (100), 77.039 (78), 91.0548 (60), 141.0103 (31), 113.0157 (26), 119.0496 (22), 121.0651 (21), 103.0548 (13), 102.0471 (10)
2,5-Dimethoxy-4-ethylphenethylamine	10 eV	193.1208 (100), 178.0974 (21)
	20 eV	178.0971 (100), 193.1204 (57), 163.0736 (29), 105.0687 (26), 135.0786 (24), 163.1071 (13)
	40 eV	91.0531 (100), 105.0685 (87), 79.0533 (68), 77.0376 (64), 163.0736 (60), 103.053 (54), 135.0787 (31), 115.0526 (30), 120.0559 (24), 133.0634 (19), 117.0684 (17), 119.0476 (16), 121.0637 (15), 107.0478 (14), 107.0837 (14)
	10 eV	225.0942 (100)

Substance	CE	Ion (Relative Abundance %)
2,5-Dimethoxy-4-ethylthiophenethylamine	20 eV	225.0942 (100), 210.0706 (42), 164.0828 (21), 134.0724 (14), 167.052 (11), 195.0816 (10), 195.0479 (10)
	40 eV	91.0541 (100), 121.0644 (40), 134.0724 (40), 119.049 (40), 58.9949 (32), 151.0208 (25), 105.0696 (20), 77.0385 (18), 167.0162 (18), 149.059 (18), 133.0642 (16), 103.0538 (14), 104.0621 (14), 135.0337 (13), 152.0288 (13), 79.054 (12), 165.0364 (12), 120.0568 (12), 123.0263 (12), 136.0511 (11)
2,5-Dimethoxy-4-iodo-N-(2-methoxybenzyl)phenethylamine	10 eV	428.07 (100), 121.0645 (43)
	20 eV	121.0644 (100), 91.0545 (12)
	40 eV	91.0543 (100), 121.0646 (67), 93.07 (21)
2,5-Dimethoxy-4-iodophenethylamine	10 eV	290.9868 (100), 275.9643 (12), 308.0131 (12)
	20 eV	275.9638 (100), 290.9872 (90), 164.0821 (23), 134.072 (16), 149.059 (14), 260.9408 (13)
	40 eV	260.9405 (100), 91.0542 (77), 106.0408 (69), 275.9634 (40), 119.0493 (36), 78.0467 (33), 104.062 (33), 121.0638 (31), 134.0715 (28), 149.0592 (25), 134.0365 (18), 77.0385 (13), 103.0543 (11)
2,5-Dimethoxy-4-isopropylthiophenethylamine	10 eV	239.1094 (100), 197.0621 (21)
	20 eV	197.0622 (100), 182.0392 (23), 239.1092 (22), 164.0822 (13)
	40 eV	167.0155 (100), 91.0537 (55), 134.0717 (36), 121.0641 (36), 182.039 (32), 149.0592 (26), 119.0481 (25), 125.0049 (16), 139.0206 (13), 152.0278 (13), 164.0819 (10)
2,5-Dimethoxy-4-methylamphetamine	10 eV	193.1209 (100), 165.0895 (20), 178.0972 (15)
	20 eV	178.097 (100), 165.0893 (87), 135.0789 (50), 163.0736 (39), 193.1205 (36), 105.0685 (15)
	40 eV	91.0531 (100), 163.0736 (67), 135.0788 (60), 79.0531 (57), 105.0686 (55), 103.0529 (52), 77.0373 (50), 115.0527 (22), 121.0632 (22), 117.0684 (18), 107.0841 (16), 131.0478 (14), 120.0553 (14), 65.0377 (12), 92.0606 (11), 107.0475 (11), 67.0531 (10), 147.0782 (10)
2,5-Dimethoxy-4-methylphenethylamine	10 eV	179.1058 (100), 164.0822 (25)
	20 eV	164.0823 (100), 179.1056 (45), 149.0588 (26), 119.0848 (20), 91.0539 (18), 117.0691 (14), 149.092 (13)
	40 eV	91.0537 (100), 77.0381 (46), 149.0587 (42), 115.0537 (27), 121.0641 (15), 103.0536 (14), 93.0694 (11), 65.0382 (10)
2,5-Dimethoxy-4-nitrophenethylamine	10 eV	210.0757 (100), 227.1012 (15)
	20 eV	151.0748 (100), 195.0508 (65), 165.0548 (50), 210.0764 (37), 121.0649 (37), 109.0648 (32), 137.058 (32), 179.0706 (30), 135.0452 (26), 119.049 (25), 133.0636 (24), 150.059 (22), 91.0545 (20), 163.0753 (19), 79.0539 (18), 209.1522 (16), 107.0488 (16), 95.0497 (16), 149.0597 (15), 93.0691 (15), 95.0856 (15), 134.0716 (13), 116.0603 (13), 148.0424 (13), 77.0388 (12), 123.082 (10), 135.0722 (10)
	40 eV	91.0544 (100), 77.0392 (87), 79.0548 (39), 103.0539 (35), 65.0391 (32), 78.0467 (19), 105.0715 (19), 119.048 (18), 121.0649 (17), 107.0492 (15)
2,5-Dimethoxy-4-n-propylphenethylamine	10 eV	207.137 (100), 192.1141 (16)
	20 eV	192.1141 (100), 207.1375 (78), 163.0749 (23), 135.0799 (17), 177.1261 (10), 165.0903 (10)
	40 eV	105.0697 (100), 91.054 (86), 163.0747 (59), 79.0541 (55), 103.054 (49), 133.0644 (48), 77.0384 (48), 117.0695 (38), 149.0597 (35), 120.0564 (32), 121.0645 (31), 115.0537 (27), 135.0796 (25), 41.0384 (17), 43.0541 (13), 119.0849 (13), 107.0487 (10), 147.0795 (10), 135.0438 (10)
2,5-Dimethoxy-4-n-propylthiophenethylamine	10 eV	239.1096 (100)
	20 eV	239.1095 (100), 197.0624 (42), 224.0859 (30), 164.0819 (20), 167.0513 (19), 182.0391 (17)

Substance	CE	Ion (Relative Abundance %)
	40 eV	167.0154 (100), 91.0538 (64), 134.0723 (57), 121.0645 (38), 119.0492 (35), 149.0593 (29), 182.038 (26), 125.0053 (20), 152.0287 (17), 135.0292 (12), 139.02 (12), 151.0211 (11), 120.0574 (11)
2,5-Dimethoxyphenethylamine	10 eV	165.0912 (100), 150.0678 (45)
	20 eV	150.0678 (100), 135.0444 (23), 105.0702 (21), 165.0911 (19)
	40 eV	77.0389 (100), 135.0443 (68), 79.0545 (45), 107.0495 (34), 91.0545 (26), 103.0547 (17)
2-Aminoindane	10 eV	117.0703 (100), 134.0967 (16)
	20 eV	117.0703 (100), 115.0548 (56), 91.0547 (27)
	40 eV	91.0548 (100), 115.0547 (79), 65.0391 (42), 89.0393 (12)
2-Diphenylmethylpyrrolidine	10 eV	238.1582 (100), 117.0699 (22), 91.0543 (18), 143.0853 (13)
	20 eV	91.0539 (100), 117.0697 (56), 143.0851 (18)
	40 eV	91.0538 (100), 115.0539 (19), 117.0695 (13), 128.0616 (11)
2-Ethylethcathinone	10 eV	188.143 (100), 206.1539 (61), 160.112 (18), 159.1042 (15)
	20 eV	159.1042 (100), 144.0809 (55), 160.1121 (49), 188.1434 (39), 132.0809 (25), 131.0732 (12), 158.0963 (11)
	40 eV	144.0806 (100), 130.0653 (24), 158.0964 (14), 128.0605 (12), 143.0732 (12)
2-Ethylmethcathinone	10 eV	174.1273 (100), 192.1383 (28), 146.0966 (22), 145.0888 (20)
	20 eV	145.0881 (100), 146.0963 (40), 144.0806 (34), 174.1274 (22), 131.073 (11), 159.1038 (11)
	40 eV	144.0802 (100), 130.065 (11)
2-Fluoroamphetamine	10 eV	109.0451 (100), 137.0766 (23)
	20 eV	109.0452 (100)
	40 eV	83.0297 (100), 109.0454 (98), 57.0141 (13), 59.0297 (11)
2-Fluoroethcathinone	10 eV	178.1028 (100), 196.1135 (94), 150.0718 (22), 149.064 (10)
	20 eV	150.0718 (100), 149.0639 (77), 178.103 (59), 123.061 (38), 135.0518 (27), 148.056 (22), 103.055 (15), 163.0793 (14)
	40 eV	148.0561 (100), 135.0485 (68), 77.0392 (55), 103.0549 (52), 115.0548 (22), 95.0296 (18), 109.0454 (17), 133.0452 (12), 108.0377 (11)
2-Fluoromethamphetamine	10 eV	109.0443 (100), 168.1179 (44), 137.0757 (29)
	20 eV	109.0441 (100)
	40 eV	109.0443 (100), 83.0289 (51)
2-Fluoromethcathinone	10 eV	164.0871 (100), 182.0979 (39), 149.0639 (20)
	20 eV	149.0636 (100), 164.0873 (41), 123.0609 (18), 148.056 (15), 103.0547 (11)
	40 eV	148.056 (100), 77.039 (41), 103.0546 (20), 149.0638 (16)
2-Methoxymethcathinone	10 eV	176.1066 (100), 161.0836 (20), 194.1178 (17), 163.0755 (11)
	20 eV	161.0833 (100), 176.1072 (34), 145.0887 (25), 146.0603 (22), 135.0805 (12)
	40 eV	118.0655 (100), 146.0603 (54), 132.081 (53), 144.081 (44), 77.0389 (34), 91.0546 (28), 117.0579 (27), 160.0757 (22)
2-Methylethcathinone	10 eV	174.1274 (100), 192.1384 (47), 146.0964 (20), 145.0885 (15)
	20 eV	145.0884 (100), 146.0963 (68), 174.1275 (46), 144.0806 (42), 159.104 (35), 131.0739 (26), 119.0853 (23)
	40 eV	144.0808 (100), 130.0651 (46), 91.0543 (38), 131.0729 (17), 115.0543 (12), 77.0387 (11), 117.0692 (10)
2-Methylmethcathinone	10 eV	160.1109 (100), 145.0876 (26), 178.1216 (19)

Substance	CE	Ion (Relative Abundance %)
	20 eV	145.0874 (100), 160.1108 (27), 144.0796 (24), 119.0844 (10)
	40 eV	144.0797 (100), 91.0533 (22), 130.0641 (11), 77.0377 (11)
2-Methyl-α-pyrrolidinobutiophenone	10 eV	232.169 (100)
	20 eV	105.0701 (100), 232.1698 (92), 112.1124 (72), 161.0961 (51), 119.0494 (48), 133.1013 (27), 70.0654 (12)
	40 eV	91.0547 (100), 105.0703 (71), 112.1123 (53), 119.0494 (32), 84.0811 (18), 70.0654 (12)
3,4-Dimethoxymethamphetamine	10 eV	179.1057 (100), 151.075 (11), 210.1487 (10)
	20 eV	151.0751 (100), 179.1065 (53), 164.0829 (20), 136.0517 (16), 138.0676 (15), 147.0804 (10)
	40 eV	91.0544 (100), 107.0492 (98), 77.0387 (73), 151.0752 (51), 121.0648 (48), 135.044 (37), 103.0542 (33), 79.0542 (25), 105.0696 (24), 147.0802 (23), 108.0568 (21), 131.0489 (20), 93.07 (20), 149.0594 (19), 95.0493 (19), 78.0465 (18), 117.0699 (18), 136.0518 (18), 115.0541 (17), 90.0464 (16), 133.0645 (14), 104.0619 (14), 58.0653 (13), 65.0387 (13), 106.0414 (12), 123.0441 (11), 105.0334 (11), 80.062 (10)
3,4-Dimethylmethcathinone	10 eV	174.1269 (100), 192.1381 (23), 159.104 (20)
	20 eV	159.1036 (100), 174.1275 (36), 158.0961 (15)
	40 eV	158.0959 (100), 144.0804 (46), 91.0541 (13), 115.0541 (12), 143.0728 (11), 105.0698 (10), 159.1038 (10)
3,4-Methylenedioxypyrovalerone	10 eV	276.1589 (100)
	20 eV	276.1587 (100), 126.1272 (87), 175.0743 (84), 205.0848 (74), 135.0436 (71), 149.0225 (35), 147.0794 (15), 174.0903 (10)
	40 eV	126.1273 (100), 135.0436 (76), 149.0227 (65), 121.0284 (36), 84.0801 (31), 65.0383 (15), 72.0803 (11), 175.0741 (11)
3,4-Methylenedioxy-α-pyrrolidinobutyrophenone	10 eV	262.1431 (100)
	20 eV	262.1438 (100), 161.0597 (94), 191.0703 (75), 112.1123 (75), 163.0753 (45), 149.0234 (27), 133.065 (10)
	40 eV	112.1123 (100), 149.0234 (57), 105.0701 (42), 121.0285 (31), 133.0648 (23), 161.0596 (22), 84.0811 (22), 135.0442 (22), 65.0388 (14), 70.0654 (12)
3,4-Methylenedioxy-α-pyrrolidinopropiophenone	10 eV	248.1274 (100)
	20 eV	98.0968 (100), 248.1284 (99), 147.0443 (81), 177.0548 (37), 149.0599 (28)
	40 eV	98.0967 (100), 91.0547 (59), 119.0494 (37), 147.0442 (28), 56.0499 (14), 149.0597 (14)
3-Ethylethcathinone	10 eV	188.1431 (100), 206.1539 (79), 160.1122 (16), 159.1044 (14)
	20 eV	159.1044 (100), 160.1125 (51), 144.0812 (48), 188.1438 (47), 132.0812 (24), 131.0738 (11), 105.0704 (11), 133.1012 (10), 158.0967 (10)
	40 eV	144.0809 (100), 130.0657 (23), 105.0703 (17), 158.0968 (14), 143.0735 (10), 117.0639 (10)
3-Ethylmethcathinone	10 eV	174.1278 (100), 192.1389 (37), 146.0969 (19), 145.0892 (18)
	20 eV	145.0891 (100), 146.0973 (41), 144.0817 (31), 174.1285 (26), 159.105 (11)
	40 eV	144.0813 (100)
3-Fluoroamphetamine	10 eV	109.0448 (100), 137.0761 (23)
	20 eV	109.0448 (100)
	40 eV	83.0295 (100), 109.0452 (84), 57.0138 (13)
3-Fluoroethcathinone	10 eV	178.1031 (100), 196.1139 (95), 150.0718 (37), 149.064 (10)
	20 eV	150.072 (100), 149.0641 (53), 178.1031 (34), 123.0611 (24), 135.0497 (24), 148.0562 (17), 103.0549 (11)

Substance	CE	Ion (Relative Abundance %)
	40 eV	148.0563 (100), 135.0486 (87), 103.0549 (51), 77.0393 (51), 95.0298 (21), 115.0547 (15), 109.0456 (15), 108.0374 (15), 133.0454 (10)
3-Fluoromethamphetamine	10 eV	109.0448 (100), 168.1182 (49), 137.0762 (30)
	20 eV	109.0447 (100)
	40 eV	109.0448 (100), 83.0294 (59)
3-Fluoromethcathinone	10 eV	164.0863 (100), 182.0973 (38.75933), 149.0635 (20.98906)
	20 eV	149.0629 (100), 164.0868 (40.39218), 148.0557 (20.80779), 123.0604 (14.65683), 103.0543 (10.34477)
	40 eV	148.0553 (100), 77.0388 (32.5626), 103.0544 (16.10737), 149.0634 (11.10015), 95.0293 (10.02891)
3-Methoxymethcathinone	10 eV	176.1056 (100), 194.1167 (32), 161.0826 (23)
	20 eV	161.0822 (100), 176.106 (32), 146.0591 (26), 145.0876 (21), 135.0795 (11)
	40 eV	118.0644 (100), 132.0798 (59), 146.059 (43), 77.0379 (29), 91.0537 (28), 117.0566 (25), 144.0796 (22), 79.0536 (15), 103.0535 (13), 160.0745 (11)
3-Methylethcathinone	10 eV	174.1268 (100), 192.1375 (57), 146.0959 (20), 145.088 (14)
	20 eV	145.0881 (100), 146.0958 (69), 174.1271 (49), 144.0802 (38), 159.1036 (32), 119.0851 (29), 131.074 (24)
	40 eV	144.0803 (100), 91.0539 (48), 130.0647 (44), 131.0724 (19), 115.0538 (13), 77.0383 (12), 117.0691 (11),
3-Methylmethcathinone	10 eV	160.1117 (100), 145.0886 (25), 178.1226 (23)
	20 eV	145.0881 (100), 160.112 (31), 144.0809 (22), 119.0856 (13)
	40 eV	144.0806 (100), 91.0545 (26), 77.0388 (12), 130.0652 (10)
3-Methyl-α-pyrrolidinobutiophenone	10 eV	232.1691 (100)
	20 eV	105.0697 (100), 232.1694 (68), 161.0958 (47), 112.112 (28), 133.1008 (26), 119.0489 (19), 70.065 (15)
	40 eV	105.0698 (100), 91.0542 (72), 112.1119 (47), 84.0807 (25), 119.0491 (25), 70.065 (13)
3-Trifluoromethylphenylpiperazine	10 eV	231.11 (100)
	20 eV	188.0677 (100), 231.11 (77), 44.0498 (24)
	40 eV	188.0679 (100), 118.0651 (91), 44.0498 (75), 145.0255 (62), 119.0725 (55), 127.0347 (43), 148.0559 (39), 168.0603 (27), 166.0461 (27), 141.0521 (24), 128.0488 (16), 174.0512 (15), 186.051 (15), 91.0542 (14), 117.0575 (13), 56.0504 (13), 104.0499 (12), 172.0361 (11), 140.0321 (10), 121.0445 (10), 161.0446 (10)
4-Ethylethcathinone	10 eV	188.1422 (100), 206.1532 (58), 160.1115 (13), 159.1037 (12)
	20 eV	159.1033 (100), 188.1426 (54), 160.1113 (52), 144.08 (45), 132.0801 (22), 133.1001 (11), 105.0694 (11), 131.0728 (10)
	40 eV	144.0797 (100), 130.0645 (21), 105.0693 (21), 158.0955 (14), 115.0537 (12), 91.0537 (11), 117.0645 (11), 143.0723 (10)
4-Ethylmethcathinone	10 eV	174.1282 (100), 192.1393 (27), 146.0973 (15), 145.0895 (15)
	20 eV	145.0893 (100), 146.0974 (41), 174.1286 (31), 144.0817 (28), 159.1051 (12), 105.0707 (10)
	40 eV	144.0814 (100)
4-Ethyl-N,N-Dimethylcathinone	10 eV	206.1533 (100), 161.0961 (24)
	20 eV	133.1009 (100), 72.081 (77), 161.096 (63), 105.0702 (57), 133.065 (47), 206.1537 (24), 143.0854 (17)
	40 eV	72.081 (100), 105.0701 (86), 79.0544 (32), 77.0388 (20), 103.0545 (19), 91.0545 (15)
4-Fluoroamphetamine	10 eV	109.0447 (100), 137.0758 (39)

Substance	CE	Ion (Relative Abundance %)
	20 eV	109.0443 (100)
	40 eV	109.0444 (100), 83.0288 (96), 57.0133 (11), 59.029 (10)
4-Fluorobenzylpiperazine	10 eV	195.1294 (100), 109.0454 (44)
	20 eV	109.0452 (100)
	40 eV	109.0453 (100), 83.0298 (31)
4-Fluoroethcathinone	10 eV	178.1021 (100), 196.1129 (64), 150.0711 (24), 149.0633 (11)
	20 eV	150.0711 (100), 149.0634 (81), 178.1024 (47), 123.0603 (31), 135.0513 (23), 148.0555 (22), 163.0789 (12), 103.0543 (11)
	40 eV	148.0555 (100), 135.0479 (55), 103.0542 (47), 77.0385 (41), 115.0541 (17), 109.0448 (15), 95.0291 (12), 108.0369 (10), 133.0448 (10)
4-Fluoroisocathinone	10 eV	151.0557 (100), 123.0609 (81), 103.0548 (11)
	20 eV	123.0609 (100), 103.0548 (91), 77.0392 (12)
	40 eV	77.0391 (100), 103.0547 (34)
4-Fluoromethamphetamine	10 eV	109.0454 (100), 137.0766 (60), 168.1185 (25)
	20 eV	109.0452 (100)
	40 eV	109.0456 (100), 83.0305 (47)
4-Fluoromethcathinone	10 eV	164.0866 (100), 149.0632 (22), 182.097 (19)
	20 eV	149.0632 (100), 164.0865 (38), 123.0601 (20), 148.0555 (18), 103.0541 (13)
	40 eV	148.0554 (100), 77.0387 (46), 103.0542 (28), 149.063 (17), 95.0291 (11)
4-Methoxy-N,N-dimethyltryptamine	10 eV	58.0659 (100), 219.1489 (42), 174.0909 (33)
	20 eV	58.0659 (100), 174.0909 (34)
	40 eV	58.0661 (100), 159.0674 (16), 115.0541 (13), 130.0648 (12)
4-Methoxy-α-pyrrolidinopropiophenone	10 eV	234.1479 (100), 98.0969 (11)
	20 eV	98.0967 (100), 163.0748 (65), 135.0802 (64), 234.1483 (41)
	40 eV	98.0967 (100), 105.0699 (50), 135.0799 (37), 79.0549 (27), 103.0544 (22), 56.0505 (22), 77.0392 (18), 120.0567 (10)
4-Methylethcathinone	10 eV	174.1267 (100), 192.1373 (31), 146.0955 (22), 145.0876 (17)
	20 eV	145.0876 (100), 146.0954 (66), 144.0799 (45), 174.1267 (43), 119.0844 (36), 159.1031 (33), 131.0737 (27), 91.0538 (13)
	40 eV	144.0797 (100), 91.0536 (57), 130.0641 (43), 115.0535 (18), 131.0724 (17), 77.0379 (15), 117.0688 (14), 103.0535 (10)
4-Methylmethcathinone	10 eV	160.1112 (100),145.0879 (28),178.1212 (14)
	20 eV	145.0877 (100),160.1108 (30),144.0797 (25),119.0847 (14)
	40 eV	144.0798 (100),91.0537 (31),77.0379 (15),130.0645 (11),103.0533 (10)
4-Methyl-α-pyrrolidinobutiophenone	10 eV	232.1688 (100), 161.0958 (10)
	20 eV	105.0705 (100), 161.0962 (65), 232.1695 (53), 112.1127 (35), 133.1014 (32), 119.0496 (22), 70.0665 (10)
	40 eV	105.0705 (100), 91.0552 (59), 112.1125 (49), 119.0494 (30), 84.0818 (22), 70.0663 (11)
4'-Methyl-α-pyrrolidinohexanophenone	10 eV	260.2001 (100)
	20 eV	105.0699 (100), 260.2005 (67), 189.1269 (48), 140.1429 (24), 119.049 (19), 133.0644 (12)
	40 eV	105.07 (100), 91.0546 (43), 140.1429 (38), 119.049 (33), 84.0814 (24)

Substance	CE	Ion (Relative Abundance %)
4'-Methyl-α-pyrrolidinopropiophenone	10 eV	218.1534 (100), 147.0804 (10)
	20 eV	119.0858 (100), 147.0807 (81), 218.1542 (66), 98.0969 (63), 70.0657 (12)
	40 eV	98.0969 (100), 91.0547 (86), 119.0858 (57), 117.0703 (36), 56.05 (25), 84.0813 (12), 70.0656 (12), 103.0546 (12), 77.039 (12), 55.0548 (10)
4-Quinolone-3-Carboxamide CB2 Ligand	10 eV	423.2635 (100)
	20 eV	135.1166 (100), 423.2639 (98), 272.1281 (28)
	40 eV	135.1164 (100), 93.0704 (10)
5-(2-Aminopropyl)benzofuran	10 eV	159.0803 (100), 131.0495 (63), 131.0826 (20)
	20 eV	131.0494 (100), 131.0829 (34), 91.055 (15)
	40 eV	91.055 (100), 131.0493 (90), 77.0397 (89), 115.0545 (43), 103.0548 (23), 116.0625 (23), 65.0398 (16)
5,6-Methylenedioxy-2-aminoindane	10 eV	161.0594 (100), 131.0492 (31), 178.0861 (18)
	20 eV	131.0492 (100), 103.0545 (64), 161.0597 (37)
	40 eV	103.0544 (100), 77.0387 (65)
5-Iodo-2-aminoindane	10 eV	242.9662 (100), 259.9928 (67), 116.0619 (32)
	20 eV	116.0619 (100), 242.966 (34)
	40 eV	116.0619 (100), 115.0541 (68)
5-Methoxy-N,N-dimethyltryptamine	10 eV	58.065 (100), 174.0905 (66), 219.1484 (18)
	20 eV	58.0649 (100), 174.0902 (73), 159.0668 (16)
	40 eV	58.0649 (100), 130.0644 (52), 131.072 (44), 159.067 (22), 143.0716 (18)
AKB48	10 eV	366.2537 (100), 135.1167 (72)
	20 eV	135.1165 (100)
	40 eV	135.1165 (100), 93.0705 (13), 107.0858 (11), 79.0551 (10)
AM1220	10 eV	383.2113 (100)
	20 eV	112.1122 (100), 98.0969 (81), 383.2119 (49), 286.1226 (43), 155.049 (38)
	40 eV	98.0968 (100), 112.1122 (36), 155.0488 (26), 127.054 (14)
AM1235	10 eV	405.1591 (100)
	20 eV	405.1587 (100)277.097 (47), 155.0487 (34)
	40 eV	155.0483 (100)127.0547 (71), 189.0288 (37), 143.0356 (28), 277.0974 (26), 231.1034 (15)
AM1241	10 eV	98.0963 (100), 112.1119 (12)
	20 eV	98.0966 (100), 504.0741 (53), 112.1119 (16)
	40 eV	504.0763 (100), 98.0966 (18)
AM1248	10 eV	391.2736 (100)
	20 eV	391.2733 (100), 135.1169 (30), 112.1125 (10)
	40 eV	135.1167 (100), 112.1124 (38), 98.0971 (32)
AM2201	10 eV	360.1745 (100)
	20 eV	360.1745 (100), 155.048 (90), 232.1126 (22)
	40 eV	127.0534 (100), 155.0483 (81), 144.0437 (17), 232.1124 (10)
AM2201 2'-naphthyl isomer	10 eV	360.1755 (100)

Substance	CE	Ion (Relative Abundance %)
	20 eV	155.0491 (100), 360.1758 (92), 232.113 (23)
	40 eV	127.0543 (100), 155.049 (83), 144.0444 (22), 232.1131 (13)
AM2201 N-(2-fluoropentyl) isomer	10 eV	360.1753 (100)
	20 eV	360.175 (100), 155.0486 (88), 232.112 (29)
	40 eV	127.0539 (100), 155.0487 (76), 232.113 (18), 144.0445 (12)
AM2201 N-(3-fluoropentyl) isomer	10 eV	360.1752 (100)
	20 eV	360.1757 (100), 155.0491 (95), 232.1136 (23)
	40 eV	127.0543 (100), 155.0492 (81), 232.1136 (12)
AM2201 N-(4-fluoropentyl) isomer	10 eV	360.1751 (100)
	20 eV	360.1748 (100), 155.0482 (93), 232.1126 (20)
	40 eV	127.0535 (100), 155.0484 (84), 144.0437 (14)
AM2232	10 eV	353.1638 (100), 155.0484 (13)
	20 eV	155.048 (100), 353.1644 (28), 225.1016 (15)
	40 eV	127.0535 (100), 155.0485 (64), 144.0437 (13), 225.1015 (11)
AM2233	10 eV	459.0913 (100), 112.1118 (10)
	20 eV	98.0965 (100), 112.1121 (78), 459.0915 (73), 362.003 (38), 230.9286 (22)
	40 eV	98.0966 (100), 112.112 (27), 230.9299 (25)
AM251	10 eV	555.0199 (100)
	20 eV	555.0203 (100), 454.9208 (59)
	40 eV	454.9205 (100)
AM630	10 eV	505.0983 (100), 135.0446 (51)
	20 eV	135.0441 (100), 505.0992 (17)
	40 eV	135.0442 (100), 114.092 (19)
AM679	10 eV	418.0658 (100)
	20 eV	230.9305 (100), 418.0668 (83), 291.1625 (16)
	40 eV	230.9307 (100), 202.9361 (53)
AM694	10 eV	436.0563 (100)
	20 eV	436.0564 (100), 230.9298 (84), 309.1527 (15)
	40 eV	230.9297 (100), 202.9353 (40)
AM694 3-iodo isomer	10 eV	436.0561 (100)
	20 eV	436.0562 (100), 230.93 (95)
	40 eV	230.93 (100), 202.9357 (56)
AM694 4-iodo isomer	10 eV	436.0563 (100)
	20 eV	230.9303 (100), 436.0568 (96)
	40 eV	230.9303 (100), 202.935 (34)
Benzylpiperazine	10 eV	177.1386 (100),91.0546 (47),85.0763 (11)
	20 eV	91.0546 (100)
	40 eV	91.0546 (100),65.0389 (35)
Buphedrone	10 eV	160.111 (100), 178.1221 (36), 132.0803 (21), 147.0799 (15), 131.0727 (13), 91.0545 (12)

Substance	CE	Ion (Relative Abundance %)
	20 eV	131.0724 (100), 132.0804 (51), 91.0546 (50), 160.1113 (32), 130.0646 (18), 145.0879 (14)
	40 eV	130.0648 (100), 91.0546 (50), 77.0391 (41), 131.0725 (25), 144.0802 (12), 117.0575 (12)
Butylone	10 eV	204.1017 (100), 174.091 (90), 222.1122 (72), 191.07 (27), 72.0808 (17), 161.0594 (12)
	20 eV	174.0908 (100), 175.0624 (29), 146.0961 (22), 204.1017 (16), 72.0807 (16), 161.059 (14)
	40 eV	131.0726 (100), 174.0548 (27), 146.0954 (26), 130.0648 (25), 72.0807 (22), 175.0623 (21), 65.0385 (19), 159.0671 (18), 105.0695 (15), 117.0573 (15), 121.0281 (14), 118.0652 (13), 174.0877 (12), 119.0725 (10), 77.0385 (10), 79.0538 (10)
Cannabipiperidiethanone	10 eV	377.2207 (100)
	20 eV	112.111 (100), 377.2213 (56), 121.0636 (45), 98.0954 (27), 229.1686 (26), 280.1322 (13)
	40 eV	98.0955 (100), 112.111 (88), 121.0637 (54), 91.0533 (30), 58.0642 (22), 70.0642 (10)
Cathinone	10 eV	132.0802 (100), 105.0695 (19), 133.0642 (19), 117.057 (16)
	20 eV	117.0568 (100), 105.0695 (48), 132.0802 (44)
	40 eV	77.0383 (100), 90.046 (80), 117.0568 (79), 89.0383 (56), 51.023 (23), 79.0539 (21), 103.0538 (14), 130.0645 (10)
CB-13	10 eV	369.1843 (100)
	20 eV	155.0492 (100), 171.0442 (71), 299.1069 (70), 369.1851 (54), 241.1222 (13)
	40 eV	171.0442 (100), 155.0493 (86), 127.0545 (75), 143.0492 (29), 115.0545 (10)
CB-25	10 eV	404.3142 (100), 58.0659 (10)
	20 eV	58.0658 (100), 181.1212 (32), 347.2572 (31), 404.315 (13)
	40 eV	58.0658 (100), 111.0436 (15), 43.0549 (14), 181.1212 (10)
CB-52	10 eV	105.0708 (100), 387.1801 (93), 404.3145 (70), 121.0646 (29), 267.1225 (23), 147.0627 (10)
	20 eV	105.0698 (100), 121.0642 (48), 58.0653 (28), 69.0343 (15)
	40 eV	105.07 (100), 93.0702 (44), 121.0632 (34), 58.0648 (28), 69.034 (18), 43.0555 (11)
CB-86	10 eV	418.3293 (100)
	20 eV	58.0644 (100), 418.3299 (37), 361.2721 (21), 275.163 (12), 182.1523 (12), 71.0845 (11), 237.1835 (10)
	40 eV	58.0644 (100), 71.0846 (15), 57.069 (12), 55.0535 (12), 43.0536 (10)
Desoxypipradrol	10 eV	252.1745 (100)
	20 eV	91.0557 (100), 252.1753 (66), 131.0863 (34), 167.086 (29), 129.0706 (19), 157.1017 (12), 143.0862 (12), 117.0709 (12), 193.1016 (11)
	40 eV	91.0556 (100), 115.0551 (19), 129.0706 (13), 165.0702 (10)
Dibenzylpiperazine	10 eV	267.1851 (100)
	20 eV	91.0545 (100), 267.1857 (59), 175.123 (51), 134.0966 (26)
	40 eV	91.0542 (100)
Dibutylone	10 eV	236.1284 (100), 191.071 (21), 86.098 (11)
	20 eV	86.0979 (100), 161.0606 (90), 149.0241 (52), 191.0711 (42), 163.076 (40), 236.1289 (22), 133.0656 (19), 135.045 (12), 105.0712 (10)
	40 eV	86.098 (100), 121.0294 (46), 149.024 (44), 105.071 (36), 65.0403 (35), 71.0746 (29), 135.0448 (15), 79.0558 (15), 133.0656 (12), 77.0401 (10)
Dimethoxybromoamphetamine	10 eV	257.0165 (100), 228.985 (21), 178.0986 (12)

Substance	CE	Ion (Relative Abundance %)
	20 eV	228.985 (100), 178.0981 (70), 241.9932 (38), 257.0164 (33), 163.0754 (18), 198.9727 (16)
	40 eV	135.0793 (100), 105.0685 (62), 226.9697 (57), 91.0532 (47), 198.9745 (43), 163.0742 (41), 105.033 (41), 77.0377 (38), 103.0542 (33), 120.057 (32), 90.0456 (24), 79.0545 (24), 148.0503 (23), 168.9648 (20), 92.0619 (18), 43.0178 (10)
Dimethylone	10 eV	222.113 (100), 72.0814 (18), 177.0552 (11), 147.0445 (10)
	20 eV	72.0814 (100), 147.0445 (76), 149.0601 (41), 222.1131 (18), 177.0549 (17), 119.0497 (14)
	40 eV	72.0814 (100), 91.0549 (91), 119.0496 (27), 65.0391 (18), 147.0446 (13)
Diphenylprolinol	10 eV	236.1428 (100), 254.154 (11)
	20 eV	236.1427 (100), 158.0964 (14), 130.0653 (12)
	40 eV	130.0654 (100), 178.0777 (31), 117.0579 (30), 91.055 (27), 165.0699 (23), 167.0855 (22), 152.062 (20), 179.0855 (15), 206.0962 (14), 158.0964 (12), 115.0545 (12)
Ethcathinone	10 eV	160.1113 (100), 178.1221 (53), 132.0806 (35), 131.0728 (16)
	20 eV	132.0806 (100), 131.0729 (94), 105.07 (42), 160.1117 (37), 130.0651 (34), 117.0595 (25), 145.0883 (11)
	40 eV	130.0651 (100), 77.0394 (51), 117.0575 (46), 79.0549 (20), 105.0701 (19), 103.0545 (17), 115.0543 (15), 91.0548 (14)
Ethylamphetamine	10 eV	91.0536 (100),119.0846 (33),164.1422 (27)
	20 eV	91.0535 (100)
	40 eV	91.0534 (100),65.0378 (38)
Ethylone	10 eV	222.1122 (100), 204.1017 (88), 174.0913 (72), 72.082 (13)
	20 eV	174.0908 (100), 204.1019 (20), 175.0626 (17), 146.0962 (16)
	40 eV	91.0551 (100), 118.0654 (68), 146.096 (58), 174.0553 (46), 117.0575 (31), 131.0731 (31), 103.0546 (28), 174.0881 (25), 146.0602 (24), 119.0501 (19), 65.0397 (18), 130.0653 (15), 72.0819 (13), 77.0398 (11), 175.0628 (10), 128.0616 (10)
Eutylone	10 eV	236.1278 (100), 218.1175 (77), 188.1069 (42), 191.0702 (17)
	20 eV	188.1066 (100), 189.0782 (49), 218.1173 (34), 161.0592 (17), 86.0973 (15), 160.1105 (11)
	40 eV	174.0547 (100), 145.0882 (28), 117.0597 (28), 105.0701 (23), 132.0805 (18), 121.0287 (18), 160.1107 (17), 65.0398 (17), 189.0779 (16), 149.0231 (14), 115.0544 (14), 86.0973 (14), 116.0499 (13), 160.0749 (13), 135.0441 (12), 130.0652 (11), 173.0833 (11), 79.0552 (11), 77.0394 (10)
HU-210	10 eV	387.2898 (100)
	20 eV	243.1379 (100), 71.0866 (86), 387.2893 (62), 85.1019 (52), 57.0713 (48), 261.1484 (32), 201.0906 (28), 43.0556 (17), 133.1013 (14), 187.0753 (13), 369.2788 (13), 95.0861 (11), 147.0438 (10)
	40 eV	43.0556 (100), 57.0711 (71), 71.0867 (59), 85.1019 (20), 201.0907 (18), 41.0399 (11), 105.0702 (11), 123.0444 (10)
HU-211	10 eV	387.2897 (100)
	20 eV	243.138 (100), 71.0865 (97), 387.2894 (65), 85.102 (51), 57.071 (49), 261.1488 (33), 201.0909 (30), 43.0556 (18), 133.1009 (15), 187.0747 (14), 369.2788 (13), 95.0862 (12), 147.0442 (10)
	40 eV	43.0554 (100), 57.0711 (78), 71.0866 (61), 85.1017 (20), 105.0698 (19), 201.091 (18), 123.0447 (11), 41.0399 (10)
HU-308	10 eV	415.3199 (100), 215.106 (24), 229.1219 (23), 271.1689 (19), 151.0751 (19)
	20 eV	151.075 (100), 215.1063 (95), 229.1223 (83), 71.0858 (53), 85.1009 (36), 57.0701 (35), 91.0533 (29), 271.1697 (24), 133.1008 (23),

Substance	CE	Ion (Relative Abundance %)
		43.0544 (16), 277.2166 (13), 415.3203 (11), 105.0689 (10), 79.0537 (10)
	40 eV	43.0544 (100), 91.0544 (100), 57.0703 (82), 71.086 (72), 151.0751 (42), 105.0693 (34), 214.0974 (26), 85.1016 (26), 200.0823 (22), 79.0539 (21), 93.0701 (20), 215.1063 (16), 41.0388 (12), 121.0636 (11), 133.1003 (11), 123.0799 (10)
HU-331	10 eV	329.2107 (100), 287.1645 (11)
	20 eV	286.1561 (100), 287.164 (86), 329.2104 (76), 259.169 (36), 209.1177 (31), 273.1487 (25), 95.0854 (20), 229.085 (19), 213.0908 (15), 233.1165 (14), 311.1998 (13), 217.0853 (12), 207.1001 (12), 247.1324 (12), 223.1315 (11), 81.07 (10), 199.0748 (10)
	40 eV	229.0856 (100), 43.0548 (19), 105.07 (16), 69.0696 (14), 41.039 (13), 153.056 (12), 91.0545 (12), 81.0704 (11), 95.0853 (10), 67.0544 (10), 79.0542 (10), 213.0898 (10)
IMMA	10 eV	427.1416 (100), 138.9947 (14), 312.0791 (11)
	20 eV	138.9946 (100), 312.079 (31), 427.1421 (20), 88.0759 (10)
	40 eV	138.9944 (100), 110.9999 (20)
JP104	10 eV	214.0867 (100), 407.2329 (59), 197.0602 (21), 390.2067 (13), 212.1648 (13)
	20 eV	214.0867 (100), 197.06 (93), 171.0804 (17)
	40 eV	197.0601 (100), 153.0704 (64), 171.0807 (55), 169.065 (13), 141.0705 (11)
JWH 007	10 eV	356.2009 (100)
	20 eV	155.0496 (100), 356.2017 (95), 228.1388 (15)
	40 eV	127.0548 (100), 155.0497 (92), 158.0605 (13)
JWH 011	10 eV	384.2319 (100)
	20 eV	384.2326 (100), 155.0494 (77)
	40 eV	155.0494 (100), 127.0548 (57), 158.0604 (27)
JWH 015	10 eV	328.1693 (100)
	20 eV	155.0481 (100), 328.1694 (48), 200.1067 (16)
	40 eV	127.0536 (100), 155.0487 (49), 158.0596 (11)
JWH 016	10 eV	342.1847 (100)
	20 eV	155.0487 (100), 342.185 (64), 214.1226 (15)
	40 eV	127.0542 (100), 155.0491 (63), 158.0601 (11)
JWH 018	10 eV	342.1838 (100)
	20 eV	155.0483 (100), 342.1846 (81), 214.122 (21)
	40 eV	127.0538 (100), 155.0485 (61), 144.0438 (14)
JWH-018 2'-naphthyl-N-(1-ethylpropyl)	10 eV	342.1848 (100)
	20 eV	155.0492 (100), 342.1856 (77), 214.1234 (11)
	40 eV	127.0547 (100), 155.0496 (80), 144.0451 (51)
JWH 018 2'-naphthyl isomer	10 eV	342.185 (100), 155.0489 (8)
	20 eV	155.0491 (100), 342.1853 (61), 214.1225 (20)
	40 eV	127.0543 (100), 155.049 (63), 144.0441 (18)
JWH 018 2'naphthyl-N-(1,1-dimethylpropyl) isomer	10 eV	342.1847 (100), 272.107 (22)
	20 eV	272.1064 (100), 155.0486 (33), 144.0438 (22), 342.1847 (13)

Substance	CE	Ion (Relative Abundance %)
	40 eV	144.0439 (100), 155.0485 (82), 127.0539 (60)
JWH 018 2'-naphthyl-N-(1,2-dimethylpropyl) isomer	10 eV	342.1841 (100)
	20 eV	155.0485 (100), 342.1844 (96), 272.1069 (12)144.0441 (10)
	40 eV	127.0541 (100), 155.0487 (96), 144.0443 (61)
JWH 018 2'-naphthyl-N-(1-methylbutyl) isomer	10 eV	342.1847 (100)
	20 eV	155.0487 (100), 342.1853 (76), 214.1229 (11)
	40 eV	127.0542 (100), 155.0491 (76), 144.0445 (43)
JWH 018 2'-naphthyl-N-(2,2-dimethylpropyl) isomer	10 eV	342.1846 (100)
	20 eV	342.1847 (100), 155.0489 (81), 214.1227 (13)
	40 eV	127.0543 (100), 155.049 (88), 144.0444 (29)
JWH 018 2'-naphthyl-N-(2-methylbutyl) isomer	10 eV	342.1849 (100)
	20 eV	155.0486 (100), 342.1852 (79), 214.1226 (17)
	40 eV	127.054 (100), 155.0489 (68), 144.0444 (21)
JWH 018 2'-naphthyl-N-(3-methylbutyl) isomer	10 eV	342.1848 (100)
	20 eV	155.0493 (100), 342.1856 (79), 214.1227 (19)
	40 eV	127.0545 (100), 155.0493 (66), 144.0443 (15)
JWH 018 6-methoxyindole analog	10 eV	372.1951 (100)
	20 eV	155.0485 (100), 372.1957 (52)
	40 eV	127.0539 (100), 155.0488 (94)
JWH 018 adamantyl analog	10 eV	350.2472 (100)
	20 eV	350.2473 (100), 135.1174 (29)
	40 eV	135.117 (100), 93.071 (15), 107.0863 (14), 79.0555 (10)
JWH 018 adamantyl carboxamide	10 eV	365.2581 (100)
	20 eV	365.2583 (100), 135.1169 (37), 214.1225 (12)
	40 eV	135.1165 (100), 93.0705 (17), 107.0858 (15), 79.0551 (11)
JWH 018 N-(1,1-dimethylpropyl) isomer	10 eV	342.185 (100)272.1077 (25)
	20 eV	272.1066 (100), 155.0493 (32), 144.0446 (17), 342.1857 (10)
	40 eV	155.0491 (100), 144.0444 (80), 127.0543 (72)
JWH 018 N-(1,2-dimethylpropyl) isomer	10 eV	342.1848 (100)
	20 eV	342.1852 (100), 155.0491 (87), 272.1075 (17), 144.0447 (11)
	40 eV	155.0492 (100), 127.0545 (97), 144.0448 (52)
JWH 018 N-(1-ethylpropyl) isomer	10 eV	342.1841 (100)
	20 eV	155.0486 (100), 342.1849 (94), 214.1227 (12), 144.0445 (10)
	40 eV	127.0542 (100), 155.049 (87), 144.0446 (46)
JWH 018 N-(1-methylbutyl) isomer	10 eV	342.1839 (100)
	20 eV	155.0479 (100), 342.1839 (92), 214.1218 (13)
	40 eV	127.0533 (100), 155.0483 (83), 144.0438 (39)
JWH 018 N-(2,2-dimethylpropyl) isomer	10 eV	342.1849 (100)
	20 eV	342.1848 (100), 155.0488 (68), 214.1225 (12)

Substance	CE	Ion (Relative Abundance %)
	40 eV	127.0541 (100), 155.049 (90), 144.0444 (26)
JWH 018 N-(2-methylbutyl) isomer	10 eV	342.1845 (100)
	20 eV	155.0486 (100), 342.1847 (94), 214.1225 (19)
	40 eV	127.0538 (100), 155.0487 (69), 144.0441 (18)
JWH 018 N-(3-methylbutyl) isomer	10 eV	342.1853 (100)
	20 eV	155.0489 (100), 342.1844 (96), 214.1229 (21)
	40 eV	127.0543 (100), 155.0491 (66), 144.0448 (12)
JWH 018 N-(4,5-epoxypentyl) analog	10 eV	356.1639 (100), 155.0489 (20)
	20 eV	155.0483 (100), 356.1643 (17)
	40 eV	127.0538 (100), 155.0486 (71)
JWH 018 N-(5-bromopentyl) analog	10 eV	420.0947 (100)
	20 eV	420.0953 (100), 155.0486 (66)
	40 eV	155.0487 (100), 127.0538 (78), 292.0327 (12), 144.0438 (10)
JWH 018 N-(5-chloropentyl) analog	10 eV	376.1449 (100)
	20 eV	376.1453 (100), 155.0488 (79), 248.0831 (20)
	40 eV	127.0542 (100), 155.0488 (96), 144.0441 (15), 248.0832 (11)
JWH 019	10 eV	356.201 (100)
	20 eV	356.2003 (100), 155.0487 (91), 228.1381 (19)
	40 eV	127.0543 (100), 155.0489 (83), 144.0443 (15)
JWH 020	10 eV	370.216 (100)
	20 eV	370.2161 (100), 155.0491 (72), 242.154 (15)
	40 eV	155.0491 (100), 127.0545 (97), 144.0445 (16)
JWH 022	10 eV	340.1685 (100)
	20 eV	155.0485 (100), 340.1693 (59), 212.1067 (20)
	40 eV	127.0541 (100), 155.0489 (52)
JWH 030	10 eV	292.1693 (100), 155.0492 (72)
	20 eV	155.0487 (100)
	40 eV	127.0542 (100), 155.0493 (21)
JWH 031	10 eV	306.1851 (100), 155.0495 (53)
	20 eV	155.0491 (100)
	40 eV	127.0546 (100), 155.0497 (30)
JWH 072	10 eV	314.1538 (100)
	20 eV	155.049 (100), 314.1544 (39), 186.0915 (22)
	40 eV	127.0543 (100), 155.0495 (34), 144.0447 (14)
JWH 073	10 eV	328.1687 (100)
	20 eV	155.0484 (100), 328.169 (55), 200.1067 (21)
	40 eV	127.0537 (100), 155.0488 (56), 144.0441 (15)
JWH 073 2-methylnaphthyl analog	10 eV	342.1846 (100)
	20 eV	342.1842 (100), 169.0636 (99), 200.106 (58)

Substance	CE	Ion (Relative Abundance %)
	40 eV	141.0689 (100), 144.0435 (47), 169.0638 (38), 200.1057 (19)
JWH 073 2'-naphthyl isomer	10 eV	328.1691 (100)
	20 eV	155.0487 (100), 328.1699 (50), 200.1071 (20)
	40 eV	127.0541 (100), 155.0493 (47), 144.0446 (17)
JWH 073 2'-naphthyl-N-(1,1-dimethylethyl) isomer	10 eV	328.1695 (100), 272.1072 (18)
	20 eV	272.1075 (100), 155.0494 (48), 144.0446 (29), 328.1696 (21)
	40 eV	144.0447 (100), 155.0493 (75), 127.0546 (67)
JWH 073 2'-naphthyl-N-(1-methylpropyl) isomer	10 eV	328.1691 (100)
	20 eV	155.0484 (100), 328.1694 (59), 200.1067 (13)
	40 eV	127.0539 (100), 155.0489 (57), 144.0443 (37)
JWH 073 2'-naphthyl-N-(2-methylpropyl) isomer	10 eV	328.1691 (100)
	20 eV	155.0491 (100), 328.1697 (60), 200.1075 (19)
	40 eV	127.0544 (100), 155.0495 (52), 144.0448 (22)
JWH 073 4-methylnaphthyl analog	10 eV	342.1846 (100)
	20 eV	169.0644 (100), 342.1851 (74), 200.107 (31)
	40 eV	141.0697 (100), 169.0648 (66), 144.0444 (24), 200.107 (12)
JWH 073 N-(1,1-dimethylethyl) isomer	10 eV	328.1684 (100), 272.1067 (17)
	20 eV	272.1062 (100), 155.0487 (40), 144.0441 (21), 328.1695 (19)
	40 eV	155.0486 (100), 127.0538 (91), 144.0439 (85)
JWH 073 N-(1-methylpropyl) isomer	10 eV	328.1687 (100)
	20 eV	155.049 (100), 328.1696 (70), 200.1074 (14)
	40 eV	127.0544 (100), 155.0495 (60), 144.0449 (31)
JWH 073 N-(2-methylpropyl) isomer	10 eV	328.1694 (100)
	20 eV	155.049 (100), 328.1696 (71), 200.1074 (20)
	40 eV	127.0544 (100), 155.0494 (53), 144.0449 (17)
JWH 081	10 eV	372.1955 (100)
	20 eV	185.0592 (100), 372.1957 (84), 214.1227 (32)
	40 eV	185.0595 (100), 157.0648 (47), 144.0444 (25), 214.1225 (14), 127.0543 (10)
JWH 081 2-methoxynaphthyl isomer	10 eV	372.195 (100), 185.0597 (38)
	20 eV	185.0587 (100)
	40 eV	185.0586 (100), 142.0408 (25), 170.0356 (13), 127.0537 (11)
JWH 081 3-methoxynaphthyl isomer	10 eV	372.1954 (100)
	20 eV	372.1952 (100), 185.0589 (86), 214.1222 (45)
	40 eV	129.0695 (100), 185.0592 (82), 144.0438 (62), 214.122 (37), 128.0616 (36), 127.0536 (36)
JWH 081 5-methoxynaphthyl isomer	10 eV	372.1952 (100), 185.06 (10)
	20 eV	185.059 (100), 372.1955 (46)
	40 eV	185.0594 (100), 157.0647 (49), 127.0543 (44), 129.07 (35), 128.0622 (19), 144.0444 (16)
	10 eV	372.1946 (100)

Substance	CE	Ion (Relative Abundance %)
JWH 081 6-methoxynaphthyl isomer	20 eV	372.1947 (100), 185.0588 (74), 214.1222 (66)
	40 eV	157.0641 (100), 185.059 (50), 144.0439 (44), 214.1219 (30), 142.0411 (16)
JWH 081 7-methoxynaphthyl isomer	10 eV	372.1952 (100), 185.0593 (92)
	20 eV	185.0588 (100)
	40 eV	170.0357 (100), 185.0594 (63)
JWH 081 8-methoxynaphthyl isomer	10 eV	372.1958 (100), 185.0597 (90)
	20 eV	185.059 (100)
	40 eV	170.0359 (100), 185.0597 (62)
JWH 098	10 eV	386.2114 (100)
	20 eV	185.0592 (100), 386.2114 (68), 228.1381 (24)
	40 eV	185.0592 (100), 157.0646 (37), 158.0598 (16), 228.138 (13)
JWH 122	10 eV	356.2009 (100)
	20 eV	356.2011 (100), 169.0649 (97), 214.1233 (30)
	40 eV	141.0703 (100), 169.0653 (86), 144.045 (24), 214.1232 (13)
JWH 122 2-methylnaphthyl isomer	10 eV	356.2003 (100)
	20 eV	356.2004 (100), 169.0647 (76), 214.1229 (42)
	40 eV	141.07 (100), 169.0649 (50), 144.0446 (46), 214.1226 (20)
JWH 122 3-methylnaphthyl isomer	10 eV	356.2 (100)
	20 eV	356.1992 (100), 169.0634 (93), 214.1214 (44)
	40 eV	141.0686 (100), 169.0638 (56), 144.0435 (30), 214.1219 (15)
JWH 122 5-methylnaphthyl isomer	10 eV	356.2003 (100)
	20 eV	169.0641 (100), 356.2004 (91), 214.1226 (22)
	40 eV	141.0696 (100), 169.0646 (66), 144.0443 (18)
JWH 122 6-methylnaphthyl isomer	10 eV	356.2006 (100)
	20 eV	356.2008 (100), 169.0648 (97), 214.123 (39)
	40 eV	141.0699 (100), 169.065 (53), 144.0447 (23), 214.1227 (11)
JWH 122 7-methylnaphthyl isomer	10 eV	356.1996 (100)
	20 eV	169.0638 (100), 356.2 (83), 214.1222 (25)
	40 eV	141.0691 (100), 169.0643 (64), 144.0441 (18)
JWH 122 8-methylnaphthyl isomer	10 eV	356.1996 (100)
	20 eV	356.2003 (100), 169.0647 (72), 214.1228 (27)
	40 eV	141.0699 (100), 169.0648 (61), 144.0446 (27), 214.1228 (13)
JWH 122 N-(4-pentenyl) analog	10 eV	354.185 (100)
	20 eV	169.0647 (100), 354.1853 (77), 212.1075 (29)
	40 eV	141.0702 (100), 169.0651 (75), 144.0449 (14), 212.1074 (11)
JWH 145	10 eV	368.2003 (100), 155.0491 (52)
	20 eV	155.0486 (100)
	40 eV	127.0541 (100), 155.049 (83)
JWH 147	10 eV	382.2159 (100), 155.0492 (46)

Substance	CE	Ion (Relative Abundance %)
	20 eV	155.0488 (100)
	40 eV	155.049 (100), 127.0542 (99)
JWH 175	10 eV	328.2059 (100), 141.0699 (88)
	20 eV	141.0698 (100)
	40 eV	141.0698 (100), 115.0542 (10)
JWH 180	10 eV	356.1995 (100)
	20 eV	356.2004 (100), 197.0954 (96), 186.0912 (37)
	40 eV	141.0695 (100), 197.096 (91), 144.0442 (47), 186.0911 (44), 169.1007 (17), 154.0774 (14)
JWH 182	10 eV	384.2311 (100)
	20 eV	384.2313 (100), 197.0955 (65), 214.1223 (23)
	40 eV	197.0957 (100), 141.0696 (63), 144.0441 (31), 214.1223 (28), 169.1006 (15)
JWH 200	10 eV	385.1912 (100), 155.0499 (18)
	20 eV	155.0492 (100), 114.0921 (37), 385.1922 (24)
	40 eV	155.0496 (100), 114.092 (96), 127.0548 (71), 70.0656 (18)
JWH 200 2'-naphthyl isomer	10 eV	385.1905 (100), 155.049 (18)
	20 eV	155.049 (100), 114.0914 (23), 385.1908 (18)
	40 eV	155.049 (100), 127.0542 (78), 114.0913 (66), 70.0652 (13)
JWH 201	10 eV	336.1945 (100)
	20 eV	121.0627 (100), 336.1939 (79), 149.0576 (40), 135.042 (31)
	40 eV	121.0626 (100), 135.042 (33), 144.0426 (13), 77.0368 (10)
JWH 203	10 eV	340.1457 (100)
	20 eV	340.1465 (100), 125.0156 (93), 188.1436 (22), 214.1227 (11)
	40 eV	125.0153 (100), 144.0445 (10)
JWH 203 3-chlorophenyl isomer	10 eV	340.1443 (100)
	20 eV	340.1448 (100), 125.0139 (79), 214.121 (52), 188.1417 (43)
	40 eV	125.0139 (100), 144.0428 (43), 214.1209 (26)
JWH 203 4-chlorophenyl isomer	10 eV	340.1456 (100)
	20 eV	340.1452 (100), 125.0147 (85), 188.1431 (28), 214.1223 (19)
	40 eV	125.0145 (100), 144.0441 (16)
JWH 210	10 eV	370.2156 (100)
	20 eV	370.2155 (100), 183.0799 (77), 214.1225 (27)
	40 eV	183.0799 (100), 155.0854 (59), 144.0442 (31), 153.0696 (27), 214.1224 (22), 154.0775 (12)
JWH 210 2-ethylnaphthyl isomer	10 eV	370.2153 (100)
	20 eV	370.2154 (100), 183.0797 (59), 214.122 (44)
	40 eV	144.0439 (100), 155.0849 (81), 183.0799 (71), 214.122 (60), 141.0694 (52), 153.0692 (26), 165.069 (15), 43.0542 (13), 154.0771 (11),
JWH 210 3-ethylnaphthyl isomer	10 eV	370.2161 (100)
	20 eV	370.2161 (100), 183.08 (72), 214.1225 (40)

Substance	CE	Ion (Relative Abundance %)
	40 eV	155.0853 (100), 183.0802 (83), 144.0442 (55), 214.1224 (36), 153.0696 (32), 154.0774 (13)
JWH 210 5-ethylnaphthyl isomer	10 eV	370.2163 (100)
	20 eV	370.2162 (100), 183.0803 (91), 214.1229 (21)
	40 eV	183.0805 (100), 155.0856 (88), 153.0701 (31), 144.0446 (27), 214.1226 (19), 154.0776 (14)
JWH 210 6-ethylnaphthyl isomer	10 eV	370.2155 (100)
	20 eV	370.2158 (100), 183.0799 (75), 214.1223 (33)
	40 eV	155.085 (100), 183.0802 (63), 144.0442 (28), 214.1222 (19)
JWH 210 7-ethylnaphthyl isomer	10 eV	370.2163 (100)
	20 eV	183.0802 (100), 370.2164 (94), 214.1229 (25)
	40 eV	155.0856 (100), 183.0806 (75), 144.0447 (21), 214.1229 (13)
JWH 210 8-ethylnaphthyl isomer	10 eV	370.2164 (100)
	20 eV	370.2162 (100), 183.0801 (93), 214.1225 (26), 165.0697 (11)
	40 eV	155.0854 (100), 183.0803 (75), 165.0696 (31), 144.0444 (29), 153.0696 (19), 214.1222 (17)
JWH 249	10 eV	384.095 (100)
	20 eV	384.0956 (100), 168.9645 (81), 188.1428 (17), 214.1222 (14)
	40 eV	168.9645 (100), 214.1222 (14), 144.0441 (13)
JWH 250	10 eV	336.1952 (100), 121.0647 (24)
	20 eV	121.0648 (100), 336.1954 (12)
	40 eV	91.0545 (100), 121.0646 (61), 93.0701 (20), 130.0648 (18), 144.0795 (13)
JWH 251	10 eV	320.2007 (100)
	20 eV	320.2004 (100), 105.0697 (94), 214.1222 (76), 188.1428 (12)
	40 eV	105.0696 (100), 144.0441 (65), 214.1221 (35), 43.0544 (10)
JWH 251 3-methylphenyl isomer	10 eV	320.1981 (100)
	20 eV	105.0693 (100), 214.1206 (99), 320.1982 (77), 188.1418 (25)
	40 eV	144.0429 (100), 105.0694 (97), 214.1207 (49), 43.0551 (17)
JWH 251 4-methylphenyl isomer	10 eV	320.2004 (100)
	20 eV	105.0695 (100), 320.2003 (95), 214.1221 (48), 119.0488 (21), 188.1428 (14)
	40 eV	105.0695 (100), 144.0439 (43), 214.122 (21), 119.0487 (15), 91.0539 (11)
JWH 302	10 eV	336.1952 (100), 121.0644 (10)
	20 eV	121.0648 (100), 214.1222 (59), 336.1948 (28), 188.1429 (27)
	40 eV	121.0647 (100), 144.044 (25), 214.1216 (61), 91.0545 (20), 43.0551 (13)
JWH 307	10 eV	386.1914 (100), 155.0494 (42)
	20 eV	155.0487 (100)
	40 eV	127.0539 (100), 155.0491 (94)
JWH 309	10 eV	418.2159 (100), 155.0493 (43)
	20 eV	155.0486 (100)
	40 eV	155.049 (100), 127.0543 (67)

Substance	CE	Ion (Relative Abundance %)
JWH 368	10 eV	386.1906 (100), 155.0487 (40)
	20 eV	155.0481 (100)
	40 eV	127.0537 (100), 155.0485 (95)
JWH 369	10 eV	402.1617 (100), 155.0493 (43)
	20 eV	155.0487 (100)
	40 eV	155.0489 (100), 127.0543 (91)
JWH 370	10 eV	382.2155 (100), 155.049 (47)
	20 eV	155.0486 (100)
	40 eV	127.0542 (100), 155.0489 (99)
JWH 398	10 eV	376.1453 (100)
	20 eV	189.0097 (100), 376.1458 (93), 214.1221 (11)
	40 eV	189.0097 (100), 161.0149 (80), 144.044 (10)
JWH 398 2-chloronaphthyl isomer	10 eV	376.146 (100)
	20 eV	376.1465 (100), 189.0102 (89)
	40 eV	189.0103 (100), 161.0154 (49)
JWH 398 3-chloronaphthyl isomer	10 eV	376.1465 (100)
	20 eV	189.0107 (100), 376.147 (98), 214.123 (10)
	40 eV	161.0156 (100), 189.0106 (91), 144.045 (11)
JWH 398 5-chloronaphthyl isomer	10 eV	376.1454 (100)
	20 eV	189.0102 (100), 376.1462 (95), 214.1226 (10)
	40 eV	161.0152 (100), 189.0103 (90)
JWH 398 6-chloronaphthyl isomer	10 eV	376.1454 (100)
	20 eV	189.0102 (100), 376.1462 (99), 214.1225 (17)
	40 eV	161.0152 (100), 189.0103 (73), 144.0445 (11)
JWH 398 7-chloronaphthyl isomer	10 eV	376.1453 (100)
	20 eV	189.0096 (100), 376.1456 (84)
	40 eV	161.0146 (100), 189.0096 (92)
JWH 398 8-chloronaphthyl isomer	10 eV	376.146 (100)
	20 eV	376.1464 (100), 189.0105 (78)
	40 eV	189.0104 (100), 161.0155 (66)
JWH 424	10 eV	420.0955 (100)
	20 eV	420.0962 (100), 232.9601 (61)
	40 eV	232.9601 (100), 204.965 (62), 214.1227 (15), 167.0491 (12), 284.1074 (11), 270.0918 (10)
JZL 195	10 eV	434.1697 (100), 183.0799 (28)
	20 eV	183.0795 (100), 434.1707 (17)
	40 eV	183.0798 (100), 155.0853 (18), 165.0695 (16), 168.0566 (15), 153.0695 (11)
MAM2201	10 eV	374.1903 (100)
	20 eV	374.1908 (100), 169.0643 (73), 232.1122 (25)
	40 eV	169.0641 (100), 141.0697 (84), 144.0443 (28), 232.1133 (20)

Substance	CE	Ion (Relative Abundance %)
MDA 19	10 eV	350.1862 (100), 105.0337 (61)
	20 eV	105.0333 (100)
	40 eV	105.0335 (100), 77.0387 (53)
MDA 77	10 eV	366.1805 (100), 105.0336 (25)
	20 eV	105.0331 (100)
	40 eV	105.0334 (100), 77.0385 (44)
MDMA methylene homolog	10 eV	208.1325 (100), 135.0441 (26)
	20 eV	135.0436 (100), 147.0803 (12)
	40 eV	77.0388 (100), 135.0441 (92), 91.0545 (29), 79.0543 (28), 105.0337 (22), 51.0232 (17)
meta-Chlorophenylpiperazine	10 eV	197.0832 (100), 154.041 (12)
	20 eV	154.0409 (100), 197.0833 (49), 119.0724 (41), 44.0493 (22), 118.0645 (12)
	40 eV	118.0646 (100), 119.0722 (25), 44.0492 (17), 110.9988 (15), 91.0539 (15), 104.0488 (12)
Methcathinone	10 eV	146.0961 (100), 131.0724 (34), 164.1067 (20)
	20 eV	131.0726 (100), 146.096 (34), 130.0646 (26), 105.0695 (26)
	40 eV	130.0647 (100), 77.0383 (58), 103.0538 (18), 79.054 (14), 131.0723 (11)
Methedrone	10 eV	176.1064 (100), 161.083 (17), 194.1168 (15), 58.0651 (14)
	20 eV	161.0827 (100), 176.1062 (45), 146.0593 (33), 145.0879 (30), 135.0799 (21), 58.0651 (20)
	40 eV	118.0648 (100), 146.0593 (88), 77.0381 (46), 144.0801 (37), 91.0539 (36), 132.0802 (33), 79.0539 (26), 58.0652 (25), 103.0536 (25), 117.057 (20), 105.0695 (19)
Methoxetamine	10 eV	203.1061 (100), 248.1638 (52), 175.1108 (17), 46.0659 (16)
	20 eV	175.1108 (100), 121.0646 (91), 203.1057 (70), 67.0547 (28), 46.0659 (18), 159.0791 (13)
	40 eV	121.0646 (100), 91.0545 (35), 67.0547 (16), 77.0392 (10)
Methylone	10 eV	160.0752 (100), 190.0857 (70), 208.0965 (42), 58.0651 (12)
	20 eV	160.0751 (100), 132.0804 (35)
	40 eV	132.0802 (100), 117.0571 (82), 91.054 (54), 131.0724 (28), 65.0383 (24), 58.065 (19), 160.0751 (14), 130.065 (11), 115.0539 (11)
N,N-Diallyl-5-methoxytryptamine	10 eV	110.0966 (100), 174.0913 (49), 271.1808 (30)
	20 eV	110.0966 (100), 174.0909 (81)
	40 eV	159.0679 (100), 131.0731 (72), 41.04 (47), 143.073 (46), 130.0654 (37), 174.0912 (36), 110.0968 (34), 79.0552 (19), 81.0708 (10), 115.0547 (10)
N,N-Diethylcathinone	10 eV	206.1533 (100)
	20 eV	105.0698 (100), 100.1123 (57), 206.153 (35), 133.0644 (314), 72.0815 (17)
	40 eV	77.0391 (100), 105.0698 (86), 100.1122 (58), 79.0548 (51), 72.0815 (37), 103.0542 (34), 58.066 (32), 44.0505 (32), 130.0647 (21), 105.0333 (19), 117.0575 (12)
N,N-Diisopropyl-5-methoxytryptamine	10 eV	114.1272 (100), 275.2113 (76), 174.0904 (46)
	20 eV	174.0903 (100), 114.127 (90), 72.0801 (10)
	40 eV	159.0668 (100), 131.072 (63), 174.0903 (50), 143.0719 (43), 72.0803 (33), 130.0644 (31), 114.1267 (17), 115.0539 (10)
N,N-Dimethylcathinone	10 eV	178.1218 (100)133.0646 (30), 105.0697 (18)

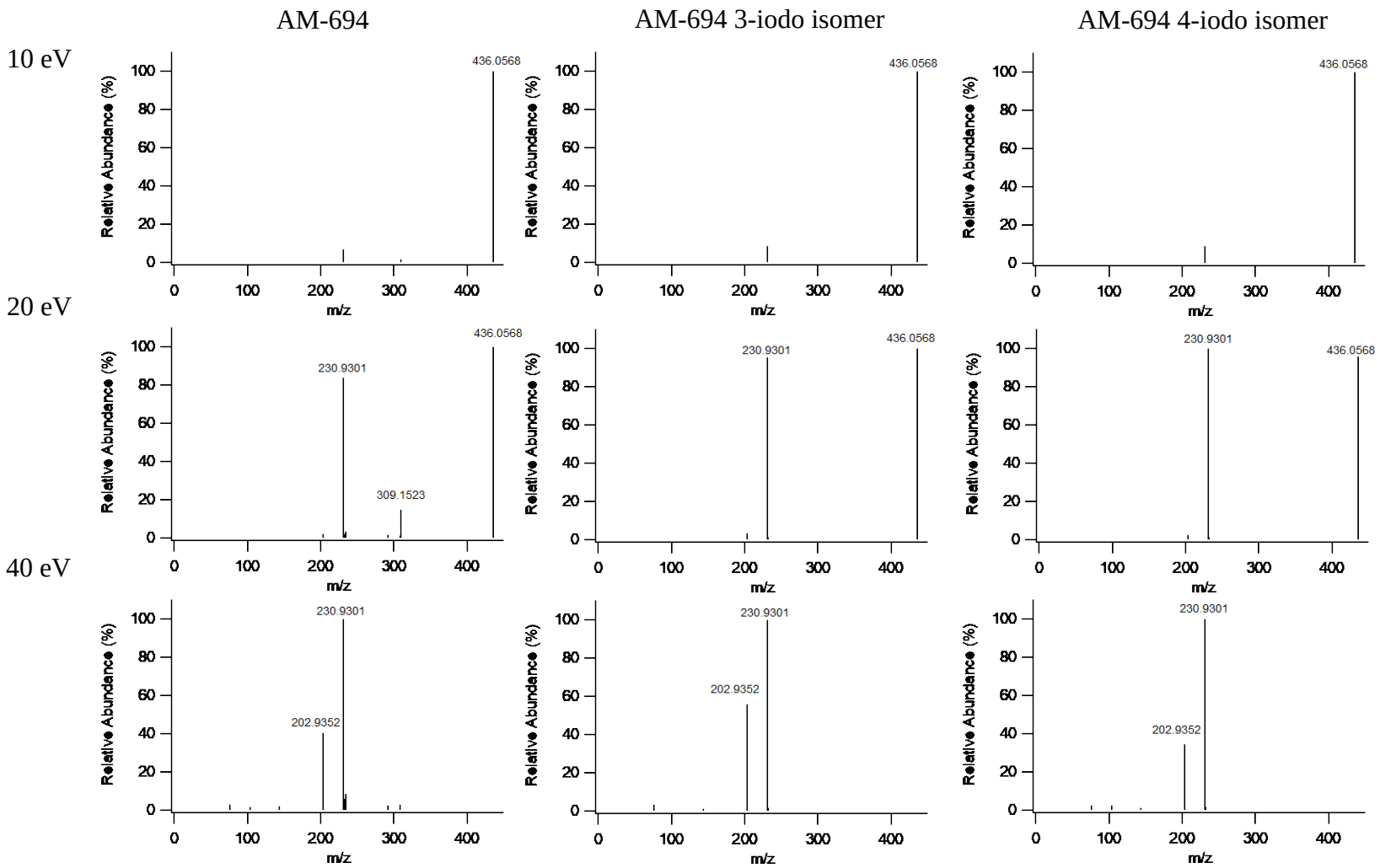
Substance	CE	Ion (Relative Abundance %)
	20 eV	105.0697 (100), 72.0808 (51), 133.0647 (24), 178.1223 (10)
	40 eV	77.0386 (100), 72.0807 (78), 79.0542 (37), 105.0696 (32), 103.0542 (23), 44.0496 (12)
N,N-Dimethyltryptamine	10 eV	58.0652 (100), 144.0804 (51), 189.1382 (15)
	20 eV	58.0651 (100), 144.0805 (84)
	40 eV	58.0651 (100), 143.0725 (37), 115.0538 (36), 117.0647 (27), 91.0543 (22), 144.0802 (19), 127.054 (18)
Naphyrone	10 eV	282.185 (100)
	20 eV	141.0693 (100), 282.185 (88), 211.1115 (78), 126.1276 (23), 155.0487 (16)
	40 eV	141.0694 (100), 127.054 (41), 126.1274 (41), 155.0488 (21), 84.0808 (18)
Naphyrone 1-naphthyl isomer	10 eV	282.1846 (100)
	20 eV	282.1849 (100), 211.1115 (81), 126.1275 (73), 141.0698 (61), 155.0489 (31), 169.0647 (12)
	40 eV	141.0697 (100), 127.0542 (92), 126.1276 (79), 155.049 (49), 84.0807 (23)
N-Isopropyl-5-methoxy-N-methyltryptamine	10 eV	91.0544 (100), 77.0392 (87), 79.0548 (39), 103.0539 (35), 65.0391 (32), 78.0467 (19), 105.0715 (19), 119.048 (18), 121.0649 (17), 107.0492 (15)
	20 eV	86.097 (100), 174.0908 (74), 44.0508 (10)
	40 eV	44.0508 (100), 131.0728 (89), 159.0675 (88), 130.065 (56), 143.0728 (48), 86.0972 (44), 174.0909 (22), 115.0542 (13), 43.0557 (11)
Nor-Mephedrone	10 eV	146.0957 (100)131.0725 (20), 147.0799 (12)
	20 eV	131.0726 (100), 146.0957 (33), 130.0647 (24), 119.085 (21)
	40 eV	130.0647 (100), 91.0539 (16), 77.0382 (13), 103.0539 (10)
para-Fluorophenylpiperazine	10 eV	181.1131 (100), 138.0713 (16)
	20 eV	138.0713 (100), 181.1134 (35), 136.0556 (15), 44.0498 (14)
	40 eV	95.0292 (100), 109.0448 (84), 96.0371 (75), 136.0556 (69), 83.0291 (59), 91.0545 (59), 44.0498 (54), 75.023 (41), 138.0713 (40), 110.0407 (37), 111.0489 (31), 101.0385 (30), 124.0556 (23), 117.0573 (23), 77.0384 (22), 97.0449 (17), 122.04 (16), 118.0648 (15), 42.0342 (14), 137.0632 (11), 56.0498 (11)
Pentedrone	10 eV	174.1274 (100), 192.1385 (61), 132.0808 (34), 161.096 (25), 91.0545 (21)
	20 eV	132.0811 (100), 91.0547 (88), 131.0732 (46), 174.1277 (28), 144.0808 (18), 117.0578 (15), 105.0339 (14), 145.0887 (12)
	40 eV	91.0546 (100), 130.0653 (64), 77.0388 (52), 144.0807 (46), 117.0578 (31), 131.073 (25), 65.0388 (14)
Pentylone	10 eV	236.1278 (100), 218.1174 (93), 188.1069 (59), 205.0857 (30), 86.0966 (16), 175.0727 (13)
	20 eV	188.1067 (100), 175.0685 (36), 218.1175 (24), 86.0967 (22), 135.0442 (19), 160.1115 (11)
	40 eV	131.0731 (100), 135.0441 (35), 175.0631 (32), 174.0548 (30), 188.0717 (227), 159.0676 (25), 121.0286 (23), 65.0389 (23), 44.0501 (22), 86.0967 (19), 118.0652 (18), 130.0652 (18), 149.0232 (17), 146.0596 (17), 119.0743 (13), 77.0387 (13), 117.0583 (13), 188.1034 (10),
Phenylpiperazine	10 eV	163.1217 (100), 120.08 (23)
	20 eV	120.0797 (100), 163.1218 (27), 118.064 (15)
	40 eV	77.0377 (100), 118.0639 (24), 91.0534 (23), 44.049 (17), 51.0224 (16), 120.0797 (15), 103.0534 (13)
Pravadoline	10 eV	379.2012 (100), 135.0441 (64)

Substance	CE	Ion (Relative Abundance %)
	20 eV	135.0438 (100)
	40 eV	135.044 (100), 114.0918 (26), 107.0495 (11), 77.039 (11)
Pyrovalerone	10 eV	246.1847 (100)
	20 eV	105.0701 (100), 175.1117 (51), 246.1855 (50), 126.1279 (26), 119.0494 (22)
	40 eV	105.0703 (100), 91.0545 (57), 126.1278 (44), 119.0495 (34), 84.081 (27)
RCS-4	10 eV	322.1794 (100), 135.044 (10)
	20 eV	135.0436 (100), 322.1802 (35)
	40 eV	135.0438 (100), 77.0388 (30), 107.0495 (22)
RCS-4 2-methoxy isomer	10 eV	322.1793 (100), 135.0439 (23)
	20 eV	135.0436 (100), 322.1802 (11)
	40 eV	135.0437 (100), 77.0388 (35)
RCS-4 3-methoxy isomer	10 eV	322.1801 (100)
	20 eV	135.0442 (100), 322.1804 (50)
	40 eV	107.0497 (100), 135.0446 (78), 77.0392 (64), 144.0448 (16), 92.0263 (15)
RCS-4-C4 Homolog	10 eV	308.1638 (100), 135.0439 (14)
	20 eV	135.0436 (100), 308.1644 (23)
	40 eV	135.0438 (100), 77.0388 (40), 107.0494 (27)
RCS-8	10 eV	376.2264 (100), 121.0645 (10)
	20 eV	121.0647 (100), 376.2258 (52)
	40 eV	121.0647 (100), 91.0546 (65), 144.0799 (26), 93.07 (20)
RCS-8 3-methoxy isomer	10 eV	376.2255 (100)
	20 eV	376.2261 (100), 121.0637 (86), 254.1532 (41), 228.1737 (30), 132.0797 (10)
	40 eV	121.0637 (100), 254.1532 (62), 144.0433 (32), 69.0689 (18), 158.0588 (13), 91.0533 (10), 132.0797 (10)
RCS-8 4-methoxy isomer	10 eV	376.2265 (100)
	20 eV	376.2258 (100), 121.0642 (37), 149.0589 (13)
	40 eV	121.0638 (100), 135.0433 (32)
STS-135	10 eV	383.2487 (100)
	20 eV	383.2488 (100), 135.1168 (25)
	40 eV	135.1167 (100), 93.0702 (14), 107.0856 (13)
Trimethoxyamphetamine	10 eV	209.1163 (100)
	20 eV	181.0849 (100), 194.0927 (98), 178.0976 (87), 209.1162 (72), 168.0771 (45), 179.0691 (37), 166.0605 (31), 163.0741 (26), 151.0743 (22), 162.0661 (22), 147.0427 (17), 165.0533 (17), 177.0893 (16), 153.054 (16), 121.0639 (15), 147.0778 (14), 135.0786 (10)
	40 eV	91.0533 (100), 107.0481 (57), 77.0379 (39), 119.0484 (39), 103.0535 (37), 121.0643 (28), 79.053 (25), 65.0377 (22), 105.0695 (22), 151.0735 (21), 147.0422 (17), 148.0502 (16), 78.0448 (16), 115.0534 (16), 136.0509 (16), 135.079 (15), 137.0595 (14), 125.0593 (11), 131.0484 (11), 93.0333 (11), 163.0737 (11), 147.0789 (10)
UR-144	10 eV	312.2317 (100)
	20 eV	312.2322 (100), 125.0964 (78), 214.123 (28), 294.222 (13)

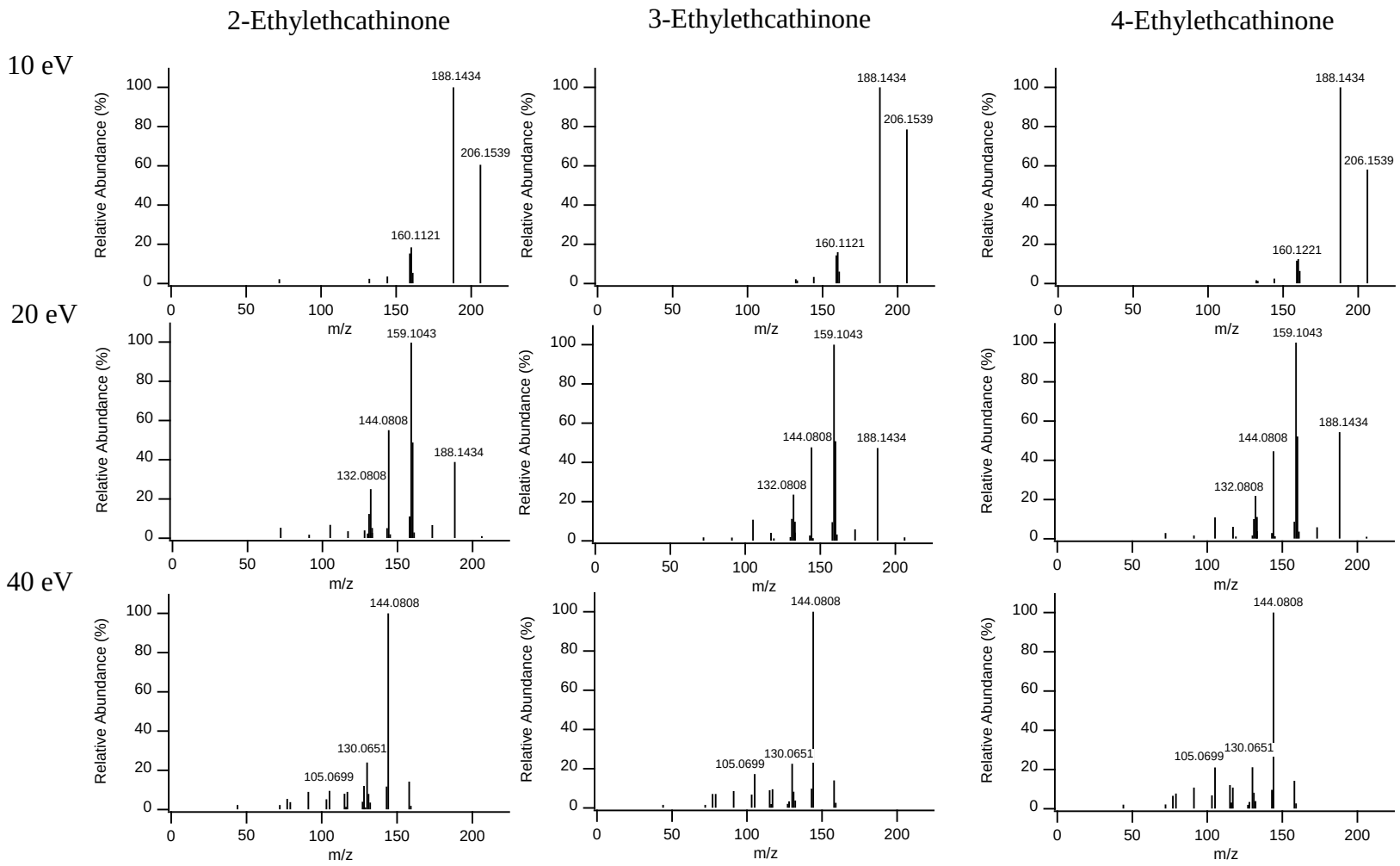
Substance	CE	Ion (Relative Abundance %)
	40 eV	55.0547 (100), 144.0447 (58), 57.0703 (45), 125.0965 (42), 97.1016 (33), 214.1228 (25), 69.0701 (25), 264.1748 (16), 43.0547 (15), 83.0857 (15), 130.0655 (13), 208.1122 (11), 222.128 (10)
URB447	10 eV	401.1411 (100)
	20 eV	105.0338 (100), 401.1416 (69), 296.1076 (42), 276.1254 (14)
	40 eV	105.0337 (100), 171.0915 (41), 77.0388 (30), 125.0154 (20), 198.0786 (10)
URB597	10 eV	214.0862 (100), 197.0594 (16)
	20 eV	197.0593 (100), 214.0858 (50), 171.0798 (24)
	40 eV	153.0692 (100), 197.0592 (45), 171.0797 (31), 141.0694 (25), 152.0616 (22), 169.0641 (20)
URB602	10 eV	214.0857 (100), 170.0956 (23), 196.0755 (13)
	20 eV	170.0959 (100), 196.0749 (63), 168.08 (30), 214.0862 (25), 153.0689 (18)
	40 eV	153.0693 (100), 152.0617 (59), 168.0801 (48), 141.0695 (28), 170.0962 (26), 151.053 (10)
URB754	10 eV	267.1136 (100), 160.0397 (27)
	20 eV	160.0392 (100), 267.1127 (12)
	40 eV	104.0497 (100), 160.0392 (46), 77.0388 (41), 106.0654 (30), 79.0544 (19)
URB937	10 eV	230.0815 (100), 213.0551 (22), 355.1672 (22)
	20 eV	213.0546 (100), 230.0816 (46), 187.0751 (12)
	40 eV	213.0547 (100), 141.0699 (57), 185.0598 (49), 157.0646 (46), 169.0655 (36), 187.0758 (26), 129.0694 (19), 167.0497 (10), 115.0535 (10)
WIN 54461	10 eV	457.1107 (100), 135.0437 (47)
	20 eV	135.0435 (100), 457.1111 (13)
	40 eV	135.0436 (100), 114.0912 (24)
WIN 55212-2	10 eV	427.2018 (100), 155.0492 (19)
	20 eV	155.0492 (100), 427.2014 (44)
	40 eV	155.0492 (100), 127.0543 (32), 100.0759 (21)
XLR11	10 eV	330.2221 (100)
	20 eV	330.2215 (100), 125.0953 (53), 232.1124 (21)
	40 eV	55.0538 (100), 144.0434 (63), 125.0952 (55), 57.0693 (43), 97.1004 (39), 232.1126 (38), 69.0691 (30), 282.1644 (21), 83.0847 (17), 130.0643 (15), 222.1269 (12), 41.0382 (11), 297.1875 (10)
α-Methyltryptamine	10 eV	158.0959 (100)
	20 eV	158.0958 (100),143.0725 (85),130.0649 (77),117.0572 (48)
	40 eV	117.0571 (100),143.0725 (84),115.054 (72),130.0649 (51),90.0464 (40),142.0648 (37),77.0385 (32),116.0612 (22),91.0537 (22),89.0382 (21),103.0541 (21),128.0507 (12)
α-Pyrrolidinobutiophenone	10 eV	218.1531 (100)
	20 eV	91.0541 (100), 218.1536 (69), 147.0801 (35), 112.1119 (32), 105.0334 (20), 70.065 (19), 119.0853 (15)
	40 eV	91.054 (100), 77.0385 (61), 112.1118 (41), 105.0333 (32), 84.0806 (24), 70.0649 (16)
α-Pyrrolidinopentiophenone	10 eV	232.1687 (100)
	20 eV	91.0546 (100), 232.1697 (75), 126.1279 (30), 161.0961 (29), 105.0339 (24), 70.0655 (18), 119.0495 (12)

Substance	CE	Ion (Relative Abundance %)
	40 eV	91.0547 (100), 77.039 (60), 126.128 (37), 105.0339 (37), 84.0811 (29), 70.0653 (10)
α-Pyrrolidinopropiophenone	10 eV	204.1374 (100)
	20 eV	105.07 (100), 204.1382 (89), 98.0966 (63), 133.0649 (50), 70.0652 (23)
	40 eV	98.0966 (100), 105.0699 (94), 77.0387 (70), 79.0544 (44), 56.0496 (31), 103.0543 (27), 70.0653 (22), 84.081 (17), 105.0336 (16), 55.0545 (13)

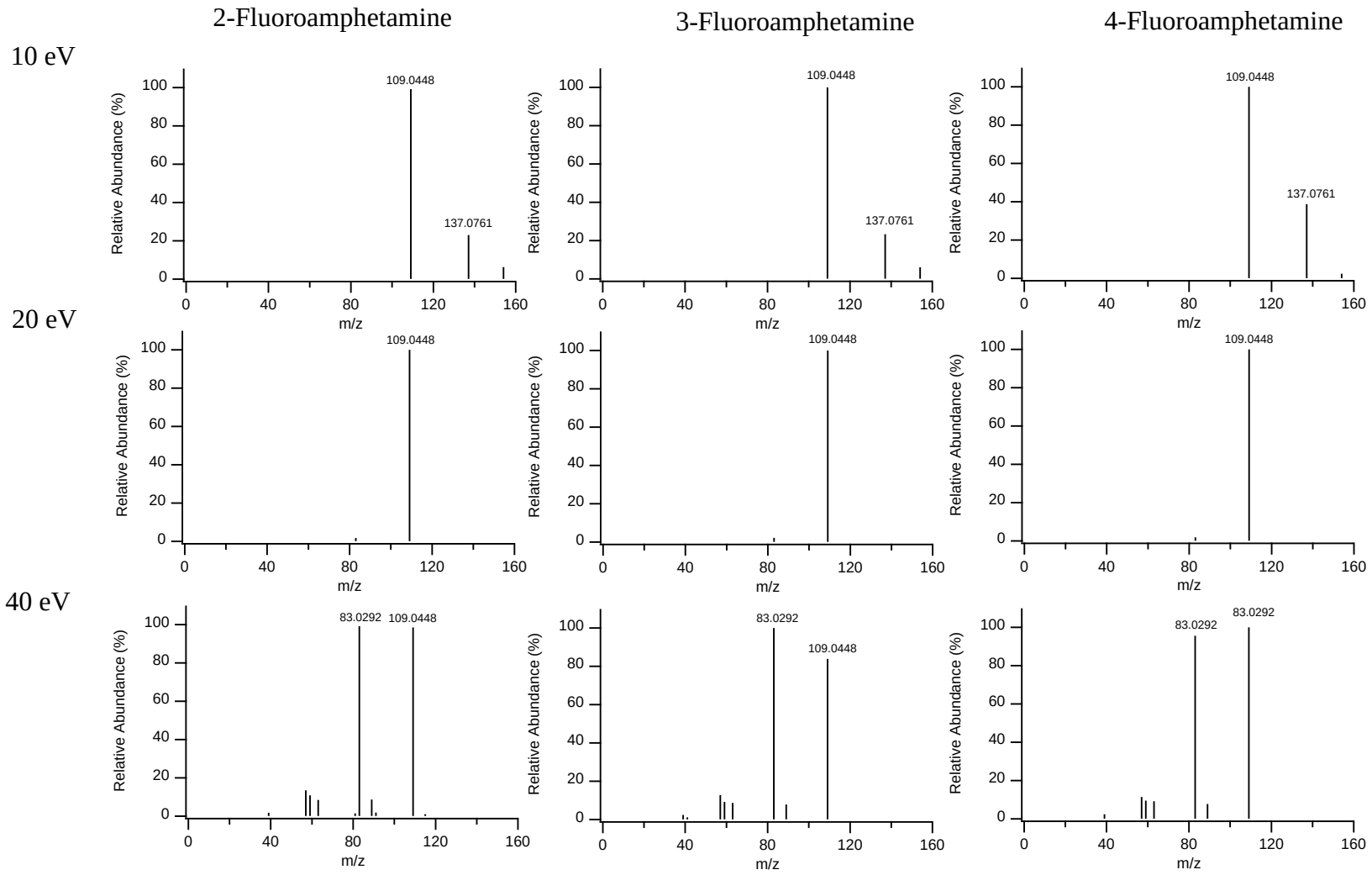
Appendix 6. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the AM 694 set of regioisomers.



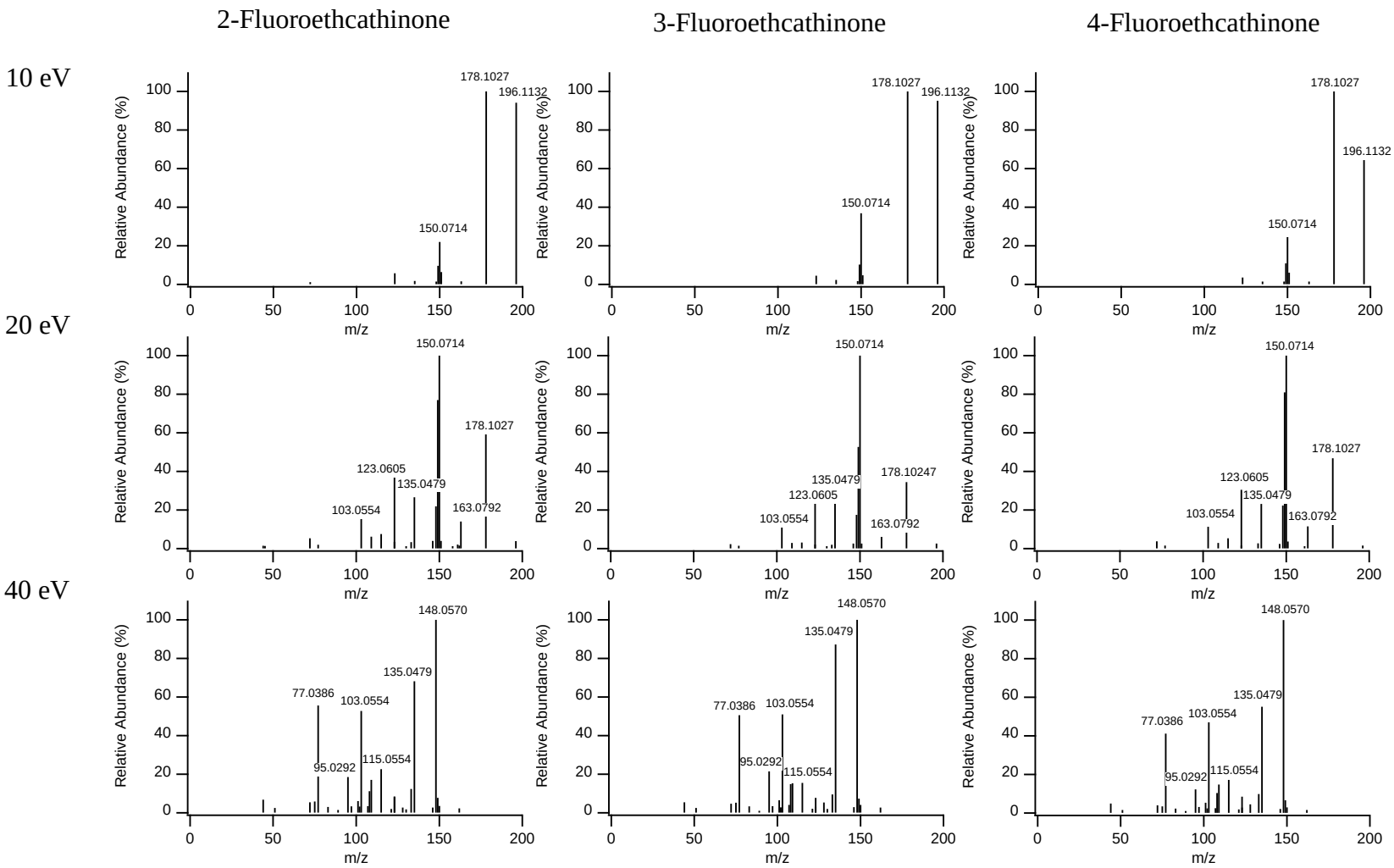
Appendix 7. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the ethylethcathinone set of regioisomers.



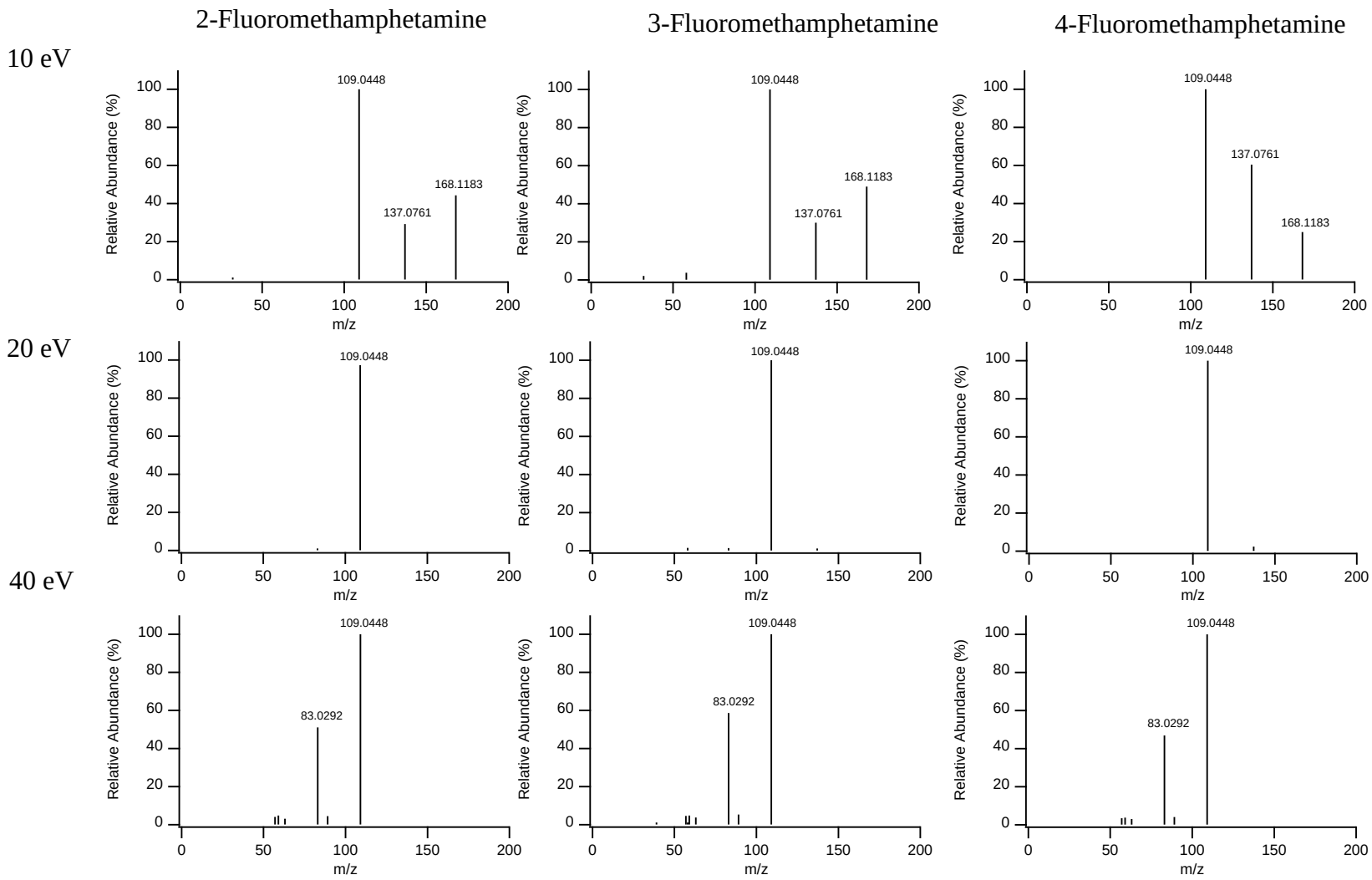
Appendix 8. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the fluoroamphetamine set of regioisomers.



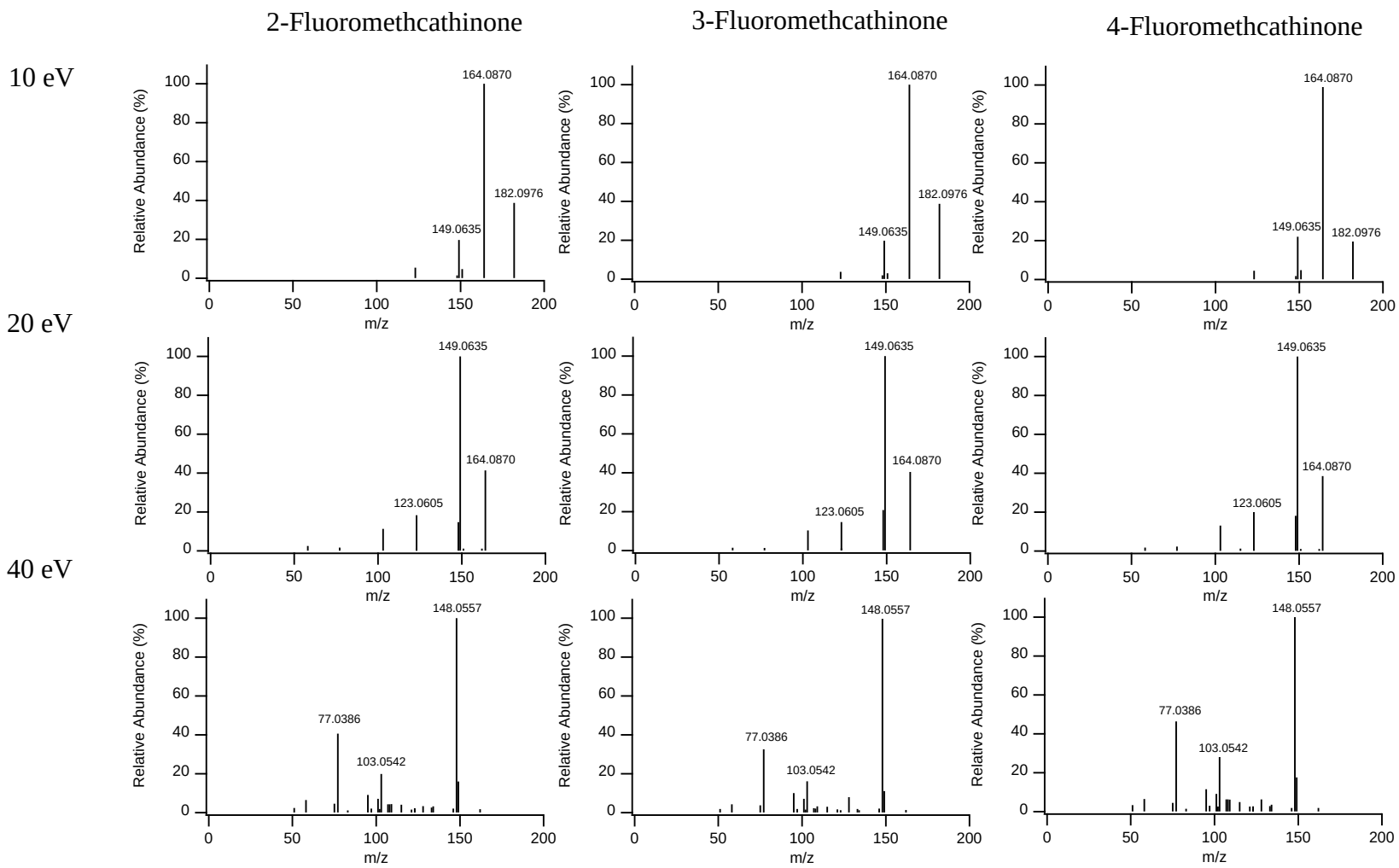
Appendix 9. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the fluoroethcathinone set of regioisomers.



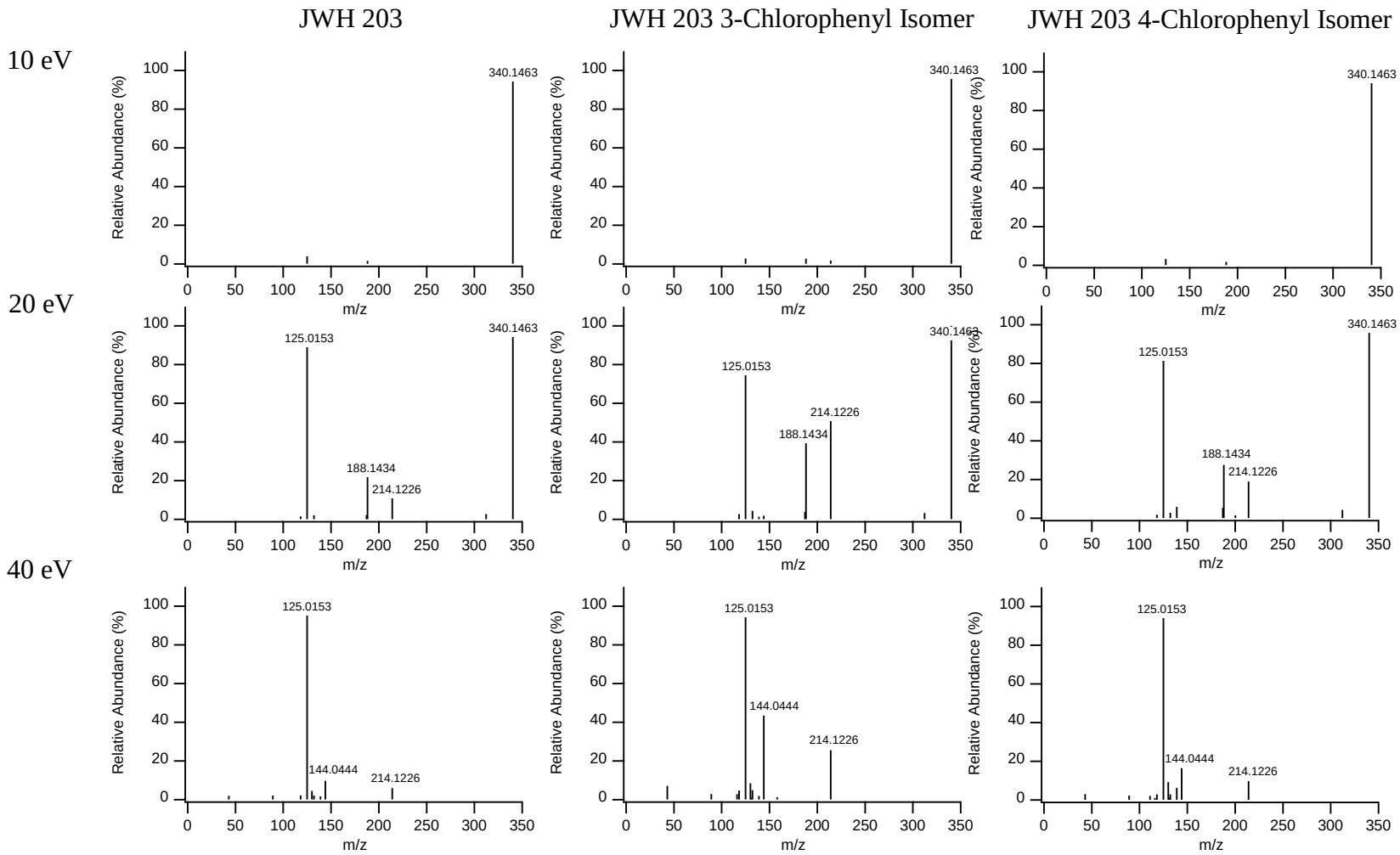
Appendix 10. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the fluoromethamphetamine set of regioisomers.



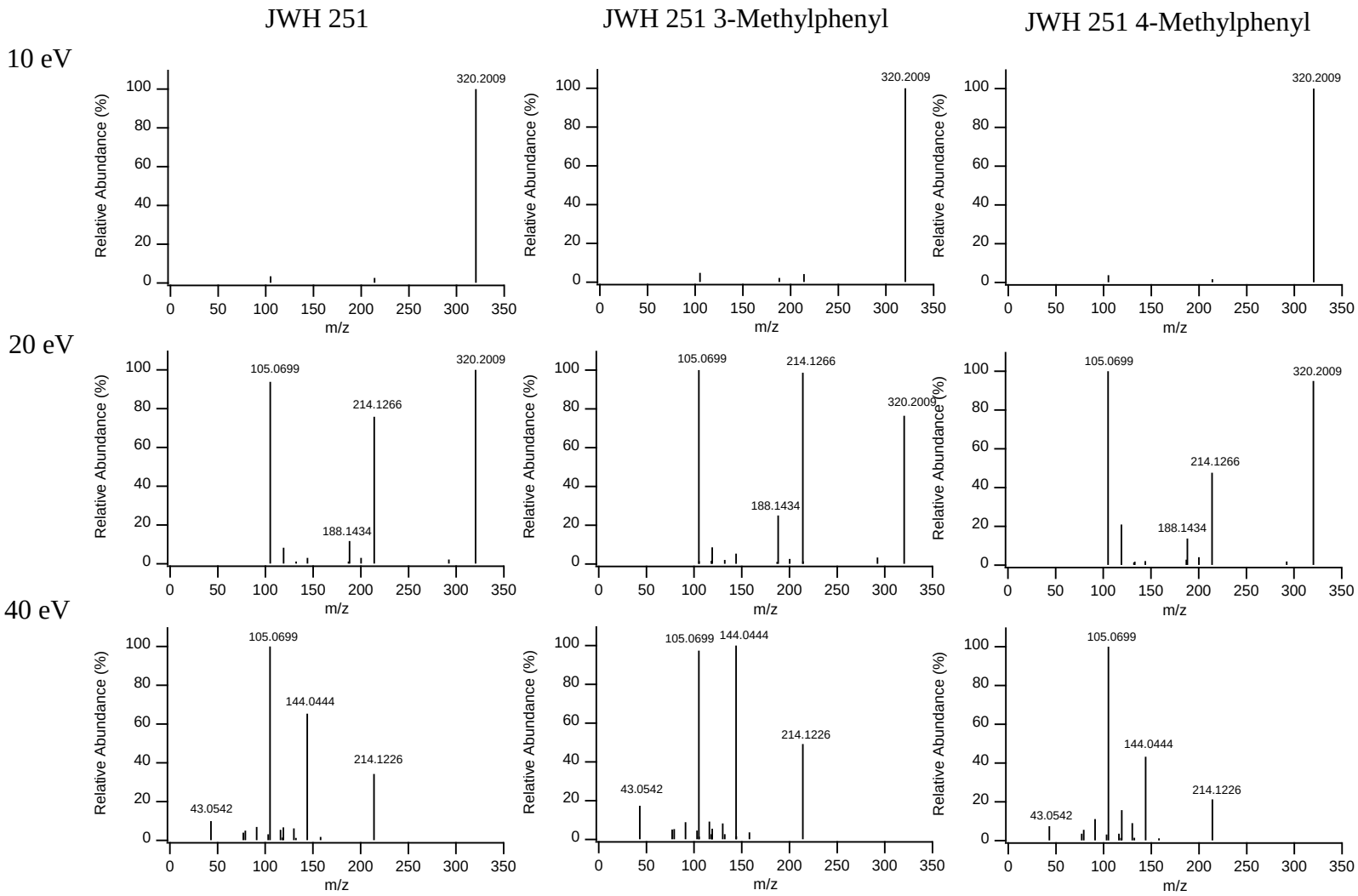
Appendix 11. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the fluoromethcathinone set of regioisomers.



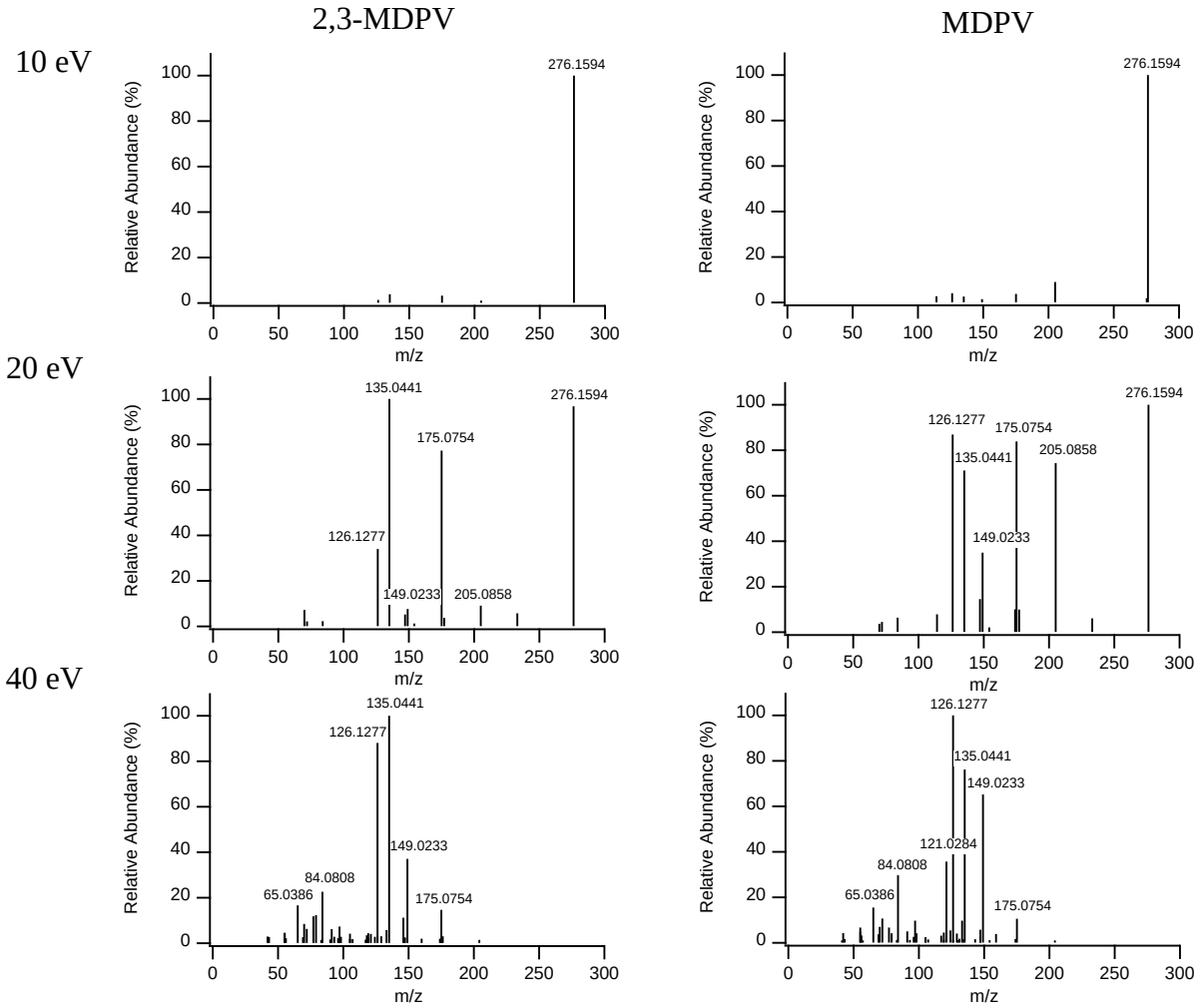
Appendix 12. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the JWH 203 set of regioisomers.



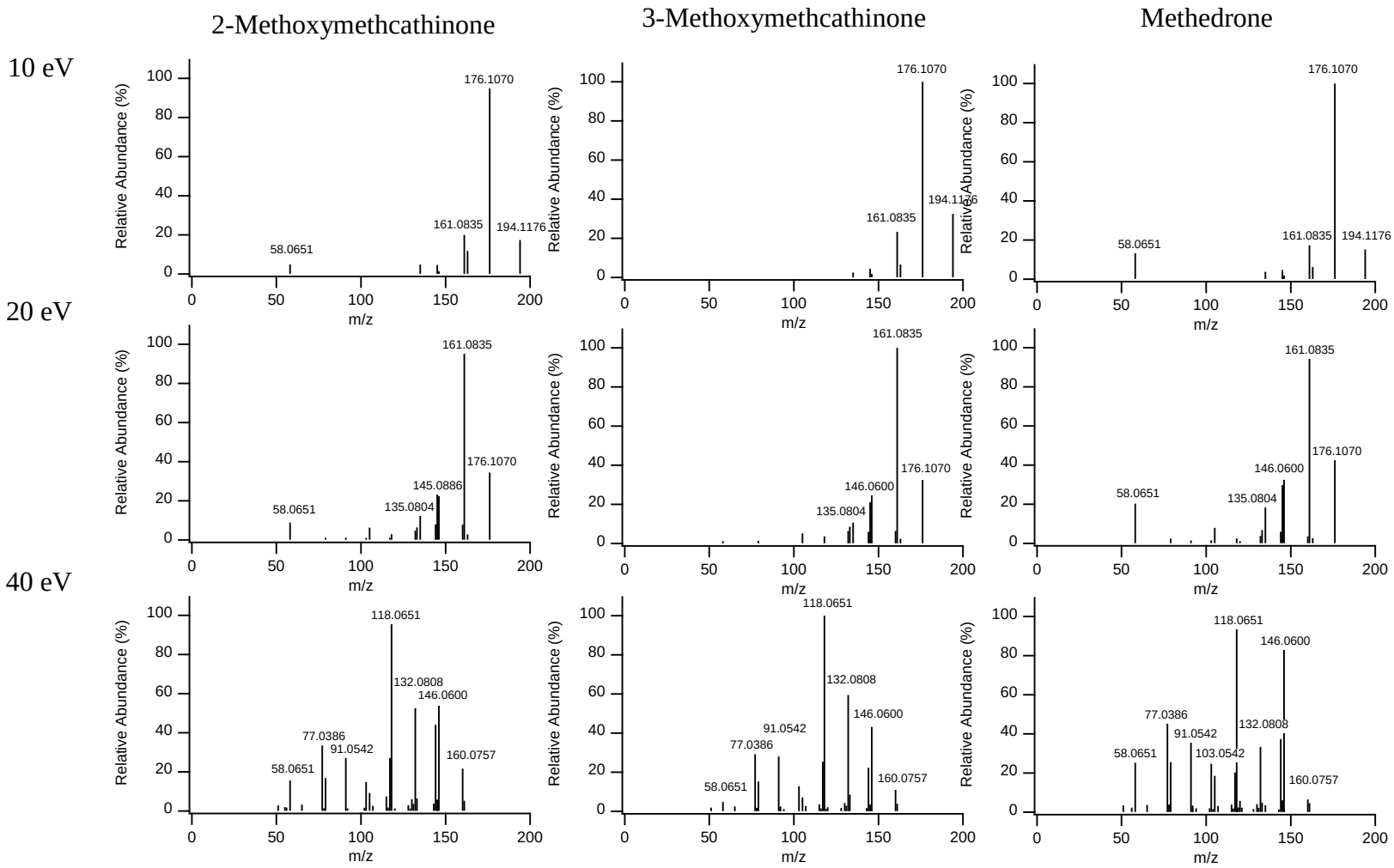
Appendix 13. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the JWH 251 set of regioisomers.



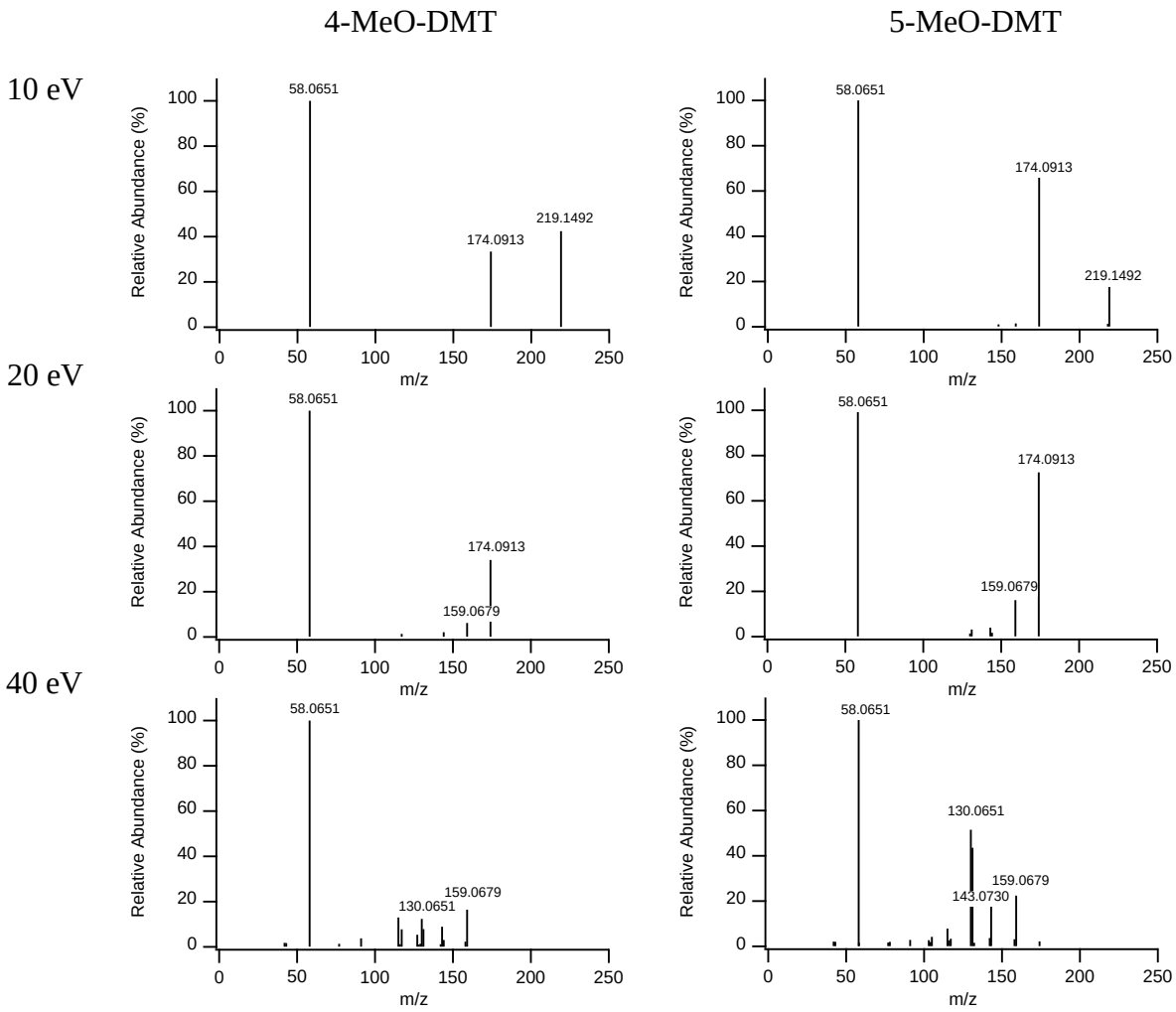
Appendix 14. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the methylenedioxy pyrovalerone set of regioisomers.



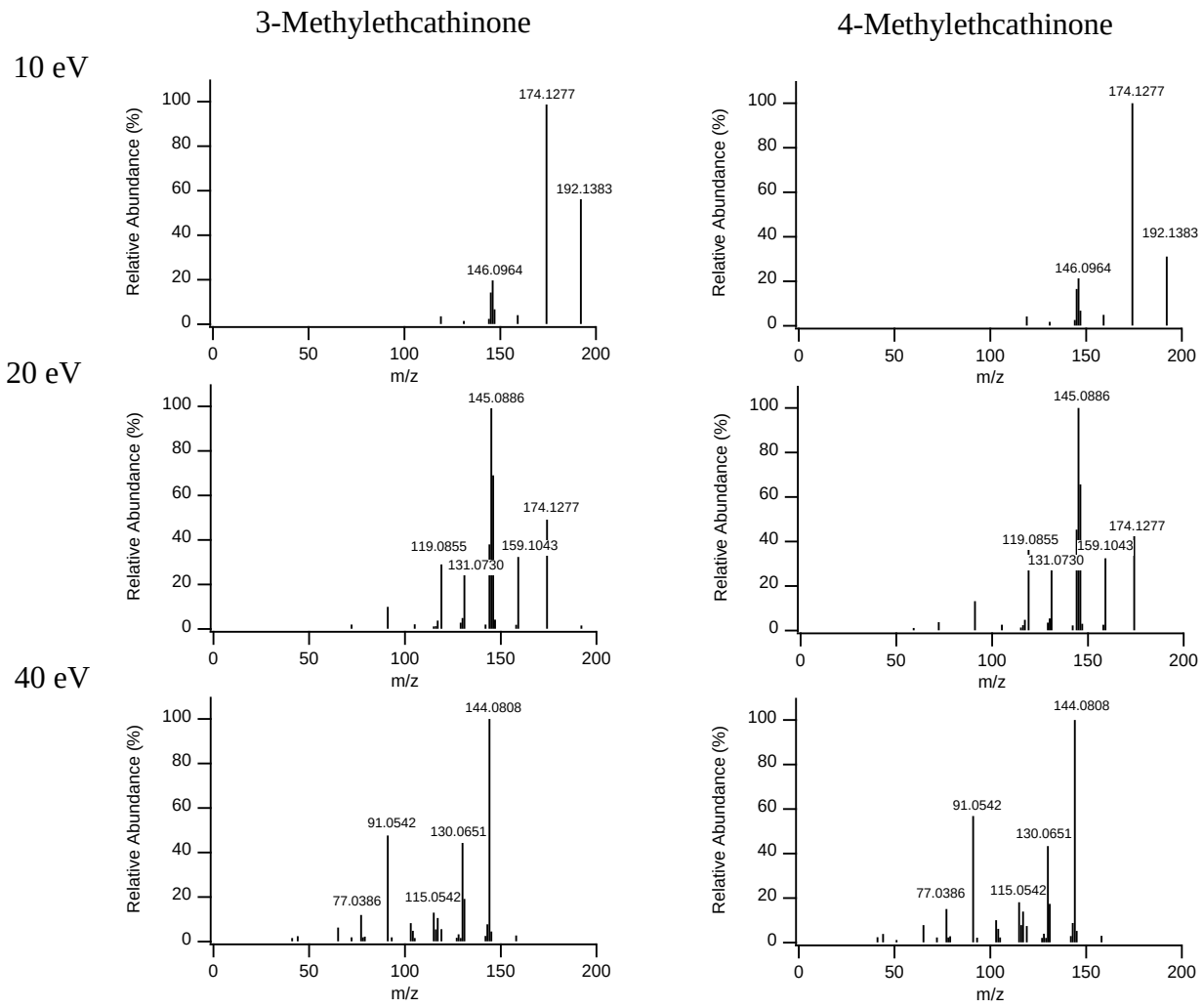
Appendix 15. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the methoxymethcathinone set of regioisomers.



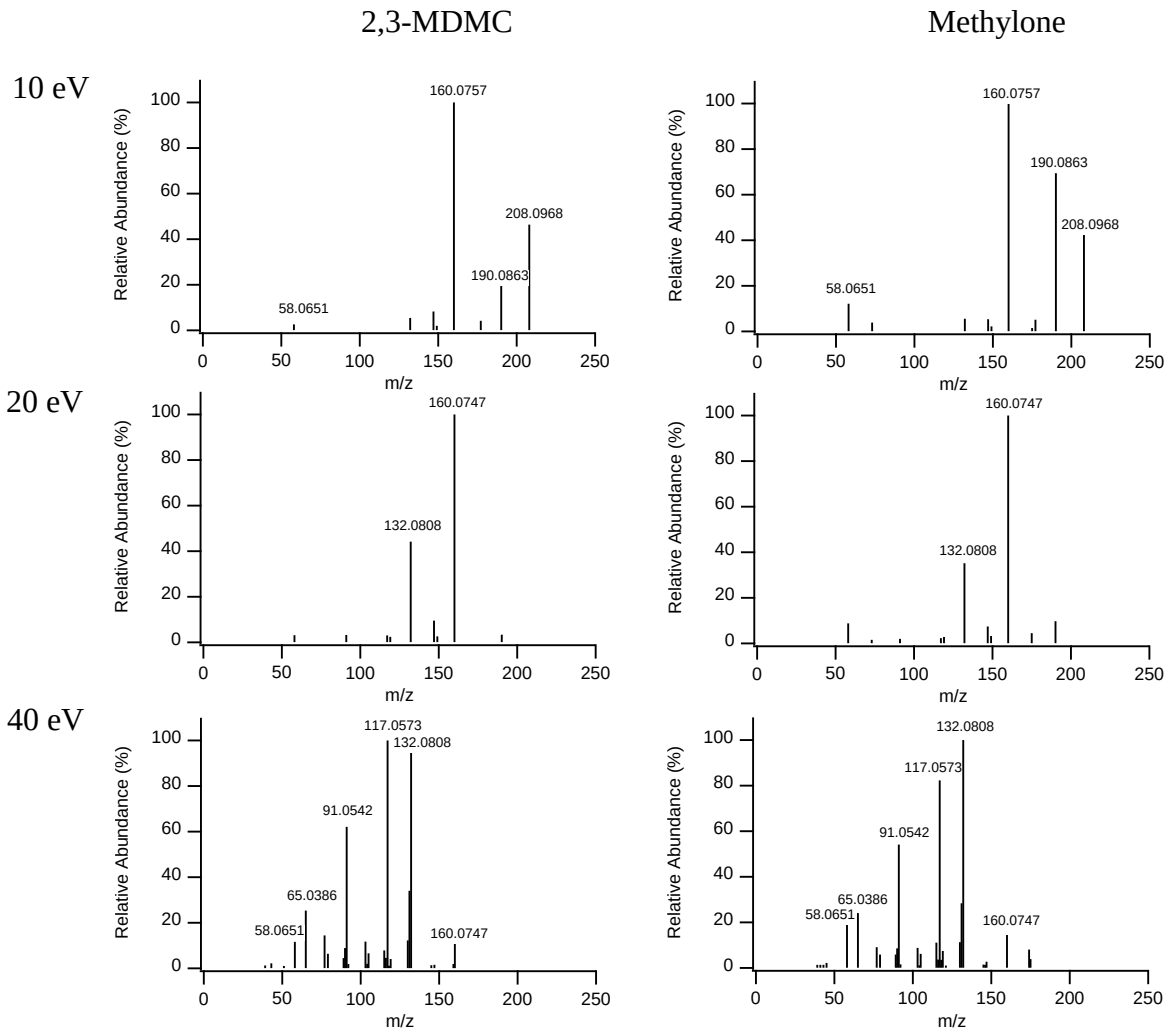
Appendix 16. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the methoxy-N,N-dimethyltryptamine set of regioisomers.



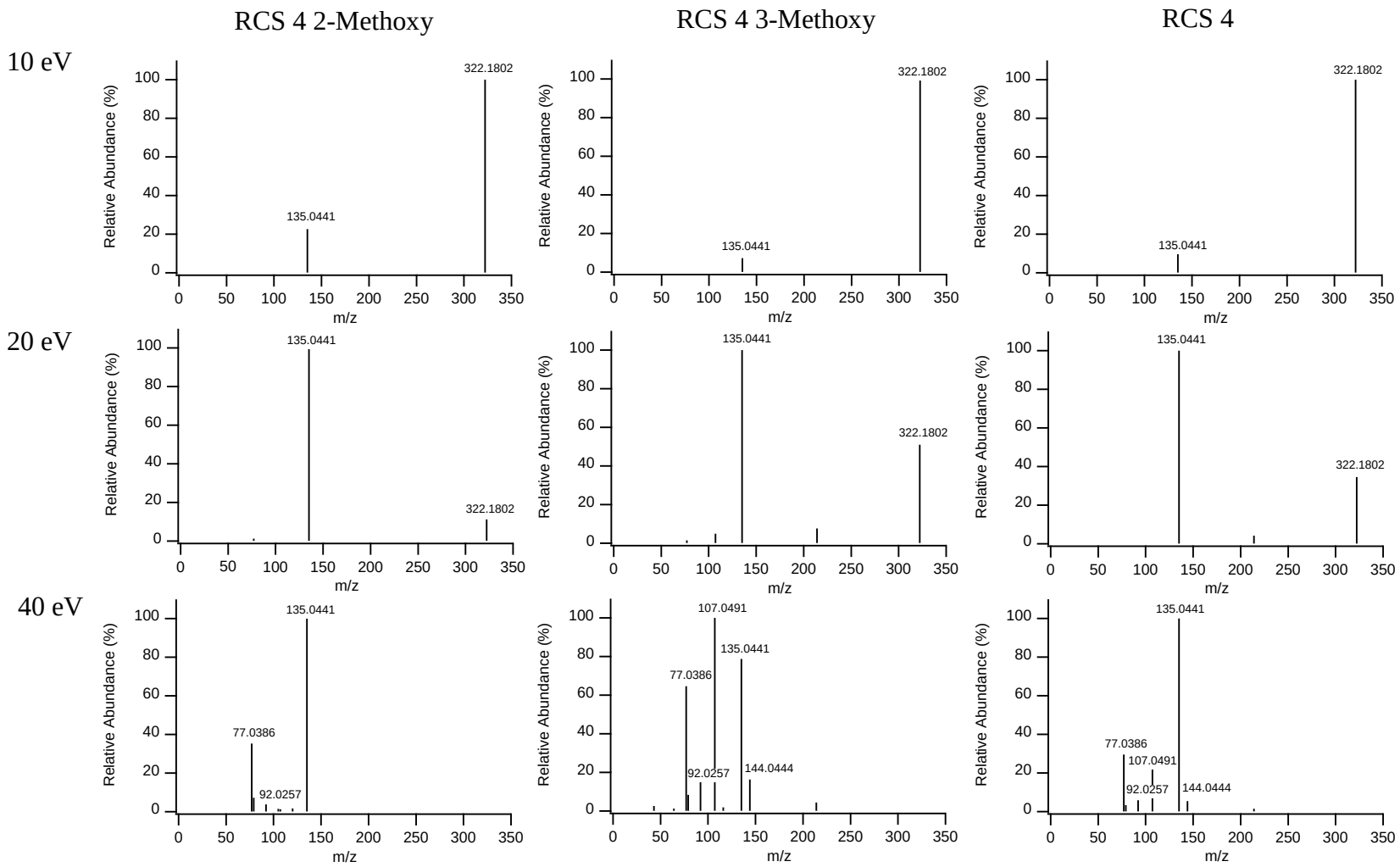
Appendix 17. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the methylethcathinone set of regioisomers.



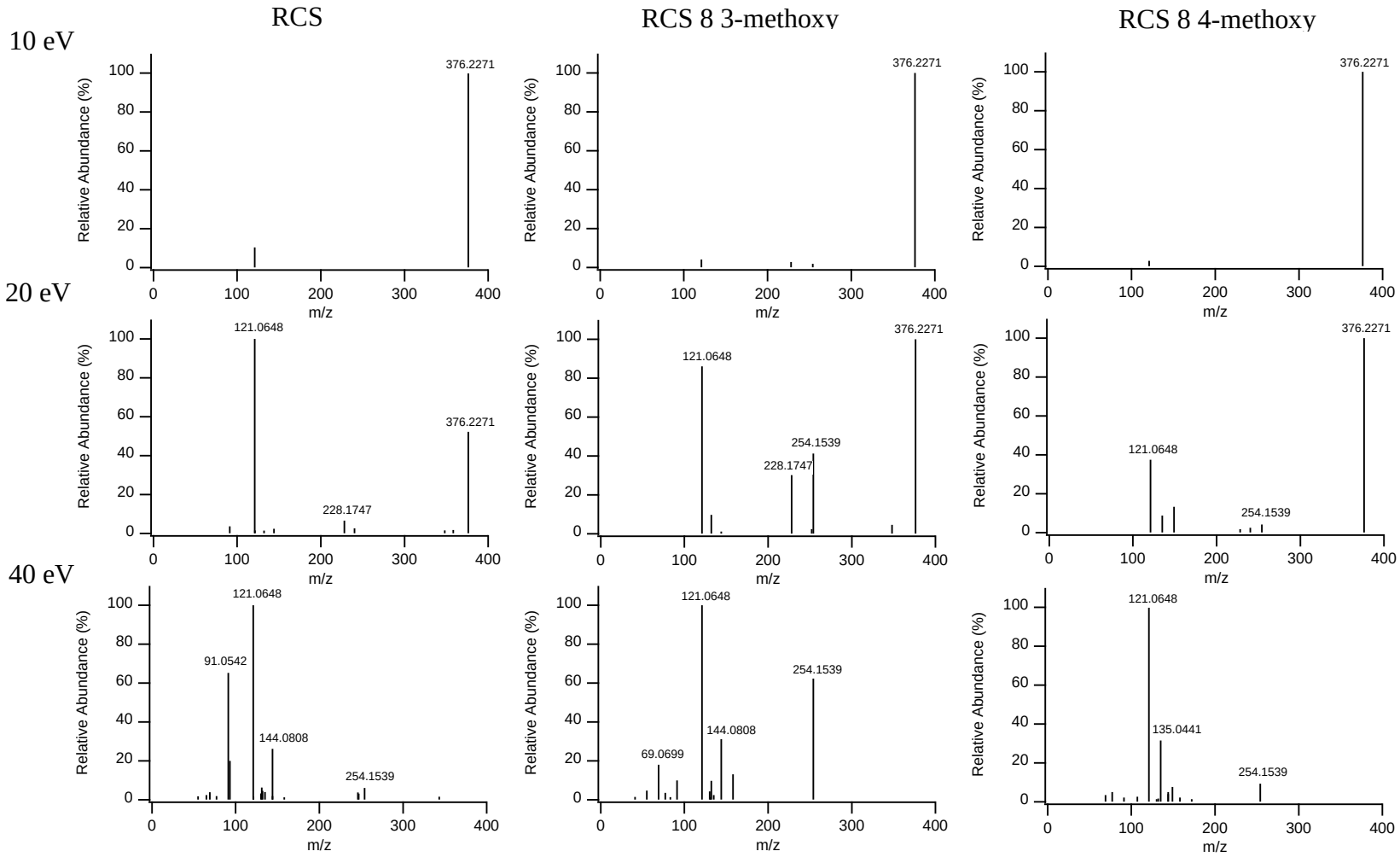
Appendix 18. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the methylenedioxymethcathinone set of regioisomers.



Appendix 19. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the RCS 4 set of regioisomers.



Appendix 20. The MS/MS spectral data collected at 10 eV, 20 eV and 40 eV collision energy levels for the RCS 8 set of regioisomers.



Appendix 21. Results of the collision induced dissociation study. The mean and relative standard deviation % is shown for the reproducibility, concentration and mobile phase experiments for all of the ions of interest. Concentration and mobile phase experiment data is not shown for ions that were not determined to be significantly different in the reproducibility experiment.

AM 694 Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
AM 694 3-iodo isomer	436.0568	10	100	0.0%												
AM 694 4-iodo isomer			100	0.0%												
AM 694			100	0.0%												
AM694 3-iodo isomer	230.9301	20	100	0.0%	93	4.8%	89	2.0%	93	7.2%	95	3.7%	99	0.9%	100	0.0%
AM694 4-iodo isomer			100	0.0%	98	3.2%	97	2.3%	98	2.7%	99	1.7%	100	0.0%	100	0.0%
AM 694			90	4.4%	91	5.4%	89	5.7%	85	3.4%	84	6.1%	84	2.8%	83	4.0%
AM 694 3-iodo isomer	309.1523	20	0	308.2%	0	128.5%	0	-	13	27.3%	5	22.0%	0	-	0	-
AM 694 4-iodo isomer			0	352.5%	0	265.0%	0	-	10	12.9%	4	31.5%	0	-	0	-
AM 694			16	6.2%	17	10.6%	16	4.9%	17	14.3%	17	12.9%	16	4.8%	16	4.9%
AM694 3-iodo isomer	436.0568	20	80	6.2%	100	1.6%	100	0.0%	99	1.5%	100	0.0%	94	6.4%	96	1.6%
AM694 4-iodo isomer			74	7.5%	97	3.4%	100	0.2%	95	5.3%	99	1.6%	83	3.7%	87	0.6%
AM 694			100	1.2%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
AM694 3-iodo isomer	202.9352	40	61	4.5%	56	6.4%	54	1.6%	48	8.2%	51	10.3%	54	11.5%	57	3.5%
AM694 4-iodo isomer			41	6.4%	37	8.2%	35	1.6%	45	8.0%	44	2.9%	38	8.8%	37	4.2%
AM 694			45	4.0%	43	3.9%	44	5.6%	42	10.8%	39	10.6%	38	1.8%	38	5.4%
AM 694 3-iodo isomer	230.9301	40	100	0.0%												
AM 694 4-iodo isomer			100	0.0%												
AM 694			100	0.0%												

Ethylethcathinone Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
2-Ethylethcathinone	159.1043	10	21	7.3%	20	3.4%	19	2.2%	18	1.0%	19	3.0%	19	0.9%	19	2.2%
3-Ethylethcathinone			19	6.0%	16	5.5%	16	2.8%	17	1.8%	17	3.3%	17	1.5%	17	1.5%
4-Ethylethcathinone			16	6.0%	14	6.9%	13	2.0%	14	0.7%	14	1.2%	15	2.6%	15	3.2%
2-Ethylethcathinone	160.1121	10	23	6.7%	21	4.3%	20	2.1%	21	2.2%	21	2.8%	21	2.2%	21	1.2%
3-Ethylethcathinone			20	7.2%	18	6.0%	17	2.1%	18	0.8%	19	2.2%	18	2.3%	19	1.1%
4-Ethylethcathinone			17	5.4%	15	6.8%	14	2.0%	15	1.0%	16	2.9%	15	1.9%	16	2.5%
2-Ethylethcathinone	188.1434	10	100	0.0%												

3-Ethylethcathinone			100	0.0%											
4-Ethylethcathinone			100	0.0%											
2-Ethylethcathinone	206.1539	10	52	5.6%	54	5.2%	53	2.6%	61	1.4%	62	2.9%	60	1.2%	60	0.9%
3-Ethylethcathinone			61	4.9%	74	3.6%	73	1.8%	77	1.3%	79	1.2%	76	0.8%	75	0.6%
4-Ethylethcathinone			44	5.3%	54	3.4%	53	1.4%	57	0.9%	60	1.5%	58	0.7%	57	2.0%
2-Ethylethcathinone	132.0808	20	27	8.1%												
3-Ethylethcathinone			26	7.5%												
4-Ethylethcathinone			23	5.3%												
2-Ethylethcathinone	144.0808	20	64	6.0%	60	2.2%	60	3.8%	57	1.5%	56	1.0%	57	0.8%	58	1.2%
3-Ethylethcathinone			56	5.8%	52	4.6%	49	1.3%	48	0.8%	49	1.7%	49	1.6%	51	2.0%
4-Ethylethcathinone			52	5.0%	47	8.5%	45	1.6%	45	2.0%	45	2.6%	46	1.0%	46	0.9%
2-Ethylethcathinone	159.1043	20	100	0.0%												
3-Ethylethcathinone			100	0.0%												
4-Ethylethcathinone			100	0.0%												
2-Ethylethcathinone	160.1121	20	46	5.5%												
3-Ethylethcathinone			47	6.3%												
4-Ethylethcathinone			47	4.8%												
2-Ethylethcathinone	188.1434	20	33	3.6%	34	6.2%	33	3.5%	39	0.9%	38	2.2%	39	1.7%	38	0.7%
3-Ethylethcathinone			38	5.9%	45	3.9%	43	1.4%	46	1.4%	47	1.4%	47	0.8%	46	1.5%
4-Ethylethcathinone			43	5.7%	52	5.6%	50	2.0%	53	1.4%	54	0.9%	53	0.7%	53	0.8%
2-Ethylethcathinone	105.0699	40	10	6.9%	10	3.4%	10	2.7%	9	3.6%	9	3.1%	9	3.8%	9	1.5%
3-Ethylethcathinone			19	8.5%	18	7.1%	17	1.5%	17	2.6%	17	1.0%	16	0.7%	17	1.6%
4-Ethylethcathinone			22	6.9%	22	8.1%	21	1.4%	21	1.7%	20	1.0%	20	0.8%	20	0.6%
2-Ethylethcathinone	130.0651	40	27	5.7%												
3-Ethylethcathinone			25	5.5%												
4-Ethylethcathinone			22	9.1%												
2-Ethylethcathinone	144.0808	40	100	0.0%												
3-Ethylethcathinone			100	0.0%												
4-Ethylethcathinone			100	0.0%												

Fluoroamphetamine Regioisomers			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
2-Fluoroamphetamine			100	0.0%												
3-Fluoroamphetamine	109.0448	10	100	0.0%												
4-Fluoroamphetamine			100	0.0%												

2-Fluoroamphetamine	137.0761	10	20	6.4%	24	10.1%	23	2.4%	28	1.9%	29	2.6%	29	4.9%	31	1.9%
3-Fluoroamphetamine			18	9.1%	24	7.7%	24	2.9%	30	6.2%	30	7.5%	31	4.0%	33	4.8%
4-Fluoroamphetamine			28	9.6%	38	8.1%	38	2.5%	47	4.5%	47	4.7%	49	3.9%	52	3.5%
2-Fluoroamphetamine	109.0448	20	100	0.0%												
3-Fluoroamphetamine			100	0.0%												
4-Fluoroamphetamine			100	0.0%												
2-Fluoroamphetamine	83.0292	40	100	0.6%	97	3.7%	99	1.2%	86	0.8%	85	1.5%	84	3.7%	83	2.3%
3-Fluoroamphetamine			100	0.0%	100	0.0%	100	0.0%	98	1.9%	97	2.4%	97	2.1%	93	3.0%
4-Fluoroamphetamine			99	2.6%	94	7.3%	93	2.1%	81	3.2%	79	4.2%	76	6.0%	79	2.4%
2-Fluoroamphetamine	109.0448	40	96	4.7%	96	5.9%	99	1.2%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
3-Fluoroamphetamine			78	8.9%	87	7.5%	87	2.1%	100	0.4%	100	0.0%	99	1.4%	100	0.0%
4-Fluoroamphetamine			94	7.5%	99	4.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%

Fluoroethcathinone Regioisomers			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
2-Fluoroethcathinone	150.0714	10	26	6.1%	25	6.7%	24	2.6%	25	2.0%	26	0.7%	26	3.8%	26	0.6%
3-Fluoroethcathinone			43	6.7%	38	8.1%	37	1.8%	38	2.8%	38	1.7%	38	1.3%	39	1.9%
4-Fluoroethcathinone			31	6.8%	27	6.1%	26	1.8%	28	1.3%	28	1.4%	29	1.6%	29	0.9%
2-Fluoroethcathinone	178.1027	10	100	0.0%												
3-Fluoroethcathinone			100	0.0%												
4-Fluoroethcathinone			100	0.0%												
2-Fluoroethcathinone	196.1132	10	84	4.0%	91	6.1%	91	1.1%	97	1.7%	99	1.1%	96	1.7%	97	0.8%
3-Fluoroethcathinone			79	4.1%	95	2.8%	95	1.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
4-Fluoroethcathinone			50	6.0%	61	3.9%	61	1.6%	66	0.9%	68	0.7%	67	1.8%	65	0.9%
2-Fluoroethcathinone	103.0554	20	19	10.9%	17	22.7%	16	3.3%	15	2.9%	15	5.2%	16	1.5%	15	1.5%
3-Fluoroethcathinone			14	11.2%	12	6.6%	11	3.1%	10	2.7%	10	2.9%	10	1.9%	10	3.9%
4-Fluoroethcathinone			15	8.3%	13	10.4%	12	3.0%	11	1.1%	11	2.8%	12	2.7%	11	1.7%
2-Fluoroethcathinone	123.0605	20	43	5.2%	42	11.7%	41	1.6%	39	1.6%	38	0.8%	39	0.9%	39	2.2%
3-Fluoroethcathinone			27	9.8%	25	5.4%	24	1.9%	23	1.9%	23	1.1%	23	3.1%	23	2.7%
4-Fluoroethcathinone			35	9.3%	33	7.1%	32	2.1%	30	1.8%	30	2.3%	30	2.4%	30	0.9%
2-Fluoroethcathinone	135.0479	20	32	5.0%												
3-Fluoroethcathinone			28	8.4%												
4-Fluoroethcathinone			28	6.7%												
2-Fluoroethcathinone	148.0557	20	26	6.5%												

3-Fluoroethcathinone			23	7.2%												
4-Fluoroethcathinone			28	6.7%												
2-Fluoroethcathinone	149.0635	20	83	2.4%	79	7.7%	81	1.8%	78	1.8%	77	1.8%	79	1.6%	78	1.5%
3-Fluoroethcathinone			58	6.1%	56	5.7%	54	1.3%	51	1.4%	51	0.8%	51	1.7%	52	2.0%
4-Fluoroethcathinone			89	4.6%	85	4.4%	84	1.0%	80	1.3%	81	0.9%	81	2.4%	80	0.5%
2-Fluoroethcathinone	150.0714	20	100	0.0%												
3-Fluoroethcathinone			100	0.0%												
4-Fluoroethcathinone			100	0.0%												
2-Fluoroethcathinone	163.0792	20	16	7.3%	15	17.8%	14	2.5%	13	4.8%	13	1.8%	14	4.9%	14	1.7%
3-Fluoroethcathinone			6	10.9%	7	9.6%	6	2.6%	6	5.2%	5	4.9%	6	3.3%	6	2.4%
4-Fluoroethcathinone			14	13.7%	13	7.7%	12	2.6%	11	2.8%	11	1.4%	12	3.9%	11	2.2%
2-Fluoroethcathinone	178.1027	20	53	3.1%	58	13.4%	56	1.6%	58	1.7%	58	0.9%	58	1.6%	56	0.7%
3-Fluoroethcathinone			30	7.4%	35	6.0%	33	2.1%	35	2.4%	34	1.6%	35	0.4%	34	1.5%
4-Fluoroethcathinone			41	7.0%	46	5.0%	45	2.2%	47	1.4%	47	1.2%	47	2.0%	46	1.6%
2-Fluoroethcathinone	77.0386	40	60	6.3%	59	13.8%	56	2.8%	54	3.6%	52	2.6%	55	3.3%	53	2.7%
3-Fluoroethcathinone			54	9.2%	50	8.2%	49	2.2%	45	2.3%	45	1.6%	46	1.2%	46	2.4%
4-Fluoroethcathinone			45	7.2%	42	8.2%	41	1.7%	38	1.7%	38	0.6%	38	3.3%	38	1.2%
2-Fluoroethcathinone	95.0292	40	20	5.4%	18	18.7%	19	2.4%	19	5.5%	18	3.2%	19	7.1%	18	4.3%
3-Fluoroethcathinone			23	11.3%	23	10.5%	22	2.7%	20	2.3%	21	1.7%	22	1.8%	21	0.6%
4-Fluoroethcathinone			14	10.8%	14	10.8%	13	3.0%	12	3.4%	12	2.8%	13	2.7%	13	2.7%
2-Fluoroethcathinone	103.0554	40	55	3.1%												
3-Fluoroethcathinone			49	8.9%												
4-Fluoroethcathinone			46	20.7%												
2-Fluoroethcathinone	108.0370	40	13	7.3%												
3-Fluoroethcathinone			15	18.7%												
4-Fluoroethcathinone			12	11.5%												
2-Fluoroethcathinone	109.0448	40	18	5.6%												
3-Fluoroethcathinone			15	8.9%												
4-Fluoroethcathinone			16	16.8%												
2-Fluoroethcathinone	115.0554	40	23	10.1%	22	16.4%	22	4.0%	23	3.9%	21	4.2%	23	4.4%	23	3.9%
3-Fluoroethcathinone			14	16.6%	15	14.9%	15	3.7%	15	4.5%	14	4.1%	15	2.5%	15	2.3%
4-Fluoroethcathinone			17	8.2%	18	10.3%	17	2.2%	16	2.6%	16	2.0%	18	4.1%	17	3.6%
2-Fluoroethcathinone	135.0479	40	71	2.3%	73	8.9%	73	2.5%	73	1.7%	71	2.1%	74	2.1%	71	1.0%
3-Fluoroethcathinone			86	6.5%	88	7.8%	87	1.7%	85	2.7%	85	1.3%	85	1.0%	86	2.0%
4-Fluoroethcathinone			55	5.5%	57	5.5%	57	1.2%	55	1.5%	55	2.2%	56	2.2%	56	2.4%
2-Fluoroethcathinone	148.0570	40	100	0.0%												

3-Fluoroethcathinone			100	0.0%											
4-Fluoroethcathinone			100	0.0%											

Fluoromethamphetamine Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
2-Fluoromethamphetamine	109.0448	10	100	0.0%												
3-Fluoromethamphetamine			100	0.0%												
4-Fluoromethamphetamine			100	0.0%												
2-Fluoromethamphetamine	137.0761	10	26	3.1%	29	4.6%	29	2.2%	32	1.7%	32	1.4%	32	2.6%	31	2.5%
3-Fluoromethamphetamine			25	5.1%	31	3.2%	30	2.1%	34	1.2%	34	1.5%	35	1.2%	33	1.8%
4-Fluoromethamphetamine			50	6.7%	62	4.7%	62	1.6%	69	0.9%	70	1.3%	72	1.6%	68	1.9%
2-Fluoromethamphetamine	168.1183	10	38	8.9%	45	5.8%	45	2.4%	53	1.5%	52	0.9%	52	2.0%	51	1.5%
3-Fluoromethamphetamine			34	6.8%	51	4.9%	49	2.4%	60	2.7%	60	2.3%	62	1.4%	57	1.2%
4-Fluoromethamphetamine			18	9.9%	28	6.2%	27	2.2%	32	2.1%	32	1.8%	35	3.4%	31	2.2%
2-Fluoromethamphetamine	109.0448	20	100	0.0%												
3-Fluoromethamphetamine			100	0.0%												
4-Fluoromethamphetamine			100	0.0%												
2-Fluoromethamphetamine	83.0292	40	56	8.7%	54	4.4%	53	1.0%	45	1.8%	45	2.2%	46	1.5%	47	1.4%
3-Fluoromethamphetamine			70	3.9%	63	5.6%	61	0.9%	52	1.4%	52	2.1%	53	1.2%	53	2.5%
4-Fluoromethamphetamine			56	5.6%	50	4.8%	49	1.4%	42	1.2%	42	1.1%	43	2.5%	43	2.5%
2-Fluoromethamphetamine	109.0448	40	100	0.0%												
3-Fluoromethamphetamine			100	0.0%												
4-Fluoromethamphetamine			100	0.0%												

Fluoromethcathinone Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
4-Fluoromethcathinone	149.0635	10	22	6.3%	19	6.1%	18	2.0%	27	1.5%	18	1.3%	19	2.9%	20	1.3%
2-Fluoromethcathinone			24	9.2%	22	13.3%	21	3.2%	22	3.1%	22	3.1%	23	2.5%	22	1.0%
3-Fluoromethcathinone			27	5.2%	23	4.2%	22	1.0%	25	7.2%	25	5.4%	25	3.5%	25	1.9%
4-Fluoromethcathinone	164.0870	10	100	0.0%												
2-Fluoromethcathinone			100	0.0%												
3-Fluoromethcathinone			100	0.0%												
4-Fluoromethcathinone	182.0976	10	20	8.7%	27	6.6%	25	1.2%	27	1.5%	27	2.6%	29	2.4%	27	1.6%

2-Fluoromethcathinone			36	7.4%	42	11.9%	40	2.1%	44	0.8%	43	1.7%	45	1.3%	42	1.5%
3-Fluoromethcathinone			31	7.0%	40	2.0%	39	1.3%	37	3.5%	37	0.5%	36	4.1%	36	3.3%
4-Fluoromethcathinone			20	7.0%	22	8.3%	20	2.1%	20	1.8%	19	1.6%	21	1.6%	20	1.1%
2-Fluoromethcathinone	123.0605	20	19	4.3%	20	14.0%	19	4.7%	19	3.2%	19	2.6%	19	1.4%	18	4.4%
3-Fluoromethcathinone			15	6.4%	16	5.1%	15	2.0%	16	1.7%	15	3.3%	15	4.4%	16	2.6%
4-Fluoromethcathinone			19	7.2%	17	6.6%	16	2.7%	15	1.9%	14	1.0%	15	2.4%	16	3.1%
2-Fluoromethcathinone	148.0557	20	18	10.2%	17	23.1%	16	3.6%	16	1.9%	15	2.5%	16	4.2%	16	2.2%
3-Fluoromethcathinone			24	2.7%	22	4.6%	21	1.2%	23	4.3%	24	7.3%	23	1.8%	24	2.5%
4-Fluoromethcathinone			100	0.0%												
2-Fluoromethcathinone	149.0635	20	100	0.0%												
3-Fluoromethcathinone			100	0.0%												
4-Fluoromethcathinone			37	4.5%												
2-Fluoromethcathinone	164.0870	20	35	7.9%												
3-Fluoromethcathinone			31	4.4%												
4-Fluoromethcathinone			47	4.2%	47	10.7%	43	2.2%	40	1.1%	39	1.6%	41	2.1%	41	3.6%
2-Fluoromethcathinone	77.0386	40	45	8.0%	44	19.7%	42	5.4%	38	2.5%	37	1.2%	39	3.5%	38	2.2%
3-Fluoromethcathinone			38	3.9%	35	7.2%	34	2.0%	37	4.4%	37	1.5%	37	1.8%	36	1.9%
4-Fluoromethcathinone			29	9.4%	31	10.4%	29	1.6%	28	2.6%	29	2.2%	30	3.7%	29	2.2%
2-Fluoromethcathinone	103.0542	40	21	4.5%	24	27.4%	22	4.9%	22	4.3%	21	2.4%	22	4.8%	22	1.4%
3-Fluoromethcathinone			17	9.4%	18	8.7%	18	2.4%	12	5.3%	18	3.8%	18	1.4%	18	4.4%
4-Fluoromethcathinone			100	0.0%												
2-Fluoromethcathinone	148.0557	40	100	0.0%												
3-Fluoromethcathinone			100	0.0%												
4-Fluoromethcathinone			16	9.9%	18	10.3%	17	2.4%	21	3.4%	20	1.7%	22	1.7%	21	1.6%
2-Fluoromethcathinone	149.0635	40	16	8.0%	20	34.9%	17	2.8%	20	4.5%	19	3.6%	20	3.0%	20	1.4%
3-Fluoromethcathinone			10	8.1%	12	7.3%	12	2.0%	12	4.8%	11	8.4%	12	4.8%	11	4.8%

JWH 203 Regioisomers			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
JWH 203 3-chlorophenyl isomer			100	0.0%												
JWH 203 4-chlorophenyl isomer	340.1463	10	100	0.0%												
JWH 203			100	0.0%												
JWH 203 3-chlorophenyl isomer	125.0153	20	91	6.3%												

JWH 203 4-chlorophenyl isomer			94	3.1%											
JWH 203			85	4.1%											
JWH 203 3-chlorophenyl isomer			47	6.1%	39	9.5%	39	1.6%	34	20.2%	32	11.1%	48	3.6%	47	2.2%
JWH 203 4-chlorophenyl isomer	188.1434	20	29	3.5%	26	2.0%	24	1.4%	30	5.6%	29	2.2%	30	1.2%	29	1.9%
JWH 203			22	3.7%	22	5.5%	20	1.1%	26	27.1%	25	3.4%	22	4.8%	22	4.3%
JWH 203 3-chlorophenyl isomer			61	4.0%	50	8.5%	48	1.9%	35	12.5%	29	9.4%	64	2.4%	63	3.6%
JWH 203 4-chlorophenyl isomer	214.1226	20	22	6.2%	18	2.7%	17	2.0%	23	3.0%	23	0.9%	23	2.6%	23	1.4%
JWH 203			11	3.8%	11	6.4%	11	1.5%	13	10.2%	16	9.1%	13	4.7%	13	3.5%
JWH 203 3-chlorophenyl isomer			100	1.2%											
JWH 203 4-chlorophenyl isomer	340.1463	20	100	0.1%											
JWH 203			100	0.0%											
JWH 203 3-chlorophenyl isomer			100	0.0%											
JWH 203 4-chlorophenyl isomer	125.0153	40	100	0.0%											
JWH 203			100	0.0%											
JWH 203 3-chlorophenyl isomer			45	6.2%	42	7.3%	43	1.3%	21	22.2%	20	6.7%	44	4.3%	43	3.9%
JWH 203 4-chlorophenyl isomer	144.0444	40	17	4.0%	17	4.6%	16	1.1%	18	2.5%	17	4.8%	17	2.7%	17	1.8%
JWH 203			10	3.5%	10	5.4%	10	1.7%	11	30.4%	13	10.2%	11	4.5%	11	3.8%
JWH 203 3-chlorophenyl isomer			25	8.7%	26	10.1%	26	2.7%	13	24.1%	12	4.5%	24	2.6%	24	4.6%
JWH 203 4-chlorophenyl isomer	214.1226	40	10	4.5%	11	6.0%	10	1.2%	10	10.4%	9	1.8%	9	4.0%	10	1.5%
JWH 203			7	5.4%	6	10.0%	6	2.4%	6	54.6%	7	10.6%	6	2.8%	6	4.0%

JWH 251 Regioisomers			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
JWH 251 3-methylphenyl isomer	320.2009	10	100	0.0%												
JWH 251 4-methylphenyl isomer			100	0.0%												
JWH-251			100	0.0%												
JWH 251 3-methylphenyl isomer	105.0699	20	99	2.7%												
JWH 251 4-methylphenyl isomer			100	0.0%												
JWH-251			100	0.0%												
JWH 251 3-methylphenyl isomer	188.1434	20	21	8.9%	22	8.6%	21	1.6%	15	17.8%	16	4.5%	20	1.5%	19	4.0%
JWH 251 4-methylphenyl isomer			13	11.2%	14	9.7%	13	1.9%	13	15.1%	14	10.6%	12	3.9%	12	3.5%
JWH-251			12	10.0%	12	7.2%	11	1.5%	13	12.6%	12	8.0%	11	2.7%	11	8.5%
JWH 251 3-methylphenyl isomer	214.1266	20	95	4.5%	95	4.3%	98	1.1%	82	10.0%	89	4.8%	98	2.3%	98	1.8%
JWH 251 4-methylphenyl isomer			50	5.5%	50	5.4%	49	1.4%	67	4.2%	74	6.8%	50	2.4%	50	3.2%

JWH-251			81	4.6%	77	4.0%	75	1.2%	85	5.1%	81	6.2%	83	0.4%	85	7.1%
JWH 251 3-methylphenyl isomer	320.2009	20	66	4.0%	79	6.1%	83	1.3%	70	5.9%	74	4.0%	61	1.8%	60	1.6%
JWH 251 4-methylphenyl isomer			80	6.0%	95	3.6%	100	0.2%	67	3.5%	73	6.9%	73	1.4%	72	2.7%
JWH-251			90	4.8%	100	0.0%	100	0.0%	87	6.1%	79	3.3%	80	1.7%	81	8.0%
JWH 251 3-methylphenyl isomer	43.0542	40	17	16.5%	15	9.6%	14	1.9%	10	20.2%	9	22.7%	12	3.4%	13	6.1%
JWH 251 4-methylphenyl isomer			7	25.3%	7	23.5%	7	3.0%	7	35.2%	9	17.0%	6	3.2%	6	6.5%
JWH-251			12	10.8%	11	9.7%	10	2.7%	7	22.9%	8	18.6%	9	3.7%	9	4.2%
JWH 251 3-methylphenyl isomer	105.0699	40	99	1.8%												
JWH 251 4-methylphenyl isomer			100	0.0%												
JWH-251			100	0.0%												
JWH 251 3-methylphenyl isomer	144.0444	40	95	5.3%	92	5.6%	94	0.9%	84	11.9%	77	1.8%	95	3.2%	97	1.8%
JWH 251 4-methylphenyl isomer			46	7.7%	46	5.4%	45	1.2%	68	8.6%	69	4.7%	47	2.9%	47	1.1%
JWH-251			72	5.7%	70	3.5%	68	1.1%	68	3.8%	69	7.0%	69	2.7%	69	4.9%
JWH 251 3-methylphenyl isomer	214.1226	40	44	5.7%	47	6.2%	47	1.1%	39	3.8%	38	4.0%	42	4.4%	42	2.5%
JWH 251 4-methylphenyl isomer			22	7.0%	24	10.2%	23	1.9%	29	9.0%	32	5.8%	21	0.6%	21	1.4%
JWH-251			35	6.3%	38	4.8%	37	1.0%	35	13.2%	34	3.5%	33	2.6%	34	4.1%

Methoxymethcathinone Regioisomers			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
Methedrone	161.0835	10	17	6.3%	17	5.6%	17	2.3%	15	1.9%	16	0.7%	16	3.0%	16	1.5%
2-Methoxymethcathinone			25	5.8%	23	3.8%	22	2.1%	21	1.8%	21	3.1%	22	1.5%	22	0.9%
3-Methoxymethcathinone			28	6.6%	26	4.6%	25	1.8%	25	1.4%	26	1.4%	25	0.6%	25	1.5%
Methedrone	176.1070	10	100	0.0%												
2-Methoxymethcathinone			100	0.0%												
3-Methoxymethcathinone			100	0.0%												
Methedrone	194.1176	10	17	6.6%	19	6.0%	18	4.6%	20	0.8%	21	1.6%	21	1.0%	20	2.9%
2-Methoxymethcathinone			15	7.9%	18	6.2%	17	1.4%	18	1.8%	18	2.4%	18	0.8%	17	1.8%
3-Methoxymethcathinone			28	6.0%	34	4.1%	32	1.2%	34	1.6%	35	0.3%	35	0.6%	34	0.6%
Methedrone	135.0804	20	21	2.3%	20	2.6%	20	1.2%	19	2.8%	19	2.5%	20	3.2%	20	2.6%
2-Methoxymethcathinone			13	2.0%	13	11.5%	13	1.6%	13	2.0%	12	1.1%	13	2.3%	12	3.0%
3-Methoxymethcathinone			11	4.8%	12	8.0%	11	2.0%	11	3.1%	10	1.5%	11	3.0%	11	1.7%
Methedrone	145.0886	20	29	4.3%	29	2.4%	28	0.9%	28	2.4%	28	2.1%	29	1.0%	28	2.3%
2-Methoxymethcathinone			27	3.9%	25	6.3%	25	2.1%	24	2.9%	24	2.2%	24	2.1%	24	0.9%
3-Methoxymethcathinone			21	2.5%	21	4.1%	20	1.2%	20	1.6%	20	1.3%	21	1.8%	20	1.5%

Methedrone	146.0600	20	34	8.6%											
2-Methoxymethcathinone			28	7.2%											
3-Methoxymethcathinone			30	7.3%											
Methedrone	161.0835	20	100	0.0%											
2-Methoxymethcathinone			100	0.0%											
3-Methoxymethcathinone			100	0.0%											
Methedrone	176.1070	20	44	2.2%	45	2.1%	46	2.4%	52	1.6%	52	1.8%	54	1.0%	52	1.2%
2-Methoxymethcathinone			31	5.1%	33	7.9%	32	2.3%	35	1.7%	35	1.3%	35	2.0%	35	2.3%
3-Methoxymethcathinone			29	3.6%	31	5.2%	31	1.2%	34	0.8%	33	1.9%	35	1.8%	33	1.0%
Methedrone	58.0651	40	28	5.1%	28	6.9%	27	2.6%	24	3.2%	23	3.2%	25	2.7%	25	5.3%
2-Methoxymethcathinone			16	10.6%	17	18.7%	16	4.6%	14	3.0%	15	3.4%	15	2.6%	15	3.7%
3-Methoxymethcathinone			6	7.8%	5	24.6%	5	4.2%	5	2.8%	5	4.4%	5	2.3%	5	6.2%
Methedrone	77.0386	40	46	5.4%	45	2.2%	43	1.8%	38	2.2%	38	1.3%	39	4.8%	40	2.8%
2-Methoxymethcathinone			35	4.2%	33	9.8%	32	3.2%	32	5.0%	31	0.9%	31	1.0%	32	2.7%
3-Methoxymethcathinone			31	2.4%	29	9.2%	28	2.8%	26	2.9%	26	2.4%	27	3.6%	27	2.6%
Methedrone	79.0542	40	29	3.9%	29	3.2%	28	2.1%	25	3.0%	25	2.6%	26	3.0%	26	2.2%
2-Methoxymethcathinone			17	7.2%	17	16.7%	17	4.2%	16	2.0%	16	3.4%	15	6.3%	16	1.8%
3-Methoxymethcathinone			15	5.3%	15	7.8%	14	2.7%	13	2.9%	13	2.7%	14	4.0%	14	3.0%
Methedrone	91.0542	40	35	2.0%	35	2.8%	34	1.7%	31	2.6%	30	1.6%	32	0.6%	32	2.7%
2-Methoxymethcathinone			30	7.2%	27	11.9%	28	3.5%	26	3.0%	27	4.1%	27	3.7%	27	1.4%
3-Methoxymethcathinone			30	3.5%	27	8.7%	27	2.9%	26	1.8%	26	2.7%	26	2.9%	26	2.9%
Methedrone	103.0542	40	27	3.3%	27	2.7%	26	1.8%	25	2.9%	25	1.3%	26	3.1%	26	3.1%
2-Methoxymethcathinone			15	5.2%	15	14.9%	15	4.4%	14	4.0%	14	3.8%	15	2.8%	15	2.3%
3-Methoxymethcathinone			14	3.8%	14	13.4%	13	2.7%	13	2.7%	13	2.9%	13	2.9%	13	3.5%
Methedrone	105.0699	40	19	9.0%	19	3.1%	18	2.8%	18	4.5%	18	3.0%	19	2.8%	19	5.1%
2-Methoxymethcathinone			9	10.3%	10	18.7%	9	5.0%	9	4.5%	9	2.8%	9	6.8%	9	1.9%
3-Methoxymethcathinone			7	6.4%	8	18.2%	7	1.8%	7	5.4%	7	2.9%	7	1.7%	7	2.6%
Methedrone	117.0573	40	19	9.4%	19		18	1.7%	16	4.5%	16	3.3%	17	2.5%	17	1.8%
2-Methoxymethcathinone			29	7.8%	27	7.9%	27	2.9%	26	4.5%	26	1.9%	27	0.6%	27	2.1%
3-Methoxymethcathinone			28	7.7%	27	6.8%	26	2.0%	25	3.7%	24	1.1%	25	3.2%	25	1.2%
Methedrone	118.0651	40	100	0.0%												
2-Methoxymethcathinone			100	0.0%												
3-Methoxymethcathinone			100	0.0%												
Methedrone	132.0808	40	33	3.6%	33	2.0%	32	1.5%	31	2.6%	31	3.6%	33	2.4%	33	2.8%
2-Methoxymethcathinone			51	3.8%	51	7.2%	51	2.6%	51	2.6%	52	1.2%	52	1.8%	51	1.6%

3-Methoxymethcathinone			59	1.5%	59	5.9%	58	0.8%	58	1.1%	58	2.2%	58	0.5%	58	1.6%
Methedrone	144.0808	40	37	4.7%	37	2.5%	35	1.7%	37	1.9%	36	1.2%	37	3.2%	37	1.7%
2-Methoxymethcathinone			44	6.7%	45	8.9%	44	1.8%	45	3.7%	46	2.8%	45	2.0%	45	2.8%
3-Methoxymethcathinone			23	4.3%	23	10.0%	22	2.0%	23	2.8%	22	1.4%	23	1.4%	22	1.5%
Methedrone	146.0600	40	95	2.6%	95	2.7%	93	3.0%	100	0.0%	100	0.0%	100	0.0%	99	0.5%
2-Methoxymethcathinone			50	4.6%	54	10.1%	54	2.0%	55	2.5%	55	2.4%	55	2.8%	54	1.4%
3-Methoxymethcathinone			42	4.5%	44	6.7%	43	1.5%	45	1.0%	45	1.9%	46	1.1%	45	2.3%
Methedrone	160.0757	40	7	10.5%	8	11.2%	7	2.8%	8	4.2%	7	3.7%	8	8.3%	8	0.8%
2-Methoxymethcathinone			22	5.1%	23	12.7%	22	3.8%	22	2.6%	22	3.6%	22	1.8%	22	2.0%
3-Methoxymethcathinone			11	7.6%	12	12.3%	11	3.0%	11	2.5%	11	1.2%	11	2.2%	11	4.5%

Methoxy-N,N-dimethyltryptamine Regioisomers			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
5-MeO-DMT	58.0651	10	100	0.0%												
4-MeO-DMT			100	0.0%												
5-MeO-DMT	174.0913	10	71	3.6%	68	2.3%	69	1.3%	80	1.9%	84	0.9%	79	1.6%	80	1.1%
4-MeO-DMT			34	3.9%	34	4.8%	34	1.4%	39	1.7%	40	1.0%	40	0.7%	39	0.6%
5-MeO-DMT	219.1492	10	20	6.8%	24	4.8%	23	2.6%	28	2.2%	29	0.9%	28	1.9%	27	2.2%
4-MeO-DMT			35	8.5%	41	4.5%	41	2.1%	49	0.9%	49	2.1%	48	1.4%	48	0.4%
5-MeO-DMT	58.0651	20	100	0.0%												
4-MeO-DMT			100	0.0%												
5-MeO-DMT	159.0679	20	14	2.9%	13	7.9%	13	2.1%	14	3.5%	15	1.8%	15	2.4%	15	1.5%
4-MeO-DMT			7	4.5%	7	5.0%	6	2.2%	7	2.6%	7	1.9%	7	1.5%	7	1.5%
5-MeO-DMT	174.0913	20	73	5.5%	73	2.5%	74	1.0%	83	2.0%	88	0.7%	81	1.3%	82	0.8%
4-MeO-DMT			34	3.4%	35	5.1%	35	1.1%	39	1.6%	39	1.8%	39	1.3%	39	1.5%
5-MeO-DMT	58.0651	40	100	0.0%												
4-MeO-DMT			100	0.0%												
5-MeO-DMT	130.0651	40	47	2.5%	43	6.1%	44	2.3%	49	1.6%	50	0.9%	49	2.2%	50	2.7%
4-MeO-DMT			14	7.0%	11	9.9%	12	2.6%	14	2.3%	13	1.0%	14	2.3%	14	2.1%
5-MeO-DMT	131.0730	40	41	3.1%	40	5.3%	39	1.2%	44	1.7%	44	1.2%	44	2.5%	44	0.8%
4-MeO-DMT			8	6.5%	7	7.1%	8	1.8%	9	2.1%	9	2.1%	9	2.5%	9	1.7%
5-MeO-DMT	143.0730	40	17	4.6%	17	9.5%	17	1.7%	18	2.1%	18	1.9%	19	2.9%	18	2.3%
4-MeO-DMT			10	5.5%	10	12.8%	9	2.9%	10	2.3%	10	4.2%	10	3.4%	10	3.1%
5-MeO-DMT	159.0679	40	21	4.9%	23	10.6%	22	1.9%	24	2.5%	24	2.3%	24	1.6%	23	2.2%

4-MeO-DMT			17	2.2%	17	9.0%	17	0.9%	18	2.0%	18	1.3%	18	2.3%	18	2.3%

Methylenedioxymethcathinone Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
Methylone	58.0651	10	13	6.6%	13	10.0%	13	1.8%	11	4.8%	10	4.7%	11	2.1%	11	2.5%
2,3-Methylenedioxymethcathinone			3	10.0%	3	11.8%	3	3.4%	2	3.9%	2	1.4%	2	7.3%	2	3.5%
Methylone	160.0757	10	100	0.0%												
2,3-Methylenedioxymethcathinone			100	0.0%												
Methylone	190.0863	10	68	2.8%	73	4.4%	72	1.3%	69	1.3%	68	1.6%	67	1.1%	67	1.1%
2,3-Methylenedioxymethcathinone			19	2.7%	20	4.3%	19	1.7%	19	0.8%	19	1.2%	18	2.7%	18	1.3%
Methylone	208.0968	10	37	6.0%	55	5.7%	54	1.2%	54	4.1%	53	1.7%	54	1.9%	52	2.3%
2,3-Methylenedioxymethcathinone			45	4.5%	44	4.6%	43	1.3%	43	0.9%	45	0.8%	44	1.0%	42	1.1%
Methylone	132.0808	20	33	4.8%	32	6.8%	30	1.3%	30	4.7%	29	1.5%	30	1.5%	30	0.6%
2,3-Methylenedioxymethcathinone			50	4.4%	45	3.4%	44	1.9%	42	1.0%	44	0.5%	42	1.2%	43	0.9%
Methylone	160.0747	20	100	0.0%												
2,3-Methylenedioxymethcathinone			100	0.0%												
Methylone	58.0651	40	12	5.5%	19	12.9%	18	2.4%	17	3.1%	16	2.9%	17	5.6%	17	3.4%
2,3-Methylenedioxymethcathinone			20	5.0%	12	9.4%	11	3.2%	11	2.9%	10	1.5%	10	3.6%	11	1.9%
Methylone	65.0386	40	29	5.8%												
2,3-Methylenedioxymethcathinone			23	6.4%												
Methylone	91.0542	40	58	1.8%	52	6.5%	53	1.4%	54	2.8%	51	2.1%	52	2.8%	53	2.5%
2,3-Methylenedioxymethcathinone			65	2.4%	64	6.6%	63	1.5%	63	1.5%	62	1.4%	63	1.9%	63	3.2%
Methylone	117.0573	40	81	2.0%	75	7.0%	77	2.0%	75	3.0%	75	1.1%	74	3.2%	76	1.7%
2,3-Methylenedioxymethcathinone			100	0.0%	100	0.9%	100	0.0%	100	0.0%	100	0.0%	100	0.5%	100	0.8%
Methylone	131.0730	40	36	4.2%	24	10.2%	24	2.8%	25	2.4%	25	2.3%	25	4.7%	25	2.5%
2,3-Methylenedioxymethcathinone			27	6.0%	35	8.1%	34	6.0%	36	1.3%	36	1.6%	36	1.2%	36	0.9%
Methylone	132.0808	40	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
2,3-Methylenedioxymethcathinone			90	3.5%	95	3.6%	94	1.5%	97	2.0%	99	1.1%	98	1.7%	98	2.1%
Methylone	160.0747	40	10	5.8%	18	8.3%	17	2.3%	17	6.3%	17	4.5%	17	3.7%	18	3.6%
2,3-Methylenedioxymethcathinone			17	4.8%	11	12.5%	10	3.4%	11	2.6%	11	2.3%	11	2.9%	11	4.1%

Methylenedioxy Pyrovalerone Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD

Methylenedioxy Pyrovalerone	276.1594	10	100	0.0%											
2,3-Methylenedioxy Pyrovalerone			100	0.0%											
Methylenedioxy Pyrovalerone	126.1277	20	69	11.6%	61	4.1%	59	1.4%	67	2.6%	67	2.2%	65	2.9%	68	1.0%
2,3-Methylenedioxy Pyrovalerone			34	3.6%	34	4.5%	33	1.1%	35	2.1%	35	1.6%	33	3.3%	36	3.5%
Methylenedioxy Pyrovalerone	135.0441	20	54	4.9%	46	3.9%	45	1.1%	54	3.6%	55	5.2%	52	1.7%	55	1.9%
2,3-Methylenedioxy Pyrovalerone			100	0.0%	97	2.8%	95	1.2%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
Methylenedioxy Pyrovalerone	147.0804	20	5	4.9%											
2,3-Methylenedioxy Pyrovalerone			8	13.4%											
Methylenedioxy Pyrovalerone	149.0233	20	28	12.2%	24	6.4%	23	1.5%	28	2.0%	28	4.1%	26	3.0%	27	4.4%
2,3-Methylenedioxy Pyrovalerone			7	4.7%	7	13.3%	7	2.7%	8	0.9%	8	7.5%	8	3.1%	8	4.2%
Methylenedioxy Pyrovalerone	175.0754	20	76	4.8%											
2,3-Methylenedioxy Pyrovalerone			68	3.2%											
Methylenedioxy Pyrovalerone	205.0858	20	67	4.5%	60	2.6%	59	0.8%	66	2.9%	65	4.1%	64	2.9%	65	0.8%
2,3-Methylenedioxy Pyrovalerone			10	4.9%	10	8.9%	9	2.0%	10	6.1%	10	4.4%	9	2.8%	10	3.5%
Methylenedioxy Pyrovalerone	276.1594	20	100	1.9%											
2,3-Methylenedioxy Pyrovalerone			90	6.0%											
Methylenedioxy Pyrovalerone	65.0386	40	19	16.0%											
2,3-Methylenedioxy Pyrovalerone			14	8.1%											
Methylenedioxy Pyrovalerone	84.0808	40	23	5.6%	30	12.6%	31	1.8%	30	1.5%	30	1.6%	30	1.8%	30	1.5%
2,3-Methylenedioxy Pyrovalerone			32	2.4%	22	6.1%	22	1.3%	22	2.6%	21	3.2%	22	3.9%	22	0.6%
Methylenedioxy Pyrovalerone	121.0284	40	4	7.4%	32	6.4%	31	1.8%	33	1.8%	33	2.5%	33	2.4%	33	2.0%
2,3-Methylenedioxy Pyrovalerone			33	3.4%	4	13.2%	4	4.3%	4	4.9%	4	3.7%	4	1.7%	4	4.2%
Methylenedioxy Pyrovalerone	126.1277	40	100	0.0%	100	0.0%	100	0.0%	83	3.0%	81	3.5%	83	1.4%	82	3.2%
2,3-Methylenedioxy Pyrovalerone			90	3.7%	90	5.8%	90	1.1%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
Methylenedioxy Pyrovalerone	135.0441	40	81	5.0%	81	7.5%	80	1.2%	83	3.0%	81	3.5%	83	1.4%	82	3.2%
2,3-Methylenedioxy Pyrovalerone			100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
Methylenedioxy Pyrovalerone	149.0233	40	69	4.6%	67	7.8%	67	1.1%	70	1.1%	70	2.3%	70	1.5%	69	1.0%
2,3-Methylenedioxy Pyrovalerone			38	4.3%	37	4.1%	37	1.4%	38	3.3%	38	2.8%	38	2.5%	38	2.8%
Methylenedioxy Pyrovalerone	175.0754	40	15	5.5%											
2,3-Methylenedioxy Pyrovalerone			15	6.9%											

Methylethcathinone Regioisomer			**Reproducibility**		**Concentration**				**Mobile Phase**							
					Low		**High**		**H20**		**5 mM AF**		**Acetonitrile**		**Methanol**	
Compound	**Ion**	**CE**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**	**Mean**	**RSD**
4-Methylethcathinone	145.0886	10	16	6.3%												

3-Methylethcathinone			18	6.4%												
4-Methylethcathinone	146.0964	10	22	5.4%												
3-Methylethcathinone			24	4.2%												
4-Methylethcathinone	174.1277	10	100	0.0%												
3-Methylethcathinone			100	0.0%												
4-Methylethcathinone	192.1383	10	32	5.7%	42	5.0%	40	1.0%	42	3.3%	44	0.7%	41	1.3%	41	0.6%
3-Methylethcathinone			44	6.2%	56	4.0%	55	0.6%	57	1.1%	60	1.5%	57	1.2%	56	0.4%
4-Methylethcathinone	119.0855	20	36	6.1%	34	8.7%	33	2.9%	32	2.2%	31	1.5%	32	2.0%	32	2.1%
3-Methylethcathinone			32	4.5%	32	6.9%	30	2.7%	29	2.8%	29	1.0%	29	2.8%	30	1.3%
4-Methylethcathinone	131.0730	20	29	5.3%												
3-Methylethcathinone			30	5.4%												
4-Methylethcathinone	144.0808	20	45	4.6%												
3-Methylethcathinone			48	6.5%												
4-Methylethcathinone	145.0886	20	100	0.0%												
3-Methylethcathinone			100	0.0%												
4-Methylethcathinone	146.0964	20	68	4.3%												
3-Methylethcathinone			65	4.3%												
4-Methylethcathinone	159.1043	20	34	7.6%												
3-Methylethcathinone			34	5.1%												
4-Methylethcathinone	174.1277	20	43	6.3%	53	7.3%	52	1.3%	57	0.7%	57	1.2%	56	1.4%	55	1.3%
3-Methylethcathinone			38	5.5%	49	5.2%	47	1.9%	51	1.9%	51	1.4%	51	0.8%	50	1.7%
4-Methylethcathinone	77.0386	40	15	8.0%												
3-Methylethcathinone			13	9.2%												
4-Methylethcathinone	91.0542	40	59	5.6%	54	5.9%	55	1.9%	51	1.2%	51	1.8%	53	2.0%	52	2.0%
3-Methylethcathinone			52	3.7%	51	5.8%	48	1.3%	46	1.8%	45	1.7%	46	1.5%	46	1.2%
4-Methylethcathinone	115.0542	40	17	11.0%												
3-Methylethcathinone			15	9.4%												
4-Methylethcathinone	130.0651	40	43	6.9%												
3-Methylethcathinone			47	6.4%												
4-Methylethcathinone	131.0730	40	18	7.5%												
3-Methylethcathinone			19	7.2%												
4-Methylethcathinone	144.0808	40	100	0.0%												
3-Methylethcathinone			100	0.0%												

RCS-4 Regioisomers	Reproducibility	Concentration	Mobile Phase

Compound	Ion	CE	Mean	RSD	Low Mean	Low RSD	High Mean	High RSD	H20 Mean	H20 RSD	5 mM AF Mean	5 mM AF RSD	Acetonitrile Mean	Acetonitrile RSD	Methanol Mean	Methanol RSD
RCS-4 2-methoxy isomer	135.0441	10	22	2.5%	22	2.8%	20	1.5%	42	5.0%	41	1.8%	41	1.1%	42	1.0%
RCS-4 3-methoxy isomer			8	3.3%	8	6.8%	7	1.9%	35	7.5%	31	3.1%	15	1.7%	16	3.0%
RCS-4			11	3.0%	11	5.0%	11	2.9%	35	4.4%	31	4.4%	24	3.6%	24	2.8%
RCS-4 2-methoxy isomer	322.1802	10	100	0.0%												
RCS-4 3-methoxy isomer			100	0.0%												
RCS-4			100	0.0%												
RCS-4 2-methoxy isomer	135.0441	20	100	0.0%												
RCS-4 3-methoxy isomer			100	0.0%												
RCS-4			100	0.0%												
RCS-4 2-methoxy isomer	322.1802	20	13	2.9%	13	4.9%	12	1.4%	10	5.3%	10	4.1%	9	1.5%	9	2.1%
RCS-4 3-methoxy isomer			51	2.2%	52	3.0%	53	1.1%	16	9.5%	18	5.6%	38	1.4%	37	2.4%
RCS-4			37	2.4%	37	4.5%	36	1.6%	29	11.5%	31	12.8%	28	4.3%	29	7.0%
RCS-4 2-methoxy isomer	77.0386	40	33	1.6%	38	2.7%	36	2.1%	36	3.0%	37	4.8%	36	2.3%	37	1.6%
RCS-4 3-methoxy isomer			64	3.4%	67	6.0%	65	2.1%	44	7.1%	45	6.5%	64	2.4%	65	3.4%
RCS-4			30	3.7%	32	7.5%	29	4.6%	40	15.9%	38	9.0%	39	2.5%	39	2.7%
RCS-4 2-methoxy isomer	92.0257	40	4	15.0%	5	10.8%	4	2.5%	5	16.1%	5	7.4%	4	7.7%	4	2.8%
RCS-4 3-methoxy isomer			15	3.6%	16	9.0%	16	2.6%	7	11.5%	7	5.3%	17	1.1%	16	4.0%
RCS-4			6	6.4%	6	5.6%	6	4.5%	6	28.6%	8	7.8%	9	9.4%	9	7.7%
RCS-4 2-methoxy isomer	107.0491	40	1	9.0%	1	37.8%	1	4.0%	1	47.0%	2	22.4%	1	2.8%	1	14.7%
RCS-4 3-methoxy isomer			100	0.0%	100	0.0%	98	9.5%	17	24.7%	24	11.8%	100	0.0%	100	0.0%
RCS-4			24	3.3%	24	4.0%	22	1.9%	27	6.2%	28	18.7%	26	2.2%	27	6.1%
RCS-4 2-methoxy isomer	135.0441	40	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
RCS-4 3-methoxy isomer			82	2.2%	79	5.0%	78	1.4%	100	0.0%	100	0.0%	75	2.8%	76	1.7%
RCS-4			100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
RCS-4 2-methoxy isomer	144.0444	40	1	101.7%	1	56.5%	0	61.8%	1	32.6%	1	54.5%	1	34.5%	1	26.4%
RCS-4 3-methoxy isomer			17	9.7%	17	9.0%	16	1.7%	4	23.8%	5	4.5%	16	10.1%	16	1.5%
RCS-4			6	22.5%	6	4.3%	6	2.1%	3	37.1%	5	19.8%	6	5.1%	6	14.4%

RCS-8 Regioisomers			Reproducibility		Concentration				Mobile Phase							
					Low		High		H20		5 mM AF		Acetonitrile		Methanol	
Compound	Ion	CE	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
RCS-8 3-methoxy isomer	376.2271	10	100	0.0%												
RCS-8 4-methoxy isomer			100	0.0%												
RCS-8			100	0.0%												

RCS-8 3-methoxy isomer	121.0648	20	76	2.5%	76	3.6%	72	0.8%	100	0.0%	100	0.0%	89	2.0%	90	0.8%
RCS-8 4-methoxy isomer			34	3.1%	35	4.5%	32	1.4%	89	5.5%	85	3.9%	40	2.2%	42	1.8%
RCS-8			100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
RCS-8 3-methoxy isomer	228.1747	20	29	2.3%	29	6.7%	27	1.0%	24	7.2%	23	5.1%	32	1.7%	32	1.7%
RCS-8 4-methoxy isomer			2	5.7%	2	18.2%	1	26.6%	19	10.0%	18	8.7%	2	7.9%	2	6.7%
RCS-8			7	3.4%	7	8.0%	7	1.6%	6	15.3%	9	28.9%	7	1.7%	7	4.3%
RCS-8 3-methoxy isomer	254.1539	20	35	2.1%	35	2.9%	33	1.2%	24	13.5%	25	4.0%	39	1.8%	40	1.4%
RCS-8 4-methoxy isomer			4	6.3%	4	13.6%	3	3.6%	20	18.7%	21	5.4%	4	2.9%	4	9.0%
RCS-8			1	13.3%	1	23.4%	1	10.2%	1	79.2%	5	80.1%	1	32.9%	1	9.7%
RCS-8 3-methoxy isomer	376.2271	20	99	3.6%	100	0.0%	100	0.0%	80	3.1%	84	3.0%	100	0.0%	100	0.0%
RCS-8 4-methoxy isomer			100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%	100	0.0%
RCS-8			57	2.3%	56	4.3%	57	0.6%	49	8.7%	54	12.8%	46	1.4%	45	1.0%
RCS-8 3-methoxy isomer	69.0699	40	19	17.9%	18	12.5%	17	4.8%	12	6.4%	12	7.5%	16	3.3%	16	2.3%
RCS-8 4-methoxy isomer			4	30.3%	4	9.8%	3	2.8%	11	30.4%	10	14.0%	3	12.4%	3	7.3%
RCS-8			4	38.2%	4	15.0%	4	3.2%	4	56.8%	5	37.7%	4	9.5%	4	4.2%
RCS-8 3-methoxy isomer	91.0542	40	10	4.5%	10	11.9%	9	1.9%	23	7.4%	22	5.6%	9	1.5%	9	3.9%
RCS-8 4-methoxy isomer			2	9.3%	2	33.8%	2	3.7%	17	20.3%	15	9.8%	2	6.2%	2	17.4%
RCS-8			61	3.7%	60	5.7%	59	0.9%	51	23.0%	43	16.1%	55	2.1%	55	2.6%
RCS-8 3-methoxy isomer	93.0699	40	0	-	0	111.4%	0	-	6	12.9%	6	12.4%	0	-	0	-
RCS-8 4-methoxy isomer			0	-	0	141.8%	0	-	4	29.6%	4	17.5%	0	-	0	-
RCS-8			20	16.3%	18	5.4%	18	1.4%	16	13.5%	14	11.0%	17	1.8%	18	3.9%
RCS-8 3-methoxy isomer	121.0648	40	100	0.0%												
RCS-8 4-methoxy isomer			100	0.0%												
RCS-8			100	0.0%												
RCS-8 3-methoxy isomer	135.0441	40	3	52.9%	3	25.1%	2	4.1%	3	58.8%	4	16.6%	3	4.2%	2	4.7%
RCS-8 4-methoxy isomer			33	7.0%	32	5.4%	31	0.7%	11	15.5%	12	9.1%	33	4.5%	32	1.4%
RCS-8			3	28.7%	4	16.8%	4	26.2%	5	13.7%	5	23.8%	4	1.7%	4	4.0%
RCS-8 3-methoxy isomer	144.0808	40	32	2.3%	30	8.8%	30	1.3%	21	8.3%	22	3.1%	31	3.0%	31	2.4%
RCS-8 4-methoxy isomer			5	4.8%	5	31.2%	5	2.3%	18	15.6%	17	6.9%	5	5.9%	5	6.7%
RCS-8			26	3.5%	25	6.2%	25	1.1%	30	17.1%	21	10.1%	25	2.6%	26	3.0%
RCS-8 3-methoxy isomer	254.1539	40	65	2.7%	62	6.3%	63	0.7%	39	10.5%	41	4.8%	60	1.5%	59	1.1%
RCS-8 4-methoxy isomer			11	3.4%	10	7.7%	10	1.3%	34	8.0%	33	7.2%	10	5.6%	9	4.7%
RCS-8			5	5.5%	5	11.9%	5	3.0%	5	11.4%	11	35.5%	5	7.8%	5	6.6%

Appendix 22. The relative abundance and the RSD % of all of the ions of interest in the four sets of regioisomers from the reproducibility experiment and the solid phase extraction experiment.

				Reproducibility		SPE	
Regioisomer Set	**Compound**	**Ion**	**CE**	**Relative Abundance Average (%)**	**RSD**	**Relative Abundance Average (%)**	**RSD**
Fluoroethcathinone	2-Fluoroethcathinone	150.0714	10	26.3	6.1%	35.7	0.1%
	3-Fluoroethcathinone			43.1	6.7%	52.5	1.7%
	4-Fluoroethcathinone			31.1	6.8%	40.9	2.3%
	2-Fluoroethcathinone	196.1132	10	84.0	4.0%	98.7	2.2%
	3-Fluoroethcathinone			78.9	4.1%	100.0	0.0%
	4-Fluoroethcathinone			50.0	6.0%	72.8	0.8%
	2-Fluoroethcathinone	103.0554	20	19.4	10.9%	22.0	0.6%
	3-Fluoroethcathinone			14.0	11.2%	14.3	2.2%
	4-Fluoroethcathinone			14.7	8.3%	17.0	4.8%
	2-Fluoroethcathinone	123.0605	20	42.9	5.2%	42.1	1.8%
	3-Fluoroethcathinone			27.3	9.8%	24.7	1.0%
	4-Fluoroethcathinone			35.5	9.3%	34.2	1.9%
	2-Fluoroethcathinone	149.0635	20	82.8	2.4%	78.5	2.9%
	3-Fluoroethcathinone			57.5	6.1%	52.5	2.4%
	4-Fluoroethcathinone			89.2	4.6%	84.9	1.6%
	2-Fluoroethcathinone	163.0792	20	15.6	7.3%	14.3	2.2%
	3-Fluoroethcathinone			6.1	10.9%	6.9	4.1%
	4-Fluoroethcathinone			13.8	13.7%	11.4	1.6%
	2-Fluoroethcathinone	178.1027	20	52.7	3.1%	61.7	6.8%
	3-Fluoroethcathinone			30.1	7.4%	38.8	1.2%
	4-Fluoroethcathinone			41.3	7.0%	53.2	2.2%
	2-Fluoroethcathinone	77.0386	40	60.1	6.3%	58.0	4.7%
	3-Fluoroethcathinone			54.3	9.2%	50.8	4.1%
	4-Fluoroethcathinone			45.0	7.2%	44.0	0.6%

	2-Fluoroethcathinone	95.0292	40	20.2	5.4%	21.0	7.0%
	3-Fluoroethcathinone			22.9	11.3%	22.8	4.8%
	4-Fluoroethcathinone			13.7	10.8%	14.3	3.8%
	2-Fluoroethcathinone	115.0554	40	23.2	10.1%	19.8	7.5%
	3-Fluoroethcathinone			14.2	16.6%	13.7	2.1%
	4-Fluoroethcathinone			17.4	8.2%	16.3	0.9%
	2-Fluoroethcathinone	135.0479	40	70.8	2.3%	69.5	5.6%
	3-Fluoroethcathinone			85.9	6.5%	82.1	6.6%
	4-Fluoroethcathinone			55.4	5.5%	55.0	0.3%
JWH 203	JWH 203 3-chlorophenyl isomer	188.1434	20	47.0	6.1%	47.2	1.9%
	JWH 203 4-chlorophenyl isomer			28.9	3.5%	28.3	2.8%
	JWH 203			21.9	3.7%	21.0	5.1%
	JWH 203 3-chlorophenyl isomer	214.1226	20	61.3	4.0%	63.8	1.6%
	JWH 203 4-chlorophenyl isomer			21.9	6.2%	21.2	4.8%
	JWH 203			11.0	3.8%	12.0	5.3%
	JWH 203 3-chlorophenyl isomer	144.0444	40	44.8	6.2%	42.5	3.4%
	JWH 203 4-chlorophenyl isomer			17.2	4.0%	16.6	0.7%
	JWH 203			10.4	3.5%	10.1	1.1%
	JWH 203 3-chlorophenyl isomer	214.1226	40	25.0	8.7%	23.5	1.3%
	JWH 203 4-chlorophenyl isomer			9.7	4.5%	9.0	2.3%
	JWH 203			7.2	5.4%	5.5	5.5%
Methoxymethcathinone	Methedrone	161.0835	10	17.3	6.3%	24.5	3.5%
	2-Methoxymethcathinone			24.6	5.8%	32.8	2.2%
	3-Methoxymethcathinone			27.8	6.6%	39.2	0.8%
	Methedrone	194.1176	10	17.3	6.6%	26.8	0.9%

	2-Methoxymethcathinone			14.7	7.9%	24.5	2.1%
	3-Methoxymethcathinone			28.3	6.0%	41.9	1.8%
	Methedrone	135.0804	20	20.6	2.3%	20.4	2.1%
	2-Methoxymethcathinone			13.4	2.0%	12.5	3.9%
	3-Methoxymethcathinone			11.0	4.8%	10.7	4.4%
	Methedrone	145.0886	20	29.0	4.3%	29.4	1.8%
	2-Methoxymethcathinone			26.7	3.9%	26.8	1.0%
	3-Methoxymethcathinone			21.1	2.5%	21.9	2.3%
	Methedrone	176.1070	20	43.7	2.2%	55.3	1.5%
	2-Methoxymethcathinone			30.7	5.1%	38.6	0.2%
	3-Methoxymethcathinone			28.6	3.6%	37.0	2.3%
	Methedrone	58.0651	40	28.0	5.1%	27.6	1.9%
	2-Methoxymethcathinone			15.7	10.6%	15.9	4.8%
	3-Methoxymethcathinone			5.6	7.8%	5.1	8.0%
	Methedrone	77.0386	40	45.6	5.4%	45.4	2.5%
	2-Methoxymethcathinone			35.2	4.2%	35.2	1.1%
	3-Methoxymethcathinone			31.3	2.4%	31.0	2.1%
	Methedrone	79.0542	40	28.8	3.9%	26.1	2.9%
	2-Methoxymethcathinone			16.6	7.2%	12.9	1.7%
	3-Methoxymethcathinone			15.1	5.3%	14.9	3.0%
	Methedrone	91.0542	40	35.4	2.0%	37.4	5.9%
	2-Methoxymethcathinone			29.8	7.2%	30.3	0.5%
	3-Methoxymethcathinone			29.7	3.5%	31.1	1.8%
	Methedrone	103.0542	40	27.1	3.2%	25.2	3.4%
	2-Methoxymethcathinone			15.0	5.2%	14.3	1.2%
	3-Methoxymethcathinone			14.1	3.8%	13.2	3.2%
	Methedrone	105.0699	40	18.5	9.0%	17.7	2.4%
	2-Methoxymethcathinone			8.8	10.3%	6.7	4.1%
	3-Methoxymethcathinone			7.1	6.4%	8.2	1.7%
	Methedrone	117.0573	40	19.4	9.4%	20.2	1.9%

	2-Methoxymethcathinone			29.4	7.8%	30.0	2.4%
	3-Methoxymethcathinone			28.4	7.7%	29.2	2.3%
	Methedrone	132.0808	40	33.4	3.6%	31.1	2.1%
	2-Methoxymethcathinone			51.2	3.8%	48.5	2.5%
	3-Methoxymethcathinone			59.5	1.5%	55.1	3.4%
	Methedrone	144.0808	40	37.2	4.7%	33.5	2.1%
	2-Methoxymethcathinone			43.9	6.7%	40.9	2.5%
	3-Methoxymethcathinone			23.1	4.2%	20.6	1.8%
	Methedrone	146.0600	40	94.6	2.6%	92.3	1.4%
	2-Methoxymethcathinone			50.2	4.6%	50.5	2.3%
	3-Methoxymethcathinone			41.5	4.5%	40.1	2.7%
	Methedrone	160.0757	40	7.5	10.5%	6.8	7.1%
	2-Methoxymethcathinone			21.6	5.1%	20.3	3.7%
	3-Methoxymethcathinone			10.9	7.6%	10.1	6.6%
RCS-8	RCS-8 3-methoxy isomer	121.0648	20	75.8	2.5%	95.3	1.1%
	RCS-8 4-methoxy isomer			33.9	3.1%	43.6	2.6%
	RCS-8			100.0	0.0%	100.0	0.0%
	RCS-8 3-methoxy isomer	228.1747	20	29.2	2.3%	31.4	0.6%
	RCS-8 4-methoxy isomer			1.8	5.7%	1.7	2.0%
	RCS-8			7.5	3.4%	6.0	4.6%
	RCS-8 3-methoxy isomer	254.1539	20	35.3	2.1%	40.7	2.4%
	RCS-8 4-methoxy isomer			3.6	6.3%	3.9	1.1%
	RCS-8			1.2	13.3%	0.7	86.6%
	RCS-8 3-methoxy isomer	376.2271	20	98.9	3.6%	100.0	0.0%
	RCS-8 4-methoxy isomer			100.0	0.0%	100.0	0.0%
	RCS-8			56.8	2.3%	44.5	3.4%
	RCS-8 3-methoxy isomer	69.0699	40	18.8	17.9%	16.7	3.5%
	RCS-8 4-methoxy isomer			3.9	30.3%	3.2	5.1%
	RCS-8			4.3	38.2%	3.7	10.6%
	RCS-8 3-methoxy isomer	91.0542	40	9.9	4.5%	8.5	3.5%
	RCS-8 4-methoxy isomer			2.1	9.3%	1.7	6.5%

	RCS-8			61.4	3.7%	57.4	3.3%
	RCS-8 3-methoxy isomer	93.0699	40	0.0	-	0.0	-
	RCS-8 4-methoxy isomer			0.0	-	0.0	-
	RCS-8			19.6	16.3%	16.9	3.8%
	RCS-8 3-methoxy isomer	135.0441	40	2.7	52.9%	2.2	9.4%
	RCS-8 4-methoxy isomer			33.4	7.0%	30.9	1.8%
	RCS-8			3.4	28.7%	3.5	0.9%
	RCS-8 3-methoxy isomer	144.0808	40	31.5	2.3%	30.4	1.4%
	RCS-8 4-methoxy isomer			5.3	4.8%	4.8	1.2%
	RCS-8			26.2	3.5%	24.5	3.1%
	RCS-8 3-methoxy isomer	254.1539	40	64.9	2.7%	57.0	2.4%
	RCS-8 4-methoxy isomer			10.8	3.4%	8.7	3.6%
	RCS-8			5.4	5.5%	4.3	5.4%

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