ANALYSIS OF DESIGNER STIMULANTS BY GC/MS

Application Compendium

The Measure of Confidence

Agilent Technologies

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Analysis of Designer Stimulants by GC/MS

Application Compendium

Introduction

By Fran Diamond, Chemistry Technical Leader, NMS Labs

A new wave of drug compounds are chemical variations of older traditional stimulant drugs. Popularly known and labeled as "bath salts," these compounds are synthetic derivatives of psychedelic chemicals known as cathinones, tryptamines, phenethylamines and piperazines. They are chemically altered so that they are not technically illegal. These new chemicals vary by slight changes to the chemical structure by placement of alkyl side-chains, replacement of methyl with ethyl groups, etc. They are packaged and sold under names such as "Ivory wave" ,"Vanilla sky", and "Tranquility", to name a few, and under the guise of "bath salts" or "plant food" and more recently "party powders". These products are legal. These are dangerous compounds. They have not been tested in humans.

Numerous states have enacted legislation banning the use of some of these drugs. The Drug Enforcement Administration (DEA) recently used its emergency authority to ban chemicals used in "bath salts", calling the chemicals an "imminent hazard" to the public; but this only addressed three of the more prevalent chemicals. There are many more of these substances and even when controlled, newer variations are readily infused. This phenomenon has given law enforcement and testing laboratories a series of challenges to overcome in order to provide testing of these new materials. As with the synthetic cannabinoids, which emerged recently, these newer variations are being manufactured and distributed worldwide.

Few legitimate suppliers of reference materials have been able to keep up with numerous analogous and homologous materials that are used. There are endless possible chemical variations. To compound the problem, there is abundant information on the internet for synthesizing these compounds.

Analytical laboratories have had a difficult time obtaining pure reference material to use for positive identification. As soon as legislation is passed banning their use, different drugs show up in the next wave. The number of variations is constantly expanding. These materials are also structurally similar in terms of chromatographic retention time and mass spectral appearance. There are many isomeric possibilities that require the analysis be capable of measuring slight variation in data. This can be chromatographic retention or slight differences in mass spectral fragmentation. Data analysis needs to be able to identify the subtle differences in these species and be able to find these substances in complex mixtures.

Sample Preparation

Extraction

These compounds are generally basic amine compounds and can be easily extracted into organic solvent under basic conditions. Since it is not uncommon to find multiple drugs of various chemical properties, we use an acid/base combined extraction. In this procedure, we acidify an aliquot of sample (approximately 25 mg of material) by adding 1 mL of de-ionized water followed by the addition of internal standard and 3 drops of 10% HCl. We next add 1 mL of extraction solvent (95% methylene chloride/5% isopropanol v/v) and mix briefly. We centrifuge the sample and remove the bottom solvent layer and keep. To the remaining aqueous mixture, we add 2 drops of concentrated ammonium hydroxide solution and add 1 mL of the above mentioned mixed solvent layer. Tubes are again mixed and centrifuged, and the lower solvent layer is again removed and combined with the initial solvent. This combined extract is then mixed briefly and transferred to an autosampler vial and capped. It is now ready for instrumental analysis.

Gas Chromatograph and Mass Spectrometer Conditions

GC

Agilent technologies 6890 with fast oven, Autoinjector and tray

Inlet	EPC Split/splitless
Mode	Constant pressure
Injection type:	Splitless
Injection volume (uL):	1.0
Inlet temperature (°C):	265
Pressure nominal (psig):	21.1
Purge flow (ml/min.):	50
Purge time (min.):	0.30
Gas type:	Helium

Oven	
Voltage (VAC):	240
Initial Oven Temp. (°C):	50
Initial oven hold (min.):	0
Ramp rate (°C/min.):	30
Final Temp. (°C):	340
Final hold (min.):	0.5
Total Run Time (min.):	10.17
Equilibration time (min.):	0.1

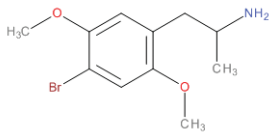
Column	
Type:	DB-1
Agilent part number:	128-1012
Length (m):	12
Diameter (mm):	0.200
Film Thickness (um):	0.33
Nominal Initial Flow (mL/min):	2.6

MSD	
Agilent Technologies 5973 network	
Vacuum pump	Turbo
Tune File	Atune.U
Mode	scan
Solvent delay (min.)	1.5
EM voltage	Atune Voltage
Low mass (amu)	40
High mass (amu)	550
Threshold	250
Sampling	1
Quad temp (°C)	150
Source temp (°C)	230
Transfer line temp (°C)	300

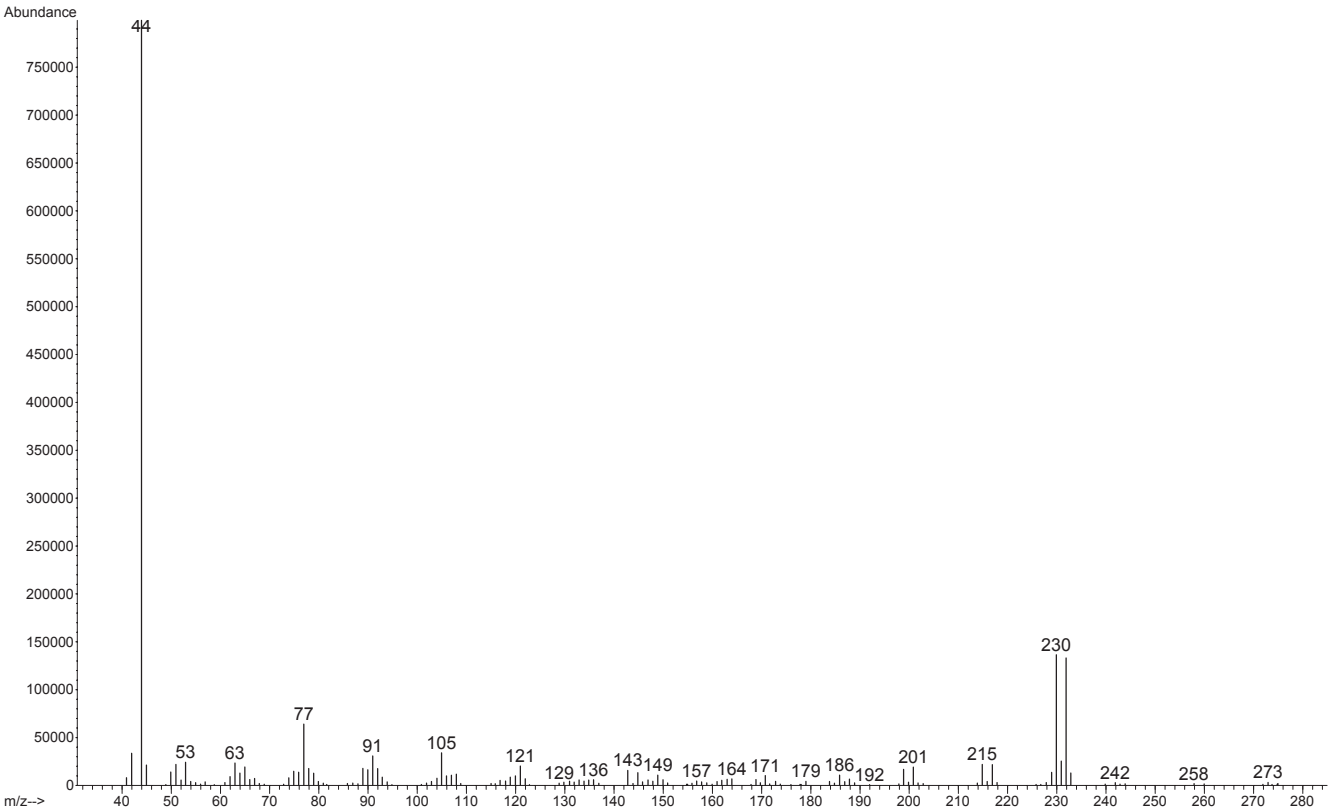
2,5-Dimethoxy-4-bromoamphetamine

Chemical name:	1-(4-Bromo-2,5-dimethoxyphenyl)-2-aminopropane	
Abbreviation:	DOB	
Molecular formula:	$C_{11}H_{16}BrNO_2$	
Molecular mass:	274.15	
Major GC/MS ions:	44, 230, 232, 77,105	
Ions used for analysis:	Target:	44
	Qualifier-1:	230
	Qualifier-2:	232
Retention time:	5.21 minutes	
LOD:	20 mcg/g	

Molecular Structure:



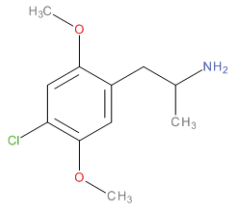
Mass Spectrum:



2,5-Dimethoxy-4-chloroamphetamine

Chemical name:	1-(4-chloro-2,5-dimethoxy-phenyl)propan-2-amine	
Abbreviation:	DOC	
Molecular formula:	$C_{11}H_{16}ClNO_2$	
Molecular mass:	229.70	
Major GC/MS ions:	44, 186, 188, 77, 171	
Ions used for analysis:	Target:	44
	Qualifier-1:	186
	Qualifier-2:	188
Retention time:	4.90 minutes	
LOD:	20 mcg/g	

Molecular Structure:



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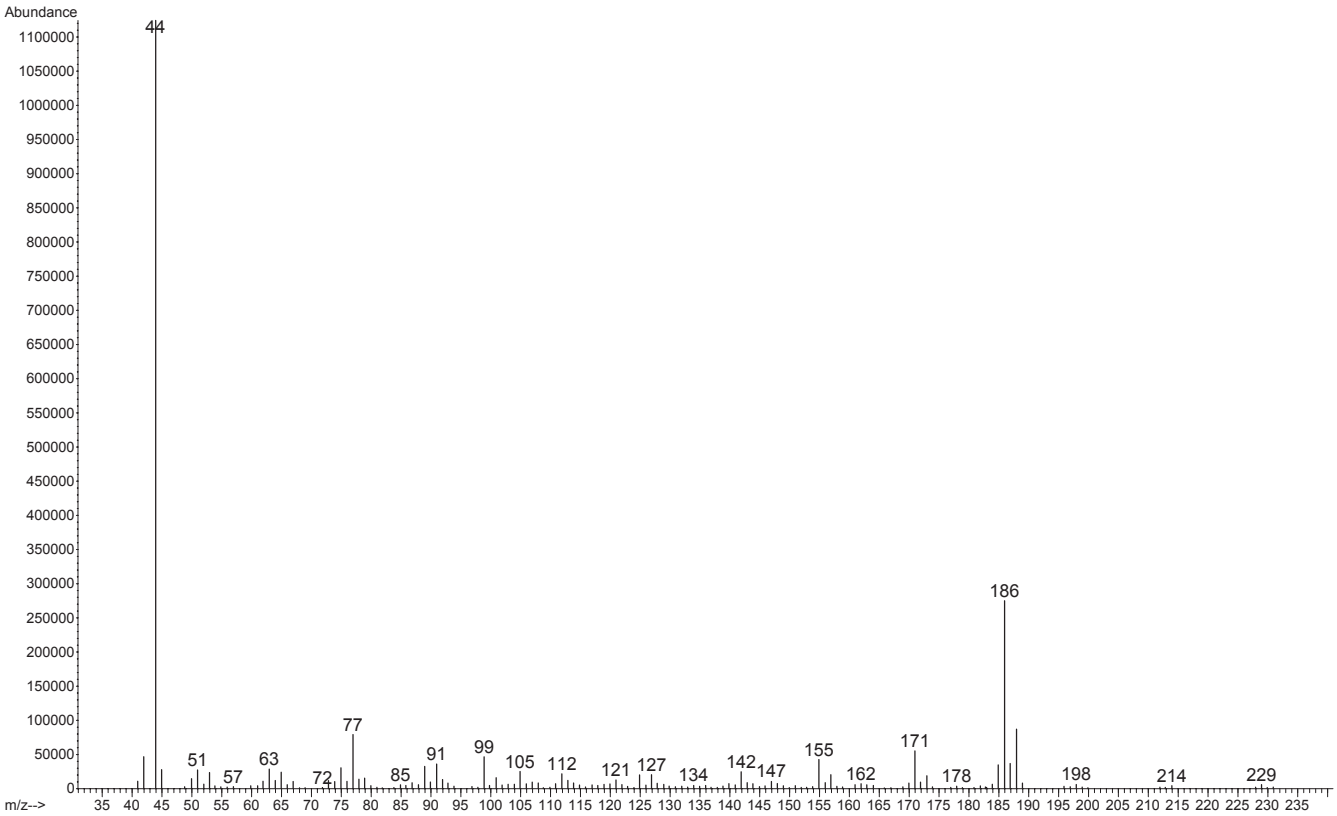
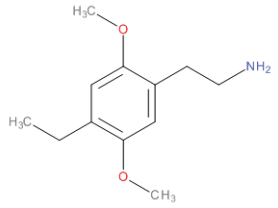


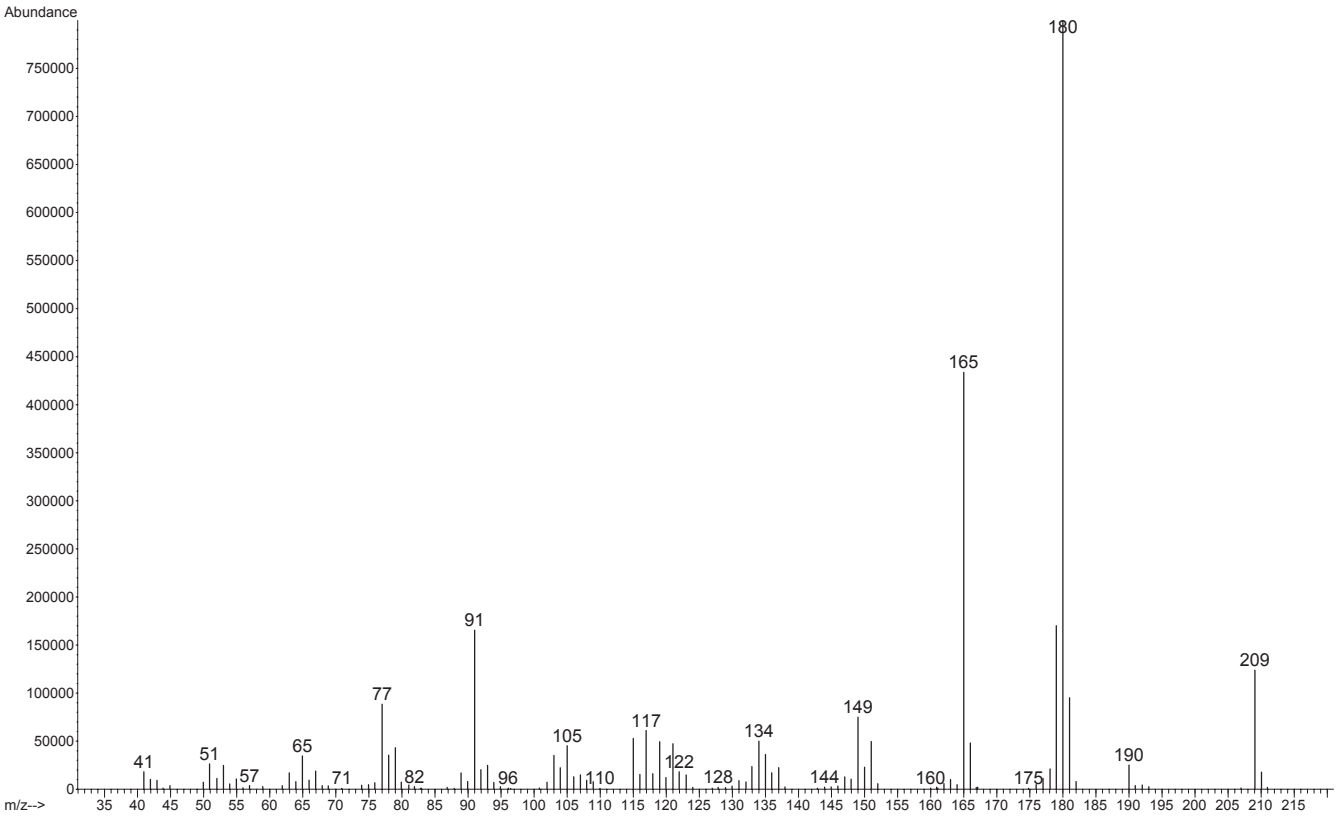
2,5-Dimethoxy-4-ethylphenethylamine

Chemical name:	1-(2,5-Dimethoxy-4-ethylphenyl)-2-aminoethane	
Abbreviation:	2C-E	
Molecular formula:	$C_{12}H_{19}NO_2$	
Molecular mass:	209.29	
Major GC/MS ions:	180, 165, 91, 179, 209	
Ions used for analysis:	Target:	180
	Qualifier-1:	165
	Qualifier-2:	209
Retention time:	4.64 minutes	
LOD:	20 mcg/g	

Molecular Structure:



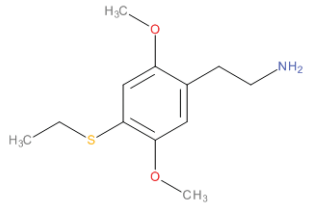
Mass Spectrum:



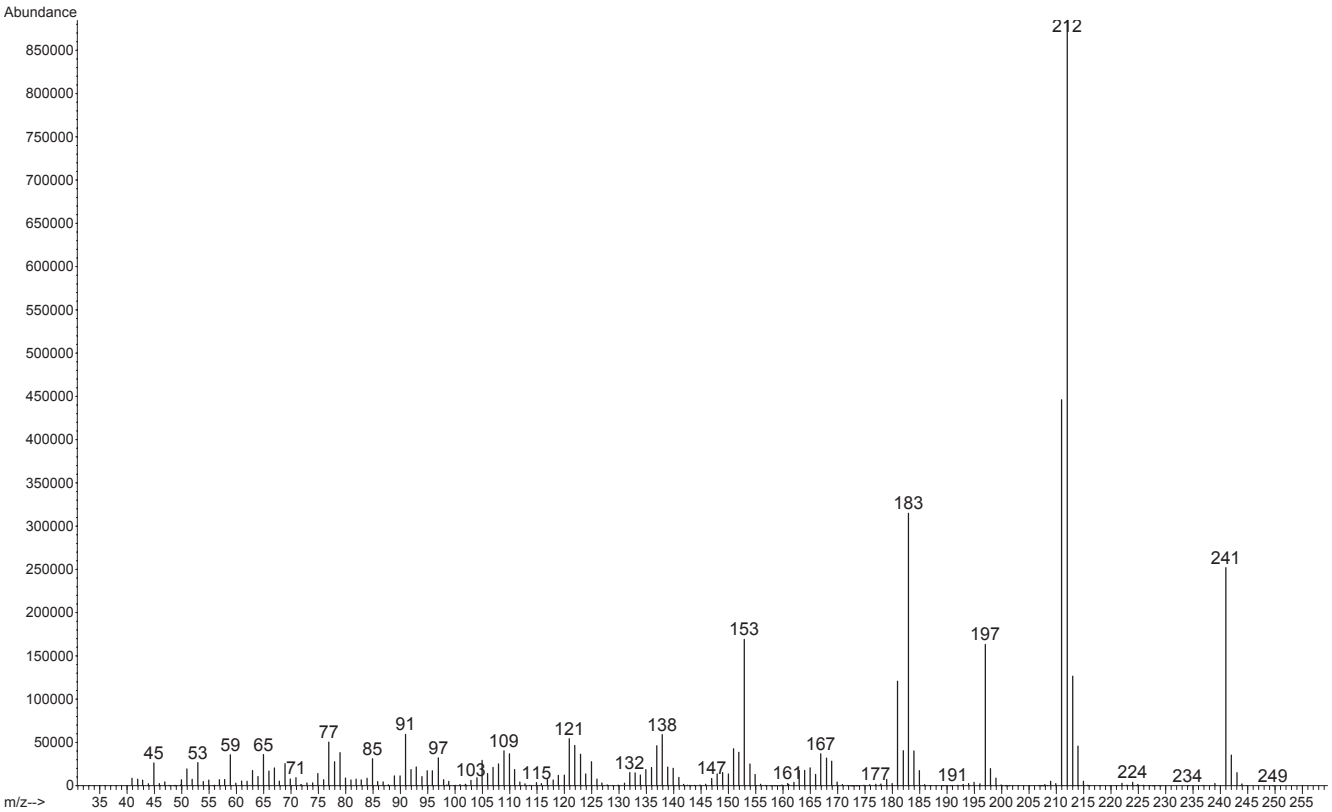
2,5-dimethoxy-4-ethylthiophenethylamine

Chemical name:	2-[4-(Ethylthio)-2,5-dimethoxyphenyl]ethanamine	
Abbreviation:	2C-T-2	
Molecular formula:	$C_{12}H_{19}NO_2S$	
Molecular mass:	241.35	
Major GC/MS ions:	212, 211, 183, 241, 153	
Ions used for analysis:	Target:	212
	Qualifier-1:	183
	Qualifier-2:	241
Retention time:	5.63 minutes	
LOD:	20 mcg/g	

Molecular Structure:



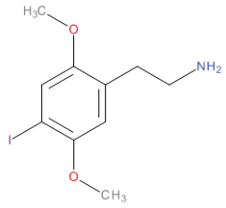
Mass Spectrum:



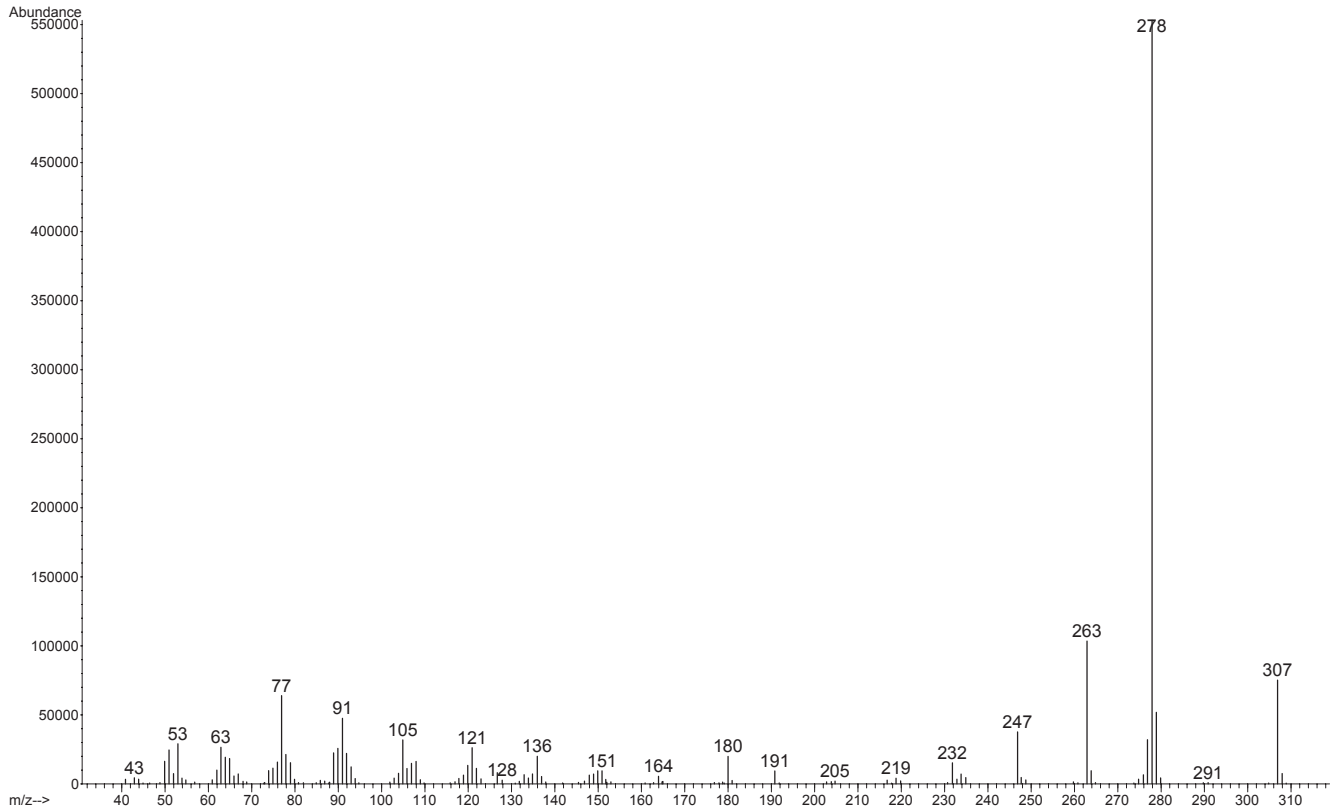
2,5-dimethoxy-4-iodophenethylamine

Chemical name:	2,5-dimethoxy-4-iodophenethylamine	
Abbreviation:	2C-I	
Molecular formula:	$C_{10}H_{14}INO_2$	
Molecular mass:	307.13	
Major GC/MS ions:	278, 263.0 307, 77, 279	
Ions used for analysis:	Target:	278
	Qualifier-1:	263
	Qualifier-2:	307
Retention time:	5.53 minutes	
LOD:	20 mcg/g	

Molecular Structure:



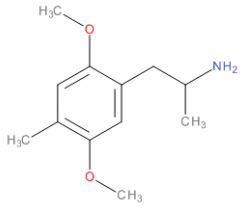
Mass Spectrum:



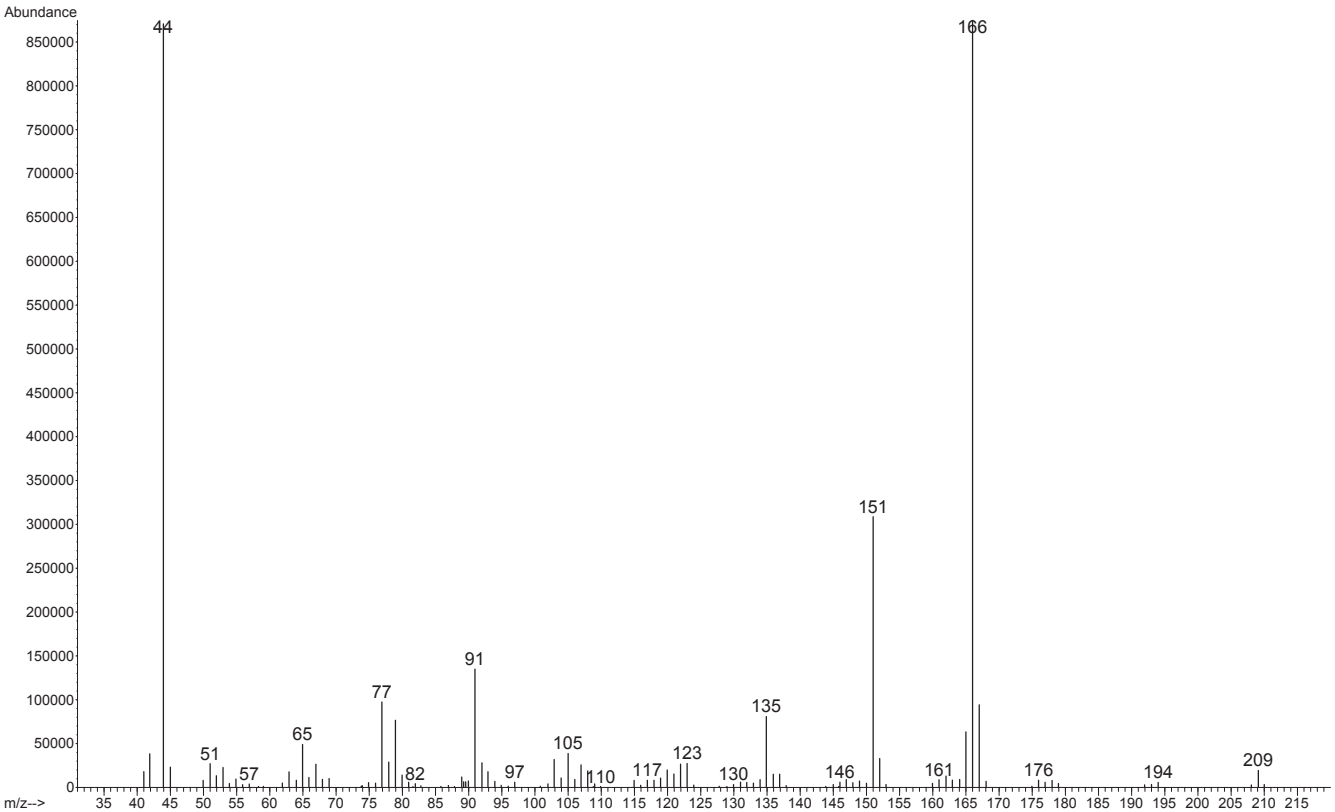
2,5-dimethoxy-4-methylamphetamine

Chemical name:	1-(2,5-Dimethoxy-4-methylphenyl)-2-aminopropane	
Abbreviation:	DOM, STP	
Molecular formula:	$C_{12}H_{19}NO_2$	
Molecular mass:	209.29	
Major GC/MS ions:	166, 44, 151, 91, 167	
Ions used for analysis:	Target:	166
	Qualifier-1:	44
	Qualifier-2:	151
Retention time:	4.45 minutes	
LOD:	20 mcg/g	

Molecular Structure:



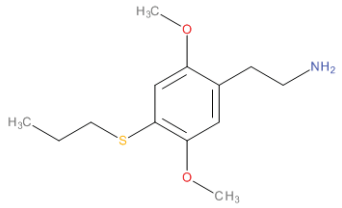
Mass Spectrum:



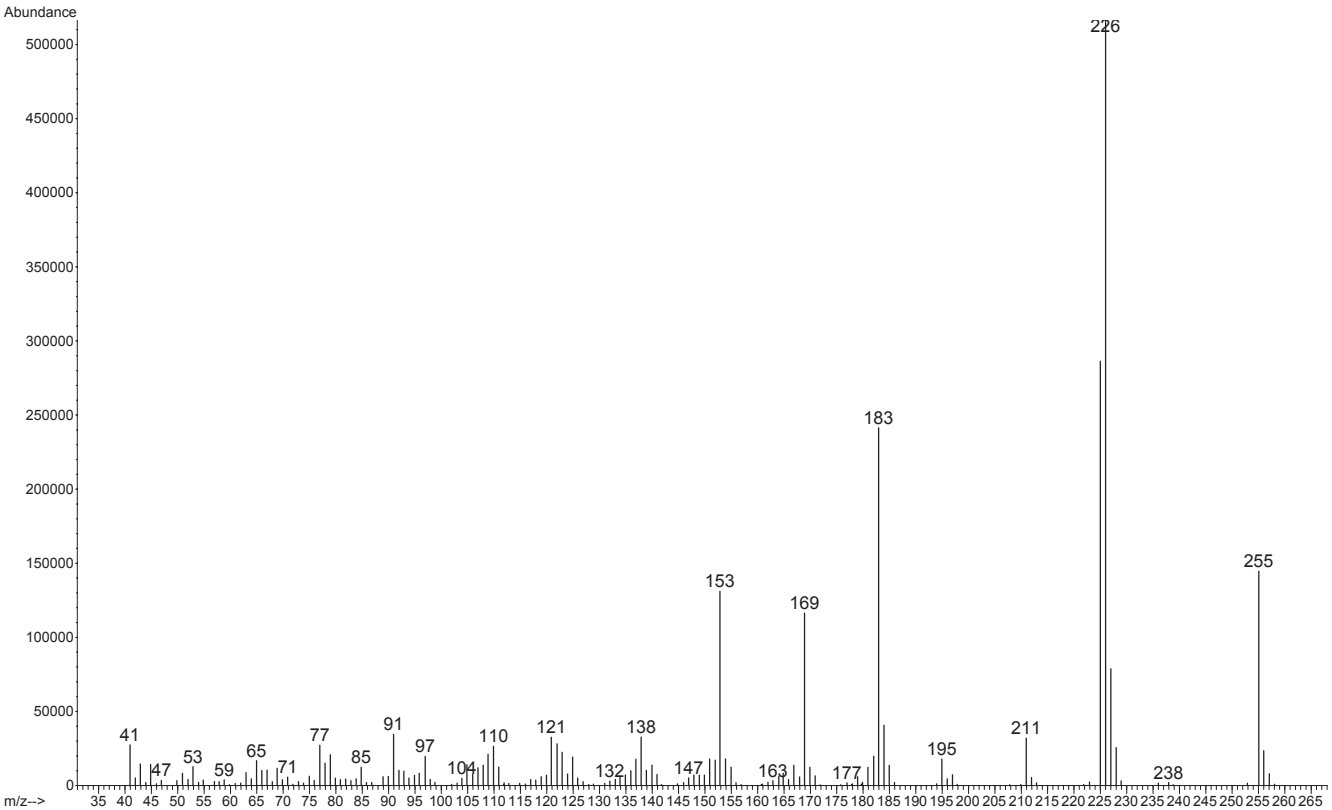
2,5-Dimethoxy-4-propylthiophenethylamine

Chemical name:	2-[2,5-Dimethoxy-4-(propylthio)phenyl]ethanamine	
Abbreviation:	2C-T-7	
Molecular formula:	$C_{13}H_{21}NO_2S$	
Molecular mass:	255.38	
Major GC/MS ions:	226, 225, 183, 255, 153	
Ions used for analysis:	Target:	226
	Qualifier-1:	183
	Qualifier-2:	255
Retention time:	5.91 minutes	
LOD:	20 mcg/g	

Molecular Structure:



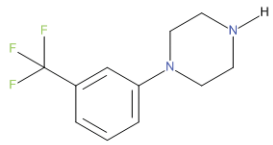
Mass Spectrum:



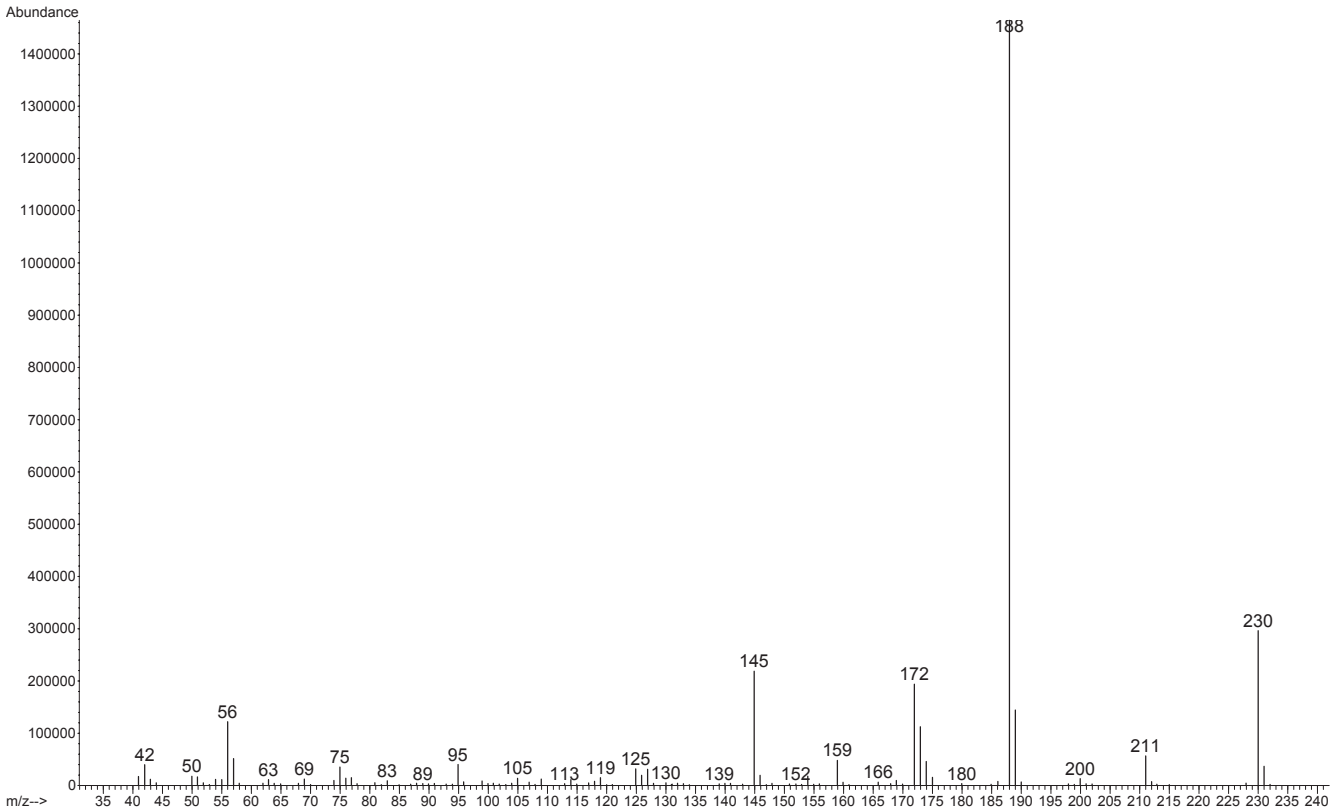
3-trifluoromethylphenylpiperazine

Chemical name:	1-[3-(trifluoromethyl)phenyl]piperazine	
Abbreviation:	TFMPP	
Molecular formula:	$C_{11}H_{13}F_3N_2$	
Molecular mass:	230.23	
Major GC/MS ions:	188, 230, 145, 172, 189	
Ions used for analysis:	Target:	188
	Qualifier-1:	230
	Qualifier-2:	145
Retention time:	4.04 minutes	
LOD:	20 mcg/g	

Molecular Structure:



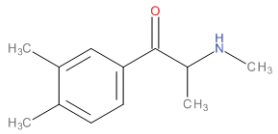
Mass Spectrum:



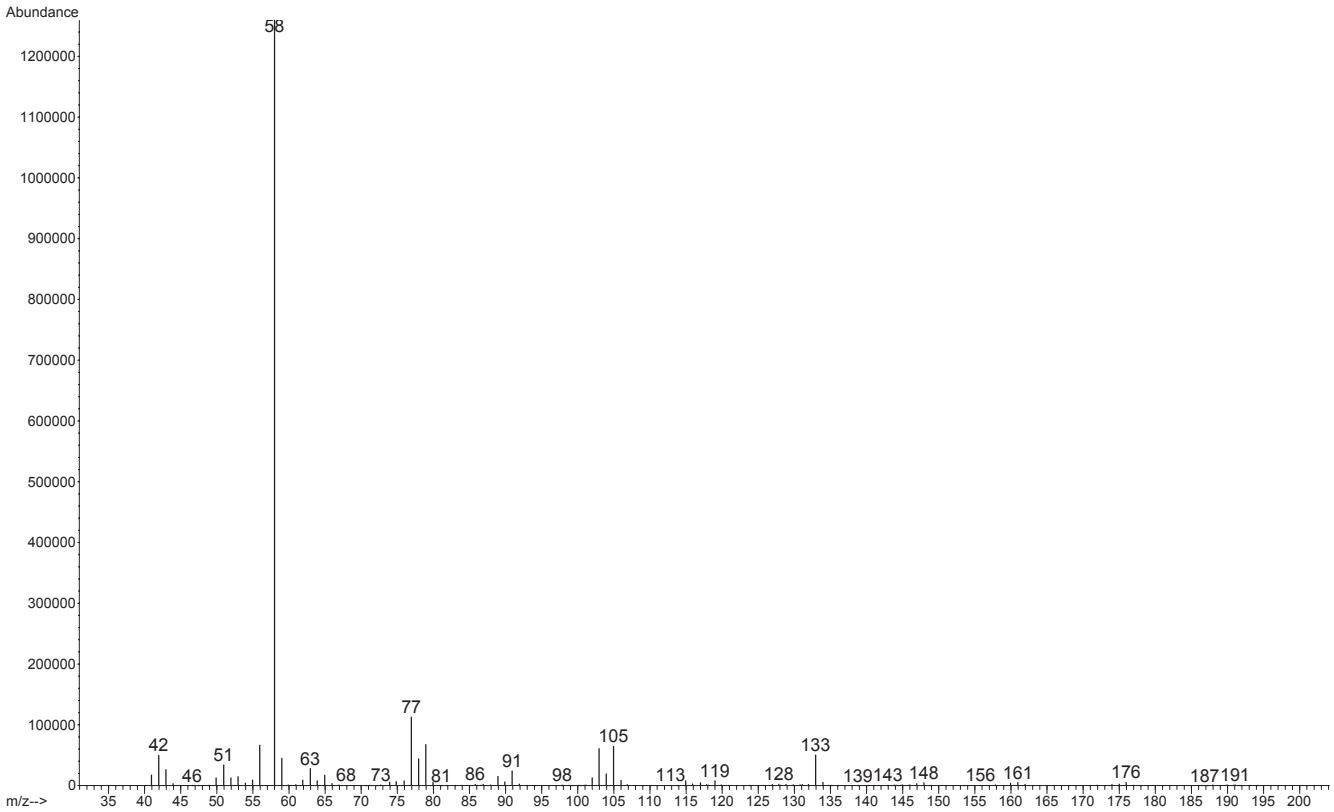
3,4-dimethylmethcathinone

Chemical name:	1-(3,4-dimethylphenyl)-2-(methylamino)propan-1-one	
Abbreviation:	3,4-DMMC	
Molecular formula:	$C_{12}H_{17}NO$	
Molecular mass:	191.27	
Major GC/MS ions:	58, 77, 79, 105, 133	
Ions used for analysis:	Target:	58
	Qualifier-1:	105
	Qualifier-2:	133
Retention time:	4.29 minutes	
LOD:	20 mcg/g	

Molecular Structure:



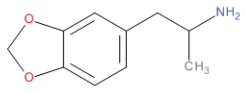
Mass Spectrum:



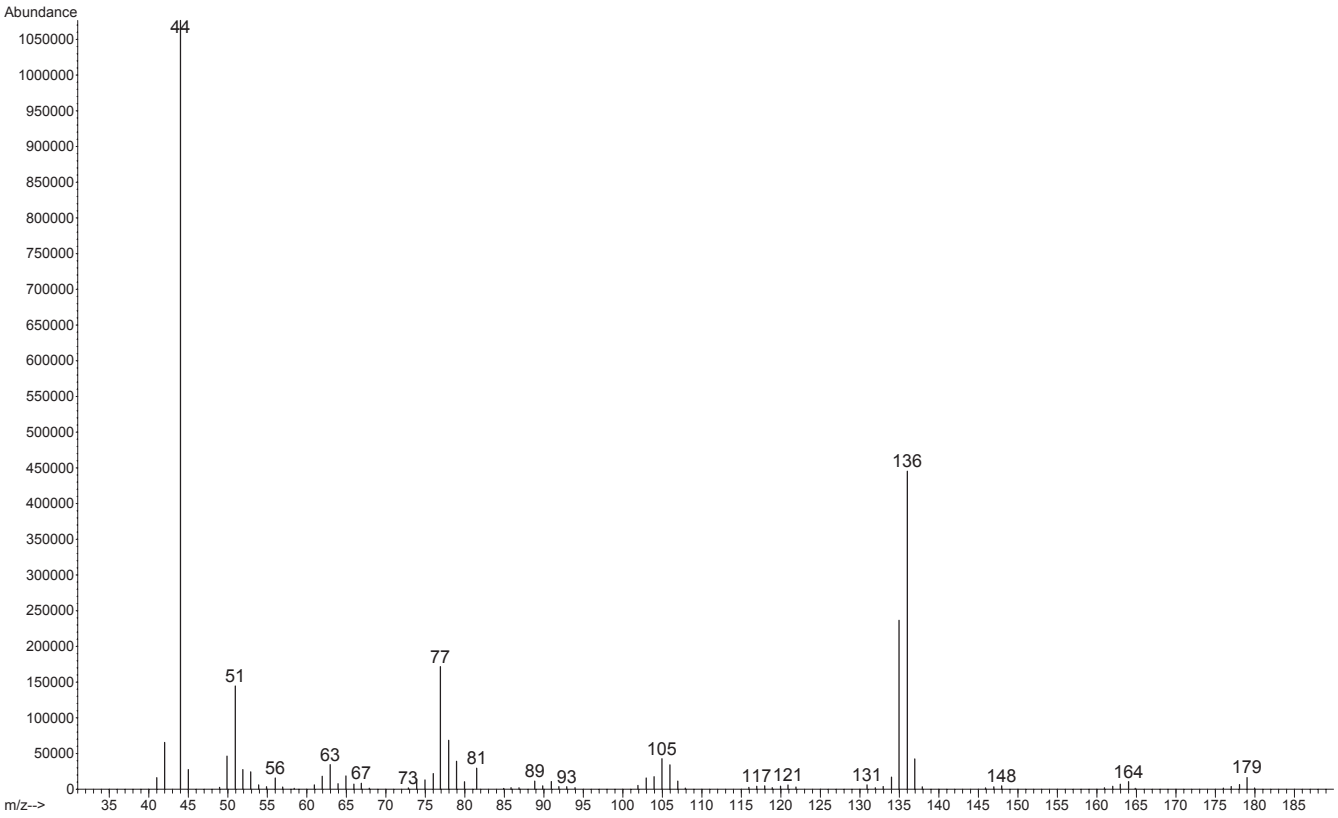
3,4-methylenedioxyamphetamine

Chemical name:	(R) 1-(benzo[1,3]dioxol-5-yl)propan-2-amine	
Abbreviation:	MDA	
Molecular formula:	$C_{10}H_{13}NO_2$	
Molecular mass:	179.22	
Major GC/MS ions:	44, 136, 135, 77, 51	
Ions used for analysis:	Target:	44
	Qualifier-1:	136
	Qualifier-2:	77
Retention time:	3.83 minutes	
LOD:	20 mcg/g	

Molecular Structure:



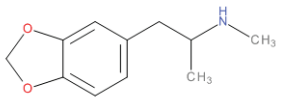
Mass Spectrum:



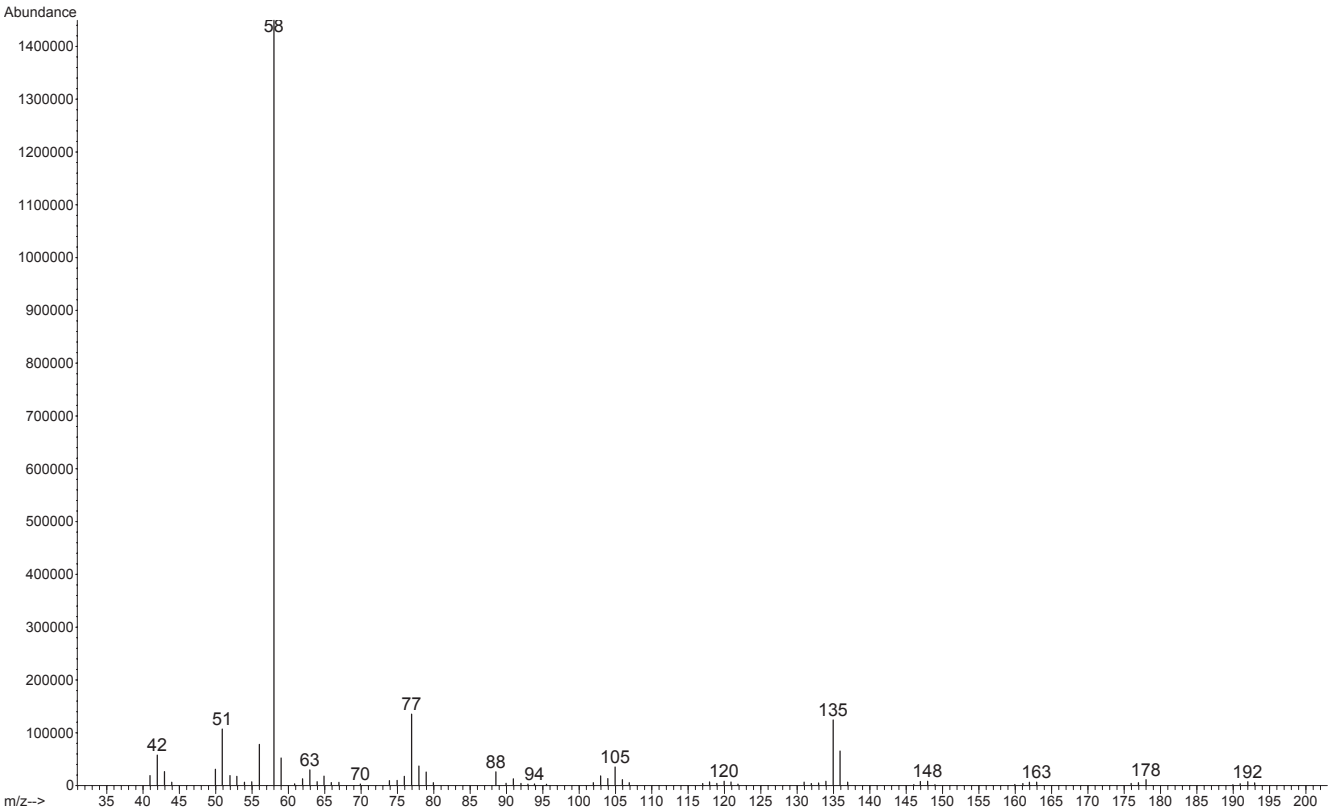
3,4-methylenedioxymethamphetamine

Chemical name:	(RS)-1-(benzo[d][1,3]dioxol-5-yl)-N-methylpropan-2-amine	
Abbreviation:	MDMA	
Molecular formula:	$C_{11}H_{15}NO_2$	
Molecular mass:	193.25	
Major GC/MS ions:	58, 77, 135, 51, 56	
Ions used for analysis:	Target:	58
	Qualifier-1:	135
	Qualifier-2:	77
Retention time:	4.08 minutes	
LOD:	20 mcg/g	

Molecular Structure:



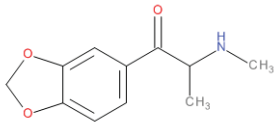
Mass Spectrum:



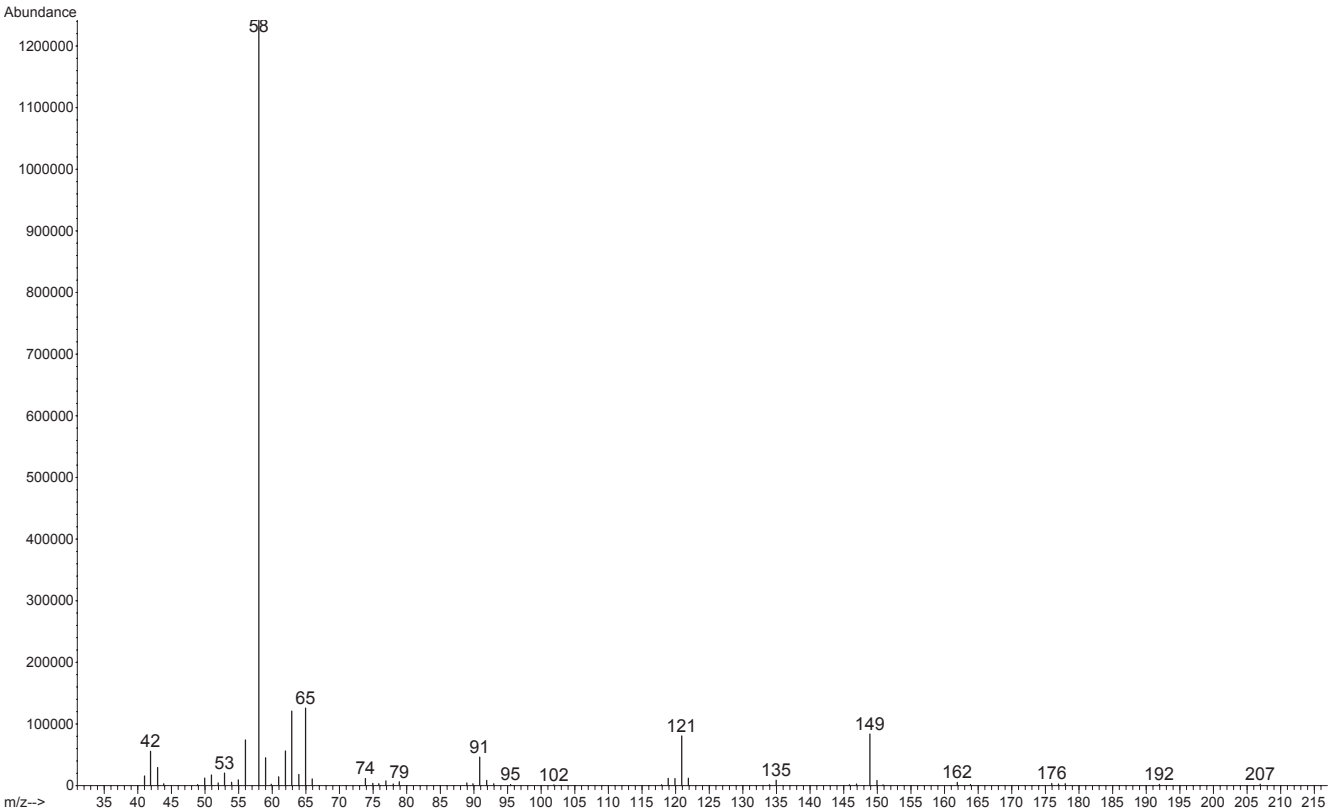
3,4-methylenedioxymethcathinone

Chemical name:	(±)-2-methylamino-1-(3,4-methylenedioxyphenyl)propan-1-one	
Abbreviation:	Methylone, bk-MDMA	
Molecular formula:	$C_{11}H_{13}NO_3$	
Molecular mass:	207.23	
Major GC/MS ions:	58, 65, 63, 149, 121	
Ions used for analysis:	Target:	58
	Qualifier-1:	121
	Qualifier-2:	149
Retention time:	4.76 minutes	
LOD:	20 mcg/g	

Molecular Structure:



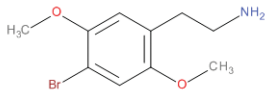
Mass Spectrum:



4-bromo-2,5-dimethoxyphenethylamine

Chemical name:	2-(4-bromo-2,5-dimethoxyphenyl)ethanamine	
Abbreviation:	2C-B	
Molecular formula:	$C_{10}H_{14}BrNO_2$	
Molecular mass:	260.13	
Major GC/MS ions:	230, 232, 215, 217, 77	
Ions used for analysis:	Target:	230
	Qualifier-1:	259
	Qualifier-2:	77
Retention time:	5.12 minutes	
LOD:	20 mcg/g	

Molecular Structure:



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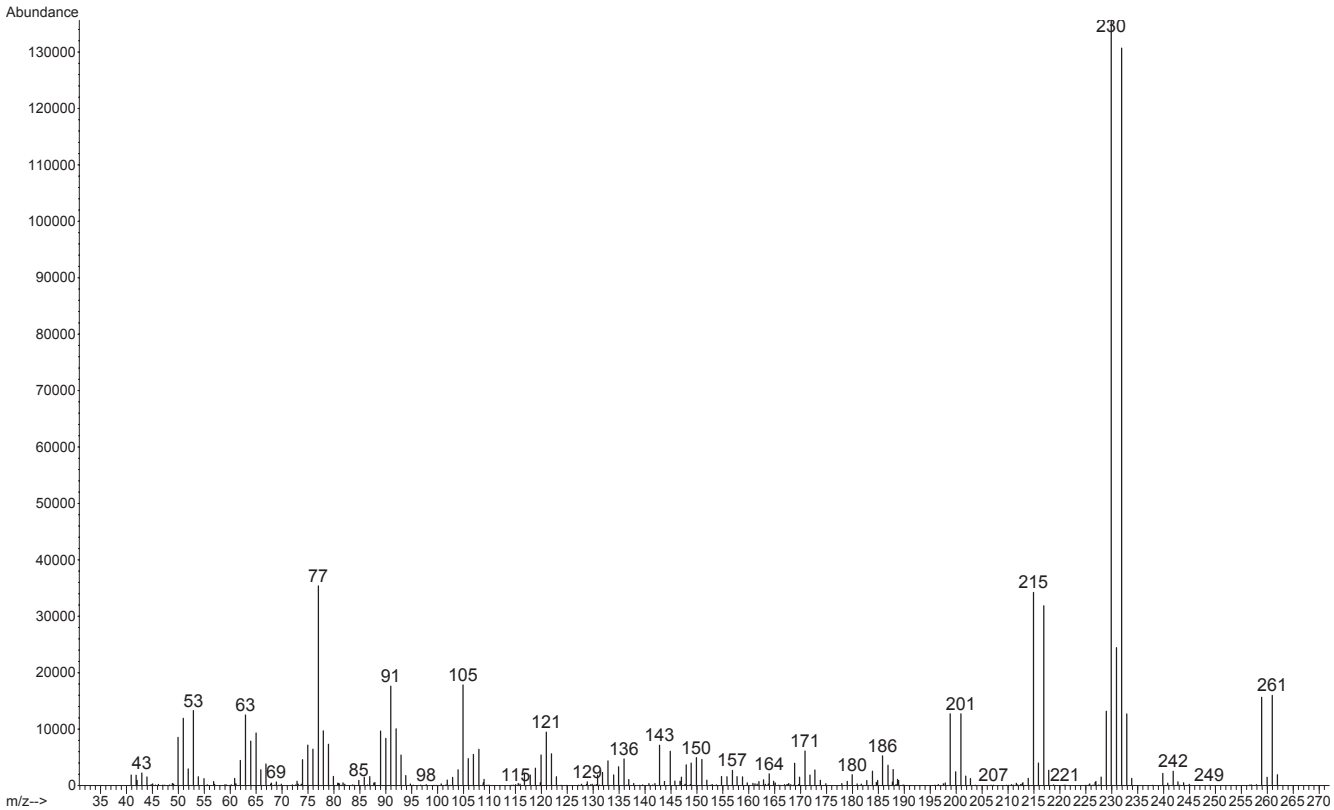
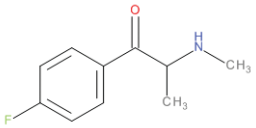


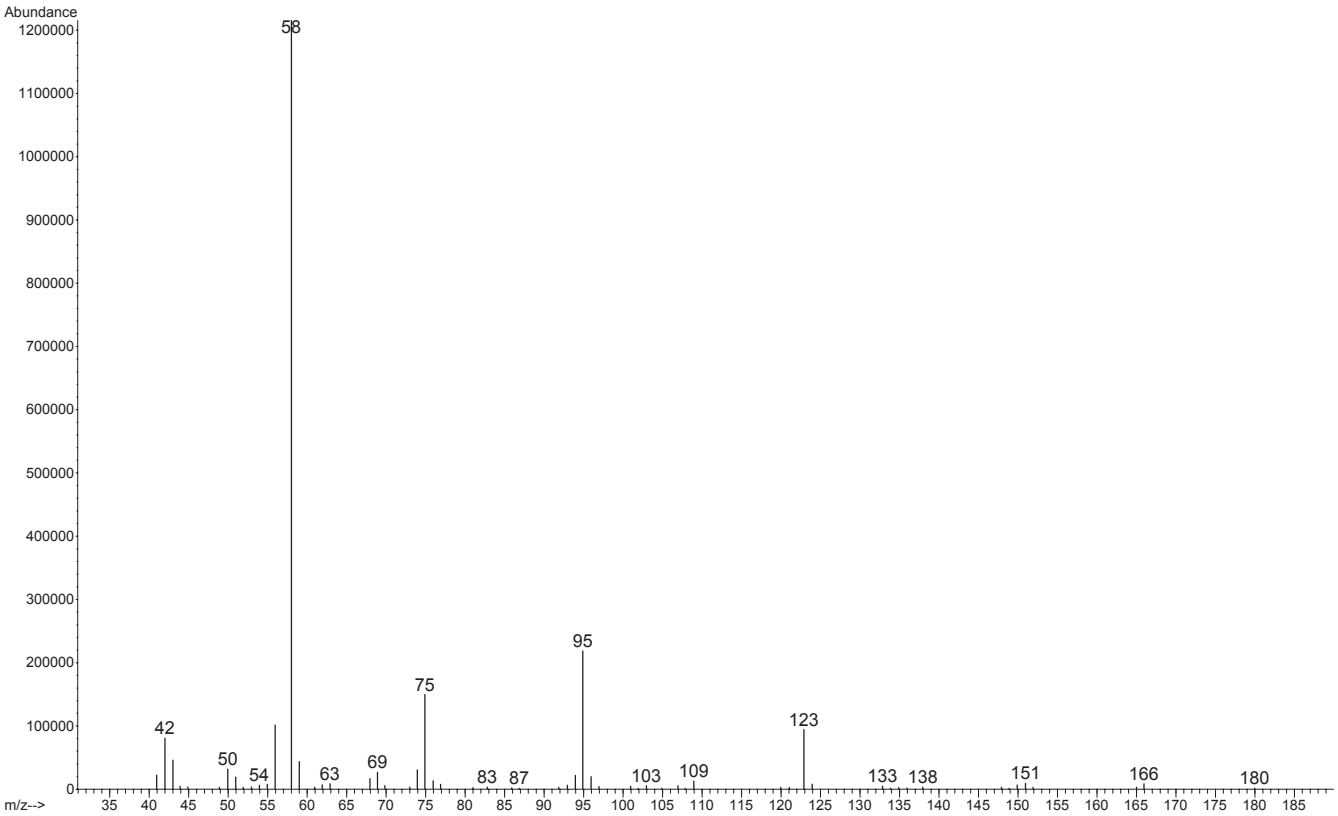
4-fluoromethcathinone

Chemical name:	(RS)-1-(4-fluorophenyl)-2-methylaminopropan-1-one	
Abbreviation:	Flephedrone, 4-FMC	
Molecular formula:	$C_{10}H_{12}FNO$	
Molecular mass:	181.206	
Major GC/MS ions:	58, 95, 75, 56, 123	
Ions used for analysis:	Target:	58
	Qualifier-1:	95
	Qualifier-2:	123
Retention time:	3.12 minutes	
LOD:	20 mcg/g	

Molecular Structure:



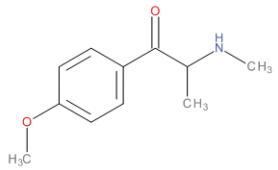
Mass Spectrum:



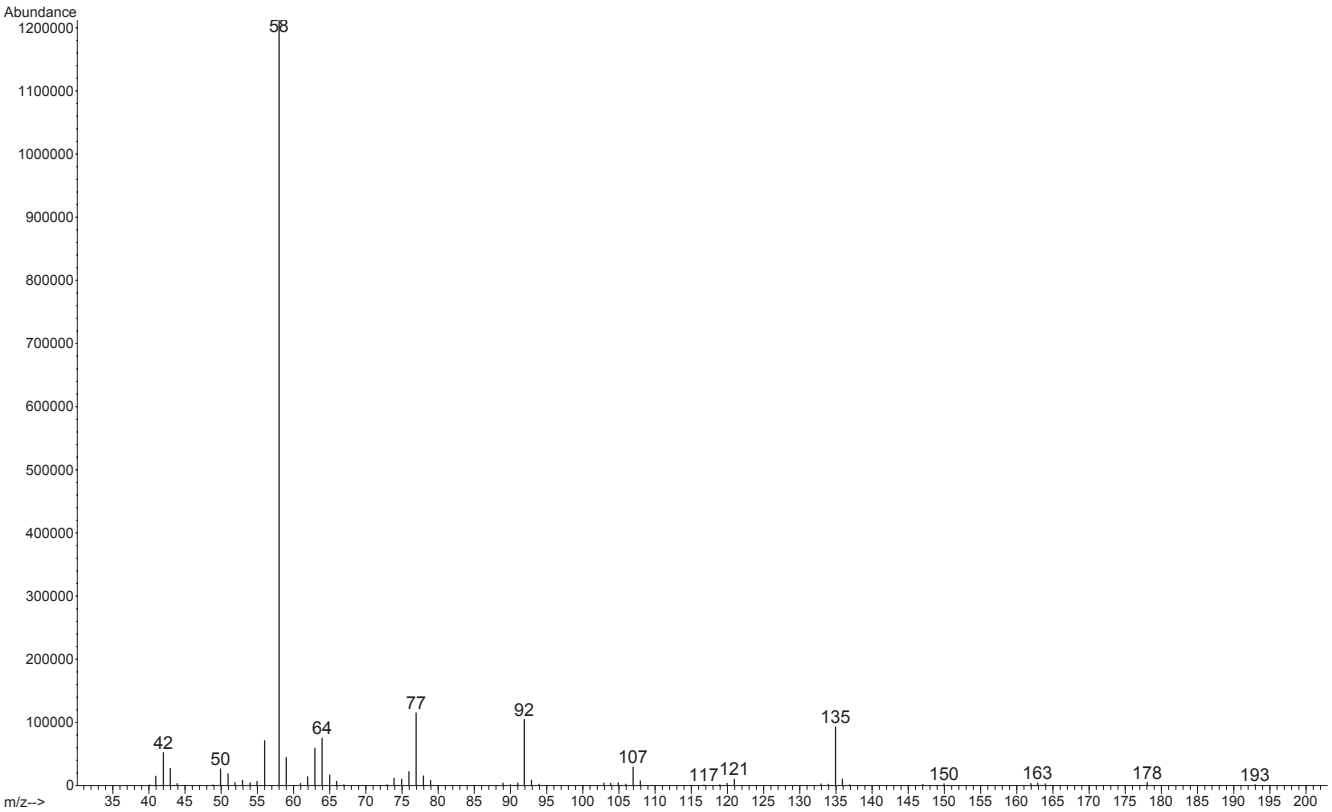
4-Methoxymethcathinone

Chemical name:	RS)-1-(4-methoxyphenyl)-2-(methylamino)propan-1-one	
Abbreviation:	Methedrone	
Molecular formula:	$C_{11}H_{15}NO_2$	
Molecular mass:	193.242	
Major GC/MS ions:	58, 77, 92, 135, 64	
Ions used for analysis:	Target:	58
	Qualifier-1:	92
	Qualifier-2:	135
Retention time:	4.43 minutes	
LOD:	20 mcg/g	

Molecular Structure:



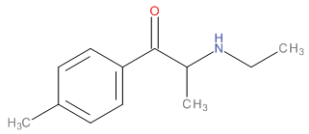
Mass Spectrum:



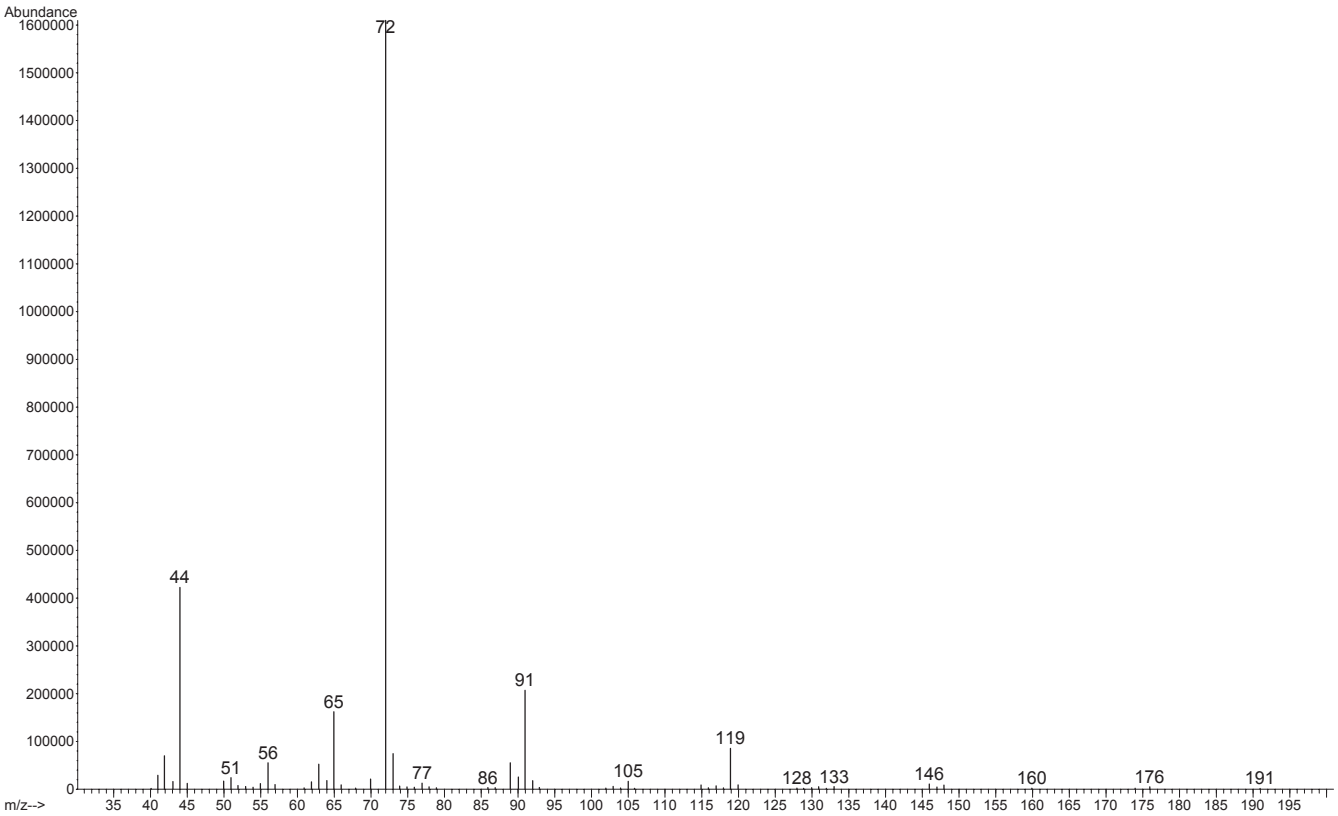
4-methyl-N-ethylcathinone

Chemical name:	(RS)-2-ethylamino-1-(4-methylphenyl)propan-1-one	
Abbreviation:	4-MEC	
Molecular formula:	$C_{12}H_{17}NO$	
Molecular mass:	191.27	
Major GC/MS ions:	72, 44, 91, 65, 119	
Ions used for analysis:	Target:	72
	Qualifier-1:	44
	Qualifier-2:	119
Retention time:	4.01 minutes	
LOD:	20 mcg/g	

Molecular Structure:



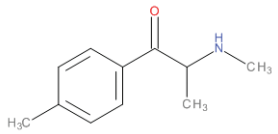
Mass Spectrum:



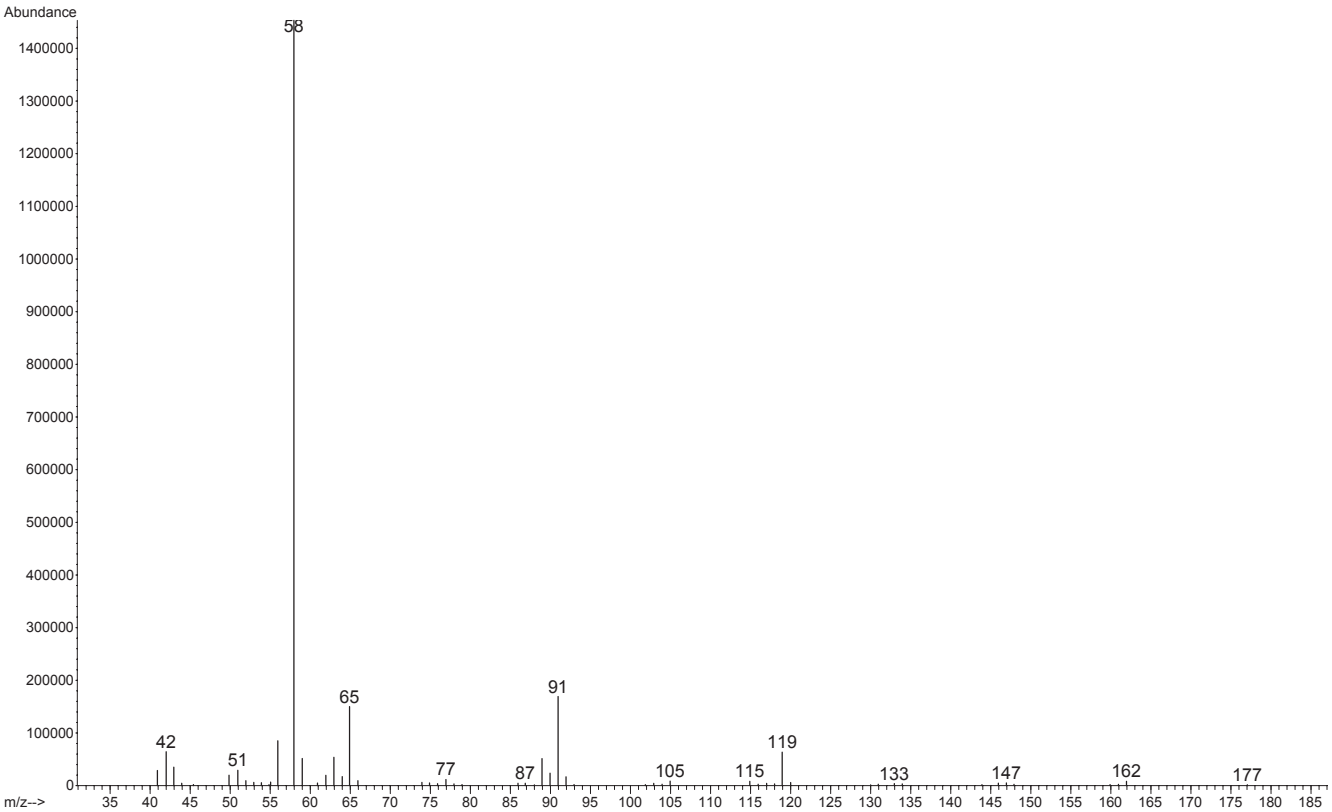
4-methylmethcathinone

Chemical name:	(RS)-2-methylamino-1-(4-methylphenyl)propan-1-one	
Abbreviation:	Mephedrone, 4-MMC	
Molecular formula:	$C_{11}H_{15}NO$	
Molecular mass:	177.242	
Major GC/MS ions:	58, 91, 65, 56, 42	
Ions used for analysis:	Target:	58
	Qualifier-1:	91
	Qualifier-2:	42
Retention time:	3.74 minutes	
LOD:	20 mcg/g	

Molecular Structure:



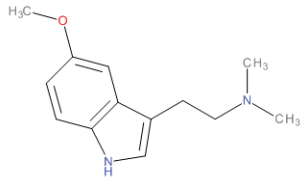
Mass Spectrum:



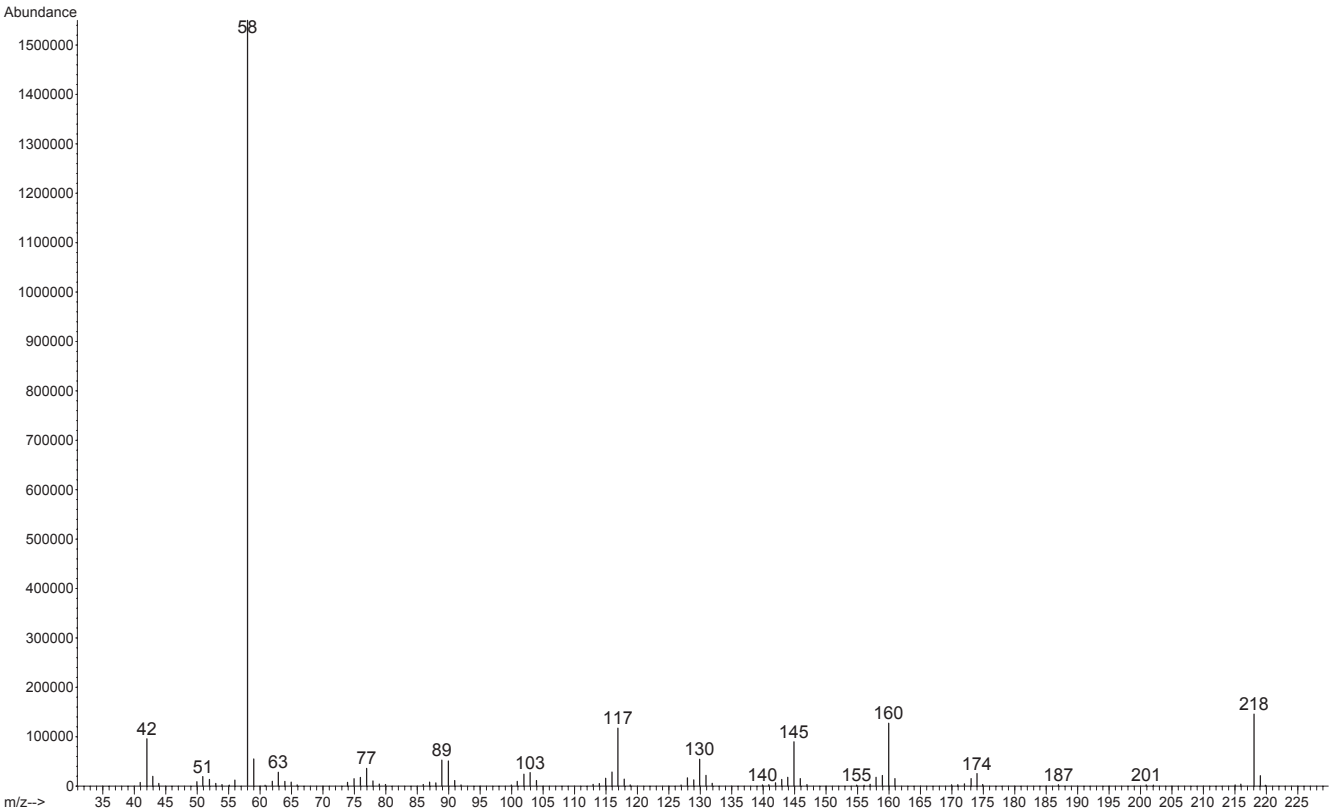
5-methoxy-dimethyltryptamine

Chemical name:	2-(5-methoxy-1H-indol-3-yl)-N,N-dimethylethanamine	
Abbreviation:	5-MeO-DMT	
Molecular formula:	$C_{13}H_{18}N_2O$	
Molecular mass:	218.298	
Major GC/MS ions:	58, 218, 160, 117, 145	
Ions used for analysis:	Target:	58
	Qualifier-1:	160
	Qualifier-2:	218
Retention time:	5.88 minutes	
LOD:	20 mcg/g	

Molecular Structure:



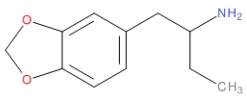
Mass Spectrum:



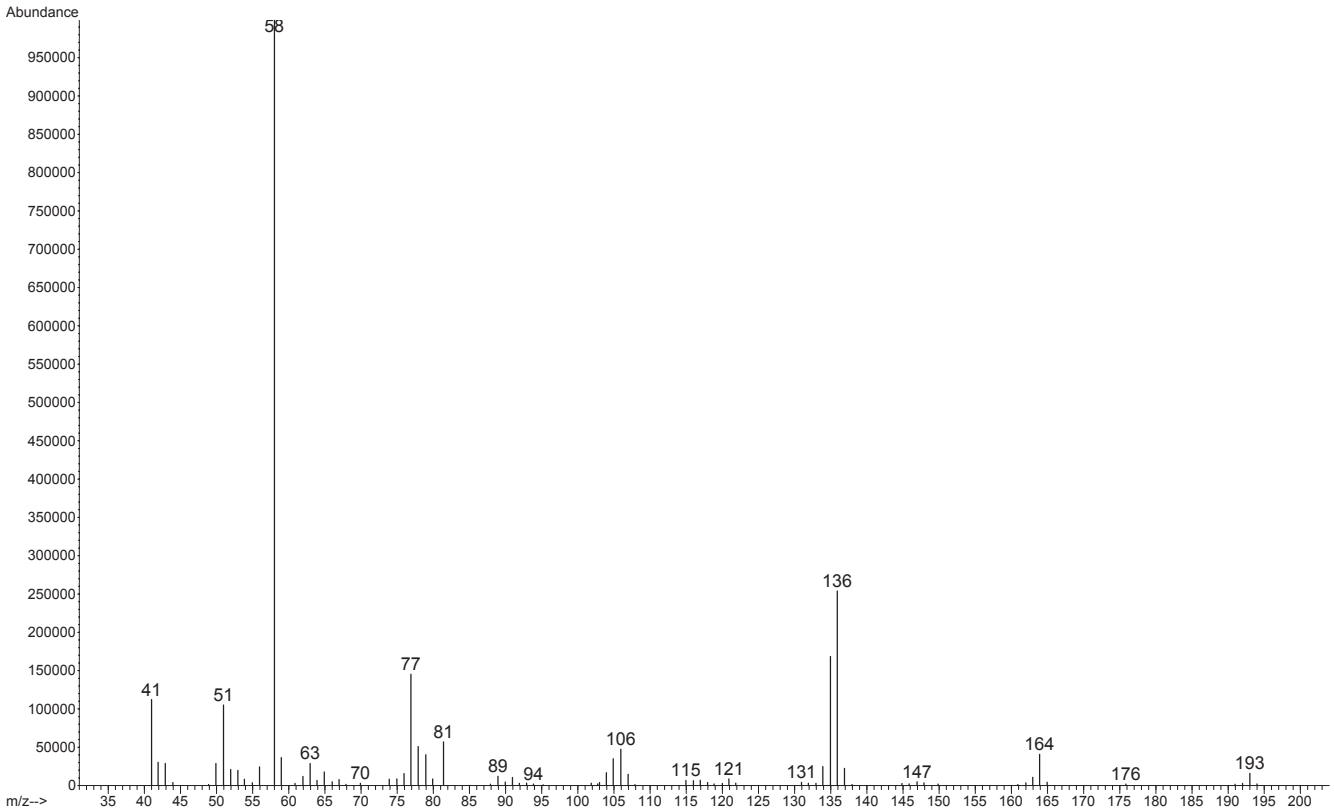
Benzodioxyolybutanamine

Chemical name:	1-(1,3-benzodioxol-5-yl)butan-2-amine	
Abbreviation:	BDB	
Molecular formula:	$C_{11}H_{15}NO_2$	
Molecular mass:	193.242	
Major GC/MS ions:	58, 136, 135, 77, 41	
Ions used for analysis:	Target:	58
	Qualifier-1:	136
	Qualifier-2:	77
Retention time:	4.29 minutes	
LOD:	20 mcg/g	

Molecular Structure:



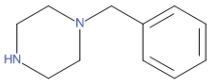
Mass Spectrum:



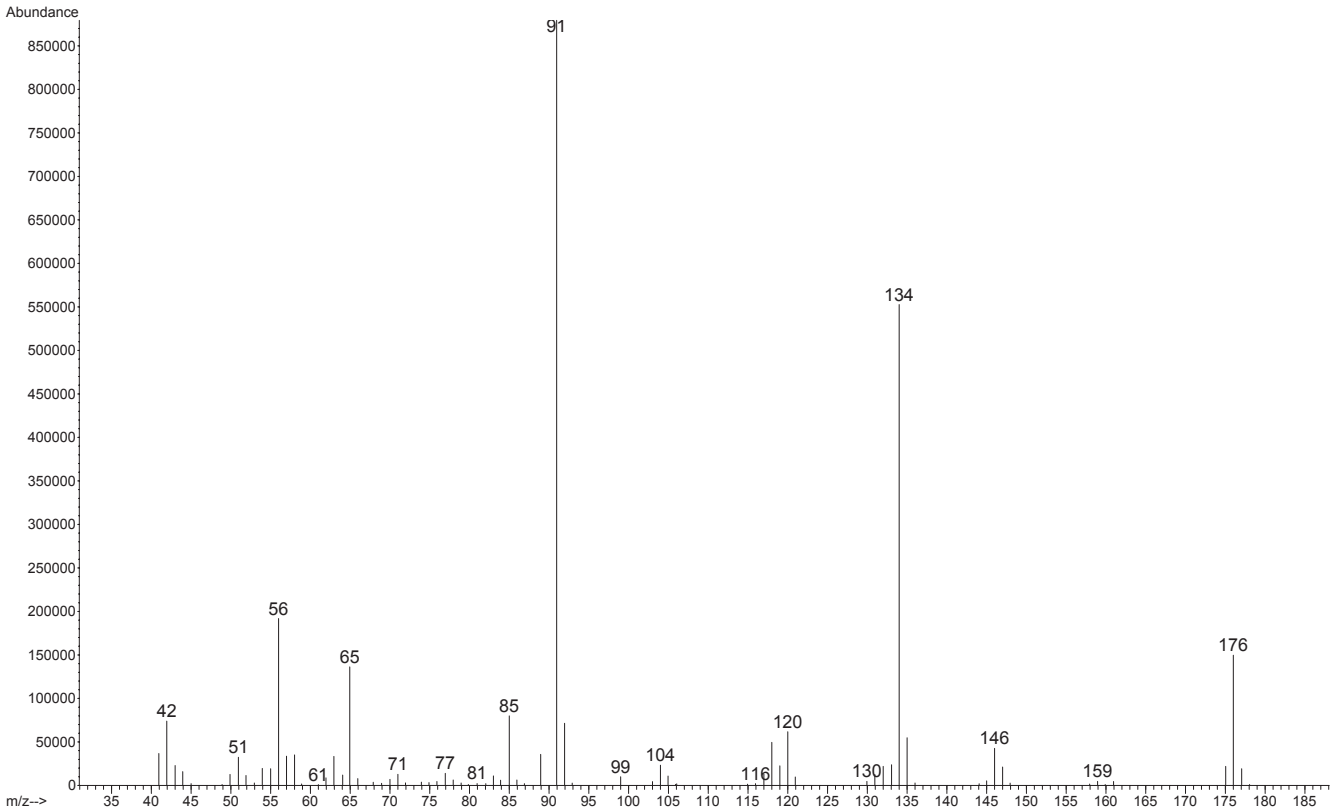
Benzylpiperazine

Chemical name:	1-benzylpiperazine	
Abbreviation:	BZP	
Molecular formula:	$C_{11}H_{16}N_2$	
Molecular mass:	176.258	
Major GC/MS ions:	91, 134, 56, 176, 65	
Ions used for analysis:	Target:	91
	Qualifier-1:	134
	Qualifier-2:	176
Retention time:	3.90 minutes	
LOD:	20 mcg/g	

Molecular Structure:



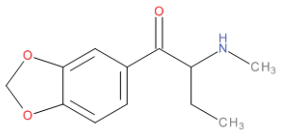
Mass Spectrum:



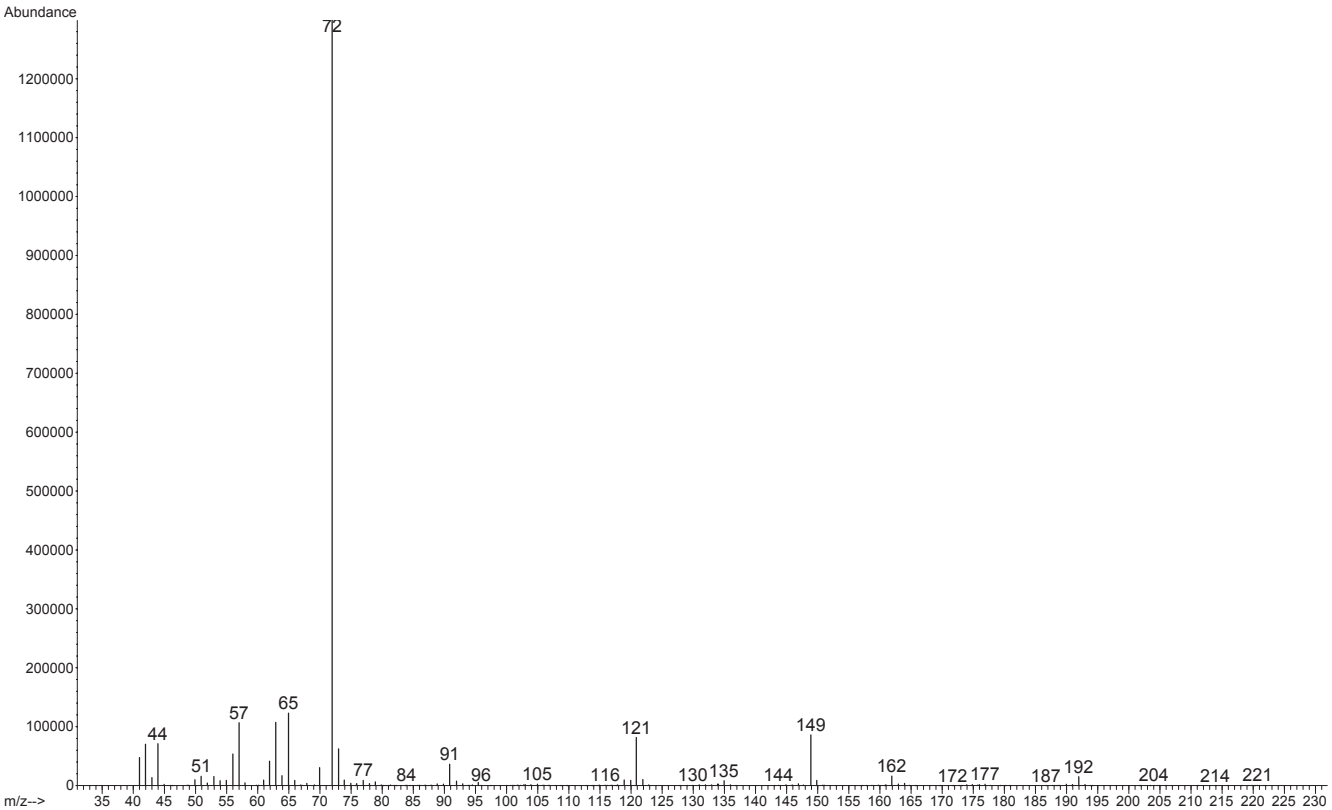
Butylone

Chemical name:	1-(1,3-benzodioxol-5-yl)-2-(methylamino)butan-1-one	
Abbreviation:	bk-MBDB	
Molecular formula:	$C_{12}H_{15}NO_3$	
Molecular mass:	221.2524	
Major GC/MS ions:	72, 65, 63, 57, 121	
Ions used for analysis:	Target:	72
	Qualifier-1:	121
	Qualifier-2:	57
Retention time:	5.05 minutes	
LOD:	20 mcg/g	

Molecular Structure:



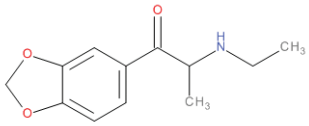
Mass Spectrum:



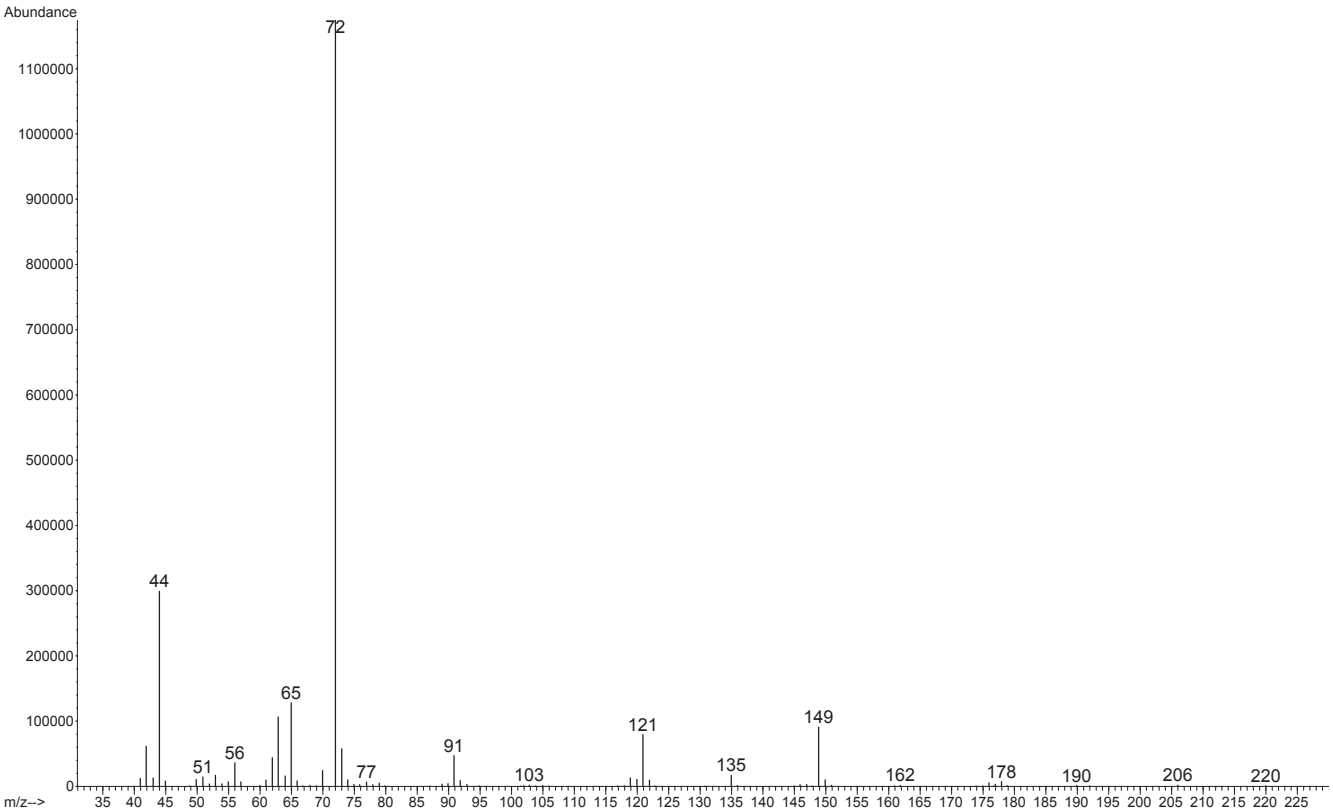
Ethylone

Chemical name:	(RS)-1-(1,3-benzodioxol-5-yl)-2-(ethylamino)propan-1-one	
Abbreviation:	bk-MDEA	
Molecular formula:	$C_{12}H_{15}NO_3$	
Molecular mass:	221.2524	
Major GC/MS ions:	72, 44, 65, 63, 149	
Ions used for analysis:	Target:	72
	Qualifier-1:	44
	Qualifier-2:	149
Retention time:	4.99 minutes	
LOD:	20 mcg/g	

Molecular Structure:



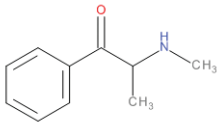
Mass Spectrum:



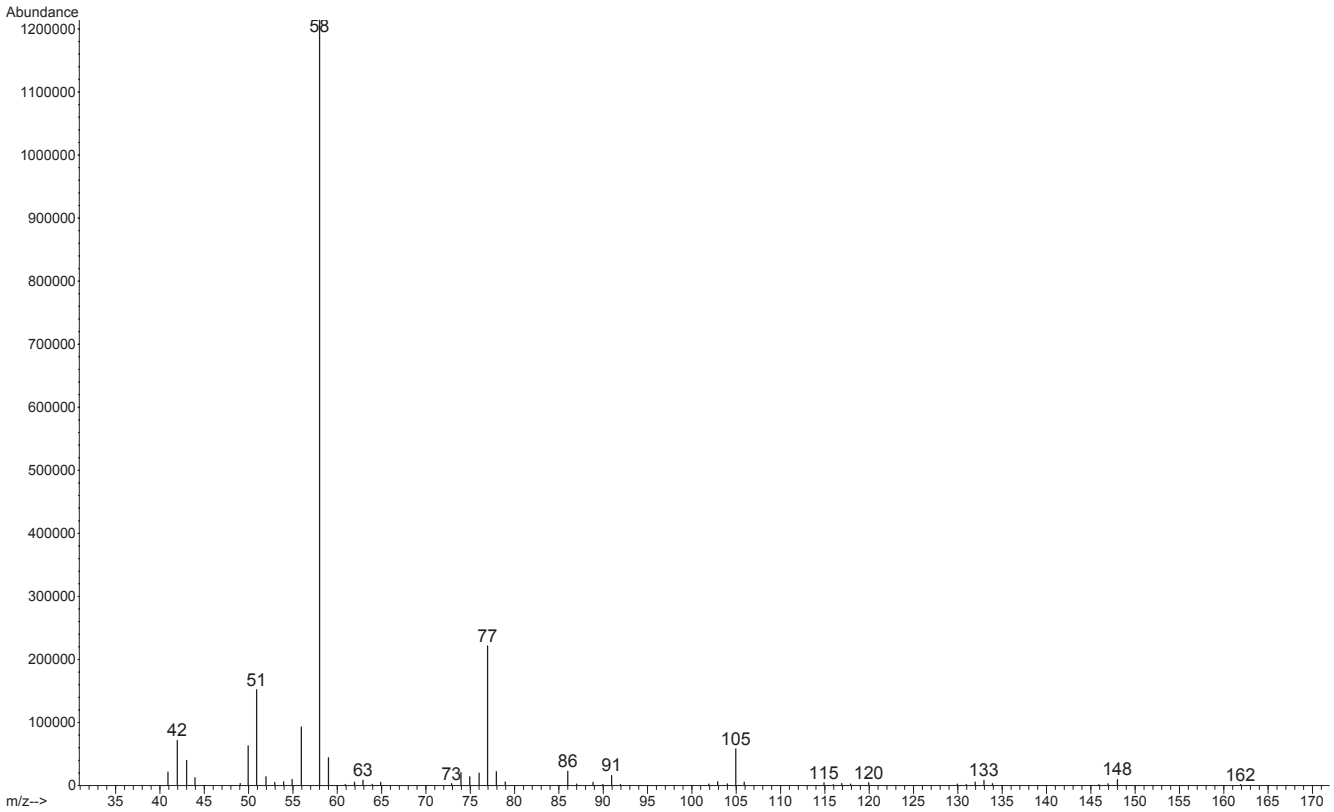
Methcathinone

Chemical name:	((RS)-2-(methylamino)-1-phenyl-propan-1-one	
Abbreviation:		
Molecular formula:	$C_{10}H_{13}NO$	
Molecular mass:	163.22	
Major GC/MS ions:	58, 77, 51, 56, 42	
Ions used for analysis:	Target:	58
	Qualifier-1:	77
	Qualifier-2:	105
Retention time:	3.19 minutes	
LOD:	20 mcg/g	

Molecular Structure:



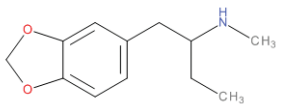
Mass Spectrum:



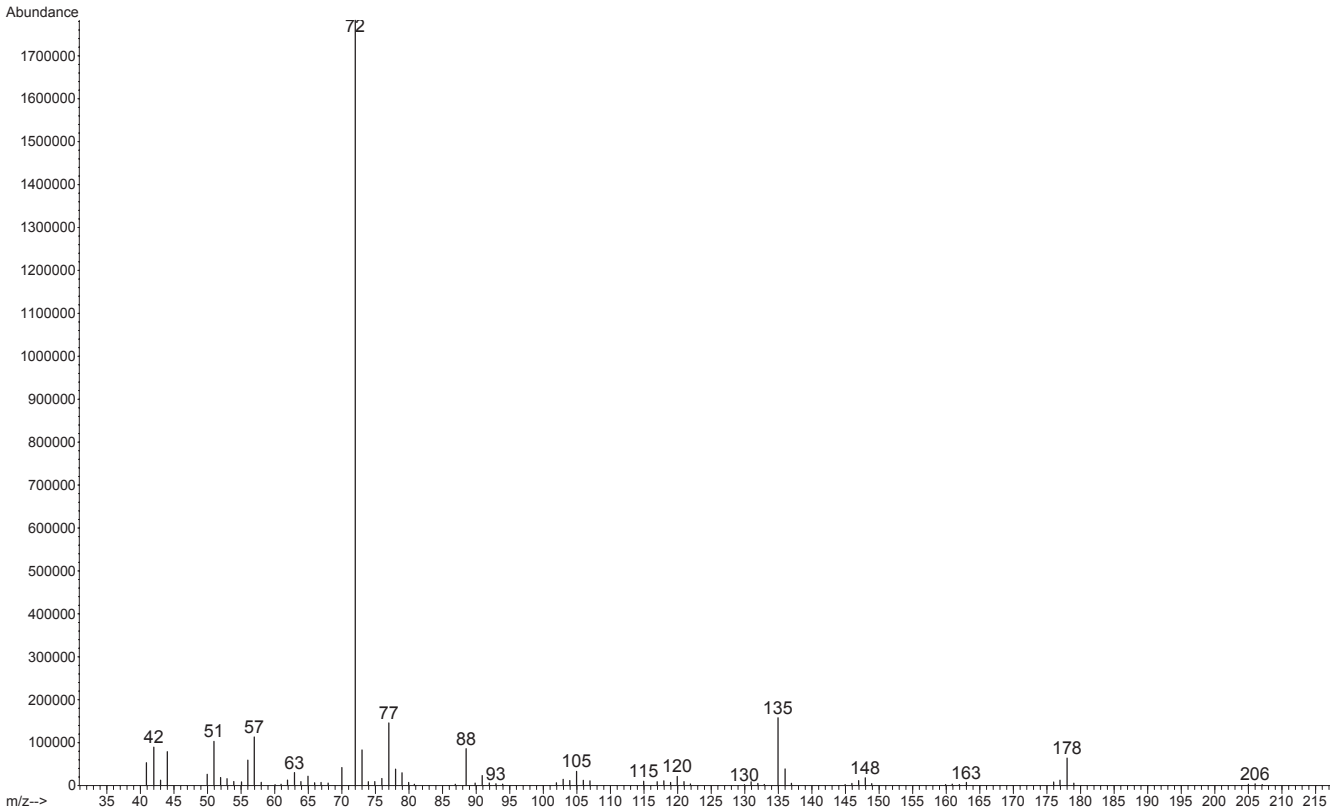
Methylbenzodioxolylbutanamine

Chemical name:	(RS)-1-(1,3-Benzodioxol-5-yl)-N-methylbutan-2-amine	
Abbreviation:	MBDB	
Molecular formula:	$C_{12}H_{17}NO_2$	
Molecular mass:	207.27	
Major GC/MS ions:	72, 135, 77, 57, 51	
Ions used for analysis:	Target:	72
	Qualifier-1:	135
	Qualifier-2:	57
Retention time:	4.47 minutes	
LOD:	20 mcg/g	

Molecular Structure:



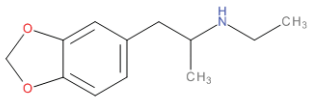
Mass Spectrum:



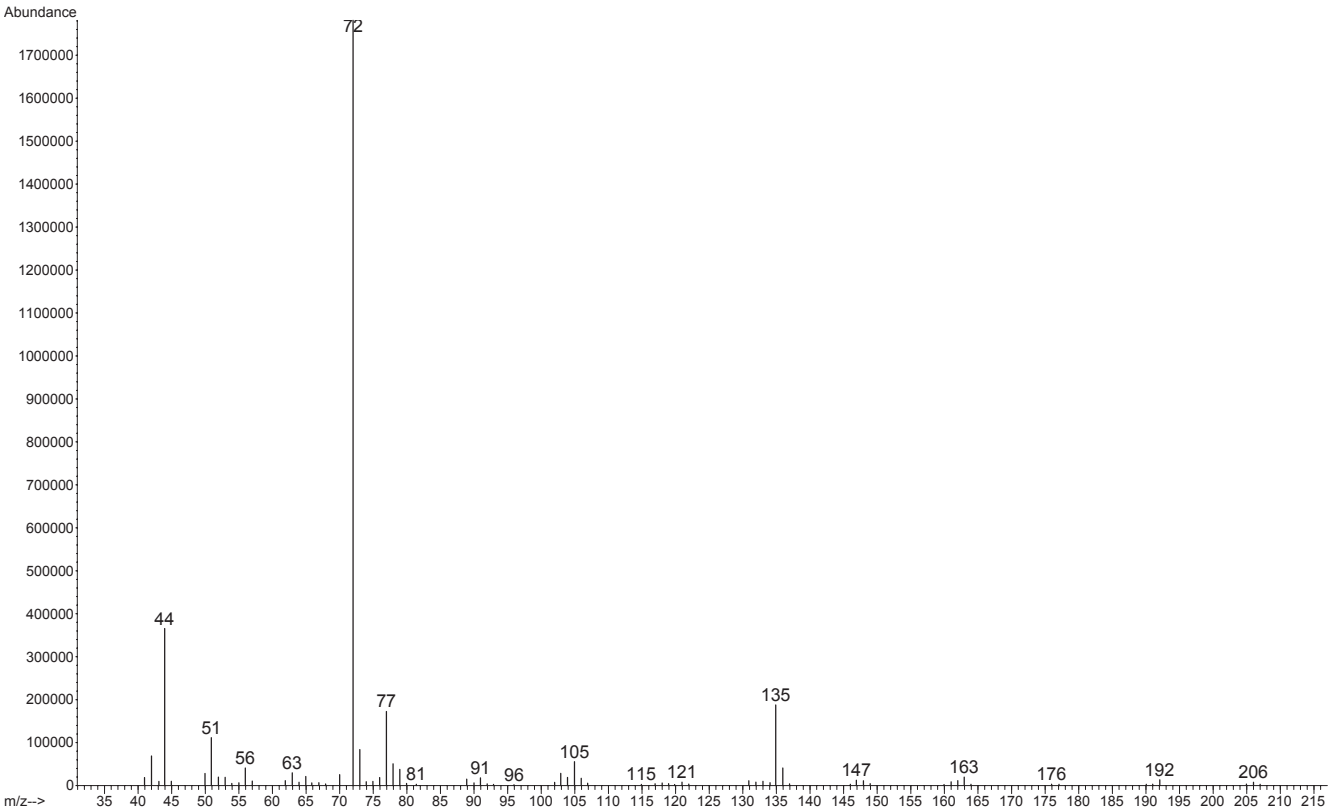
Methylenedioxyethylamphetamine

Chemical name:	1-(1,3-benzodioxol-5-yl)-N-ethyl-propan-2-amine	
Abbreviation:	MDEA	
Molecular formula:	$C_{12}H_{17}NO_2$	
Molecular mass:	207.27	
Major GC/MS ions:	72, 44, 135, 77, 51	
Ions used for analysis:	Target:	72
	Qualifier-1:	135
	Qualifier-2:	44
Retention time:	4.29 minutes	
LOD:	20 mcg/g	

Molecular Structure:



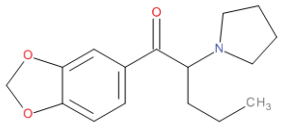
Mass Spectrum:



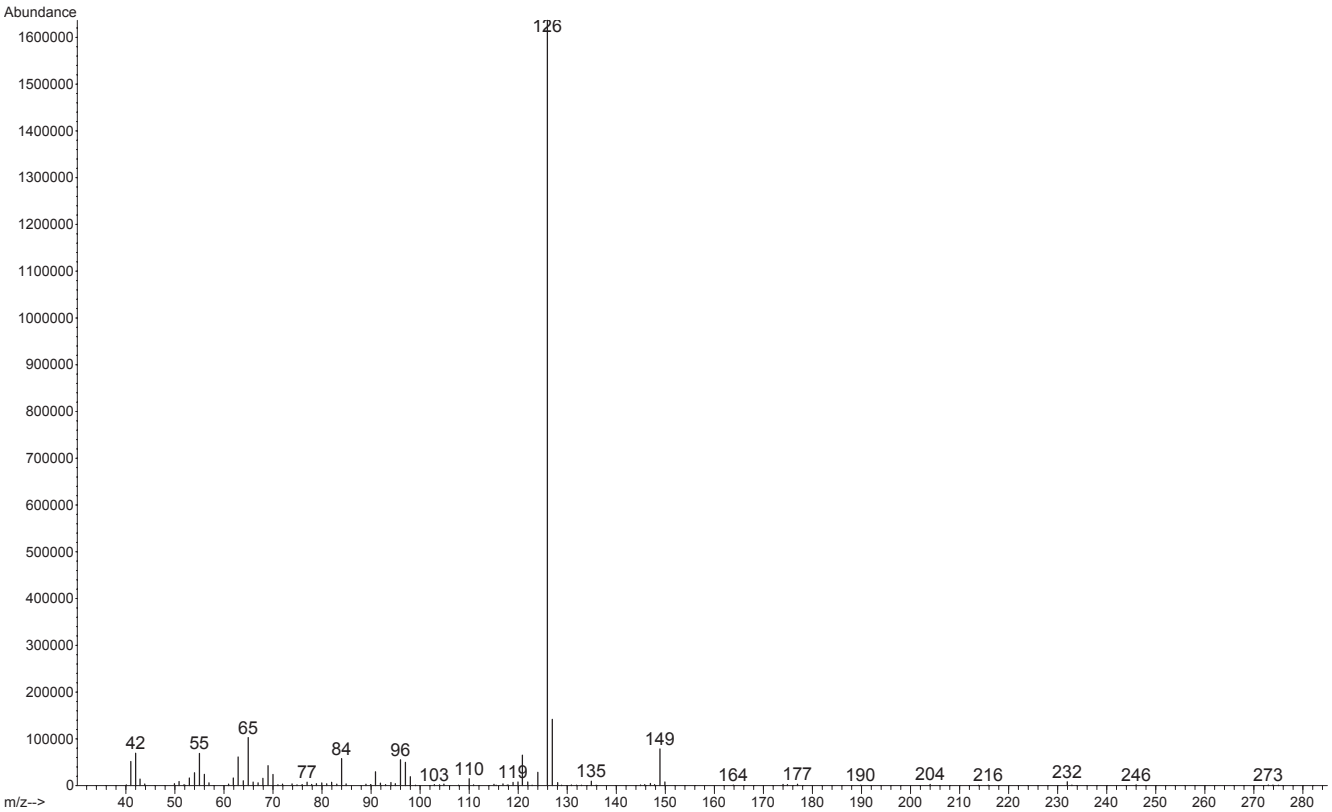
Methylenedioxypyrovalerone

Chemical name:	(RS)-1-(Benzo[d][1,3]dioxol-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one	
Abbreviation:	MDPV	
Molecular formula:	$C_{16}H_{21}NO_3$	
Molecular mass:	275.343	
Major GC/MS ions:	126, 127, 65, 149, 55	
Ions used for analysis:	Target:	126
	Qualifier-1:	65
	Qualifier-2:	149
Retention time:	6.34 minutes	
LOD:	20 mcg/g	

Molecular Structure:



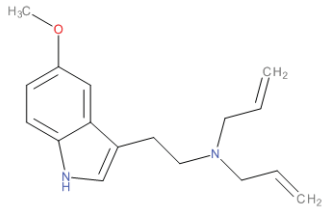
Mass Spectrum:



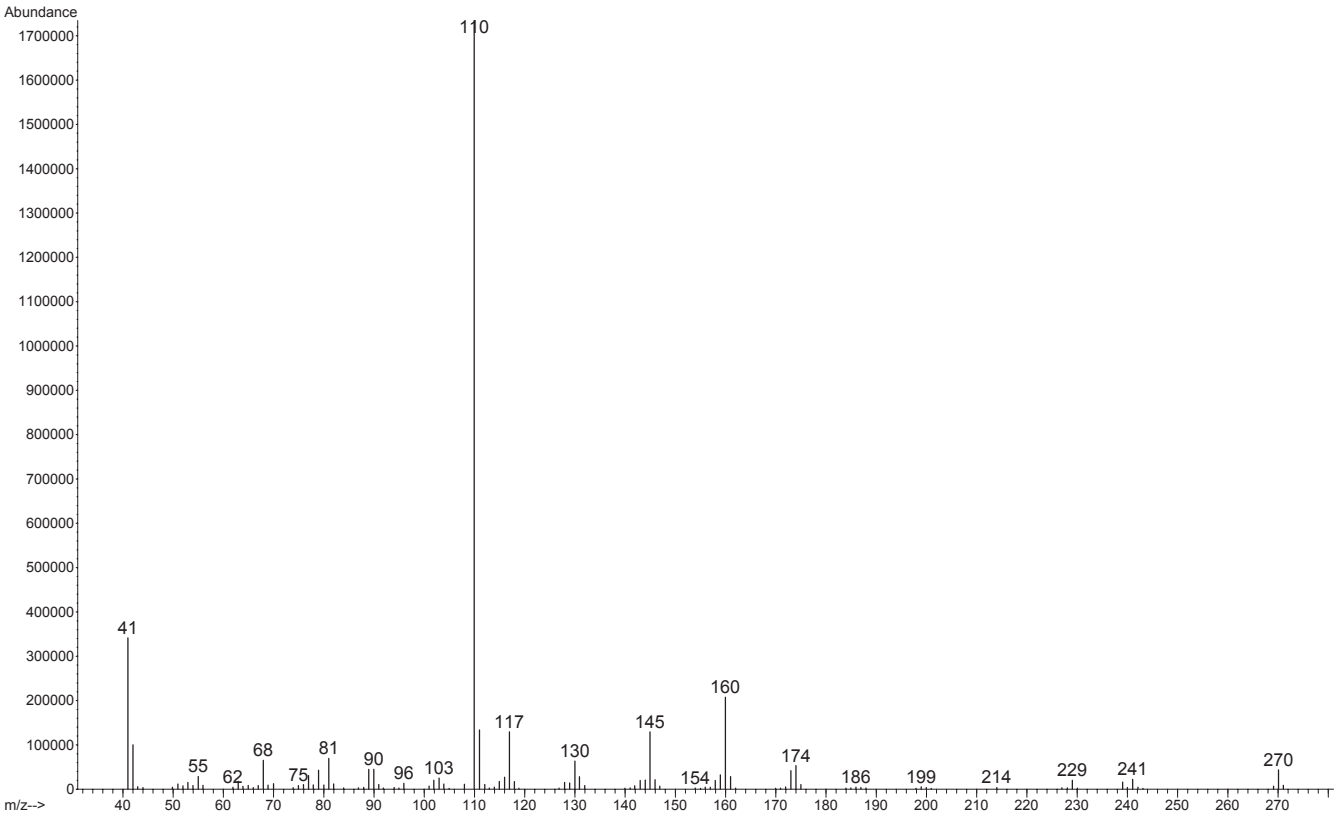
N,N-diallyl-5-methoxytryptamine

Chemical name:	N-allyl-N-[2-(5-methoxy-1H-indol-3-yl)ethyl]prop-2-en-1-amine	
Abbreviation:	5-MeO-Dalt	
Molecular formula:	$C_{17}H_{22}N_2O$	
Molecular mass:	270.375	
Major GC/MS ions:	110, 41, 160, 111, 117	
Ions used for analysis:	Target:	110
	Qualifier-1:	160
	Qualifier-2:	41
Retention time:	6.81 minutes	
LOD:	20 mcg/g	

Molecular Structure:



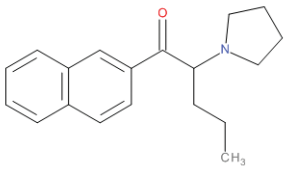
Mass Spectrum:



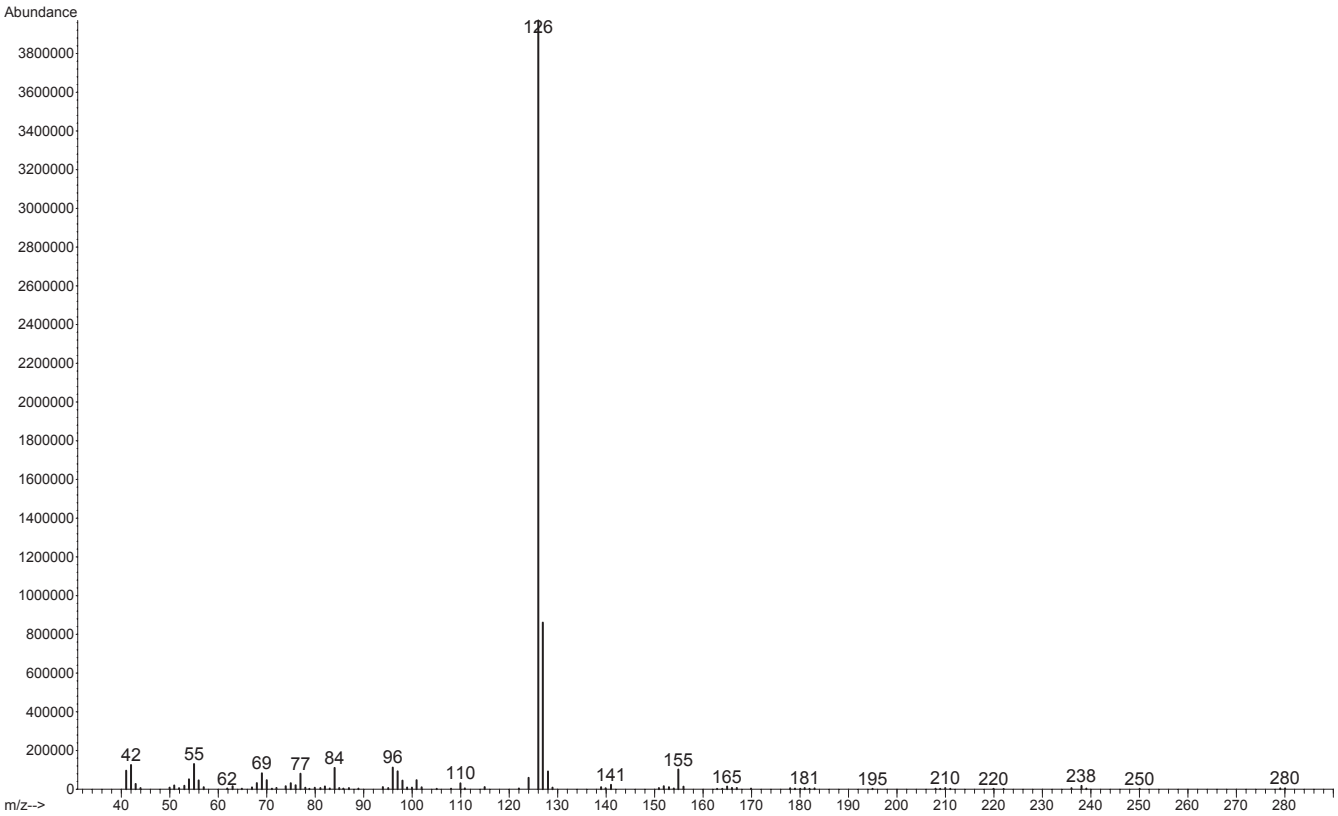
Naphyrone

Chemical name:	1-naphthalen-2-yl-2-pyrrolidin-1-ylpentan-1-one	
Abbreviation:	NRG-1	
Molecular formula:	$C_{19}H_{23}NO$	
Molecular mass:	281.391	
Major GC/MS ions:	126, 127, 55, 42, 96	
Ions used for analysis:	Target:	126
	Qualifier-1:	127
	Qualifier-2:	55
Retention time:	6.92 minutes	
LOD:	20 mcg/g	

Molecular Structure:



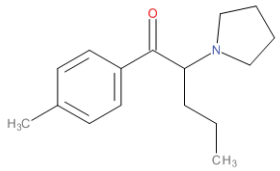
Mass Spectrum:



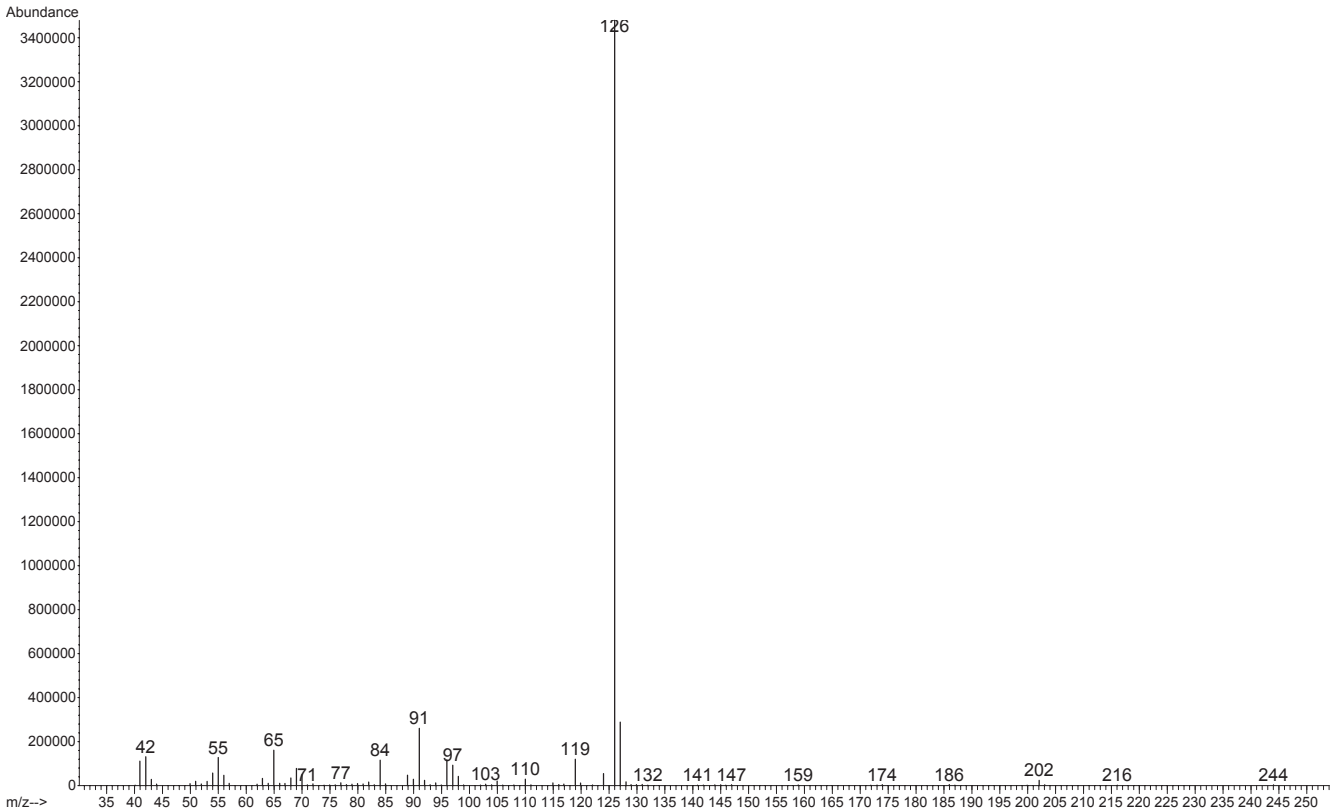
Pyrovalerone

Chemical name:	(RS)-1-(4-methylphenyl)-2-(1-pyrrolidinyl)pentan-1-one	
Abbreviation:		
Molecular formula:	$C_{16}H_{23}NO$	
Molecular mass:	245.36	
Major GC/MS ions:	126, 127, 91, 65, 55	
Ions used for analysis:	Target:	126
	Qualifier-1:	91
	Qualifier-2:	65
Retention time:	5.49 minutes	
LOD:	20 mcg/g	

Molecular Structure:



Mass Spectrum:

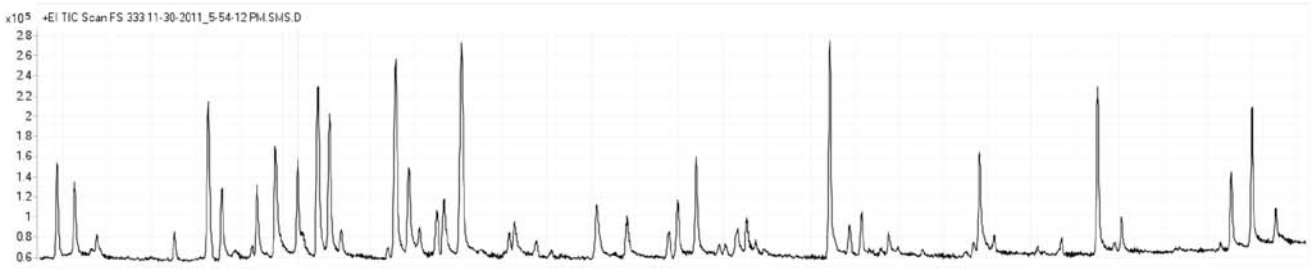


Bath Salts Analysis

Introduction

Spectra obtained for all bath salts on the Agilent 240 Ion Trap GC/MS are comparable to spectra generated on the Agilent 5973 GC/MSD. The bath salts Designer Drugs Library created using spectra from the Agilent 5973 GC/MSD were used to accurately identify all analytes of interest in this study. Chromatograms and spectra obtained on the Agilent Technologies 240 Ion Trap GC/MS were seamlessly interpreted using Agilent's MassHunter Workstation Software for qualitative and quantitative analysis. LOD for most analytes of interest was 1ppb in Full Scan mode. Whether you want to analyze bath salts by Quadruple or Ion Trap GC/MS, Agilent Technologies has the solution to your laboratory's cutting-edge and complex forensic problems.

Bath Salts Analysis



Full Scan Total Ion Chromatogram of Bath Salts Mixture (100ppb in MeoH) on the Agilent 240 Ion Trap GC/MS

Bath Salt Analyte	R.T. (min)	Bath Salt Analyte	R.T. (min)
1: 4-Fluoromethcathinone	6.935	16: 3,4-methylenedioxymethcathinone	13.064
2: Methcathinone	7.135	17: 2,5-Dimethoxy-4-chloroamphetamine	13.412
3: 3,4-Dimethylmethcathinone	8.272	18: Ethylone	13.986
4: 4-Methylmethcathinone	8.804	19: Butylone	14.198
5: Methylenedioxyamphetamine (MDA)	9.208	20: 4-Bromo-2,5-dimethoxyphenethylamine	14.647
6: Benzylpiperazine (BZP)	9.418	21: 2,5-Dimethoxy-4-bromoamphetamine	14.773
7: 4-Methyl-N-ethylcathinone	9.671	22: Methylenedioxypyrovalerone (MDPV)	15.715
8: 3-Trifluoromethylphenylpiperazine (TFMPP)	9.899	23: 2,5-Dimethoxy-4-iodophenethylamine	16.081
9: Methylenedioxymethamphetamine (MDMA)	10.03	24: 2,5-Dimethoxy-4-ethylthiophenethylamine	16.383
10: Methylenedioxyethylamphetamine (MDEA)	10.776	25: 2,5-Dimethoxy-4-propylthiophenethylamine	17.35
11: Benzodioxolylbutanamine	10.934	26: 5-Methoxy-dimethyltryptamine	17.416
12: 2,5-Dimethoxy-4-methylamphetamine	11.331	27: Methylenedioxypyrovalerone (MDPV)	18.76
13: 4-Methoxymethcathinone	11.521	28: Benzylpiperazine (BZP)	19.033
14: Methylbenzodioxolylbutanamine	11.531	29: N,N-diallyl-5-methoxytryptamine	20.278
15: 2,5-Dimethoxy-4-ethylphenethylamine	12.132	30: Naphyrone	20.513

Bath Salts Analysis

Baths Salts Anlysis: Agilent 240 Ion Trap MS Conditions:

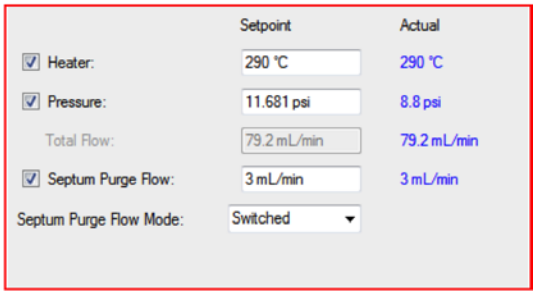
Scan type:	Full Scan
Ionization:	EI
Scan Mode:	Fast
uScan Averaged:	1uScans
Count Threshold:	1
Target TIC:	40000 Counts
Emission Current:	10uAmps
Mass Range:	43 – 350 m/z
Tune Type:	Auto
Solvent Delay:	3 min
Trap Temperature:	200 °C
Manifold Temperature:	100 °C

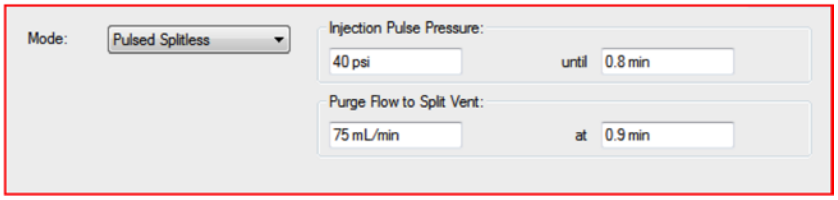
Bath Salts Analysis: Agilent 7890A GC Conditions:

Column:	Agilent J&W Factor Four VF-5ms 30m x 0.250mm x 0.25um (p/n: CP8944)
Carrier gas:	Helium, 1.2mL/min, Constant Flow
Oven:	Temperature Programmed

	Rate °C/min	Value °C	Hold Time min	Run Time min
(Initial)		80	0	0
Ramp 1	10	150	0	7
Ramp 2	5	180	0	13
Ramp 3	10	300	0	25

Inlet: Multi Mode Inlet, 1.0uL injection volume





Inlet Liner:	2 mm Dimpled Deactivated Liner (Part No 5190-2296)
MS Transfer Line:	300 °C

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