

# IDENTIFICATION OF SYNTHETIC CANNABINOIDS IN HERBAL INCENSE BLENDS BY GC/MS

Application Compendium

The Measure of Confidence



Agilent Technologies



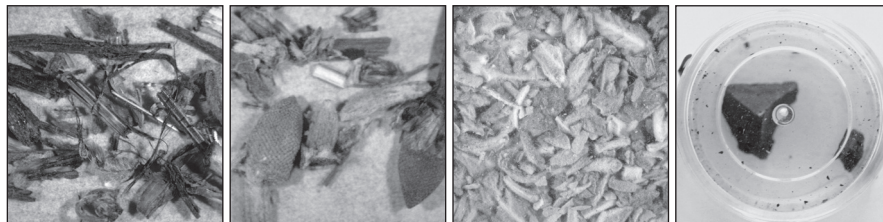
# Table of Contents

Introduction.....	3
Sample Preparation.....	4
Gas Chromatograph and Mass Spectrometer Conditions.....	5
GC/MS Total Ion Chromatogram of the Synthetic Cannabinoids Evaluated.....	6
JWH-007.....	7
JWH-015.....	8
JWH-018.....	9
JWH-018 1-methylhexyl homolog.....	10
JWH-018 6-methoxyindole analog.....	11
JWH-019.....	12
JWH-073.....	13
JWH-073 2-methylbutyl homolog.....	14
JWH-081.....	15
JWH-098.....	16
JWH-122.....	17
JWH-133.....	18
JWH-200.....	19
JWH-201.....	20
JWH-203.....	21
JWH-210.....	22
JWH-250.....	23
JWH-251.....	24
JWH-302.....	25
JWH-398.....	26
HU-210.....	27
HU-210-di-TMS derivative.....	28
HU-211.....	29
HU-211-di-TMS derivative.....	30
HU-308.....	31
HU-308-mono-TMS derivative.....	32
HU-331.....	33
HU-331-tri-TMS derivative.....	34
CB-25.....	35
CB-25-di-TMS derivative.....	36
CB-52.....	37
CB-52-di-TMS derivative.....	38
CP47,497 (C7 analog).....	39
CP47,497 (C7 analog)-di-TMS derivative.....	40
CP47,497 (C8 analog).....	41
CP47,497 (C8 analog)-di-TMS derivative.....	42
CP55,940.....	43
CP55,940-tri-TMS derivative.....	44
AM-694.....	45
AM-2201.....	46
RCS-4.....	47
RCS-8.....	48
WIN55,212-2.....	49
WIN55-212-3.....	50



# Identification of Synthetic Cannabinoids in Herbal Incense Blends by GC/MS

## Application Compendium



## Introduction

By Fran Diamond, Chemistry Technical Leader, NMS Labs

The recent phenomenon of synthetic cannabinoid usage has given law enforcement and testing laboratories a series of challenges to overcome in order to provide testing of these new materials. These emerging substances are being manufactured and distributed worldwide, but few legitimate certified synthetic laboratories have been able to keep up with numerous analogous and homologous materials that are used. Analytical laboratories have had a difficult time obtaining pure reference material to use for positive identification. The sheer number of different chemicals has also thwarted the attempts of law-enforcement to crack down on the distribution and use. These are legal drugs. As soon as legislation is passed banning their use, different drugs show up in the next wave. These chemicals have different function group chemistry that dictates a sample extraction procedure that will capture the various chemical functionalities. Some of these new compounds are extremely potent in terms of dosage so that they may only be present at trace levels. This necessitates the ability to analyze the complex chromatographic data in the presence of large amounts of co-extractant material. These materials are also structurally similar in terms of chromatographic retention time and mass spectral appearance. Data analysis needs to be able to identify the subtle differences in these species and be able to detect these substances in complex mixtures.

Test development and validation was completed at the Criminalistics division of NMS labs. For 40 years, NMS Labs has been setting the standard for excellence in forensic testing with state-of-the-art tests that other labs don't or can't provide. A national reference laboratory, NMS Labs is unsurpassed in its scope of tests, accuracy of results, client service, scientific expertise, and innovation.

# Sample Preparation

## Homogenization

These synthetic cannabinoid preparations are produced by preparing a solution of the pure chemical in acetone. Next, this acetone solution is sprayed onto the botanical matrix. The botanical material is then air-dried, and is soft and light. These properties make it difficult to crush into a homogeneous material to allow for proper representative sampling. We tested numerous methods such as crushing in a mortar and pestle, an herb grinder, and even electrical grinders and mills. These procedures did not produce acceptable results. We finally developed a method of grinding by applying approximately 500 mg of material between two 5 in. x 5in. sheets of sandpaper (grit#100) and rubbing the two sheets together until a finely divided powder was obtained.

## Extraction

The chemicals in this class contain various functional groups that require we use a generalized method of extraction. We have used two basic strategies: an acid/base combined extraction and a simple methanol incubation followed by centrifugation. In the acid/base extraction, we acidify an aliquot of sample (between 50 and 100 mg of ground material) by adding 1 mL of de-ionized water followed by the addition of 3 drops of 10% HCl. We next add 1 mL of solvent extraction (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. Tubes are again mixed and centrifuged, and the lower solvent layer is 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.

## Derivatization

Some of the chemicals used in production contain active, polar functional groups such as alcohols, phenols, amides and ketones that negatively impact the GC/MS analysis in their native form. To enhance sensitivity and detectability, we will employ a derivatization procedure to shield these polar groups.

We employ the use of BSTFA with 1% TMCS. The procedure is performed as follows: The above mentioned extracts are evaporated to dryness at room temperature under a gentle stream of nitrogen. It is crucial that these extracts are completely dry and free from residual water or alcohol as this will neutralize the derivatizing agent. Next, 50  $\mu$ L of SELECTRA-SIL® (BSTFA with 1% TMCS) was added and the tube capped. Tube is incubated at 70 °C for thirty minutes. Upon cooling, the derivatized mixture is transferred to an autosampler vial with a 200  $\mu$ L insert, capped, and sealed. Samples are now ready for instrumental analysis.

# Gas Chromatograph and Mass Spectrometer Conditions

## GC

Agilent technologies 6890 with fast oven, Autoinjector and tray

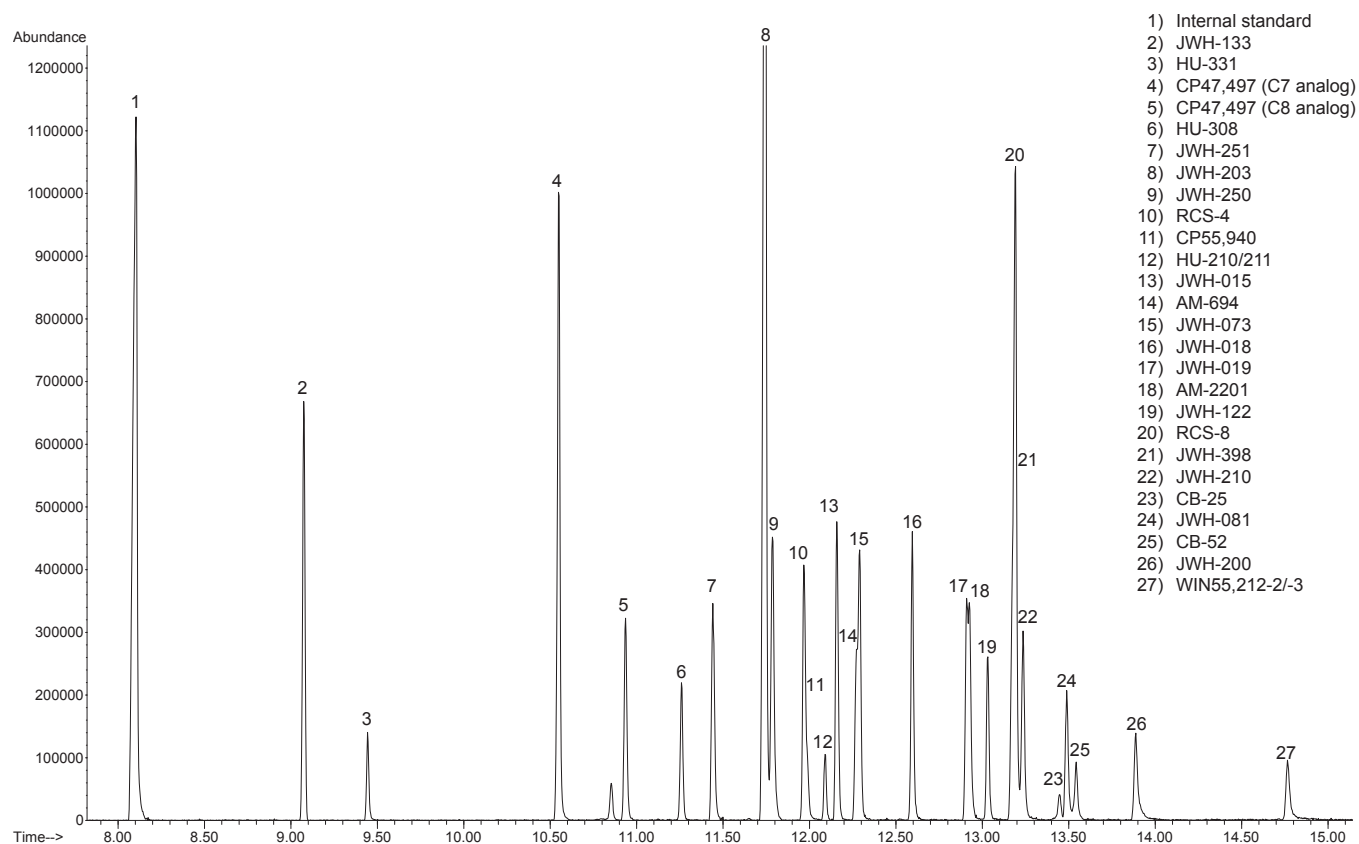
<b>Inlet</b>	EPC Split/splitless
Mode	Constant pressure
Injection type	Splitless
Injection volume (uL)	1.0
Inlet temperature (°C)	265
Pressure nominal (psig)	20.70
Purge flow (ml/min.)	50
Purge time (min.)	0.30
Gas type	Helium

<b>Oven</b>	
Voltage (VAC)	240
Initial Oven Temp. (°C)	50
Initial oven hold (min.)	0
Ramp rate (°C/min.)	20
Final Temp. (°C)	340
Final hold (min.)	2.0
Total Run Time (min.)	16.50
Equilibration time (min.)	0.1

<b>Column</b>	
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

<b>MSD</b>	
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)	620
Threshold	250
Sampling	1
Quad temp (°C)	150
Source temp (°C)	230
Transfer line temp (°C)	300

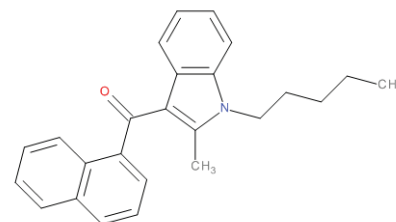
# GC/MS Total Ion Chromatogram of the Synthetic Cannabinoids Evaluated



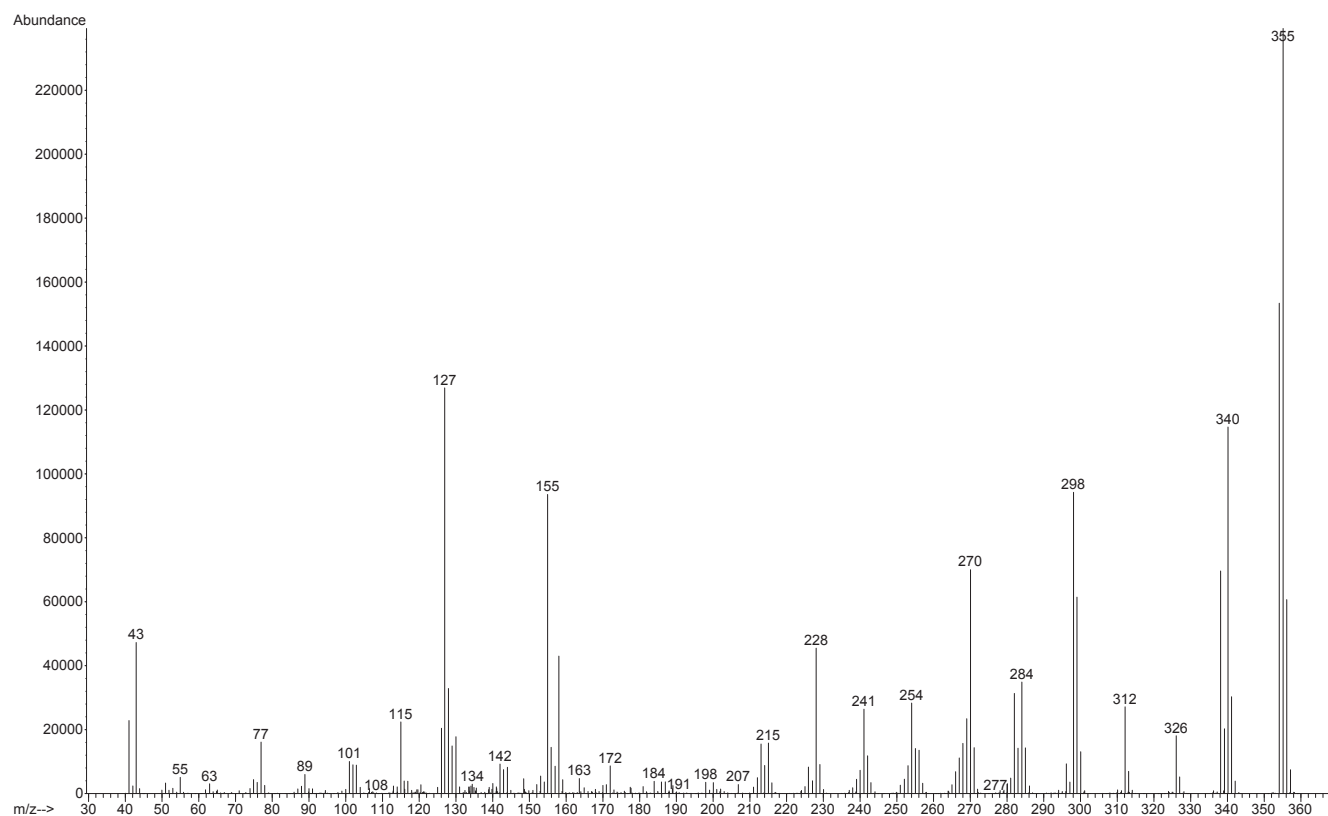
# JWH-007

Chemical name	1-pentyl-2-methyl-3-(1-naphthoyl)indole	
Molecular formula	C <sub>25</sub> H <sub>25</sub> NO	
Molecular mass	355.471	
Major GC/MS ions	355.2, 354.2, 127.0, 340.1, 298.1	
Ions used for analysis	Target	355
	Qualifier-1	340
	Qualifier-2	127
Retention time	12.97 minutes	
LOD	Not yet established	

## Molecular Structure:



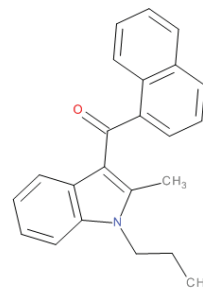
## Mass Spectrum:



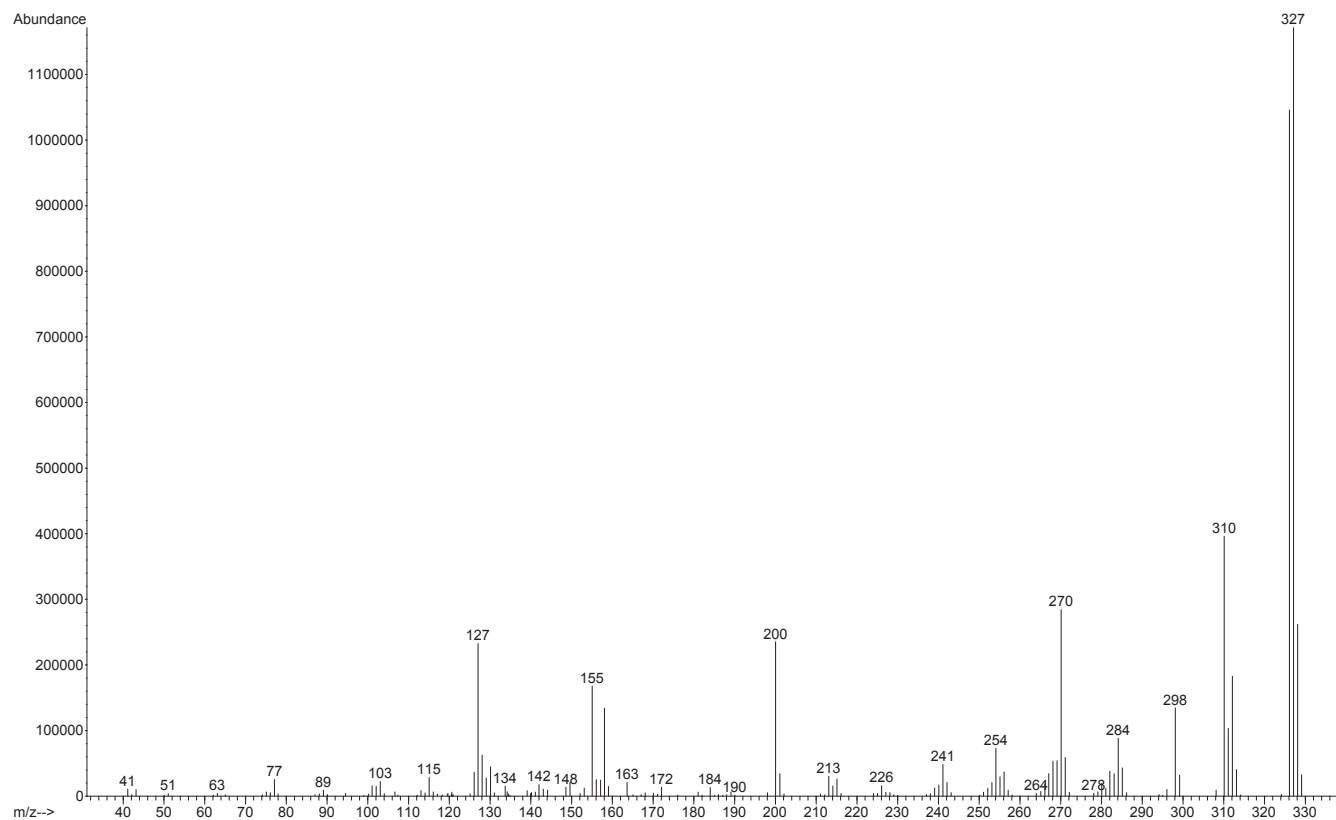
# JWH-015

Chemical name	(2-Methyl-1-propyl-1H-indol-3-yl)-1-naphthalenylmethanone	
Molecular formula	C <sub>23</sub> H <sub>21</sub> NO	
Molecular mass	327.16	
Major GC/MS ions	327.3, 326.3, 310.3, 270.2, 200.2, 127.1	
Ions used for analysis	Target	327.3
	Qualifier-1	310.3
	Qualifier-2	270.2
Retention time	12.62 minutes	
LOD	Not yet established	
Additional comments	JWH-015 does not derivatize. JWH-015 and JWH-073 are formula isomers. They have similar fragmentation patterns with slight differences in retention time.	

## Molecular Structure:



## Mass Spectrum:

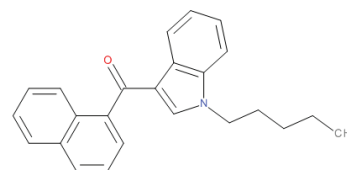




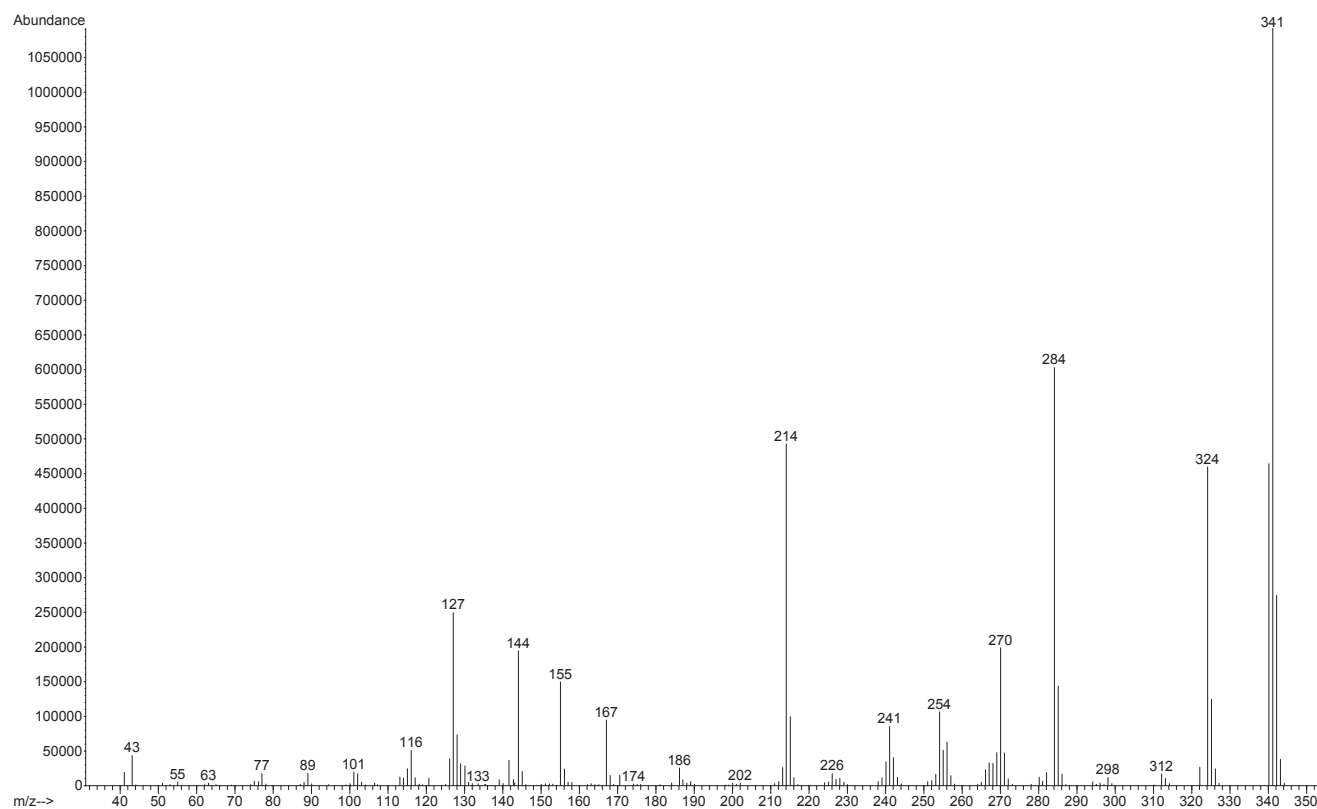
# JWH-018

Chemical name	Naphthalen-1-yl-(1-pentylindol-3-yl)methanone	
Molecular formula	C <sub>24</sub> H <sub>23</sub> NO	
Molecular mass	341.18	
Major GC/MS ions	341.3, 324.3, 284.2, 270.2, 214.2, 127.1	
Ions used for analysis	Target	341.3
	Qualifier-1	324.3
	Qualifier-2	284.2
Retention time	13.05 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-018 will not derivatize	

## Molecular Structure:



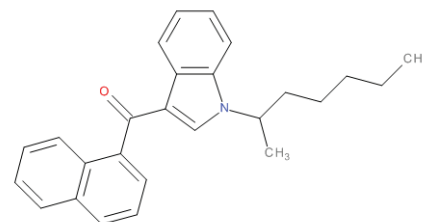
## Mass Spectrum:



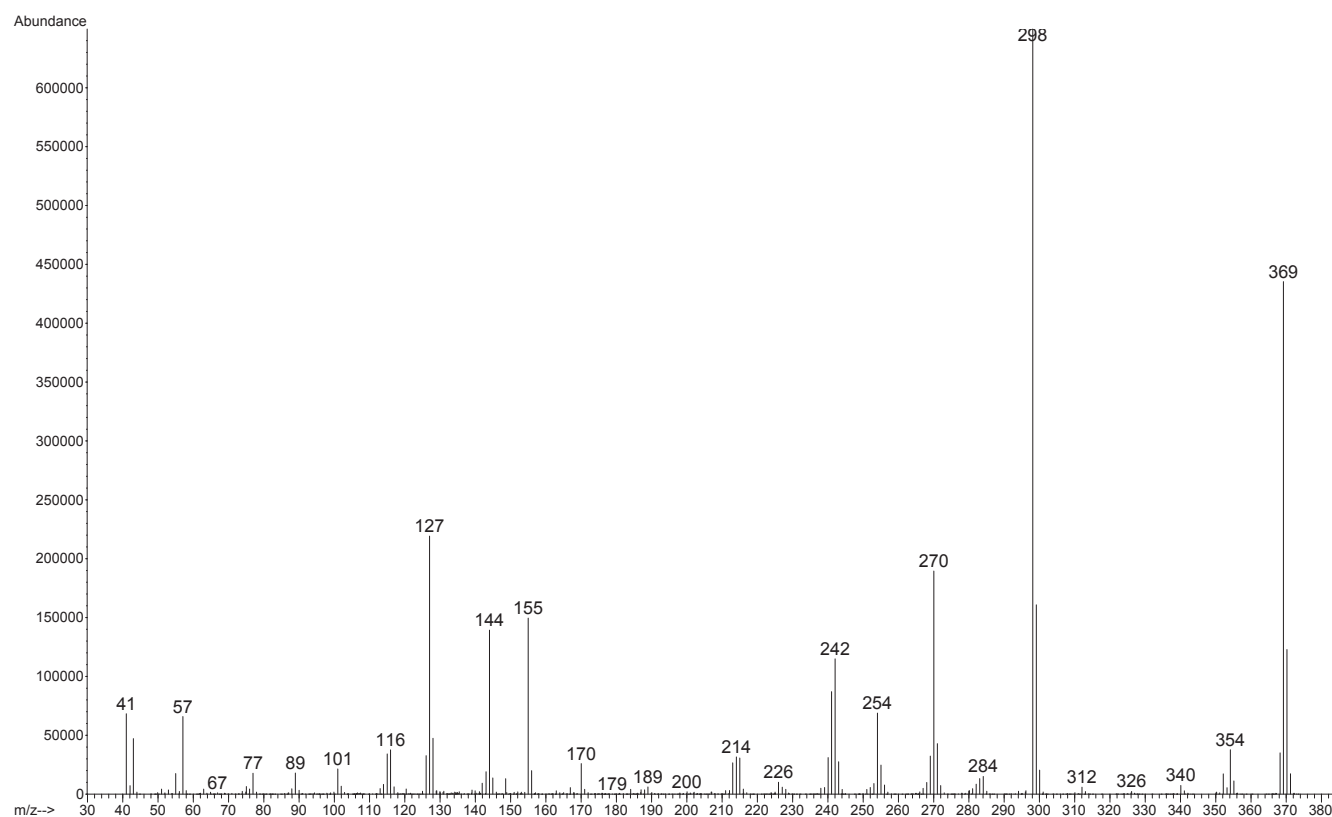
# JWH-018 1-methylhexyl homolog

Chemical name	(1-(Heptan-2-yl)-1H-indol-3-yl)(naphthalen-1-yl)methanone (racemate)	
Molecular formula	$C_{26}H_{27}NO$	
Molecular mass	369.50	
Major GC/MS ions	298.1, 369.2, 127.0, 270.1, 299.1	
Ions used for analysis	Target	298
	Qualifier-1	369
	Qualifier-2	127
Retention time	12.94 minutes	
LOD	Not yet established	

## Molecular Structure:



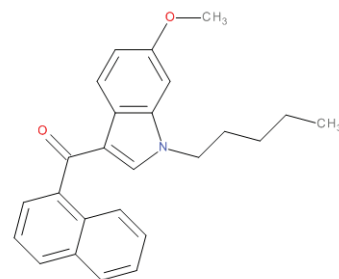
## Mass Spectrum:



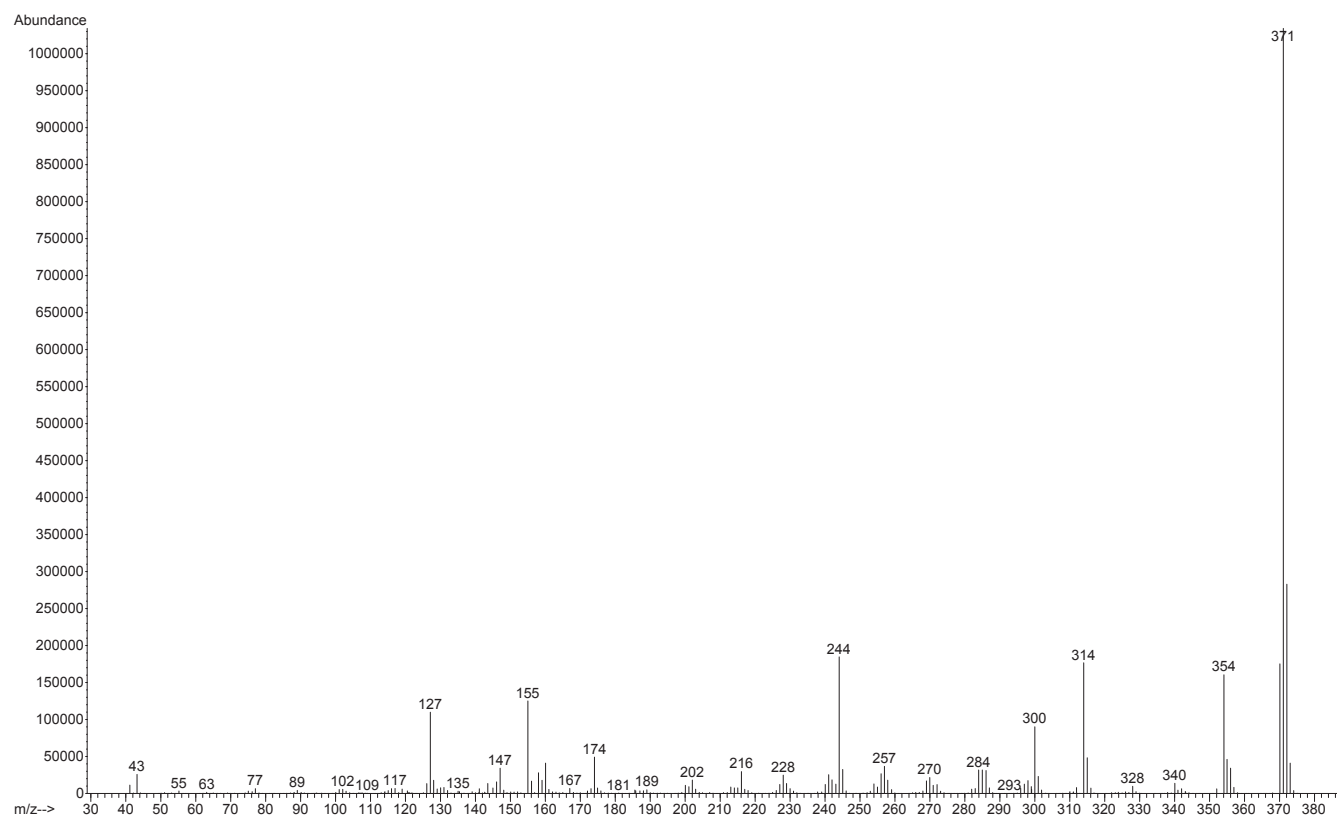
# JWH-018 6-methoxyindole analog

Chemical name	(6-methoxy-1-pentyl-1H-indol-3-yl)(naphthalen-1-yl)-methanone	
Molecular formula	$C_{25}H_{25}NO_2$	
Molecular mass	371.5	
Major GC/MS ions	371.1, 372.1, 244.1, 370.1, 314.0	
Ions used for analysis	Target	371
	Qualifier-1	244
	Qualifier-2	314
Retention time	13.68 minutes	
LOD	Not yet established	

## Molecular Structure:



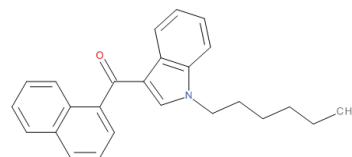
## Mass Spectrum:



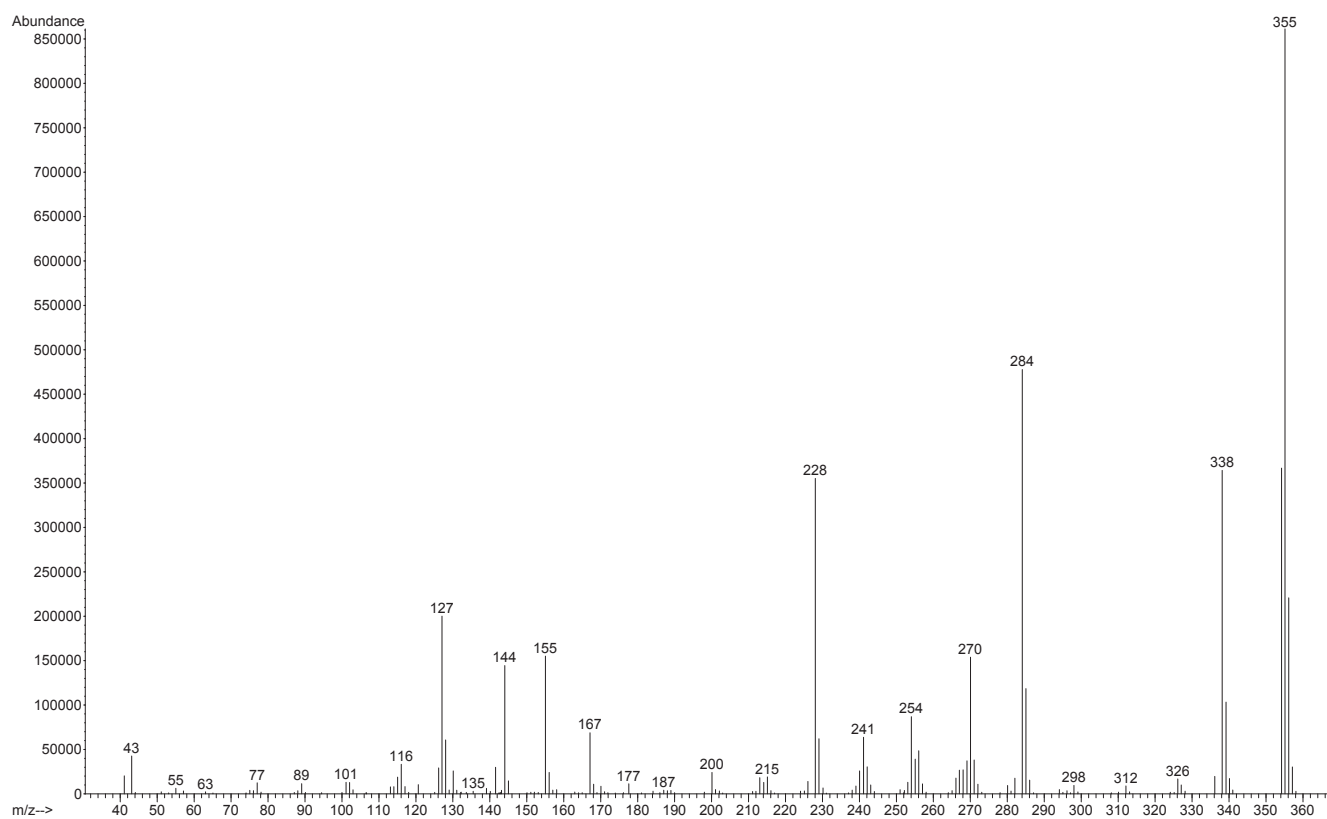
# JWH-019

Chemical name	Naphthalen-1-yl-(1-pentylindol-3-yl)methanone	
Molecular formula	C <sub>25</sub> H <sub>25</sub> NO	
Molecular mass	355.19	
Major GC/MS ions	355.3, 338.3, 284.2, 228.2, 127.1, 155.1	
Ions used for analysis	Target	355.3
	Qualifier-1	284.2
	Qualifier-2	338.3
Retention time	13.37 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-019 will not derivatize. JWH-019 is a formula isomer of JWH-122 and has similar fragmentation pattern with only a slight difference in retention time.	

## Molecular Structure:



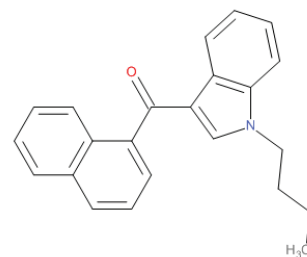
## Mass Spectrum:



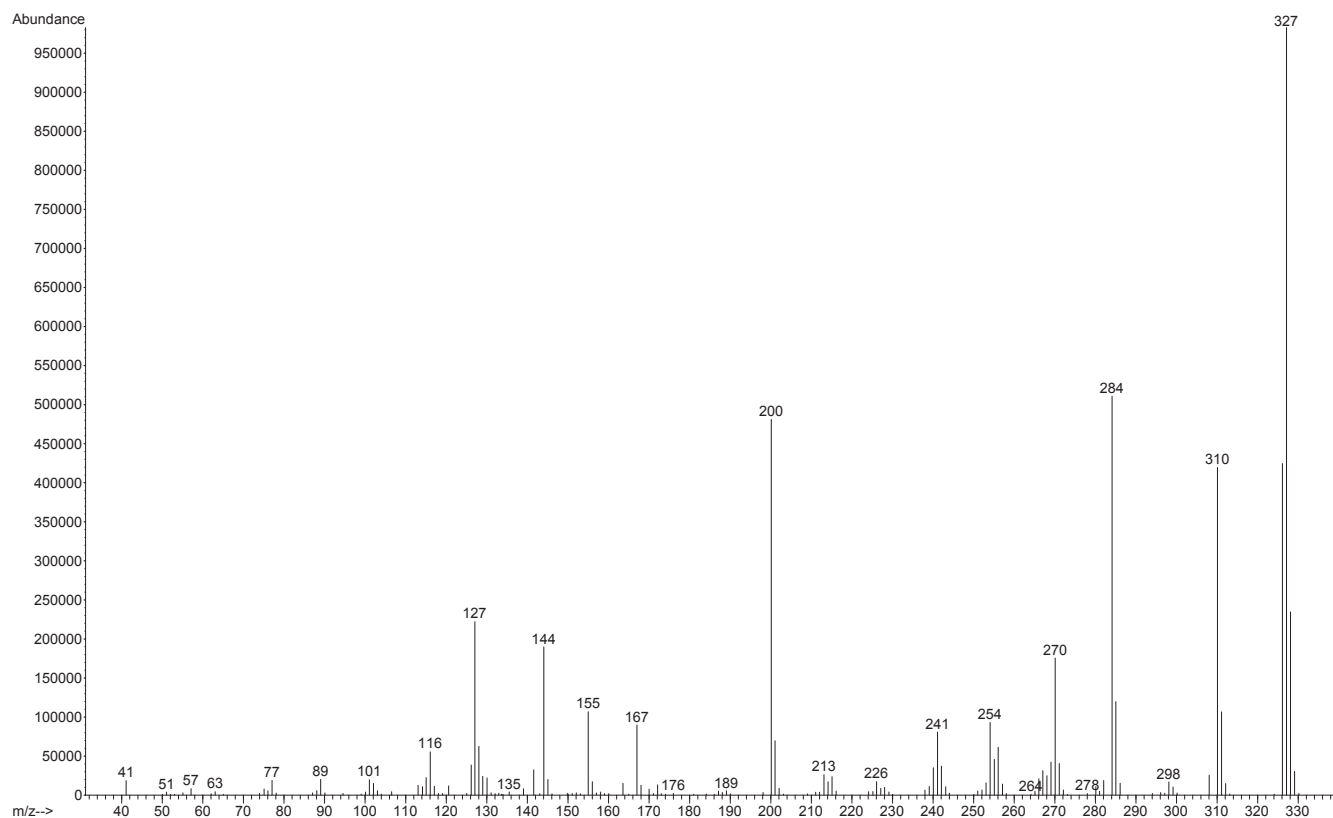
# JWH-073

Chemical name	naphthalen-1-yl-(1-butylindol-3-yl)meth	
Molecular formula	C <sub>23</sub> H <sub>21</sub> NO	
Molecular mass	327.16	
Major GC/MS ions	327.3, 310.3, 284.2, 200.2, 127.1, 144.1	
Ions used for analysis	Target	327.3
	Qualifier-1	310.3
	Qualifier-2	284.2
Retention time	12.75 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-073 does not derivatize. JWH-073 is a structural isomer of JWH-015 with similar fragmentation and a slight difference in retention time.	

## Molecular Structure:



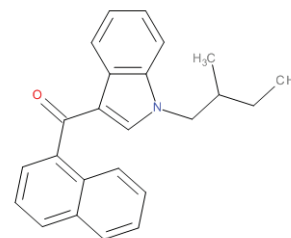
## Mass Spectrum:



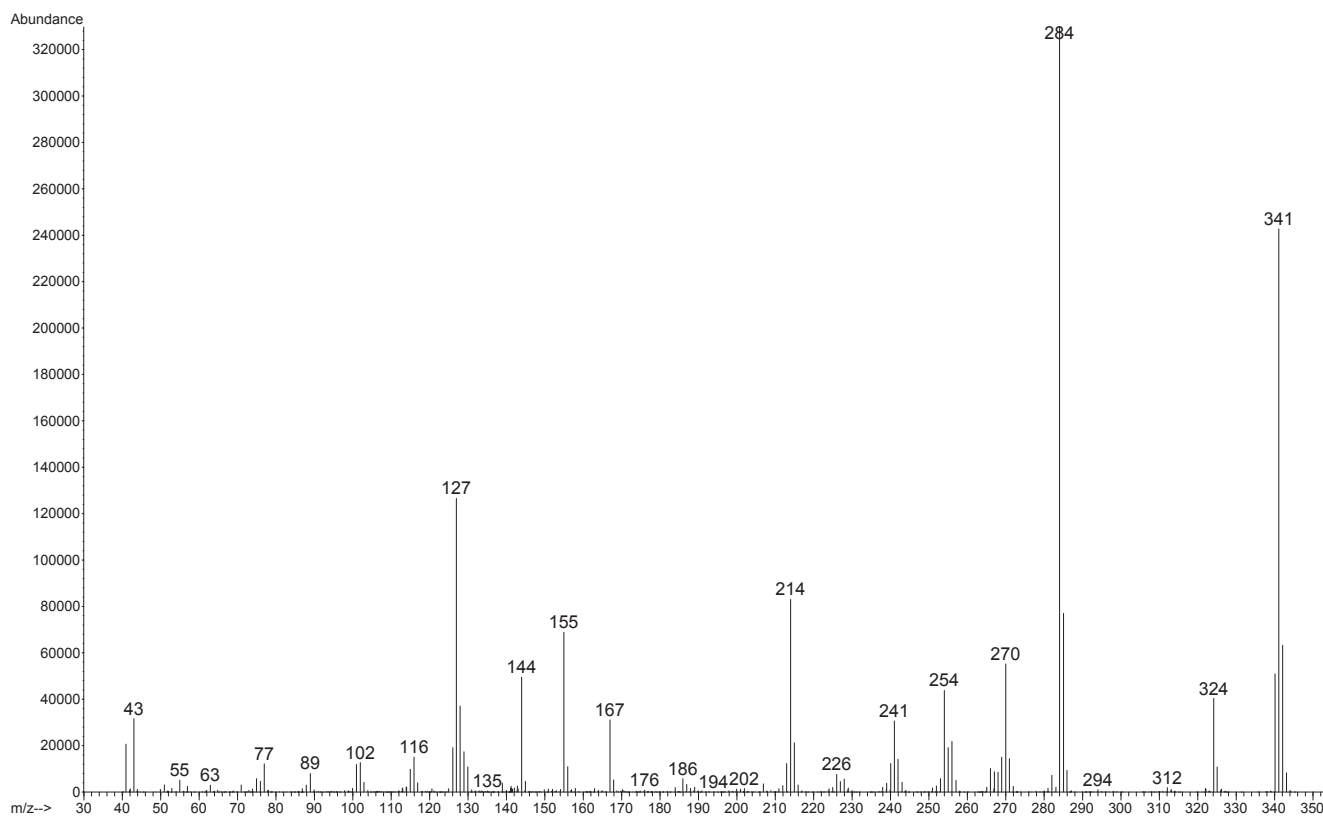
# JWH-073 2-methylbutyl homolog

Chemical name	N-(2-methylbutyl)-3-(1-naphthoyl)-indole	
Molecular formula	C <sub>24</sub> H <sub>23</sub> NO	
Molecular mass	341.5	
Major GC/MS ions	284.0, 341.1, 127.0, 214.0, 285.0	
Ions used for analysis	Target	284
	Qualifier-1	341
	Qualifier-2	127
Retention time	12.65 minutes	
LOD	Not yet established	

## Molecular Structure:



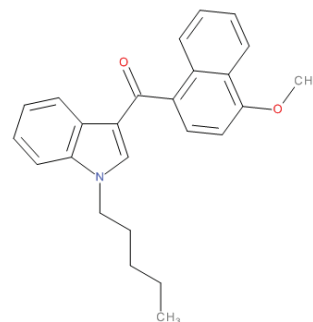
## Mass Spectrum:



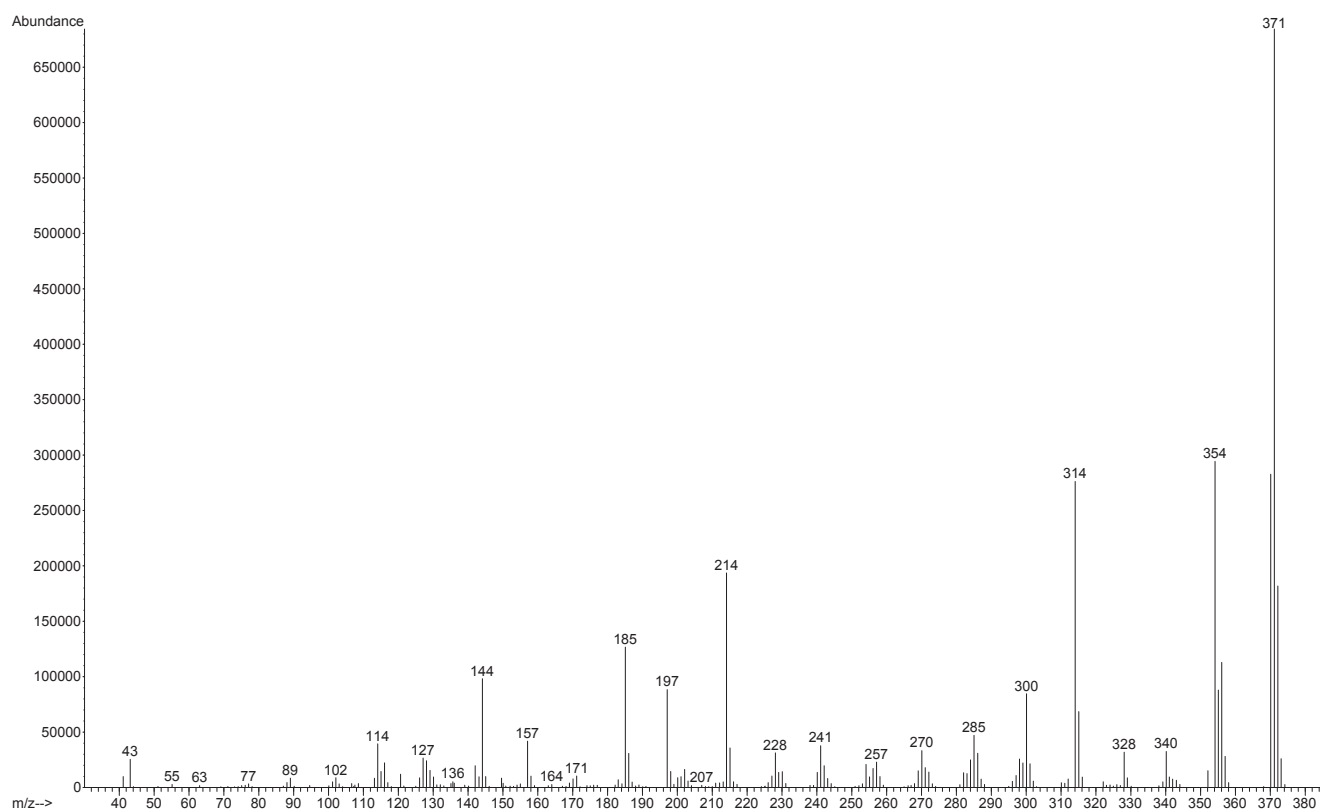
# JWH-081

Chemical name	4-methoxynaphthalen-1-yl- (1-pentylindol-3-yl)methanone	
Molecular formula	C <sub>25</sub> H <sub>25</sub> NO <sub>2</sub>	
Molecular mass	371.19	
Major GC/MS ions	371.3, 354.3, 314.3, 370.3, 214.2, 185.1	
Ions used for analysis	Target	371.3
	Qualifier-1	354.3
	Qualifier-2	314.3
Retention time	13.99 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-081 will not derivatize	

## Molecular Structure:



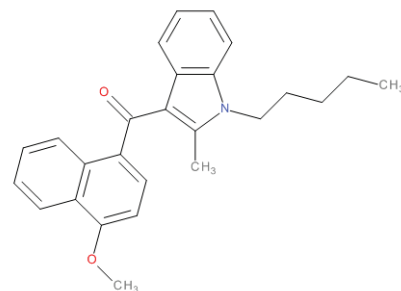
## Mass Spectrum:



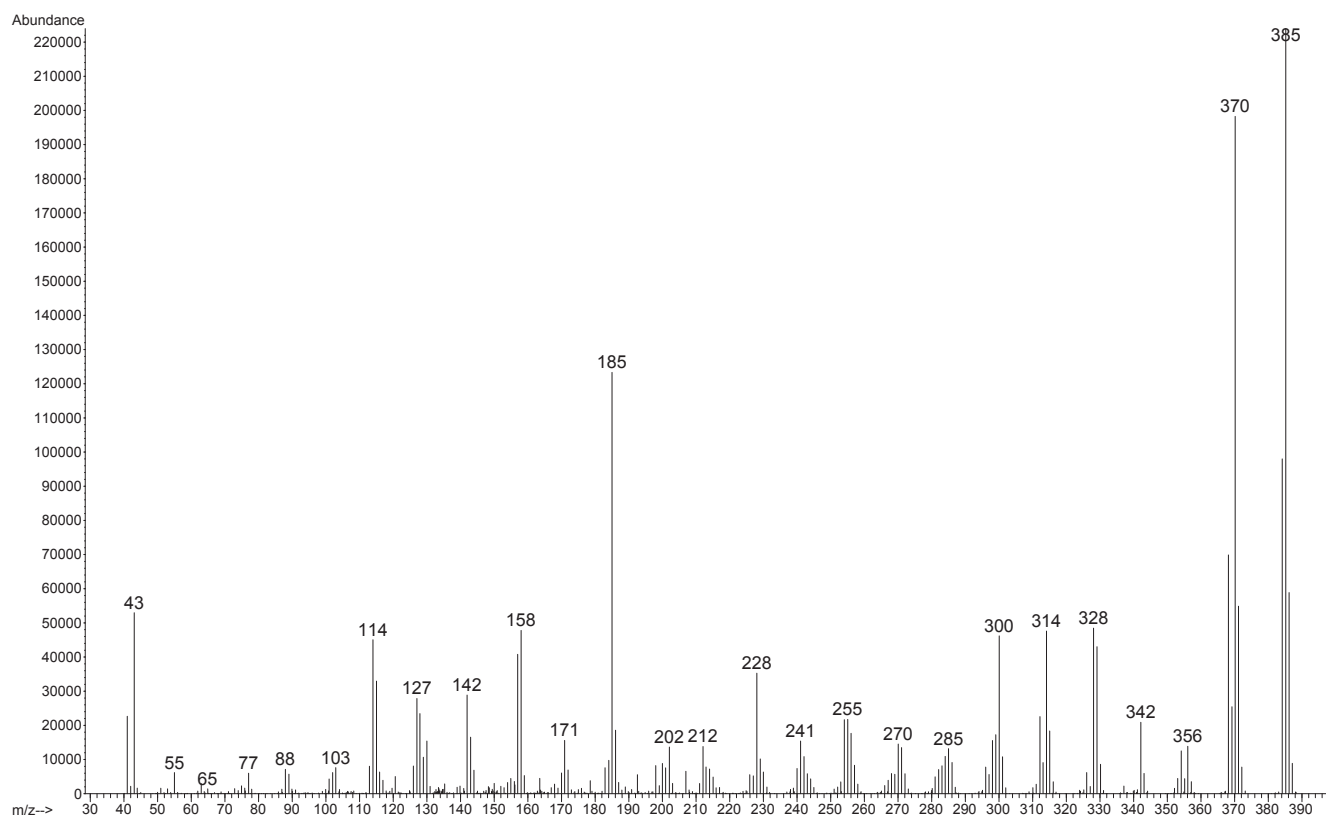
# JWH-098

Chemical name	4-methoxynaphthalen-1-yl-(1-pentyl-2-methylindol-3-yl) methanone	
Molecular formula	C <sub>26</sub> H <sub>27</sub> NO <sub>2</sub>	
Molecular mass	385.497	
Major GC/MS ions	385.2, 370.2, 185.0, 384.2, 368.2	
Ions used for analysis	Target	385
	Qualifier-1	370
	Qualifier-2	185
Retention time	13.82 minutes	
LOD	Not yet established	

## Molecular Structure:



## Mass Spectrum:

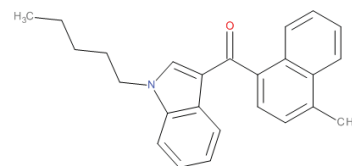




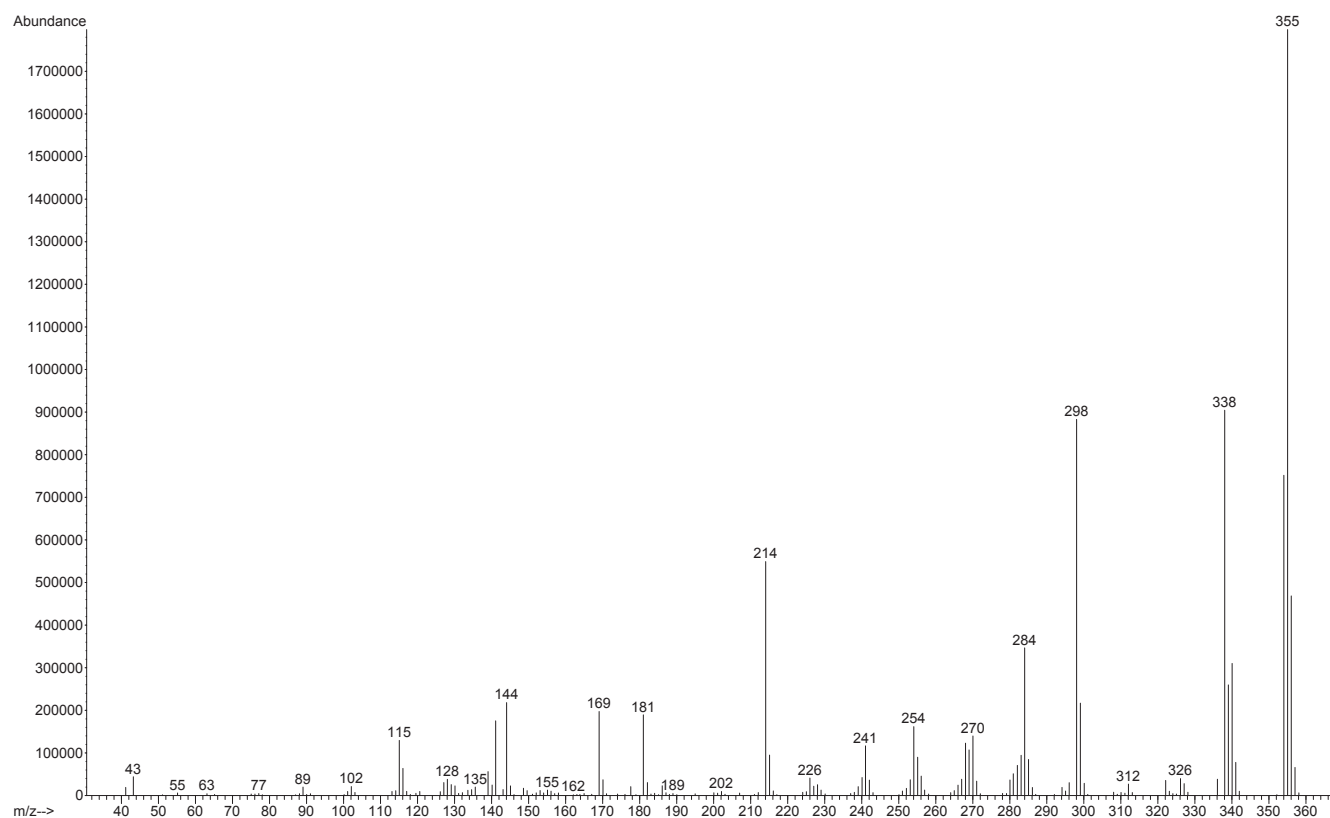
# JWH-122

Chemical name	1-Pentyl-3-(4-methyl-1-naphthoyl)indole	
Molecular formula	C <sub>25</sub> H <sub>25</sub> NO	
Molecular mass	355.19	
Major GC/MS ions	355.3, 338.3, 298.2, 284.2, 214.2, 144.1	
Ions used for analysis	Target	355.3
	Qualifier-1	338.3
	Qualifier-2	298.2
Retention time	13.46 minutes	
LOD	not yet established	
Additional comments	JWH-122 will not derivatize. JWH-122 is a structural isomer of JWH-019 with similar fragmentation and slight difference in retention time.	

## Molecular Structure:



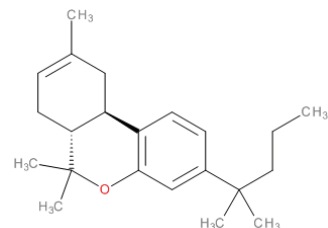
## Mass Spectrum:



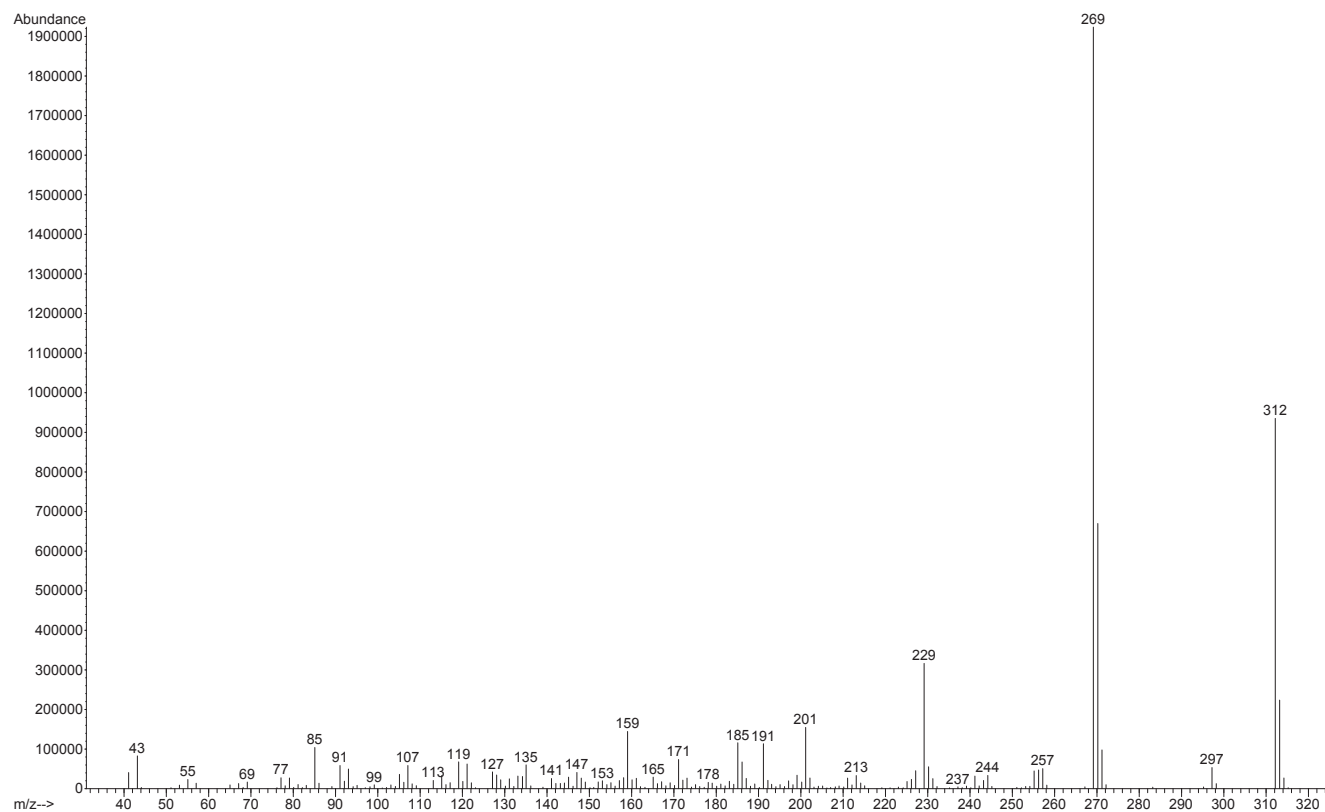
# JWH-133

Chemical name	(6aR,10aR)-3-(1,1-Dimethylbutyl)-6a,7,10,10a-tetrahydro-6,6,9-trimethyl-6H-dibenzo[b,d]pyran	
Molecular formula	C <sub>22</sub> H <sub>32</sub> O	
Molecular mass	312.24	
Major GC/MS ions	312.3, 269.2, 229.2, 270.2, 201.2, 159.1	
Ions used for analysis	Target	312.3
	Qualifier-1	269.2
	Qualifier-2	229.2
Retention time	9.47 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-133 will not derivatize	

## Molecular Structure:



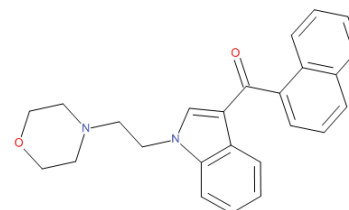
## Mass Spectrum:



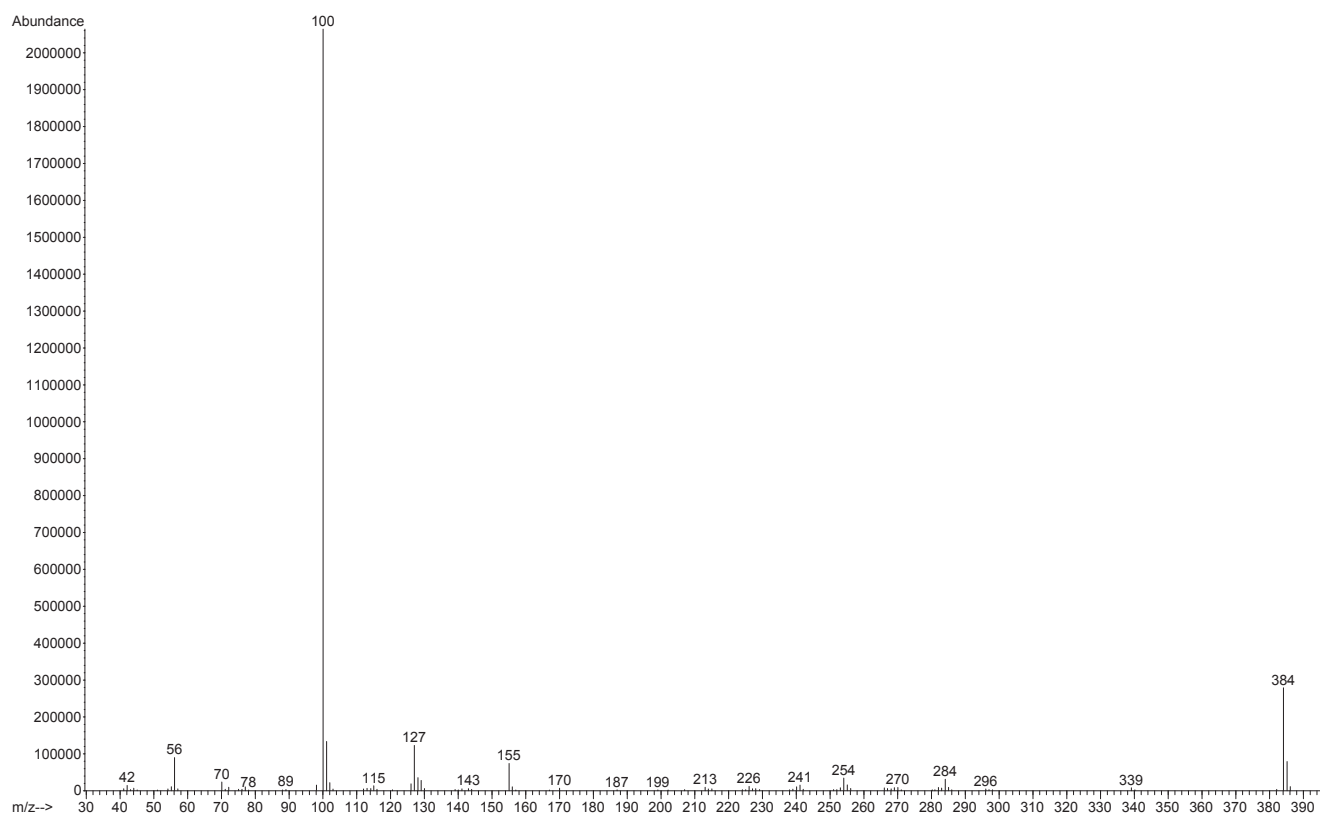
# JWH-200

Chemical name	(1-(2-morpholin-4-ylethyl)indol-3-yl)-naphthalen-1-ylmethanone	
Molecular formula	C <sub>25</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>	
Molecular mass	384.18	
Major GC/MS ions	100.0, 384.3, 127.1, 155.1, 56	
Ions used for analysis	Target	384.3
	Qualifier-1	100.0
	Qualifier-2	127.1
Retention time	14.38 minutes	
LOD	0.05 mg/g	
Additional comments	JWH-200 will not derivatize	

## Molecular Structure:



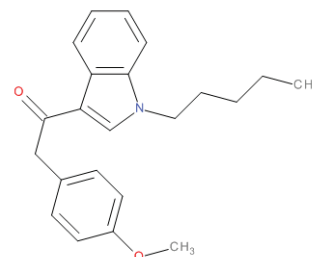
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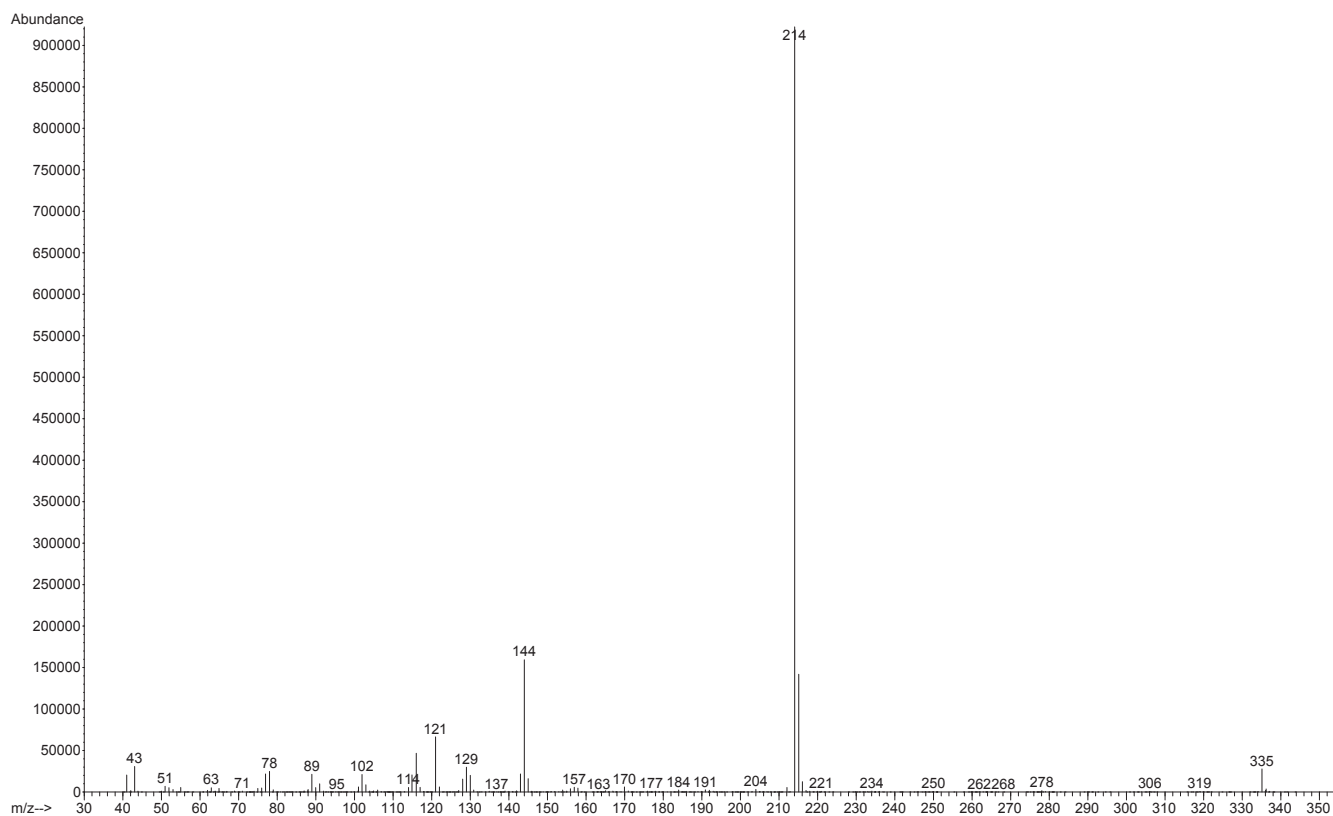
# JWH-201

Chemical name	2-(4-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl)-ethanone	
Molecular formula	C <sub>22</sub> H <sub>25</sub> NO <sub>2</sub>	
Molecular mass	335.4	
Major GC/MS ions	214.1, 144.0, 215.1, 121.0, 116.0	
Ions used for analysis	Target	214
	Qualifier-1	144
	Qualifier-2	335
Retention time	12.27 minutes	
LOD	Not yet established	

## Molecular Structure:



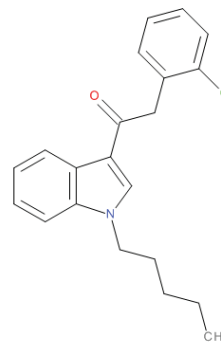
## Mass Spectrum:



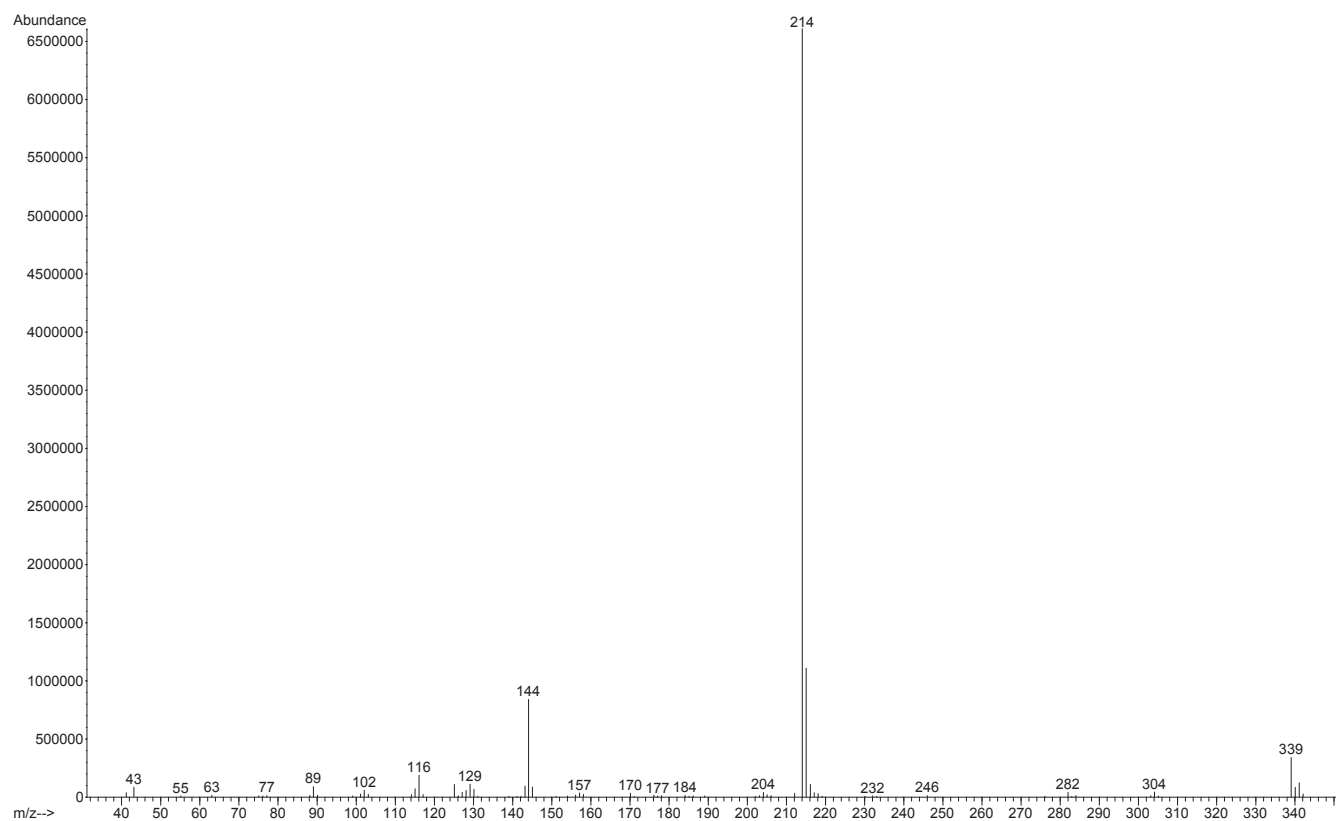
# JWH-203

Chemical name	2-(2-chlorophenyl)-1-(1-pentylindol-3-yl)ethanone	
Molecular formula	C <sub>21</sub> H <sub>22</sub> ClNO	
Molecular mass	339.14	
Major GC/MS ions	214.2, 144.1, 339.3	
Ions used for analysis	Target	214.2
	Qualifier-1	144.1
	Qualifier-2	339.3
Retention time	12.15 minutes	
LOD	not yet established	
Additional comments	JWH-203 will not derivatize	

## Molecular Structure:



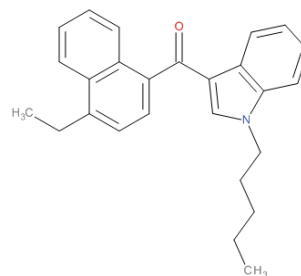
## Mass Spectrum:



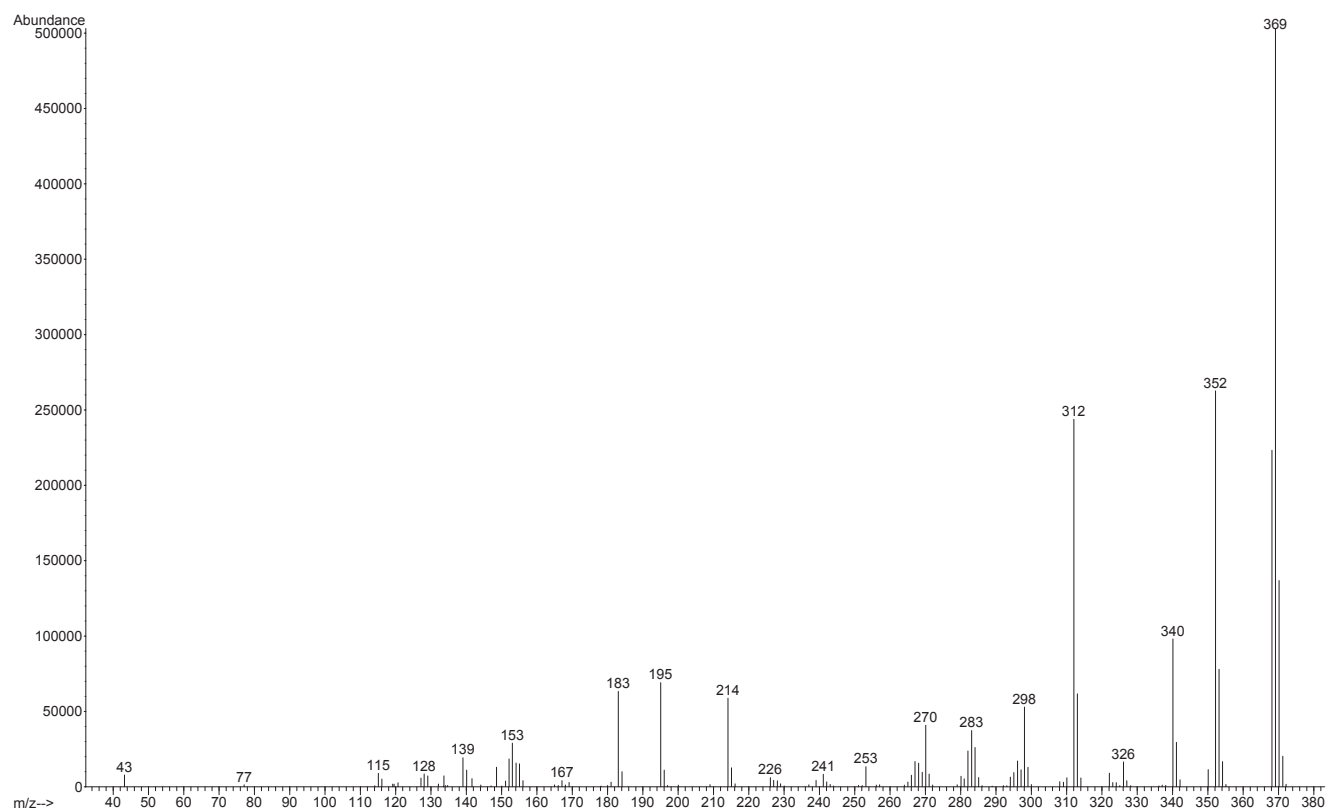
# JWH-210

Chemical name	4-ethylnaphthalen-1-yl-(1-pentylindol-3-yl)methanone	
Molecular formula	C <sub>26</sub> H <sub>27</sub> NO	
Molecular mass	369.21	
Major GC/MS ions	369.3, 352.3, 340.3, 312.3, 183.1, 195.1	
Ions used for analysis	Target	369.3
	Qualifier-1	352.3
	Qualifier-2	312.3
Retention time	13.72 minutes	
LOD	not yet established	
Additional comments	JWH-210 will not derivatize	

## Molecular Structure:



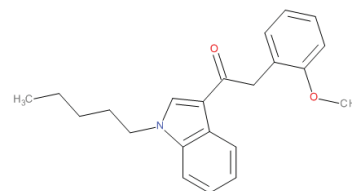
## Mass Spectrum:



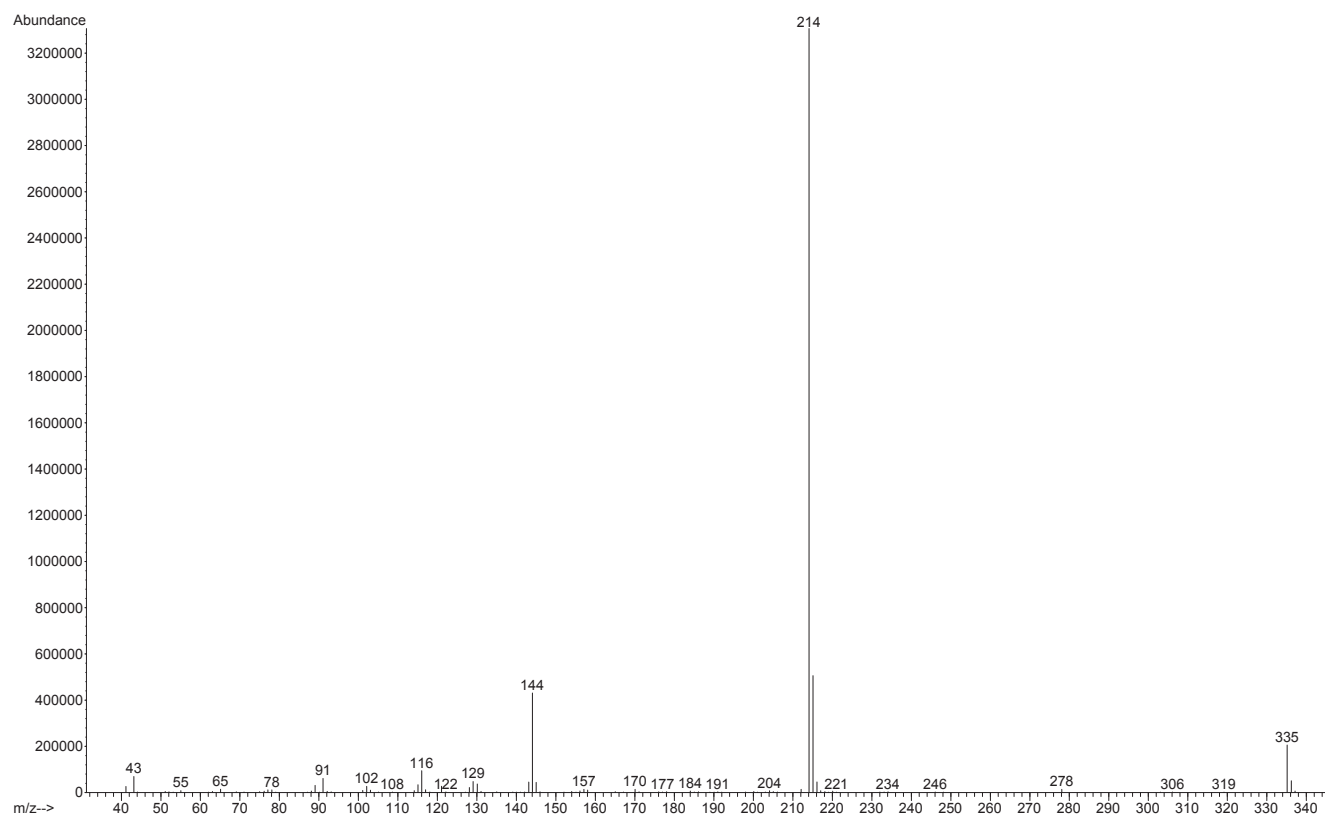
# JWH-250

Chemical name	2-(2-methoxyphenyl)-1-(1-pentylindol-3-yl)ethanone	
Molecular formula	C <sub>22</sub> H <sub>25</sub> NO <sub>2</sub>	
Molecular mass	335.19	
Major GC/MS ions	214.2, 144.1, 335.3	
Ions used for analysis	Target	214.2
	Qualifier-1	144.1
	Qualifier-2	335.3
Retention time	12.22 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-250 will not derivatize	

## Molecular Structure:



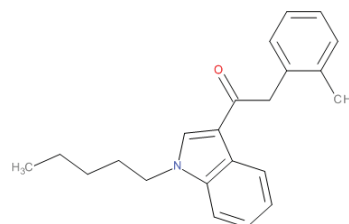
## Mass Spectrum:



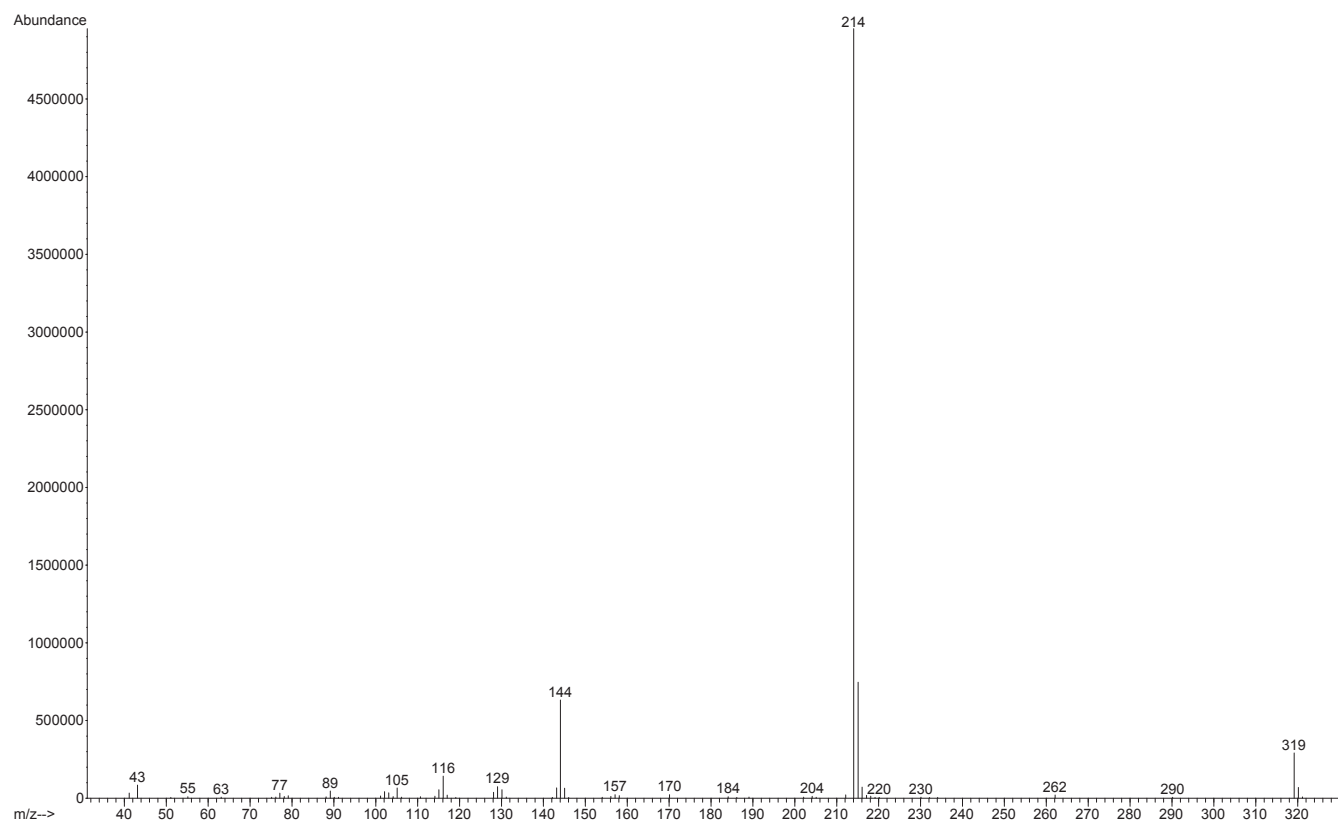
# JWH-251

Chemical name	2-(2-methylphenyl)-1-(1-pentyl-1H-indol-3-yl)ethanone	
Molecular formula	C <sub>22</sub> H <sub>25</sub> NO	
Molecular mass	319.19	
Major GC/MS ions	214.2, 319.3, 144.1	
Ions used for analysis	Target	214.2
	Qualifier-1	319.3
	Qualifier-2	144.1
Retention time	11.92 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-251 will not derivatize	

## Molecular Structure:



## Mass Spectrum:

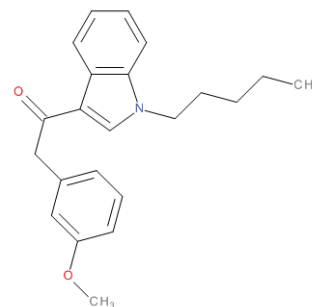




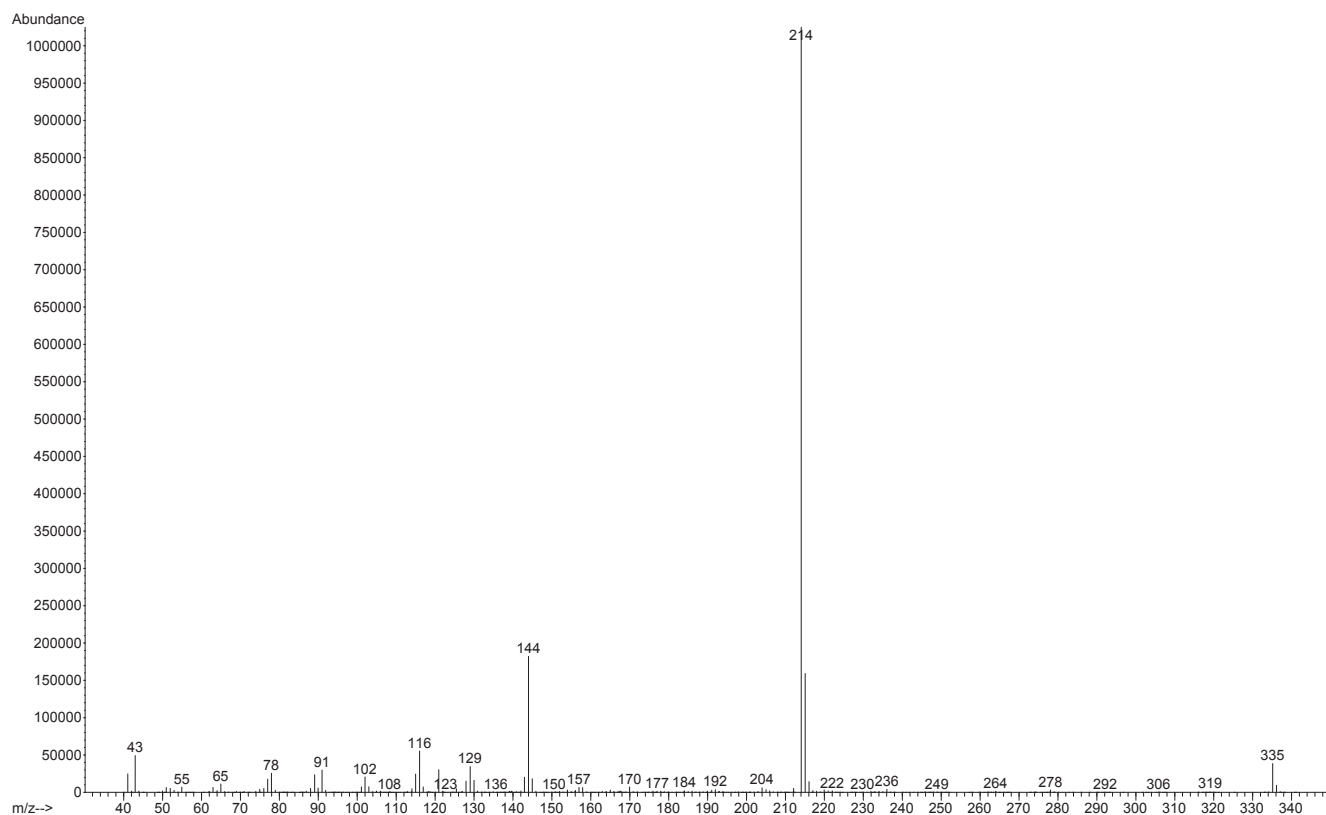
# JWH-302

Chemical name	2-(3-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl)-ethanone	
Molecular formula	C <sub>22</sub> H <sub>25</sub> NO <sub>2</sub>	
Molecular mass	335.4	
Major GC/MS ions	214.1, 144.0, 215.1, 116.0, 335	
Ions used for analysis	Target	214
	Qualifier-1	144
	Qualifier-2	335
Retention time	12.09 minutes	
LOD	Not yet established	

## Molecular Structure:



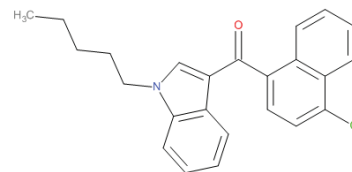
## Mass Spectrum:



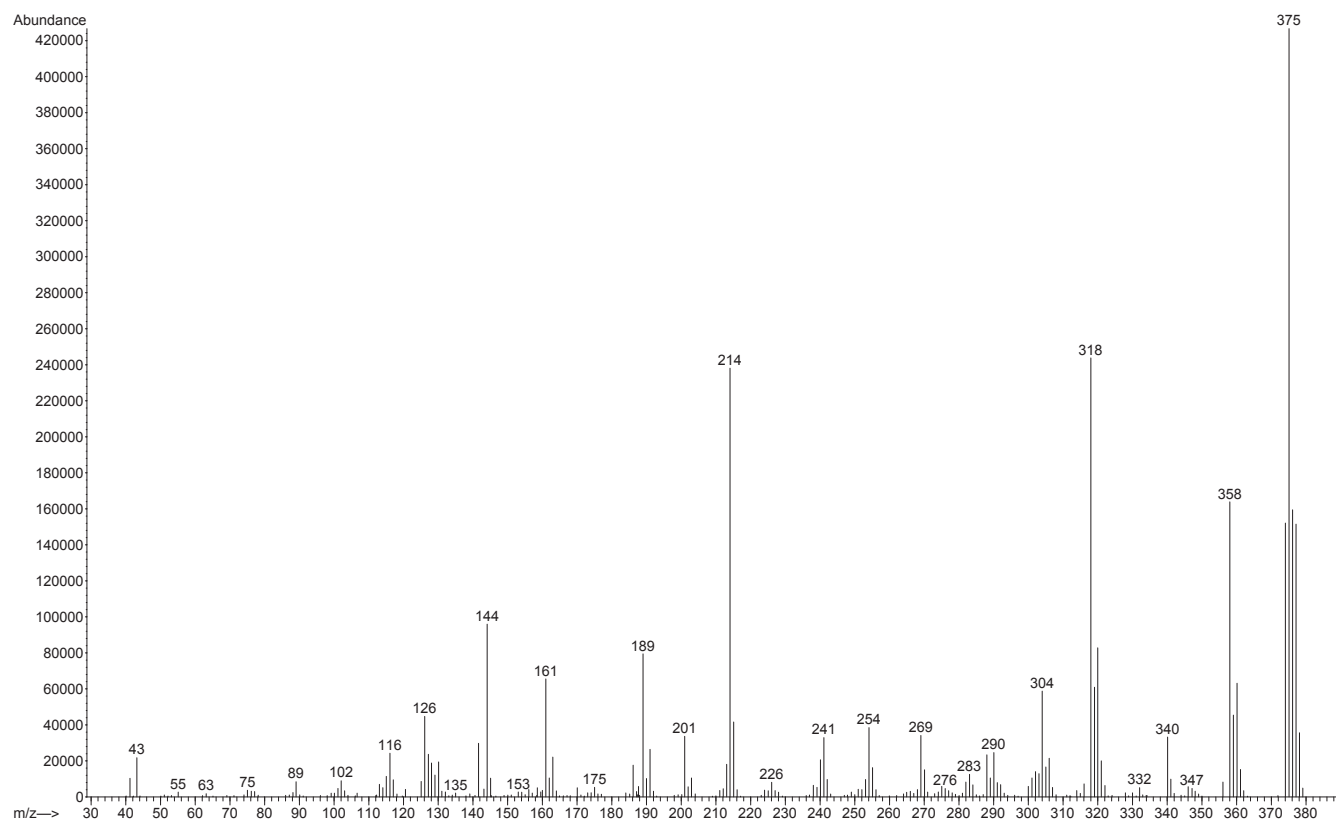
# JWH-398

Chemical name	1-pentyl-3-(4-chloro-1-naphthoyl)indole	
Molecular formula	C <sub>24</sub> H <sub>22</sub> ClNO	
Molecular mass	375.14	
Major GC/MS ions	375.3, 358.3, 318.3, 214.2, 189.1, 144.1	
Ions used for analysis	Target	375.3
	Qualifier-1	358.3
	Qualifier-2	318.3
Retention time	13.69 minutes	
LOD	0.02 mg/g	
Additional comments	JWH-398 will not derivatize	

## Molecular Structure:



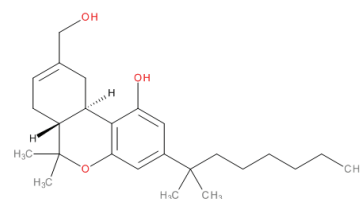
## Mass Spectrum:



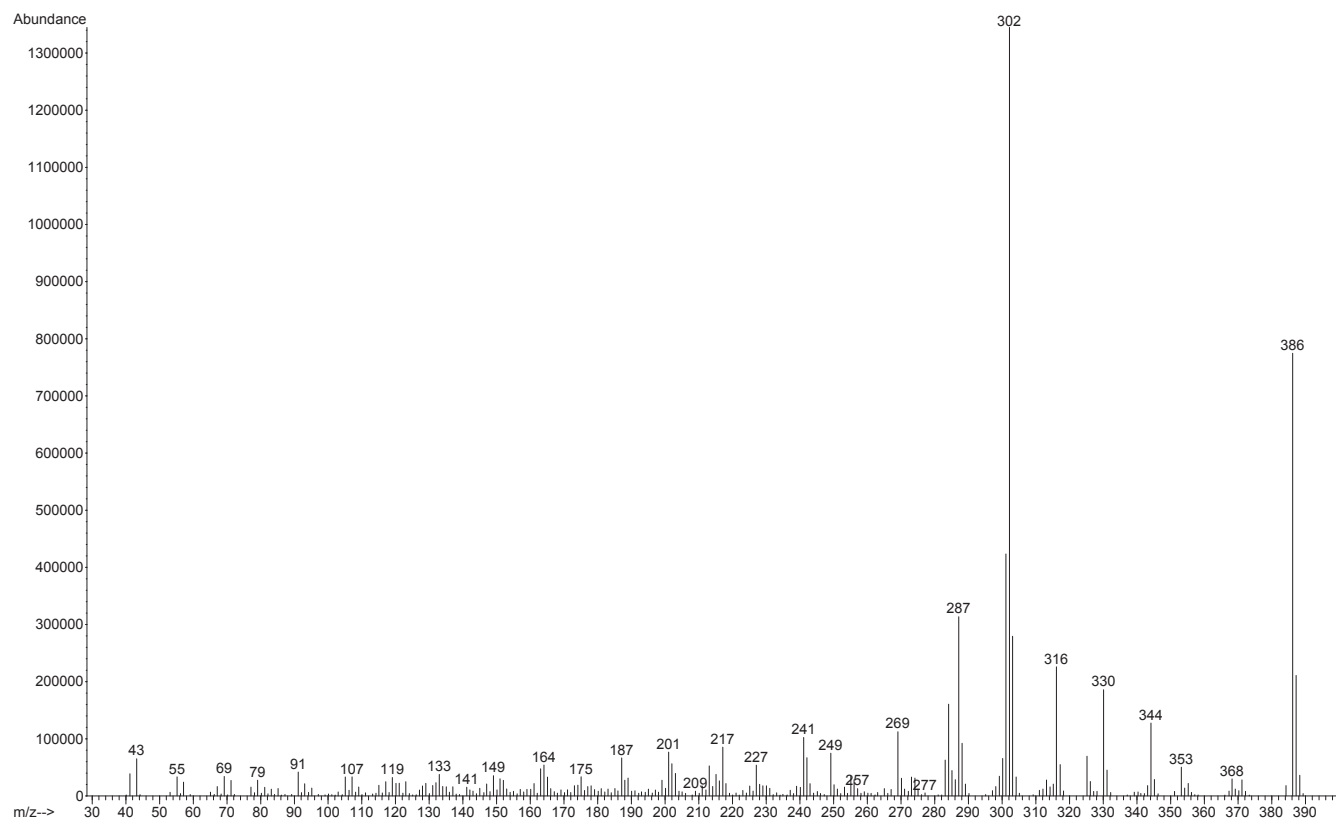
# HU-210

Chemical name	(6aR,10aR)- 9-(Hydroxymethyl)- 6,6-dimethyl-3-(2-methyloctan-2-yl)- 6a,7,10,10a-tetrahydrobenzo [c] chromen- 1-ol	
Molecular formula	C <sub>25</sub> H <sub>38</sub> O <sub>3</sub>	
Molecular mass	386.28	
Major GC/MS ions	386.3, 302.3, 287.2, 316.3, 330.3, 344.3	
Ions used for analysis	Target	386.3
	Qualifier-1	302.3
	Qualifier-2	287.2
Retention time	12.56 minutes	
LOD	0.02 mg/g	
Additional comments	Forms di-TMS derivative with BSTFA	

## Molecular Structure:



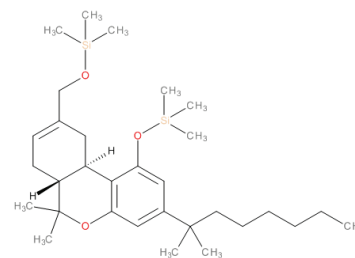
## Mass Spectrum:



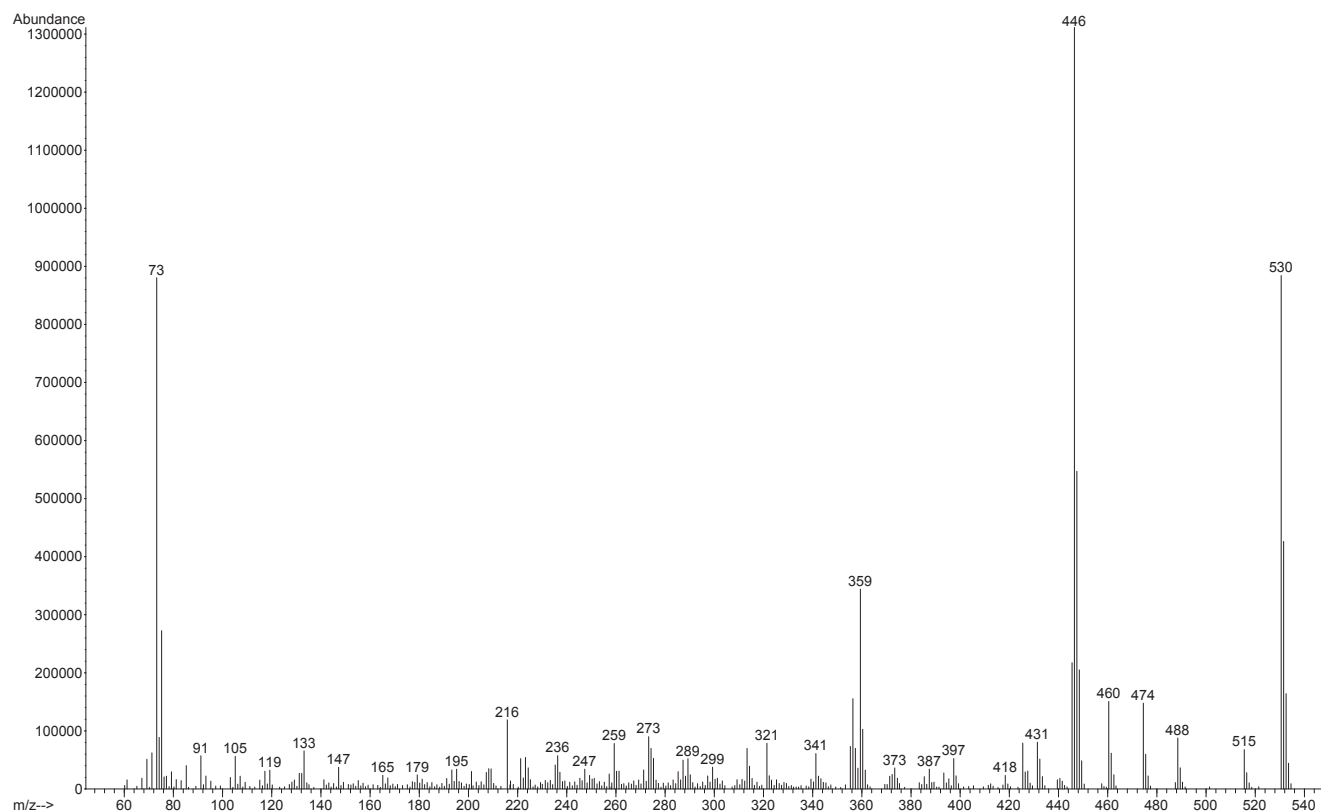
# HU-210 di-TMS derivative

Chemical name	(6aR,10aR)- 9-(Hydroxymethyl)- 6,6-dimethyl-3-(2-methyloctan-2-yl)- 6a,7,10,10a-tetrahydrobenzo [c] chromen- 1-ol-di-TMS derivative	
Molecular formula	C <sub>31</sub> H <sub>54</sub> O <sub>3</sub> Si <sub>2</sub>	
Molecular mass	530.36	
Major GC/MS ions	530.5, 446.4, 531.5, 359.3, 460.4, 474.4	
Ions used for analysis	Target	530.5
	Qualifier-1	446.4
	Qualifier-2	359.3
Retention time	8.35 minutes	
LOD	0.004 mg/g	
Additional comments	HU-210 is indistinguishable from HU-211.	

## Molecular Structure:



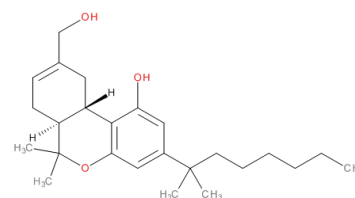
## Mass Spectrum:



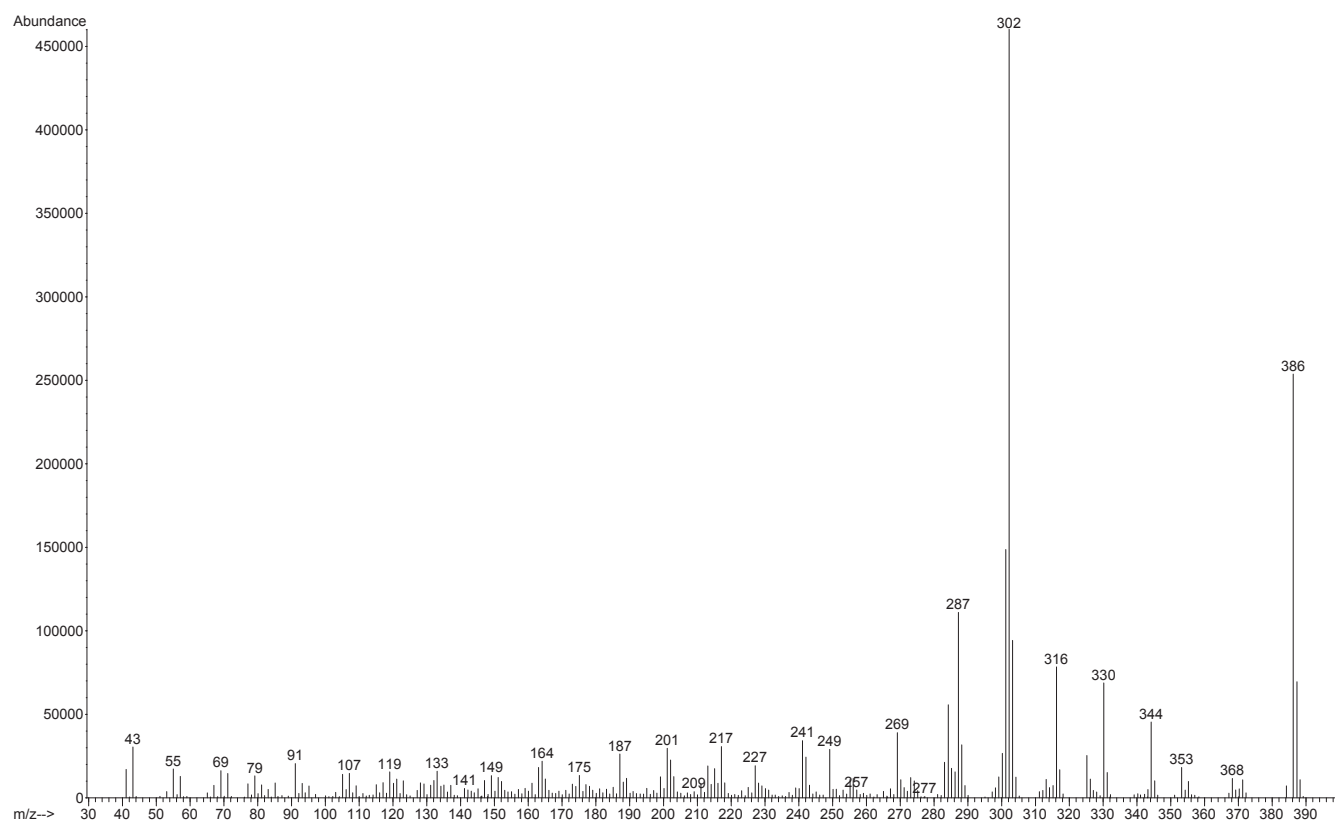
# HU-211

Chemical name	(6aS,10aS)-9-(Hydroxymethyl)- 6,6-dimethyl-3-(2-methyloctan-2-yl)- 6a,7,10,10a-tetrahydrobenzo [c] chromen-1-ol	
Molecular formula	C <sub>25</sub> H <sub>38</sub> O <sub>3</sub>	
Molecular mass	386.28	
Major GC/MS ions	386.3, 302.3, 287.2, 316.3, 330.3, 344.3	
Ions used for analysis	Target	386.3
	Qualifier-1	302.3
	Qualifier-2	287.2
Retention time	12.56 minutes	
LOD	0.02 mg/g	
Additional comments	Forms di-TMS derivative with BSTFA HU-211 is indistinguishable from HU-210	

## Molecular Structure:



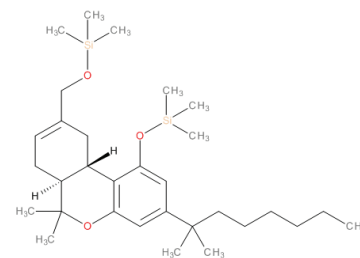
## Mass Spectrum:



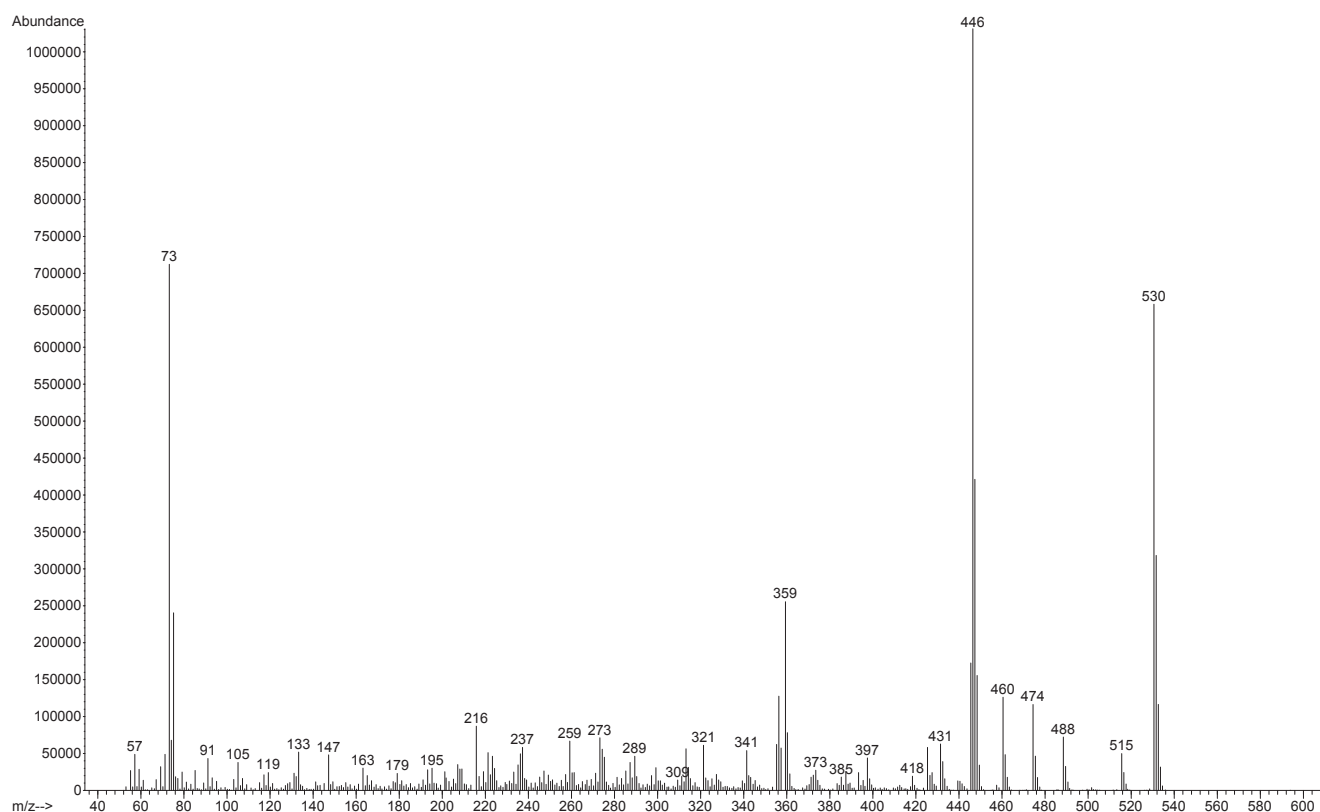
# HU-211-di-TMS derivative

Chemical name	(6aS,10aS)-9-(Hydroxymethyl)- 6,6-dimethyl-3-(2-methyloctan-2-yl)- 6a,7,10,10a-tetrahydrobenzo [c] chromen-1-ol-di-TMS derivative		
Molecular formula	C <sub>31</sub> H <sub>54</sub> O <sub>3</sub> Si <sub>2</sub>		
Molecular mass	530.36		
Major GC/MS ions	530.5, 446.4, 531.5, 359.3, 460.4, 474.4		
Ions used for analysis	Target	530.5	
	Qualifier-1	446.4	
	Qualifier-2	359.3	
Retention time	8.35 minutes		
LOD	0.004 mg/g		
Additional comments	HU-211 is indistinguishable from HU-210		

## Molecular Structure:



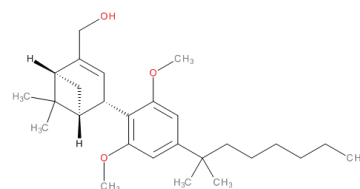
## Mass Spectrum:



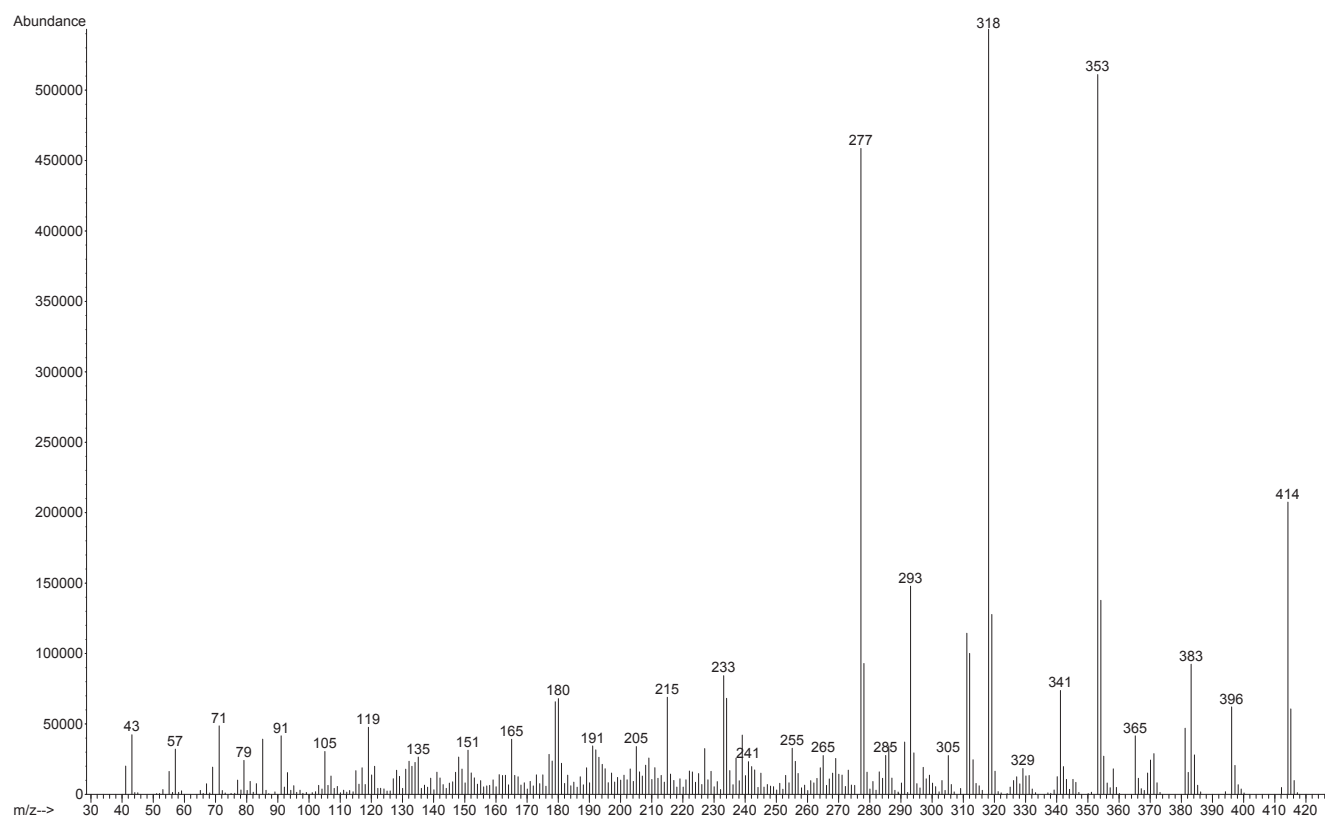
# HU-308

Chemical name	[(1R,2R,5R)-2-[2,6-dimethoxy-4-(2-methyloctan-2-yl)phenyl]-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enyl] methanol	
Molecular formula	C <sub>27</sub> H <sub>42</sub> O <sub>3</sub>	
Molecular mass	414.31	
Major GC/MS ions	277.2, 318.3, 353.3, 414.4, 293.2, 383.3	
Ions used for analysis	Target	414.4
	Qualifier-1	318.3
	Qualifier-2	353.3
Retention time	11.69 minutes	
LOD	Not yet established	
Additional comments	Forms mono-TMS derivative with BSTFA	

## Molecular Structure:



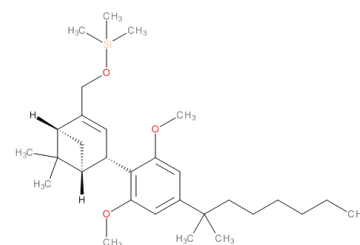
## Mass Spectrum:



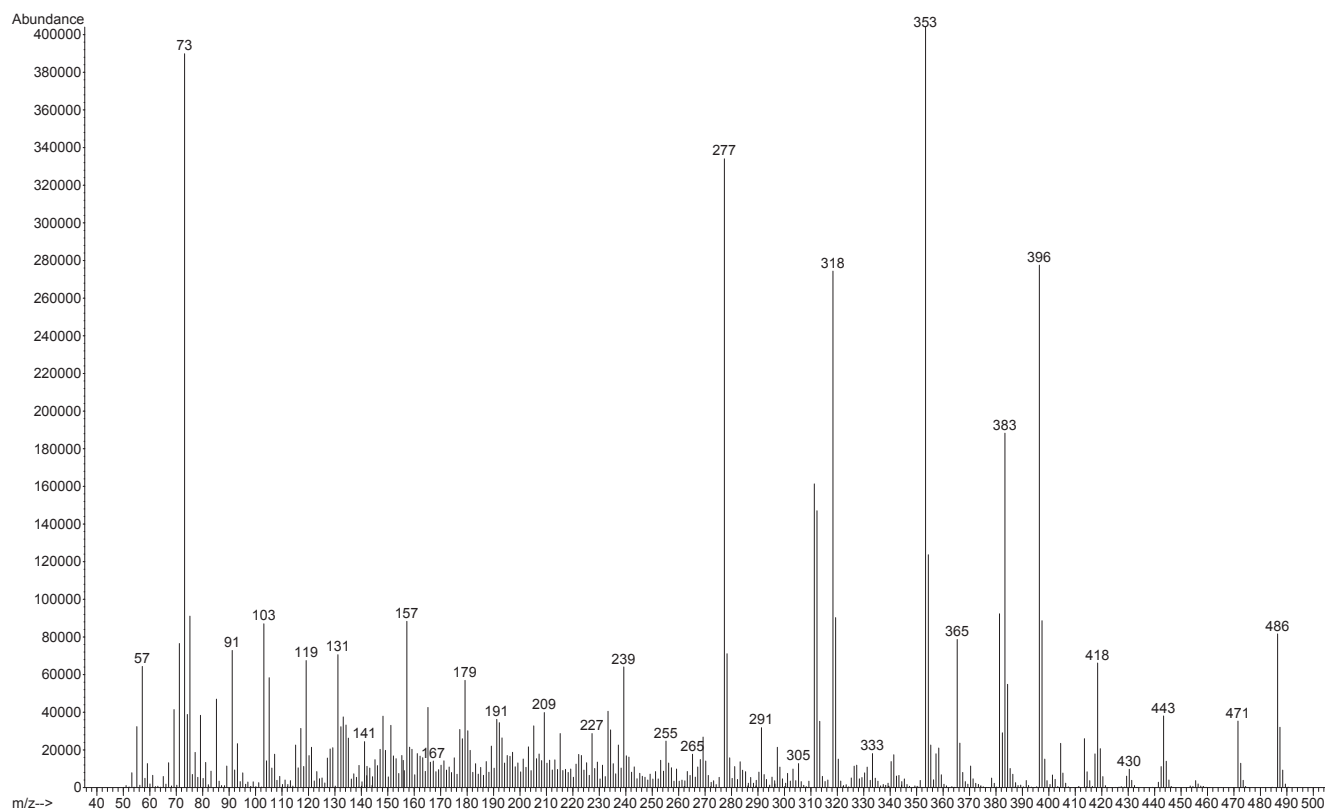
# HU-308-mono-TMS derivative

Chemical name	[(1R,2R,5R)-2-[2,6-dimethoxy-4-(2-methyloctan-2-yl)phenyl]-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enyl] methanol-mono-TMS derivative	
Molecular formula	C <sub>30</sub> H <sub>50</sub> O <sub>3</sub> Si	
Molecular mass	486.35	
Major GC/MS ions	277.2, 318.3, 353.3, 383.3, 396.3, 486.4	
Ions used for analysis	Target	486.4
	Qualifier-1	396.3
	Qualifier-2	353.3
Retention time	8.20 minutes	
LOD	Not yet established	

## Molecular Structure:



## Mass Spectrum:

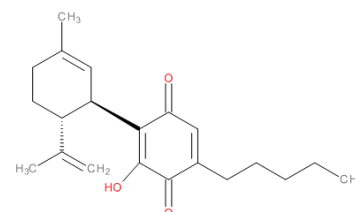




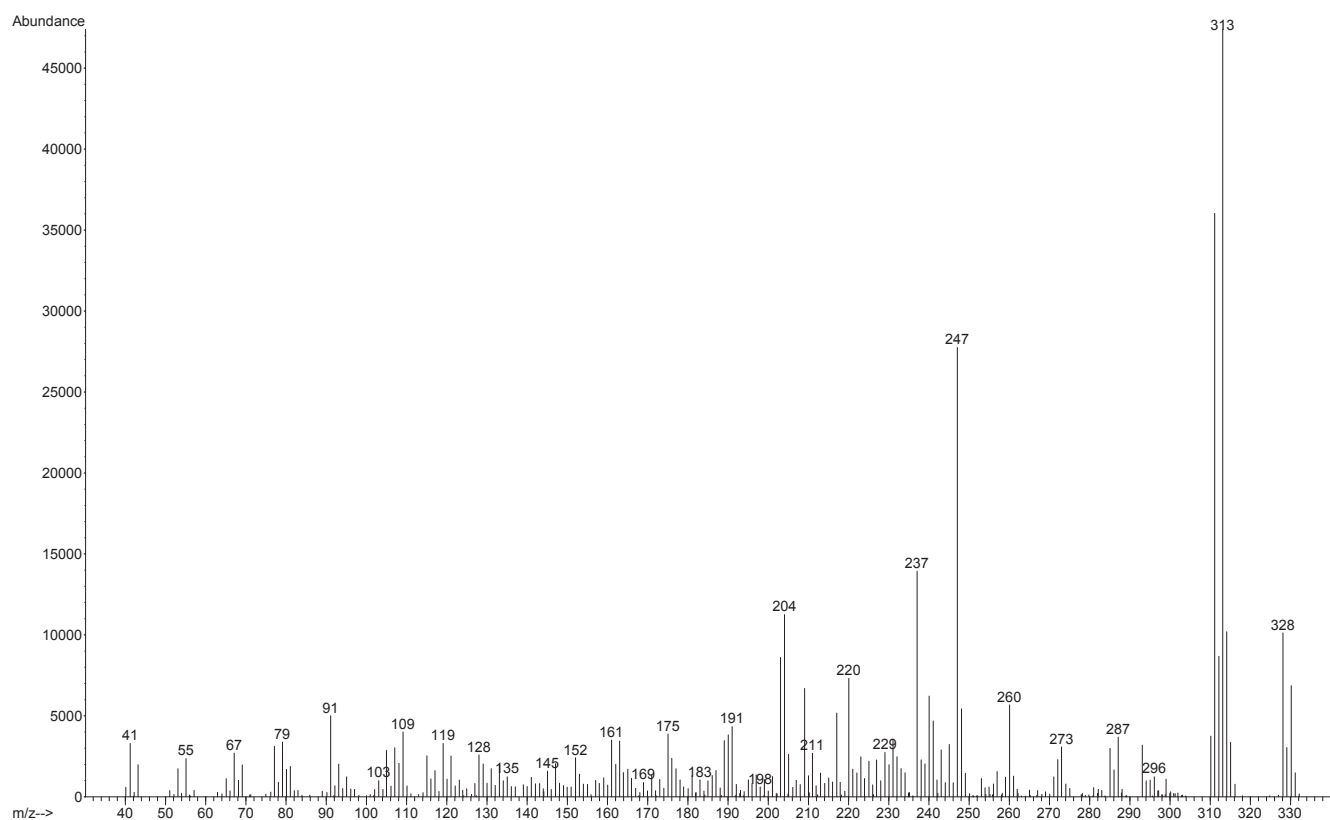
# HU-331

Chemical name	3-hydroxy-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-2,5-cyclohexadiene-1,4-dione	
Molecular formula	C <sub>21</sub> H <sub>28</sub> O <sub>3</sub>	
Molecular mass	328.203	
Major GC/MS ions	313.3, 311.3, 328.3, 247.2, 237.2, 204.2	
Ions used for analysis	Target	328.3
	Qualifier-1	313.3
	Qualifier-2	247.2
Retention time	9.84 minutes	
LOD	Not yet established	
Additional comments	Forms tri-TMS derivative with BSTFA	

## Molecular Structure:



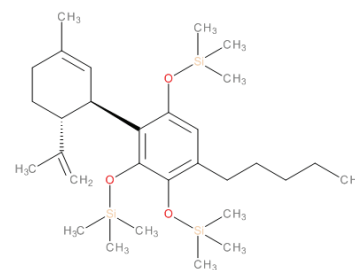
## Mass Spectrum:



# HU-331-tri-TMS derivative

Chemical name	3-hydroxy-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-2,5-cyclohexadiene-1,4-dione-tri-TMS derivative	
Molecular formula	$C_{30}H_{52}O_3Si_3$	
Molecular mass	544.32	
Major GC/MS ions	455.4, 384.3, 529.5, 544.4	
Ions used for analysis	Target	455.4
	Qualifier-1	384.3
	Qualifier-2	544.5
Retention time	7.18 minutes	
LOD	Not yet established	

## Molecular Structure:



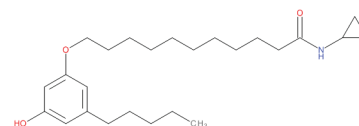
## Mass Spectrum:



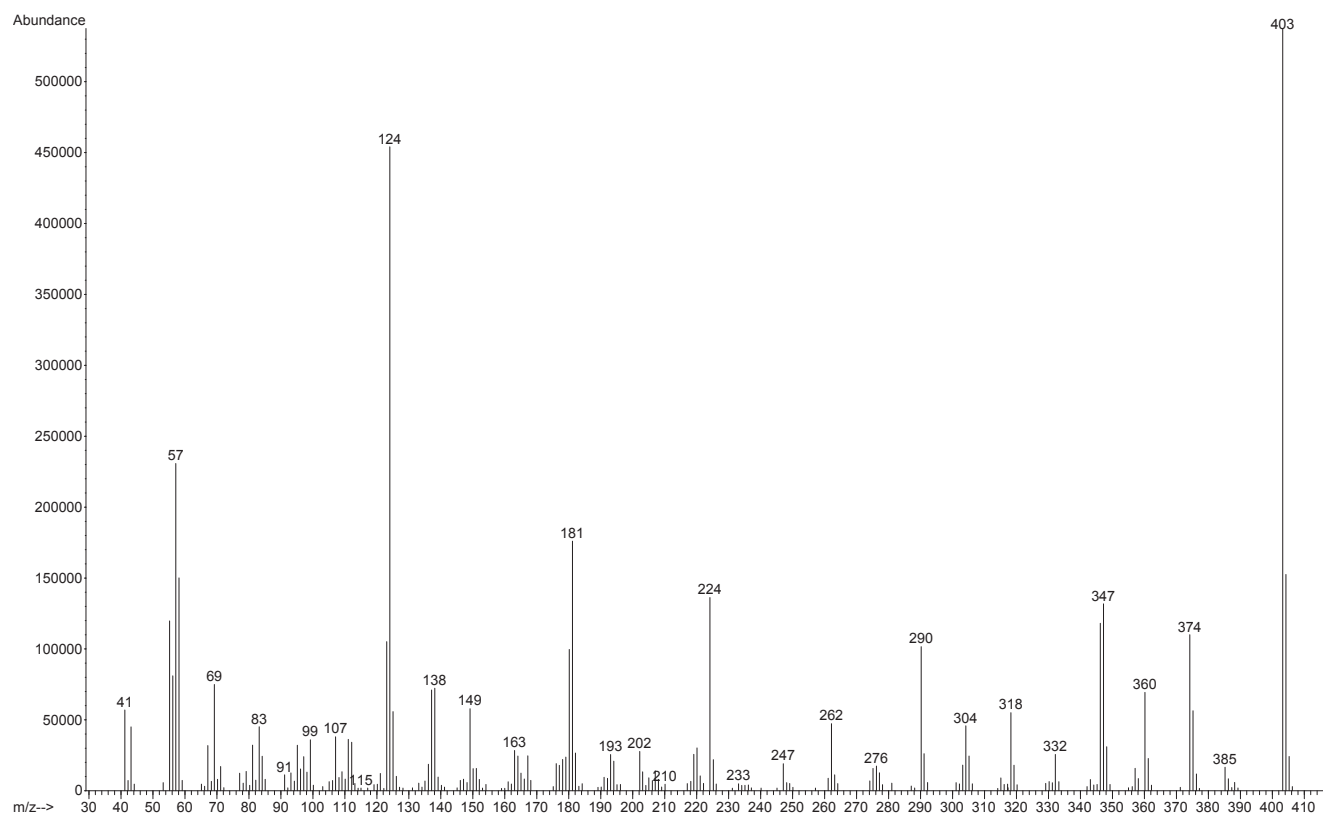
# CB-25

Chemical name	N-cyclopropyl-11-(3-hydroxy-5-pentylphenoxy)-undecanamide	
Molecular formula	C <sub>25</sub> H <sub>41</sub> NO <sub>3</sub>	
Molecular mass	403.31	
Major GC/MS ions	403.4, 124.1, 57.0, 181.1, 347.3, 374.3	
Ions used for analysis	Target	403.4
	Qualifier-1	124.1
	Qualifier-2	57.0
Retention time	13.88 minutes	
LOD	not yet established	
Additional comments	Forms di-TMS derivative with BSTFA	

## Molecular Structure:



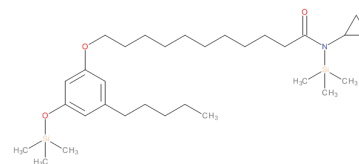
## Mass Spectrum:



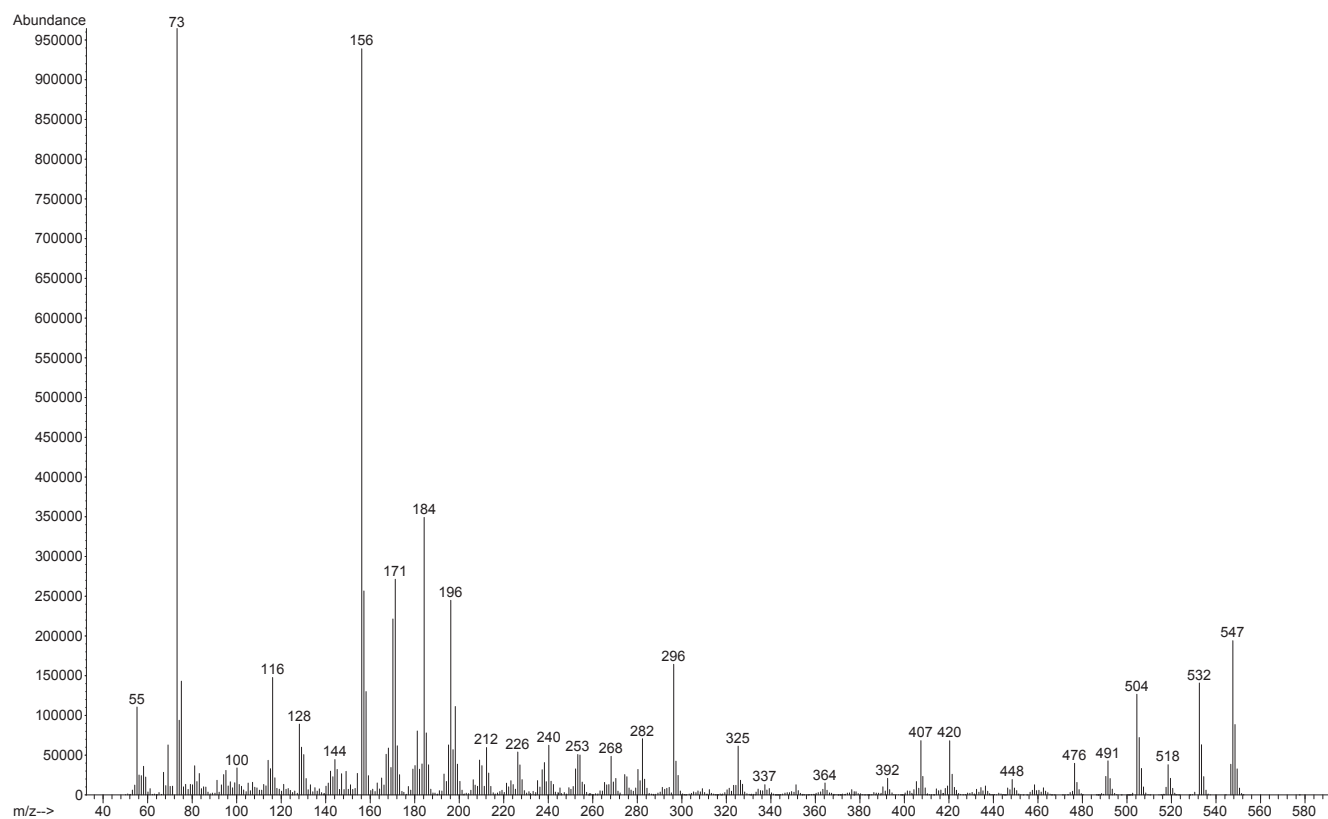
# CB-25-di-TMS derivative

Chemical name	N-cyclopropyl-11-(3-hydroxy-5-pentylphenoxy)-undecanamide di-TMS derivative	
Molecular formula	$C_{31}H_{57}NO_3Si_2$	
Molecular mass	547.39	
Major GC/MS ions	547, 532, 504, 156, 184, 196	
Ions used for analysis	Target	547.5
	Qualifier-1	532.5
	Qualifier-2	504.5
Retention time	9.22 minutes	
LOD	not yet established	

## Molecular Structure:



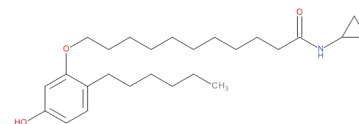
## Mass Spectrum:



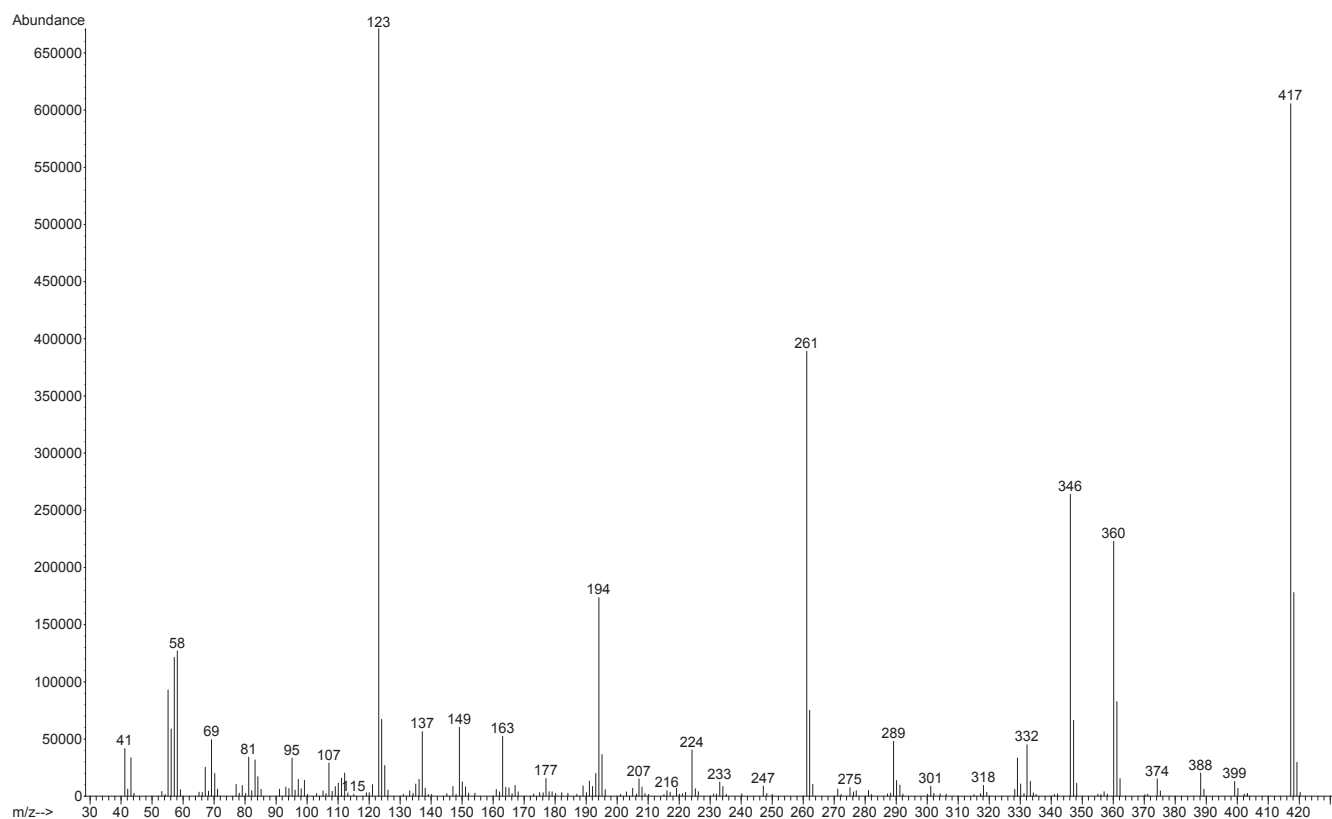
# CB-52

Chemical name	N-cyclopropyl-11-(2-hexyl-5-hydroxyphenoxy)-undecanamide	
Molecular formula	C <sub>26</sub> H <sub>43</sub> NO <sub>3</sub>	
Molecular mass	417.32	
Major GC/MS ions	417.4, 123.1, 261.2, 346.3, 360.3, 194.1	
Ions used for analysis	Target	417.4
	Qualifier-1	261.2
	Qualifier-2	346.3
Retention time	13.88 minutes	
LOD	not yet established	
Additional comments	Forms di-TMS derivative with BSTFA	

## Molecular Structure:



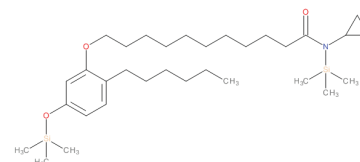
## Mass Spectrum:



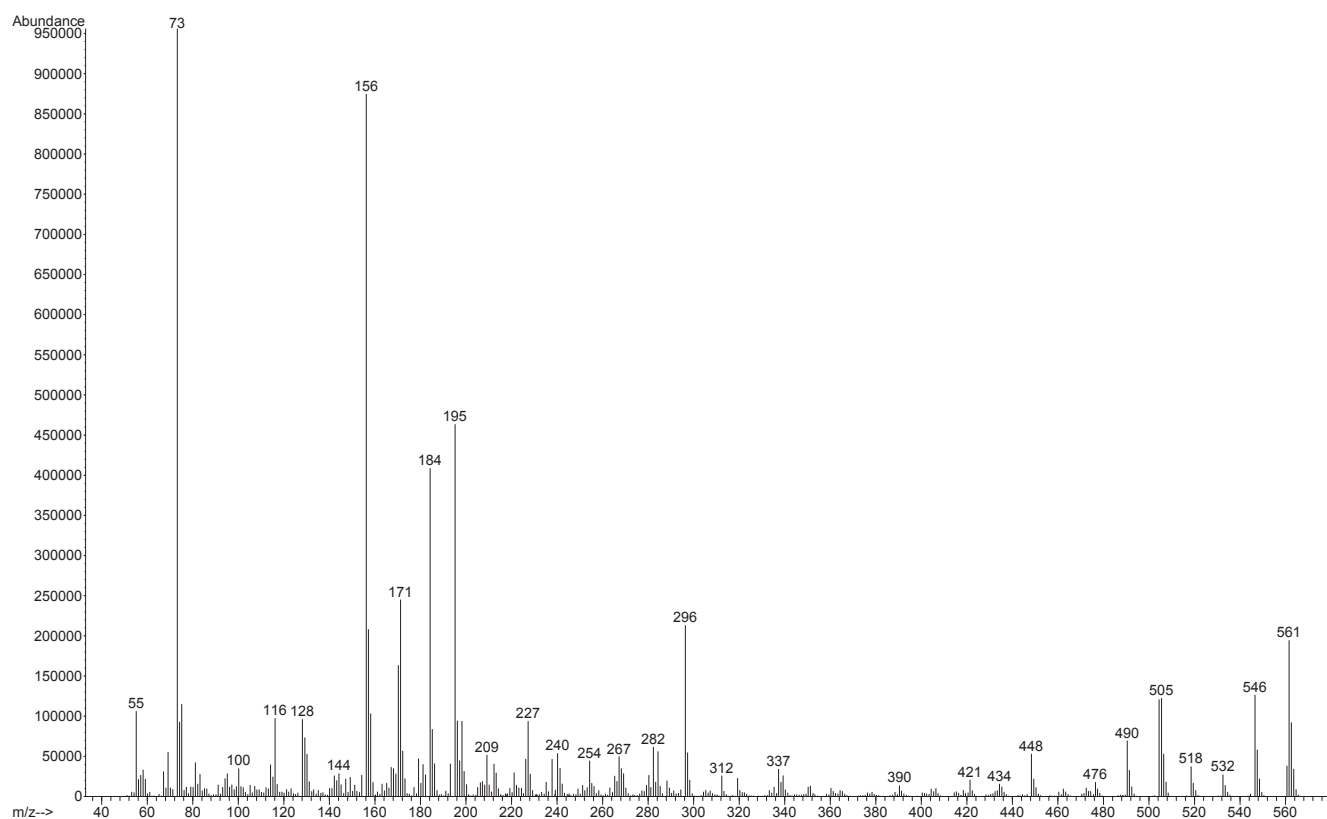
# CB-52-di-TMS derivative

Chemical name	N-cyclopropyl-11-(2-hexyl-5-hydroxyphenoxy)-undecanamide di-TMS derivative	
Molecular formula	$C_{32}H_{59}NO_3Si_2$	
Molecular mass	561.4	
Major GC/MS ions	561.5, 546.5, 505.5, 296.2, 195.1, 156.1	
Ions used for analysis	Target	561.5
	Qualifier-1	546.5
	Qualifier-2	505.5
Retention time	9.31 minutes	
LOD	not yet established	

## Molecular Structure:



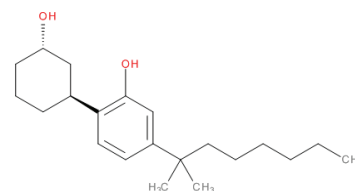
## Mass Spectrum:



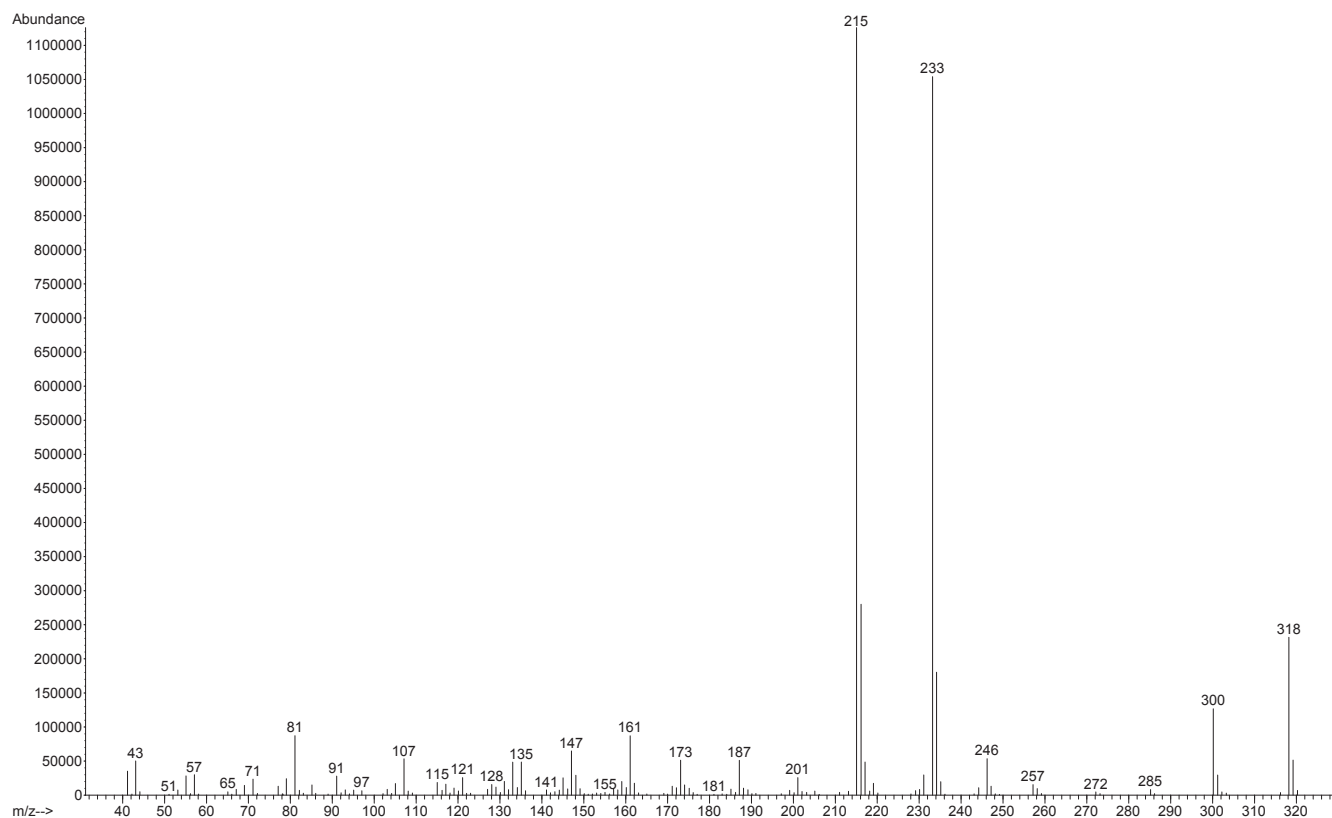
# CP47,497 (C7 analog)

Chemical name	2-[(1R,3S)-3-hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol	
Molecular formula	C <sub>21</sub> H <sub>34</sub> O <sub>2</sub>	
Molecular mass	318.26	
Major GC/MS ions	215.2, 233.2, 318.3, 300.3	
Ions used for analysis	Target	318.3
	Qualifier-1	215.2
	Qualifier-2	233.2
Retention time	10.96 minutes	
LOD	0.01 mg/g	
Additional comments	Forms di-TMS derivative with BSTFA	
	Compound shares some common ions with the C8 analog.	

## Molecular Structure:



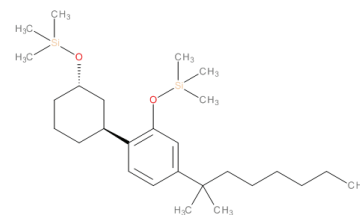
## Mass Spectrum:



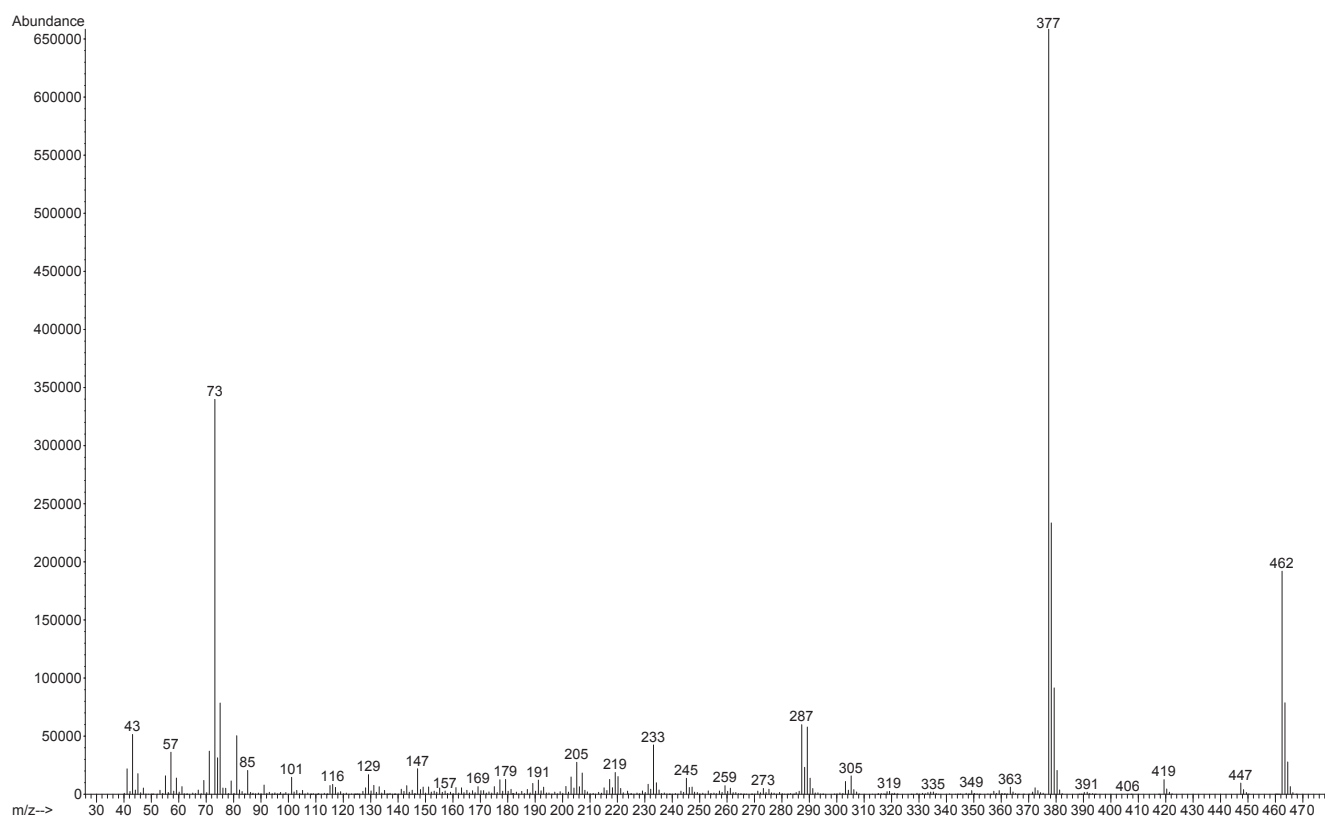
# CP47,497 (C7 analog)-di-TMS derivative

Chemical name	2-[(1R,3S)-3-hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol-di-TMS derivative	
Molecular formula	$C_{27}H_{50}O_2Si_2$	
Molecular mass	462.33	
Major GC/MS ions	377, 462, 378, 463	
Ions used for analysis	Target	377.3
	Qualifier-1	462.4
	Qualifier-2	378.3
Retention time	7.43 minutes	
LOD	0.002 mg/g	
Additional comments	Compound shares some common ions with the C8 analog.	

## Molecular Structure:



## Mass Spectrum:

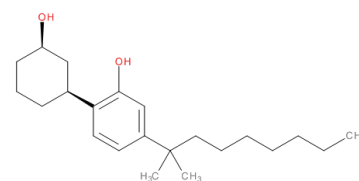




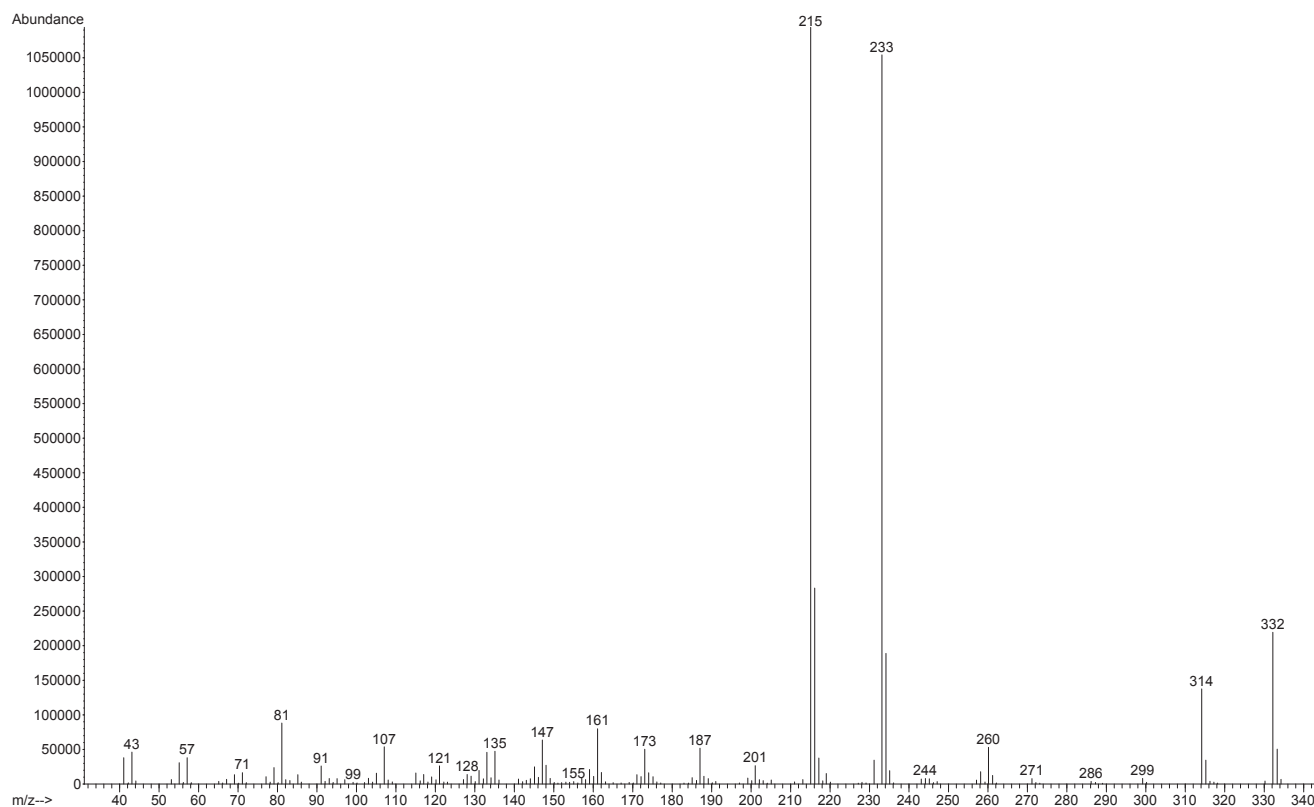
# CP47,497 (C8 analog)

Chemical name	2-[(1R,3S)-3-hydroxycyclohexyl]-5-(2-methylnonan-2-yl)phenol	
Molecular formula	C <sub>22</sub> H <sub>36</sub> O <sub>2</sub>	
Molecular mass	332.27	
Major GC/MS ions	215.2, 233.2, 314.3, 332.3	
Ions used for analysis	Target	332.3
	Qualifier-1	215.2
	Qualifier-2	233.2
Retention time	11.35 minutes	
LOD	0.02 mg/g	
Additional comments	Forms di-TMS derivative with BSTFA	
	Compound shares some common ions with the C7 analog.	

## Molecular Structure:



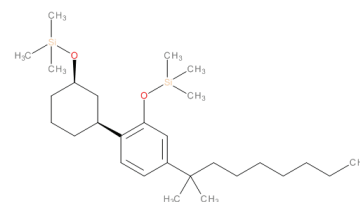
## Mass Spectrum:



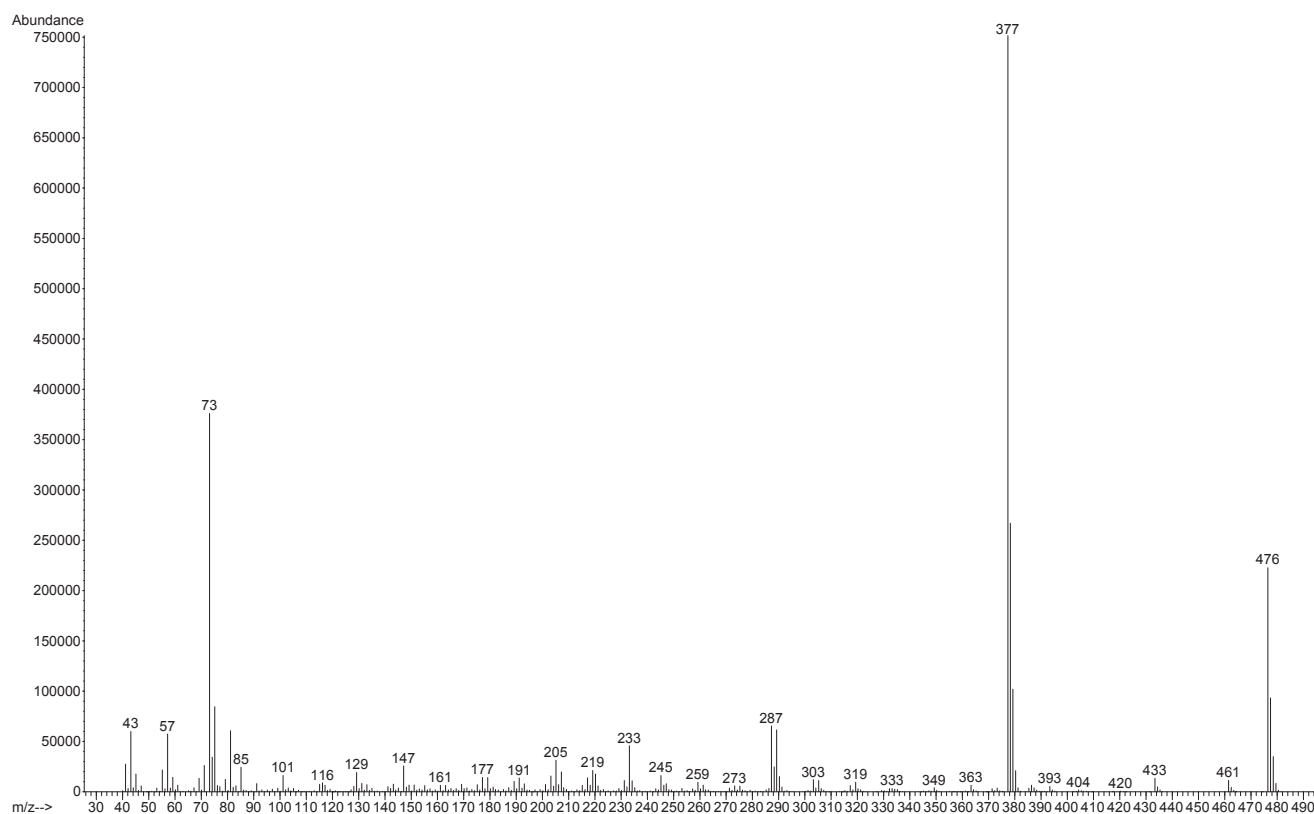
# CP47,497 (C8 analog)-di-TMS derivative

Chemical name	2-[(1R,3S)-3-hydroxycyclohexyl]-5-(2-methylnonan-2-yl)phenol-di-TMS derivative	
Molecular formula	$C_{28}H_{52}O_2Si_2$	
Molecular mass	476.35	
Major GC/MS ions	377.3, 476.4, 378.3, 477.4	
Ions used for analysis	Target	476.4
	Qualifier-1	377.3
	Qualifier-2	378.3
Retention time	7.67 minutes	
LOD	0.004 mg/g	
Additional comments	Compound shares some common ions with the C7 analog.	

## Molecular Structure:



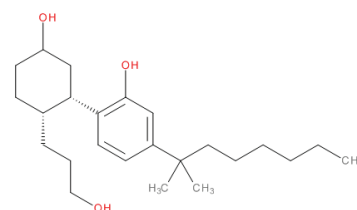
## Mass Spectrum:



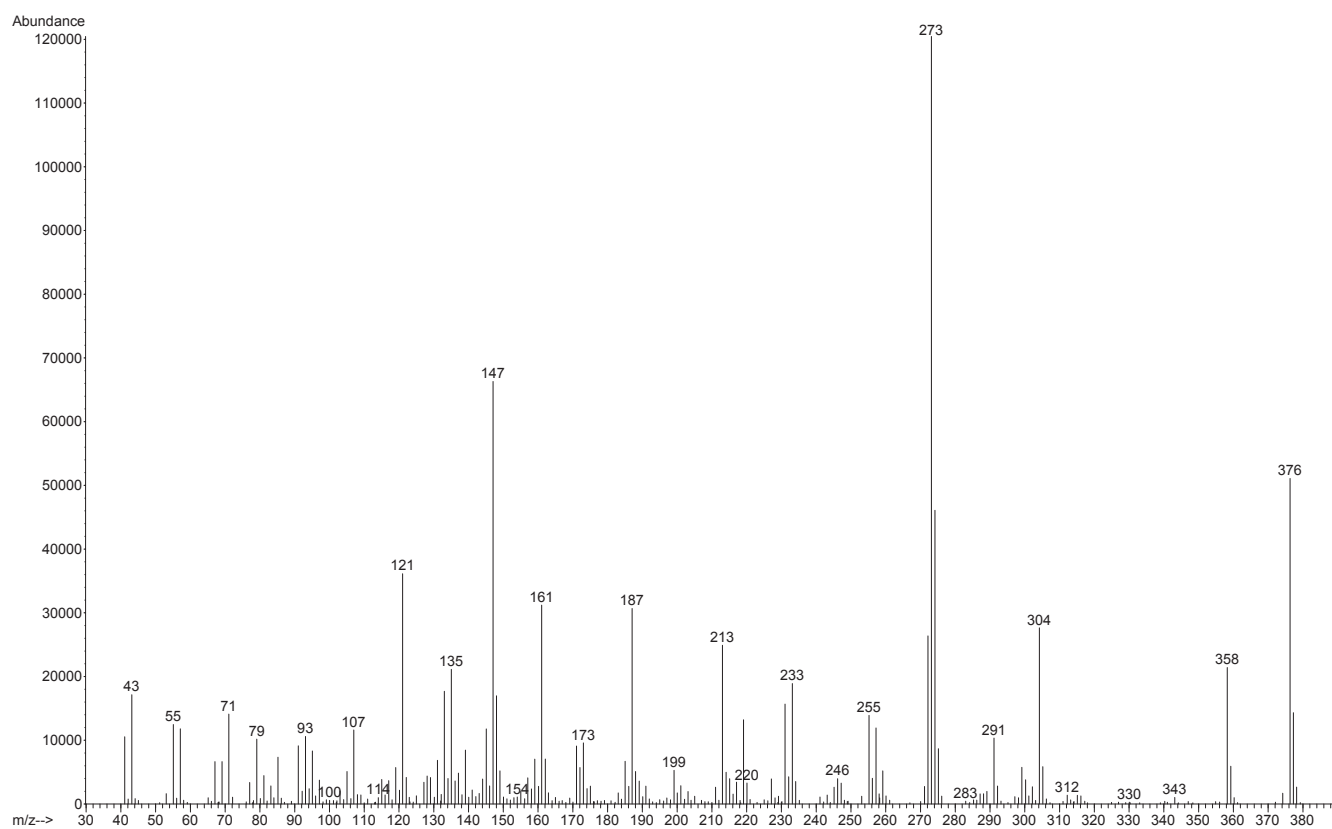
# CP55,940

Chemical name	2-[(1R,2R,5R)-5-hydroxy-2-(3-hydroxypropyl) cyclohexyl]-5-(2-methyloctan-2-yl)phenol	
Molecular formula	C <sub>24</sub> H <sub>40</sub> O <sub>3</sub>	
Molecular mass	376.3	
Major GC/MS ions	273.2, 147.1, 376.3, 121.1, 304.3, 358.3	
Ions used for analysis	Target	376.3
	Qualifier-1	273.2
	Qualifier-2	358.3
Retention time	12.43 minutes	
LOD	0.05 mg/g	
Additional comments	Forms tri-TMS derivative with BSTFA	

## Molecular Structure:



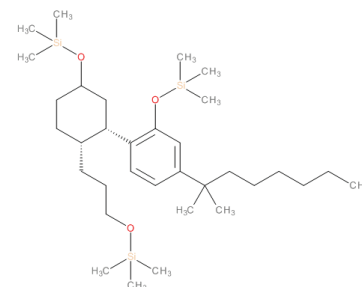
## Mass Spectrum:



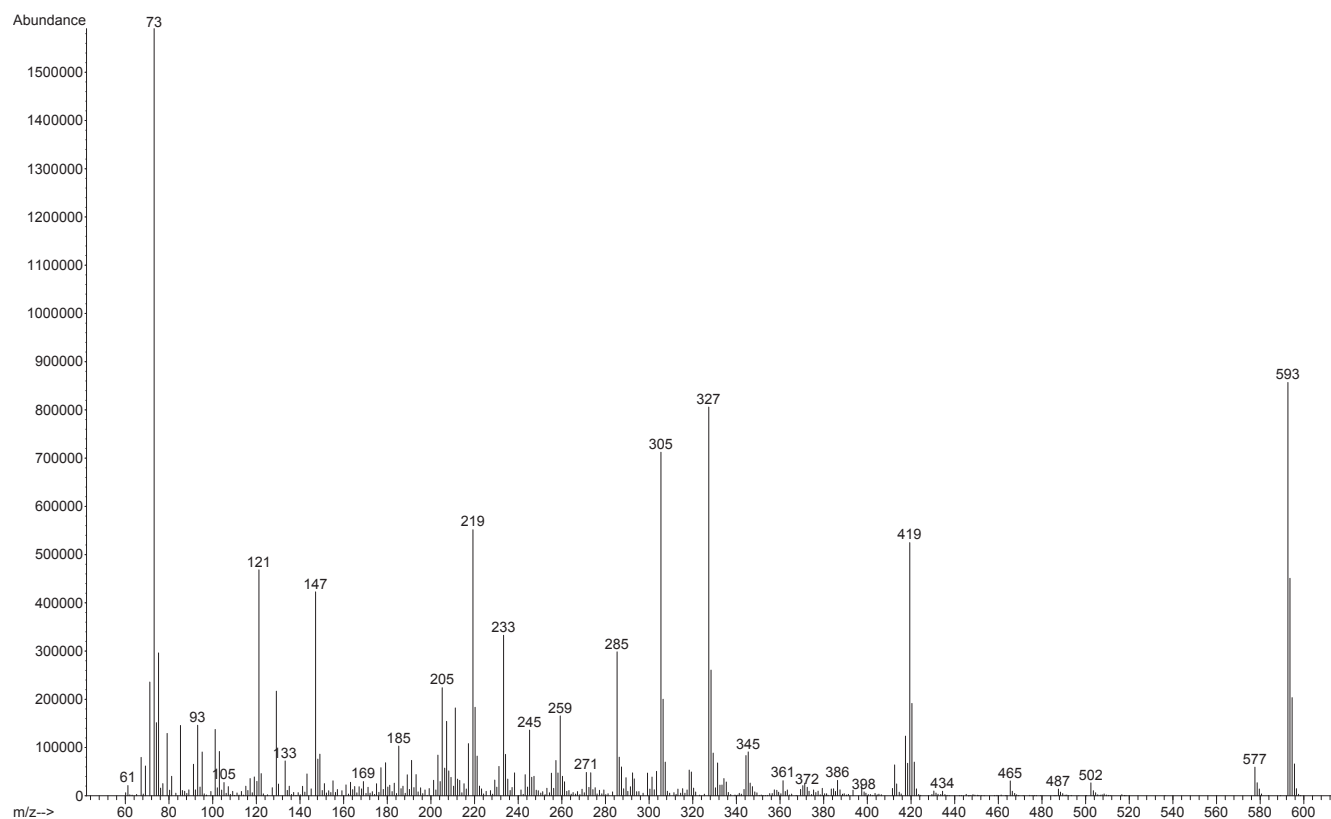
# CP55,940-tri-TMS derivative

Chemical name	2-[(1R,2R,5R)-5-hydroxy-2-(3-hydroxypropyl) cyclohexyl]-5-(2-methyloctan-2-yl)phenol-tri-TMS derivative	
Molecular formula	$C_{33}H_{64}O_3Si_3$	
Molecular mass	592.41	
Major GC/MS ions	593.5, 419.4, 327.3, 305.3, 219.2, 121.1	
Ions used for analysis	Target	593.5
	Qualifier-1	419.4
	Qualifier-2	327.3
Retention time	8.27 minutes	
LOD	0.01 mg/g	

## Molecular Structure:



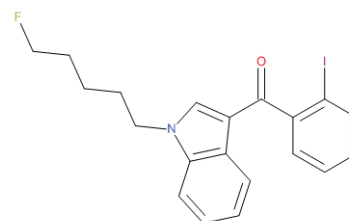
## Mass Spectrum:



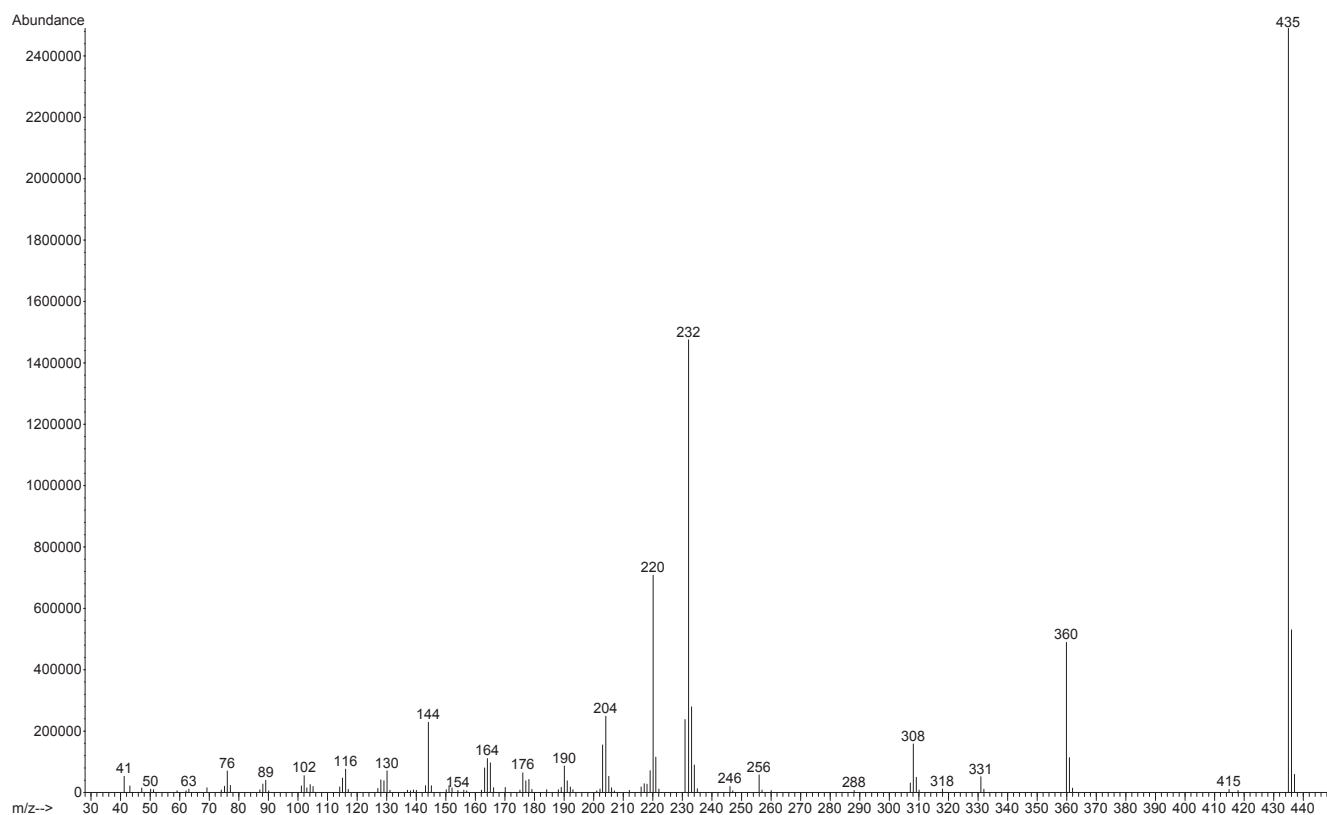
# AM-694

Chemical name	1-[(5-fluoropentyl)-1H-indol-3-yl]-(2-iodophenyl)methanone	
Molecular formula	C <sub>20</sub> H <sub>19</sub> FI <sub>1</sub> O	
Molecular mass	435.05	
Major GC/MS ions	435.3, 232.1, 220.1, 360.2	
Ions used for analysis	Target	435.3
	Qualifier-1	232.1
	Qualifier-2	220.1
Retention time	12.66 minutes	
LOD	not yet established	
Additional comments	Does not form derivative	

## Molecular Structure:



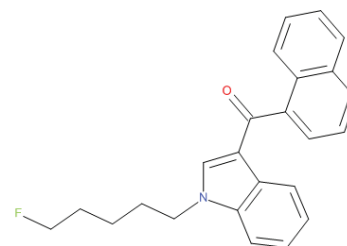
## Mass Spectrum:



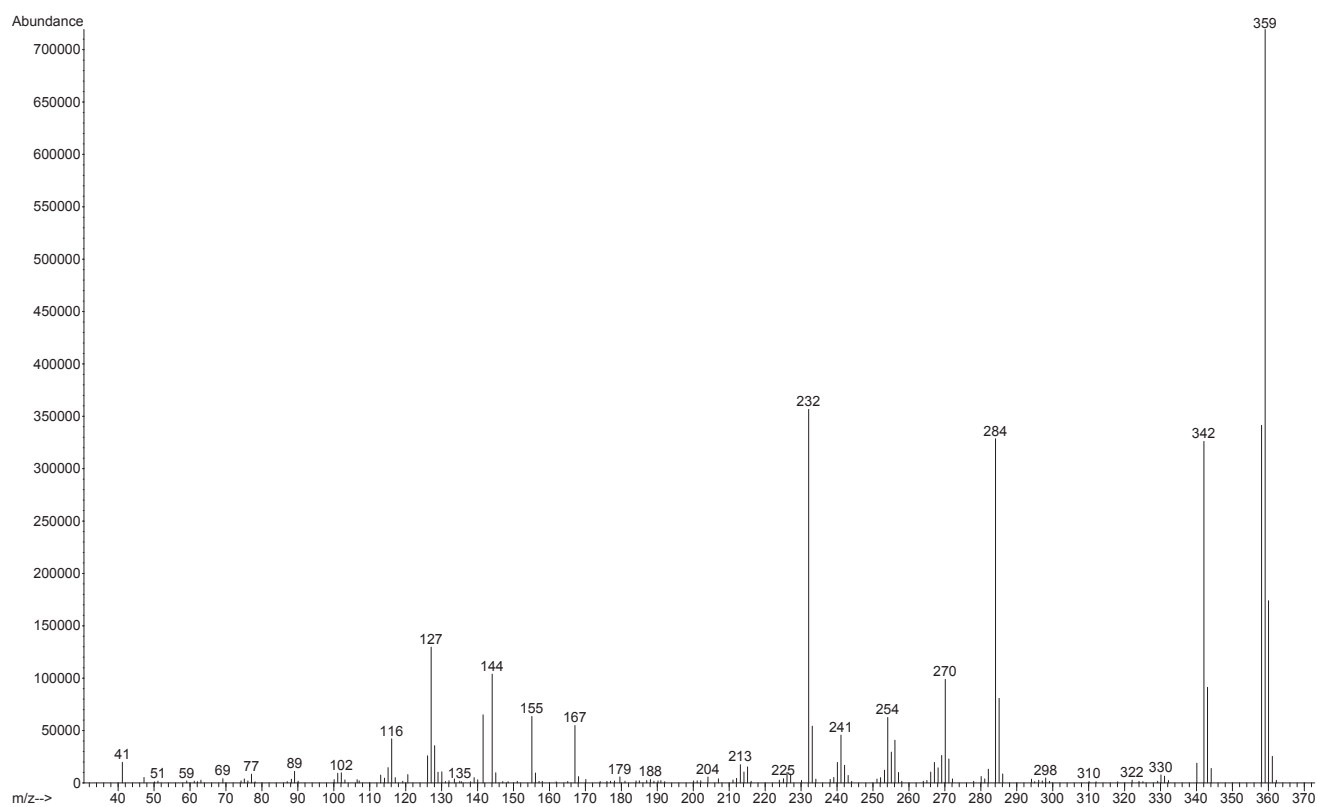
# AM-2201

Chemical name	1-[(5-fluoropentyl)-1H-indol-3-yl]-(naphthalen-1-yl)methanone	
Molecular formula	C <sub>24</sub> H <sub>22</sub> FO	
Molecular mass	359.17	
Major GC/MS ions	127.1, 232.2, 284.2, 359.3	
Ions used for analysis	Target	359.3
	Qualifier-1	232.2
	Qualifier-2	284.2
Retention time	13.41 minutes	
LOD	not yet established	
Additional comments	Does not form derivative	
	AM-2201 is the fluoro-analog of JWH-018	

## Molecular Structure:



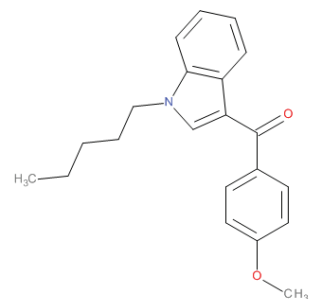
## Mass Spectrum:



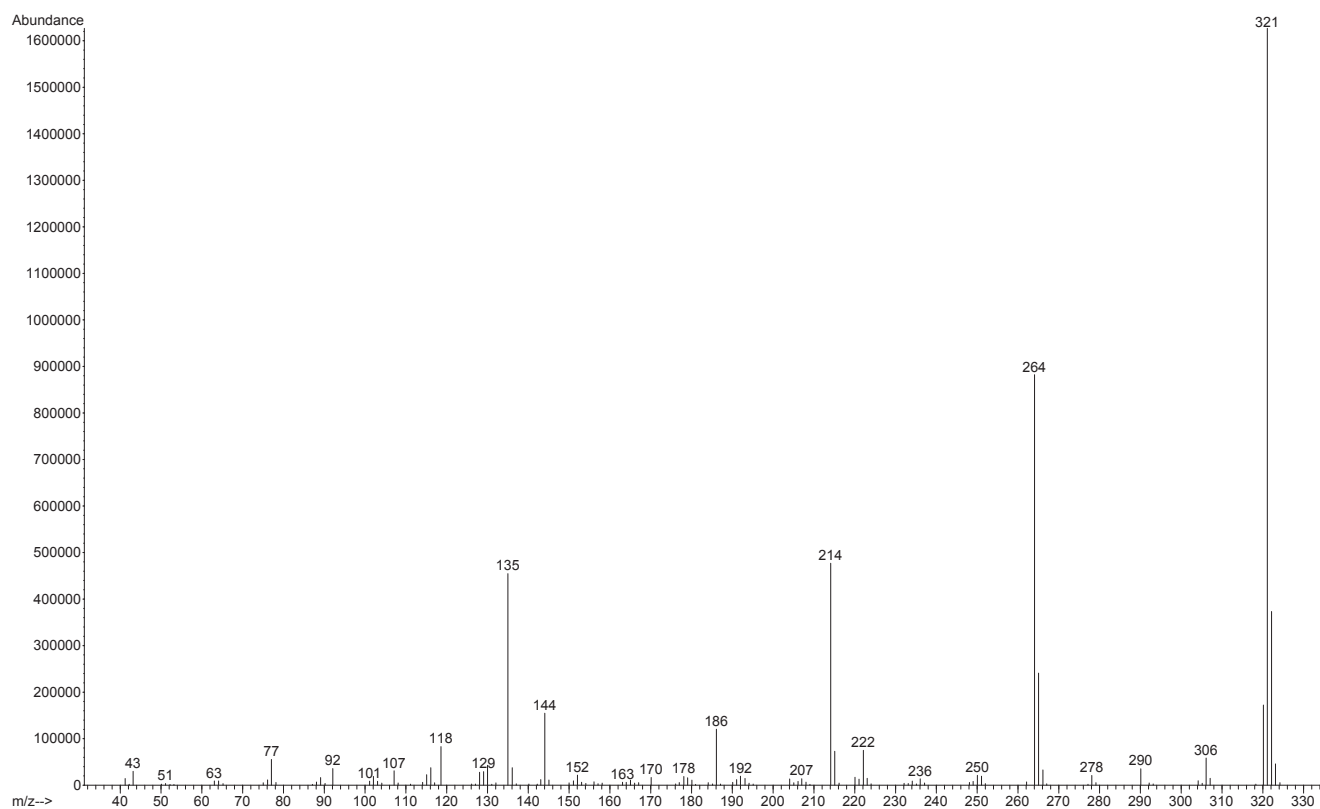
# RCS-4

Chemical name	((4-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone)	
Molecular formula	C <sub>21</sub> H <sub>23</sub> NO <sub>2</sub>	
Molecular mass	321.17	
Major GC/MS ions	321.3, 264.2, 214.2, 135.1, 144.1, 186.1	
Ions used for analysis	Target	321.3
	Qualifier-1	264.2
	Qualifier-2	214.2
Retention time	12.43 minutes	
LOD	not yet established	
Additional comments	RCS-4 will not derivatize	

## Molecular Structure:



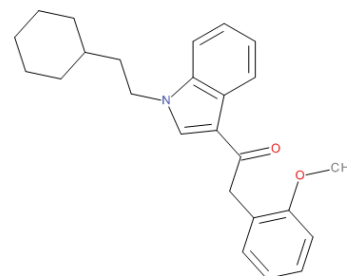
## Mass Spectrum:



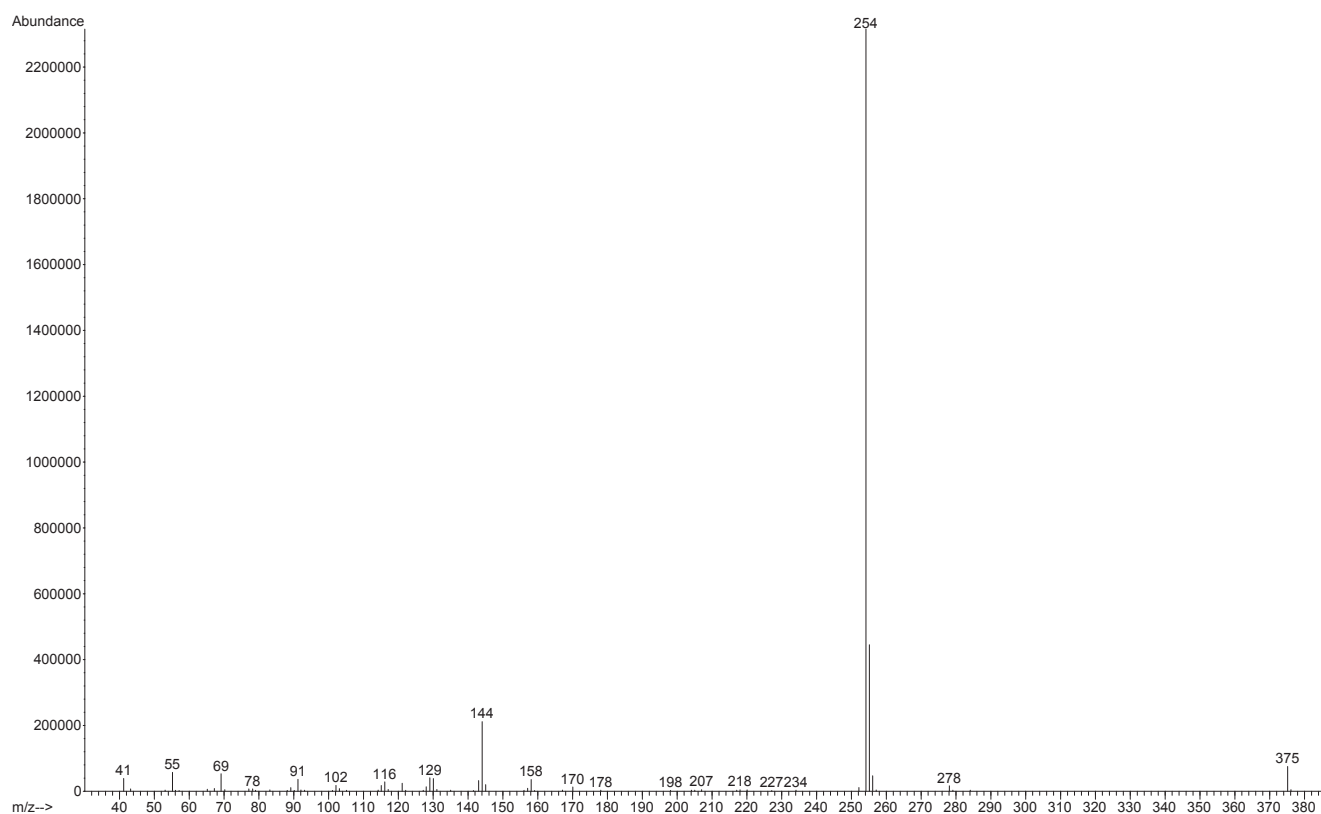
# RCS-8

Chemical name	1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(2-methoxyphenyl)ethanone	
Molecular formula	C <sub>25</sub> H <sub>29</sub> NO <sub>2</sub>	
Molecular mass	375.22	
Major GC/MS ions	254.2, 144.1, 375.3	
Ions used for analysis	Target	254.2
	Qualifier-1	144.1
	Qualifier-2	375.3
Retention time	13.66 minutes	
LOD	not yet established	
Additional comments	RCS-8 will not derivatize	

## Molecular Structure:



## Mass Spectrum:

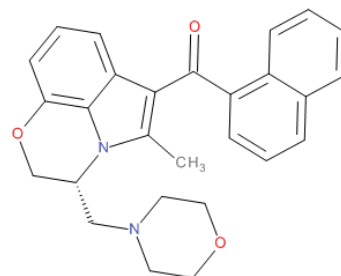




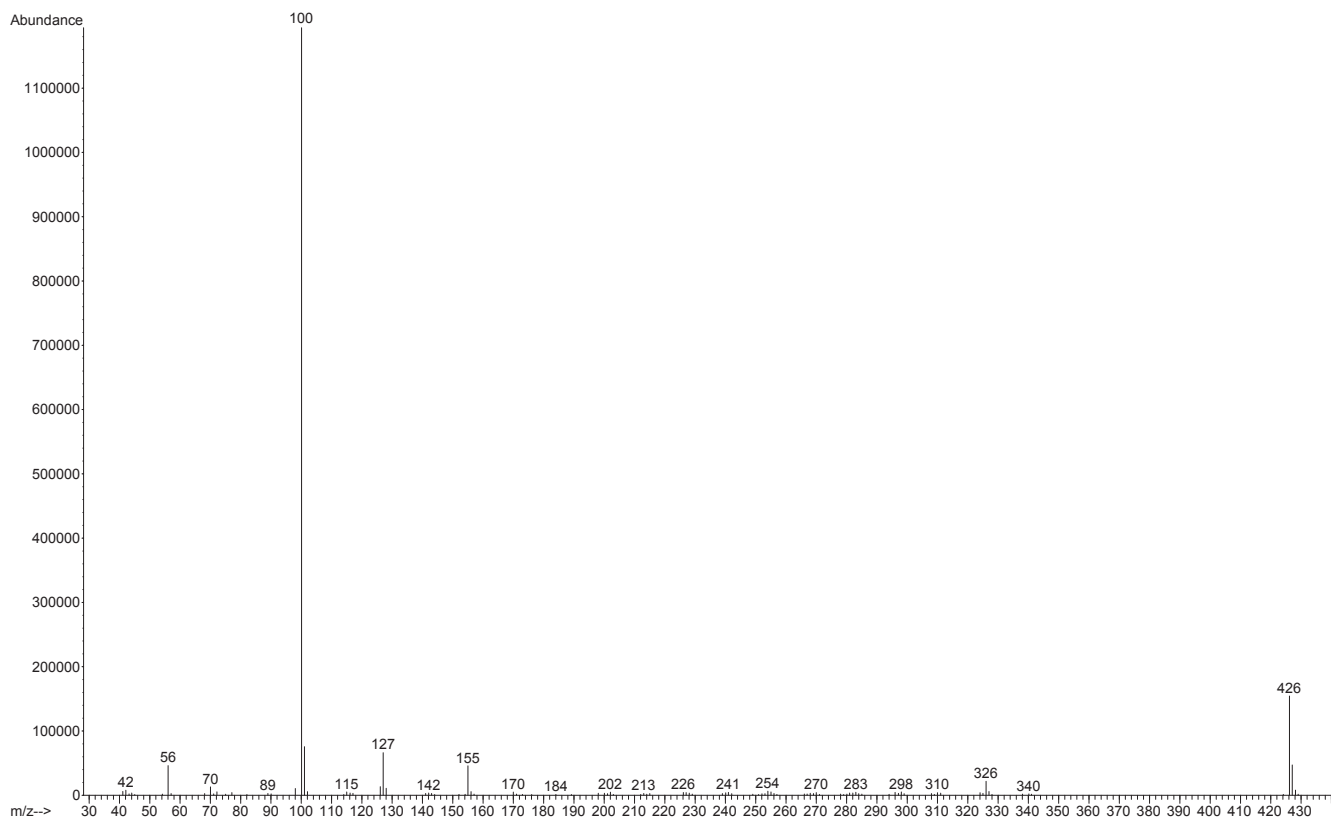
# WIN55,212-2

Chemical name	(R)-(+)-[2,3-Dihydro-5-methyl-3-(4-morpholinylmethyl)pyrrolo [1,2,3-de]-1,4-benzoxazin-6-yl]-1-napthalenylmethanone		
Molecular formula	C <sub>27</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>		
Molecular mass	426.19		
Major GC/MS ions	100.0, 127.1, 155.1, 326.3, 426.4, 56.0		
Ions used for analysis	Target	100.0	
	Qualifier-1	426.4	
	Qualifier-2	127.1	
Retention time	15.38 minutes		
LOD	0.12 mg/g		
Additional comments	WIN55,212-2 will not derivatize. WIN55,212-2 and WIN55,212-3 are isomers and are indistinguishable.		

## Molecular Structure:



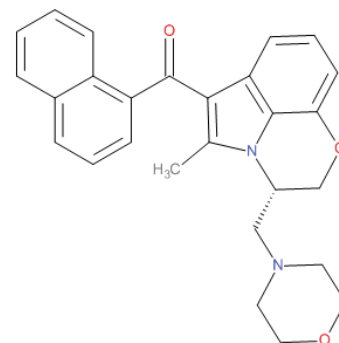
## Mass Spectrum:



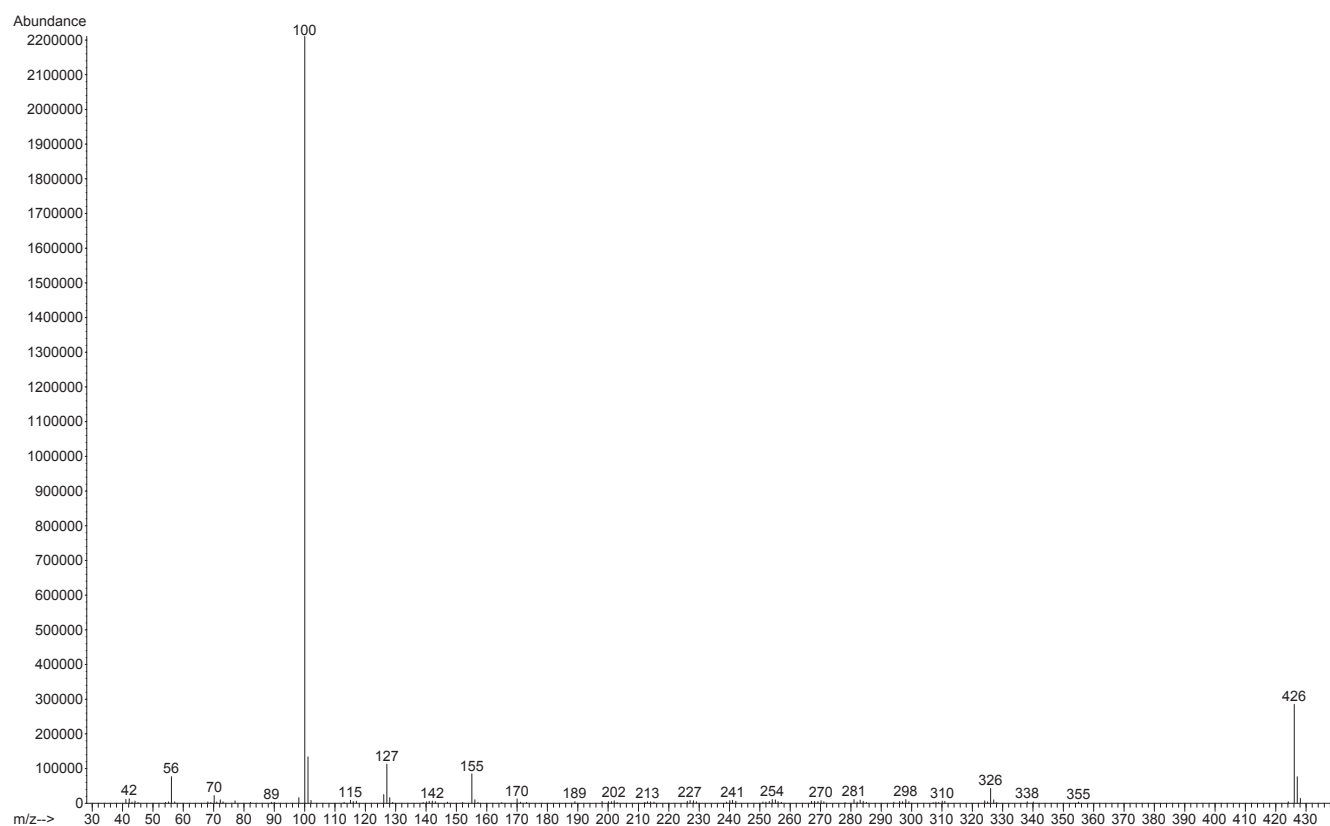
# WIN55,212-3

Chemical name	[(3S)-2,3-Dihydro-5-methyl-3-(4-morpholinylmethyl)pyrrolo[1,2,3-de]-1,4-benzoxazin-6-yl]-1-naphthalenyl-methanone	
Molecular formula	C <sub>27</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>	
Molecular mass	426.19	
Major GC/MS ions	100.0, 127.1, 155.1, 326.3, 426.4, 56.0	
Ions used for analysis	Target	100.0
	Qualifier-1	426.4
	Qualifier-2	127.1
Retention time	15.38 minutes	
LOD	0.12 mg/g	
Additional comments	WIN55,212-2 will not derivatize. WIN55,212-2 and WIN55,212-3 are isomers and are indistinguishable.	

## Molecular Structure:



## Mass Spectrum:



## For more information

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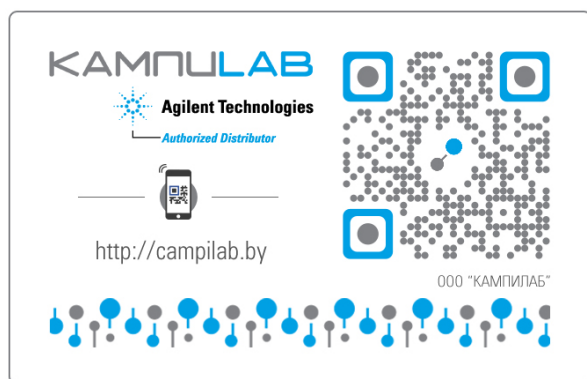
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