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

Application Compendium

The Measure of Confidence

Agilent Technologies

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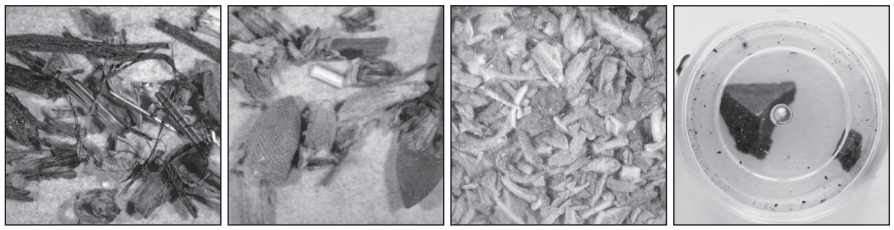
# Identification of Synthetic Cannabinoids in Herbal Incense Blends by GC/MS

Application Compendium



## Introduction

By Fran Diamond, Chemistry Technical Leader, NMS Labs

The recent phenomenon of synthetic cannabinoid usage has given law enforcement and forensic laboratories a series of challenges to overcome in order to provide testing of these new materials. Few certified synthetic laboratories have been able to keep up with numerous analogous and homologous materials that are used. Forensic laboratories have had a difficult time obtaining pure reference material to use for positive identifi cation. 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 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, scientifi c 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 the production of these drugs contain active, polar funtional 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 uL 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 µL 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

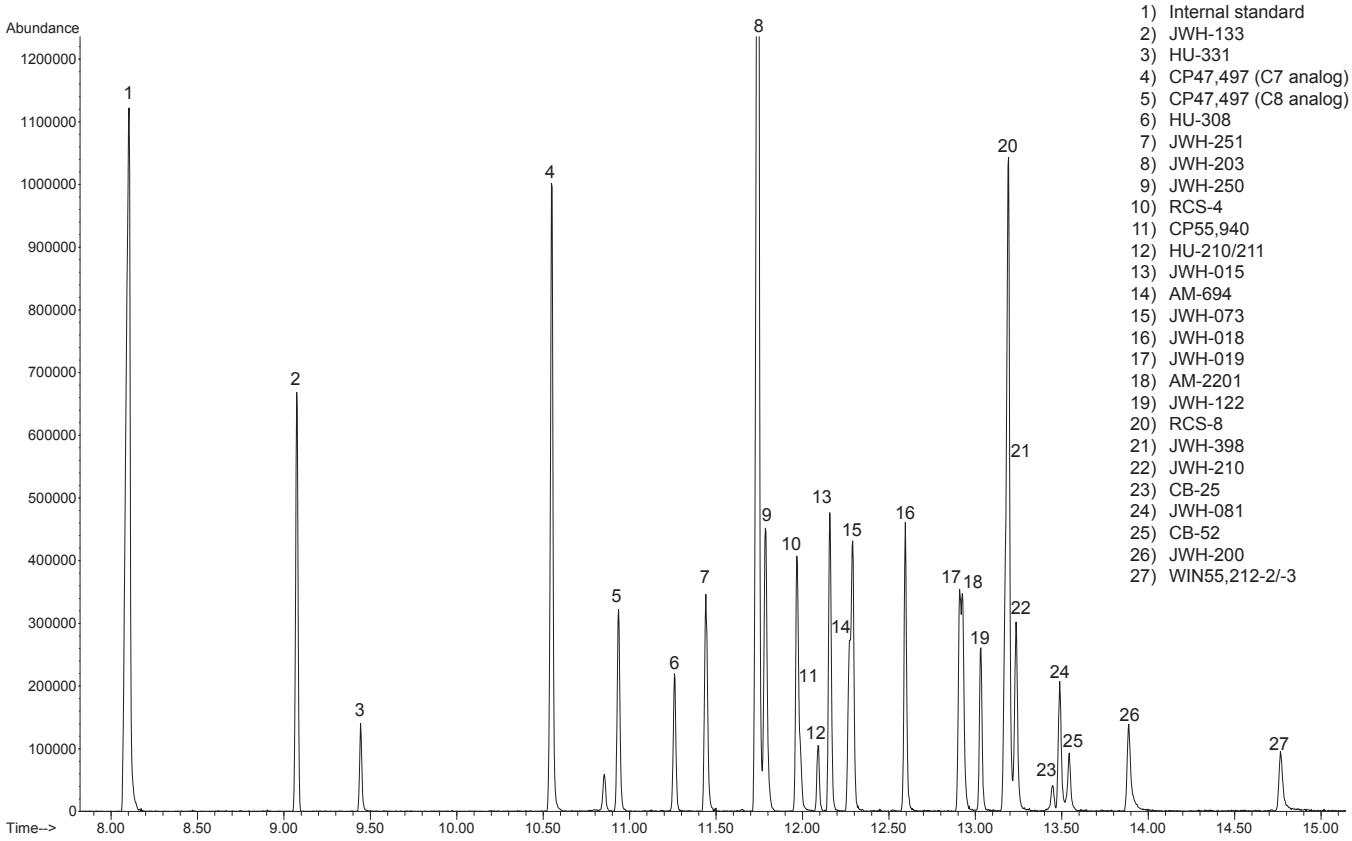
| **Inlet** | EPC Split/splitless |
|---|---|
| Mode | Constant pressure |
| Injection type | Splitless |
| Injection volume (uL) | 1.0 |
| Inlet temperature (°C) | 265 |
| Pressure nominal (psig) | 20.70 |
| Purge flow (ml/min.) | 50 |
| Purge time (min.) | 0.30 |
| Gas type | Helium |

| **Oven** | |
|---|---|
| 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 |

| **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) | 620 |
| Threshold | 250 |
| Sampling | 1 |
| Quad temp (°C) | 150 |
| Source temp (°C) | 230 |
| Transfer line temp (°C) | 300 |

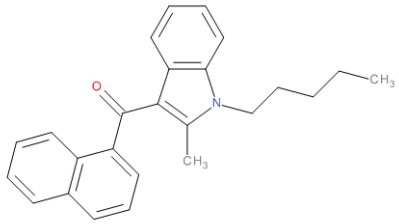
# GC/MS Total Ion Chromatogram of the Synthetic Cannabinoids Evaluated



# JWH-007

| | | |
|---|---|---|
| Chemical name | 1-pentyl-2-methyl-3-(1-naphthoyl)indole | |
| Molecular formula | $C_{25}H_{25}NO$ | |
| 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:**

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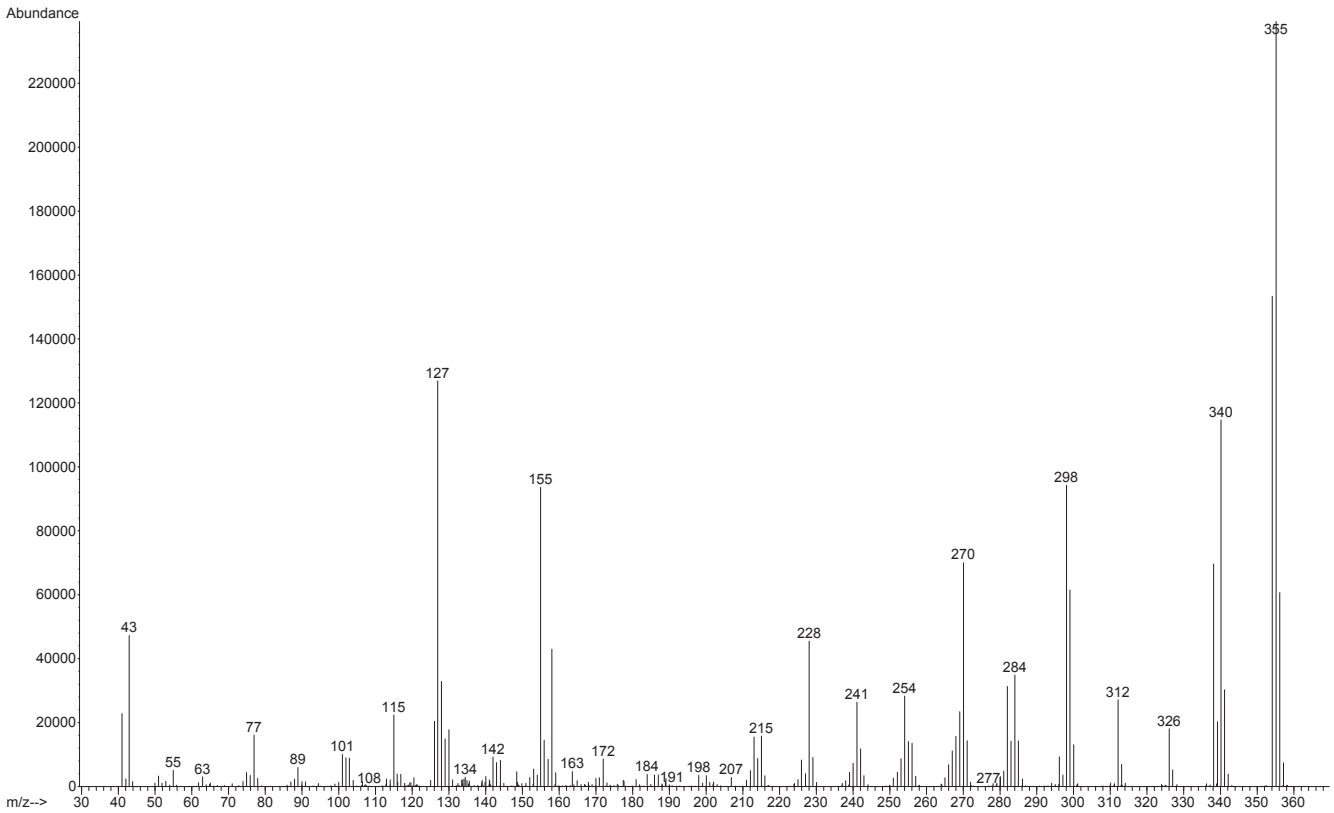
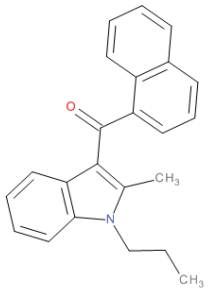


# JWH-015

| | | |
|---|---|---|
| Chemical name | (2-Methyl-1-propyl-1H-indol-3-yl)-1-naphthalenylmethanone | |
| Molecular formula | $C_{23}H_{21}NO$ | |
| 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.<br>JWH-015 and JWH-073 are formula isomers. They have similar fragmentation patterns with slight differences in retention time. | |

**Molecular Structure:**

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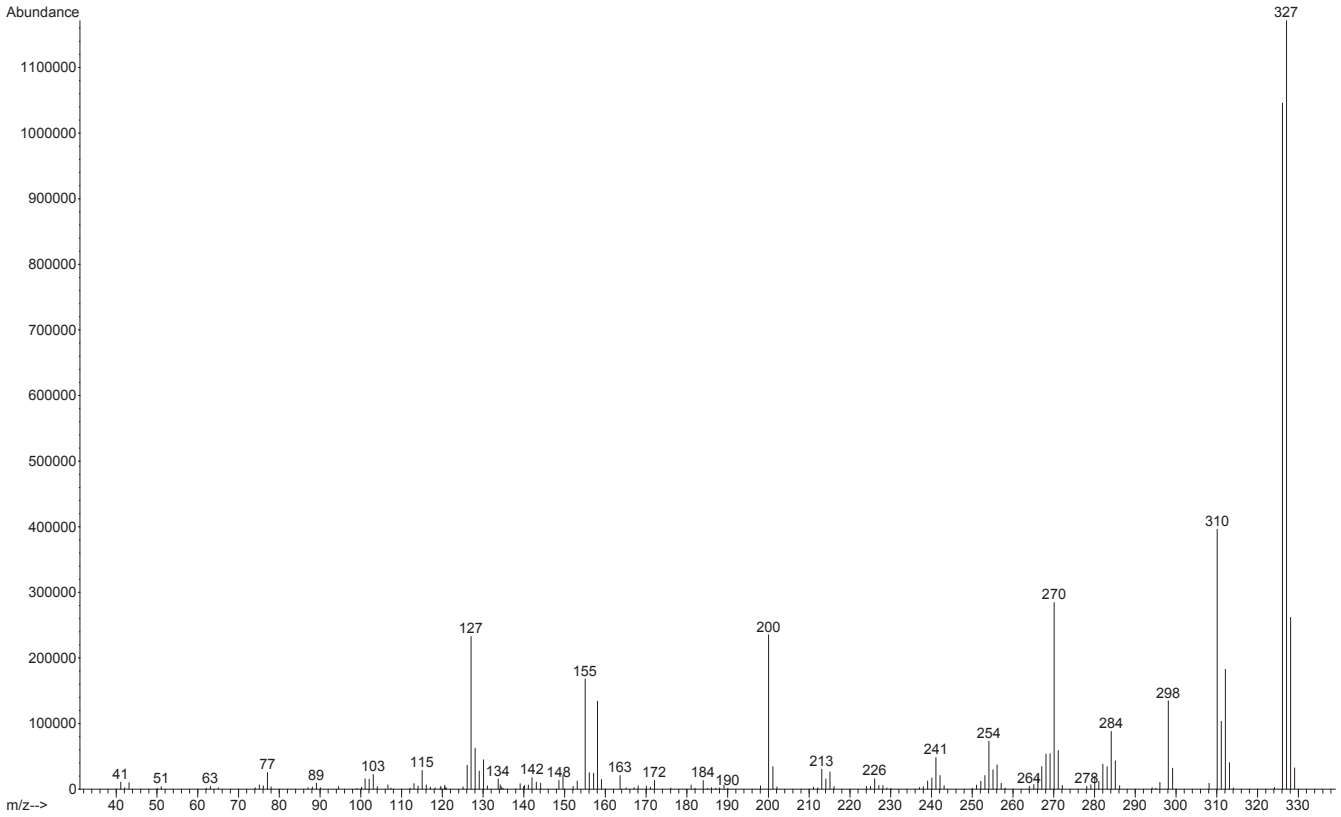
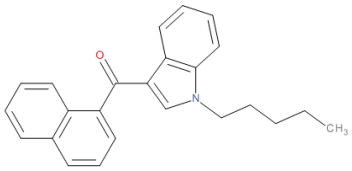


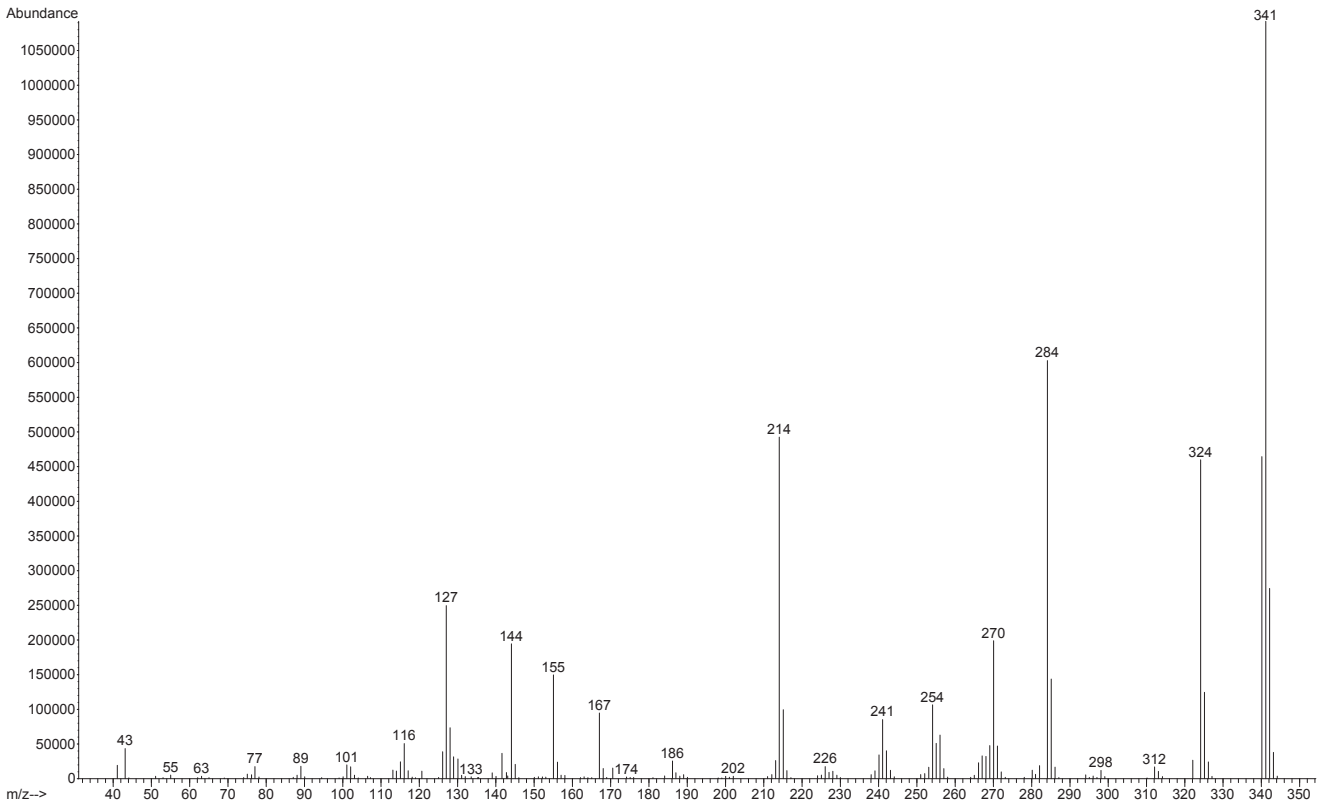
# JWH-018

| | | |
|---|---|---|
| Chemical name | Naphthalen-1-yl-(1-pentylindol-3-yl)methanone | |
| Molecular formula | $C_{24}H_{23}NO$ | |
| 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:**



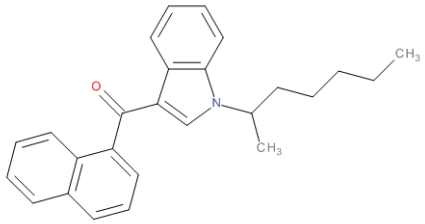

**Mass Spectrum:**



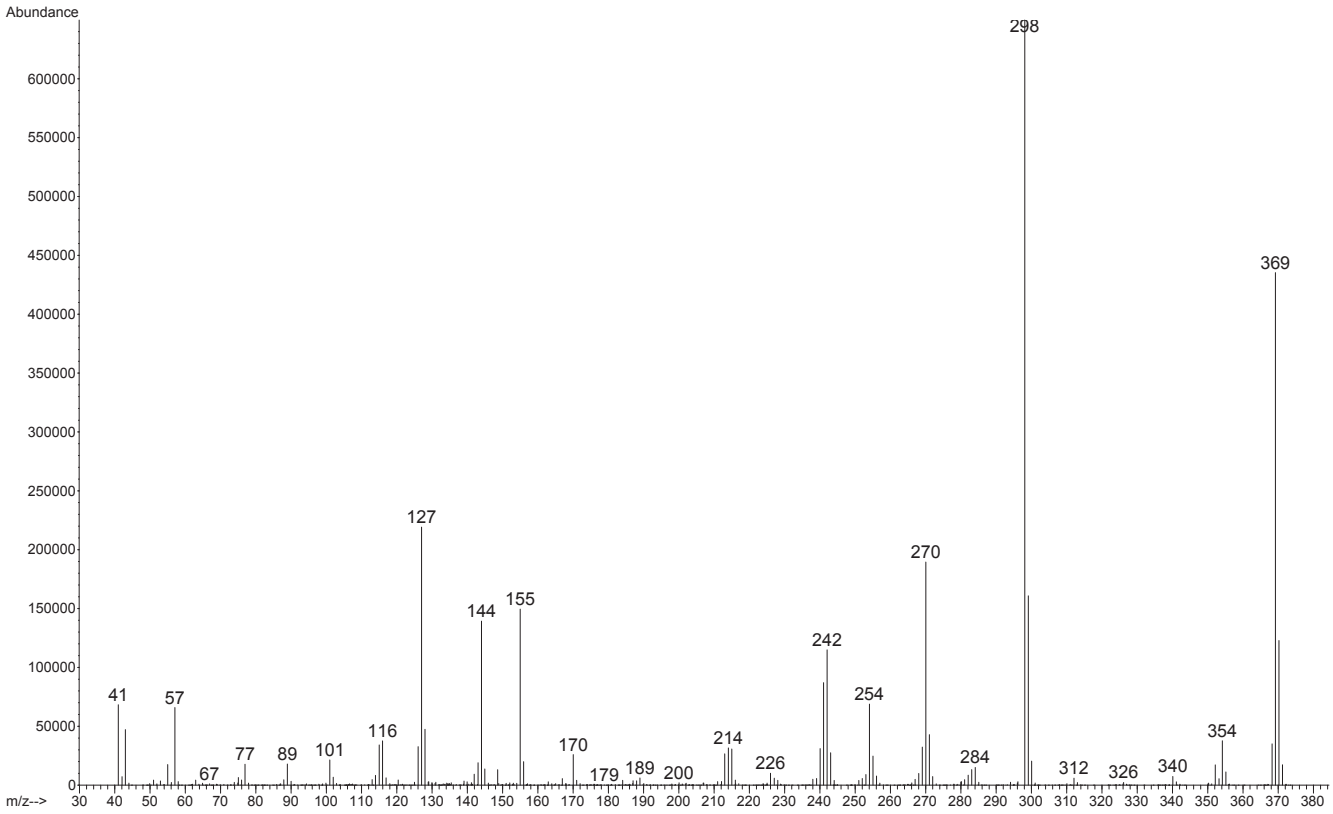
# JWH-018 1-methylhexyl homolog

| | | |
|---|---|---|
| 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:**



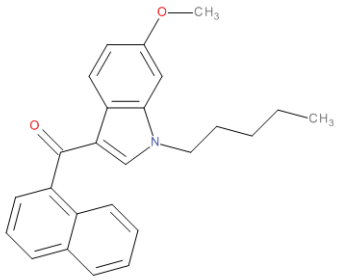

**Mass Spectrum:**



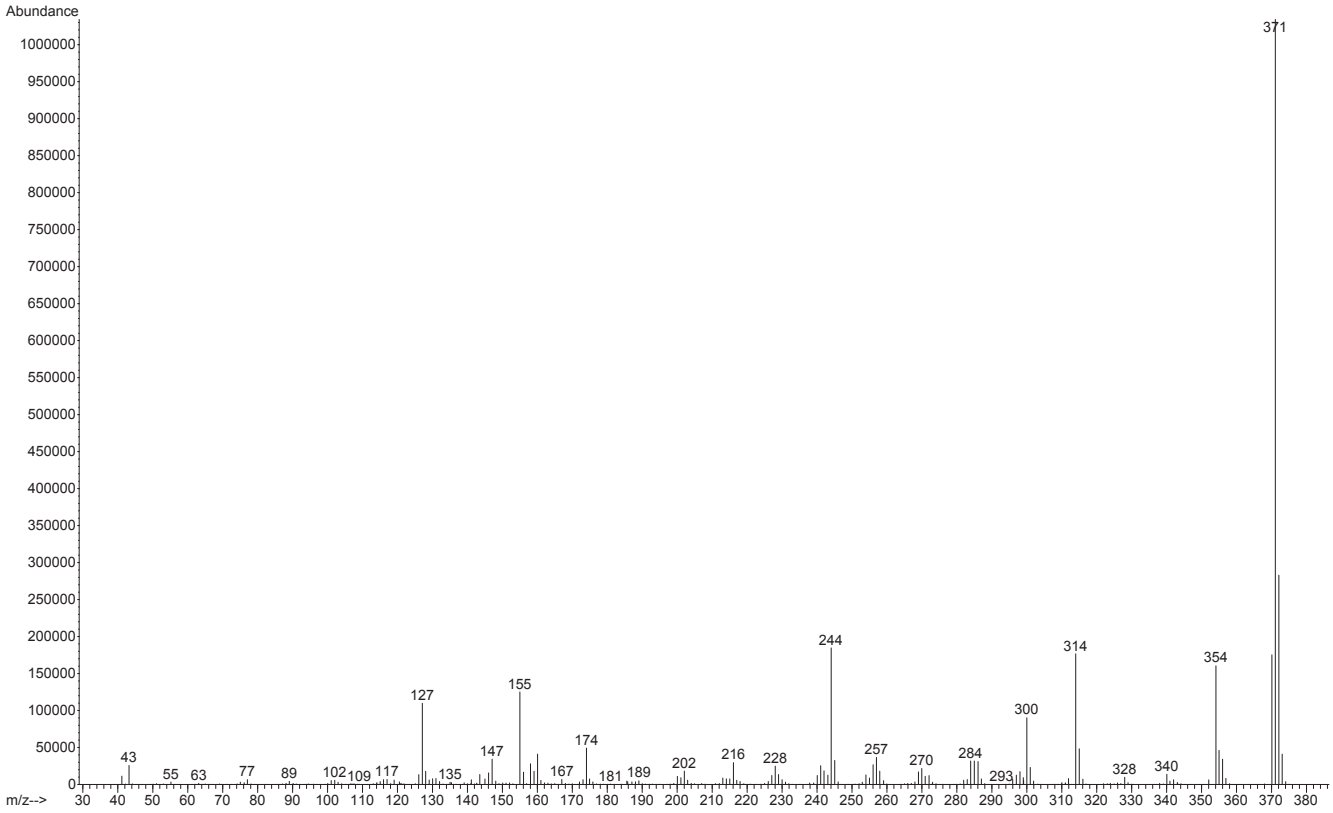
# JWH-018 6-methoxyindole analog

| | | |
|---|---|---|
| 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:**



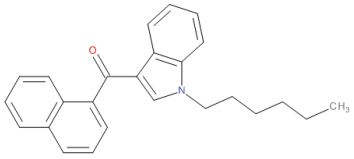

**Mass Spectrum:**



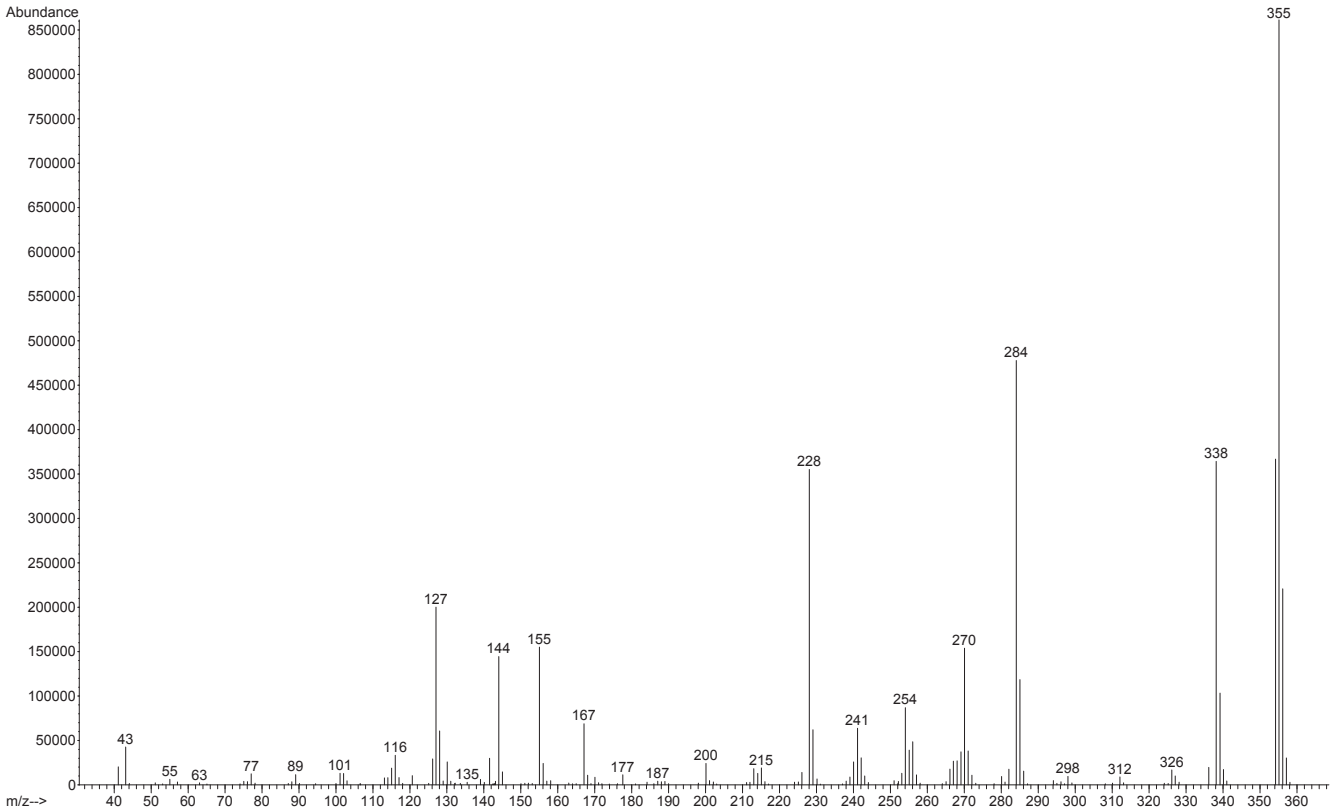
# JWH-019

| | | |
|---|---|---|
| Chemical name | Naphthalen-1-yl-(1-pentylindol-3-yl)methanone | |
| Molecular formula | $C_{25}H_{25}NO$ | |
| 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:**



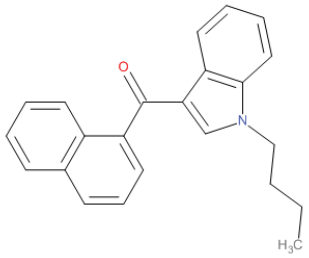

**Mass Spectrum:**



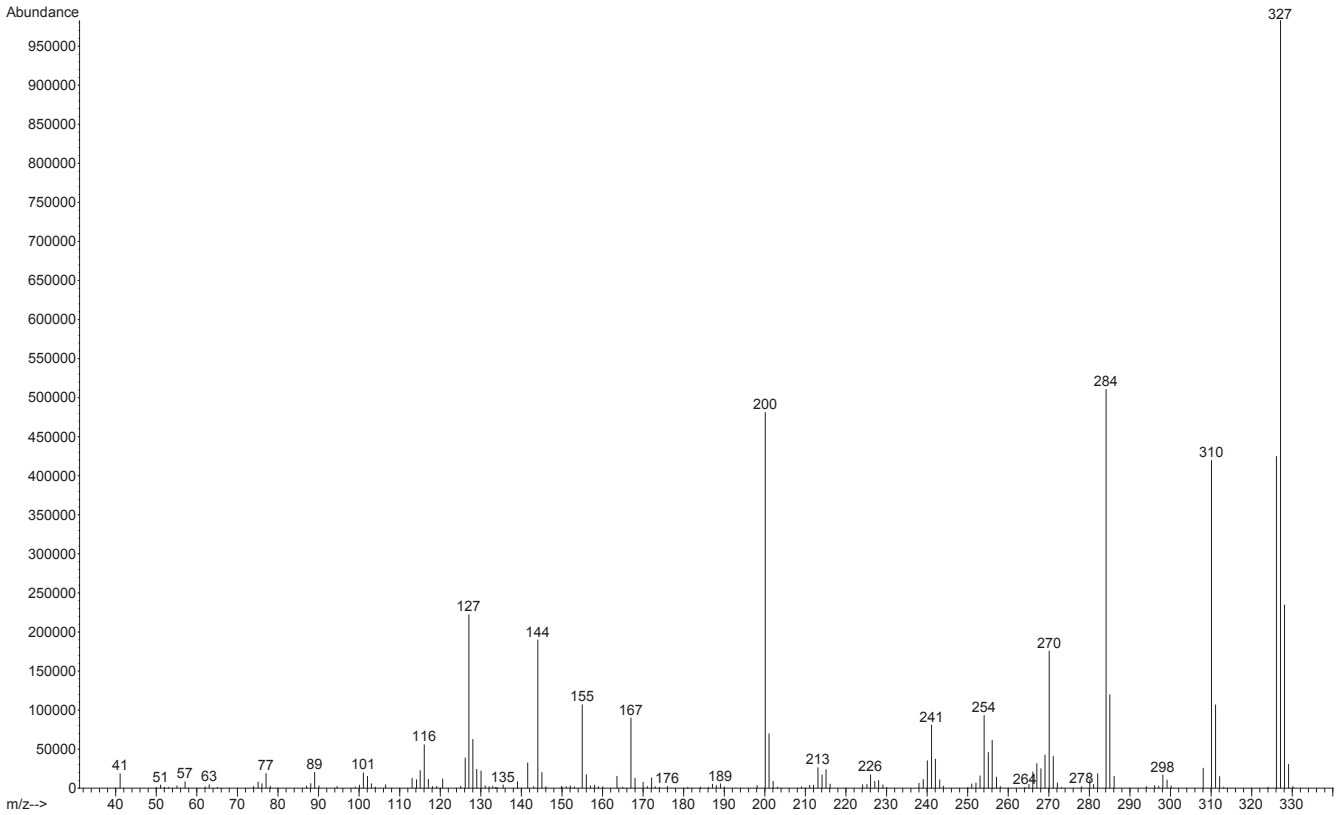
# JWH-073

| | | |
|---|---|---|
| Chemical name | naphthalen-1-yl-(1-butylindol-3-yl)meth | |
| Molecular formula | $C_{23}H_{21}NO$ | |
| 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:**



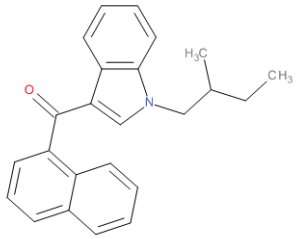

**Mass Spectrum:**



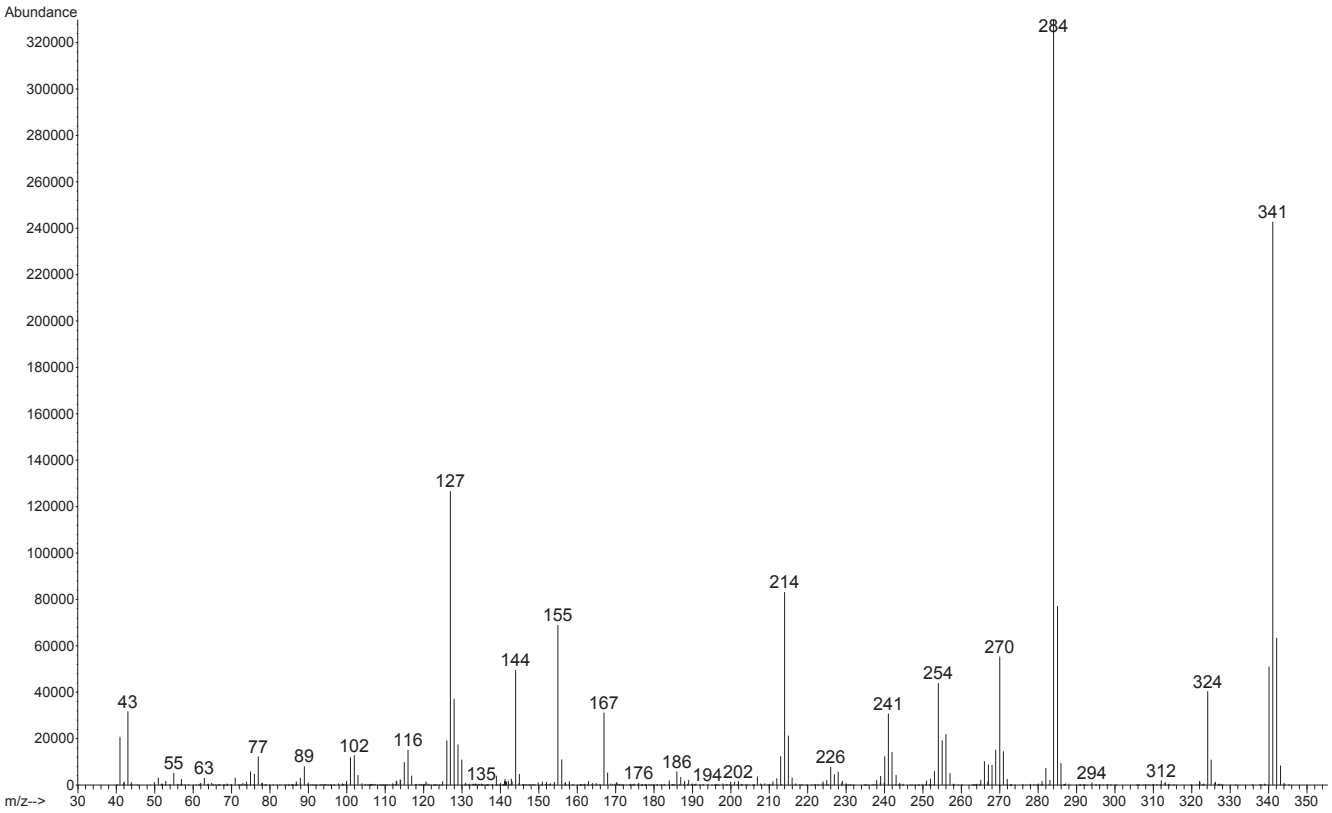
# JWH-073 2-methylbutyl homolog

| | | |
|---|---|---|
| Chemical name | N-(2-methylbutyl)-3-(1-naphthoyl)-indole | |
| Molecular formula | $C_{24}H_{23}NO$ | |
| 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:**



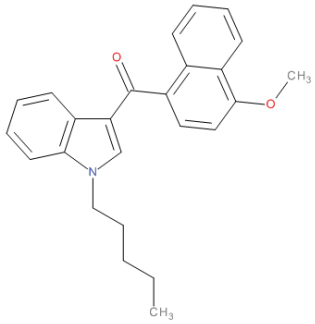

**Mass Spectrum:**



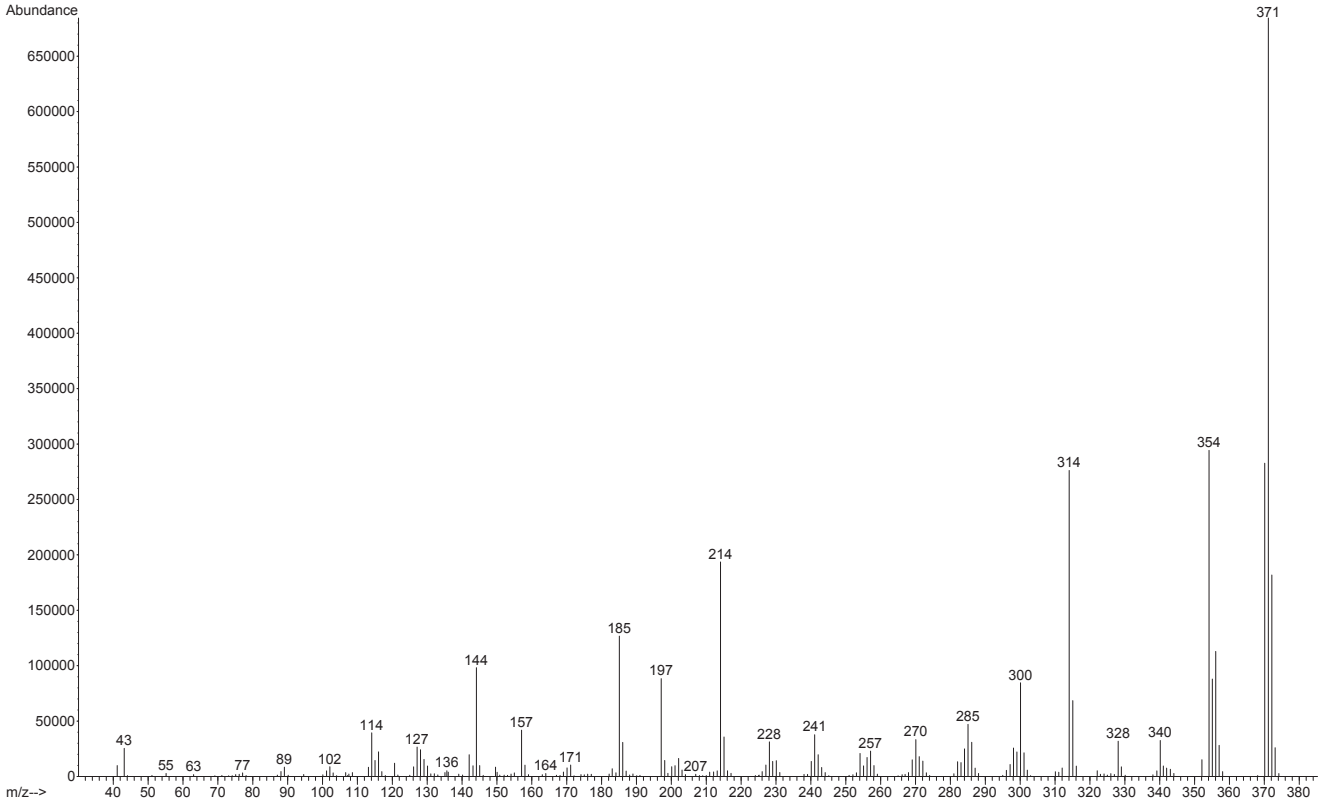
# JWH-081

| | | |
|---|---|---|
| Chemical name | 4-methoxynaphthalen- 1-yl- (1-pentylindol- 3-yl)methanone | |
| Molecular formula | $C_{25}H_{25}NO_2$ | |
| 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:**



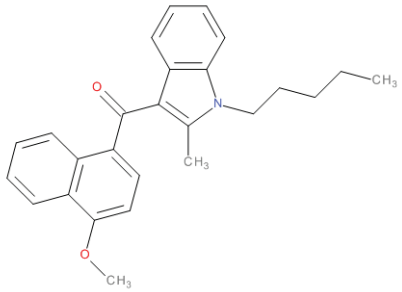

**Mass Spectrum:**



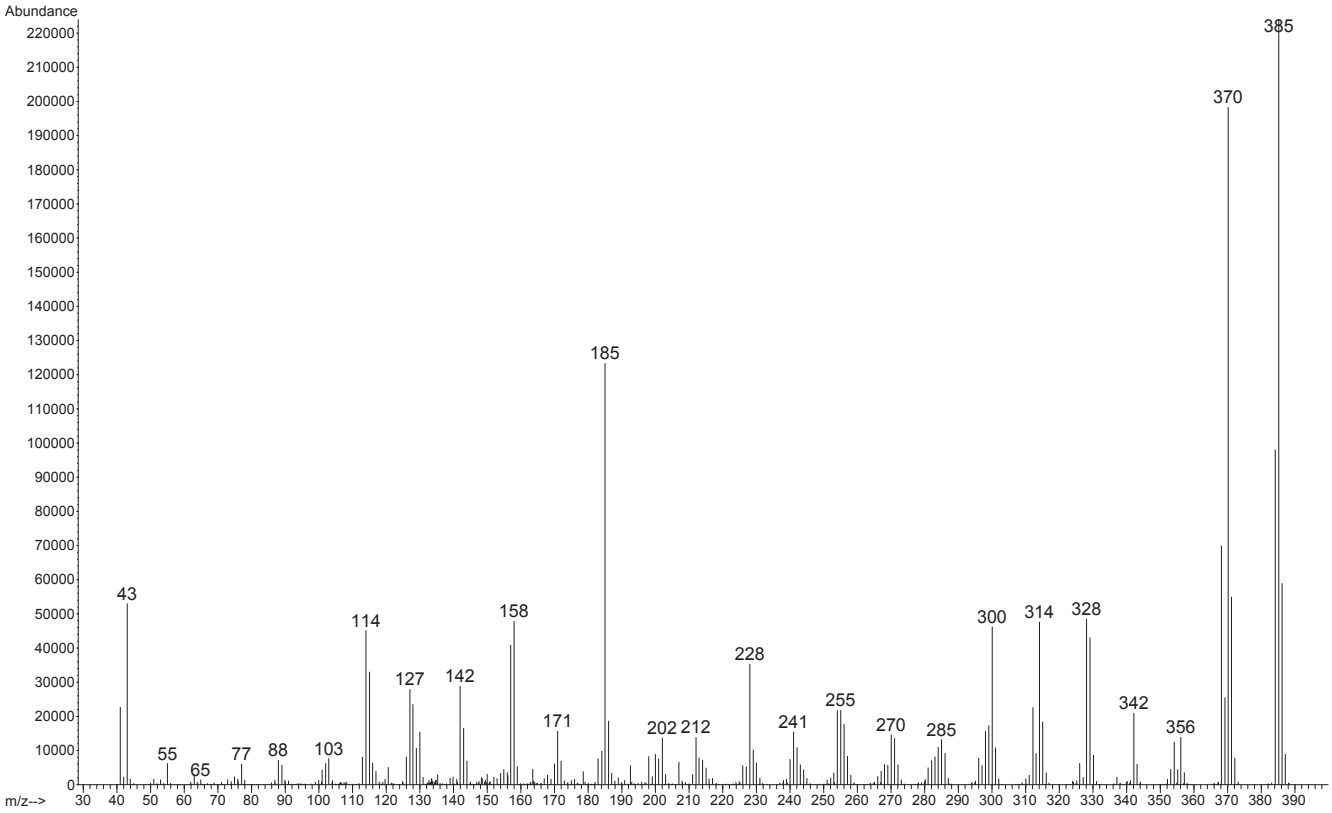
# JWH-098

| | | |
|---|---|---|
| Chemical name | 4-methoxynaphthalen-1-yl-(1-pentyl-2-methylindol-3-yl) methanone | |
| Molecular formula | $C_{26}H_{27}NO_2$ | |
| 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:**



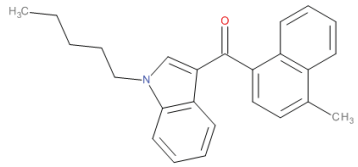

**Mass Spectrum:**



# JWH-122

| | | |
|---|---|---|
| Chemical name | 1-Pentyl-3-(4-methyl-1-naphthoyl)indole | |
| Molecular formula | $C_{25}H_{25}NO$ | |
| 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:**

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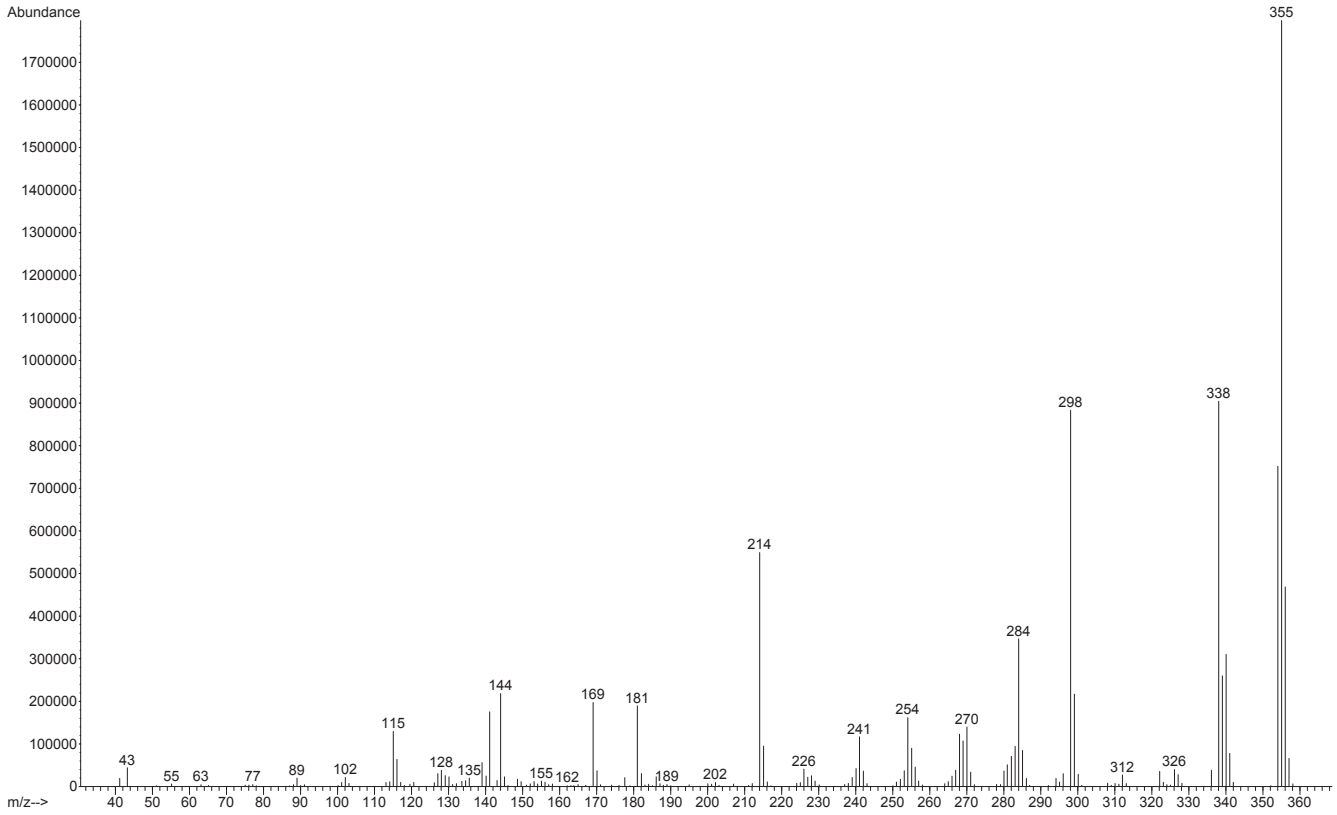
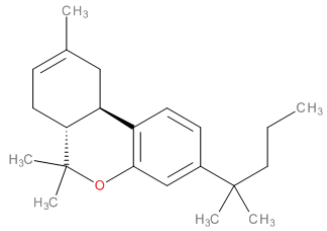


# JWH-133

| | | |
|---|---|---|
| Chemical name | (6aR,10aR)-3-(1,1-Dimethylbutyl)-6a,7,10,10a-tetrahydro -6,6,9-trimethyl-6H-dibenzo[b,d]pyran | |
| Molecular formula | $C_{22}H_{32}O$ | |
| 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:**

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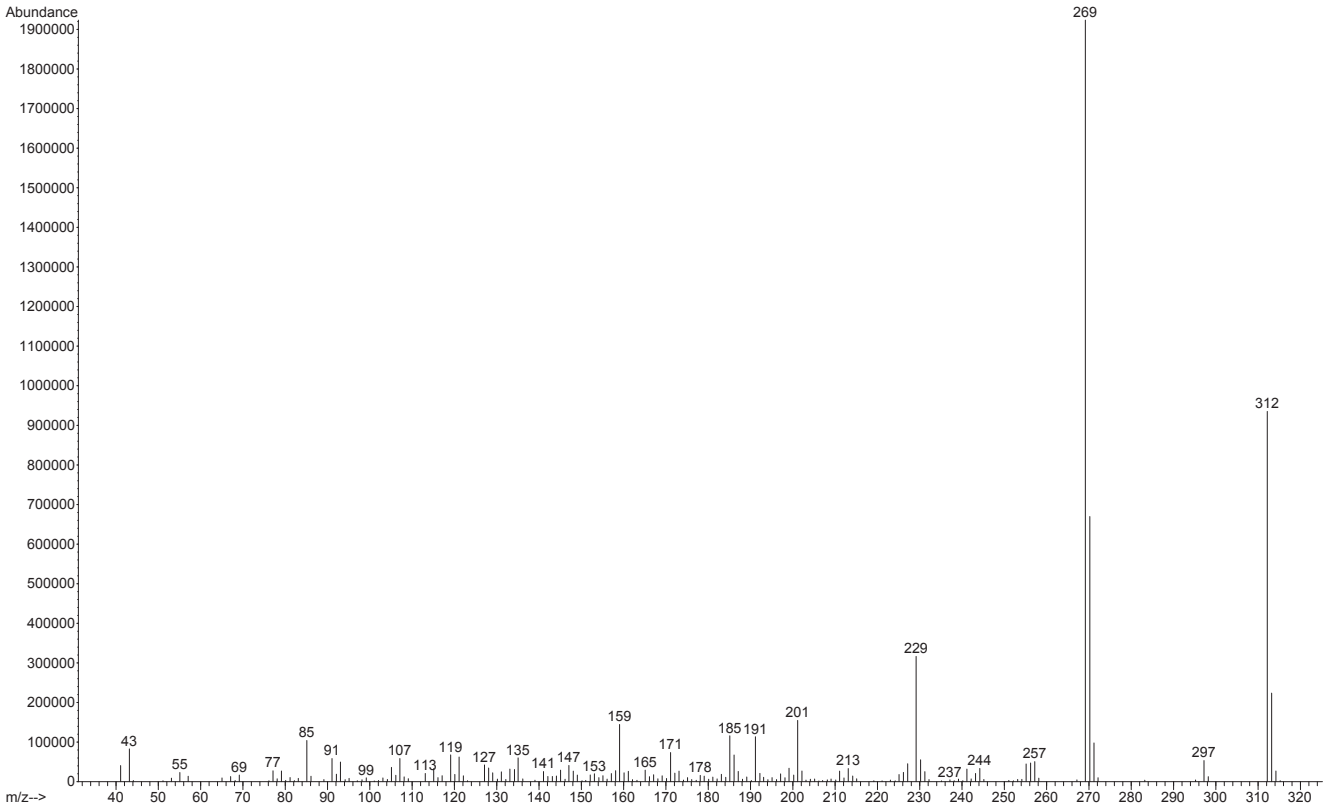
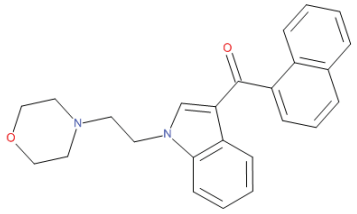


# JWH-200

| | | |
|---|---|---|
| Chemical name | (1-(2-morpholin-4-ylethyl)indol-3-yl)-naphthalen-1-ylmethanone | |
| Molecular formula | $C_{25}H_{24}N_2O_2$ | |
| 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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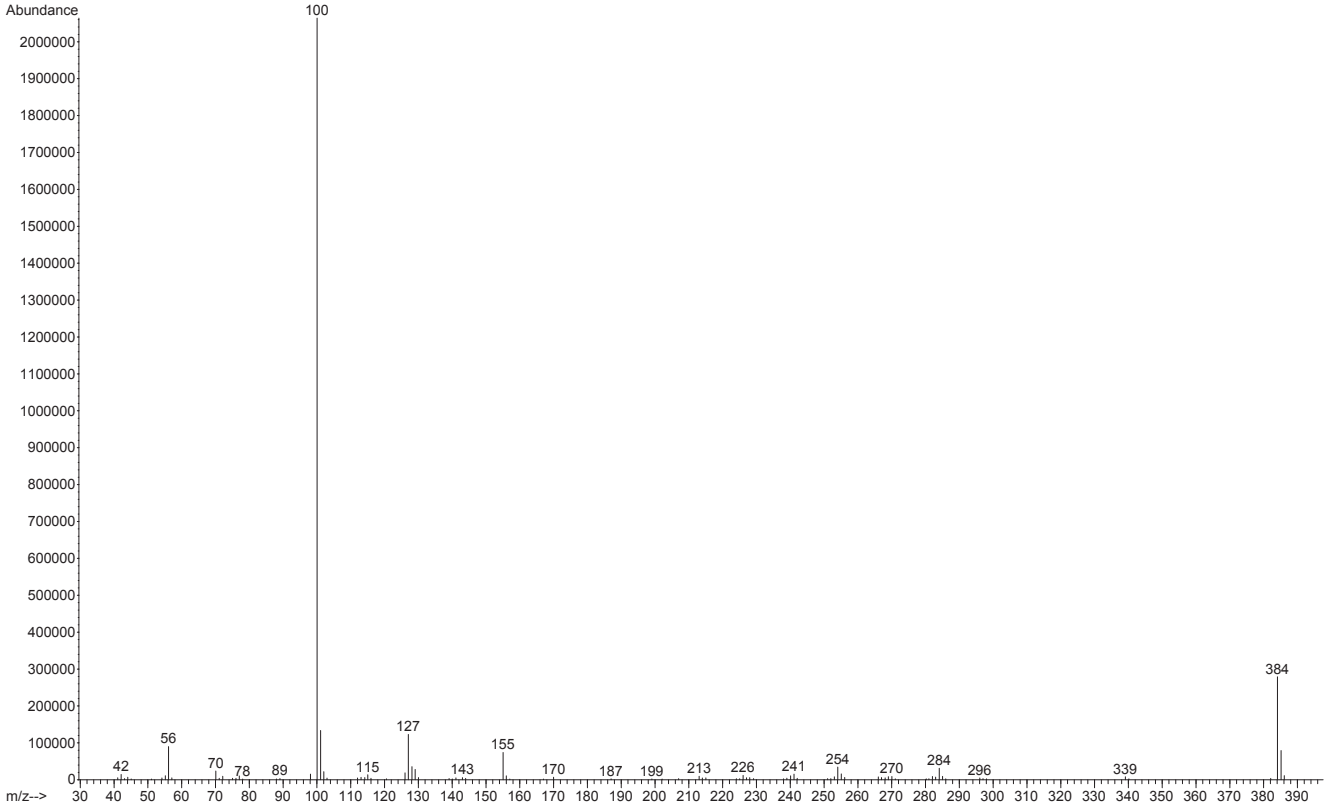
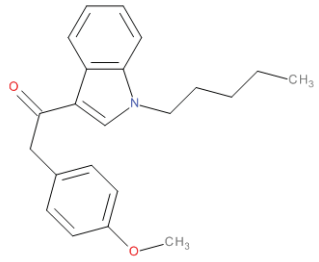


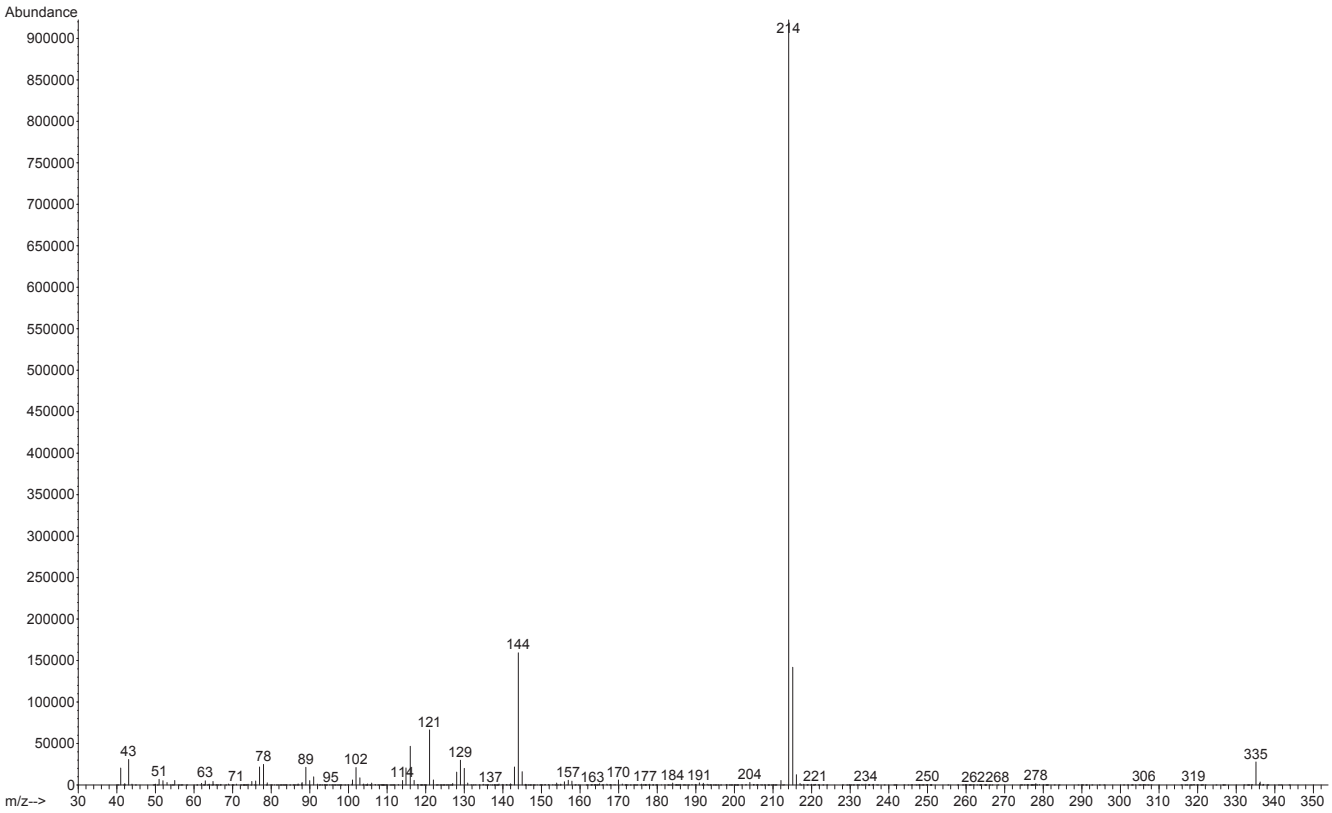
# JWH-201

| | | |
|---|---|---|
| Chemical name | 2-(4-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl)-ethanone | |
| Molecular formula | $C_{22}H_{25}NO_2$ | |
| 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:**



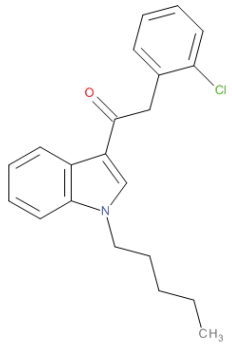

**Mass Spectrum:**



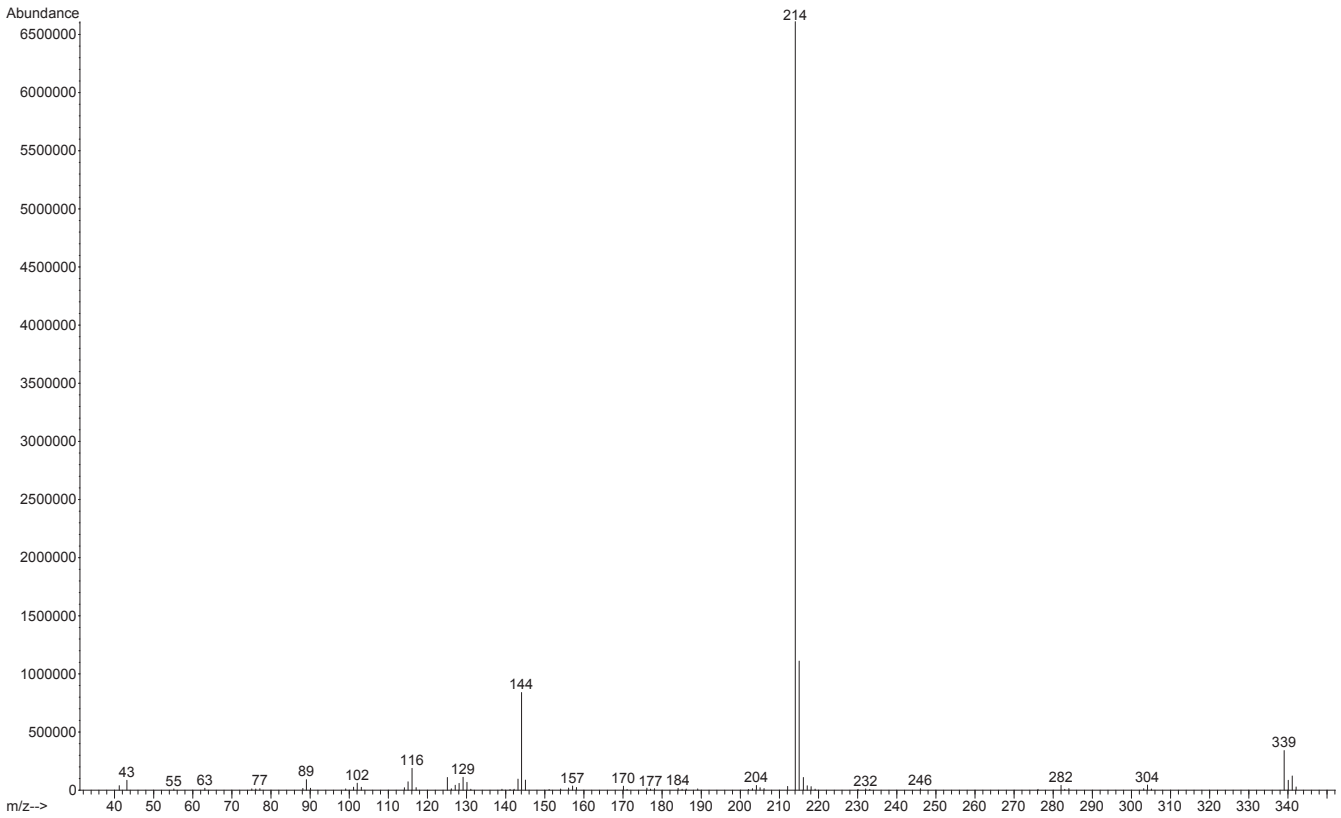
# JWH-203

| | | |
|---|---|---|
| Chemical name | 2-(2-chlorophenyl)-1-(1-pentylindol-3-yl)ethanone | |
| Molecular formula | $C_{21}H_{22}ClNO$ | |
| 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:**



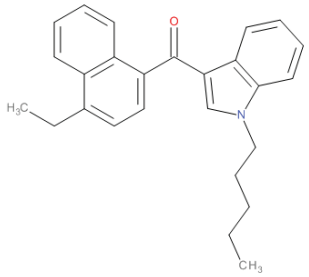

**Mass Spectrum:**



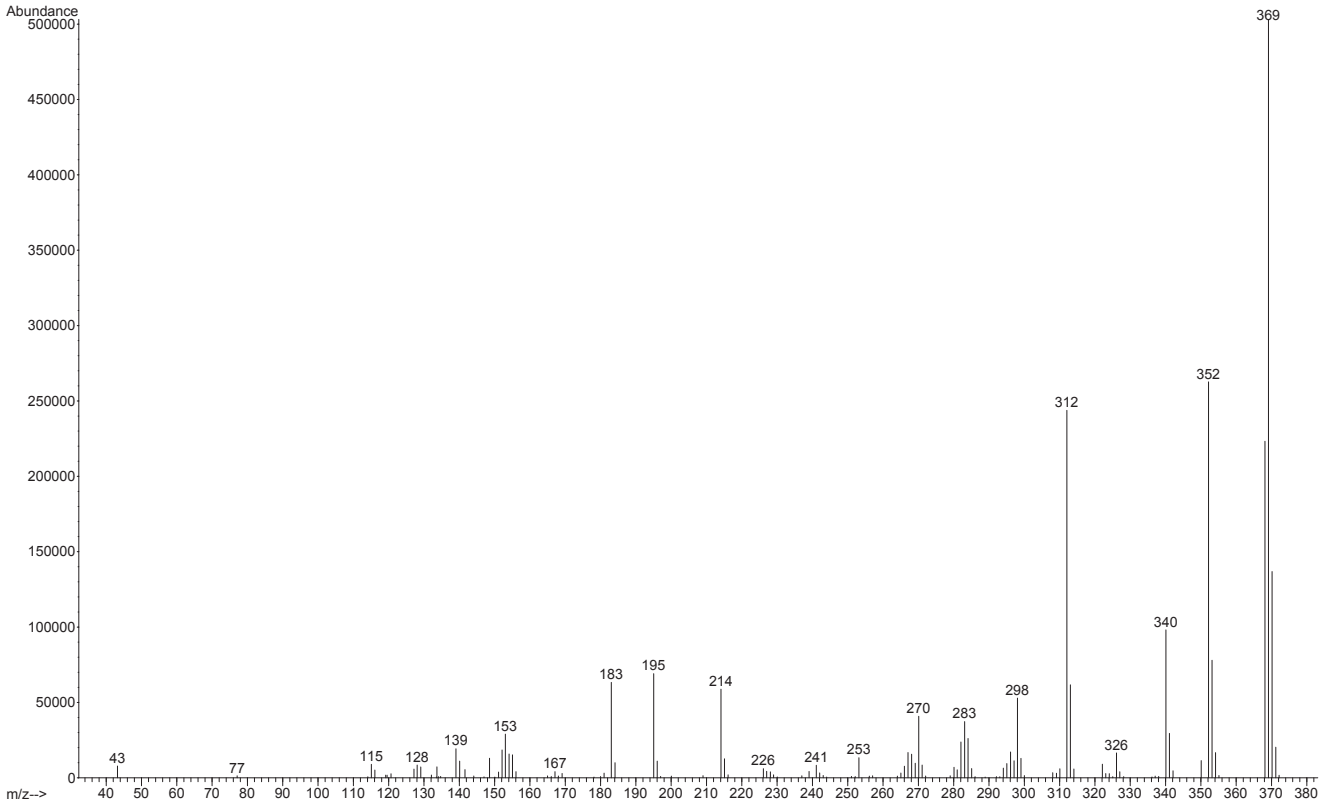
# JWH-210

| | | |
|---|---|---|
| Chemical name | 4-ethylnaphthalen-1-yl-(1-pentylindol-3-yl)methanone | |
| Molecular formula | $C_{26}H_{27}NO$ | |
| 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:**



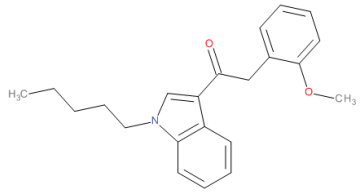

**Mass Spectrum:**



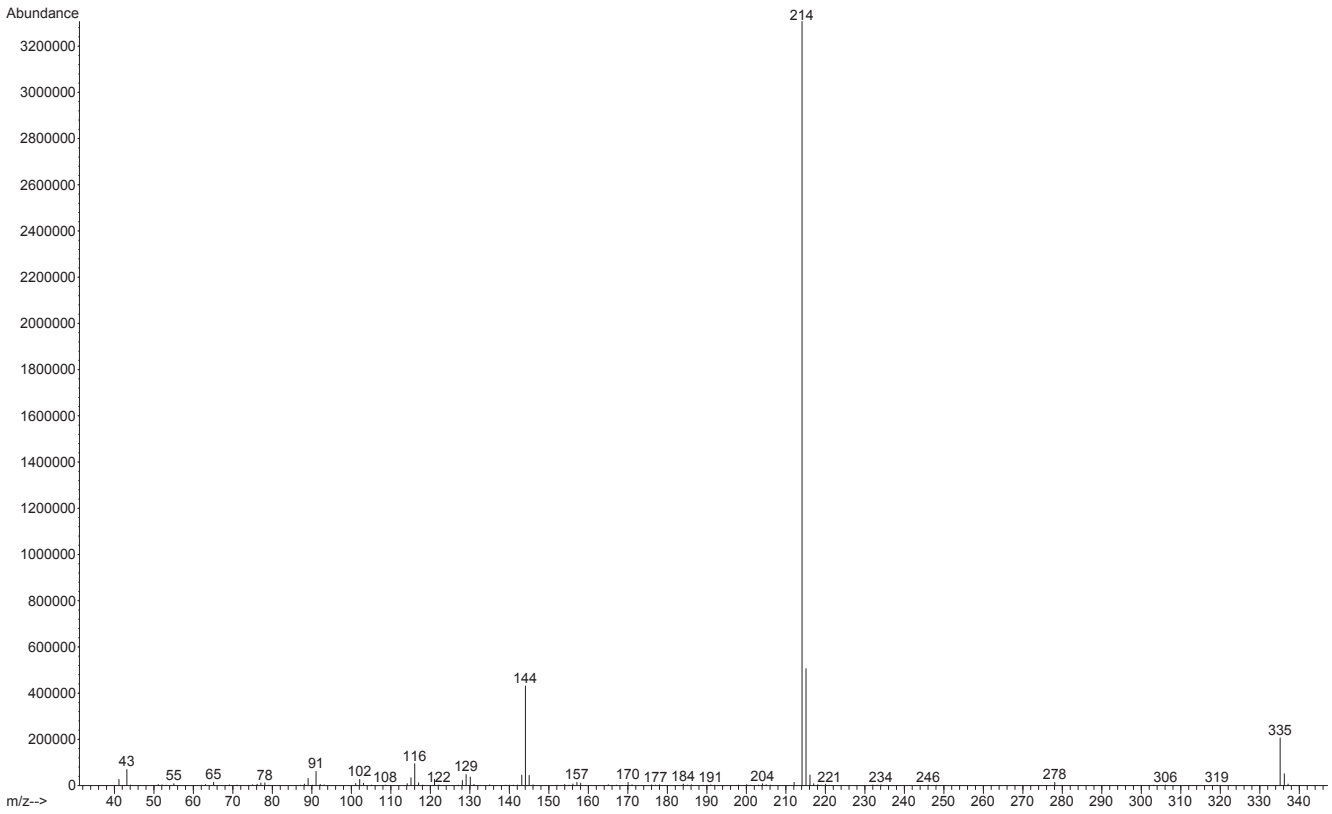
# JWH-250

| | | |
|---|---|---|
| Chemical name | 2-(2-methoxyphenyl)-1-(1-pentylindol-3-yl)ethanone | |
| Molecular formula | $C_{22}H_{25}NO_2$ | |
| 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:**



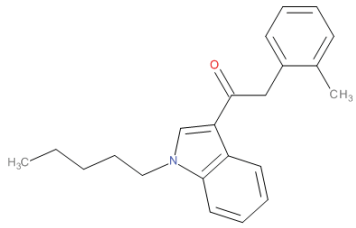

**Mass Spectrum:**



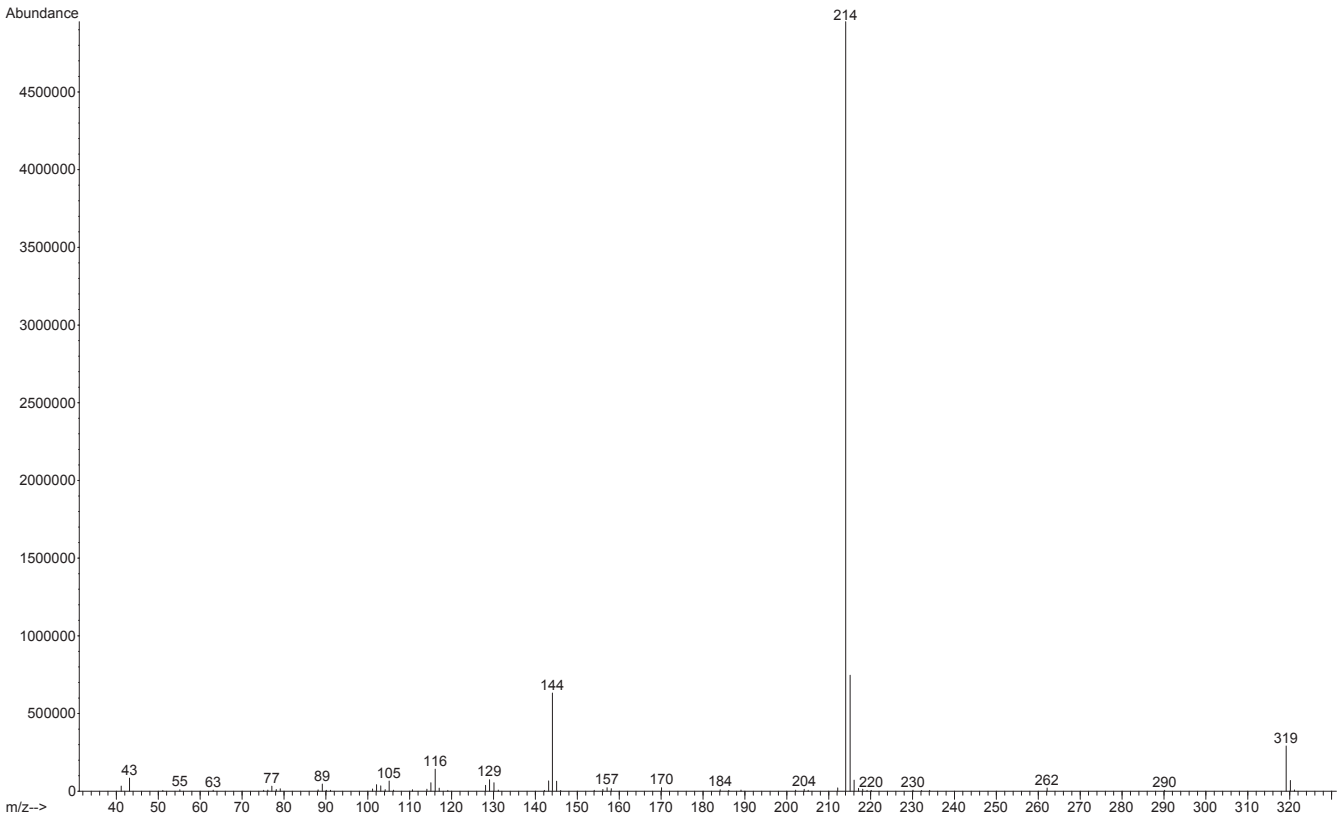
# JWH-251

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

**Molecular Structure:**



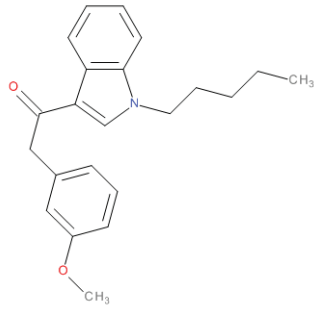

**Mass Spectrum:**



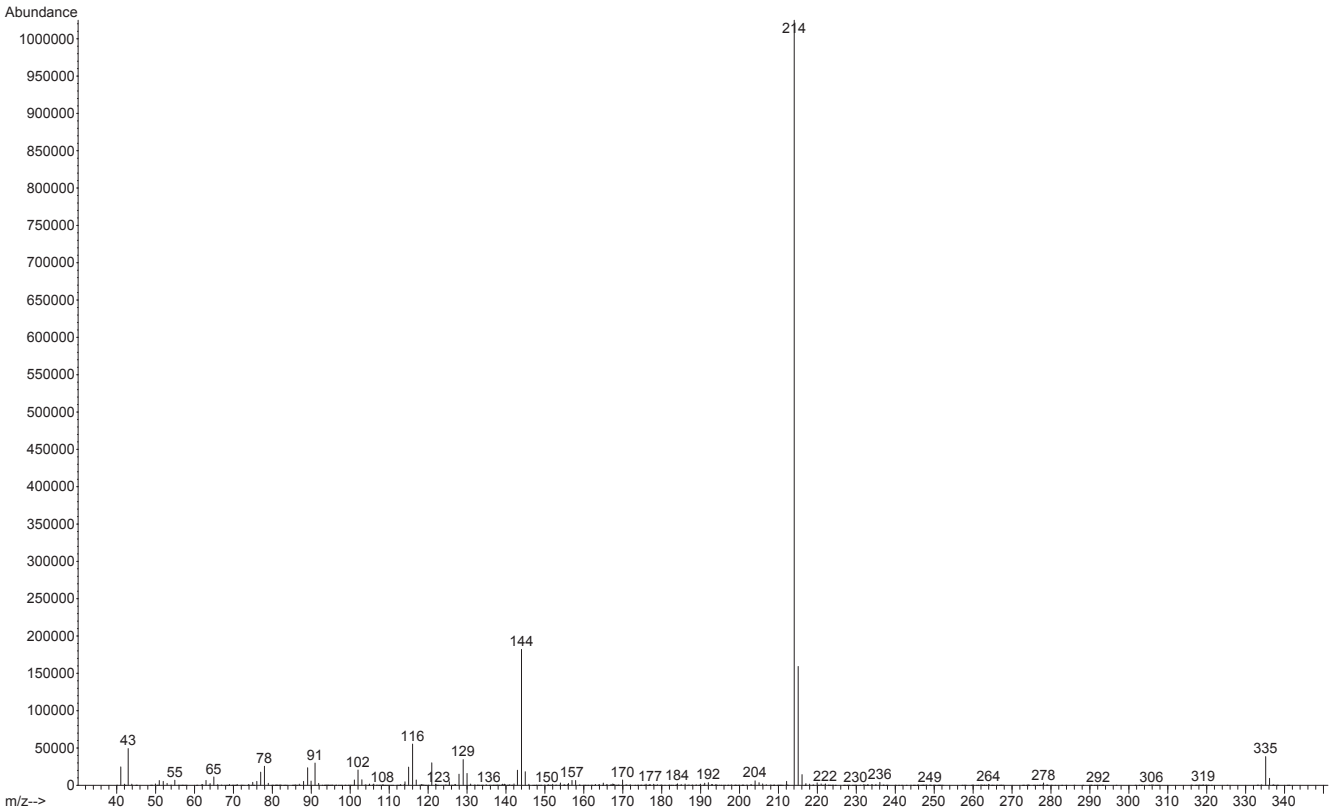
# JWH-302

| | | |
|---|---|---|
| Chemical name | 2-(3-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl)-ethanone | |
| Molecular formula | $C_{22}H_{25}NO_2$ | |
| 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:**



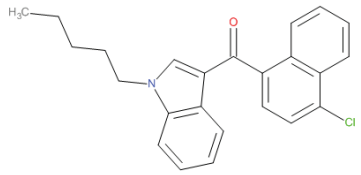

**Mass Spectrum:**



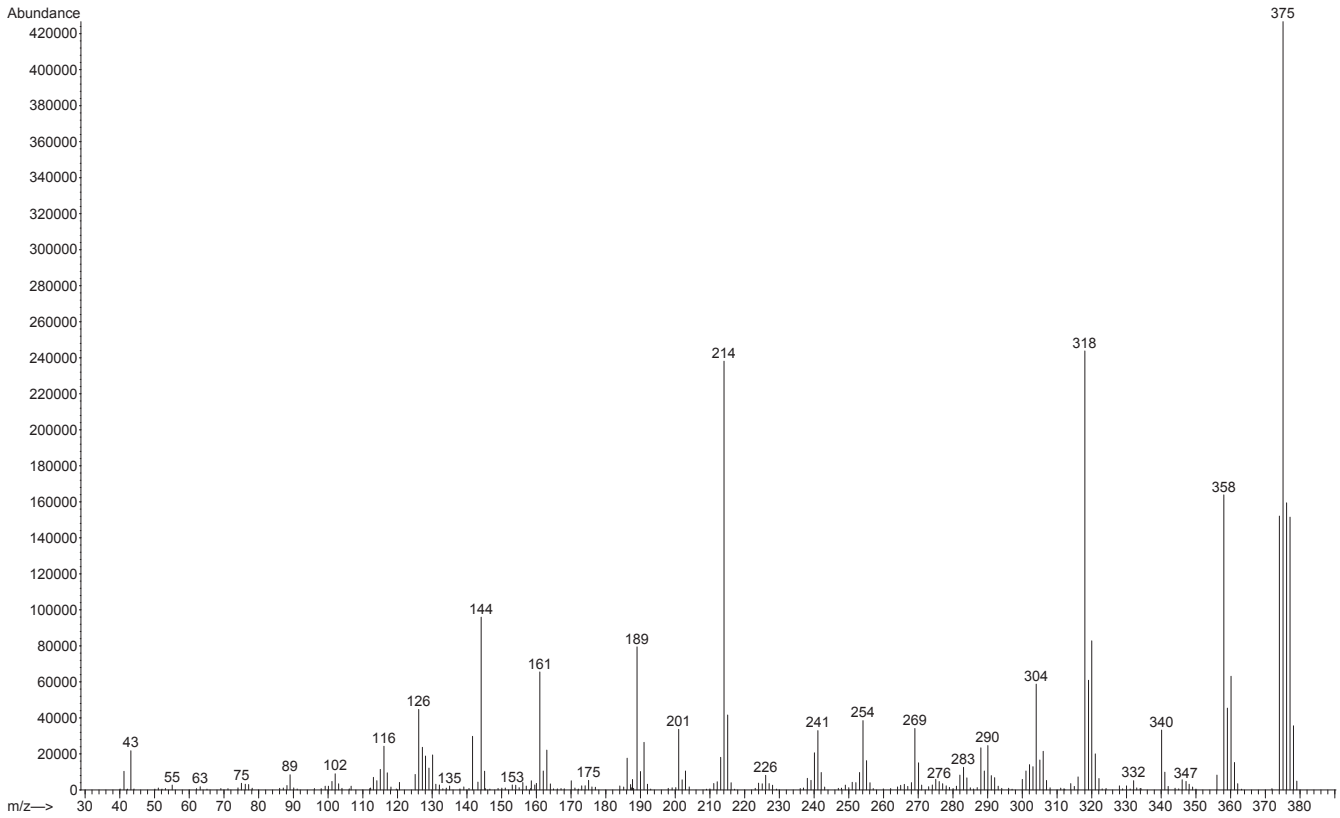
# JWH-398

| | | |
|---|---|---|
| Chemical name | 1-pentyl-3-(4-chloro-1-naphthoyl)indole | |
| Molecular formula | $C_{24}H_{22}ClNO$ | |
| 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:**



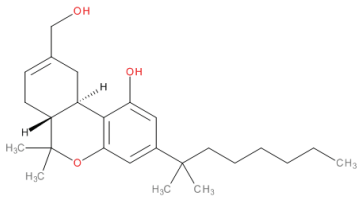

**Mass Spectrum:**



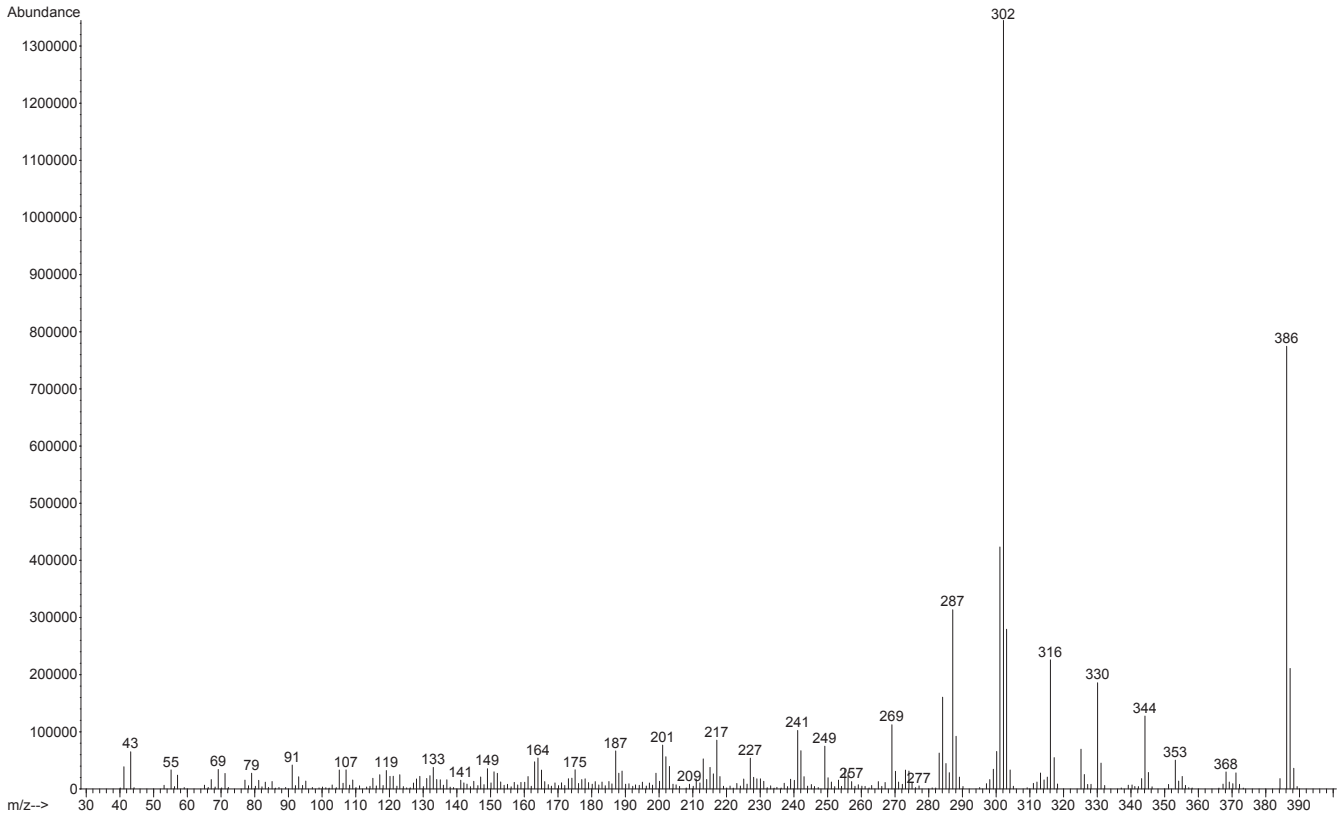
# HU-210

| | | |
|---|---|---|
| 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 | $C_{25}H_{38}O_3$ | |
| 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:**



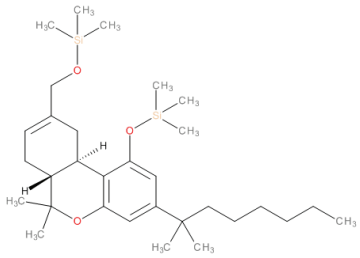

**Mass Spectrum:**



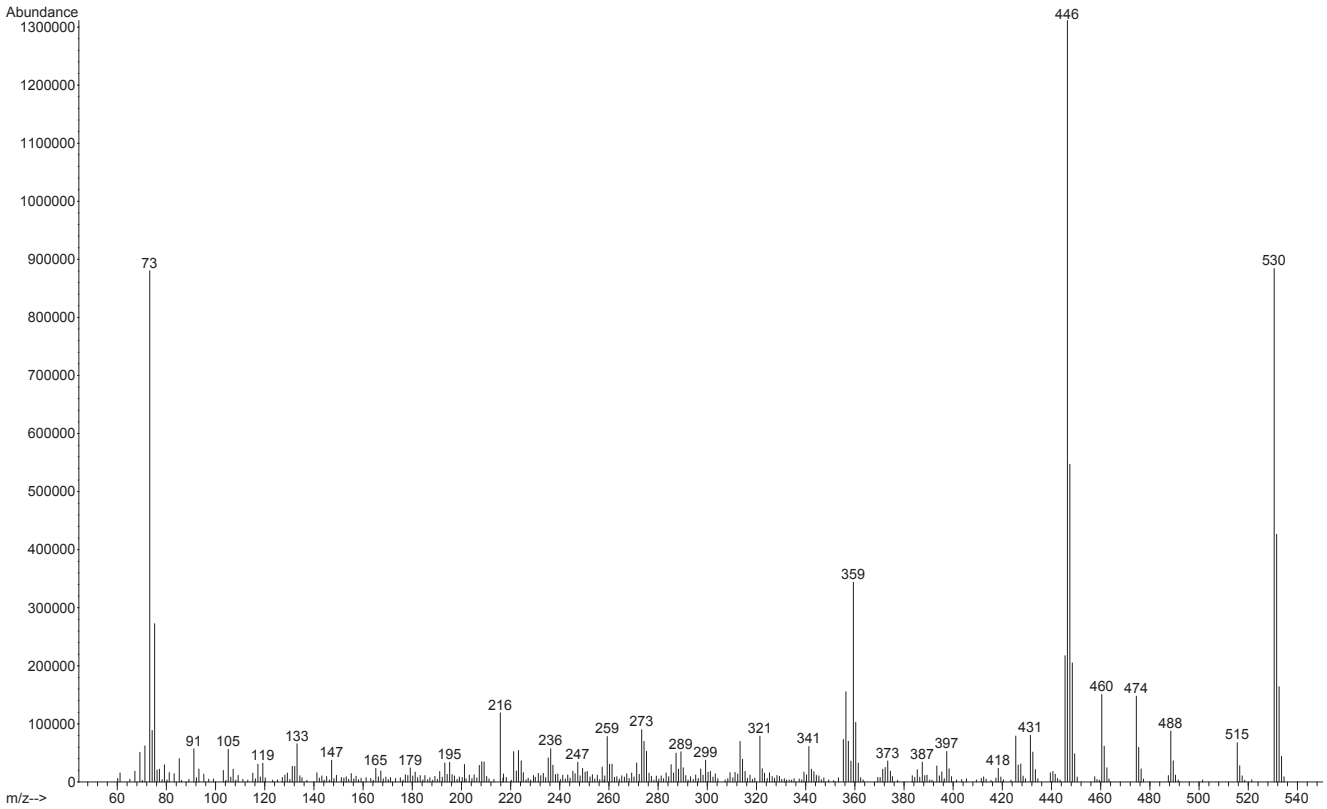
# HU-210 di-TMS derivative

| | | |
|---|---|---|
| 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 | $C_{31}H_{54}O_3Si_2$ | |
| 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:**



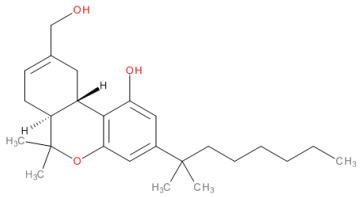
**Mass Spectrum:**



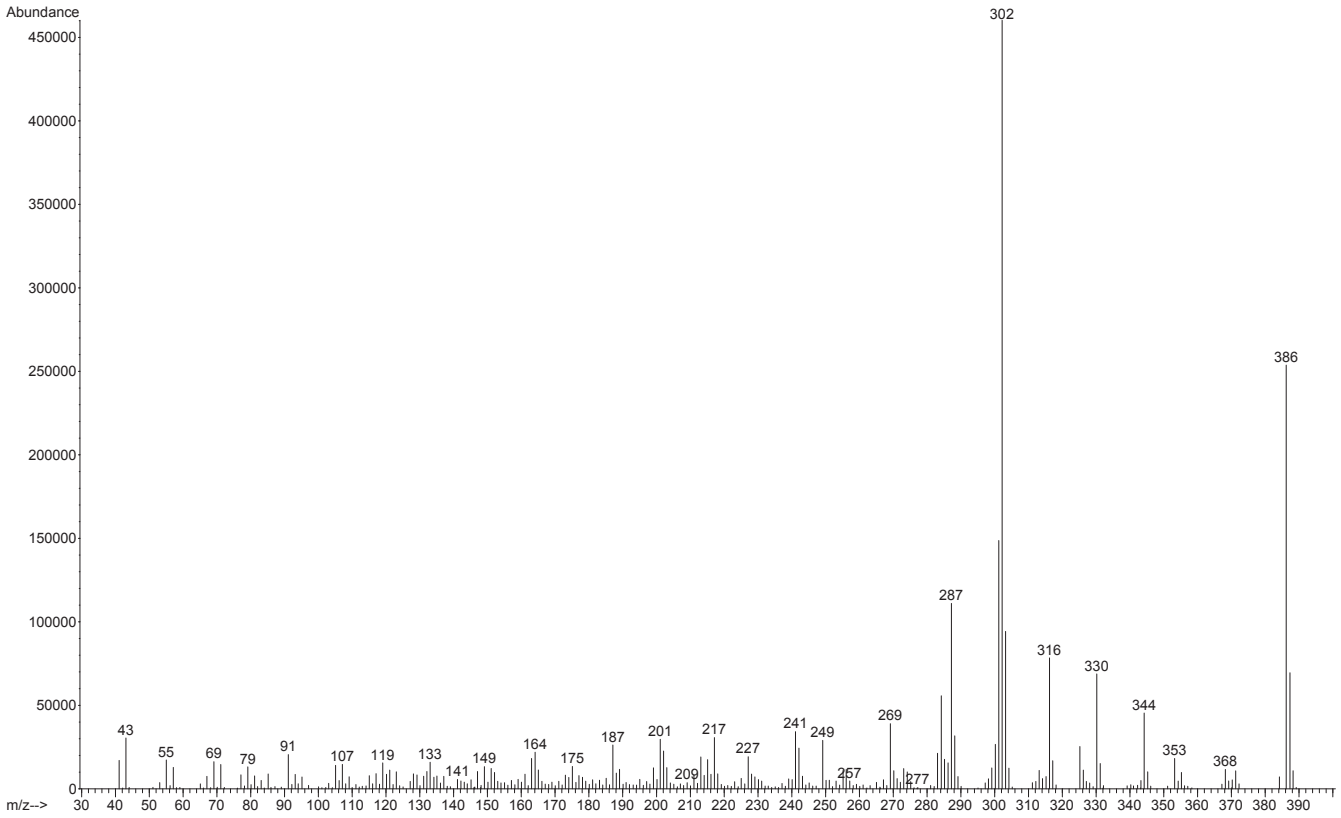
# HU-211

| | | |
|---|---|---|
| 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 | $C_{25}H_{38}O_3$ | |
| 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<br>HU-211 is indistinguishable from HU-210 | |

**Molecular Structure:**



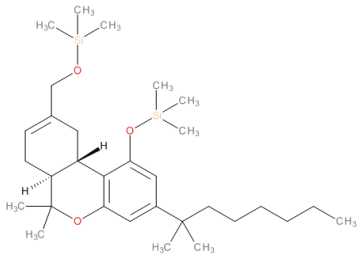

**Mass Spectrum:**



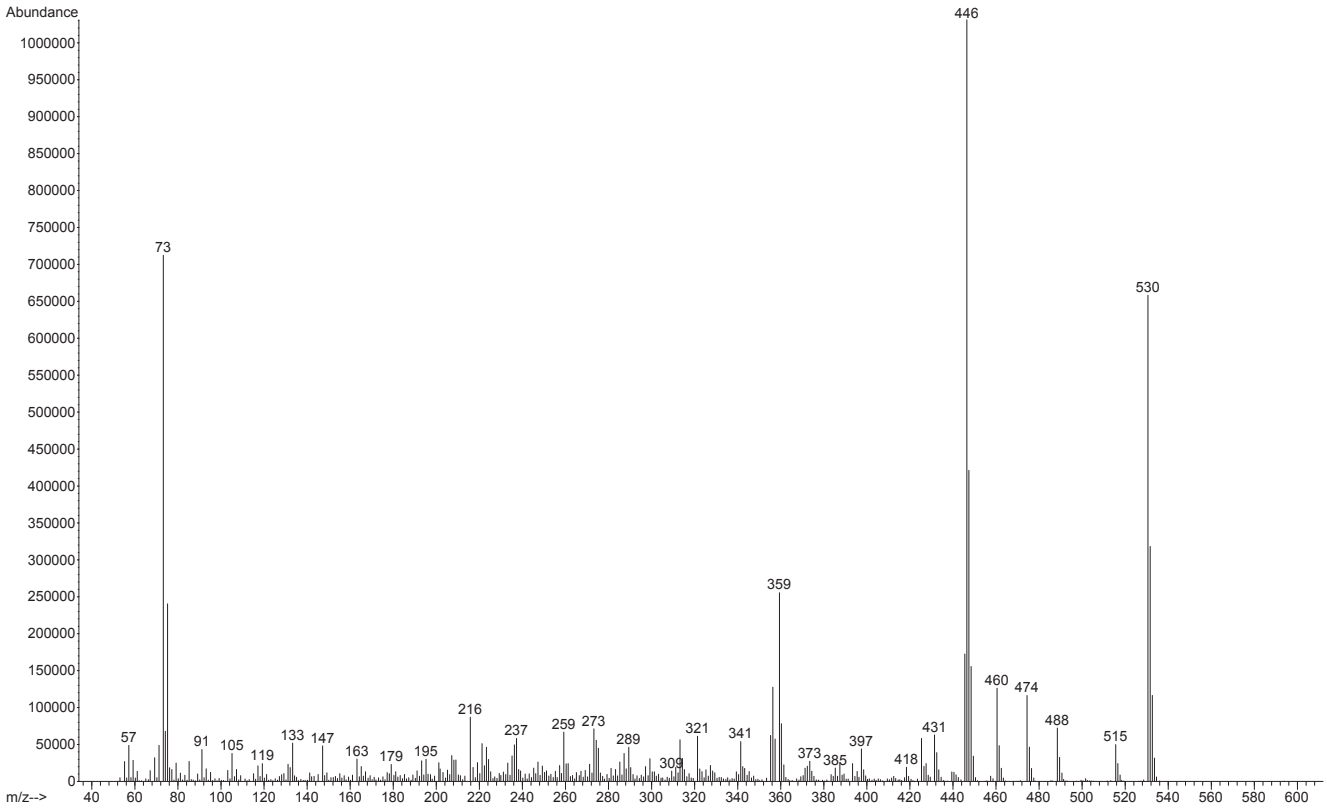
# HU-211-di-TMS derivative

| | | |
|---|---|---|
| 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 | $C_{31}H_{54}O_3Si_2$ | |
| 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:**



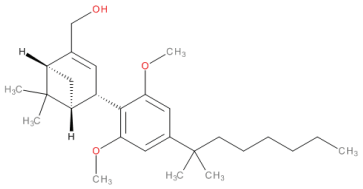
**Mass Spectrum:**



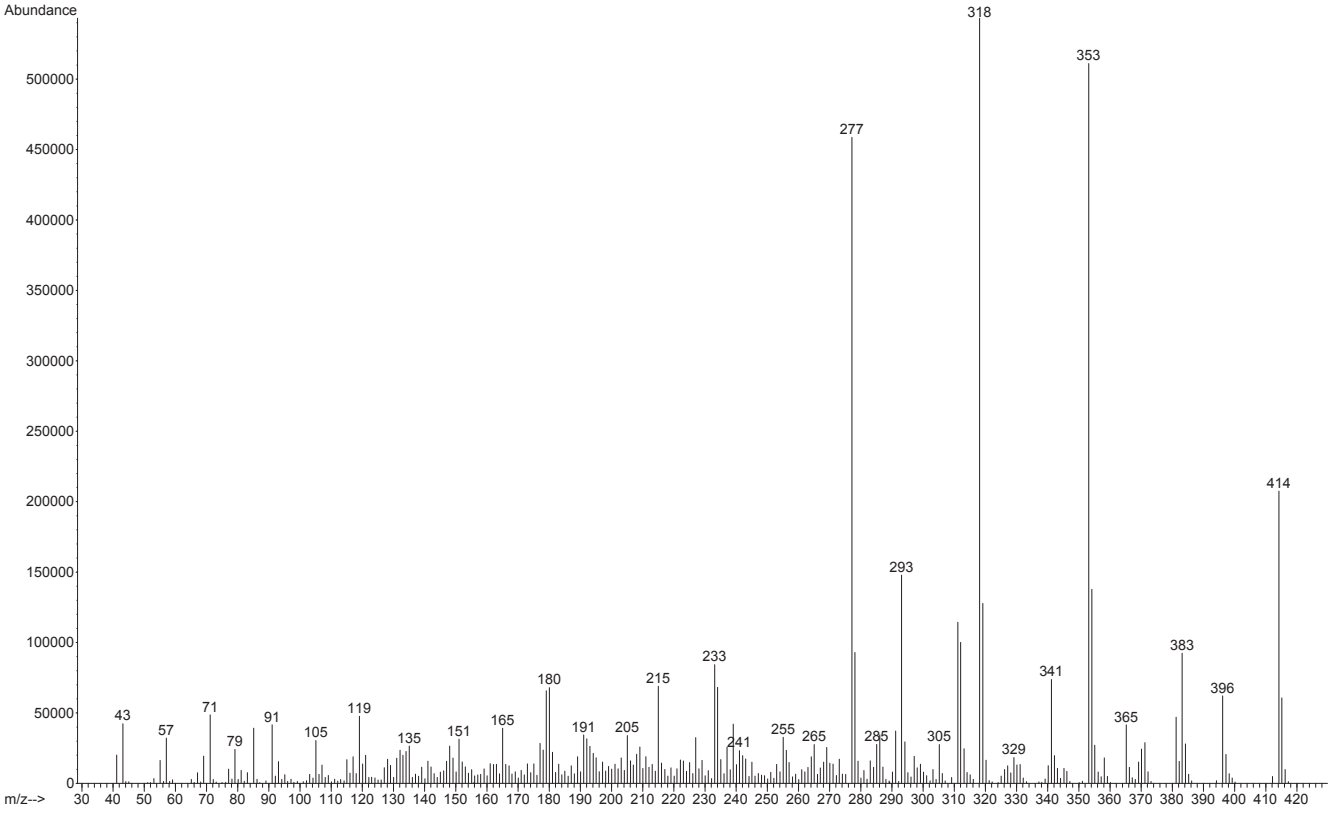
# HU-308

| | | |
|---|---|---|
| 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 | $C_{27}H_{42}O_3$ | |
| 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:**



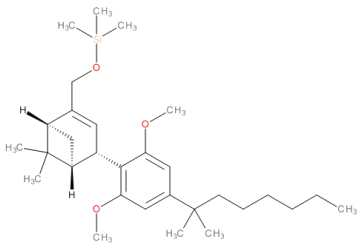

**Mass Spectrum:**



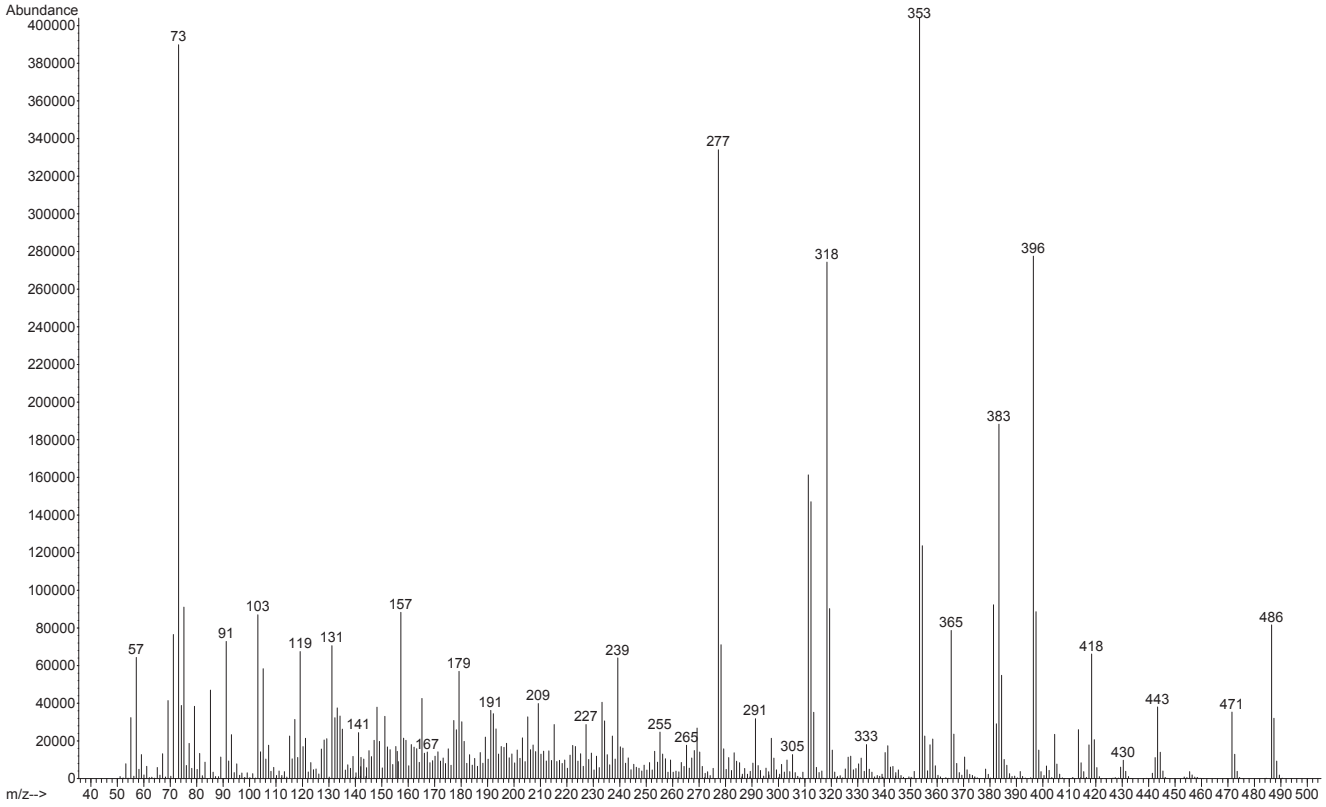
# HU-308-mono-TMS derivative

| | | |
|---|---|---|
| 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 | $C_{30}H_{50}O_3Si$ | |
| 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:**



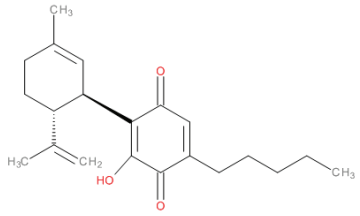
**Mass Spectrum:**



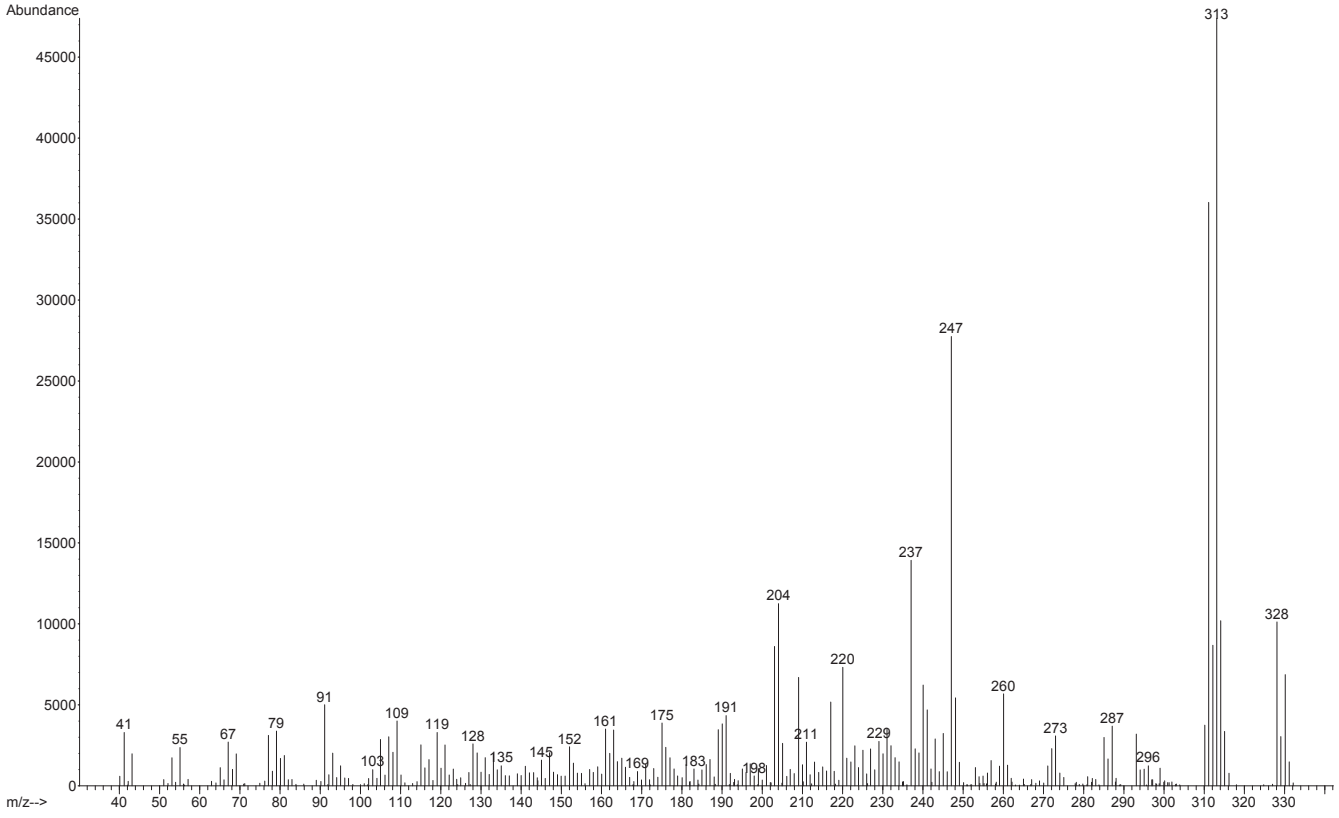
# HU-331

| | | |
|---|---|---|
| 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 | $C_{21}H_{28}O_3$ | |
| 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:**



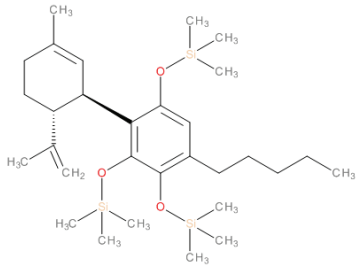

**Mass Spectrum:**



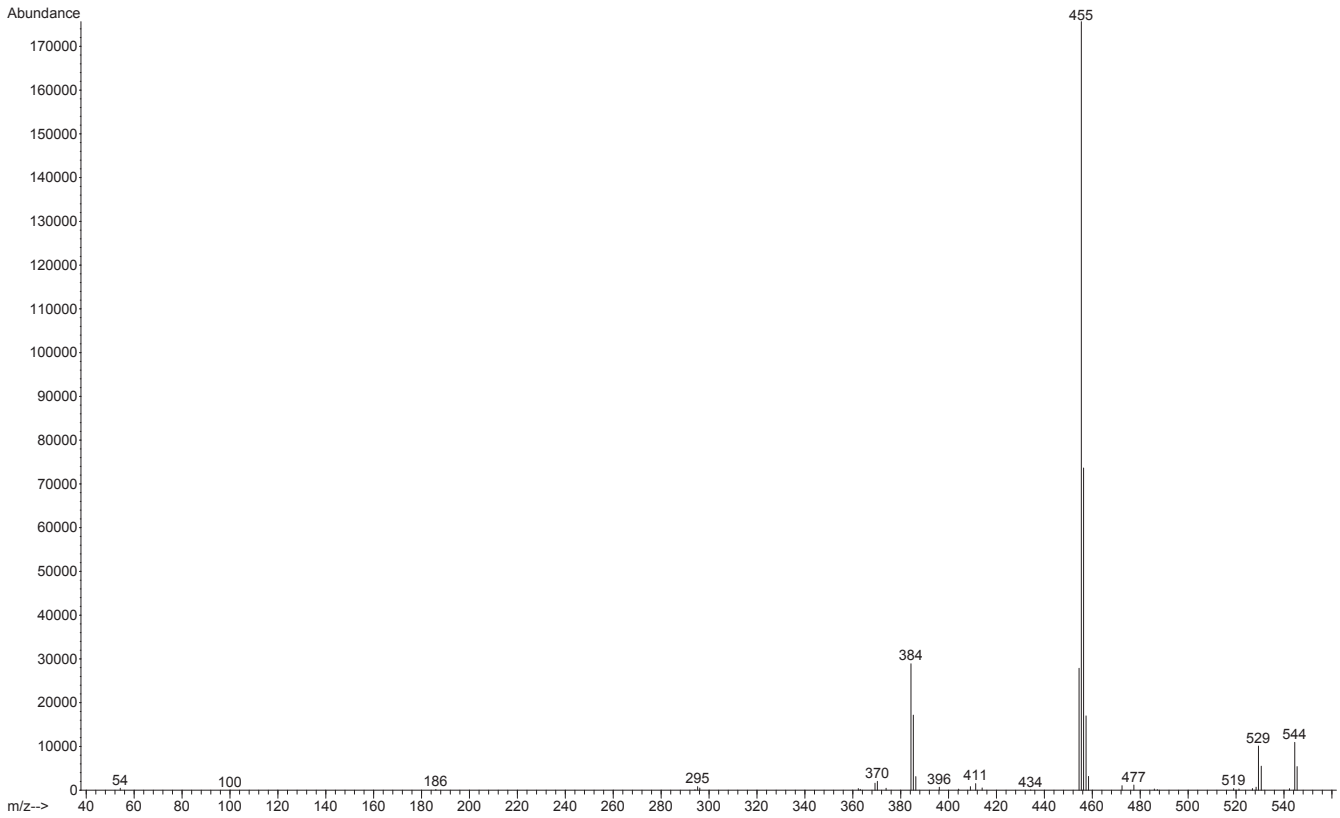
# HU-331-tri-TMS derivative

| | | |
|---|---|---|
| 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:**



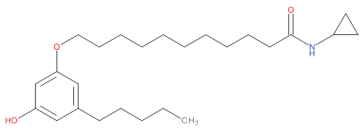
**Mass Spectrum:**



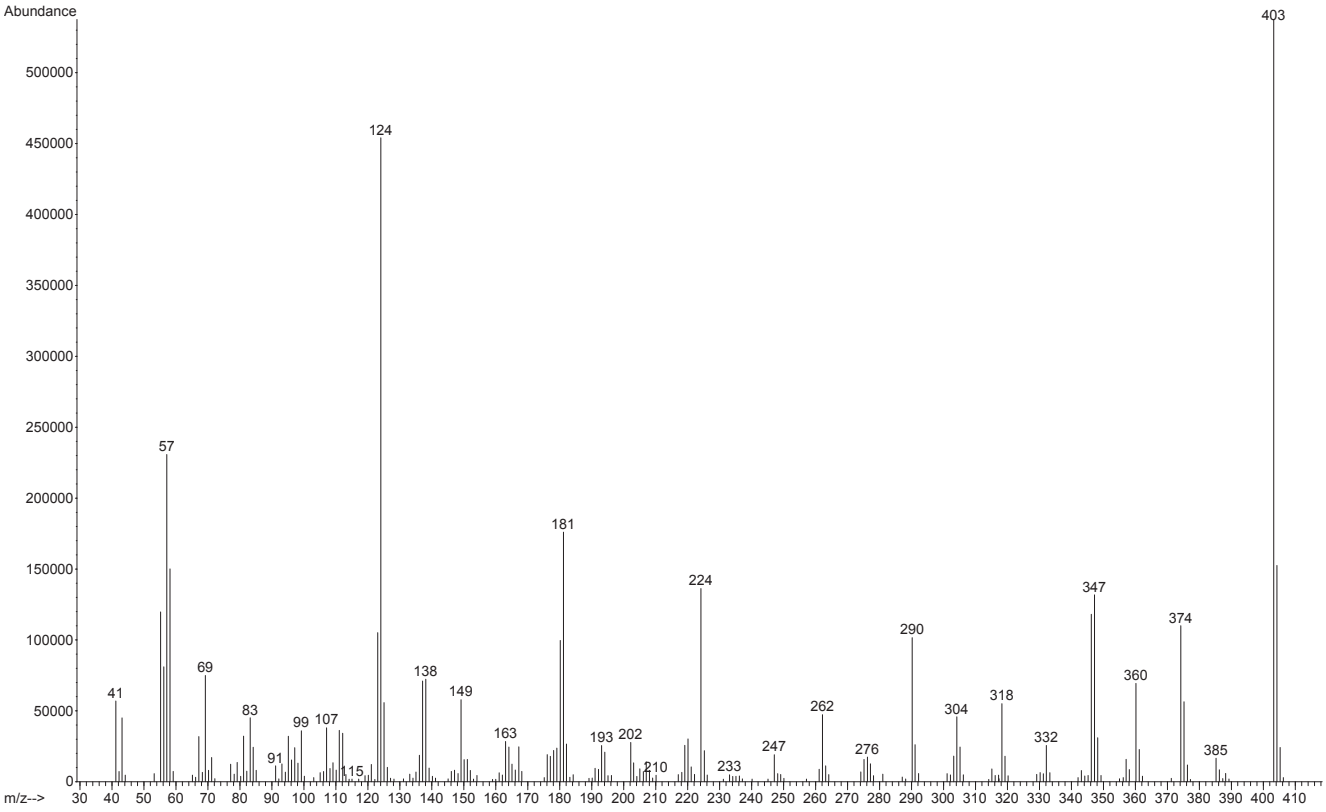
# CB-25

| | | |
|---|---|---|
| Chemical name | N-cyclopropyl-11-(3-hydroxy-5-pentylphenoxy)-undecanamide | |
| Molecular formula | $C_{25}H_{41}NO_3$ | |
| 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:**



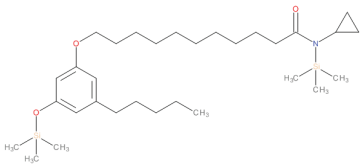
**Mass Spectrum:**



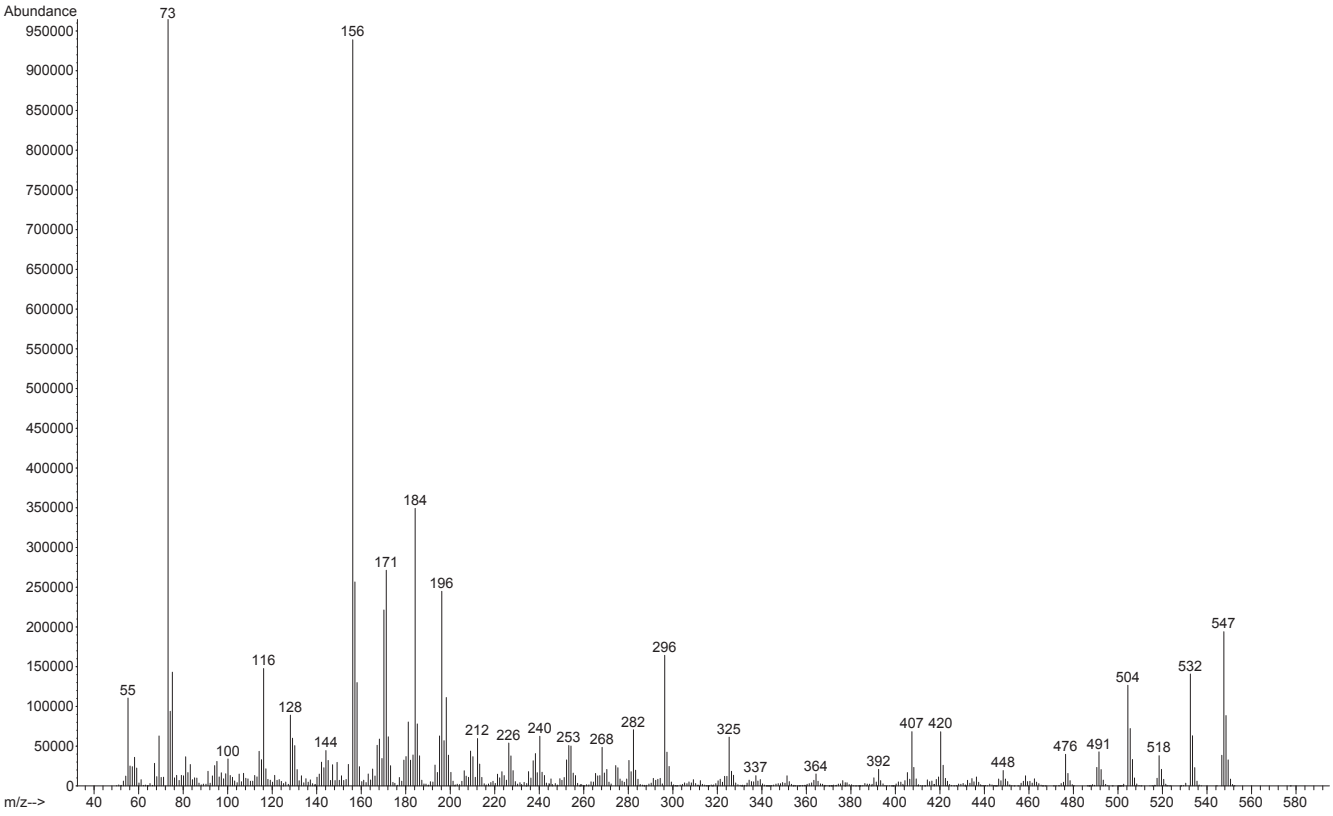
# CB-25-di-TMS derivative

| | | |
|---|---|---|
| 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:**



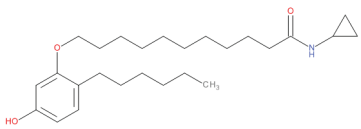
**Mass Spectrum:**



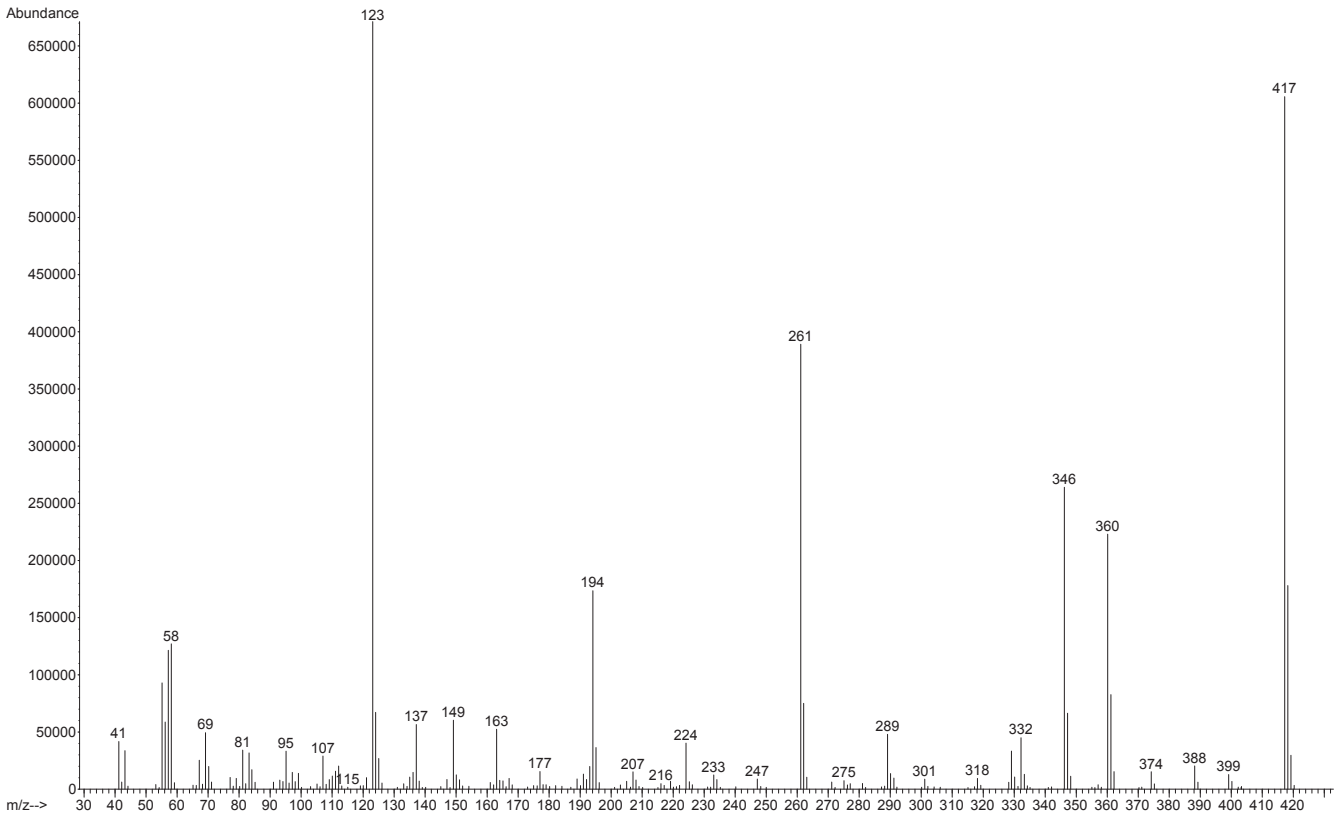
# CB-52

| | | |
|---|---|---|
| Chemical name | N-cyclopropyl-11-(2-hexyl-5-hydroxyphenoxy)-undecanamide | |
| Molecular formula | $C_{26}H_{43}NO_3$ | |
| 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:**



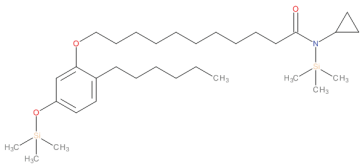
**Mass Spectrum:**



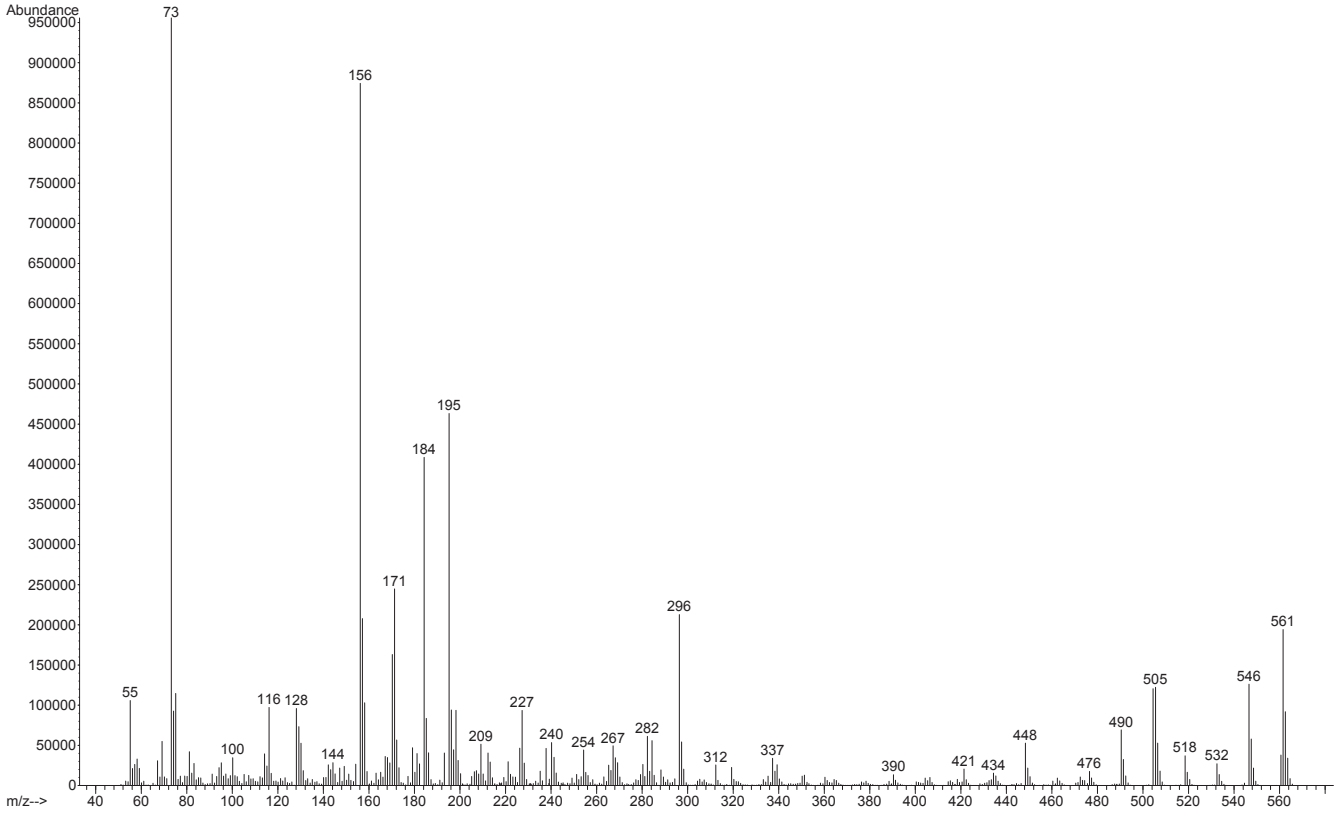
# CB-52-di-TMS derivative

| | | |
|---|---|---|
| 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:**



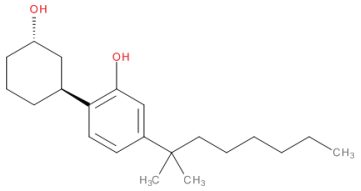
**Mass Spectrum:**



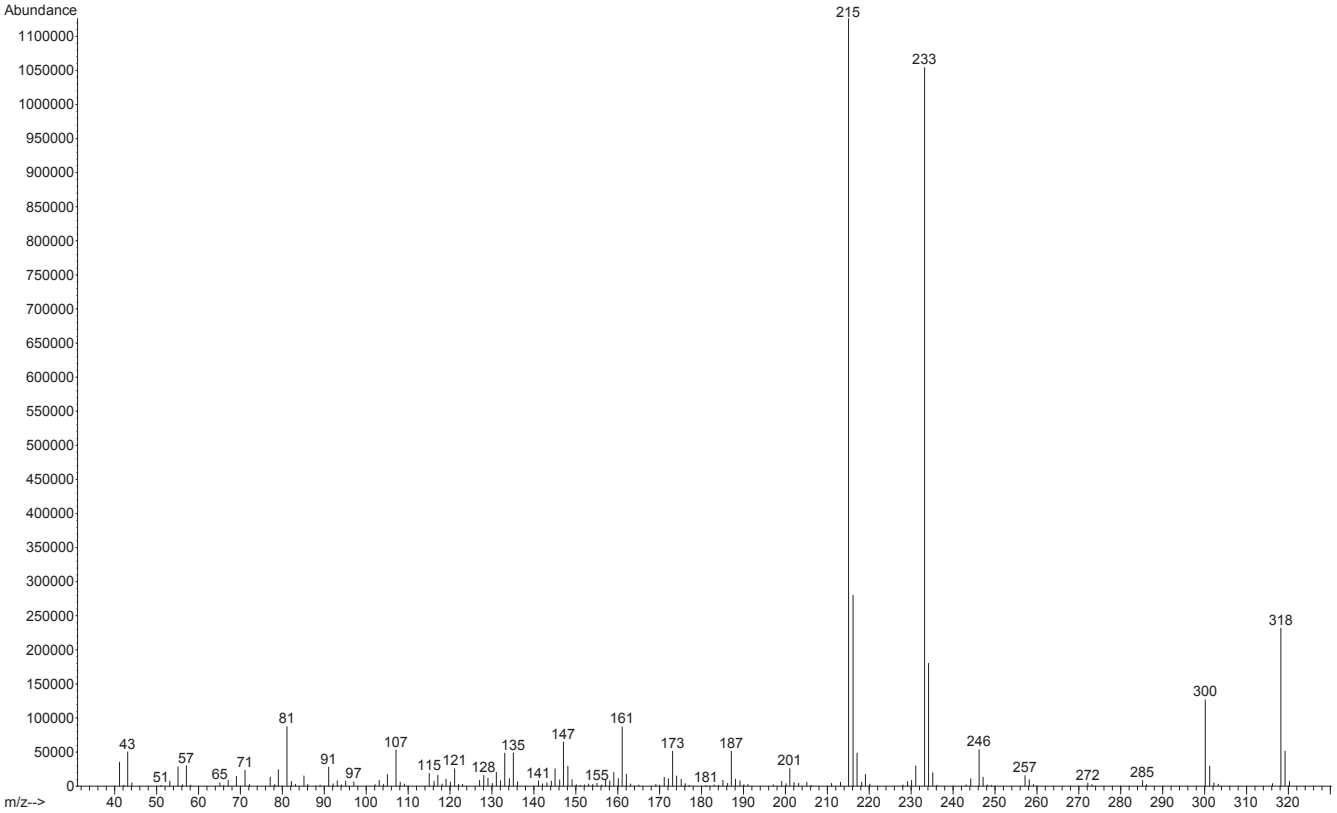
# CP47,497 (C7 analog)

| | | |
|---|---|---|
| Chemical name | 2-[(1R,3S)-3-hydroxycyclohexyl]- 5-(2-methyloctan-2-yl) phenol | |
| Molecular formula | $C_{21}H_{34}O_2$ | |
| 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<br>Compound shares some common ions with the C8 analog. | |

**Molecular Structure:**



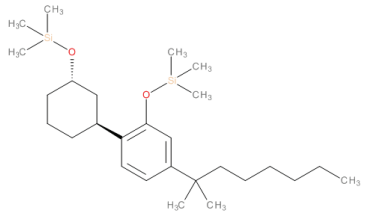

**Mass Spectrum:**



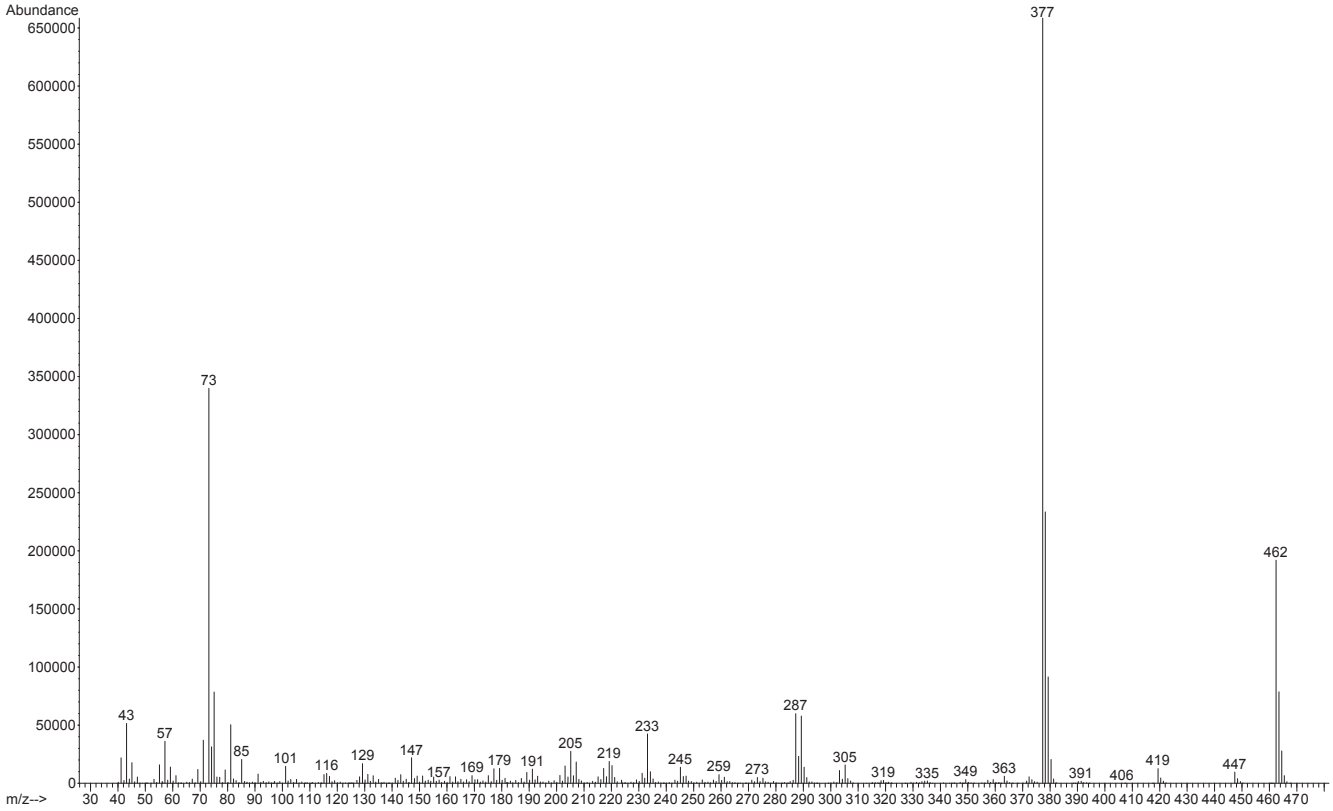
# CP47,497 (C7 analog)-di-TMS derivative

| | | |
|---|---|---|
| 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:**



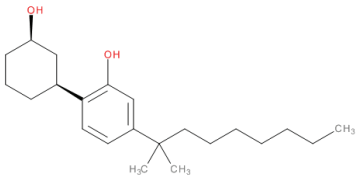
**Mass Spectrum:**



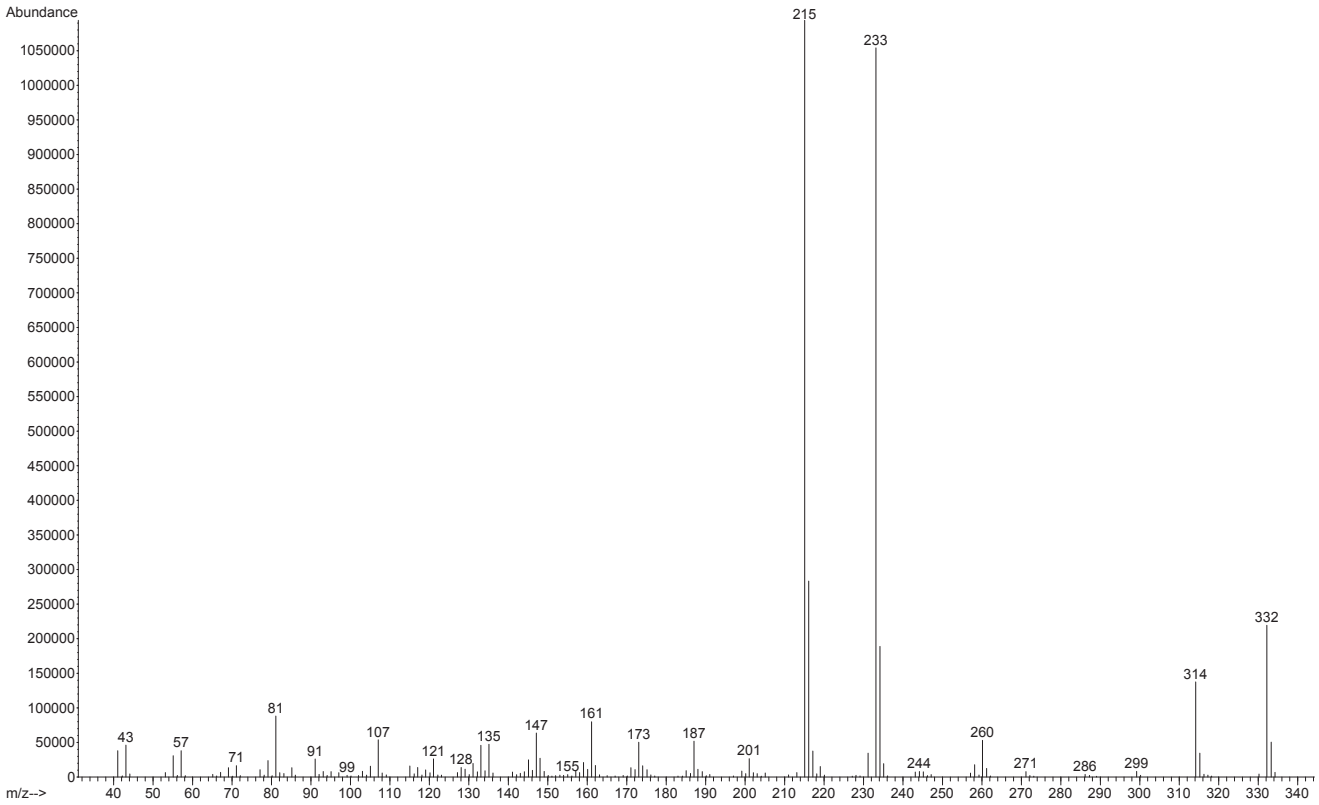
# CP47,497 (C8 analog)

| | | |
|---|---|---|
| Chemical name | 2-[(1R,3S)-3-hydroxycyclohexyl]- 5-(2-methylnonan-2-yl) phenol | |
| Molecular formula | $C_{22}H_{36}O_2$ | |
| 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<br>Compound shares some common ions with the C7 analog. | |

**Molecular Structure:**



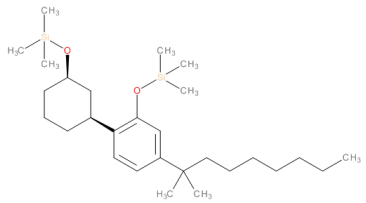

**Mass Spectrum:**



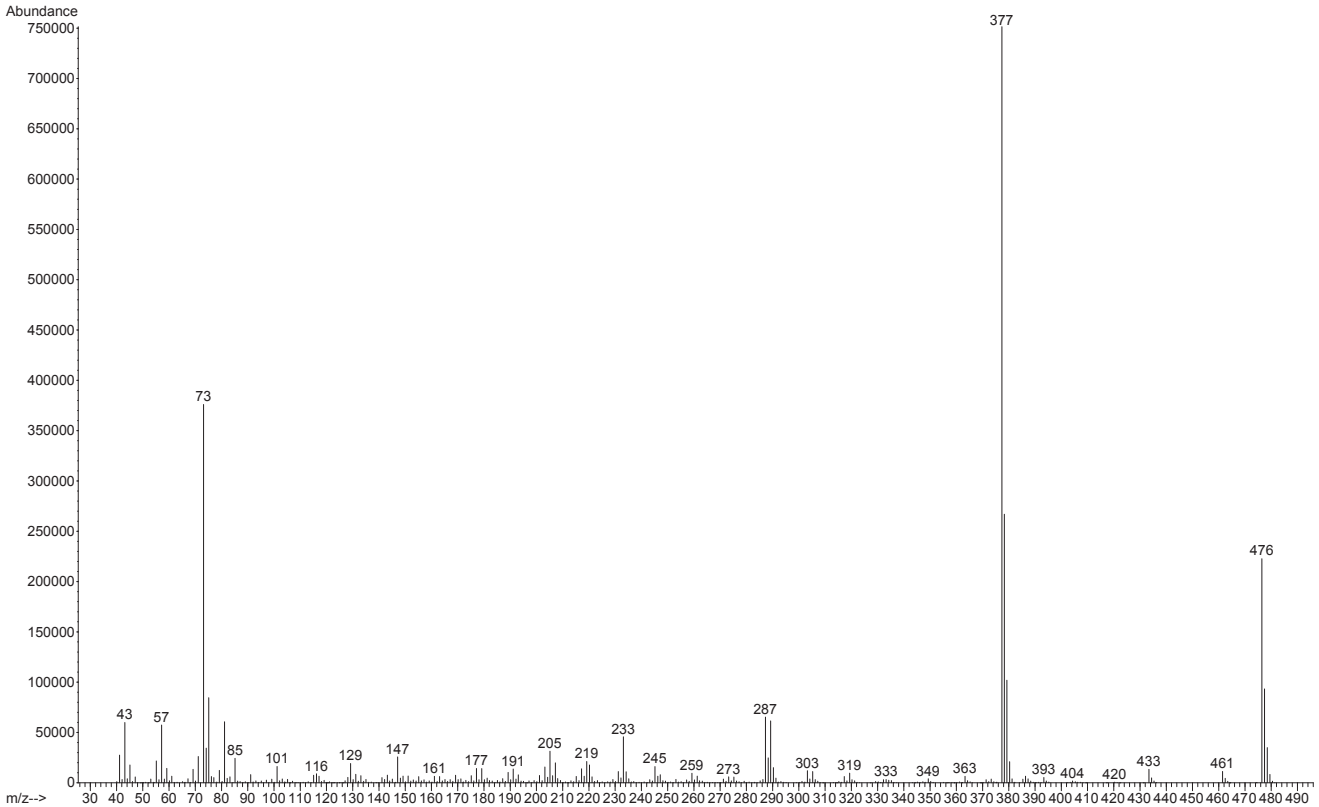
# CP47,497 (C8 analog)-di-TMS derivative

| | | |
|---|---|---|
| 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:**



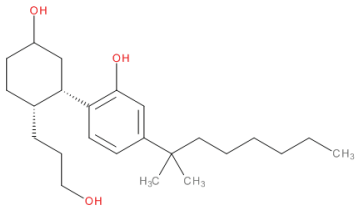
**Mass Spectrum:**



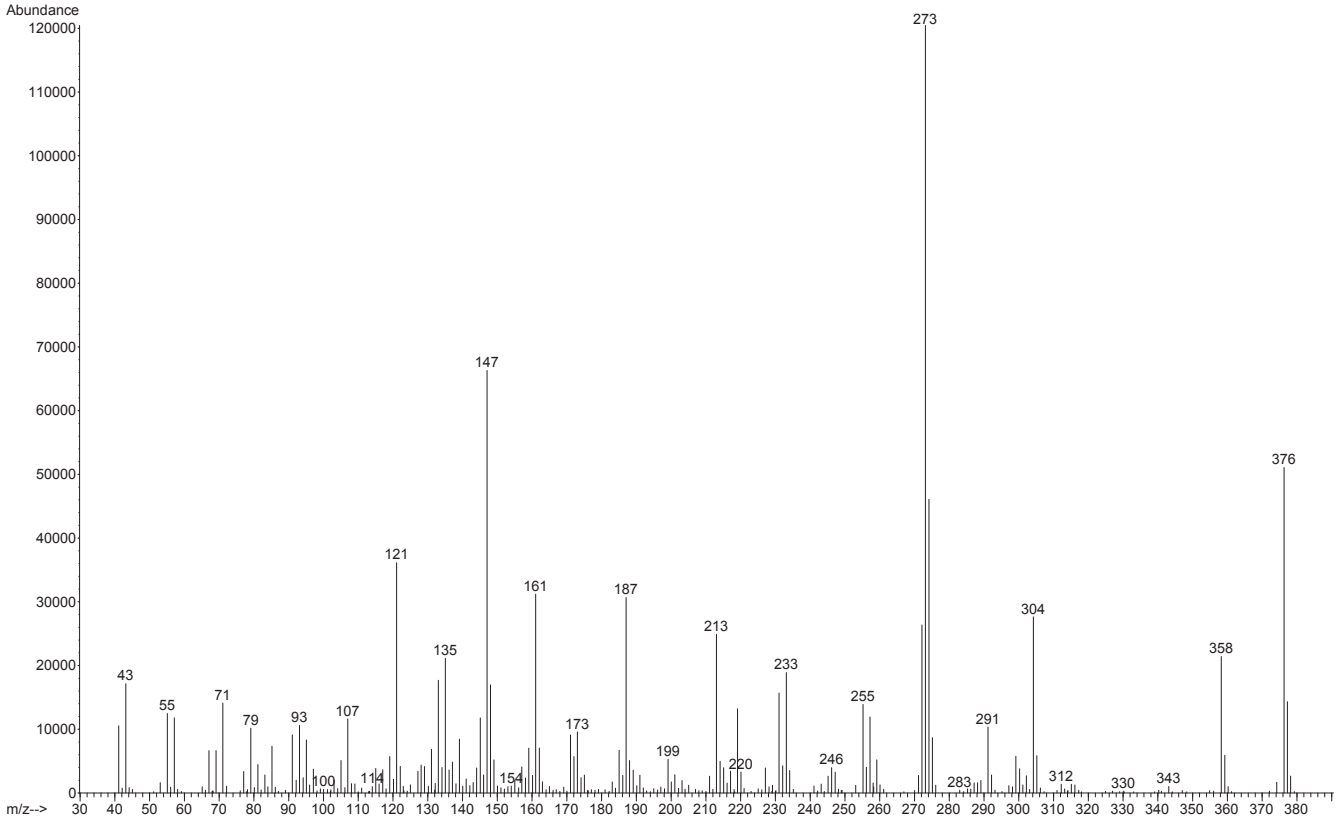
# CP55,940

| | | |
|---|---|---|
| Chemical name | 2-[(1R,2R,5R)-5-hydroxy-2-(3-hydroxypropyl) cyclohexyl]-5-(2-methyloctan-2-yl)phenol | |
| Molecular formula | $C_{24}H_{40}O_3$ | |
| 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:**



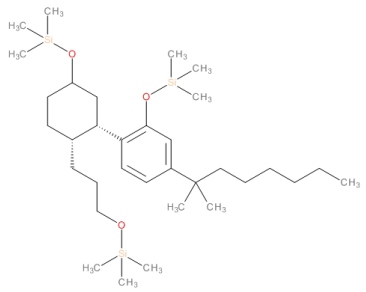

**Mass Spectrum:**



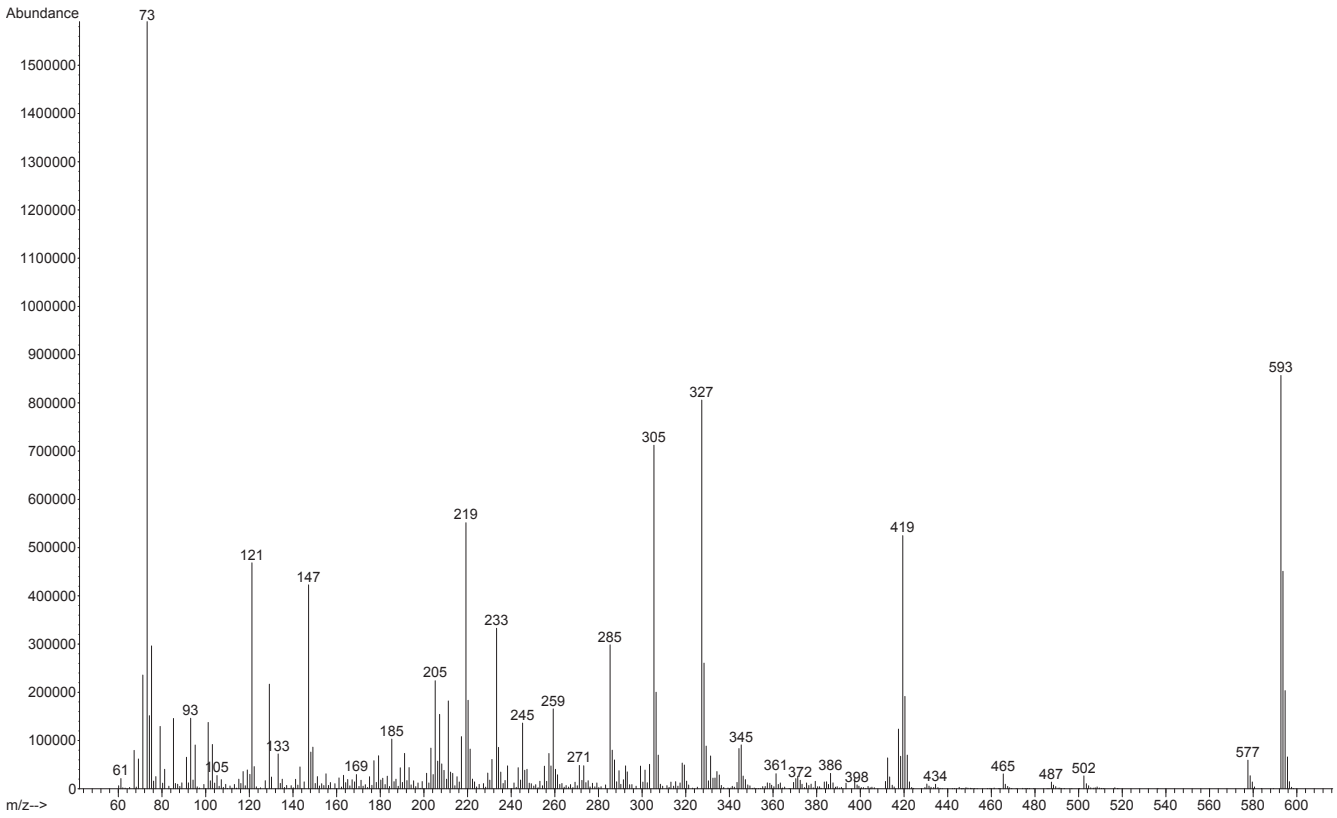
# CP55,940-tri-TMS derivative

| | | |
|---|---|---|
| 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:**



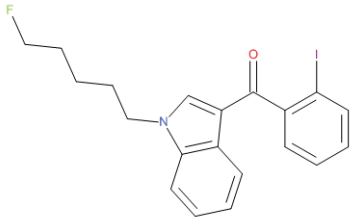
**Mass Spectrum:**



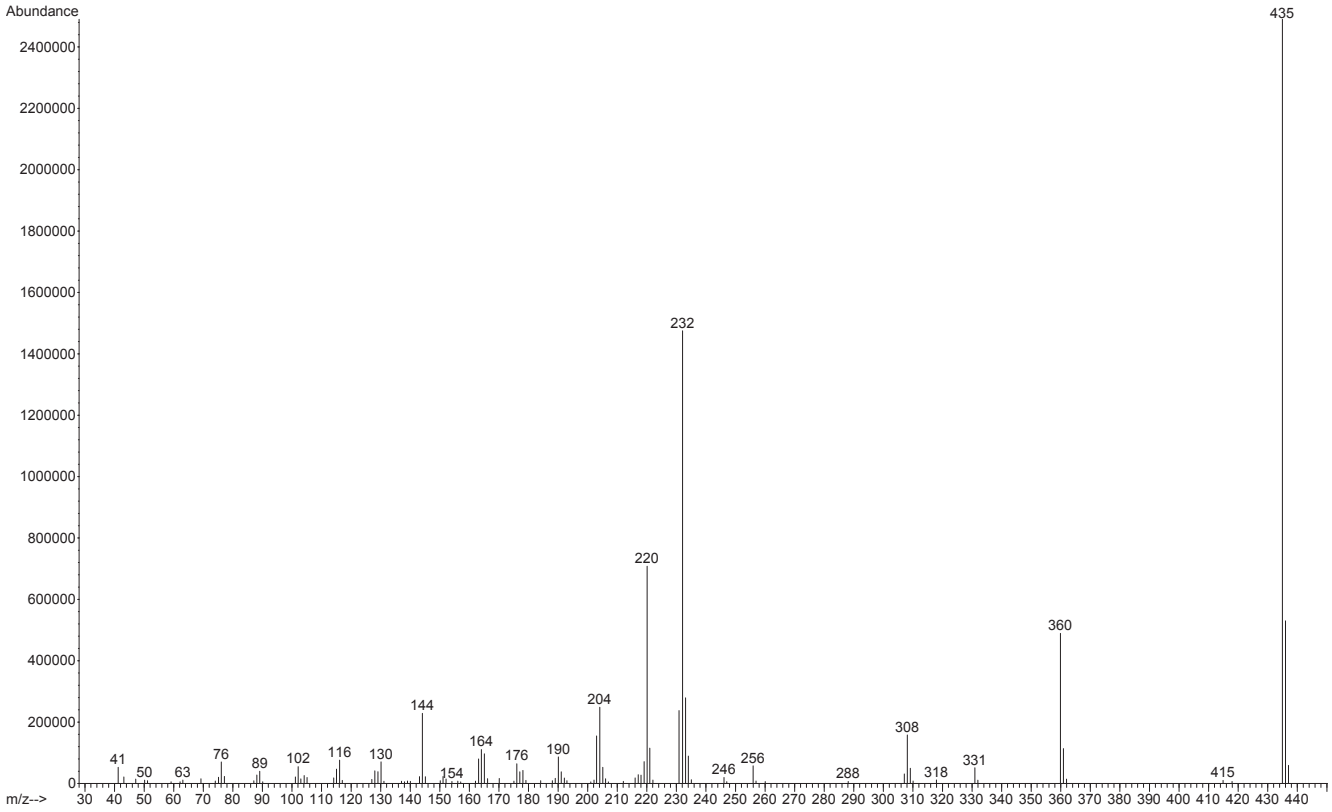
# AM-694

| | | |
|---|---|---|
| Chemical name | 1-[(5-fluoropentyl)-1H-indol-3-yl]-(2-iodophenyl)methanone | |
| Molecular formula | $C_{20}H_{19}FINO$ | |
| 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:**



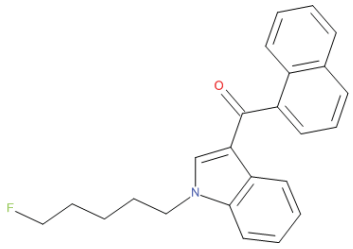

**Mass Spectrum:**



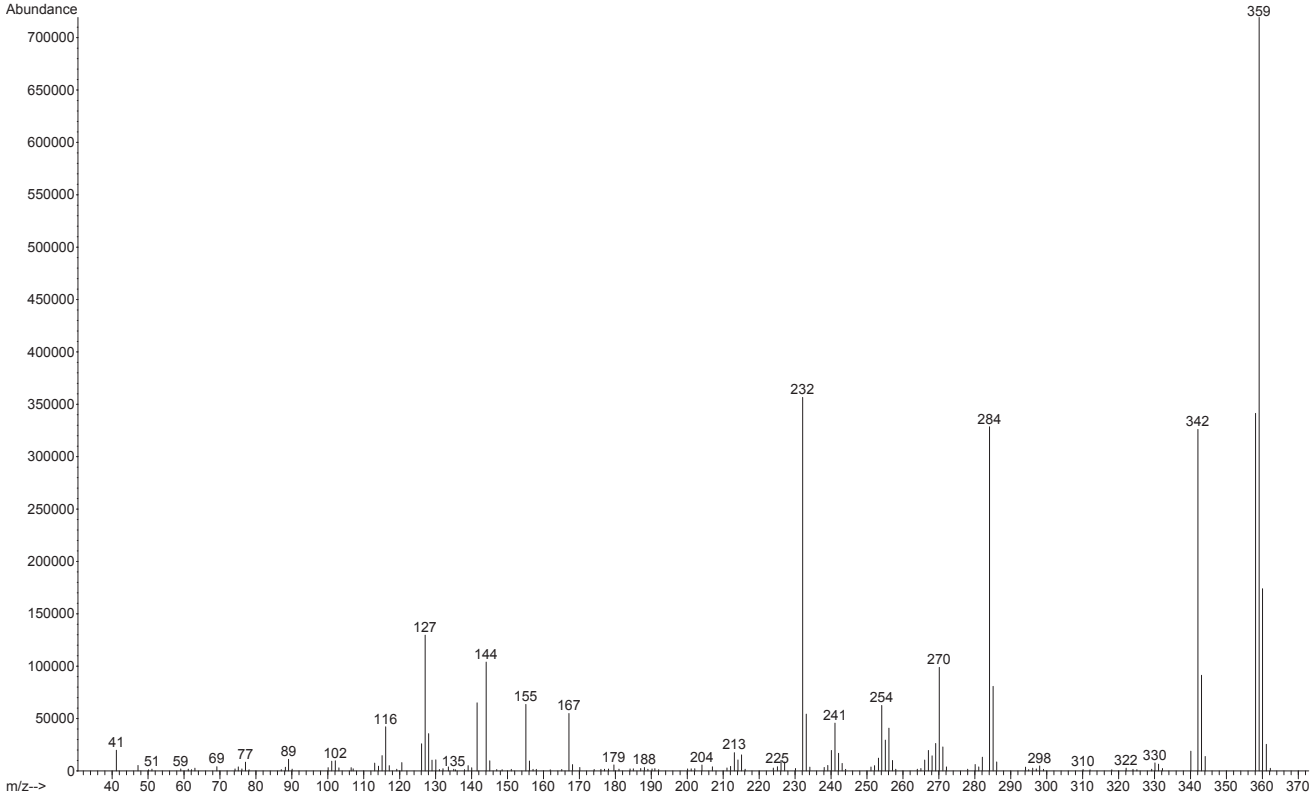
# AM-2201

| | | |
|---|---|---|
| Chemical name | 1-[(5-fluoropentyl)-1H-indol-3-yl]-(naphthalen-1-yl)methanone | |
| Molecular formula | $C_{24}H_{22}FNO$ | |
| 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<br>AM-2201 is the fluoro-analog of JWH-018 | |

**Molecular Structure:**



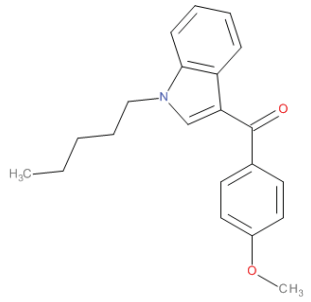

**Mass Spectrum:**



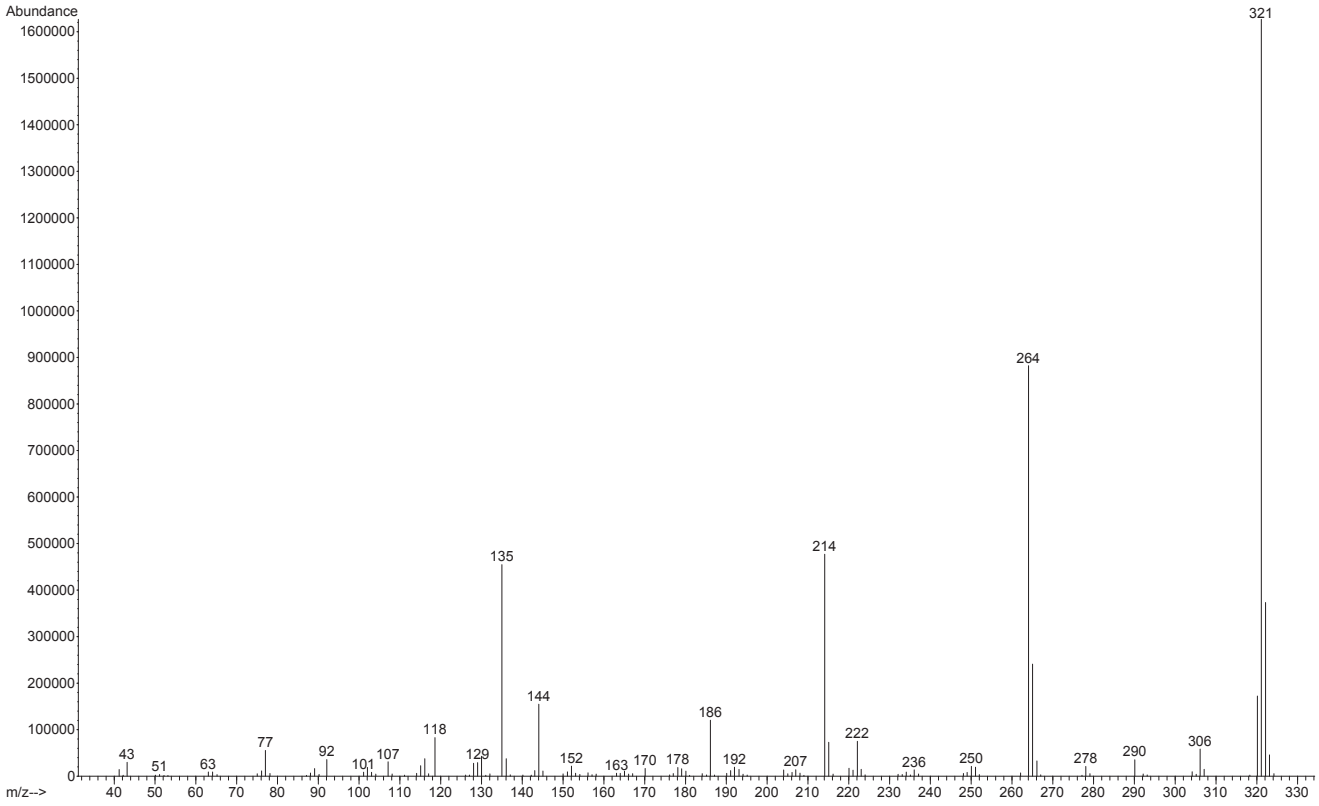
# RCS-4

| | | |
|---|---|---|
| Chemical name | ((4-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone) | |
| Molecular formula | $C_{21}H_{23}NO_2$ | |
| 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:**



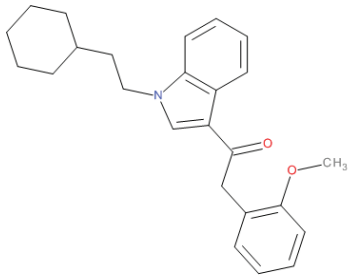

**Mass Spectrum:**



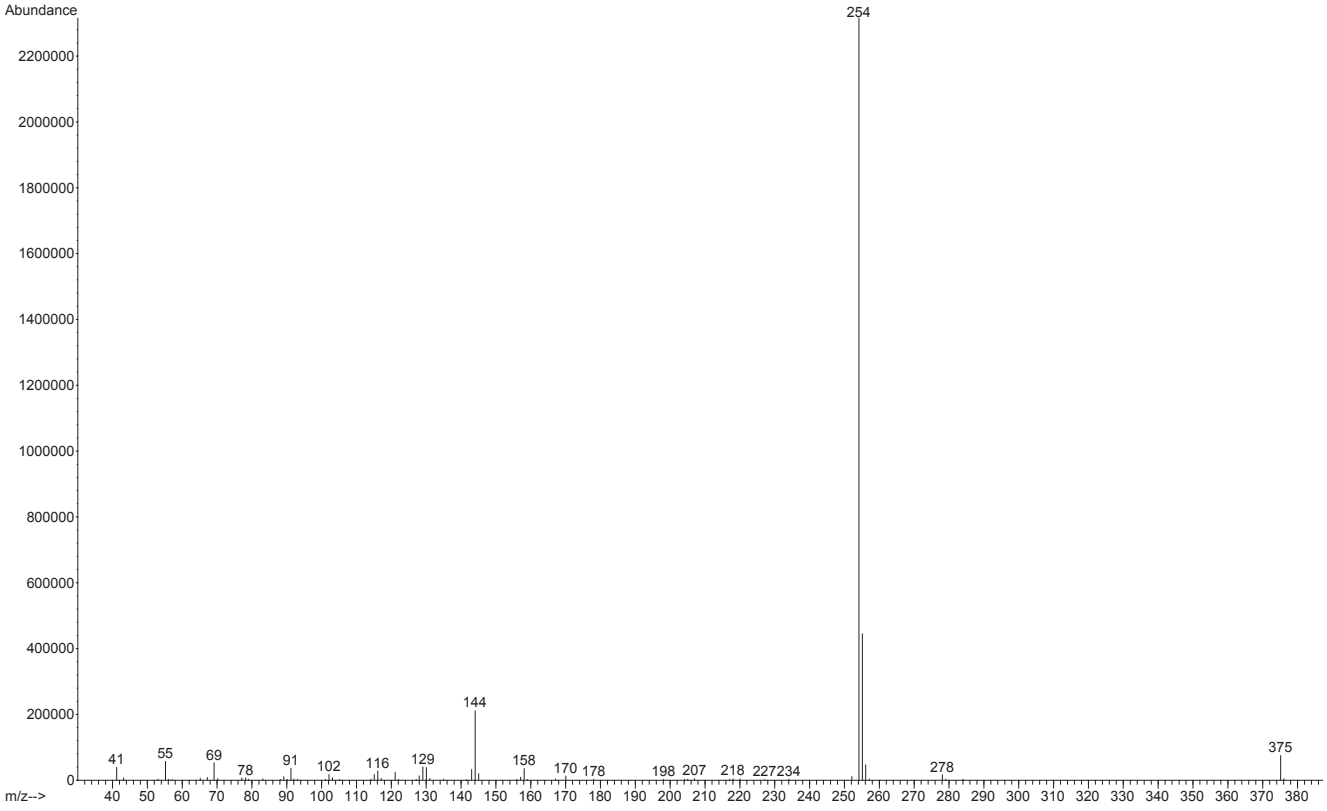
# RCS-8

| | | |
|---|---|---|
| Chemical name | 1-(1-(2-cyclohexylethyl)-1H-indol-3-yl)-2-(2-methoxyphenyl) ethanone | |
| Molecular formula | $C_{25}H_{29}NO_2$ | |
| 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:**



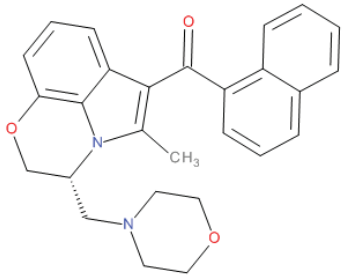

**Mass Spectrum:**



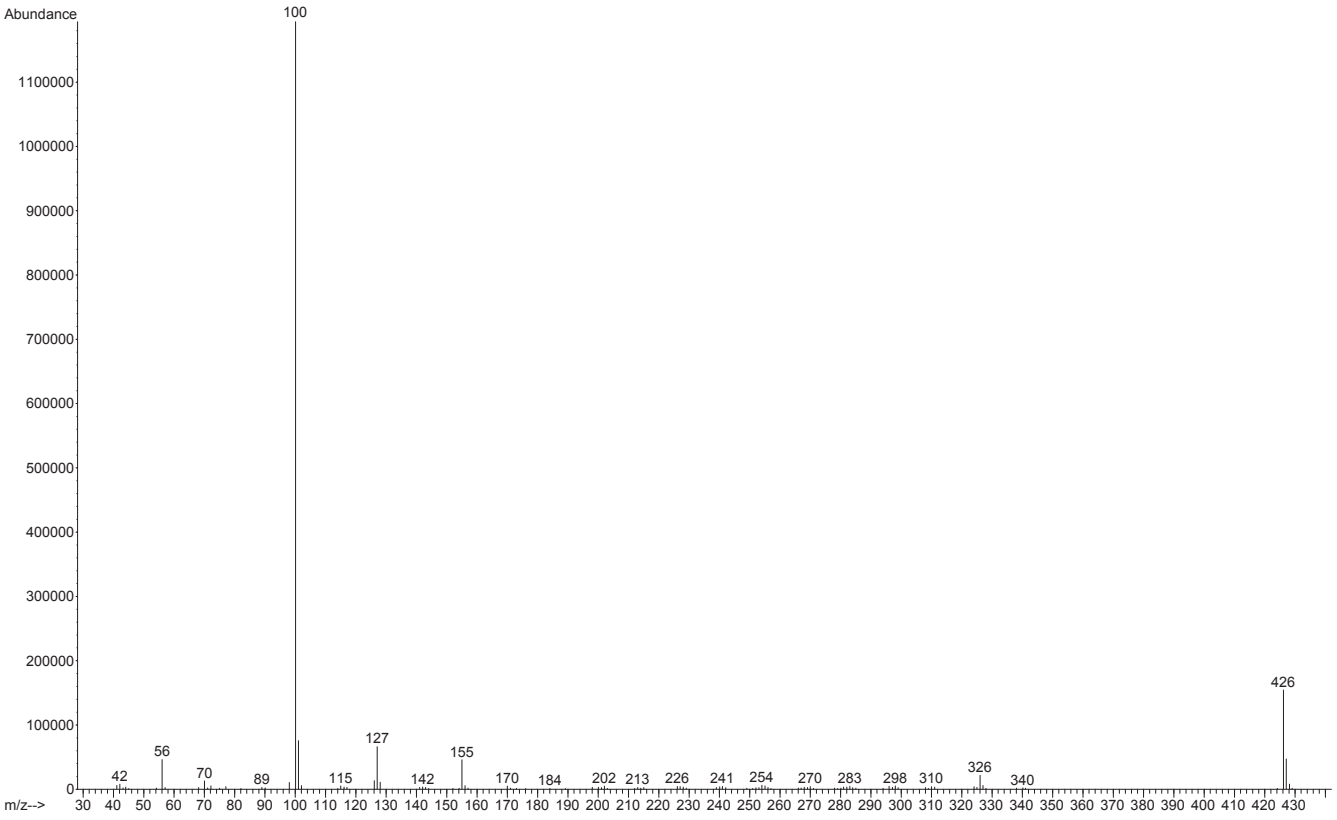
# WIN55,212-2

| | | |
|---|---|---|
| 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 | $C_{27}H_{26}N_2O_3$ | |
| 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:**



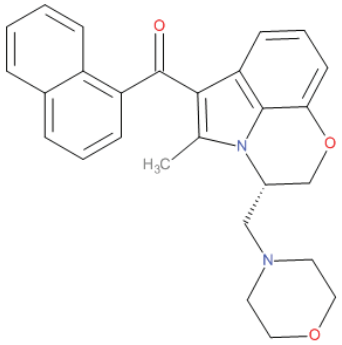

**Mass Spectrum:**



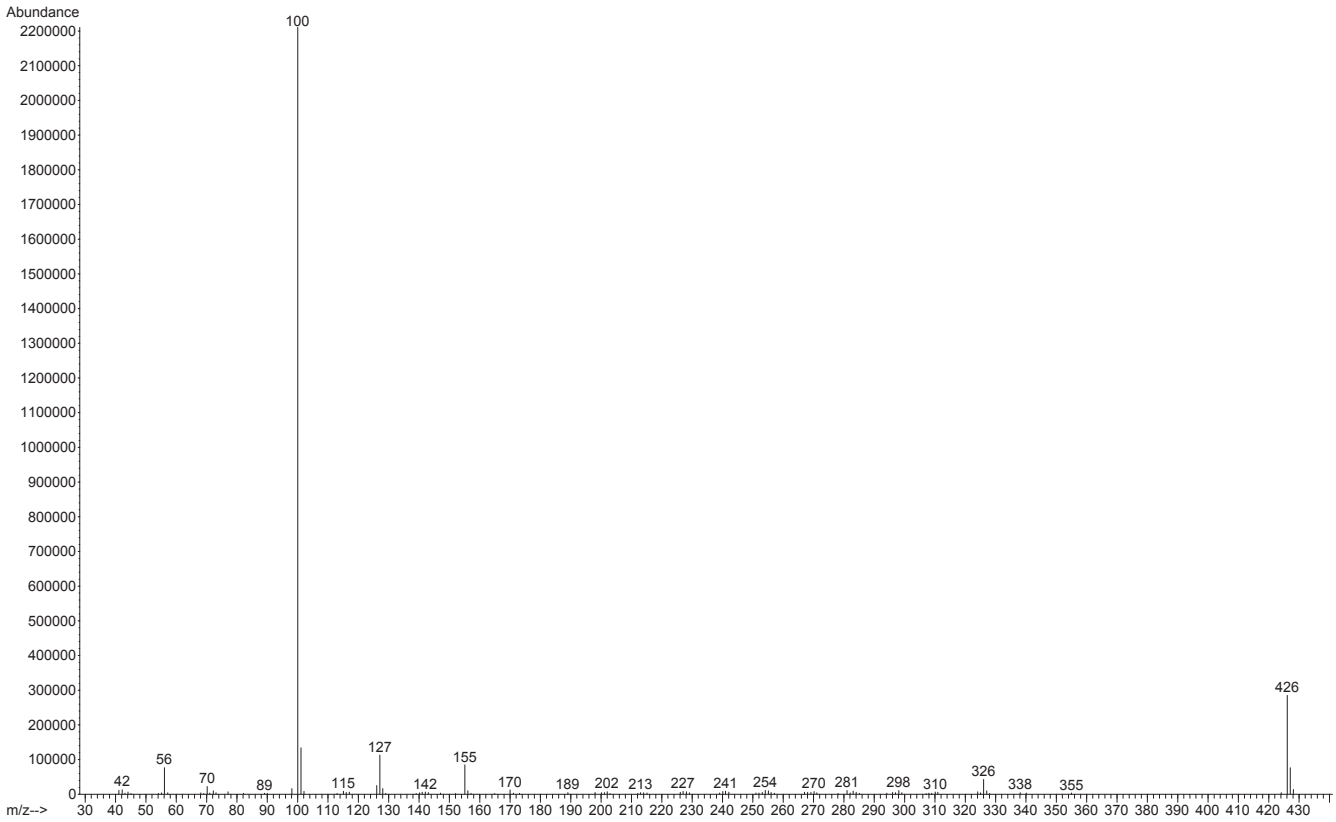
# WIN55,212-3

| | |
|---|---|
| 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 | $C_{27}H_{26}N_2O_3$ |
| 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<br>Qualifier-1 426.4<br>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:**



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