

JWH 015 JWH 250 HU-210 HU-231 HU-331 JWH 018



C hemistry

orensic



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The use of synthetic designer drugs targeting cannabinoids (referred to as "spice") has exploded in the last few years. There were more than 6,000 calls to Poison Control Centers in 2011 reporting symptoms atypical of natural marijuana use, and it was reported that one in nine high school seniors admitted to trying synthetic cannabinoids (CBs) in 2011.¹ "Spice" consists of any dried, leafy plant material laced with synthetic chemicals including the JWH, AM, CP, HU, RCS, and UR-families of CB analogs. More than 200 distinct chemical species have appeared in these mixtures.² Little is known of the pharmacokinetics, metabolism, or even toxicology associated with their consumption, making it incredibly difficult for medical providers to treat acute symptoms. Cayman scientists were first alerted to the issue in 2009 when a bulk request for the potent central CB1 agonist CP 47,497 was received from an unknown, off-shore customer. Our subsequent investigations and collaborations with law enforcement agencies revealed an elaborate network of shadowy bulk suppliers, manufacturers (cooks), and distributors racing to stay ahead of formal DEA listings of banned substances.

This Forensic Chemistry mini-catalog is devoted to showcasing our collection of synthetic CB reference standards. These include all of the main families of abused compounds as well as their metabolites, isomers, and deuterated forms.* Throughout these pages you will also find a wide variety of cathinones (bath salts), phenethylamines, amphetamines, indanes, and tryptamines. The JWH Metabolite ELISA, designed by our scientists to quickly detect synthetic CB metabolites in human urine, is also featured. Cayman's forensic product line is continually evolving. The most current availability will always be listed at www.caymanchem.com/forensics. We are dedicated to working with the forensic and academic communities to identify emerging new drugs and to quickly make authentic reference standards available. Please contact our sales department (sales@caymanchem.com) for your custom requests and to share your new product ideas.

1. Johnston, L.D., O.M.P., Bachman, J.G., and Schulenberg, J.E. (2011) Marijuana use continues to rise among U.S. teens, while alcohol use hits historical lows. Univ. Michigan News Serv., www.monitoringthefuture.org

2. Variously named Master Puff, Kryptonite, Colorado Chronic, Bazinga, Pandora Platinum, Flawless, Berry Twist, Purple Dank, Ice, Kush, Baha Blast, Slow Motion Potion, Baked, Destiny, Buddha's Belly, Paralyzing Passion Fruit, Hot Hawaiian, Daisy, Supaman Black, Supaman Silver, Hush, King, Extreme potpourri, Funkey Monkey, Jamaican potpourri, Deadman, Venom, BC, Bliss-blueberry, Bliss-strawberry, Passion, Juiced, MJ, K2, K3, Black Mamba, Mr. Smiley, Wyoming Sky, Texas Sky, Deadman Walking, Smiley Dog, Red velvet, Blindman, Naked Lady, Red Magic, Green Buddha, Grape Ape, Nuke, High Times, Dark Lotus, Headee Confetti, Karma-Bubble gum, Oz potpourri, XXL2 Tropic Hypnotic, Bocomo True Gold, Pandora Morpheus, Bocomo Kind, Spush, Chili, Wildcat, Bocomo Blue Lotus, Flame Boy, Cloud 10X, Metamorphosis, California 10X, Green Grass, Junale Booaie, California 7X, Dirty Blonde, Crazy Lab Monkey Evolution, Purple Dragon, Code Red, High Volt, FUBAR, Mind Eraser, M@ary Joy, Paco,

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Forensic Chemistry

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AEA	Arachidonoyl Ethanolamine; Anandamide
AMT	α-Methyltryptamine
BZP	Benzylpiperazine
СВ	Cannabinoid
СҮР	Cytochrome P450
EC ₅₀	50% Effective Concentration
ED ₅₀	50% Effective Dose
FAAH	Fatty Acid Amide Hydrolase
GC	Gas Chromatography
GTΡγS	Guanosine 5'-O-(gamma-thio) triphosphate
IC ₅₀	50% Inhibitory Concentration
K _i	Dissociation Constant
MAGL	Monoacylglycerol Lipase
MDA	3,4-Methylenedioxyamphetamin
MDMA	3,4-Methylenedioxy-N- methylamphetamine
MS	Mass Spectrometry
LC	Liquid Chromatography
pEC ₅₀	Negative logarithm of the EC ₅₀ value
рК _і	Negative logarithm of the K _i value
РМА	<i>para-</i> Methoxyamphetamine
тнс	Tetrahydrocannabinol

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Thomas G. Brock, Ph.D.

Fc

Synthetic Cannabinoids: From JWH 018 to Marinol[®]

Marijuana (*Cannabis* spp.) is usually marketed as dried leaves and buds. These plant parts are rich in chemicals, with over 60 compounds which are unique to this genus and thus are called 'cannabinoids' (CB). Many, including cannabidiol and cannabigerol, have diverse, pronounced physiological effects in mammalian systems.^{1,2} One CB in particular, Δ^9 -tetrahydrocannabinol (THC), has drawn interest because of its psychoactive and analgesic effects. The remarkable mixture of CBs and other phytochemicals in marijuana has driven its use throughout the world for medical, recreational, and spiritual purposes for five millennia.3

The Pursuit of Synthetic CBs

Legal, commercial, and medical issues support the development of synthetic CBs. In the United States, the FDA, which supervises the approval of new drugs, must evaluate each active compound with its associated inactive ingredients, which may, for example, affect pharmacokinetics. As may be expected, different varieties of *Cannabis* have unique ratios of CBs and other chemicals, and, like distinct formulations of prescription drugs, have discrete physiological effects. Marijuana simply cannot be evaluated as a drug by the FDA. Botanical preparations may, in FDA parlance, be called 'dietary supplements' and may claim to offer health benefits, but they must also explicitly disclaim ability to treat or prevent disease.

While inhaling the smoke of marijuana has negative respiratory effects and many purported benefits of cannabis are anecdotal or less effective than existing therapies, it is clear that marijuana and THC analogs affect pain, nausea, appetite, immunity, memory, and mood.⁴ Although medications or treatments exist for each of these conditions, there is significant room for improvement and each represents a huge commercial market. The challenge is developing an FDA-approvable formulation using an active compound or compounds from marijuana, or their analogs. The search skyrocketed after the elucidation of the molecular structure and actions of THC.

The primary receptors targeted by THC are G_i protein-coupled receptors known as CB1 and CB2. As with other Gi-linked receptors, the activation of CB₁ or CB₂ typically blocks the activation of adenvlate cyclase, preventing signaling through cyclic AMP. Significantly, CB1 and CB2 differ in their distribution, so they subserve distinct roles. CB1 is predominantly localized in the central nervous system (CNS) and has critical actions in suppressing neuronal signaling, particularly that related to mood, stress, appetite, and



memory.5 The receptor was the first one described to be involved in retrograde neuronal signaling: it is localized, within neuronal junctions, on the presynapse. Its activation can produce a reduction in the release of neurotransmitters. Normally, signaling through the synapse by neurotransmitters can result in the synthesis of natural endocannabinoids, with their subsequent secretion into the synapse, leading to retrograde signaling back to terminate neurotransmitter release. CB₂, on the other hand, is primarily found on immune cells, both throughout the peripheral vascular system and in the CNS. Activation of this Gi-linked receptor profoundly suppresses immune cell function and pain.⁵ It is important to note that, beyond these generalizations, there is some overlap in the distributions and actions of the two receptors. CB1 can be found peripherally and CB₂ has neuronal sites and both are involved in nociception.¹

Synthetic THC Analogs and Synthetic Cannabinoids

The first THC analogs, including HU-210 and CP 47,497 (Figure 2), were developed in the 1980s. Their introduction allowed characterization of the localization and types of responses evoked by THC analogs and, subsequently in the early 1990s, the discovery of CB1 and CB2. Cannabimimetic actions of CP-47,497 included analgesic, motor depressant, anticonvulsant, and hypothermic effects, as well as increased vocalization in dogs.⁶ An independent search for novel antinociceptive compounds, based on known NSAIDs, introduced the structurally distinct (aminoalkyl)indoles, like WIN 55,212-2.7 Surprisingly, WIN 55,212-2 binds both CB_1 and CB_2 (K_i = 1.9 and 0.28 nM, respectively) with higher affinities than does THC (K_i = 41 and 36 nM, respectively). This breakthrough molecule led John W. Huffman, working at Clemson University, to conclude after some modeling that "a simple alkyl chain could replace the aminoalkyl group" (personal communication). The investigation of hundreds of related "JWH compounds", characterized primarily by their binding affinities for CB receptors, ensued.

JWH 018 is the prototypical JWH compound (Figure 2). Its high potency $(CB_1:K_i = 9.0 \text{ nM}, CB_2:K_i = 2.94 \text{ nM})$ and non-THC structure made it a desirable component of many Spice/K2-type herbal blends.^{8,9} Typically, these herbal samples, commonly promoted as 'incense' and 'not for human consumption', contain multiple synthetic CBs (e.g., JWH 018, JWH 073, or a C8 homolog of CP 47,497), natural endocannabinoids (e.g., oleamide), as well as other substances (e.g., eucalyptol, α -tocopherol).^{8,10,11} In an effort to develop generic legislation to control all synthetic CBs, the Advisory Council on the Misuse of Drugs (ACMD; United Kingdom) developed a structural classification of JWH compounds.¹² The Group 1 naphthoylindoles are typified by JWH 018 and includes 73 other compounds. The related Group 2 naphthylmethylindoles contain 9 compounds (e.g., JWH 175 ($CB_1:K_i =$ 22 nM)).13 Several of the 32 known naphthoylpyrroles (Group 3) are potent CB receptor agonists (JWH 147: $CB_1:K_i = 11 \text{ nM}$, $CB_2:K_i = 7.1 \text{ nM}$)¹⁴ and therefore have a high abuse potential. The Group 4 napthylmethylindenes have 3 members, like IWH 176 (CB₁:K₁ = 26 nM).¹³ Finally, the Group 5 phenylacetylindoles cover 28 synthetic CBs, like JWH 203 (CB1:Ki = 8 nM, $CB_2:K_i = 7 \text{ nM})^{15}$, some of which have been detected in blends.¹⁶⁻¹⁹

THC analogs, like HU-210 and CP 47,497, and certain first-generation synthetic CBs, like JWH 018 and JWH 073, have largely been regulated worldwide. They have been replaced by similarly potent JWH compounds, including naphthoylindoles (e.g., JWH 081, JWH 122, JWH 200, JWH 210, JWH 398) and phenylacetylindoles (e.g., JWH 203, JWH 250, JWH 251).16,20,21 In addition, AM2201 (Figure 3), an "AM-type" compounds described in a patent by Alexandros Makrivannis, has emerged.²² This patent also introduced benzoylindoles, like AM679. Also common is UR-144, developed by scientists at Abbott, who included a tetramethylcyclopropyl group to confer selectivity for the CB₂ receptor.²³ While selective for CB₂, this



Figure 2. Examples of four major classes of JWH compounds

compound still binds CB₁ effectively (K_i = 150 nM), presumably explaining its popularity. Both the Makriyannis patent and the Abbott report describe dozens of additional compounds which are candidates for abuse.

Several additional synthetic CBs are structurally distinctive. The replacement of the indole core of the JWH CBs with a benzimidazole core, as in AZ-11713908 (Figure 3), gives significant CB₂ selectivity.^{24,25} A series of compounds using a quinolone core also have high affinities for CB receptors, as well as effectiveness *in vivo*.^{26,27} The addition of an adamantylamino group to a quinolone base, as in SER-601, confers selectivity for CB_2 over CB_1 (CB_2 : $K_i = 6.3$ nM, CB_1 : $K_i =$ 1220 nM).²⁷ The adamantylamino group also appears on newer synthetic CBs, replacing the naphthyl groups of JWH 018 and AM2201 to generate 2NE1 and STS-135, respectively. The combination of a tetramethylcyclopropyl group and a thiazolylidene base gives A-836,339, which, although CB2-selective $(CB_1:K_i = 270 \text{ nM}, CB_2:K_i = 0.64 \text{ nM})$, activates CNS CB_1 in vivo at higher doses.²⁸ The combination of neuronal pain suppression via CB₂ with milder psychoactive effects through CB1 distinguishes A-836,339 from the synthetic cannabinoids with higher affinities for CB₁.

An Eye to the Future

Marijuana provides clinical benefits, including reducing neuropathic pain and muscle spasticity.²⁹ Efforts to provide an FDA-approvable marijuana has led to the development (and approval) of Marinol® (active ingredient: dronabinol, *aka* Δ^9 -THC), which can be legally prescribed to reduce nausea and vomiting



Figure 3. Structures of some non JWH-type synthetic CBs

or increase appetite. The potential side effects of Marinol®, aside from feeling "high", are listed as: seizure, paranoia, tachycardia (fast heart rate), fainting, unusual thoughts or behavior, mood changes, dizziness, drowsiness, anxiety, confusion, nausea, and vomiting. Attempts at 'taming THC' include mixing it with other CBs, like cannabidiol, or, more recently, terpenoids.² The idea is that certain combinations will benefit from an entourage effect.

The American Association of Poison Control Centers received 6,959 calls about exposures to synthetic CBs in 2011. Adverse effects of synthetic CB exposures, compiled from the National Poison Data System in 2010, were tachycardia, agitation/irritability, vomiting, drowsiness/lethargy, confusion, nausea, hallucination/delusion, hypertension, dizziness, and chest pain.³⁰ In short, the side effects of synthetic CBs parallel those of Marinol®. According to websites like erowid.org and drugs-forum.com, users are experimenting with mixtures to provide the ideal entourage effect. Forensic screeners and toxicologists should expect an increase in blends of CBs and, perhaps, terpenoids, in the future.

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IIR-144



AZ-11713908





STS-135

6

Synthetic Cannabinoids **AKB** Series

AKB48	11566
[1345973-53-6] APINAC	A
MF: C ₂₃ H ₃₁ N ₃ O FW: 365	5.5 Purity: ≥98%
A crystalline solid Stabilit	y: ≥2 years at -20°C
Summary: A pentyl inda	azole that mimics synthetic CBs that may be sold for
recreational use; intended	for research and forensic applications
1 mg	
5 mg	$\langle \rangle$
10 mg	$\rightarrow = \langle$



AM Series

AM251

AKB48

[183232-66-8] **MF:** C₂₂H₂₁Cl₂IN₄O **FW:** 555.2 **Purity:** ≥98% A crystalline solid **Stability:** ≥1 year at -20°C Summary: A selective CB_1 receptor antagonist (K_i = 7.5 nM)

5 mg 10 mg

50 mg

100 mg



AM630

[164178-33-0] Iodopravadoline

MF: C₂₃H₂₅IN₂O₃ **FW:** 504.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A selective CB₂ receptor antagonist that binds to CB₁ and CB₂ receptors with K, values of 5.2 μM and 31.2 nM, respectively; behaves as an inverse agonist at CB₂ receptors and as a weak partial agonist at CB₁ receptors

5 mg 10 ma 50 mg 100 mg



AM679

[335160-91-3]

MF: C₂₀H₂₀INO **FW:** 417.3 **Purity:** ≥98% A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A potent synthetic CB with K_i values of 13.5 and 49.5 nM for the CB₁ and CB2 receptors, respectively; intended for research and forensic applications

5 mg 10 mg 25 mg







AM694 3-iodo isomer

MF: C₂₀H₁₉FINO **FW:** 435.3 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: An analog of AM694; intended for forensic applications

1 mg 5 mg 10 mg

11566

71670

10006974



AM694 4-iodo isomer **MF:** C₂₀H₁₀FINO **FW:** 435.3 **Purity:** ≥97%

A solution in methanol **Stability:** ≥ 1 year at -20°C Summary: An analog of AM694; intended for forensic applications



10 mg



AM1220

5 mg

10 mg

25 mg

[137642-54-7]

MF: C₂₆H₂₆N₂O **FW:** 382.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A potent synthetic CB with preference for the central CB₁ receptor (K_i = 3.88 nM) over the CB₂ receptor ($K_i = 73.4 \text{ nM}$)



AM1220 azepane isomer

MF: C₂₆H₂₆N₂O **FW:** 382.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An isomer of AM1220 in which the piperidine group has been replaced with azepane; intended for forensic and research applications



AM1235 [335161-27-8] **MF:** C₂₄H₂₁FN₂O₃ **FW:** 404.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: A potent synthetic CB with K_i values of 1.5 and 20.4 nM for the CB₁ and CB₂ receptors, respectively; intended for research and forensic applications 10 mg



AM1241

10869

9001055

1 mg

5 mg

10 mg

1 mg

5 mg

[444912-48-5] **MF:** C₂₂H₂₂IN₃O₃ **FW:** 503.3 **Purity:** ≥97% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: CB₂ receptor agonist with a K_i value of 2 nM and greater than 100-fold selectivity over the CB1 receptor



AM1248

[335160-66-2] **MF:** C₂₆H₃₄N₂O **FW:** 390.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An adamantoylindole derivative with an N-methylpiperidin-2-ylmethyl substitution at the indole 1-position that reportedly acts as a moderately potent agonist for both the CB₁ and CB₂ receptors ($K_s = 11.9$ and 4.8 nM, respectively)

5 mg 10 mg 25 mg



11583

9001094

10010118

11282

AM2201 [335161-24-5]

MF: C₂₄H₂₂FNO **FW:** 359.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C Summary: A potent synthetic CB with K, values of 1.0 and 2.6 nM for the CB₁ and CB₂ receptors, respectively

5 mg 10 mg 25 mg



Summary: An internal standard for the quantification of AM2201 by GC- or LC-MS

500 µg 1 mg 5 mg

AM2201-d₅

AM2201 N-(2-fluoropentyl) isomer **MF:** C₂₄H₂₂FNO **FW:** 359.4 **Purity:** ≥95%

A solution in acetonitrile **Stability:** ≥ 1 year at -20°C

Summary: Differs structurally from AM2201 by having a fluoro atom at the 2 postion rather than the 5 position of the pentyl chain; intended for forensic applications

100 µg 500 µg 1 mg

AM2201 N-(3-fluoropentyl) isomer

MF: C₂₄H₂₂FNO **FW:** 359.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: Differs structurally from AM2201 by having a fluoro atom at the 3 position rather than the 5 position of the pentyl chain; intended for forensic applications

100 µg 500 µg 1 mg







AM-series

10706

9001031



MF: C₂₄H₂₂FNO **FW:** 359.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A derivative of AM2201, a potent synthetic CB with K_i values of 1.0 and 2.6 nM for the CB₁ and CB₂ receptors, respectively



AM2201 2-hydroxyindole metabolite

MF: C₂₄H₂₂FNO₂ **FW:** 375.4 **Purity:** ≥98%

A solution in acetonitrile **Stability:** ≥ 1 year at -20° C

Summary: A potential monohydroxylated urinary metabolite of AM2201, a potent synthetic cannabinoid ($K_1s = 1.0$ and 2.6 nM for the CB₁ and CB₂ receptors, respectively)



AM2201 5-hydroxyindole metabolite

MF: C₂₄H₂₂FNO₂ **FW:** 375.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An expected phase I metabolite of AM2201, detectable in serum or as a glucuronidated derivative in urine

1 mg 5 mg 10 mg

1 mg

5 mg

10 mg

100 µg

500 µg

1 mg

1 mg

5 mg

10 mg



AM2201 6-hydroxyindole metabolite

MF: C₂₄H₂₂FNO₂ **FW:** 375.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: An expected metabolite of AM2201 generated during phase I metabolism, detectable in blood and urine; intended for forensic applications





A solution in acetonitrile **Stability:** ≥1 year at -20°C

Summary: An expected minor monohydroxylated urinary metabolite of AM2201, a potent synthetic cannabinoid ($K_s = 1.0$ and 2.6 nM for the CB₁ and CB₂ receptors, respectively)

1 mg 5 mg 10 mg

100 µg

500 µg

1 mg

9001029

11194

11196

11192



11193

AM2201 N-(4-hydroxypentyl) metabolite 10203

MF: C₂₄H₂₂FNO₂ **FW:** 375.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥1 year at -20°C

Summary: An expected urinary metabolite of AM2201



AM2201 N-(4-hydroxypentyl) metabolite-d₅ 11457

MF: C₂₄H₁₇D₅FNO₂ **FW:** 380.5 **Chemical Purity:** ≥98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀ A solution in methanol **Stability:** ≥ 2 years at -20° C Summary: An internal standard for the quantification of AM2201 N-(4-hydroxypentyl) metabolite by GC- or LC-MS



AM2201 2'-naphthyl isomer

MF: C₂₄H₂₂FNO **FW:** 359.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from AM2201 by having the naphthyl group attached at the 2' position

1 mg 5 mg 10 mg



AM2232 11503 [335161-19-8]

MF: C₂₄H₂₀N₂O **FW:** 352.4 **Purity:** ≥95%

A solution in acetonitrile **Stability:** ≥1 year at -20°C

Summary: A potent synthetic CB with K, values of 0.28 and 1.48 nM for the CB₁ and CB2 receptors, respectively; intended for research and forensic applications



AM2233

1 mg

5 mg

10 mg

25 mg

1 mg

5 mg

10862

10 mg

5 mg

10 mg

25 mg

[444912-75-8]

MF: C₂₂H₂₃IN₂O **FW:** 458.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A full agonist of the CB_1 receptor (K_i = 2.8 nM); the (R)-enantiomer exhibits a K_i value of 0.2 nM and has ~8-fold higher affinity for CB₁ compared to WIN 55,212-2 (K = 1.6 nM); intended for forensic applications



AM2233 azepane isomer

11584

11008

MF: C₂₂H₂₃IN₂O **FW:** 458.3 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An isomer of AM2233 in which the piperidine group has been replaced with azepane; intended for forensic and research applications



MAM2201

1 mg 5 mg 10 ma 9001219

[1354631-24-5] AM2201 4-methylnaphthyl analog, JWH 122 N-(5-fluoropentyl) analog **MF:** C₂₅H₂₄FNO **FW:** 373.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: An analog of AM2201 that is methylated at the 4 position of the naphthyl group; intended for research and forensic purposes

11619

MAM2201-d₅

AM2201 4-methylnaphthyl analog-d₅ [WH 122 N-(5-fluoropentyl) analog-d₅ **MF:** C₂₅H₁₉D₅FNO **FW:** 378.5 **Purity:** ≥98%

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An internal standard for the quantification of MAM2201 by GC- or LC-MS

500 µg 1 mg 5 mg



MAM2201 N-(4-fluoropentyl) isomer

11782

MF: C₂₅H₂₄FNO **FW:** 373.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥ 1 year at -20° C Summary: A derivative of MAM2201, a synthetic cannabinoid structurally related

to AM2201 and JWH 122, two compounds which display high affinities for both CB receptors

100 µg 500 µg 1 mg



MAM2201 N-pentanoic acid metabolite 11779

JWH 122 N-pentanoic acid metabolite

MF: C₂₅H₂₃NO₃ **FW:** 385.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential phase 1 metabolite of MAM2201 or JWH 122; intended for forensic and research applications

1 mg 5 mg 10 mg



CB Series

CB-13

[432047-72-8] CRA-13

MF: C₂₆H₂₄O₂ **FW:** 368.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A dual agonist of the CB_1 (IC₅₀ = 15 nM) and CB_2 (IC₅₀ = 98 nM) receptors; potently blocks CB1-dependent neuropathic mechanical hyperalgesia in



CB-25

[869376-63-6]

MF: C₂₅H₄₁NO₃ **FW:** 403.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A stable analog of Δ^9 -THC; exhibits high affinity for the CB₁ and CB₂ receptors with K_i values of 5.2 and 13 nM, respectively, also it behaves as an inverse agonist for the CB₁ receptor as assessed in a cyclic AMP functional assay



CB-52

[869376-90-9]

MF: C₂₆H₄₃NO₃ **FW:** 417.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A stable analog of Δ^9 -THC and AEA; exhibits high-affinity for the CB₁ and CB₂ receptors (K_i = 210 and 30 nM, respectively); behaves primarily as a CB₁ receptor partial agonist and a CB2 receptor neutral antagonist in vitro



CB-86

[1150586-64-3]

MF: C₂₆H₄₃NO₃ **FW:** 417.6 **Purity:** ≥98%

A solution in ethanol **Stability:** ≥ 1 year at -20° C

Summary: A partial agonist for the CB1 receptor and a neutral antagonist for the CB₂ receptor with K_i values of 5.6 and 7.9 nM, respectively; at 1 mg/kg, exhibits antinociceptive effects in mice treated with formalin



CP Series (±)-CP 47,497

[70434-82-1]

10010398

10010117

13289

MF: $C_{21}H_{34}O_2$ **FW:** 318.5 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A cannabimimetic compound that binds the CB₁ receptor with a K_i value of 2.2 nM



•Also Available: (±)-CP 47,497 (solution) (16851)

(±)-epi CP 47,497

3-trans CP 47,497

Summary: An epimer of (±)-CP 47,497; intended to be used as an analytical standard



(±)-epi CP 47,497 (solution)

3-trans CP 47,497

MF: C₂₁H₃₄O₂ **FW:** 318.5 **Purity:** ≥98% A solution in methanol **Stability:** ≥2 years at -20°C Summary: An epimer of (±)-CP 47,497; intended to be used as an analytical standard



(±)-CP 47,497-d₁₁ (solution)

MF: C₂₁H₂₃D₁₁O₂ **FW:** 329.6 **Chemical Purity:** ≥98%

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₁₁); \leq 1% d₀ A solution in methanol **Stability:** ≥ 1 year at -20° C Summary: An internal standard for the quantification of (±)-CP 47,497 by GC- or



5 ma

10 mg

25 mg





(+)-CP 47,497

[1.34.308-14-8] **MF:** C₂₁H₃₄O₂ **FW:** 318.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A bicyclic CB analog with potent analgesic activity; comparable or more potent than Δ^9 -THC in analgesic motor depressant, anticonvulsant, and hypothermic effects; avidly binds the CB_1 receptor (K_i = 4.15 nM)



(+)-CP 47,497 (solution)

[134308-14-8]

MF: $C_{21}H_{34}O_2$ **FW:** 318.5 **Purity:** \ge 98%

A solution in methanol **Stability:** ≥ 2 years at -20° C

Summary: A bicyclic CB analog with potent analgesic activity; comparable or more potent than Δ^9 -THC in analgesic motor depressant, anticonvulsant, and hypothermic effects; avidly binds the CB_1 receptor (K_i = 4.15 nM)



[114753-51-4]

MF: $C_{21}H_{34}O_2$ **FW:** 318.5 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A bicyclic CB analog with potent analgesic activity; comparable or more potent than Δ^9 -THC in analgesic motor depressant, anticonvulsant, and hypothermic effects; avidly binds the CB_1 receptor ($K_i = 2.1$ nM)



[114753-51-4]

MF: $C_{21}H_{34}O_2$ **FW:** 318.5 **Purity:** \ge 98%

A solution in methanol **Stability:** ≥2 years at -20°C

Summary: A bicyclic CB analog with potent analgesic activity; comparable or more potent than Δ^9 -THC in analgesic motor depressant, anticonvulsant, and hypothermic effects; avidly binds the CB_1 receptor ($K_i = 2.1 \text{ nM}$)



500 µg 1 mg

10910

13219

10913

10919

10687





MF: C₂₁H₃₄O₂ **FW:** 318.5 **Purity:** ≥98%

A crystalline solid **Stability:** \geq 2 years at -20°C



•Also Available: (±)-CP 47,497-C8-homolog (solution) (13216) DEA-exempt formulation

(±)-CP	47,49	7-C8-ho	molog-d7 (solution)	10686

Cannabicvclohexanol-d-

MF: $C_{22}H_{29}D_7O_2$ **FW:** 339.6 Chemical Purity: \ge 98%

Deuterium Incorporation: \ge 99% deuterated forms (d₁-d₇); \le 1% d₀

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An internal standard for the quantification of (±)-CP 47,497-C8homolog by GC- or LC-MS

100 µg 500 µg 1 mg



(±)3-epi CP 47,497-C8-homolog

10918

MF: $C_{22}H_{22}O_2$ **FW:** 332.5 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥1 year at -20°C Summary: A by-product generated in the synthesis of (+)-CP 47,497-C8-homolog; for use as an analytical standard

5 mg 10 mg 25 mg



(±)3-epi CP 47,497-C8-homolog (solution)

MF: C₂₂H₃₆O₂ **FW:** 332.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A by-product generated in the synthesis of (+)-CP 47,497-C8-homolog; for use as an analytical standard

CP 47,497-C8-homolog

C-8-hydroxy metabolite

MF: C₂₂H₃₆O₃ **FW:** 348.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A potential metabolite of CP 47,497-C8-homolog; intended for forensic purposes



CP 47,497-para-quinone analog

MF: C₂₁H₂₂O₂ **FW:** 332.5 **Purity:** ≥90%

A solution in methanol **Stability:** ≥1 year at -20°C Summary: A potential metabolite of CP 47,497

500 µg 1 mg

5 mg

10 mg

25 mg



(±)-CP 55,940

[83003-12-7]

MF: C₂₄H₄₀O₃ **FW:** 376.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: One of the first bicyclic mimetics of Δ^9 -THC found to have superior analgesic properties; 20- to 100-fold more effective than Δ^9 -THC in altering the reactions to thermal, mechanical, and chemical pain in mice; used to characterize the capacity of novel cannabimimetics to bind the CB₁ receptor in rat brain preparations





13802 (+)-CP 55,940

MF: C₂₄H₄₀O₃ **FW:** 376.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: An enantiomer purified from the (±)-CP 55,940 racemic mixture; the functional characteristics of this isomer have not been studied



(-)-CP 55,940

[83002-04-4]

1 mg

5 mg

10 mg

25 mg

5 mg

10 mg

25 mg

9000773

10889

13241

MF: C₂₄H₄₀O₃ **FW:** 376.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A potent, non-selective CB receptor agonist with K_i values of 0.58 and 0.69 nM for human recombinant CB1 and CB2, respectively



(±)5-epi CP 55,940

MF: C₂₄H₄₀O₃ **FW:** 376.6 **Purity:** ≥98%

Summary: A by-product generated in the synthesis of (±)-CP 55,940; intended to be used as an analytical standard



HU Series

HU-210

13608

13803

(DEA Schedule | Regulated Compound) 90082

[112830-95-2]

MF: C₂₅H₃₈O₃ **FW:** 386.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic agonist analog of Δ^9 -THC, which is the primary psychoactive component of marijuana; a potent CB1 and CB2 receptor agonist that binds to neuroblastoma cell membrane CB1 receptors with about the same affinity as CP 55,940; demonstrates ED₅₀ values of 5-20 µg/kg in mouse hypothermia, analgesia, hypoactivity, and catalepsy models

1 mg 5 mg 10 mg 25 ma



• Also Available: HU-210 (solution) (90083) DEA-exempt formulation

HU-211

1 mg

5 mg

10 mg

25 mg

10006350

90086

10005673

[112924-45-5] Dexanabinol **MF:** C₂₅H₂₀O₂ **FW:** 386.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic terpene-based CB devoid of CB1 and CB2 receptor agonist activity; exhibits neuroprotective, antioxidant, and anti-inflammatory properties



HU-308

[256934-39-1]

MF: C₂₇H₄₂O₃ **FW:** 414.6 **Purity:** ≥98%

A solution in methyl acetate **Stability:** ≥1 year at -20°C

Summary: A potent, selective agonist for the CB_2 receptor (K_i = -20 nM compared to that of $CB_1:K_i = >10 \ \mu M$; elicits hypotensive, analgesic, and anti-inflammatory activity, but none of the behavioral tetrad of psychomotor responses characteristic of the phenolic components of hemp, such as Δ^9 -THC when administered to whole animals

1 mg 5 mg 10 mg 25 mg



HU-331

[137252-25-6]

MF: C₂₁H₂₈O₃ **FW:** 328.5 **Purity:** ≥95%

A solution in methyl acetate **Stability:** ≥ 1 year at -20° C Summary: A hydroxylquinone CB analog that exhibits potent antineoplastic activity on a variety of human cancer cell lines



For current European or other overseas pricing, see caymaneurope.com or contact your local distributor.



JWH Series

JWH 007 [155471-10-6]

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98% A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A potent CB receptor agonist that avidly binds to both CB1 and CB2 (K_i = 9.5 and 2.9 nM, respectively); performs comparably to Δ^9 -THC in mouse studies on spontaneous activity, antinociception, hypothermia, and catalepsy

5 mg 10 mg 25 mg



JWH 007-d。

MF: $C_{35}H_{16}D_{0}NO$ **FW:** 364.5 **Chemical Purity:** \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀ A solution in methyl acetate Stability: ≥1 year at -20°C Summary: An internal standard for the quantification of JWH 007 by GC- or LC-MS

500 µg 1 mg 5 mg



JWH 011

[155471-13-9] JWH 004 1-methylhexyl analog

MF: C₂₇H₂₉NO **FW:** 383.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A synthetic CB that is analogous to the N-hexyl JWH 004, which has high affinities for both central CB1 and peripheral CB2 receptors (Ki = 48 and 4.02 nM, respectively)

1 mg 5 mg 10 mg



JWH 015

10009018

9001058

[155471-08-2] **MF:** C₂₃H₂₁NO **FW:** 327.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: A selective CB2 receptor agonist with K, values of 13.8 and 383 nM for human recombinant CB2 and CB1 receptors, respectively

5 mg 10 mg 25 mg



10266

JWH 015-d₇

MF: C₂₃H₁₄D₇NO **FW:** 334.5 **Chemical Purity:** ≥98%

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₇); \leq 1% d₀

A crystalline solid **Stability:** ≥2 years at -20°C

 $\ensuremath{\textit{Summary:}}$ An internal standard for the quantification of JWH 015 by GC- or LC-MS

500 µg

1 mg 5 mg



JWH 016

[155471-09-3]

MF: C₂₄H₂₃NO **FW:** 341.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A cannabimimetic indole that potently activates both CB receptors, with K_i values of 22.0 and 4.29 nM for CB₁ and CB₂, respectively

5 mg

10 mg 25 mg



JWH 018

57711010

[209414-07-3] AM678 **MF:** C₂₄H₂₃NO **FW:** 341.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: A selective agonist of the CB_2 receptor with K_1 values of 9.0 and 2.94 nM for CB_1 and CB_2 , respectively



•Also Available: **JWH 018 (solution)** (13169) DEA-exempt formulation

JWH 018-d₉ (solution)

AM678

MF: C₂₄H₁₄D₉NO **FW:** 350.5 **Chemical Purity:** ≥98%

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀

A solution in methanol **Stability:** ≥ 1 year at -20°C **Summary:** An internal standard for the quantification of JWH 018 by GC- or LC-MS

500 µg







JWH 018 adamantyl analog

AB-001

MF: $C_{24}H_{31}$ NO **FW:** 349.5 **Purity:** \ge 97% A crystalline solid **Stability:** \ge 2 years at -20°C

Summary: An analog of JWH 018, a mildly selective agonist of the peripheral cannabinoid receptor, where the naphthalene ring is substituted with an adamantyl group



JWH 018 adamantyl carboxamide 9001193

[1345973-50-3] APICA, 2NE1

MF: $C_{24}H_{32}N_2O$ **FW:** 364.5 **Purity:** $\ge 98\%$

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A structural analog of JWH 018 where the naphthalenyl-methanone portion has been replaced by adamantyl carboxamide; may retain high affinity for the CB_2 receptor with reduced affinity for the CB_1 receptor; intended for research and forensic applications



JWH 018 N-(5-bromopentyl) analog 11047

MF: C₂₄H₂₂BrNO **FW:** 420.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C **Summary:** Differs structurally from JWH 018 by having bromine added at the 5 position of the pentyl chain; intended for forensic and research applications



JWH 018 N-(5-chloropentyl) analog

MF: $C_{24}H_{22}$ ClNO **FW:** 375.9 **Purity:** \ge 95% A crystalline solid **Stability:** \ge 2 years at -20°C

Summary: Differs structurally from JWH 018 by having chlorine added to the 5 position of the pentyl chain; intended for forensic and research applications



JWH 018 N-(1,1-dimethylpropyl) isomer

MF: $C_{24}H_{23}$ NO **FW:** 341.5 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs from JWH 018 structurally by having a 1,1-dimethylpropyl group, rather than a pentyl chain, extending from the indole group; intended for forensic purposes



9000799



JWH 018 N-(1,2-dimethylpropyl) isomer

MF: C₂₄H₂₃NO **FW:** 341.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C **Summary:** Differs from JWH 018 structurally by having a 1,2-dimethylpropyl

group, rather than a pentyl chain, extending from the indole group; intended for forensic purposes

1 mg 5 mg 10 mg

1 mg

5 mg

10 mg

JWH 018 N-(2,2-dimethylpropyl) isomer

MF: C₂₄H₂₃NO **FW:** 341.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C **Summary:** Differs from JWH 018 structurally by having a 2,2-dimethylpropyl

Summary: Differs from JWH 018 structurally by having a 2,2-dimethylpropyl group, rather than a pentyl chain, extending from the indole group



JWH 018 N-(4,5-epoxypentyl) analog

JWH 018 epoxide

MF: $C_{24}H_{21}NO_2$ **FW:** 355.4 **Purity:** \ge 98% A solution in methanol **Stability:** \ge 1 year at -20°C

Summary: An analog of JWH 018 distinguished by a terminal epoxide group on the alkyl chain



10521





10900

13824

1 mg 5 mg

10 ma

1 mg 5 mg 10 mg

10660

10849

11585

JWH 018 N-(1-ethylpropyl) isomer

MF: C₂₄H₂₃NO **FW:** 341.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An isomer of JWH 018, differing by having an ethylpropyl group in place of the crucial pentyl chain; intended for research and forensic applications

1 mg 5 mg 10 mg

9001000

9001003

9001001

11075



JWH 018 2-hydroxyindole metabolite

9000844

MF: $C_{24}H_{23}NO_2$ **FW:** 357.4 **Purity:** \ge 98% A crystalline solid **Stability:** \ge 2 years at -20°C

Summary: A potential monohydroxylated urinary metabolite of JWH 018

1 mg 5 mg 10 mg



JWH 018 2-hydroxyindole metabolite-d₉

10711

MF: $C_{24}H_{14}D_9NO_2$ **FW:** 366.5 **Chemical Purity:** $\ge 98\%$ **Deuterium Incorporation:** $\ge 99\%$ deuterated forms $(d_1-d_9); \le 1\% d_9$

A solution in methanol **Stability:** \geq 1 year at -20°C **Summary:** An internal standard for the quantification of JWH 018 2-hydroxyindole

metabolite by GC- or LC-MS

100 µg 500 µg 1 mg



JWH 018 4-hydroxyindole metabolite 9000851

MF: C₂₄H₂₃NO₂ **FW:** 357.4 **Purity:** ≥98% A solution in ethanol **Stability:** ≥1 year at -20°C **Summary:** A major urinary metabolite of JWH 018

1 mg 5 mg 10 mg



JWH 018 4-hydroxyindole metabolite-d₉

10712

MF: $C_{24}H_{14}D_9NO_2$ **FW:** 366.5 **Chemical Purity:** \ge 98%

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀

A solution in ethanol **Stability:** ≥1 year at -20°C

Summary: An internal standard for the quantification of JWH 018 4-hydroxyindole metabolite by GC- or LC-MS

100 µg 500 µg 1 mg



Thomas G. Brock, Ph.D.

Fc

Today's Designer Drugs and Recreational Drugs of Abuse

In the past, the war on drugs was traditional warfare, a battle against easily recognizable foes, like heroin, cocaine, and marijuana. Their detection by crime labs was relatively straightforward, scientists could evaluate their actions and toxicology, and even the public knew what they should look and act like. Today, the enemy is much more elusive. Some drugs are chemical variations on old compounds, legal largely by design. Many are unrecognizable by name, except to the well-informed. Some appear under the guise of dietary supplements, while others are hidden in everyday products, like bath salts, plant foods, or foot powders (Figure 1). The rapid innovation in the design of drugs of abuse challenges legal systems to keep apace, while the blending of novel compounds tests the skills of forensic scientists. Research laboratories don't have the money or manpower to evaluate the physiological or neurological properties of most designer drugs, so most of the testing is done by the curious public and reported through online drug forums. The following is an overview of some of the major designer and recreational drugs that are currently of concern.



Figure 1. Some party pills, dietary supplements, and plant food samples

Phenethylamines and Tryptamines

Phenethylamines (or phenylethylamines) were popularized in the 1990s by Dr. Alexander Shulgin and Ann Shulgin in their book, PiHKAL: A Chemical Love Story, where PiHKAL stands for 'Phenethylamines I Have Known and Loved'. This book includes, among other things, synthesis procedures and dosages for over 200 psychedelic compounds. The simplest compound, phenethylamine (Figure 2), is a natural compound which is rapidly metabolized by monoamine oxidases to phenylacetic acid. Its structural similarity to the neurotransmitter dopamine (Figure 2) is readily apparent. The most commonly abused phenethylamines have methoxy groups in positions 2 and 5 of the aromatic ring plus distinct lipophilic substituents (alkyl, halogen, alkylthio, etc.) at the 4 position. The separation of the primary amine from the phenyl ring by two carbons defines these '2C' compounds. An addition at the para position is denoted in the name by a single letter (e.g., Cl, 2C-C; ethyl, 2C-E). Phenethylamines can activate a variety of receptors, most notably the serotonin 5-HT_{2A} and 5-HT_{2C} receptors.^{2,3} While only certain phenethylamines (e.g., 2C-B) are regulated in the United States, most would be illegal under the Federal Analog Act, but only if intended for human consumption. Several, such as 2C-E and 2C-I, were popularized by PiHKAL, while other compounds, like 25I-NBOMe, have been developed more recently. They are often combined with monoamine oxidase inhibitors to reduce metabolism and prolong psychoactivity.



Figure 2. Some phenethylamines (left) and tryptamines (right) compared to the neurotransmitters dopamine and serotonin (bottom)

The Shulgins followed PiHKAL with TiHKAL: The Continuation, which includes dosages, effects, and synthetic pathways of 55 tryptamines which they knew and loved. The simplest tryptamine (or indoleamine) has two carbons separating a primary amine from an indole ring structure (Figure 2). Serotonin, or 5-hydroxytryptamine (5-HT), is a natural tryptamine that has diverse effects throughout the body. In general, tryptamines that are abused act as hallucinogens, activating 5-HT₂ receptors and altering the re-uptake of monoamines, like serotonin, dopamine, and norepinephrine.⁴⁻⁶ Most commonly, the tryptamines differ in the number and types of amino-terminal alkyl groups and the presence of a hydroxy or methoxy group at the 4 or 5 indole position. All are metabolized by cytochrome P450 isoenzymes.³ Some, like N,N-dimethyltryptamine (DMT), 5-MeO-DMT, and the mushroom psychedelic psilocin (4-OH-DMT), are naturally occurring compounds found in plants and animals. DMT, the prototypical tryptamine, is regulated in the US. A commonly abused designer drug is 5-methoxy-diisopropyltryptamine (5-MeO-DIPT, foxy, or foxy methoxy). Despite legislation, phenethylamines and tryptamines remain commonly abused.7

Amphetamines and Cathinones

The simple addition of a methyl group to the α -carbon converts phenethylamine to amphetamine (Figure 3). The result is anything but subtle. While phenethylamines and tryptamines were known and loved, mostly as psychedelics and entactogens, amphetamines are potent psychostimulants. These drugs have value as medications, as in the use of Adderall for the treatment of attention deficit hyperactivity disorder and narcolepsy. However, amphetamines are known and abused worldwide, in spite of their proclivities for tolerance and dependence. Some of the most commonly abused amphetamines are modified on the primary amine, as in methamphetamine, or on the phenyl group, as in 3,4-methylenedioxy-N-methylamphetamine (MDMA, or ecstasy). Halogenated amphetamines, such as 4-fluoroamphetamine (4-FA), are also used recreationally. Many amphetamines profoundly increase dopamine concentrations in the CNS.⁶ They can also increase serotonin and norepinephrine release and inhibit their re-uptake.⁶

Adding a β -keto group to the basic amphetamine structure gives cathinone, named after khat or qat, two great Scrabble words that refer to *Catha edulis*, a flowering plant whose leaves contain the monoamine alkaloid cathinone. The chewing of khat leaves has long been popular and commonplace in parts of Africa and the Arabian peninsula. However, recent widespread abuse of cathinones as the true designer drugs of the twenty-first century has led to the ban of the plant, as well as the compounds, in the US and other countries. The cathinone family includes a variety of β -keto analogs of



Figure 3. The structures of some amphetamines, compared with norepinephrine and epinephrine (adrenaline)

the amphetamines (Figure 4). Typical alterations include a variation of the α -carbon substituent (R₁), N-alkylation or inclusion of the nitrogen atom in a ring structure (*e.g.*, pyrrolidine) at R₂ and R₃, or an addition at the aromatic ring (R₄). 4-Methylmethcathinone, commonly known as mephedrone, Meow, or M-Cat, has been one of the most commonly detected products in bath salts and has been associated with sympathomimetic adverse effects (neurological CNS issues including headache, bruxism, seizures; psychiatric disturbances like anxiety, confusion, hallucinations; gastrointestinal, cardiovascular and renal problems).⁸⁻¹⁰

Piperazines and Plant Products

Piperazines contain a six-membered ring with two nitrogen atoms at opposite positions in the ring (Figure 5). Interestingly, some piperazines act as antihelmintics, anti-histamines, anti-depressants, anti-psychotics, or hardeners for epoxy resins and plastics. Other piperazines, like 1-benzylpiperazine (BZP), are used as recreational drugs, often distributed in party pills. Many mimic the actions of amphetamines, both physiologically and psychoactively, to the point that piperazines and amphetamines are indistinguishable to both



Common Name	R1	R2	R3	R4
Cathinone	CH ₃	Н	Н	Н
Methcathinone (Ephedrone)	CH3	CH ₃	Н	Н
Ethcathinone	CH_3	$\rm CH_2 CH_3$	Н	н
4-Methylmethcathinone (Mephedrone)	CH_3	CH ₃	Н	4-CH ₃
4-Methylethcathinone	CH3	$\rm CH_2 CH_3$	Н	4-CH ₃
4-Fluoromethcathinone (Flephedrone)	CH ₃	CH_3	Н	4-F
3-Fluoromethcathinone	CH33	CH ₃	Н	3-F
4-Methoxymethcathinone (Methedrone)	CH_3	CH_3	Н	4-0CH ₃
Buphedrone	$\rm CH_2 CH_3$	CH ₃	Н	Н
Methylone (bk-MDMA)	CH_3	CH3	Н	3,4-methylenedioxy
Ethylone (bk-MDEA)	CH3	$\rm CH_2 CH_3$	Н	3,4-methylenedioxy
Butylone (bk-MBDB)	$\rm CH_2 CH_3$	CH3	Н	3,4-methylenedioxy
Pentylone	$\rm CH_2 CH_2 CH_3$	CH ₃	Н	3,4-methylenedioxy
MPPP	CH_3	pyrrol	idinyl	4-CH ₃
Pyrovalerone	$\rm CH_2\rm CH_2\rm CH_3$	pyrrol	idinyl	4-CH ₃
MDPV (3,4-Methylenedioxypyrovalerone)	$\rm CH_2CH_2CH_3$	pyrrol	idinyl	3,4-methylenedioxy

Figure 4. Chemical structures of some common cathinones; adapted from Kikura-Hanajiri *et al.*¹⁷

animal and human subjects.^{6,11} Piperazines that are currently abused can be divided into two sub-classes, the benzylpiperazines, which includes BZP and its derivatives, and the phenylpiperazines, like 1-(*m*-trifluoromethylphenyl) piperazine (TFMPP).^{12,13}

Salvia divinorum is a plant from the mint family whose growth range is limited to the cloud forests of Oaxaca, Mexico. Its leaves have long been used by shamans of the area to evoke altered states of consciousness. The primary psychoactive compound in salvia is salvinorin A (Figure 5), a diterpenoid which acts as a potent agonist of κ opioid and dopamine D₂ receptors.¹⁴⁻¹⁶ Salvia is commonly claimed to be in herbal mixtures sold online, as it remains legal in many countries and is restricted in only a few states in the U.S.^{17,18}

From the other side of the world comes *Mitragyna speciosa*, a tree that is phylogenetically related to coffee and jasmine and indigenous to Southeast Asia. The leaves of *Mitragyna* are commonly known as kratom and used for medicinal purposes, namely as a mild stimulant at lower doses and as a sedative at higher levels, as well as a substitute for opium. The leaves contain several biologically-active alkaloids, including mitragynine (Figure 5). This compound activates noradrenergic, serotonergic, and opioid receptors, with a higher affinity for the μ -opioid receptor over the δ or κ receptors.^{19,20} 7-Hydroxymitragynine is a natural derivative of mitragynine that is less abundant in the mitragyna leaves but more potent than the parent compound. Leaves and alkaloids are available online and have been detected in herbal blends distributed as incense.¹⁷



Figure 5. Piperazines (above) and two psychoactive plant products (below)

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10 mg

JWH 018 N-(5-hydroxypentyl) metabolite

MF: C₂₄H₂₃NO₂ **FW:** 357.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A major urinary metabolite of JWH 018, characterized by monohydroxylation of the N-alkyl chain

1 mg 5 mg 10 mg



JWH 018 N-(5-hydroxypentyl) metabolite-d₅ 10933

MF: $C_{24}H_{18}D_5NO_2$ **FW:** 362.5 **Chemical Purity:** \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀ A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An internal standard for the quantification of JWH 018 N-(5-hydroxypentyl) metabolite by GC- or LC-MS

100 µg 500 µg 1 mg

10920

10921

JWH 018 6-methoxyindole analog

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A solution in methyl acetate **Stability:** ≥ 1 year at -20° C Summary: Analog of JWH 018 6-hydroxyindole metabolite, a urinary metabolite of the CB receptor agonist JWH 018

1 mg 5 mg 10 mg



JWH 018 N-(1-methylbutyl) isomer

9001002

10697

IWH 073 1-methylbutyl homolog

MF: C₂₄H₂₃NO **FW:** 341.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 1 year at -20° C

Summary: Differs from JWH 018 structurally by having a methylbutyl chain, rather than a pentyl chain, extending from the indole group

1 mg 5 mg 10 mg





5 mg 10 mg

JWH 018 N-pentanoic acid metabolite-d₅ 11748

MF: $C_{24}H_{14}D_5NO_3$ FW: 376.5 Chemical Purity: \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An internal standard for the quantification of JWH 018 N-pentanoic acid metabolite by GC- or LC-MS

1 mg 5 mg 10 mg



JWH 019

[209414-08-4]

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A cannabimimetic indole that shows high-affinity for both CB1 $(K_i = 9.8 \text{ nM})$ and CB_2 $(K_i = 5.6 \text{ nM})$ receptors

5 mg 10 mg 25 mg



JWH 019 N-(6-hydroxyhexyl) metabolite

9000765

MF: C₂₅H₂₅NO₂ **FW:** 371.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An expected metabolite of JWH 019, detectable both in serum and urine

1 ma 5 mg 10 mg



JWH 019 5-hydroxyindole metabolite 9000764

JWH 019-M2

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: Expected to be a major metabolite, detectable in serum and urine, of JWH 019, based on the metabolism of the closely related compounds JWH 015 and JWH 018; biological effects are not known

1 mg 5 mg 10 mg



JWH 020

5 mg

10 mg

25 mg

[209414-09-5]

MF: C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A cannabimimetic indole derived from WIN 55,212-1; affinities for CB_1 and CB_2 receptors (128 and 205 nM, respectively) are significantly weaker than those of WIN 55,212-2 (1.89 and 0.28 nM, respectively)



JWH 022

[209414-16-4] AM2201 N-(4-pentenyl) analog

MF: C₂₄H₂₁NO **FW:** 339.4 **Purity:** ≥98%

A solution in methanol Stability: ${\geq}1$ year at -20°C Summary: A cannabimimetic indole that is structurally related to JWH 018, a

mildly selective agonist of the CB_2 receptor $1\ \text{mg}$

5 mg

10 mg



JWH 030

[162934-73-8]

MF: C₂₀H₂₁NO **FW:** 291.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A naphthoyl pyrrole cannabimimetic which activates the CB₁ receptor (EC₅₀ = 30.5 nM for rat, K_i = 87 nM for mouse) better than CB₂ (EC₅₀ = 552 nM for human CB₂); potent *in vivo* in the mouse spontaneous activity and tail flick (antinociception) assays (ED₅₀ = 26.8 μ M/kg)





JWH 031

[162934-74-9]

MF: C₂₁H₂₃NO **FW:** 305.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A synthetic CB with a relatively low binding affinity for the central CB_1 receptor ($K_i = 399 \text{ nM}$); efficacious in reducing spontaneous activity and increasing antinociception in mice; intended for forensic and research applications

5 mg









5 mg

10 mg

25 mg

10850

9001056

10831

10824

MF: $C_{22}H_{19}$ NO **FW:** 313.4 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic CB that displays a higher affinity for the peripheral CB_2 receptor (K_i = 170 nM) than the central CB_1 receptor (K_i = 1,050 nM); intended for research and forensic purposes



JWH 073 [208987-48-8]

MF: $C_{23}H_{21}$ NO **FW:** 327.4 **Purity:** \ge 97%

A crystalline solid **Stability:** ≥ 1 year at -20°C

Summary: A selective agonist of the CB_1 receptor with K_i values of 8.9 and 38 nM for CB_1 and CB_2 , respectively



• Also Available: **JWH 073 (solution)** (13170) *DEA-exempt formulation*

JWH 073-d₇ (solution)

MF: C₂₃H₁₄D₇NO **FW:** 334.5 **Chemical Purity:** ≥98%

Deuterium Incorporation: \ge 99% deuterated forms (d₁-d₇); \le 1% d₀ A solution in methanol **Stability:** \ge 1 year at -20°C

 ${\bf Summary:}$ An internal standard for the quantification of JWH 073 by GC- or LC-MS



JWH 073 N-butanoic acid metabolite

MF: C₂₃H₁₉NO₃ FW: 357.4 Purity: ≥98% A crystalline solid Stability: ≥2 years at -20°C Summary: Expected urinary metabolite of JWH 073





JWH 073 N-butanoic acid metabolite-d₅

MF: $C_{23}H_{14}D_5NO_3$ **FW:** 362.4 **Chemical Purity:** ≥98% **Deuterium Incorporation:** ≥99% deuterated forms (d₁-d₅); ≤1% d₀

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An internal standard for the quanitification of JWH 073 N-butanoic acid metabolite by GC- or LC-MS



9001201

10904

9000868

9000866



JWH 073 N-(1,1-dimethylethyl) isomer

MF: $C_{23}H_{21}NO$ **FW:** 327.4 **Purity:** \ge 98% A crystalline solid **Stability:** \ge 2 years at -20°C

Summary: Differs structurally from JWH 073 by having a 1,1-dimethylethyl group, rather than a butyl chain, extending from the indole group; intended for forensic and research applications



(±)-JWH 073 N-(3-hydroxybutyl) metabolite 10795

MF: $C_{23}H_{21}NO_2$ **FW:** 343.4 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Expected product of the metabolism of JWH 073 by human liver microsomes *in vitro*, generated by the oxidation of the aminoalkyl chain; biological actions are unknown





(±)-JWH 073 N-(3-hydroxybutyl) metabolite-d₅ 10927

MF: C₂₃H₁₆D₅NO₂ **FW:** 348.5 **Chemical Purity:** ≥98%

Deuterium Incorporation: \ge 99% deuterated forms (d₁-d₅); \le 1% d₀ A solution in methanol **Stability:** \ge 1 year at -20°C **Summary:** An internal standard for the quanitification of (±)-JWH 073 N-(3-hydroxybutyl) metabolite by GC- or LC-MS





(S)-(+)-JWH 073 N-(3-hydroxybutyl) metabolite 10898

MF: C₂₃H₂₁NO₂ **FW:** 343.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 1 year at -20° C

Summary: A purified single enantiomer of a major metabolite of JWH 073, produced by human liver microsomes *in vitro* and detected, as a glucuronidated form, in urine

100 µg 500 µg 1 mg

9000870

9001013



(R)-(-)-JWH 073 N-(3-hydroxybutyl) metabolite 10899

MF: C₂₃H₂₁NO₂ **FW:** 343.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C **Summary:** A purified single enantiomer of a major metabolite of JWH 073, produced by human liver microsomes *in vitro* and detected, as a glucuronidated form, in urine

100 µg 500 µg 1 mg



JWH 073 N-(4-hydroxybutyl) metabolite

9000865

MF: $C_{23}H_{21}NO_2$ **FW:** 343.4 **Purity:** $\ge 98\%$ A crystalline solid **Stability:** ≥ 2 years at $-20^{\circ}C$ **Summary:** Expected to be a major urinary metabolite of JWH 073

1 mg 5 mg 10 mg



JWH 073 N-(4-hydroxybutyl) metabolite-d₅ 10934

 $\begin{array}{l} \textbf{MF:} C_{23}H_{16}D_5NO_2 \ \textbf{FW:} \ 348.5 \ \textbf{Chemical Purity:} \geq 98\% \\ \textbf{Deuterium Incorporation:} \geq 99\% \ deuterated \ forms \ (d_1-d_5); \leq 1\% \ d_0 \\ A \ solution \ in \ methanol \ \textbf{Stability:} \geq 1 \ year \ at \ -20^\circ\text{C} \\ \textbf{Summary:} \ An \ internal \ standard \ for \ the \ quantification \ of \ JWH \ 073 \end{array}$

N-(4-hydroxybutyl) metabolite by GC- or LC-MS

100 µg 500 µg 1 mg





MF: $C_{23}H_{21}NO$ **FW:** 327.4 **Purity:** $\ge 98\%$

JWH 073 N-(1-methylpropyl) isomer

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 073 by having a methylpropyl chain, rather than a butyl group, extending from the indole group

1 mg 5 mg 10 mg



JWH 073 N-(2-methylpropyl) isomer

MF: C₂₃H₂₁NO **FW:** 327.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: Differs structurally from JWH 073 by having a methylpropyl chain, rather than a butyl group, extending from the indole group

1 mg 5 mg 10 mg

10 mg



JWH 073 2'-naphthyl isomer

MF: $C_{23}H_{21}NO$ **FW:** 327.4 **Purity:** \geq 97% A crystalline solid **Stability:** \geq 2 years at -20°C **Summary:** Differs structurally from JWH 073 by having the naphthyl group attached at the 2' position

1 mg 5 mg 10 mg



JWH 073 2'-naphthyl-N-

(1,1-dimethylethyl) isomer

MF: C₂₃H₂₁NO **FW:** 327.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 073 by having the naphthyl group attached at the 2 position and a 1,1-dimethylethyl group in place of a butyl chain; intended for forensic and research applications

1 mg 5 mg 10 mg



9001012

JWH-series

25

9001014

9001011

JWH 073 2'-naphthyl-N-9001016 (1-methylpropyl) isomer **MF:** C₂₃H₂₁NO **FW:** 327.4 **Purity:** ≥98% A solution in methanol **Stability:** ≥1 year at -20°C and in urine Summary: Differs structurally from JWH 073 by having the naphthyl group attached at the 2' position and a 1-methylpropyl group in place of a butyl chain 1 mg 5 mg 1 mg 10 mg 5 mg 10 mg JWH 073 2'-naphthyl-N-9001015 (2-methylpropyl) isomer

MF: C₂₃H₂₁NO **FW:** 327.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 073 by having the naphthyl group attached at the 2' position and a 2-methylpropyl group in place of a butyl chain



JWH 081

[210179-46-7]

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A cannabimimetic indole with selectivity for the CB1 receptor $(K_i = 1.2 \text{ nM})$ and ten-fold reduced affinity for the CB₂ receptor $(K_i = 12.4 \text{ nM})$



25 mg



JWH 081-do

MF: C₂₅H₁₆D₉NO₂ **FW:** 380.5 **Chemical Purity:** ≥98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀ A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An internal standard for the quantification of JWH 081 by GC- or LC-MS







MF: C₂₅H₂₅NO₃ **FW:** 387.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: Expected metabolite of JWH 081 that would be detectable both in serum



JWH 081 2-methoxynaphthyl isomer 9001044

[824960-76-1] [WH 267

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: Differs structurally from JWH 081 by having the methoxy group attached to the naphthyl rings at the 2' position





JWH 081 3-methoxynaphthyl isomer

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: Differs structurally from JWH 081 by having the methoxy group attached to the naphthyl rings at the 3 position, instead of the 4 position; intended for forensic and research purposes

1 mg	
5 mg	
10 mg	

1 mg

5 mg

10 mg

10579



JWH 081 5-methoxynaphthyl isomer 9001046

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 081 by having the methoxy group attached to the naphthyl rings at the 5 position, instead of the 4 position



JWH 081 6-methoxynaphthyl isomer

[824961-41-3] [WH 166

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 2 years at -20° C

Summary: Differs structurally from JWH 081 by having the methoxy group attached to the naphthyl rings at the 6 position, instead of the 4 position ; intended for forensic and research purposes



1 mg

5 mg

10 mg



JWH 081 7-methoxynaphthyl isomer

[824961-61-7] IWH 164

9001048

9001047

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: Differs structurally from JWH 081 by having the methoxy group attached to the naphthyl rings at the 7 position, instead of the 4 position



JWH 081 8-methoxynaphthyl isomer

9001049

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C Summary: Differs structurally from JWH 081 by having the methoxy group attached to the naphthyl rings at the 8 position, instead of the 4 position; intended for forensic and research purposes



JWH 098

1 mg

5 mg

10 mg

10680

[316189-74-9]

MF: C₂₆H₂₇NO₂ **FW:** 385.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent synthetic CB, activating the CB₁ receptor with a K₁ value of 4.5 nM and the CB2 receptor with a K, value of 1.88 nM; effects in cells and animals are unknown



9001045

10591

10512

JWH 122

[619294-47-2] **MF:** C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98% A crystalline solid **Stability:** ≥1 year at -20°C **Summary:** A CB that displays high-affinities for both CB_1 (K_i = 0.69 nM) and CB_2 $(K_i = 1.2 \text{ nM})$ receptors

5 mg 10 mg 25 mg



JWH 122-d。

MF: $C_{25}H_{16}D_9NO$ **FW:** 364.5 **Chemical Purity:** \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀ A solution in methanol **Stability:** ≥1 year at -20°C Summary: An internal standard for the quantification of JWH 122 by GC- or LC-MS

500 µg 1 mg 5 mg



JWH 122 N-(4-hydroxypentyl) metabolite 11784

MF: C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An expected phase I metabolite of JWH 122, detectable in serum and urine; intended for research and forensic applications

1 mg 5 mg 10 mg



JWH 122 N-(5-hydroxypentyl) metabolite

10925

MAM2201 N-(5-hydroxypentyl) metabolite **MF:** C₂₅H₂₅NO₂ **FW:** 371.5 **Purity:** ≥98% A solution in methanol **Stability:** ≥ 1 year at -20°C Summary: A metabolite of JWH 122 that is characterized by monohydroxylation of the N-alkyl chain

1 mg 5 mg 10 mg





MF: $C_{25}H_{20}D_5NO_2$ FW: 376.5 Chemical Purity: $\ge 98\%$ **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀

A solution in methanol **Stability:** ≥1 year at -20°C Summary: An internal standard for the quantification of JWH 122 N-(5-

hydroxypentyl) metabolite by GC- or LC-MS

100 µg 500 µg 1 mg

JWH 122 2-methylnaphthyl isomer

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 1 year at -20° C Summary: Differs from JWH 122 in that the methyl group is attached to the

naphthyl rings at the 2, rather than the 4, position 1 mg



JWH 122 3-methylnaphthyl isomer

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: Differs from JWH 122 in that the methyl group is attached to the naphthyl rings at the 3, rather than the 4, position; intended for forensic purposes

1 mg 5 mg

5 mg

10 mg



JWH 122 5-methylnaphthyl isomer

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs from JWH 122 in that the methyl group is attached to the naphthyl rings at the 5, rather than the 4, position; intended for forensic purposes

1 mg 5 mg 10 mg



JWH 122 6-methylnaphthyl isomer

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: Differs from JWH 122 in that the methyl group is attached to the naphthyl rings at the 6, rather than the 4, position



9001035

9001036

9001037

11611

JWH 122 7-methylnaphthyl isomer

[824960-56-7]

1 mg

5 mg

10 mg

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs from JWH 122 in that the methyl group is attached to the naphthyl rings at the 7, rather than the 4, position



9001032

9001033

9001034



JWH 122 8-methylnaphthyl isomer

MF: C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: Differs from JWH 122 in that the methyl group is attached to the naphthyl rings at the 8, rather than the 4, position

1 mg 5 mg 10 mg

1 mg

5 mg

10 mg



JWH 122 N-(4-pentenyl) analog

JWH 022 4-methylnaphthyl analog, MAM2201 N-(4-pentenyl) analog **MF:** C₂₅H₂₃NO **FW:** 353.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: Structurally related to JWH 122, differing only by the presence of a terminal double bond on the acyl chain; intended for forensic and research applications

JWH 145 10825 [914458-19-8]

MF: C₂₆H₂₅NO **FW:** 367.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: A (1-naphthoyl)pyrrole analog of JWH 018 that potently activates both CB1 and CB2 receptors (K; values of 14 and 6.4 nM, respectively)



5 mg

10 mg

25 mg

[914458-20-1] **MF:** C₂₇H₂₇NO **FW:** 381.5 **Purity:** ≥95%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A synthetic CB with a high affinity for both the central CB1 receptor $(K_i = 11 \text{ nM})$ and the peripheral CB₂ receptor $(K_i = 7.1 \text{ nM})$; intended for research and forensic applications



JWH 175

[619294-35-8]

MF: C₂₄H₂₅N **FW:** 327.5 **Purity:** ≥98%

A solution in acetonitrile **Stability:** ≥1 year at -20°C Summary: A synthetic CB that potently activates the central CB_1 receptor (K_i = 22 nM); intended for forensic and research purposes



JWH 180

9001205

11201

[824959-87-7] **MF:** C₂₅H₂₅NO **FW:** 355.5 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent synthetic CB that binds both the central CB_1 receptor (K_i = 26 nM) and the peripheral CB_2 receptor (K_i = 9.6 nM); intended for research and forensic applications

5 mg

10 ma 25 mg

10643

10902

JWH 182

[824960-02-3]

MF: C₂₇H₂₉NO **FW:** 383.5 **Purity:** ≥97%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent synthetic CB, activating the central CB₁ receptor with a K, value of 0.65 nM and the peripheral CB2 receptor with a K1 value of 1.1 nM; effects in cells and animals are unknown

1 mg 5 mg 10 mg



JWH 200

[103610-04-4]

MF: C₂₅H₂₄N₂O₂ **FW:** 384.5 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An aminoalkylindole that acts as a CB receptor ligand, binding the CB1 receptor with high-affinity (IC₅₀ = 7.8-42 nM)

5 mg 10 mg 25 mg



JWH 200-d₅

MF: $C_{25}H_{10}D_5N_2O_2$ **FW:** 389.5 **Chemical Purity:** \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀ A crystalline solid **Stability:** ≥2 years at -20°C Summary: An internal standard for the quantification of JWH 200 by GC- or LC-MS

500 µg 1 mg 5 mg



• Also Available: **IWH 200-d**₅ (solution) (10682) DEA-exempt formulation

JWH 200 4-hydroxyindole metabolite 10744

MF: C₂₅H₂₄N₂O₃ **FW:** 400.5 **Purity:** ≥98%

A solution in methanol Stability: ≥1 year at -20°C Summary: Expected to be a urinary metabolite of JWH 200 based on the metabolism of the closely-related JWH 015 and JWH 018

1 mg 5 mg 10 mg



Fc

Regulating Endocannabinoid Levels Olivia L. May, Ph.D. CB receptor ligands, MAGL, FAAH

THC, the active ingredient in marijuana, and the body's own natural forms of THC, anandamide (or arachidonyl ethanolamide (AEA)) and 2-arachidonoyl glycerol (2-AG) produce effects by binding to and activating the cannabinoid (CB)₁ receptor and the CB₂ receptor.

CB1 is one of the most widely expressed receptors on cells throughout the body, and it is particularly abundant in the brain where it is responsible for mediating the well-known effects of the typical marijuana high (including pain control, memory blocking, and appetite enhancement). In general, however, CB1 modulates the activity of other systems in the brain. CB1 receptors are distributed across the terminals of an axon, which delivers signals to another neuron across a synapse. Greater activity in the synapse tends to produce an upsurge of the brain's endogenous cannabinoids (endocannabinoids), which bind to CB₁ and trigger a change in the flow of signals across the synapse (Figure 1). CB1 receptors are found on two broad classes of nerve terminals: excitatory, which increase the activity of target neurons, and inhibitory, which reduce activity. CB1, therefore, can either enhance or diminish synaptic signaling depending on which of these systems it modulates. Thus, any manipulation with CB1 agonists or antagonists could potentially have a host of effects, depending on the systems affected.

The other cannabinoid receptor, CB2, was long considered a peripheral cannabinoid receptor, meaning that CB₂ receptors weren't present in the central nervous system, but were, however, abundant in the immune system, and seemed to be involved in inflammation as well as pain responses.¹ CB₂ receptors, though, have now been located in the central nervous system, and have been shown to be active in the brain during certain kinds of inflammatory responses.²

Cannabinoid receptor ligands

As the brain's main endocannabinoid activating CB1, anandamide (named for the Sanskrit word for bliss) has been shown to have analgesic,



anti-anxiety and antidepressant roles, as well as connections to feeding control and obesity. In addition to the reinforcing influence on brain reward processes, CB₁ agonists have a number of other effects, particularly on movement, through receptors in the basal ganglia, and on cognition, by altering sensory perception through receptors in the cerebral cortex, and impacting memory by means of receptors in the hippocampus.³

Direct pharmacological CB1 agonists have been sought after to produce medicinally useful effects, such as pain relief, but a number of undesirable side effects, including locomotor and cognitive impairments, as well as abuse liability, prove hard to avoid. Additionally, many synthetic CB1 ligands, modeled after metabolically labile AEA or 2-AG, are difficult to work with due to rapid degradation, polymerization, or high lipophilicity.⁴ CB-25 and CB-52, derived from olivetol, the biosynthetic precursor of THC, were designed as analogs with promising analgesic activity that overcome the instability of AEA and its analogs.⁵ With high affinity and specificity for CB₁ and CB₂ receptors, CB-25 and CB-52, behave *in vitro* mostly as CB₁ indirect agonists (inhibiting inactivation) and CB₂ neutral (inactive) antagonists, demonstrating efficacy in models of pain.⁶ Little has been reported to clarify their activity in vivo. Invariably though, it has proved complicated to uncouple beneficial and negative properties of direct CB1 agonists, limiting their therapeutic utility.

A somewhat similar complication surfaced with rimonabant, a CB1 receptor inverse agonist, pursued for its utility in reducing food intake and body-weight gain. Rimonabant was quickly suspended from distribution when serious psychiatric side effects were attributed to its indiscriminate activity on CB receptors in the CNS.7 To circumvent these issues, a comparable compound, URB447, a mixed CB1 receptor antagonist/CB2 receptor agonist that does not cross the blood-brain barrier (to antagonize CB1 receptors in the CNS), was developed to selectively block peripheral CB1 receptors located in the gastrointestinal tract.8

FAAH Inhibitors

Anandamide is degraded fairly quickly by fatty acid amide hydrolase (FAAH) near the synapses it activates. Genetic deletion of the *faah* gene in mice elevates brain anandamide levels and amplifies its antinociceptive effects.⁹ Likewise, pharmacological blockade of FAAH activity reduces nocifensive behavior in animal models of acute and inflammatory pain.^{10,11} Daniele Piomelli at the University of California-Irvine together with research teams at the Universities of Urbino and Parma in Italy developed URB597 (formulated for potential human use under the name KDS-4103), which prevents the breakdown of anandamide by specifically blocking the FAAH enzyme at low nanomolar concentrations.¹²⁻¹⁴ Theoretically without degradation by FAAH, anandamide accumulates in tissues to levels sufficient to selectively activate more cannabinoid receptors. Under these conditions, a higher level of activity is maintained primarily where anandamide already signals and to a lesser extent in other areas of the CNS and periphery where the boosting of such activity could produce undesired side effects. When URB597 was administered in chronically

able 1. Cannabinoid Receptor Ligands				
10010116 CB-25 exclusive		CB_1 receptor partial agonist (K _i = 210 nM) and a CB_2 receptor neutral antagonist (K _i = 30 nM)		
10010117 CB-52 exclusive		CB_1 receptor partial agonist (K_i = 210 nM) and a CB_2 receptor neutral antagonist (K_i = 30 nM)		
13261 URB447		mixed CB_1 receptor antagonist ($IC_{50} = 313 \text{ nM}$) and a CB_2 receptor agonist ($IC_{50} = 41 \text{ nM}$) that does not cross the blood-brain barrier		

stressed lab rodents, anandamide levels indeed increased and produced a in models of drug abuse, such as drug discrimination assays.²⁰⁻²² Therefore, physiological effect similar to that produced by certain antidepressant drugs selective blockade of FAAH or MAGL can be used to tease apart some of the by reducing inhibitory controls on a midbrain region where neurons deliver beneficial and undesirable effects of CB1 activation. the neurotransmitters serotonin and noradrenaline.¹⁵ By boosting the levels Dually Inhibiting both FAAH and MAGL of these neurotransmitters in the brain of rodents and monkeys, URB597 On the other hand, pharmacologically inhibiting both FAAH and MAGL activities simultaneously to elevate brain levels of both AEA and 2-AG can

provoked measurable antidepressant, anti-anxiety, and analgesic effects within 1-4 weeks of treatment.¹⁵ give combined effects. Selective blockade of both FAAH and MAGL is Importantly, FAAH inhibition does not reinforce other drug-taking behaviors, sufficient to produce additive endocannabinoid activity in pain and catalepsy as THC and certain CB1 agonists are known to do.¹⁶ That is, the effects of assays.²³ These behaviors include catalepsy and THC-like drug discrimination anandamide were selectively targeted without inducing a potentially addictive, responses, indicating that some of the undesirable effects of direct CB1 agonists psychotropic high, like in cases of marijuana use. To circumvent activation of derive from crosstalk between AEA and 2-AG signaling pathways. JZL195 is CB_1 receptors in the brain all-together, these same investigators developed the one such inhibitor that inactivates both FAAH and MAGL with high efficacy peripherally restricted inhibitor URB937. URB937 doesn't cross the bloodand selectivity in vivo.23 It simultaneously augments brain levels of both AEA brain barrier, but it is still able to lessen pain by preventing the deactivation and 2-AG, producing antinociceptive, cataleptic, and hypomotility effects like of anandamide at the site of an injury.¹⁷ Anandamide has been shown to those produced by direct CB1 agonists. JZL195 was developed to improve on exert analgesic actions in various pain research models by binding strictly to shortcomings of the fluorophosphonate IDFP, another dual inhibitor of both peripheral CB₁ receptors.¹⁸ Notably, there is likely little to no recreational FAAH and MAGL that proved too promiscuous, inhibiting many additional effect with either URB597 or URB937. serine hydrolases and was toxic to mice when tested in vivo.24

MAGL Inhibitors

Despite the structural similarities shared between AEA and 2-AG, a different serine hydrolase, monoacylglycerol lipase (MAGL) is the main enzyme responsible for inactivating 2-AG. Mice treated with the selective MAGL inhibitor IZL184 show 8- to 10-fold increases in brain 2-AG levels without changes in AEA content.¹⁹ Distinct enzymes preferentially inactivating either anandamide or 2-AG have revealed key points of control over different endocannabinoid signaling events and produce only a subset of the behavioral effects observed with direct CB1 agonists. For instance, inhibition of MAGL, but not FAAH, causes CB1-dependent hypomotility.¹⁹ Neither FAAH nor MAGL inhibitors have been shown to induce the cataleptic behavioral responses observed with direct CB1 agonists and have largely proved inactive

Table 2. FA	AH Inhibitors			
10046 URB597		inhibits FAAH ($IC_{50} = 4.6$ nM in brain membranes and 0.5 nM in intact neurons) resulting in reduced sensation of pain in <i>in</i> <i>vivo</i> mouse models		
10674 URB937 exclusive		peripherally-specific FAAH inhibitor (IC $_{50}$ = 26.8 nM, <i>in vitro</i>) that does not cross the blood-brain barrier		
10008661 JP104		irreversible FAAH inhibitor of the carbamate class ($IC_{50} = 7.3$ nM for the human recombinant enzyme)		
10010908 PF-750		irreversible FAAH inhibitor (IC ₅₀ s = 0.6 and 0.016 μM when preincubated with FAAH for 5 and 60 minutes, respectively)		
13279 PF-3845		potent, selective, irreversible FAAH inhibitor (K_i = 0.23 $\mu M)$		
10010032 CAY10570		reversible, competitive FAAH inhibitor (IC_{50} = 1.3 μM) with no affinity for the human CB_1 receptor		
Table 3. MAGL Inhibitors				
10007457 URB602	H H C C C C C C C C C C C C C C C C C C	selectively inhibits MAGL (IC_{50} = 28 μM for the rat brain enzyme) and does not inhibit FAAH at concentrations up to 100 μM		
13158 JZL 184		selectively inhibits MAGL (IC_{\rm 50} = 8 nM) over FAAH IC_{\rm 50} = 4 μM) in mouse brain membranes		

Figure 1. Endocannabinoid signaling at the synapse. Glut = excitatory; GABA = inhibitory

Conclusion

Unfortunately due to their potential to elicit psychoactive effects, many of these compounds have piqued the interest of recreational chemists and experimental drug users. Cayman is dedicated to working with forensic agencies to identify emerging new drugs by providing authentic reference standards, as well as with academic communities exploring the therapeutic opportunities that arise from regulating endocannabinoid levels. As such, the cannabinoid receptor ligands and FAAH/MAGL inhibitors listed in tables 1-4 are available for forensic and research purposes only.





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JWH 210 10644 JWH 210 3-ethylnaphthyl isomer [824959-81-1] **MF:** C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98% **MF:** C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A potent cannabimimetic alkylindole, binding the CB1 and CB2 receptors with K_i values of 0.46 and 0.69 nM, respectively; effects of JWH 210 in whole cells or organisms have not been evaluated



JWH 210-d。

1 mg 5 mg 10510

MF: $C_{26}H_{10}D_9NO$ FW: 378.6 Chemical Purity: \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀ A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An internal standard for the quantification of JWH 210 by GC- or LC-MS



JWH 210 N-(5-carboxypentyl) metabolite

MF: C₂₆H₂₅NO₃ **FW:** 399.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An expected metabolite of JWH 210, detectable primarily in the urine



JWH 210 2-ethylnaphthyl isomer

MF: C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A positional isomer of JWH 210, having the ethyl side chain at the 2 position rather than at the 4 position of the naphthyl group; intended for forensic purposes





9001039

A solution in methanol **Stability:** ≥ 1 year at -20° C

Summary: A positional isomer of JWH 210, having the ethyl side chain at the 3 position rather than at the 4 position of the naphthyl group; intended for forensic purposes

1 mg 5 mg 10 mg



JWH 210 5-ethylnaphthyl isomer

MF: C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A positional isomer of JWH 210, having the ethyl side chain at the 5 position rather than at the 4 position of the naphthyl group; intended for forensic purposes

1 mg 5 mg 10 mg



MF: C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A positional isomer of JWH 210, having the ethyl side chain at the 6 position rather than at the 4 position of the naphthyl group; intended for forensic purposes

1 mg 5 mg 10 mg



JWH 210 7-ethylnaphthyl isomer

9001042

9001041

[824960-64-7] JWH 234

MF: C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20°C

Summary: A positional isomer of JWH 210, having the ethyl side chain at the 7 position rather than at the 4 position of the naphthyl group; intended for forensic purposes

1 mg 5 mg 10 mg



JWH 210 8-ethylnaphthyl isomer

MF: C₂₆H₂₇NO **FW:** 369.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: A positional isomer of JWH 210, having the ethyl side chain at the 8 position rather than at the 4 position of the naphthyl group; intended for forensic purposes

1 mg



10 mg



JWH 210 5-hydroxyindole metabolite

MF: C₂₆H₂₇NO₂ **FW:** 385.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An expected metabolite of JWH 210, detectable both in serum and urine



JWH 210 N-(4-hydroxypentyl) metabolite

MF: C₂₆H₂₇NO₂ **FW:** 385.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C Summary: An expected metabolite of JWH 210, detectable in the serum and urine

1 mg 5 mg 10 mg

1 mg

5 mg

10 mg



JWH 210 N-(5-hydroxypentyl) metabolite 9000772

MF: C₂₆H₂₇NO₂ **FW:** 385.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An expected metabolite of JWH 210, detectable in the serum and urine; intended for forensic purposes





9001043

9000771

10940

MF: C₂₇H₂₉NO FW: 383.5 Purity: ≥98% A solution in methanol **Stability:** ≥ 2 years at -20° C

Summary: A naphthoylindole-class synthetic cannabinoid (CB) which strongly binds both the central CB1 and peripheral CB2 receptor (K, values of 1.5 and 0.42 nM, respectively); intended for forensic and research applications



JWH 249

5 mg

10 mg 25 mg

[864445-60-3]

MF: C₂₁H₂₂BrNO **FW:** 384.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A synthetic CB that potently activates the central CB1 and peripheral CB₂ receptors (K_i = 8.4 and 20 nM, respectively); intended for forensic and research purposes



MF: C₂₂H₂₅NO₂ **FW:** 335.2 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: A cannabimimetic indole that shows high affinity for both CB_1 (K_i = 11 nM) and CB_2 (K_i = 33 nM) receptors



JWH	25	0-d ₅	
ME.C	ц	D NO	EW/. 2/0 5 Cha

MF: $C_{22}H_{20}D_5NO_2$ FW: 340.5 Chemical Purity: $\ge 98\%$

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀ A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An internal standard for the quantification of JWH 250 by GC- or LC-MS

500 µg 1 mg 5 mg

5 mg 10 mg

25 mg



JWH 250 N-(5-carboxypentyl) metabolite

JWH 250 5-hydroxyindole metabolite

MF: C₂₂H₂₅NO₃ **FW:** 351.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Expected to be a metabolite of JWH 250 that would be detectable both in serum and in urine

1 mg 5 mg 10 mg

11659

11153

10661



JWH 250 N-(4-hydroxypentyl) metabolite

MF: C₂₂H₂₅NO₃ **FW:** 351.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C Summary: Expected to be a cytochrome P450 phase I metabolite of JWH 250, detectable both in serum and urine



JWH 250 N-(4-hydroxypentyl) metabolite-d₅ 11749

MF: C₂₂H₂₀D₅NO₃ **FW:** 356.5 **Purity:** ≥98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀ A solution in methanol **Stability:** ≥ 1 year at -20°C Summary: Intended for use as an internal standard for GC- or LC-MS

100 µg 500 µg 1 mg





9000767

JWH 250 N-(5-hydroxypentyl) metabolite

MF: C₂₂H₂₅NO₃ **FW:** 351.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: Expected metabolite of JWH 250 that would be detectable both in serum and in urine

1 mg 5 mg 10 mg

10938

9000766

10939



JWH 250 N-(5-hydroxypentyl) metabolite-d₅ 11474

MF: $C_{22}H_{20}D_5NO_3$ FW: 356.5 Chemical Purity: $\ge 98\%$ **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₅); \leq 1% d₀ A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: An internal standard for the quantification of JWH 250 N-(5hydroxypentyl) metabolite by GC- or LC-MS

100 µg 500 µg 1 mg



JWH 251

10578

[864445-39-6]

MF: C₂₂H₂₅NO **FW:** 319.4 **Purity:** ≥98%

A solution in methyl acetate **Stability:** ≥1 year at -20°C

Summary: A cannabimimetic indole with selectivity for the CB_1 receptor (K_i = 29 and 146 nM, for CB1 and CB2, respectively); stimulates GTPYS binding of CB1 and CB₂ receptors with EC₅₀ values of 29 and 8.3 nM, respectively

5 mg 10 mg 25 mg



JWH 251 3-methylphenyl isomer

9001021

JWH 251 3-methyl isomer

MF: C₂₂H₂₅NO **FW:** 319.4 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: Differs from JWH 251 by having the methyl group at the 3 position, rather than the 2 position, on the phenyl group

5 mg 10 mg 25 mg



CANNABINOID FORENSIC ANALYSIS CAYMAN LEADS THE WAY IN SYNTHETIC

Synthetic Cannabinoid HPLC Mixtures Screen for Compounds most often Found in Designer Drugs AM • CP • JWH • HU • WIN

Synthetic Cannabinoid HPLC Mixture I				I 1383	
Purity: ≥95	% for each co	mpound S	Supplied as	A solution	n in methanol
Summary:	Contains	(±)-CP	47,497,	(±)-CP	47,497-C8-homolog

(±)-CP 55,940, HU-308, HU-331, JWH 015, JWH 018, JWH 019, JWH 073, JWH 200, JWH 250, and WIN 55212-2 (100 µg each) 1.2 mg

Synthetic Cannabinoid HPLC Mixture II	13850
Purity: >95% for each compound Supplied as: A solution in methanol	

Summary: Contains (±)-CP 47,497, (±)-CP 47,497-C8-homolog, HU-210, JWH 018, JWH 073, and JWH 200 (100 µg each) 600 µg

Synthetic Cannabinoid HPLC Mixture III

Purity: ≥95% for each compound Supplied as: A solution in methanol Summary: Contains JWH 081, AM2201, JWH 210, RCS-4, RCS-8, JWH 201, JWH 398, JWH 251, JWH 016, and JWH 370

11335

11337

1 ea

11336 Synthetic Cannabinoid HPLC Mixture IV

Purity: ≥95% for each compound Supplied as: A solution in methanol Summary: Contains JWH 020, JWH 302, JWH 203, AM2233, JWH 098, Pravadoline, JWH 011, JWH 182, JWH 122, and JWH 022 1 ea

Synthetic Cannabinoid HPLC Mixture V (AM Series)

Purity: ≥95% for each compound Supplied as: A solution in methanol Summary: Contains AM630, AM694, AM1220, AM1241, AM2201, and AM2233 (100 µg each)

1 ea



Detect K2/Spice Metabolites in Urine

Specificity: Anglyte	Cross Reactivity	Analyte	Cross Reactivity
JWH 018 N-pentanoic acid metabolite (Item No. 9000856)	100%	JWH 022 (Item No. 9001056)	30%
JWH 200 (Item No. 10902)	156%	JWH 018 (Item No. 10900)	15%
(±)-JWH 073 N-(3-hydroxybutyl) metabolite (Item No. 10795)	142%	MAM2201 (Item No. 9001219)	13%
JWH 073 N-butanoic acid metabolite (Item No. 9000866)	131%	JWH 210 N-(5-carboxypentyl) metabolite (Item No. 10941)	11%
JWH 073 N-(4-hydroxybutyl) metabolite (Item No. 9000865)	102%	JWH 015 (Item No. 10009018)	4.2%
(+)-JWH 018 N-(4-hydroxypentyl) metabolite (Item No. 10920)	97%	JWH 122 (Item No. 10591)	3.6%
JWH 018 N-(5-hydroxypentyl) metabolite (Item No. 9000855)	76%	JWH 081 N-(5-hydroxypentyl) metabolite (Item No. 9000768)	3.2%
JWH 018 N-(4-hydroxypentyl) β-D-Glucuronide (Item No. 10959)	73%	JWH 020 (Item No. 10850)	2.5%
JWH 019 N-(6-hydroxyhexyl) metabolite (Item No. 9000765)	59%	JWH 398 (Item No. 13636)	2.4%
AM2201 N-(4-hydroxypentyl) metabolite (Item No. 10203)	58%	JWH 250 N-(5-carboxypentyl) metabolite (Item No. 10938)	0.6%
JWH 073 (Item No. 10904)	51%	JWH 210 (Item No. 10644)	0.5%
AM2201 (Item No. 10707)	39%	Arachidonoyl Ethanolamide (Item No. 90050)	*
JWH 018 N-(5-hydroxypentyl) β-D-Glucuronide (Item No. 10958)	38%	2-Arachidonoyl Glycerol (Item No. 62160)	*
JWH 122 N-(5-hydroxypentyl) metabolite (Item No. 10925)	32%	STS-135 (Item No. 11564)	*
JWH 398 N-(5-hydroxypentyl) metabolite (Item No. 9000770)	32%	XLR11 (Item No. 11565)	*
		* Not Detected	

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FORENSIC CHEMISTRY

EOBENSIC CHEMISTRY

Cayman has developed this assay to detect a structural feature common to the urinary metabolites of many of the most popular synthetic cannabinoids (CBs), including JWH 018, JWH 073, JWH 200, JWH 122, JWH 398, AM2201, MAM2201, JWH 019, and JWH 022. This kit is intended to be used as a rapid, inexpensive, high-throughput screening tool for the detection of synthetic CB metabolites in urine. Because specific chemical modifications in various synthetic CB urinary metabolites can alter the relative strength of the signal in this assay, it is not possible to use this assay as a quantitative assay to determine the specific amounts of an individual CB in urine. Rather, it is designed to generate a qualitative positive versus negative answer. It is recommended that samples testing positive in Cayman's assay be confirmed and quantified using LC/MS. This assay has been validated with human urine samples, and demonstrates a high degree of correlation with LC/MS analysis.

More time and cost effective than LC/MS • Rapid results in just a few hours Optimized to minimize false positives • Highly accurate with nanomolar sensitivity

FORENSIC CHEMISTRY

FORE

JWH 251 4-methylphenyl isomer

[864445-41-0] [WH 251 4-methyl isomer

MF: C₂₂H₂₅NO **FW:** 319.4 **Purity:** ≥98% A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: Differs from JWH 251 by having the methyl group at the 4 position,

rather than the 2 position, on the phenyl group

5 mg 10 mg 25 mg

JWH 302

[864445-45-4]

MF: C₂₂H₂₅NO₂ **FW:** 335.4 **Purity:** ≥95%

A solution in methyl acetate **Stability:** ≥1 year at -20°C

Summary: A cannabimimetic indole with 5-fold selectivity for the CB1 receptor $(K_i = 17 \text{ nM})$ compared to the CB₂ receptor $(K_i = 89 \text{ nM})$; stimulates GTP γ S binding

of CB1 and CB2 receptors with EC50 values of 29.3 and 24.4 nM, respectively

5 mg 10 mg 25 mg



JWH 307

1 mg

5 mg

10 mg

[914458-26-7]

MF: C₂₆H₂₄FNO **FW:** 385.5 **Purity:** ≥96%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A (1-naphthoyl)pyrrole cannabimimetic that potently activates both CB1 and CB2 receptors (Ki values of 7.7 and 3.3 nM, respectively)



JWH 309

[914458-42-7]

MF: C₃₀H₂₇NO **FW:** 417.6 **Purity:** ≥98%

A solution in methyl acetate **Stability:** ≥1 year at -20°C

Summary: A synthetic CB that displays high affinities for both the central CB1 receptor (K_i = 41 nM) and the peripheral CB_2 receptor (K_i = 49 nM); intended for forensic and research applications

1 ma 5 mg

10 mg





JWH 368 [914458-.

9001022

10722

10797

10830

MF: C₂₆H₂₄FNO **FW:** 385.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A (1-naphthoyl)pyrrole cannabimimetic that potently activates both CB1 and CB2 receptors (Ki values of 16 and 9.1 nM, respectively); intended for forensic and research applications



JWH 369

1 mg

5 mg

10 mg

[914458-27-8]

MF: C₂₆H₂₄ClNO **FW:** 401.9 **Purity:** ≥95%

A solution in methanol **Stability:** ≥ 1 year at -20° C

Summary: A synthetic CB that potently activates the central CB1 and peripheral CB_2 receptors (K_i = 7.9 and 5.2 nM, respectively); intended for forensic and research purposes





1 mg

5 mg

10 mg 25 mg

Summary: A (1-naphthoyl)pyrrole analog of JWH 018 that potently activates both



JWH 398

1 mg

5 mg

10 mg

MF: C₂₄H₂₂ClNO **FW:** 375.9 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An agonist at both the CB_1 receptor and the CB_2 receptor (K_is = 2.3 and 2.8 nM, respectively)



JWH 398-d。

MF: C₂₄H₁₃D₉ClNO **FW:** 385.0 **Purity:** ≥95% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀

A solution in methanol **Stability:** ≥ 1 year at -20° C

Summary: An internal standard for the quantification of JWH 398 by GC- or LC-MS





JWH 398 2-chloronaphthyl isomer

MF: C₂₄H₂₂ClNO **FW:** 375.9 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: Differs structurally from JWH 398 by having the chloro group attached to the naphthyl rings at the 2, rather than the 4, position; intended for forensic purposes



1 mg

5 mg

10 mg



JWH 398 3-chloronaphthyl isomer

MF: C₁₄H₁₂ClNO **FW:** 375.9 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 398 by having chlorine positioned on the naphthyl rings at the 3, rather than the 4, position; intended for forensic purposes



JWH 398 5-chloronaphthyl isomer

9001025

MF: C₂₄H₂₂ClNO **FW:** 375.9 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 398 by having the chloro group attached to the naphthyl rings at the 5, rather than the 4, position







10514

9001023

9001024

10828

13636

10829





IW

[914458-22-3]

MF: C₂₇H₂₇NO **FW:** 381.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

CB1 and CB2 receptors (Ki values of 5.6 and 4.0 nM, respectively)

JWH 398 6-chloronaphthyl isomer

MF: C₂₄H₂₂ClNO **FW:** 375.9 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs structurally from JWH 398 by having the chloro group attached to the naphthyl rings at the 6, rather than the 4, position; intended for forensic purposes

1 mg 5 mg 10 mg



JWH 398 7-chloronaphthyl isomer

MF: C₂₄H₂₂ClNO **FW:** 375.9 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: Differs structurally from JWH 398 by having the chloro group attached

to the naphthyl rings at the 7, rather than the 4, position; intended for forensic purposes

1 mg 5 mg 10 mg

JWH 398 8-chloronaphthyl isomer

MF: C₂₄H₂₂ClNO **FW:** 375.9 **Purity:** ≥98% A solution in methanol **Stability:** ≥1 year at -20°C Summary: Differs structurally from JWH 398 by having chlorine positioned on the naphthyl rings at the 8, rather than the 4, position; intended for forensic purposes

1 mg 5 mg 10 mg



JWH 398 N-(5-hydroxypentyl) metabolite

9000770

9001028

MF: C₂₄H₂₂ClNO₂ **FW:** 391.9 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: A potential metabolite of JWH 398, detectable in urine

1 mg 5 mg 10 mg



9001026

JWH 424

MF: C₂₄H₂₂BrNO **FW:** 420.3 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An 8-bromonaphthyl derivative of JWH 018 which shows a reduced selectivity for CB_1 over CB_2 (K₁ = 20.9 and 5.4, respectively); intended for forensic and research applications

5 mg 10 mg 25 mg



MDA Series

MDA 19

9001203

13158

13668

[1048973-47-2]

MF: C₂₁H₂₃N₃O₂ **FW:** 349.4 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A selective agonist of the CB2 receptor, with an EC50 value for CB2 activation (63.4 nM) that is 14-fold lower than that for CB_1 activation (EC₅₀ = 867 nM); dose-dependently reduces tactile allodynia in rats and in CB2*/+ mice but not in CB2-/- mice





MDA 77

[1103774-21-5] **MF:** C₂₁H₂₃N₃O₃ **FW:** 365.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A selective inverse agonist of the human CB2 receptor that demonstrates an EC₅₀ value of 5.8 nM at CB₂ and no activity at CB₁

1 mg 5 mg 10 mg 50 mg



RCS Series

RCS-4

1 mg

5 mg

10 mg

10563

10639

BTM-4, E-4, OBT-199, SR-19 **MF:** C₂₁H₂₃NO₂ **FW:** 321.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥1 year at -20°C Summary: A synthetic JWH 018 CB analog identified as a component of several different 'herbal incense' products

RCS-4-d₉

10513

10645

BTM-4-do E-4-do OBT-199-do SR-19-do **MF:** $C_{21}H_{14}D_9NO_2$ **FW:** 330.5 **Chemical Purity:** \ge 98% **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₉); \leq 1% d₀ A solution in methanol **Stability:** ≥1 year at -20°C Summary: An internal standard for the quantification of RCS-4 by GC- or LC-MS



RCS-4-C4 homolog

10798

BTM-4, E-4, OBT-199, SR-19 **MF:** C₂₀H₂₁NO₂ **FW:** 307.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: Identical to RCS-4 except the N-1 alkyl chain length has been shortened from C5 to C4; detected in herbal blends

1 mg 5 mg 10 mg



10937

MF: C₂₁H₂₁NO₄ **FW:** 351.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: An expected metabolite of RCS-4, which should be detectable in the urine



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JZL 195

MF: C₂₄H₂₃N₃O₅**FW:** 433.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

5 mg

10 mg 50 mg 100 mg



JZL 184

[1101854-58-3]

MF: C₂₇H₂₄N₂O₉ **FW:** 520.2 **Purity:** ≥97%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent and selective inhibitor of MAGL that displays IC₅₀ values of 8 nM and $4\ \mu\text{M}$ for inhibition of MAGL and FAAH, respectively in mouse brain membranes

5 mg 10 mg 50 mg

100 mg

NOTE: Sold under license from The Scripps Research Institute

[121004-12-8]

Summary: A potent inhibitor of both FAAH and MAGL ($IC_{50} = 2$ and 4 nM,

respectively); poorly inhibits other brain serine hydrolases

NOTE: Sold under license from The Scripps Research Institute



Summary: An analog of RCS-4 that differs only in the location of the methoxy group on the phenyl ring; structurally resembles JWH 250, which shows a high-affinity for both CB_1 and CB_2 (K_i = 11 and 33 nM, respectively)

1 mg 5 mg 10 mg



10866

RCS-4 3-methoxy isomer

MF: C₂₁H₂₃NO₂ **FW:** 321.4 **Purity:** ≥98% A solution in methanol **Stability:** ≥1 year at -20°C Summary: An RCS-4 analog whose design is based on the structure of the synthetic CB JWH 018 whose biological activity has not been reported

1 mg 5 mg 10 mg





[1345970-42-4] BTM-8, SR-18 **MF:** C₂₅H₂₉NO₂ **FW:** 375.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A synthetic CB identified as a component of several different herbal incense products; an analog of JWH 250

1 mg

5 mg

10 mg



RCS-8 3-methoxy isomer

MF: C₂₅H₂₉NO₂ **FW:** 375.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Differs from RCS-8 by having a methoxy group at the 3, rather than 2, position of its phenylacetyl group

1 mg 5 mg 10 mg



RCS-8 4-methoxy isomer

10863

MF: C₂₅H₂₉NO₂ **FW:** 375.5 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: Differs from RCS-8 by having a methoxy group at the 4, rather than 2, position of its phenylacetyl group

1 mg 5 mg 10 mg



STS Series

STS-135

10636

10864

[1354631-26-7] N-adamantyl-1-fluoropentylindole-3-Carboxamide

MF: C₂₄H₂₁FN₂O **FW:** 382.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A designer drug purported to be found in herbal blends; intended for research and forensic applications





UR-Series

AB-005

11564

[895155-25-6]

MF: C₂₃H₃₂N₂O **FW:** 352.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic CB built on a 1-[(1-methylpiperidin-2-yl)methyl]-indole base that is characteristic of a series of potent CBs; may have selectivity for the CB2 receptor; intended for forensic and research applications



UR-144

11502

[1199943-44-6] KM-X1 **MF:** C₂₁H₂₉NO **FW:** 311.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent synthetic CB which preferentially binds the peripheral CB2 receptor ($K_i = 1.8$ nM) over the central CB₁ receptor ($K_i = 150$ nM); intended for research and forensic applications

1 mg 5 mg 10 mg



(±)-UR-144 N-(4-hydroxypentyl) metabolite 11774

MF: C₂₁H₂₉NO₂ **FW:** 327.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: An expected phase I metabolite of UR-144; should be detectable in either serum or urine; intended for forensic and research applications



UR-144 N-(5-hydroxypentyl) metabolite

[895155-95-0]

MF: C₂₁H₂₉NO₂ **FW:** 327.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: An expected phase I metabolite of UR-144, based on the metabolism of similar cannabimimetics; should be detectable in either serum or urine; intended for forensic and research applications

1 mg 5 mg 10 mg



11766

11773

43

UR-144 N-pentanoic acid metabolite

MF: C₂₁H₂₇NO₃ **FW:** 341.5 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: An expected phase I metabolite of UR-144; should be detectable in either serum or urine; intended for forensic and research applications

1 mg 5 mg 10 mg



URB Series

URB447

13261

[1132922-57-6]

MF: C₂₅H₂₁ClN₂O **FW:** 400.9 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A mixed CB1 receptor antagonist/CB2 receptor agonist with IC50 values of 313 and 41 nM, respectively; reduces food intake and body-weight gain in ob/ob mice and Swiss mice (20 mg/kg) with an efficacy comparable to rimonabant; does not penetrate the blood-brain barrier

5 mg 10 mg 25 mg 50 mg



URB597

10046

10007457

[546141-08-6]

MF: C₁₀H₁₁N₂O₂ **FW:** 338.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent and selective inhibitor of FAAH with an IC₅₀ value of 4.6 nM in brain membranes and 0.5 nM in intact neurons; exhibits anti-nociceptive and anxiolytic effects in vivo

5 mg 10 mg 50 mg 100 ma



URB602

11775

[565460-15-3]

MF: C₁₉H₂₁NO₂ **FW:** 295.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A selective inhibitor of MAGL, exhibiting an IC₅₀ value of 28 µM for the rat brain enzyme

5 mg 10 mg 50 mg 100 ma



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Thomas G. Brock, Ph.D.

Fc

The Metabolism of JWH-type **Synthetic Cannabinoids**

For most users, the appeal of "Spice/K2" blends and synthetic cannabinoids (CBs) centers on drug testing: the active compounds do not score positive on standard tests for drugs of abuse. This is particularly important to those users who prefer cannabis, since the relatively long half-lives of metabolites of the key compound, Δ^9 -tetrahydrocannabinol (THC), leave users vulnerable to drug testing for days to weeks after partaking. The guarantee of a negative drug test can make an experimental herbal mixture, even a potentially nasty one, a little more attractive.

There are two issues regarding the synthetic CBs used in Spice/K2 blends that make them challenging for forensic testing. First, the diverse variety of potent CBs that can be interchanged and mixed together (see Related Article, page 4) makes it hard to zero in on offending compounds. Perhaps more critically, tests must detect the metabolites of all of these compounds, since synthetic CBs, like THC, are rapidly processed by the body. Several recent studies on the metabolism of the most popular synthetic CBs provide a valuable foundation for understanding the challenges to forensic testing of these drugs of abuse.

Lessons from Cannabis

What have we learned from marijuana? Although the bud from C. sativa contains over 400 chemicals, forensic testing has focused on THC, a major component which most potently produces the psychoactive effect of interest. Remarkably, marijuana contains some 65 other structurally- and functionally-related compounds which are unique to this plant genus and are truly 'cannabinoids', including cannabinol and cannabidiol. Something that should certainly be kept in mind is that the physiological and toxicological effects of using cannabis must be the integrated impact of all of these chemicals, not just THC.

Still, the testing for cannabis use centers on the presence of THC and its metabolites. Δ^9 -THC is rapidly metabolized in the body to a number of oxygenated products.¹ In the primary route of metabolism, a methyl group at carbon 11 is metabolized by liver cytochrome P450 to produce 11-hydroxy-THC (Figure 1). This intermediate is subsequently converted to an acid, 11-COOH-THC, known also as THC-COOH or more formally as 11-nor-



 Δ^9 -THC-9-carboxylic acid. Either the hydroxylated or carboxylated metabolite may be glucuronidated, facilitating urinary excretion. While THC has a short half-life in serum, 11-COOH-THC has a half-life of days to weeks due to accumulation in fatty tissue and delayed elimination, making it the ideal target for forensic testing. Metabolites are most commonly detected in urine samples after deglucuronidation, but detection of both THC and 11-COOH-THC in oral fluids is possible after concentration and derivatization.² Assessment of oral fluid obviates the possibility of substituting 'clean' samples; measuring both compounds minimizes the potential for misidentifying individuals passively exposed to marijuana smoke.

Other metabolites of THC are produced, although they are less abundant than 11-COOH-THC and aren't used in forensic tests. These metabolites are produced by oxidation along the five carbon side chain as well as at C-8 (Figure 1). Many different combinations may be detected in serum; COOH residues are subject to glucuronidation, with these products detectable in urine.

The term 'metabolite' may be misleading by suggesting lack of activity: many compounds derived from THC have diverse actions which may mimic THC or be pharmacologically distinct. Perhaps of greatest interest, the primary metabolite 11-COOH-THC, which clearly lacks the psychoactive actions of THC, may significantly contribute to the analgesic properties of marijuana and may, in fact, limit the psychoactive effects of THC.¹

Metabolism of JWH 018

Although JWH 018 has been banned and is now less commonly found in current herbal blends, it remains the archetypical naphthoylalkylindole type of synthetic CB. When exposed to human liver microsomes (to mimic phase I metabolism), diverse products are obtained, including mono-, di-, and trihydroxylated, N-dealkylated, carboxylated, and/or dehydrogenated forms.³ However, the majority of the metabolites are monohydroxylated on one of many carbons throughout the molecule, while a second group consists of dihydrodiols resulting from arene oxidation of the naphthalene ring system.³ Analyses of human urine samples, using predominantly LC-MS/MS, confirmed that the prevailing metabolite is monohydroxylated, typically on the terminal (ω) carbon of the alkyl group (Figure 2), and that essentially all monohydroxylated products are glucuronidated.⁴⁻⁷ Also commonly detected in human urine are metabolites that are monohydroxylated on the ω-1 alkyl site, monohydroxylated on the indole group, or carboxylated on the ω alkyl site (JWH 018-COOH). Reminiscent of the long serum half-life of 11-COOH-THC, JWH 018-COOH is poorly glucuronidated,^{5,6} suggesting that this metabolite might be less efficiently excreted than the hydroxylated metabolites. Interestingly, N-dealkylated and N-dealkyl monohydroxylated metabolites of JWH 018 are abundant in rat urine but rare in human samples.⁷

The metabolism of THC, as noted earlier, occurs predominantly in the liver, with a high clearance rate that reflects a high degree of first-pass metabolism. The rate of plasma clearance of THC varies greatly between individuals and may be higher in females than males and in regular THC users than in naïve users.⁸ The metabolism of JWH 018 is comparably rapid (Figure 2). Both a female regular smoker and male occasional smoker showed an approximately 80% reduction in the maximum measurable serum JWH 018 one hour after inhalation; JWH 018 was still detectable in the serum of both subjects after 24 h.9 This very small study suggests that clearance of this synthetic CB is fast, regardless of sex or experience of the consumer.

The activity of metabolites of JWH 018 may be important. As seen with THC vs. 11-COOH-THC, CB metabolites may mimic, oppose, or have distinct actions from parent compounds. Remarkably, the monohydroxylated metabolites of JWH 018 bind the central CB1 receptor with high affinity



and act as full agonists.¹⁰ This indicates that, for this CB, phase I metabolism glucuronidated) at the ω site of the chain. With increasing time after may not significantly diminish action. This finding does not generalize to consumption, this product may be less abundant, replaced in prevalence all synthetic CBs, as phase I metabolites of JWH 073 exhibit only neutral by either a dihydroxylated metabolite or an ω-carboxylated product. The antagonist or partial agonist activity, although they still strongly bind the ω-monohydroxylated metabolite, often referred to as 'M1' in the literature, has CB1 receptor.¹¹ Furthermore, glucuronidated metabolites can act as neutral been called the 'most convenient compound for establishing consumption',¹⁴ antagonists at CB₁ receptors, blocking receptor activation.¹² because of its abundance and apparent universality across synthetic CBs.

Metabolism of Other JWH-type CBs

Different studies have been published on the metabolism of JWH 015 in vitro using rat liver microsomes,¹³ JWH 073 in humans,⁵⁻⁷ and JWH 250 in humans and rats.¹⁴ Like JWH 018, each of these contains an aminoalkylindole group; JWH 015 and JWH 073 also have a naphthoyl group in common with JWH 018 (Figure 3). The in vitro metabolism of JWH 015 produces 22 products reminiscent of those detected following similar treatment of JWH 018.¹³ The diversity of products generated by this method greatly exceeds those typically reported from urine, as in the studies examining the human urinary metabolites of JWH 073. As JWH 073 differs structurally from JWH 018 solely in alkyl chain length (butyl for pentyl), the human urinary metabolites are naturally comparable: monohydroxylation of the indole group or alkyl ω site or ω-carboxylation of the alkyl chain.^{5,6} Again, all monohydroxylated forms are fully glucuronidated while only a fraction (<50%) of the carboxylated products are glucuronidated.

The analysis of JWH 250 metabolism in humans and rats used GC-MS as well as LC-MS/MS, examined urine samples from eleven different human subjects, and also evaluated metabolites in human serum.¹⁴ By GC-MS, which is relatively more sensitive than LC-MS/MS, some 20 different metabolites of JWH 250 can be detected in human urine, although many are of very low abundance. Native JWH 250 is not detectable. Unlike the case for JWH 018, N-dealkylated JWH 250 is detected in both rat and human urine, although the levels in human samples are low. Mono- and dihydroxylated metabolites are the most prevalent metabolites detected in human urine by LC-MS/MS, with monohydroxylation occurring on the terminal alkyl carbon and the second hydroxylation on the methoxybenzyl moiety (Figure 3). The ratios between these two metabolites differs between individuals, the second hydroxylation assumed to reflect increased time between JWH 250 administration and urine collection. Evaluation of the serum sample by GC-MS reveals five metabolites. All of these are hydroxylated on the alkyl chain, on the methoxybenzyl group, or on both sites. No carboxylated metabolites of JWH 250 are identified in either human urine or serum samples.

Summary

Over a decade ago, Aung et al. demonstrated that, for a variety of cannabimimetics, an alkyl chain of 3-6 carbons is sufficient for high affinity binding to the CB receptors.¹⁵ The most common human urinary metabolite for synthetic CBs having this tail is monohydroxylated (and



Figure 2. Metabolism of JWH 018. A.) Sites of modification in major metabolites detected in human urine. B.) Time course of metabolism of JWH 018 in human subjects following inhalation.



Figure 3. The metabolism of JWH compounds 015, 073, and 250; major metabolites are given in larger font.

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MF: C₁₆H₁₄N₂O₂ **FW:** 266.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Reported to be a potent, noncompetitive inhibitor of MAGL; conflicting data indicates that it does not inhibit human recombinant, rat brain, or mouse brain MAGL at concentrations up to 100 μM

5 mg 10 mg

50 mg 100 mg



URB937 10674 [1357160-72-5]

MF: C₂₀H₂₂N₂O₄ **FW:** 354.4 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent FAAH inhibitor (IC50 = 26.8 nM, in vitro) that does not penetrate the blood-brain barrier; ED₅₀ value for FAAH inhibition in brain is 200fold higher than the ED₅₀ value for FAAH inhibition in liver when administered systemically in mice; attenuates behavioral responses elicited in mouse models of visceral (ED₅₀ = 0.1 mg/kg), neuropathic, and inflammatory pain





JP104	10008661
MF: CarHanNaOa FW: 406 5 Purity: >98%	

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An irreversible FAAH inhibitor with an IC₅₀ value of 7.3 nM for the human recombinant enzyme

5 mg 10 mg 50 mg 100 mg



WIN Series

Pravadoline

10007691

[92623-83-1] WIN 48,098

MF: C₂₃H₂₆N₂O₃ **FW:** 378.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A nonacidic, aminoalkylindole analgesic agent that inhibits COX; inhibits PG synthesis (IC₅₀ = 5 μ M in mouse brain microsomes) and displays antinociceptive activity (ED₅₀ = 26 mg/kg in an ACh-induced writhing assay in mice); inhibits neuronally stimulated contractions in mouse vas deferens preparations $(IC_{50} = 0.45 \ \mu M)$

5 mg 10 mg 25 mg

9001204

WIN 54,461

1 mg

5 mg 10 mg

[166599-63-9] 6-Bromopravadoline

MF: $C_{23}H_{25}BrN_{2}O_{3}$ **FW:** 457.4 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An aminoalikylindole which acts as a CB mimetic, displacing WIN 55,212-2 from CB receptors on rat cerebellum membranes (IC₅₀ = 515 nM); antagonizes the inhibition of electrically-induced contractions in isolated mouse vas deferens preparations by tetrahydrocannabinol or pravadoline; intended for research and forensic applications



(±)-WIN 55,212 (mesylate)

[137795-17-6]

MF: C₂₇H₂₆N₂O₃ • CH₃SO₃H **FW:** 522.6 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A mixture of the two enantiomers, (+)-WIN 55,212-2 and (-)-WIN 55,212-3



(+)-WIN 55,212-2 (mesylate)

[131543-23-2]

5 mg

10 mg

25 mg

50 mg

10006973

10736

MF: C₂₇H₂₆N₂O₃ • CH₃SO₃H **FW:** 522.6 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: A potent aminoalkylindole CB receptor agonist with K values of 62.3

and 3.3 nM for human recombinant CB1 and CB2 receptors, respectively



XLR Series

XLR11

11565

11769

[1364933-54-9] 5-fluoro UR-144 **MF:** C₂₁H₂₈FNO **FW:** 329.5 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: An aminoalkylindole compound that is expected to be a CB mimetic; intended for forensic and research applications



XLR11 N-(4-fluoropentyl) isomer

MF: C₂₁H₂₈FNO **FW:** 329.5 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An isomer of XLR11 which has the fluorine atom placed on the 4 position, rather than the terminal 5 position, of the alkyl group; intended for forensic and research purposes



11688 XLR11 N-(4-pentenyl) analog UR-144 N-(4-pentenyl) analog

MF: C₂₁H₂₇NO **FW**: 309.5 **Purity**: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A variant of XLR11 which replaces the N-(5-fluoropentyl) chain with N-(4-pentenyl); commonly observed component of herbal mixtures containing synthetic CBs with the 5-fluoropentyl moiety; intended for forensic and research applications





10009023

Miscellaneous

Cannabidiol

(DEA Schedule I Regulated Compound)

[13956-29-1] CBD

MF: C₂₁H₃₀O₂ **FW:** 314.5 **Purity:** ≥99%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: Displays antioxidant activity when administered at relatively high doses without undesired toxic or psychological effects seen with Δ^9 -THC; is neuroprotective against both excitatory neurotransmitter (glutamate) and oxidant (hydroperoxide) induced neurotoxicity at a concentration of 10 µM

1 mg 5 mg 10 mg 50 mg



• Also Available: Cannabidiol (solution) (90081) DEA-exempt formulation

Cannabipiperidiethanone

11655

90080

[1.345970-43-5]

MF: C₂₄H₂₈N₂O₂ **FW:** 376.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A synthetic cannabinoid that binds to the cannabinoid receptors CB1 and CB2 with IC50 values of 591 and 968 nM, respectively; this product is intended for forensic purposes and research applications

5 mg 10 mg 25 mg



IMMA

70275

BML-190, Indomethacin Morpholinylamide **MF:** $C_{23}H_{23}ClN_2O_4$ **FW:** 426.9 **Purity:** \ge 98% A crystalline solid **Stability:** ≥1 year at -20°C Summary: A selective CB2 receptor agonist with Ki values of >20,000 and 435 nM for the CB₁ and CB₂ receptors, respectively

5 mg 10 mg 50 mg 100 mg



KM 233

[628263-22-9]

MF: C₂₅H₃₀O₂ **FW:** 362.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Δ^8 -THC analog with 13-fold selectivity for the CB₂ receptor (K_is = 12.3) and 0.91 nM, for CB1 and CB2 respectively); its CB agonist activity inhibits human U87 glioma cell proliferation in vitro (IC₅₀ = 1.4 μ M) and in vivo (2 mg/kg in a severe combined immunodeficiency mouse xenograft side-pocket model)

1 mg 5 mg 10 mg 25 mg



1'-Naphthoyl Indole

[109555-87-5]

MF: C₁₉H₁₃NO **FW:** 271.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Represents the simplest form of a large group of related synthetic CBs; should have no appreciable affinity for either CB receptor; intended for forensic and research applications







90375

11687

[301-02-0] cis-9-Octadecenamide, Oleamide **MF:** C₁₉H₃₅NO **FW:** 281.5 **Purity:** ≥98%

9-Octadecenamide

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: The amide of oleic acid found in cerebrospinal fluid; induces physiological sleep when injected into rats intraperitoneally at 5 to 50 mg doses

50 mg 100 mg 500 mg

1 g



(-)-11-nor-9-carboxy- Δ^{9} -THC (solution) 10009897

[56354-06-4]

MF: C₂₁H₂₈O₄ **FW:** 344.4 **Purity:** ≥98% A solution in methanol **Stability:** ≥1 year at -20°C

Summary: The major metabolite of Δ^9 -THC, used as an internal standard in various analytical procedures to unequivocally confirm its presence in biological fluids

500 µg 1 mg 5 mg 10 mg



(-)-11-nor-9-carboxy- Δ^{9} -THC-d₃ (solution) 10009898

[130381-15-6]

MF: $C_{21}H_{25}D_3O_4$ FW: 347.5 Chemical Purity: $\ge 98\%$ **Deuterium Incorporation:** \geq 99% deuterated forms (d₁-d₃); \leq 1% d₀ A solution in methanol **Stability:** ≥ 1 year at -20°C

Summary: An internal standard for the quantification of (-)-11-nor-9-carboxy- Δ^9 -THC by GC- or LC-MS



5 mg



4-Quinolone-3-Carboxamide CB₂ Ligand

[1314230-69-7] 4Q3C CB, Ligand

MF: $C_{26}H_{34}N_2O_3$ **FW:** 422.6 **Purity:** \ge 98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A selective, high affinity ligand of the CB_2 receptor (K_i = 0.6 nM v. CB_1 binding at a K_i >10,000 nM in vitro) that may behave as an inverse agonist; displays antinociceptive activity in a formalin test in mice at a dose of 6 mg/kg

1 mg 5 mg 25 mg



Alkaloids

Harmaline

[304-21-2]

MF: C₁₃H₁₄N₂O **FW:** 214.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychoactive indole found naturally in certain plants; inhibitor of monoamine oxidases; induces tremor in mice through the N-methyl-D-aspartate receptor; intended for forensic or research purposes

5 mg 10 mg 25 mg



Mitragynine

[4098-40-2] 9-methoxy Corynantheidine, Kratom **MF:** $C_{23}H_{30}N_2O_4$ **FW:** 398.5 **Purity:** \ge 95%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: An indole alkaloid that has stimulatory, antinociceptive, and opiate-like effects, acting through noradrenergic, serotonergic, and opioid receptors; has a higher affinity for the μ -opioid receptor than the δ - or κ -opioid receptors (pK_i = 8.14, 7.22, and 5.96, respectively); intended for forensic applications

1 mg 5 mg 10 mg





11151

10 mg

Amphetamines

5-APB (hydrochloride)

[286834-80-8] 5-(2-Aminopropyl) Benzofuran **MF:** C₁₁H₁₃NO • HCl **FW:** 211.7 **Purity:** ≥95% A crystalline solid **Stability:** ≥ 2 years at -20° C Summary: An analog of MDA where the 3,4-methylenedioxyphenyl ring system has been replaced with a benzofuran ring; intended for forensic purposes

1 mg 5 mg 10 mg



6-APB (hydrochloride)

[286834-84-2] Benzo-Fury, 6-(2-aminopropyl)Benzofuran

MF: C₁₁H₁₃NO • HCl **FW:** 211.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A phenethylamine designer drug analog to the amphetamine MDA in that the 3,4-methylendioxyphenyl ring system has been replaced with a benzofuran ring; intended for forensic and research applications



D2PM (hydrochloride)

[172152-19-1] Diphenylprolinol, Diphenyl-2-pyrrolidinemethanol **MF:** $C_{17}H_{19}NO \bullet HCl$ **FW:** 289.8 **Purity:** $\ge 98\%$

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychoactive designer drug; also used in organic synthesis to prepare the Corey-Bakshi-Shibata catalyst; intended for forensic purposes

5 mg 10 mg 25 mg



(S)-Desoxy-D2PM (hydrochloride)

9001095

[188398-87-0] (S)-2-Diphenylmethylpyrrolidine **MF:** C₁₇H₁₉N • HCl **FW:** 273.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Most commonly used as a chiral solvating agent for NMR analysis of chiral compounds; structurally related to desoxypipradrol, a dopamine transporter inhibitor and psychoactive stimulant

5 mg 10 mg 25 mg



11079

11160

• HCI





3,4-Dimethoxymethamphetamine

(hydrochloride)

[70932-18-2] 3,4-DMMA

MF: C₁₂H₁₉NO₂ • HCl **FW:** 245.7 **Purity:** ≥97%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An MDMA analog that appears to act as a serotonin-norepinephrinedopamine releasing agent binding to and inhibiting uptake at noradrenalin and serotonin transporters (K_is = 22.8 and 7.7 μ M and IC₅₀s = 253.4 and 108 μ M, respectively); significantly less potent than MDMA

5 mg 10 mg 50 mg



DOET

[22004-32-6]

5 mg

MF: C₁₃H₂₁NO₂ **FW:** 223.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent, long-acting psychedelic drug of the phenethylamine and amphetamine chemical classes that likely acts as a serotonin 5-HT₂ receptor partial agonist; intended only for research and forensic applications



2-Fluoroamphetamine (hydrochloride) 11419 **MF:** C₀H₁₂FN • HCl **FW:** 189.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥ 2 years at -20° C Summary: A structural isomer of 4-FA, having the fluorine at the 2, rather than the 4, position; intended for research and forensic applications 3-Fluoroamphetamine (hydrochloride) 9001191 **MF:** C₉H₁₂FN • HCl **FW:** 189.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: A structural isomer of 4-FA, having the fluorine at the 3, rather than the 4, position; intended for research and forensic applications

para-Fluoroamphetamine (hydrochloride) 11156

MF: C₉H₁₂FN • HCl **FW:** 189.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Inhibits the uptake of dopamine, serotonin, and norepinephrine with IC_{50} values of 0.77, 6.8, and 0.42 μ M, respectively, indicating potency comparable to cocaine or methamphetamine; intended for forensic purposes



2-Fluoromethamphetamine (hydrochloride) 11420

MF: C₁₀H₁₄FN • HCl **FW:** 203.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A stimulant drug related to methamphetamine and 2-fluroamphetamine that has been identified as a component of designer drugs sold as "legal high" replacements for restricted substances; intended for use as a standard for the forensic analysis of samples that may contain this compound



3-Fluoromethamphetamine (hydrochloride) 9001185

3-FMA

5 mg

10 mg

50 mg

11128

11141

MF: C₁₀H₁₄FN • HCl **FW:** 203.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: An isomer of 4-FMA characterized by having fluorine at the 3 position of the phenyl group; intended for forensic and research applications







• HCI

4-Fluoromethamphetamine (hydrochloride) 9001070 [52063-62-4] 4-FMA

MF: C₁₀H₁₄FN • HCl **FW:** 203.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A stimulant drug related to methamphetamine and 4-fluoroamphetamine that has been identified as a component of designer drugs sold as "legal high" replacements for restricted substances; intended for use as a standard for the forensic analysis of samples that may contain this compound



10979 MDMA methylene homolog (hydrochloride)

3,4-Methylenedioxymethamphetamine methyl homolog **MF:** C₁₂H₁₇NO₂ • HCl **FW:** 243.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential designer drug created by inserting a methylene group in the methylamphetamine portion of MDMA



Methiopropamine (hydrochloride)

[7464-94-0] MPA, NSC 400137

MF: C₈H₁₃NS • HCl **FW:** 191.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A structural analog of methamphetamine in which the phenyl group has been replaced with thiophene; intended for forensic and research applications



Methoxetamine (hydrochloride)

[1239908-48-5] MXE

MF: C₁₅H₂₁NO₂ • HCl **FW:** 283.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A 3-methoxy, N-ethyl analog of ketamine which, like ketamine, has been abused recreationally; intended for forensic and research applications

1 mg 5 mg 10 mg

Methylhexanamine (hydrochloride)



11161

11139

[13803-74-2] Dimethylamylamine, DMAA, Floradrene, Forthane, Geranamine, NSC 1106

MF: C₇H₁₇N • HCl **FW:** 151.2 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A simple aliphatic amine that was once marketed as a nasal decongestant but is now sold as a bodybuilding supplement; sold as a mild stimulant in the form of party pills; intended for forensic or research purposes



2-FMA

11144

4-MTA

[14116-06-4] 4-Methylthioamphetamine, P 1882 **MF:** C₁₀H₁₅NS **FW:** 181.3 **Purity:** ≥98% A solution in ethanol **Stability:** ≥1 year at -20°C Summary: A methylthio analog of PMA, a hallucinogenic drug that has been scheduled in many countries; intended for forensic applications

1 mg 5 mg 10 mg



TMA-2

[1083-09-6] 2,4,5-Trimethoxysmphetamine **MF:** C₁₂H₁₉NO₃ **FW:** 225.3 **Purity:** ≥95% A solution in ethanol **Stability:** ≥ 1 year at -20° C

Summary: A psychedelic hallucinogen which has appeared on the illicit drug market; intended for research and forensic applications

5 mg 10 mg 50 mg



Benzodiazepines

Phenazepam

[51753-57-2] BD 98, Fenazepam

MF: C₁₅H₁₀BrClN₂O FW: 349.6 Purity: >98% A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A benzodiazepine agonist of the GABAA-benzodiazepine receptor chloride channel complex; has been shown to exhibit strong anxiolytic, sedative, anticonvulsive, and hypnotic properties; has been shown to act as an anxioselective tranquilizer at very low doses (10-5 to 10-10 mg/kg)

5 mg 10 mg

50 mg 100 mg



Cathinones



[166593-10-8] α-methylamino-Butyrophenone, MABP

MF: C₁₁H₁₅NO • HCl **FW**: 213.7 **Purity**: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: A substituted cathinone characterized by an ethyl group at the alpha position

and an N-terminal methyl group; intended for forensic applications

5 mg 10 mg 50 mg



Butylone (hydrochloride)

[17762-90-2] β-keto MBDB

MF: C₁₂H₁₅NO₃ • HCl **FW:** 257.7 **Purity:** ≥97%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A B-keto derivative of MBDB that has been identified in designer drugs sold as bath salts; a cathinone, intended to be used for forensic applications



Diethylcathinone (hydrochloride)

[134-80-5] Menutil, Moderatan, Tenuate

MF: C₁₃H₁₉NO • HCl **FW:** 241.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A stimulant drug of the phenethylamine, amphetamine, and cathinone chemical classes that is used as an appetite suppressant; functions as an inactive prodrug to ethcathinone, a selective norepinephrine releasing agent



N,N-Dimethylcathinone (hydrochloride) 9001144

[10105-90-5] Metamfepramone

MF: C₁₁H₁₅NO • HCl **FW**: 213.7 **Purity**: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychotropic compound of the phenethylamine and cathinone classes; slightly less potent than methcathinone and essentially equipotent with cathinone, in behavioral studies involving rats; intended for forensic purposes

5 mg

10 mg 50 mg



4-ethyl-N,N-Dimethylcathinone (hvdrochloride)

MF: C₁₃H₁₉NO • HCl **FW:** 241.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential stimulatory designer drug of the amphetamine and cathinone chemical classes; intended for forensic purposes



4-methoxy-N,N-Dimethylcathinone

(hydrochloride)

[1089307-23-2] N-Methylmethedrone

MF: C₁₂H₁₇NO₂ • HCl **FW**: 243.7 **Purity**: ≥98% A crystalline solid **Stability:** ≥1 year at -20°C Summary: An analog of methedrone, differing by the presence of a second

aminomethyl group; intended for forensic and research applications

5 mg 10 mg 50 mg

5 mg

10 mg

50 mg

9000849



3,4-DMEC

MF: C₁₃H₁₉NO • HCl **FW:** 241.8 **Purity:** ≥95%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A substituted cathinone with potential for abuse; intended for forensic and research applications

5 mg 10 mg 50 mg

5 mg

10 mg

50 mg

10393

11333

2,3-Dimethylmethcathinone (hydrochloride) 11225

2,3-DMMC

MF: C₁₂H₁₇NO • HCl **FW:** 227.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential designer drug that is structurally related to 4-MMC; intended for research and forensic applications



3,4-Dimethylmethcathinone (hydrochloride) 9001098

[1081772-06-6] 3.4-DMMC

MF: C₁₂H₁₇NO • HCl **FW:** 227.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C Summary: A potential designer drug that is structurally related to 4-MMC; intended

for research and forensic applications









11207

11666

[17763-12-1] Dibutylone **MF:** C₁₃H₁₇NO₃ • HCl **FW:** 271.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential psychotropic designer drug of the phenethylamine, amphetamine, and cathinone chemical classes; intended for forensic purposes



Ethcathinone (hydrochloride)

[51553-17-4] N-Ethylcathinone, RMI 8201A

MF: C₁₁H₁₅NO • HCl **FW:** 213.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted cathinone that produces amphetamine-like stimulus effects in rats trained to discriminate amphetamine from vehicle; intended for research and forensic applications





9001125

11241

11665

11199

11198

N-Ethylbuphedrone (hydrochloride) NEB

MF: C₁₂H₁₇NO • HCl **FW:** 227.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted cathinone characterized by an ethyl group at the alpha position as well as an N-terminal ethyl group; intended for forensic and research applications



2-Ethylethcathinone (hydrochloride)

2-EEC

MF: C₁₃H₁₉NO • HCl **FW:** 241.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted cathinone with potential for abuse; intended for forensic and research applications

5 mg	0 1
10 mg	Ń.
50 mg	
	• HCI

3-Ethylethcathinone (hydrochloride)

3-EEC

MF: C₁₃H₁₉NO • HCl **FW:** 241.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted cathinone with potential for abuse; intended for forensic applications









2-Fluoroethcathinone (hydrochloride) 11229 2-FEC **MF:** C₁₁H₁₄FNO • HCl **FW:** 231.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥ 2 years at -20° C Summary: A fluorine-substituted synthetic cathinone that has potential for abuse; intended for forensic and research applications

5 mg 10 mg 50 ma







that may contain this compound

5 mg 10 mg







4-Fluoromethcathinone (hydrochloride) 10859

[7589-35-7] Flephedrone, 4-FMC **MF**: C₁₀H₁₂FNO • HCl **FW**: 217.7 **Purity**: ≥98% A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A cathinone derivative identified in several designer drugs that are marketed as plant feeders; intended for use as a standard for the forensic analysis of samples that may contain this compound



bk-MDDMA (hydrochloride)

[109367-07-9] Dimethylone

MF: $C_{12}H_{15}NO_3 \bullet HCl$ **FW:** 257.7 **Purity:** \ge 98% A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A potential psychotropic designer drug of the phenethylamine, amphetamine, and cathinone chemical classes; intended for forensic purposes



bk-MDEA (hydrochloride)



MF: C₁₂H₁₅NO₃ • HCl **FW**: 257.7 **Purity**: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychotropic designer drug of the phenethylamine, amphetamine, and cathinone chemical classes; detected in products marketed as bath salts, plant food, and tablets; intended for forensic purposes



nor-Mephedrone (hydrochloride)

[6941-17-9] Mephedrone Metabolite, NSC 60487 **MF:** $C_{10}H_{13}NO \bullet HCl$ **FW:** 199.7 **Purity:** \ge 98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A metabolite of mephedrone that can be detected in the urine; formed by the N-demethylation of the primary amine



Methedrone (hydrochloride)

[879665-92-6] 4-Methedrone, para-Methoxymethcathinone, Methoxyphedrine, PMMC **MF**: C₁₁H₁, NO₂ • HCl **FW**: 229.7 **Purity**: ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A phenethylamine, amphetamine, and cathinone derivative that acts as a triple reuptake/release/reversible MAO inhibitor; intended for use as a standard for the forensic analysis of samples that may contain this compound







2-Methoxymethcathinone (hydrochloride) 9001186 2-MMC

MF: C₁₁H₁₅NO₂ • HCl **FW:** 229.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A positional isomer of methedrone, having the methoxy group at the 2 rather than the 4 position; intended for forensic and research applications



3-Methoxymethcathinone (hydrochloride) 9001187 3-MeOMC

5 mg

10 mg

50 mg

5 mg

10 mg

50 ma

9001124

9001123

9000940

10529

• HCI

MF: C₁₁H₁₅NO₂ • HCl **FW:** 229.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A positional isomer of methedrone, having the methoxy group at the 3 rather than the 4 position; intended for forensic and research applications



4'-Methoxy- α -pyrrolidinopropiophenone (tosylate)

4'-MeO-α-PPP, 4'-MeOPPP

MF: C₁₄H₁₉NO₂ • C₇H₈O₃S **FW:** 405.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A structural analog of α -PPP, differing by the addition of a methoxy group in the para position of the phenyl ring; metabolites that are detectable in rat urine have been described; intended for forensic testing





4-Methylbuphedrone (hydrochloride)

[1336911-98-8] BZ-6378, 4-MeBP **MF:** C₁₂H₁₇NO • HCl **FW:** 227.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A para-methyl analog of buphedrone; intended for forensic applications



1 mg

5 mg

10 mg

50 mg

4-methyl-N-Methylbuphedrone (hvdrochloride)

4-methyl- α -Methylaminobutiophenone

MF: C₁₃H₁₉NO • HCl **FW:** 241.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: A para-methyl analog of buphedrone with an aminomethyl addition; intended for research and forensic applications

5 mg 10 mg 50 mg



N-ethyl-N-Methylcathinone (hydrochloride) 11604

[1157739-24-6]

MF: C₁₂H₁₇NO • HCl **FW:** 227.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted cathinone structurally similar to the designer drugs mephedrone and methylone; intended for forensic and research applications

5 mg 10 mg 50 mg



2,3-Methylenedioxymethcathinone (hydrochloride)

2.3-MDMC

MF: C₁₁H₁₃NO₃ • HCl **FW:** 243.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A positional isomer of methylone, having the methylenedioxy group attached to the 2 and 3, rather than the 3 and 4, positions; intended for forensic and research applications

5 mg 10 mg 50 mg

10449

11486



Methylenedioxy Pyrovalerone

[687603-66-3] MDPV

MF: C₁₆H₂₁NO₃ **FW:** 275.3 **Purity:** ≥98%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An analog of pyrovalerone which includes the 3,4-methylenedioxy moiety found on MDMA: physiological, neurological, and toxicological actions have not been characterized; reported by the DEA to be abused as a CNS stimulant; intended to be used in the forensic analysis of samples that may contain this compound

5 mg 10 mg 50 mg



Methylenedioxy Pyrovalerone (hydrochloride) 10684

[24622-62-6] MDPV **MF:** C₁₆H₂₁NO₃ • HCl **FW:** 311.8 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: A more aqueous soluble form of MDPV

5 ma 10 mg 50 mg



11667

9001133

Thomas G. Brock, Ph.D.

Fc

Analysis of Synthetic Cannabinoids and Designer Drugs

Designer drugs are creating opportunities. Herbal blends advertised as "100% legal" are popular with students and young adults, although the ingredients aren't listed. That creates an opportunity for companies to develop ways to accurately detect synthetic cannabinoids (CBs) and designer drugs that might be mixed with flavorings and scents in plant material. There are opportunities for manufacturers of equipment to produce instruments that can detect parent compounds and metabolites in urine, saliva, serum, or hair. Also generating opportunities are those off-white powders that are found in foil packets, marketed as bath salts, plant food, or anything else that would not normally be for human consumption. These mystery mixtures might contain any of the usual controlled substances or their analogs, or they may have something quite different and unexpected. Most likely, they will contain a mixture of active compounds, as well as some filler or camouflaging compound. Several companies are developing devices to analyze these powders in the lab. Finally, an opportunity exists in the field, where bulk powders and liquids are being transported alongside legal goods. Point-and-shoot identification of designer drugs is needed there.

Of course, these opportunities are generated by designer CBs, cathinones, and other compounds, currently being marketed to a curious public. In fact, the public is very accepting of pills, formulations, and herbal remedies that might alleviate any discomfort. Many have tried products to lose weight or increase their energy, knowing little about the ingredients. The phrase "100% legal" may suggest that the contents have been approved by authorities, which, in turn, indicates that the products are safe for consumption. Unfortunately, diverse stimulants, relaxants, entactogens, anxiolytics, and hallucinogens, which are commonly chemical isomers or analogs of known controlled substances, constitute the biological activity of many of these "100% legal" products currently available online, as well as at gas stations, head shops, and other commercial outlets. The magnitude of this problem is underscored by the number of users admitted to emergency rooms around the world.^{1,2}

Synthetic Cannabinoids and Their Metabolites

It seemed like a good idea at the time: develop stable analogs of THC, the most potent ingredient in cannabis, that might be able to reduce pain or stimulate appetite without the psychoactive effects. Several laboratories accepted the challenge during the 1990s and 2000s, developing an array of structurally distinct compounds which avidly activate one or both of the CB receptors (see related article on page 4). Unfortunately, certain entrepreneurs had a different idea, to create synthetic marijuana by adding these synthetic CBs to dried plant material. Originally known as Spice or K2 and marketed as incense, these products contain varying mixes of synthetic CBs in uncharacterized concentrations. The use of these cannabimimetics translates, often, into hospital admissions due to cannabinoid toxicity and other adverse effects. Still, because the synthetic CBs are structurally distinct from THC, users who anticipate being tested for smoking weed have an added incentive: the synthetic CBs and their metabolites are not detected by marijuana tests.

Enter the Cayman JWH Metabolite ELISA. This assay detects urinary metabolites of many of the most popular synthetic CBs, including JWH 018, IWH 073, IWH 019, IWH 200, and AM2201. It has been validated with human urine samples and demonstrates a high degree of correlation with LC/MS analysis. This assay is designed as a rapid and inexpensive screening tool that generates a positive vs. negative answer (Figure 1). Samples testing positive in Cayman's assay should be confirmed by quantitative analysis, such as LC/MS.



Figure 1. The Cayman JWH Metabolite ELISA kit (top) selectively and sensitively detects several JWH metabolites, like JWH 018 N-pentanoic acid (bottom).

Analysis at the Bench

The analysis of samples which might contain one or more forensic compounds can be performed using a variety of related techniques. Gas chromatography (GC) paired with mass spectroscopy (MS) has long been the gold standard for forensic analysis. In GC/MS, chemicals in a mixture are separated by GC, ionized, and then the mass to charge ratio (m/z) of each compound is determined by MS. The mass spectrum is then compared with a spectral library of known compounds for identification. While MS provides the m/z of a compound, tandem mass spectrometry (MS/MS) involves fragmenting the compound after initial MS and then determining the m/z of each piece, providing important information when parent compounds have identical mass. Different types of mass analyzers may be used, including quadrupole and time of flight (TOF), which differ in their sensitivity and selectivity. Tandem MS often combines sequential quadrupole devices (triple quadrupole, or QQQ) or quadrupole followed by TOF (QTOF). Other types of detectors may also follow GC (e.g., flame ionization detectors (FID)) or LC (e.g., photodiode array detectors (PDA, DAD)).

Different equipment is suited to different goals in analysis. In some cases, analysis is targeted, seeking to specifically test whether a particular substance is present in a given sample. For this purpose, both the analytical hardware and the acquisition software should be optimized to avoid false positives. For this goal, Agilent's 6400 series Triple Quadrupole LC/MS systems with triggered MRM (tMRM) acquisition software would be an excellent match: this system

produces quantitative data and a searchable library spectrum in a single injection in order to avoid false positive identification. Alternatively, the goal Sir Chandrasekhara Venkata Raman was a Nobel Prize winning physicist from may be to identify a variety of compounds, some novel, in a complex mixture, India. He discovered that, when light traverses a transparent material, some of as is often the case in designer drug preparations. In this case, the appropriate the light that is deflected changes in wavelength (Raman scattering). In one hardware must be combined with software that can scan an extensive library current approach, laser light is directed at a sample and is scattered by specific of compounds. Here, one might choose from Agilent's 6500 series Q-TOF molecules in the sample. A sensor then measures the intensity of light at each LC/MS platforms which combine accurate mass analysis with the ability to wavelength and converts it to a spectrum that fingerprints those molecules. retrospectively mine data for new compounds without reinjection. In addition, Raman spectroscopy may be used in diverse applications, including profiling Agilent offers high quality accurate mass databases and libraries across all of molecular components of cells and tissues (e.g., for cancer detection), studying its GC/MS and LC/MS instruments for thousands of compounds related static and changing chemical structure, and analyzing liquids for explosives. to Forensic Toxicology. Cayman is actively synthesizing new and expected Raman spectroscopy is rapid and does not require processing or labeling of analytical reference standards, including synthetic CBs, cathinones, and others, samples. Certain forms of Raman spectroscopy show low sensitivity to surface to help develop these forensic libraries. layers and can be used without opening packaging, including plastic bags, glass Synthetic CBs and cathinones provide a unique challenge for MS analysis: containers, and gel caps.

many isomers have identical masses and cannot be distinguished by MS or MS/MS. One example would be flephedrone (4-fluoromethcathinone, 4-FMC) and 3-FMC, which are, respectively, para- and ortho-substituted isomers of a cathinone that may be found in bath salt-type pouders. The DiscovIR-GC[™] from Spectra Analysis couples Fourier transform infrared spectroscopy (FTIR) with gas chromatography (Figure 2). The DiscovIR-GC[™] provides a high resolution solid phase transmission spectrum for each component of a sample. Infrared spectroscopy can resolve ortho-, meta- and para-substituted isomers; even diastereomers can be resolved by infrared spectroscopy. FTIR can differentiate isomers based on spectral differences, so the DiscovIR-GC[™] does not rely on retention time, a crucial capability



Figure 2. The DiscovIR-GC[™] from Spectra Analysis differentiates isomers based on spectral erences.

when the mass spectra are identical and retention times are similar. Please visit www.Spectra-Analysis.com for more information.

Not Outstanding in the Field

The curious can find designer drugs online, but where are they made? The answer is often some variation on 'Clandestine labs in other countries, most likely China or India'. This means that the front line of defense is at the borders, where evaluation of imported powders and liquids for drugs must be performed rapidly and accurately, often in the field. One contemporary option is the portable Raman Spectrometer, a handheld device which offers point-and-shoot analysis.

Portable or handheld Raman spectrometers are available in a variety of formats for forensic analysis in the field. Four devices were recently evaluated by the National Forensic Science Technology Center (nfstc.org). It is worth noting that previous evaluations of portable GC-MS, near infrared (NIR) or FTIR devices revealed numerous drawbacks, most notably failure to identify compounds in samples accurately and reproducibly. The overall review of portable Raman spectrometers is somewhat favorable: testing is rapid and non-destructive, units are easy to operate, and very little sample preparation is required prior to analysis. However, accuracy remains a limitation, with only 50% accuracy being typical for mixtures of controlled substances (although the Thermo FirstDefender RM attained 70% accuracy). Reproducibility was less than 50% for all devices. Moreover, Raman spectrometry does not work well with trace amounts or with highly fluorescent or pigmented samples. In short, field testing remains an area for opportunity.

This brings us back to GC/MS. Companies have engineered instruments to be operated under field conditions, some with internal gas cylinders and vacuum pumps, capacities for rapid sample processing, and integrated software analysis. Torion Technologies has an extremely rugged and truly portable unit that combines GC with toroidal ion trap MS which offers both sample preparation (extraction) and sample injection in one device, its Solid Phase Micro Extraction (SPME) syringe. FLIR Systems offers several portable MS devices, including the Griffin 400 and 460 GC/MS models for mobile forensic investigations. These instruments also have SPME capacity and are MS/MS capable. Cayman Chemical is collaborating with FLIR Systems by providing analytical reference standards of known and anticipated designer drugs to produce a Mass Spectral Library that can be used with the Griffin GC/MS systems.

Schifano, F., Albanese, A., Fergus, S., et al. Psychoparmacol. (Berl). 214(3), 593-602 (2011).

James, D., Adams, R.D., Spears, R., et al. Emerg. Med. J. 28(8), 686-689 (2011).





3-Methylethcathinone (hydrochloride) 11222







4-Methylethcathinone (hydrochloride) 9001069

[1266688-86-1] 4-methyl-N-ethyl Cathinone, 4-MEC

MF: C₁₂H₁₇NO • HCl **FW:** 227.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A cathinone derivative identified in several designer drugs that are sold as "legal high" replacements for controlled stimulants such as methamphetamine and MDMA; intended for use as a standard for the forensic analysis of samples that may contain this compound

5 mg 10 mg



11489

4-Methyl-α-ethylaminobutiophenone

(hydrochloride) [18268-19-4]

MF: C₁₃H₁₉NO • HCl FW: 241.8 Purity: ≥98% A crystalline solid **Stability:** ≥1 year at -20°C Summary: A para-methyl analog of buphedrone with an ethyl group replacing

methyl at the alpha position; intended for forensic and research applications



2-Methylmethcathinone (hydrochloride) 11223

[1246815-51-9] 2-MeMC MF: C₁₁H₁₅NO • HCl FW: 213.7 Purity: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential major impurity in the preparation of 4-MMC; may be marketed as a designer drug; intended for forensic and research applications



3-Methylmethcathinone (hydrochloride) 11224

[1246816-62-5] 3-MeMC **MF:** C₁₁H₁₅NO • HCl **FW:** 213.7 **Purity:** ≥97%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potential major impurity in preparations of 4-MMC; may be marketed as a designer drug; intended for forensic and research applications





[1189726-22-4] 4-Methylephedrone, 4-MeMC

MF: C₁₁H₁₅NO • HCl **FW:** 213.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A designer drug of the phenethylamine class that shares substantial structural similarities with methcathinone and methamphetamine; intended to be used to facilitate the identification of 4-MMC in complex mixtures





[186028-80-8] M1, bk-MDMA, 3,4-Methylenedioxy-N-methylcathinone **MF:** C₁₁H₁₃NO₃ • HCl **FW:** 243.1 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A designer drug that is structurally similar to MDMA, differing by having a β -keto group; detected in products marketed as bath salts, plant food, and tablets



2-Methyl-a-pyrrolidinobutiophenone (hydrochloride)

9001188

2-Me-a-PBP. 2-MePBP

MF: C₁₅H₂₁NO • HCl **FW:** 267.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An isomer of 4-Me-α-PBP, having the methyl group attached at the 2 position of the phenyl ring, instead of the 4 position; intended for forensic and research applications

5 mg 10 mg 50 mg



3-Methyl-a-pyrrolidinobutiophenone (hydrochloride)

9001189

3-Me-a-PBP, 3-MePBP

MF: C₁₅H₂₁NO • HCl **FW:** 267.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An isomer of 4-MBPB, having the methyl group attached at the 3 position of the phenyl ring, instead of the 4 position; intended for forensic and research applications

5 mg 10 mg 50 mg

5 mg

10 mg 50 mg



4-Methyl-α-pyrrolidinobutiophenone (hydrochloride)

9001190

[1214-15-9] F 1938, 4-Me-a-PBP, 4-MePBP **MF:** C₁₅H₂₁NO • HCl **FW:** 267.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic cathinone with psychoactive properties which has recently been identified in party pills and powders; intended for forensic and research applications



10 mg

50 mg





4'-Methyl-a-pyrrolidinohexanophenone (hvdrochloride)

4'-Me-α-PHP. 4'-MePHP

MF: C₁₇H₂₅NO • HCl **FW:** 295.9 **Purity:** ≥98%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: An α -PPP derivative, homologous to MPPP; assumed to be a psychostimulant; intended to be used for forensic purposes

5 mg 10 mg 50 mg

10801



2-Methyl-a-pyrrolidinopropiophenone

(hydrochloride)

2-Me-α-PPP, 2-MePPP **MF:** C₁₄H₁₉NO • HCl **FW:** 253.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥1 year at -20°C

Summary: Shares structural features with the stimulant α -PPP and is a positional isomer of 4-MeMPPP, which has been detected in bath salts and other formulations; this product is intended to be used for forensic and research applications

5 mg 10 mg 50 mg

3-Methyl-a-pyrrolidinopropiophenone

(hydrochloride)

3-Me-α-PPP, 3-MePPP

MF: C₁₄H₁₉NO • HCl **FW:** 253.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A structural isomer of 4'Me- α -PPP, having the methyl group at the 3 position, rather than the 4 position, of the phenyl group; intended for forensic and research applications

5 mg 10 mg 50 mg

4'-Methyl-α-pyrrolidinopropiophenone

(hydrochloride)

[1313393-58-6] 4' Me-a-PPP, 4'-MePPP

MF: C₁₄H₁₉NO • HCl **FW**: 253.8 **Purity**: ≥97%

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: A cathinone that shares structural features with the stimulant α -PPP; intended to be used for forensic applications

5 mg 10 mg 50 mg



• HCI

59 Cathinones



11485

10446

Naphyrone (hydrochloride)

[850352-11-3] Naphpyrovalerone, β-Naphyrone, NRG-1, O-2482 **MF:** C₁₉H₂₃NO • HCl **FW:** 317.9 **Purity:** ≥97% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An analog of pyrovalerone that is characterized by the substitution of the methylphenyl group of pyrovalerone with a naphthyl group; potently inhibits dopamine, serotonin, and norepinephrine transporters (IC₅₀ = 20, 33, and 136 nM, respectively); intended for forensic and research purposes



Naphyrone 1-naphthyl isomer (hydrochloride) 11240

MF: C₁₉H₂₃NO • HCl **FW:** 317.9 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

1 mg

5 mg

10 mg

Summary: A structural isomer of naphyrone, having the napthyl group attached at the 1, rather than 2, position; intended for forensic and research applications





Pentedrone (hydrochloride)

[879669-95-1] α -methylamino-Valerophenone

MF: C₁₂H₁₇NO • HCl **FW**: 227.7 **Purity**: ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted cathinone that is structurally similar to methcathinone



Pentylone (hydrochloride)

[17763-01-8]

MF: C₁₃H₁₇NO₃ • HCl **FW:** 271.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A cathione derivative abused as a central nervous system stimulant; for the forensic analysis of samples that may contain this compound



2,3-Pentylone isomer (hydrochloride)

MF: C₁₃H₁₇NO₃ • HCl **FW:** 271.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A structural isomer of pentylone, having the methylenedioxy group attached at carbons 2 and 3 of the terminal phenyl group; intended for forensic and research applications









[3563-49-3] Centroton, Thymergix, Valerophenone

MF: C₁₆H₂₃NO **FW:** 245.4 **Purity:** ≥95%

A solution in methanol **Stability:** ≥1 year at -20°C

Summary: An inhibitor of the transporters for certain monoamine neurotransmitters, including dopamine and norepinephrine, preventing their uptake; for use in the forensic analysis of samples that may contain this compound



Pyrovalerone (hydrochloride)

[1147-62-2] Centroton, Thymergix, Valerophenone MF: C₁₆H₂₃NO • HCl FW: 281.8 Purity: ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An inhibitor of the transporters for certain monoamine neurotransmitters, including dopamine and norepinephrine, preventing their uptake; for use in the forensic analysis of samples that may contain this compound



α -Pyrrolidinobutiophenone (hydrochloride) 9001195

[13415-54-8] α-PBP **MF:** C₁₄H₁₉NO • HCl **FW:** 253.8 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic cathinone/butyrophenone that has potential for abuse; intended for forensic and research applications



11011

11463

5 mg



α -Pyrrolidinopentiophenone (hydrochloride) 9001083

[5485-65-4] O-2387, α-PVP, 2-(1-pyrrolidinyl)-Valerophenone MF: C₁₅H₂₁NO • HCl FW: 267.8 Purity: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An analog of pyrovalerone, lacking only the methyl group that is found on the phenyl moiety of pyrovalerone; expected to be a psychoactive stimulant; intended for forensic applications



α-Pyrrolidinopropiophenone (hydrochloride) 10445

[92040-10-3] α*-PPP*

MF: C₁₃H₁₇NO • HCl **FW:** 239.7 **Purity:** ≥97%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An analog of the appetite suppressant diethylcathinone related to the designer drug MPPP; metabolized to a variety of products, including cathinone; intended to be used for forensic applications

HCI





10817

10836

2-AI (hydrochloride)

[2338-18-3] 2-Aminoindane, SU 8629

MF: C₀H₁₁N • HCl **FW:** 169.7 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An aminoindane that serves as the starting point for the synthesis of psychoactive compounds, such as 5,6-methylenedioxy-2-aminoindane; has modest analgesic and stimulatory properties; intended for forensic applications



5-IAI (hydrochloride)

5-iodo-2-Aminoindan

5 mg

10 ma

50 mg

MF: C₉H₁₀IN • HCl **FW:** 295.6 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychoactive analog of p-iodoamphetamine that is indistinguishable, in its physiological effects, from MDMA in rats; significantly reduces both serotonin uptake sites and hippocampal serotonin levels in rats; intended for forensic applications



MDAI (hydrochloride)

[155344-90-4] 5,6-Methylenedioxy-2-aminoindane **MF:** C₁₀H₁₁NO₂ • HCl **FW:** 213.7 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C Summary: An indane analog of MDA; produces significant serotonin neurotoxicity

when given with dopaminergic agents; intended for forensic purposes





11048

11035

9001102

11735

11888

Phenethylamines

2C-C (hydrochloride)

[88441-15-0]



A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A member of a family of 2,5-dimethoxy-phenethylamines, substituted on the 4-position of the aromatic ring with chlorine; potently alters monoamine re-uptake





2C-D (hydrochloride)

[25505-65-1]

MF: C₁₁H₁₇NO₂ • HCl **FW:** 231.7 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A member of a family of 2,5-dimethoxy-phenethylamines, substituted on the 4-position of the aromatic ring with a methyl group; weakly alters monoamine re-uptake

5 mg 10 mg 50 mg



2C-E (hydrochloride)

[923013-67-6] 2,5-Dimethoxy-4-ethylphenethylamine **MF**: C₁₂H₁₀NO₂ • HCl **FW**: 245.7 **Purity**: ≥95% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent monoamine oxidase inhibitor, blocking the uptake of serotonin and norepinephrine (IC50 values of 72 and 89 µM, respectively), but not dopamine; intended for forensic applications

5 mg 10 mg 50 mg



2C-H (hydrochloride)

[3166-74-3] **MF:** C₁₀H₁₅NO₂ • HCl **FW:** 217.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: Described formally as 2,5-dimethoxyphenethylamine; has little effect on serotonin receptors; intended for research and forensic applications

5 mg 10 ma 50 mg



2C-I (hydrochloride)

[64584-32-3]

MF: C₁₀H₁₄INO₂ • HCl **FW**: 343.6 **Purity**: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A monoamine oxidase inhibitor, blocking the uptake of serotonin and norepinephrine (IC50 values of 79 and 37 µM, respectively), but not dopamine; intended for forensic applications

5 mg 10 mg 50 mg



10395

11889



[868738-44-7]

MF: C₁₃H₂₁NO₂S • HCl **FW:** 291.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A member of a family of 2,5-dimethoxy-phenethylamines, substituted on the 4-position of the aromatic ring with an isopropylthio group

5 mg

10 mg 50 ma



25I-NBOMe

[1043868-97-8]

MF: C₁₈H₂₂INO₃ • HCl **FW:** 463.7 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A derivative of the phenethylamine hallucinogen 2C-I that acts as a highly potent agonist for the human 5-HT_{2A} receptor ($K_i = 0.044$ nM)

1 mg 5 mg

10 mg



9001128

Piperazines

1,4-Dibenzylpiperazine (hydrochloride) 11206

[2298-55-7] DBZP

MF: C₁₈H₂₂N₂ • 2HCl FW: 339.3 Purity: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A common impurity produced as a reaction byproduct during the synthesis of BZP; intended for forensic applications



2-DPMP (hydrochloride)

[5807-81-8] Desoxypipradrol, 2-Diphenylmethylpiperidine

MF: C₁₈H₂₁N • HCl FW: 287.8 Purity: ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: Structurally related to pipradrol and methylphenidate (Ritalin), which are psychostimulatory piperadines that inhibit monoamine transporters; identified in recreational drugs; intended for research and forensic applications

1-(m-Trifluoromethylphenyl) piperazine

(hydrochloride) [76835-14-8] TFMPP

MF: C₁₁H₁₃F₃N₂ • 2HCl **FW:** 303.2 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An entactogenic drug which selectively promotes the release of serotonin; in combination with BZP, increases both serotonin and dopamine, mirroring the effects of MDMA; has been identified in party pills and powders and is intended for forensic applications



11481



1-(4-Fluorobenzyl) piperazine (hydrochloride) 11112

MF: $C_{11}H_{15}FN_2 \bullet 2HCl$ **FW:** 267.2 **Purity:** $\ge 98\%$ A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted benzylpiperazine with a potential for abuse; intended for forensic and research applications



1-(p-Fluorophenyl) piperazine (hydrochloride) 11204

[64090-19-3] pFPP, NSC 149515 **MF:** $C_{10}H_{13}FN_2 \bullet 2HCl$ **FW:** 253.1 **Purity:** $\ge 98\%$ A crystalline solid **Stability:** ≥2 years at -20°C Summary: A substituted phenylpiperazine with a potential for abuse; intended for forensic and research applications

10 mg 50 mg 100 mg

Phenylpiperazine (hydrochloride)

11203

[4004-95-9] NSC 38914, NSC 150847

MF: C₁₀H₁₄N₂ • 2HCl **FW:** 235.2 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C Summary: The base compound from which bioactive drugs, such as the entactogen meta-chlorophenylpiperazine, are derived; intended for forensic applications



10 mg

50 mg

100 mg

11205

Terpenoids

Meconin

[569-31-3] NSC 35547, Opianyl **MF:** $C_{10}H_{10}O_4$ **FW:** 194.2 **Purity:** $\ge 95\%$ A crystalline solid **Stability:** ≥2 years at -20°C Summary: A noscapine metabolite used to detect illicit opiates in urine samples; intended for use as a forensic standard





Meconin-da

NSC 35547-d₃, Opianyl-d₃

MF: $C_{10}H_7D_3O_4$ FW: 197.2 Chemical Purity: $\ge 98\%$

Deuterium Incorporation: \geq 99% deuterated forms (d₁-d₃); \leq 1% d₀

A crystalline solid **Stability:** ≥ 2 years at -20° C

Summary: An internal standard for the quantification of meconin by GC- or LC-MS

1 mg 5 mg 10 mg



Salvinorin A

[83729-01-5] Divinorin A

MF: C₂₃H₂₈O₈ **FW:** 432.5 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent, selective K opioid receptor agonist with potential for recreational abuse; it is intended for forensic and research applications

5 mg 10 mg 50 mg 100 mg



Salvinorin B

[92545-30-7] Divinorin B

MF: C₂₁H₂₆O₇ **FW:** 390.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: The major deacetylated metabolite of Salvinorin A, a potent, selective κ opioid receptor agonist with potential for recreational abuse; though it lacks pharmacological activity, alkoxymethyl ether derivatives have been designed to develop selective κ opioid receptor antagonists or partial agonists with potential research utility in the treatment of depression and the study of κ opioid receptor signaling

5 mg 10 mg 50 mg 100 mg



9001141

9001140

11487

Tryptamines

5-methoxy AMT

[1137-04-8] 5-MeO AMT

MF: C₁₂H₁₆N₂O **FW:** 204.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A potent psychoactive analog of 5-methoxy DiPT and AMT that inhibits re-uptake (IC₅₀s = 0.18, 2.9, and 3.37 μ M) and stimulates release (EC₅₀s = 1.5, 460, and 8.9 μ M) of dopamine, serotonin, and norepinephrine, respectively from rat brain synaptosomes

5 mg

10 mg 25 mg



5-methoxy DALT

[928822-98-4] N,N-Diallyl-5-Methoxytryptamine

MF: C₁₇H₂₂N₂O **FW:** 270.4 **Purity:** ≥95% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A tryptamine derivative with psychoactive effects used as a component in

'bath salts'; intended as an analytical standard for the forensic analysis of samples that may contain this compound



DiPT

5 mg

10 mg

25 mg

5 mg

10 mg 25 mg

[14780-24-6] N,N-Diisopropyltryptamine

MF: C₁₆H₂₄N₂ **FW:** 244.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: An uncommonly abused psychedelic drug related to 5-MeO DiPT; intended for forensic and research applications



4-hydroxy DiPT (hydrochloride)

[63065-90-7] 4-OH DiPT

MF: C₁₆H₂₄N₂O • HCl **FW:** 296.8 **Purity:** ≥95%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic tryptamine derivative with structural and functional similarities to psilocin; intended for forensic and research applications



5-methoxy DiPT

[4021-34-5] 5-methoxy-N,N-Diisopropyltryptamine, FOXY, 5-MeO DiPT

MF: C₁₇H₂₆N₂O **FW:** 274.4 **Purity:** ≥98% A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A tryptamine-type designer drug with pronounced psychoactive and physiological effects; inhibits the re-uptake of monoamines (IC₅₀ = 0.65, 2.2, and 8.2 µM for dopamine, serotonin, and norepinephrine, respectively) while not affecting their release; intended for forensic applications



4-methoxy DMI

5 mg

10 mg

25 mg

[3965-97-7] 4-methoxy-N,N-Dimethyltryptamine, 4-MeO DMT **MF:** $C_{13}H_{18}N_2O$ **FW:** 218.3 **Purity:** $\ge 98\%$

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A substituted form of DMT that binds 5-HT receptors with comparable affinity (pA2 = 6.17 for 4-methoxy DMT vs. 6.00 for DMT); also has behavior disruption activity in rats that is similar to that of DMT; intended for forensic and research applications



[1019-45-0] 5-methoxy-N,N-Dimethyltryptamine, 5-MeO DMT

MF: $C_{13}H_{18}N_2O$ **FW:** 218.3 **Purity:** $\ge 98\%$ A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A naturally-occurring hallucinogenic indolealkylamine that potently activates serotonin receptors; inactivated by monoamine oxidases; intended for forensic applications



DPT (hydrochloride)

5 mg

10 mg

25 mg

[16382-06-2] N,N-Dipropyltryptamine **MF:** C₁₆H₂₄N₂ • HCl **FW:** 280.8 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychedelic drug of the tryptamine class; inhibits the re-uptake of dopamine, serotonin, and norepinephrine (IC₅₀ = 23, 2.9, and 9.1 μ M); intended for forensic and research applications



4-hydroxy MET

[77872-41-4] 4-OH MET, Metocin

MF: C₁₃H₁₈N₂O **FW:** 218.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychoactive synthetic tryptamine with structural and functional similarities to psilocin; intended for forensic and research applications



11135 α -Methyltryptamine (hydrochloride)

MF: $C_{11}H_{14}N_2 \bullet HCl$ **FW:** 210.7 **Purity:** $\ge 98\%$

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychedelic drug that is scheduled in the United States; potently stimulates the release of monoamines from synaptosomes and inhibits their re-uptake (IC₅₀s = 0.73, 0.38, and 0.4 μ M for dopamine, serotonin, and norepinephrine, respectively); intended for forensic uses



4-hydroxy MiPT

[77872-43-6] 4-OH MiPT

MF: C₁₄H₂₀N₂O **FW:** 232.3 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A synthetic tryptamine derivative with structural and functional similarities to psilocin; intended for forensic and research applications



5-methoxy MiPT

11482

11552

11148

[96096-55-8] 5-MeO MiPT

MF: C₁₅H₂₂N₂O **FW:** 246.4 **Purity:** ≥98%

A crystalline solid **Stability:** ≥2 years at -20°C

Summary: A psychedelic tryptamine which potently inhibits the re-uptake of the monoamines serotonin and norepinephrine (IC₅₀s = 6.4 and 2.6 μ M, respectively), but does not affect dopamine re-uptake; intended for forensic and research applications





[879-36-7] Indopan, α-MT

5 mg

10 mg

25 mg

9000895

11551

11865



10729

11550

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