Forensic Technology
CENTER OF EXCELLENCE
A program of the National Institute of Justice

Published May 2022

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Disclaimer: The FTCoE, led by RTI International, is supported through a Cooperative Agreement with the NIJ (2016-MU-BX-K110), Office of Justice Programs, U.S. Department of Justice. Neither the U.S. Department of Justice nor any of its components operate, control, are responsible for, or necessarily endorse, this technical note.

TECHNICAL NOTE

Currently Applied Naming Conventions for Various Subclassifications of Novel Psychoactive Substances

Purpose

This document outlines recommended naming conventions for several popular novel psychoactive substances (NPS) subclassifications; however, it is not all-inclusive. NPS classes are broken down into commonly encountered subclassifications,[1, 2] which are defined by core structural features. Example figures and the currently used or existing naming conventions are included for each.

Disclaimer: Further evaluation to develop recommended naming conventions is on-going.

Scope

The National Institute of Justice (NIJ), in partnership with its Forensic Technology Center of Excellence (FTCoE; 2016-MU-DX-K110) at RTI International and the Center for Disease Control and Prevention, convened a virtual Medicolegal Death Investigation Data Exchange Working Group (MDI-Data-WG) over 12 months, beginning in September 2020. The MDI-Data-WG was formed to advance forensic science and ensure communication between medical examiners and coroners (ME/Cs), death investigators, forensic scientists, and other stakeholders. An MDI-Data-WG subcommittee focused on methods of capturing and disseminating information on the types of drugs involved in deaths, including drug taxonomy and other categorizations and classification needs concerning drug naming, drug terms, drug mappings, and drug classification. The goal is to disseminate information to all relevant stakeholders to facilitate information

exchange of data related to drug overdose mortality. The work of the MDI-Data-WG resulted in a final report published by NIJ's FTCoE and the Centers for Disease Control and Prevention that included guidance on moving toward consistency, data standards, and best practices for improving the process of handling novel psychoactive substances. The efforts of this working group resulted in various user case profiles, presentations, implementation forums, further research, and process mapping and evaluations of the various processes. This document is part of the final report.

1. Synthetic Cannabinoids

a. Introduction: Synthetic cannabinoids (SCs) can be broken down into core, tail, linker, and head (or linked) groups, which help define structure and naming convention.[3]

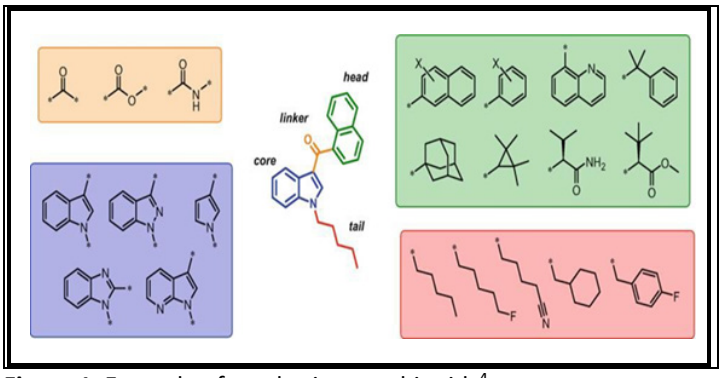

Figure 1. Example of synthetic cannabinoids[4]

b. Naphthoylindoles, Naphthoylindazoles, Naphthoylcarbazoles, Naphthylmethylindoles, Naphthylmethylindazoles, and Naphthylmethylcarbazoles

i. Definition: Contains head naphthyl moiety (red) accompanied by either core indole, indazole, carbazole, or methyl version moiety (blue)

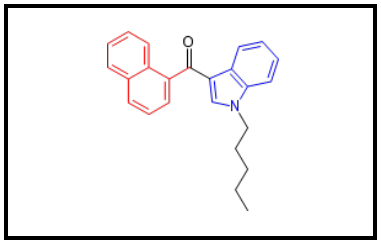

Figure 2. JWH-018

ii. Examples: JWH-018 (Figure 2), JWH-122, AM-2201, THJ-2201, MAM-2201, WIN55,212

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

c. Phenylacetylindoles and Phenylacetylindazoles

i. Definition: Contains head/linker phenylacetyl moiety (red) accompanied by either core indole or indazole moiety (blue)

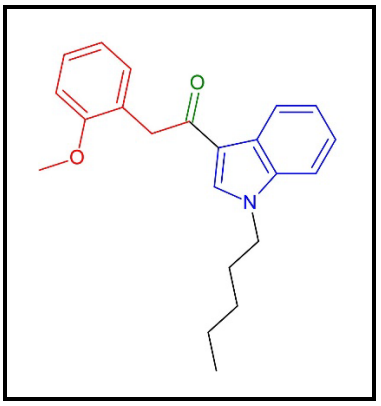

Figure 3. JWH-250

ii. Examples: JWH-250 (Figure 3), RCS-8

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

d. Cyclohexylphenols

i. Definition: Contains core cyclohexylphenol moiety (red) accompanied by a lipophilic tail moiety (blue)

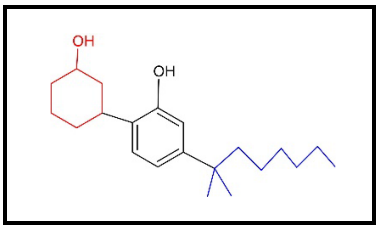

Figure 4. CP 47,497

ii. Examples: CP 47,497 (Figure 4); CP 55,490

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

e. Benzoylindoles and Benzoylindazoles

i. Definition: Contains head/linker benzoyl moiety (red) accompanied by either core indole or indazole moiety (blue)

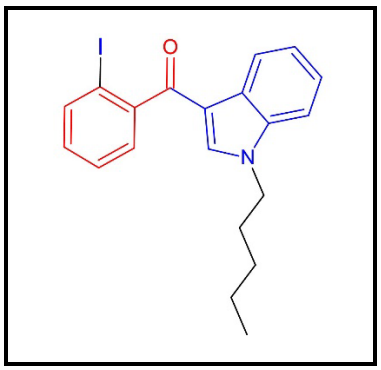

Figure 5. AM-679

ii. Examples: AM-679 (Figure 5), Pravadoline (WIN 48,098), RCS-4

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

f. Tetramethylcyclopropanoylindoles and Tetramethylcyclopropanoylindazoles

i. Definition: Contains head/linker tetramethylcyclopropanoyl moiety (red) accompanied by either core indole or indazole moiety (blue)

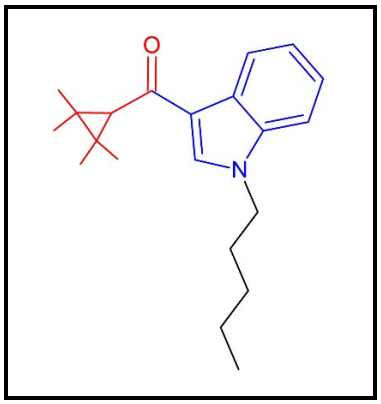

Figure 6. UR-144

ii. Examples: UR-144 (Figure 6), XLR-11, FUB-144

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

g. Adamantoylindoles, Adamantoylindazoles, Adamantylindole carboxamides, and Adamantylindazole carboxamides

i. Definition: Contains head adamantyl moiety (red) accompanied by either indole or indazole moiety (blue) with amide or ester linker (green)

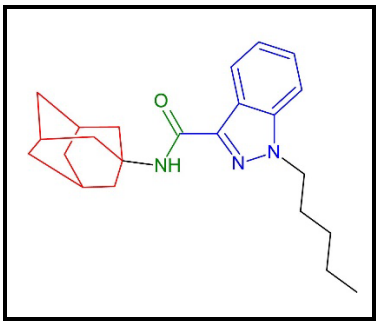

Figure 7. APINACA (AKB48)

ii. Examples: APINACA (AKB48) (Figure 7), APICA

iii. Naming Convention: Modified Uchiyama (Alpha-numeric sequence)

h. Quinolinylindolecarboxylates, Quinolinylindazolecarboxylates, Quinolinylindolecarboxamides, and Quinolinylindazolecarboxamides

i. Definition: Contains head quinolinyl or isoquinolinyl moiety (red) accompanied by core indole or indazole moiety (blue) with amide or ester linker (green)

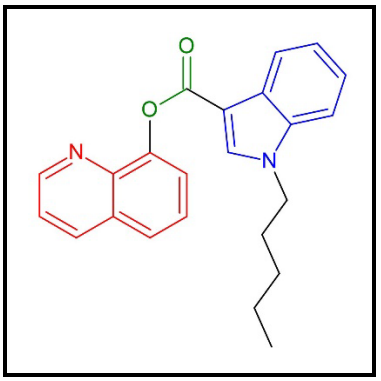

Figure 8. PB-22

ii. Example: PB-22 (Figure 8), THJ-2201

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

i. Naphthylindolecarboxylates, Naphthylindazolecarboxylates, Naphthylindole carboxamides, and Naphthylindazole carboxamides

i. Definition: Contains head naphthyl moiety (red) accompanied by either core indole or indazole (blue) with amide or ester linker (green)

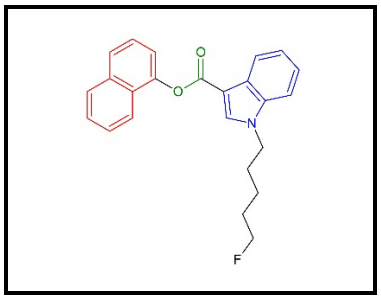

Figure 9. NM-2201

ii. Examples: NM-2201 (Figure 9), SDB-005, FDU-PB-22, NNEI, MN-18

iii. Naming Convention: Historical SC Convention (XX-### based on inventor)

j. Alkylcarbonyl indole carboxamides, Alkylcarbonyl indazole carboxamides, Alkylcarbonyl indole carboxylates, and Alkylcarbonyl indazole carboxylates

i. Definition: Contains head alkylcarbonyl moiety (red) accompanied by either core indole or indazole (blue) with amide or ester linker (green)[5]

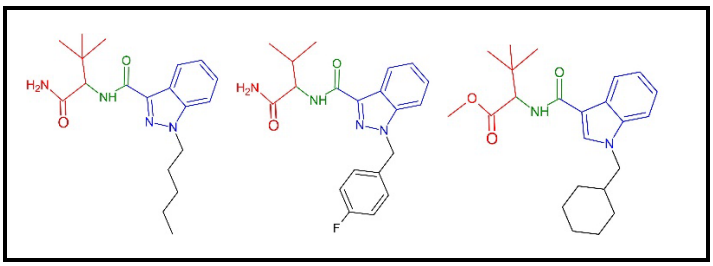

Figure 10. ADB-PINACA (left), AB-FUBINACA (center), MDMB-CHMICA (right)[5]

ii. Examples: AB-PINACA, ADB-PINACA (Figure 10, left); AB-FUBINACA (Figure 10, center), ADB-FUBINACA, AB-CHMINACA, MMB-FUBINACA (FUB-AMB), MDMB-FUBINACA,MDMB-CHMICA (Figure 10, right), PX-1, PX-2, 5F-MDMB-PINACA (5F-ADB)

iii. Naming Convention: Modified Uchiyama (Alpha-numeric sequence)

k. Cumylindolecarboxamides and Cumylindazolecarboxamides

i. Definition: Contains head N-(2-phenylpropan-2-yl) moiety (red) accompanied by either core indole, indazole, or other (blue) with amide or ester linker (green)

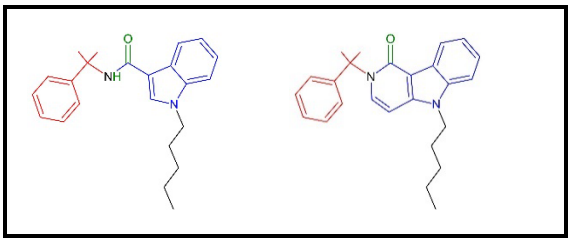

Figure 11. CUMYL-PICA (left), CUMYL-PeGACLONE (right)

ii. Examples: CUMYL-PICA (Figure 11, left), 4CN-CUMYL-BINACA, CUMYL-PeGACLONE (Figure 11, right)

iii. Naming Convention: Modified Uchiyama (Alpha-numeric sequence)

l. Oxindole Hydrazides

i. Definition: Contains head alkylcarbonyl moiety (red) accompanied by a core 2-oxindole (blue) and hydrazide linker (green)

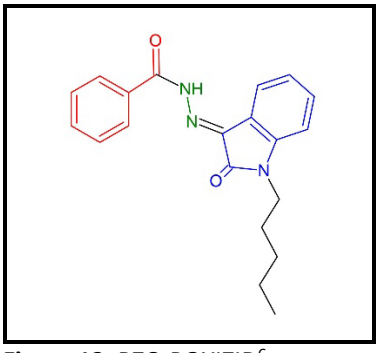

Figure 12. BZO-POXIZID[6]

ii. Examples: BZO-POXIZID (Figure 12), BZO-HEXOXIZID, 5F-BZO-POXIZID

iii. Naming Convention: Modified Uchiyama (Alpha-numeric sequence)

m. Several new subclasses of synthetic cannabinoids are emerging and were not included here; further discussion and review of these subclasses is needed.

2. Stimulants & Hallucinogens:

a. Simple Substituted phenethylamines

i. Definition: Contains phenethylamine core structure (in red) but with no substitutions on the α or β carbon; the amine may or may not have an alkyl group or groups

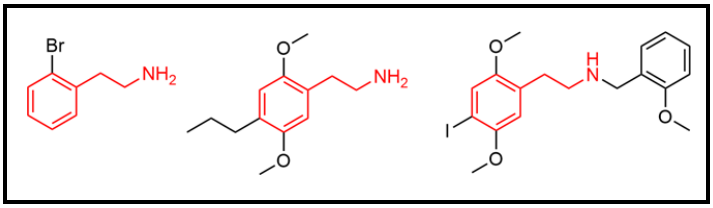

Figure 13. 2-bromophenethylamine (left), 2C-P (center), and 25I-NBOMe (right)

ii. Examples: 2-bromophenethylamine (Figure 13, left), 2C-P (Figure 13, center), and 25I-NBOMe (Figure 13, right)

iii. Naming Conventions: Varied depending on specific substitution patterns

- For example, if the core is specifically substituted with 2,5-dimethoxy groups, the "2C-X" convention is used (based on the work of Dr. Alexander Shulgin)
- If the phenethylamine is also further substituted with an ortho- methoxybenzyl moiety on the amine, the "25X-NBOMe" system is used
- Other substitution-specific naming conventions exist

b. Simple Substituted Amphetamines

i. Definition: Contains the phenethylamine core structure and an alkyl substitution on the α, but no β carbonyl (in red); the amine may or may not have an alkyl group or groups

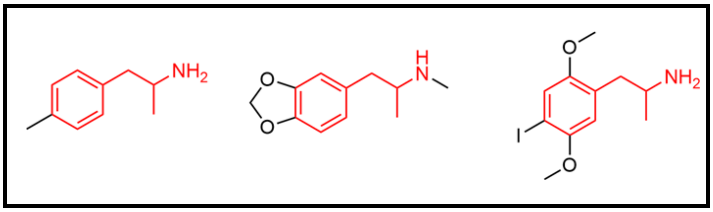

Figure 14. 4-Methylamphetamine (left), 3,4-MDMA (center), and DOI (right)

ii. Examples: 4-Methylamphetamine (Figure 14, left), 3,4-MDMA (Figure 14, center), and DOI (Figure 14, right)

iii. Naming Conventions: Varied depending on specific substitution patterns

- Sometimes names are spelled out and sometimes common acronymsare used ("methylenedioxymethamphetamine" is abbreviated to "MDMA")
- One example of a naming convention used for a site-specific core substitution is the "DOX" naming system that is used for amphetamines with a 2,5-dimethoxy substitution on the aryl ring where X is a letter describing the 4-position substituent

c. Substituted Cathinones

i. Definition: Contains the phenethylamine core structure, at least one-carbon- chain off the α carbon, and a β carbonyl (in red); the amine may or may nothave an alkyl group or groups

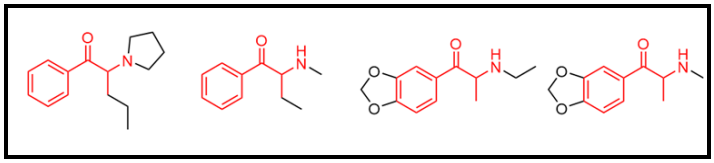

Figure 15. α-Pyrrolidinovalerophenone (far left), Buphedrone (center left), bk-MDEA (center right), and Methylone (far right)

ii. Examples: α-Pyrrolidinovalerophenone (Figure 15 far left), Buphedrone (Figure 15, center left), bk-MDEA (Figure 15, center right), and Methylone (Figure 15, far right)

iii. Naming Conventions: Varied depending on specific substitution patterns

- Sometimes names are spelled out and sometimes common acronyms are used ("pyrrolidinovalerophenone" is abbreviated to "PVP")
- Some cathinones are named as "beta-keto" ("bk") versions of their corresponding amphetamines as in bk-MDEA (where MDEA stands formethylenedioxyethamphetamine)

- Many cathinones can have a name with the suffix of “drone” or “ylone”as well; the “ylones” have a methylenedioxy ring fused to the aryl ring and the “drones” do not

d. Substituted Tryptamines

i. Definition: Contains tryptamine core structure (red); the amine may or may not have an alkyl group or groups

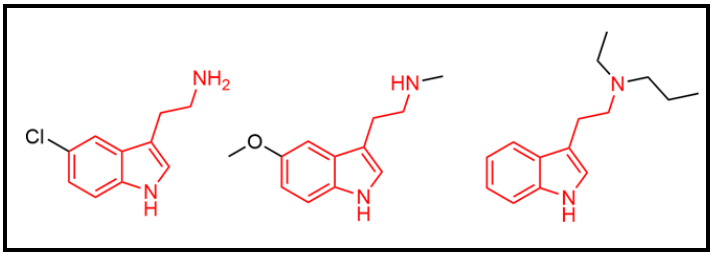

Figure 16. 5-Chloro Tryptamine (left), 5-Methoxy NMT (center), and EPT (right)

ii. Examples: 5-Chloro Tryptamine (Figure 16, left), 5-Methoxy NMT (Figure 16, center), and EPT (Figure 16, right)

iii. Naming Convention: Letter code acronyms are often used to abbreviate substituents; for example, “N-Methyl Tryptamine” is abbreviated to “NMT” and “*N*-Ethyl-*N*-Propyl Tryptamine” is abbreviated to EPT

e. Lysergamides

i. Definition: Contains core structure similar to LSD

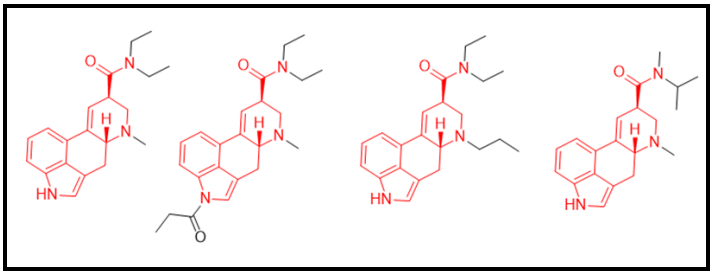

Figure 17. LSD (left), 1P-LSD (center left), PRO-LAD (center right), and MIPLA (right)

ii. Examples: LSD (Figure 17, left), 1P-LSD (Figure 17, center left), PRO-LAD (Figure 17, center right), and MIPLA (Figure 17, right)

iii. Naming Convention: Letter code acronyms are often used to abbreviate substituents to the core

- “LSD” is widely known to stand for “Lysergic acid diethylamide” (also abbreviated “LAD”); modifications to LSD where the indole nitrogen issubstitution have a designation before the letters “LSD” as in “1P-LSD”, where “P” represents “Propionyl”
- Other typical points of modification are at the other nitrogen atoms; letter code acronyms are used to designate the modifications using “LAD” instead of “LSD”; “PRO-LAD” indicates that a propyl (“PRO”) substitution has made to the typical methyl moiety on the piperidine nitrogen
- The letters MIP in “MIPLA” stand for the “methyl” and “isopropyl” alkyl groups that replace the prototypical diethyl substitution

f. Substituted Arylcyclohexylamines

i. Definition: Contains arylcyclohexylamine core structure (red); there may or may not be a ketone in the 2-position on cyclohexane ring

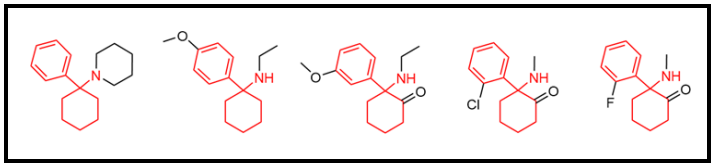

Figure 18. PCP (left), 4-MeO-PCE (center left), Methoxetamine (center),Ketamine (center right), and 2F-Deschloroketamine (right)

ii. Examples: PCP (Figure 18, left), 4-MeO-PCE (Figure 18, center left), Methoxetamine (Figure 18, center), Ketamine (Figure 18, center right), and 2F-Deschloroketamine (Figure 18, right)

iii. Naming Conventions: Varied

- “PCP” is an acronym of ”phenyl cyclohexyl piperidine,” but it is alsoknown as phencyclidine
- Analogues with a ketone in the 2-postion on the cyclohexane are oftennamed with ”2-oxo” before the ”PCP” designation
- The change from ”PCP” to the ”PCE” acronym represents the swapping ofthe piperidine ring to an *N*-ethyl group

- Many of these compounds have multiple synonyms, for example, “Methoxetamine” is also known as “MXE” and “3-MeO-2'-oxo-PCE”
- Because Phencyclidine and Ketamine are well-known names, manyanalogues are named as derivatives of those drugs as in ”2F-Deschloroketamine” whose name denotes that the prototypical chlorinewas replaced with a fluorine

3. Opioids

a. Fentanyl Derivatives

i. Definition: Contain core structure similar to fentanyl

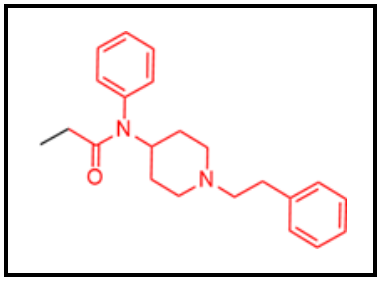

Figure 20. Fentanyl

ii. Examples: Acetylfentanyl, Carfentanil, para-Fluoroisobutyrylfentanyl

iii. Naming Convention: Scheme developed by Cayman Chemicals

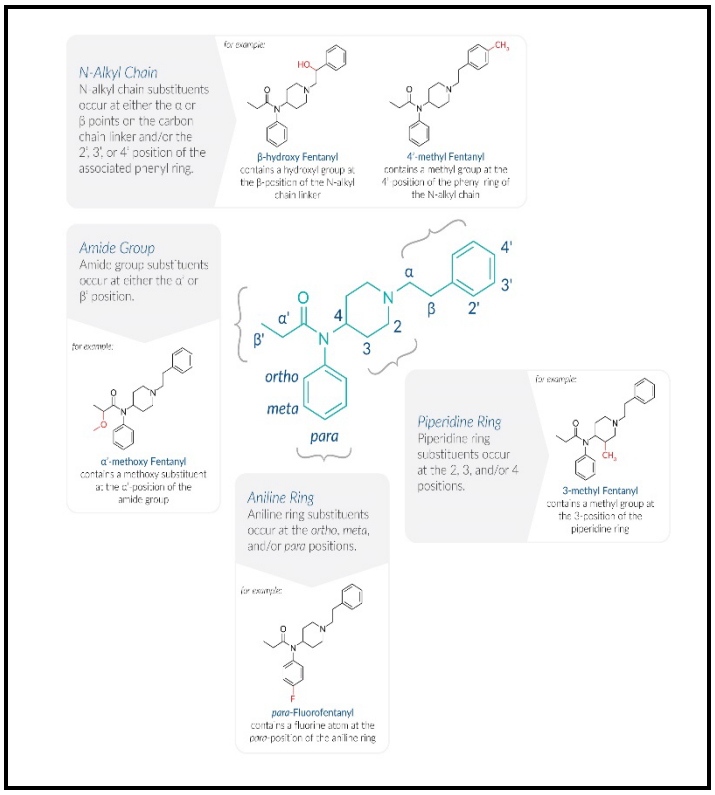

Figure 21. Naming convention developed by Cayman Chemical for fentanyl analogues[7]

b. U-Series Derivatives

i. Definition: Contains cyclohexylamino group and benzyl or phenyl group connected by an amide

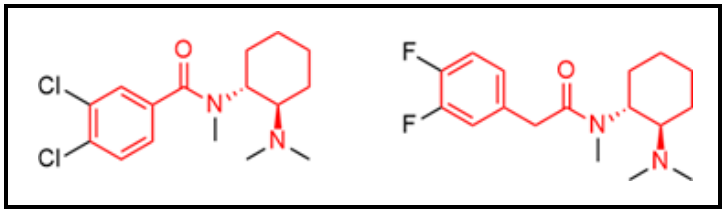

Figure 22. U-47700 (left), Difluoro U-48800 (right)

ii. Examples: U-47700 (Figure 22, left), U-49900, N-ethyl U-47700, Napthyl U-47700, Difluoro U-48800 (Figure 22, right)

iii. Naming Convention: Historical convention (XX-###) based on inventor OR names developed for recreational use/sale; new modifications are named based on U-47700 or others

c. Benzimidazoles (Nitazenes)

i. Definition: Contains benzimidazole core (with or without nitro group),substituted benzyl group, and substituted ethylamino group

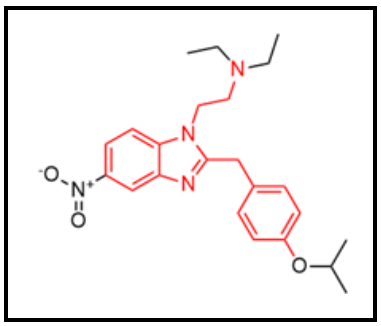

Figure 23. Isotonitazene

ii. Examples: Etonitazene, Isotonitazene (Figure 23), Metonitazene, Clonitazene, Etodesnitazene, 5-Amino isotonitazene, 4'-Hydroxy nitazene, N-pyrrolidinoetonitazene

iii. Naming Convention: Named based on structural modifications in relation to "etonitazene"

d. Benzimidazolones

i. Definition: Contains benzimidazolone, piperidine, and benzyl group

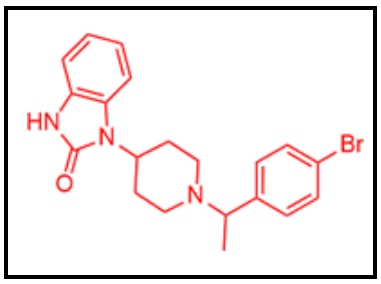

Figure 24. Brorphine

ii. Examples: Brorphine (Figure 24)

iii. Naming Convention: Named based on structural modifications in relation to "brorphine"

e. Cinnamylpiperazines (AP Series)

i. Definition: Contains cinnamylpiperazine and alkylcarbonyl

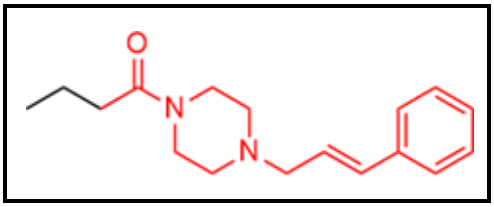

Figure 25. AP-237

ii. Examples: AP-237 (Figure 25), 2-Methyl AP-237, AP-238, para-Methyl AP-237

iii. Naming Convention: Historical convention (XX-###) based on inventor OR names developed for recreational use/sale; new modifications are namedbased on AP-237 or others

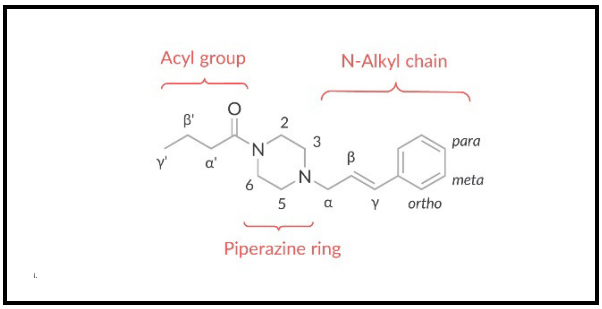

Figure 26. Naming convention developed by Cayman Chemical for AP-237 analogues.[8]

f. Thiambutenes

i. Definition: Substituted (RS)-4,4-dithiophen-2-yl-but-3-en-2-amine

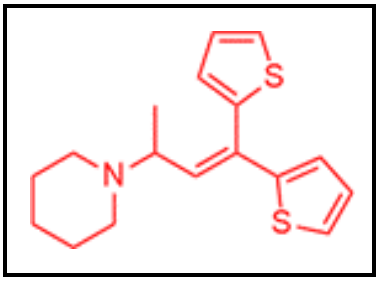

Figure 27. Piperidylthiambutene

ii. Examples: Piperidylthiambutene (Figure 27)

iii. Naming Convention: Named based on structural modifications in relation to "thiambutene"

g. MTs

i. Definition: 1-substituted-4-(1,2-diphenylethyl)piperazine derivatives

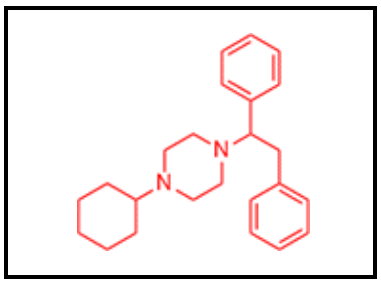

Figure 28. MT-45

ii. Example: MT-45 (Figure 28)

iii. Naming Convention: Named based on structural modifications in relation to "MT-45"

h. Viminols

i. Definition: Based on the core of viminol – 1-[1-[(2-Chlorophenyl)methyl]pyrrol-2-yl]-2-[di(butan-2-yl)amino]ethanol

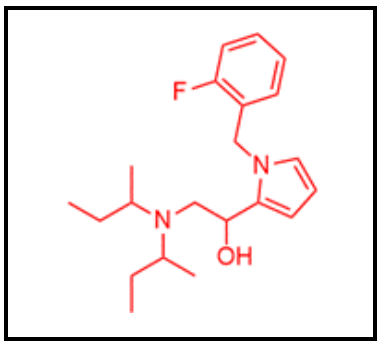

Figure 29. 2F-Viminol

ii. Example: 2F-Viminol (Figure 29)

iii. Naming Convention: Named based on structural modifications in relation to "viminol"

i. Bromadol

i. Definition: Arylcyclohexylamine containing benzyl group and phenethyl group

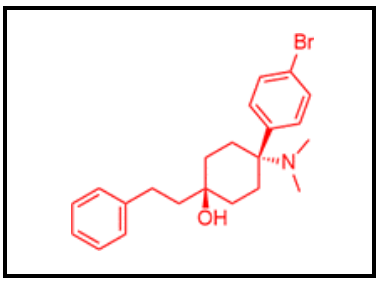

Figure 30. Bromadol

ii. Example: Bromadol (Figure 30)

iii. Naming Convention: Named based on structural modifications in relation to "bromadol"

4. Benzodiazepines

a. 2-Keto

i. Definition: Contains carbonyl in position 2 of the benzodiazepine ring

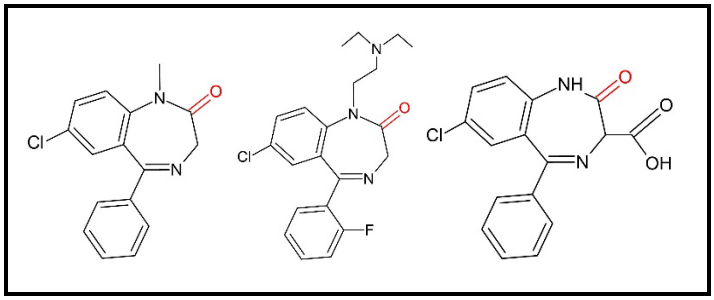

Figure 31. Diazepam (left), Flurazepam (middle), Clorazepate (right)

ii. Examples: Diazepam (Figure 31, left), Flurazepam (Figure 31, center), Clorazepate (Figure 31, right), Halazepam, Prazepam, Chlordiazepoxide

iii. Naming Convention: Historical nomenclature, ending with the suffix "azepam"

b. 3-Hydroxy

i. Definition: Contains a hydroxy group in the third position

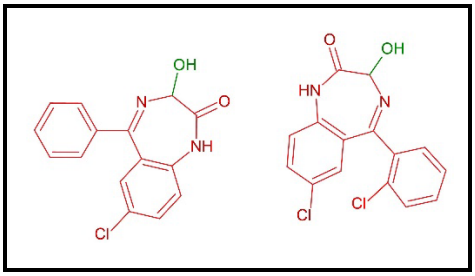

Figure 32. Oxazepam (left), Lorazepam (right)

ii. Examples: Oxazepam (Figure 32, left), Lorazepam (Figure 32, right), 3-Hydroxyphenazepam, Lormetazepam, Temazepam

iii. Naming Convention: Historical nomenclature, ending with the suffix "azepam" like 2-keto benzodiazepines but name modified based on added group

c. 7-Nitro / 8-Nitro

i. Definition: Contain a nitro group in the 7 or 8 position

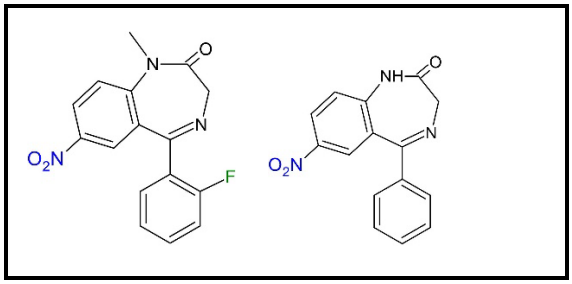

Figure 33. Flunitrazepam (left), Nitrazepam (right)

ii. Examples: Flunitrazepam (Figure 33, left), Nitrazepam (Figure 33, right), Nimetazepam, Clonazepam

iii. Naming Convention: Historical nomenclature, can end in "azepam" or "azolam," may contain "nitr" within the name to signify the nitro group

d. Triazolo

i. Triazolo ring added to positions 1 and 2

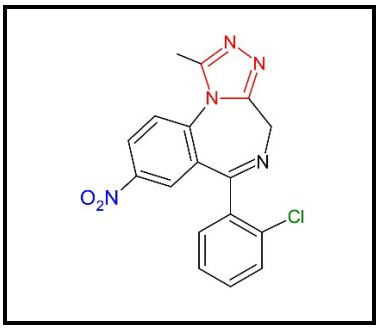

Figure 34. Clonazolam

ii. Examples: Clonazolam (Figure 34), Alprazolam, Adinazolam, Flubromazolam, Estazolam, Triazolam

iii. Naming Convention: Historical nomenclature, ending with the suffix "azolam"

e. Imidazo

i. Definition: Contains a five-membered ring with only 2 nitrogens

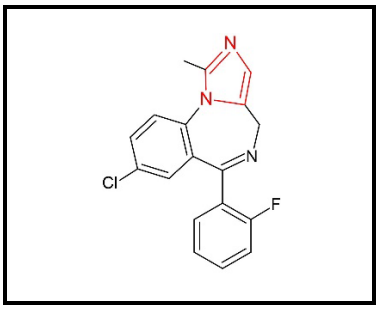

Figure 35. Midazolam

ii. Examples: Midazolam (Figure 35), Imidazenil, Flumazenil, Bretazenil, Climazolam, Loprazolam

iii. Naming Convention: Historical nomenclature, ending with the suffix "azolam" or"azenil"

f. 1,5-Benzodiazepines

i. Definition: Contains two nitrogen atoms at positions 1 and 5 in a seven-membered diazepine ring fused to a benzene ring; they are 2,3-benzo-fused derivatives of the dihydrodiazepines

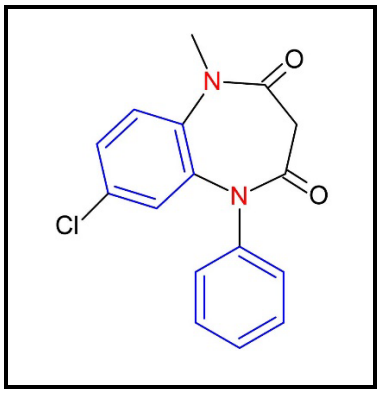

Figure 36. Clobazam

ii. Examples: Clobazam (Figure 36), Arfendazam, Lofendazam, CP-1414S

iii. Naming Convention: Historical nomenclature, ending with the suffix "azam"

g. Thienodiazepine

i. Definition: Contain a thiophene ring fused to the diazepine ring

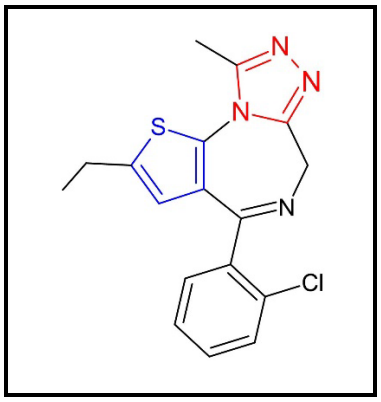

Figure 37. Etizolam

ii. Examples: Etizolam (Figure 37), Deschloroetizolam, Brotizolam, Metizolam, Fluclotizolam

iii. Naming Convention: Historical nomenclature, usually ending in "azolam" due to addition of triazole ring, usually contains "tiz" within the name to signify the thiophene ring

5. Others

a. Additional NPS subclassifications will be added as the document is further revised.

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Suggested Citation

Krotulski, A. J., Iula, D. M., & Winokur, A. D. (2021, November). *Currently applied naming conventions for various subclassifications of novel psychoactive substances (NPS)*. Research Triangle Park, NC: RTI International.