

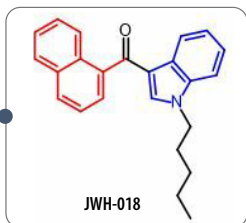
Appendix C. Drug Taxonomy: Framework for Subclassification and Naming of Novel Psychoactive Substances

This framework tool can assist forensic scientists seeking to better understand how drugs are classified by structural components. It is broken down by NPS classes (e.g., opioids) and then further subdivided by subclassifications of each NPS class (e.g., fentanyl analogs). This framework provides potential names for a substance, a figure with a drug structure from the subclass (with core components highlighted), and an example substance that fits within this subclassification. Users of this framework can easily follow this layout to understand how NPS are subclassified and how those drug molecules could be named. The framework was created to be a standalone poster to use as a reference. This alleviates scientists of the need to check multiple sources and allows for quicker association with naming convention and nomenclature. **Although this framework tool helps users understand the drug-naming process, it does not provide a means to predict and name future unknown substances by simply following this subclassification scheme and framework.**

Drug Taxonomy: Framework for Subclassification and Naming of Novel Psychoactive Substances (NPS)

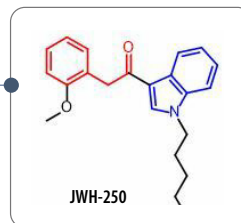
Naphthoylindoles
Naphthoylindazoles
Naphthylcarbazoles
Naphthylmethylindoles
Naphthylmethylindazoles
Naphthylmethylcarbazoles

Contain head naphthyl moiety (red) accompanied by either core indole, indazole, carbazole, or methyl moiety (blue)



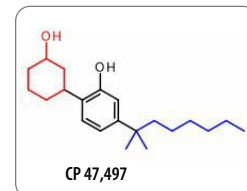
Phenylacetylindoles
Phenylacetylindazoles

Contain head/linker phenylacetyl moiety (red) accompanied by either core indole or indazole moiety (blue)



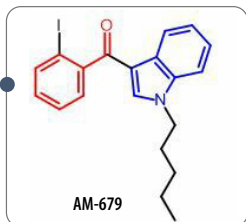
Cyclohexylphenols

Contain core cyclohexylphenol moiety (red) accompanied by a lipophilic tail moiety (blue)



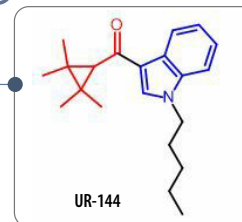
Benzoylindoles
Benzoylindazoles

Contain head/linker benzoyl moiety (red) accompanied by either core indole or indazole moiety (blue)



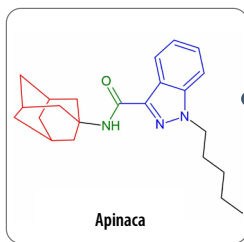
Tetramethylcyclopropanoylindoles
Tetramethylcyclopropanoylindazoles

Contain head/linker tetramethylcyclopropanoyl moiety (red) accompanied by either core indole or indazole moiety (blue)



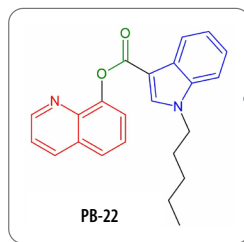
Adamantylindoles
Adamantylindazoles
Adamantylindole carboxamides
Adamantylindazole carboxamides

Contain head adamantyl moiety (red) accompanied by either core indole or indazole moiety (blue) with amide or ester linker (green)



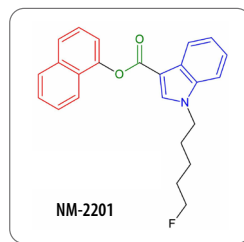
Quinolinyndolecarboxylates
Quinolinyndazolecarboxylates
Quinolinyndolecarboxamides
Quinolinyndazolecarboxamides

Contain head quinoliny or isoquinoliny moiety (red) accompanied by core indole or indazole moiety (blue) with amide or ester linker (green)



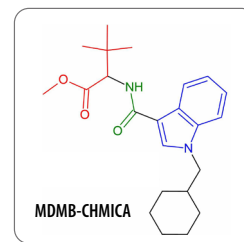
Naphthylindolecarboxylates
Naphthylindazolecarboxylates
Naphthylindole carboxamides
Naphthylindazole carboxamides

Contain head naphthyl moiety (red) accompanied by either core indole or indazole (blue) with amide or ester linker (green)



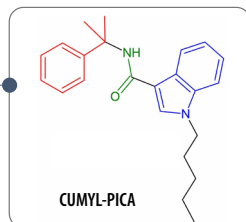
Alkylcarbonyl indole carboxamides
Alkylcarbonyl indazole carboxamides
Alkylcarbonyl indole carboxylates
Alkylcarbonyl indazole carboxylates

Contain head alkylcarbonyl moiety (red) accompanied by either core indole or indazole (blue) with amide or ester linker (green)



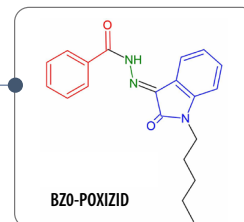
Cumylindolecarboxamides
Cumylindazolecarboxamides

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



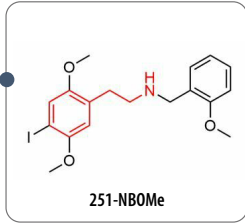
Oxidole Hydrazides

Contain head alkylcarbonyl moiety (red) accompanied by a core 2-oxindole (blue) and hydrazide linker (green)



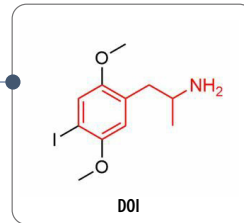
Substituted Phenethylamines

Contain the phenethylamine core structure (in red) but with no substitutions on the alpha or beta carbon; the amine may or may not have an alkyl group or groups



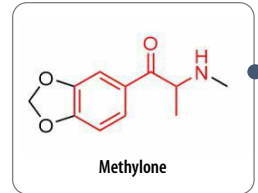
Simple Substituted Amphetamines

Contain the phenethylamine core structure and an alkyl substitution on the alpha, but no beta carbonyl (in red); the amine may or may not have an alkyl group or groups



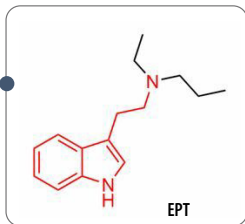
Substituted Cathinones

Contain the phenethylamine core structure, at least one carbon-chain off the alpha carbon, and a beta carbonyl (in red); the amine may or may not have an alkyl group or groups



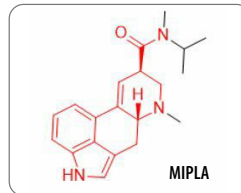
Substituted Tryptamines

Contain tryptamine core structure (red); the amine may or may not have an alkyl group or groups



Lysergamides

Contain core structure similar to LSD



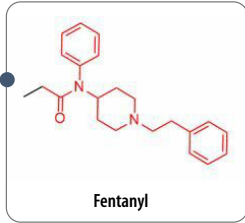
Substituted Arylcyclohexylamines

Contain arylcyclohexylamine core structure; there may or may not be a ketone in the 2-position on the cyclohexane ring



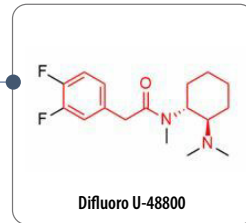
Fentanyl Derivatives

Contain core structure similar to fentanyl



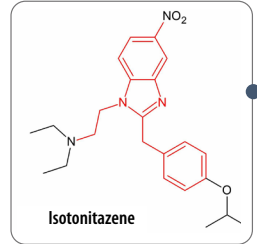
U-series Derivatives

Contain cyclohexylamino group and benzyl or phenyl group connected by an amide



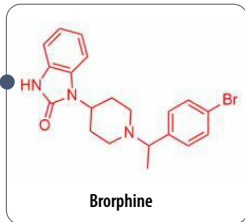
Benzimidazoles (Nitazenes)

Contain benzimidazole core (with or without nitro group), substituted benzyl group, and substituted ethylamino group



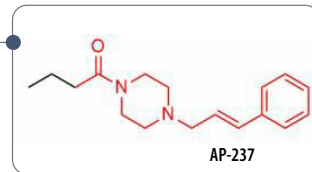
Benzimidazolones

Contain benzimidazolone, piperidine, and benzyl group



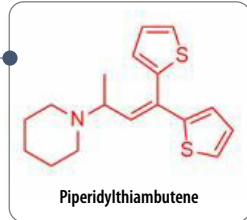
Cinnamylpiperazines (APs)

Contain cinnamylpiperazine and alkylcarbonyl



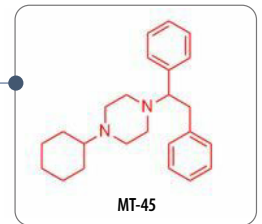
Thiambutenes

Substituted (RS)-4,4-dithiophen-2-yl-but-3-en-2-amine



Benzimidazolones

1-substituted-4-(1,2-diphenylethyl)piperazine derivatives



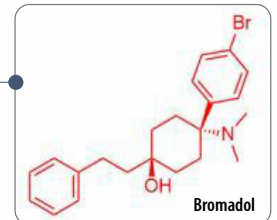
Viminols

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



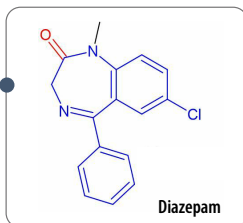
Bromadol

Arylcyclohexylamine containing benzyl group and phenethyl group

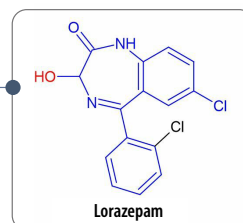


2-Keto

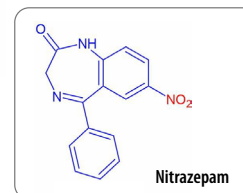
Contain a carbonyl (red) in position 2 of the benzodiazepine ring (blue)

**3-Hydroxy**

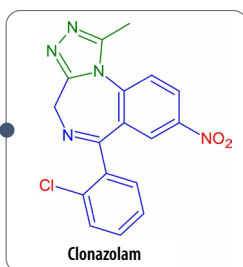
Contain a hydroxy group (red) in the third position of the benzodiazepine ring (blue)

**7-Nitro / 8-Nitro**

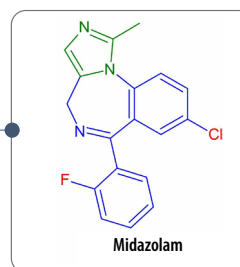
Contain a nitro group (red) in the 7 or 8 position of the benzodiazepine ring (blue)

**Triazolo**

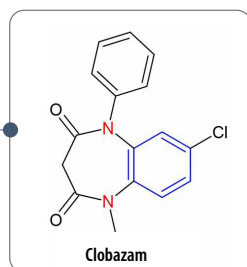
Tricyclic benzodiazepines that contain an additional fused triazole ring (green)

**Imidazo**

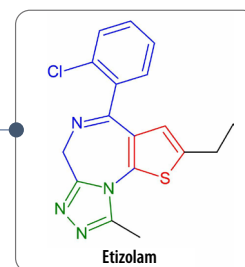
Contain a five-member ring with 2 nitrogens (imidazole group) (green)

**1,5-Benzodiazepines**

Bicyclic compounds with nitrogen atoms at 1 and 5 positions (red) in a seven-membered ring fused to a benzene (green), rather than the 1,4 positions

**Thienodiazepine**

Contains a diazepine ring (blue) fused to a thiophene ring (red) and a triazole group (green)



From Roper-Miller, Jeri, Nichole Bynum, Kelly Keyes, Erica Fornaro, and Micaela Ascolese. *Data Exchange Practices of Medicolegal Death Investigation*. Research Triangle Park, NC: RTI International, December 2022.