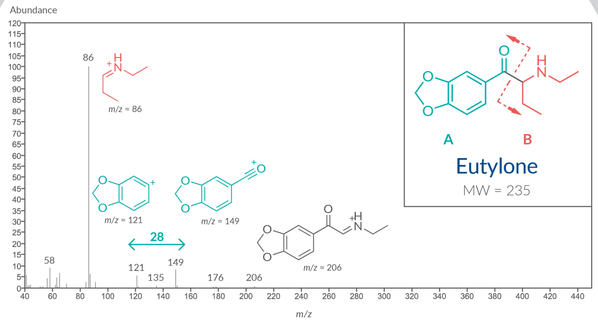
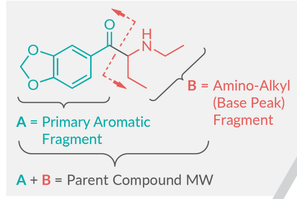
Laboratory Guide for CATHINONE Identification and Naming

Mass Spectrum of Eutylone and Tips for Interpretation



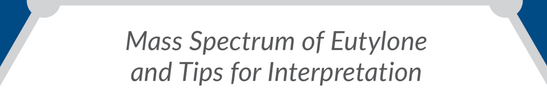
Tips for EI-MS Interpretation:

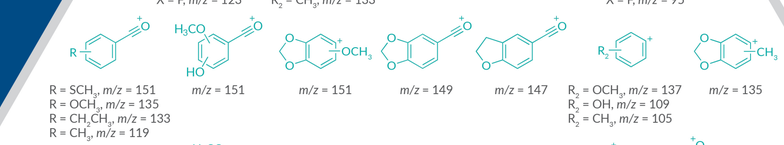
- Fragmentation often results in no molecular weight ion.
- Fragmentation occurs *via* α-cleavage to yield the primary aromatic (A) and amino-alkyl (B) fragments.
- The sum of the A and B fragments results in the parent compound molecular weight (MW).
- Base peak is always the amino-alkyl fragment (B), which may also be observed in amphetamines.
- Fragment A, the acylium ion, further cleaves to yield a subsequent fragment minus 28 (A-28), also common to amphetamines.
- IR spectroscopy and/or NMR can be used in addition to GC-MS to differentiate amphetamines from cathinones.
- Multiple positional isomers are possible for cathinones.

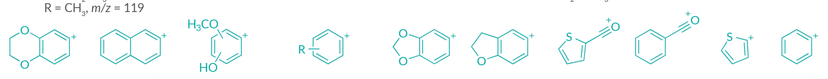


Common Mass Spec Fragments

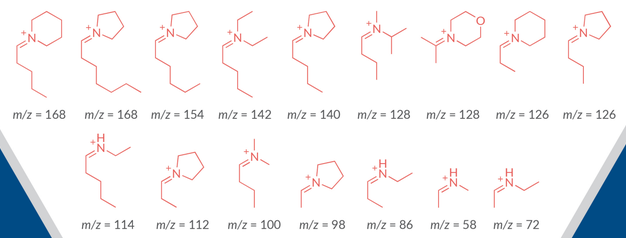
Aromatic Fragments (in descending *m/z* order)







Amino-Alkyl (Base Peak) Fragments (in descending *m/z* order)



Please note that multiple isomers can exist for all mass spec fragments.

Common Substitutions

PHENYL RING

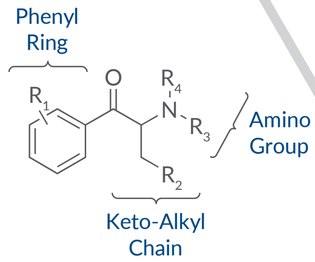
R_1 denotes hydrogen or one or more substitutions on the phenyl ring (alkoxy groups, halides, alkyl/aryl groups, etc.)

KETO-ALKYL CHAIN

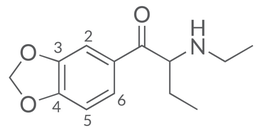
R_2 denotes hydrogen or increased carbon chain length, which can also be branched

AMINO GROUP

R_3/R_4 denotes hydrogen, alkyl groups, or a ring system



Substituted Cathinone Example: Eutylone



Eutylone

Molecular Formula: $C_{13}H_{17}NO_3$
Molecular Weight: 235.28
DEA Schedule: I

SYNONYMS

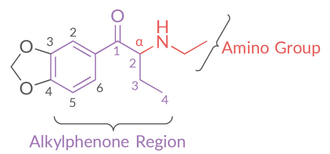
β-keto-Ethylbenzodioxolylbutanamine, 3,4-Methylenedioxy-α-Ethylaminobutiophenone, bk-EBDB, "Ethyl Butylone"

SUBSTITUTIONS

Contains a methylenedioxy on the phenyl ring; **R_2** is a methyl group, **R_3** is an ethyl group, and **R_4** is a hydrogen

Standardized Alkylphenone Naming System

- The first step in using this naming system is recognition of the alkylphenone region. Alkylphenones are named "propiophenone," "butiophenone," "pentio/valerophenone," etc. based on the keto-alkyl chain length (see **Table**).
- The α-amino group is then identified, such as "α-methylamino," "α-ethylamino," etc. The α-amino group name is positioned before the alkylphenone name in the naming order sequence. If the amine group is a ring system such as a pyrrolidine or piperidine, then "α-pyrrolidino" and "α-piperidino" are used.
- Substituents on the phenyl ring and their location designation ("4-fluoro," "3,4-methylenedioxy," etc.) are positioned at the beginning of the name.



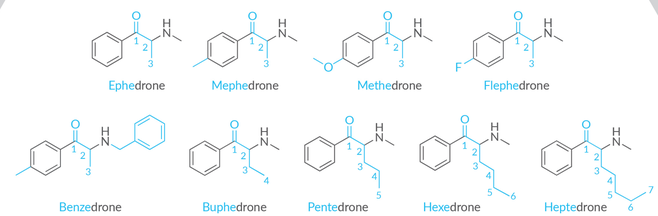
Alkylphenone Region Naming	Keto-Alkyl Chain (# of Carbons)
Propiophenone	3
Butyro/Butano/Butiophenone	4
Pentio/Valerophenone	5
Hexio/Hexanophenone	6
Heptanophenone	7
Octanophenone	8
Nonanophenone	9
Decanophenone	10

Final Naming Order Sequence: Phenyl ring substituents *then* α-amino group *then* alkylphenone region

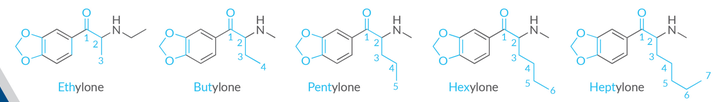
Examples: 3-fluoro-α-Ethylaminobutiophenone or 4-methyl-α-Isopropylaminovalerophenone

Other Common Naming Conventions

"drone" Naming: The suffix "drone" commonly represents a cathinone without a methylendioxy group, and the prefix typically represents the length of the alkyl chain. Please note that there are exceptions to this trend such as in the case of the first five examples below.



"ylone" Naming: The suffix "ylone" commonly represents a cathinone with a methylenedioxy group fused to the aryl ring, and the prefix typically corresponds to the length of the alkyl chain.



β-keto Naming: Some cathinones are named after their corresponding amphetamine analogs as "β-keto" (bk) versions.

Scan to download the NPS Metabolism Monograph for N-butyl Pentylone