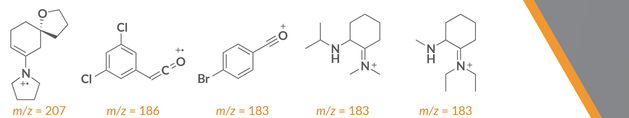
Laboratory Guide for UTOPIOID Identification, Naming, and Metabolism

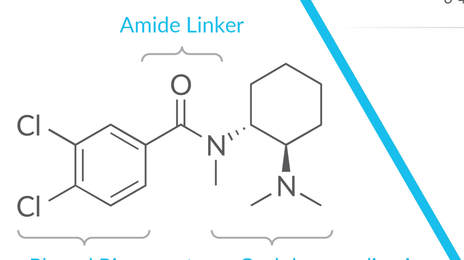
Common EI-GC-MS Utopioid Fragments



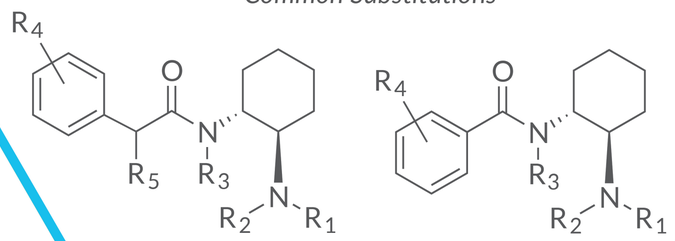
Defining Utopioids

U-type opioids, also known as U-drugs or U-compounds, and their metabolites are characterized by a *trans*-cyclohexanediamine moiety and their substituted phenyl ring, linked together by an amide carbonyl group.

Commonly detected utopioids:
U-47700, U-48800, U-49900, U-51754, 3,4-Methylenedioxy U-47700, Isopropyl U-47700



Common Substitutions

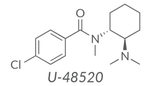


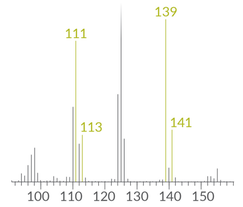
- Groups R_1-R_3 and R_5 denote cyclic or acyclic alkyl group substitutions
- R_4 denotes one or more substitutions on the phenyl ring (halides, alkoxy groups, alkyl/aryl groups, etc.)

Halogen Isotope Patterns

Monochloro

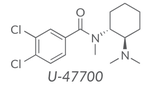
The high natural abundance of ^{37}Cl gives characteristic ions in the spectra with a 3:1 peak height ratio of M:M+2 (111/113, 139/141).

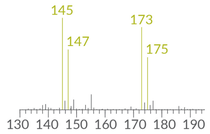




Dichloro

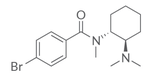
Compounds with 2 chlorines exhibit ions with a 3:2 peak height ratio of M:M+2 (145/147, 173/175).

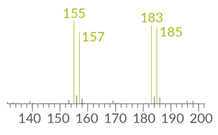




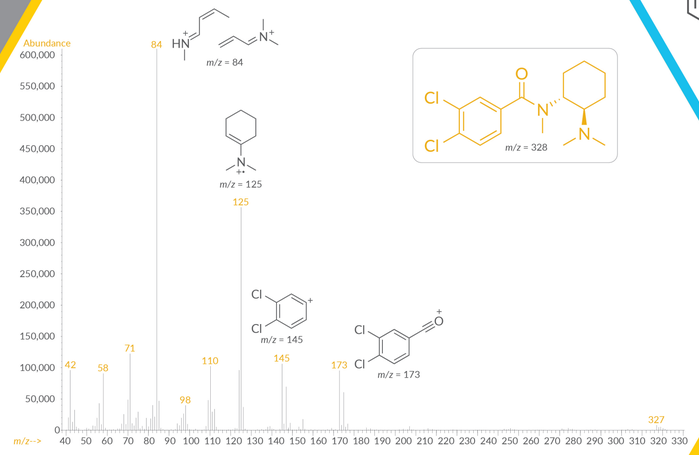
Monobromo

The high natural abundance of ^{81}Br gives characteristic ions in the spectra with a 1:1 peak height ratio of M:M+2 (155/157, 183/185).



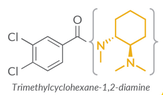


Mass Spectrum of U-47700 and Tips for Interpretation

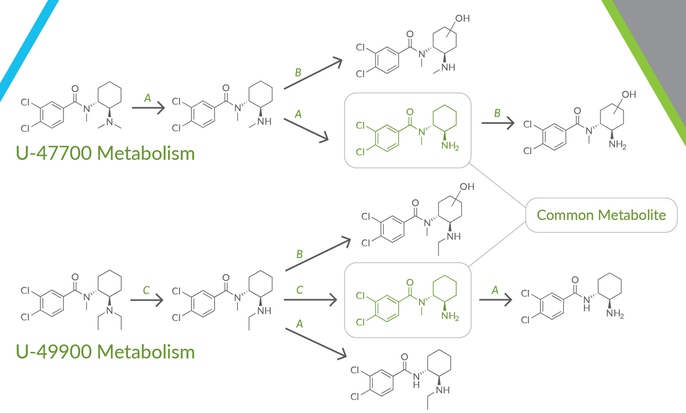


Tips for GC-MS Interpretation:

- The 84 and 125 ions are indicative of the trimethylcyclohexane-1,2-diamine moiety *(right)*
- Isotope patterns can help identify chlorine or bromine substituents on the phenyl ring
- The molecular ion (or the M-1 ion) is usually present but very minor



Utopioid Metabolism



Biotransformation Pathway:
A) N-Demethylation B) Hydroxylation C) N-Deethylation

- Utopioids can undergo dealkylation at both the amine and the amide
- Hydroxylation can occur at several positions on the cyclohexane ring
- U-47700 and U-49900 share a common metabolite, N-(2-aminocyclohexyl)-3,4-dichloro-N-methylbenzamide

References

Krotulski, A.J., Mohr, A.L.A., Papsun, D.M., *et al. Drug Test Anal.* **10(1)**, 127-136 (2018).
Fleming, S.W., Cooley, J.C., Johnson, L., *et al. J. Anal. Toxicol.* **41(3)**, 173-180 (2017).

Learn more about the need for standardized naming at **www.caymanchem.com/utopioids**