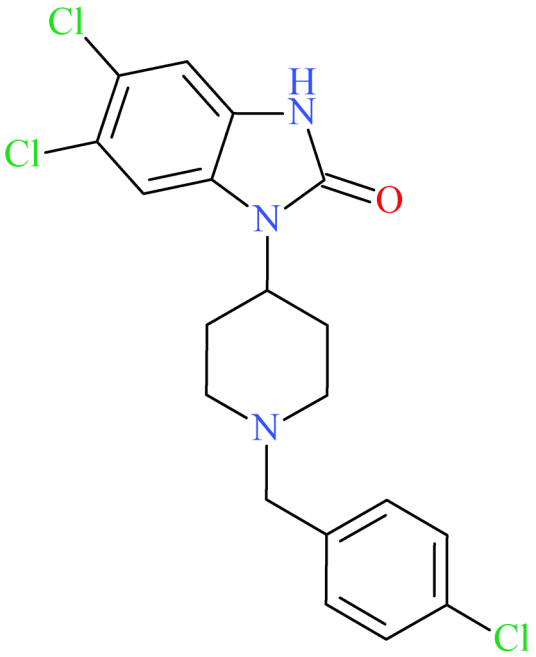
5,6-Dichloro Desmethylchlorphine



NPS SUBCLASS
Opioid
REPORT DATE
August 23, 2024
SAMPLE RECEIVED
May 8, 2024
SAMPLE TYPE
Drug Material

Preferred Name	5,6-Dichloro Desmethylchlorphine
Synonyms	SR 17018, SR-17018, 5,6-Dichlorodesmethylchlorphine
Formal Name	5,6-dichloro-3-[1-[(4-chlorophenyl)methyl]-4-piperidyl]-1H-benzimidazol-2-one
InChI Key	LAGUDYUGRSQDKS-UHFFFAOYSA-N
CAS Number	2134602-45-0
Chemical Formula	$C_{19}H_{18}Cl_3N_3O$
Molecular Weight	410.7
Molecular Ion [M⁺]	409
Exact Mass [M+H]⁺	410.0588

Characterization & Intelligence

The following information was compiled in August 2024 and is subject to change as new research is conducted and as new information becomes available:

Description: 5,6-Dichloro desmethylchlorphine is a novel synthetic opioid with structural similarity to other benzimidazolones (e.g., brorphine, chlorphine, etc.). 5,6-Dichloro desmethylchlorphine (also known as SR-17018) was first evaluated as a potential mu opioid receptor agonist via bias factor calculations in 2017.[1] 5,6-Dichloro desmethylchlorphine was first identified by our laboratory in a sample designated for recreational use in May 2024 and was confirmed in June 2024 after acquiring standard reference material.

Sample Source: Unknown (United States)

Sample Appearance: White powder

Pharmacology: 5,6-Dichloro desmethylchlorphine is described as a biased mu opioid receptor agonist with less respiratory depression compared to other opioid agonists.[1,2] 5,6-Dichloro desmethylchlorphine was determined to have similar potency to morphine with a half-life of 6-8 hours.[3]

Toxicology: 5,6-Dichloro desmethylchlorphine has not been identified in toxicology cases at the CFSRE.

Drug Materials: 5,6-Dichloro desmethylchlorphine has been detected in one drug material at the CFSRE.

Demographics / Geographics: The drug material sample containing 5,6-dichloro desmethylchlorphine for originated from the United States.

Legal Status: 5,6-Dichloro desmethylchlorphine is not currently a scheduled drug in the United States.

References:

- Cayman Chemical: 5,6-Dichloro Desmethylchlorphine
- [1]Schmid et al. (2017) Bias factor and therapeutic window correlate to predict safer opioid analgesics
- [2]Kudla et al. (2021) Comparison of an addictive potential of mu-opioid receptor agonists...
- [3]Pantouli et al. (2020) Comparison of morphine, oxycodone and the biased MOR agonist SR-17018...

About: In collaboration with medical examiner and coroner offices, crime laboratories, clinical partners, and other stakeholders, the Center for Forensic Science Research and Education (CFSRE) is documenting first confirmations of NPS through analysis of drug materials and/or toxicology samples. These reports are generated using comprehensive analytical techniques (e.g., GC-MS, LC-QTOF-MS, NMR) and include available information about the new substances identified at the time of reporting, as well as the analytical data generated during testing. Our new drug monographs are intended to assist with the rapid identification of NPS in forensic casework and related disciplines, and should not be used for confirmatory purposes alone.

Analytical Notes: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF-MS) in comparison to analysis of acquired reference material.

Acknowledgements: This report was prepared by Sara E. Walton, Max T. Denn, Alexis D. Quinter, Joshua S. DeBord, Barry K. Logan, and Alex J. Krotulski at the Center for Forensic Science Research and Education (CFSRE) at the Fredric Rieders Family Foundation. The authors acknowledge scientists at the CFSRE for their involvements and contributions. For more information, contact npsdiscovery@cfsre.org or visit www.npsdiscovery.org.

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Gas Chromatography Mass Spectrometry (GC-MS)

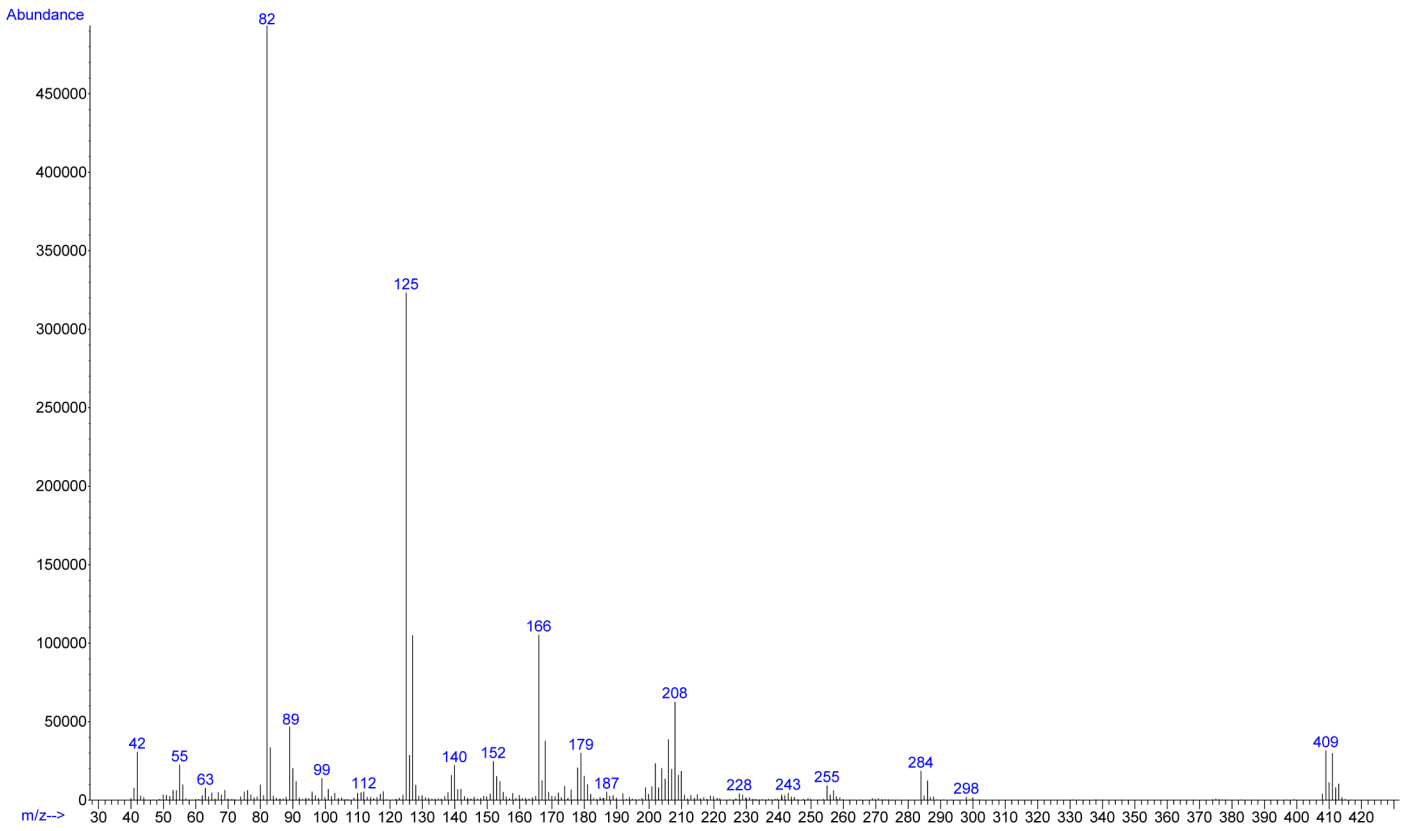
Laboratory: Center for Forensic Science Research and Education (CFSRE, Horsham, PA, USA)

Sample Preparation: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD

Methods: GC-MS Method Details & Monographs

GC-MS: Mass Spectrum (EI 70 eV)



Confirmation Using Drug Standard: *Reference material (Batch: 0579244-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 5,6-dichloro desmethylchlorphine based on retention time (sample: 9.83 min vs. standard: 9.66 min) and mass spectral data comparisons.*

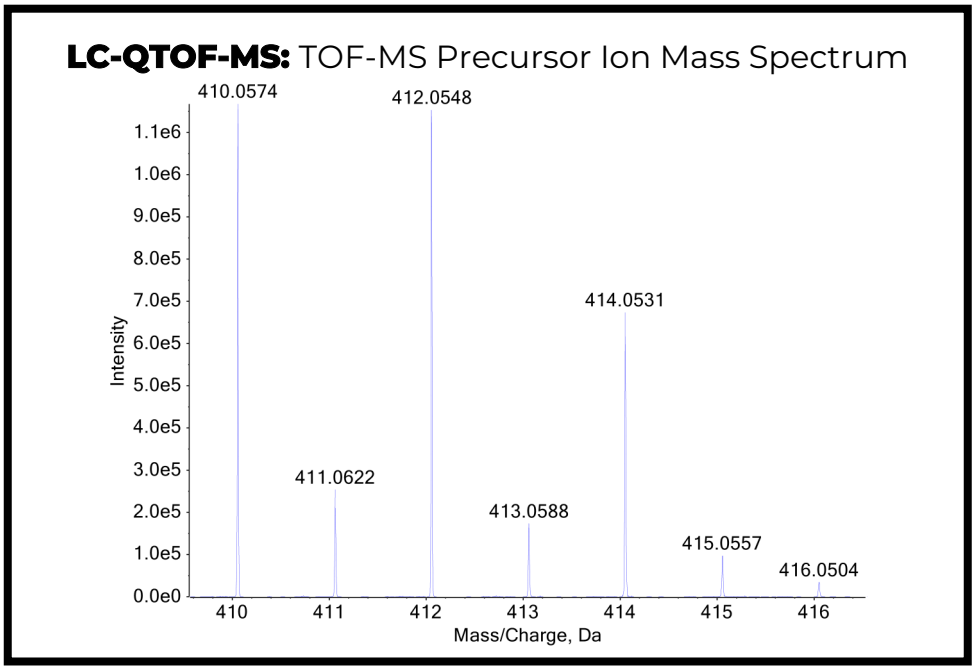
Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

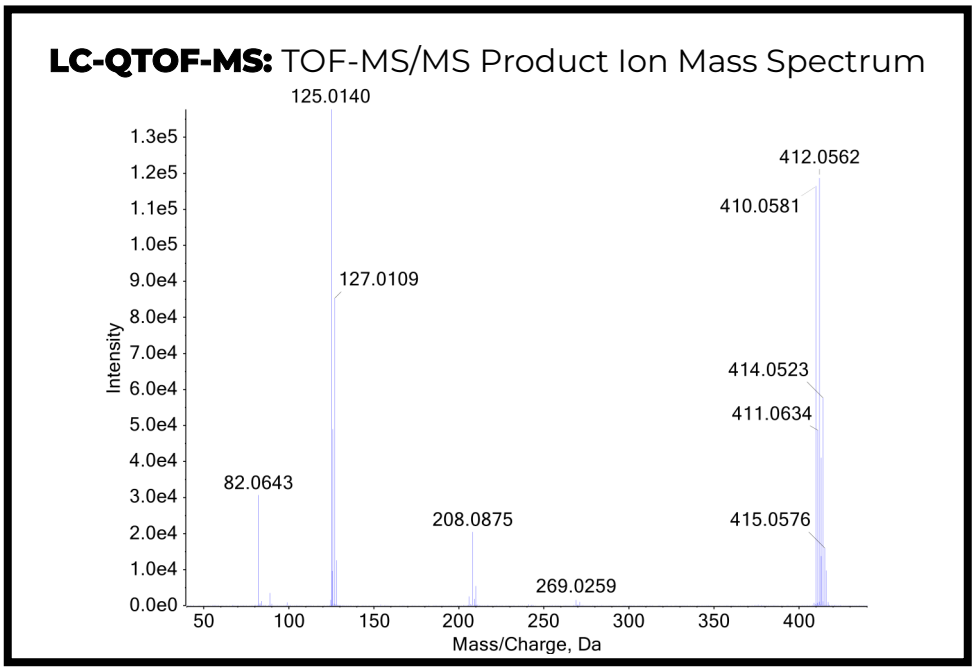
Laboratory: Center for Forensic Science Research and Education (CFSRE, Horsham, PA, USA)

Sample Preparation: Dilution in mobile phase

Instrument: Sciex 5600+ LC-QTOF-MS

Methods: LC-QTOF-MS Method Details & Monographs





Confirmation Using Drug Standard: *Reference material (Batch: 0579244-1 was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 5,6-dichloro desmethylchlorphine based on retention time (sample: 7.21 min vs. standard: 7.41 min) and mass spectral data comparisons.*