

This information was derived from drug materials experimentally and without analytical standard.
This monograph was compiled in April 2026 and is subject to revision.

Compound Information

Proposed Name: Chloro Desmethylchlorphine
(regioisomer not assigned)

Chemical Formula: C₁₉H₁₉Cl₂N₃O

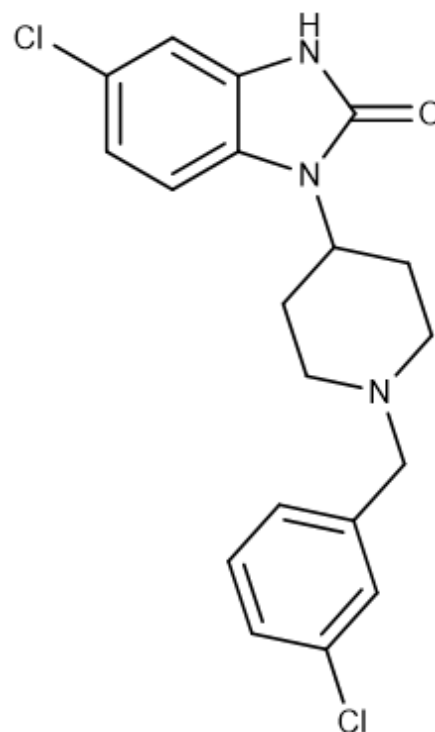
Molecular Weight: 376.28

Molecular Ion [M]⁺: 375.0905

Exact Mass [M+H]⁺: 376.0978

First detection of novel orphine analog by Substance Drug Checking was made in February 2026 in white powder drug material received from unknown location by mail. Compound detections to date have been made, primarily, in samples expected to contain **SR-17018 (5,6-dichloro Desmethylchlorphine)**.

Literature documentation of candidate regioisomers is limited to patents and key publications^{2,3}. Repeat observations prompted compound characterization for insight mobilization.



Structure of regioisomer 5-chloro-1-(1-(5-chlorobenzyl)piperidin-4-yl)-1H-benzo[d]imidazol-2(3H)-one

Proposed candidates are regioisomers of:

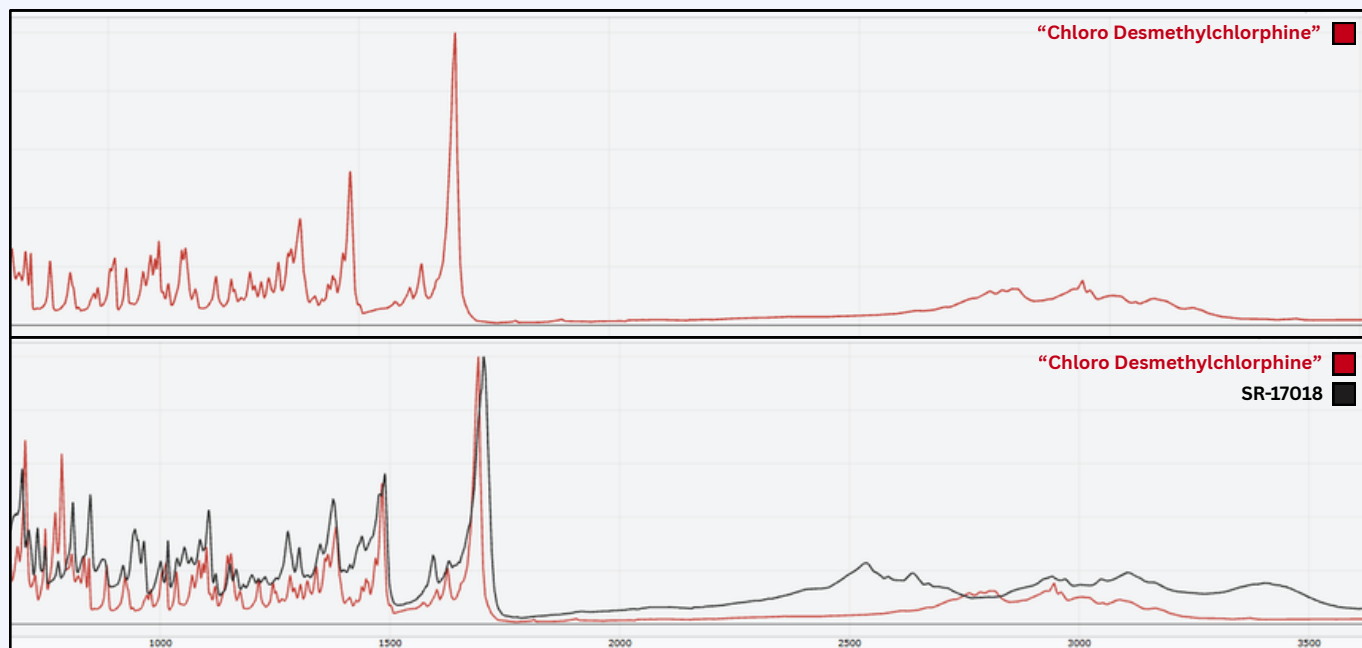
4-chloro-1-(1-(2-chlorobenzyl)piperidin-4-yl)-1H-benzo[d]imidazol-2(3H)-one; (SR-11099)^{2,3} where:

1. **One** of the 4-, 5-, 6-, 7- positions of the benzimidazole core is chlorinated **AND**
2. **One** of the 2-, 3-, 4-, 5-, 6- positions on the benzylpiperidyl moiety is chlorinated.

Literature used in Identification

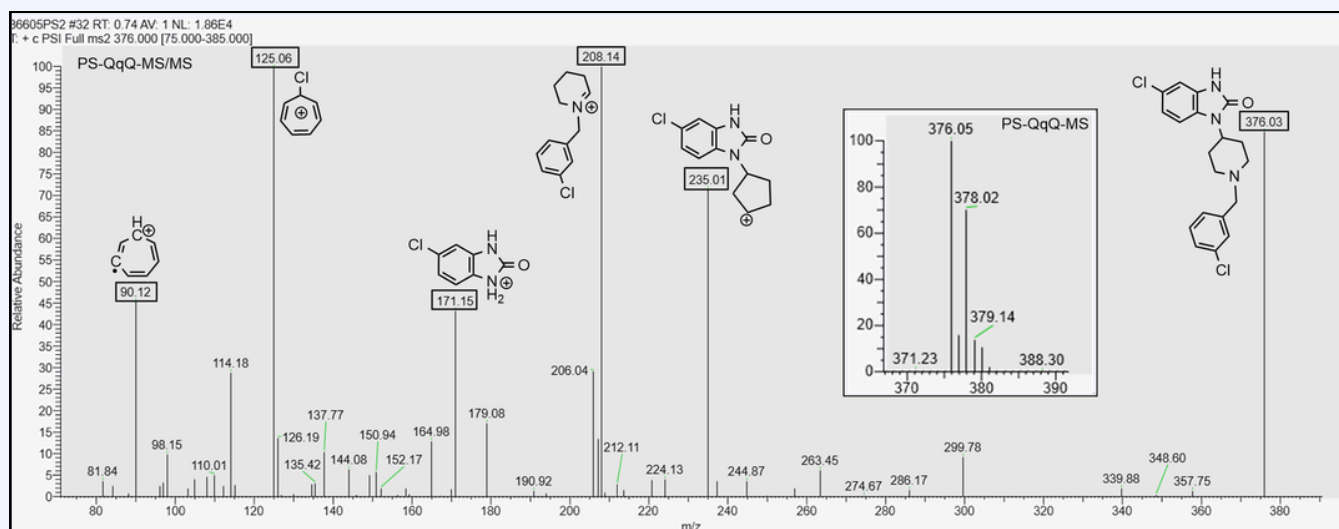
1. Grafinger, K. E.; Wilde, M.; Otte, L.; Volker Auwärter. Pharmacological and Metabolic Characterization of the Novel Synthetic Opioid Brorphine and Its Detection in Routine Casework. *Forensic Science International* 2021, 327, 110989–110989. <https://doi.org/10.1016/j.forsciint.2021.110989>.
2. Kennedy, N. M.; Schmid, C. L.; Ross, N. C.; Lovell, K. M.; Yue, Z.; Yen Ting Chen; Cameron, M. D.; Bohn, L. M.; Bannister, T. D. Optimization of a Series of Mu Opioid Receptor (MOR) Agonists with High G Protein Signaling Bias. *Journal of Medicinal Chemistry* 2018, 61 (19), 8895–8907. <https://doi.org/10.1021/acs.jmedchem.8b01136>.
3. Bannister, T. D.; Bohn, L. M.; Schmid, C. L. Benzimidazolones as Signaling-Biased MuOpioid Receptor Agonists and their Preparation. U.S. Patent 62,308,333, 2017.
4. SR-17018 (CAS 2134602-45-0). Caymanchem.com. https://www.caymanchem.com/product/24480/sr-17018?srsltid=AfmBOop9YjytJrPOF5Zyrd4mipOwqp5_Egy2EEmkmlWadV_UFq-4EWuh (accessed 2026-05-06).
5. LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS). https://www.cfsre.org/images/samples/CFSRE_NPS_Discovery_LC-QTOF-MS_Method_Details.pdf.

FTIR



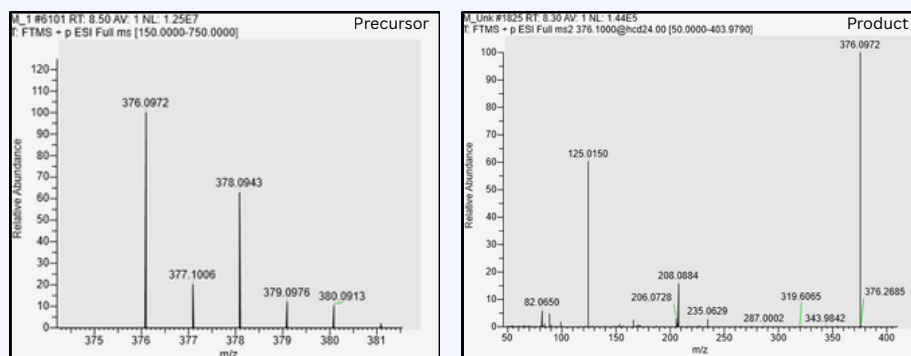
IR absorption scans of query compound (top figure) and query compound overlaid with SR-17018 spectrum (bottom figure).

PS-MS



Precursor (MS) and product ion (MS/MS) scans of query compound accompanied by proposed fragments observed. Structural elucidation was not performed to confirm exact compound and fragment structure. Characterization methods used are unable to distinguish between regioisomers.

Orbitrap LC - HRMS



Precursor (left) and product ion (right) scans of query compound.

Immunoassay



1. FYL-1S48; (20 ng/ml)
2. BZO-1S3; (300ng/ml)
3. MED-18S2; (1000ng/ml)
4. XYL-18S2; (1000ng/ml)
5. NTZ-18S26; (2000ng/ml)

Methodology

Fourier-Transform Infrared Spectroscopy

Acquisition: Agilent 4500a Series Portable FTIR with dTGS detector and single-bounce diamond ATR accessory. Spectral data was compiled over 32 scans in the 650-4000 (cm^{-1}) range with a spectral resolution of 4(cm^{-1}) and zero fill factor of 4.

Paper Spray Mass Spectrometry

Instrument:

Thermo Scientific TSQ Fortis™ triple quadrupole mass spectrometer with a VeriSpray™ paper spray ion source.

Aquisition:

Mode: Positive ion mode, $[\text{M}+\text{H}]^+$
Spray Voltage: 3800V,
Ion transfer tube temp: 300 °C
Scan Rate: 250 Da/s.

MS/MS:

Precursor: 376.0
Collision Energy Ramp: 10-30V
Scan range: m/z 75-385.

Orbitrap Liquid Chromatography-High Resolution Mass Spectrometry

Instrument:

Orbitrap Exploris™ 120 with Thermo Scientific Vanquish™ HPLC

Column:

Thermo Scientific Accucore™ aQ C18 polar endcapped column (100 x 2.1 mm, 2.6 μm pore size)

Mobile Phase:

A: HPLC Grade Water + 0.1% Formic Acid
B: HPLC Grade Acetonitrile + 0.1% Formic Acid
Flow rate: 200 $\mu\text{L}/\text{min}$

Gradient:

0 min: 20% B, 3 min: 20% B, 13 min: 65% B, 14 min: 20% B, 15 min: End

Temperatures:

Autosampler: 5 °C (sample storage temp)
Column Chamber and Precolumn Chamber: 30 °C
ESI Source: 275 °C

Targeted Aquisition Parameters:

1 μL Injection
MS²: Precursor 376.1, 120 000 resolution
HCD: (5, 15, 20, 30, 50V)
DDMS²: Full Scan 150-750, 120 000 resolution

Lateral Flow Immunoassay Strip Tests

Immunoassay strip tests were conducted on powder sample with BTNX strips in 38°C sterile water at a concentration of 1mg/ml. Results were Interpreted after 5 minutes.