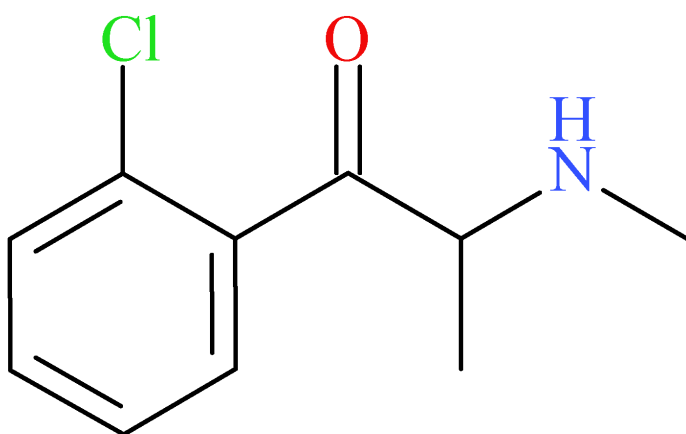


## Chloromethcathinone



*Note: The structure of 2-chloromethcathinone was used for illustrative purposes only. The exact isomer configuration was not determined based on analysis performed.*

| NPS SUBCLASS    | Stimulant       |
|-----------------|-----------------|
| REPORT DATE     | August 27, 2024 |
| SAMPLE RECEIVED | March 27, 2024  |
| SAMPLE TYPE     | Toxicology      |

|                                 |   |
|---------------------------------|---|
| Preferred Name                  | 2-Chloromethcathinone / 3-Chloromethcathinone / 4-Chloromethcathinone |
| Synonyms                        | 2-CMC, 3-CMC, 4-CMC   |
| Formal Name                     | 1-(2-chlorophenyl)-2-(methylamino)propan-1-one                        |
| InChI Key                       | UHVGPBZWPKWNT-UHFFFAOYSA-N  |
| CAS Number                      | 90869-66-2 (2-CMC), 1607439-32-6 (3-CMC), 2319878-22-1 (4-CMC)        |
| Chemical Formula                | C <sub>10</sub> H <sub>12</sub> ClNO                                  |
| Molecular Weight                | 197.7   |
| Molecular Ion [M <sup>+</sup> ] | 197   |
| Exact Mass [M+H] <sup>+</sup>   | 198.0680  |

## 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:** Chloromethcathinone (CMC) is a novel synthetic stimulant with structural similarity to methcathinone. Chloromethcathinone exists in three isomeric forms: 2-, 3-, and 4-chloromethcathinone. The position of the chlorine was not confirmed during analysis. Chloromethcathinone was first detected in March 2024 by our laboratory and was confirmed in comparison to standard reference material.

**Sample Source:** NYU Langone Health (New York City, NY)

**Sample Appearance:** Oral fluid specimen

**Pharmacology:** *In vitro* pharmacological data available for chloromethcathinone show that this substituted cathinone is an active stimulant at the dopamine, serotonin, and norepinephrine transporters with comparable potency to methyl-substituted counterparts (e.g., mephedrone or 4-MMC).<sup>1</sup>

**Toxicology:** Chloromethcathinone has been detected in three toxicology cases to date at the CFSRE.

**Drug Materials:** Chloromethcathinone has not yet been identified in drug materials to date at the CFSRE.

**Demographics / Geographics:** Toxicology specimens were collected in New York City, New York. Chloromethcathinone was found alongside other substituted cathinones (e.g., methylmethcathinone) and traditional stimulants/hallucinogens (e.g., MDMA, ketamine, methamphetamine).

**Legal Status:** No isomer of chloromethcathinone is explicitly scheduled in the United States; however, 3- and 4-chloromethcathinone are both controlled internationally as Schedule II substances.

### References:

- ▶ Cayman Chemical: [2-Chloromethcathinone](#), [3-Chloromethcathinone](#), and [4-Chloromethcathinone](#)
- ▶ <sup>1</sup>Walther *et al.* (2018) [Systematic structure-activity studies on selected 2-, 3-, and 4-monosubstituted synthetic methcathinone analogs as monoamine transporter releasing agents](#)

**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, Joseph J. Palamar, Patricia Acosta, Nina Abukahok, Brianna N. Stang, Alyssa G. Reyes, 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 and staff at the CFSRE and NYU Langone Health for their involvements and contributions. For more information, contact [npsdiscovery@cfsre.org](mailto:npsdiscovery@cfsre.org) or visit [www.npsdiscovery.org](http://www.npsdiscovery.org).

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**Suggested Citation:** Walton, SE; Palamar, JJ; Acosta, P; Abukahok, N; Stang, BN; Reyes, AG; Logan, BK; Krotulski, AJ. (2024) *Chloromethcathinone — NPS Discovery New Drug Monograph*, Center for Forensic Science Research and Education, United States.

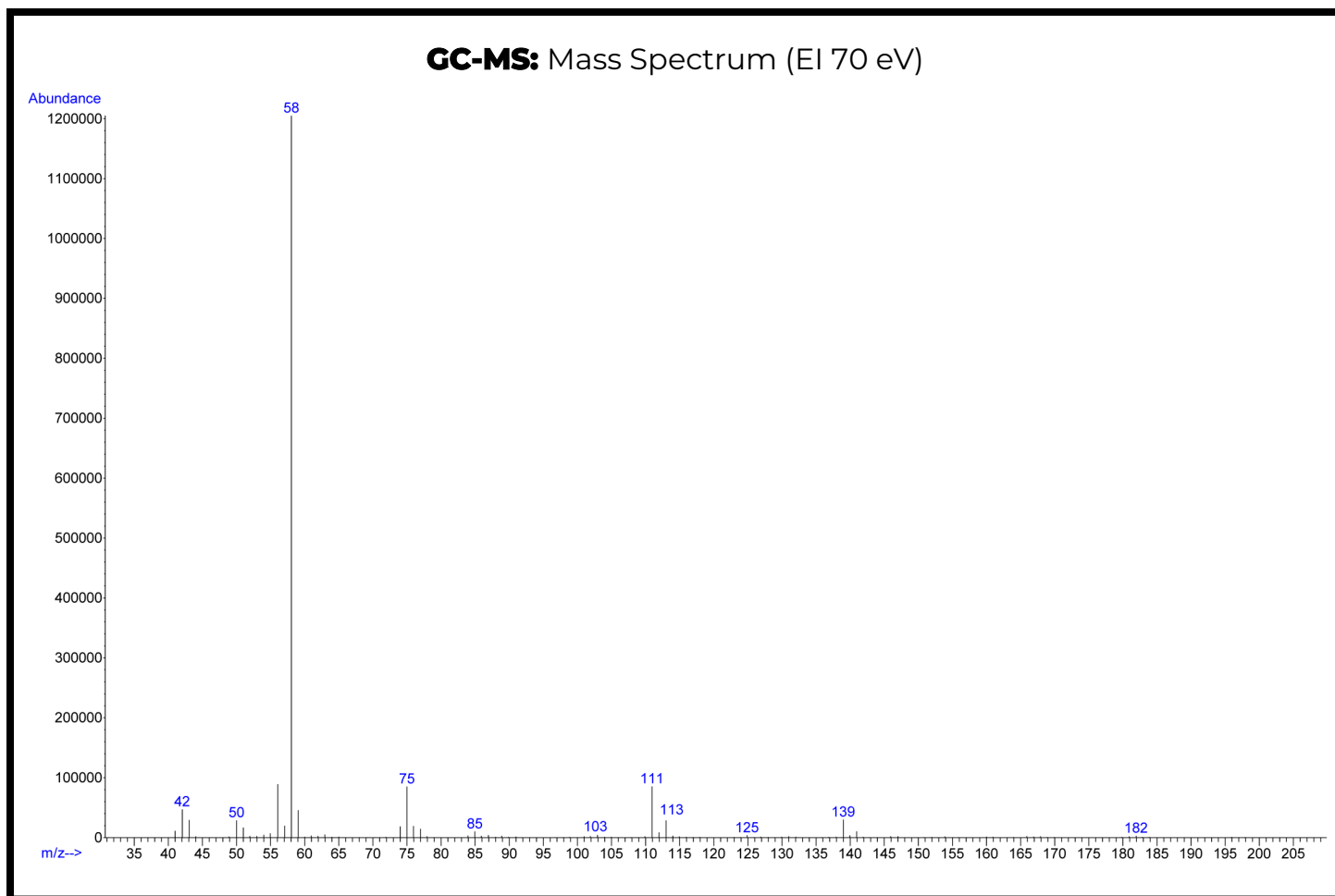
## Gas Chromatography Mass Spectrometry (GC-MS)

**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Instrument:** Agilent 5975 Series GC/MSD

**Methods:** [GC-MS Method Details](#) & [Monographs](#)

**Sample Preparation:** Standard diluted in methanol



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

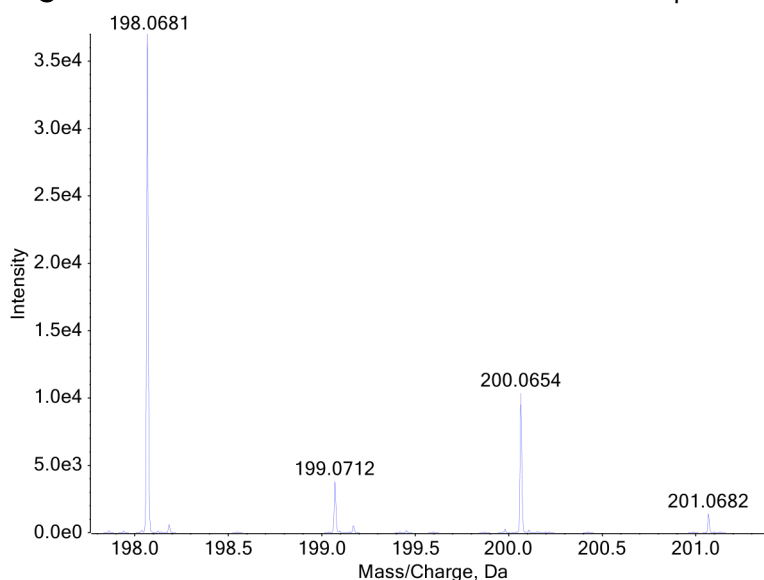
**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Instrument:** Sciex X500R LC-QTOF-MS

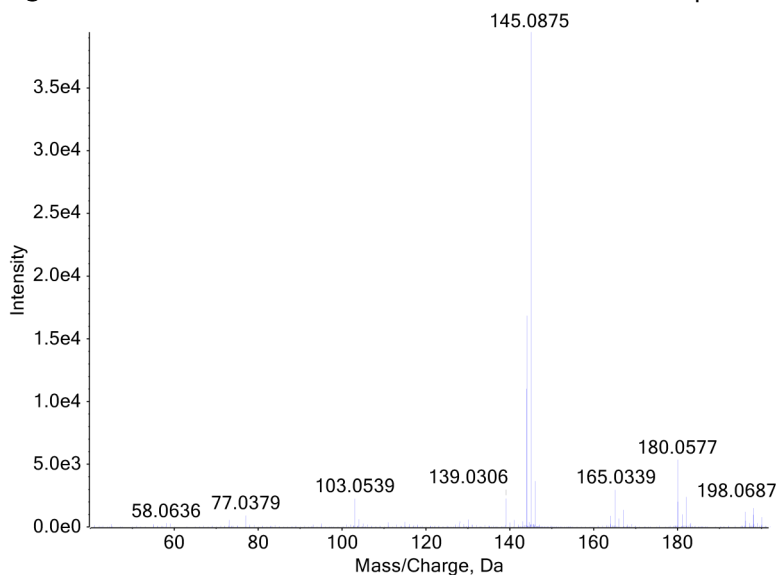
**Methods:** [LC-QTOF-MS Method Details](#) & [Monographs](#)

**Sample Preparation:** Liquid-liquid extraction

**LC-QTOF-MS: TOF-MS Precursor Ion Mass Spectrum**



**LC-QTOF-MS: TOF-MS/MS Product Ion Mass Spectrum**



**Confirmation Using Drug Standard:** Reference material (Batch: 0467004-52) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be chloromethcathinone based on retention time (sample: 4.34 min vs. standard: 4.39 min) and mass spectral data comparisons.