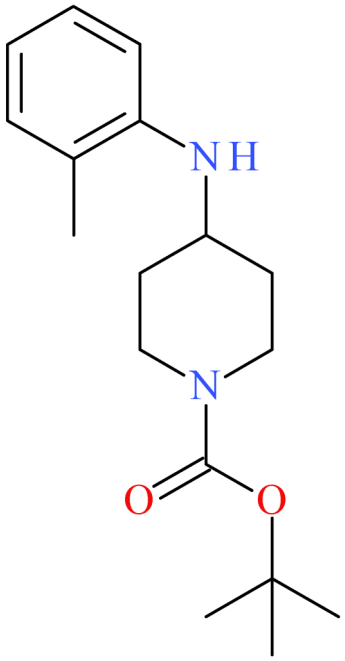
ortho-Methyl Boc-4-AP



NPS SUBCLASS
Opioid
REPORT DATE
August 30, 2024
SAMPLE RECEIVED
April 2, 2024
SAMPLE TYPE
Drug Material

Preferred Name	*ortho*-Methyl Boc-4-AP
Synonyms	*ortho*-Methyl 4-Anilino-1-Boc-piperidine, 4-(*ortho*-tolylamino)-1-Boc-piperidine
Formal Name	*tert*-butyl 4-(2-methylanilino)piperidine-1-carboxylate
InChI Key	HIVZJTXXEISBPZ-UHFFFAOYSA-N
CAS Number	1154101-90-2
Chemical Formula	$C_{17}H_{26}N_2O_2$
Molecular Weight	290.40
Molecular Ion [M⁺]	290
Exact Mass [M+H]⁺	291.2067

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: *ortho*-Methyl boc-4-AP is a synthetic opioid precursor that can be used in the synthesis of *ortho*-methylfentanyl. *ortho*-Methyl boc-4-AP bears structural similarity to *N*-boc 4-AP and other related fentanyl precursors. *ortho*-Methyl boc-4-AP was first detected in May 2024 by our laboratory and was confirmed through comprehensive chemical analysis.

Sample Source: Reuters (Media Agency)

Sample Appearance: White powder

Pharmacology: Based on our understanding of fentanyl analogue precursor pharmacology, it is hypothesized that *ortho*-methyl boc-4-AP is not an active opioid or exhibits very low potency compared to fentanyl and other synthetic opioids. *Ortho*-methyl boc-4-AP can be used to produce *ortho*-methylfentanyl, an active mu opioid agonist with potency similar to that of fentanyl.[1]

Toxicology: *ortho*-Methyl boc-4-AP has not been identified in toxicology cases to date at the CFSRE.

Drug Materials: *ortho*-Methyl boc-4-AP has been detected in one drug material to date at the CFSRE.

Demographics / Geographics: The drug material originated from China. *Ortho*-Methyl boc-4-AP was detected in the absence of other substances.

Legal Status: *ortho*-Methyl boc-4-AP is not explicitly scheduled in the United States.

References:

- Cayman Chemical: *ortho*-Methyl Boc-4-AP
- [1]Hassanien *et al.* (2020) *In vitro* pharmacology of fentanyl analogs at the human mu opioid receptor...

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, LC-QTOF-MS, and NMR) 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 and staff at the CFSRE and IteraMed (Doylestown, PA) 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)

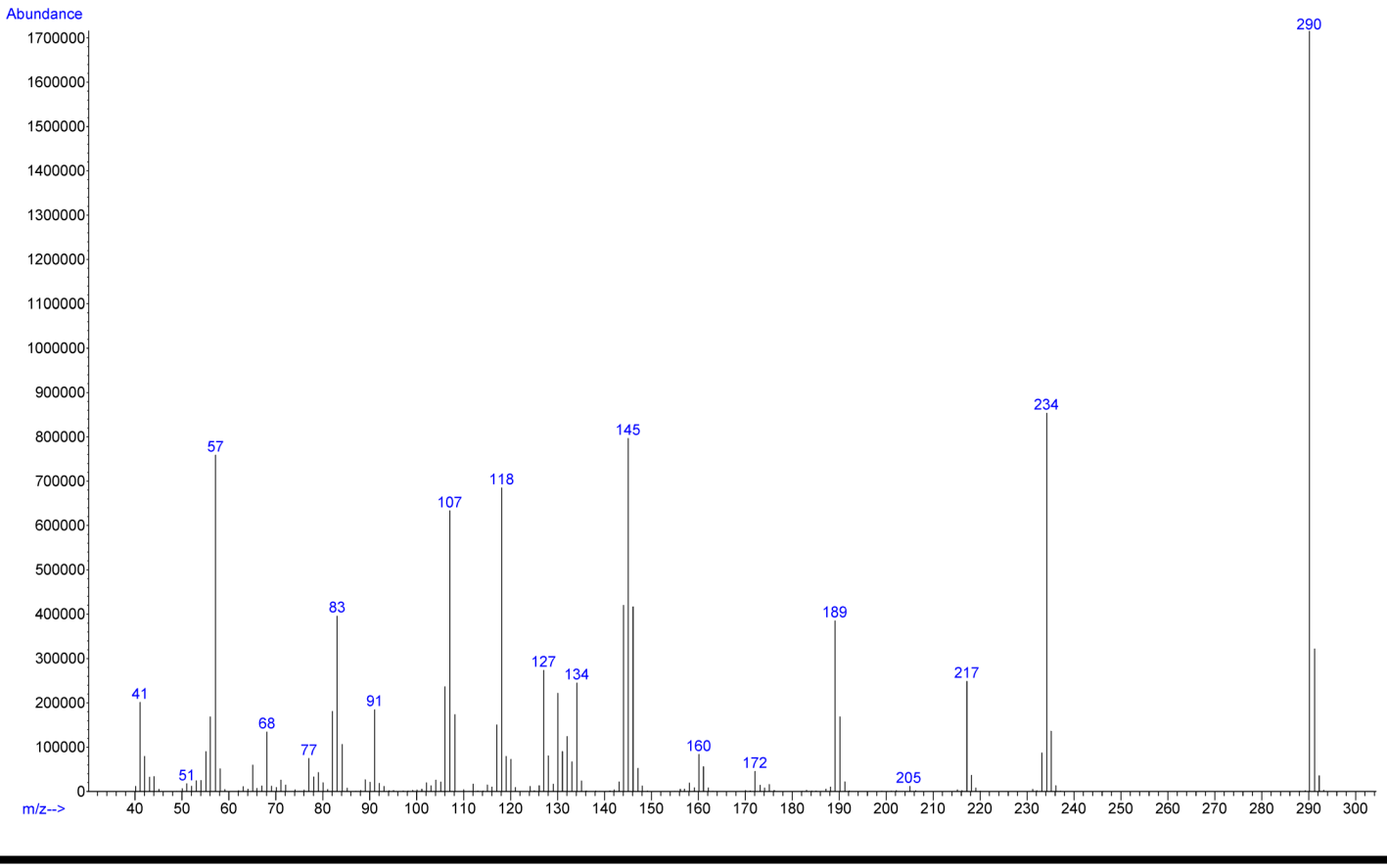
Laboratory: Center for Forensic Science Research and Education (CFSRE, Horsham, PA, USA)

Sample Preparation: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD

Methods: GC-MS Method Details & Monographs

GC-MS: Mass Spectrum (EI 70 eV)



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

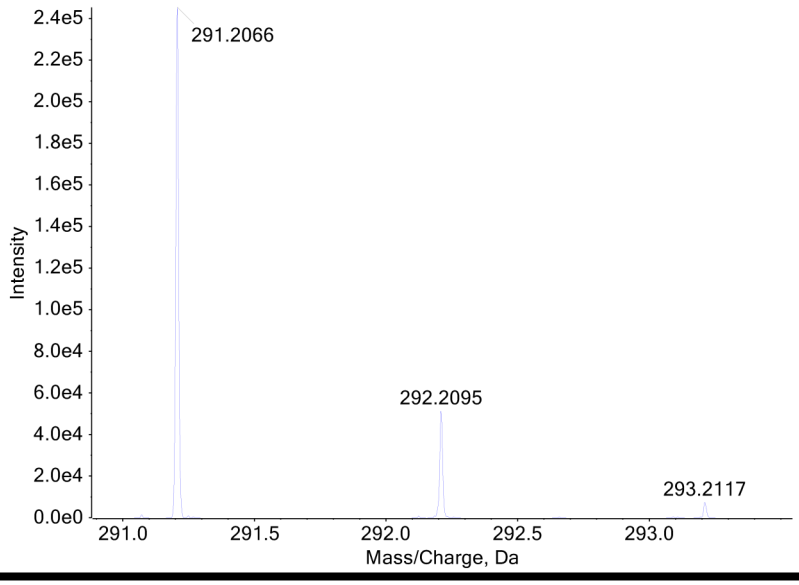
Laboratory: Center for Forensic Science Research and Education (CFSRE, Horsham, PA, USA)

Sample Preparation: Dilution in mobile phase

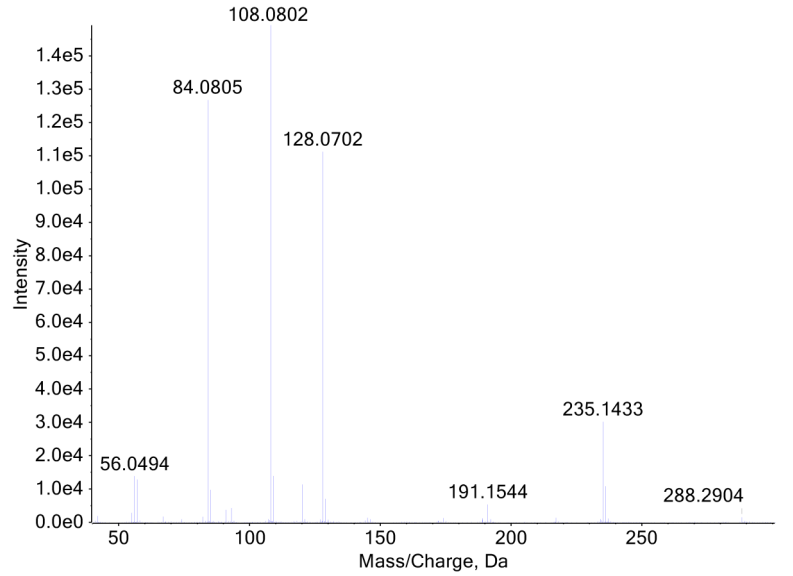
Instrument: Sciex X500R LC-QTOF-MS

Methods: LC-QTOF-MS Method Details & Monographs

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



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



Nuclear Magnetic Resonance (NMR) Spectroscopy

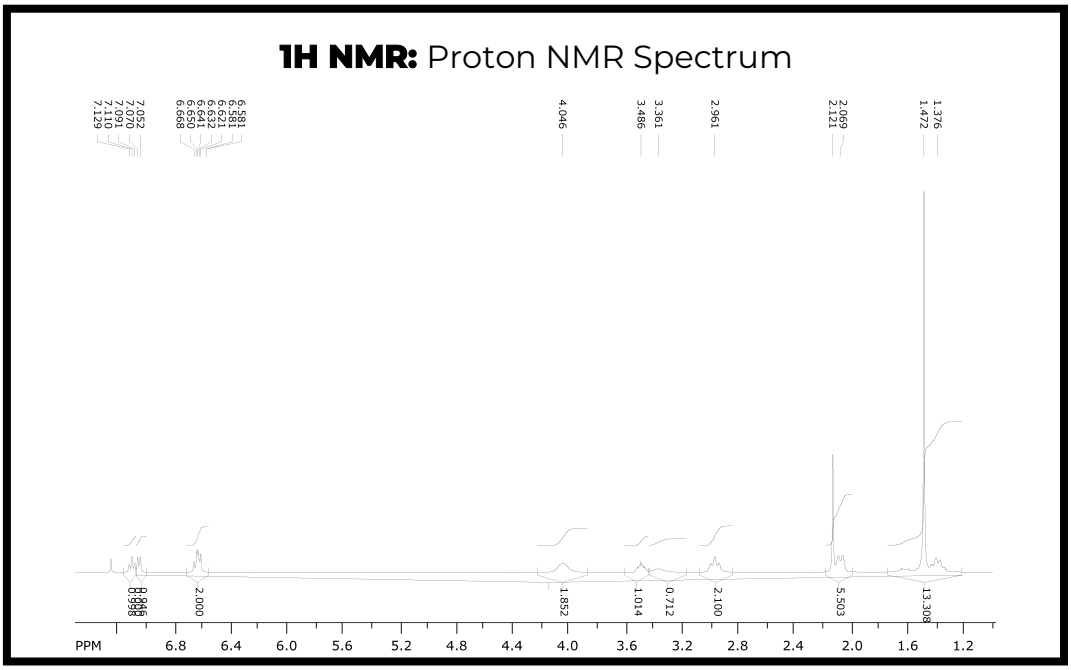
Laboratory: IteraMed™ (Doylestown, PA, USA)

Instrument: Various (See Link Below)

Sample Preparation: Dilution in $CDCl_3$

Methods: NMR Method Details & Monographs

1H NMR: Proton NMR Spectrum



COSY: ^{1}H-^{1}H COSY NMR Spectrum