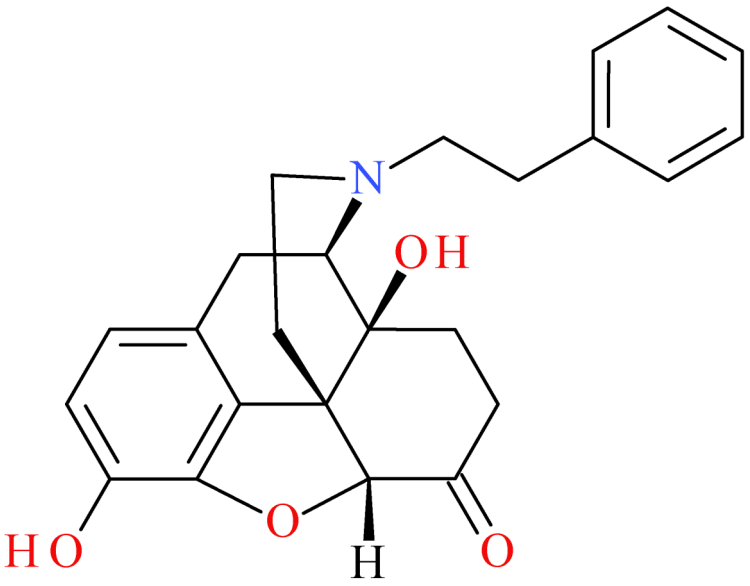
N-Phenethyl Noroxymorphone



NPS SUBCLASS
Opioid
REPORT DATE
August 21, 2024
SAMPLE RECEIVED
October 20, 2023
SAMPLE TYPE
Drug Material

Preferred Name	*N*-Phenethyl Noroxymorphone
Synonyms	*N*-Phenethylnoroxymorphone, (+)-Phenethylnoroxymorphone
Formal Name	(4R,4aS,7aR,12bS)-4a,9-dihydroxy-3-(2-phenylethyl)-2,4,5,6,7a,13-hexahydro-1H-4,12-methanobenzofuro[3,2-e]isoquinolin-7-one
InChI Key	NDHIGBQXQCVRAU-QLBRKBSLSA-N
CAS Number	4778-94-3
Chemical Formula	$C_{24}H_{25}NO_4$
Molecular Weight	391.5
Molecular Ion [M⁺]	391
Exact Mass [M+H]⁺	392.1856

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: *N*-Phenethyl noroxymorphone is a novel synthetic opioid with structural similarity to oxymorphone and naltrexone. *N*-Phenethyl noroxymorphone was first synthesized in the 1960s as a potential analgesic.[1] *N*-Phenethyl noroxymorphone was first identified in October 2023 by our laboratory and was confirmed in February 2024 after acquiring standard reference material.

Sample Source: PA Groundhogs (Pennsylvania)

Sample Appearance: White powder

Pharmacology: *N*-Phenethyl noroxymorphone is reported to be an active and potent drug at the mu-opioid receptor.[2] Compared to oxymorphone, *N*-phenethyl noroxymorphone was determined to have 2x higher affinity and potency at the mu-opioid receptor *in vitro* and is highly selective for the mu-opioid receptor over the kappa-opioid receptor (EC_{50}: 2.63±1.06 nM, Ki: 0.54±0.03 nM).[2]

Toxicology: *N*-Phenethyl noroxymorphone has not been identified toxicology cases to date at the CFSRE.

Drug Materials: *N*-Phenethyl noroxymorphone has been detected in 1 drug material to date at the CFSRE.

Demographics / Geographics: The drug material positive for *N*-phenethyl noroxymorphone originated from Pennsylvania and was identified alone without the presence of other drugs.

Legal Status: *N*-Phenethyl noroxymorphone is not currently a scheduled drug in the United States.

References:

- Cayman Chemical: *N*-Phenethyl Noroxymorphone
- [1]Seki *et al.* (1964) Pharmacological studies on morphine derivatives.
- [2]Haddou *et al.* (2014) Pharmacological investigations of N-substituent variation in morphine and oxymorphone...

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, Christopher Moraff, 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)

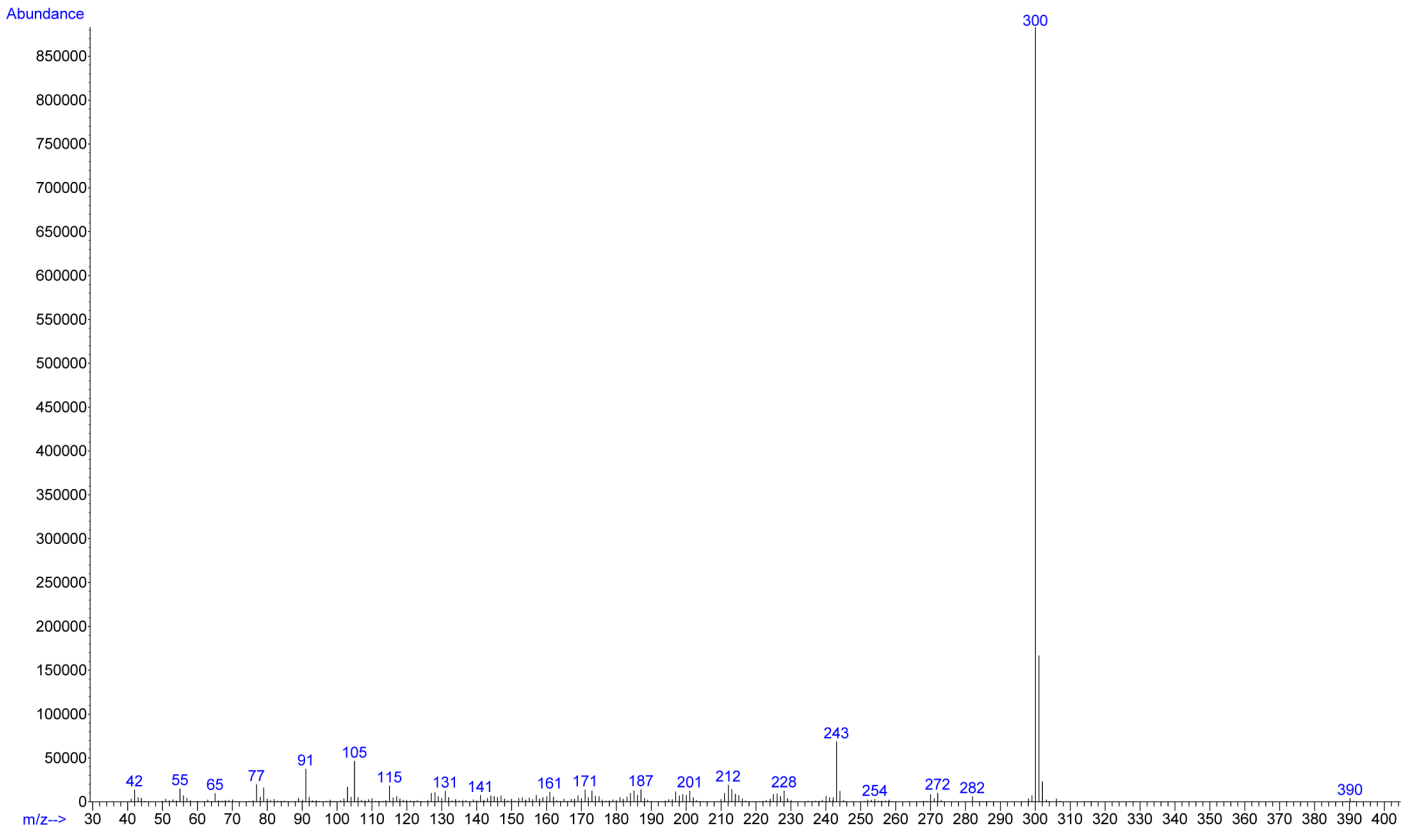
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

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: 0696945-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be N-phenethyl noroxymorphone based on mass spectral data comparisons.*

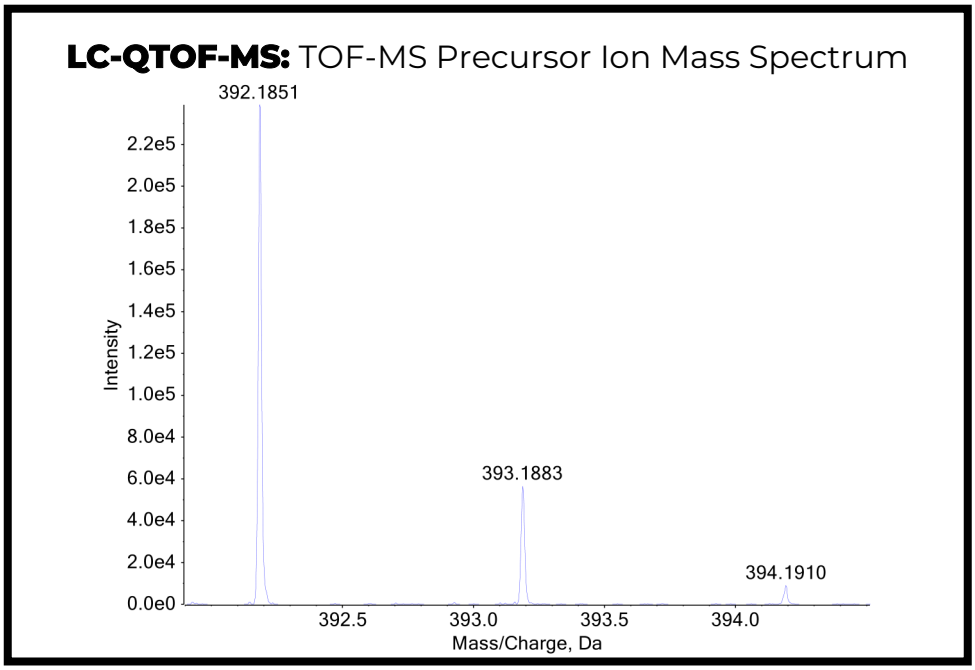
Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

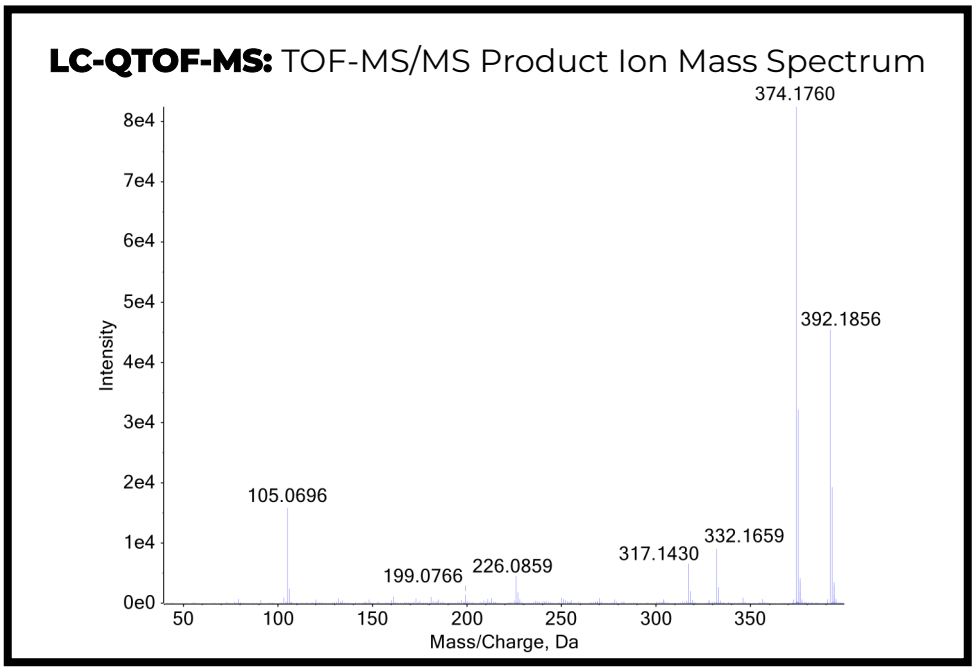
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

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: 0696945-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be N-phenethyl noroxymorphone based on retention time (sample: 5.30 min vs. standard: 5.41 min) and mass spectral data comparisons.*