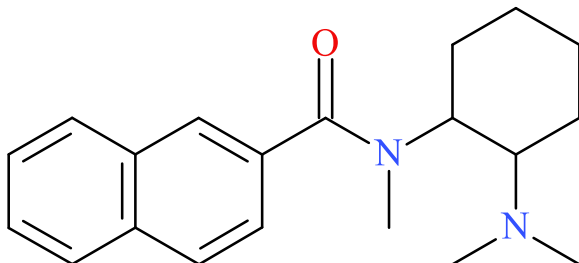


Naphthyl-U-47700

Sample Type: **Drug Material**



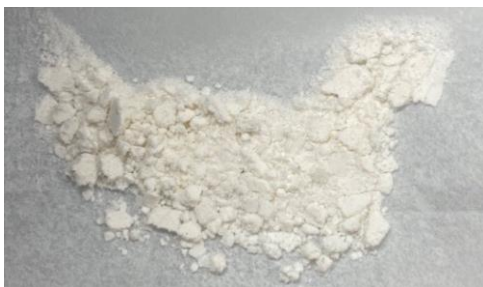
Latest Revision: **December 16, 2021**

Date Received: **June 29, 2021**

Date of Report: **December 16, 2021**

1. GENERAL INFORMATION

| | |
|----------------------|--|
| IUPAC Name: | N-[2-(dimethylamino)cyclohexyl]-N-methyl-naphthalene-2-carboxamide |
| InChI String: | InChI=1S/C20H26N2O/c1-21(2)18-10-6-7-11-19(18)22(3)20(23)17-13-12-15-8-4-5-9-16(15)14-17/h4-5,8-9,12-14,18-19H,6-7,10-11H2,1-3H3 |
| CFR: | Not Scheduled (12/2021) |
| CAS# | 67579-80-0 |
| Synonyms: | 1-Naphthyl U-47700, 2-Naphthyl U-47700 |
| Source: | Columbus Police Crime Laboratory |



Important Note: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The “2-naphthyl” configuration was used for structural purposes; however, position of the naphthyl group was not confirmed during analysis.

Prepared By: Prepared By: Alex J. Krotulski, PhD; Erica Miller; Sara E. Walton, MS; Melissa F. Fogarty, MSFS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

| Drug | Chemical Formula | Molecular Weight | Molecular Ion [M ⁺] | Exact Mass [M+H] ⁺ |
|------------------|--|------------------|---------------------------------|-------------------------------|
| Naphthyl-U-47700 | C ₂₀ H ₂₆ N ₂ O | 310.4 | 310 | 311.2118 |

3. BRIEF DESCRIPTION

Naphthyl-U-47700 is classified as a novel opioid. Novel opioids have been reported to cause psychoactive effects similar to heroin, fentanyl, and other opioids. Novel opioids in the trans-N-[2-(methylamino)cyclohexyl]-benzamide class (e.g. U-47700) and similar classes (e.g. U-49900) have caused adverse events, including deaths, as described in the literature. U-47700 is a Schedule I substance in the United States; no other U-series analogues are explicitly scheduled.

4. ADDITIONAL RESOURCES

Drug Enforcement Administration (2021). Announcement of an Emerging Synthetic Opioid 2-Naphthyl U-47700. https://www.nflis.deadiversion.usdoj.gov/nflisdata/docs/NFLIS_Synth-Opioids_2-naphthyl_U47700.pdf

<https://www.caymanchem.com/product/33872/2-naphthyl-u-47700>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

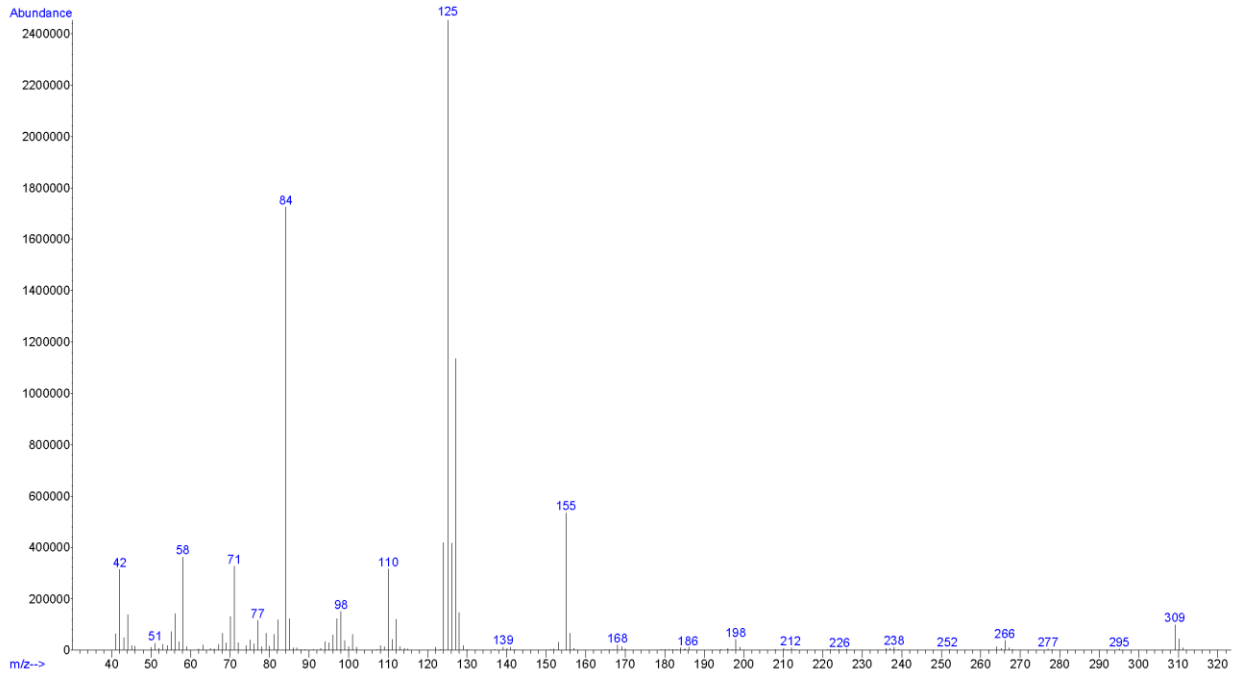
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for 2-Naphthyl-U-47700 (Batch: 0611555-2) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (<https://www.caymanchem.com/product/33872/2-naphthyl-u-47700>)

EI (70 eV) Mass Spectrum: 2-Naphthyl-U-47700 (Standard)



5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Dilution in methanol followed by 1:100 dilution in mobile phase

Instrument: Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

Column: Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)

Mobile Phase: A: Ammonium formate (10 mM, pH 3.0)
B: Methanol/acetonitrile (50:50)
Flow rate: 0.4 mL/min

Gradient: Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min

Temperatures: Autosampler: 15 °C
Column Oven: 30 °C

Source Heater: 600 °C

Injection Parameters: Injection Volume: 10 µL

QTOF Parameters: TOF MS Scan Range: 100-510 Da

Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collision Energy Spread (35±15 eV)

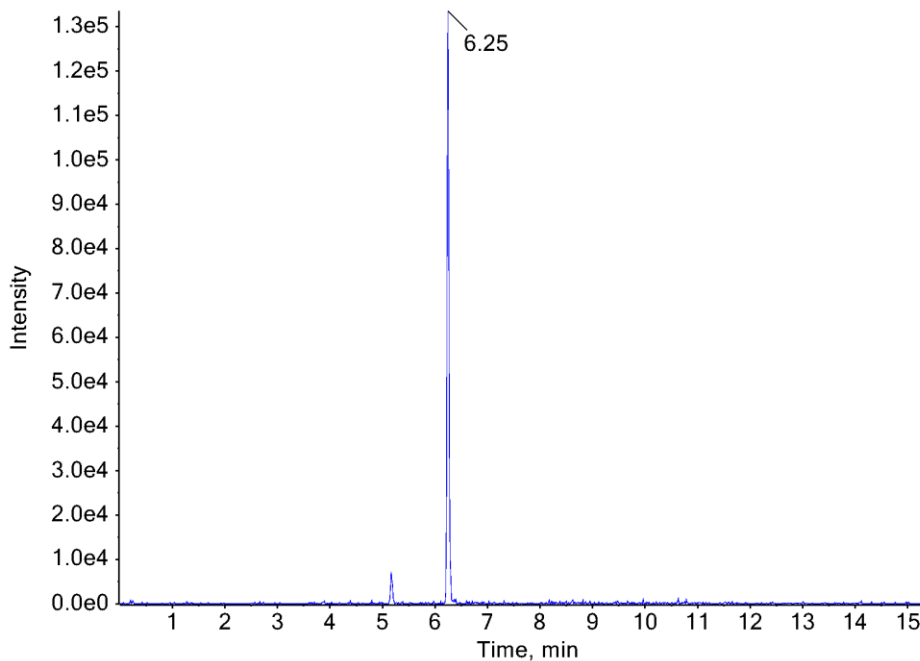
MS/MS Scan Range: 50-510 Da

Retention Time: 6.25 min

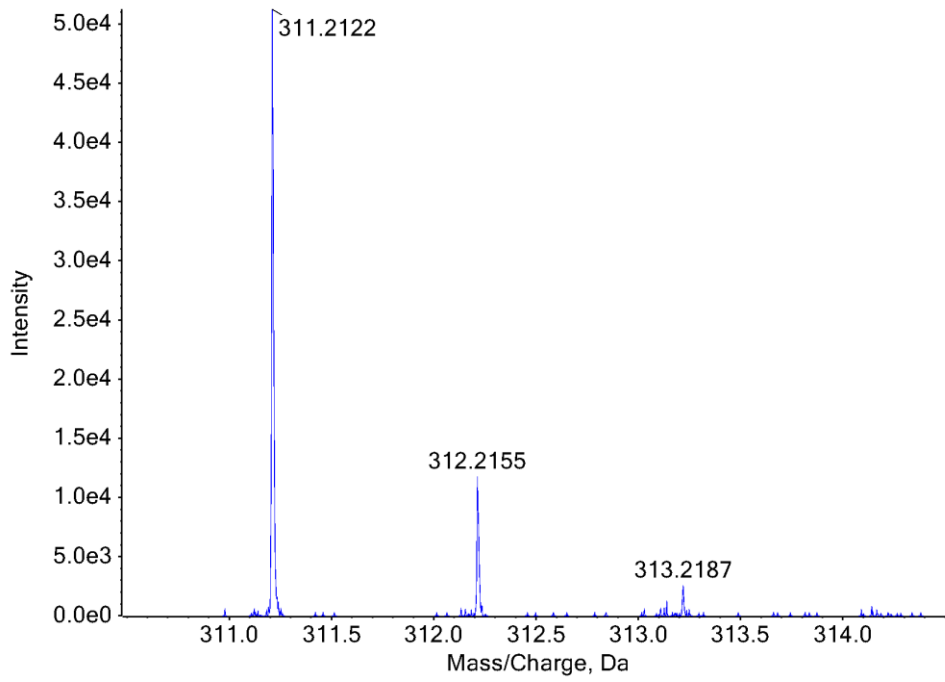
Standard Comparison: Reference material for 2-Naphthyl-U-47700 (Batch: 0611555-2) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Naphthyl-U-47700, based on retention time (6.10 min) and mass spectral data; however, absolute configuration of the structure as 1-Naphthyl-U-47700 vs. 2-Naphthyl-U-47700 was not determined.

<https://www.caymanchem.com/product/33872/2-naphthyl-u-47700>

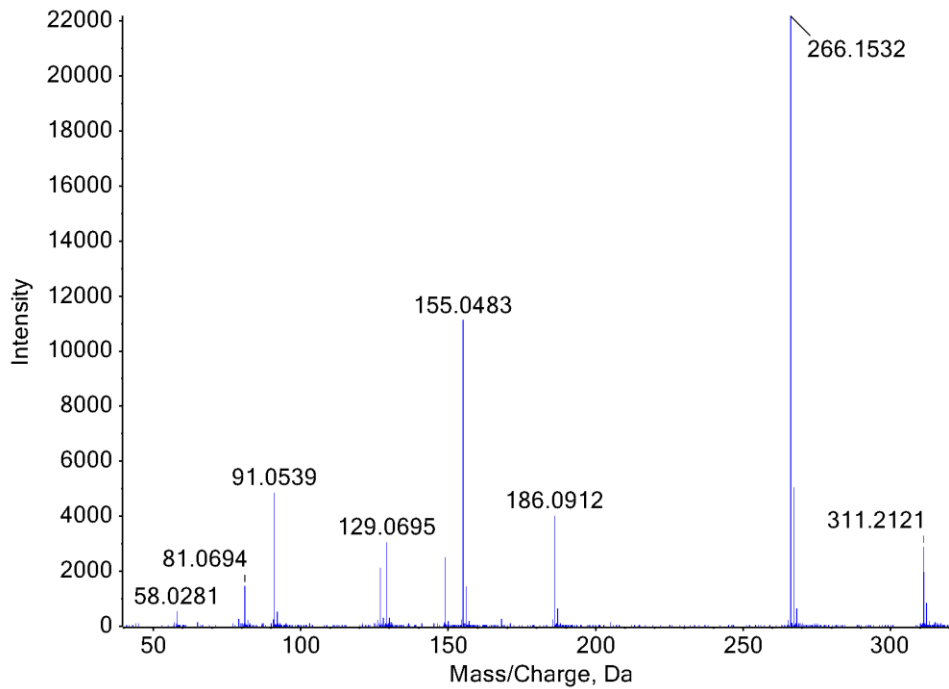
Extracted Ion Chromatogram: Naphthyl-U-47700



TOF MS Spectra: Naphthyl-U-47700



MS/MS Spectra: Naphthyl-U-47700



6. FUNDING

NPS Discovery is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, “Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect those of the DOJ.