I. 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,6-7,10-11H2,1H3

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.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Drug</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthyl-U-47700</td>
<td>C₂₀H₂₄N₂O</td>
<td>310.4</td>
<td>310</td>
<td>311.2118</td>
</tr>
</tbody>
</table>

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


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: Collison 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.