1. GENERAL INFORMATION

IUPAC Name: N-(1-methyl-1-phenyl-ethyl)-1-(p-tolylsulfonyl)indazole-3-carboxamide

InChI String: InChI=1S/C24H23N3O3S/c1-17-13-15-19(16-14-17)31(29,30)27-21-12-8-7-11-20(21)22(26-27)23(28)25-24(2,3)18-9-5-4-6-10-18/h4-16H,1-3H3,(H,25,28)

CFR: Not Scheduled (12/2022)

CAS#: Not Available

Synonyms: Cumyl-tosyl-indazole-3-carboxamide

Source: ACMT’s Toxicology Investigators Consortium (ToxIC)

Important Note: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material.

Prepared By: Alex J. Krotulski, PhD; Alex Manini, MD; Jeff Brent, MD, PhD; Paul Wax, MD; Kim Aldy, MD; 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

<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>CUMYL-TsINACA</td>
<td>C_{24}H_{23}N_{3}O_{3}S</td>
<td>433.5</td>
<td>433</td>
<td>434.1533</td>
</tr>
</tbody>
</table>

3. SAMPLE HISTORY

To date, CUMYL-TsINACA was identified in one clinical case since October 2022. The geographical and demographical breakdown is below:

Geographical Location: Los Angeles (n=1)

Biological Sample: Plasma (n=1)

Date of First Receipt: October 2022

Other Notable Findings: MDMB-INACA, BZO-CHMOXIZID, 4F-MDMB-BINACA

4. BRIEF DESCRIPTION

CUMYL-TsINACA is classified as a synthetic cannabinoid. Synthetic cannabinoids have been reported to cause psychoactive effects similar to delta-9-tetrahydrocannabinol (THC). Synthetic cannabinoids have caused adverse events, including deaths, as described in the literature. Little to no information is currently available regarding CUMYL-TsINACA. CUMYL-TsINACA is not explicitly scheduled in the United States.

5. ADDITIONAL RESOURCES


6. QUALITATIVE DATA

6.1 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 CUMYL-TsINACA (Batch: 0647276-2) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/36834/cumyl-tsinaca)

EI (70 eV) Mass Spectrum: CUMYL-TsINACA (Standard)
6.2 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: Liquid-liquid extraction (LLE)

Instrument: Sciex X500R, Sciex ExionLC

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: 10.01 min

Standard Comparison: Reference material for CUMYL-TsINACA (Batch: 0647276-2) 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 CUMYL-TsINACA, based on retention time (10.08 min) and mass spectral data. (https://www.caymanchem.com/product/36834/cumyl-tsinaca)
Extracted Ion Chromatogram: CUMYL-TsINACA

TOF MS Spectra: CUMYL-TsINACA
7. FUNDING

Funding for sample collection and analysis was received from the National Institute on Drug Abuse (NIDA) from the National Institutes of Health (NIH), Award Number: R01DA048009. The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the authors and do not necessarily reflect those of the NIH.

NPS Discovery at the CFSRE 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 represent the official position or policies of the U.S. Department of Justice.