

NMS Labs 2300 Stratford Ave Willow Grove, PA 19090

5F-CUMYL-PINACA



Sample Type: Seized Material

Latest Revision: May 29, 2020

Date Received: March 3, 2020

Date of Report: May 29, 2020

1. GENERAL INFORMATION

IUPAC Name:	1-(5-fluoropentyl)-N-(1-methyl-1-phenyl-ethyl)indazole-3- carboxamide
InChI String:	InChI=1S/C22H26FN3O/c1-22(2,17-11-5-3-6-12-17)24-21(27)20- 18-13-7-8-14-19(18)26(25-20)16-10-4-9-15-23/h3,5-8,11-14H,4,9- 10,15-16H2,1-2H3,(H,24,27)
CFR:	21 CFR 1308: Temporary Placement of 5F-CUMYL-PINACA into Schedule I (04/16/2019)
CAS#	1400742-16-6
Synonyms:	5-fluoro CUMYL-PINACA, CUMYL-5F-PINACA, SGT-25
Source:	Department of Homeland Security
Appearance:	Plant-like Material

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

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical	Molecular	Molecular Ion	Exact Mass
	Formula	Weight	[M ⁺]	[M+H] ⁺
Base	C ₂₂ H ₂₆ FN ₃ O	367.5	367	368.2133

3. BRIEF DESCRIPTION

5F-CUMYL-PINACA 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. 5F-CUMYL-PINACA is an active and potent synthetic cannabinoid.¹ The synthesis of 5F-CUMYL-PINACA was patented in 2013 by researchers in New Zealand.² 5F-CUMYL-PINACA was first reported in seized drug casework by Sweden in 2014.³ Subsequently, this emerging synthetic cannabinoid was identified in e-cigarette liquid.⁴ Forty-five cases involving 5F-CUMYL-PINACA have been uploaded into the United Nations Office of Drugs and Crime (UNODC) Early Warning Advisory on New Psychoactive Substances Portal dating back to 2014; one case was submitted from an agency in the United States in 2018. Through our monitoring program for synthetic cannabinoids in toxicology casework, NPS Discovery has not identified any positive cases for 5F-CUMYL-PINACA in the United States since our program began in mid-2018 - this is our first encounter with this substance, for which no reference monograph is available. CUMYL-PINACA, 4CN-CUMYL-BINACA, and other "CUMYL-" analogues are structurally similar synthetic cannabinoids. 5F-CUMYL-PINACA and 4-CN-CUMYL-BINACA are Schedule I substances in the United States.⁵

4. ADDITIONAL RESOURCES

- Longworth M, Banister SD, Boyd R, Kevin RC, Connor M, McGregor IS, Kassiou M (2017). Pharmacology of Cumyl-Carboxamide Synthetic Cannabinoid New Psychoactive Substances (NPS) CUMYL-BICA, CUMYL-PICA, CUMYL-5F-PICA, CUMYL-5F-PINACA, and Their Analogues. ACS Chemical Neuroscience. 8 (10): 2159–2167.
- Bowden MJ, Williamson, JPB. (2013). Patent WO 2014167530 Cannabinoid compounds. New Zealand Patent Application 623626. International Publication Number WO2014/167530A. <u>https://patents.google.com/patent/WO2014167530A1</u>

4. ADDITIONAL RESOURCES (CONTINUED)

- 3. European Monitoring Centre for Drugs and Drug Addiction (2015), EMCDDA–Europol 2014 Annual Report on the implementation of Council Decision 2005/387/JHA, Implementation reports, Publications Office of the European Union, Luxembourg. <u>http://www.emcdda.europa.eu/system/files/publications/1018/TDAN15001ENN.pdf</u>
- 4. Angerer V, Franz F, Moosmann B, Bisel P, Auwärter V. (2019) 5F-Cumyl-PINACA in 'eliquids' for electronic cigarettes: comprehensive characterization of a new type of synthetic cannabinoid in a trendy product including investigations on the in vitro and in vivo phase I metabolism of 5F-Cumyl-PINACA and its non-fluorinated analog Cumyl-PINACA. *Forensic Toxicology*, **37** (1): 186-196.
- 5. Drug Enforcement Administration. (April 16, 2019) Schedules of Controlled Substances: Temporary Placement of 5F-EDMB-PINACA, 5F-MDMB-PICA, FUB-AKB48, 5F-CUMYL-PINACA, and FUB-144 into Schedule I. *Federal Register*, 84, 15505-15511. https://www.deadiversion.usdoj.gov/fed_regs/rules/2019/fr0416.htm

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/CUMYL-5F-PINACA-ID-1155-report_final.pdf

https://www.caymanchem.com/product/17726/5-fluoro-cumyl-pinaca-(crm)

https://en.wikipedia.org/wiki/5F-CUMYL-PINACA

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebron TM Inferno TM ZB-35HT (15 m x 250 μ m x 0.25 μ m)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C

	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	8.22 min
Standard Comparison:	Reference material for 5F-CUMYL-PINACA (Batch: 0493225) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-CUMYL-PINACA, based on retention time (8.22 min) and mass spectral data. (<u>https://www.caymanchem.com/product/17726/5-fluoro-cumyl- pinaca-(crm)</u>)

Chromatogram: 5F-CUMYL-PINACA



Additional peaks present in chromatogram: internal standard (6.30 min)



EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-CUMYL-PINACA

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

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)	
Sample Preparation:	1:100 dilution of acid/base extraction 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:	9.76 min	
Standard Comparison:	Reference material for 5F-CUMYL-PINACA (Batch: 0520119) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-CUMYL-PINACA, based on retention time (9.73 min) and mass spectral data. (https://www.caymanchem.com/product/17726/5-fluoro-cumyl-pinaca-(crm))	





TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-CUMYL-PINACA

