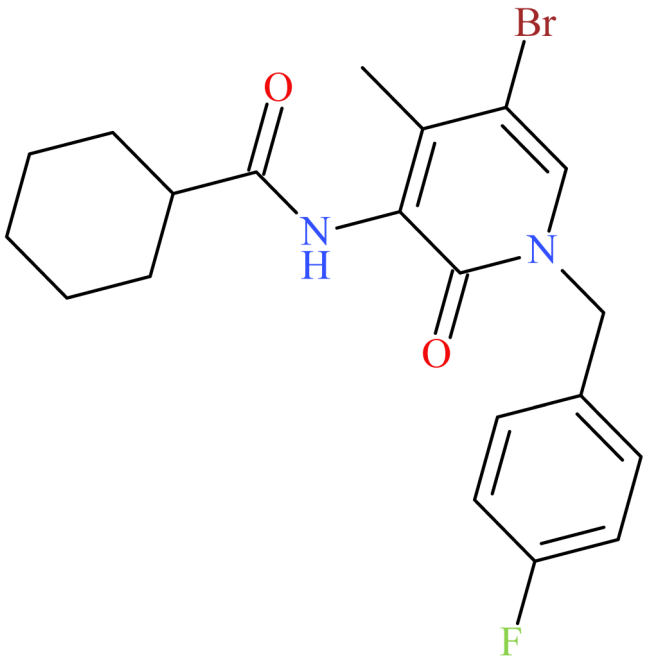
CHO-4'Me-5'Br-FUBOXPYRA



NPS SUBCLASS
Synthetic Cannabinoid
REPORT DATE
June 28, 2023
SAMPLE RECEIVED
March 10, 2023
SAMPLE TYPE
Drug Material

Preferred Name	CHO-4'Me-5'Br-FUBOXPYRA
Synonyms	CH-FUBBMPDORA, 6TP
Formal Name	N-[5-bromo-1-[(4-fluorophenyl)methyl]-4-methyl-2-oxo-3-pyridyl]cyclohexanecarboxamide
InChI Key	CKYYASUICQFJPH-UHFFFAOYSA-N
CAS Number	Not Available
Chemical Formula	$C_{20}H_{22}BrFN_2O_2$
Molecular Weight	421.30
Molecular Ion [M⁺]	420
Exact Mass [M+H]⁺	421.0921

Characterization & Intelligence

The following information was compiled in June 2023 and is subject to change as new research is conducted and as new information becomes available:

Description: CHO-4'Me-5'Br-FUBOXPYRA is a novel synthetic cannabinoid. To date, no structurally similar drugs to CHO-4'Me-5'Br-FUBOXPYRA have been identified in the recreational drug supply. However, medicinal chemistry literature documents the synthesis and evaluation of other molecules from the its synthetic cannabinoid subclass, including an analogue with a cycloheptyl-containing head group. In early 2023, forensic laboratories in the United States shared their identifications of this novel synthetic cannabinoid, although the structure of CHO-4'Me-5'Br-FUBOXPYRA was not previously confirmed or reported. Due to its novelty, little information is currently known about CHO-4'Me-5'Br-FUBOXPYRA.

Sample Source: Pinellas County Forensic Lab (Largo, FL, USA).

Sample Appearance: Drug material – white powder.

Pharmacology: No information is available at this time.

Toxicology: CHO-4'Me-5'Br-FUBOXPYRA has not been detected in toxicology samples at the CFSRE.

Drug Materials: CHO-4'Me-5'Br-FUBOXPYRA has been identified in one drug material at the CFSRE.

Demographics / Geographics: The drug material originated from the state of Florida.

Legal Status: CHO-4'Me-5'Br-FUBOXPYRA is not explicitly scheduled in the United States.

References:

- Cayman Chemical: CHO-4'Me-5'Br-FUBOXPYRA
- National Forensic Laboratory (Slovenia): CHO-4'Me-5'Br-FUBOXPYRA (referred to as "CH-FUBBMPDORA")
- Gado et al. Identification of the First Synthetic Allosteric Modulator of the CB2 Receptors and Evidence of Its Efficacy for Neuropathic Pain Relief. *Journal of Medicinal Chemistry*, 2019, 62 (1), 276-287.

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, LC-QTOF-MS, NMR), as reference material was not available at the time of initial analysis.

Acknowledgements: This report was prepared by Alex J. Krotulski, Reta Newman, Michael Gilbert, Robert M. Schelkun, Donna M. Iula, Sara E. Walton, Joshua DeBord, Melissa F. Fogarty, and Barry K. Logan at the Center for Forensic Science Research and Education (CFSRE) at the Fredric Rieders Family Foundation. The authors acknowledge scientists at the CFSRE and NMS Labs for their involvements and contributions. For more information, contact npsdiscovery@cfsre.org or visit www.npsdiscovery.org.

Funding: CFSRE's NPS Discovery is supported by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 15PNIJ-22-GG-04434-MUMU, "Implementation of NPS Discovery – An Early Warning System for Novel Drug Intelligence, Surveillance, Monitoring, Response, and Forecasting using Drug Materials and Toxicology Populations in the US"). 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.

Suggested Citation: Krotulski, AJ; Newman, R; Gilbert, M; Schelkun, RM; Iula, DM; Walton, SE; DeBord, J; Fogarty, MF; Logan, BK. (2023) *CHO-4'Me-5'Br-FUBOXPYRA — NPS Discovery New Drug Monograph*, Center for Forensic Science Research and Education, United States.

Gas Chromatography Mass Spectrometry (GC-MS)

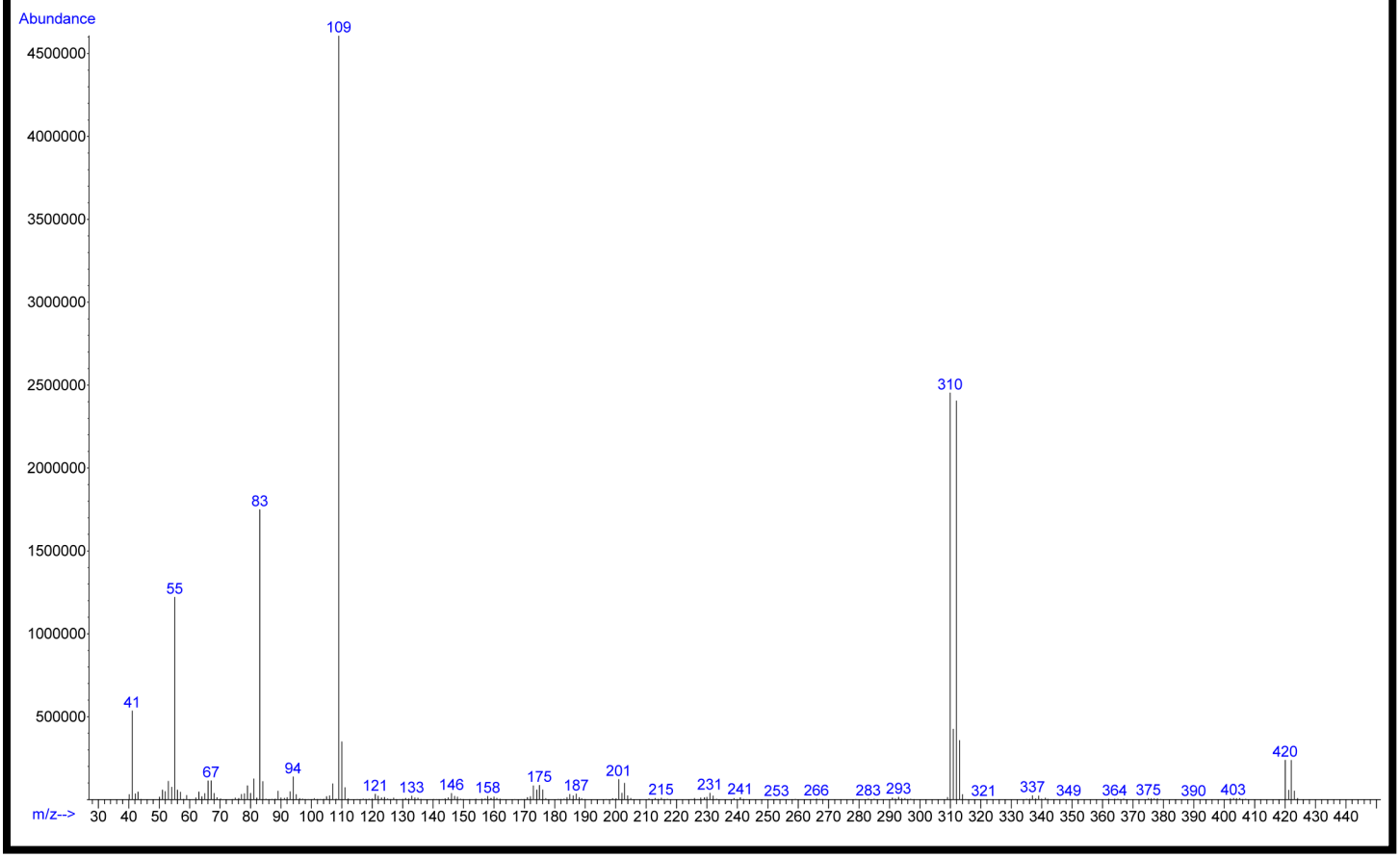
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

Sample Preparation: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD

Methods: www.cfsre.org/nps-discovery/monographs

GC-MS: Mass Spectrum (EI 70 eV)



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

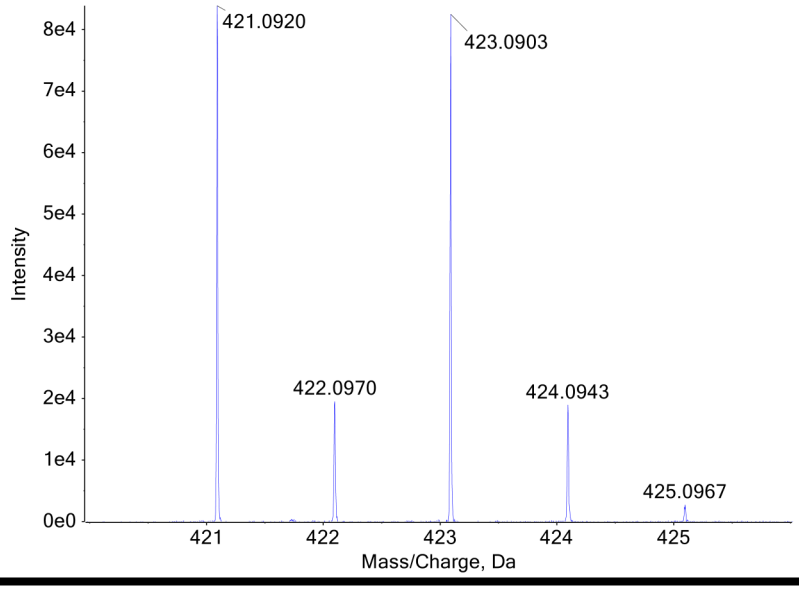
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

Sample Preparation: Dilution in mobile phase

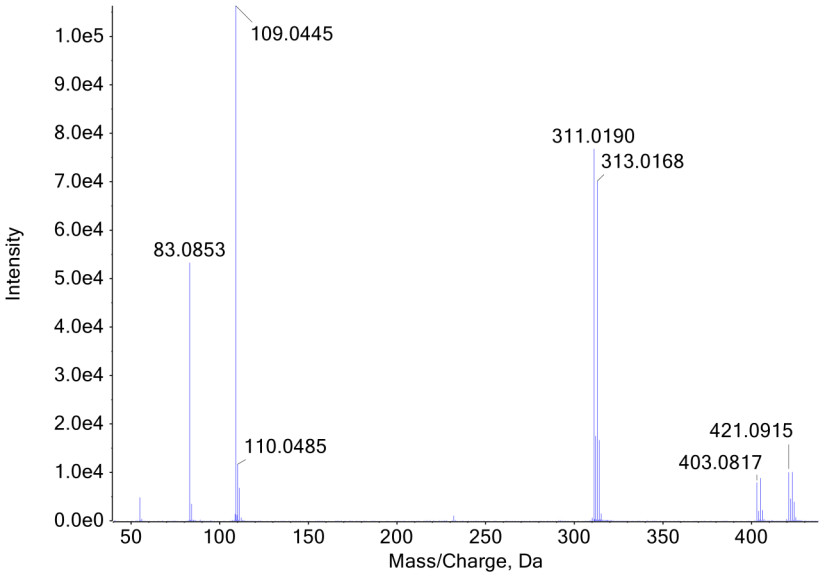
Instrument: Sciex TripleTOF® 5600+ LC-QTOF-MS

Methods: www.cfsre.org/nps-discovery/monographs

LC-QTOF-MS: TOF-MS Precursor Ion Mass Spectrum



LC-QTOF-MS: TOF-MS/MS Product Ion Mass Spectrum



Nuclear Magnetic Resonance (NMR) Spectroscopy

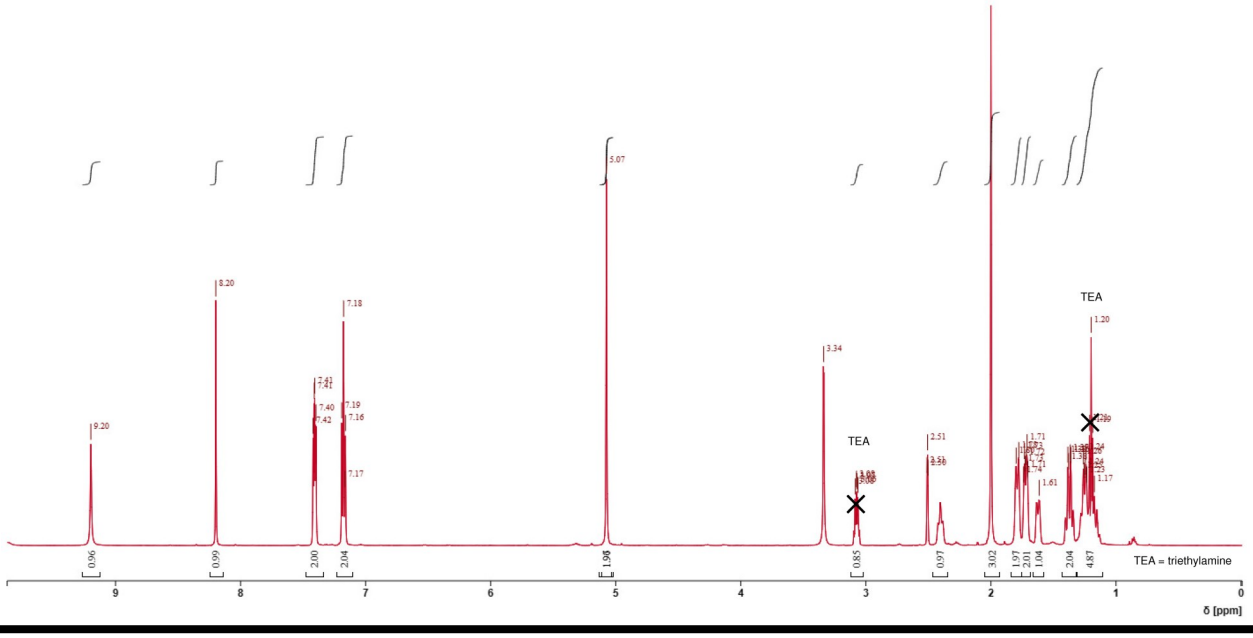
Laboratory: IteraMed™ (Doylestown, PA, USA)

Instrument: Various (See Link Below)

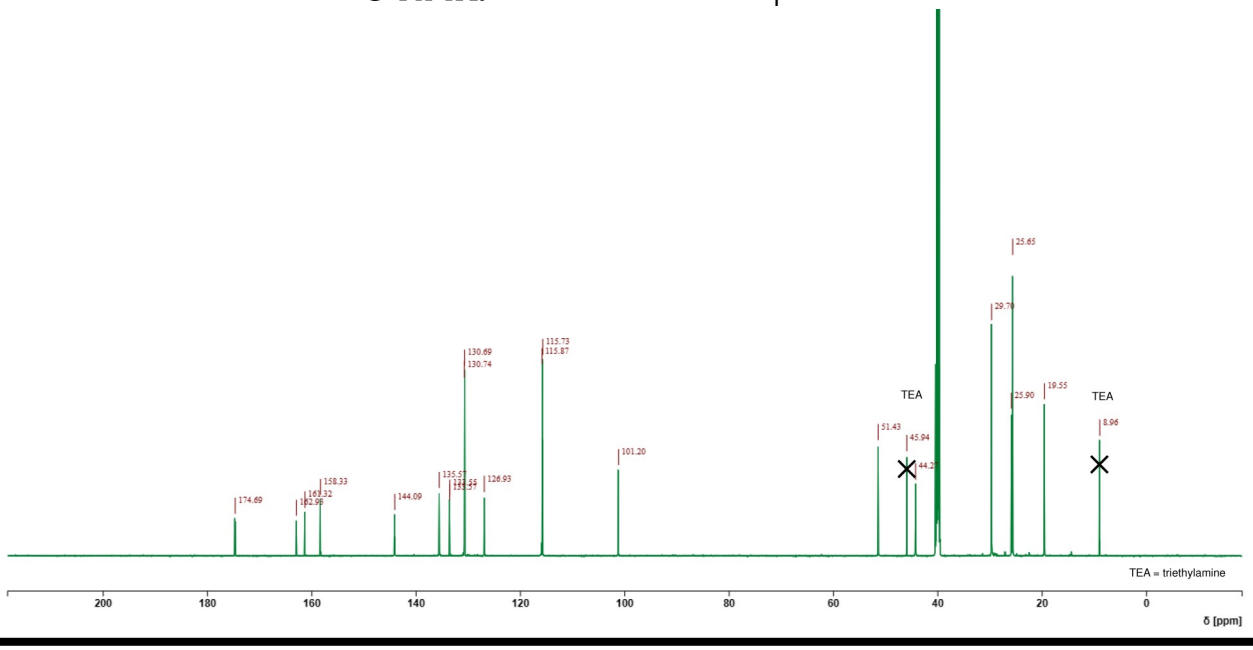
Sample Preparation: Dilution in DMSO-D6

Methods: www.cfsre.org/nps-discovery/monographs

^{1}H-NMR: Proton NMR Spectrum



^{13}C-NMR: Carbon-13 NMR Spectrum



Nuclear Magnetic Resonance (NMR) Spectroscopy

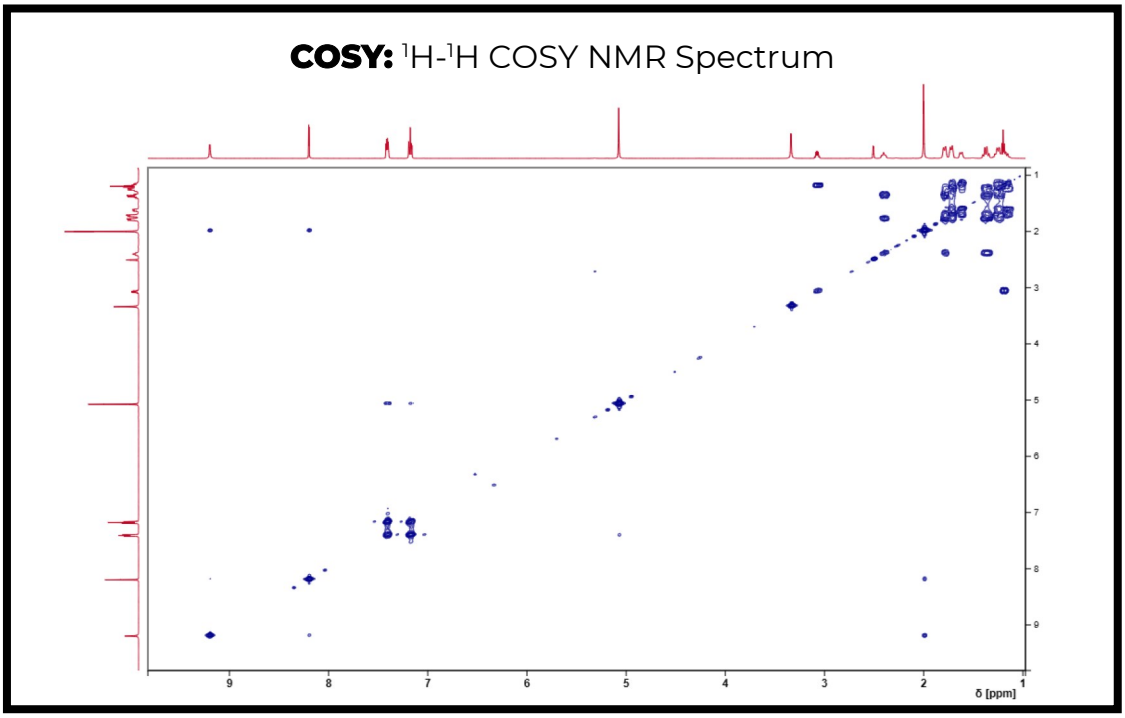
Laboratory: IteraMed™ (Doylestown, PA, USA)

Instrument: Various (See Link Below)

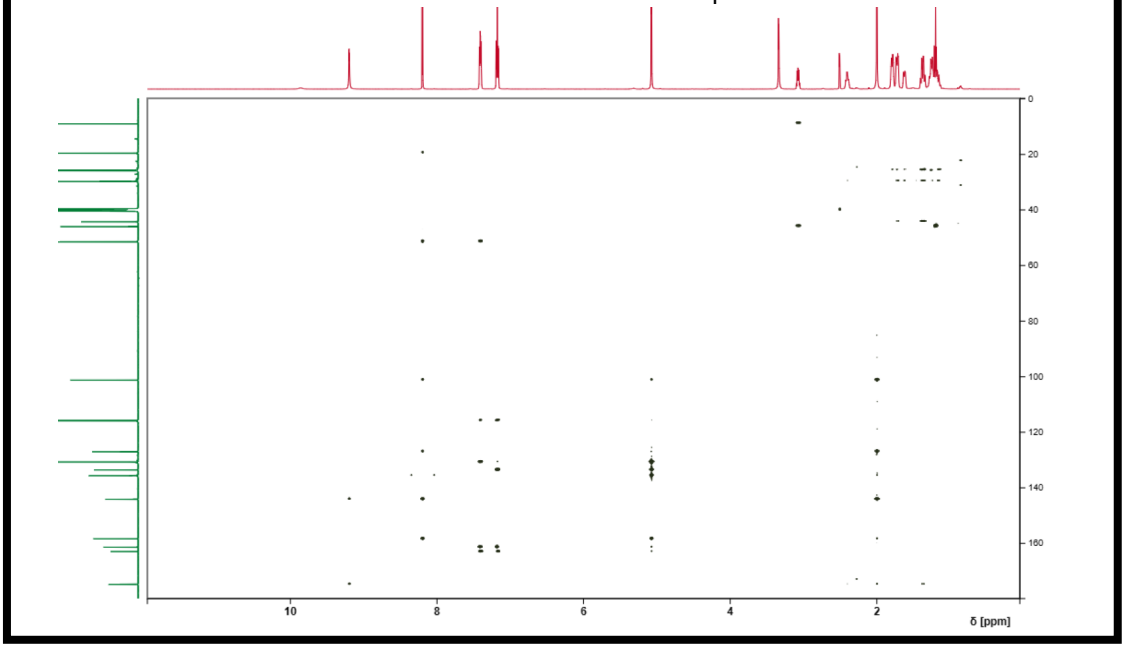
Sample Preparation: Dilution in DMSO-D6

Methods: www.cfsre.org/nps-discovery/monographs

COSY: ^{1}H-^{1}H COSY NMR Spectrum



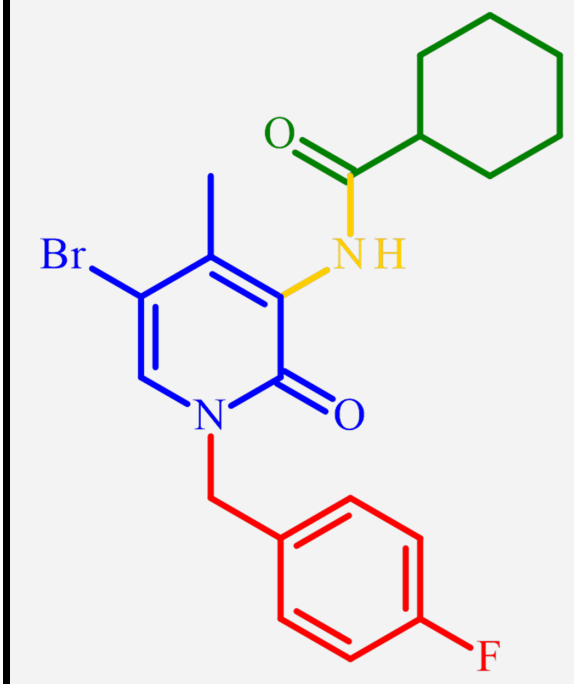
HMBC: ^{1}H-^{13}C HMBC NMR Spectrum



Systematic Nomenclature

As new drugs emerge for the first time and their structures are characterized, scientists are faced with the difficult decision of selecting a commonly preferred name — a process that encompasses evaluation of prior peer-reviewed literature, historical naming conventions, and future considerations. Scientists at the Center for Forensic Science Research and Education (CFSRE) and Cayman Chemical continue to develop and expand appropriate naming conventions using systematic approaches pertaining to a variety of NPS subclasses. The products of this work continue to be codified within our collective publications, reports, and other work products.

Preferred names for synthetic cannabinoids are often determined by the use of alpha-numeric sequences correlating to components of the drug's formal name and molecular features (e.g., **core**, **tail**, **head**, **linker**). The name ***CHO-4'Me-5'Br-FUBOXPYRA*** was established based on the details outlined below.



Formal Name:

N-(5-Bromo-1-(4-FlUoroBenzyl)-4-Methyl-2-OXo-1,3-dihydroPYRidin-3-yl)CycloHexanecarbOxAmide

Preferred Name:

CHO-4'Me-5'Br-FUBOXPYRA