DEA TOX
DRUG ENFORCEMENT ADMINISTRATION
TOXICOLOGY TESTING PROGRAM

UCSF Clinical Toxicology and Environmental Biomonitoring Laboratory

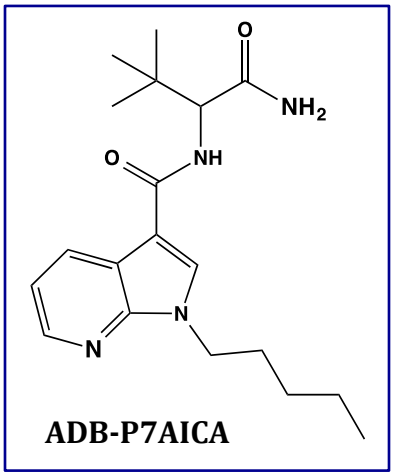
Announcement of a Newly Identified Synthetic Cannabinoid ADB-P7AICA – February 25, 2021

The US Drug Enforcement Administration in collaboration with the University of California San Francisco Clinical Toxicology and Environmental Biomonitoring (CTEB) Laboratory has identified a new synthetic cannabinoid, ADB-P7AICA, in urine samples submitted to our New Psychoactive Substances (NPS) surveillance program.[1]

Cohort: In November 2020, prisoners under a work release program in Alabama were suspected of using tianeptine and a suspected synthetic cannabinoid-laced drug product inmates referred to as "No Show".

Drugs Detected: ADB-P7AICA was detected, confirmed and quantified in the cohort. The majority of urine samples from these individuals contained tianeptine and 4-CN-AMB-BUTINACA. Other prominent substances detected in these samples include cathinones (pentedrone, N-butylpentylone and N-ethylbuphedrone (NEB)), amphetamines (ethylamphetamine and PMMA[2]), and phenibut.

ADB-P7AICA: 7-azaindole synthetic cannabinoid receptor agonists such as 5F-Cumyl-P7AICA were first identified in 2015.[3] 5F-Cumyl-P7AICA is a potent CB_1 agonist (EC_{50}=4.7 nM) that can induce significant hypothermia in mice (6°C, 3 mg/kg) through a CB_1-dependent mechanism.[4] This new synthetic cannabinoid (ADB-P7AICA) is related to a number of previously reported 7-azaindole synthetic cannabinoids including 5F-AB-P7AICA, which was first reported by the European Monitoring Center for Drugs and Drug Addiction (EMCDDA) in 2018.[5]



ADB-P7AICA

Analysis: ADB-P7AICA was detected, confirmed and quantified in urine samples using liquid chromatography-quadrupole time-of-flight mass spectrometry. Details of the method used along with the chromatogram and mass spectra associated with the compound are presented below.

Reference Standard: There is currently no commercially available reference standard for ADB-P7AICA. A reference standard of this substance was synthesized by our program collaborator at the University of Sydney, Dr. Samuel Banister. Chemical characterization of the reference standard was performed by Mr. Eric Sparkes and Dr. Adam Ametovski and is detailed below. This reference standard is part of the prophetic cannabinoids standards library proactively synthesized to allow our surveillance to identify and confirm previously unreported NPS in real time.

Pharmacological Data: The Banister Lab at the University of Sydney is currently acquiring pharmacological data for this compound and will publish the results as soon as it becomes available.

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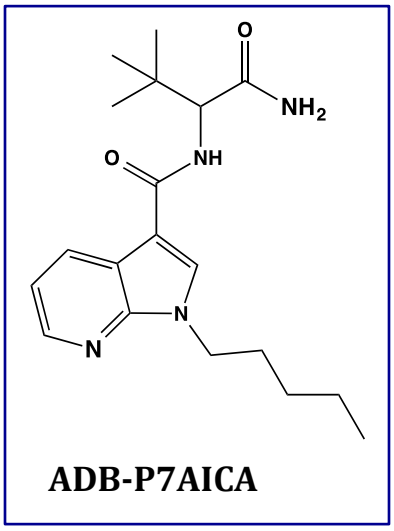
[1] This report was prepared by Roy Gerona, Ross Ellison, Eric Sparkes, Adam Ametovski, Shuli Chen, Michelle Glass, Samuel Banister and Jordan Trecki.
[2] PMMA [1-(4-methoxyphenyl)-*N*-methylpropan-2-amine; *para*-methoxymethamphetamine
[3] Europol. 2015. Annual Report on the implementation of Council Decision 2005/387/JHA
[4] Banister SD, Adams A, Kevin RC, Macdonald C, Glass M, Boyd R, Connor M, McGregor IS, Havel CM, Bright SJ, Ventura Vilamala M, Gil Lladanosa C, Barratt MJ, Gerona RR (August 2018). Synthesis and pharmacology of new psychoactive substance 5F-CUMYL-P7AICA, a scaffold-hopping analog of synthetic cannabinoid receptor agonists 5F-CUMYL-PICA and 5F-CUMYL-PINACA. Drug Testing and Analysis. 11 (2): 279–291
[5] EMCDDA. 2018. Formal notification of N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl)-1H-pyrrolo[2,3-b]pyridine-3-carboxamide (5F-AB-P7AICA) by Germany as a new psychoactive substance under the terms of Council Decision 2005/387/JHA, In EU Early Warning System Formal Notification, European Monitoring Centre for Drugs and Drug Addiction, Lisbon, Portugal.

ADB-P7AICA

I General Information



Synonyms: ADB-P7AICA

IUPAC Name: (*S*)-*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1*H*-pyrrolo[2,3-*b*]pyridine-3-carboxamide

InChi String: InChI=1S/C19H28N4O2/c1-5-6-7-11-23-12-14(13-9-8-10-21-17(13)23)18(25)22-15(16(20)24)19(2,3)4/h8-10,12,15H,5-7,11H2,1-4H3,(H2,20,24)(H,22,25)/t15-/m1/s1

InChi Key: QDZHLYBDQFZWCJ-OAHLLOKOSA-N

SMILES:
O=C(N[C@@H](C(C)(C)C)C(N)=O)C1=CN(CCCCC)C2=C1C=CC=N2

CAS Number: Not available

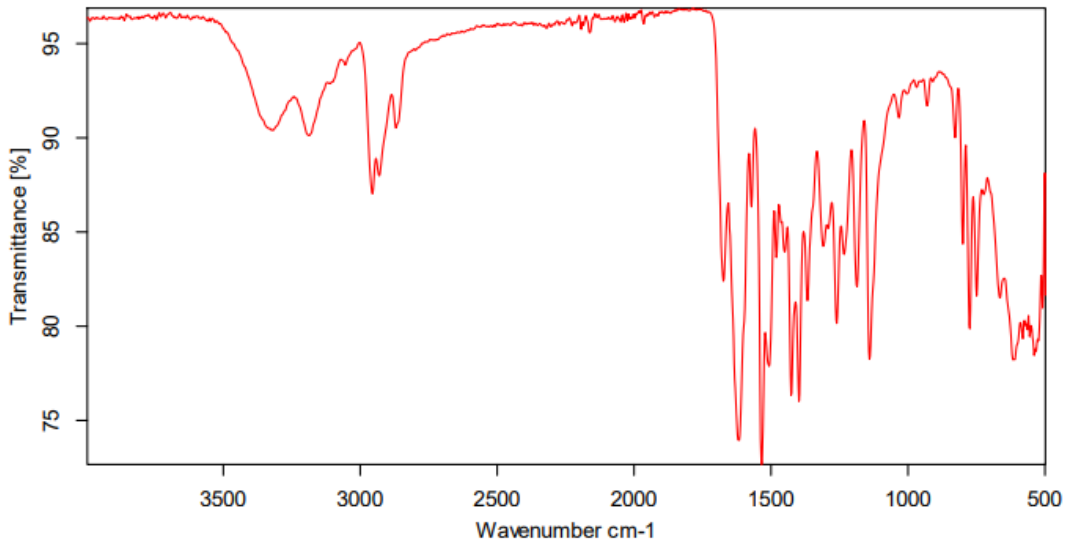
CFR: Not scheduled (02/2021)

II Physical Properties

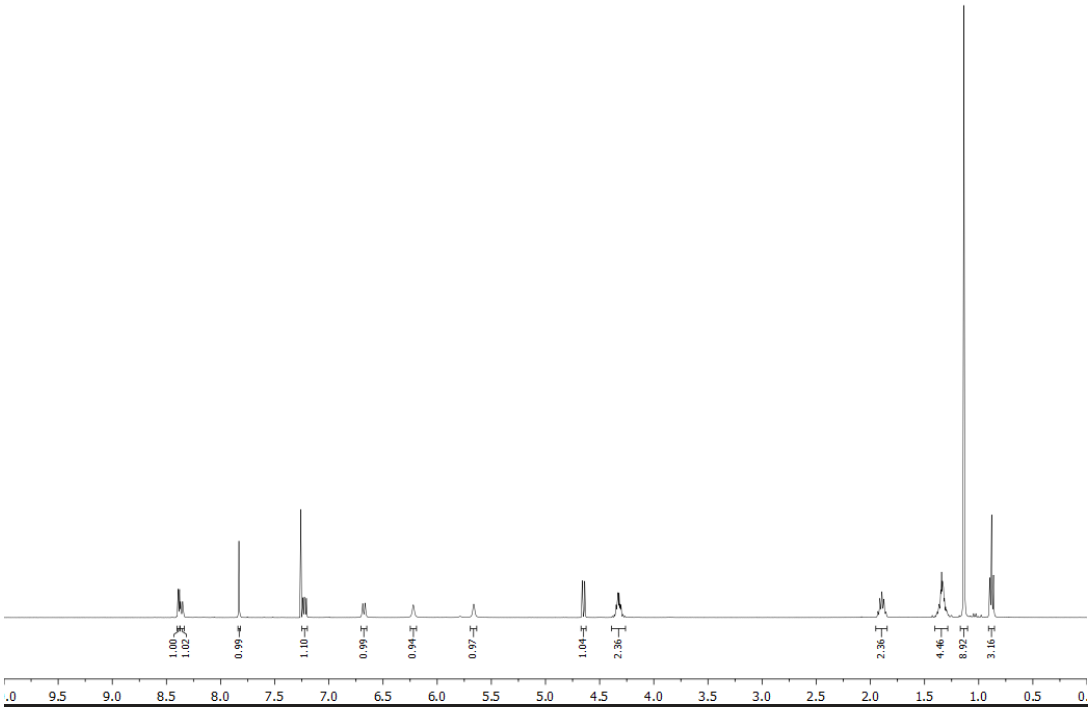
Melting Point: 87 – 88 °C

III Chemical Characterization

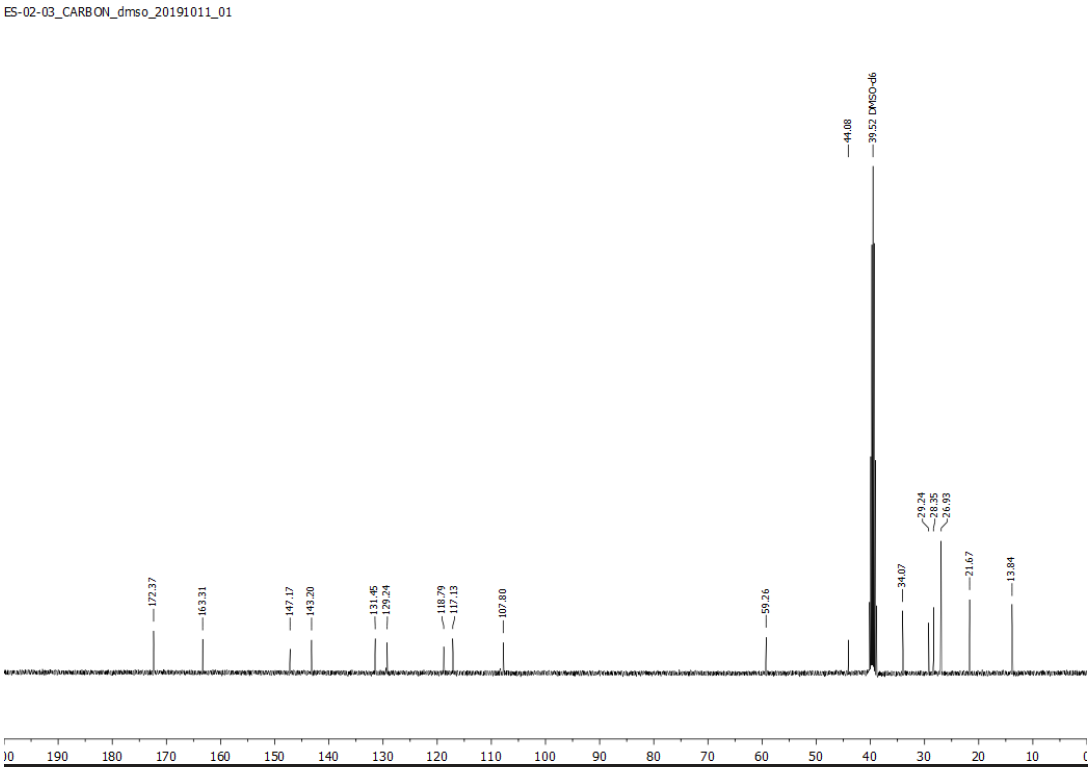
FTIR Spectrum: ν_{max} (cm^{-1}): 3186, 2955, 1674, 1617, 1534, 1426, 1398, 1367, 1260, 1187, 1140, 800, 775, 749, 610.



^{1}H NMR Spectrum: (400 MHz, $CDCl_3$) δ 8.43 – 8.32 (m, 2H), 7.83 (s, 1H), 7.22 (dd, J = 8.0, 4.8 Hz, 1H), 6.68 (d, J = 9.1 Hz, 1H), 6.22 (s, 1H), 5.68 – 5.64 (m, 1H), 4.65 (d, J = 9.2 Hz, 1H), 4.33 (td, J = 7.1, 3.4 Hz, 2H), 1.95 – 1.83 (m, 2H), 1.42 – 1.23 (m, 4H), 1.14 (s, 9H), 0.93 – 0.84 (m, 3H)



^{13}C NMR Spectrum: (101 MHz, DMSO-d_6) δ 172.4 ($(CO)NH_2$), 163.3 (CO), 147.2 (quat.), 143.2 (CH), 131.5 (CH), 129.2 (CH), 118.8 (quat.), 117.1 (CH), 107.8 (quat.), 59.3 (NHCH), 44.1 (NCH_2), 34.1 (CH), 29.2 (CH_2), 28.4 (CH_2), 26.9 (3 × CH_3), 21.7 (CH_2), 13.8 (CH_3)



IV LC-QTOF/MS Analysis

Instrument: Agilent 1260 Infinity, Agilent 6550 QTOF-MS/MS

Sample Preparation: Enzymatic deconjugation with *H pomatia* glucuronidase followed by dilution

Chromatography

***Column*:** Agilent Poroshell 120 EC-C18 (100 mm x 2.1 mm, 2.7 µm)

Column Temperature: 50 °C

Injection Volume: 2.5 µL

***Mobile Phase*:** A: Ammonium formate (5 mM) and Formic Acid (12.6 mM) in H_2O

B: Formic Acid (12.6mM) in acetonitrile

***Flow rate*:** 0.5 mL/min

***Elution Profile*:** Gradient- 95A:5B initially; 70A:30B from 0.5 to 1.5 min; 30A:70B from 1.5 to 4.5 min; 0A:100B from 4.5 to 7.5min; 95A:5B from 10.0 to 14.0 min

Run Time: 12 min

Mass Spectrometry

***Ion Source*:** Dual Jet Stream Electrospray Ionization

***Polarity*:** Positive

***TOF MS Scan Range*:** 75-1000 Da

***MS/MS Scan Range*:** 50-510 Da

Gas Temperature: 225 °C

Drying Gas Flow Rate: 14L/min

Sheath Gas Temperature: 350 °C

Sheath Gas Flow Rate: 11L/min

Nebulizer pressure: 14psi

Capillary Voltage: 3000 V

Nozzle Voltage: 500 V

Skimmer Voltage: 65 V

Octopole RF: 750 V

Fragmentor Voltage: 380 V

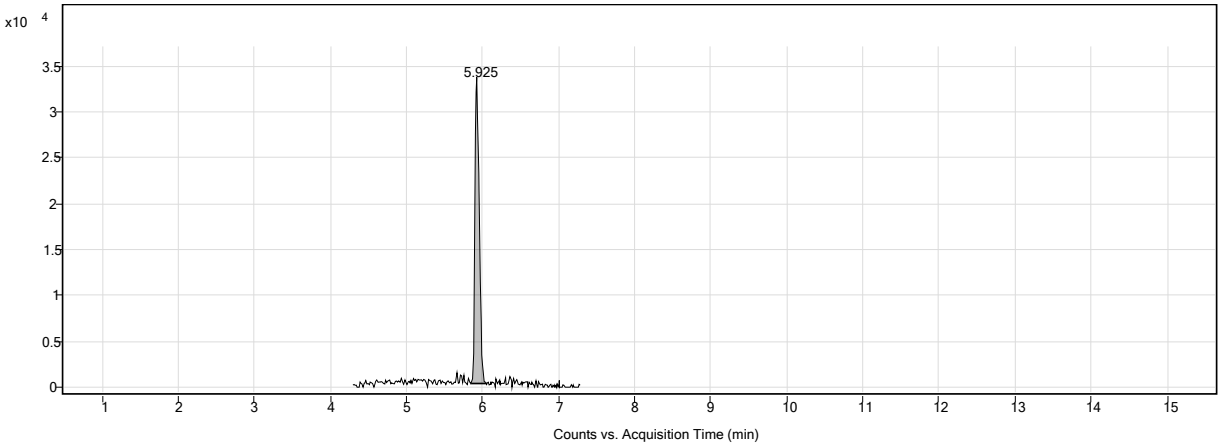
Internal Reference Masses: Purine at m/z 121.0509; HP-921 at m/z 922.0098

Data Acquisition: 2GHz, extended dynamic range

Fragmentation: Auto MS/MS, three maximum precursors (threshold: 500 counts) per cycle with active exclusion after 1 spectrum at a 30s release time

Extracted Ion Chromatogram

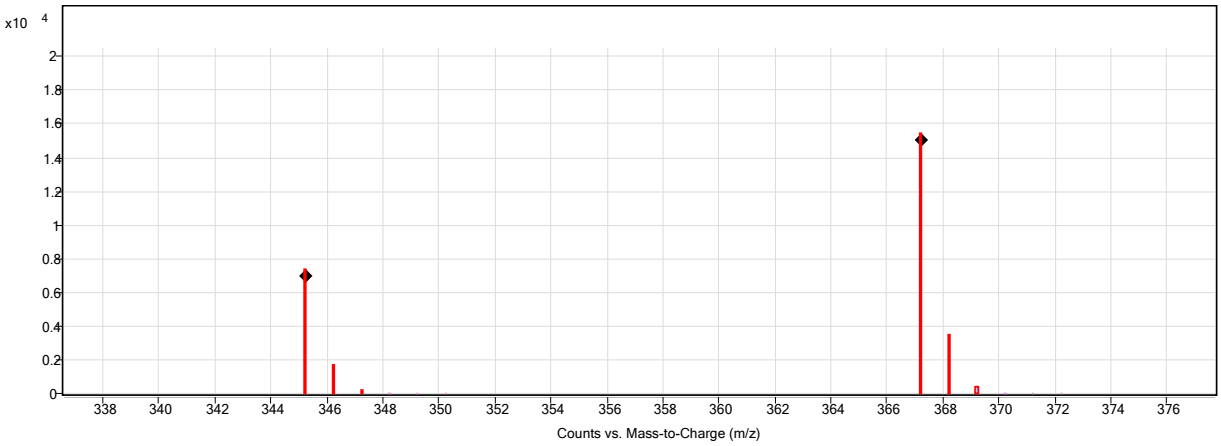
***Retention Time*:** 5.925 min



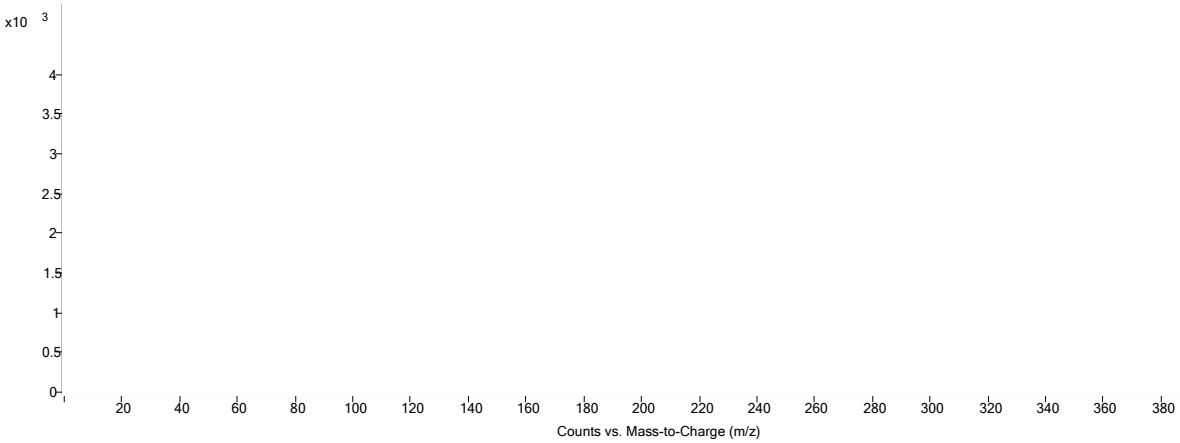
TOF-MS Spectrum

***Exact Mass*:** 344.2212

***Accurate Mass*:** $[M+H]^+$= 345.2287 (mass error= 0.26ppm); $[M+Na]^+$=367.2102 (mass error= -0.82 ppm)



MS/MS Spectrum



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TOXICOLOGY TESTING PROGRAM

U. S. Department of Justice
Drug Enforcement Administration
Diversion Control Division
Drug & Chemical Evaluation Section
Toxicology Testing Program
DEATOX@USDOJ.GOV

www.dea.gov

In response to the ongoing synthetic drug epidemic, the Drug Enforcement Administration (DEA) has initiated a contract with the University of California at San Francisco (UCSF) whereby biological samples generated from overdose victims of synthetic drugs can be further analyzed. In many cases, it can be difficult to ascertain the specific substance responsible for the overdose. In the future, we invite you to contact our program if you encounter an overdose of a suspected synthetic drug and desire to have any leftover biological samples (blood preferred) analyzed further for such synthetic substances.

- **Sample Qualifications:**
  - Patients thought to have ingested a synthetic drug, where the traditional drug screen has produced little or no viable options to explain the symptoms exhibited by the patient (alcohol and THC are exempted)
- **How to Contact Us and Send Your Samples:**
  - Once the above qualifications are satisfied:
    - Email DEATOX@USDOJ.GOV with a brief description of the case (including initial toxicology screen and history) and a request for testing.
    - DEA will respond to each inquiry, and if approved, will send the instructions for packing and shipping of sample(s) to UCSF.
      - The main reason for disapproval of a case would be the identification of substances including methamphetamine, heroin, fentanyl, cocaine, LSD, PCP etc. in a routine toxicology screening at your facility.
      - This program's goal is to connect symptom causation to abuse of newly emerging synthetic drugs (i.e. synthetic cannabinoids, synthetic cathinones, fentanyl-related substances, other hallucinogens etc.).
    - Ensure that you de-identify and label the sample with a numerical value, sex, date of birth or age, and the date and time the sample was collected in accordance with the labeling instructions (sent with shipping instructions).
    - Keep a master list of the patients and the numerical values you allocated to each sample at your institution.
- **Cost of sample analysis:**
  - DEA will cover the full cost of testing the patient samples.
  - The sender will only be responsible for paying for packing and shipping samples to UCSF.
- **Turn-around Time:**
  - Results are expected within three weeks of receipt of the sample at UCSF except in rare occurrences when a novel substance is identified.

Public Domain Notice

Suggested citation:
U.S. Drug Enforcement Administration, Diversion Control Division. (2021). *DEA-TOX: Announcement of a Newly Identified Synthetic Cannabinoid ADB-P7AICA – February XX, 2021*. Springfield, VA: U.S. Drug Enforcement Administration.

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DEA PRB 02-24-21-16