DEA TOX

DRUG ENFORCEMENT ADMINISTRATION

TOXICOLOGY TESTING PROGRAM

UCSF Clinical Toxicology and Environmental Biomonitoring Laboratory

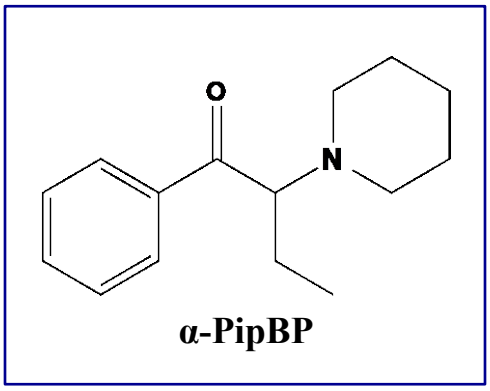
# Announcement of a Newly Identified Cathinone alpha-Piperidinobutiophenone (α-PipBP)– March 23, 2021

The US Drug Enforcement Administration (DEA) in collaboration with the University of California San Francisco Clinical Toxicology and Environmental Biomonitoring (CTEB) Laboratory has identified a new cathinone, alpha-piperidinobutiophenone (α-PipBP), in a urine sample submitted to our New Psychoactive Substances (NPS) surveillance program[1].

**Cohort**: In January 2021, samples from individuals under court-ordered urinalysis in Alabama were submitted.

**Drugs Detected**: alpha-Piperidinobutiophenone was confirmed and quantified in one of the submitted samples. The major substances detected in the cohort include 1-(4-Chlorophenyl)piperazine (p-CPP), methamphetamine, and morphine. Other drugs confirmed within this cohort included N-butyl pentylone, N-ethyl hexylone, NRG-3, sufentanil, and tianeptine.

**α-PipBP**: This cathinone is related to a number of previously reported cathinones such as alpha-pyrrolidinobutiophenone (α-PBP), a popular butyrophenone. α-PBP is a stimulant developed in the 1960s[2] that has been reported as an NPS in the previous decade.[3] α-PBP, similar to other cathinones including α-PVP and MDPV, is reported to block dopamine and norepinephrine transporters and is demonstrated to have locomotor stimulant activity in mice.[4] Our search of the published literature indicate that there have been no previous reports of α-PipBP being detected in biologic samples.



α-PipBP

**National Forensic Laboratory Information System (NFLIS)[5]:** Three exhibits submitted to NFLIS confirmed the presence of α-PipBP. The first two exhibits were submitted in August of 2017, while the third exhibit was submitted in February of 2018. All three exhibits were reported to be in liquid form and were seized in Georgia.

**Analysis**: α-PipBP was detected, confirmed and quantified in urine sample 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 in the attached supporting documents.

**Reference Standard**: A reference standard for α-PipBP is currently available.[6]

**Pharmacological Data**: No pharmacological data for α-PipBP is currently available.

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[1] This report was prepared by Roy Gerona, Ross Ellison, and Jordan Trecki.

[2] Ernst Seeger. A-Pyrrolidinyl ketones. US Patent 3314970.

[3] Wurita A, Hasegawa K, Minakata K, Gonmori K, Nozawa H, Yamagishi I, Suzuki O, Watanabe K. 2014. Postmortem distribution of alpha-pyrrolidinobutiophenone in body fluids and solid tissues of a human cadaver. Leg Med 16(5): 241-6.

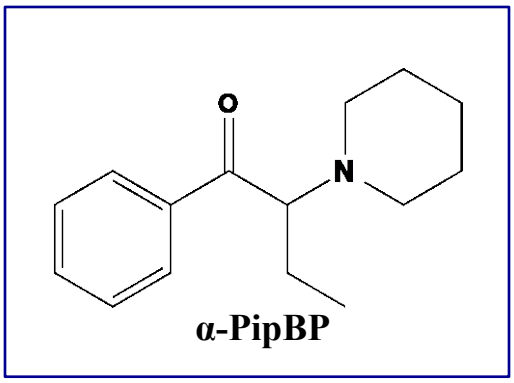
[4] Marusich JA, Antonazzo KR, Wiley JL, Blough BE, Partilla JS, Baumann MH. 2014. Pharmacology of novel synthetic stimulants structurally related to the "bath salts" constituent 3,4-methylenedioxypyrovalerone (MDPV). Neuropharmacol 87: 206-13.

[5] NFLIS is a national forensic laboratory reporting system that systematically collects results from drug chemistry analyses conducted by Federal, State, and local forensic laboratories in the United States.

[6] https://www.caymanchem.com/product/9001513/%CE%B1-piperidinobutiophenone-(hydrochloride)

# alpha-Piperidinobutiophenone

## I General Information




**Synonyms**: α-PipBP

**IUPAC Name**: 1-phenyl-2-(1-pyrrolidinyl)-1-butanone

**InChi String**: InChI=1S/C15H21NO/c1-2-14(16-11-7-4-8-12-16)15(17)13-9-5-3-6-10-13/h3,5-6,9-10,14H,2,4,7-8,11-12H2,1H3

**InChi Key**: VFLPICJWFQLLSY-UHFFFAOYSA-N
**SMILES:** O=C(C(N1CCCC1)CC)C2=CC=CC=C2

**CAS Number:** 92728-82-0

**CFR:** Not scheduled (03/2021)

## II Physical Properties

**Solubility**: DMSO: 0.5 mg/mL

Ethanol: 1mg/mL

## III Chemical Characterization

**GC-MS:** The GC-MS spectrum for α-PipBP is available at Cayman Chemical- https://www.caymanchem.com/gcms/9001513-0453871-GCMS.pdf

## 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

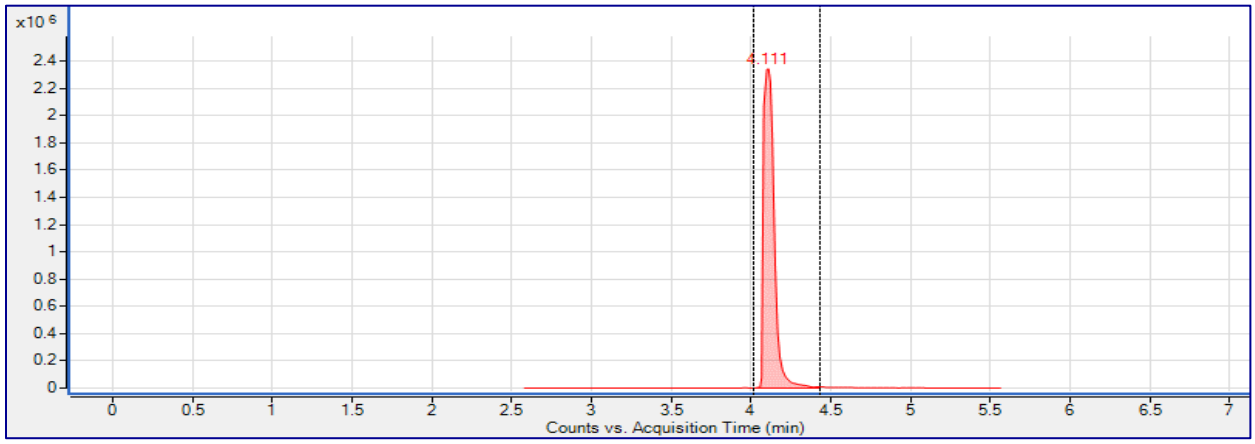
***MS/MS Scan Range*:** 50-510 Da

***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**

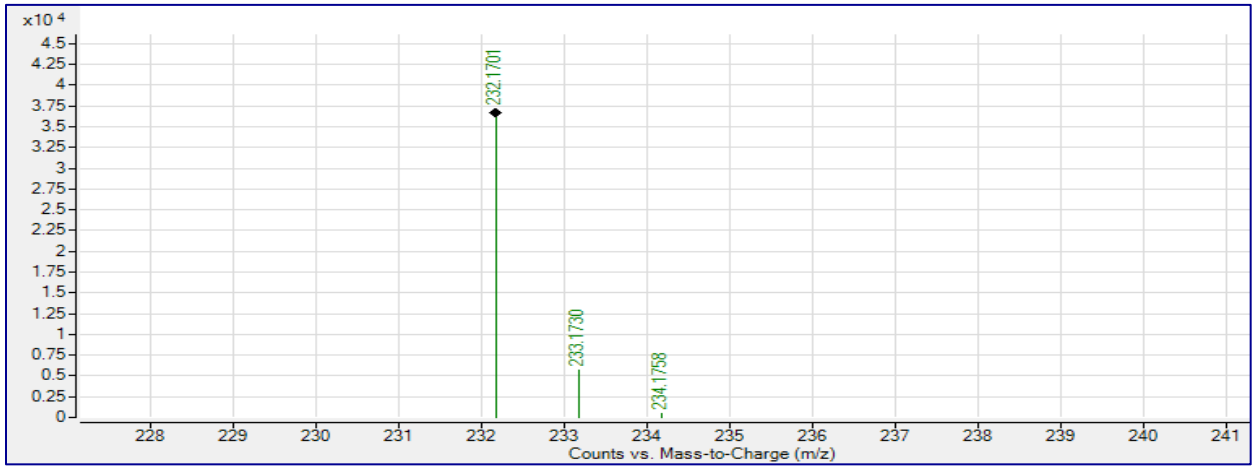
***Retention Time*****:** 4.11 min



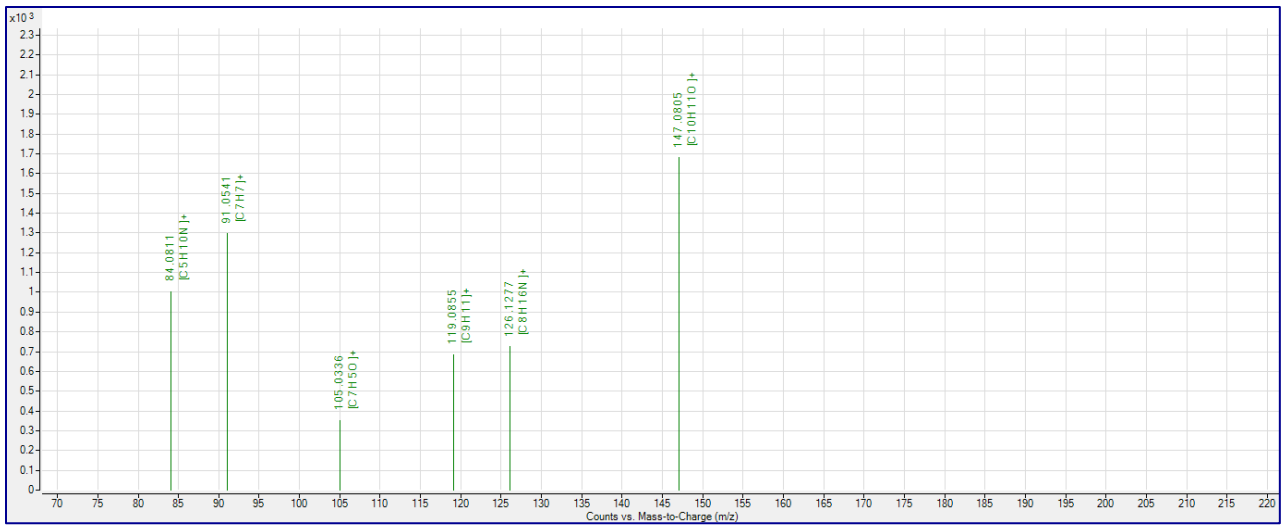

**TOF-MS Spectrum**

***Exact Mass*****:** 231.1628

***Accurate Mass*****:** $[M+H]^+$= 232.1701 (mass error = -1.93 ppm)




**MS/MS Spectrum**


x10 3
84.0811
[C5H10N]+
91.0541
[C7H7]+
105.0336
[C7H5O]+
119.0855
[C9H11]+
126.1277
[C8H16N]+
147.0805
[C10H11O]+
Counts vs. Mass-to-Charge (m/z)

**DEA TOX**
DRUG ENFORCEMENT ADMINISTRATION
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:**
  - The 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:*
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# Obtaining Copies of This Publication

Electronic copies of this publication can be downloaded from the DEA-TOX website at https://www.deadiversion.usdoj.gov/dea_tox/index.html.

This report was produced in conjunction with the CTEB laboratory at UCSF.


Clinical Toxicology
and Environmental Biomonitoring Laboratory

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