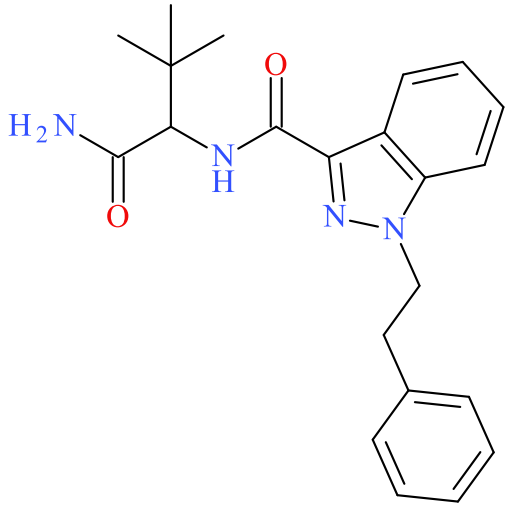
# ADB-PHETINACA

Sample Type: **Biological Sample**



Latest Revision: **November 19, 2021**

Date Received: **October 18, 2021**

Date of Report: **November 19, 2021**

## 1. GENERAL INFORMATION

| | |
|---|---|
| **IUPAC Name:** | N-(1-carbamoyl-2,2-dimethyl-propyl)-1-(2-phenylethyl)indazole-3-carboxamide |
| **InChI String:** | InChI=1S/C22H26N4O2/c1-22(2,3)19(20(23)27)24-21(28)18-16-11-7-8-12-17(16)26(25-18)14-13-15-9-5-4-6-10-15/h4-12,19H,13-14H2,1-3H3,(H2,23,27)(H,24,28) |
| **CFR:** | Not Scheduled (11/2021) |
| **CAS#** | Not Available |
| **Synonyms:** | ADB-PHTINACA |
| **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.*

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## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

| Drug | Chemical Formula | Molecular Weight | Molecular Ion $[M^+]$ | Exact Mass $[M+H]^+$ |
|---|---|---|---|---|
| ADB-PHETINACA | $C_{22}H_{26}N_4O_2$ | 378.5 | 378 | 379.2129 |

## 3. SAMPLE HISTORY

To date, ADB-PHETINACA was identified in one case in October 2021. The geographical and demographical breakdown is below:

**Geographical Location:** New Jersey

**Biological Sample:** Serum

**Date of First Receipt:** October 2021

**Other Notable Findings:** Fentanyl

## 4. BRIEF DESCRIPTION

ADB-PHETINACA 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 regarding ADB-PHETINACA is currently available, specifically regarding activity and potency. “PHET” is used in the name of this synthetic cannabinoid to represent the phenethyl tail group compared to prior “P” used for pentyl or “FUB” used for fluorobenzyl. ADB-PINACA and ADB-FUBINACA are structurally similar synthetic cannabinoids. ADB-PINACA and ADB-FUBINACA are Schedule I substances in the United States; currently, ADB-PHETINACA is not a scheduled substance.

## 5. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/ADB-PHETINACA-ID-2996-21_report.pdf

https://www.caymanchem.com/product/33194/adb-phetinaca

## 6. QUALITATIVE DATA

### 6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

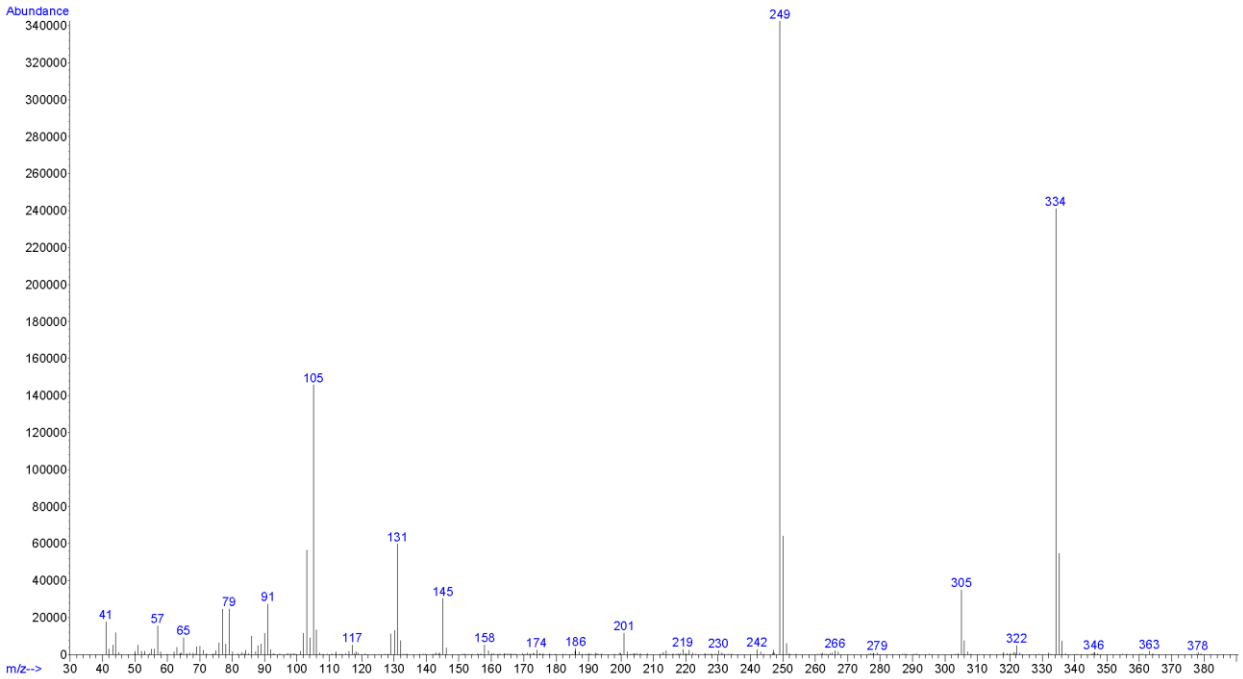
**Testing Performed At:** The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

**Sample Preparation:** Standard diluted in methanol

**Instrument:** Agilent 5975 Series GC/MSD System

**Standard:** Reference material for ADB-PHETINACA (Batch: 0610717-2) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/33194/adb-phetinaca)

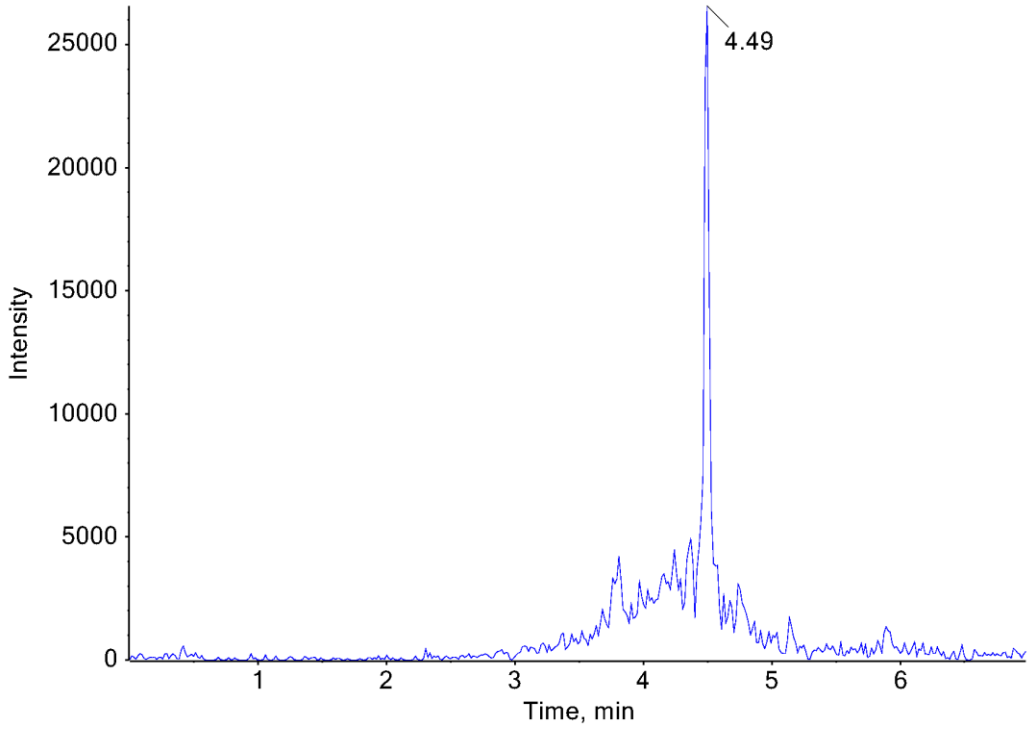
**EI (70 eV) Mass Spectrum: ADB-PHETINACA (Standard)**



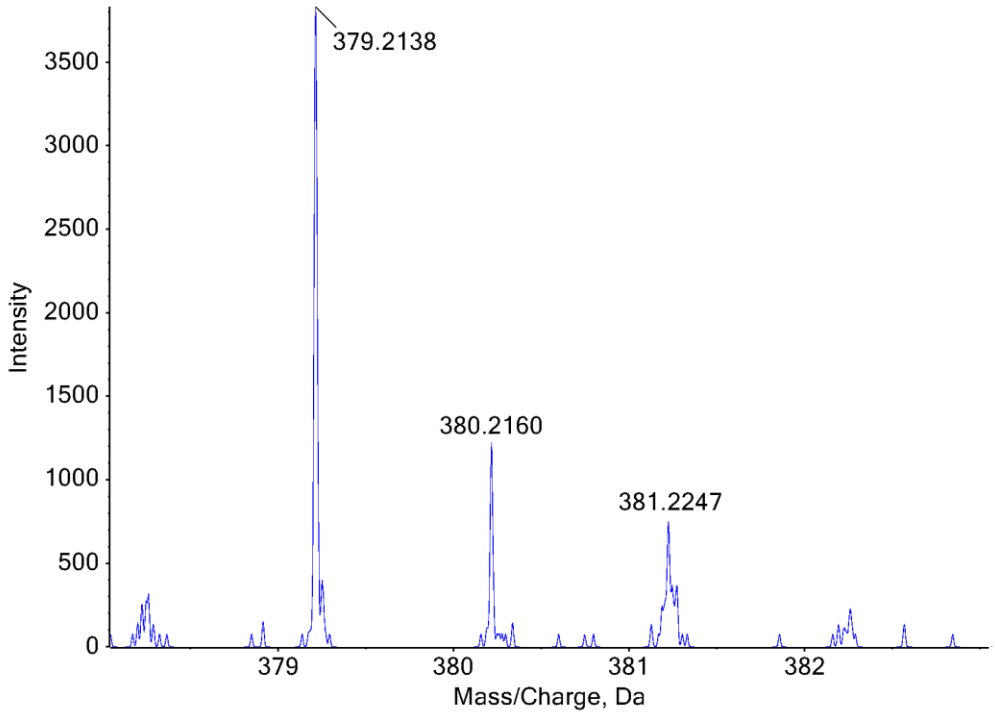
## 6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

| | |
|---|---|
| **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) – diluted 3+2 with DI $H_2O$ |
| **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) with 0.1% formic acid |
| | Flow rate: 0.5 mL/min |
| **Gradient:** | Initial: 95A:5B; 5A:95B over 4 min, hold 2 min; 95A:5B at 7 min |
| **Temperatures:** | Autosampler: 15 °C |
| | Column Oven: 30 °C |
| | Source Heater: 600 °C |
| **Injection Parameters:** | Injection Volume: 20 µL |
| **QTOF Parameters:** | TOF MS Scan Range: 100-550 Da |
| | Precursor Isolation: SWATH® acquisition (10-25 Da) |
| | Fragmentation: Collison Energy Spread (35±15 eV) |
| | MS/MS Scan Range: 50-550 Da |
| **Retention Time:** | 4.49 min |
| **Standard Comparison:** | Reference material for ADB-PHETINACA (Batch: 0610717-2) 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 ADB-PHETINACA, based on retention time (4.51 min) and mass spectral data. (https://www.caymanchem.com/product/33194/adb-phetinaca) |

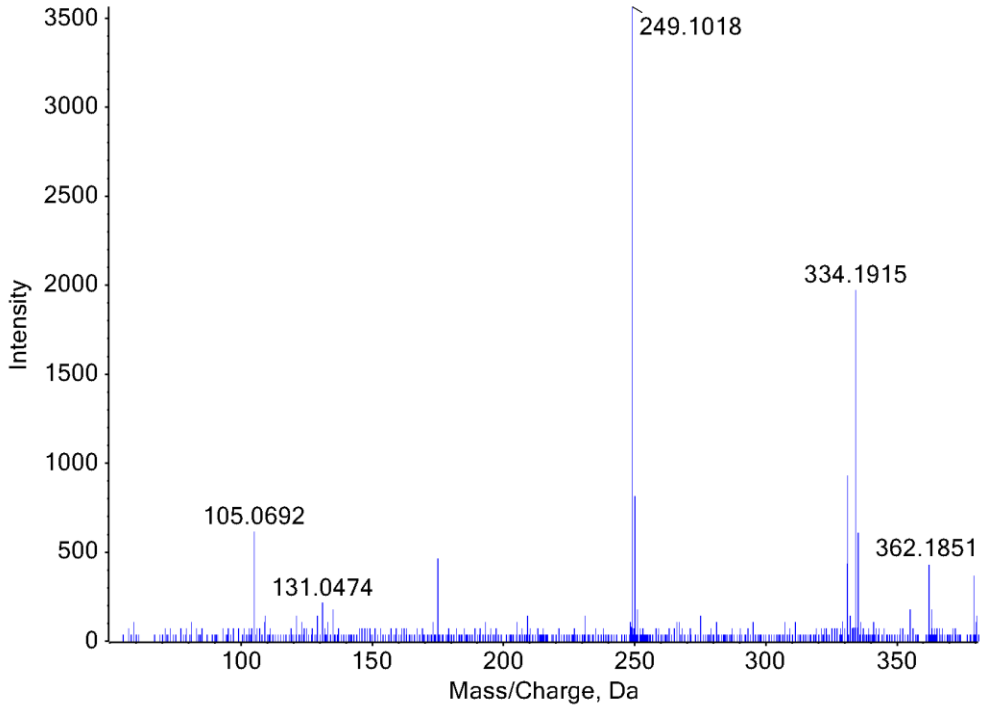
**Extracted Ion Chromatogram: ADB-PHETINACA**




**TOF MS Spectra: ADB-PHETINACA**



**MS/MS Spectra: ADB-PHETINACA**




## 7. FUNDING

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