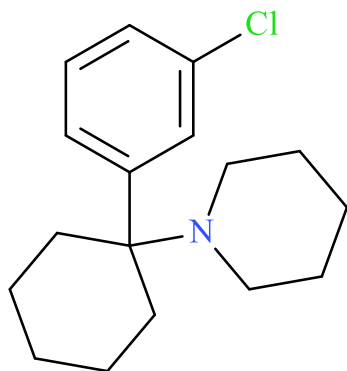


## Cl-PCP

Sample Type: **Biological Fluid**

Latest Revision: **February 4, 2021**

Date of Report: **February 4, 2021**



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-[1-(3-chlorophenyl)cyclohexyl]piperidine
<b>InChI String:</b>	InChI=1S/C17H24ClN/c18-16-9-7-8-15(14-16)17(10-3-1-4-11-17)19-12-5-2-6-13-19/h7-9,14H,1-6,10-13H2
<b>CFR:</b>	Not Scheduled (02/2021)
<b>CAS#</b>	1934-43-6 (3Cl-PCP)
<b>Synonyms:</b>	3Cl-PCP, 3-Chloro-PCP, 3-Chloro Phencyclidine, 4Cl-PCP, 4-Chloro-PCP, 4-Chloro Phencyclidine
<b>Source:</b>	NMS Labs – Toxicology Department

**Important Notes:** All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The “3-chloro” configuration was used for structural purposes; however, position of the chlorine atom was not confirmed during analysis.

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## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>17</sub> H <sub>24</sub> ClN	277.8	277	278.1670

### 3. SAMPLE HISTORY

Cl-PCP has been identified in at least two toxicology cases since December 2020. The geographical and demographical breakdown is below:

<b>Case Type:</b>	Postmortem (n=2)
<b>Geographical Location:</b>	Indiana (n=2)
<b>Biological Sample:</b>	Femoral Blood (n=2)
<b>Date of First Collection:</b>	November 2020
<b>Additional NPS Findings:</b>	Metonitazene (n=2), Fentanyl (n=2)

### 4. BRIEF DESCRIPTION

Cl-PCP is classified as a novel hallucinogen. Novel hallucinogens have been reported to cause effects similar to ketamine and phencyclidine (PCP). Novel hallucinogens have caused adverse events, including death, as described in the literature. Structurally similar compounds include PCP, MeO-PCP, and HO-PCP. PCP is a Schedule II substance in the United States; however, MeO-PCP, HO-PCP, and Cl-PCP are not explicitly scheduled.

### 5. ADDITIONAL RESOURCES

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/3Cl-PCP-ID-2201-20\\_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/3Cl-PCP-ID-2201-20_report.pdf)

[https://www.caymanchem.com/product/31475/3-chloro-pcp-\(hydrochloride\)](https://www.caymanchem.com/product/31475/3-chloro-pcp-(hydrochloride))

## 6. QUALITATIVE DATA

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

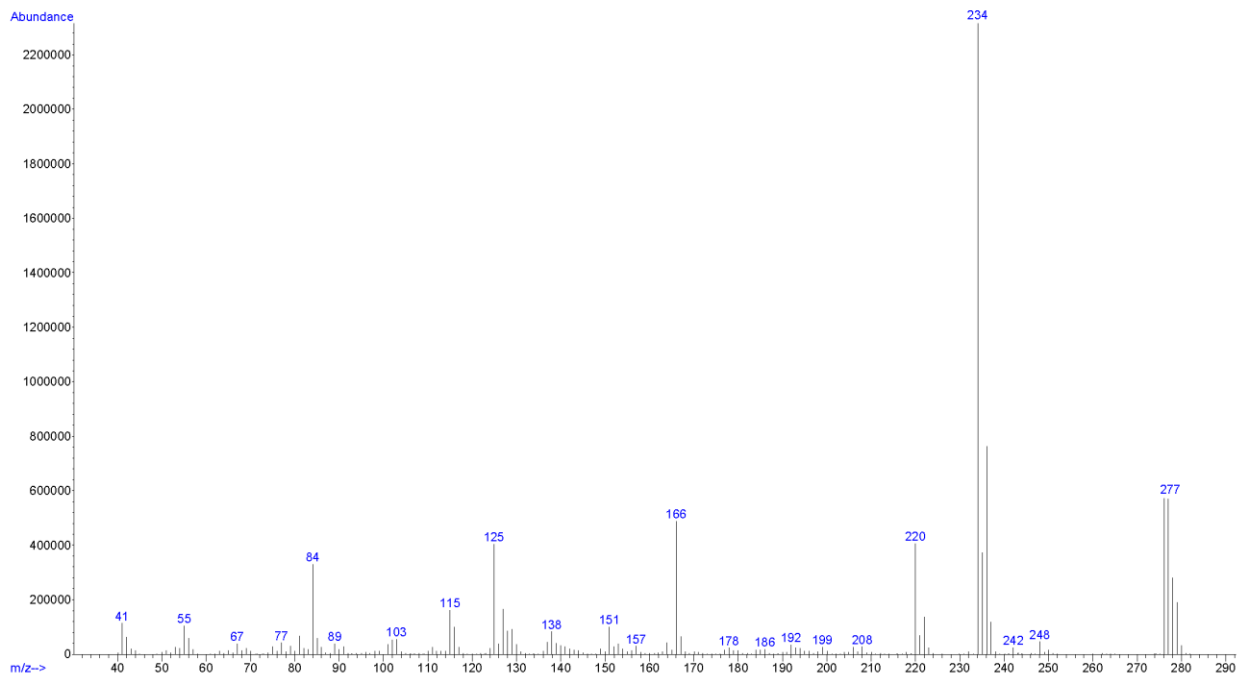
**Testing Performed At:** The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

**Sample Preparation:** Standard diluted in methanol

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

**Standard:** Reference material for 3Cl-PCP (Batch: 0594732-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (<https://www.caymanchem.com/product/31475/3-chloro-pcp-hydrochloride>)

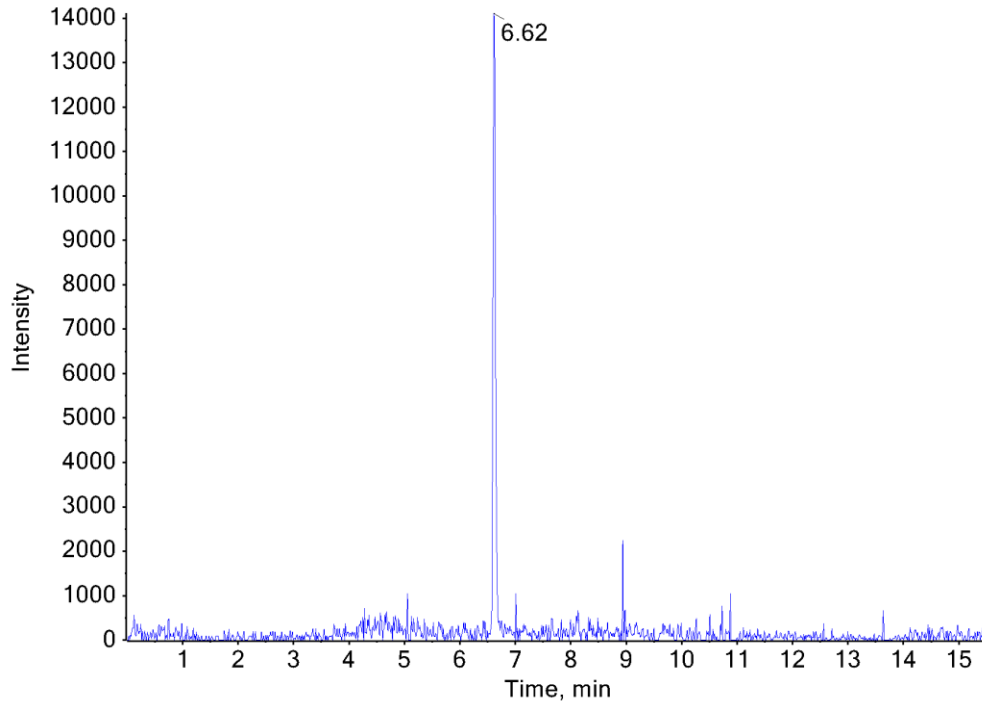
#### EI (70 eV) Mass Spectrum: 3Cl-PCP (Standard)



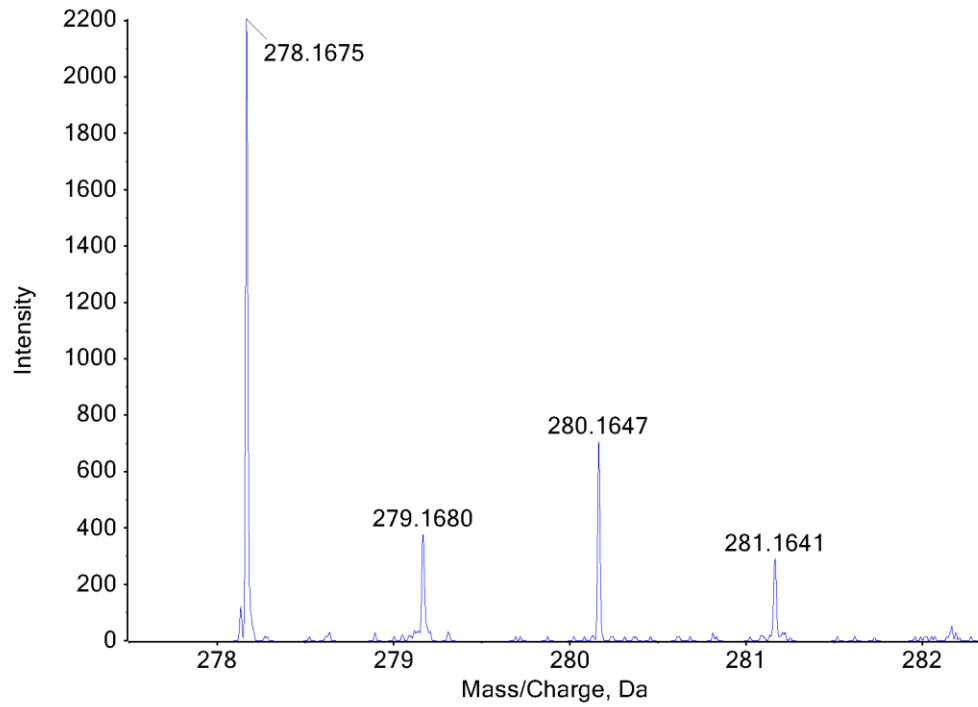
## 6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	No additional preparation - direct analysis of sample extract
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	TOF MS Scan Range: 100-510 Da Precursor Isolation: SWATH® acquisition (27 windows) Fragmentation: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
<b>Retention Time:</b>	6.62 min
<b>Standard Comparison:</b>	Reference material for 3Cl-PCP (Batch: 0594732-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Cl-PCP, based on retention time (6.57 min) and mass spectral data; however, absolute configuration of the structure as 3Cl-PCP vs. 4Cl-PCP was not determined. ( <a href="https://www.caymanchem.com/product/31475/3-chloro-pcp-hydrochloride">https://www.caymanchem.com/product/31475/3-chloro-pcp-hydrochloride</a> )

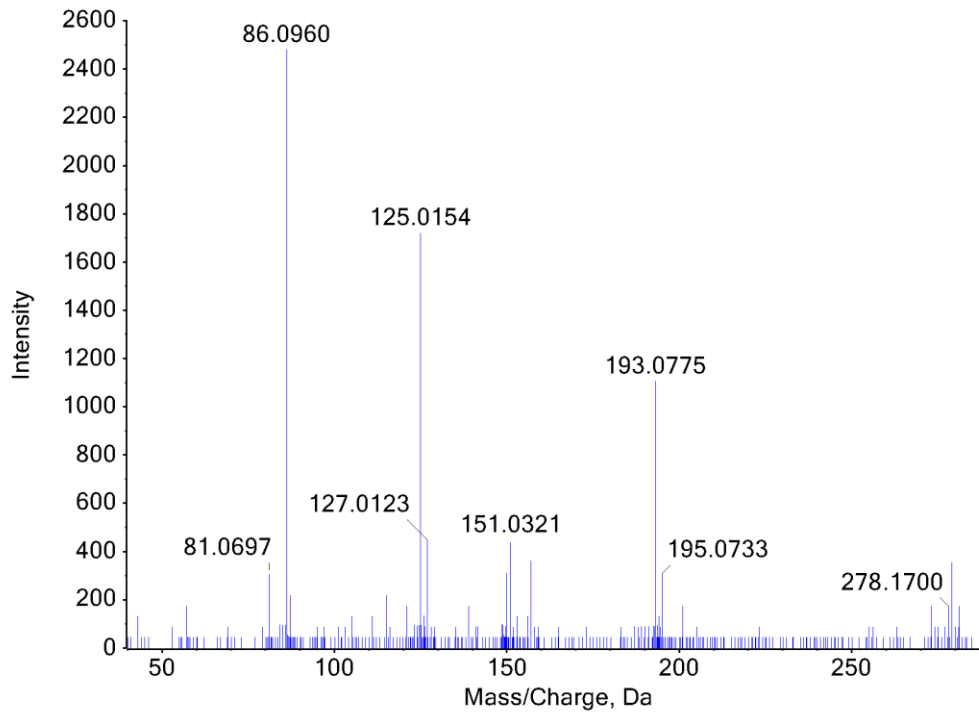
### Extracted Ion Chromatogram: Cl-PCP (Biological Sample)



### TOF MS Spectrum: Cl-PCP (Biological Sample)



## MS/MS Spectrum: Cl-PCP (Biological Sample)



## 7. FUNDING

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