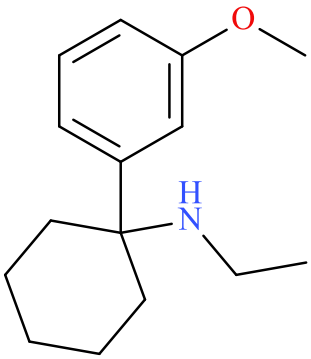
NPS Discovery at CFSRE
2300 Stratford Avenue
Willow Grove, PA 19090

MeO-PCE

Sample Type: **Biological Fluid**



Latest Revision: **December 10, 2020**

Date of Report: **December 10, 2020**

1. GENERAL INFORMATION

IUPAC Name:	N-ethyl-1-(3-methoxyphenyl)cyclohexanamine
InChI String:	InChI=1S/C15H23NO/c1-3-16-15(10-5-4-6-11-15)13-8-7-9-14(12-13)17-2/h7-9,12,16H,3-6,10-11H2,1-2H3
CFR:	Not Scheduled (12/2020)
CAS#	1933-15-9 *(4-MeO-PCE)*
Synonyms:	3-MeO-PCE, 3-methoxy-PCE, 4-MeO-PCE, 4-methoxy-PCE, 3-Methoxyeticyclidine, 4-Methoxyeticyclidine
Source:	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-methoxy" configuration was used for structural purposes; however, position of the methoxy moiety 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 $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{15}H_{23}NO$	233.4	233	234.1852

3. SAMPLE HISTORY

MeO-PCE has been identified in at least one toxicology case since September 2020. The geographical and demographical breakdown is below:

Case Type: Postmortem (n=1)

Geographical Location: Washington (n=1)

Biological Sample: Peripheral Blood (n=1)

Date of First Collection: September 2020

Additional NPS Findings: HO-PCE, 2F-Deschloroketamine, 2-Methyl AP-237, 8-Aminoclonazolam, Flualprazolam, Etizolam

4. BRIEF DESCRIPTION

MeO-PCE 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 deaths, as described in the literature. Structurally similar compounds include PCE (eticyclidine) and HO-PCE. PCE is a Schedule I substance in the United States. 3-HO-PCE was previously reported by NPS Discovery in December 2019. HO-PCE is a suspected metabolite of MeO-PCE.

5. ADDITIONAL RESOURCES

Roth, BL; Gibbons, S; Arunotayanun, W; Huang, XP; Setola, V; Treble, R; Iversen, L. The Ketamine Analogue Methoxetamine and 3- and 4-Methoxy Analogues of Phencyclidine Are High Affinity and Selective Ligands for the Glutamate NMDA Receptor. *PLoS One*. 2013, 8(3), e59334. https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0059334

De Paoli, G; Brandt, SD; Wallach, J; Archer, RP; Pounder, DJ. From the Street to the Laboratory: Analytical Profiles of Methoxetamine, 3-Methoxyeticyclidine and 3-Methoxyphencyclidine and their Determination in Three Biological Matrices. *Journal of Analytical Toxicology*. 2013, 37, 277-283. https://academic.oup.com/jat/article/37/5/277/786406

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/3-MeO-PCE-ID-1732-16_report-final.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-MeO-PCE-ID-1969-18_report.pdf

https://www.caymanchem.com/product/9001355/3-methoxy-pce-(hydrochloride)

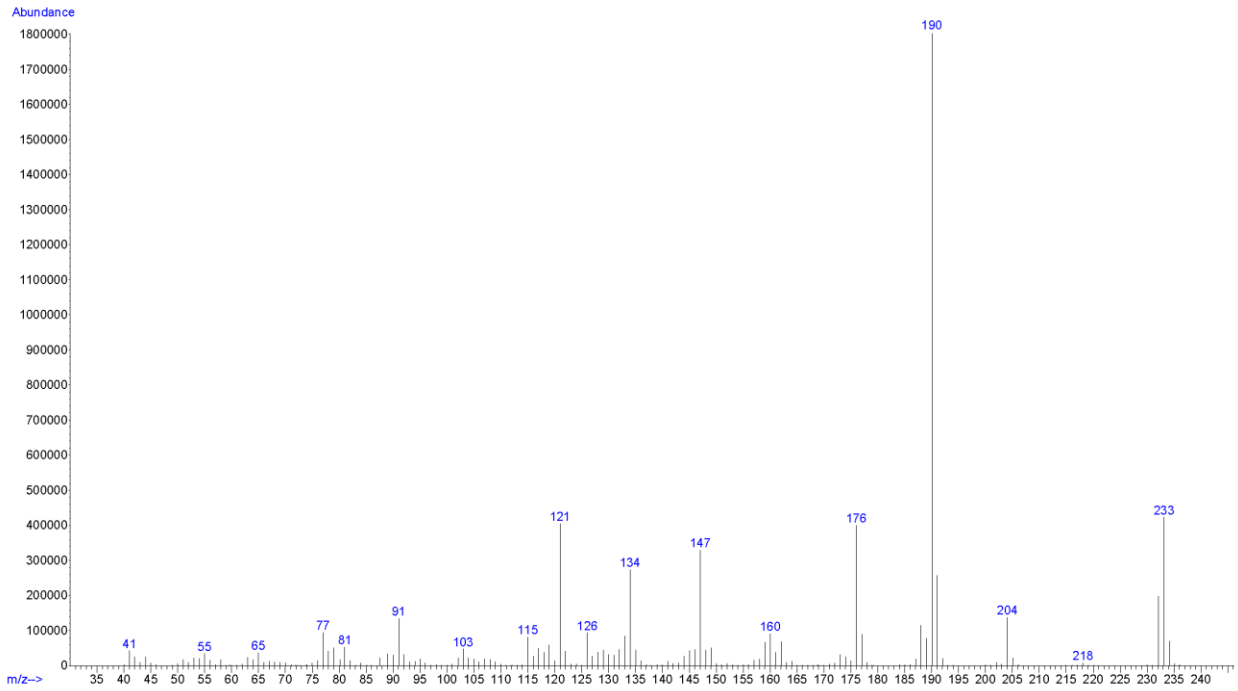
https://www.caymanchem.com/product/9001356/4-methoxy-pce-(hydrochloride)

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 3-MeO-PCE (Batch: 0459577-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/9001355/3-methoxy-pce-(hydrochloride))

EI (70 eV) Mass Spectrum: MeO-PCE

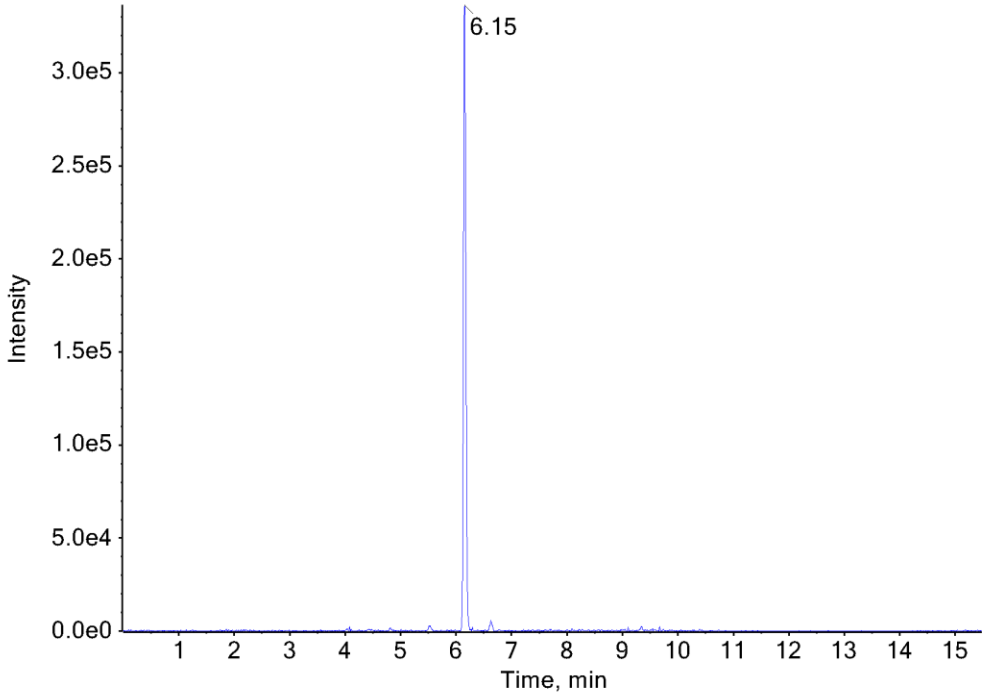


6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	No additional preparation - direct analysis of sample extract
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)
	Flow rate: 0.4 mL/min
Gradient:	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
Temperatures:	Autosampler: 15 °C
	Column Oven: 30 °C

	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	TOF MS Scan Range: 100-510 Da
	Precursor Isolation: SWATH® acquisition (27 windows)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	6.15 min
Standard Comparison:	Reference material for 3-MeO-PCE (Batch: 0459577-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as MeO-PCE, based on retention time (6.00 min) and mass spectral data; however, absolute configuration of the structure as 3-MeO-PCE was not determined. (https://www.caymanchem.com/product/9001355/3-methoxy-pce-(hydrochloride))

Extracted Ion Chromatogram (XIC): MeO-PCE



TOF MS (Top) and MS/MS (Bottom) Spectra: MeO-PCE