

# 4-Acetoxy-MALT

Sample Type: Seized Material

HN

Latest Revision: **February 4, 2019**Date Received: **November 2, 2018** 

Date of Report: February 4, 2019

#### 1. GENERAL INFORMATION

**IUPAC Name:** [3-[2-[allyl(methyl)amino]ethyl]-1H-indol-4-yl] acetate

**InChI String:** InChI=1S/C16H20N2O2/c1-4-9-18(3)10-8-13-11-17-14-6-5-7-

15(16(13)14)20-12(2)19/h4-7,11,17H,1,8-10H2,2-3H3

**CFR:** Not Scheduled (02/2019)

CAS# Not Available

**Synonyms:** 4-AcO-MALT, 4-Acetyloxy-*N*-methyl-*N*-allyltryptamine

**Source:** Department of Homeland Security

**Appearance:** Tan Solid Material

Important Note: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

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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	$C_{16}H_{20}N_2O_2$	272.3	272	273.1598

#### 3. BRIEF DESCRIPTION

4-Acetoxy-MALT is classified as a novel tryptamine analogue. Tryptamine analogues are modified based on the structure of tryptamine. Tryptamine is found at low concentrations endogenously in the brain, suspected of playing a role in neurological functions, and exogenously in some plant species. Tryptamine analogues have been reported to cause hallucinogenic effects, often associated with "psychedelic mushrooms." Tryptamine analogues have caused adverse events, including agitation, tachyarrhythmias, hyperpyrexia, and death, as described in the literature. Structurally similar compounds include psilocin, *O*-acetylpsilocin (4-acetoxy-DMT), and 5-MeO-MALT, among several other tryptamine analogues. Psilocin is a Schedule I substance in the United States.

#### 4. ADDITIONAL RESOURCES

No resources available.

### **5. QUALITATIVE DATA**

## **5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)**

**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/base extraction

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

Column: Zebron<sup>TM</sup> Inferno<sup>TM</sup> ZB-35HT (15 m x 250  $\mu$ m x 0.25  $\mu$ m)

Carrier Gas: Helium (Flow: 1 mL/min)

**Temperatures:** Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

**Injection Parameters:** Injection Type: Splitless

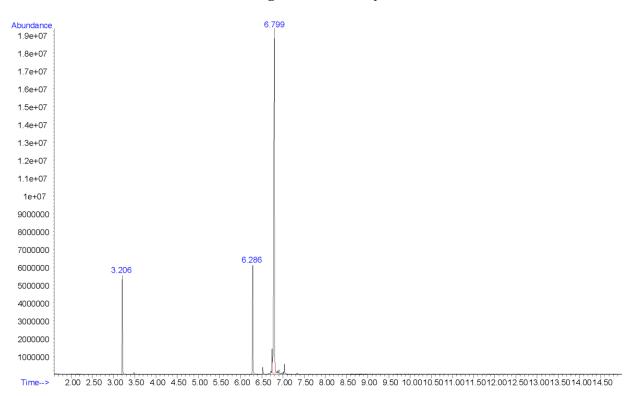
Injection Volume: 1 µL

**MS Parameters:** Mass Scan Range: 40-550 m/z

Threshold: 250

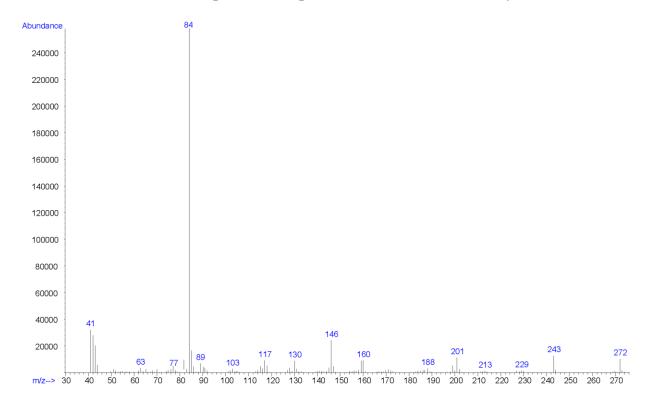
**Retention Time:** 6.799 min

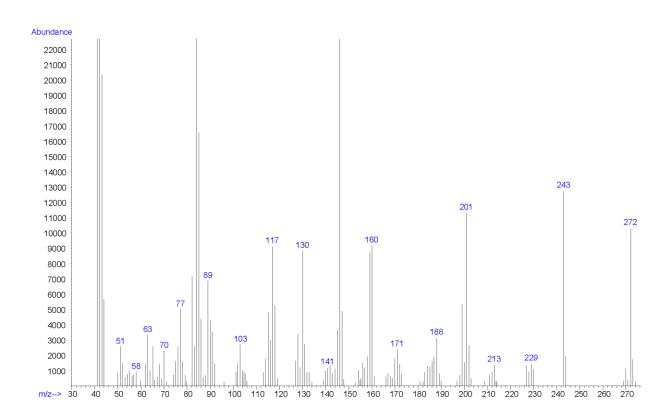
# **Chromatogram: 4-Acetoxy-MALT**



Additional peaks present in chromatogram: internal standards (3.206 min and 6.286 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-Acetoxy-MALT





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

**Testing Performed At:** The Center for Forensic Science Research and Education at the

Fredric Rieders Family Foundation (Willow Grove, PA)

**Sample Preparation:** 1:100 dilution of acid/base extraction in mobile phase

**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

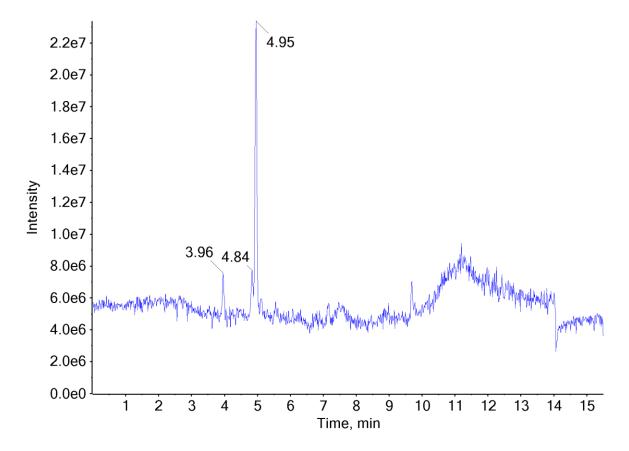
Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

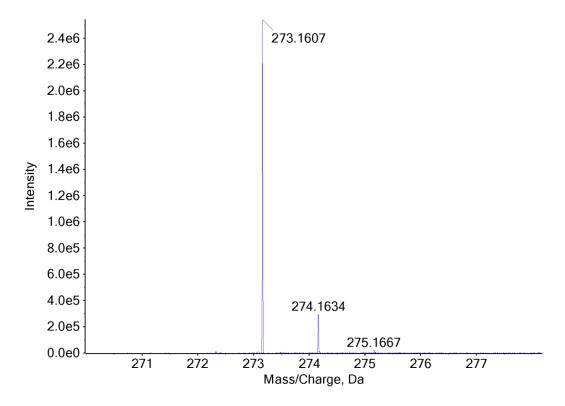
**Retention Time:** 4.95 min

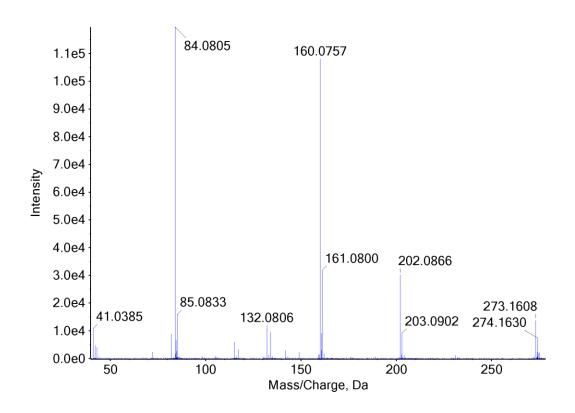
# **Extracted Ion Chromatogram: 4-Acetoxy-MALT**



Additional peak present in chromatogram: not a controlled substance (3.96 mins), internal standard (4.84 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 4-Acetoxy-MALT





# **5.3 NUCLEAR MAGNETIC RESONANCE (NMR)**

**Testing Performed At:** IteraMed<sup>TM</sup> (Doylestown, PA)

**Sample Preparation:** Dilute powder in DMSO-D6

**Instrument:** 300 MHz INOVA VARIAN Spectrometer

**Parameters:** Pulse Sequence: Proton

Solvent: DMSO-D6

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

# <sup>1</sup>H NMR: 4-Acetoxy-MALT

 $^{1}$ H NMR (300 MHz, DMSO-d<sub>6</sub>) ä 11.02-11.14 (m, 1H), 7.20-7.24 (m, 1H), 7.15 (d, J=2.52 Hz, 1H), 7.02 (t, J=7.87 Hz, 1H), 6.63-6.69 (m, 1H), 6.56 (s, 2H), 5.79-5.93 (m, 1H), 5.17-5.29 (m, 2H), 3.21 (d, J=6.44 Hz, 2H), 2.80-2.88 (m, 2H), 2.68-2.77 (m, 2H), 2.56 (s, 1H), 2.34 (d, J=2.93 Hz,

