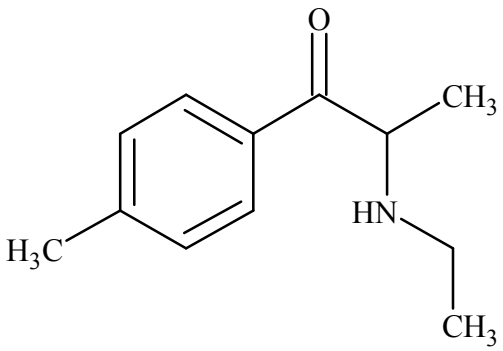
4-methylethcathinone

Latest Revision: April 15, 2013



1. GENERAL INFORMATION

IUPAC Name: 2-(ethylamino)-1-(4-methylphenyl)propan-1-one

CFR: Not Scheduled (4/2013)

CAS#: 1225617-18-4 (base), 1266688-86-1 (HCl)

Synonyms: 4-MEC, 4-methyl-N-ethylcathinone

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}: 262.8

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{12}H_{17}NO$	191	Not Determined
HCl	$C_{12}H_{17}NO \cdot HCl$	227	210.4

3. ADDITIONAL RESOURCES

Swortwood MJ, Boland DM, DeCaprio AP. Determination of 32 cathinone derivatives and other designer drugs in serum by comprehensive LC-QQQ-MS/MS analysis. *Anal Bioanal Chem*. 2013; 405: 1383-1397.

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Mohr S, Taschwer M, Schmid MG. Chiral separation of cathinone derivatives used as recreational drugs by HPLC-UV using a CHIRALPAK® AS-H column as stationary phase. *Chirality*. 2012; 24: 486-492.

Mohr S, Pilaj S, Schmid MG. Chiral separation of cathinone derivatives used as recreational drugs by cyclodextrin-modified capillary electrophoresis. *Electrophoresis.* 2012; 33: 1624-1630.

O'Byrne PM, Kavanagh PV, McNamara SM, Stokes SM. Screening of stimulants including designer drugs in urine using a liquid chromatography tandem mass spectrometry system. *J Anal Toxicology*. 2013; 37: 64-73.

Mohr S, Weiß JA, Spreitz J, Schmid MG. Chiral separation of new cathinone- and amphetamine-related designer drugs by gas chromatography-mass spectrometry using trifluoroacetyl-l-prolyl chloride as chiral derivatization reagent. *J Chromatogr A*. 2012; 1269: 352-359.

Strano-Rossi S, Anzillotti L, Castrignanò E, Romolo FS, Chiarotti M. Ultra high performance liquid chromatography-electrospray ionization-tandem mass spectrometry screening method for direct analysis of designer drugs, "spice" and stimulants in oral fluid. *J Chromatogr A*. 2012; 1258: 37-42.

Mayer M, Benko A, Huszár A, et al. Simultaneous determination of 4-substituted cathinones (4-MMC, 4-MEC and 4-FMC) in human urine by HPLC-DAD. *J Chromatogr Sci*. 2012; 1-6. doi:10.1093/chromsci/bms183.

Khreit OIG, Irving C, Schmidt E, Parkinson JA, Daeid NN, Sutcliffe OB. Synthesis, full chemical characterisation and development of validated methods for the quantification of the components found in the evolved "legal high" NRG-2. *J Pharm Biomed Anal*. 2012; 61: 122-135.

Lopez-Avila V, Gao W, Urdahl R. Mass spectral fragmentation of cathinones by high-resolution TOFMS using a soft ionization source. *J Pharm Sci Innov*. 2012; 1(6): 44-53.

Power JD, McDermott SD, Talbot B, O'Brien JE, Kavanagh P. The analysis of amphetamine-like cathinone derivatives using positive electrospray ionization with in-source collision-induced dissociation. *Rapid Commun Mass Spectrom*. 2012, 26, 2601-2611.

Zuba D. Identification of cathinones and other active components of 'legal highs' by mass spectrometric methods. *Trends Anal Chem*. 2012; 32: 15-30.

Jankovics P, Váradi A, Tölgyesi L, Lohner S, Németh-Palotás J, Kőszegi-Szalai H. Identification and characterization of the new designer drug 4'-methylethcathinone (4-MEC) and elaboration of a novel liquid chromatography-tandem mass spectrometry (LC-MS/MS) screening method for seven different methcathinone analogs. *Forensic Sci Int*. 2011; 210: 213-220.

Forendex

Wikipedia

4. QUALITATIVE DATA

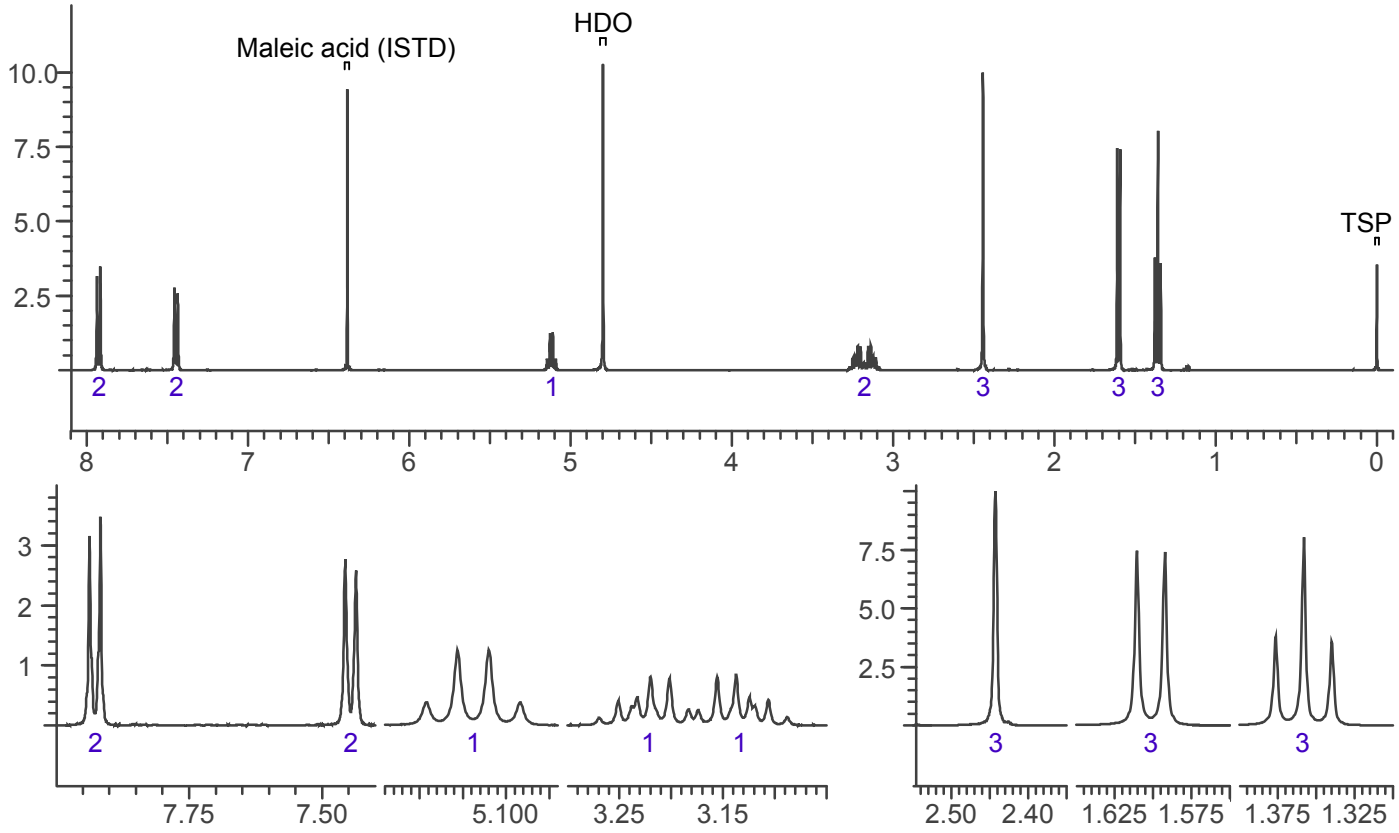
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

Sample Preparation: Dilute analyte to ~10 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}H NMR: 4-methylethcathinone HCl; lot TAD0311; D_2O, 400 MHz

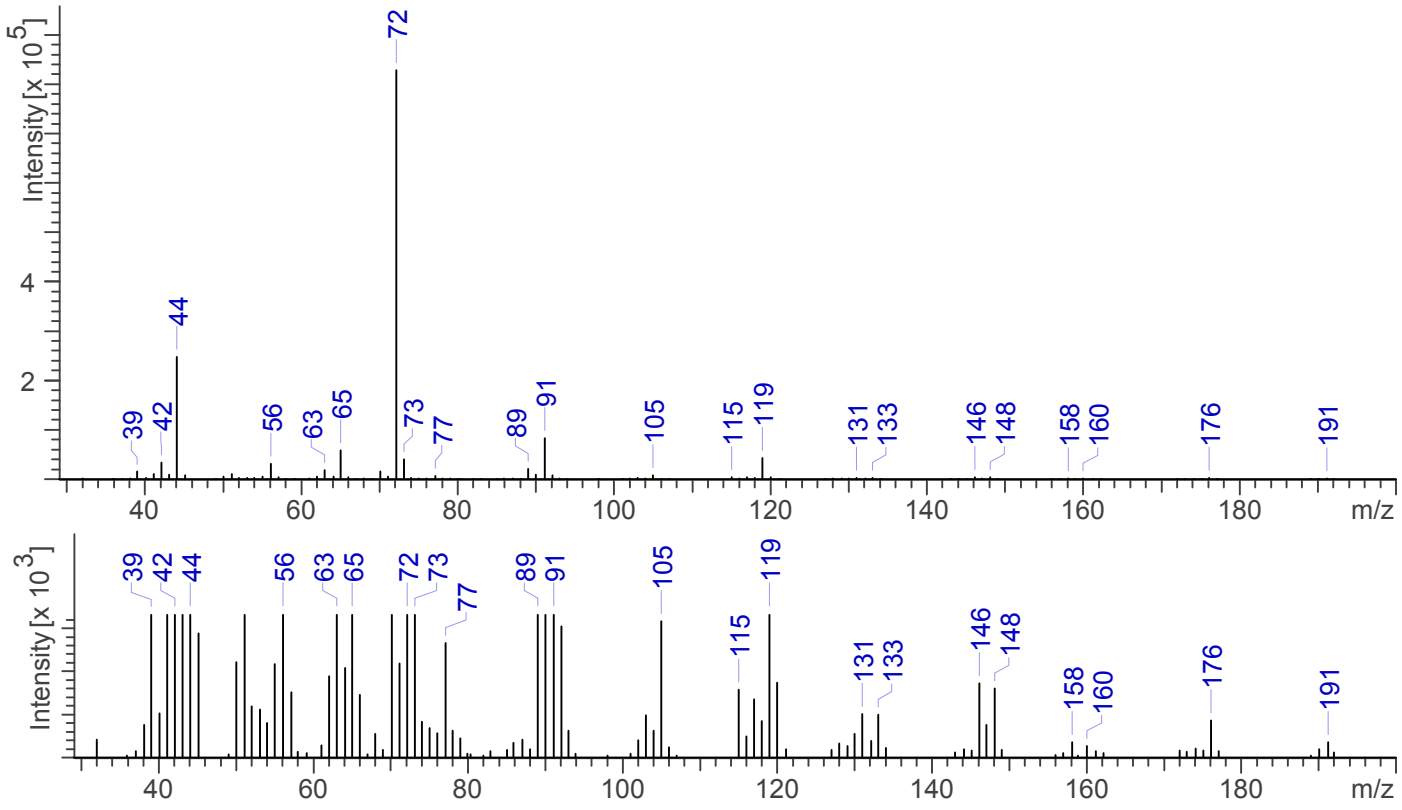


4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~1 mg/mL base extracted into chloroform.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12 °C/min 3) Hold final temperature for 9.0 min
Injection Parameters:	Split Ratio = 20:1, 1 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	7.747 min

EI Mass Spectrum: 4-methylethcathinone HCl; lot TAD0311



4.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 bounce): 4-methylethcathinone HCl; lot TAD0311