



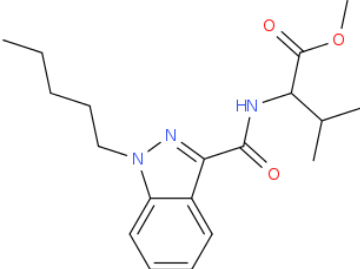
ANALYTICAL REPORT¹

AMB (C19H27N3O3)

methyl 3-methyl-2-[(1-pentyl-1H-indazol-3-yl)formamido]butanoate

Remark – other NPS detected: **none**

Sample ID:	1462-16
Sample description:	powder - white
Sample type:	collected /Institute of Forensic medicine, University Freiburg, Germany
Date of sample receipt (M/D/Y):	1/14/2016
Date of entry (M/D/Y) into NFL database:	3/9/2016
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ² (base form)	
Systematic name	methyl 3-methyl-2-[(1-pentyl-1H-indazol-3-yl)formamido]butanoate
Other names	AMP; methyl (1-pentyl-1H-indazole-3-carbonyl)-valinate
Formula (per base form)	C19H27N3O3
M _w (g/mol)	345.44
Salt form/anions detected	base
StdInChIKey	KTTMFFHXDMTTOB-UHFFFAOYSA-N
Compound Class	Cannabinoids
Other NPS detected	none
Add.info (purity..)	impurities not detected

¹ This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

² Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50) . Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N₂) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

3. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

4. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above (**1**). Split MS : IR = 1:9.

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

IR (condensed phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

5. IC (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30°C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

Supporting information

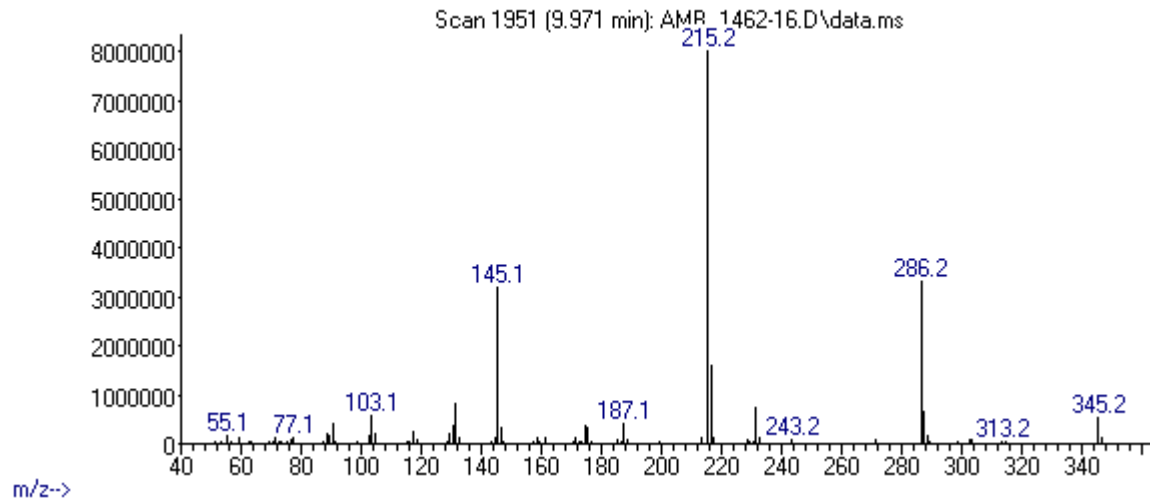
Solubility in	result/remark
CH ₂ Cl ₂	soluble
MeOH	soluble
H ₂ O	partially

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 9.97 BP(1): 215; BP(2): 286,BP(3) :145,
HPLC-TOF	+	Exact mass (theoretical): 345.2052; measured value Δppm:-0.27; formula:C19H27N3O3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	-	
NMR (in FKKT)	-	
validation		MS consistent by SWGDRUG.L entry
other		

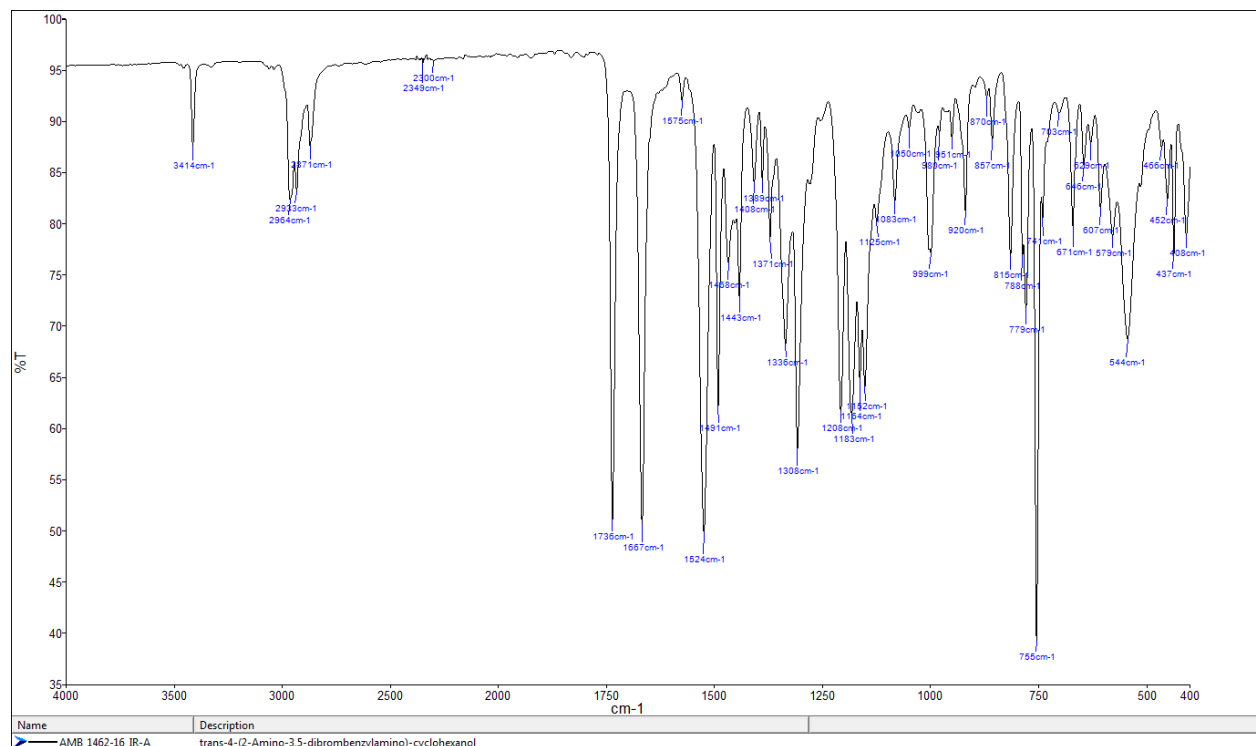
ANALYTICAL RESULTS

MS (EI)

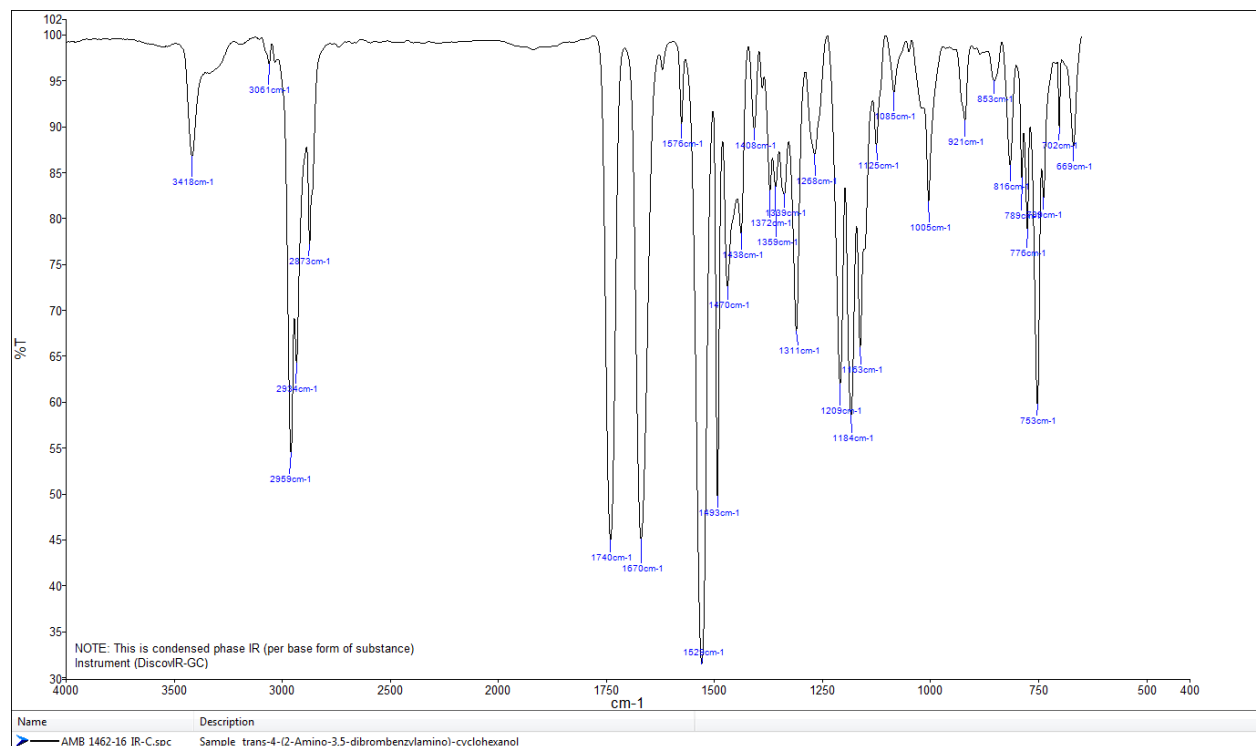
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



HPLC-TOF report

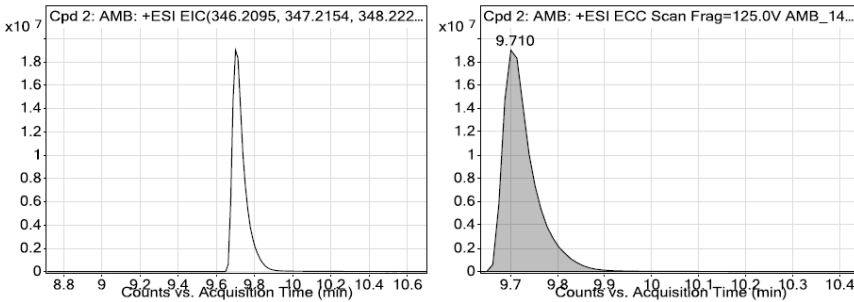
Data File	AMB_1462--16_TOF.d	Sample Name	ID_1462-16
Sample Type	Sample	Position	P2-C9
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-1512015-XDB-C18-ESI-poz-pod.m	Acquired Time	2/26/2016 9:48:38 AM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	extract in MeOH		

Compound Table

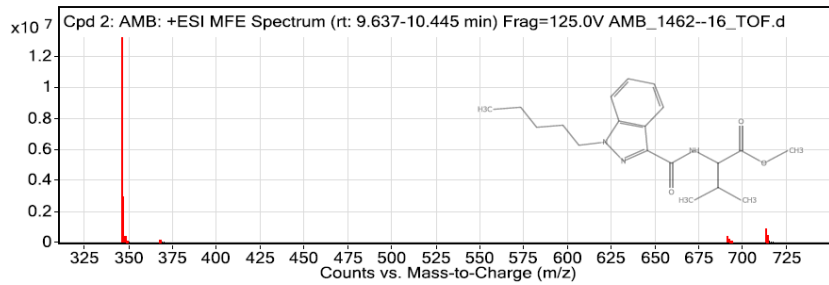
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: AMB	AMB	C19 H27 N3 O3	9.71	345.2053

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
AMB	346.2126	9.71	345.2053	9.71	C19 H27 N3 O3	345.2052	-0.27

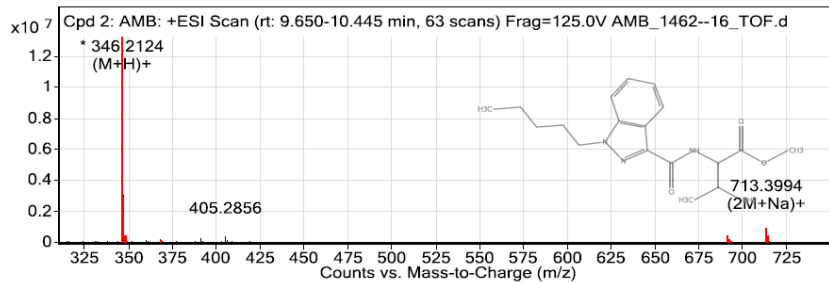
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
346.2126	1	13235116	C19 H27 N3 O3	(M+H)+
347.2158	1	2940199.1	C19 H27 N3 O3	(M+H)+
348.2189	1	357670.04	C19 H27 N3 O3	(M+H)+
368.1945	1	117030.09	C19 H27 N3 O3	(M+Na)+
691.418	1	411107.78	C19 H27 N3 O3	(2M+H)+
692.4209	1	168776.12	C19 H27 N3 O3	(2M+H)+
693.4231	1	37062.41	C19 H27 N3 O3	(2M+H)+
713.4004	1	903061.94	C19 H27 N3 O3	(2M+Na)+
714.4032	1	383765.81	C19 H27 N3 O3	(2M+Na)+
715.4054	1	82921.7	C19 H27 N3 O3	(2M+Na)+

--- End Of Report ---