



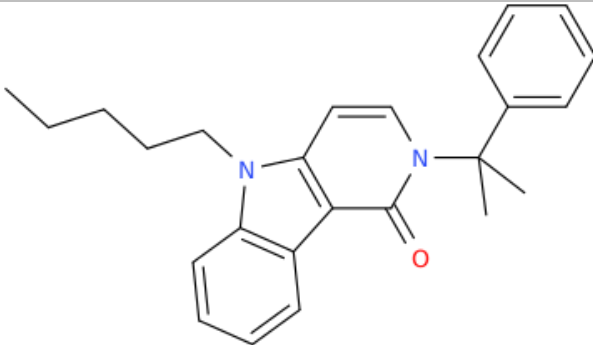
ANALYTICAL REPORT

Cumyl-Pegaclone (C₂₅H₂₈N₂O)

5-pentyl-2-(2-phenylpropan-2-yl)-1H,2H,5H-pyrido[4,3-b]indol-1-one

Remark – other NPS detected:

Sample ID:	1905-18
Sample description:	powder
Sample type:	test purchase /ISF projekt (NFL-SI)
Date of sample receipt (M/D/Y):	1/4/2018
Date of entry (M/D/Y) into NFL database:	1/18/2018
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ¹ (base form)	
Systematic name	5-pentyl-2-(2-phenylpropan-2-yl)-1H,2H,5H-pyrido[4,3-b]indol-1-one
Other names	2-(1-methyl-1-phenyl-ethyl)-5-pentyl-pyrido[4,3-b]indol-1-one; Cumyl pegaclone; SGT-151
Formula (per base form)	C ₂₅ H ₂₈ N ₂ O
M _w (g/mol)	372,51
Salt form/anions detected	base
StdInChIKey (per base form)	AWHWTKXMUJLSRM-UHFFFAOYSA-N
Other NPS detected	
Additional info (purity..)	unidentified compound C ₂₆ H ₂₈ N ₂ O ₂ (<1%) was detected by HPLC-TOF

¹ 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 (9.258 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 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 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 until 6 min) 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 (solid) 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

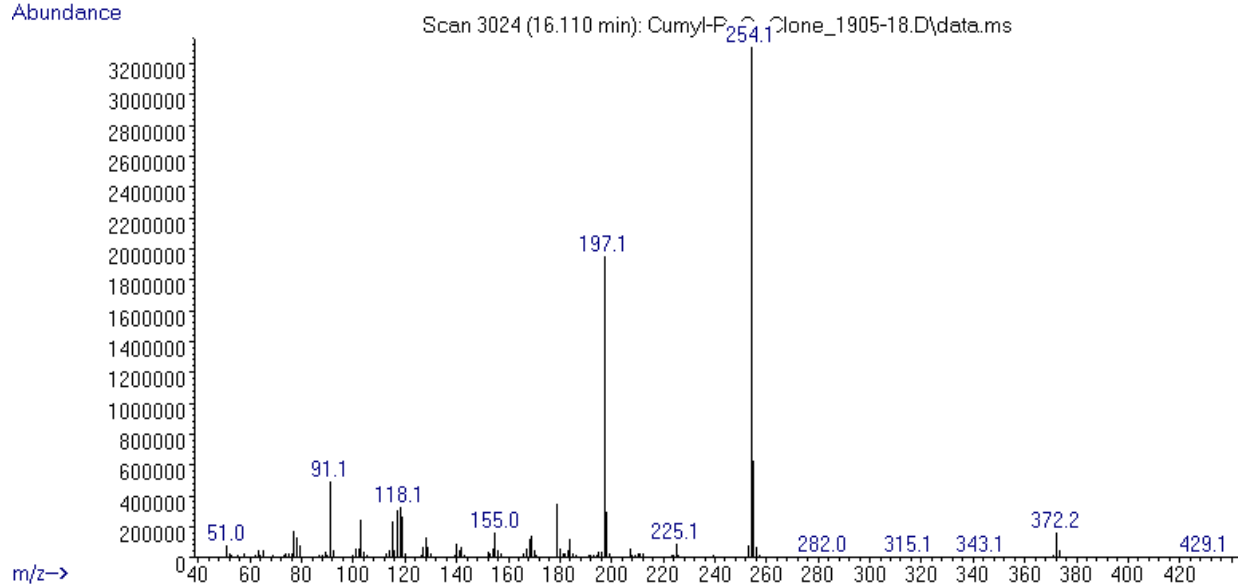
Solubility in	result/remark
CH ₂ Cl ₂	soluble
MeOH	soluble
H ₂ O	partially

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 16,11 BP(1): 254; BP(2): 197,BP(3) :255,
HPLC-TOF	+	Exact mass (theoretical): 372,2202; measured value Δppm:0,21; formula:C25H28N2O
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		confirmed by the RESPONSE project entry ID-1860-17 https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Cumyl-PeGaClone-ID-1860-17_report.pdf
other - reference		Angerer V. et al: Structural characterization and pharmacological evaluation of the new synthetic cannabinoid CUMYL-PEGACLONE, <i>Drug Test Anal.</i> 2017 Jul 3., DOI: 10.1002/dita.2237

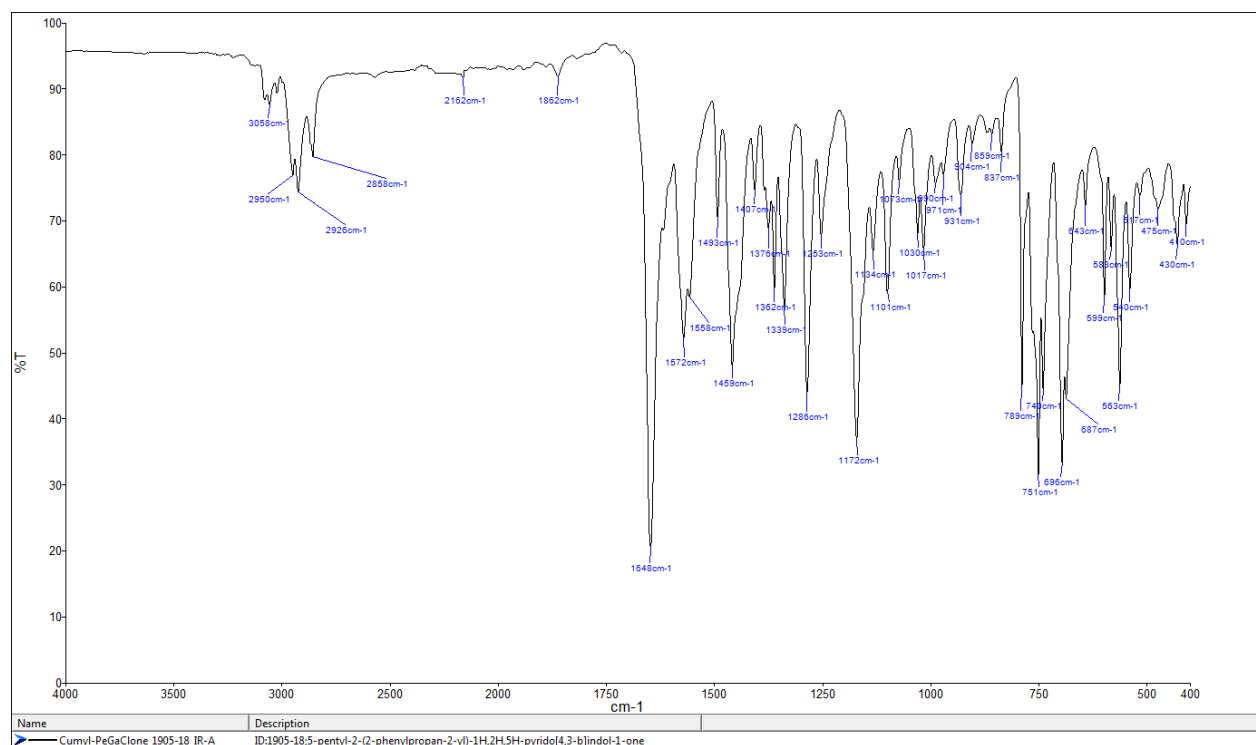
ANALYTICAL RESULTS

MS (EI)

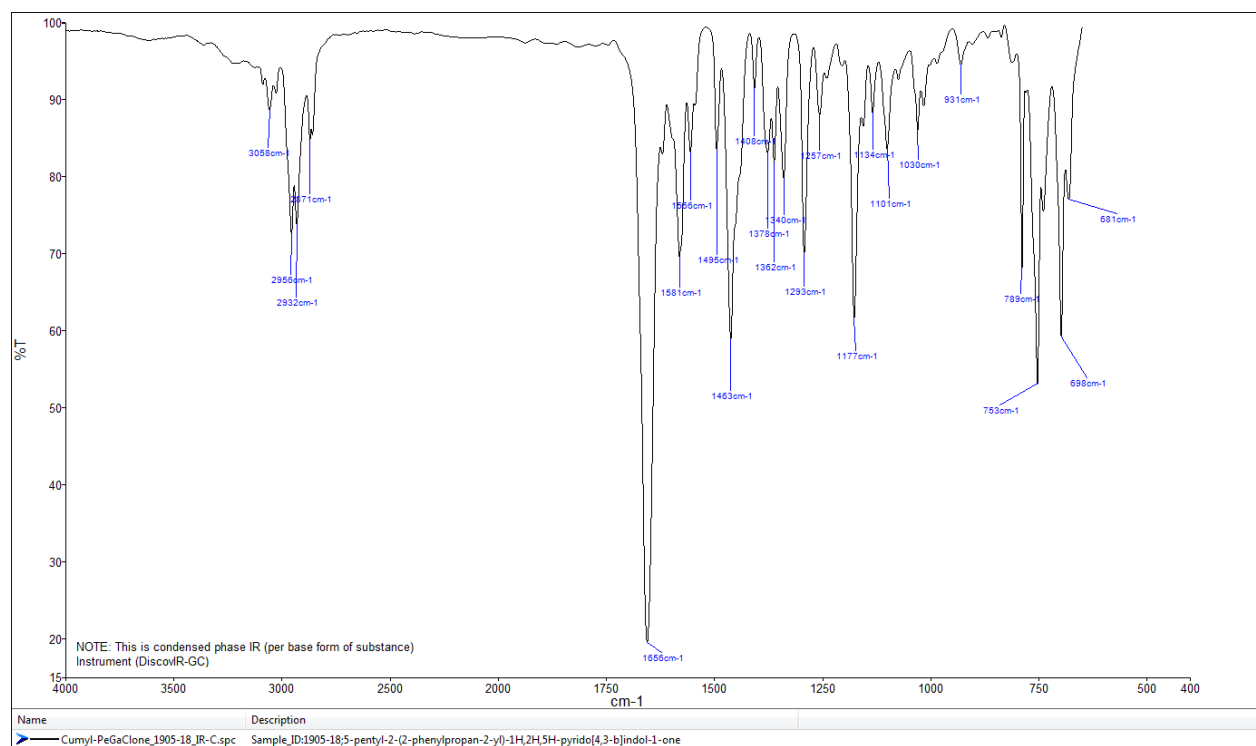
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

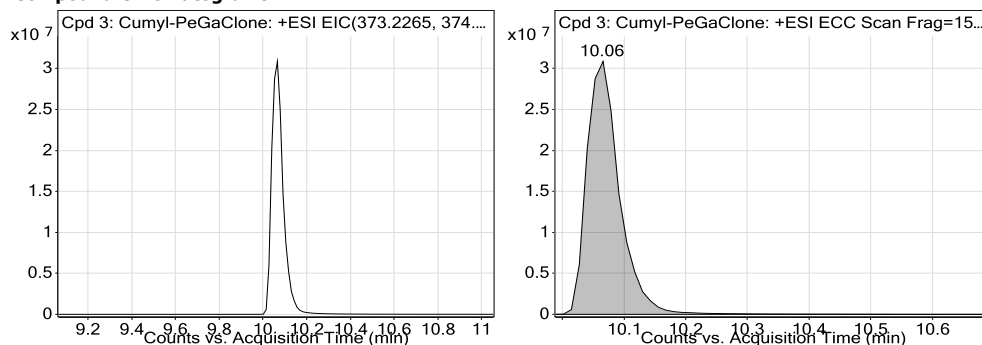
Data File	Cumyl PeGaClone_1905_18.d	Sample Name	1905-18
Sample Type	Sample	Position	P1-F2
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-04_12_2017-XDB-C18-ESI+.m	Acquired Time	1/19/2018 12:04:54 PM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	MeOH		

Compound Table

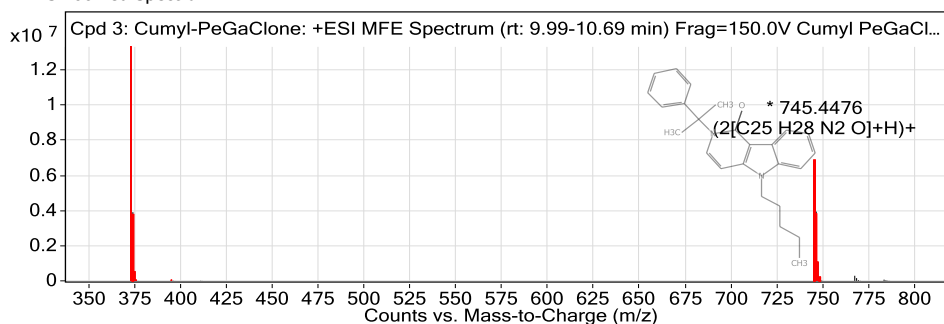
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 3: Cumyl-PeGaClone	Cumyl-PeGaClone	C25 H28 N2 O	10.06	372.2201

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
Cumyl-PeGaClone	373.2275	10.06	372.2201	10.06	C25 H28 N2 O	372.2202	0.21

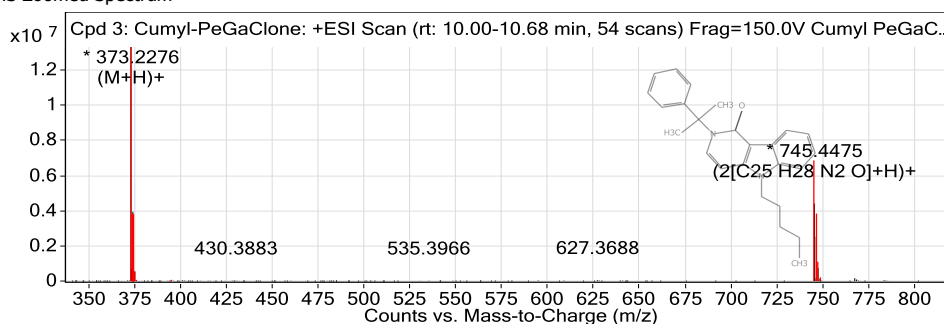
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
373.2275	1	13318992	C25 H28 N2 O	(M+H)+
374.2311	1	3911197.5	C25 H28 N2 O	(M+H)+
375.2346	1	476342.19	C25 H28 N2 O	(M+H)+
745.4476	1	6855018	C25 H28 N2 O	(2M+H)+
746.4508	1	3943522.75	C25 H28 N2 O	(2M+H)+
747.4551	1	1064149.66	C25 H28 N2 O	(2M+H)+
748.4578	1	188554	C25 H28 N2 O	(2M+H)+
767.4301	1	289489.94		(2M+Na)+
768.4332	1	156174.96		(2M+Na)+
783.4032	1	69031.3		(2M+K)+

--- End Of Report ---