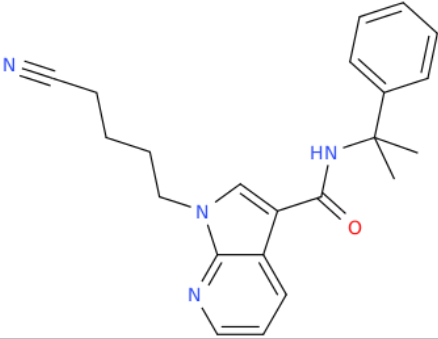


ANALYTICAL REPORT¹Cumyl-4CN-B7AICA (C₂₂H₂₄N₄O)**1-(4-cyanobutyl)-N-(2-phenylpropan-2-yl)-1H-pyrrolo[2,3-b]pyridine-3-carboxamide**Remark – other NPS detected: **none**

Sample ID:	1859-17
Sample description:	powder - white off
Sample type:	collected /FSI Zurich, Switzerland
Date of sample receipt (M/D/Y):	10/11/2017
Date of entry (M/D/Y) into NFL database:	10/20/2017
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	1-(4-cyanobutyl)-N-(2-phenylpropan-2-yl)-1H-pyrrolo[2,3-b]pyridine-3-carboxamide
Other names	N-Cumyl-1-(4-cyanobutyl)-7-azaindol-3-carboxamide; 1-(4-cyanobutyl)-N-(1-methyl-1-phenyl-ethyl)pyrrolo[2,3-b]pyridine-3-carboxamide; 1-(4-cyanobutyl)-N-(2-phenylpropan-2-yl)-7-azaindol-3-carboxamide
Formula (per base form)	C ₂₂ H ₂₄ N ₄ O
M _w (g/mol)	360,46
Salt form/anions detected	base
StdInChIKey (for base form)	DYPZVGXELGJCHD-UHFFFAOYSA-N
Other NPS detected	none
Add.info (purity..)	>95 % (FSI Zurich data)
References:	1) Michael Bovens, Christian Bissig, Sandra N.Staeheli, Michael Poetzsch, Bernhard Pfeiffer, Thomas Kraemer, Structural Characterization of the New Synthetic Cannabinoids CUMYL-PINACA, 5F-CUMYL-PINACA, CUMYL-4CN-BINACA, 5F-CUMYL-P7AICA and CUMYL-4CN-B7AICA; Forensic Science International https://doi.org/10.1016/j.forsciint.2017.10.020 (accessed 20 October 2017) 2) Sandra N. Staeheli, Michael Poetzsch, Veronica P. Veloso, Michael Bovens, Christian Bissig, Andrea E. Steuer, Thomas Kraemer, In Vitro Metabolism of the Synthetic Cannabinoids CUMYL-PINACA, 5F-CUMYL-PINACA, CUMYL-4CN-BINACA, 5F-CUMYL-P7AICA and CUMYL-4CN-B7AICA, http://onlinelibrary.wiley.com/doi/10.1002/dta.2298/full (accessed 20 October 2017)

¹ Acknowledgement: Sample (NMR confirmed) was kindly provided by FSI Zurich, Switzerland. Measurements shown in this report were done in NFL.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 (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

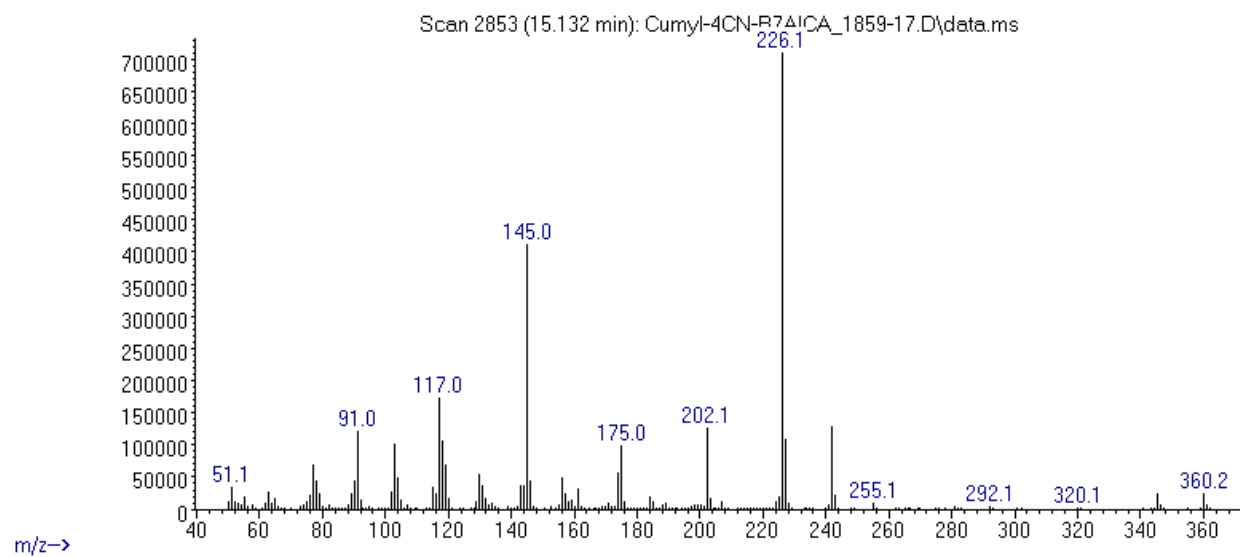
Solubility in	result/remark
CH ₂ Cl ₂	soluble
MeOH	soluble
H ₂ O	partially

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 15,13 BP(1): 226; BP(2): 145,BP(3) :117,
HPLC-TOF	+	Exact mass (theoretical): 360,195; measured value Δppm:-0,91; formula:C22H24N4O
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		See reference 1: https://doi.org/10.1016/j.forsciint.2017.10.020 (accessed 20 October 2017)
other		

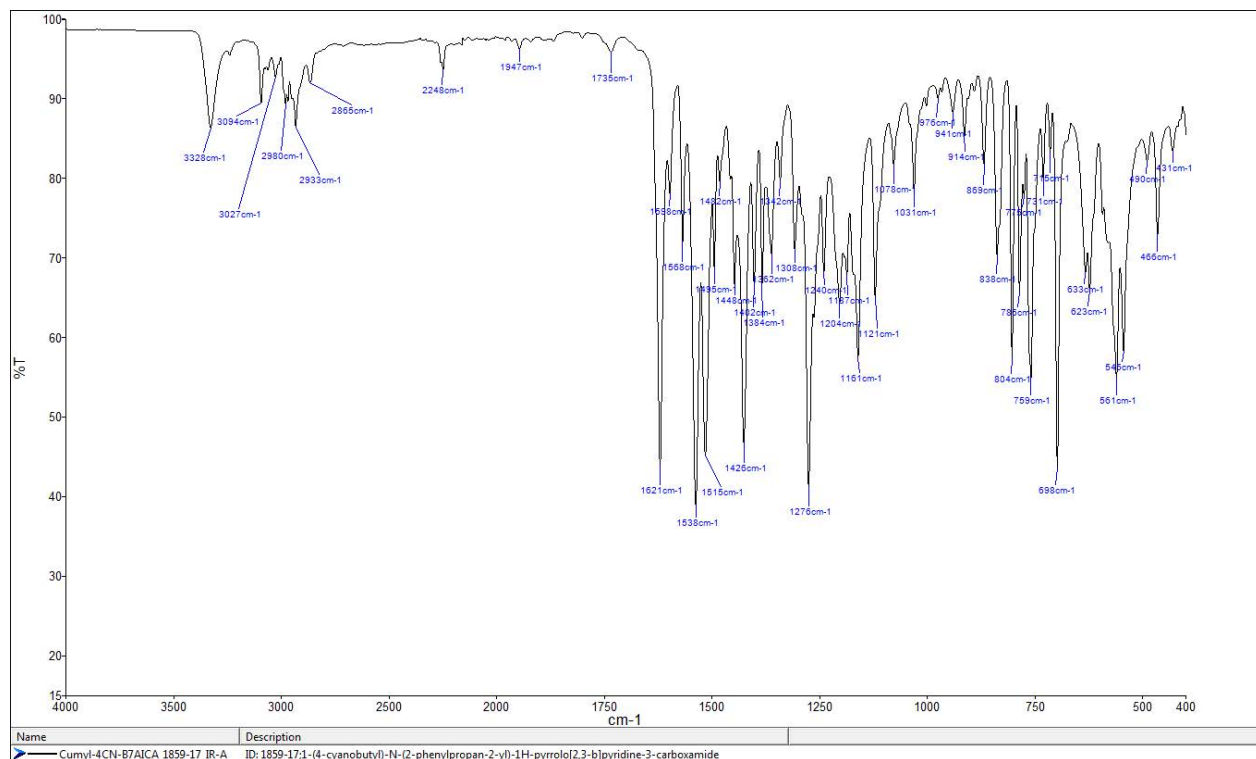
ANALYTICAL RESULTS

MS (EI)

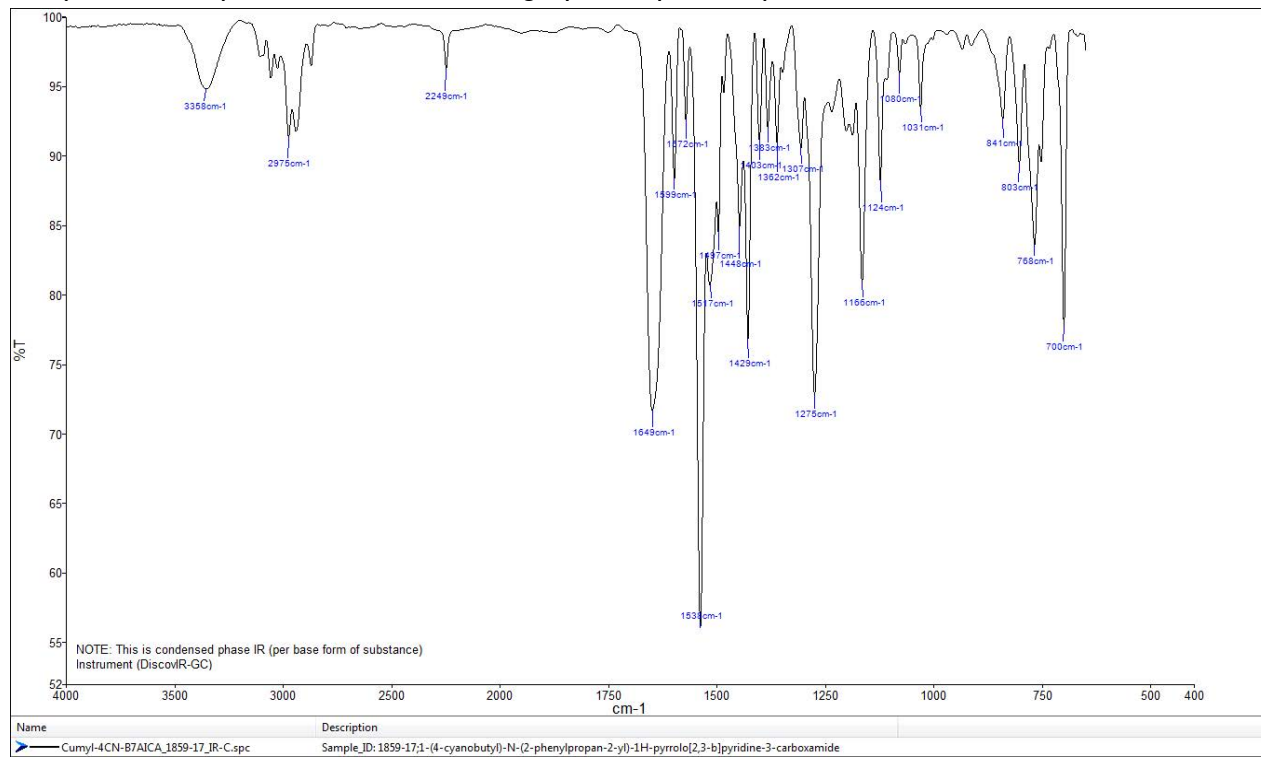
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

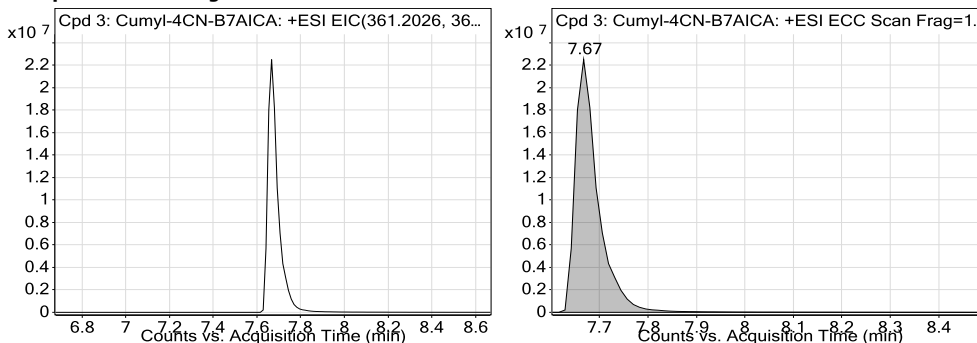
Data File	Cumyl-4CN-B7AICA_1859_17.d	Sample Name	1859-17
Sample Type	Sample	Position	P1-A9
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-19_07_2017-XDB-C18-ESI-final.m	Acquired Time	10/17/2017 12:39:53 PM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	MeOH		

Compound Table

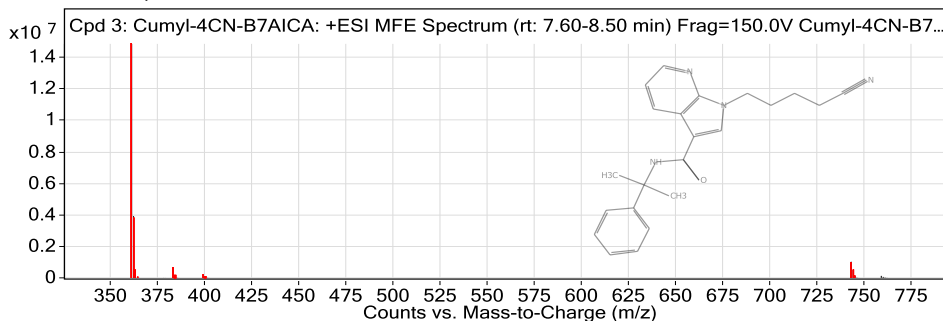
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 3: Cumyl-4CN-B7AICA	Cumyl-4CN-B7AICA	C22 H24 N4 O	7.67	360.1953

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
Cumyl-4CN-B7AICA	361.2026	7.67	360.1953	7.67	C22 H24 N4 O	360.195	-0.91

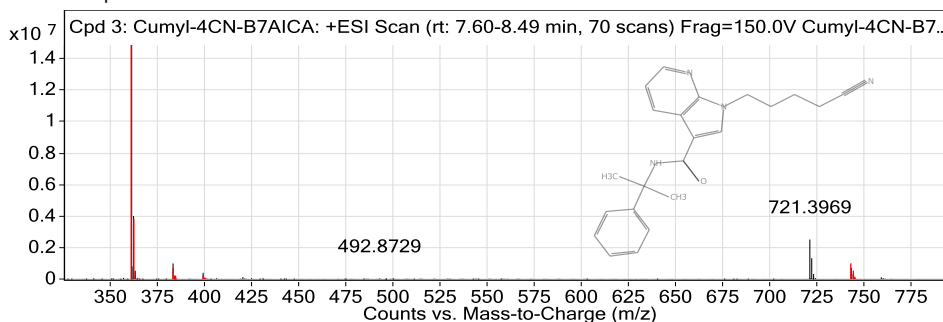
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
361.2026	1	14861194	C22 H24 N4 O	(M+H)+
362.2058	1	3920818.88	C22 H24 N4 O	(M+H)+
363.2092	1	441539.75	C22 H24 N4 O	(M+H)+
383.185	1	668231.38	C22 H24 N4 O	(M+Na)+
384.1877	1	156541.8	C22 H24 N4 O	(M+Na)+
399.1585	1	234274.94	C22 H24 N4 O	(M+K)+
743.3797	1	1023044	C22 H24 N4 O	(2M+Na)+
744.3826	1	496695.31	C22 H24 N4 O	(2M+Na)+
745.385	1	116160.29	C22 H24 N4 O	(2M+Na)+
759.3529	1	126245.71		(2M+K)+

--- End Of Report ---

Peak Integration Report

Sample Name:	1859-17	Inj. Vol.:	25,00
Injection Type:	Unknown	Dilution Factor:	1,0000
Program:	ANIONI	Operator:	kemija
Inj. Date / Time:	17-okt-2017 / 18:49	Run Time:	42,00

No.	Time min	Peak Name	Peak Type	Area $\mu\text{S} \cdot \text{min}$	Height μS	Amount n.a.
		TOTAL:		0,00	0,00	0,00

