



NACIONALNI FORENZIČNI LABORATORIJ
NATIONAL FORENSIC LABORATORY

Vodovodna 95
1000 Ljubljana
SLOVENIJA

T: +386 (0)1 428 44 93
E: nfl@policija.si
www.policija.si

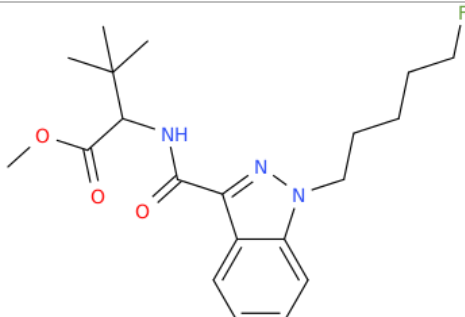
ANALYTICAL REPORT

5F-MDMB-PINACA (C₂₀H₂₈FN₃O₃)

methyl 2-[[1-(5-fluoropentyl)-1H-indazol-3-yl]formamido]-3,3-dimethylbutanoate

Remark – other NPS detected: **none**

Sample ID:	1749-16
Sample description:	powder - white
Sample type:	test purchase /RESPONSE -purchasing
Date of sample receipt (M/D/Y):	12/20/2016
Date of entry (M/D/Y) into NFL database:	3/6/2017
Report ¹ 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 2-[[1-(5-fluoropentyl)-1H-indazol-3-yl]formamido]-3,3-dimethylbutanoate
Other names	5F-ADB5, F-methyl-AMB, 5-fluoro-MAMB, 5-fluoro ADB
Formula (per base form)	C ₂₀ H ₂₈ FN ₃ O ₃
M _w (g/mol)	377,46
Salt form/anions detected	base
StdInChIKey (for base form)	PWEKNGSNNAKWBL-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	minor impurity observed by GC-MS, HPLC TOF, and FTIR

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 (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

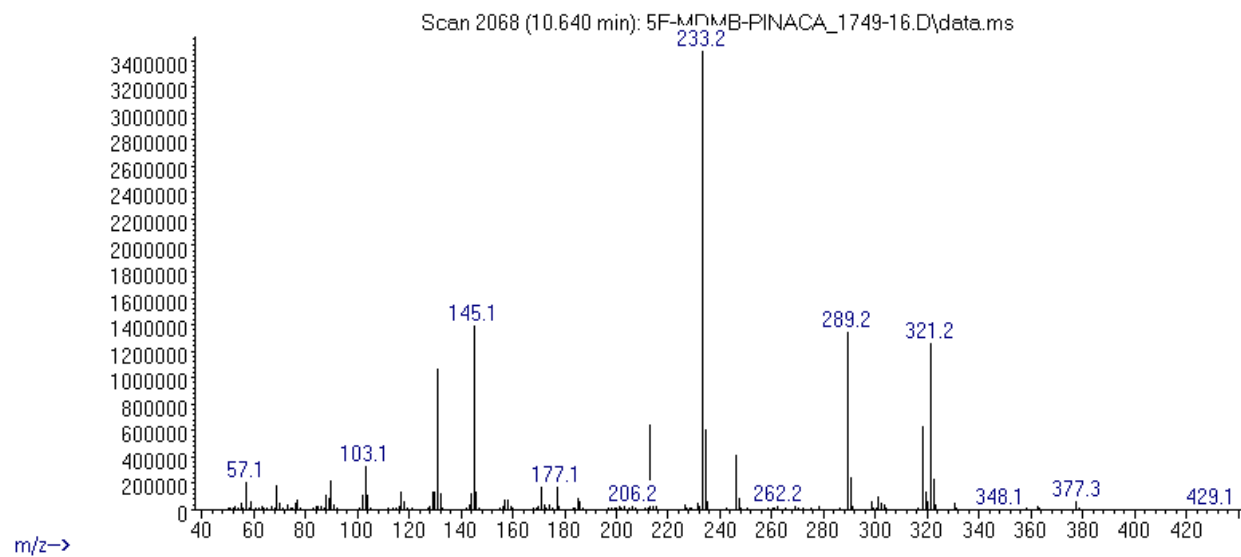
Solubility in	result/remark
CH ₂ Cl ₂	soluble
MeOH	soluble
H ₂ O	partially

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 10,64 BP(1): 233; BP(2): 145,BP(3) :289,
HPLC-TOF	+	Exact mass (theoretical): 377,2115; measured value Δppm:0,59; formula:C20H28FN3O3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		confirmed by reference material from Chiron Lot#16293
other		

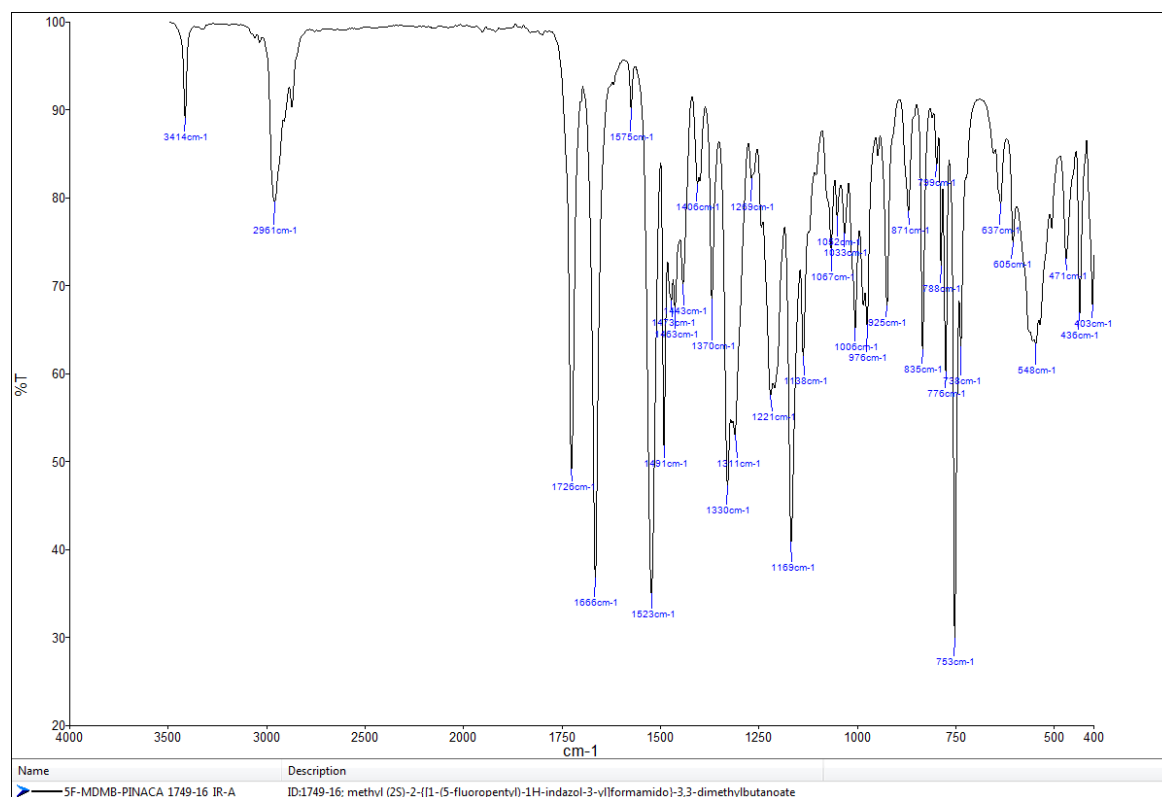
ANALYTICAL RESULTS

MS (EI)

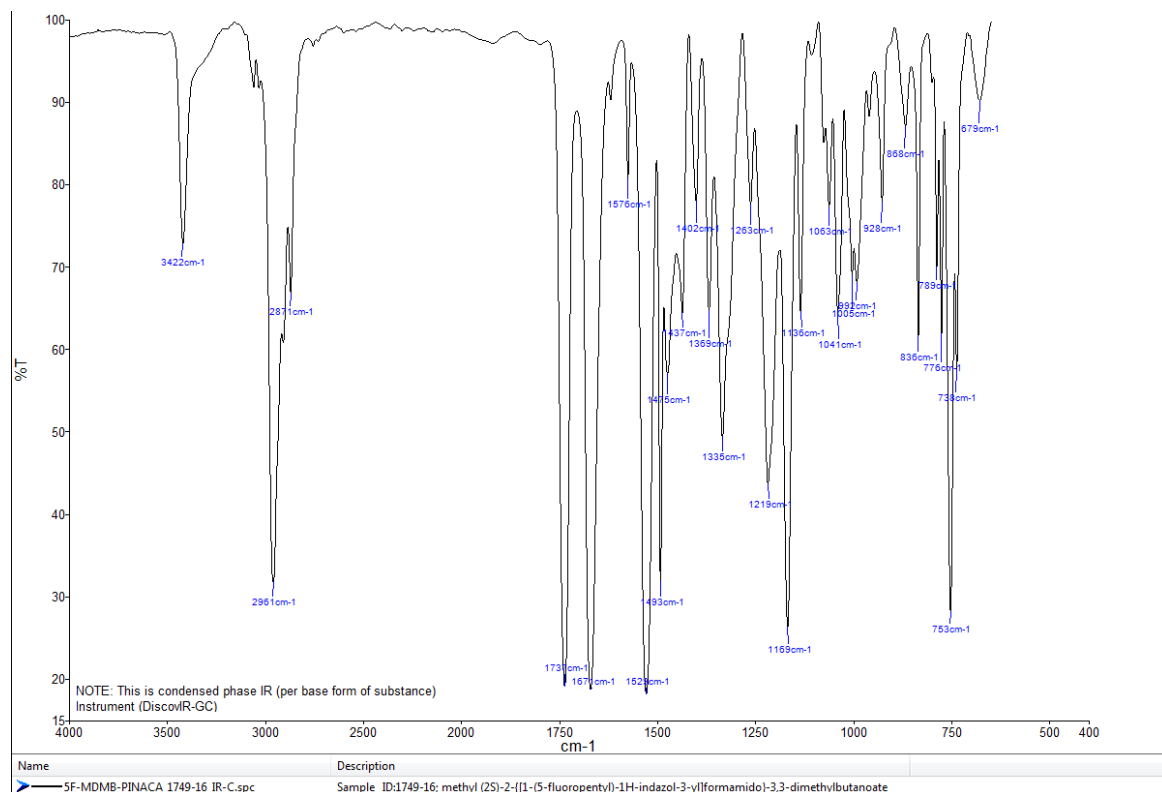
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

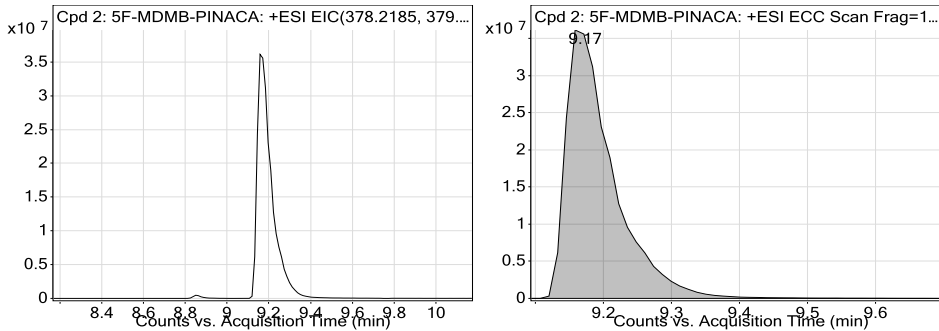
Data File	5F-MDMB-PINACA_1749-16.d	Sample Name	ID_1749-16
Sample Type	Sample	Position	P1-C7
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-20_12_2016-XDB-C18-ESI-poz-soft.m	Acquired Time	12/29/2016 9:50:23 AM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	extract in MeOH		

Compound Table

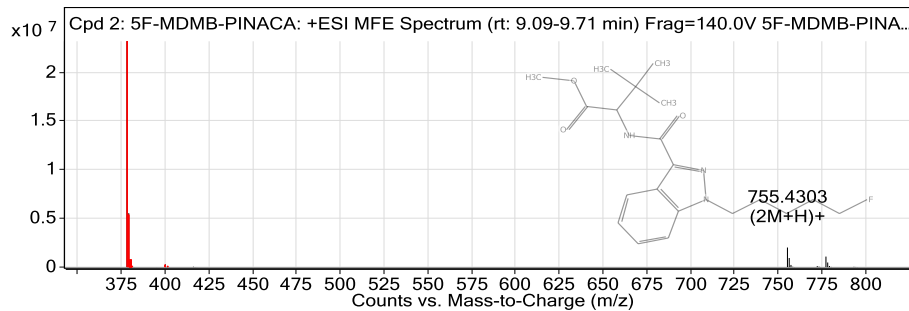
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: 5F-MDMB-PINACA	5F-MDMB-PINACA	C20 H28 F N3 O3	9.17	377.2112
Cpd 3: C20 H27 N3 O3		C20 H27 N3 O3	9.72	357.2047
Cpd 6: C35 H46 N6 O6		C35 H46 N6 O6	10.56	646.3476
Cpd 8: C35 H65 N O3		C35 H65 N O3	13.4	547.4965

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
5F-MDMB-PINACA	378.2185	9.17	377.2112	9.21	C20 H28 F N3 O3	377.2115	0.59

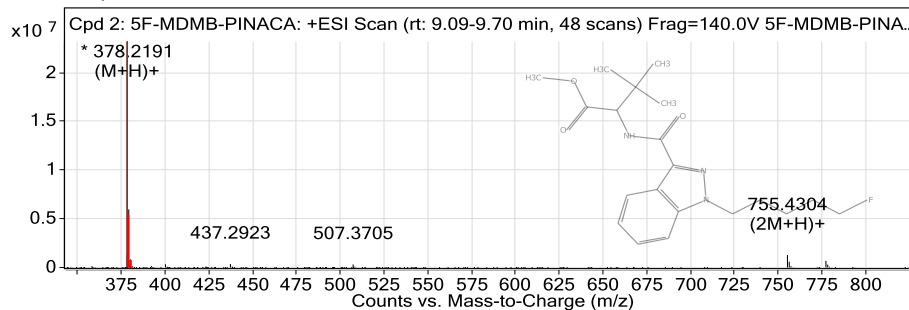
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



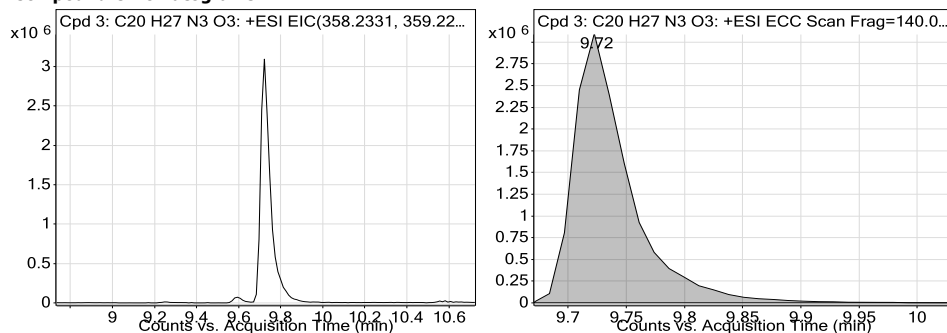
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
378.2185	1	23168446	C20 H28 F N3 O3	(M+H)+
379.2217	1	5527522.98	C20 H28 F N3 O3	(M+H)+
380.2251	1	690657.87	C20 H28 F N3 O3	(M+H)+
400.2007	1	270446.97	C20 H28 F N3 O3	(M+Na)+
755.4303	1	2006634.63		(2M+H)+
756.4342	1	930501.03		(2M+H)+
757.4367	1	220643.54		(2M+H)+
777.4131	1	1077440		(2M+Na)+
778.4159	1	469464.61		(2M+Na)+
779.4184	1	112127.32		(2M+Na)+

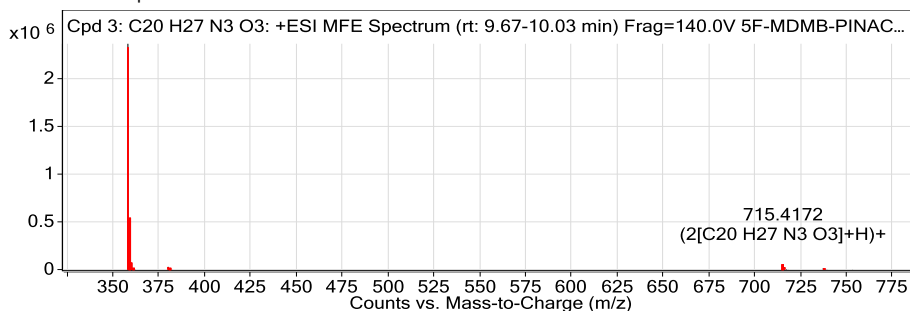
TOF REPORT

Obs. m/z	Obs. RT	Obs. Mass
358.2124	9.72	357.2047

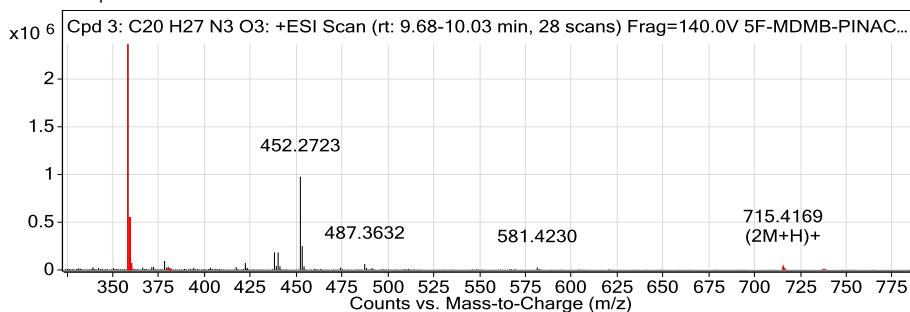
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



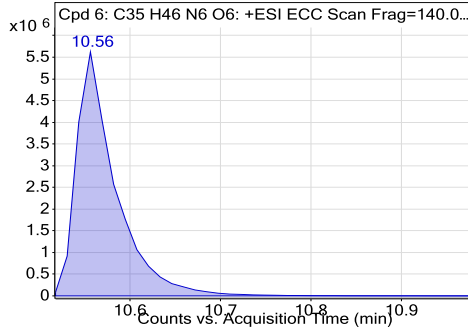
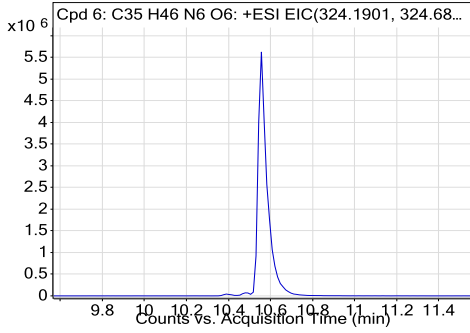
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
358.2124	1	2363017	C20 H27 N3 O3	(M+H)+
359.2159	1	515775.4	C20 H27 N3 O3	(M+H)+
360.218	1	65607.21	C20 H27 N3 O3	(M+H)+
361.2199	1	8343.6	C20 H27 N3 O3	(M+H)+
380.1945	1	28679.45	C20 H27 N3 O3	(M+Na)+
381.1977	1	7171.01	C20 H27 N3 O3	(M+Na)+
715.4172	1	44609.41	C20 H27 N3 O3	(2M+H)+
716.4203	1	20346.54	C20 H27 N3 O3	(2M+H)+
737.3992	1	14114.15	C20 H27 N3 O3	(2M+Na)+
738.4021	1	6407.83	C20 H27 N3 O3	(2M+Na)+

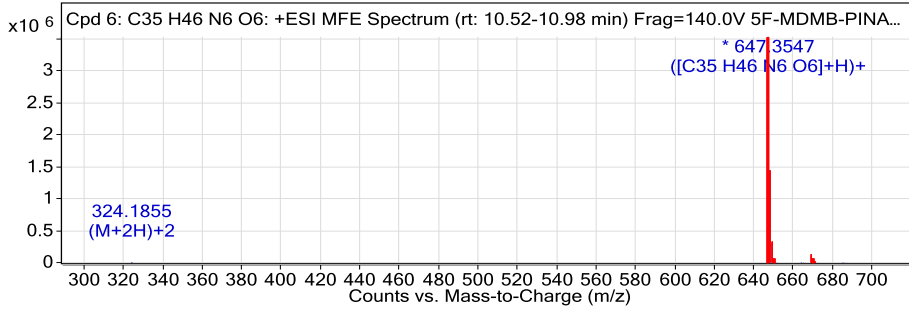
Obs. m/z	Obs. RT	Obs. Mass
647.3547	10.56	646.3476

Compound Chromatograms

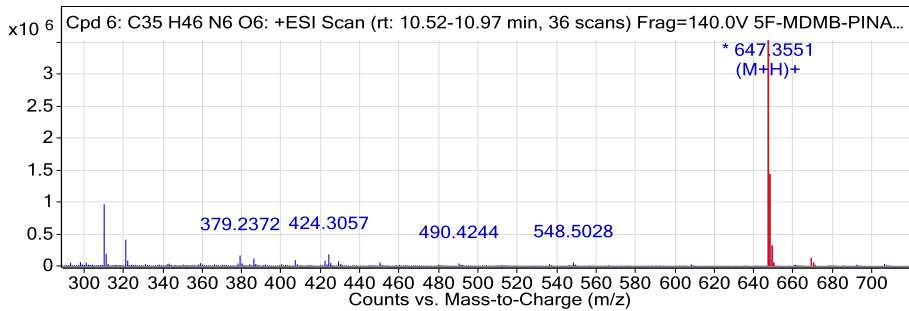
TOF REPORT



MFE MS Zoomed Spectrum



MS Zoomed Spectrum

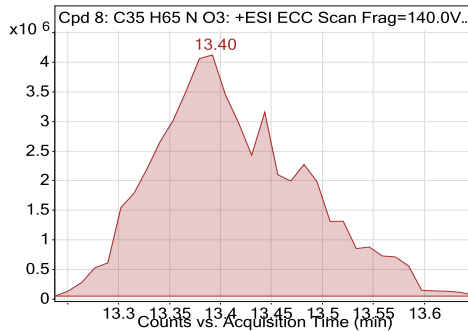
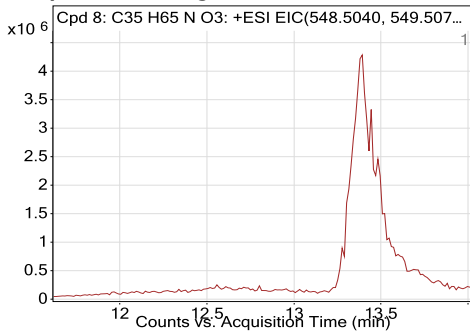


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
324.1855	2	9213.35		(M+2H)+2
647.3547	1	3537319.5	C35 H46 N6 O6	(M+H)+
648.3581	1	1448303.12	C35 H46 N6 O6	(M+H)+
649.3613	1	312773.63	C35 H46 N6 O6	(M+H)+
650.3633	1	48490.4	C35 H46 N6 O6	(M+H)+
664.3823	1	6853.55	C35 H46 N6 O6	(M+NH4)+
669.3367	1	125766.54	C35 H46 N6 O6	(M+Na)+
670.3395	1	49387.77	C35 H46 N6 O6	(M+Na)+
671.3421	1	11346.39	C35 H46 N6 O6	(M+Na)+
685.3102	1	6193.84	C35 H46 N6 O6	(M+K)+

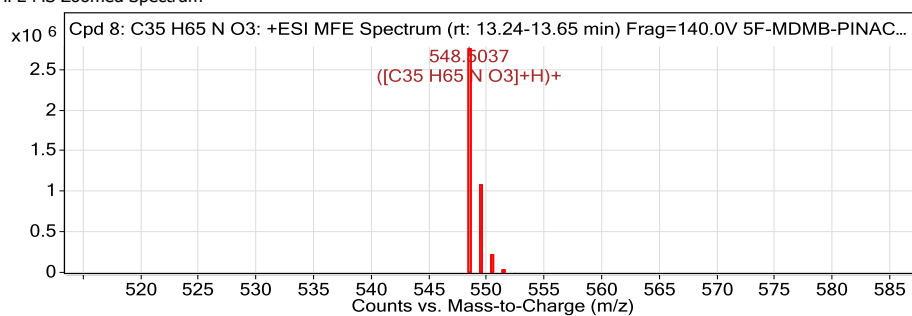
Obs. m/z	Obs. RT	Obs. Mass
548.5037	13.4	547.4965

Compound Chromatograms

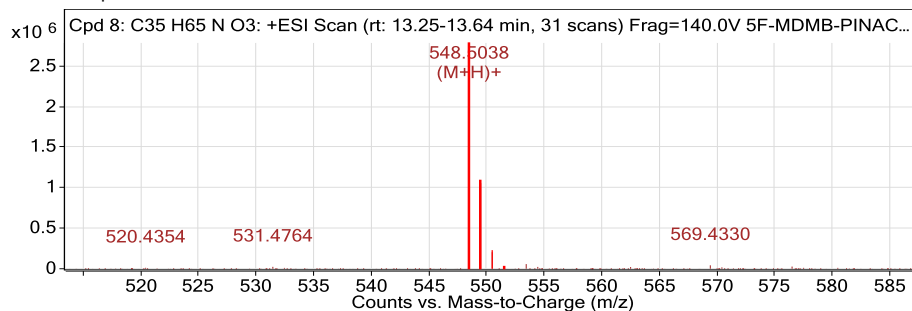


TOF REPORT

MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
548.5037	1	2781649	C ₃₅ H ₆₅ N O ₃	(M+H)+
549.5075	1	1060451.1	C ₃₅ H ₆₅ N O ₃	(M+H)+
550.5103	1	203322.46	C ₃₅ H ₆₅ N O ₃	(M+H)+
551.5128	1	27850.87	C ₃₅ H ₆₅ N O ₃	(M+H)+
552.5137	1	3213.64	C ₃₅ H ₆₅ N O ₃	(M+H)+

--- End Of Report ---

Peak Integration Report

Sample Name:	ID-1749-16	Inj. Vol.:	25,00
Injection Type:	Unknown	Dilution Factor:	1,0000
Program:	ANIONI	Operator:	kemija
Inj. Date / Time:	29-dec-2016 / 10:02	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

