

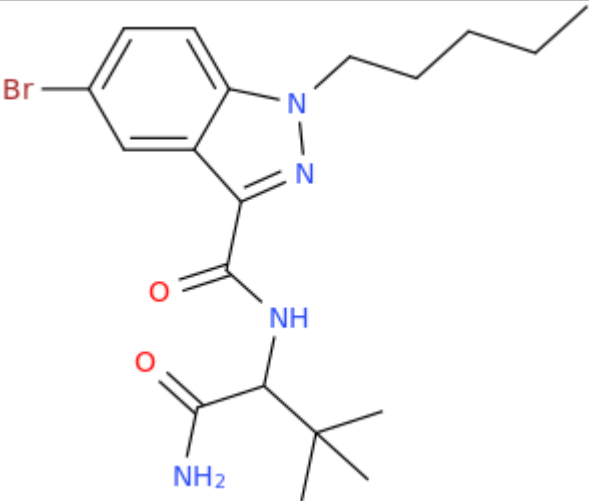
ANALYTICAL REPORT

ADB-P-5Br-INACA (C₁₉H₂₇BrN₄O₂)

2-[(5-bromo-1-pentyl-1H-indazol-3-yl)formamido]-3,3-dimethylbutanamide

Remark – other NPS detected: **ADB-5Br-INACA, JWH-210**

Sample ID:	3236-23
Sample description:	plant material
Sample type:	seized /NM
Date of entry (DD/MM/YYYY) into NFL database:	22/05/2023
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	2-[(5-bromo-1-pentyl-1H-indazol-3-yl)formamido]-3,3-dimethylbutanamide
Other names	N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-5-bromo-1-pentyl-1H-indazole-3-carboxamide; ADB-5Br-PINACA; ADMB-P-5Br-INACA
Formula (per base form)	C ₁₉ H ₂₇ BrN ₄ O ₂
M _w (g/mol)	423,36
Salt form/anions detected	/
StdInChIKey (per base form)	OUVBRTCXLMBRLT-UHFFFAOYSA-N
Other NPS detected	ADB-5Br-INACA, JWH-210
Additional info (purity..)	herbal incense

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 µl 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 6.1 min, then heating at 50 °C/min up to 325 °C and finally 9.1 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 solid phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

GC-method: Injection volume 1 µl 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 KOH 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

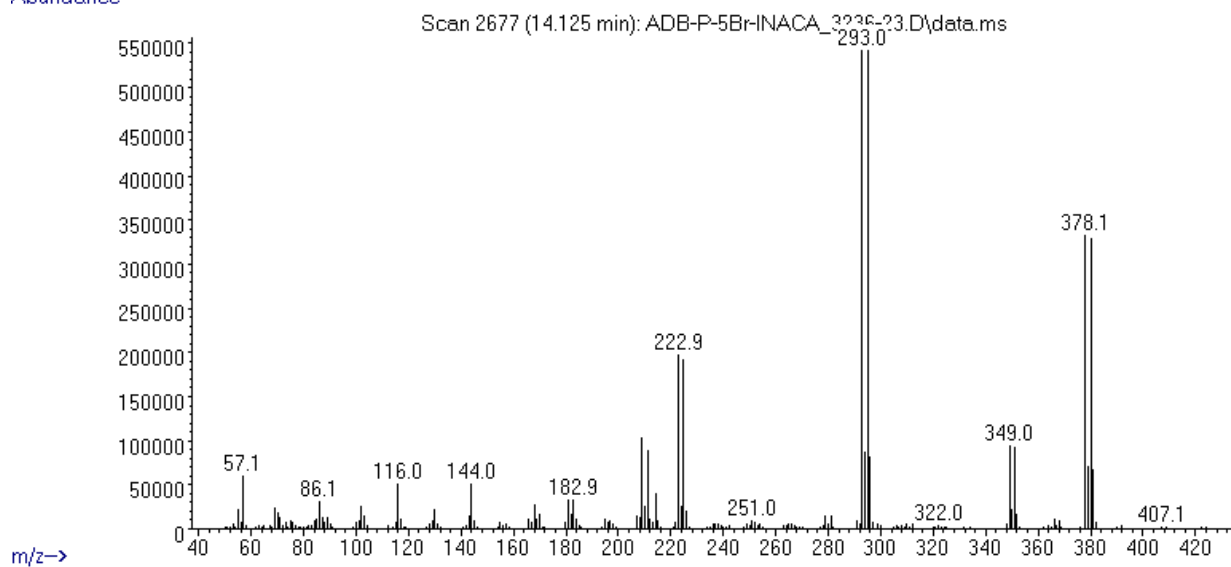
Solubility in	result/remark
CH ₂ Cl ₂	soluble
MeOH	soluble
H ₂ O	/

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 14,13 BP(1): 293; BP(2): 295,BP(3) :378,
HPLC-TOF	+	Exact mass (theoretical): 422,1317; measured value Δppm:-0,88; formula:C19H27BrN4O2
FTIR-ATR	-	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	-	
NMR (in FKKT)	-	
validation		
other		

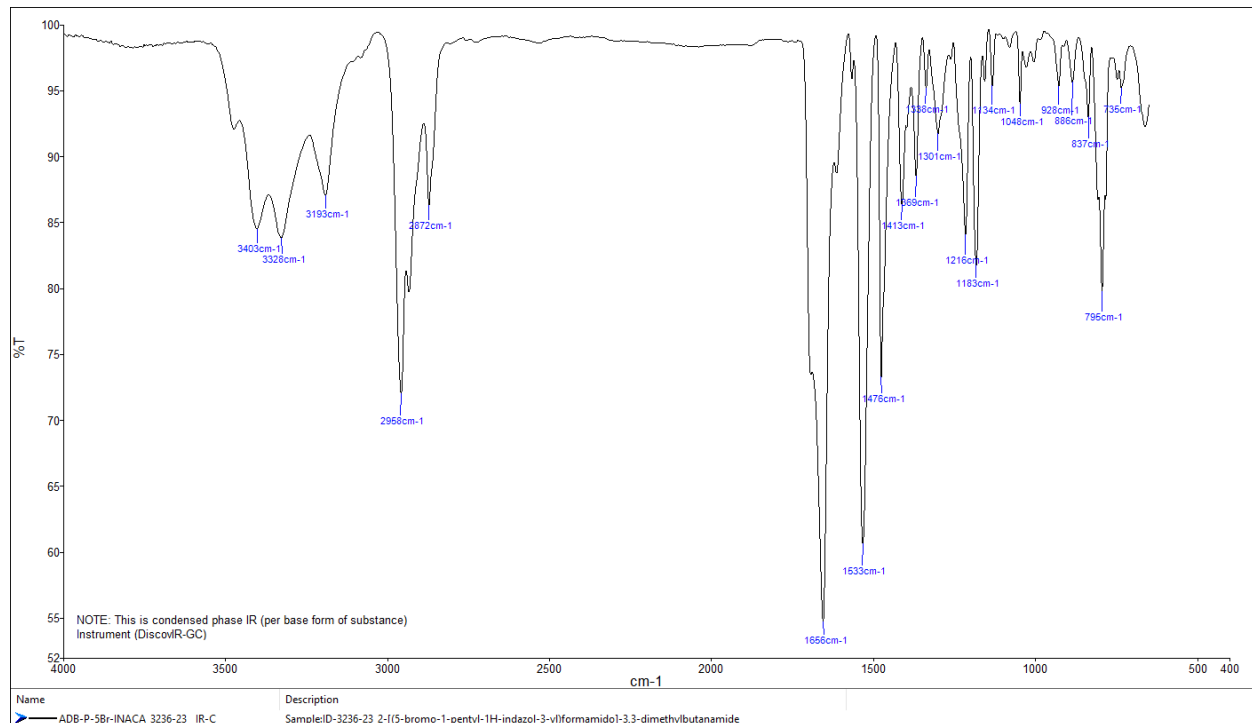
ANALYTICAL RESULTS

MS (EI)

Abundance



IR (solid phase – after chromatographic separation)



TOF REPORT

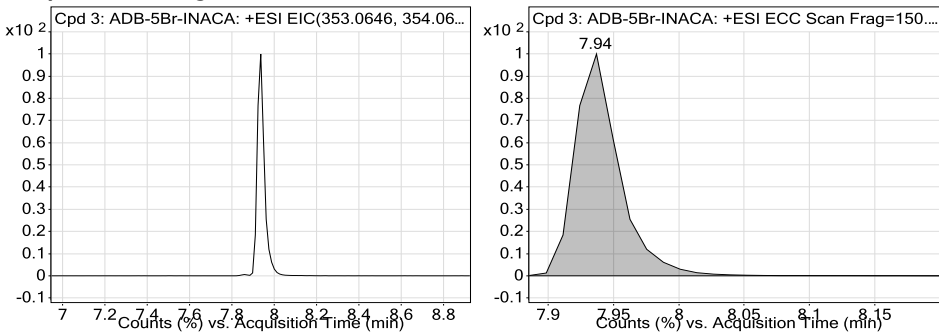
Data File	ADB-P-5Br-INACA_3236-23.d	Sample Name	ID-3236-23
Sample Type	Sample	Position	P1-A5
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-13_03_2023-XDB-C18-ESI+.m	Acquired Time	4/25/2023 10:12:09 AM
IRM Calibration Status	Success	DA Method	0-NPS in sorodne snovi.m
Comment	extract in MeOH		

Compound Table

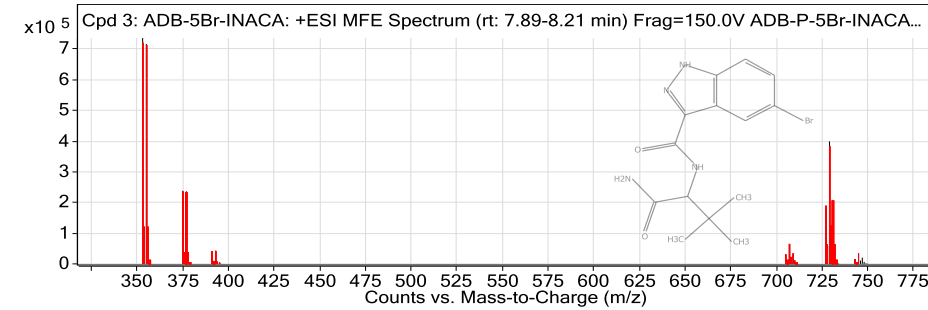
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 3: ADB-5Br-INACA	ADB-5Br-INACA	C14 H17 Br N4 O2	7.94	352.0535
Cpd 7: ADB-5'Br-PINACA	ADB-5'Br-PINACA	C19 H27 Br N4 O2	9.96	422.1321
Cpd 8: JWH-210	JWH-210	C26 H27 N O	11.07	369.2099

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
ADB-5Br-INACA	353.0617	7.94	352.0535	7.98	C14 H17 Br N4 O2	352.0535	-0.11

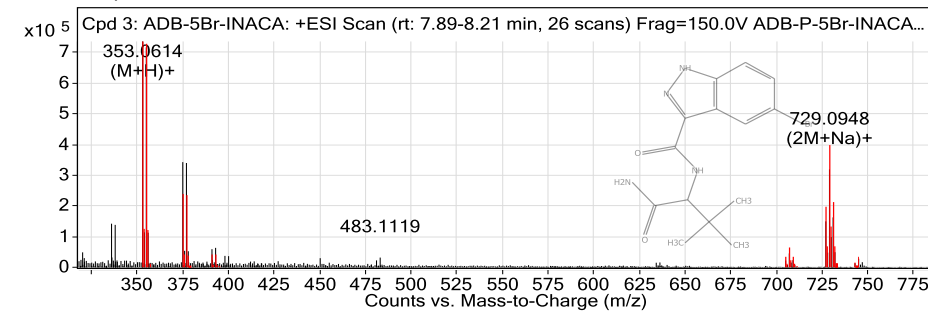
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

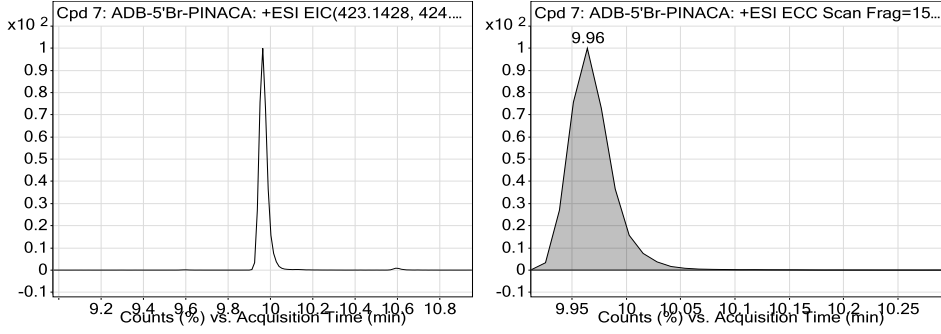
Obs. m/z	Charge	Abund	Formula	Ion/Isotope
353.0617	1	735789.56	C14 H17 Br N4 O2	(M+H)+
354.064	1	113023.79	C14 H17 Br N4 O2	(M+H)+
355.0597	1	716305.78	C14 H17 Br N4 O2	(M+H)+
356.0621	1	112729.63	C14 H17 Br N4 O2	(M+H)+
375.0431	1	238254.22	C14 H17 Br N4 O2	(M+Na)+
377.0413	1	236293.26	C14 H17 Br N4 O2	(M+Na)+
727.0966	1	186614.14	C14 H17 Br N4 O2	(2M+Na)+
729.0954	1	398888.91	C14 H17 Br N4 O2	(2M+Na)+
730.0972	1	122993.29	C14 H17 Br N4 O2	(2M+Na)+
731.0936	1	202859.21	C14 H17 Br N4 O2	(2M+Na)+

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
ADB-5Br-INACA	353.0617	7.94	352.0535	7.98	C14 H17 Br N4 O2	352.0535	-0.11

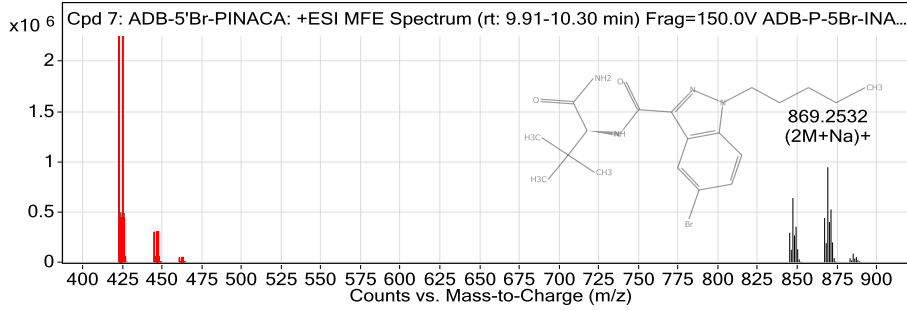
TOF REPORT

ADB-5'Br-PINACA	423.14	9.96	422.1321	9.98	C19 H27 Br N4 O2	422.1317	-0.88
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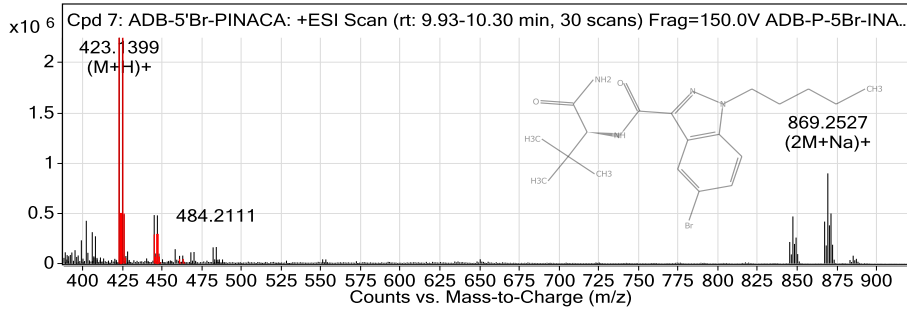
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



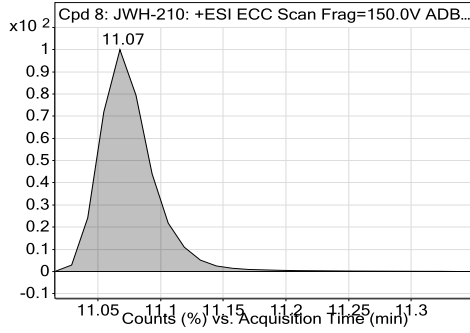
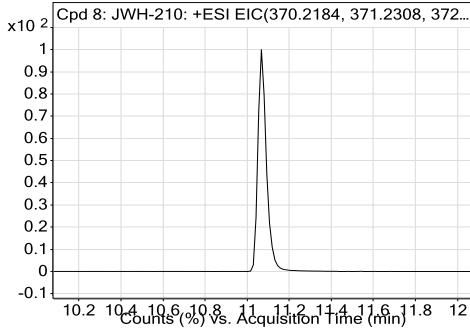
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
423.14	1	2248130.75	C19 H27 Br N4 O2	(M+H)+
424.1433	1	495936.73	C19 H27 Br N4 O2	(M+H)+
425.1381	1	2239518.14	C19 H27 Br N4 O2	(M+H)+
426.1415	1	490312.48	C19 H27 Br N4 O2	(M+H)+
847.2711	1	639056.88		(2M+H)+
849.2698	1	352338.23		(2M+H)+
867.2543	1	439847.7		(2M+Na)+
869.2532	1	945197.88		(2M+Na)+
870.2556	1	400245.35		(2M+Na)+
871.2521	1	525366.36		(2M+Na)+

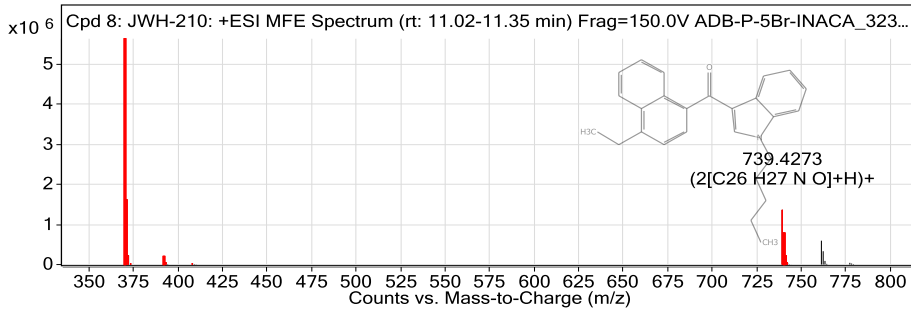
Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
JWH-210	370.2171	11.07	369.2099	10.98	C26 H27 N O	369.2093	-1.85

Compound Chromatograms

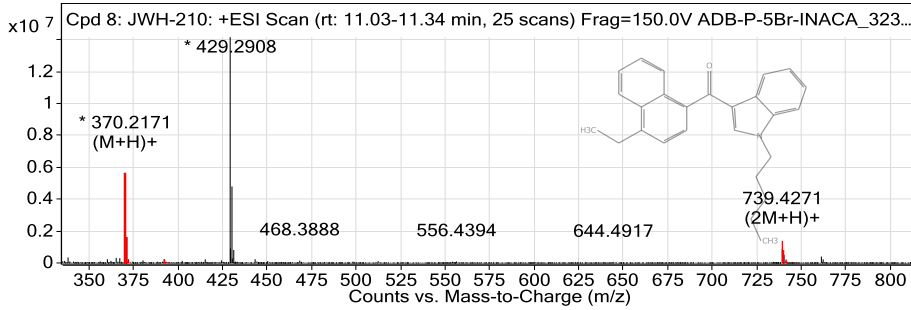
TOF REPORT



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
370.2171	1	5627417.5	C ₂₆ H ₂₇ N O	(M+H) ⁺
371.2209	1	1633393.55	C ₂₆ H ₂₇ N O	(M+H) ⁺
372.224	1	229053.47	C ₂₆ H ₂₇ N O	(M+H) ⁺
392.1992	1	211532.56	C ₂₆ H ₂₇ N O	(M+Na) ⁺
739.4273	1	1363735	C ₂₆ H ₂₇ N O	(2M+H) ⁺
740.431	1	803865.17	C ₂₆ H ₂₇ N O	(2M+H) ⁺
741.4334	1	223792.48	C ₂₆ H ₂₇ N O	(2M+H) ⁺
761.4094	1	595263.81		(2M+Na) ⁺
762.4128	1	332588.56		(2M+Na) ⁺
763.4157	1	90768.42		(2M+Na) ⁺

--- End Of Report ---