

Chemistry - maXis HPLC-ESI Accurate Mass Report

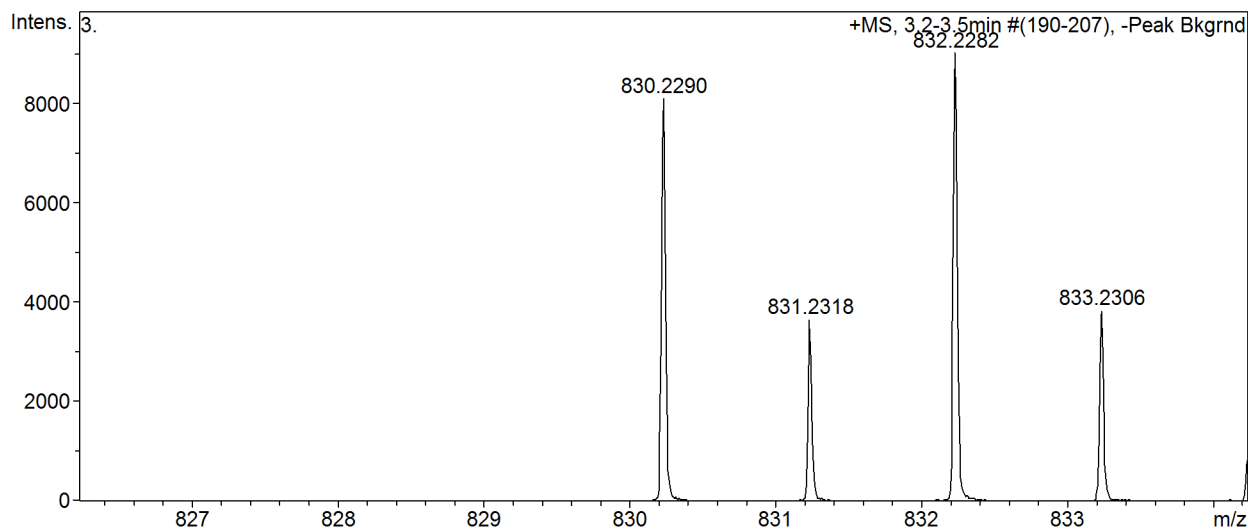
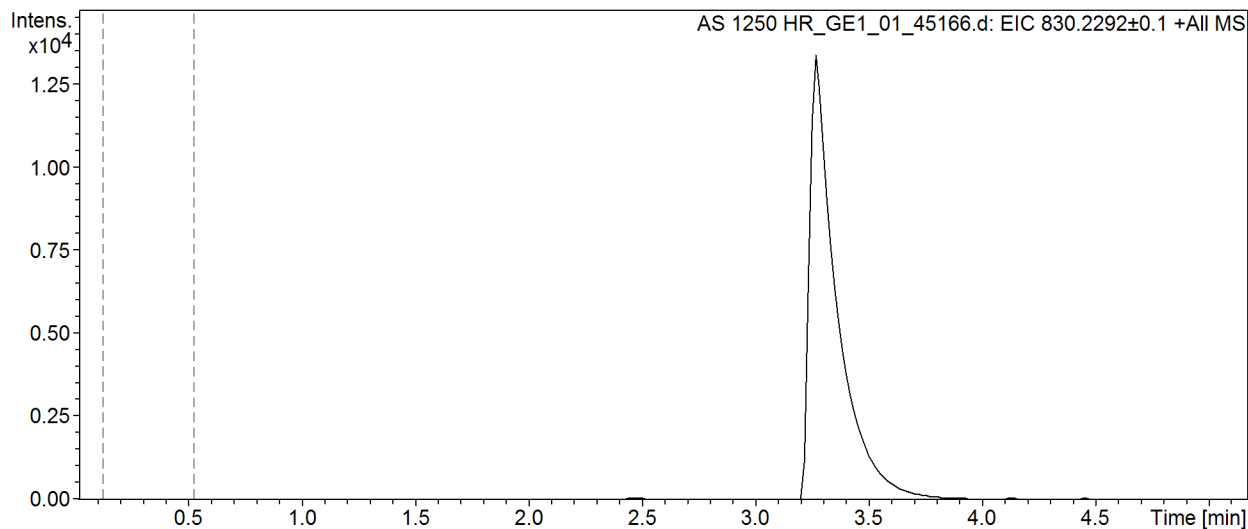
Analysis Info

Analysis Name	D:\Data\Chemistry\2023\March\AS 1250 HR_GE1_01_45166.d	Acquisition Date	14/03/2023 09:34:38
Method	soton lcms pos 150 to 1500.m	Operator	MSWEB@SOTON.AC.UK
Sample Name	AS 1250 HR	Instrument / Ser#	maXis 17
Comment	Analyst: JMH		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	230 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

Cmpd 3, 3.3 min



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Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e ⁻ Conf	N-Rule
830.2290	C 42 H 45 Br N 3 O 10	830.2283	-0.8	-0.7	1	15.6	21.5	even	ok
	C 43 H 41 Br N 7 O 6	830.2296	0.8	0.6	2	24.6	26.5	even	ok
	C 45 H 46 Br N Na O 8	830.2299	1.1	0.9	3	24.6	22.5	even	ok
	C 42 H 38 Br N 11 Na O 2	830.2286	-0.5	-0.4	4	26.5	28.5	even	ok
	C 40 H 33 Br N 17	830.2283	-0.9	-0.7	5	27.1	32.5	even	ok
852.2105	C 40 H 32 Br N 17 Na	852.2102	-0.3	-0.3	1	12.4	32.5	even	ok
	C 39 H 36 Br N 13 Na O 4	852.2089	-1.9	-1.6	2	14.3	27.5	even	ok
	C 41 H 35 Br N 13 O 4	852.2113	0.9	0.8	3	15.8	30.5	even	ok
	C 43 H 40 Br N 7 Na O 6	852.2116	1.3	1.1	4	18.2	26.5	even	ok
	C 40 H 39 Br N 9 O 8	852.2099	-0.6	-0.5	5	18.7	25.5	even	ok
	C 42 H 44 Br N 3 Na O 10	852.2102	-0.3	-0.3	6	20.5	21.5	even	ok
	C 56 H 39 Br N O 3	852.2108	0.4	0.3	7	61.3	37.5	even	ok

Samples were analysed using a MaXis (Bruker Daltonics, Bremen, Germany) time of flight (TOF) mass spectrometer. Samples were introduced to the mass spectrometer via a Dionex Ultimate 3000 autosampler and uHPLC pump. Ultrahigh performance liquid chromatography was performed using a Waters, Acquity UPLC BEH C18 (50 mm x 2.1 mm 1.7µm) column. Gradient elution from 5% acetonitrile (0.2% formic acid) to 100% acetonitrile (0.2% formic acid) was performed in five minutes at 0.6 mL/min. High resolution positive/negative ion electrospray ionisation mass spectra were recorded.

Please use the calculated m/z for the formula of each ion as reported here, as this takes into account the mass of the electron.