

Chemistry - maXis HPLC-ESI Accurate Mass Report

Analysis Info

Analysis Name D:\Data\chemistry\2015\nov 15\RL-Ligand A_GA2_01_20529.d
Method soton lcms pos 120 to 1500.m
Sample Name RL-Ligand A
Comment Analyst: JMH

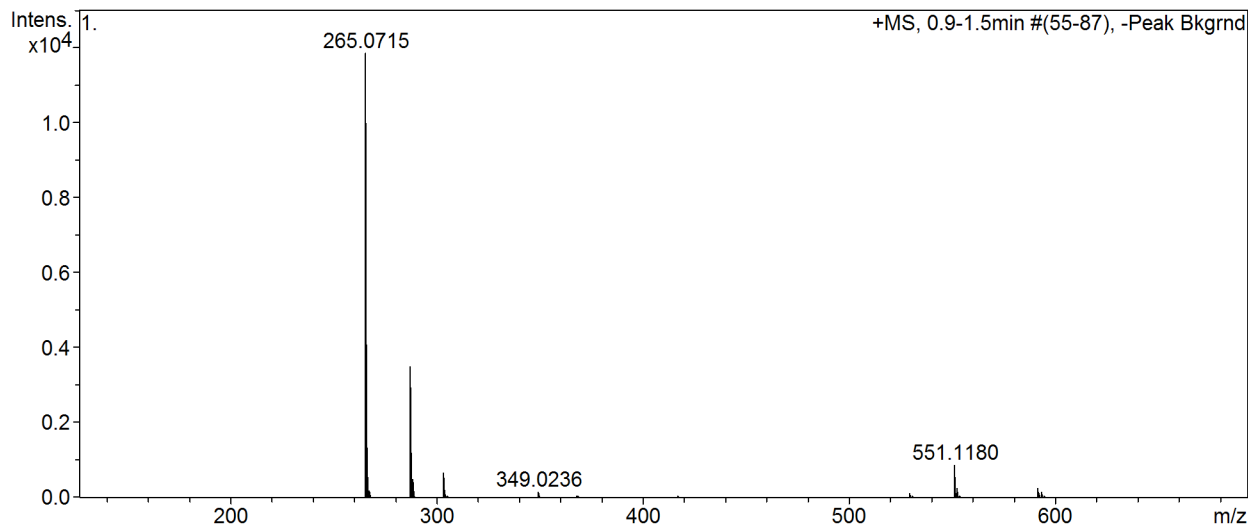
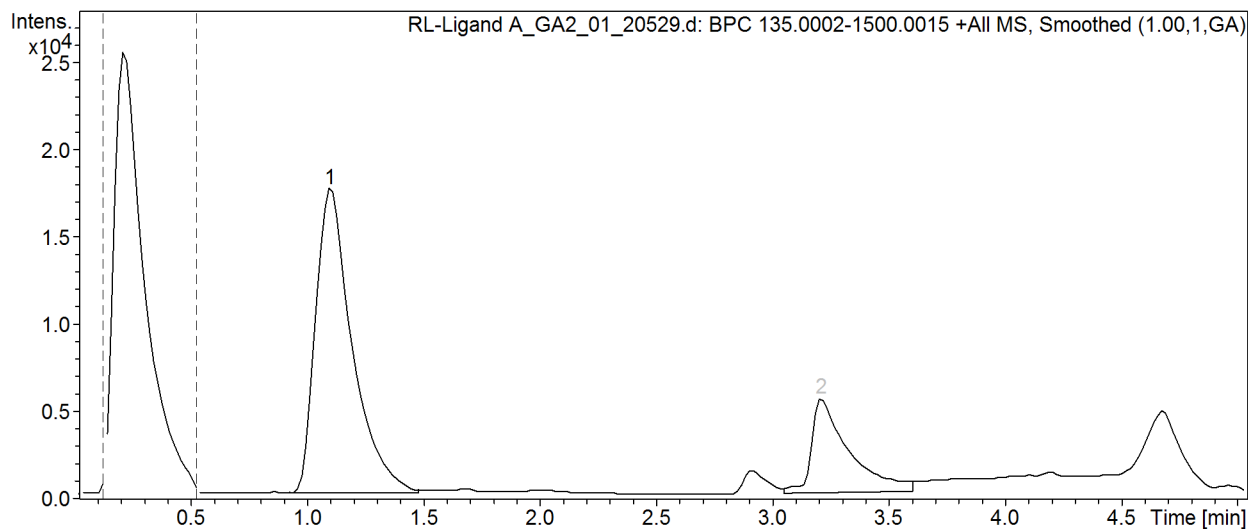
Acquisition Date 18/11/2015 14:28:20

Operator MSWEB@SOTON.AC.UK
Instrument / Ser# maXis 17

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	120 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 1, 1.1 min



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Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e ⁻ Conf	N-Rule
265.0715	C 13 H 13 O 6	265.0707	-3.0	-0.8	1	6.6	7.5	even	ok
	C 14 H 9 N 4 O 2	265.0720	2.1	0.6	2	19.8	12.5	even	ok
	C 7 H 9 N 10 S	265.0727	4.7	1.2	3	29.0	8.5	even	ok
	C 8 H 18 Na O 6 S	265.0716	0.7	0.2	4	34.7	-0.5	even	ok
	C 6 H 13 N 6 O 4 S	265.0714	-0.4	-0.1	5	38.5	3.5	even	ok
287.0532	C 11 H 7 N 6 O 4	287.0523	-3.0	-0.9	1	10.2	11.5	even	ok
	C 13 H 12 Na O 6	287.0526	-2.0	-0.6	2	12.5	7.5	even	ok
	C 12 H 3 N 10	287.0537	1.7	0.5	3	18.5	16.5	even	ok
	C 14 H 8 N 4 Na O 2	287.0539	2.6	0.8	4	19.3	12.5	even	ok
	C 7 H 15 N 2 O 8 S	287.0544	4.1	1.2	5	45.0	1.5	even	ok
	C 19 H 11 O S	287.0525	-2.4	-0.7	6	50.9	14.5	even	ok

Samples were analysed using a MaXis (Bruker Daltonics, Bremen, Germany) mass spectrometer equipped with a Time of Flight (TOF) analyser. Samples were introduced to the mass spectrometer via a Dionex Ultimate 3000 autosampler and uHPLC pump. Gradient 20% acetonitrile (0.2% formic acid) to 100% acetonitrile (0.2% formic acid) in five minutes at 0.6 mL min. Column, Acquity UPLC BEH C18 (Waters) 1.7 micron 50 x 2.1mm. High resolution mass spectra were recorded using positive/negative ion electrospray ionisation.

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.