

Chemistry - maXis HPLC-ESI Accurate Mass Report

Analysis Info

Analysis Name D:\Data\chemistry\2015\nov 15\RL-Ligand B_GA3_01_20530.d
Method soton lcms pos 120 to 1500.m
Sample Name RL-Ligand B
Comment Analyst: JMH

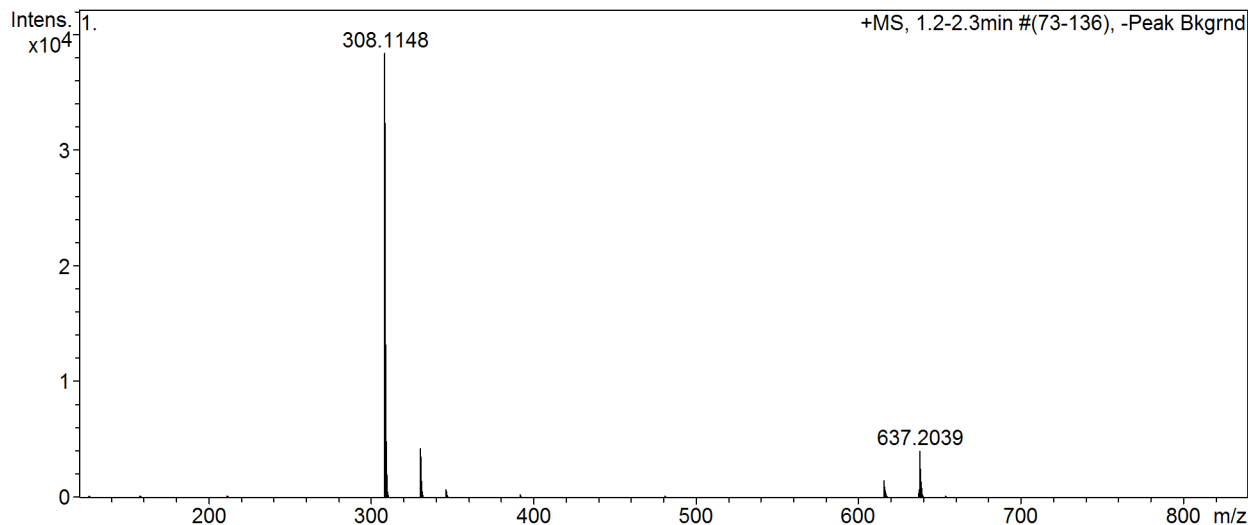
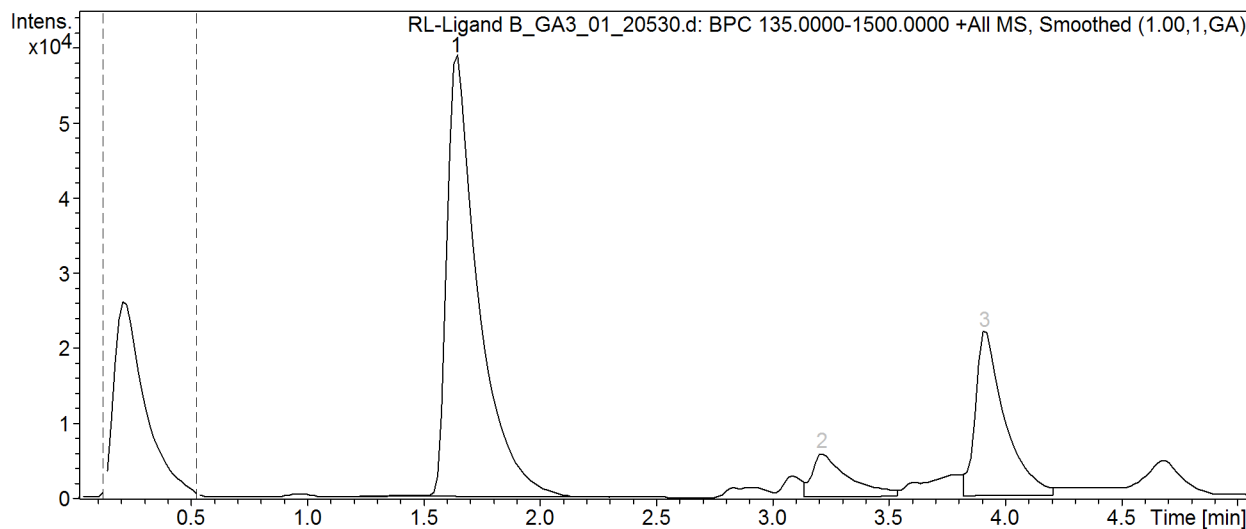
Acquisition Date 18/11/2015 14:34:44

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, 1.6 min



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Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e ⁻ Conf	N-Rule
308.1148	C 16 H 14 N 5 O 2	308.1142	-2.0	-0.6	1	24.8	12.5	even	ok
	C 9 H 14 N 11 S	308.1149	0.2	0.1	2	27.5	8.5	even	ok
	C 11 H 19 N 5 Na O 2 S	308.1152	1.1	0.3	3	29.8	4.5	even	ok
	C 8 H 18 N 7 O 4 S	308.1135	-4.1	-1.3	4	31.8	3.5	even	ok
	C 12 H 22 N O 6 S	308.1162	4.6	1.4	5	33.8	2.5	even	ok
	C 10 H 23 N Na O 6 S	308.1138	-3.2	-1.0	6	35.4	-0.5	even	ok
	C 19 H 15 N 3 Na	308.1158	3.2	1.0	7	39.2	13.5	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.