

Chemistry - maXis HPLC-ESI Accurate Mass Report

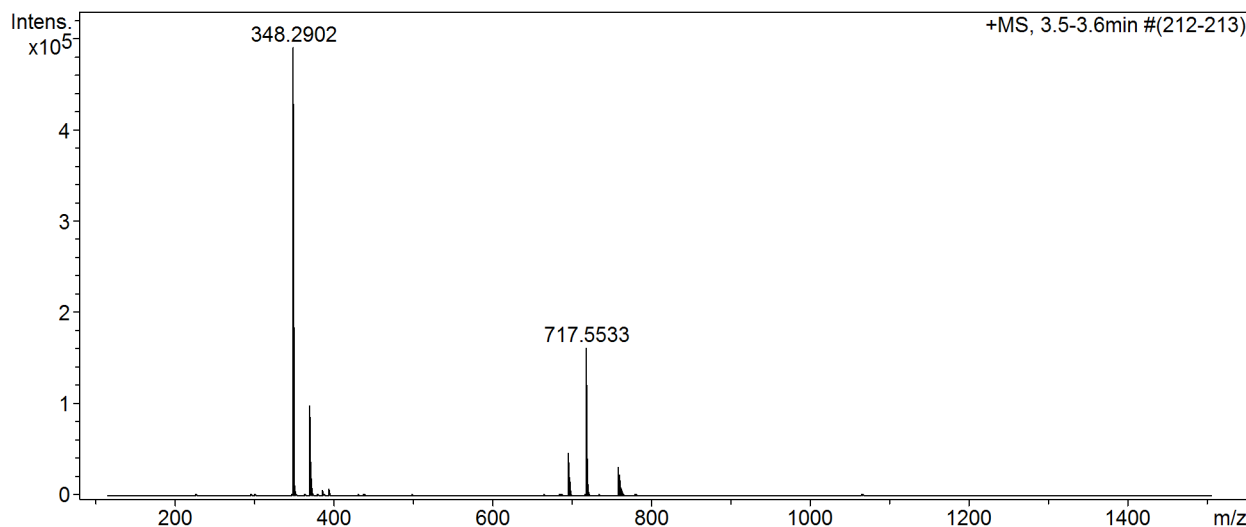
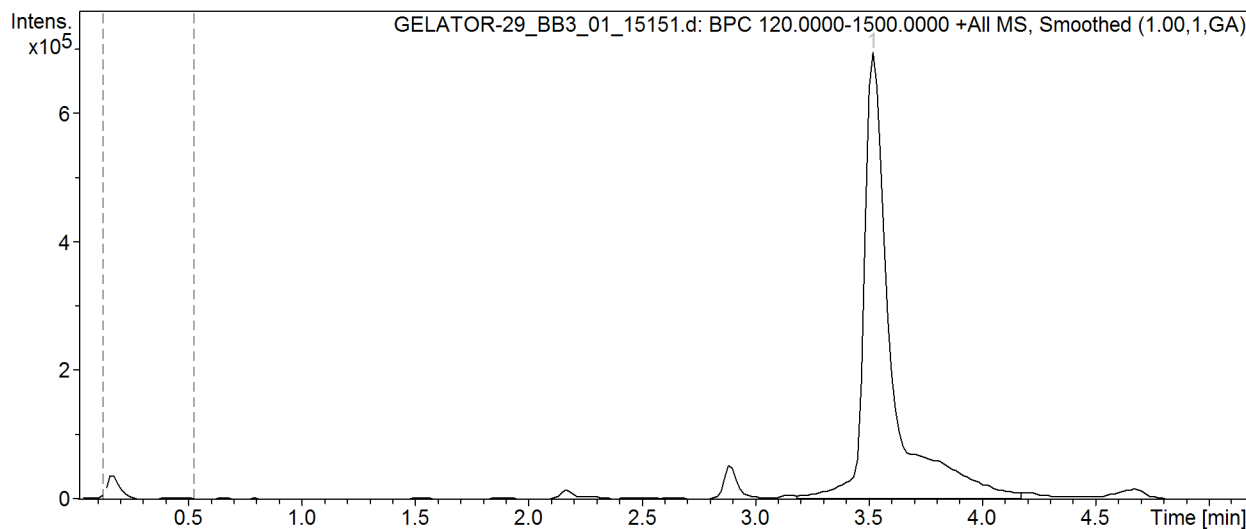
Analysis Info

Analysis Name	D:\Data\Chemistry\2014\Dec 14\GELATOR-29_BB3_01_15151.d	Acquisition Date	10/12/2014 18:29:40
Method	soton lcms pos 120 to 1500.m	Operator	MSWEB@SOTON.AC.UK
Sample Name	GELATOR-29	Instrument / Ser#	maXis 17
Comment	Analyst: JMH		

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	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

+MS, 3.5-3.6min #(212-213)



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Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e ⁻ Conf	N-Rule
348.2902	C 22 H 38 N O 2	348.2897	-1.4	-0.5	1	7.7	4.5	even	ok
370.2719	C 20 H 32 N 7	370.2714	-1.4	-0.5	1	18.2	8.5	even	ok
	C 22 H 37 N Na O 2	370.2717	-0.7	-0.2	2	18.6	4.5	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.