

Chemistry - maXis HPLC-ESI Accurate Mass Report

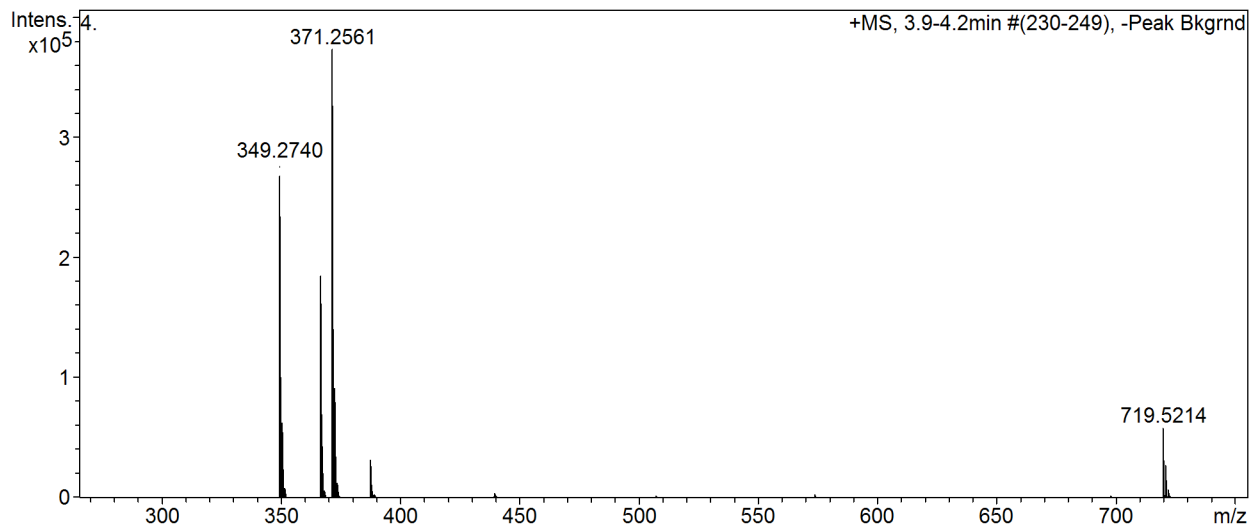
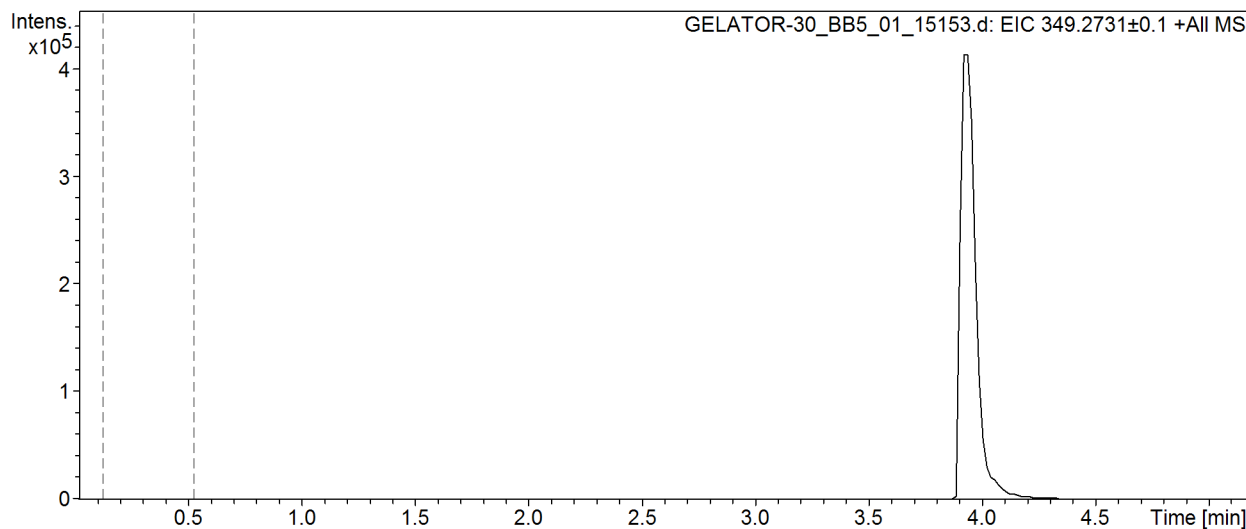
Analysis Info

Analysis Name	D:\Data\Chemistry\2014\Dec 14\GELATOR-30_BB5_01_15153.d	Acquisition Date	10/12/2014 18:42:28
Method	soton lcms pos 120 to 1500.m	Operator	MSWEB@SOTON.AC.UK
Sample Name	GELATOR-30	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

Cmpd 4, 3.9 min



Chemistry - maXis HPLC-ESI Accurate Mass Report

Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e ⁻ Conf	N-Rule
349.2740	C 22 H 37 O 3	349.2737	-0.9	-0.3	1	7.1	4.5	even	ok
371.2561	C 22 H 36 Na O 3	371.2557	-1.1	-0.4	1	1.8	4.5	even	ok
	C 20 H 31 N 6 O	371.2554	-1.9	-0.7	2	1.9	8.5	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.