

Chemistry - maXis HPLC-ESI Accurate Mass Report

Analysis Info

Analysis Name D:\Data\Chemistry\2014\Oct 14\Gelator 11_GA7_01_14969.d
Method soton lcms pos 120 to 1500.m
Sample Name Gelator 11
Comment Analyst: JMH

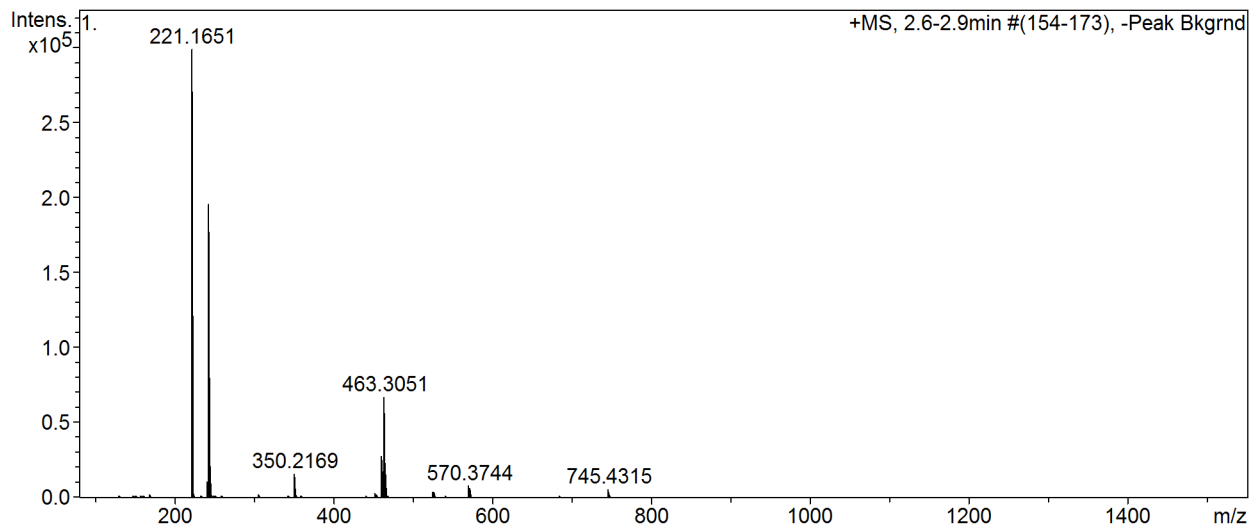
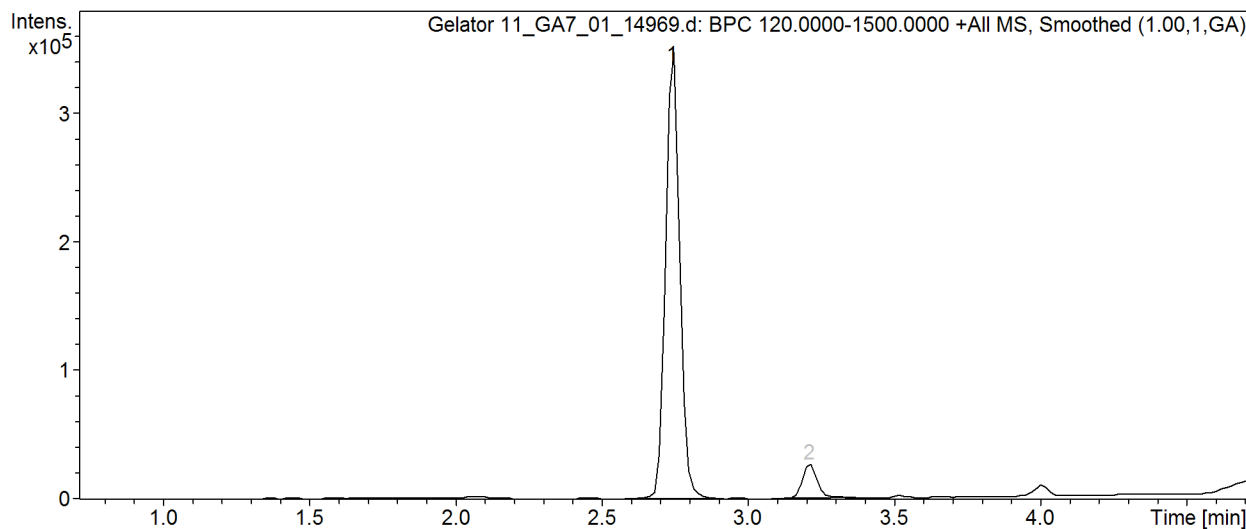
Acquisition Date 23/10/2014 12:59:46

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

Cmpd 1, 2.7 min



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Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e ⁻ Conf	N-Rule
221.1651	C 13 H 21 N 2 O	221.1648	-1.3	-0.3	1	0.1	4.5	even	ok
243.1471	C 13 H 20 N 2 Na O	243.1468	-1.4	-0.3	1	16.8	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 2% methanol (0.1% formic acid) to 100% methanol (0.1% formic acid) in seven minutes. Column, Kinetex C18 (Phenomenex) 1.7 micron 50 x 2.1mm. High resolution mass spectra were recorded using positive/negative ion electrospray ionisation.