

Chemistry - maXis HPLC-ESI Accurate Mass Report

Analysis Info

Analysis Name D:\Data\Chemistry\2014\Oct 14\Gelator 26_GB2_01_14972.d
Method soton lcms pos 120 to 1500.m
Sample Name Gelator 26
Comment Analyst: JMH

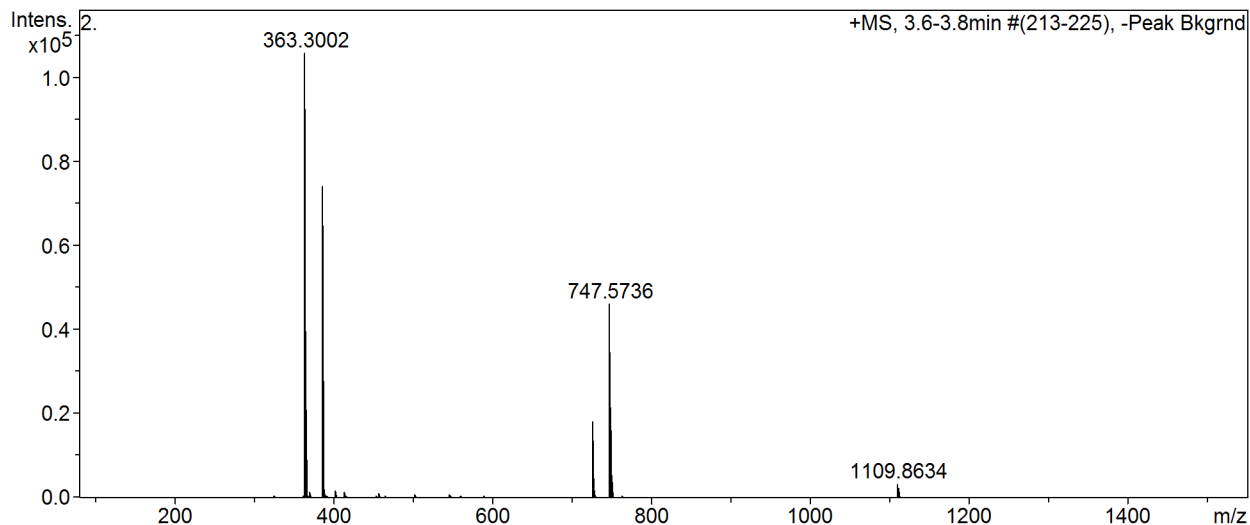
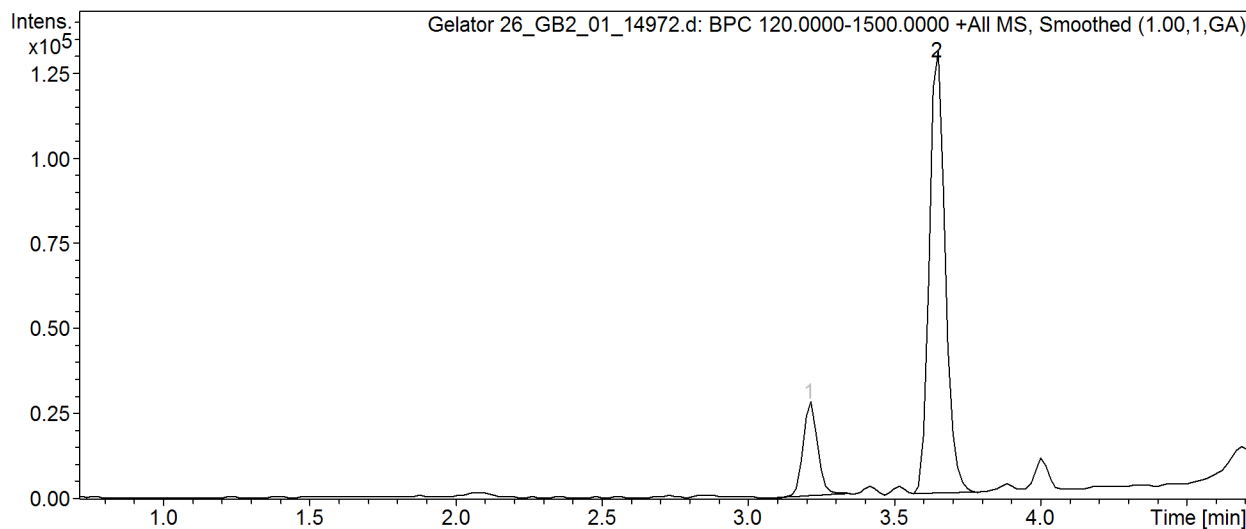
Acquisition Date 23/10/2014 13:19:02

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 2, 3.6 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
363.3002	C ₂₂ H ₃₉ N ₂ O ₂	363.3006	1.2	0.4	1	14.7	4.5	even	ok
385.2822	C ₂₂ H ₃₆ F ₃ N ₂	385.2825	0.7	0.3	1	16.3	4.5	even	ok
	C ₂₀ H ₃₃ N ₈	385.2823	0.1	0.0	2	16.4	8.5	even	ok
	C ₂₂ H ₃₈ N ₂ NaO ₂	385.2825	0.8	0.3	3	16.7	4.5	even	ok
	C ₁₉ H ₄₀ F ₂ N ₂ NaSi	385.2821	-0.3	-0.1	4	41.1	0.5	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.