

## Chemistry - maXis HPLC-ESI Accurate Mass Report

### Analysis Info

Analysis Name D:\Data\Chemistry\2014\Oct 14\Gelator 14\_GA6\_01\_14968.d  
Method soton lcms pos 120 to 1500.m  
Sample Name Gelator 14  
Comment Analyst: JMH

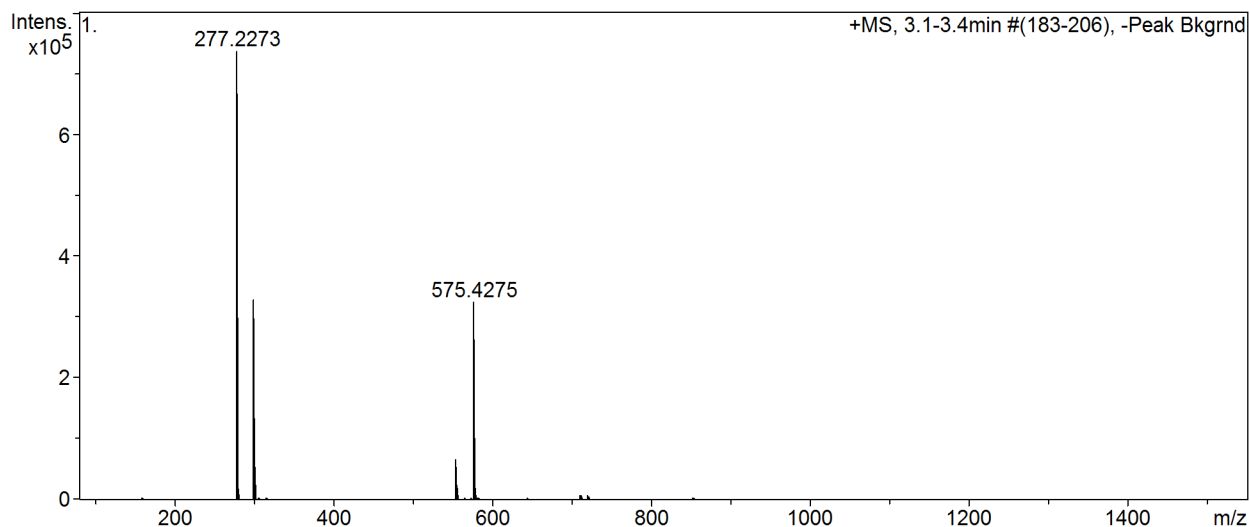
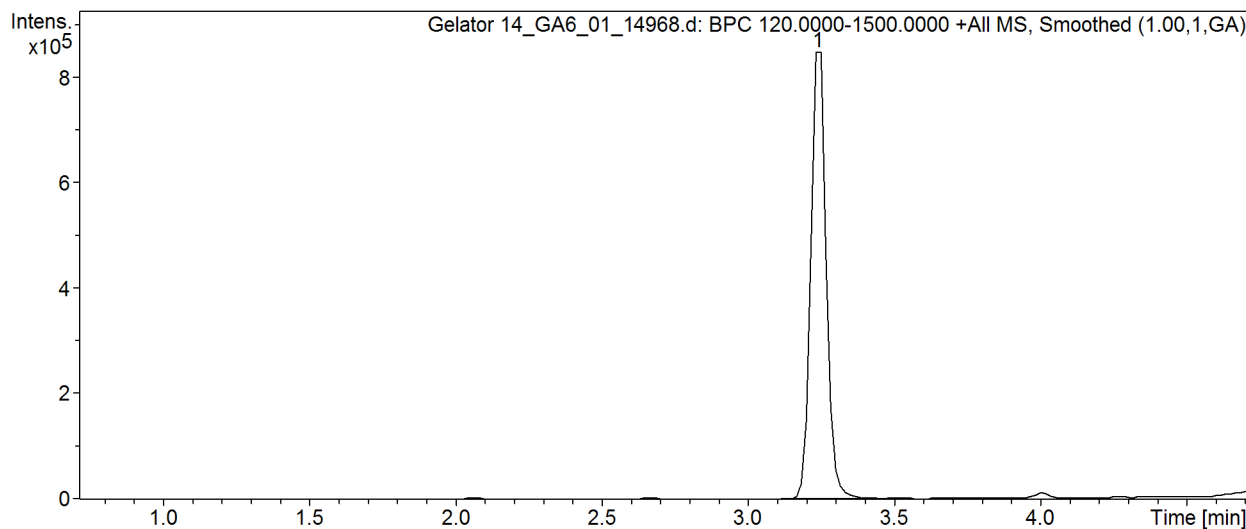
Acquisition Date 23/10/2014 12:53:22

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, 3.2 min



## Chemistry - maXis HPLC-ESI Accurate Mass Report

---

Meas. m/z	Formula	m/z	err [ppm]	err [mDa]	# Sigma	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
277.2273	C 17 H 29 N 2 O	277.2274	0.6	0.2	1	64.4	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.