

rc5-635-A MW=280?

ASAP (SOLID)

C₁₅H₂₀O₃S

IMPBUL-AYEWR-WR-A 261 (2.427) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (214:276)

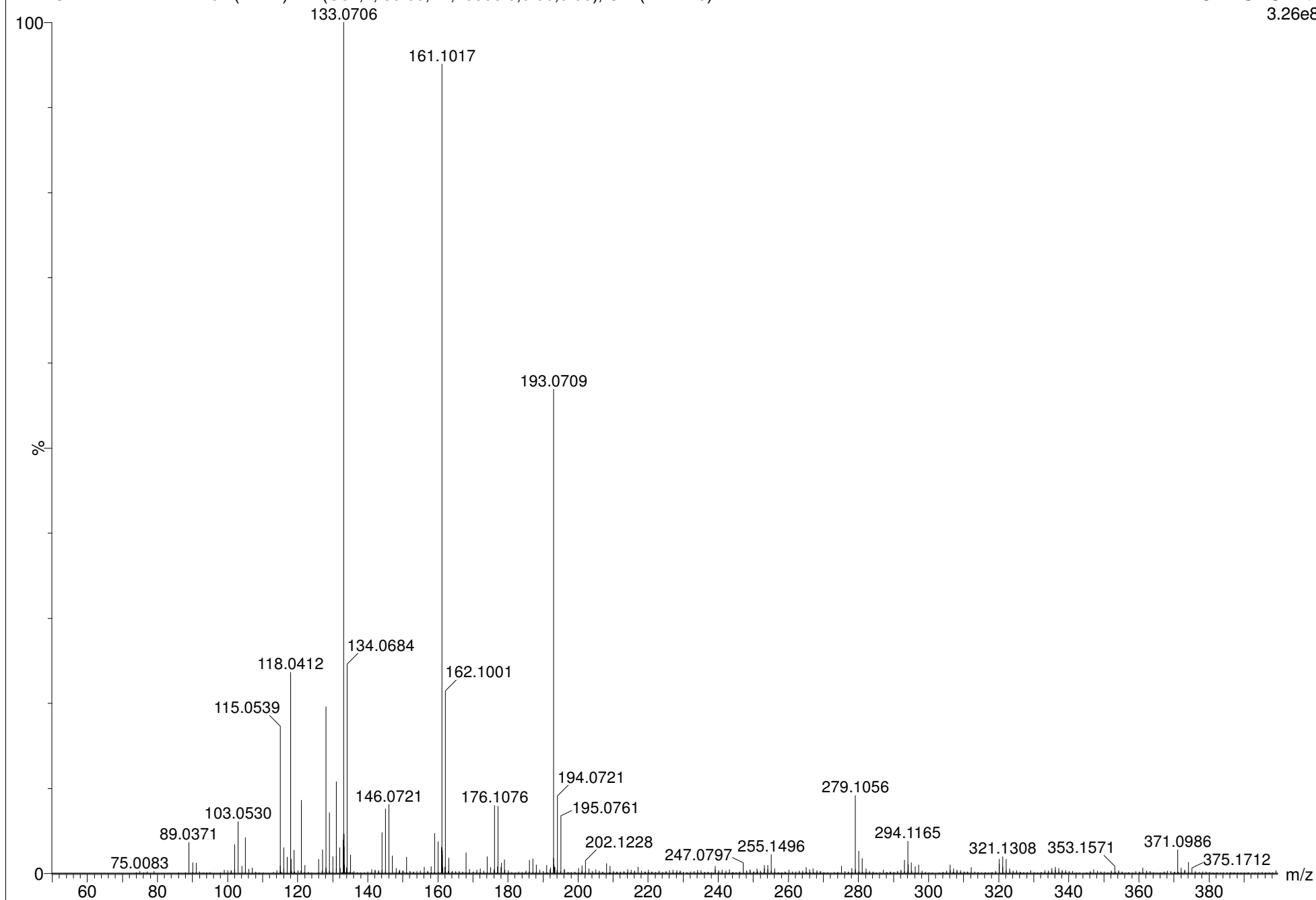
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Rosie Croft

07-Apr-2017

1: TOF MS ASAP+
3.26e8



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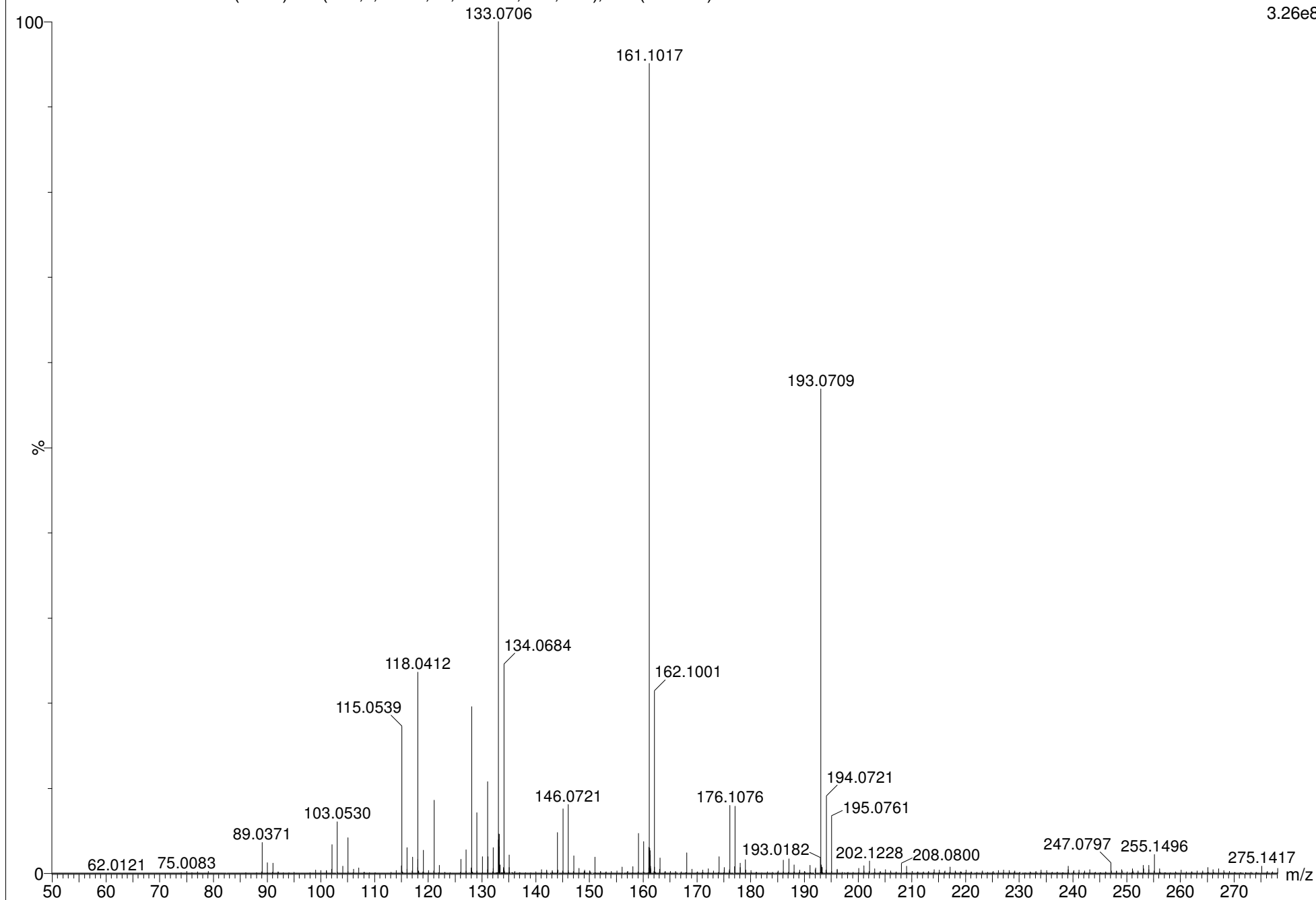
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3.26e8



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IMPBUL-AYEWR-WR-A (0.037) Is (1.00,0.05) C₁₅H₁₉O₃S

National Mass Spectrometry Facility, Swansea

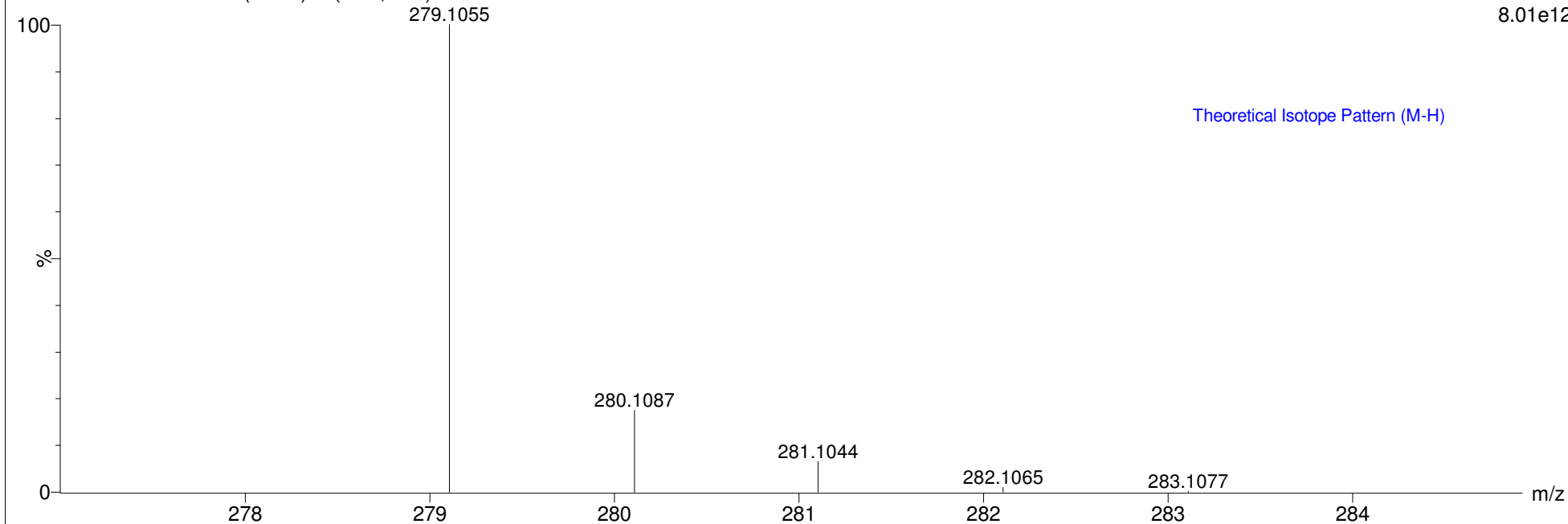
Xevo G2-S

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1: TOF MS ASAP+

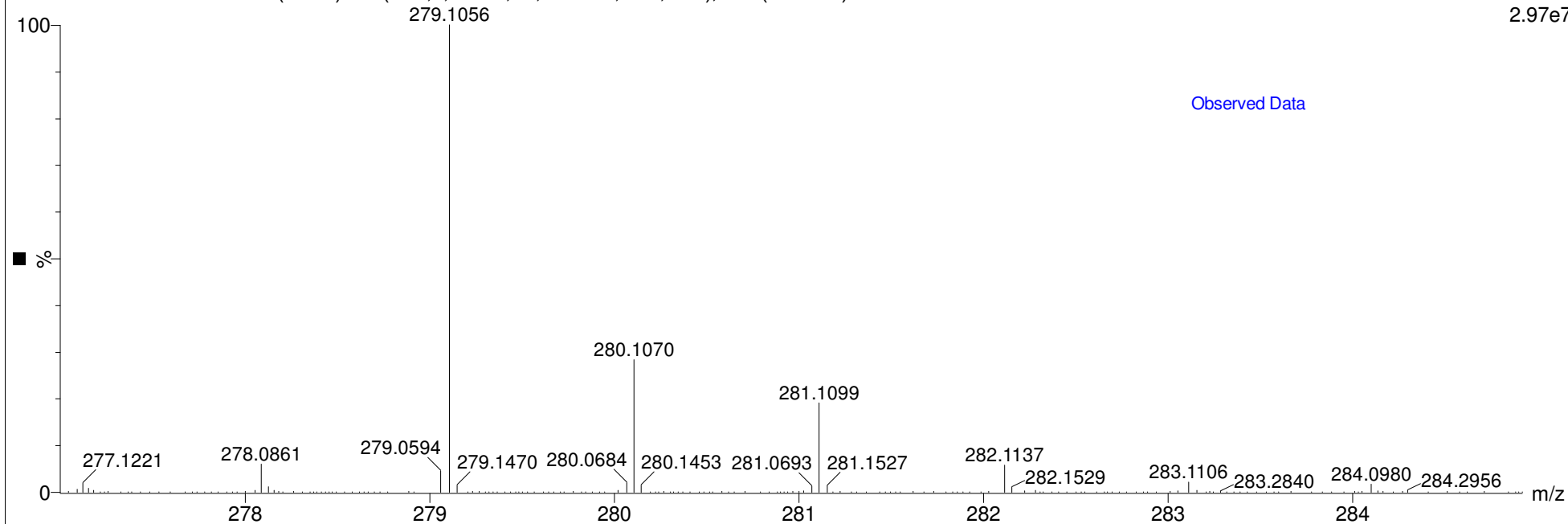
8.01e12



IMPBUL-AYEWR-WR-A 261 (2.427) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (214:276)

1: TOF MS ASAP+

2.97e7



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -150.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions

2128 formula(e) evaluated with 10 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-10 O: 0-13 S: 0-2

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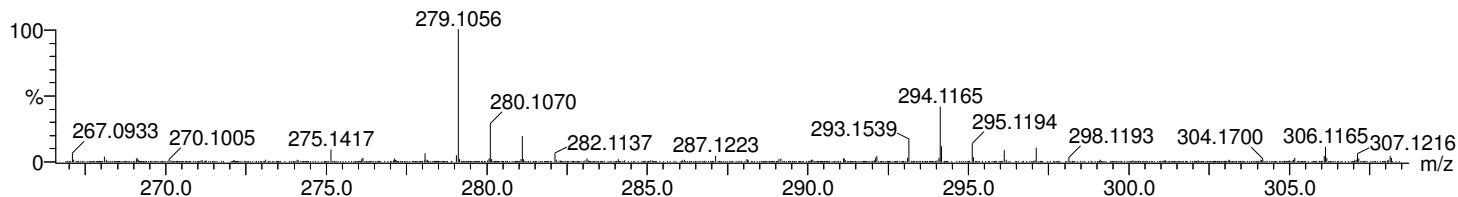
07-Apr-2017

C₁₅H₂₀O₃S

IMPBUL-AYEWR-WR-A 261 (2.427) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (214:276)

1: TOF MS ASAP+

2.98e+007



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
279.1056	279.1055	0.1	0.4	6.5	2213.8	3.355	3.49	C ₁₅ H ₁₉ O ₃ S
	279.1053	0.3	1.1	3.5	2211.9	1.357	25.74	C ₇ H ₁₅ N ₆ O ₆
	279.1060	-0.4	-1.4	-6.0	2216.2	5.684	0.34	C H ₂₁ N ₅ O ₉ S
	279.1062	-0.6	-2.1	2.5	2216.2	5.680	0.34	C ₈ H ₁₉ N ₆ O S ₂
	279.1048	0.8	2.9	16.0	2213.5	2.998	4.99	C ₂₁ H ₁₃ N
	279.1048	0.8	2.9	3.0	2216.9	6.433	0.16	C ₆ H ₁₇ N ₉ S ₂
	279.1048	0.8	2.9	-2.5	2216.2	5.660	0.35	C ₇ H ₂₃ N ₂ O ₅ S ₂
	279.1047	0.9	3.2	-11.0	2215.2	4.678	0.93	H ₂₅ N O ₁₃ S
	279.1066	-1.0	-3.6	3.0	2212.0	1.551	21.21	C ₉ H ₁₇ N ₃ O ₇
	279.1066	-1.0	-3.6	8.5	2211.4	0.857	42.45	C ₈ H ₁₁ N ₁₀ O ₂