

rc5-640-A MW=312?

ASAP (SOLID)

C15H20O5S

IMPBUL-AYMH9-WR-A 415 (3.850) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (413:434)

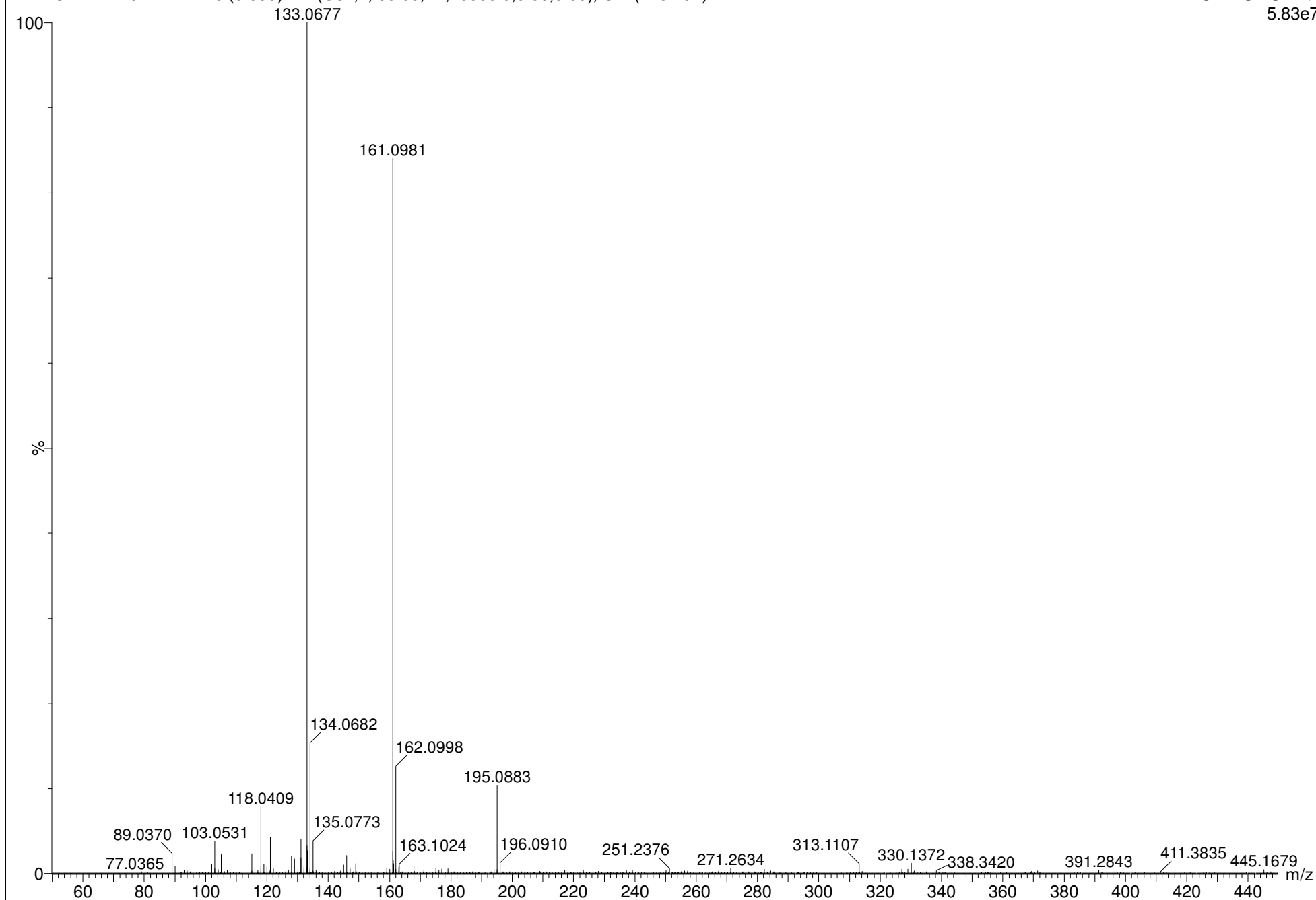
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Rosie Croft

07-Apr-2017

1: TOF MS ASAP+  
5.83e7



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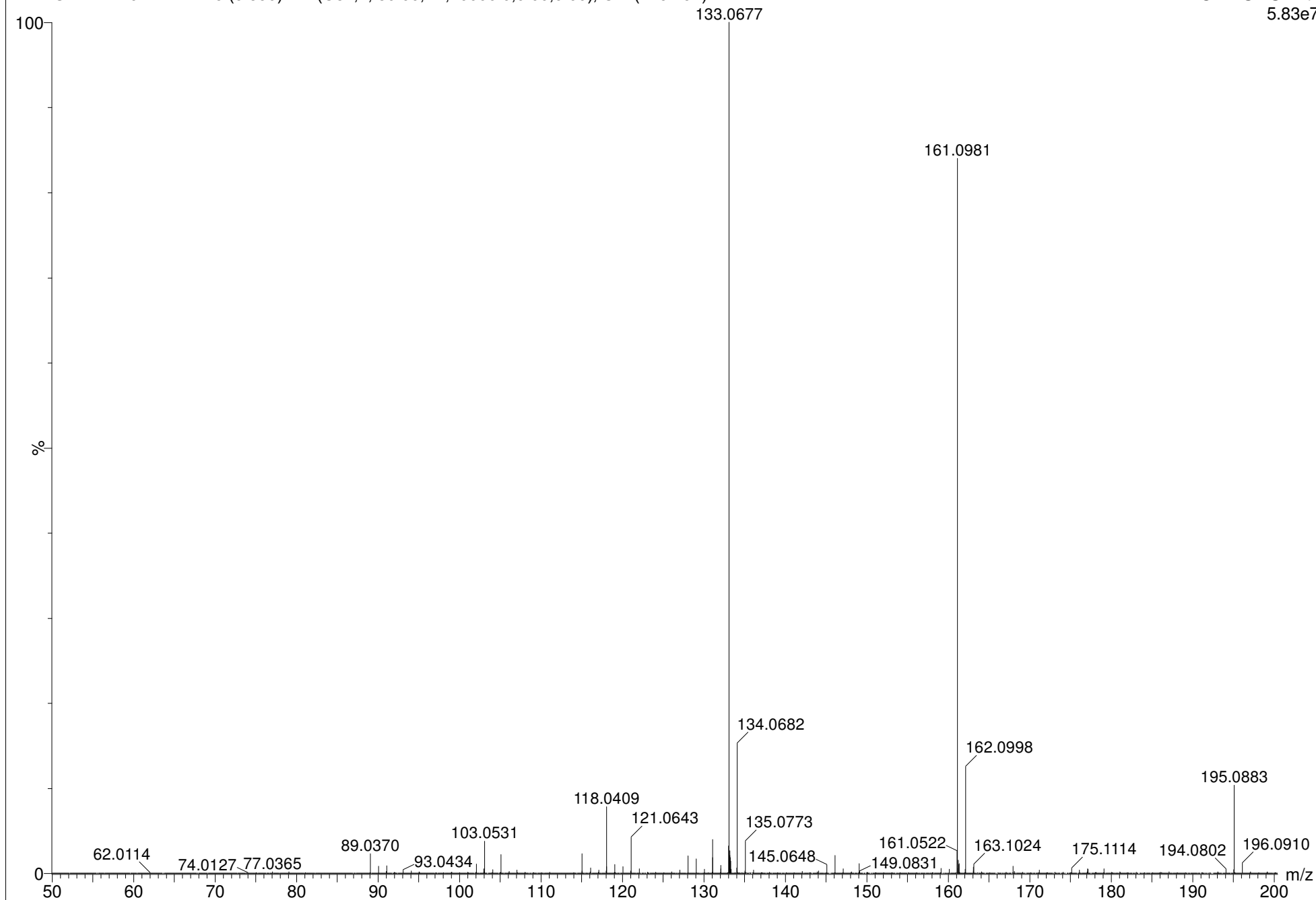
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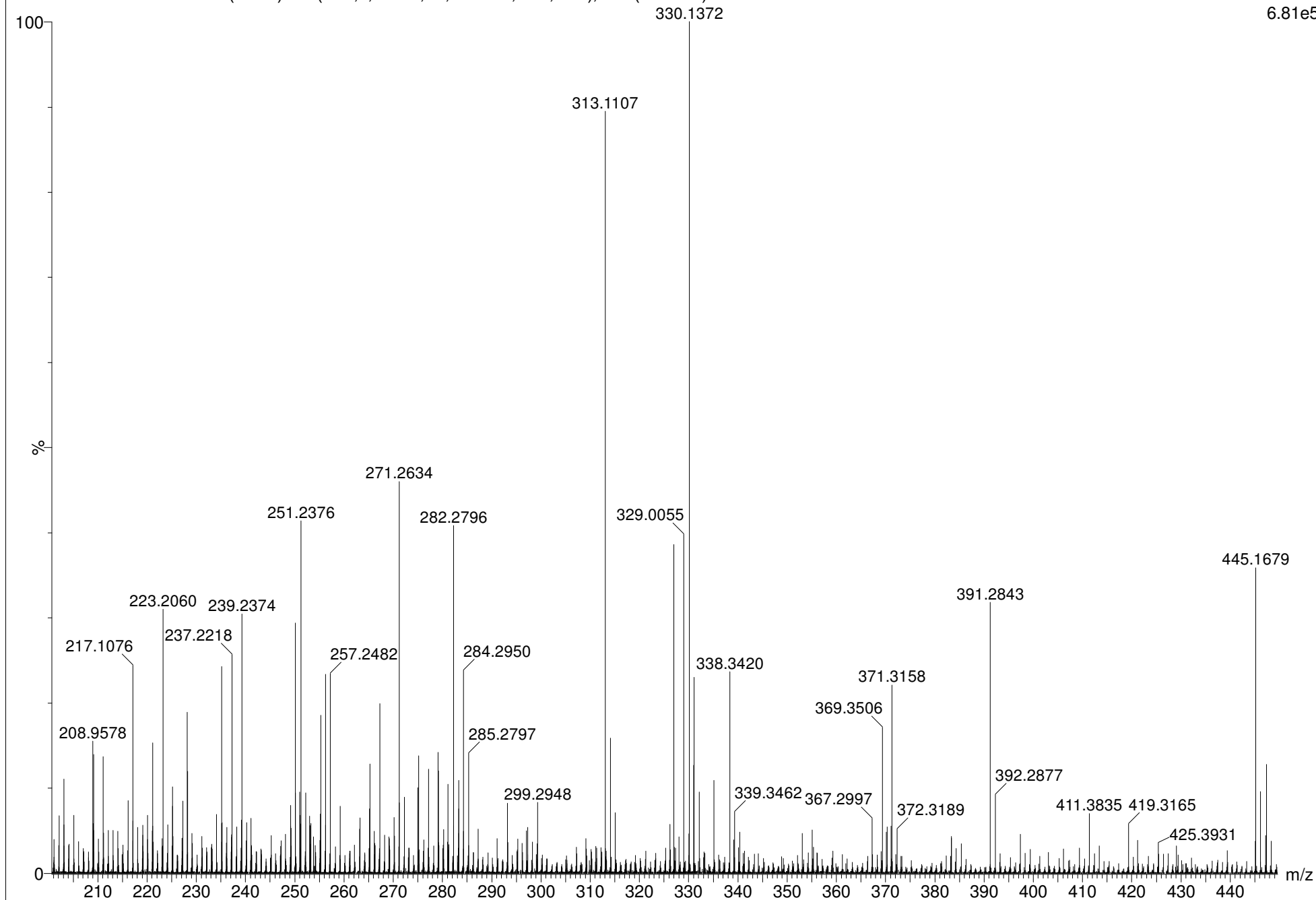
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1: TOF MS ASAP+  
6.81e5



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IMPBUL-AYMH9-WR-A (0.037) Is (1.00,0.05) C<sub>15</sub>H<sub>20</sub>O<sub>5</sub>SH

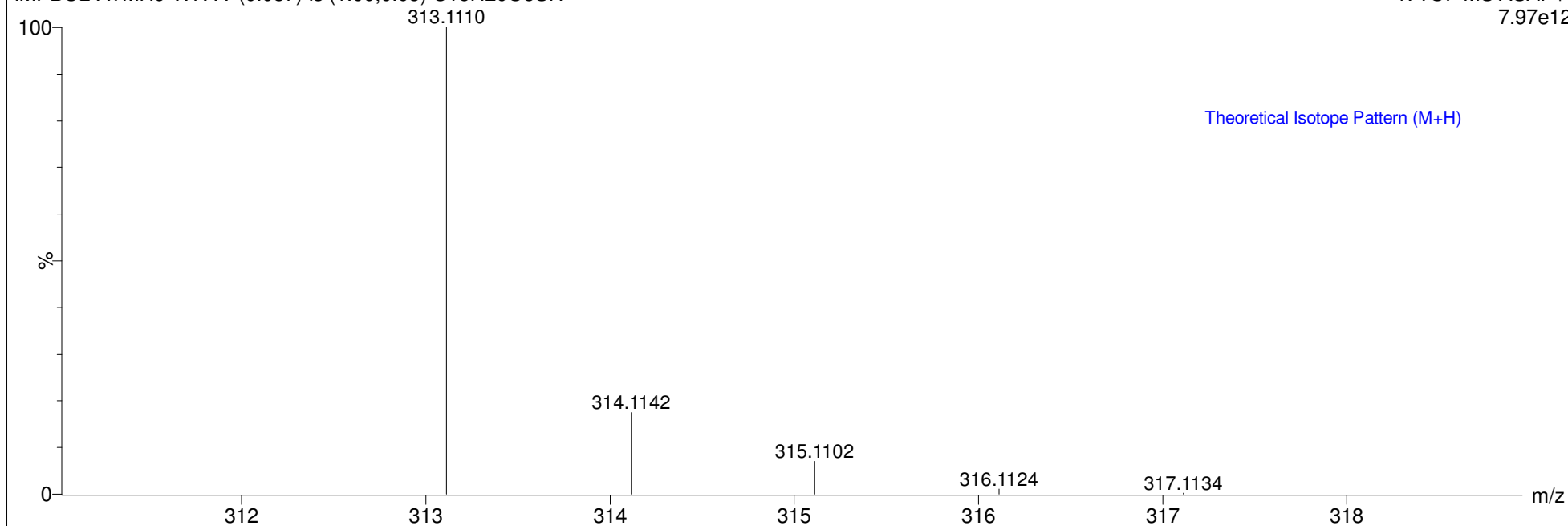
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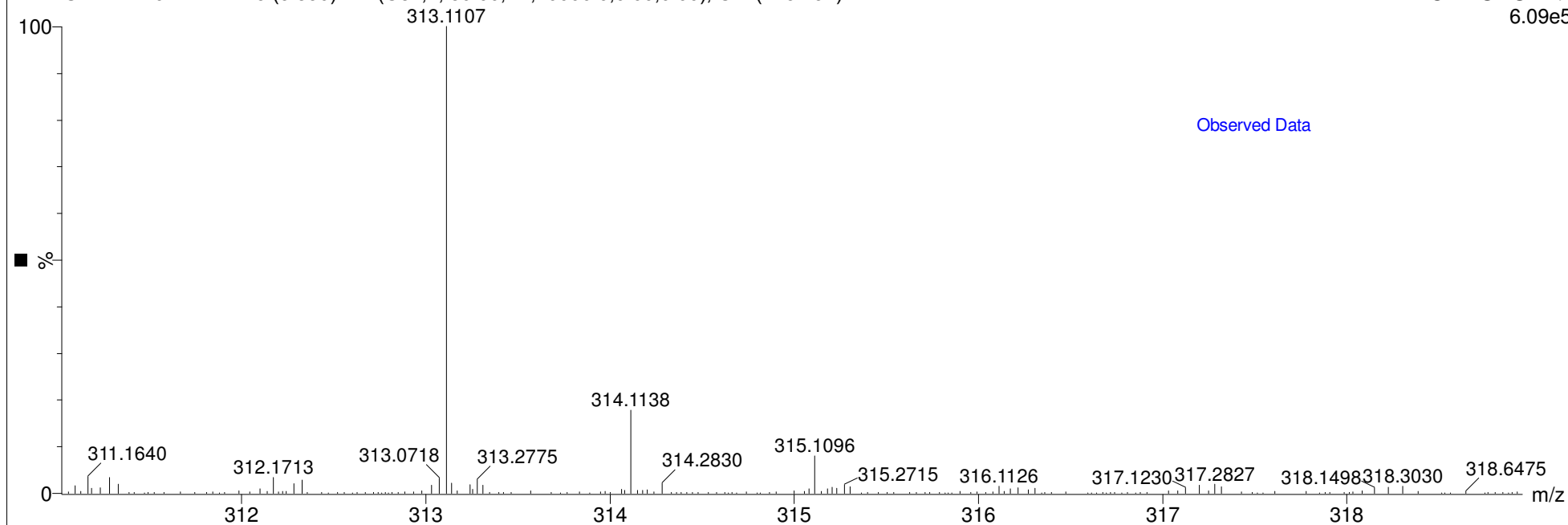
07-Apr-2017

1: TOF MS ASAP+  
7.97e12



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1: TOF MS ASAP+  
6.09e5



## 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

2596 formula(e) evaluated with 14 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-10 O: 0-15 S: 0-2

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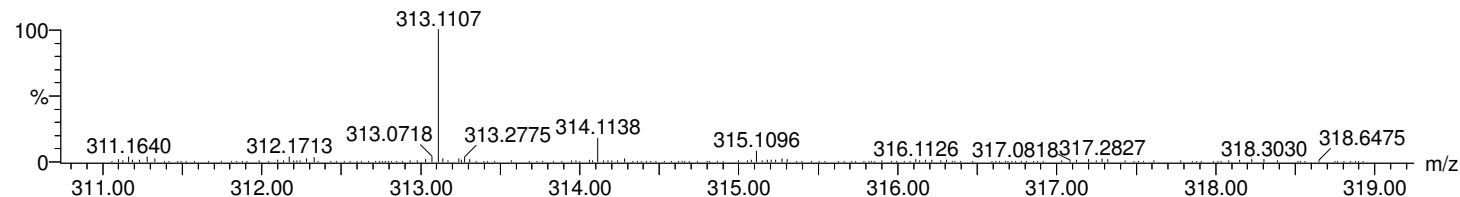
07-Apr-2017

C15H20O5S

IMPBUL-AYMH9-WR-A 415 (3.850) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (413:434)

1: TOF MS ASAP+

6.09e+005



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
313.1107	313.1108	-0.1	-0.3	2.5	1481.0	6.059	0.23	C7 H17 N6 O8
	313.1110	-0.3	-1.0	5.5	1475.4	0.429	65.09	C15 H21 O5 S
	313.1110	-0.3	-1.0	11.0	1477.3	2.336	9.67	C14 H15 N7 S
	313.1103	0.4	1.3	-3.5	1482.4	7.450	0.06	C7 H25 N2 O7 S2
	313.1103	0.4	1.3	15.0	1480.4	5.440	0.43	C21 H15 N O2
	313.1103	0.4	1.3	2.0	1481.8	6.881	0.10	C6 H19 N9 O2 S2
	313.1101	0.6	1.9	-12.0	1483.8	8.878	0.01	H27 N O15 S
	313.1115	-0.8	-2.6	-7.0	1482.8	7.868	0.04	C H23 N5 O11 S
	313.1117	-1.0	-3.2	1.5	1481.0	6.032	0.24	C8 H21 N6 O3 S2
	313.1096	1.1	3.5	6.0	1476.4	1.459	23.24	C13 H19 N3 O4 S
	313.1094	1.3	4.2	3.0	1481.6	6.594	0.14	C5 H15 N9 O7
	313.1094	1.3	4.2	-2.5	1481.5	6.528	0.15	C6 H21 N2 O12
	313.1121	-1.4	-4.5	2.0	1480.6	5.655	0.35	C9 H19 N3 O9
	313.1121	-1.4	-4.5	7.5	1480.9	5.977	0.25	C8 H13 N10 O4