

AB4-446 MW=259??

ASAP (SOLID)

C₁₀H₈F₃N₃O₂

IMPBUL-CM377-WR-A 228 (2.121) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (228:247)

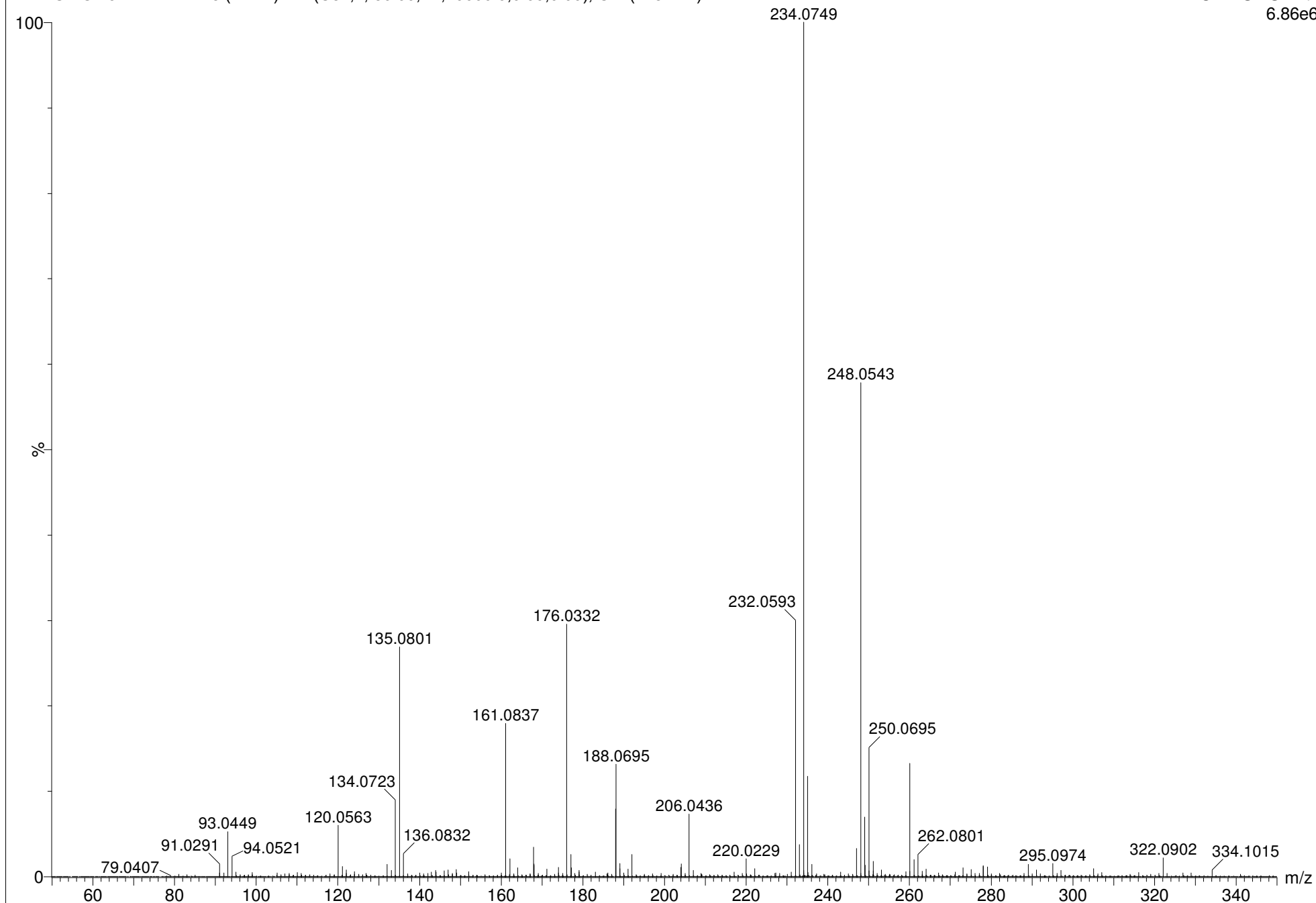
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Alexander Boddy

25-Jun-2018

1: TOF MS ASAP+
6.86e6



AB4-446 MW=259??

ASAP (SOLID)

C₁₀H₈F₃N₃O₂

IMPBUL-CM377-WR-A 228 (2.121) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (228:247)

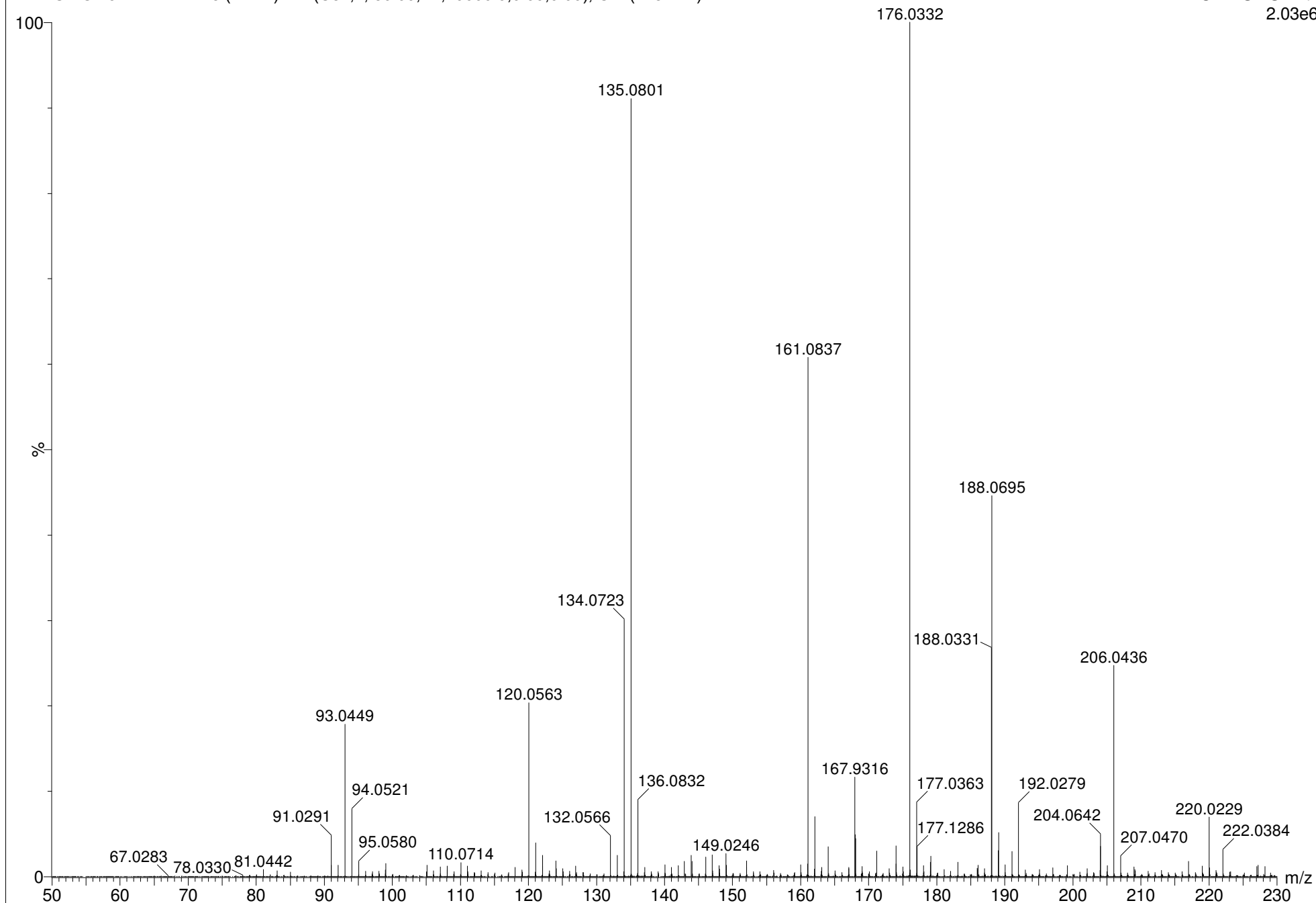
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Alexander Boddy

25-Jun-2018

1: TOF MS ASAP+
2.03e6



AB4-446 MW=259??

ASAP (SOLID)

C₁₀H₈F₃N₃O₂

IMPBUL-CM377-WR-A 228 (2.121) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (228:247)

National Mass Spectrometry Facility, Swansea

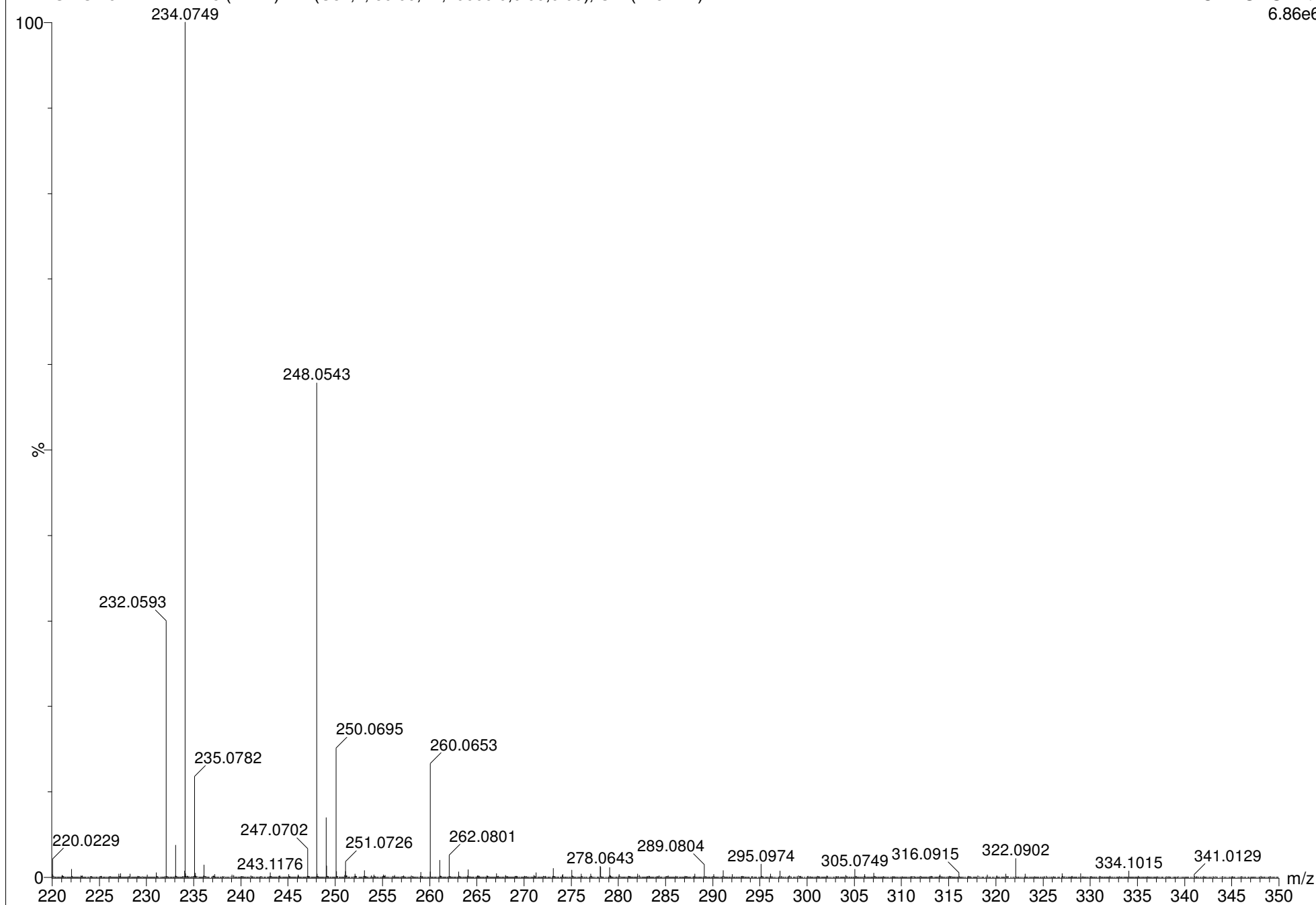
Xevo G2-S

Alexander Boddy

25-Jun-2018

1: TOF MS ASAP+

6.86e6



AB4-446 MW=259??

ASAP (SOLID)

C₁₀H₈F₃N₃O₂

IMPBUL-CM377-WR-A (0.037) Is (1.00,0.01) C₁₀H₈F₃N₃O₂H

National Mass Spectrometry Facility, Swansea

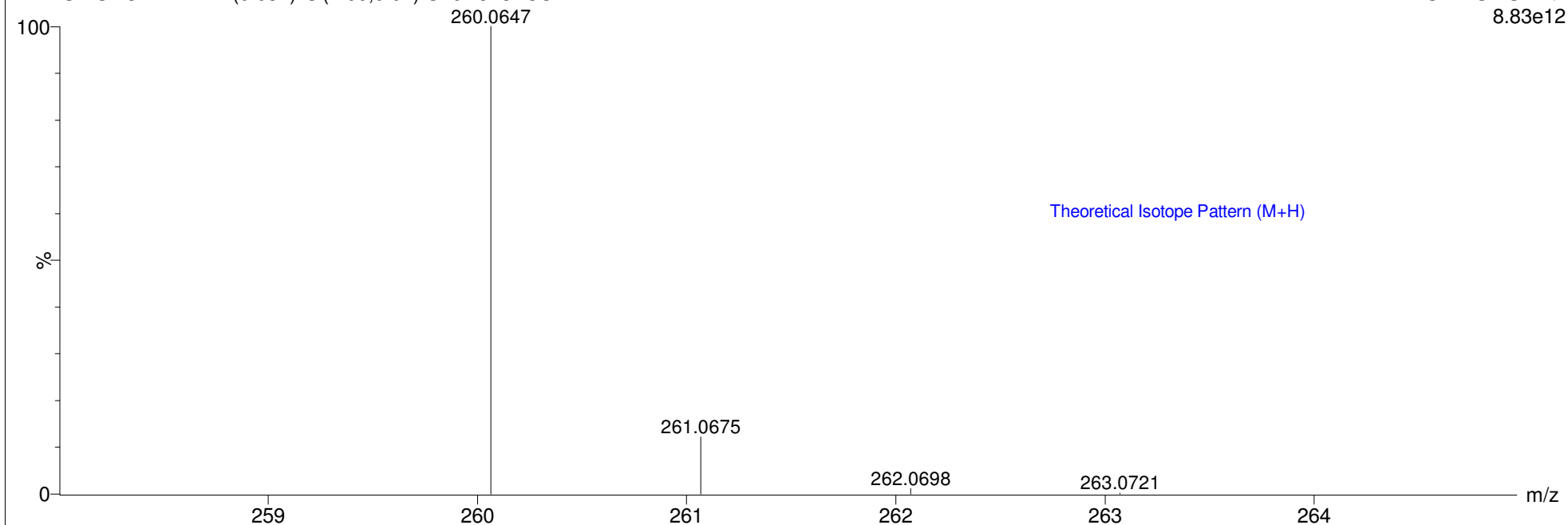
Xevo G2-S

Alexander Boddy

25-Jun-2018

1: TOF MS ASAP+

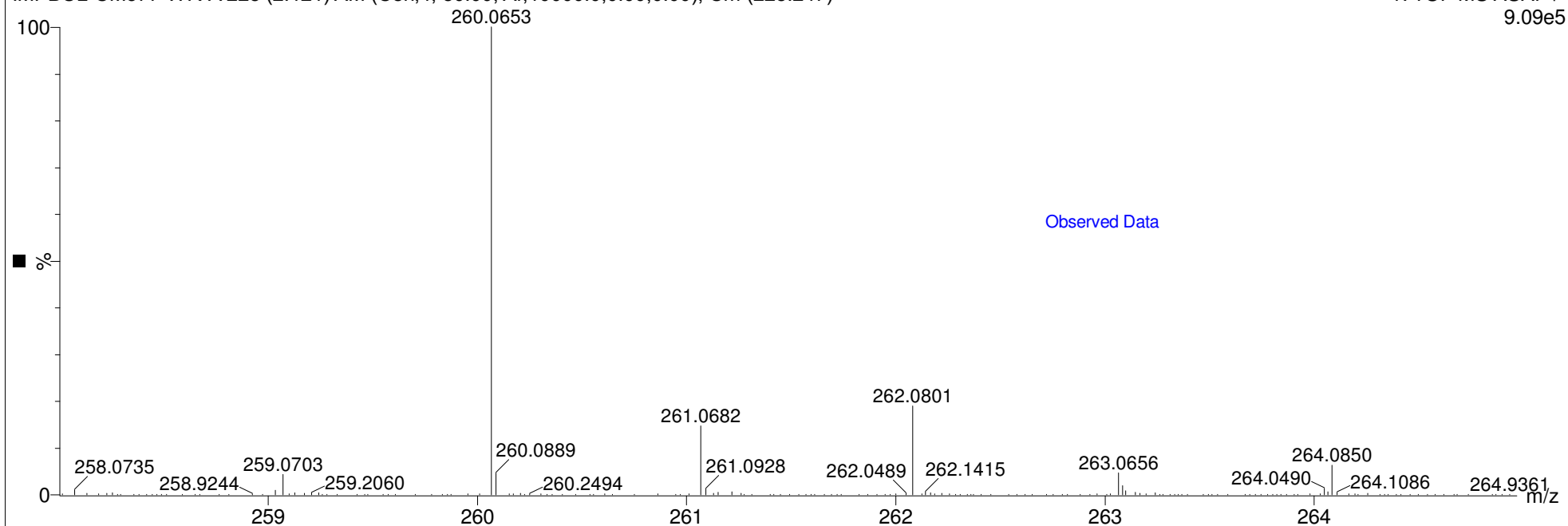
8.83e12



IMPBUL-CM377-WR-A 228 (2.121) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (228:247)

1: TOF MS ASAP+

9.09e5



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -50.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Odd and Even Electron Ions

3731 formula(e) evaluated with 17 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-10 O: 0-12 F: 0-7

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National Mass Spectrometry Facility, Swansea

Alexander Boddy

ASAP (SOLID)

Xevo G2-S

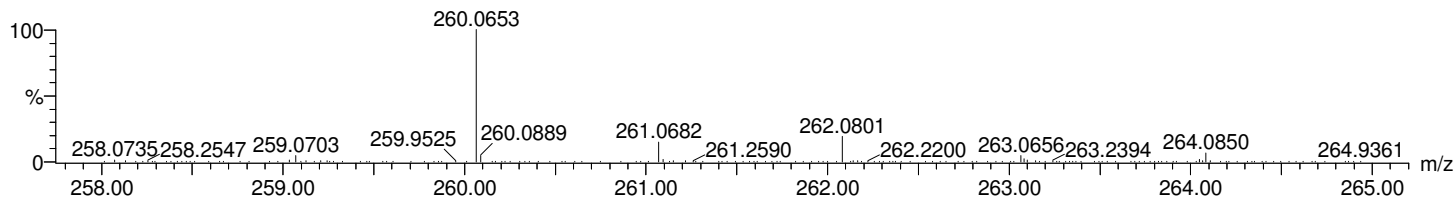
25-Jun-2018

C₁₀H₈F₃N₃O₂

IMPBUL-CM377-WR-A 228 (2.121) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (228:247)

1: TOF MS ASAP+

9.09e+005



Minimum: -50.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
260.0653	260.0654	-0.1	-0.4	-2.5	1118.7	2.899	5.51	C H12 N5 O8 F2
	260.0656	-0.3	-1.2	1.0	1118.7	2.923	5.38	C6 H13 N2 O8 F
	260.0656	-0.3	-1.2	6.5	1118.6	2.783	6.19	C5 H7 N9 O3 F
	260.0656	-0.3	-1.2	-1.0	1118.9	3.080	4.60	C2 H9 N6 O3 F5
	260.0649	0.4	1.5	10.0	1118.1	2.278	10.25	C15 H10 O2 F2
	260.0658	-0.5	-1.9	2.5	1118.7	2.930	5.34	C7 H10 N3 O3 F4
	260.0658	-0.5	-1.9	10.0	1118.3	2.532	7.95	C10 H8 N6 O3
	260.0647	0.6	2.3	-1.0	1119.0	3.189	4.12	C7 H11 O2 F7
	260.0647	0.6	2.3	6.5	1118.5	2.684	6.83	C10 H9 N3 O2 F3
	260.0660	-0.7	-2.7	6.0	1118.3	2.528	7.98	C12 H11 O3 F3
	260.0645	0.8	3.1	3.0	1118.8	3.028	4.84	C5 H8 N6 O2 F4
	260.0645	0.8	3.1	5.0	1118.4	2.623	7.26	C9 H12 N2 O7
	260.0644	0.9	3.5	10.5	1118.4	2.658	7.01	C8 H6 N9 O2
	260.0643	1.0	3.8	-0.5	1118.7	2.910	5.45	H7 N9 O2 F5
	260.0643	1.0	3.8	1.5	1118.7	2.902	5.49	C4 H11 N5 O7 F
	260.0643	1.0	3.8	-6.0	1119.3	3.478	3.09	C H13 N2 O7 F5
	260.0641	1.2	4.6	-7.5	1119.4	3.602	2.73	H16 N O12 F2