

EM033 MW=526?

ASAP (SOLID)

C30H20F6O2

STATAY-CWEHC-WG-A 534 (4.939) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (521:534)

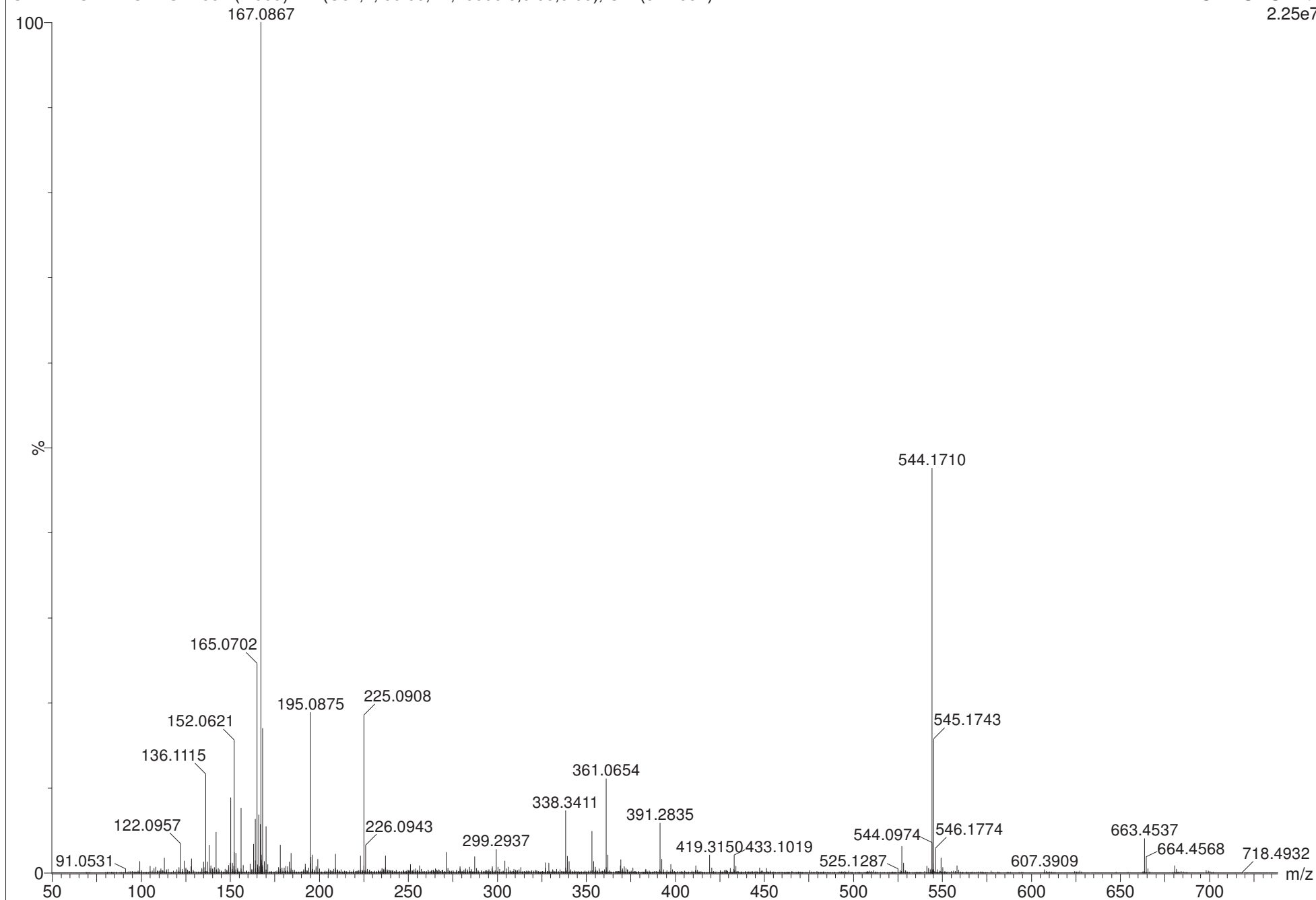
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Taylor

19-Jul-2017

1: TOF MS ASAP+  
2.25e7



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C<sub>30</sub>H<sub>20</sub>F<sub>6</sub>O<sub>2</sub>

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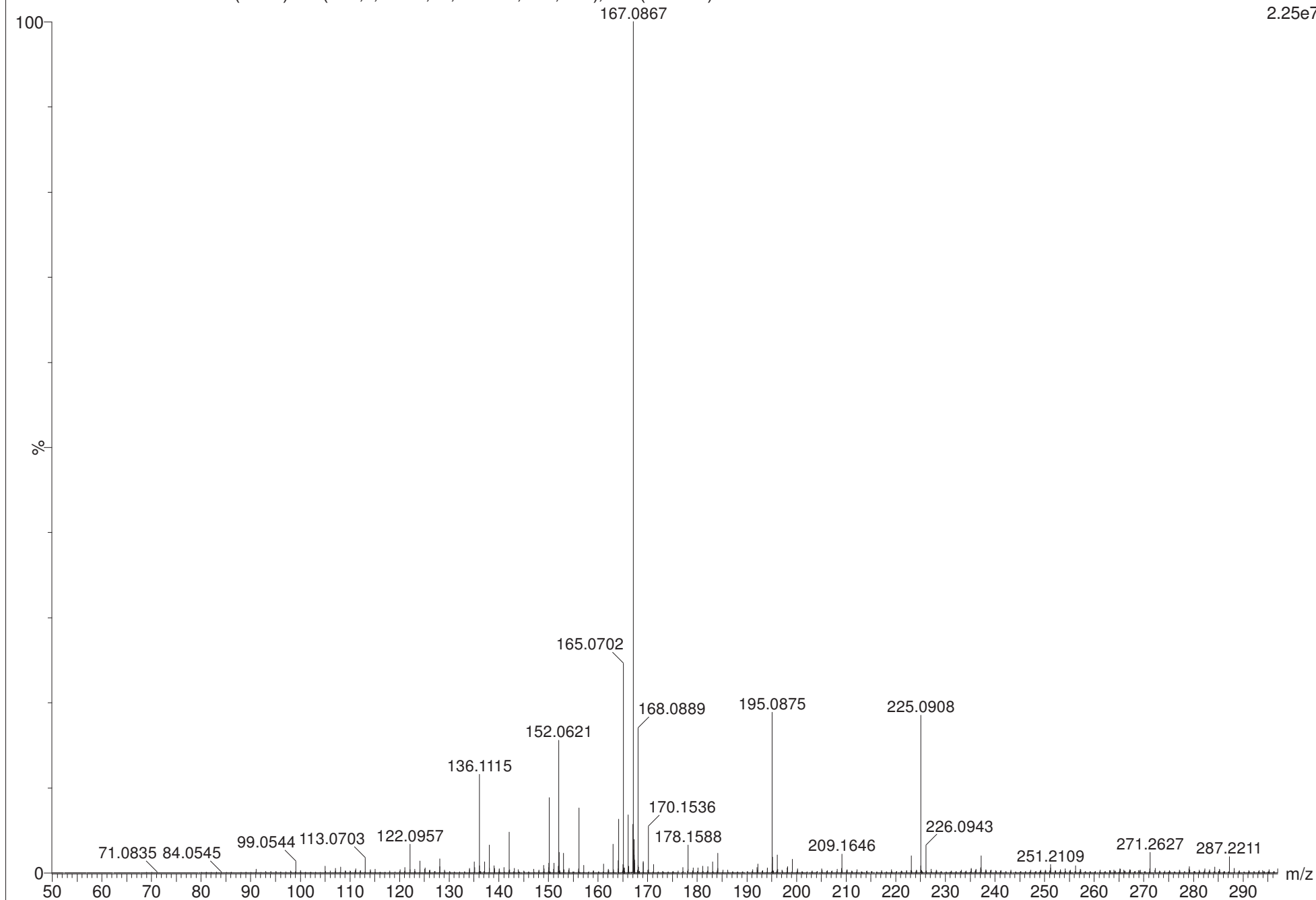
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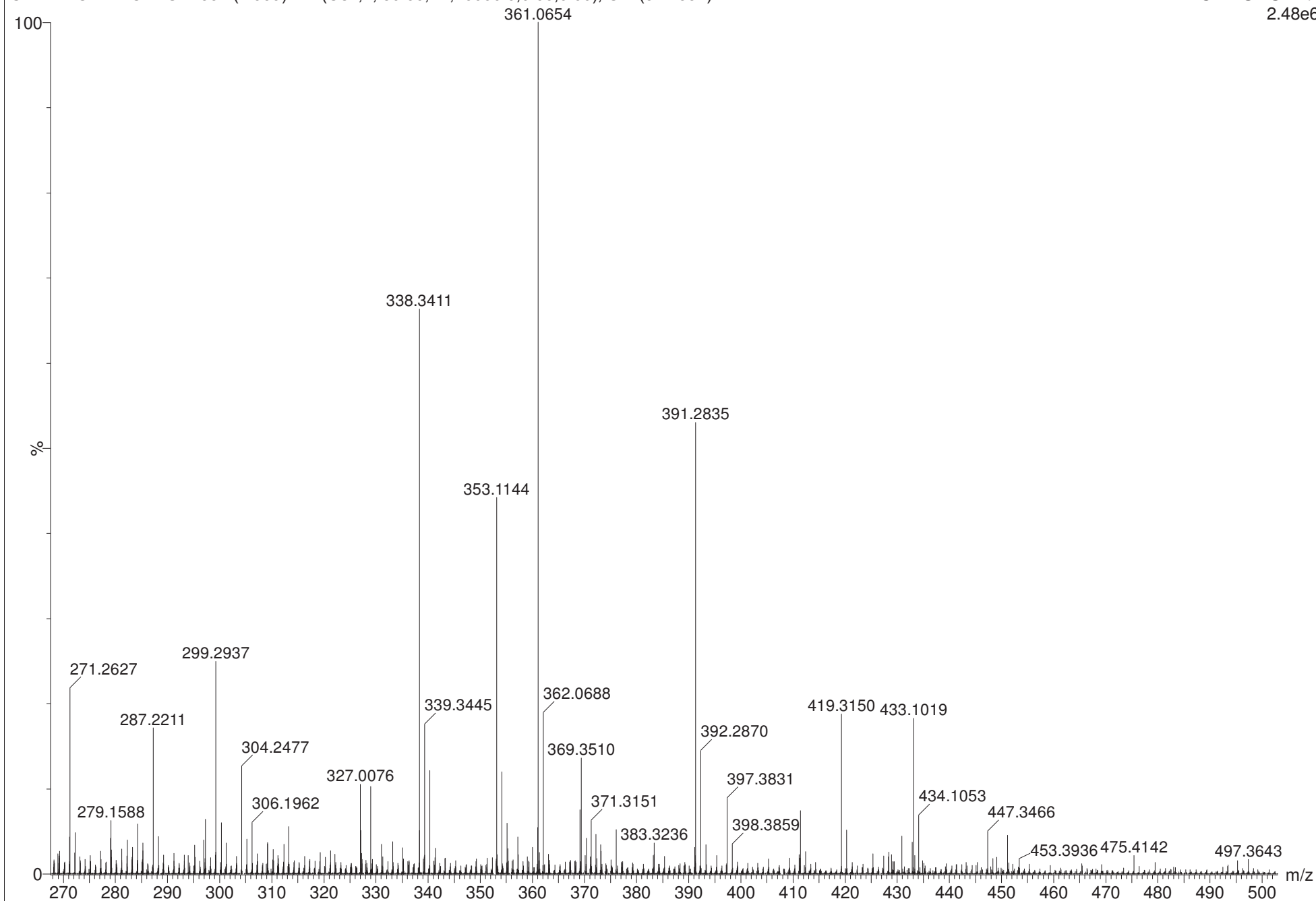
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1: TOF MS ASAP+  
2.48e6



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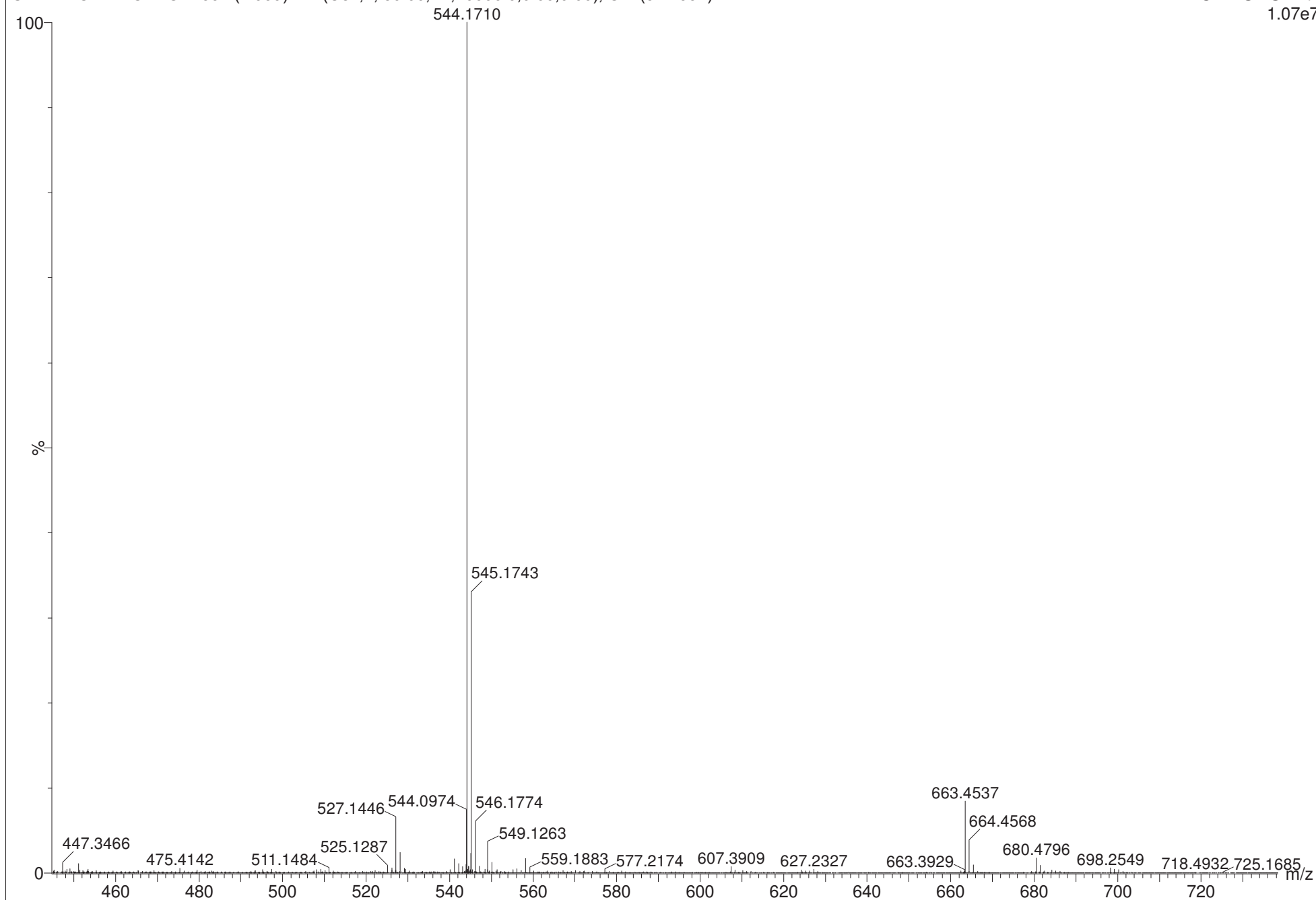
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1: TOF MS ASAP+  
1.07e7



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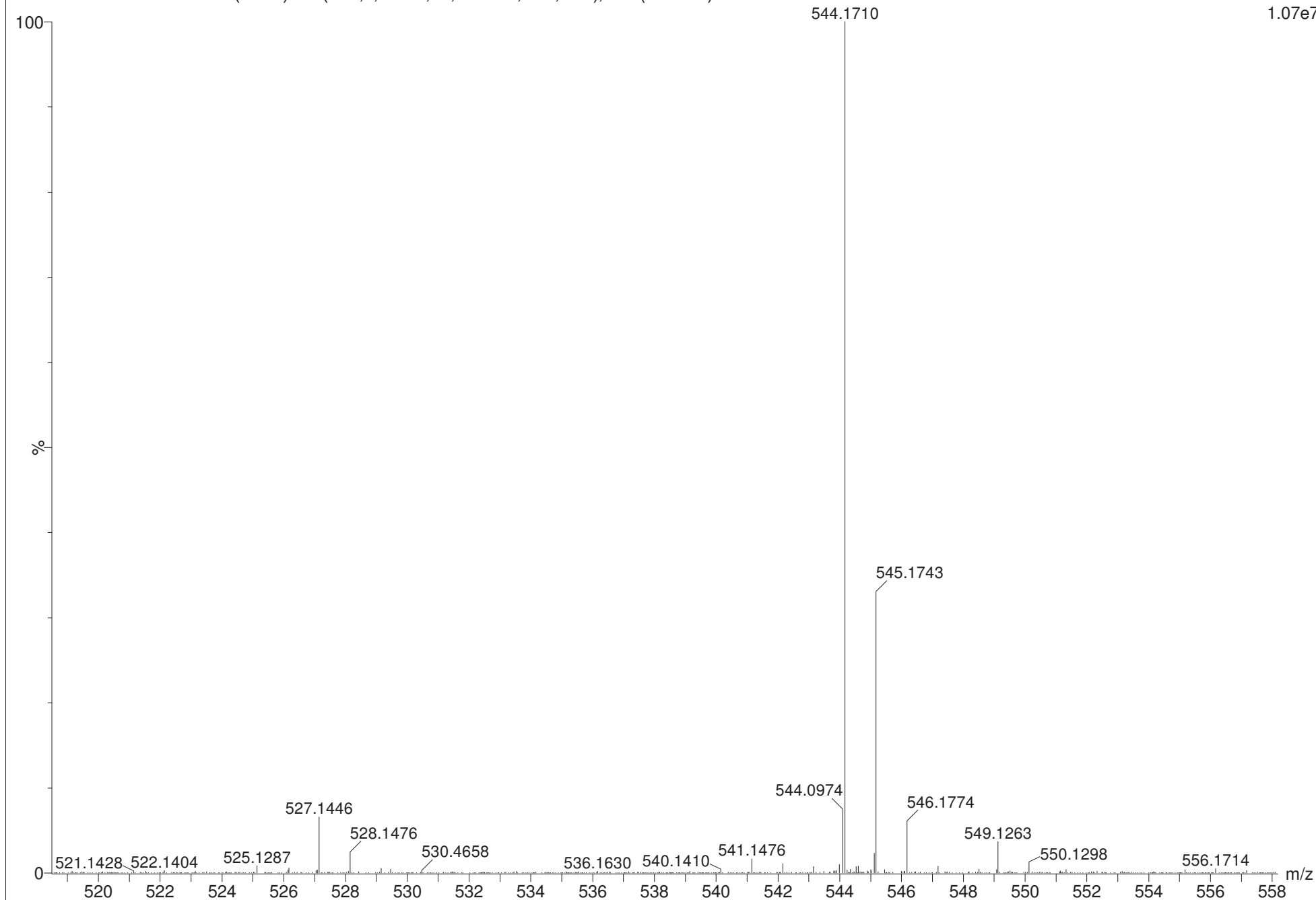
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1: TOF MS ASAP+  
1.07e7



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C<sub>30</sub>H<sub>20</sub>F<sub>6</sub>O<sub>2</sub>

STATAY-CWEHC-WG-A (0.037) Is (1.00,0.05) C<sub>30</sub>H<sub>20</sub>F<sub>6</sub>O<sub>2</sub>NH<sub>4</sub>

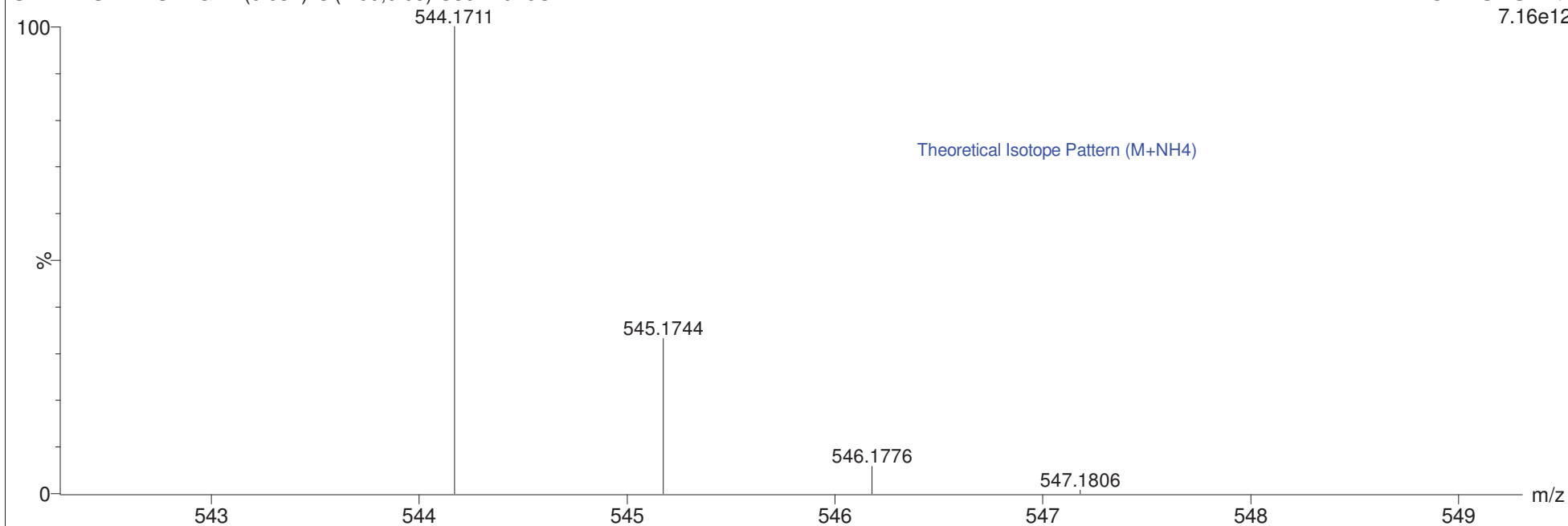
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Xevo G2-S

Taylor

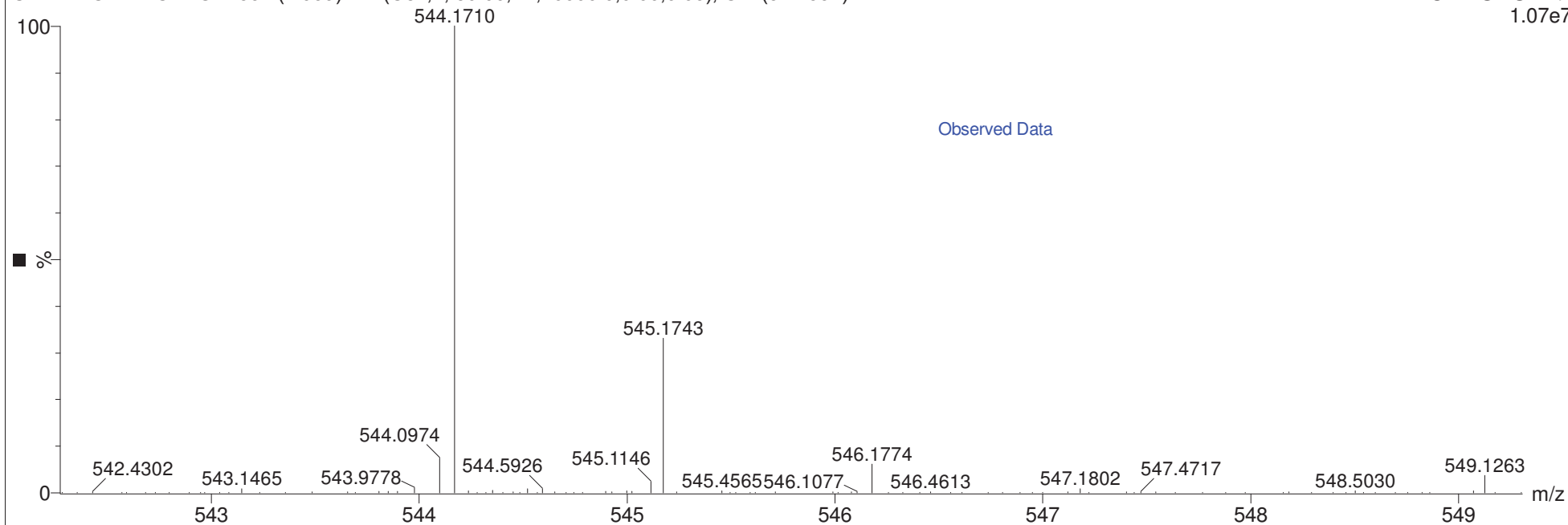
19-Jul-2017

1: TOF MS ASAP+  
7.16e12



STATAY-CWEHC-WG-A 534 (4.939) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (521:534)

1: TOF MS ASAP+  
1.07e7



## 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, Even Electron Ions

3375 formula(e) evaluated with 13 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-10 O: 0-14 F: 5-7

EM033 MW=526?

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ASAP (SOLID)

Xevo G2-S

C30H20F6O2

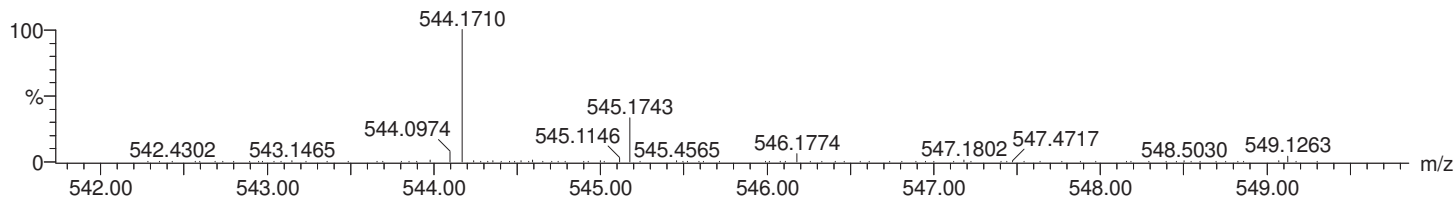
STATAY-CWEHC-WG-A 534 (4.939) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (521:534)

Taylor

19-Jul-2017

1: TOF MS ASAP+

1.07e+007



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
544.1710	544.1711	-0.1	-0.2	16.5	1037.7	0.003	99.75	C30 H24 N O2 F6
	544.1714	-0.4	-0.7	0.5	1061.7	24.022	0.00	C11 H25 N9 O8 F7
	544.1703	0.7	1.3	4.5	1060.3	22.652	0.00	C14 H24 N9 O7 F6
	544.1718	-0.8	-1.5	7.5	1054.4	16.703	0.00	C21 H27 N3 O8 F5
	544.1701	0.9	1.7	-4.5	1062.1	24.403	0.00	C10 H29 N5 O12 F7
	544.1700	1.0	1.8	20.5	1043.7	6.050	0.24	C33 H23 N O F5
	544.1723	-1.3	-2.4	12.5	1046.6	8.880	0.01	C27 H25 N O3 F7
	544.1696	1.4	2.6	13.5	1053.3	15.641	0.00	C23 H21 N7 O F7
	544.1691	1.9	3.5	8.5	1058.7	21.057	0.00	C17 H23 N9 O6 F5
	544.1690	2.0	3.7	-0.5	1060.9	23.246	0.00	C13 H28 N5 O11 F6
	544.1730	-2.0	-3.7	3.5	1057.0	19.301	0.00	C18 H28 N3 O9 F6
	544.1732	-2.2	-4.0	12.5	1053.6	15.896	0.00	C22 H23 N7 O4 F5
	544.1684	2.6	4.8	17.5	1050.0	12.370	0.00	C26 H20 N7 F6

EM033 MW=526?

ASAP (SOLID)

C30H20F6O2

STATAY-CWEHC-WG-A (0.037) Is (1.00,0.05) C30H20F6O2H

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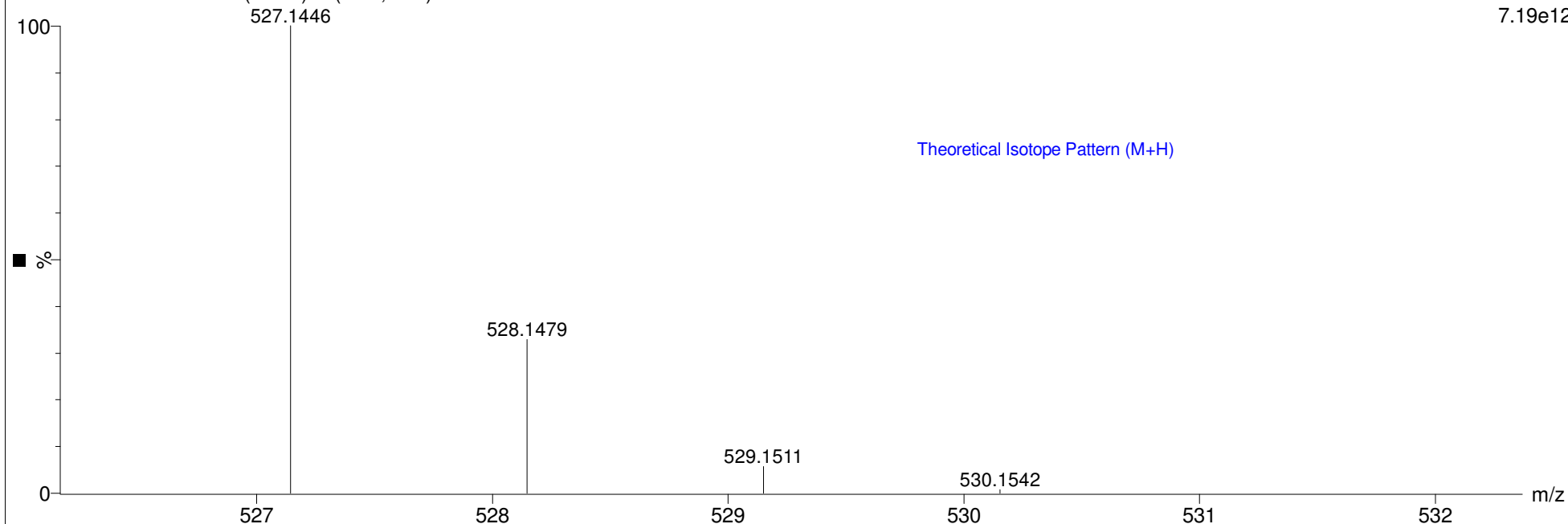
Xevo G2-S

Taylor

19-Jul-2017

1: TOF MS ASAP+

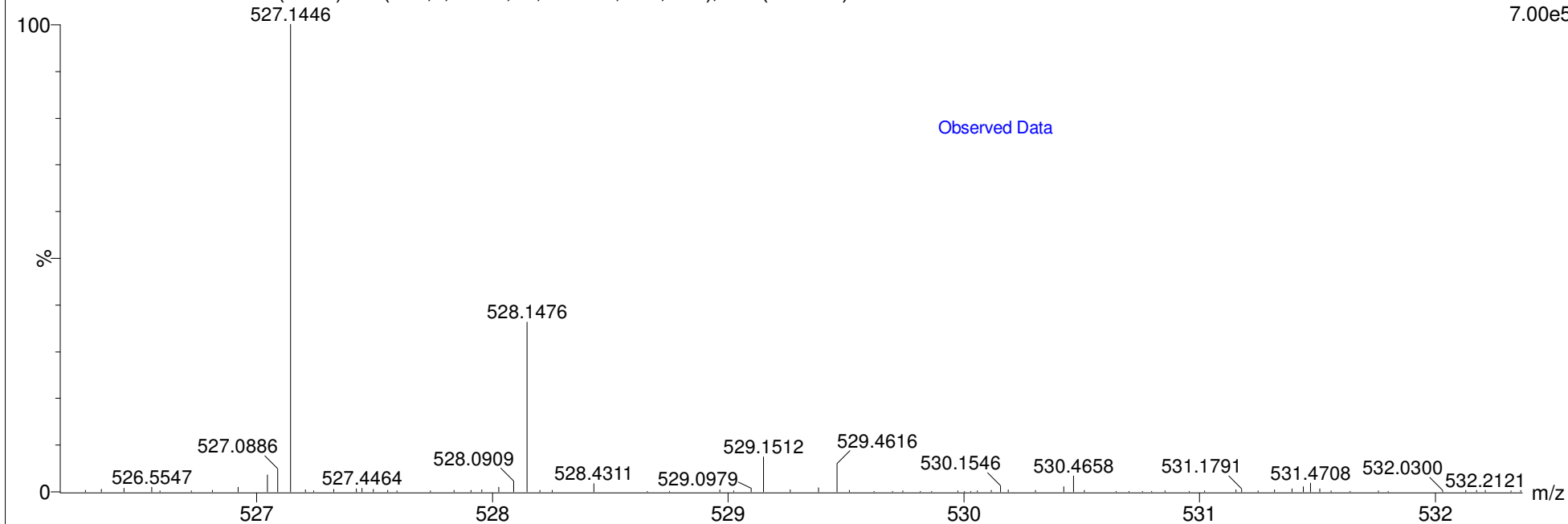
7.19e12



STATAY-CWEHC-WG-A 534 (4.939) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (521:534)

1: TOF MS ASAP+

7.00e5





## 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, Even Electron Ions

3364 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: 0-14 F: 5-7

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ASAP (SOLID)

Xevo G2-S

Taylor

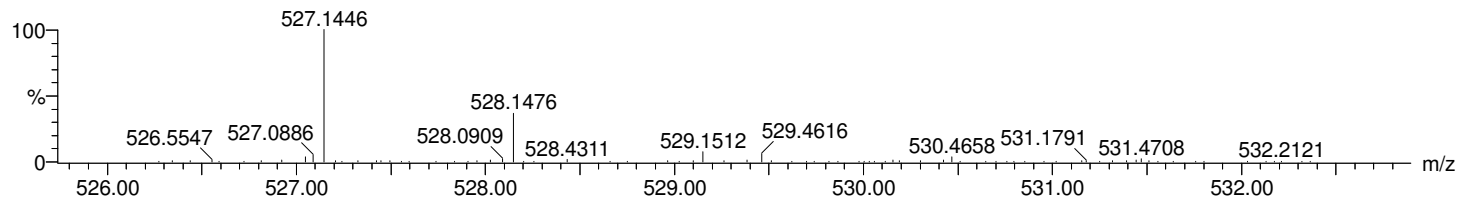
19-Jul-2017

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STATAY-CWEHC-WG-A 534 (4.939) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (521:534)

1: TOF MS ASAP+

7.00e+005



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
527.1446	527.1446	0.0	0.0	17.5	854.3	1.723	17.85	C30 H21 O2 F6
	527.1444	0.2	0.4	-3.5	868.3	15.802	0.00	C5 H24 N10 O13 F5
	527.1449	-0.3	-0.6	1.5	865.7	13.198	0.00	C11 H22 N8 O8 F7
	527.1453	-0.7	-1.3	8.5	859.2	6.622	0.13	C21 H24 N2 O8 F5
	527.1437	0.9	1.7	5.5	864.6	12.107	0.00	C14 H21 N8 O7 F6
	527.1456	-1.0	-1.9	-7.5	869.8	17.281	0.00	C2 H25 N10 O14 F6
	527.1435	1.1	2.1	-3.5	865.9	13.362	0.00	C10 H26 N4 O12 F7
	527.1457	-1.1	-2.1	13.5	856.4	3.866	2.09	C27 H22 O3 F7
	527.1434	1.2	2.3	21.5	852.8	0.228	79.64	C33 H20 O F5
	527.1430	1.6	3.0	14.5	859.2	6.625	0.13	C23 H18 N6 O F7
	527.1464	-1.8	-3.4	4.5	861.3	8.800	0.02	C18 H25 N2 O9 F6
	527.1426	2.0	3.8	9.5	863.6	11.091	0.00	C17 H20 N8 O6 F5
	527.1466	-2.0	-3.8	13.5	859.1	6.613	0.13	C22 H20 N6 O4 F5
	527.1424	2.2	4.2	0.5	865.2	12.648	0.00	C13 H25 N4 O11 F6