

ACS650 MW=330?

ASAP (SOLID)

C<sub>14</sub>H<sub>23</sub>BrO<sub>2</sub>Si

BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452:464)

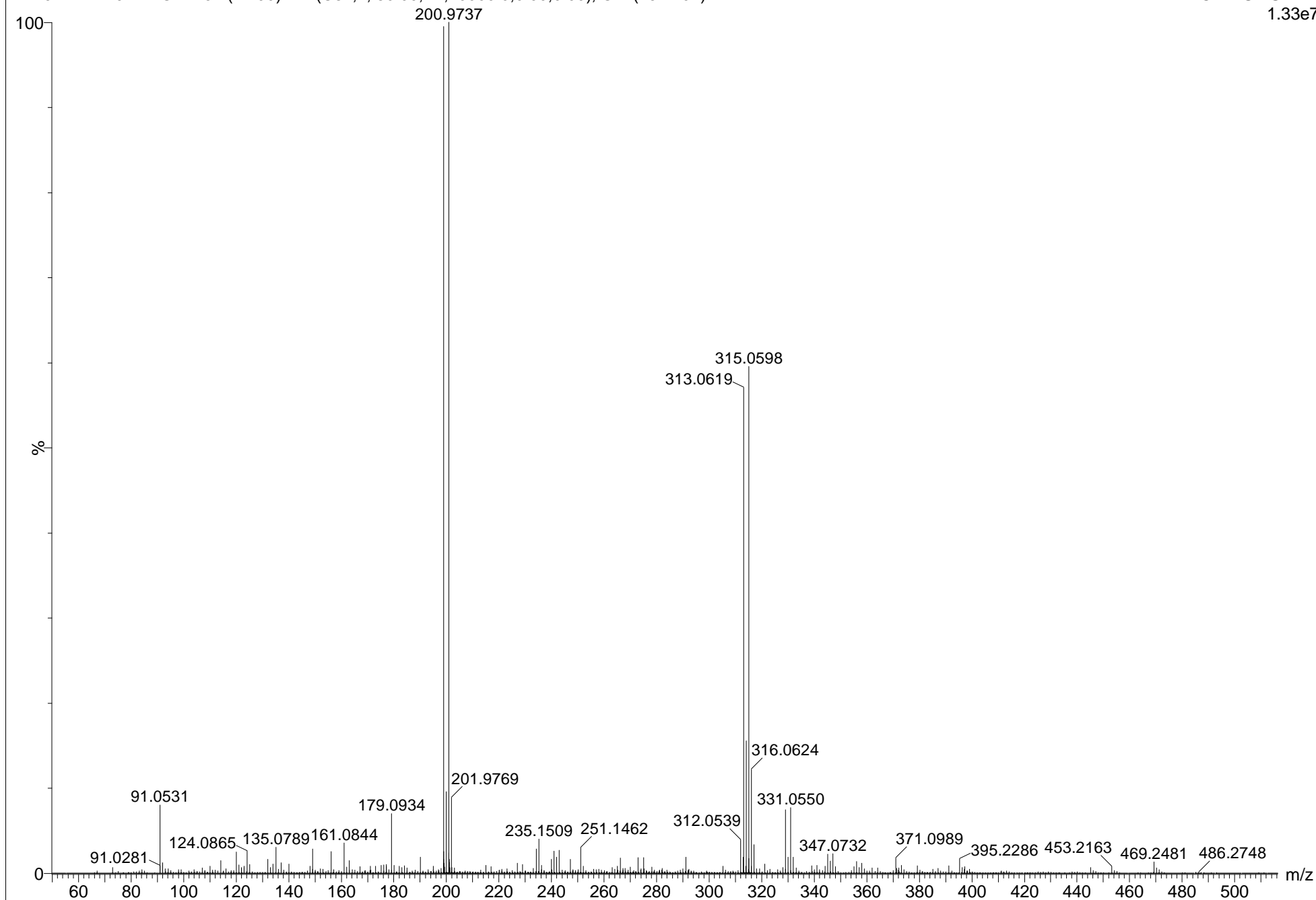
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Sedgewick

21-Feb-2017

1: TOF MS ASAP+  
1.33e7



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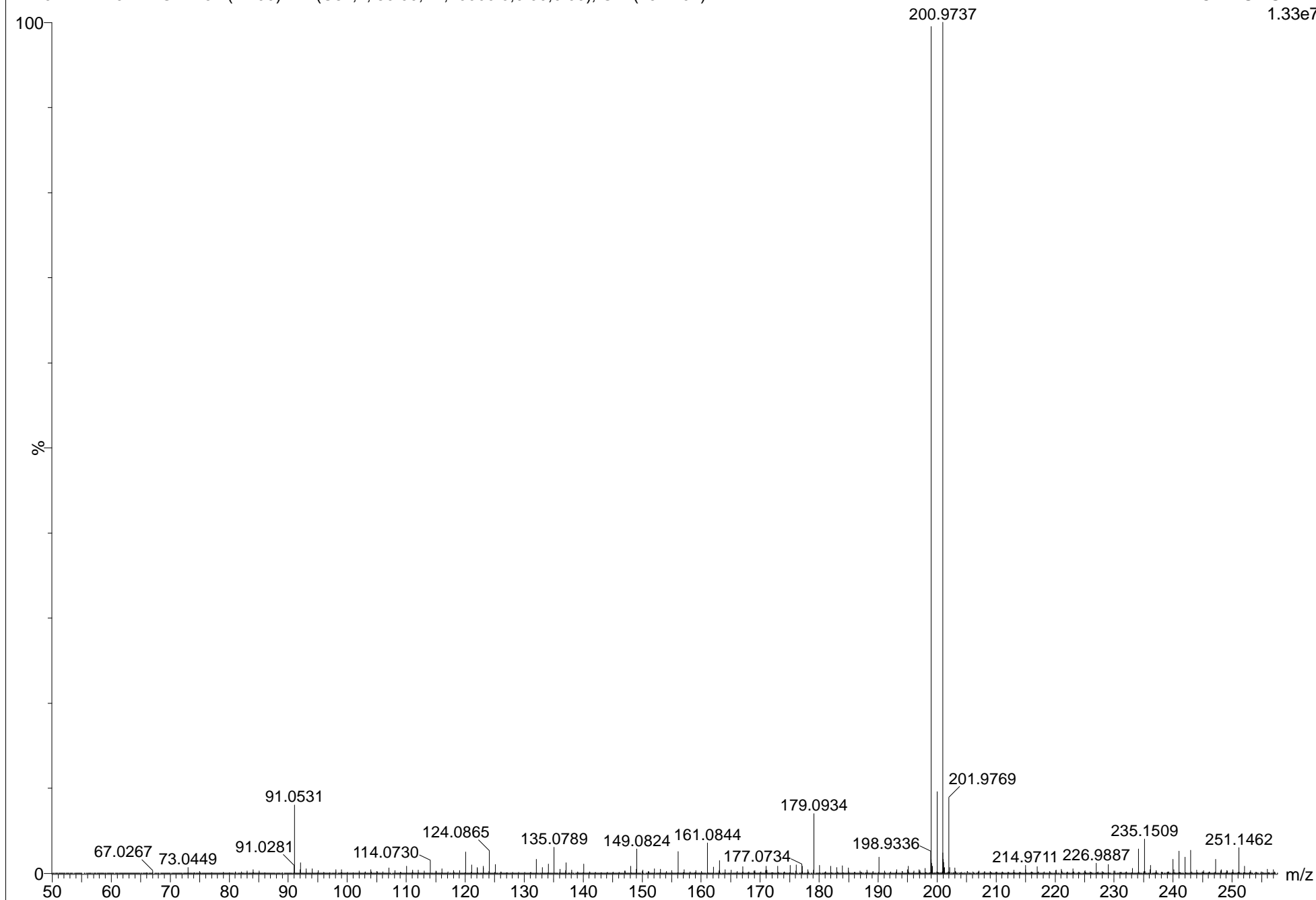
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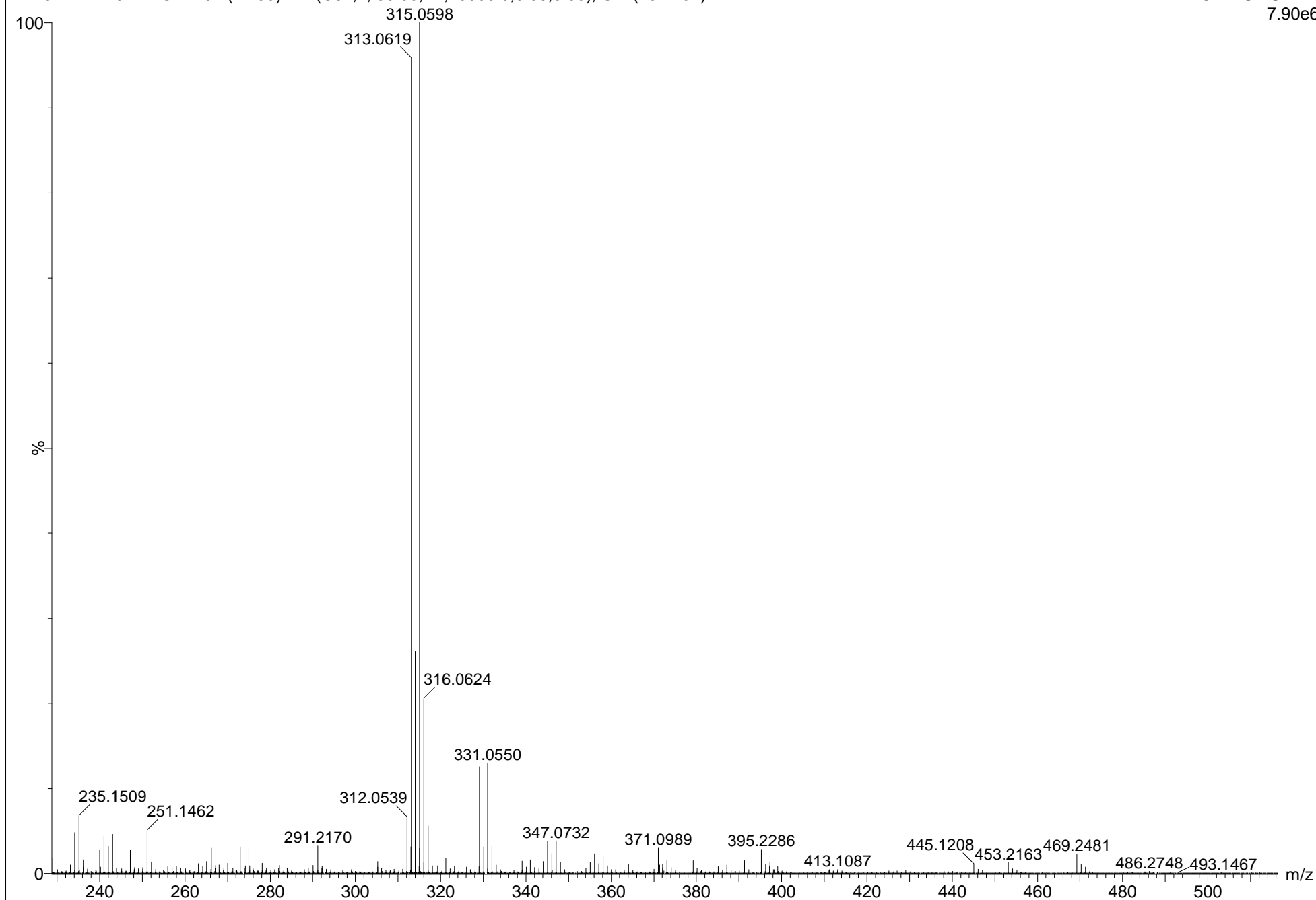
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1: TOF MS ASAP+  
7.90e6



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BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452:464)

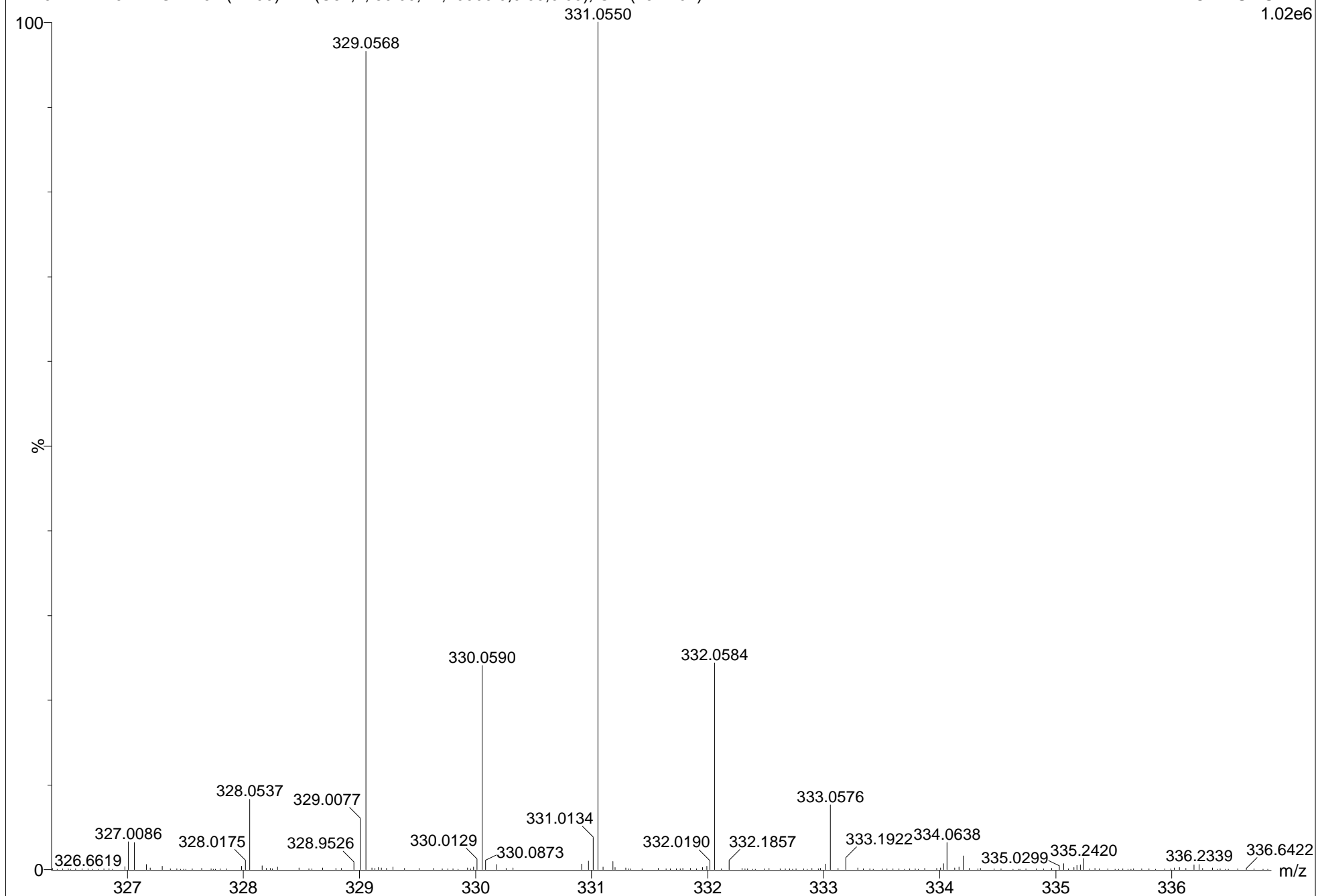
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1: TOF MS ASAP+  
1.02e6



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C<sub>14</sub>H<sub>23</sub>BrO<sub>2</sub>Si

BATJAM-7LRJN-WG-A (0.037) Is (1.00,0.05) C<sub>14</sub>H<sub>22</sub>BrO<sub>2</sub>Si

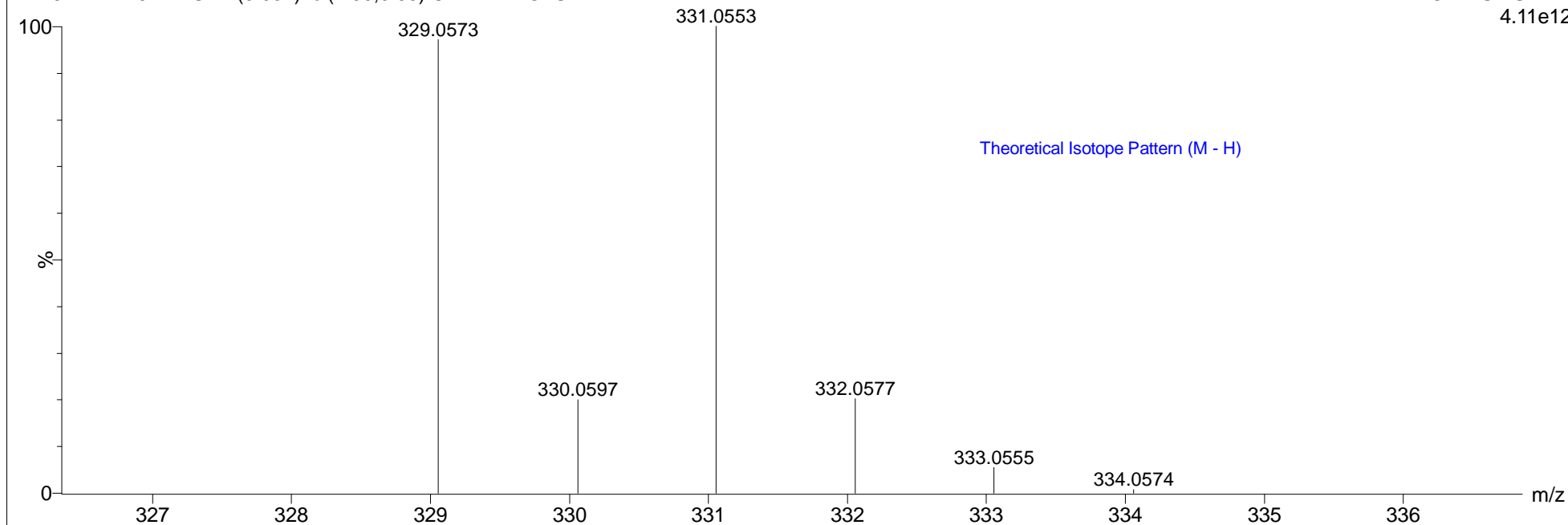
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Sedgewick

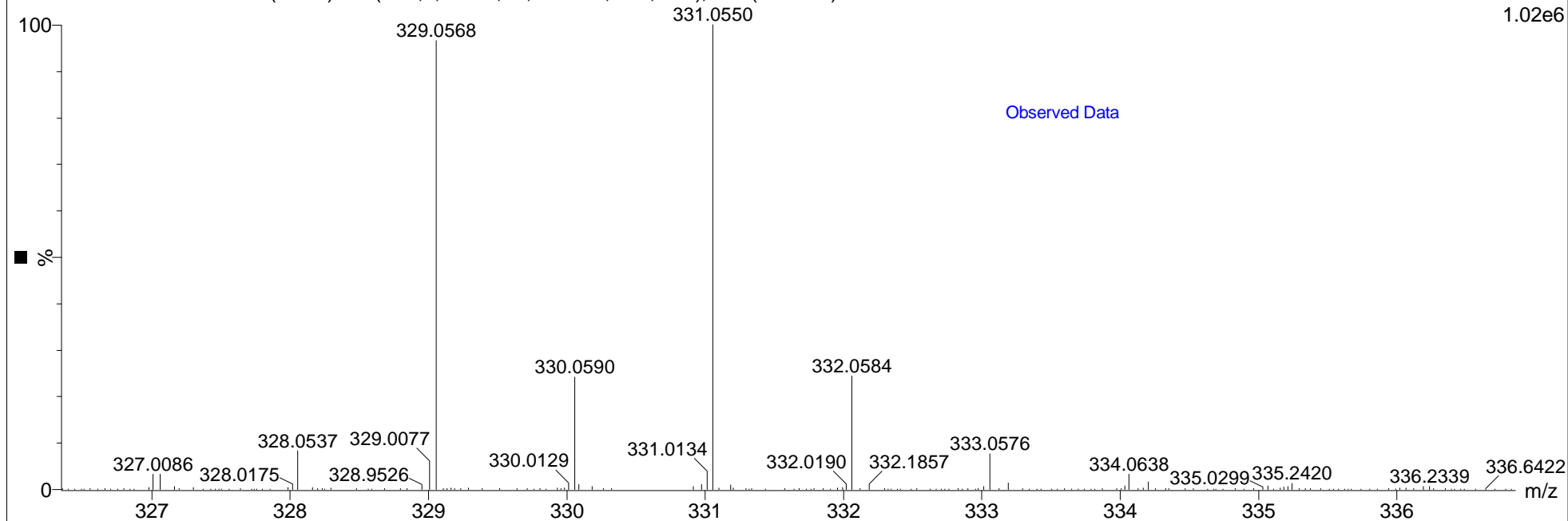
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1: TOF MS ASAP+  
4.11e12



BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452:464)

1: TOF MS ASAP+  
1.02e6



## 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

1089 formula(e) evaluated with 3 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-12 O: 0-12 Si: 1-2 Br: 1-1

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ASAP (SOLID)

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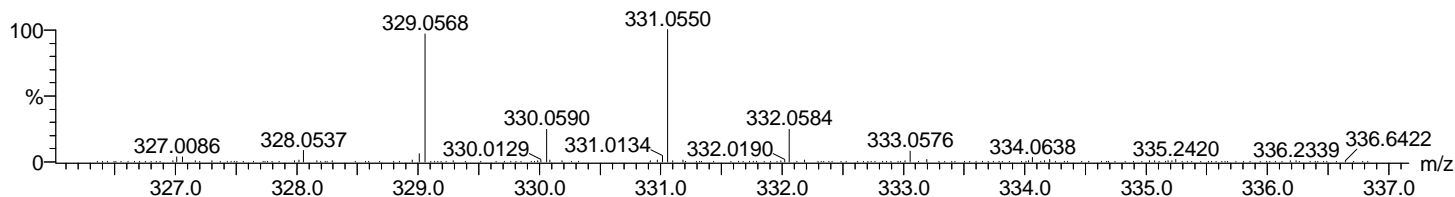
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C<sub>14</sub>H<sub>23</sub>BrO<sub>2</sub>Si

BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452.464)

1: TOF MS ASAP+

1.02e+006



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
329.0568	329.0572	-0.4	-1.2	4.5	1015.7	0.016	98.37	C14 H22 O2 Si Br
	329.0564	0.4	1.2	-4.5	1021.7	6.002	0.25	C5 H26 N2 O5 Si2 Br
	329.0577	-0.9	-2.7	0.5	1020.0	4.284	1.38	C6 H22 N6 O Si2 Br

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ASAP (SOLID)

C<sub>14</sub>H<sub>23</sub>BrO<sub>2</sub>Si

BATJAM-7LRJN-WG-A (0.037) Is (1.00,0.05) C<sub>14</sub>H<sub>21</sub>BrOSiH

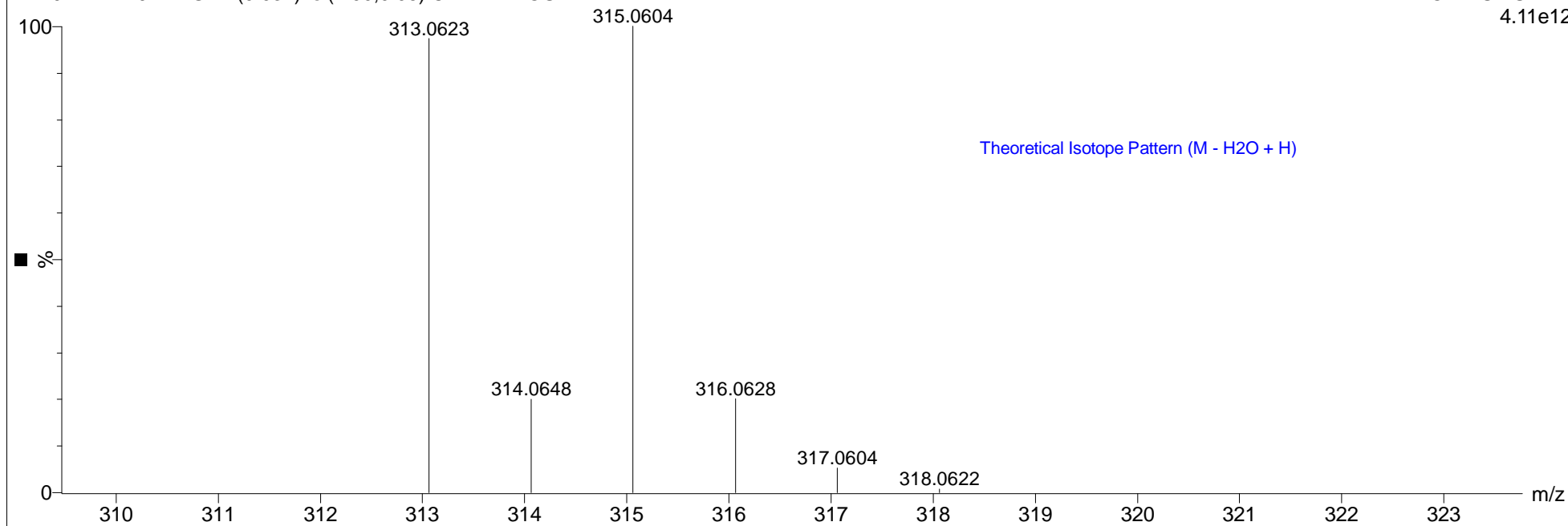
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Xevo G2-S

Sedgewick

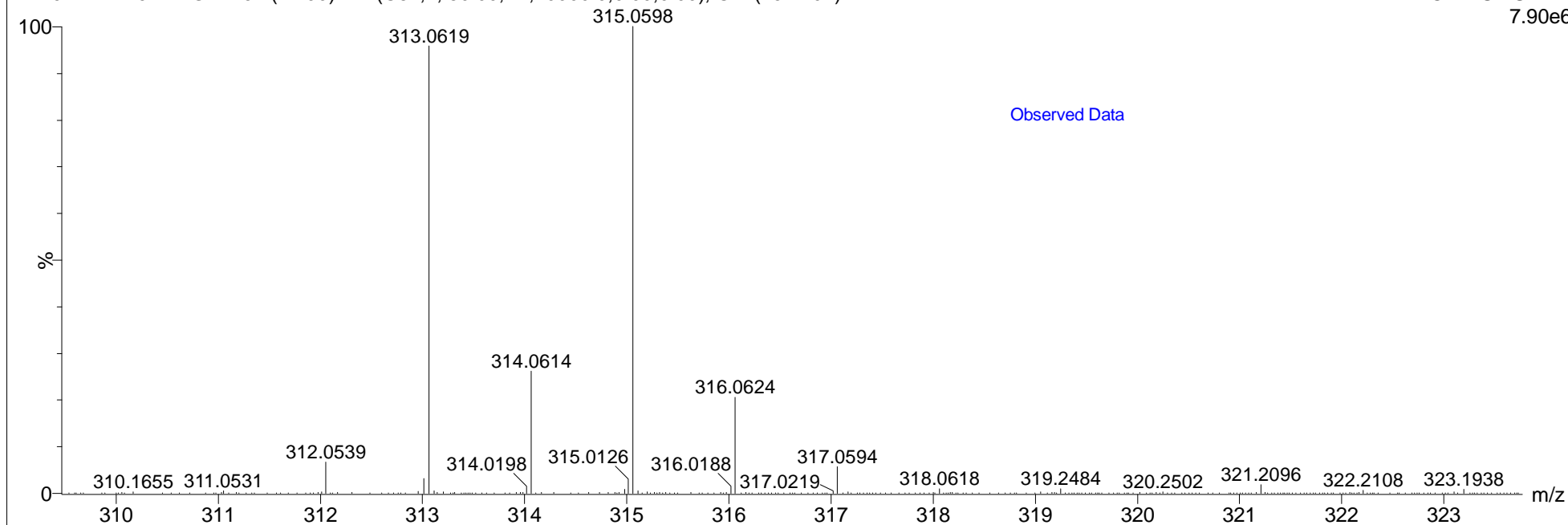
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1: TOF MS ASAP+  
4.11e12



BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452:464)

1: TOF MS ASAP+  
7.90e6



## 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

927 formula(e) evaluated with 3 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-12 O: 0-12 Si: 1-2 Br: 1-1

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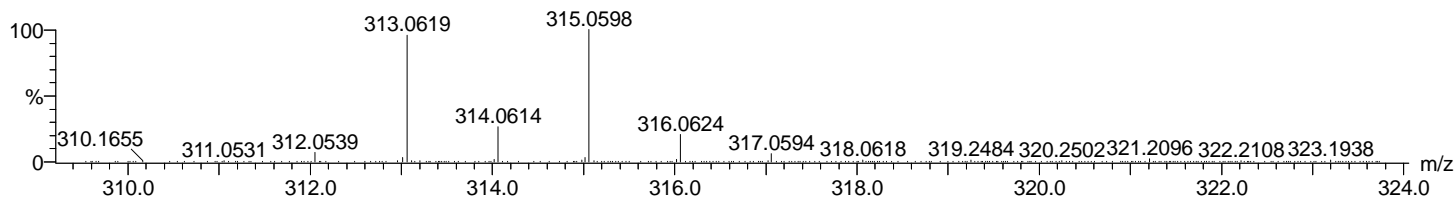
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C<sub>14</sub>H<sub>23</sub>BrO<sub>2</sub>Si

BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452:464)

1: TOF MS ASAP+

7.90e+006



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
313.0619	313.0623	-0.4	-1.3	4.5	1518.7	0.091	91.33	C14 H22 O Si Br
	313.0614	0.5	1.6	-4.5	1522.4	3.856	2.11	C5 H26 N2 O4 Si2 Br
	313.0628	-0.9	-2.9	0.5	1521.3	2.725	6.55	C6 H22 N6 Si2 Br



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C<sub>14</sub>H<sub>23</sub>BrO<sub>2</sub>Si

BATJAM-7LRJN-WG-A (0.037) Is (1.00,0.05) C<sub>8</sub>H<sub>8</sub>BrO

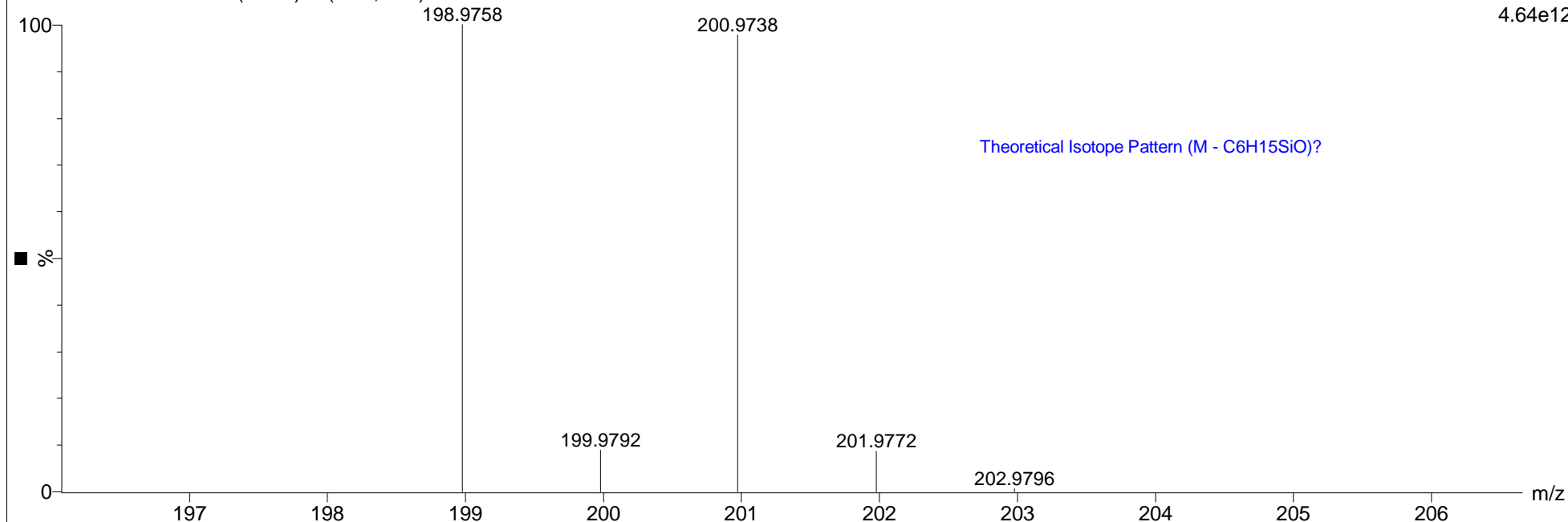
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Sedgewick

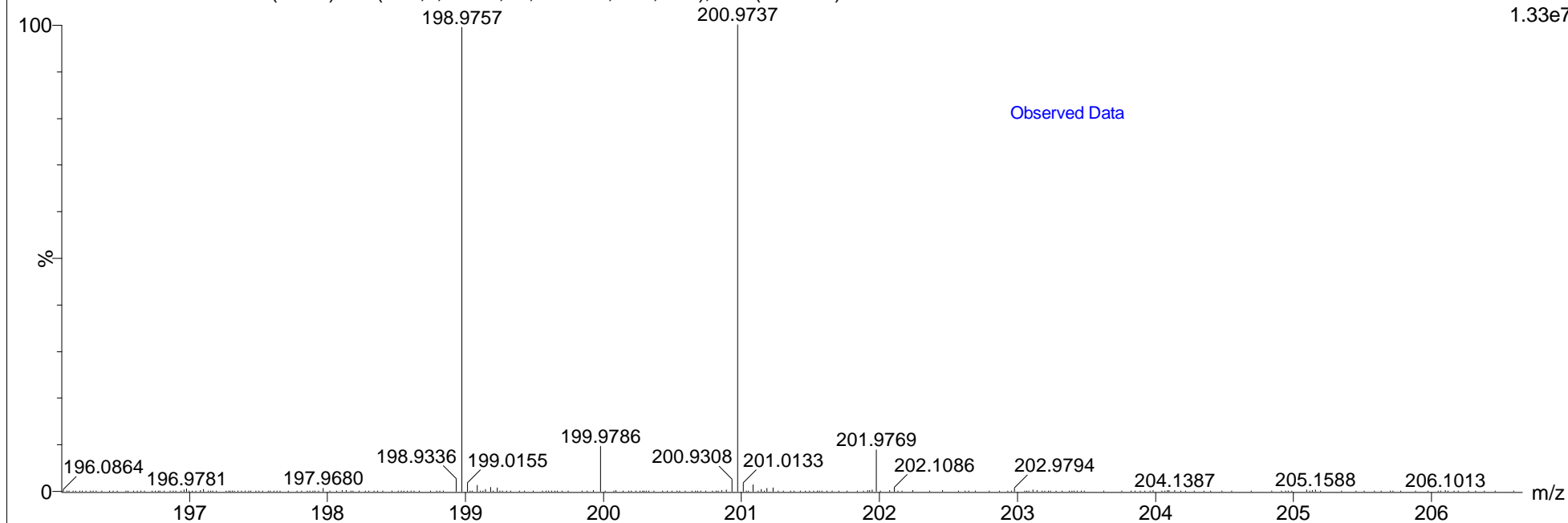
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1: TOF MS ASAP+  
4.64e12



BATJAM-7LRJN-WG-A 452 (4.190) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (452:464)

1: TOF MS ASAP+  
1.33e7



## 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

254 formula(e) evaluated with 2 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-12 O: 0-12 Si: 0-1 Br: 1-1

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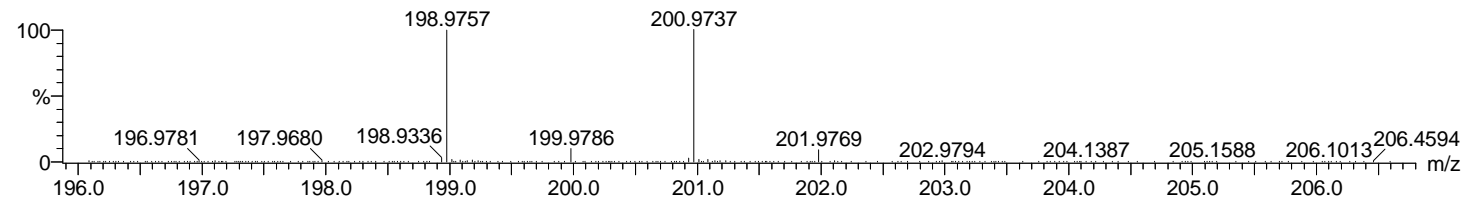
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1: TOF MS ASAP+

1.33e+007



Minimum: -150.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
198.9757	198.9759	-0.2	-1.0	4.5	1994.5	0.000	100.00	C8 H8 O Br
	198.9763	-0.6	-3.0	0.5	2026.1	31.562	0.00	H8 N6 Si Br