

EM307 MW=297?

ASAP(SOLID)

C<sub>16</sub>H<sub>12</sub>BrN

HERLEE-ECUWR-WG-A 203 (1.895) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (203:229)

National Mass Spectrometry Facility, Swansea

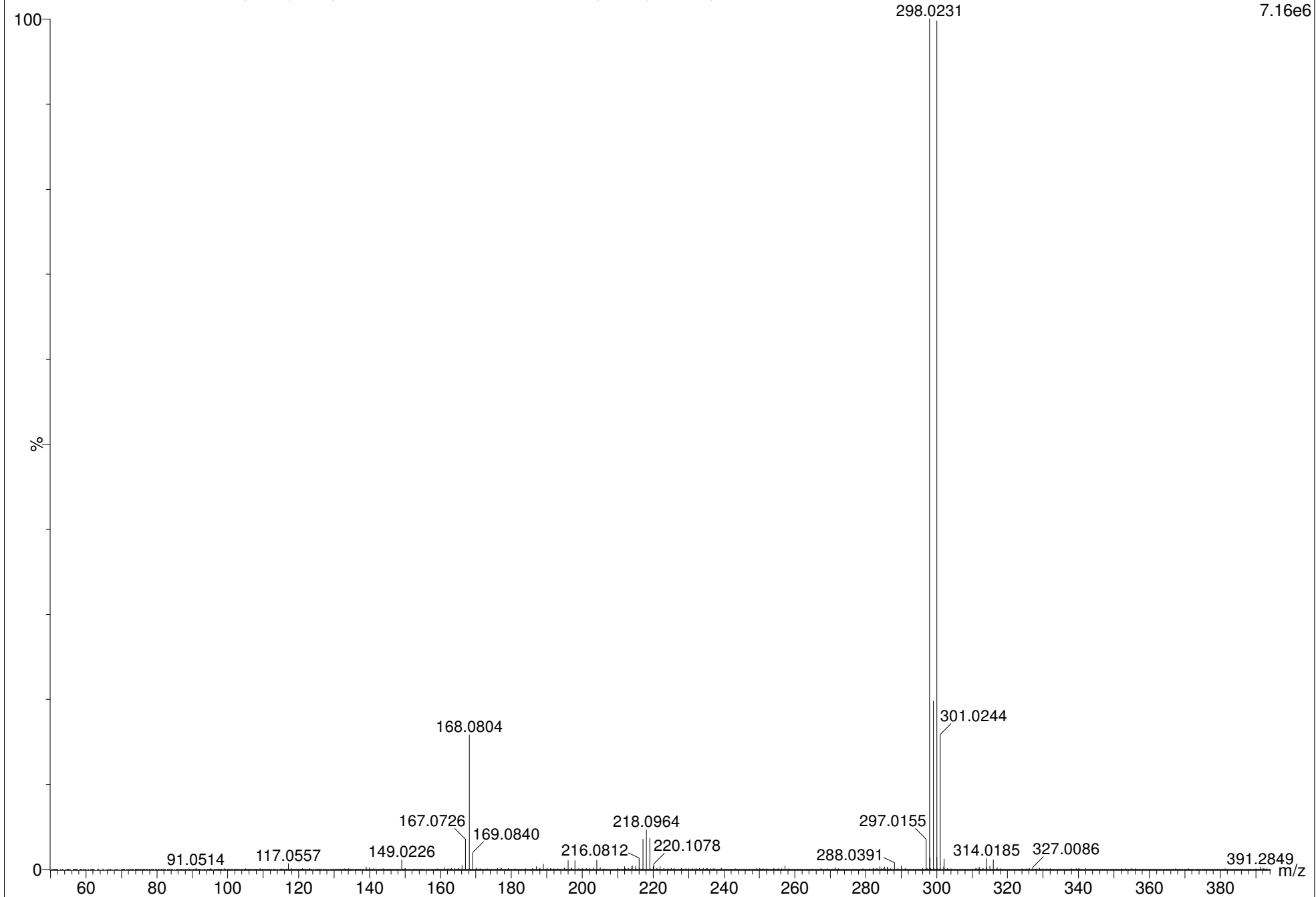
Xevo G2-S

McLean

31-Oct-2019

1: TOF MS ASAP+

7.16e6



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National Mass Spectrometry Facility, Swansea

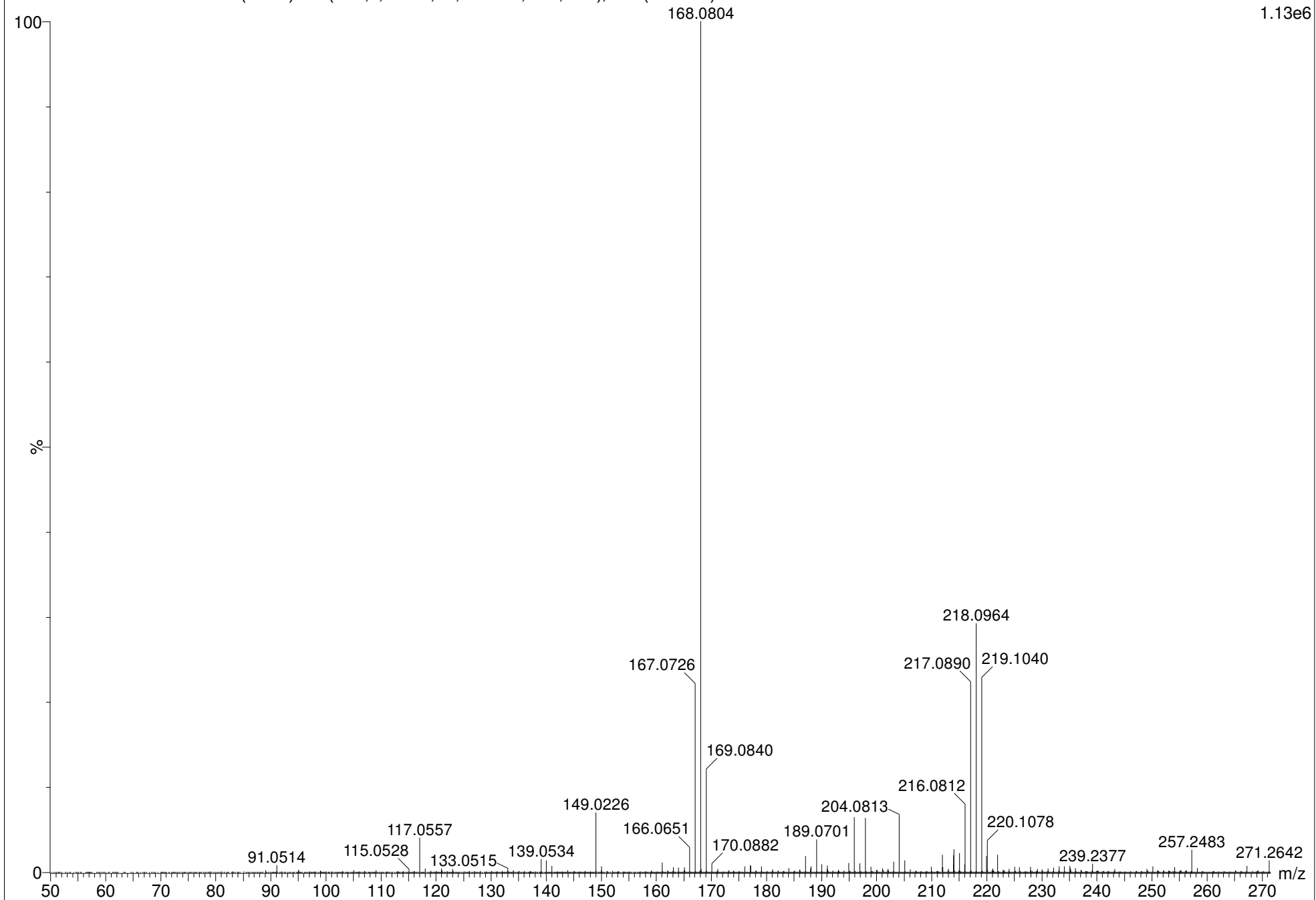
Xevo G2-S

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1: TOF MS ASAP+

1.13e6



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HERLEE-ECUWR-WG-A 203 (1.895) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (203:229)

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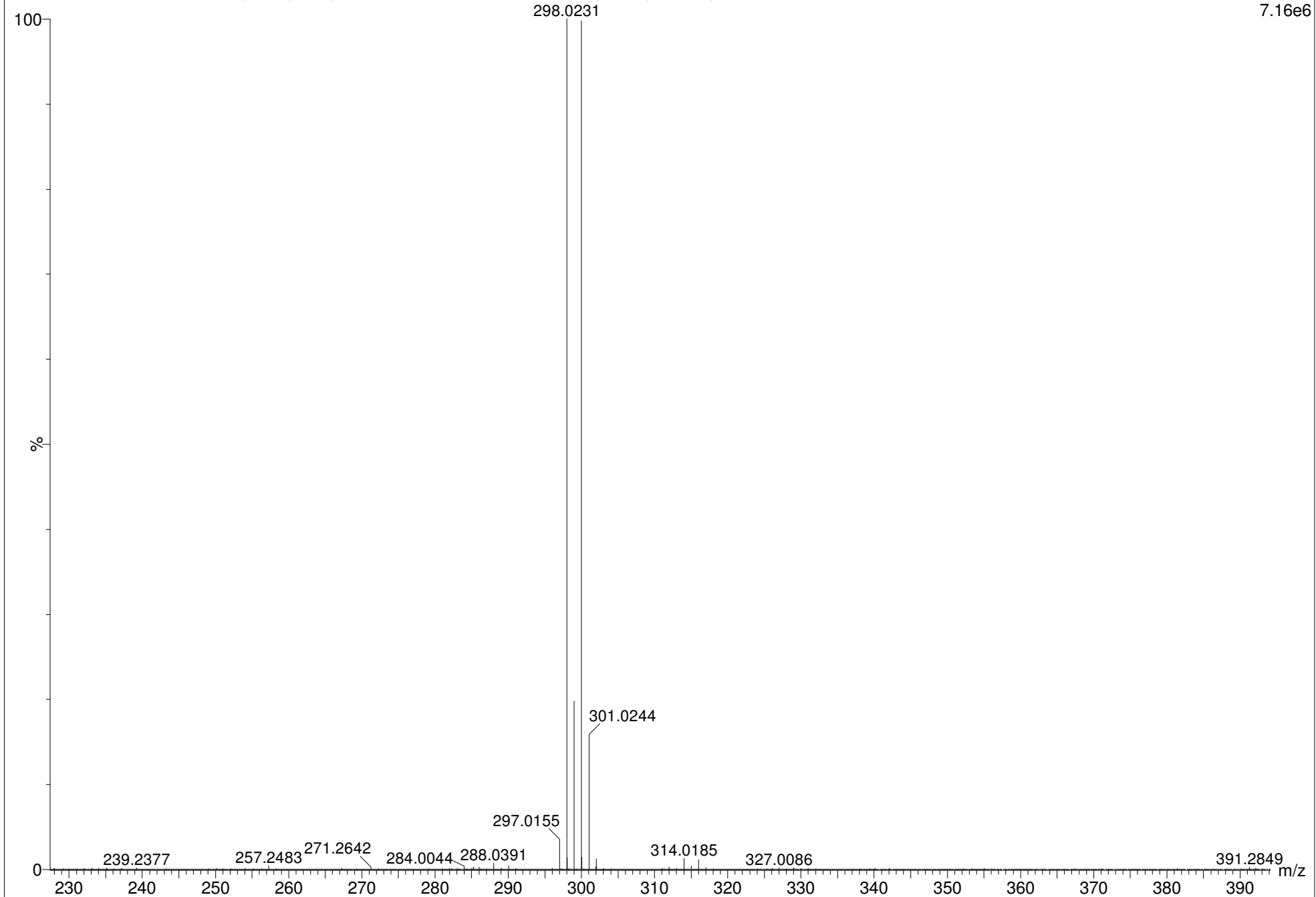
Xevo G2-S

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31-Oct-2019

1: TOF MS ASAP+

7.16e6



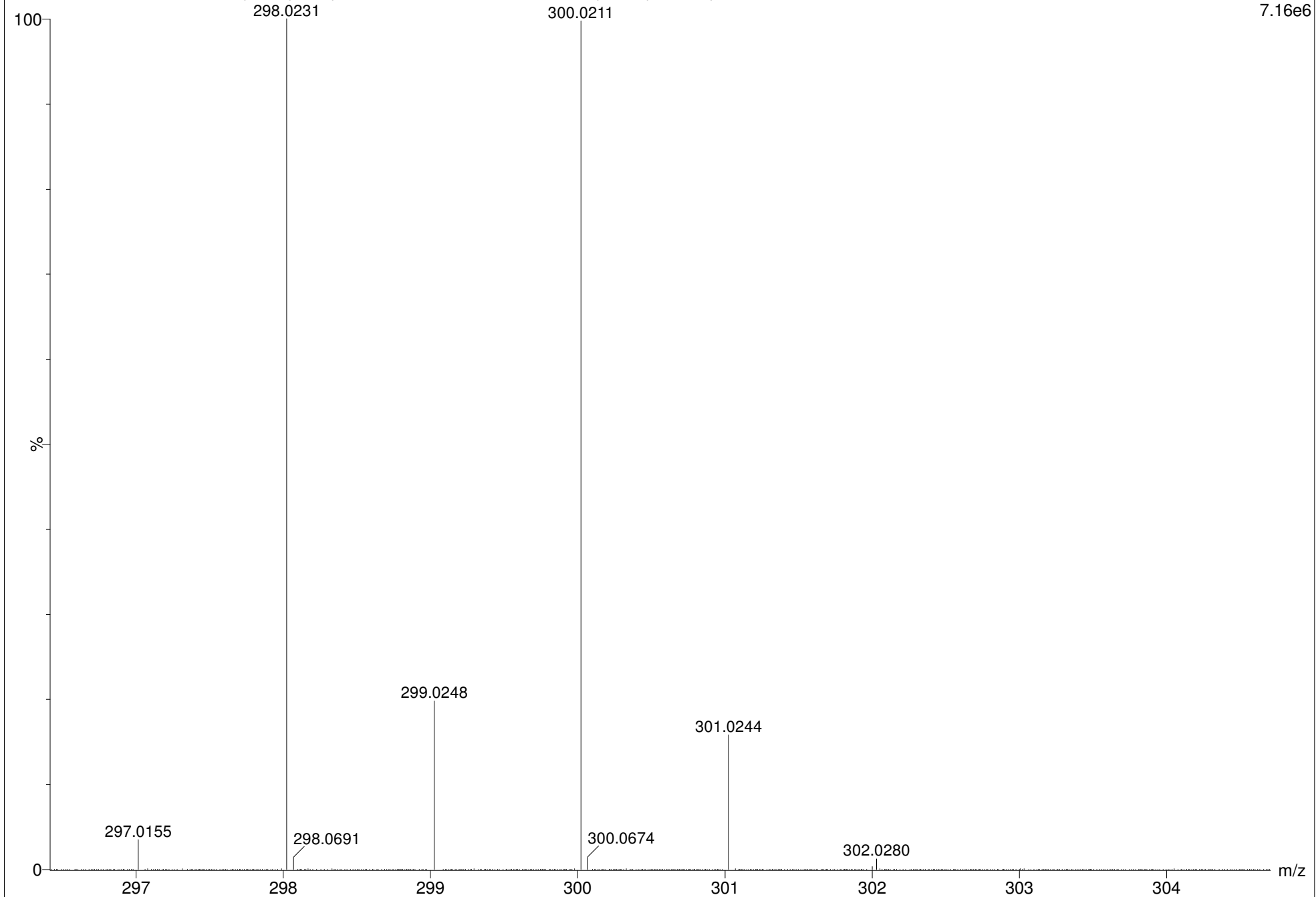
EM307 MW=297?  
ASAP(SOLID)  
C16H12BrN

National Mass Spectrometry Facility, Swansea  
Xevo G2-S

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31-Oct-2019

HERLEE-ECUWR-WG-A 203 (1.895) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (203:229)

1: TOF MS ASAP+  
7.16e6



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C<sub>16</sub>H<sub>12</sub>BrN

HERLEE-ECUWR-WG-A (0.037) Is (1.00,0.01) C<sub>16</sub>H<sub>12</sub>BrNH

National Mass Spectrometry Facility, Swansea

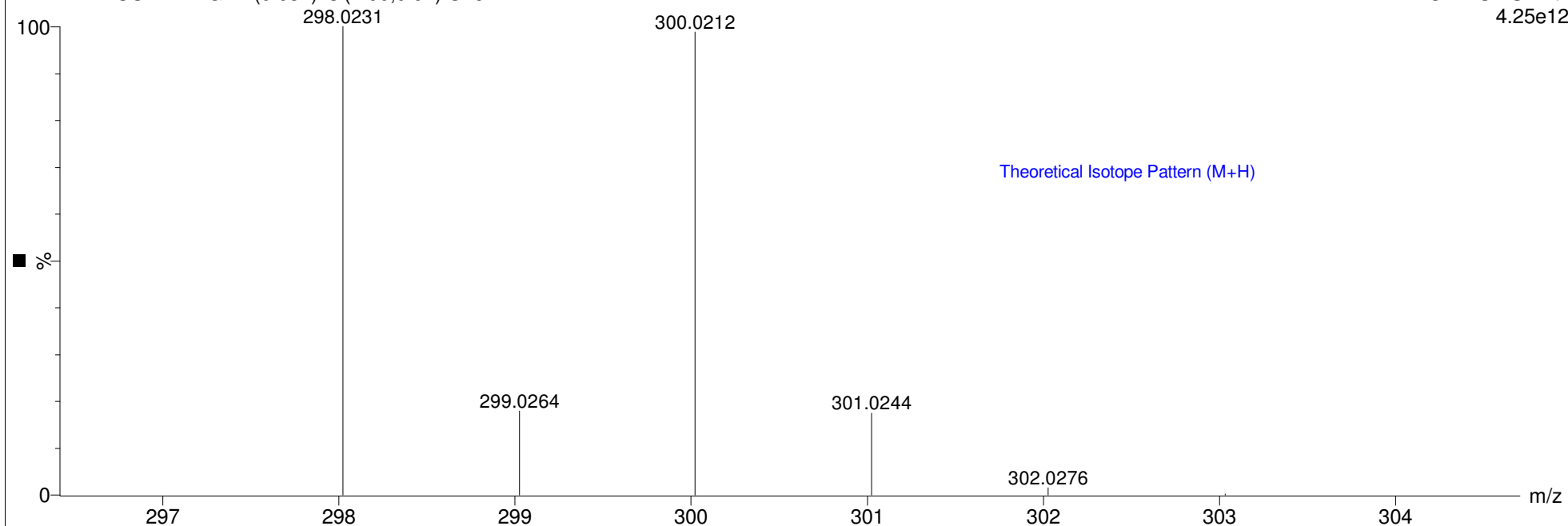
Xevo G2-S

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1: TOF MS ASAP+

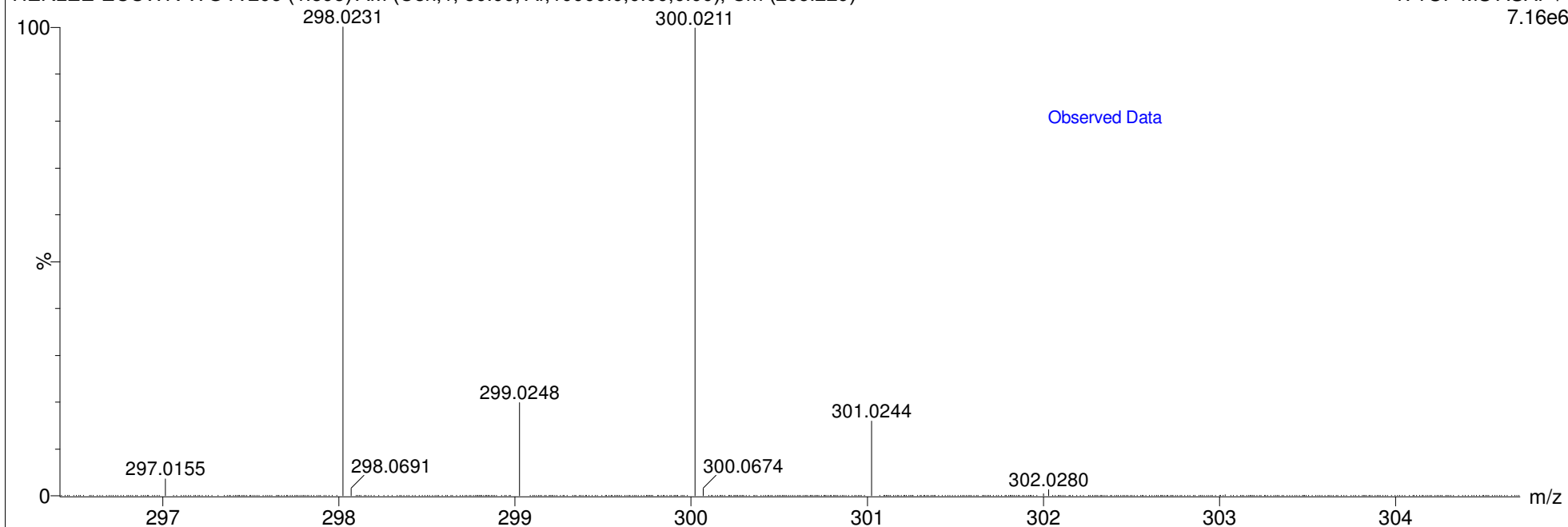
4.25e12



HERLEE-ECUWR-WG-A 203 (1.895) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (203:229)

1: TOF MS ASAP+

7.16e6



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

385 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-12 O: 0-14 Br: 1-1

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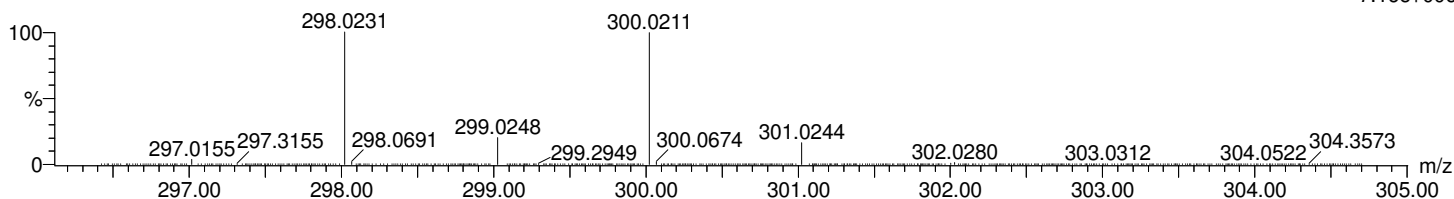
C16H12BrN

HERLEE-ECUWR-WG-A 203 (1.895) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (203:229)

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Xevo G2-S

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1: TOF MS ASAP+  
7.16e+006



Minimum: -10.0  
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
<b>298.0231</b>	<b>298.0231</b>	<b>0.0</b>	<b>0.0</b>	<b>10.5</b>	<b>2110.7</b>	<b>0.009</b>	<b>99.08</b>	<b>C16 H13 N Br</b>
	298.0236	-0.5	-1.7	-2.0	2118.0	7.268	0.07	C2 H15 N6 O6 Br
	298.0223	0.8	2.7	-7.0	2115.5	4.769	0.85	C H19 N2 O10 Br
	298.0223	0.8	2.7	-1.5	2123.4	12.705	0.00	H13 N9 O5 Br