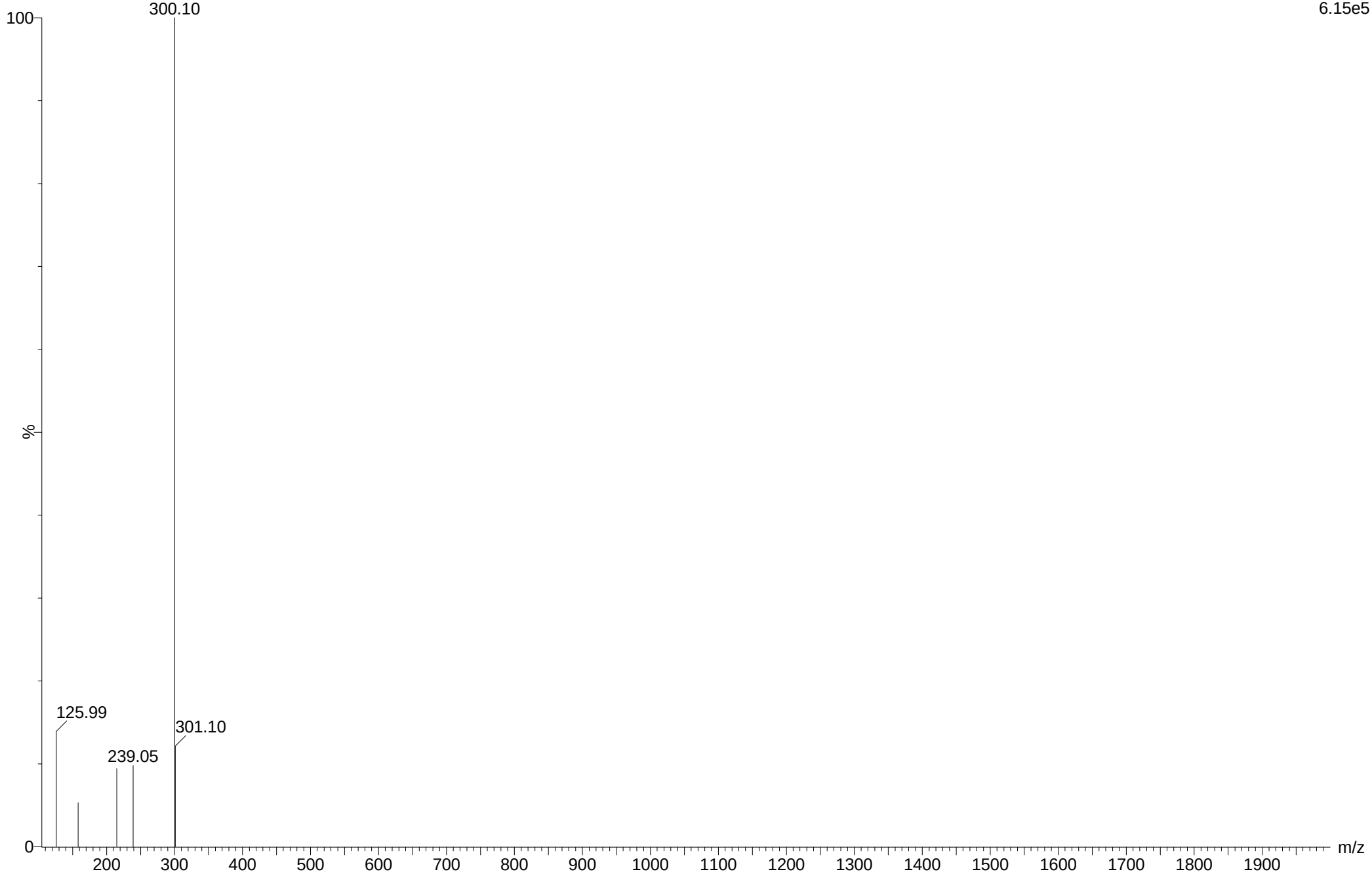
LNB0367-132-P C12H17N3O4S MW=299
Methanol
LRC-DXK-3UCJC-ESI-Pos-1 8 (0.552) AM2 (Ar,30000.0,0.00,0.00); ABS

University of Birmingham, School of Chemistry
Waters Xevo G2-XS

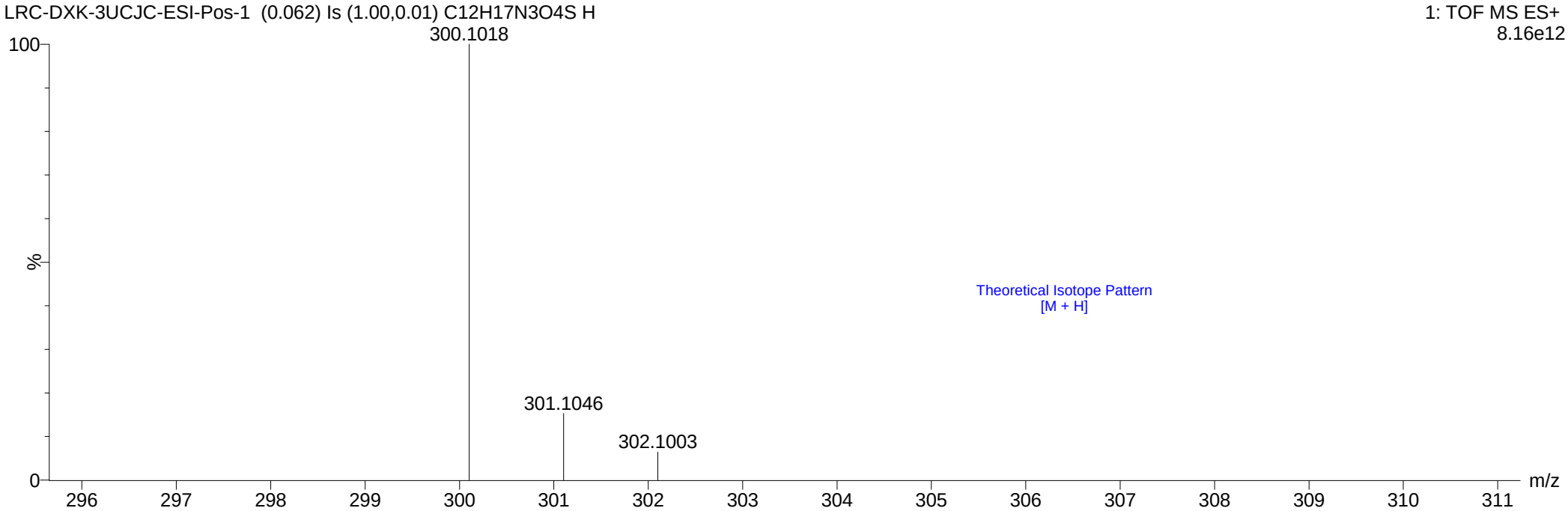
Daniel Kovari
12-Dec-2020 01:13:52
1: TOF MS ES+
6.15e5

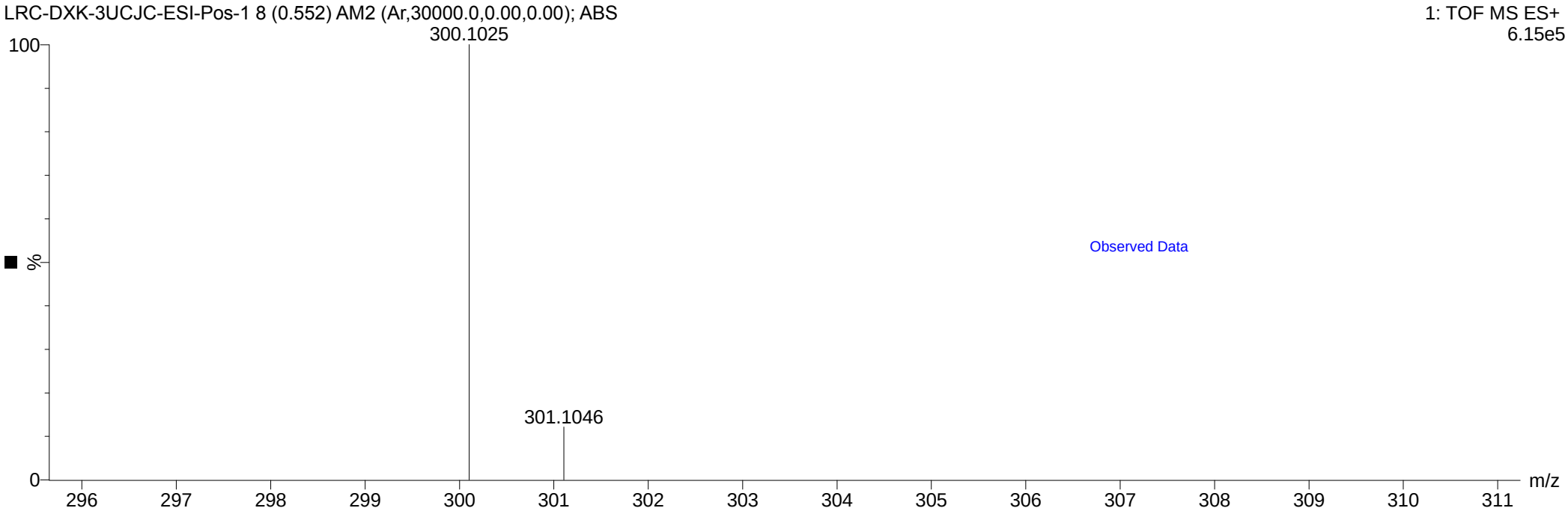


LNB0367-132-P C12H17N3O4S MW=299
Methanol

University of Birmingham, School of Chemistry
Waters Xevo G2-XS

Daniel Kovari
12-Dec-2020 01:13:52



## 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 = 4

Monoisotopic Mass, Even Electron Ions
459 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-60 N: 0-10 O: 0-10 S: 1-1

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -10.0 | | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
| 300.1025 | 300.1031 | -0.6 | -2.0 | 10.5 | 45.3 | 0.409 | 66.46 | C13 H14 N7 S |
| | 300.1018 | 0.7 | 2.3 | 5.5 | 46.0 | 1.092 | 33.54 | C12 H18 N3 O4 S |