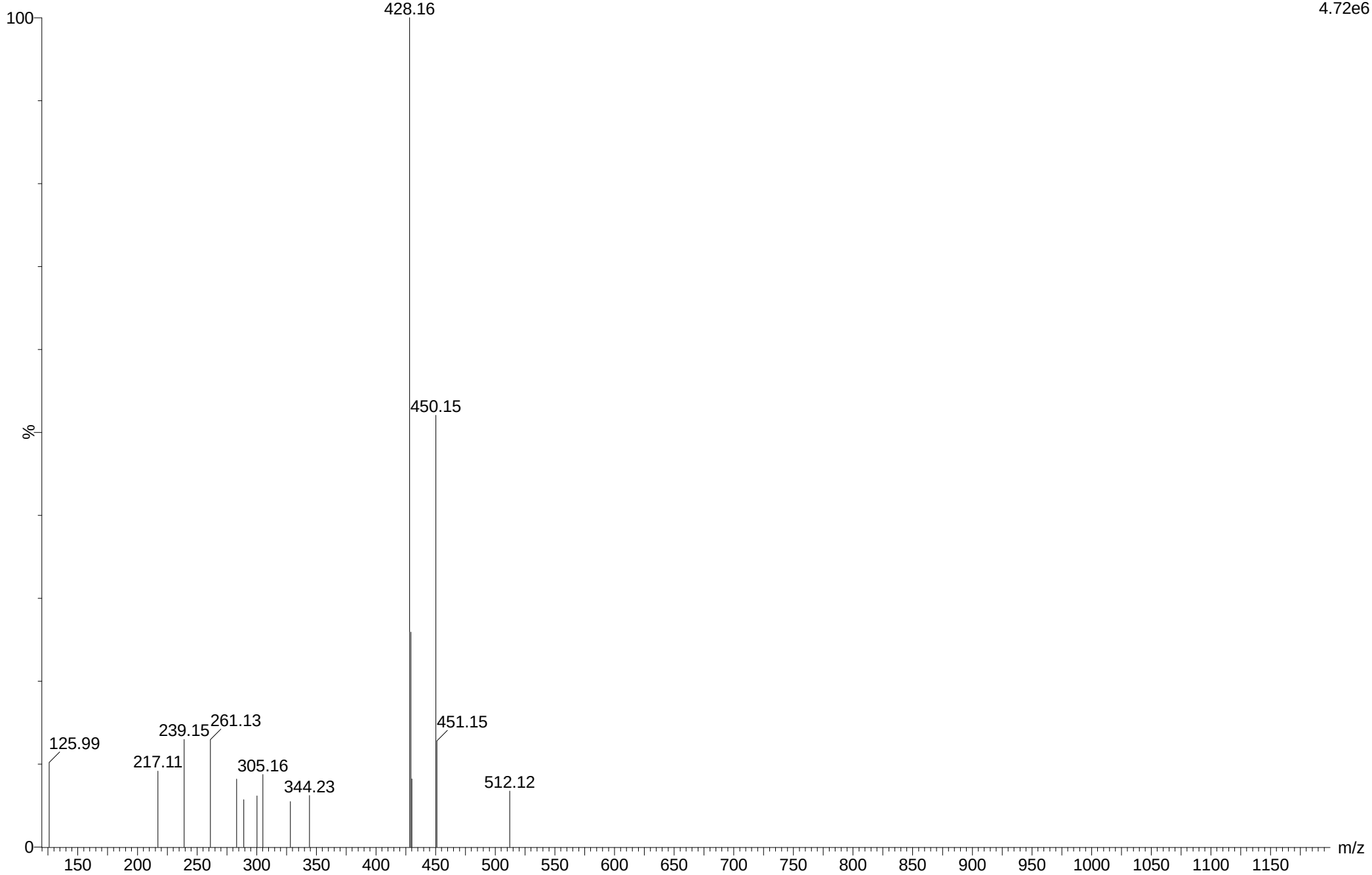
NAT384-652614 C22H25N3O4S MW=428
Methanol:Water
LRC-HVA-4TXW9-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS

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

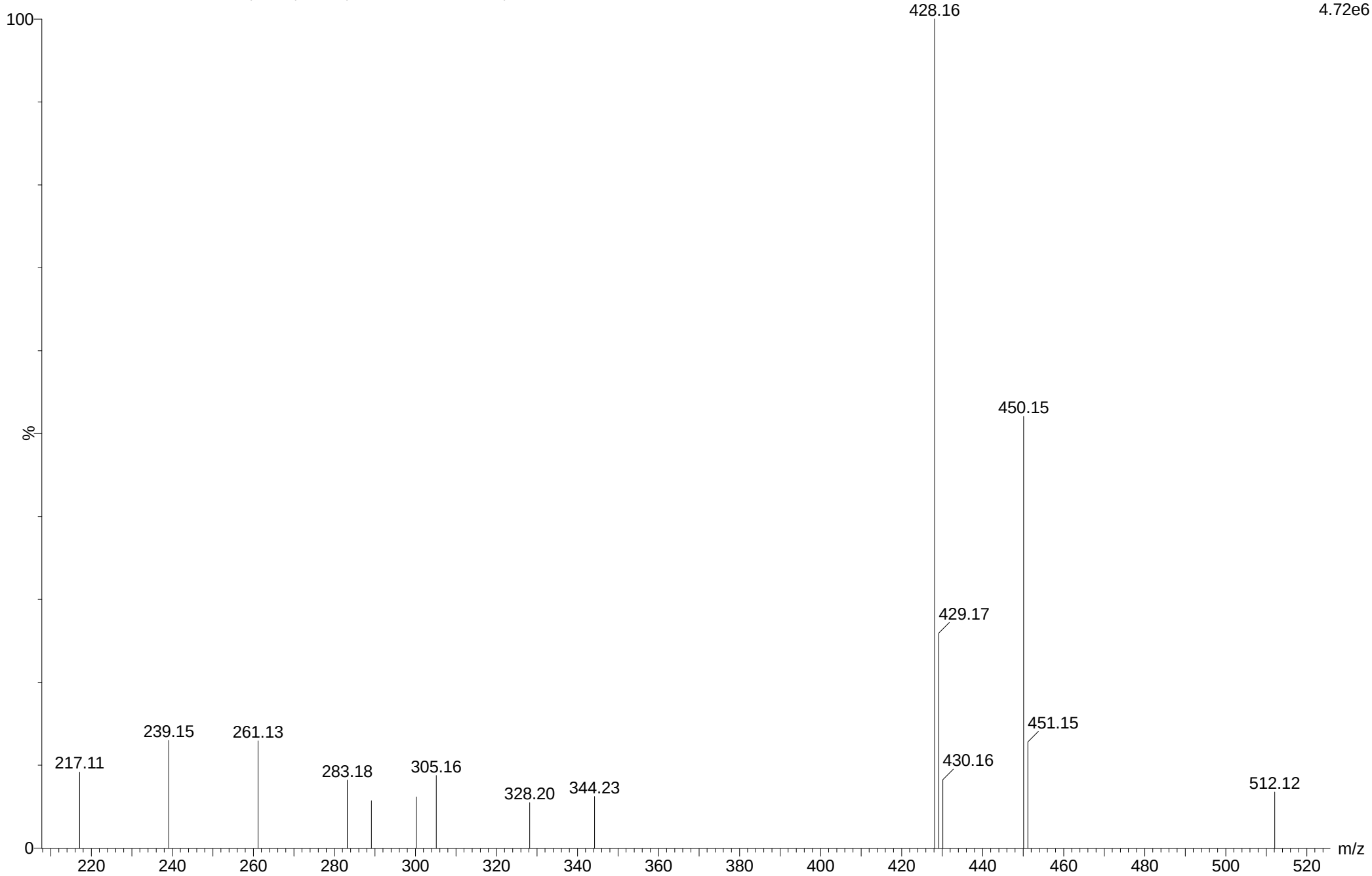
Holly Adcock
16-Apr-2021 17:03:49
2: TOF MS ES+
4.72e6



NAT384-652614 C22H25N3O4S MW=428
Methanol:Water
LRC-HVA-4TXW9-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS

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

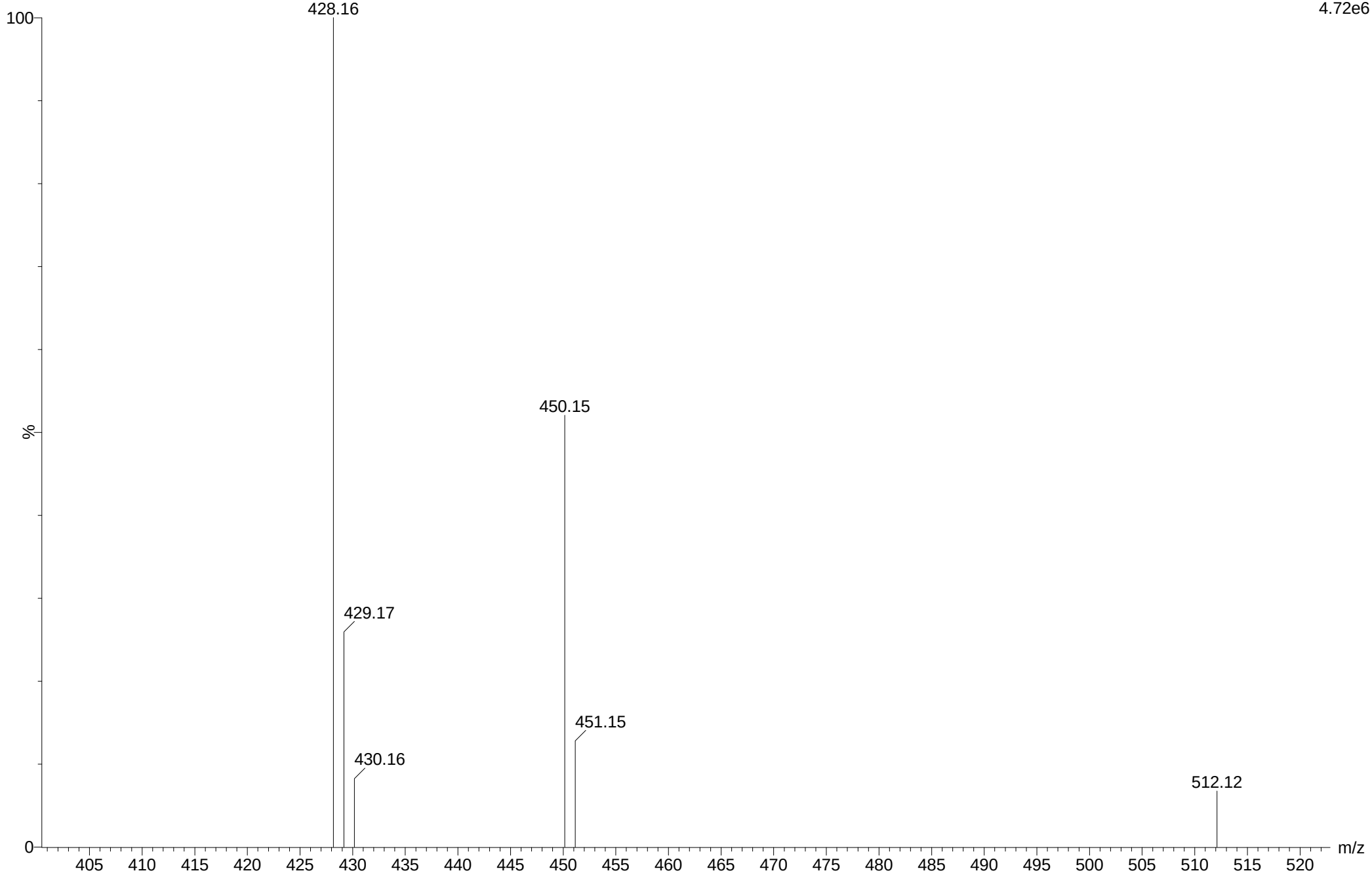
Holly Adcock
16-Apr-2021 17:03:49
2: TOF MS ES+
4.72e6



NAT384-652614 C22H25N3O4S MW=428
Methanol:Water
LRC-HVA-4TXW9-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS

University of Birmingham, School of Chemistry
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Holly Adcock
16-Apr-2021 17:03:49
2: TOF MS ES+
4.72e6



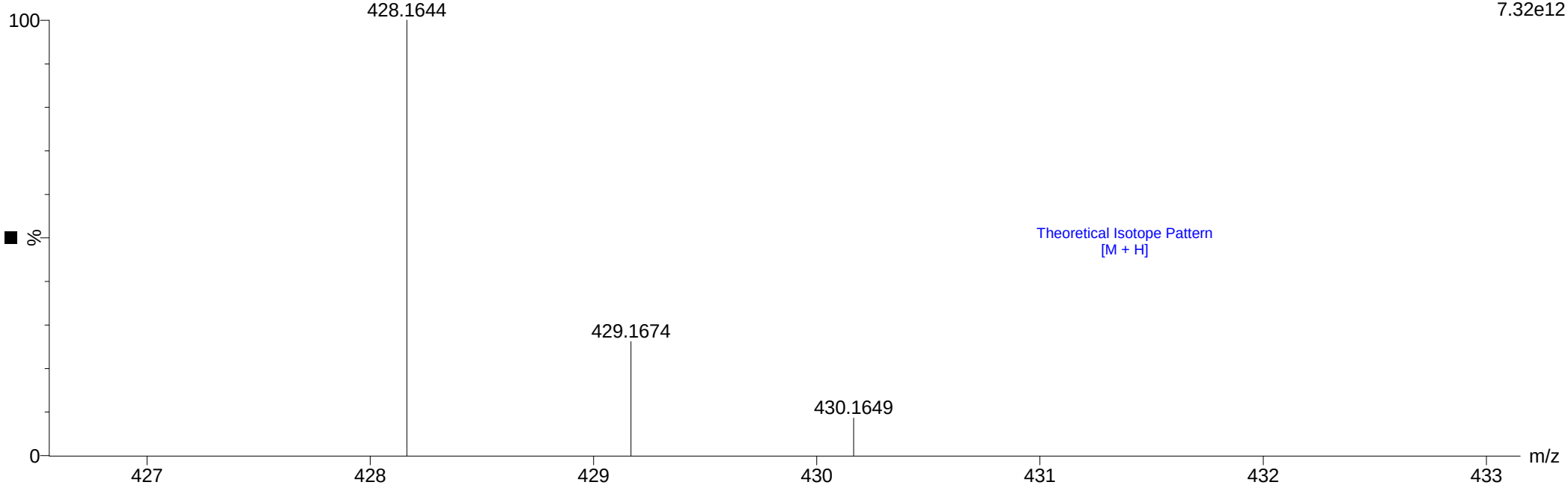
NAT384-652614 C22H25N3O4S MW=428
Methanol:Water

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

Holly Adcock
16-Apr-2021 17:03:49

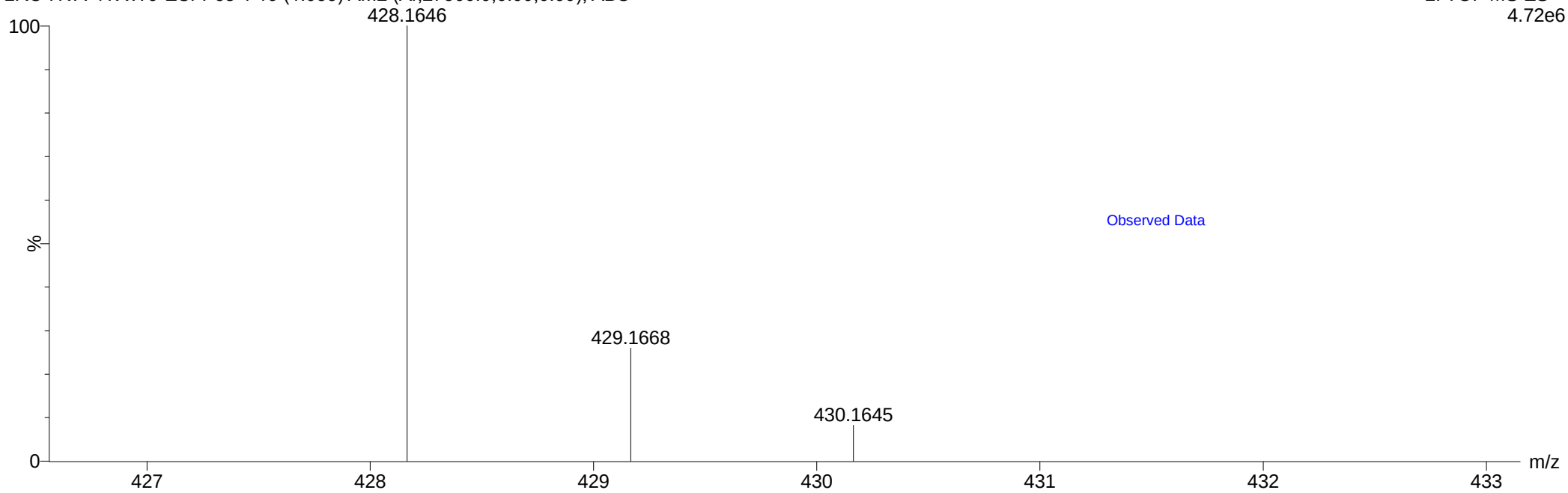
LRC-HVA-4TXW9-ESI-Pos-1 (0.290) Is (1.00,0.01) C22H25N3O4S H

2: TOF MS ES+
7.32e12




LRC-HVA-4TXW9-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS

2: TOF MS ES+
4.72e6



## Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -4.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1637 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-40 H: 0-60 N: 0-10 O: 0-10 S: 0-2

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -4.0 | | | | |
| Maximum: | | 3.0 | 3.0 | 100.0 | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
| 428.1646 | 428.1644 | 0.2 | 0.5 | 11.5 | 23.4 | 0.001 | 99.91 | C22 H26 N3 O4 S |
| | 428.1642 | 0.4 | 0.9 | 8.5 | 41.4 | 18.007 | 0.00 | C14 H22 N9 O7 |
| | 428.1651 | -0.5 | -1.2 | 20.5 | 41.6 | 18.218 | 0.00 | C30 H22 N O2 |
| | 428.1651 | -0.5 | -1.2 | 7.5 | 36.8 | 13.478 | 0.00 | C15 H26 N9 O2 S2 |
| | 428.1638 | 0.8 | 1.9 | 2.5 | 38.2 | 14.886 | 0.00 | C14 H30 N5 O6 S2 |
| | 428.1657 | -1.1 | -2.6 | 16.5 | 30.4 | 7.055 | 0.09 | C23 H22 N7 S |