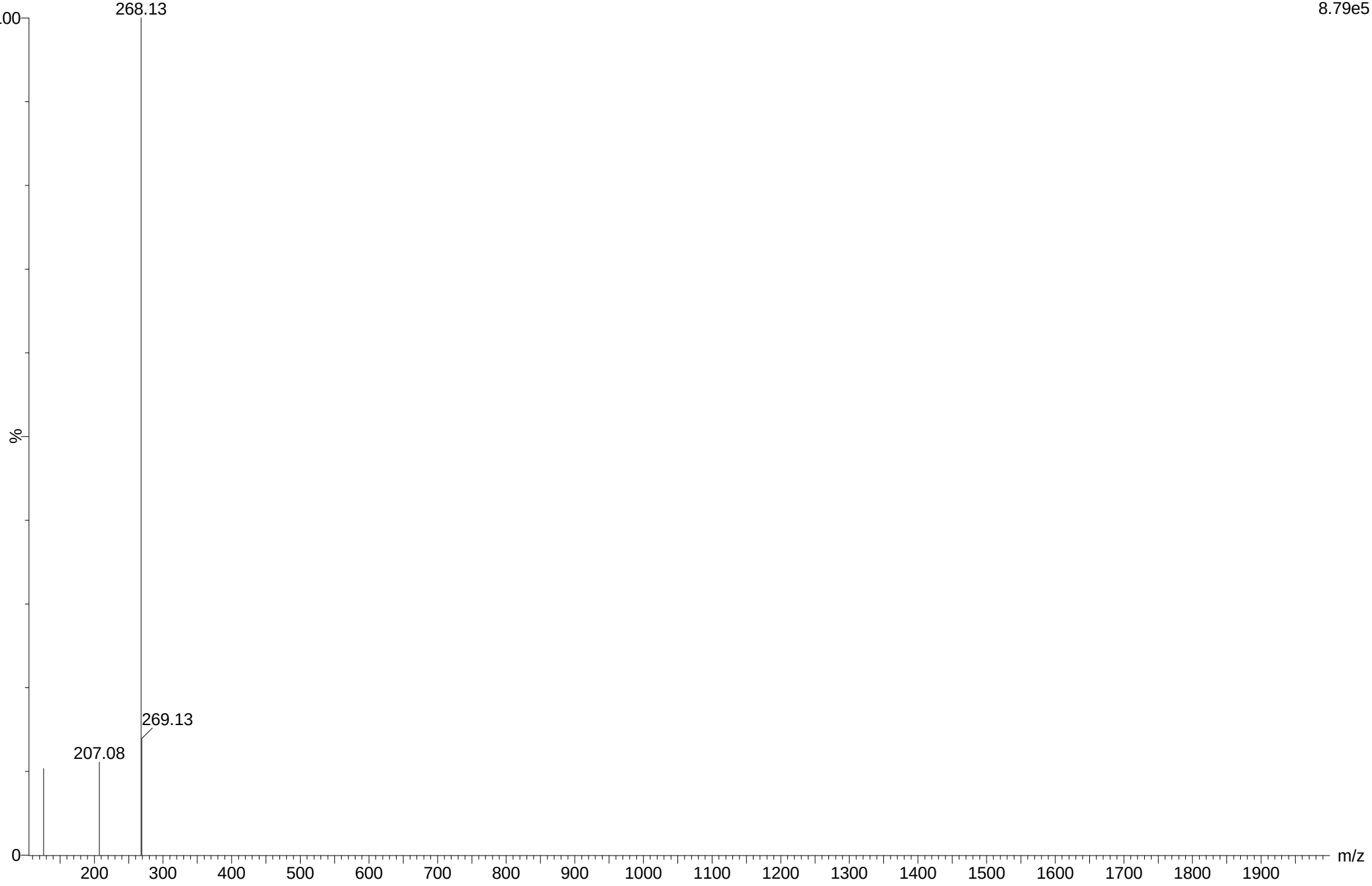
LNB0367-145-P C12H17N3O4 MW=267
Methanol

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

Daniel Kovari
12-Dec-2020 00:54:36

LRC-DXK-3U4R3-ESI-Pos-1 8 (0.552) AM2 (Ar,30000.0,0.00,0.00); ABS

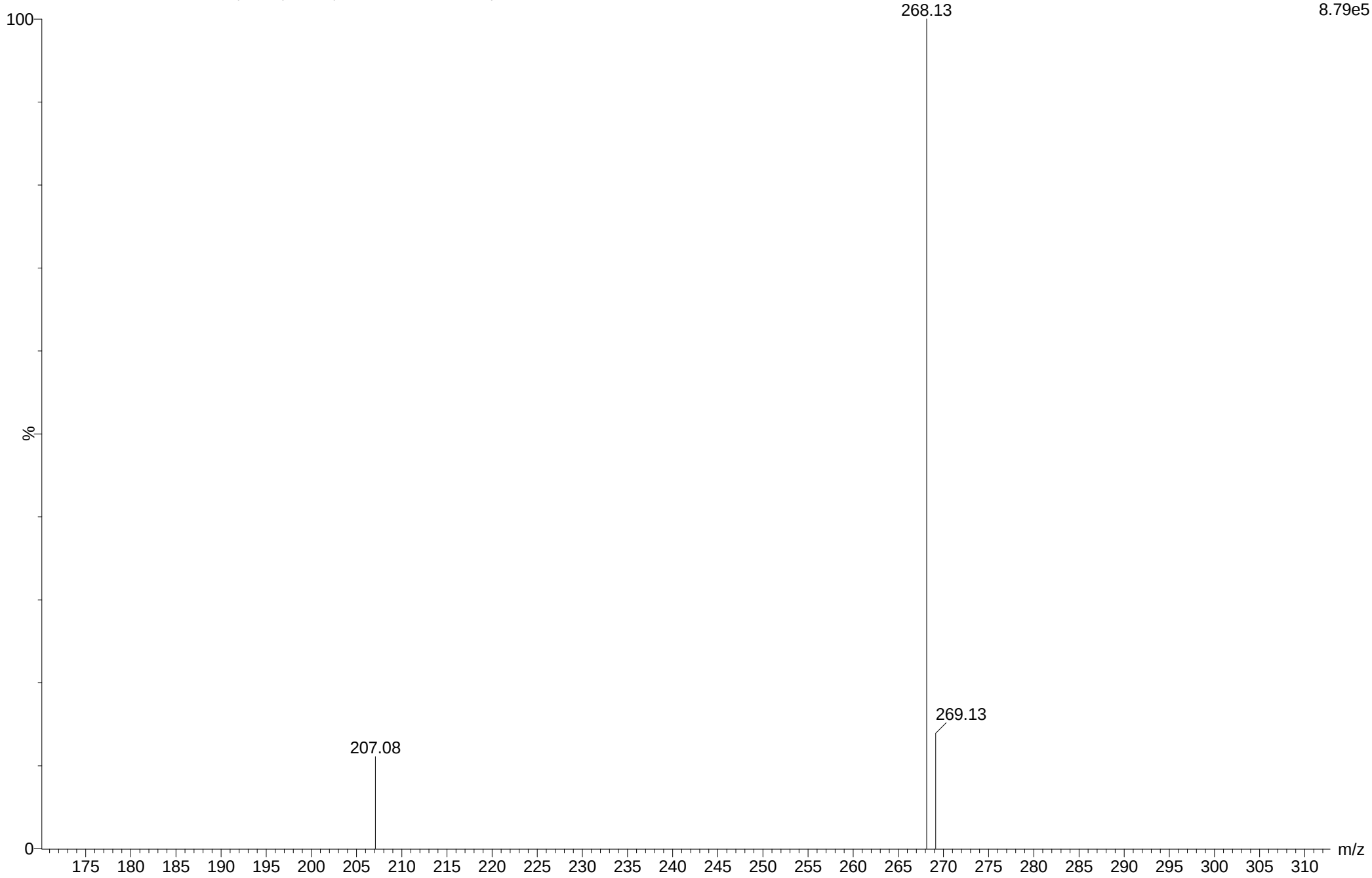
1: TOF MS ES+
8.79e5



LNB0367-145-P C12H17N3O4 MW=267
Methanol
LRC-DXK-3U4R3-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 00:54:36
1: TOF MS ES+
8.79e5



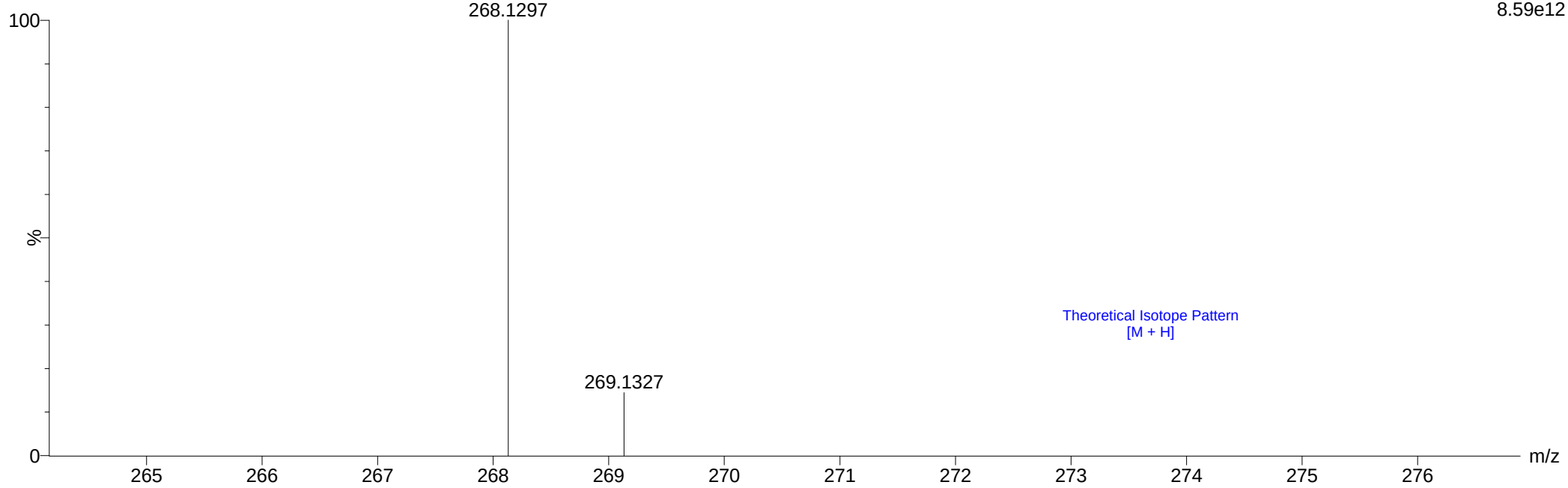
LNB0367-145-P C12H17N3O4 MW=267
Methanol

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

Daniel Kovari
12-Dec-2020 00:54:36

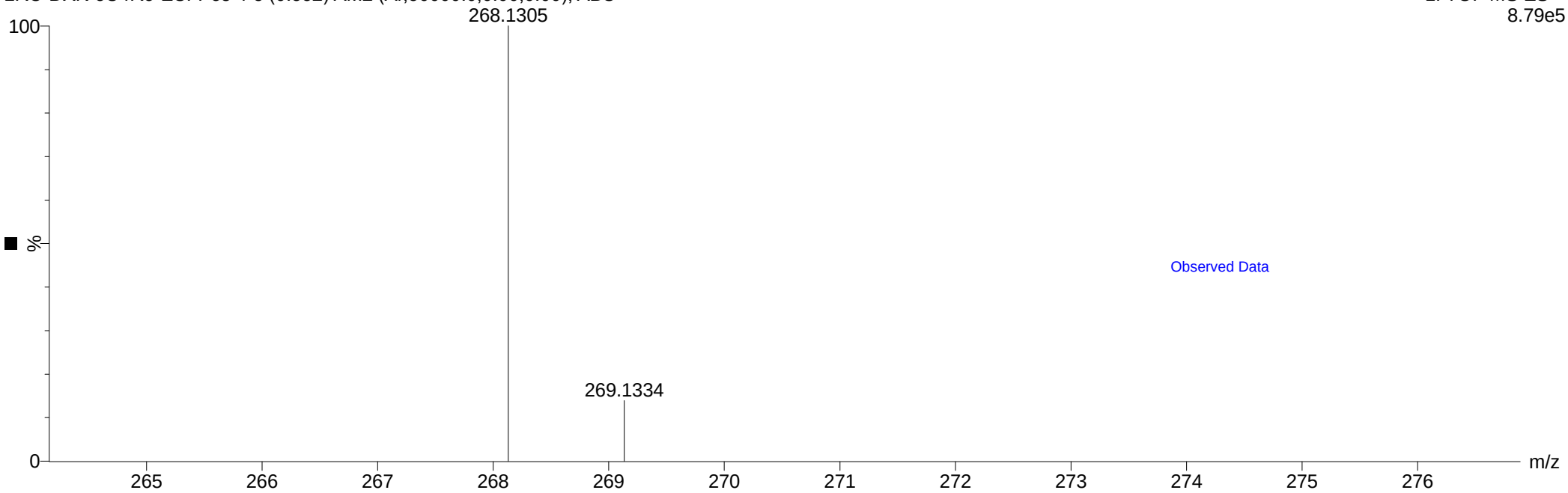
LRC-DXK-3U4R3-ESI-Pos-1 (0.062) Is (1.00,0.01) C12H17N3O4 H

1: TOF MS ES+
8.59e12




LRC-DXK-3U4R3-ESI-Pos-1 8 (0.552) AM2 (Ar,30000.0,0.00,0.00); ABS

1: TOF MS ES+
8.79e5



## 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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -10.0 | | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
| 268.1305 | 268.1311 | -0.6 | -2.2 | 10.5 | 45.2 | 0.583 | 55.81 | C13 H14 N7 |
| | 268.1297 | 0.8 | 3.0 | 5.5 | 45.5 | 0.817 | 44.19 | C12 H18 N3 O4 |