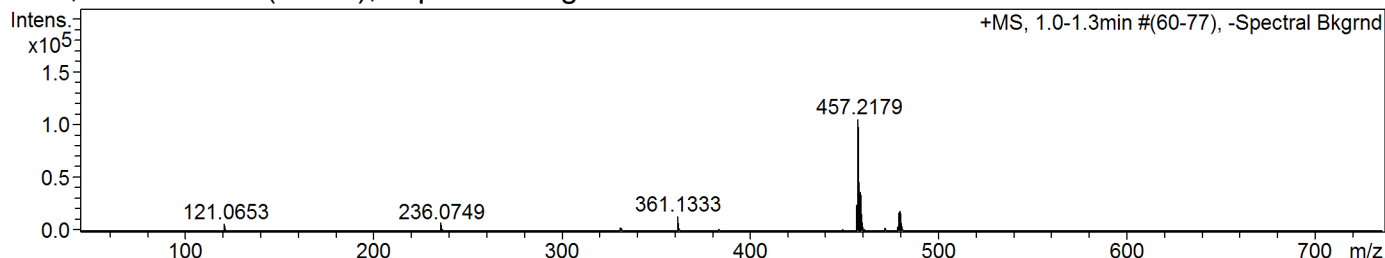


Confirmation of Expected Formula

Sample-ID acs_sdb_acs311 Submitter Adam Sedgwick
 Analysis Name acs_sdb_acs311_346008_32_01_50629.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 06/01/2016 16:59:15
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



| # | m/z | I | I % | Area | S/N |
|----|----------|--------|-------|------|---------|
| 1 | 121.0653 | 6171 | 5.9 | 79 | 17487.8 |
| 2 | 236.0749 | 6372 | 6.1 | 248 | 4990.2 |
| 3 | 361.1333 | 13602 | 13.0 | 992 | 9676.7 |
| 4 | 456.2171 | 24717 | 23.7 | 2462 | 2811.3 |
| 5 | 457.2179 | 104497 | 100.0 | 8279 | 11988.5 |
| 6 | 458.2169 | 31485 | 30.1 | 3162 | 3643.6 |
| 7 | 459.2148 | 9359 | 9.0 | 974 | 1092.5 |
| 8 | 478.1961 | 3715 | 3.6 | 415 | 520.7 |
| 9 | 479.1963 | 17978 | 17.2 | 1990 | 2546.3 |
| 10 | 480.1995 | 5507 | 5.3 | 579 | 788.4 |

Generate Molecular Formula Parameters

| Charge | Tolerance | SearchRadius | H/C Ratio min. | H/C Ratio max. | Electron Conf. | Nitrogen Rule | sigma limit |
|----------|-----------|--------------|----------------|----------------|----------------|---------------|-------------|
| positive | 10 ppm | 0.05 m/z | 0 | 3 | both | true | 0.05 |

Expected Formula C₂₇ H₂₉ B N₂ O₂ S Adduct(s): H, Na

| # | meas. m/z | theo. m/z | Err[ppm] | Sigma | Formula |
|---|-----------|------------|----------|--------|---|
| 1 | 479.1963 | 479.194049 | -4.90 | 0.0218 | C ₂₇ H ₂₉ B N ₂ Na O ₂ S ₁ |

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication