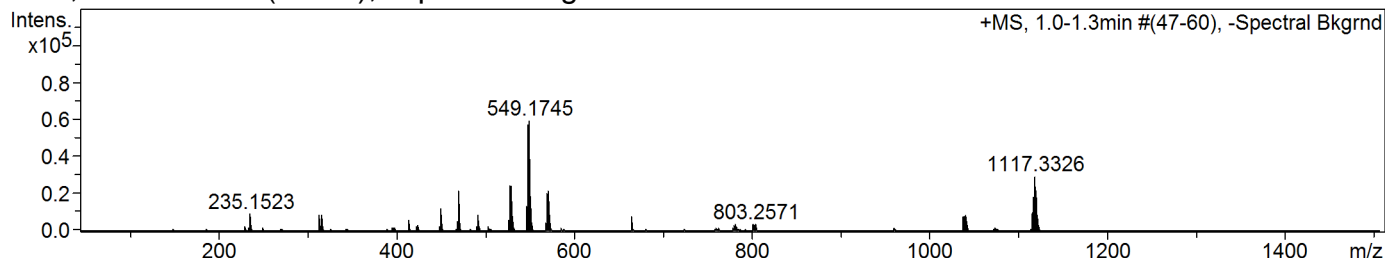


Confirmation of Expected Formula

Sample-ID acs_sdb_acs237 Submitter Adam Sedgwick
 Analysis Name acs_sdb_acs237_344349_12_01_48804.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 20/07/2015 09:48:38
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(47-60), -Spectral Bkgrnd



| # | m/z | I | I % | Area | S/N |
|----|-----------|-------|-------|------|--------|
| 1 | 469.2657 | 21748 | 36.6 | 2178 | 1186.0 |
| 2 | 527.1711 | 24096 | 40.6 | 2446 | 1165.2 |
| 3 | 529.1690 | 24102 | 40.6 | 2629 | 1165.0 |
| 4 | 547.1768 | 57070 | 96.1 | 5494 | 2749.1 |
| 5 | 548.1782 | 32430 | 54.6 | 3419 | 1561.9 |
| 6 | 549.1745 | 59361 | 100.0 | 5815 | 2858.3 |
| 7 | 569.1607 | 20512 | 34.6 | 2192 | 983.9 |
| 8 | 571.1619 | 21463 | 36.2 | 2307 | 1029.1 |
| 9 | 1117.3326 | 29321 | 49.4 | 4855 | 2068.0 |
| 10 | 1118.3330 | 21752 | 36.6 | 3832 | 1536.0 |

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 C26 H34 B Br F2 N2 O Si

Adduct(s): H, Na

| # | meas. m/z | theo. m/z | Err[ppm] | Sigma | Formula |
|---|-----------|------------|----------|--------|--|
| 1 | 547.1768 | 547.176315 | -1.00 | 0.0098 | C 26 H 35 B 1 Br 1 F 2 N 2 O 1 Si 1 |
| 1 | 569.1607 | 569.158259 | -4.30 | 0.0246 | C 26 H 34 B 1 Br 1 F 2 N 2 Na 1 O 1 Si 1 |

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