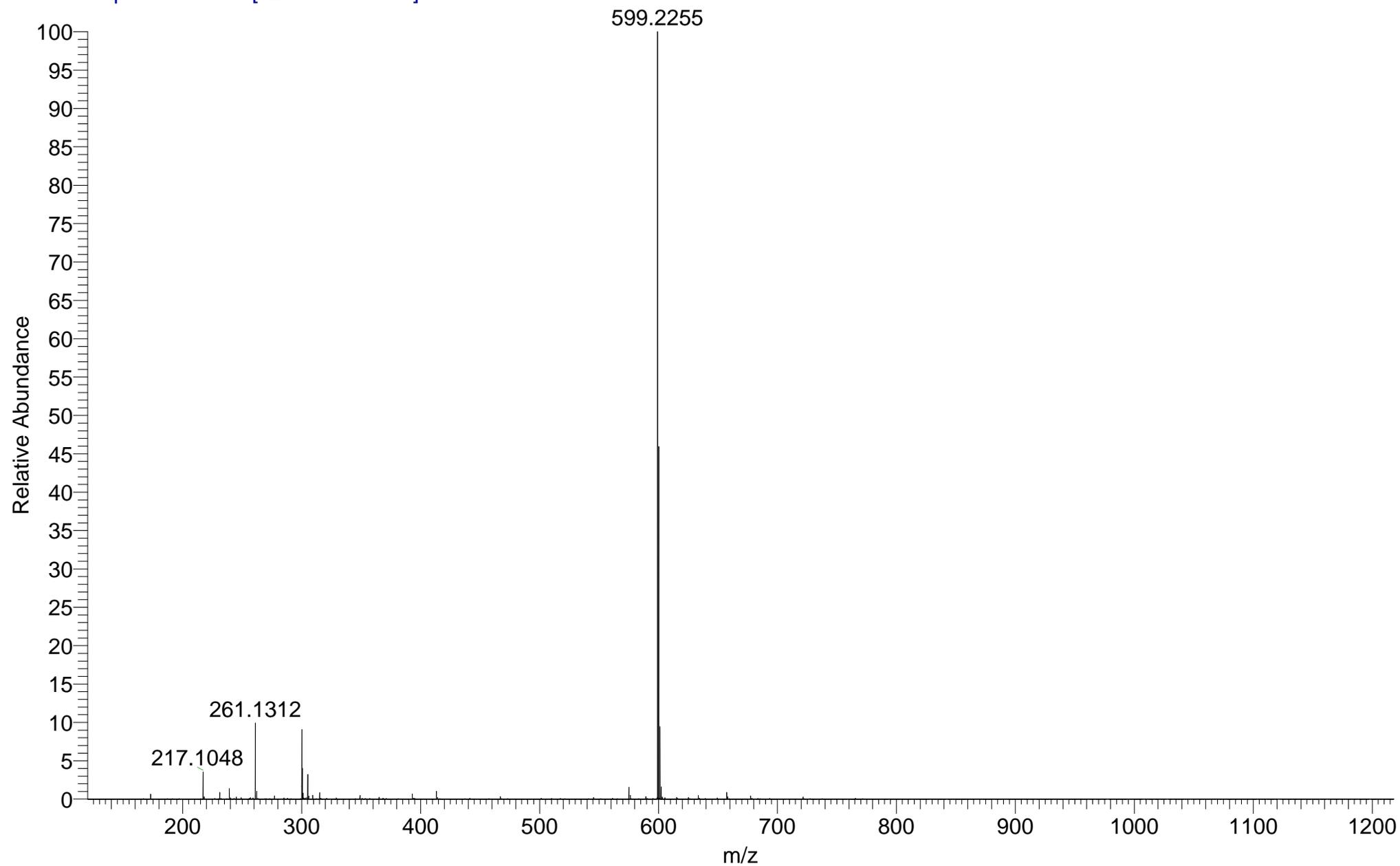


MAR-58
(MeCN)/(MeOH)
C40H31F6N4PS

EPSRC National Facility Swansea
LTQ Orbitrap XL

UEAFIL
10/25/16 14:26:50

UEAFIL_4PCUZ_95 #9-16 RT: 0.20-0.53 AV: 7 SM: 7G NL: 3.42E7
T: FTMS + p NSI Full ms [120.00-1935.00]



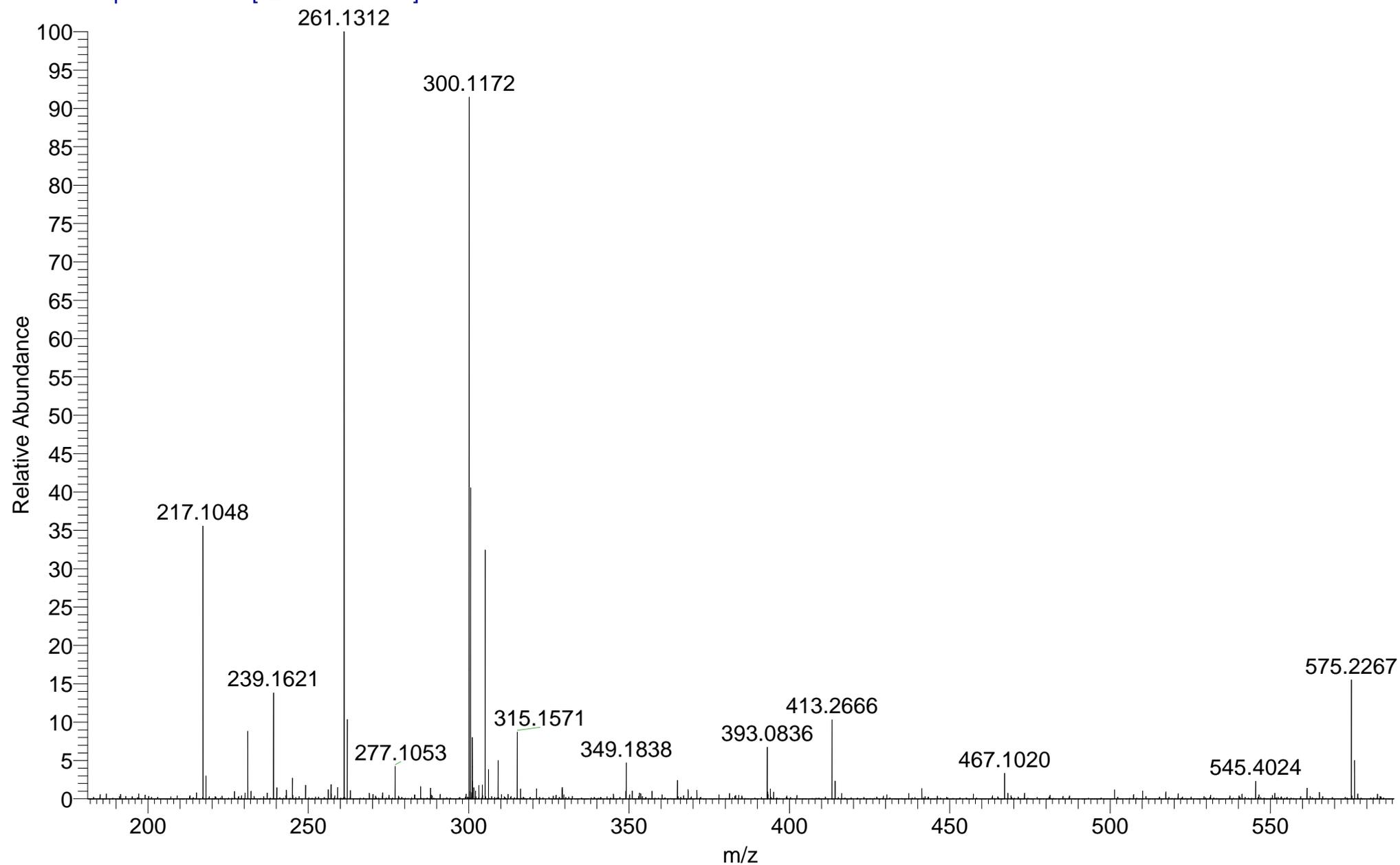
MAR-58
(MeCN)/(MeOH)
C40H31F6N4PS

EPSRC National Facility Swansea
LTQ Orbitrap XL

UEAFIL
10/25/16 14:26:50

UEAFIL_4PCUZ_95 #9-16 RT: 0.20-0.53 AV: 7 SM: 7G NL: 3.39E6

T: FTMS + p NSI Full ms [120.00-1935.00]

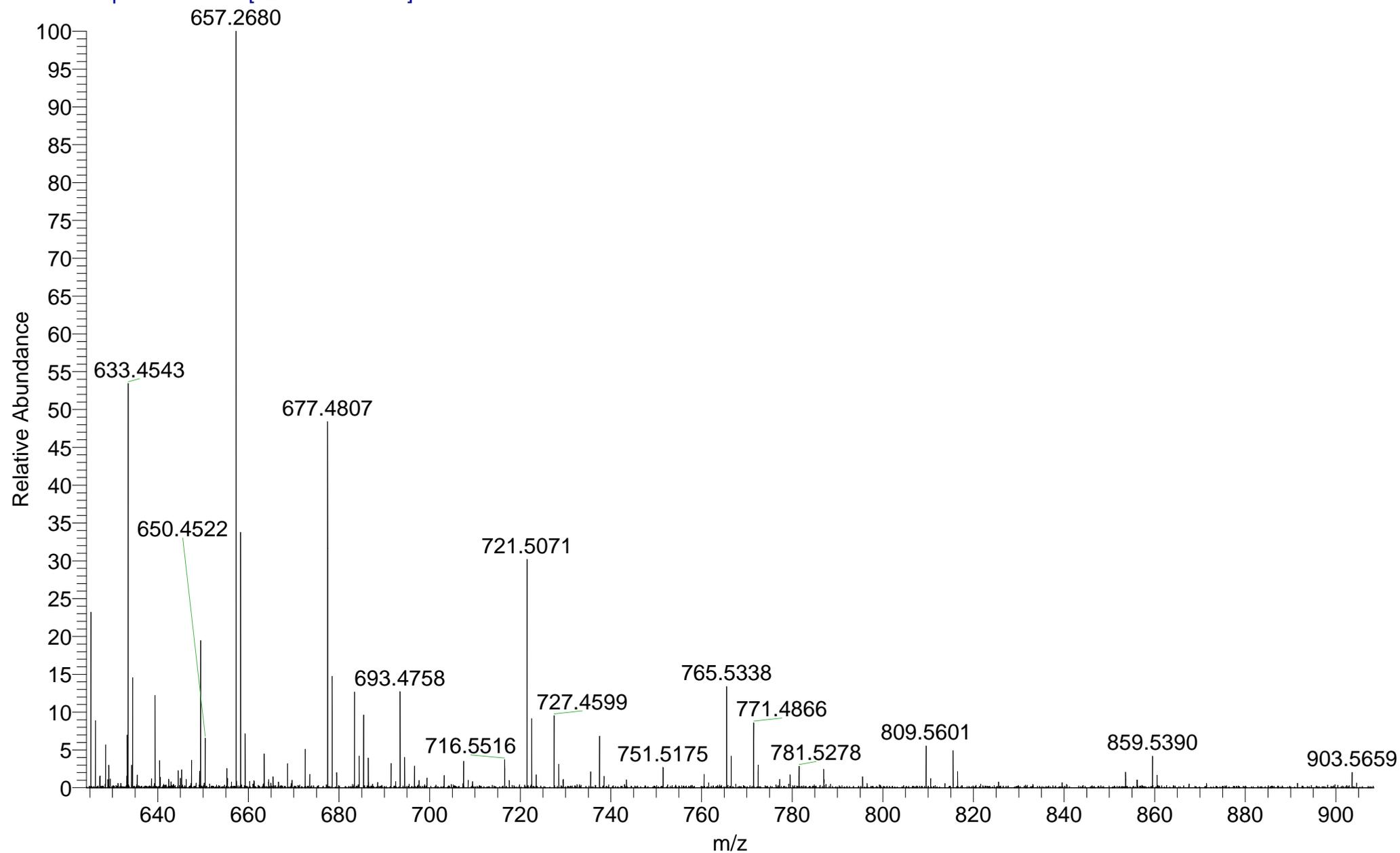


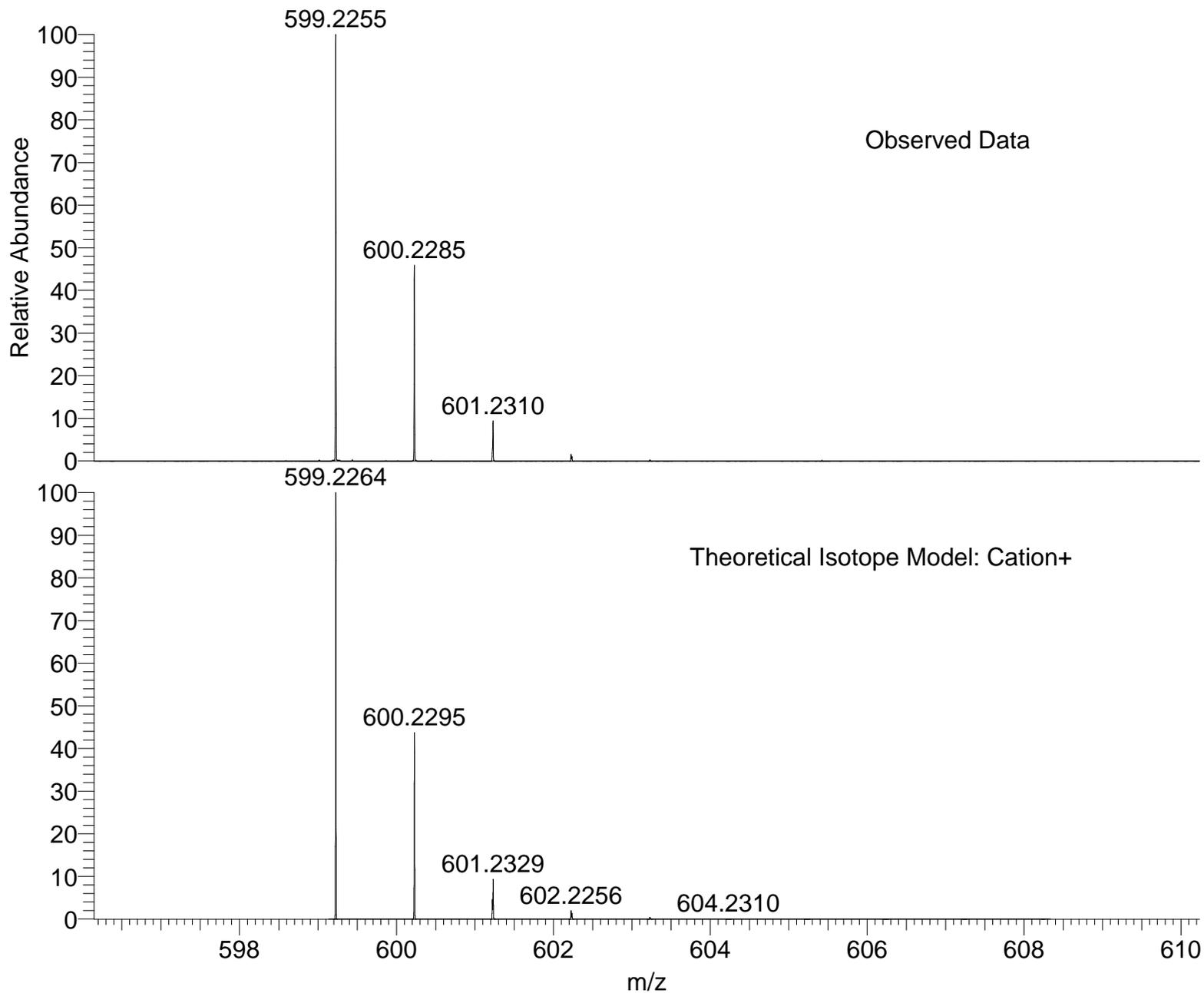
MAR-58
(MeCN)/(MeOH)
C40H31F6N4PS

EPSRC National Facility Swansea
LTQ Orbitrap XL

UEAFIL
10/25/16 14:26:50

UEAFIL_4PCUZ_95 #9-16 RT: 0.20-0.53 AV: 7 SM: 7G NL: 3.00E5
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
3.42E7
UEAFIL_4PCUZ_95#9-16 RT:
0.20-0.53 AV: 7 T: FTMS + p
NSI Full ms [120.00-1935.00]

NL:
1.42E4
C₄₀ H₃₁ N₄ S:
C₄₀ H₃₁ N₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....50
 1 H 0....70
 23 Na 0....0
 32 S 0....5
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

| Mass | Theoretical Mass | Delta [ppm] | RDB | Composition |
|----------|---------------------|----------------|------|--|
| 599.2255 | 599.2256 | -0.1 | 15.5 | C ₂₄ H ₃₁ O ₅ N ₁₂ S ₁ |
| | 599.2256 | -0.1 | 10.0 | C ₂₅ H ₃₇ O ₁₀ N ₅ S ₁ |
| | 599.2256 | -0.2 | -3.0 | C ₁₀ H ₄₁ O ₁₀ N ₁₃ S ₃ |
| | 599.2254 | 0.2 | 7.0 | C ₁₇ H ₃₃ O ₁₃ N ₁₁ |
| | 599.2253 | 0.4 | 12.5 | C ₃₂ H ₄₃ O ₁ N ₂ S ₄ |
| | 599.2257 | -0.4 | 18.5 | C ₃₂ H ₃₅ O ₂ N ₆ S ₂ |
| | 599.2258 | -0.5 | 5.5 | C ₁₇ H ₃₉ O ₂ N ₁₄ S ₄ |
| | 599.2258 | -0.5 | 0.0 | C ₁₈ H ₄₅ O ₇ N ₇ S ₄ |
| | 599.2251 | 0.7 | 4.0 | C ₂₅ H ₄₅ O ₉ N ₁ S ₃ |
| | 599.2251 | 0.7 | 9.5 | C ₂₄ H ₃₉ O ₄ N ₈ S ₃ |
| | 599.2251 | 0.7 | 22.5 | C ₃₉ H ₃₅ O ₄ S ₁ |
| | 599.2260 | -0.8 | 3.0 | C ₂₆ H ₄₉ O ₄ N ₁ S ₅ |
| | 599.2249 | 1.0 | 1.0 | C ₁₇ H ₄₁ O ₁₂ N ₇ S ₂ |
| | 599.2249 | 1.0 | 6.5 | C ₁₆ H ₃₅ O ₇ N ₁₄ S ₂ |
| | 599.2249 | 1.0 | 19.5 | C ₃₁ H ₃₁ O ₇ N ₆ |
| | 599.2249 | 1.1 | 25.0 | C ₃₀ H ₂₅ O ₂ N ₁₃ |
| | 599.2262 | -1.2 | 24.5 | C ₃₂ H ₂₇ O ₃ N ₁₀ |
| | 599.2262 | -1.2 | 19.0 | C ₃₃ H ₃₃ O ₈ N ₃ |
| | 599.2262 | -1.3 | 6.0 | C ₁₈ H ₃₇ O ₈ N ₁₁ S ₂ |
| | 599.2263 | -1.3 | 0.5 | C ₁₉ H ₄₃ O ₁₃ N ₄ S ₂ |
| | 599.2247 | 1.3 | -2.0 | C ₉ H ₃₇ O ₁₅ N ₁₃ S ₁ |
| | 599.2246 | 1.5 | 3.5 | C ₂₄ H ₄₇ O ₃ N ₄ S ₅ |
| | 599.2264 | -1.5 | 27.5 | C ₄₀ H ₃₁ N ₄ S ₁ |
| | 599.2264 | -1.5 | 14.5 | C ₂₅ H ₃₅ N ₁₂ S ₃ |
| | 599.2264 | -1.6 | 9.0 | C ₂₆ H ₄₁ O ₅ N ₅ S ₃ |
| | 599.2244 | 1.8 | 0.5 | C ₁₆ H ₄₃ O ₆ N ₁₀ S ₄ |
| | 599.2244 | 1.8 | 13.5 | C ₃₁ H ₃₉ O ₆ N ₂ S ₂ |
| | 599.2244 | 1.8 | 19.0 | C ₃₀ H ₃₃ O ₁ N ₉ S ₂ |
| | 599.2244 | 1.9 | 32.0 | C ₄₅ H ₂₉ O ₁ N ₁ |
| | 599.2267 | -2.0 | 12.0 | C ₁₈ H ₂₉ O ₉ N ₁₅ |
| | 599.2267 | -2.0 | 6.5 | C ₁₉ H ₃₅ O ₁₄ N ₈ |

| Mass | Theoretical Mass | Delta [ppm] | RDB | Composition |
|----------|---------------------|----------------|------|--|
| 599.2242 | 599.2242 | 2.1 | 5.0 | C ₂₄ H ₄₁ O ₁₄ N ₁ S ₁ |
| 599.2242 | 599.2242 | 2.1 | 10.5 | C ₂₃ H ₃₅ O ₉ N ₈ S ₁ |
| 599.2242 | 599.2242 | 2.1 | 16.0 | C ₂₂ H ₂₉ O ₄ N ₁₅ S ₁ |
| 599.2269 | 599.2269 | -2.3 | 15.0 | C ₂₆ H ₃₃ O ₆ N ₉ S ₁ |
| 599.2269 | 599.2269 | -2.3 | 9.5 | C ₂₇ H ₃₉ O ₁₁ N ₂ S ₁ |
| 599.2240 | 599.2240 | 2.4 | 7.5 | C ₁₅ H ₃₁ O ₁₂ N ₁₄ |
| 599.2239 | 599.2239 | 2.6 | 13.0 | C ₃₀ H ₄₁ N ₅ S ₄ |
| 599.2271 | 599.2271 | -2.6 | 18.0 | C ₃₄ H ₃₇ O ₃ N ₃ S ₂ |
| 599.2271 | 599.2271 | -2.7 | 5.0 | C ₁₉ H ₄₁ O ₃ N ₁₁ S ₄ |
| 599.2271 | 599.2271 | -2.7 | -0.5 | C ₂₀ H ₄₇ O ₈ N ₄ S ₄ |
| 599.2238 | 599.2238 | 2.9 | 4.5 | C ₂₃ H ₄₃ O ₈ N ₄ S ₃ |
| 599.2237 | 599.2237 | 2.9 | 10.0 | C ₂₂ H ₃₇ O ₃ N ₁₁ S ₃ |
| 599.2237 | 599.2237 | 3.0 | 23.0 | C ₃₇ H ₃₃ O ₃ N ₃ S ₁ |
| 599.2273 | 599.2273 | -3.0 | 8.0 | C ₂₇ H ₄₅ N ₅ S ₅ |
| 599.2274 | 599.2274 | -3.2 | 2.5 | C ₁₂ H ₃₅ O ₁₂ N ₁₄ S ₁ |
| 599.2236 | 599.2236 | 3.2 | 1.5 | C ₁₅ H ₃₉ O ₁₁ N ₁₀ S ₂ |
| 599.2235 | 599.2235 | 3.3 | 14.5 | C ₃₀ H ₃₅ O ₁₁ N ₂ |
| 599.2235 | 599.2235 | 3.3 | 20.0 | C ₂₉ H ₂₉ O ₆ N ₉ |
| 599.2276 | 599.2276 | -3.4 | 24.0 | C ₃₄ H ₂₉ O ₄ N ₇ |
| 599.2276 | 599.2276 | -3.4 | 18.5 | C ₃₅ H ₃₅ O ₉ |
| 599.2276 | 599.2276 | -3.5 | 11.0 | C ₁₉ H ₃₃ O ₄ N ₁₅ S ₂ |
| 599.2276 | 599.2276 | -3.5 | 5.5 | C ₂₀ H ₃₉ O ₉ N ₈ S ₂ |
| 599.2276 | 599.2276 | -3.5 | 0.0 | C ₂₁ H ₄₅ O ₁₄ N ₁ S ₂ |
| 599.2233 | 599.2233 | 3.7 | -1.5 | C ₂₃ H ₅₁ O ₇ S ₅ |
| 599.2233 | 599.2233 | 3.7 | 4.0 | C ₂₂ H ₄₅ O ₂ N ₇ S ₅ |
| 599.2277 | 599.2277 | -3.7 | 27.0 | C ₄₂ H ₃₃ O ₁ N ₁ S ₁ |
| 599.2278 | 599.2278 | -3.8 | 14.0 | C ₂₇ H ₃₇ O ₁ N ₉ S ₃ |
| 599.2278 | 599.2278 | -3.8 | 8.5 | C ₂₈ H ₄₃ O ₆ N ₂ S ₃ |
| 599.2231 | 599.2231 | 4.0 | 1.0 | C ₁₄ H ₄₁ O ₅ N ₁₃ S ₄ |
| 599.2231 | 599.2231 | 4.1 | 14.0 | C ₂₉ H ₃₇ O ₅ N ₅ S ₂ |
| 599.2231 | 599.2231 | 4.1 | 19.5 | C ₂₈ H ₃₁ N ₁₂ S ₂ |
| 599.2230 | 599.2230 | 4.1 | 32.5 | C ₄₃ H ₂₇ N ₄ |
| 599.2281 | 599.2281 | -4.3 | 11.5 | C ₂₀ H ₃₁ O ₁₀ N ₁₂ |
| 599.2281 | 599.2281 | -4.3 | 6.0 | C ₂₁ H ₃₇ O ₁₅ N ₅ |
| 599.2229 | 599.2229 | 4.4 | 5.5 | C ₂₂ H ₃₉ O ₁₃ N ₄ S ₁ |
| 599.2229 | 599.2229 | 4.4 | 11.0 | C ₂₁ H ₃₃ O ₈ N ₁₁ S ₁ |
| 599.2282 | 599.2282 | -4.6 | 20.0 | C ₂₇ H ₂₉ O ₂ N ₁₃ S ₁ |
| 599.2282 | 599.2282 | -4.6 | 14.5 | C ₂₈ H ₃₅ O ₇ N ₆ S ₁ |
| 599.2283 | 599.2283 | -4.6 | 1.5 | C ₁₃ H ₃₉ O ₇ N ₁₄ S ₃ |
| 599.2226 | 599.2226 | 4.9 | 8.0 | C ₂₉ H ₄₅ O ₄ N ₁ S ₄ |
| 599.2284 | 599.2284 | -4.9 | 17.5 | C ₃₆ H ₃₉ O ₄ S ₂ |
| 599.2285 | 599.2285 | -4.9 | 4.5 | C ₂₁ H ₄₃ O ₄ N ₈ S ₄ |
| 599.2285 | 599.2285 | -5.0 | -1.0 | C ₂₂ H ₄₉ O ₉ N ₁ S ₄ |