D:\Data\...\Apotteri_HDX 10/12/17 19:11:36 1 ug/ul in H2O/ACN 3:1 + 0.05% TFA RT: 0.00 - 22.01 Apotteri HDX#601 RT: 3.86 T: FTMS + p ESI Full ms [100.00-1500.00] NL: 1.69E8 3.09 3.11 m/z = 457.00000 - 458.00000100 7.31 7<u>.3</u>4 Base Peak m/z= 3.06 3.14 Intensity Relative Delta Composition 6.38 100.00000-1500.00000 F: FTMS + p (mqq) 9.77 1.66 50⁻ ESI Full ms [100.00-1500.00] MS 457.39310 3786912.8 100.00 1.42 C 24 H 43 ²H 4 O 3 N 5 20.25 -1.97 C₂₄ H₄₅ ²H₃ O₃ N₅ Apotteri_HDX Relative Abundance 4.80 C24 H41 2H5 O3 N5 NL: 4.03E6 3.86 Base Peak m/z= 457.38916-457.39374 F: FTMS + p ESI Full ms [100.00-1500.00] MS Apotteri_HDX NL: 8.22E6 3.84 Base Peak m/z= 229.70163-229.70393 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Apotteri_HDX 0-NL: 1.62E5 3.86 100-Base Peak m/z= 572.38773-572.39345 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Apotteri_HDX 10 15 20 Time (min) Apotteri_HDX #601 RT: 3.86 AV: 1 NL: 2.18E7 Apotteri_HDX #601 RT: 3.86 AV: 1 NL: 3.71E6 T: FTMS + p ESI Full ms [100.00-1500.00] T: FTMS + p ESI Full ms [100.00-1500.00] 457.39310 157.08432 90-90-462.41339 80-80-70-70-Relative Abundance Relative Abundance 60 60-50 50-235.00119 40 40-30-30-276.02798 459.39853 464.42026 20 457.39310 20-586.31232 10 10 442.90945 449.95096 454.37112

200

400

600

800

m/z

1000

1200

1400

440

445

450

m/z

455

460

465