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#1031 RT: 6.45 T: FTMS + p ESI Full ms [100.00-1500.00] 3.09 3.11 NL: 1.69E8 m/z = 511.00000 - 512.00000100 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 511.42621 5355508.5 100.00 -1.20 C 27 H 47 ²H 4 O 3 N 6 20.25 1.83 C₂₇ H₄₅ ²H₅ O₃ N₆ Apotteri_HDX Relative Abundance -4.23 C27 H49 2H3 O3 N6 6.44 6.45 NL: 5.36E6 4.85 C₂₇ H₄₃ ²H₆ O₃ N₆ Base Peak m/z= 511.42172-511.42684 F: FTMS + p ESI Full ms [100.00-1500.00] MS Apotteri_HDX -NL: 1.13E7 6.44 Base Peak m/z= 256.71791-256.72047 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Apotteri_HDX 0 NL: 8.64E4 6.43 100 Base Peak m/z= 626.42029-626.42655 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Apotteri_HDX 10 15 20 Time (min) Apotteri_HDX #1031 RT: 6.45 AV: 1 NL: 2.74E7 Apotteri_HDX #1031 RT: 6.45 AV: 1 NL: 5.35E6 T: FTMS + p ESI Full ms [100.00-1500.00] T: FTMS + p ESI Full ms [100.00-1500.00] 511.42621 157.08424 90-90-80-80-70-70-Relative Abundance Relative Abundance 60 60-532.44141 50-50-367.32123 256.71964 40-512.42987 30-30-20 20-640.34497 10 10 500.93518 513.43311 509.39636 501.93915

200

400

600

800

m/z

1000

1200

1400

505

500

510

m/z

516.44708 518.94666

520

515