D:\Data\...\Pluctuosa HDX 10/12/17 18:38:24 1 ug/ul in H2O/ACN 3:1 + 0.05% TFA RT: 0.00 - 22.01 Pluctuosa HDX#602 RT: 3.86 T: FTMS + p ESI Full ms [100.00-1500.00] 6.66 6.67 NL: 1.25E8 m/z = 457.00000 - 458.00000100 6.70 Base Peak m/z= Intensity Relative Delta Composition 3.02 100.00000-1500.00000 F: FTMS + p (mqq) 6.74 50⁻ 1.06 ESI Full ms [100.00-1500.00] MS 457.39145 5620816.0 100.00 1.20 C₂₄ H₄₁ ²H₅ O₃ N₅ 20.24 7.41 -2.19 C₂₄ H₄₃ ²H₄ O₃ N₅ Pluctuosa HDX Relative Abundance 4.58 C24 H39 2H6 O3 N5 NL: 7.03E6 3.86 Base Peak m/z= 457.38916-457.39374 F: FTMS + p ESI Full ms [100.00-1500.00] MS Pluctuosa HDX _ NL: 1.35E7 3.86 Base Peak m/z= 229.70163-229.70393 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Pluctuosa HDX 0-NL: 2.92E5 3.87 100-Base Peak m/z= 572.38773-572.39345 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Pluctuosa HDX 10 15 20 5 Time (min) Pluctuosa_HDX #602 RT: 3.86 AV: 1 NL: 2.04E7 Pluctuosa_HDX #602 RT: 3.86 AV: 1 NL: 5.44E6 T: FTMS + p ESI Full ms [100.00-1500.00] T: FTMS + p ESI Full ms [100.00-1500.00] 457.39145 157.08377 90-90-80-80-70-70-Relative Abundance Relative Abundance 229.70255 60 60-50 50-40-30-457.39145 30-459.39828 276.02701 20 20-586.31024 10 10 461.93973 465.92404 454.36926

200

400

600

800

m/z

1000

1200

1400

442.90775 446.88873

445

440

450

m/z

455

460

465