D:\Data\...\Eagrestis HDX 10/12/17 18:05:07 1 ug/ul in H2O/ACN 3:1 + 0.05% TFA RT: 0.00 - 22.01 Eagrestis HDX#613 RT: 3.87 T: FTMS + p ESI Full ms [100.00-1500.00] NL: 1.58E8 4.03 m/z = 457.00000 - 458.00000100 Base Peak m/z= Intensity Relative Delta Composition 6.67 6.69 3.01 100.00000-1500.00000 F: FTMS + p (mqq) 1.18 50⁻ ESI Full ms [100.00-1500.00] MS 457.39276 6963927.0 100.00 0.68 C₂₄ H₄₃ ²H₄ O₃ N₅ 20.26 6.77 Eagrestis_HDX -2.70 C₂₄ H₄₅ ²H₃ O₃ N₅ Relative Abundance 4.07 C24 H41 2H5 O3 N5 NL: 6.96E6 3.87 Base Peak m/z= 3.85 457.38916-457.39374 F: FTMS + p ESI Full ms [100.00-1500.00] MS Eagrestis_HDX NL: 1.23E7 3.87 Base Peak m/z= 229.70163-229.70393 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Eagrestis_HDX 0 NL: 2.58E5 3.87 100 Base Peak m/z= 3.85 572.38773-572.39345 F: FTMS + p 50-ESI Full ms [100.00-1500.00] MS Eagrestis_HDX 20 10 15 5 Time (min) Eagrestis_HDX #613 RT: 3.87 AV: 1 NL: 2.18E7 Eagrestis_HDX #613 RT: 3.87 AV: 1 NL: 6.72E6 T: FTMS + p ESI Full ms [100.00-1500.00] T: FTMS + p ESI Full ms [100.00-1500.00] 457.39276 157.08421 90-90-80-80-70-70-Relative Abundance Relative Abundance 60 60-229.70322 50-50-40-457.39276 30-30-459.39944 586.31195 276.02780 20 20-10 10 462.41306

200

400

600

800

m/z

1000

1200

1400

465.92511

465

460

454.37091

455

450

m/z

442.90942 448.20013

445

440