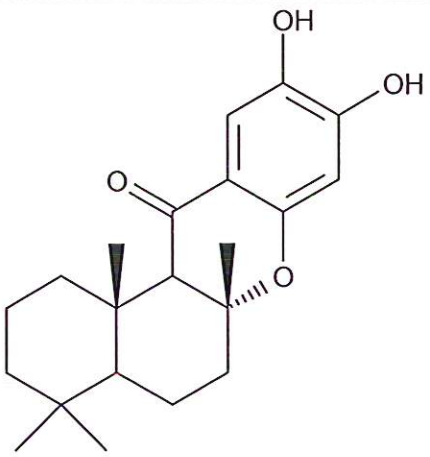
HARBOR BRANCH

FLORIDA ATLANTIC UNIVERSITY

| HBOI-32 |  |
|---|---|
| PETROSIA QUINOL | |
| $C_{21}H_{28}O_4$ | 344.45 |
| Petrosiidae | |
| | |

☑ hplc (trace attached)

Method: Vydac C18 Protein and Peptide, 4.6 x 250mm, 10µ
flow 1 ml/min, detection: PDA: UV (extracted at 220 nm); ELSD (green dotted)
A: $H_2O$:$CH_3CN$ (95:5,v/v), B: $CH_3CN$
t=0 min A:B (90:10,v/v), t=20 min (100%B) , t=28 min (100%B)

☑ LC-MS (spectrum attached)

Method: Vydac C18 Protein and Peptide, 2.1x150 mm, flow 0.2 ml/min
A: $H_2O$ (0.1% formic acid), B:$CH_3CN$ (0.1% formic acid)
t= 0 min A:B (90:10, v/v), t=15 min (100%B), t=21 min (100%B), t=22.1 min A:B(90:10, v/v)
using a linear gradient

☑ $^1H$ (600 MHz) ☐ $CDCL_3$ ☑ $CD_3OD$ (Methanol-$d_4$) ☐ $CDCl_3/CD_3OD$

☑ $^{13}C$ (150 MHz) ☐ $CDCL_3$ ☑ $CD_3OD$ (Methanol-$d_4$) ☐ $CDCl_3/CD_3OD$

☑ solubility ☐ $CHCl_3$/MeOH (9:1) ☑ MeOH ☐ DMSO

☑ estimated purity _>90_%

☑ sample weight _20.6_mg

For further information contact:
Amy E. Wright, PhD, HBOI@FAU, 5600 US 1, North, Fort Pierce, FL 34946
awrigh33@hboi.fau.edu, 772-242-2459

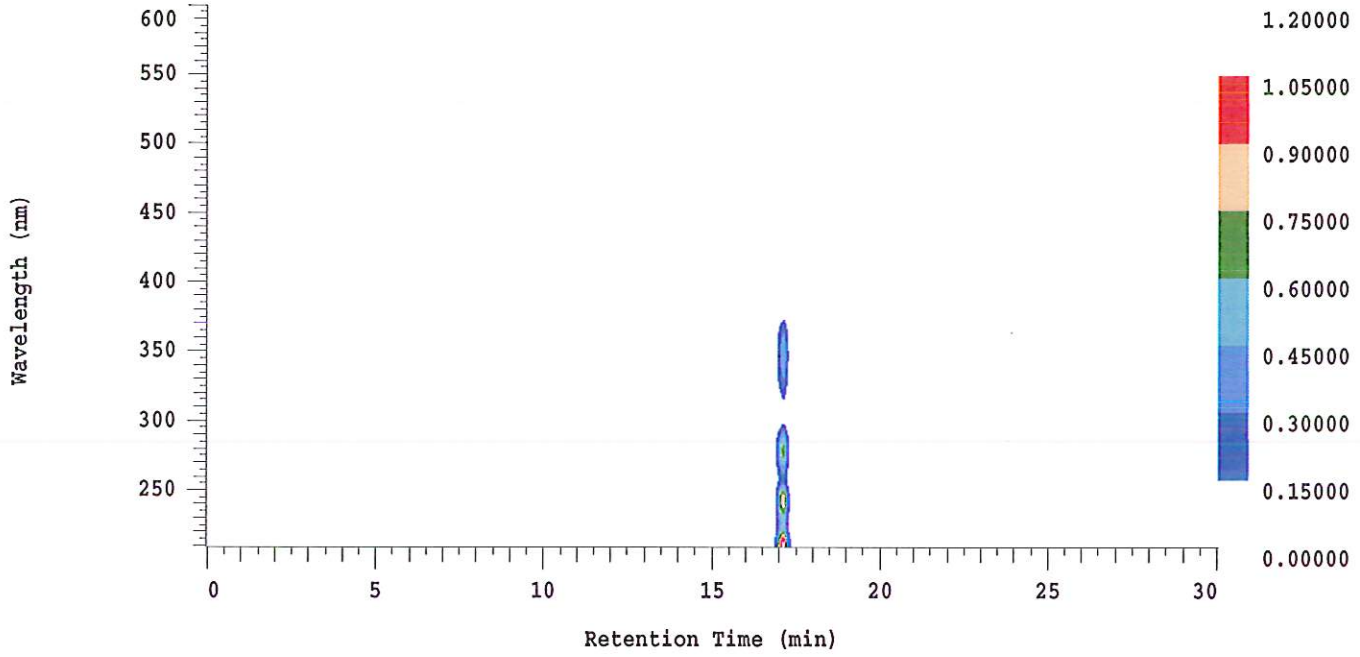
Date: 1/28/13

# D-2000 Elite HPLC System Manager Report

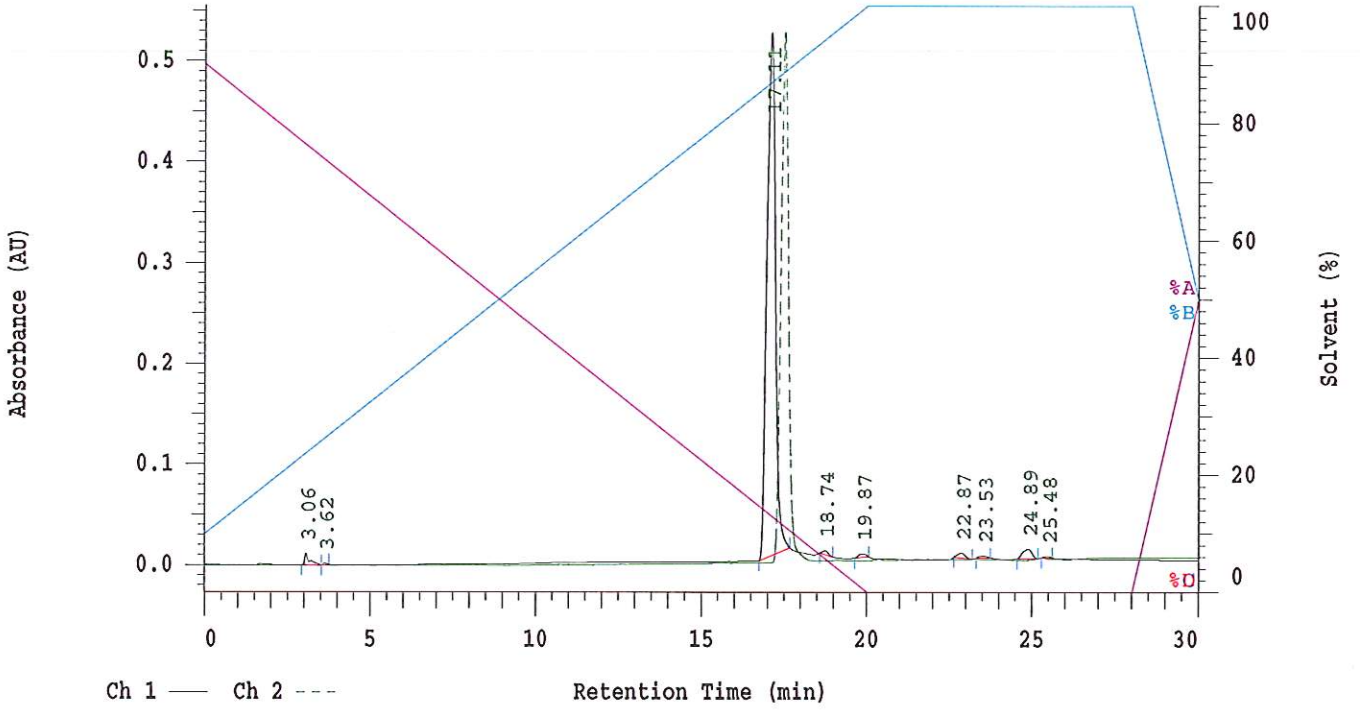
Analyzed: 01/23/2013 06:16 PM Reported: 01/24/2013 10:41 AM

Sample Name: HBOI-32

Sample Description: HBOI-32




Channel 1 Chrom Type: Fixed WL Chromatogram, 230 nm



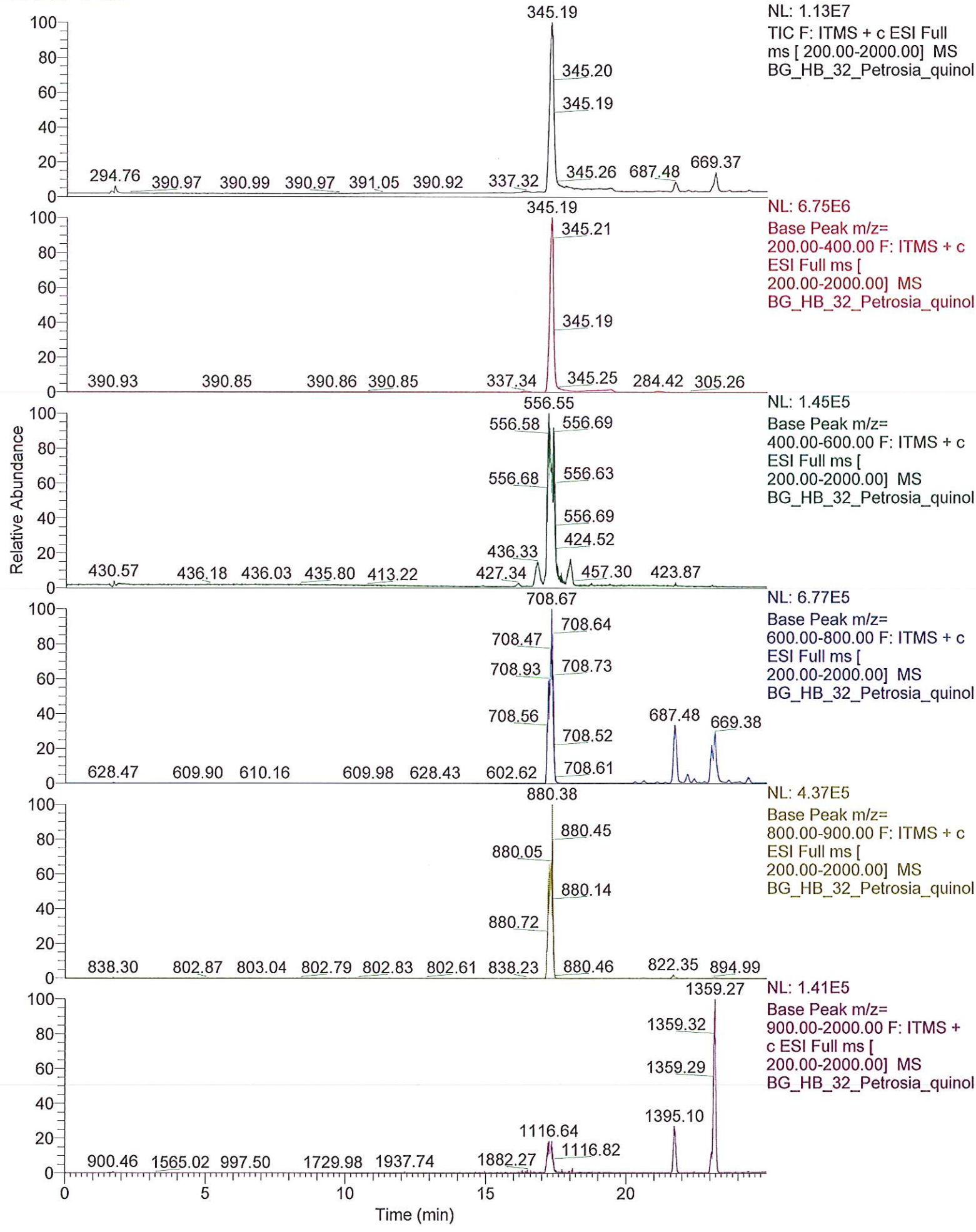

Acquisition Method: autosamp_30mn_UV220_wELSD

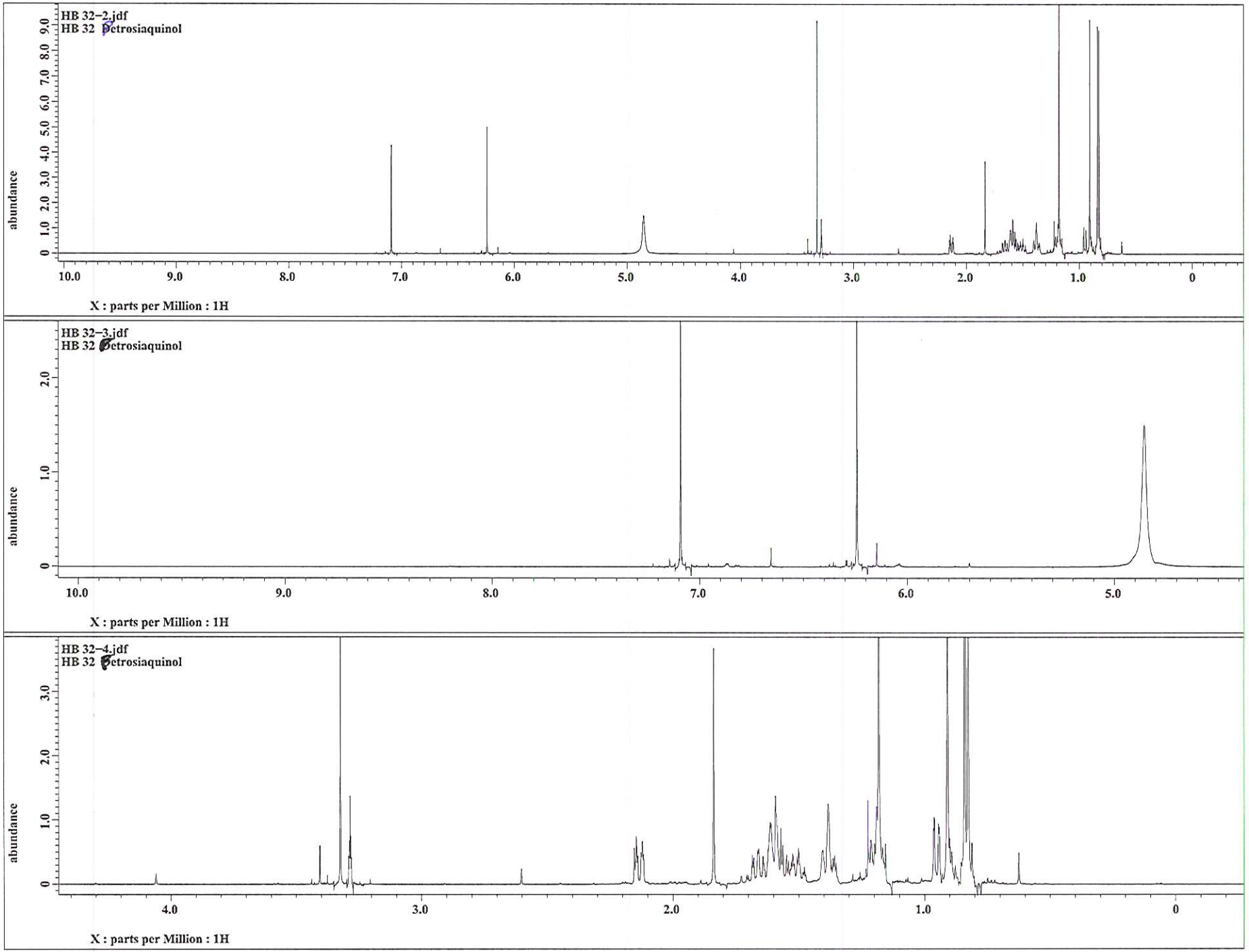
Column Type: Vydac C18

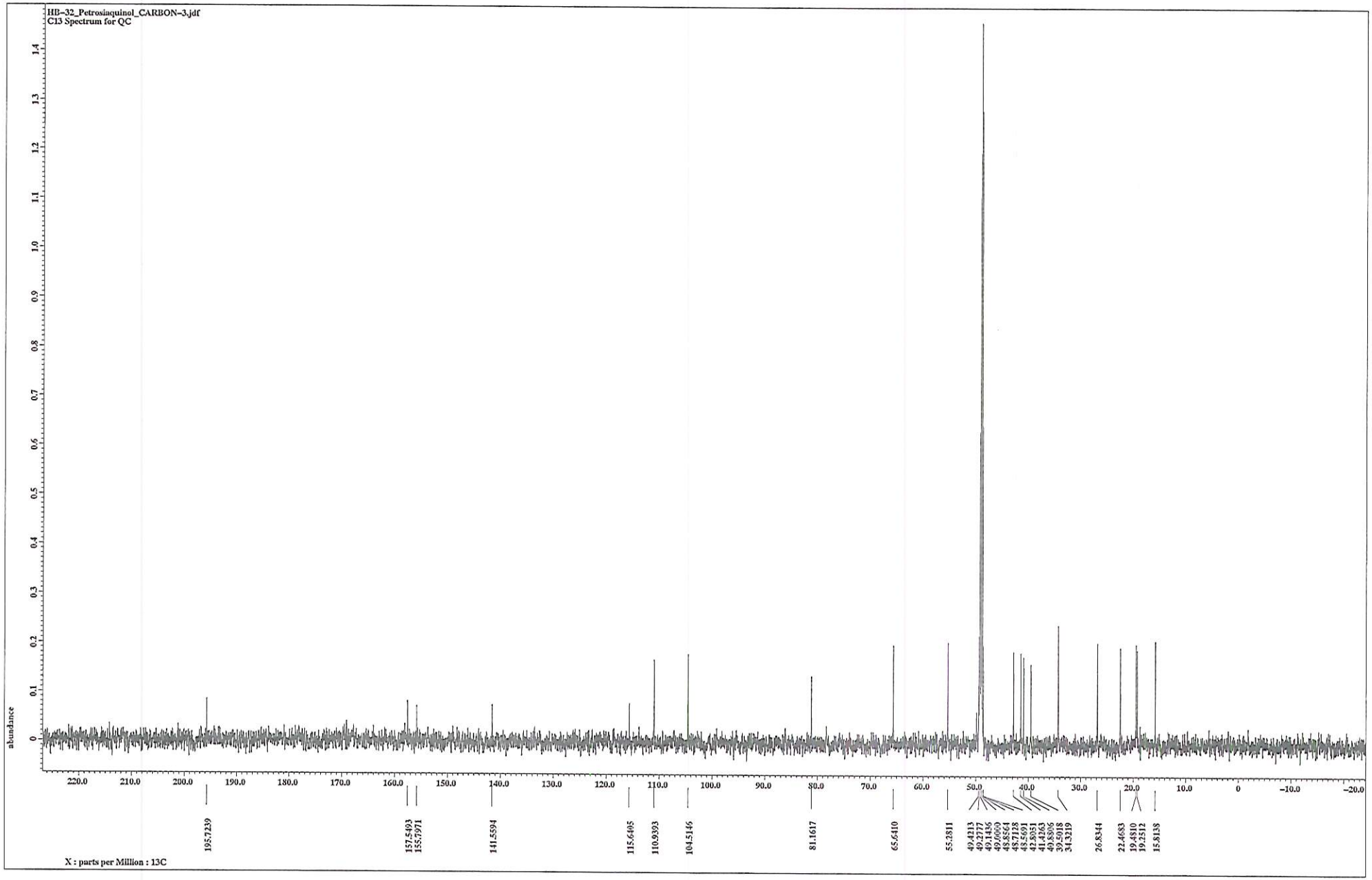
Pump A Solvent A: H2O/5% ACN Pump A Solvent B: ACN

Method Description:

RT: 0.00 - 24.99


345.19
345.20
345.19
294.76
390.97
390.99
390.97
391.05
390.92
337.32
345.26
687.48
669.37
NL: 1.13E7
TIC F: ITMS + c ESI Full ms [ 200.00-2000.00] MS BG_HB_32_Petrosia_quinol
345.19
345.21
345.19
390.93
390.85
390.86
390.85
337.34
345.25
284.42
305.26
NL: 6.75E6
Base Peak m/z= 200.00-400.00 F: ITMS + c ESI Full ms [ 200.00-2000.00] MS BG_HB_32_Petrosia_quinol
556.55
556.58
556.69
556.68
556.63
556.69
424.52
436.33
430.57
436.18
436.03
435.80
413.22
427.34
457.30
423.87
NL: 1.45E5
Base Peak m/z= 400.00-600.00 F: ITMS + c ESI Full ms [ 200.00-2000.00] MS BG_HB_32_Petrosia_quinol
Relative Abundance
708.67
708.64
708.47
708.93
708.73
708.56
687.48
669.38
708.52
628.47
609.90
610.16
609.98
628.43
602.62
708.61
NL: 6.77E5
Base Peak m/z= 600.00-800.00 F: ITMS + c ESI Full ms [ 200.00-2000.00] MS BG_HB_32_Petrosia_quinol
880.38
880.45
880.05
880.14
880.72
838.30
802.87
803.04
802.79
802.83
802.61
838.23
880.46
822.35
894.99
NL: 4.37E5
Base Peak m/z= 800.00-900.00 F: ITMS + c ESI Full ms [ 200.00-2000.00] MS BG_HB_32_Petrosia_quinol
1359.27
1359.32
1359.29
1395.10
1116.64
1116.82
900.46
1565.02
997.50
1729.98
1937.74
1882.27
NL: 1.41E5
Base Peak m/z= 900.00-2000.00 F: ITMS + c ESI Full ms [ 200.00-2000.00] MS BG_HB_32_Petrosia_quinol
0
5
10
15
20
Time (min)


HB 32-2.jdf
HB 32 petrosiaquinol
abundance
X : parts per Million : 1H
HB 32-3.jdf
HB 32 petrosiaquinol
abundance
X : parts per Million : 1H
HB 32-4.jdf
HB 32 petrosiaquinol
abundance
X : parts per Million : 1H


HB-32_Petrosiaquinol_CARBON-3.jdf
C13 Spectrum for QC
abundance
X : parts per Million : 13C
195.7239
157.5493
155.7971
141.5594
115.6405
110.9393
104.5146
81.1617
65.6410
55.2811
49.4213
49.2777
49.1436
49.0060
48.8554
48.7128
48.5691
42.8051
41.4263
40.8895
39.5018
34.3219
26.8344
22.4683
19.4810
19.2512
15.8138