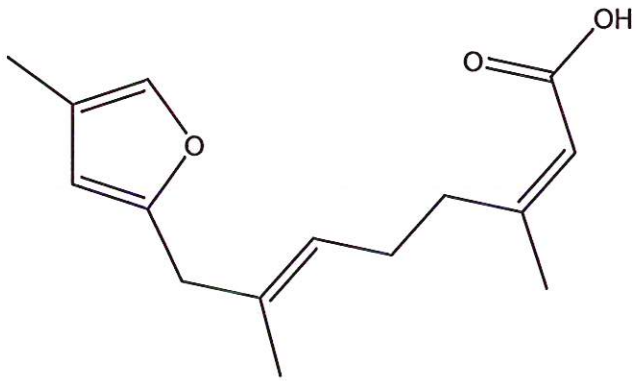
HARBOR BRANCH
FLORIDA ATLANTIC UNIVERSITY

HBOI-353	
MCOO1-38-4 FURAN	
$C_{15}H_{20}O_3$	248.32
Poecilosclerida	

☑ isolation scheme (Visio)

☑ 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, black); 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 _19.0_mg

For further information contact:
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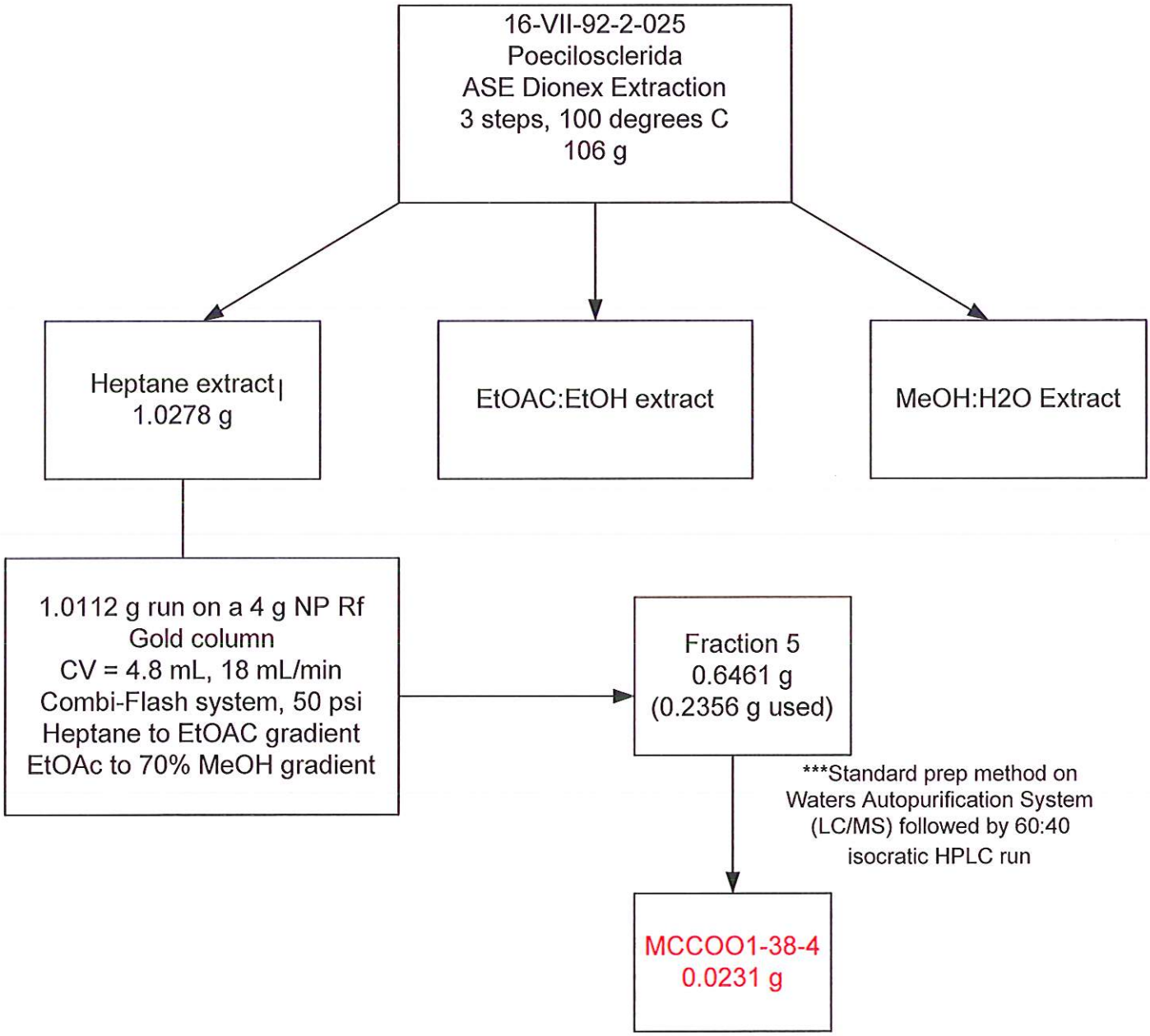
awrigh33@hboi.fau.edu, 772-242-2459

Date: 1/28/13



Combi-Flash
A:heptane, B: EtoAc, C: MeOH
t=0 min (100%A), t=1.5 min (100% A), t=11.5min (100% B), t=13 min (100% B), t= 17 min B:C (30:70)

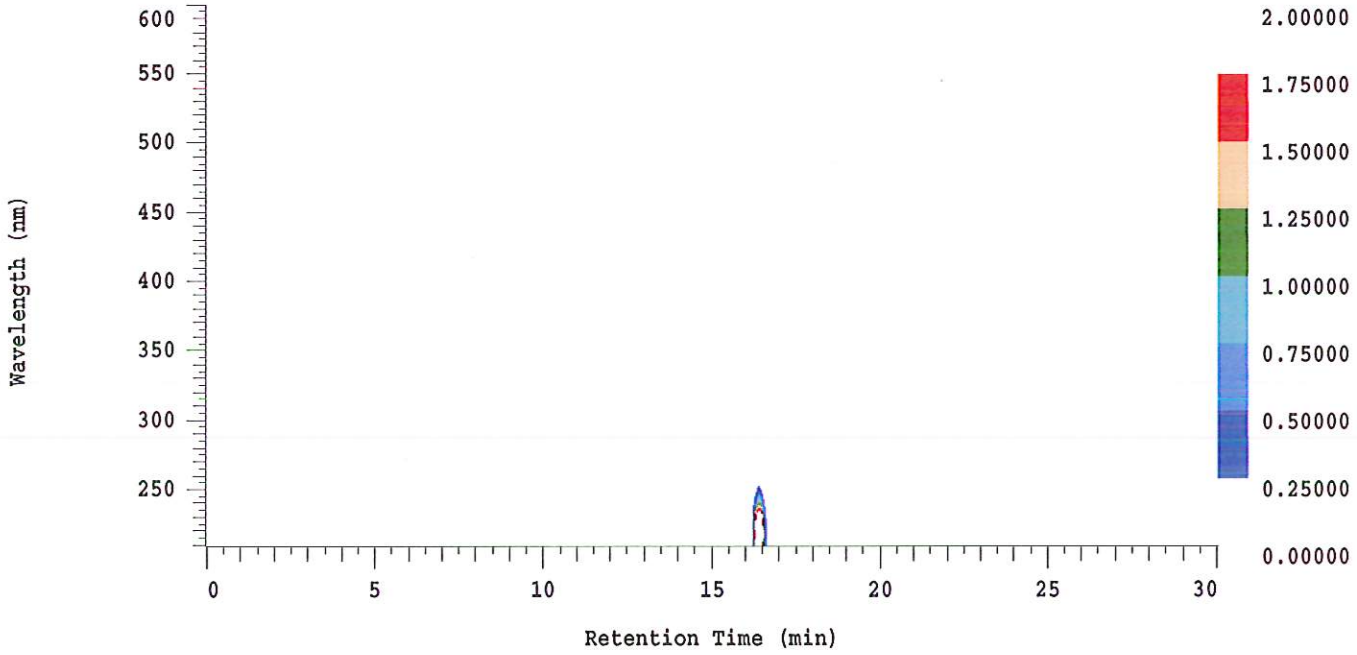
LC/MS:
A: H_2O:CH_3CN (95:5) - 0.1% TFA B: CH_3CN - 0.1% TFA
t=0 min A:B (95:5), t=20 min (100% B), t=23 min (100%B)

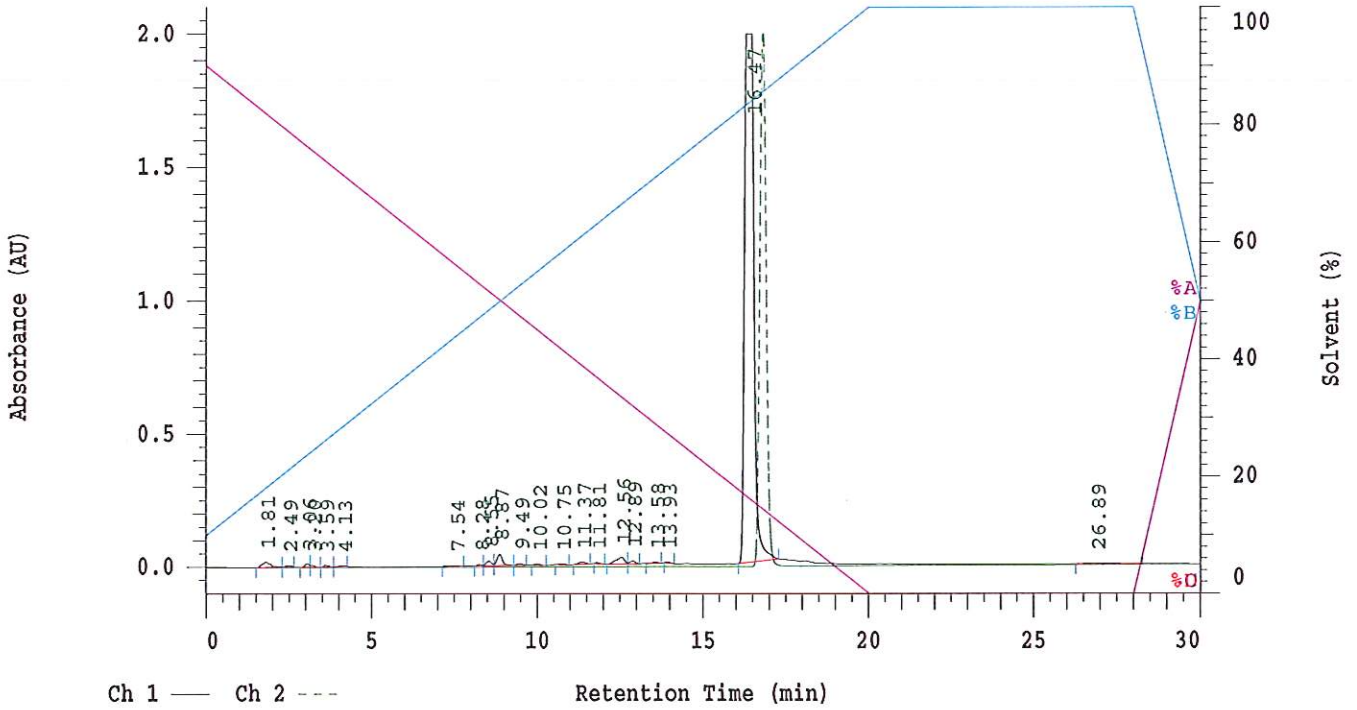
D-2000 Elite HPLC System Manager Report

Analyzed: 01/24/2013 10:52 AM Reported: 01/24/2013 11:26 AM

Sample Name: HBOI-353

Sample Description: HBOI-353





Ch 1 —— Ch 2 ---

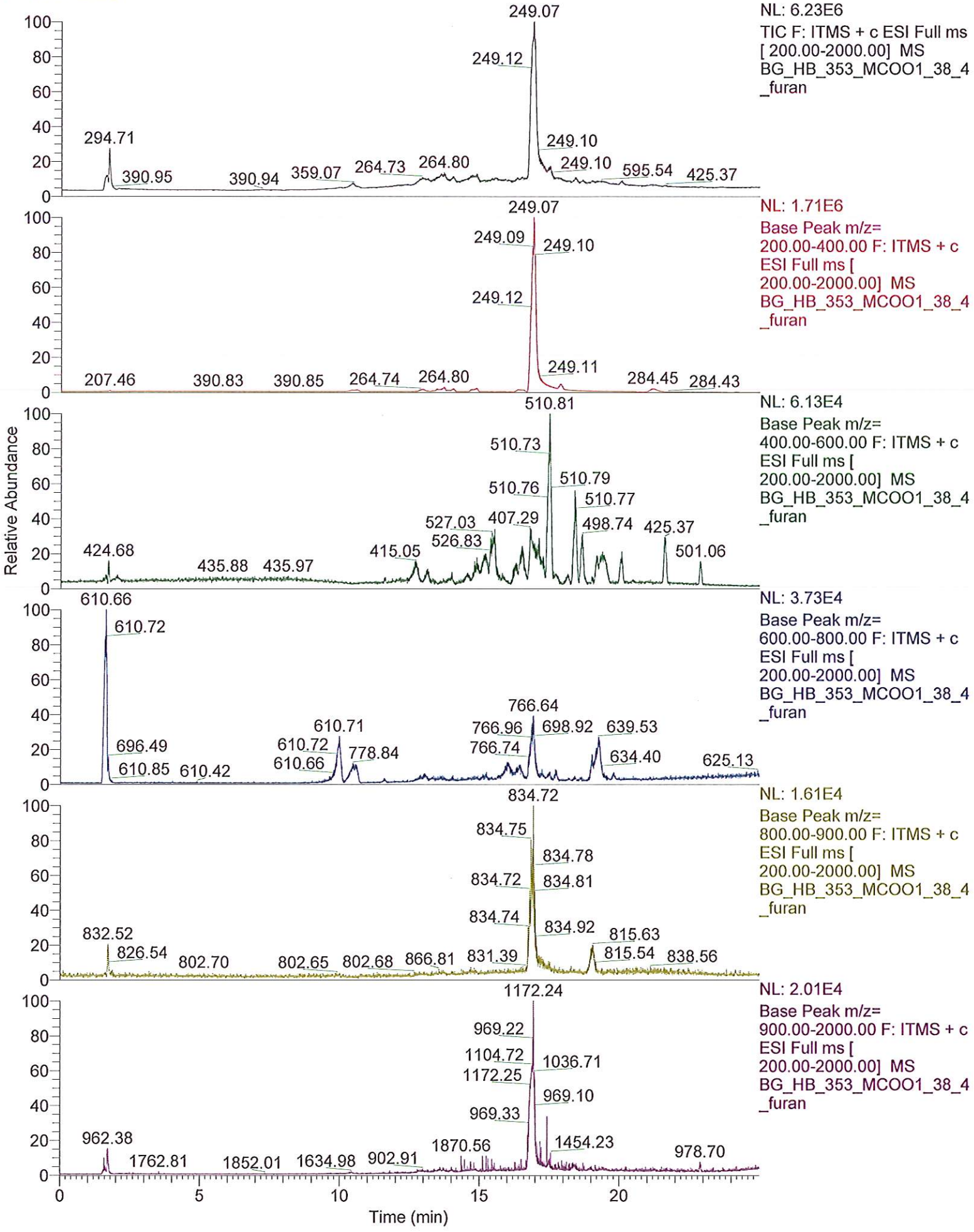
Acquisition Method: autosamp_30mn_UV220_wELSD

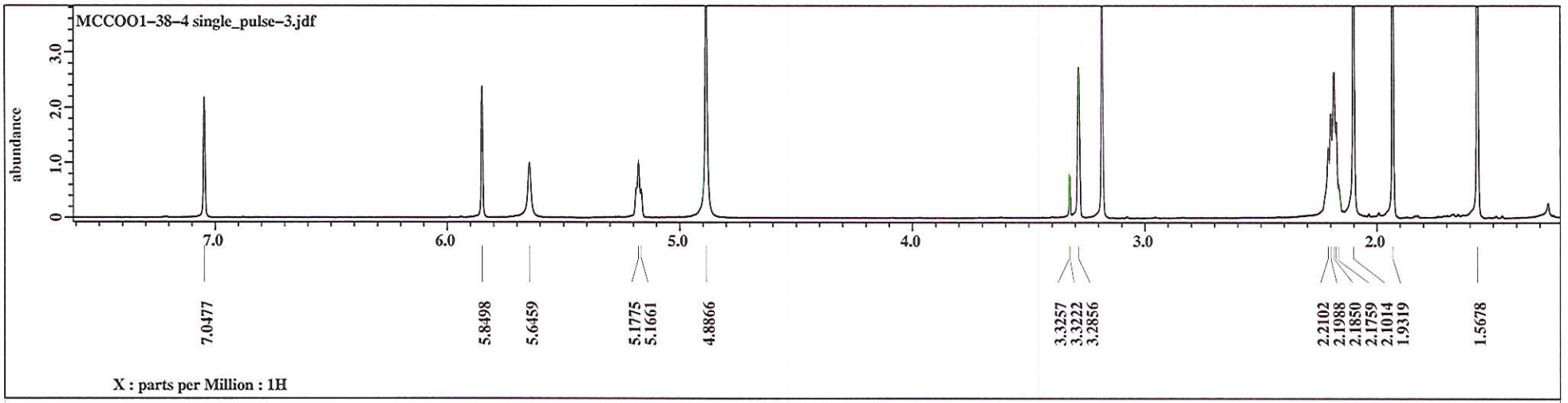
Column Type: Vydac C18

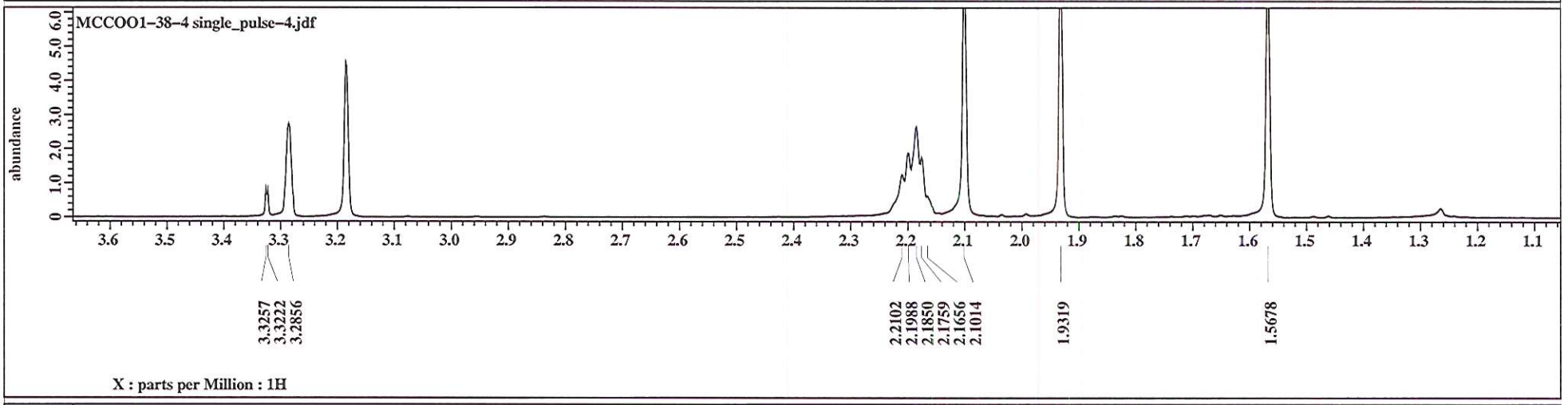
Pump A Solvent A: H2O/5% ACN Pump A Solvent B: ACN

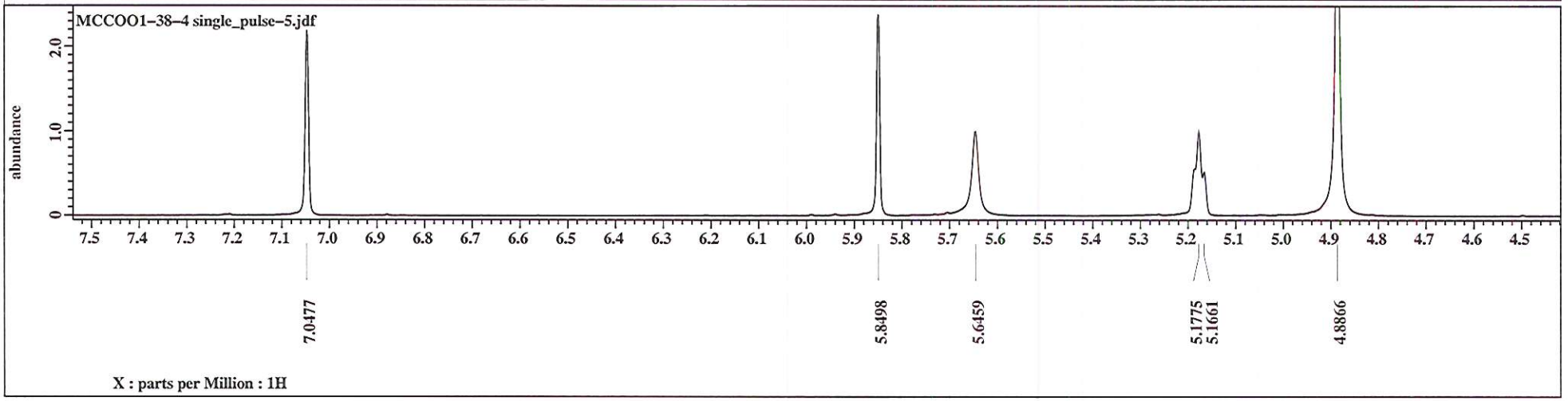
Method Description:

RT: 0.00 - 24.99

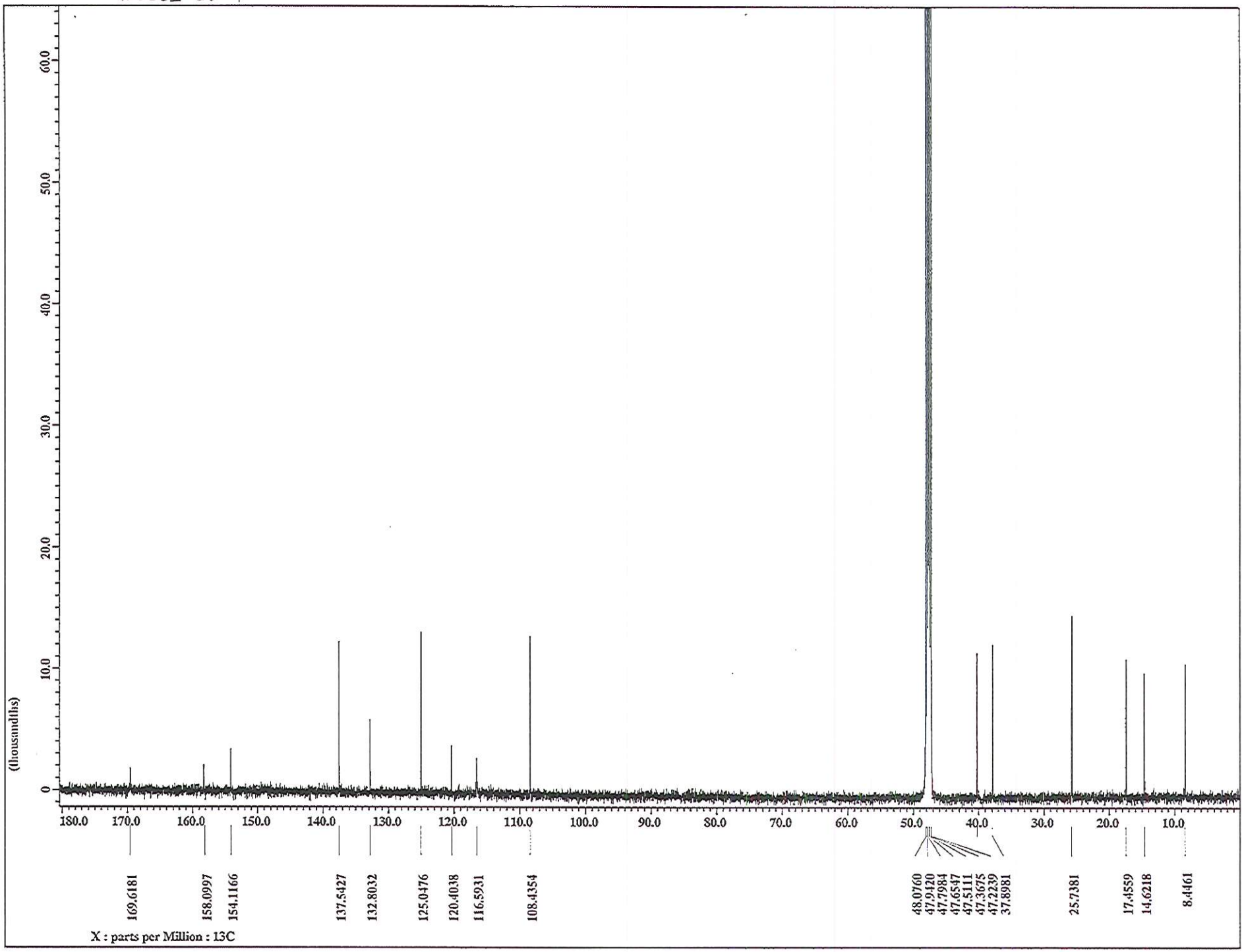

NL: 6.23E6
TIC F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_353_MCOO1_38_4 _furan
249.07
249.12
294.71
249.10
390.95
390.94
359.07
264.73
264.80
249.10
595.54
425.37
NL: 1.71E6
Base Peak m/z= 200.00-400.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_353_MCOO1_38_4 _furan
249.07
249.09
249.10
249.12
249.11
207.46
390.83
390.85
264.74
264.80
284.45
284.43
NL: 6.13E4
Base Peak m/z= 400.00-600.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_353_MCOO1_38_4 _furan
510.81
510.73
510.76
510.79
510.77
527.03
407.29
498.74
425.37
526.83
424.68
415.05
501.06
435.88
435.97
NL: 3.73E4
Base Peak m/z= 600.00-800.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_353_MCOO1_38_4 _furan
610.66
610.72
766.64
610.71
766.96
698.92
639.53
696.49
610.72
778.84
766.74
634.40
625.13
610.85
610.42
610.66
NL: 1.61E4
Base Peak m/z= 800.00-900.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_353_MCOO1_38_4 _furan
834.72
834.75
834.78
834.72
834.81
834.74
834.92
815.63
832.52
826.54
815.54
838.56
802.70
802.65
802.68
866.81
831.39
NL: 2.01E4
Base Peak m/z= 900.00-2000.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_353_MCOO1_38_4 _furan
1172.24
969.22
1104.72
1036.71
1172.25
969.10
969.33
962.38
1870.56
1454.23
978.70
1762.81
1852.01
1634.98
902.91
Relative Abundance
Time (min)
0
5
10
15
20


MCCOO1-38-4 single_pulse-3.jdf
abundance
7.0477
5.8498
5.6459
5.1775
5.1661
4.8866
3.3257
3.3222
3.2856
2.2102
2.1988
2.1850
2.1759
2.1014
1.9319
1.5678
X : parts per Million : 1H


MCCOO1-38-4 single_pulse-4.jdf
abundance
3.3257
3.3222
3.2856
2.2102
2.1988
2.1850
2.1759
2.1656
2.1014
1.9319
1.5678
X : parts per Million : 1H


MCCOO1-38-4 single_pulse-5.jdf
abundance
7.0477
5.8498
5.6459
5.1775
5.1661
4.8866
X : parts per Million : 1H

MCC001-38-4


(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
169.6181
158.0997
154.1166
137.5427
132.8032
125.0476
120.4038
116.5931
108.4354
48.0760
47.9420
47.7984
47.6547
47.5111
47.3675
47.2239
37.8981
25.7381
17.4559
14.6218
8.4461
X : parts per Million : 13C