

## Supplementary Data

Synthesis and Biological Evaluation of Indole-based, Anti-cancer Agents Inspired by the Vascular Disrupting Agent 2-(3'-Hydroxy-4'-methoxyphenyl)-3-(3'',4'',5''-trimethoxybenzoyl)-6-methoxyindole (OXi8006)

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\*Corresponding Author: Kevin G. Pinney

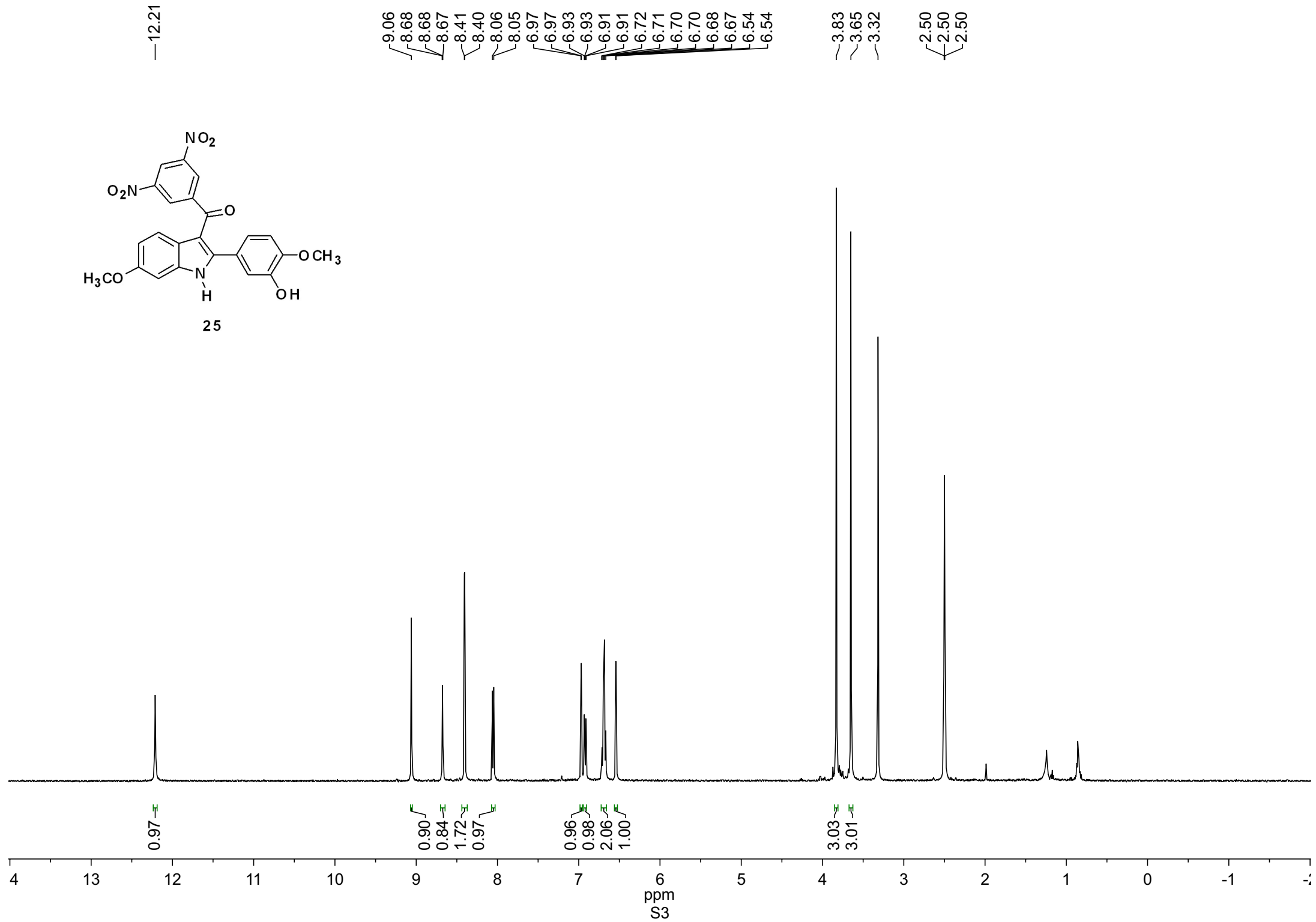
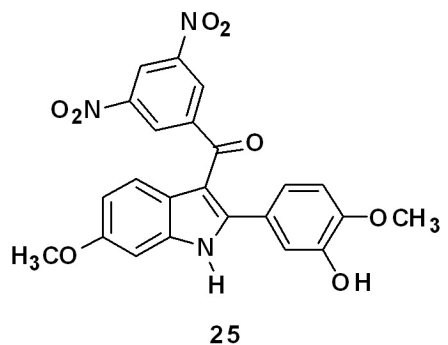
Telephone: 1-254-710-4117

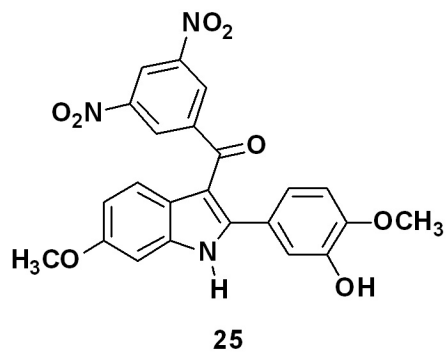
Fax: 1-254-710-4272

Email: [Kevin.Pinney@baylor.edu](mailto:Kevin.Pinney@baylor.edu)

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— 186.67

— 156.84

148.23

147.08

146.68

146.13

142.76

136.72

128.48

123.26

121.75

121.75

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111.73

111.14

— 95.02

55.67

55.34

40.02

39.85

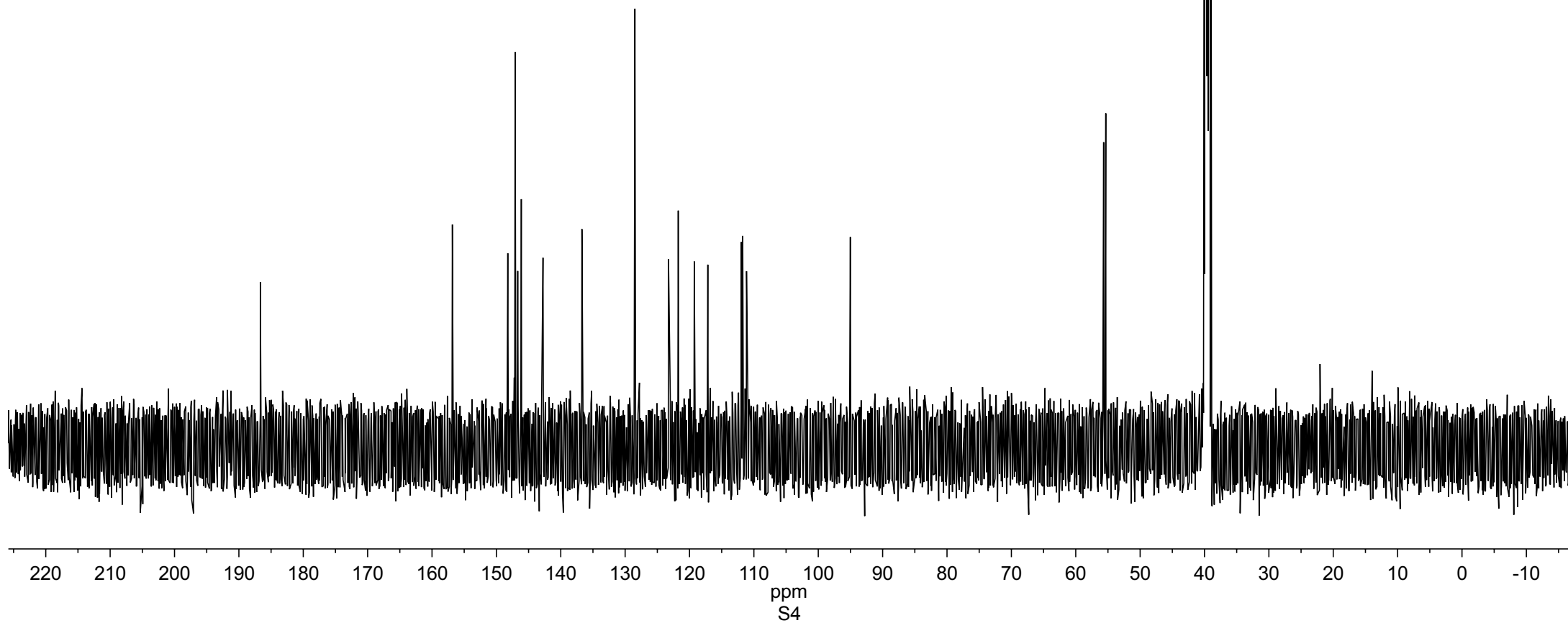
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39.52

39.35

39.19

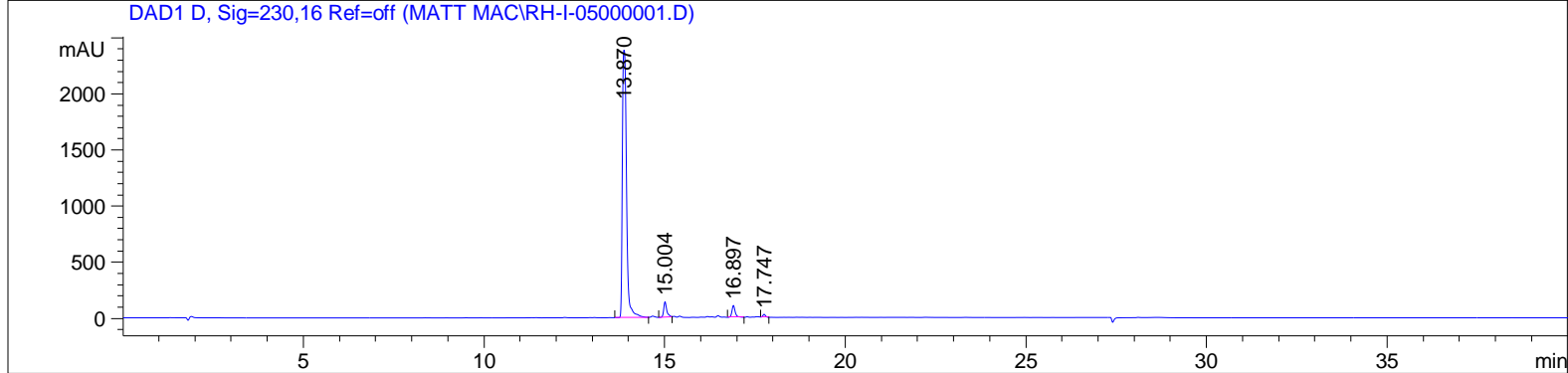
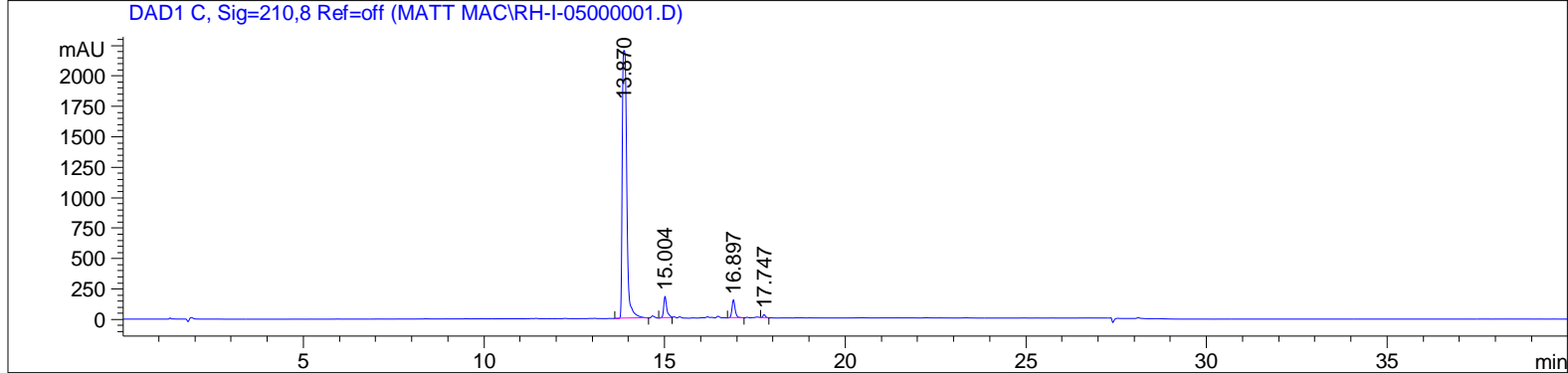
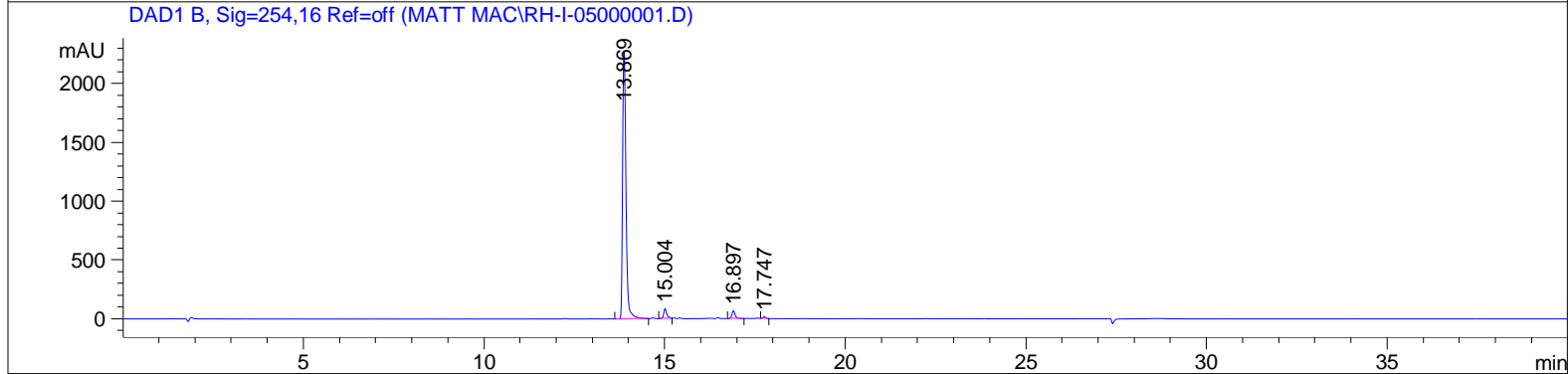
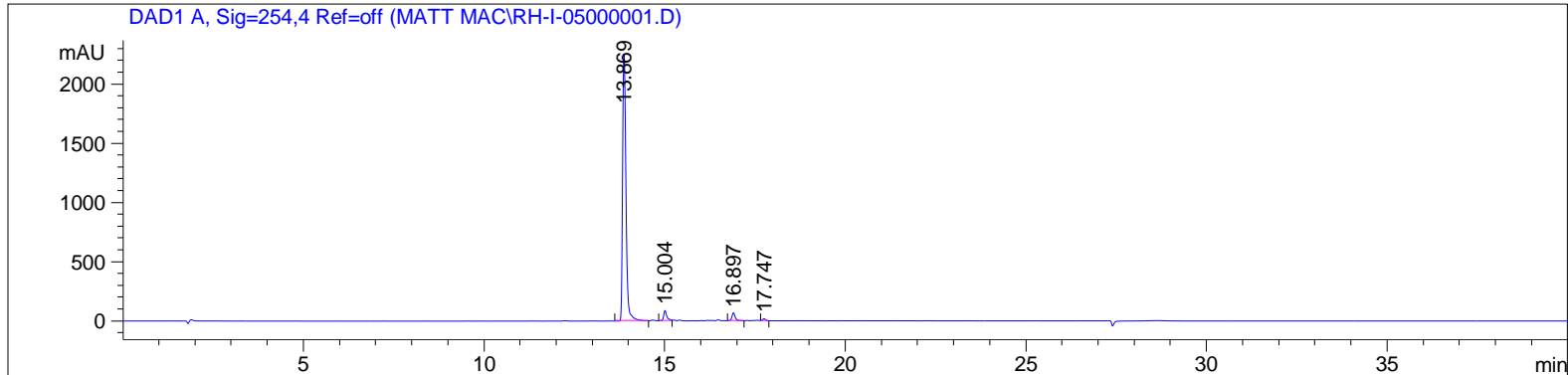
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Sample Name: run1

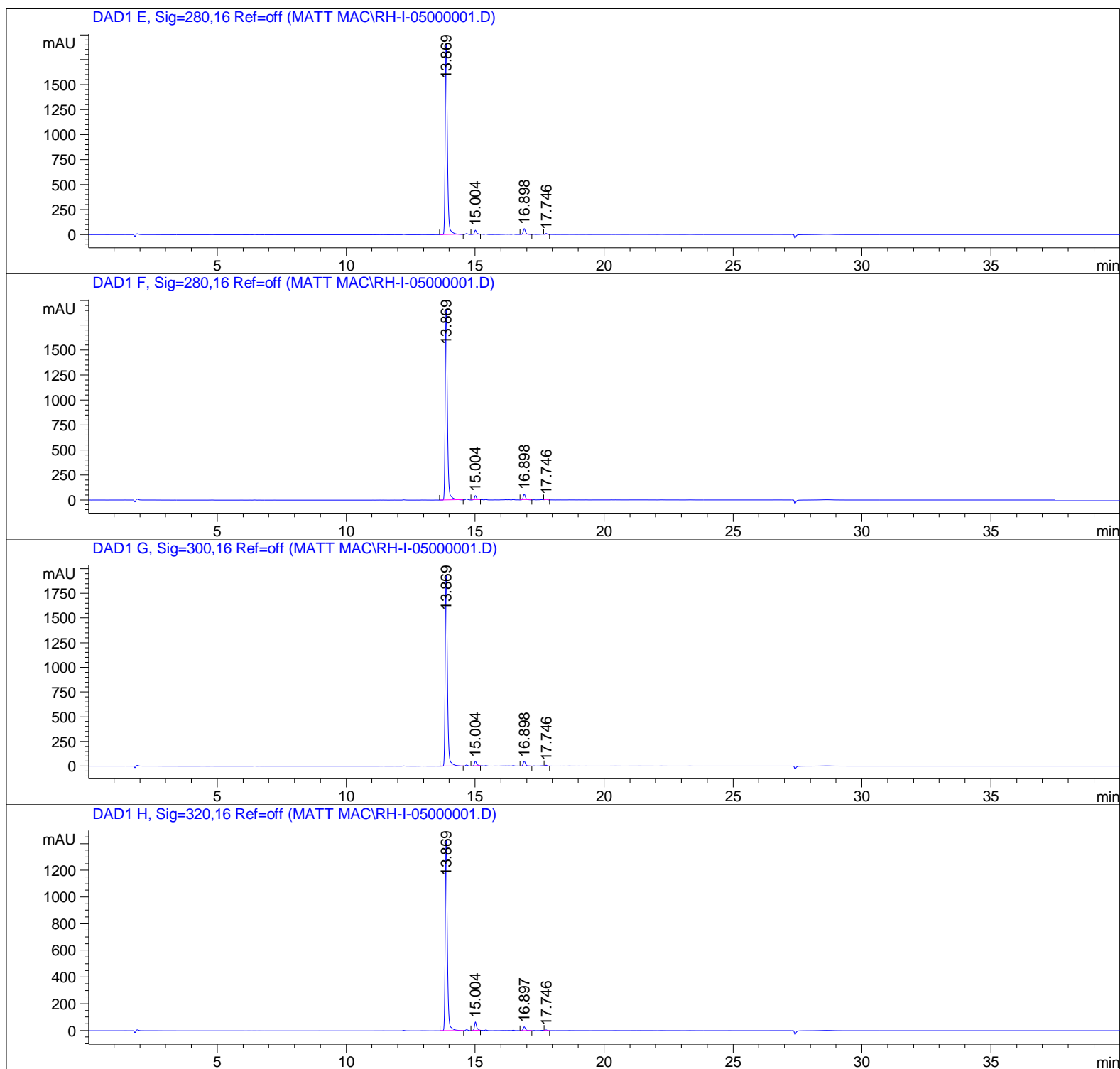
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Acq. Instrument : Instrument 1 Location : -  
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Last changed : 1/9/2013 5:30:58 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:04:11 PM by Matt Mac  
(modified after loading)



Sample Name: run1

## HPLC traces of compound 25

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

### HPLC traces of compound 25

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.869	BV	0.0999	1.47072e4	2260.91943	93.3598
2	15.004	BV	0.0927	533.26215	85.62164	3.3851
3	16.897	BB	0.0934	422.24030	67.12388	2.6803
4	17.747	VB	0.0792	90.54961	17.25830	0.5748

Totals : 1.57532e4 2430.92325

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.869	BV	0.0999	1.48180e4	2276.77466	93.4310
2	15.004	BV	0.0925	527.65247	84.90611	3.3270
3	16.897	BB	0.0934	423.42865	67.28013	2.6698
4	17.747	VB	0.0792	90.75919	17.31082	0.5723

Totals : 1.58598e4 2446.27172

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.870	BV	0.1375	1.91453e4	2200.73096	89.8328
2	15.004	BV	0.0924	1104.12341	177.90869	5.1807
3	16.897	BV	0.0923	923.61694	148.94827	4.3337
4	17.747	VB	0.0799	139.10408	26.22550	0.6527

Totals : 2.13122e4 2553.81342

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.870	BV	0.1274	1.90738e4	2383.21851	92.0747
2	15.004	BV	0.0912	840.35529	137.73363	4.0566
3	16.897	BB	0.0935	663.92902	105.42035	3.2050
4	17.747	VB	0.0790	137.49413	26.29313	0.6637

Sample Name: run1

## HPLC traces of compound 25

Totals : 2.07156e4 2652.66561

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.869	BV	0.0915	1.14248e4	1918.42883	94.3685
2	15.004	BV	0.0925	267.09799	42.97807	2.2062
3	16.898	BB	0.0918	361.20950	58.69957	2.9836
4	17.746	VB	0.0793	53.48040	10.17261	0.4417

Totals : 1.21066e4 2030.27908

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.869	BV	0.0915	1.14248e4	1918.42883	94.3685
2	15.004	BV	0.0925	267.09799	42.97807	2.2062
3	16.898	BB	0.0918	361.20950	58.69957	2.9836
4	17.746	VB	0.0793	53.48040	10.17261	0.4417

Totals : 1.21066e4 2030.27908

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.869	BV	0.0926	1.17744e4	1945.19104	94.6889
2	15.004	BV	0.0924	307.58649	49.56367	2.4736
3	16.898	BB	0.0924	309.97372	49.95343	2.4928
4	17.746	VB	0.0794	42.87123	8.13978	0.3448

Totals : 1.24348e4 2052.84792

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.869	BV	0.0868	8205.55176	1432.52271	93.2305
2	15.004	BV	0.0903	388.63116	64.46502	4.4156



Sample Name: run1

HPLC traces of compound **25**

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
3	16.897	BB	0.0936	179.76132	28.50370	2.0424
4	17.746	VB	0.0795	27.41720	5.20166	0.3115

Totals :                                   8801.36144 1530.69308

=====  
\*\*\* End of Report \*\*\*

# HRMS of compound 25

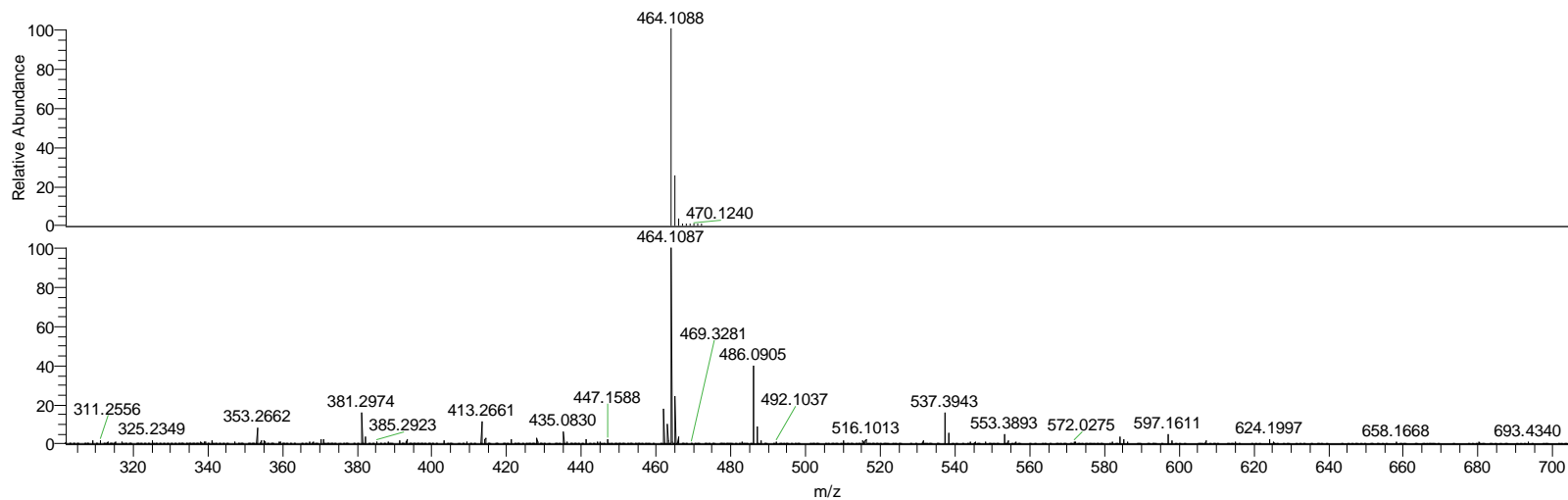
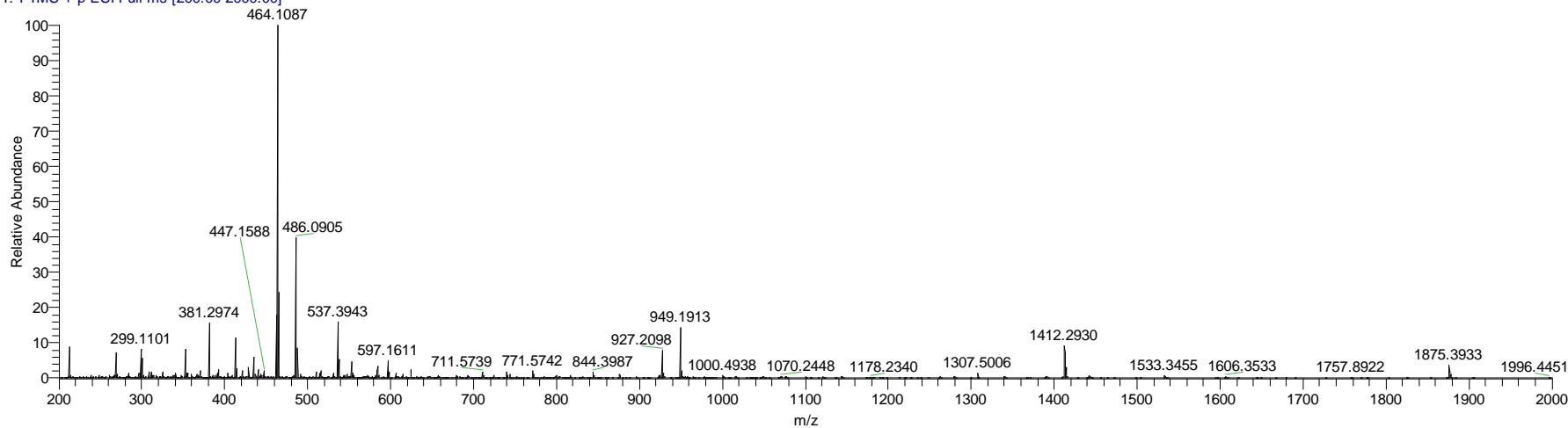
C:\Xcalibur...\Matt2-10-2013\RH-I-05

2/10/2013 5:57:30 PM

RH-I-05

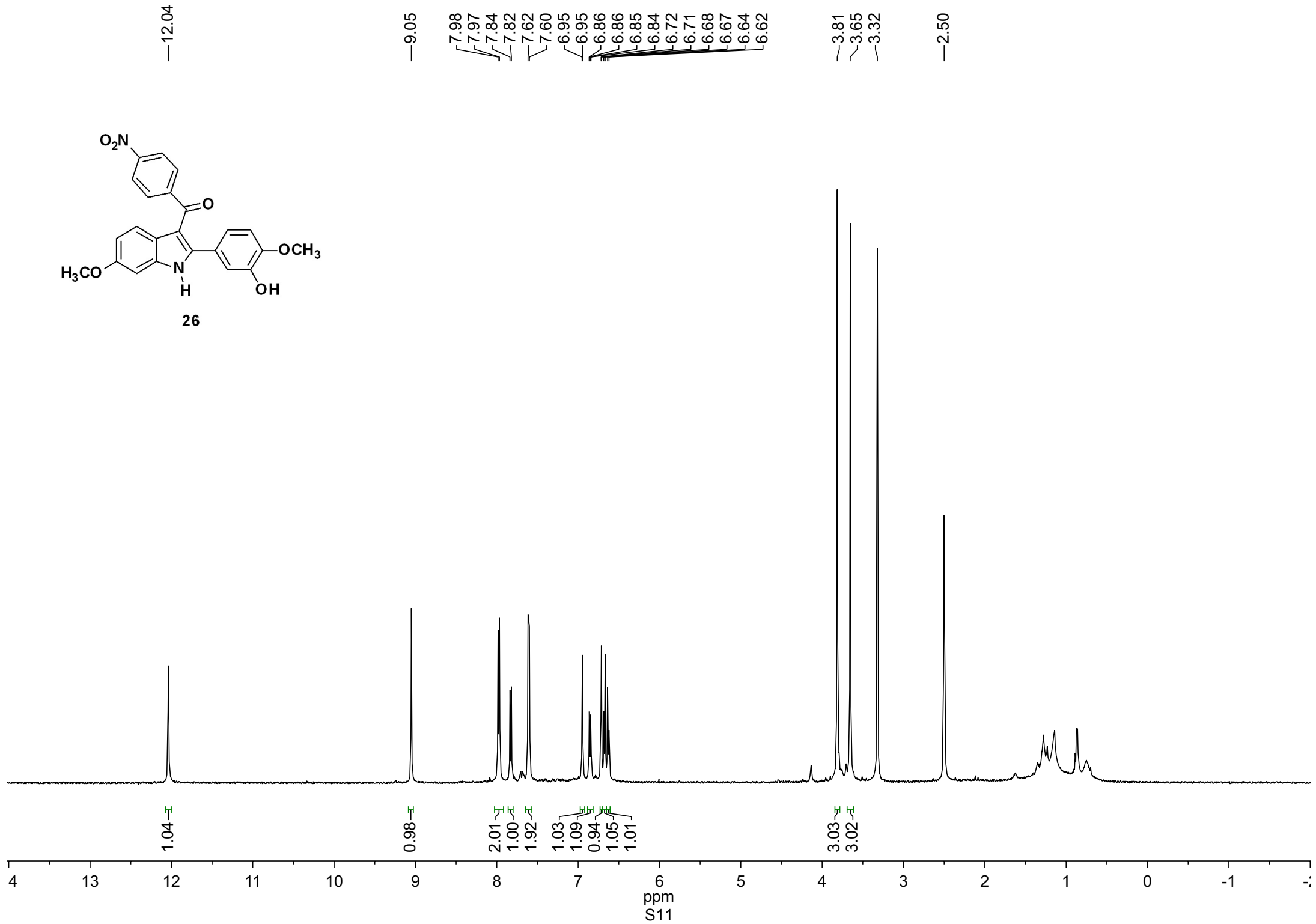
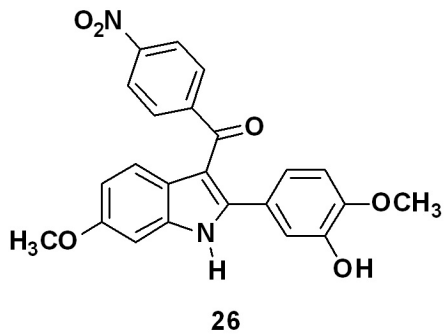
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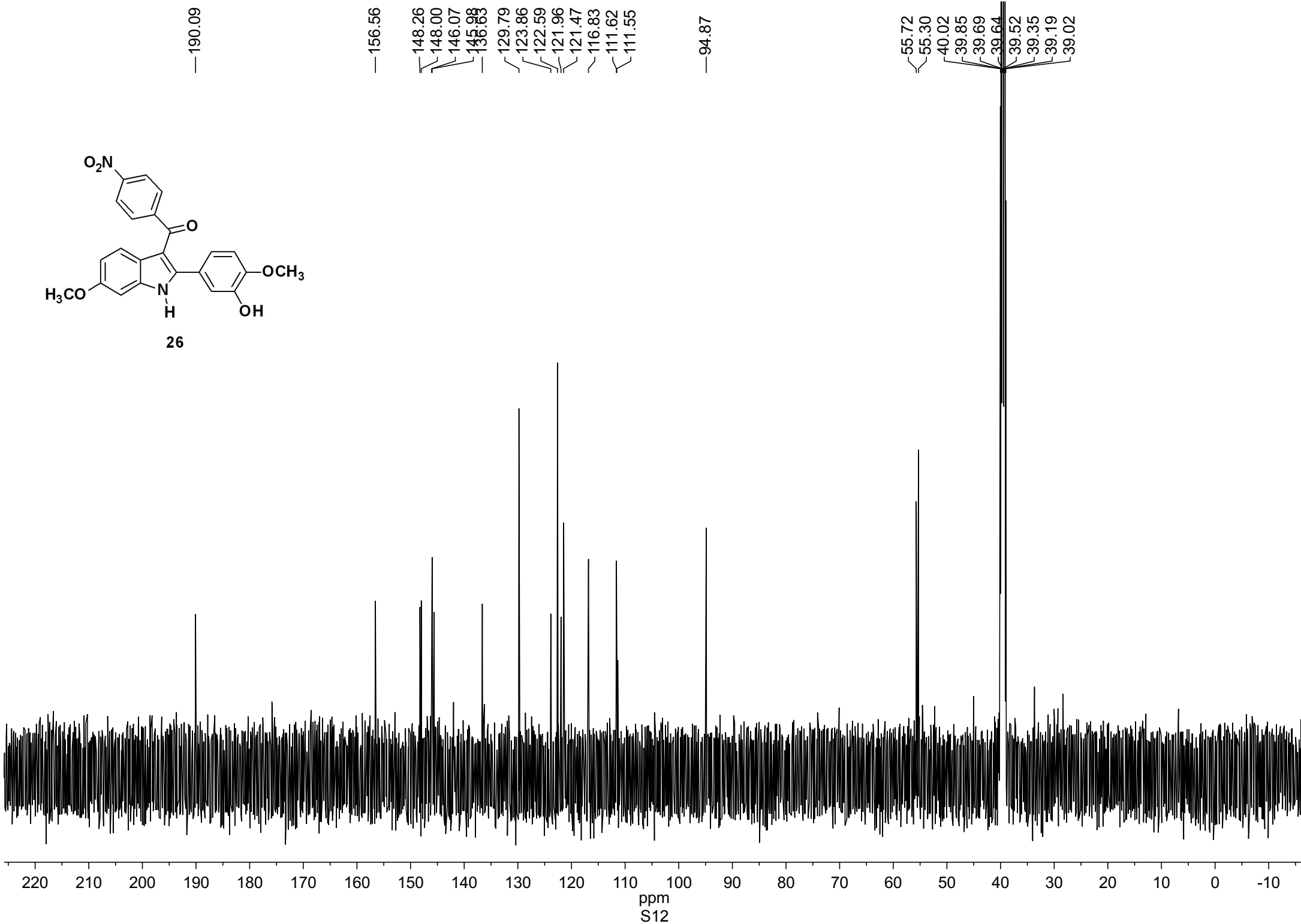
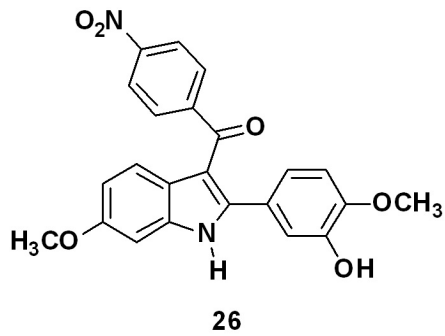
T: FTMS + p ESI Full ms [200.00-2000.00]



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7.56E5  
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C<sub>23</sub>H<sub>18</sub>O<sub>8</sub>N<sub>3</sub>  
pa Chrg 1

NL:  
2.11E7  
RH-I-05#17 RT:  
0.14 AV: 1 T:  
FTMS + p ESI  
Full ms  
[200.00-2000.00]



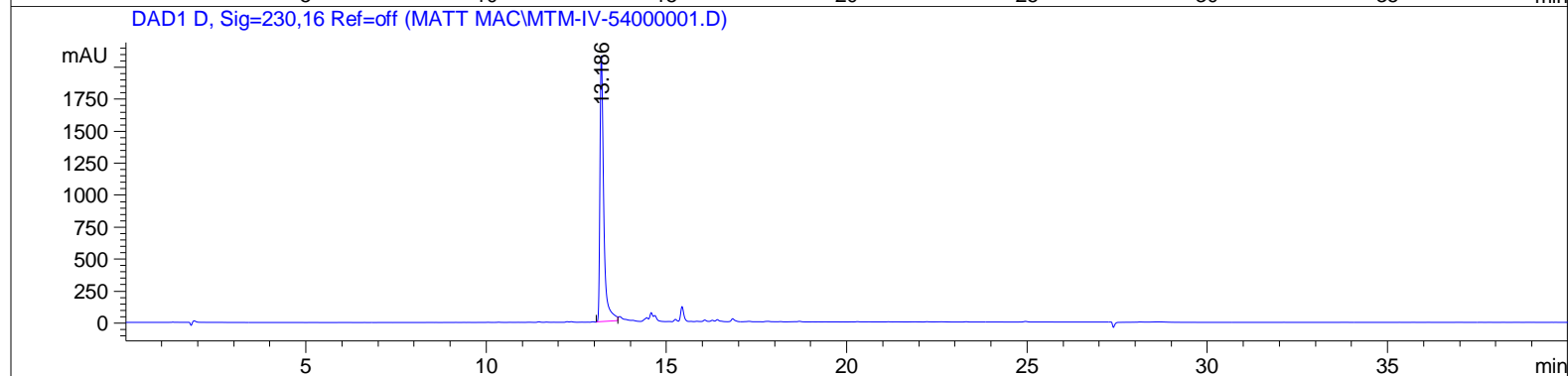
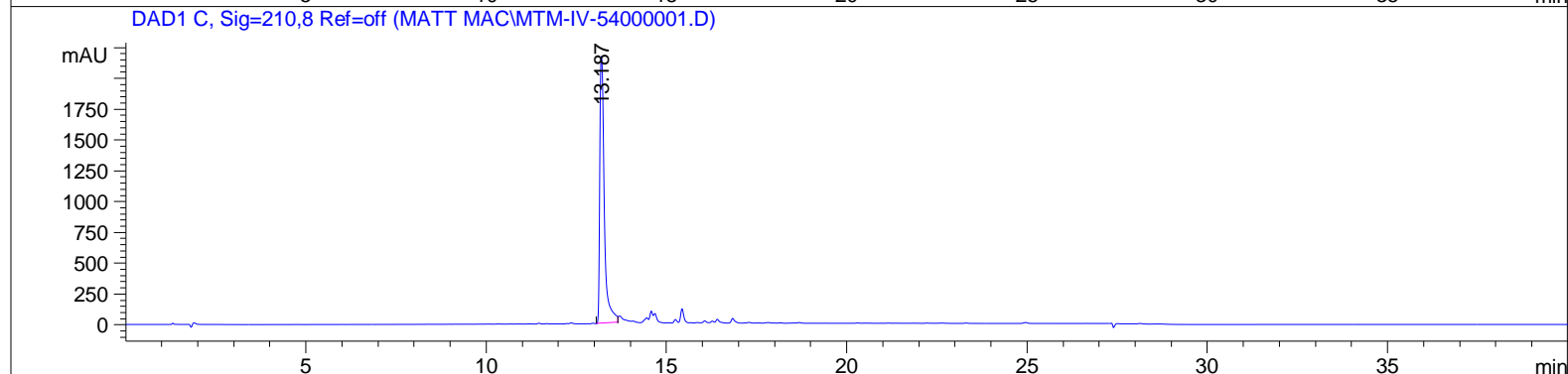
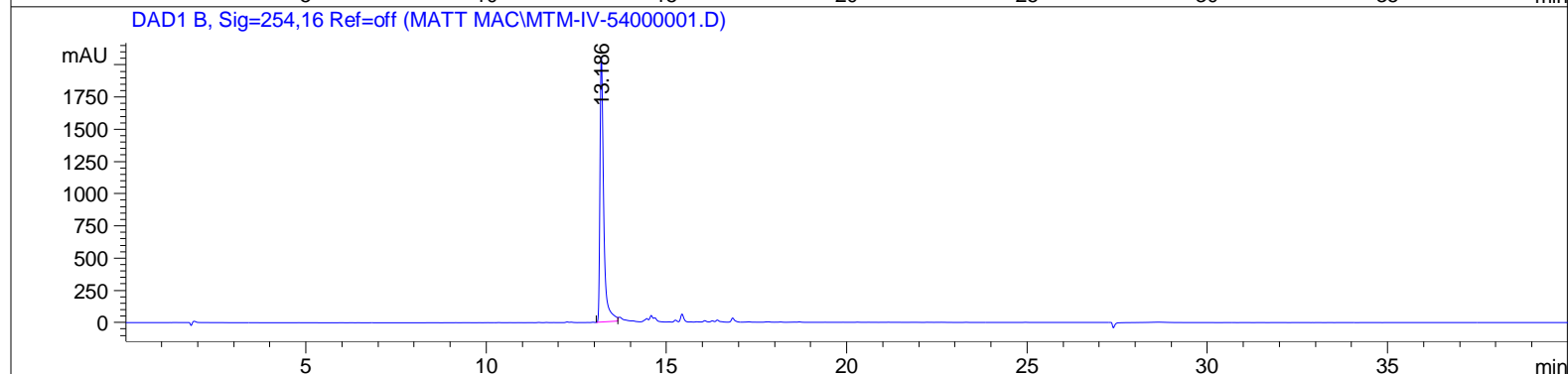
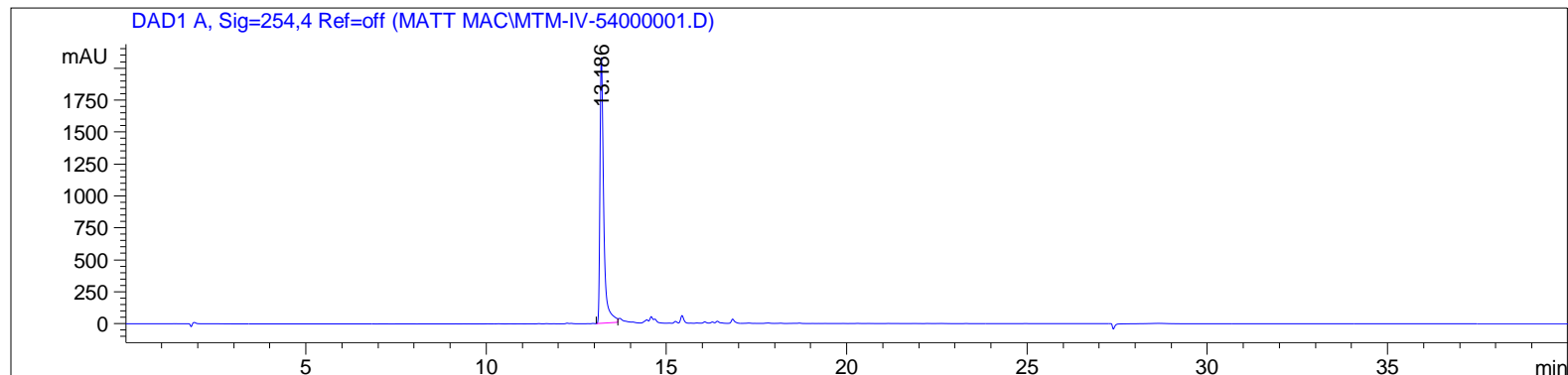


Sample Name: run1

## HPLC traces of compound 26

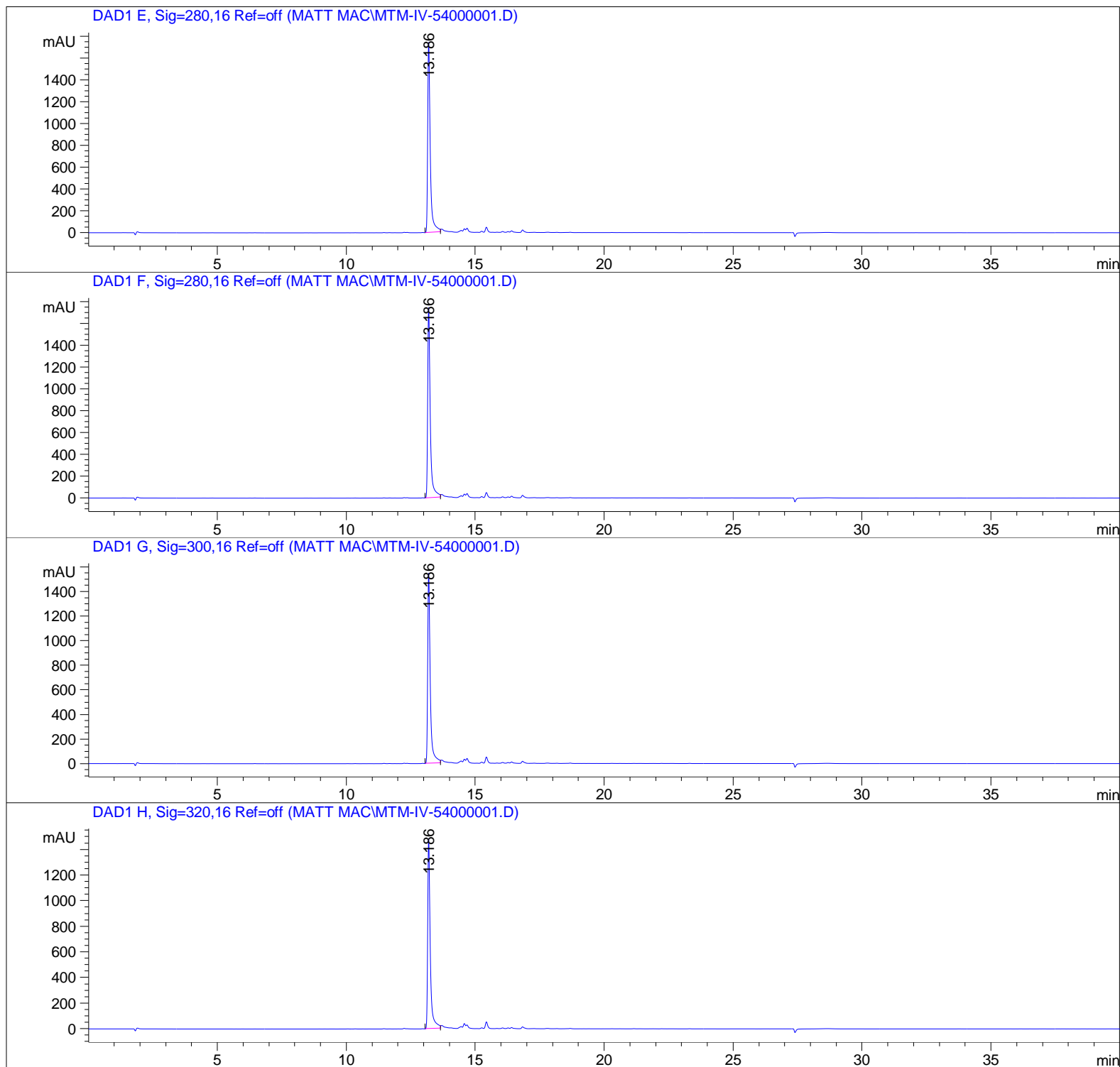
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Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:04:11 PM by Matt Mac  
(modified after loading)



Sample Name: run1

## HPLC traces of compound 26

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 26

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1094	1.52234e4	2080.05469	100.0000

Totals : 1.52234e4 2080.05469

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1089	1.50116e4	2063.30054	100.0000

Totals : 1.50116e4 2063.30054

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.187	BV	0.1346	1.90632e4	2167.22290	100.0000

Totals : 1.90632e4 2167.22290

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1104	1.54060e4	2079.89819	100.0000

Totals : 1.54060e4 2079.89819

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1036	1.22133e4	1745.71863	100.0000

Totals : 1.22133e4 1745.71863

Sample Name: run1

## HPLC traces of compound 26

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1036	1.22133e4	1745.71863	100.0000

Totals : 1.22133e4 1745.71863

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1009	1.07514e4	1549.86780	100.0000

Totals : 1.07514e4 1549.86780

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BV	0.1004	1.02645e4	1488.61096	100.0000

Totals : 1.02645e4 1488.61096

=====  
\*\*\* End of Report \*\*\*



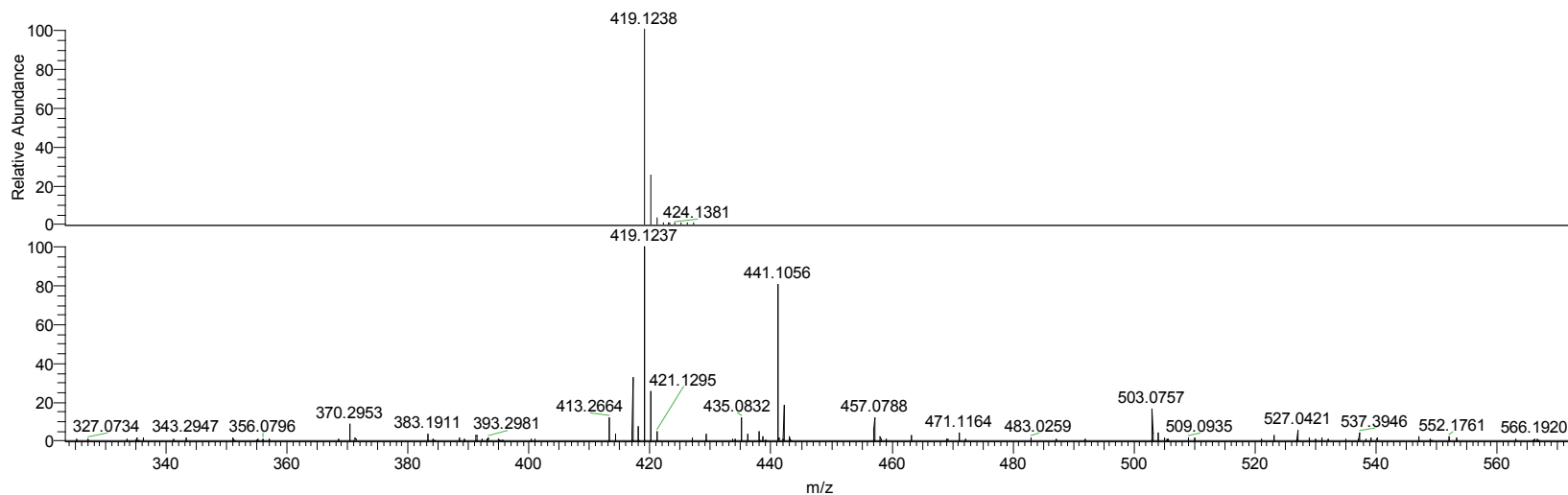
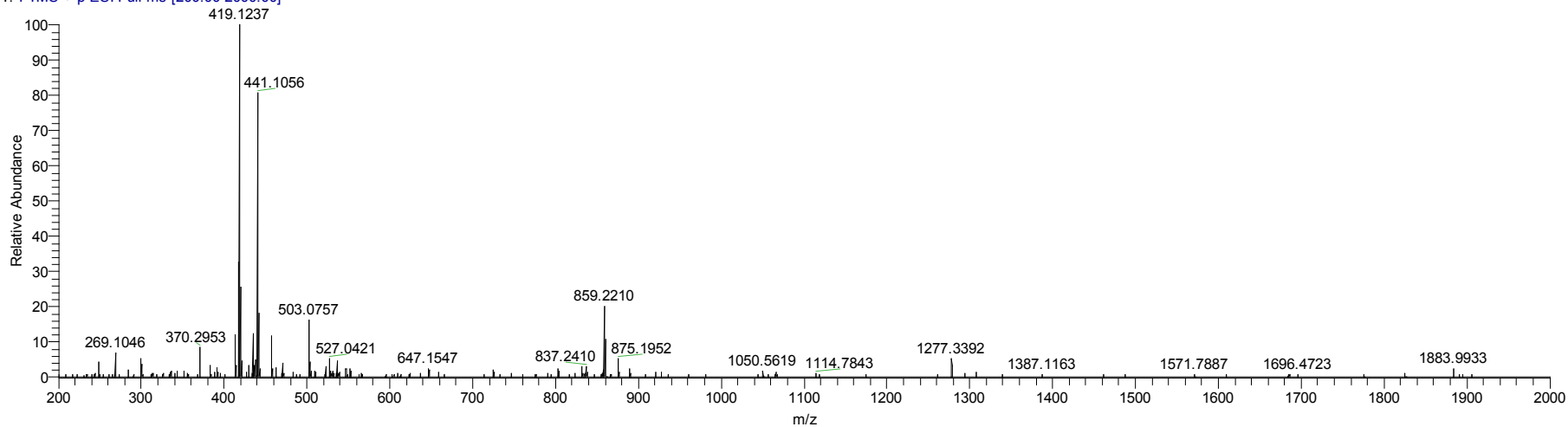
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2/10/2013 4:33:04 PM

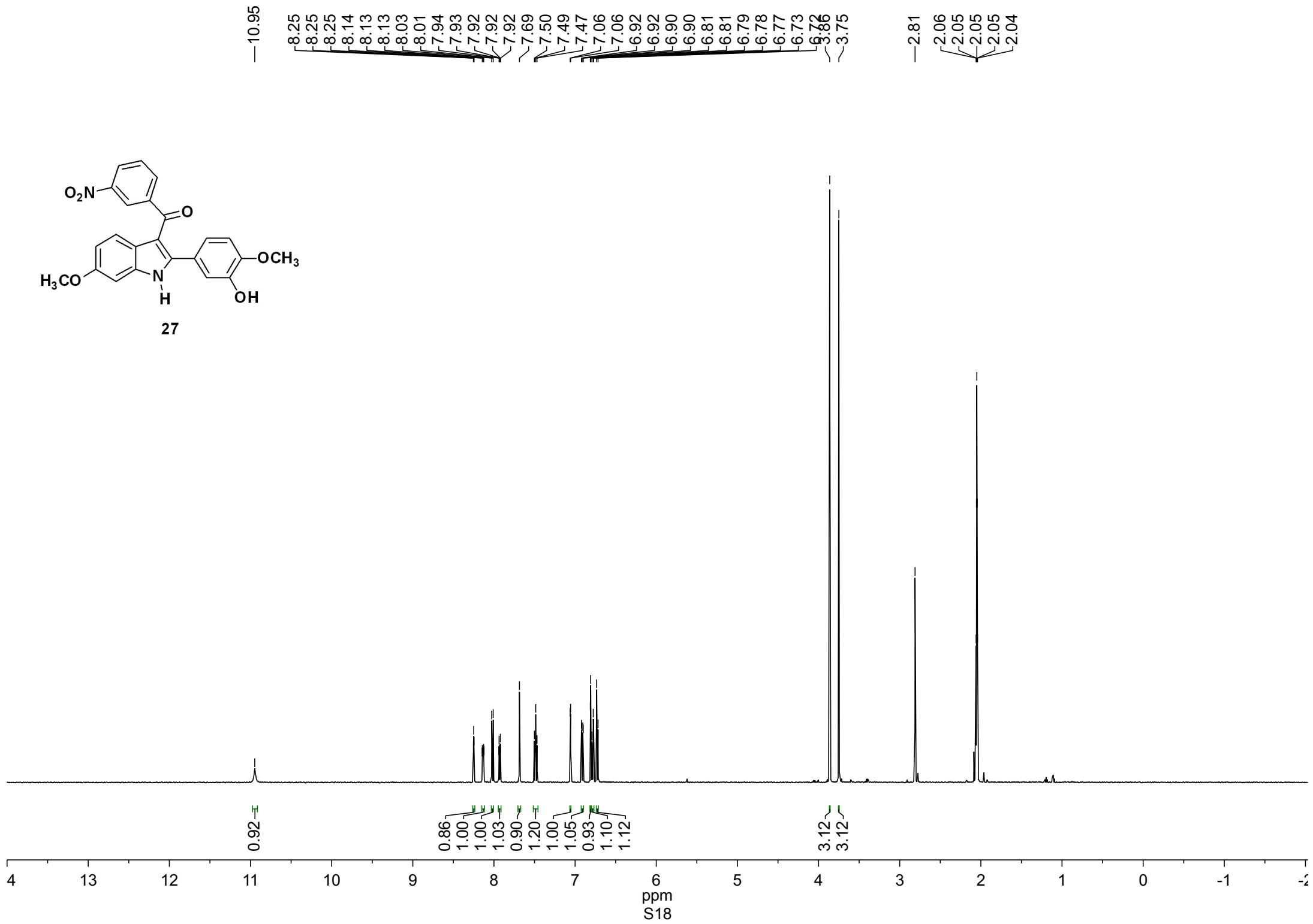
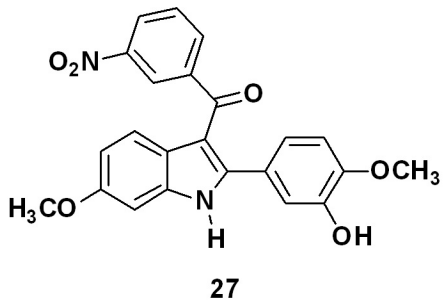
MTM-IV-54

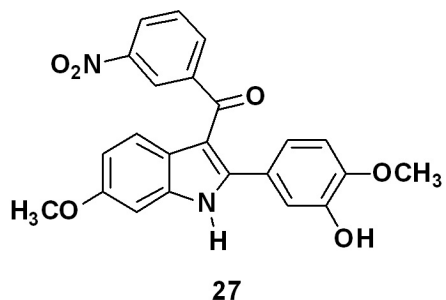
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NL:  
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C<sub>23</sub>H<sub>19</sub>O<sub>6</sub>N<sub>2</sub>:  
C<sub>23</sub>H<sub>19</sub>O<sub>6</sub>N<sub>2</sub>:  
pa Chrg 1

NL:  
2.49E6  
MTM-IV-54#20  
RT: 0.20 AV: 1 T:  
FTMS + p ESI Full  
ms  
[200.00-2000.00]





206.42  
206.27  
206.26  
206.25  
206.25  
206.10

190.51

158.52

149.15

147.40

145.95

143.10

138.04

135.88

130.11

125.82

125.69

124.84

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112.73

112.25

95.75

56.48

55.97

30.46

30.31

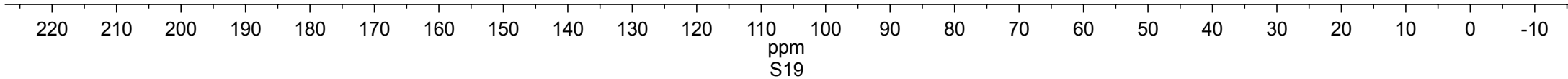
30.15

30.00

29.84

29.69

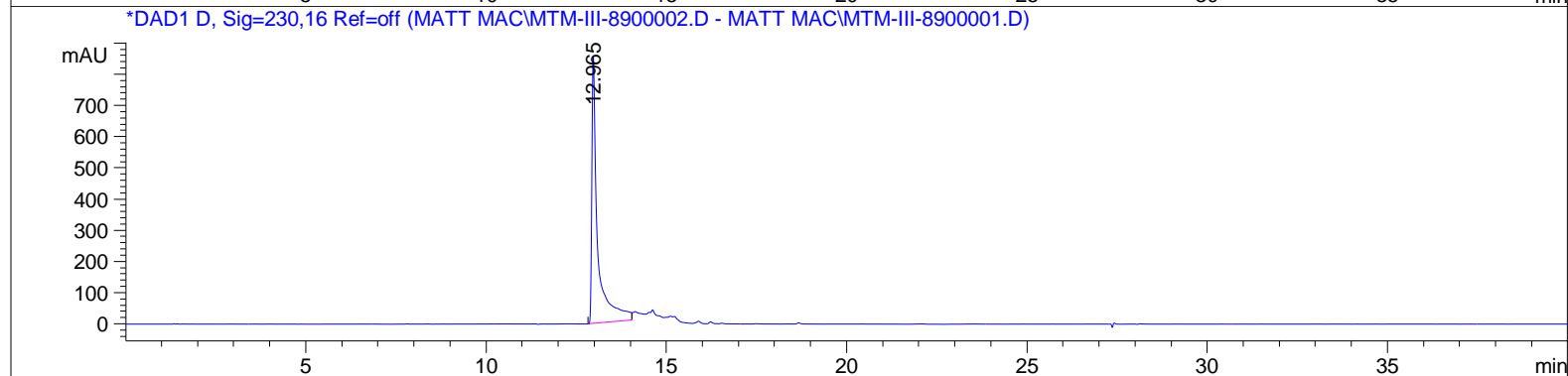
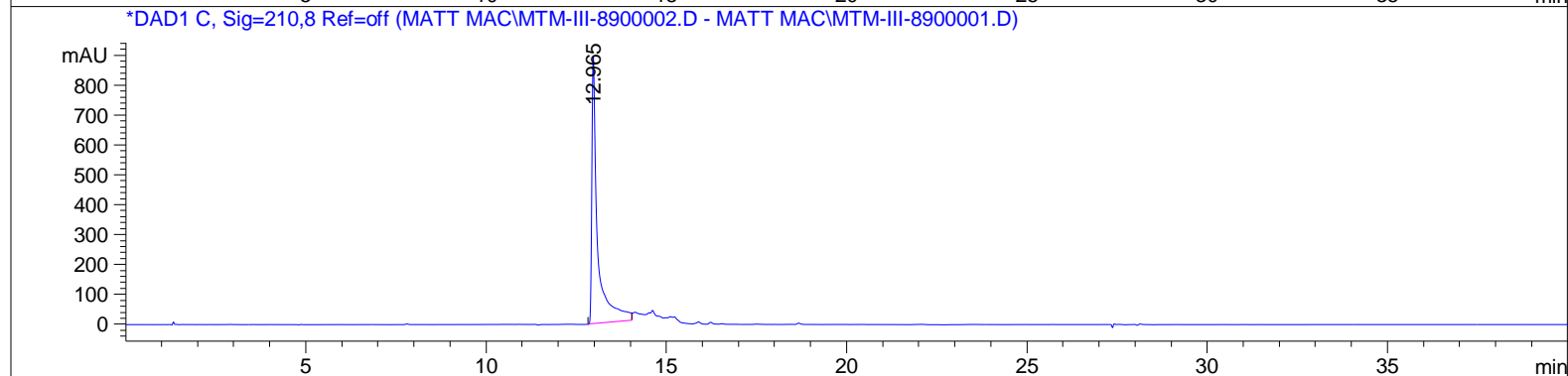
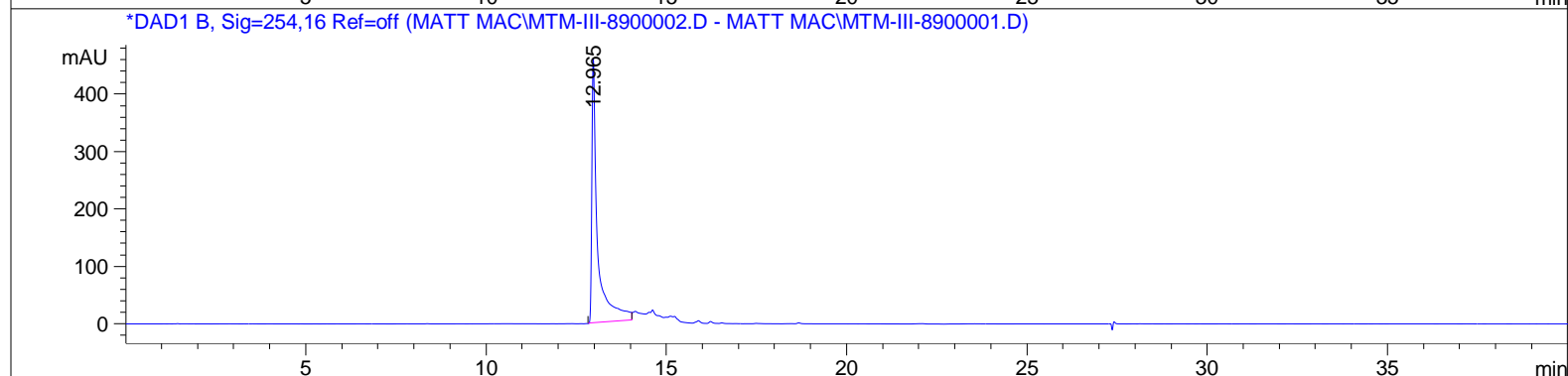
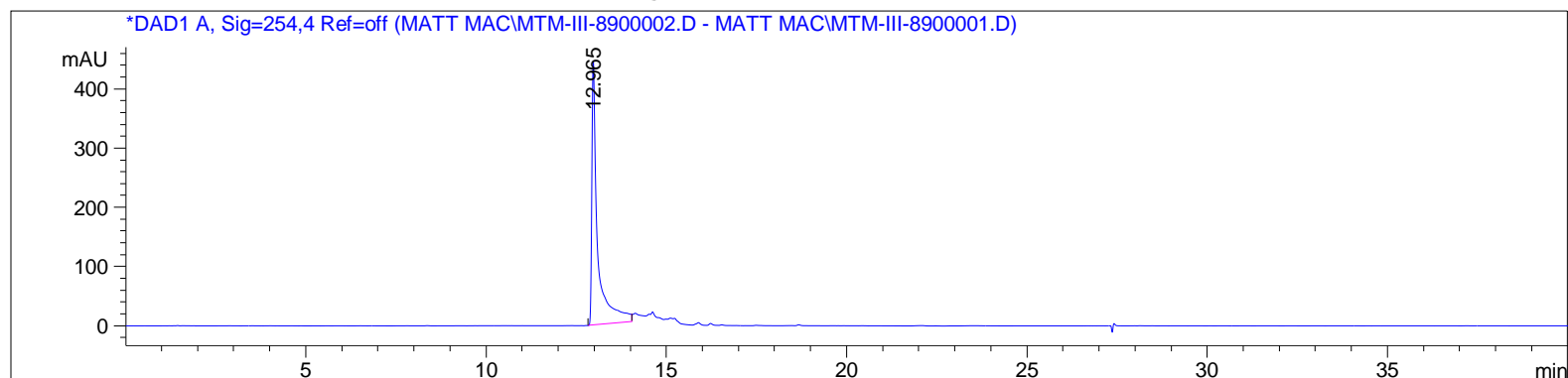
29.54



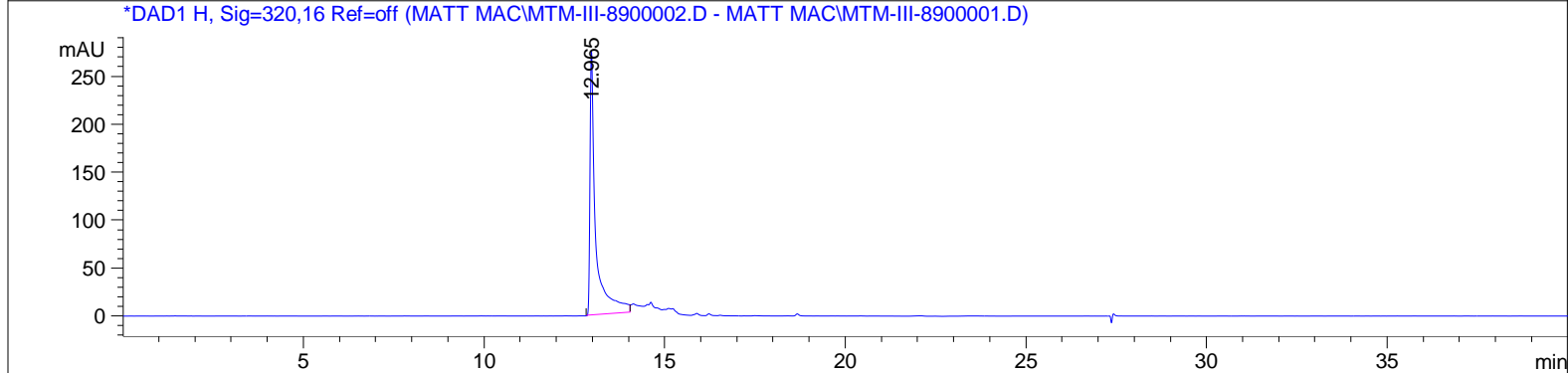
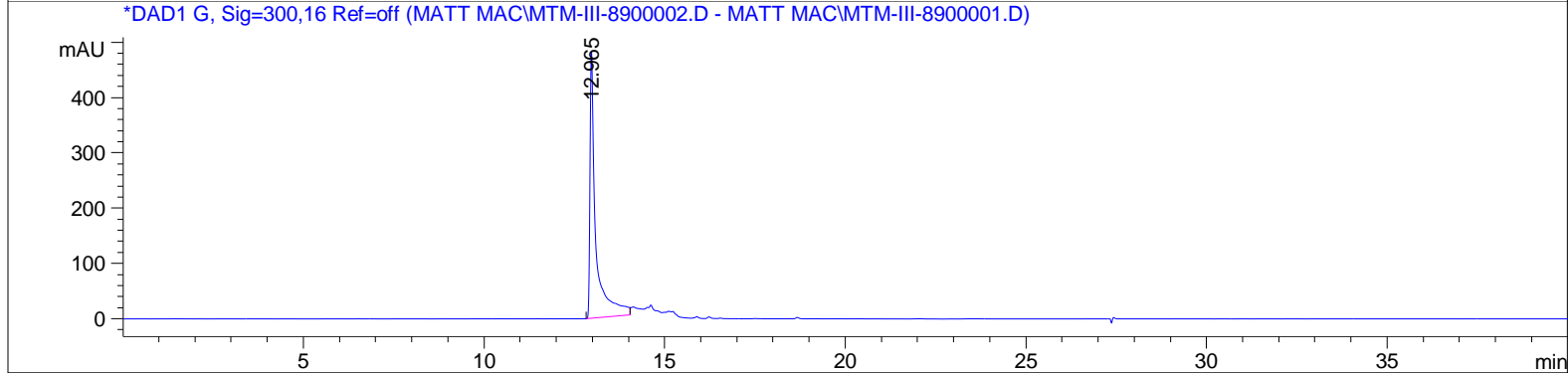
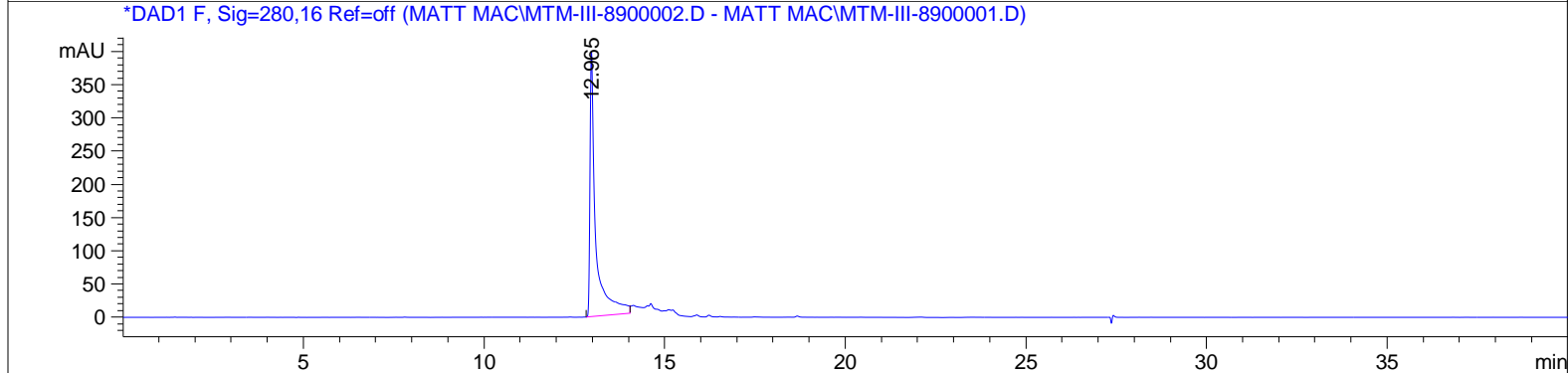
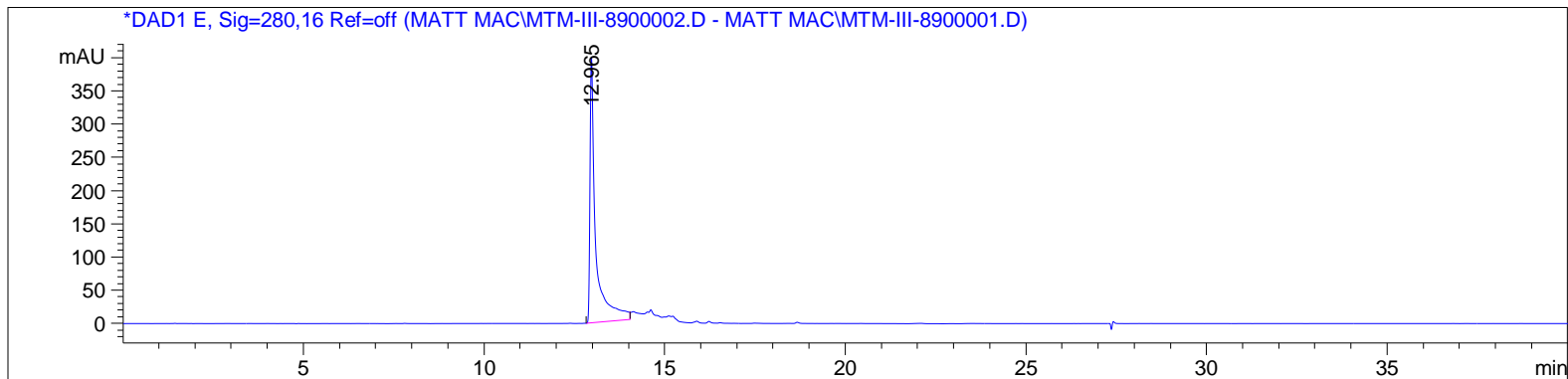
Sample Name: run1

## HPLC traces of compound 27

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Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/8/2013 7:19:42 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/8/2013 7:13:43 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/8/2013 8:58:30 AM by Matt Mac  
(modified after loading)



Sample Name: run1



=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 27

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1527	5005.44141	446.85699	100.0000

Totals : 5005.44141 446.85699

Signal 2: DAD1 B, Sig=254,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1526	5166.09326	461.32089	100.0000

Totals : 5166.09326 461.32089

Signal 3: DAD1 C, Sig=210,8 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1532	1.00692e4	895.34930	100.0000

Totals : 1.00692e4 895.34930

Signal 4: DAD1 D, Sig=230,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1531	9635.51758	857.25806	100.0000

Totals : 9635.51758 857.25806

Sample Name: run1

## HPLC traces of compound 27

Signal 5: DAD1 E, Sig=280,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1523	4463.91895	399.77322	100.0000

Totals :                                   4463.91895   399.77322

Signal 6: DAD1 F, Sig=280,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1523	4463.91895	399.77322	100.0000

Totals :                                   4463.91895   399.77322

Signal 7: DAD1 G, Sig=300,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1524	5404.95215	483.64343	100.0000

Totals :                                   5404.95215   483.64343

Signal 8: DAD1 H, Sig=320,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.965	BV	0.1526	3091.80371	276.23389	100.0000

Totals :                                   3091.80371   276.23389

=====  
\*\*\* End of Report \*\*\*

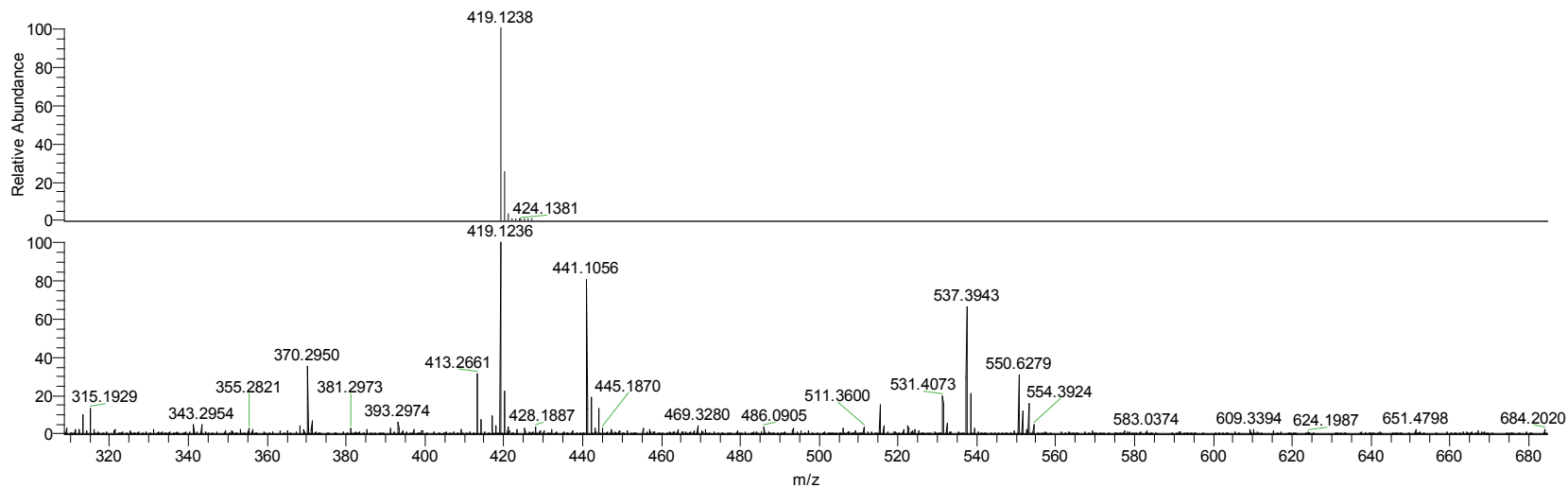
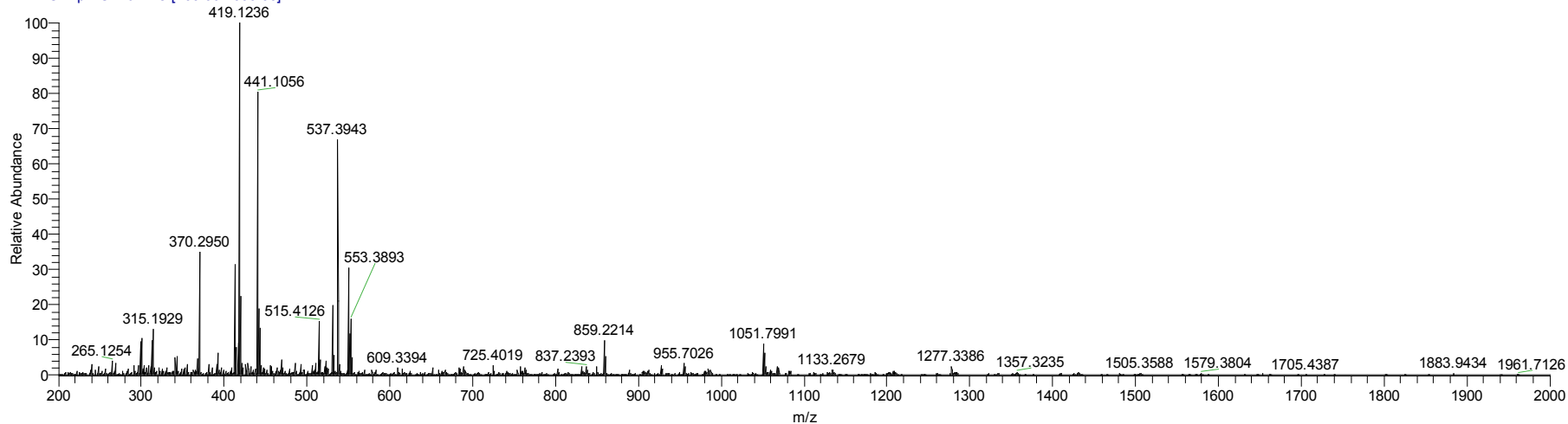
# HPLC traces of compound 27

C:\Xcalibur...12-10-2013\MTM-III-89

2/10/2013 6:58:21 PM

MTM-III-89

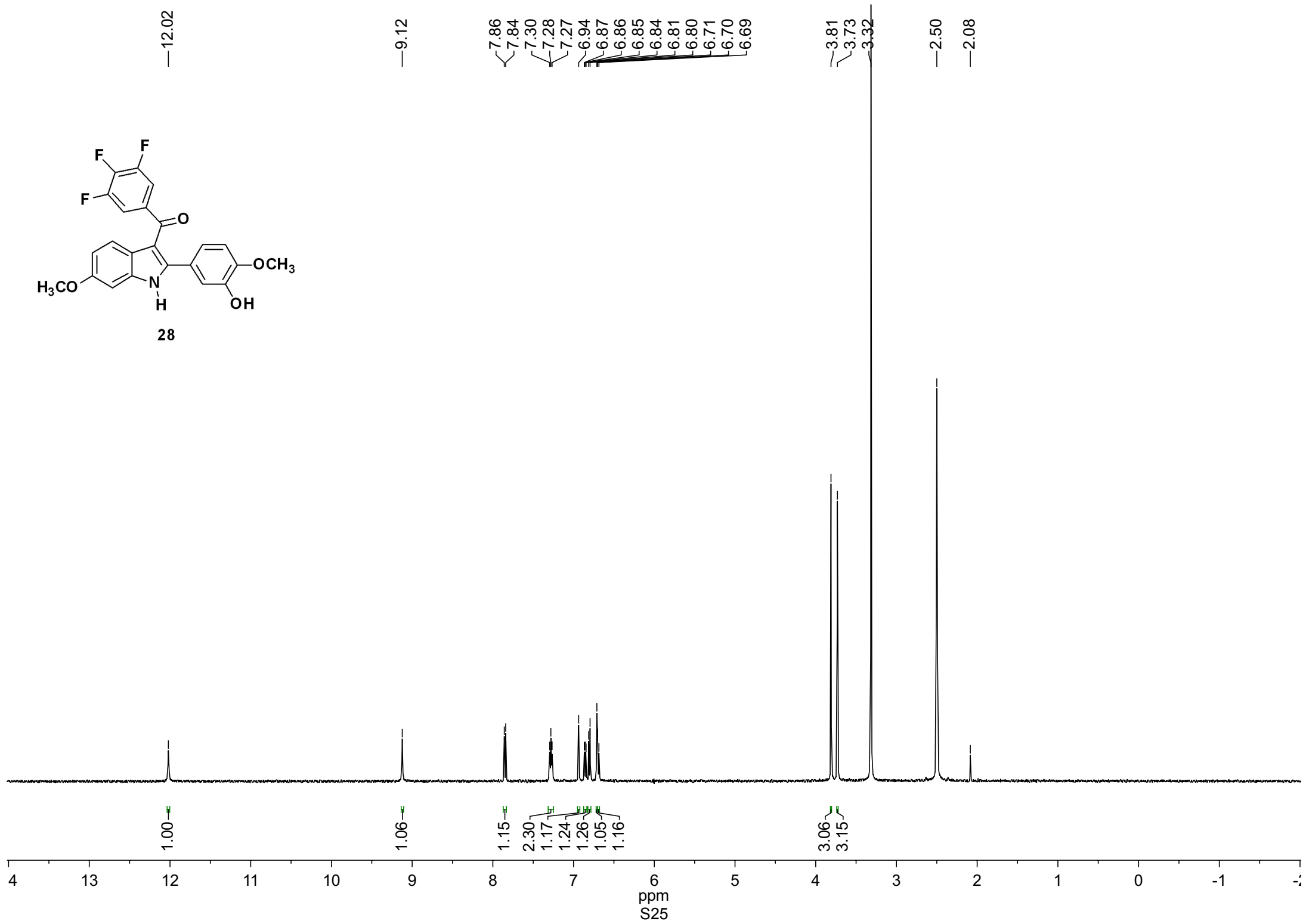
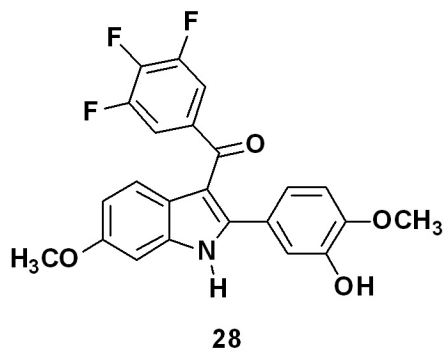
MTM-III-89 #20 RT: 0.19 AV: 1 NL: 8.65E6  
T: FTMS + p ESI Full ms [200.00-2000.00]

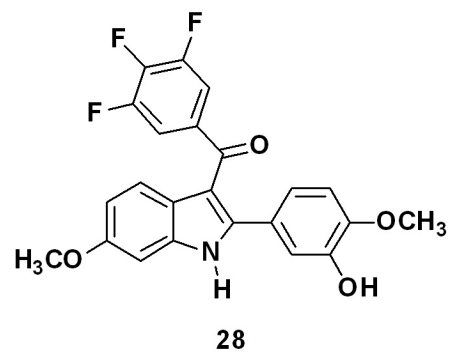


NL:  
7.62E5  
C<sub>23</sub>H<sub>19</sub>O<sub>6</sub>N<sub>2</sub>:  
C<sub>23</sub>H<sub>19</sub>O<sub>6</sub>N<sub>2</sub>  
pa Chrg 1

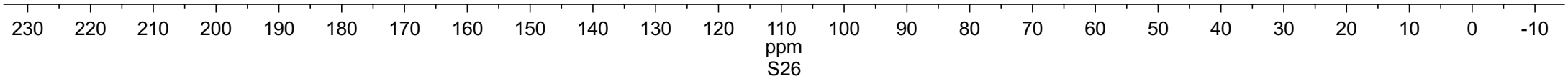
NL:  
8.65E6  
MTM-III-89#20 RT:  
0.19 AV: 1 T:  
FTMS + p ESI Full  
ms  
[200.00-2000.00]

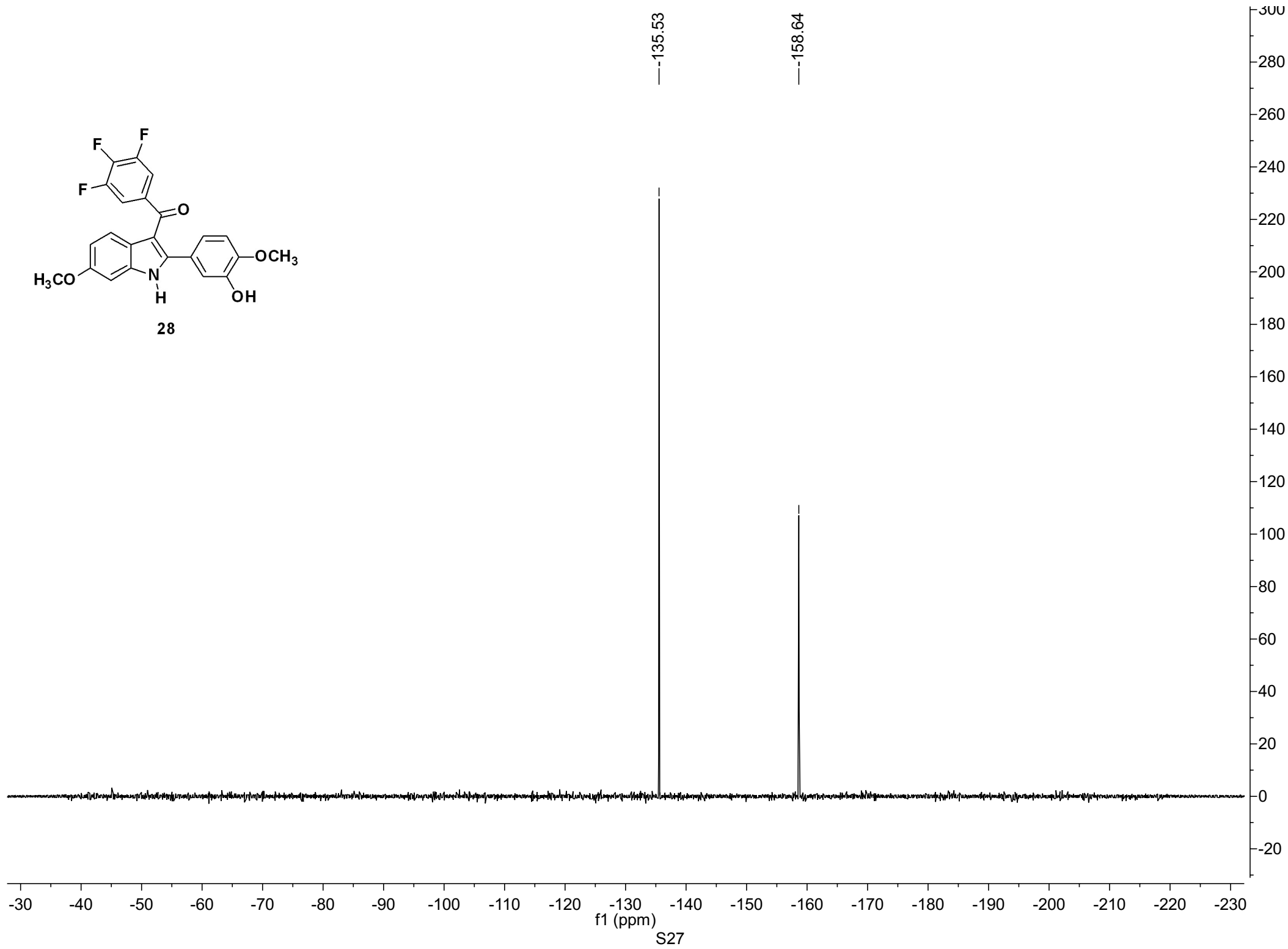
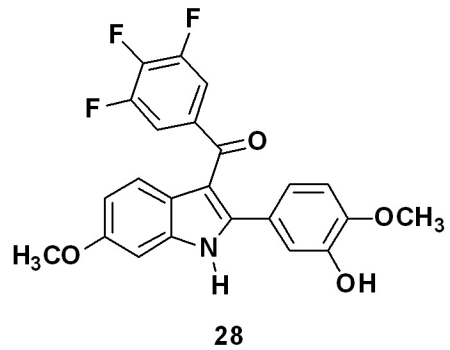






188.00  
156.58  
150.48  
150.42  
148.50  
148.45  
148.23  
146.14  
145.46  
141.15  
141.03  
139.14  
139.01  
138.89  
136.74  
136.69  
136.65  
124.16  
122.03  
121.43  
121.21  
116.75  
113.63  
111.76  
111.53  
110.81  
94.87  
55.82  
55.30  
40.02  
39.85  
39.69  
39.52  
39.35  
39.19  
39.02



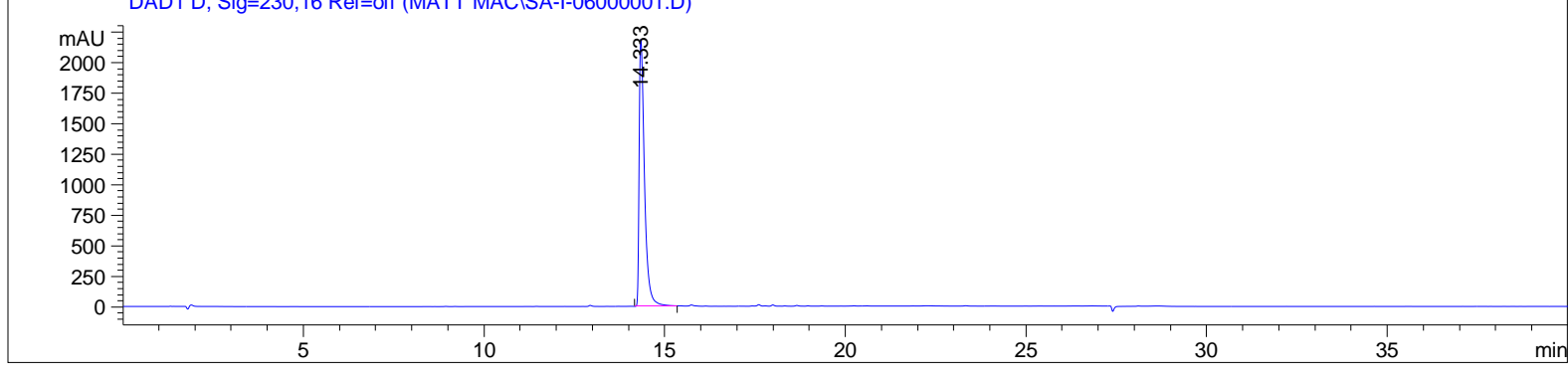
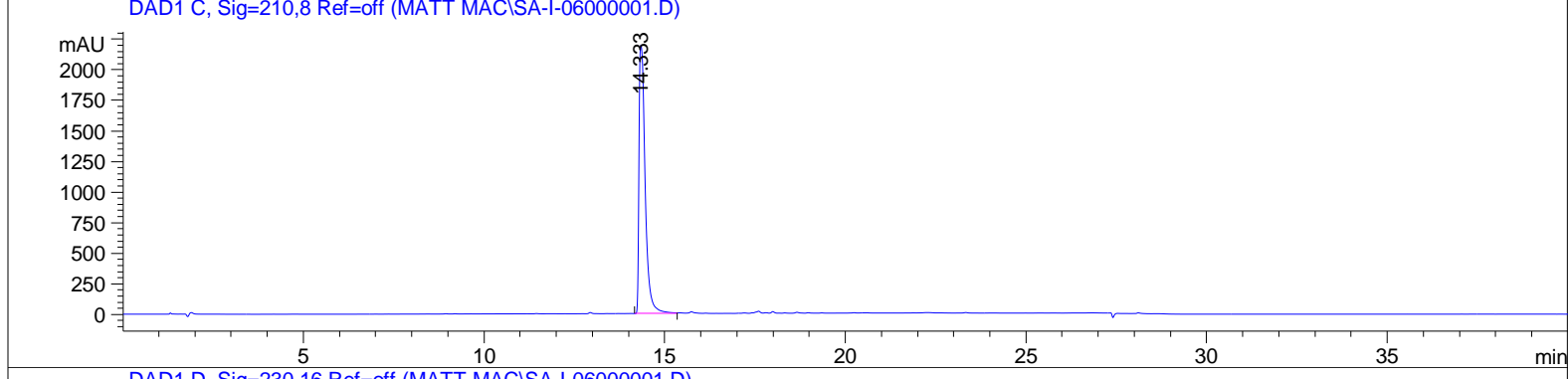
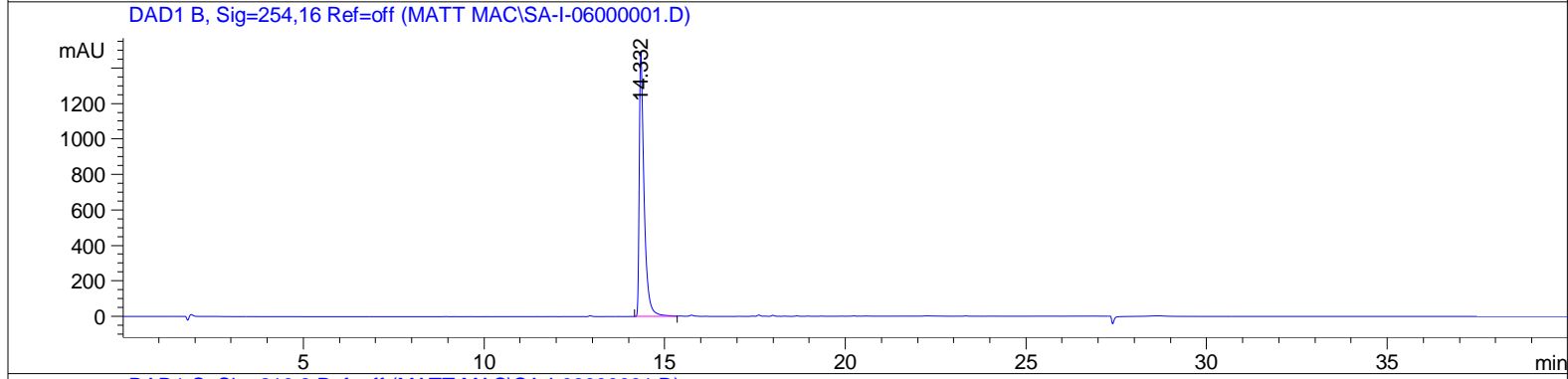
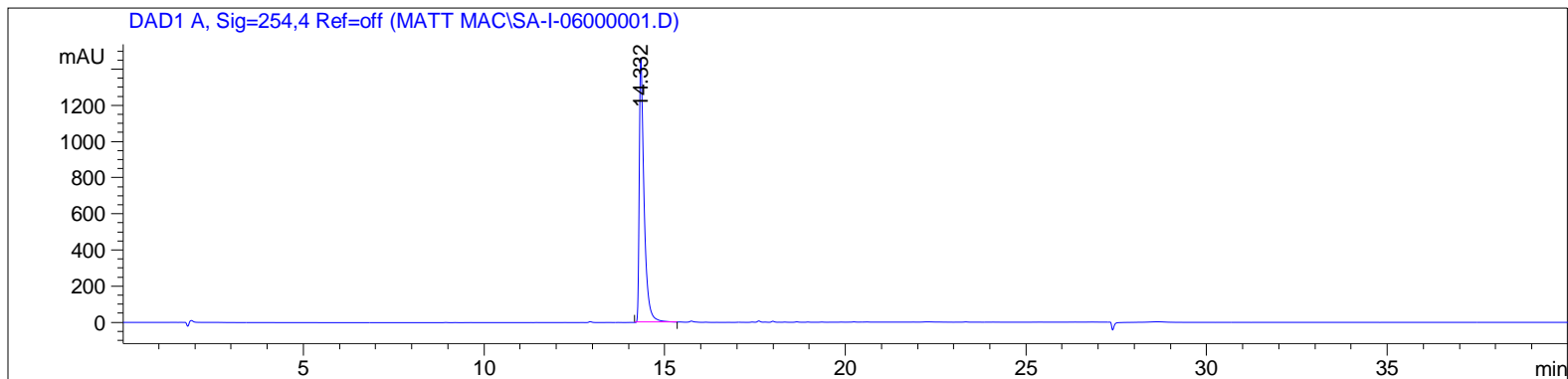


Sample Name: run1

### HPLC traces of compound 28

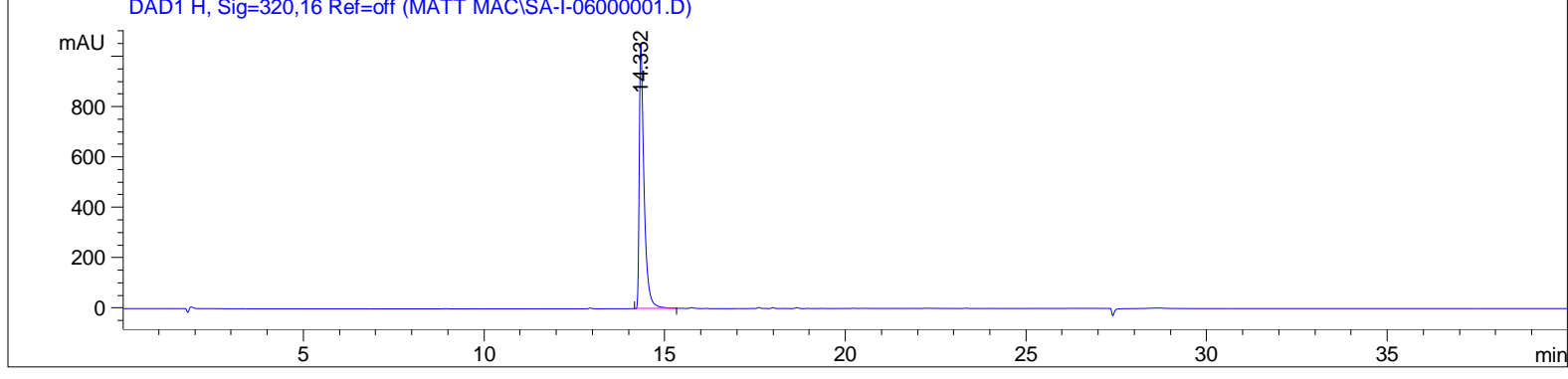
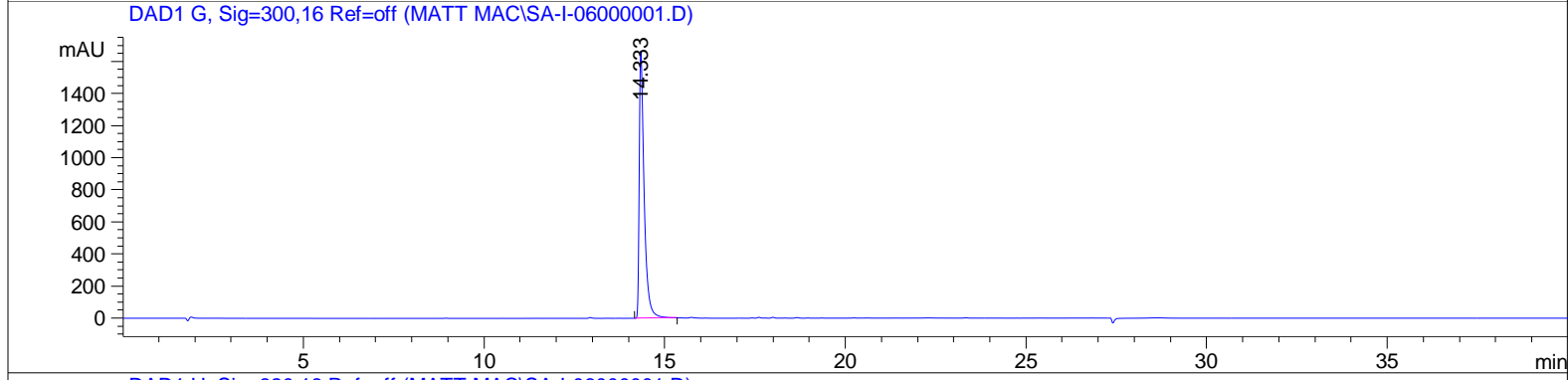
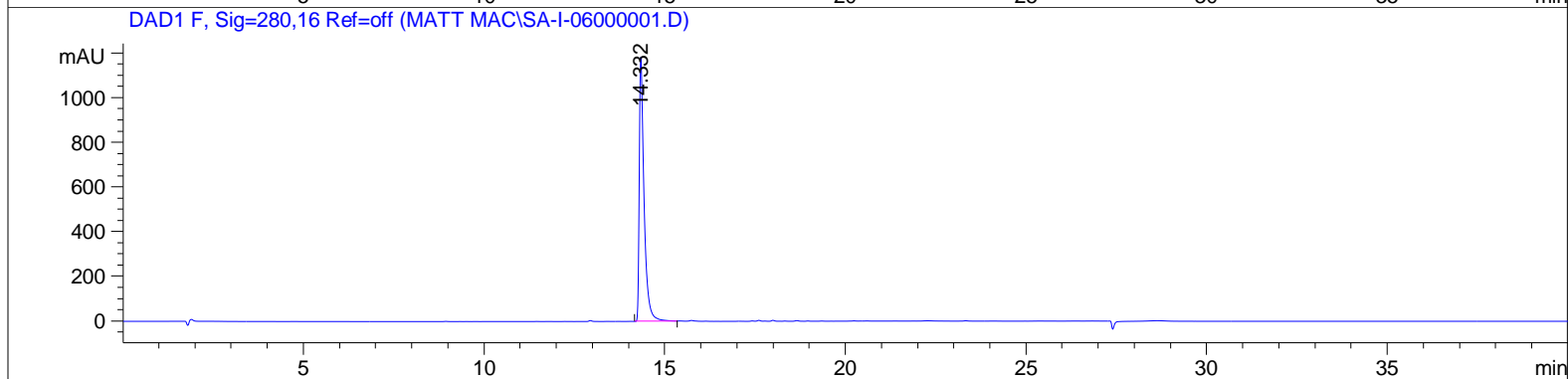
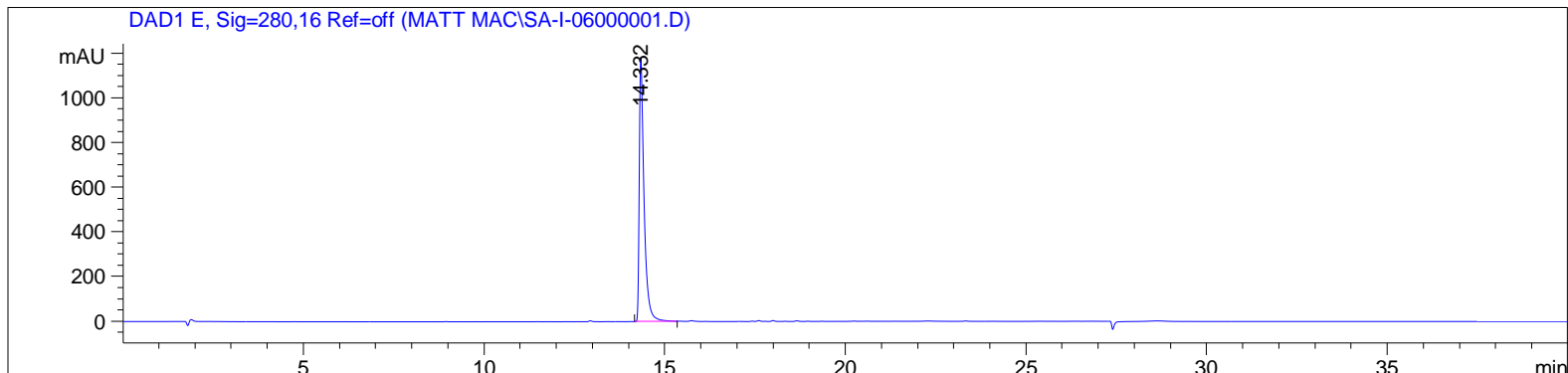
=====

Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/9/2013 2:09:32 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:01:45 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:04:11 PM by Matt Mac  
(modified after loading)



Sample Name: run1

### HPLC traces of compound 28



=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

HPLC traces of compound 28

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.332	BV	0.1353	1.37124e4	1463.69946	100.0000

Totals : 1.37124e4 1463.69946

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.332	BV	0.1354	1.39932e4	1492.83130	100.0000

Totals : 1.39932e4 1492.83130

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.333	BV	0.1830	2.61008e4	2190.66382	100.0000

Totals : 2.61008e4 2190.66382

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.333	BV	0.1573	2.27137e4	2185.28418	100.0000

Totals : 2.27137e4 2185.28418

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.332	BV	0.1345	1.10130e4	1183.79114	100.0000

Totals : 1.10130e4 1183.79114

Sample Name: run1

### HPLC traces of compound 28

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.332	BV	0.1345	1.10130e4	1183.79114	100.0000

Totals : 1.10130e4 1183.79114

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.333	BB	0.1388	1.58261e4	1666.54199	100.0000

Totals : 1.58261e4 1666.54199

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.332	BV	0.1344	9783.57031	1052.70361	100.0000

Totals : 9783.57031 1052.70361

=====  
 \*\*\* End of Report \*\*\*

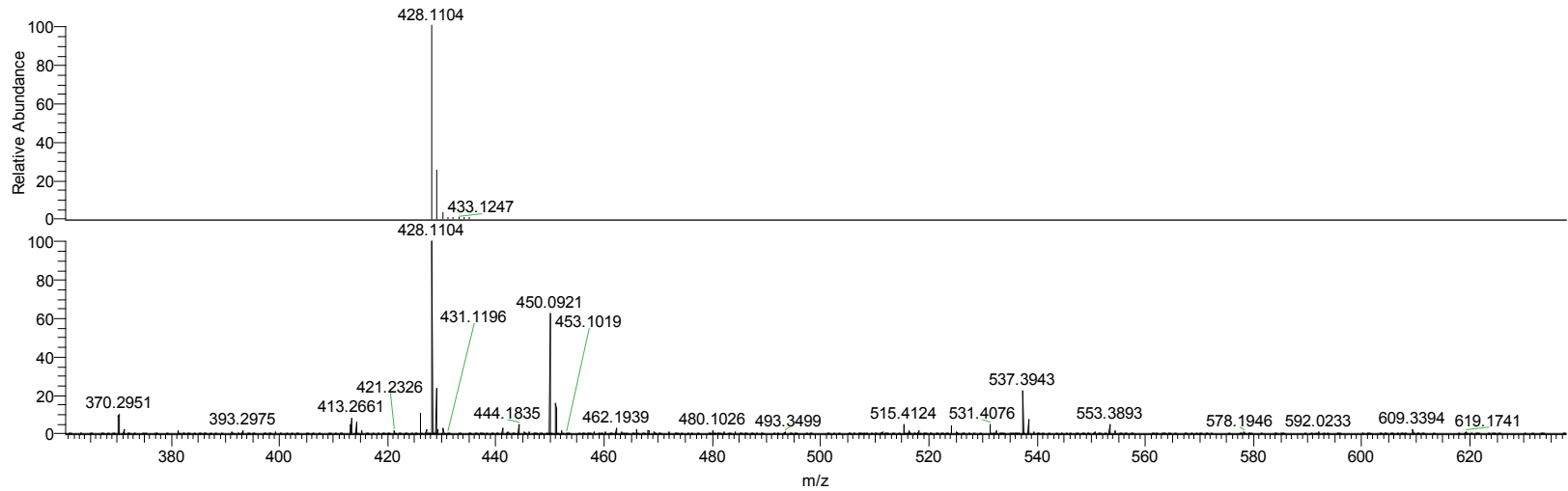
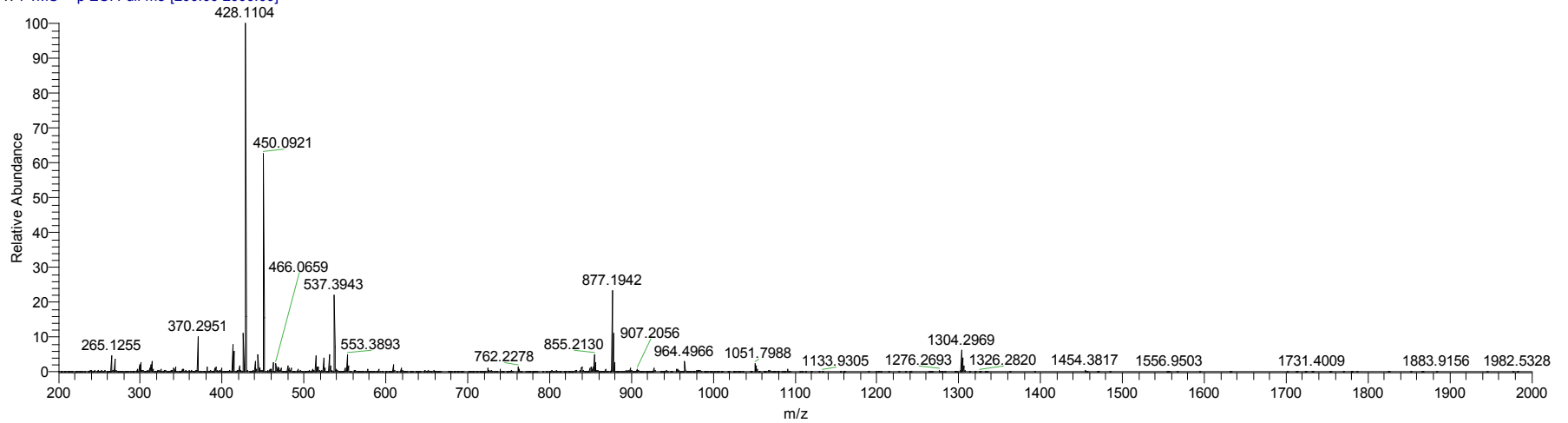
# HRMS of compound 28

C:\Xcalibur\...Matt\2-10-2013\SA-I-06

2/10/2013 5:04:20 PM

SA-I-06

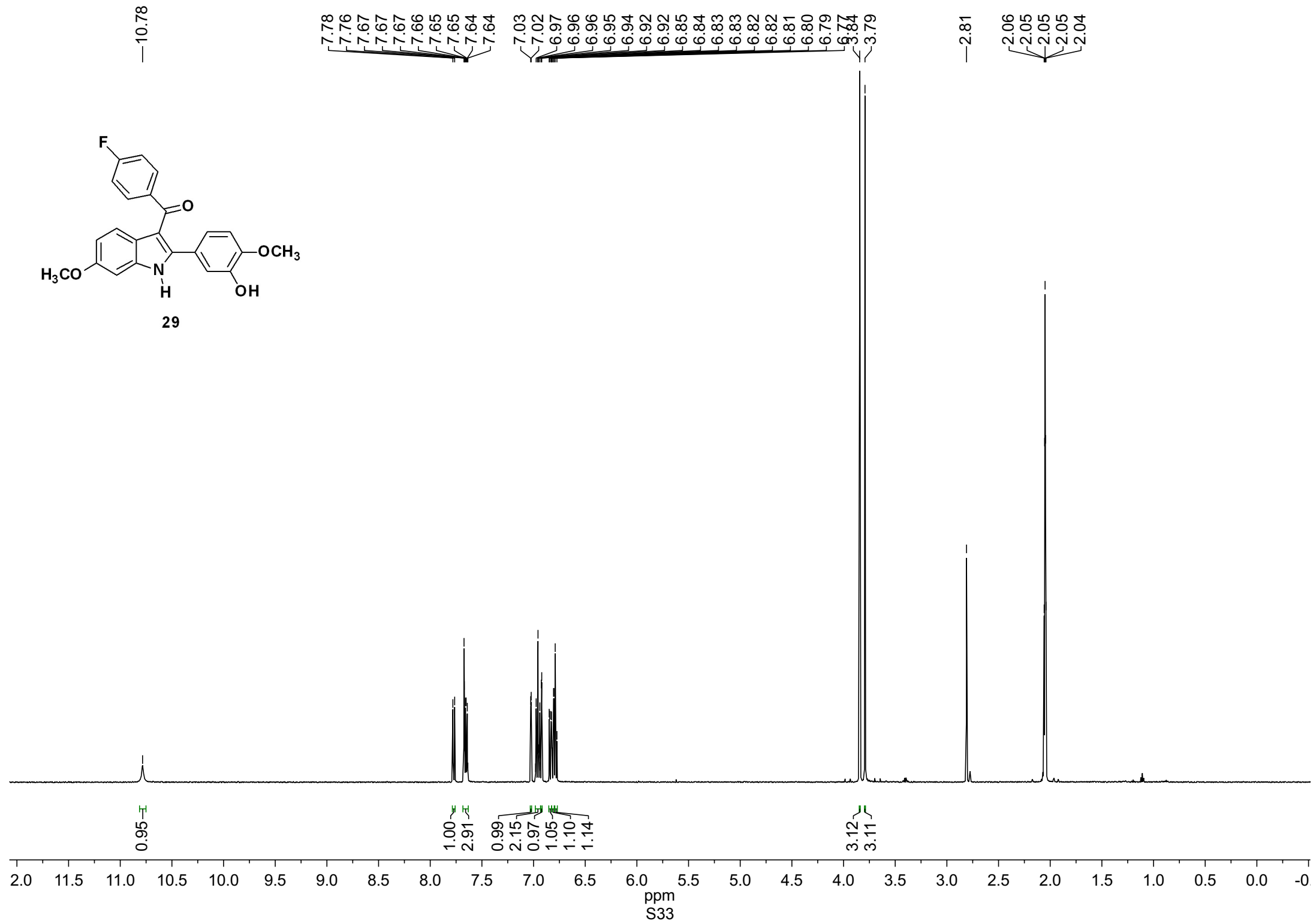
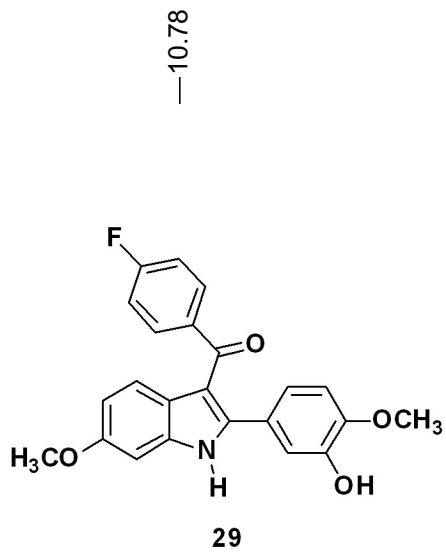
SA-I-06 #20 RT: 0.16 AV: 1 NL: 3.19E7  
T: FTMS + p ESI Full ms [200.00-2000.00]

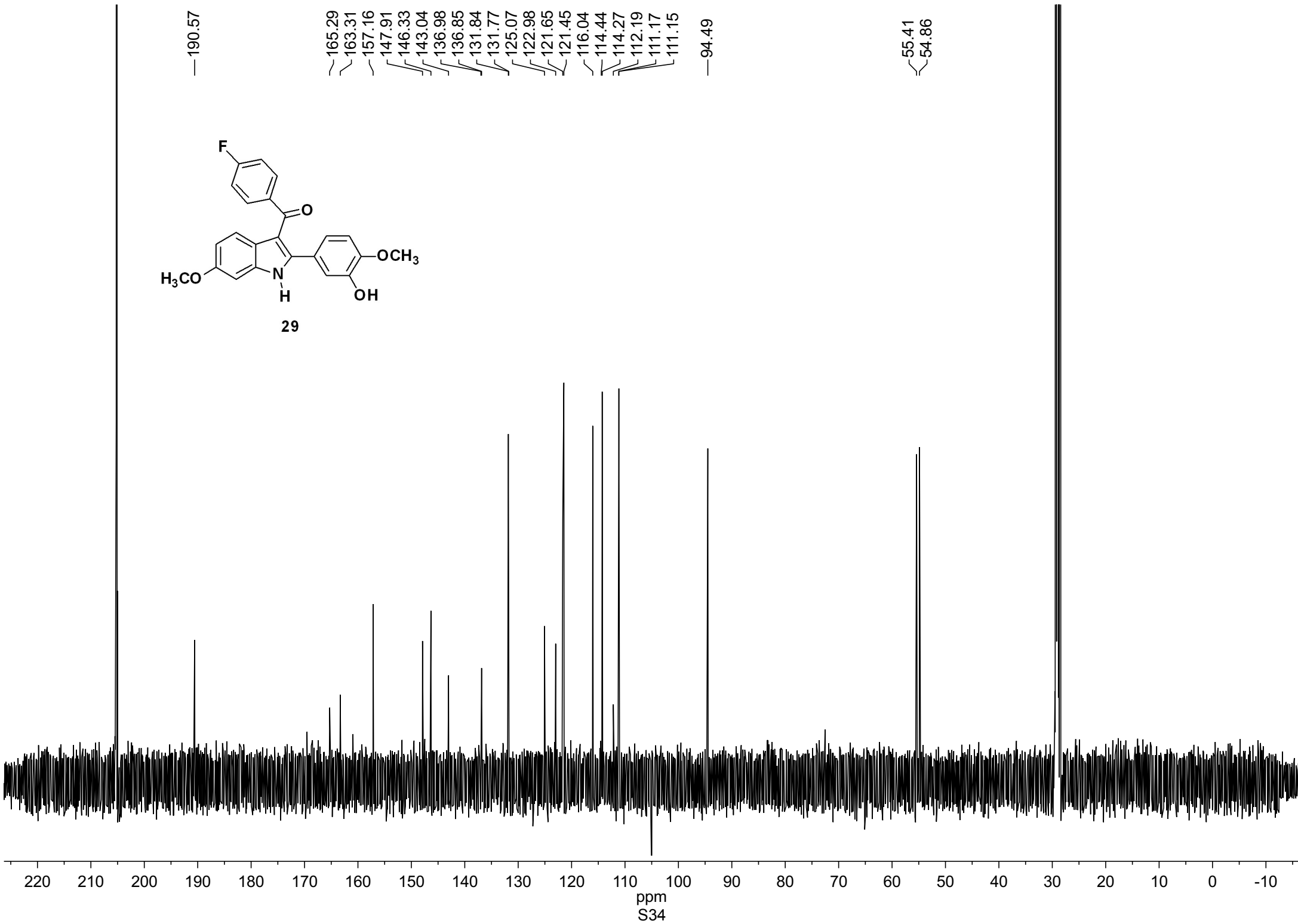
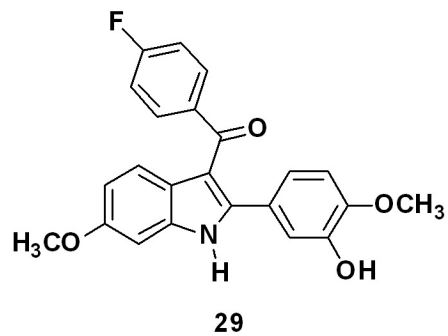


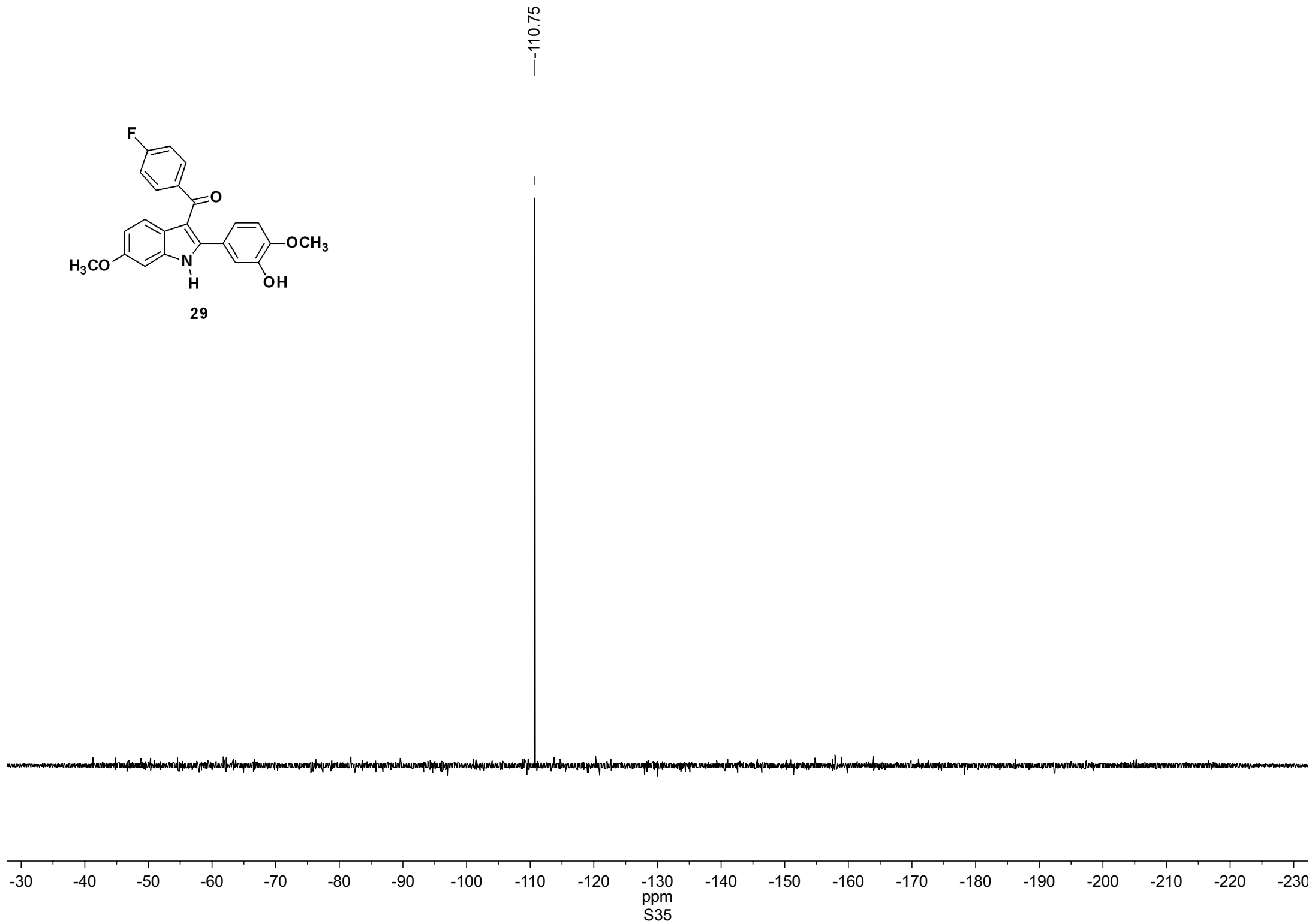
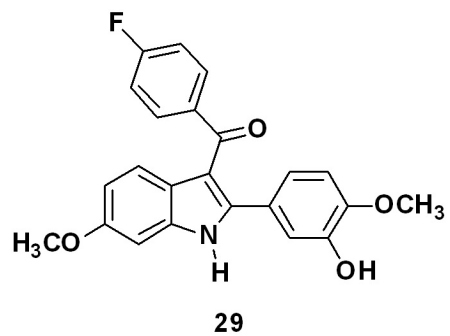
NL:  
7.69E5  
C<sub>23</sub>H<sub>17</sub>O<sub>4</sub>NF<sub>3</sub>:  
C<sub>23</sub>H<sub>17</sub>O<sub>4</sub>N<sub>1</sub>F<sub>3</sub>  
pa Chrg 1

NL:  
3.19E7  
SA-I-06#20 RT:  
0.16 AV: 1 T:  
FTMS + p ESI  
Full ms  
[200.00-2000.00]





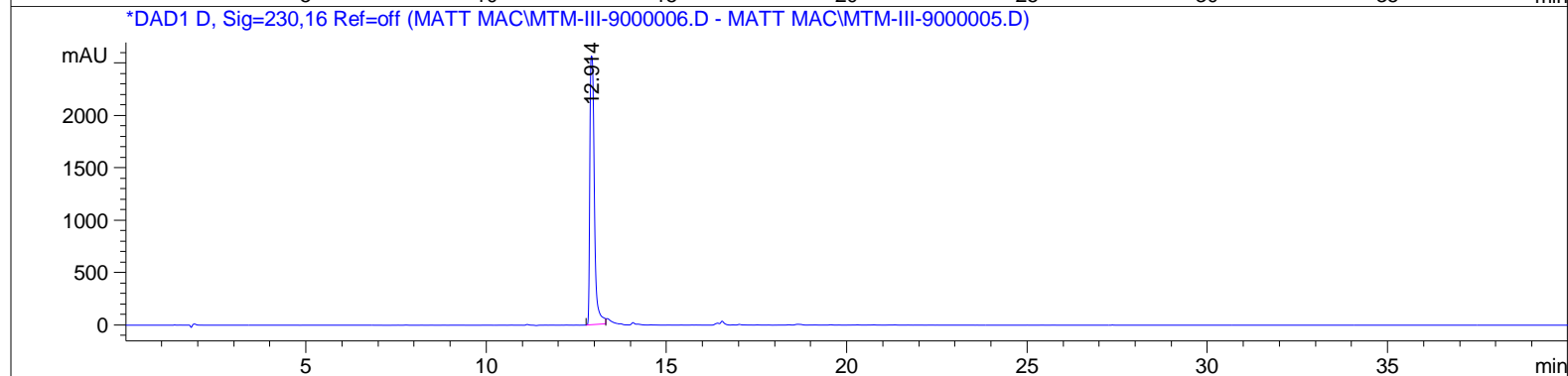
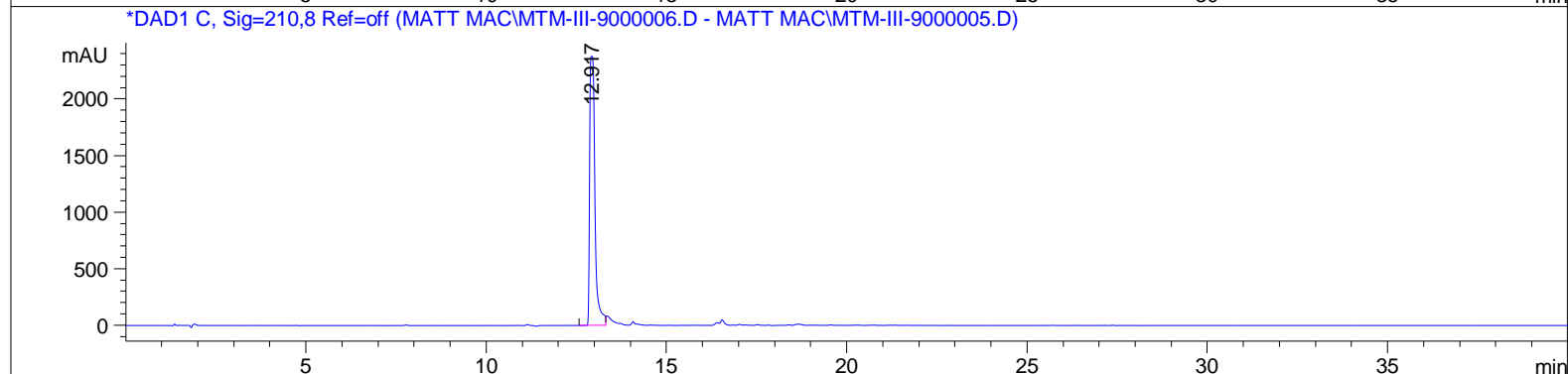
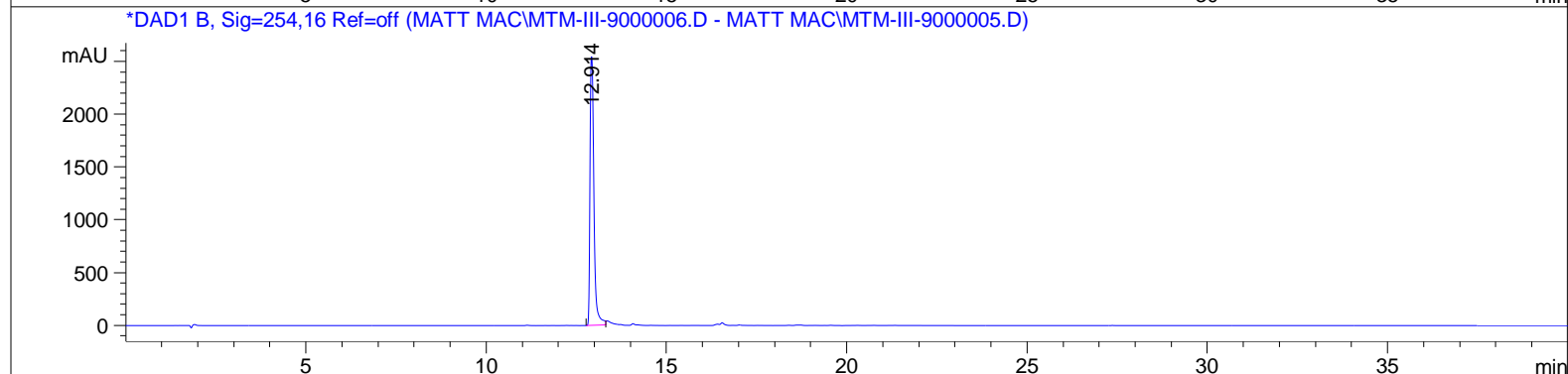
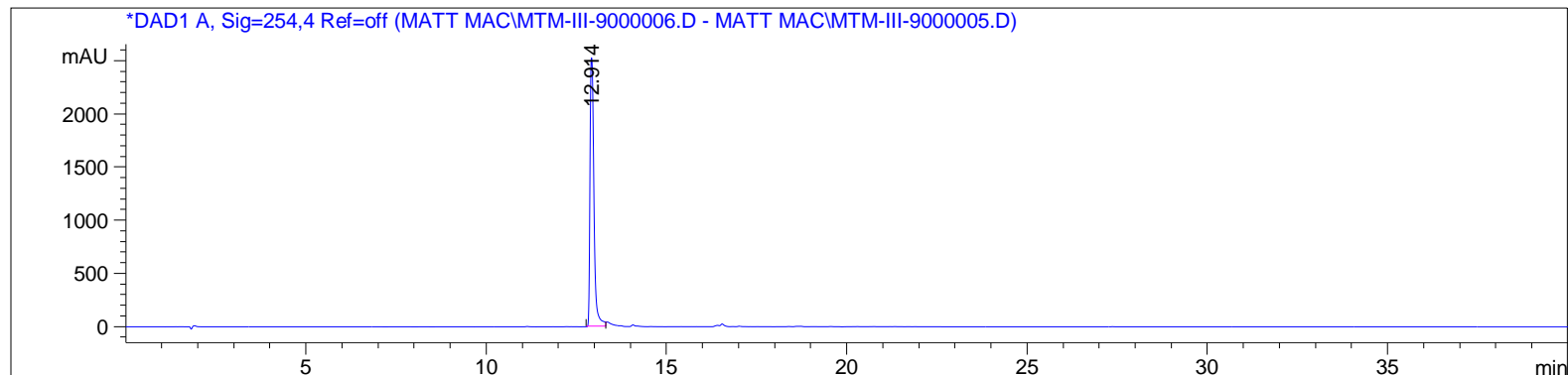




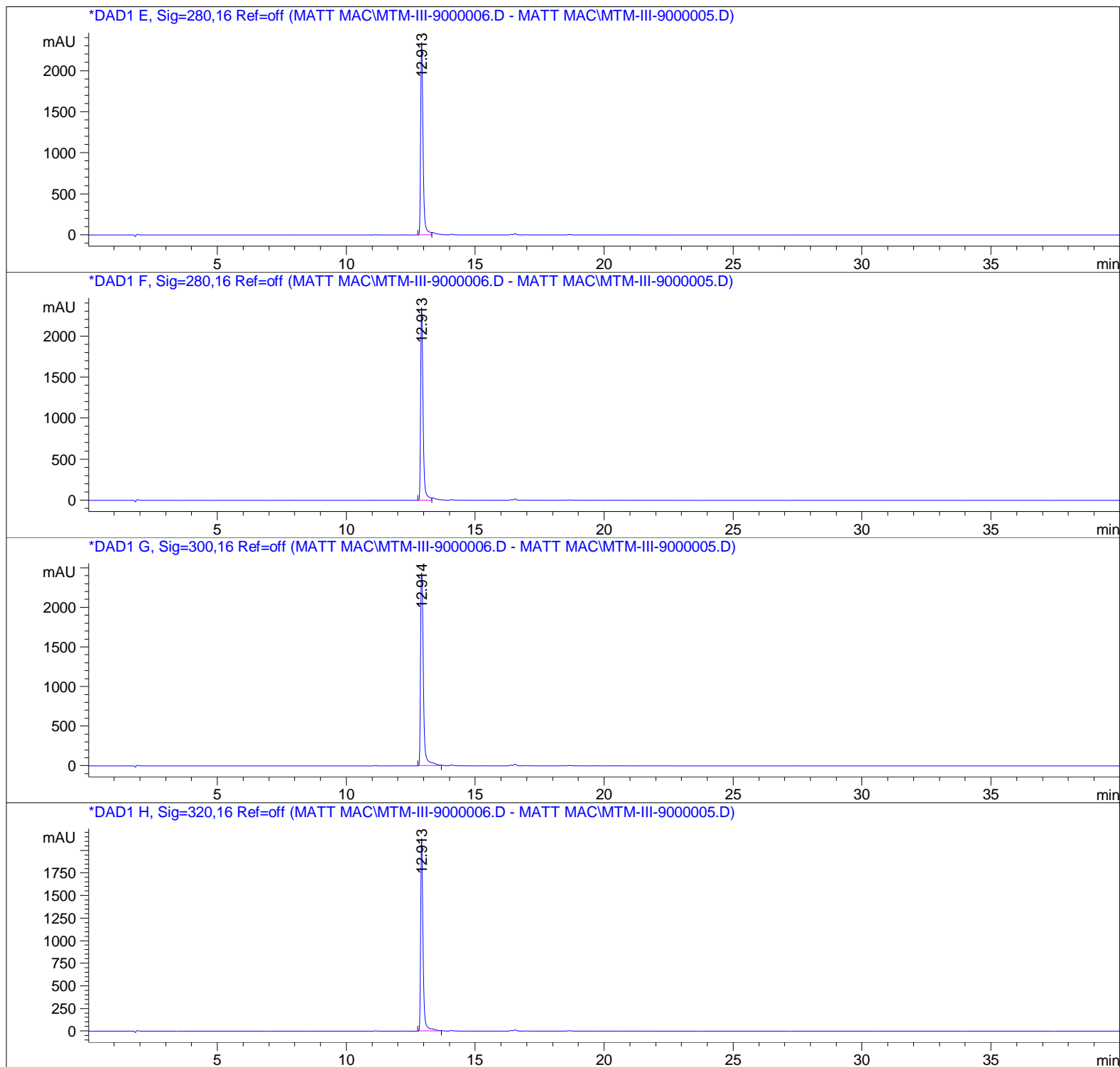
Sample Name: run1

## HPLC traces of compound 29

=====  
Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/8/2013 3:01:17 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/8/2013 2:20:25 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/8/2013 8:58:30 AM by Matt Mac  
(modified after loading)



## HPLC traces of compound 29

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 29

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.914	BV	0.1192	1.93264e4	2528.52637	100.0000

Totals : 1.93264e4 2528.52637

Signal 2: DAD1 B, Sig=254,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.914	BV	0.1185	1.93178e4	2547.96143	100.0000

Totals : 1.93178e4 2547.96143

Signal 3: DAD1 C, Sig=210,8 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.917	BV	0.1595	2.43604e4	2378.69629	100.0000

Totals : 2.43604e4 2378.69629

Signal 4: DAD1 D, Sig=230,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.914	BV	0.1364	2.25143e4	2565.28882	100.0000

Totals : 2.25143e4 2565.28882

Sample Name: run1

## HPLC traces of compound 29

Signal 5: DAD1 E, Sig=280,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.913	BV	0.1006	1.53996e4	2346.69971	100.0000

Totals : 1.53996e4 2346.69971

Signal 6: DAD1 F, Sig=280,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.913	BV	0.1006	1.53996e4	2346.69971	100.0000

Totals : 1.53996e4 2346.69971

Signal 7: DAD1 G, Sig=300,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.914	BV	0.1206	1.89096e4	2435.48779	100.0000

Totals : 1.89096e4 2435.48779

Signal 8: DAD1 H, Sig=320,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.913	BV	0.0976	1.38327e4	2135.87988	100.0000

Totals : 1.38327e4 2135.87988

\*\*\* End of Report \*\*\*

# HRMS of compound 29

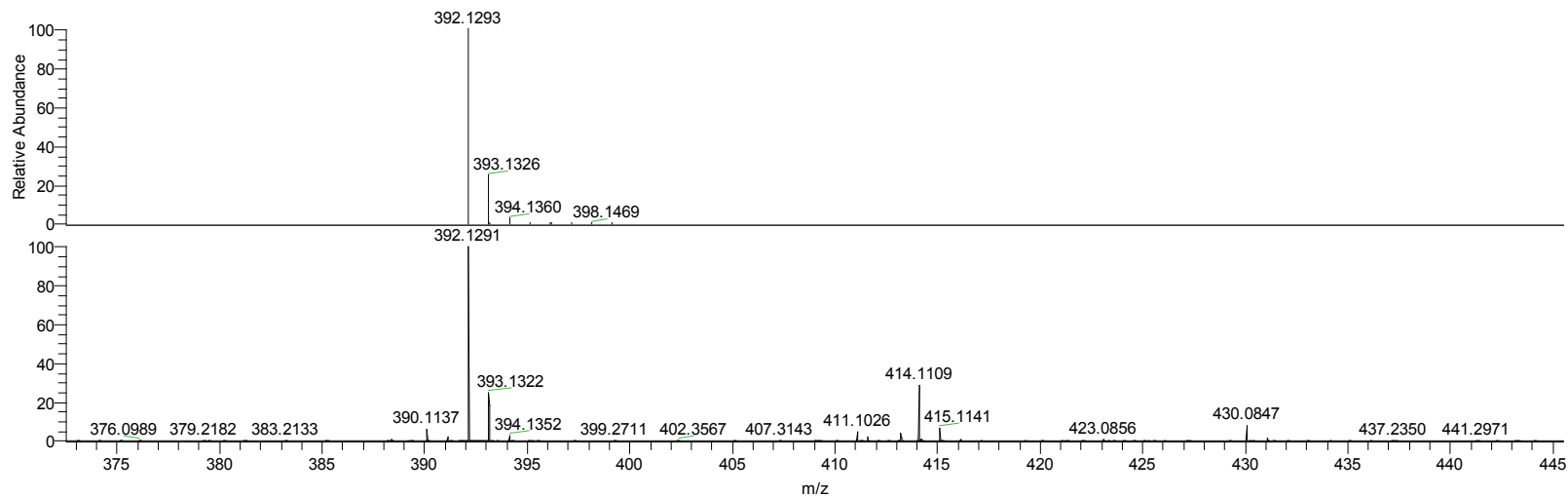
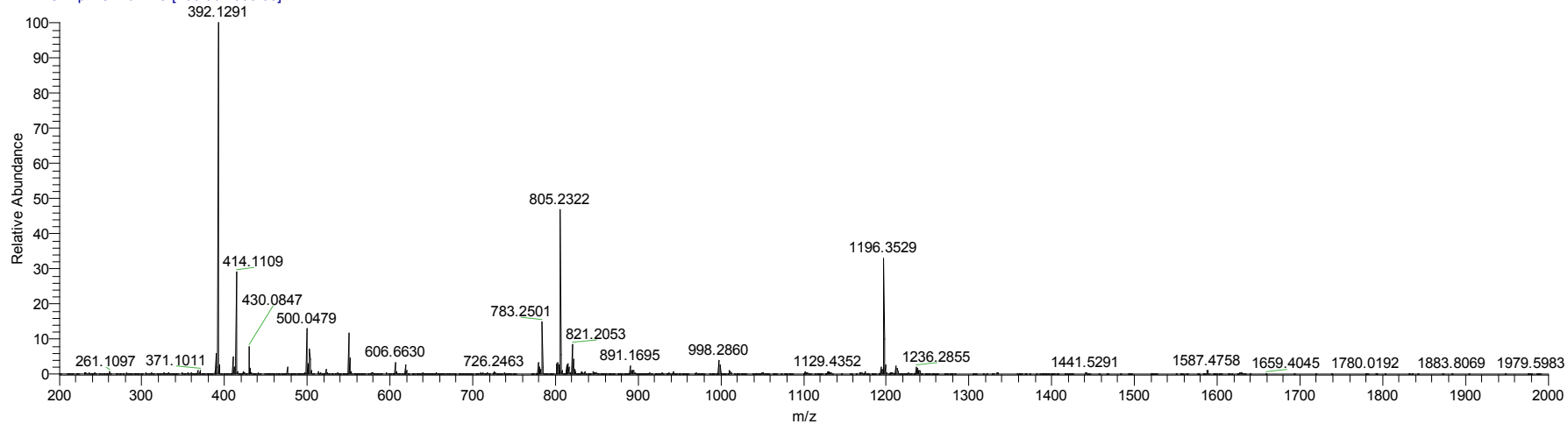
C:\Xcalibur\...MTM-III-90\_+ESI

2/10/2013 10:32:12 AM

MTM-III-90

MTM-III-90\_+ESI #20 RT: 0.15 AV: 1 NL: 2.27E8

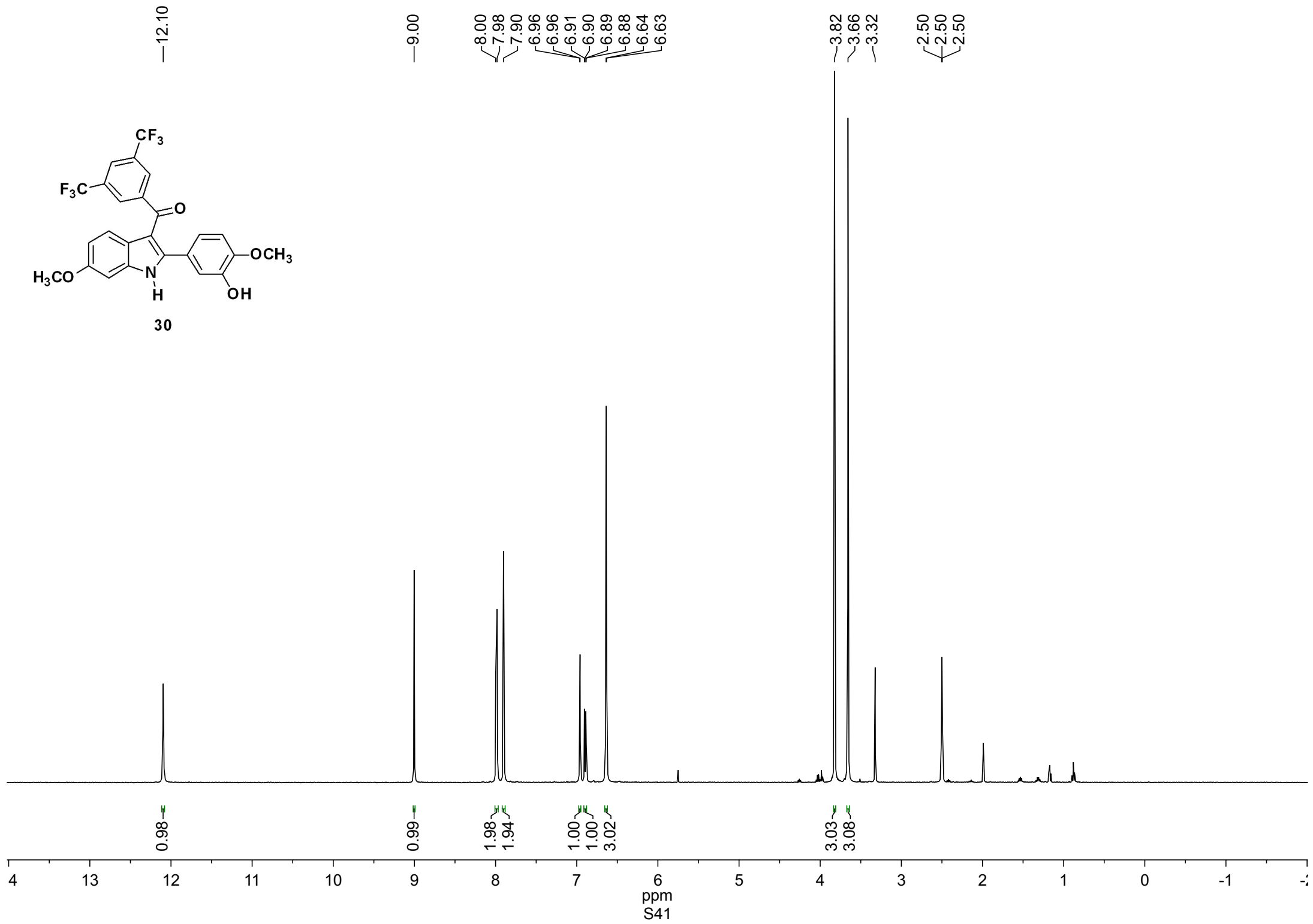
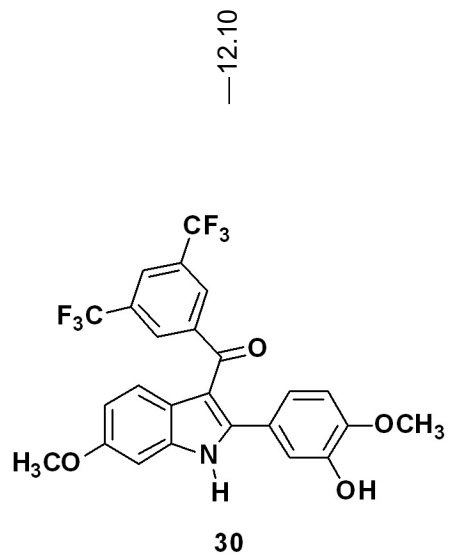
T: FTMS + p ESI Full ms [200.00-2000.00]

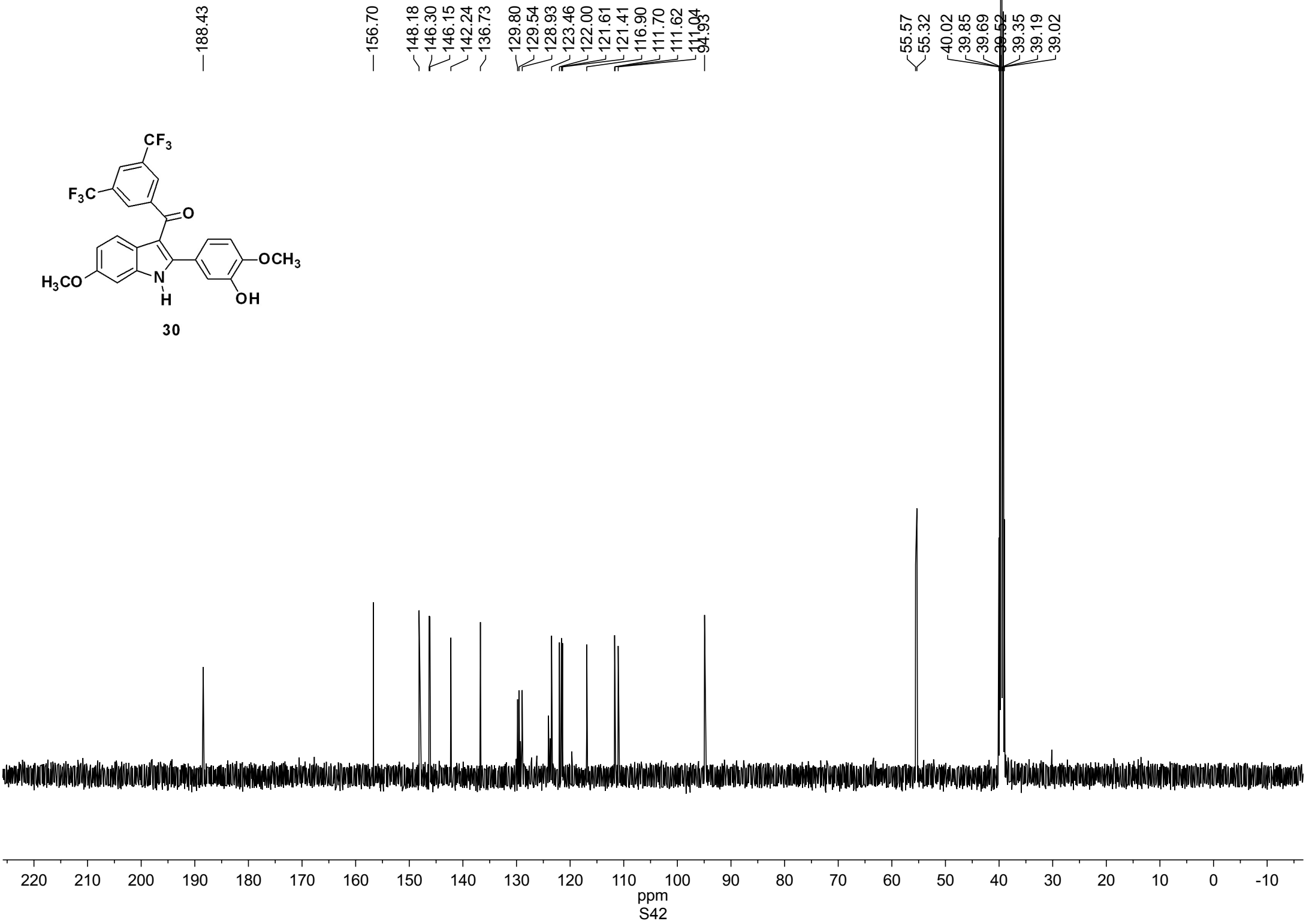
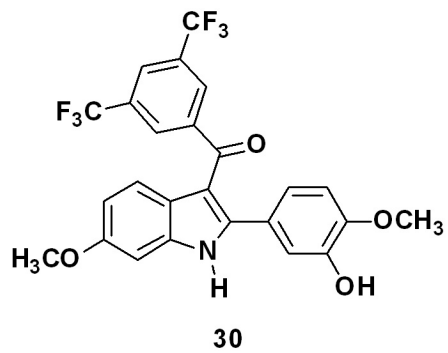


NL:  
7.69E5  
C<sub>23</sub>H<sub>19</sub>O<sub>4</sub>NF:  
C<sub>23</sub>H<sub>19</sub>O<sub>4</sub>N<sub>1</sub>F<sub>1</sub>  
pa Chrg 1

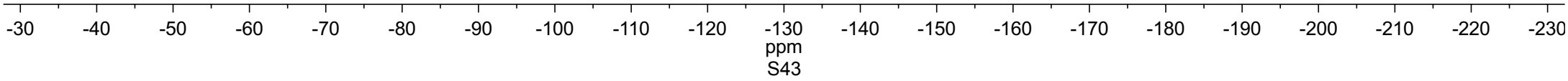
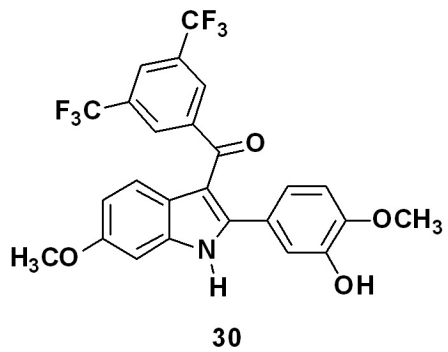
NL:  
2.27E8  
MTM-III-90\_+ESI#20  
RT: 0.15 AV: 1 T:  
FTMS + p ESI Full  
ms [200.00-2000.00]







—61.41

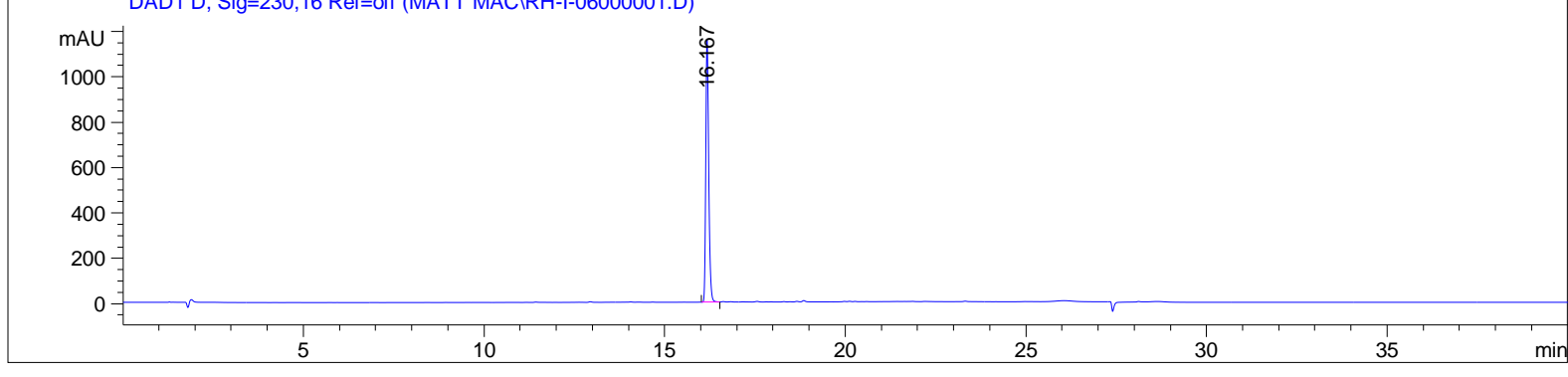
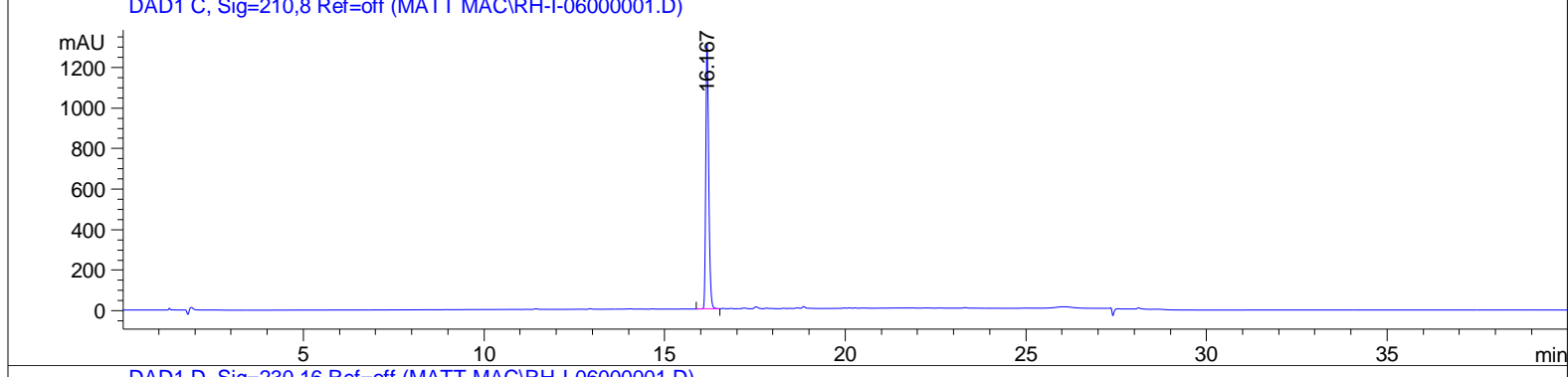
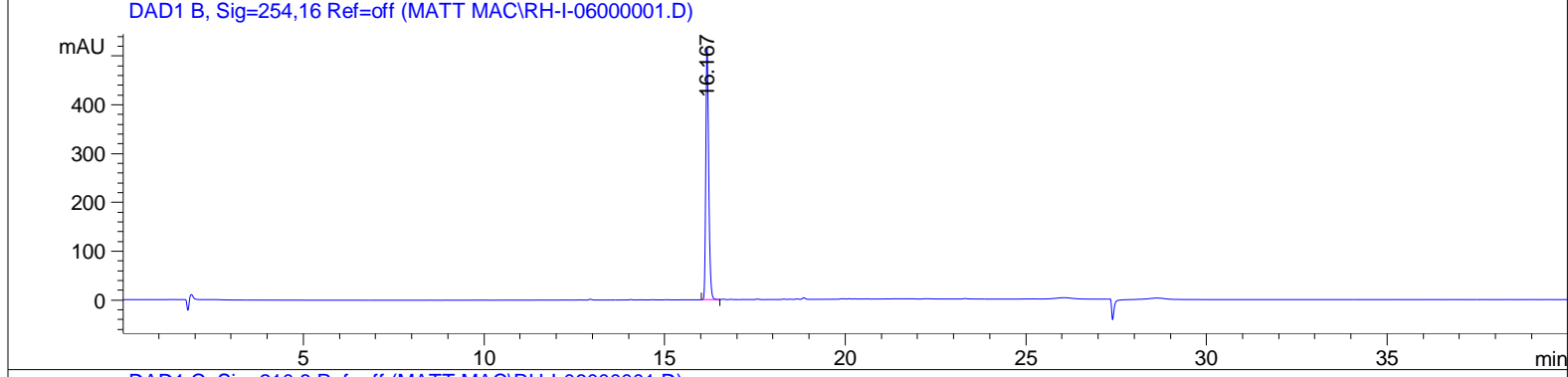
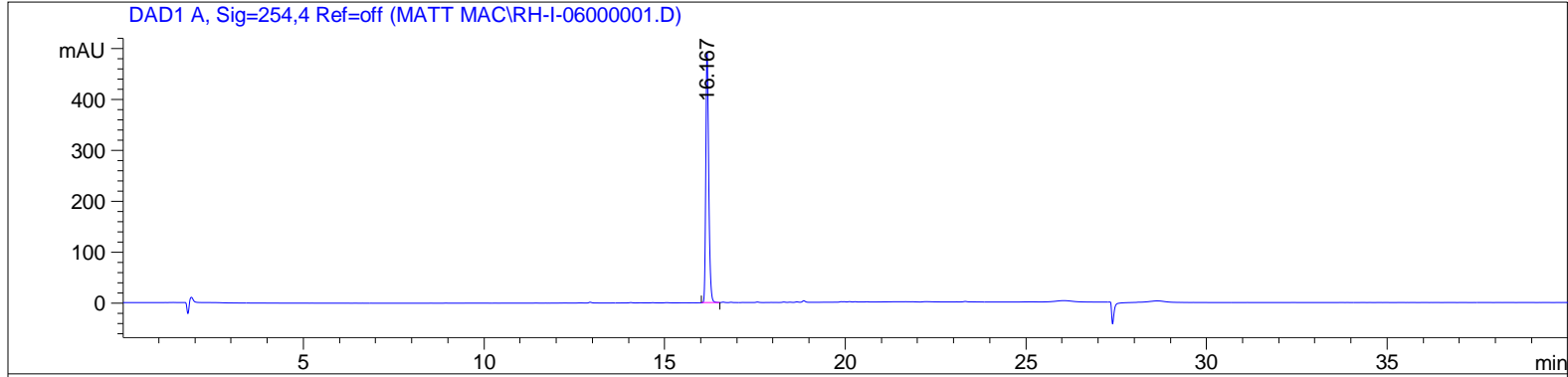


Sample Name: run1

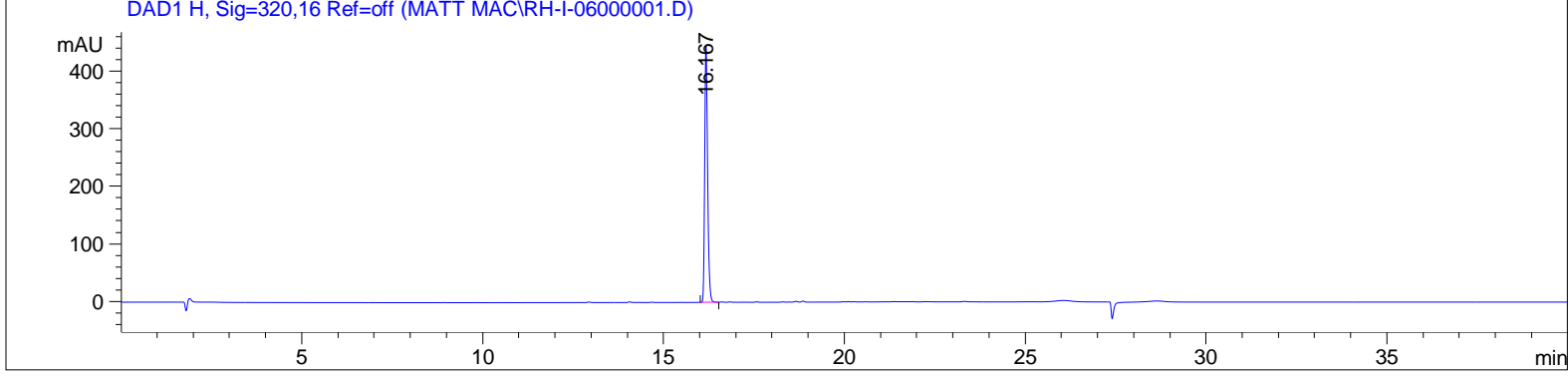
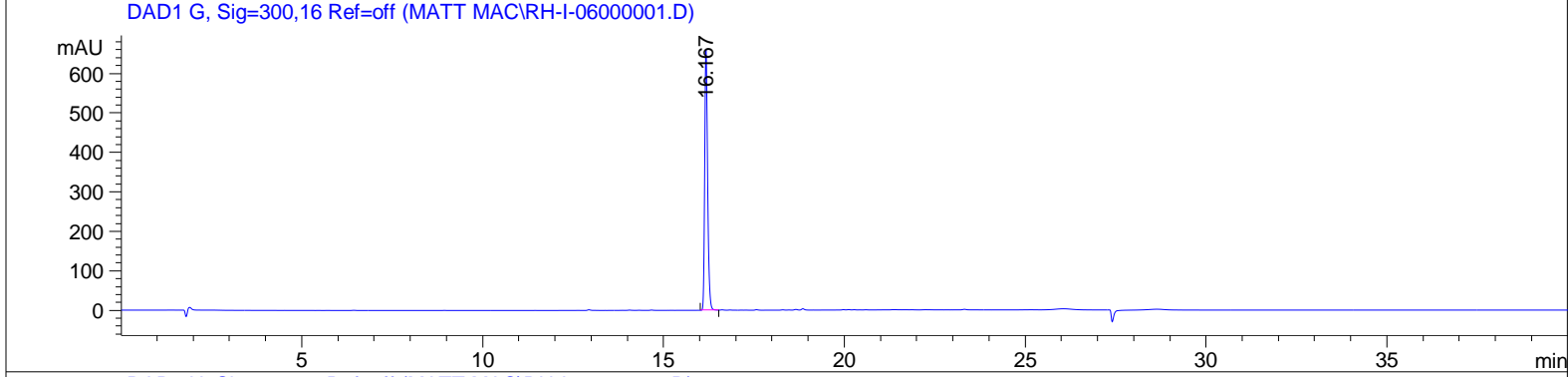
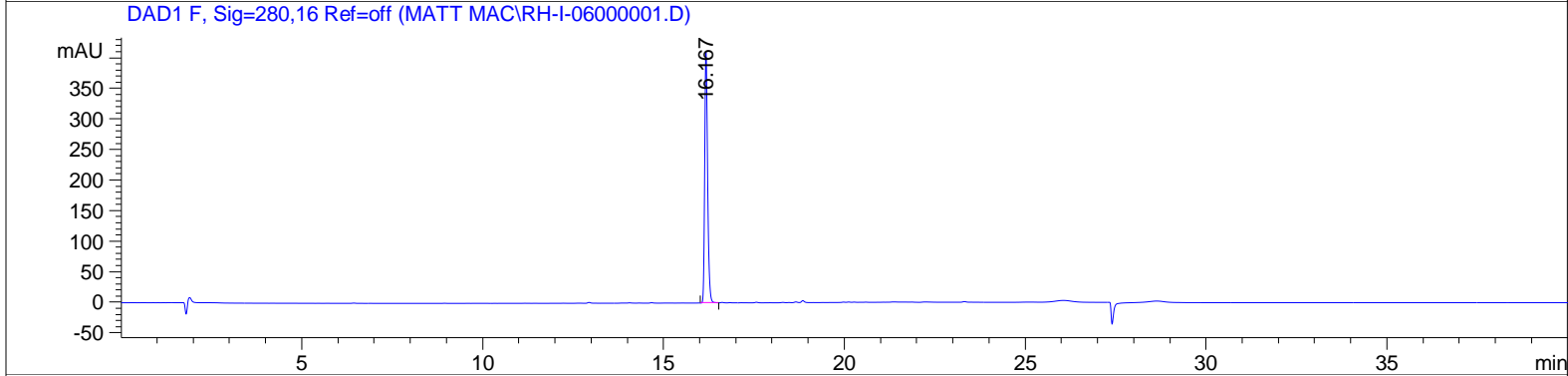
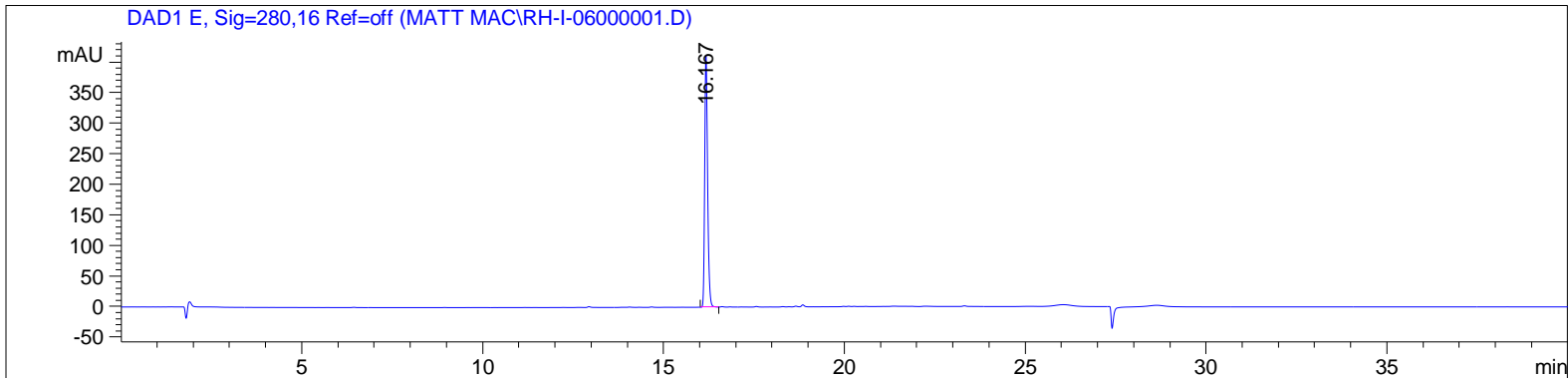
### HPLC traces of compound 30

=====

Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/9/2013 3:45:45 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:59:47 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:04:11 PM by Matt Mac  
(modified after loading)



### HPLC traces of compound 30



=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

### HPLC traces of compound 30

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0852	2759.49121	493.87103	100.0000

Totals : 2759.49121 493.87103

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0852	2894.88745	518.10498	100.0000

Totals : 2894.88745 518.10498

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0860	7422.78369	1312.45374	100.0000

Totals : 7422.78369 1312.45374

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0856	6530.87451	1161.71985	100.0000

Totals : 6530.87451 1161.71985

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0851	2305.04321	413.06256	100.0000

Totals : 2305.04321 413.06256

Sample Name: run1

### HPLC traces of compound 30

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0851	2305.04321	413.06256	100.0000

Totals : 2305.04321 413.06256

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0852	3709.70337	663.46100	100.0000

Totals : 3709.70337 663.46100

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.167	BV	0.0852	2500.62109	447.69040	100.0000

Totals : 2500.62109 447.69040

=====  
 \*\*\* End of Report \*\*\*

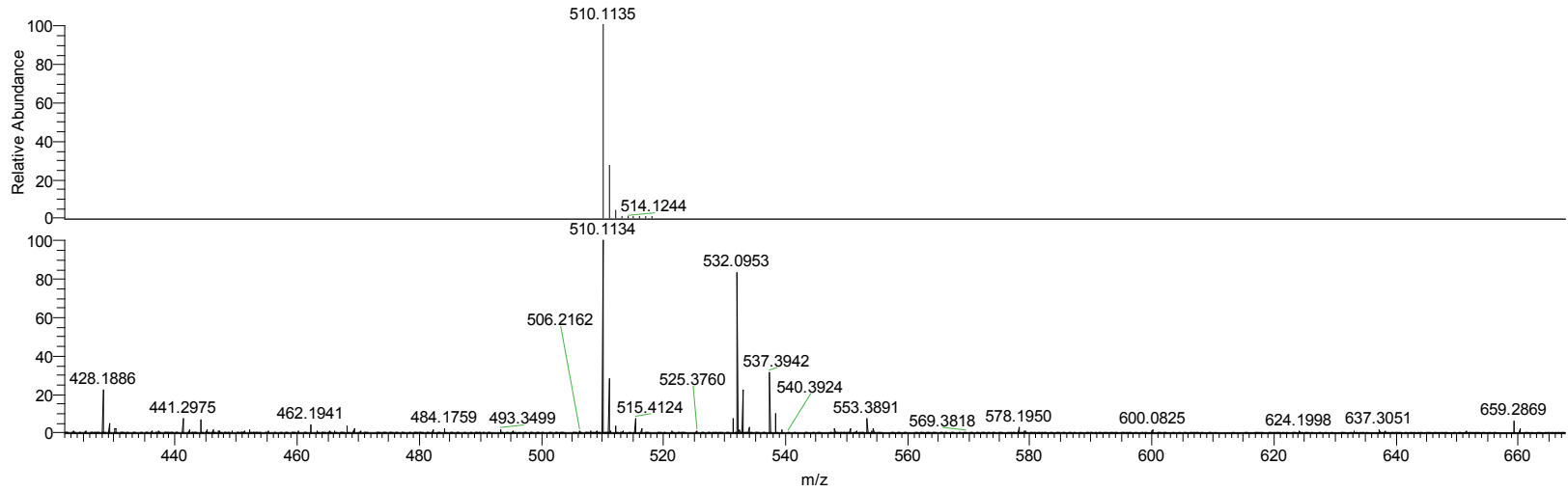
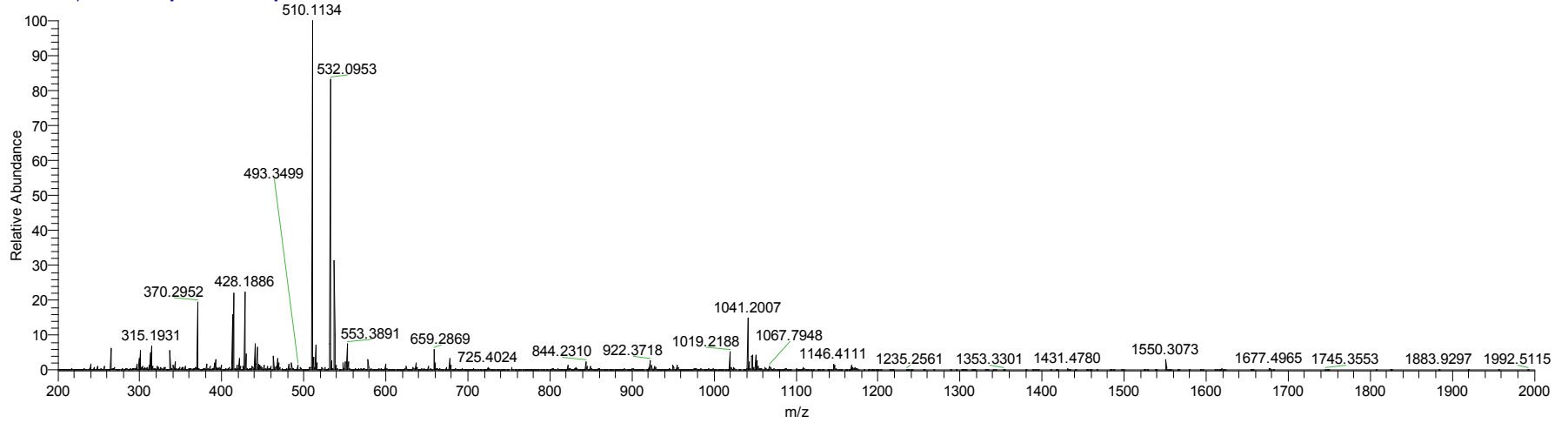
# HRMS of compound 30

C:\Xcalibur\...Matt\2-10-2013\RH-I-06

2/10/2013 3:37:45 PM

RH-I-06

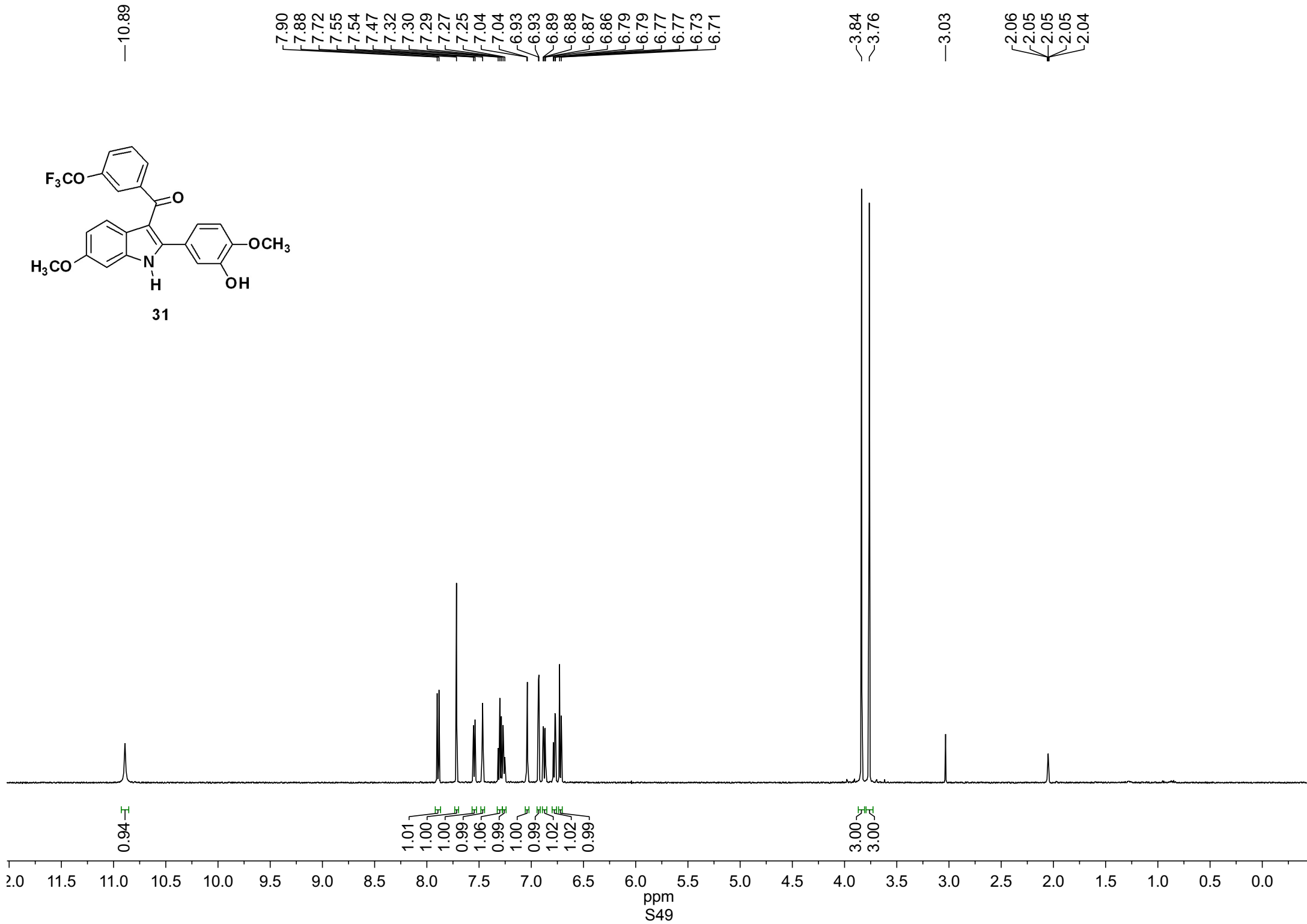
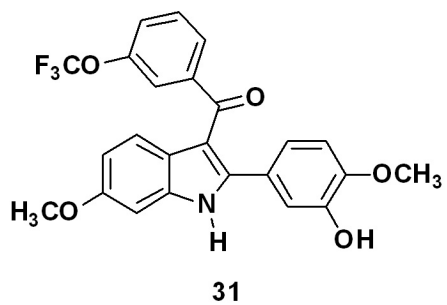
RH-I-06 #14 RT: 0.14 AV: 1 NL: 1.05E7  
T: FTMS + p ESI Full ms [200.00-2000.00]

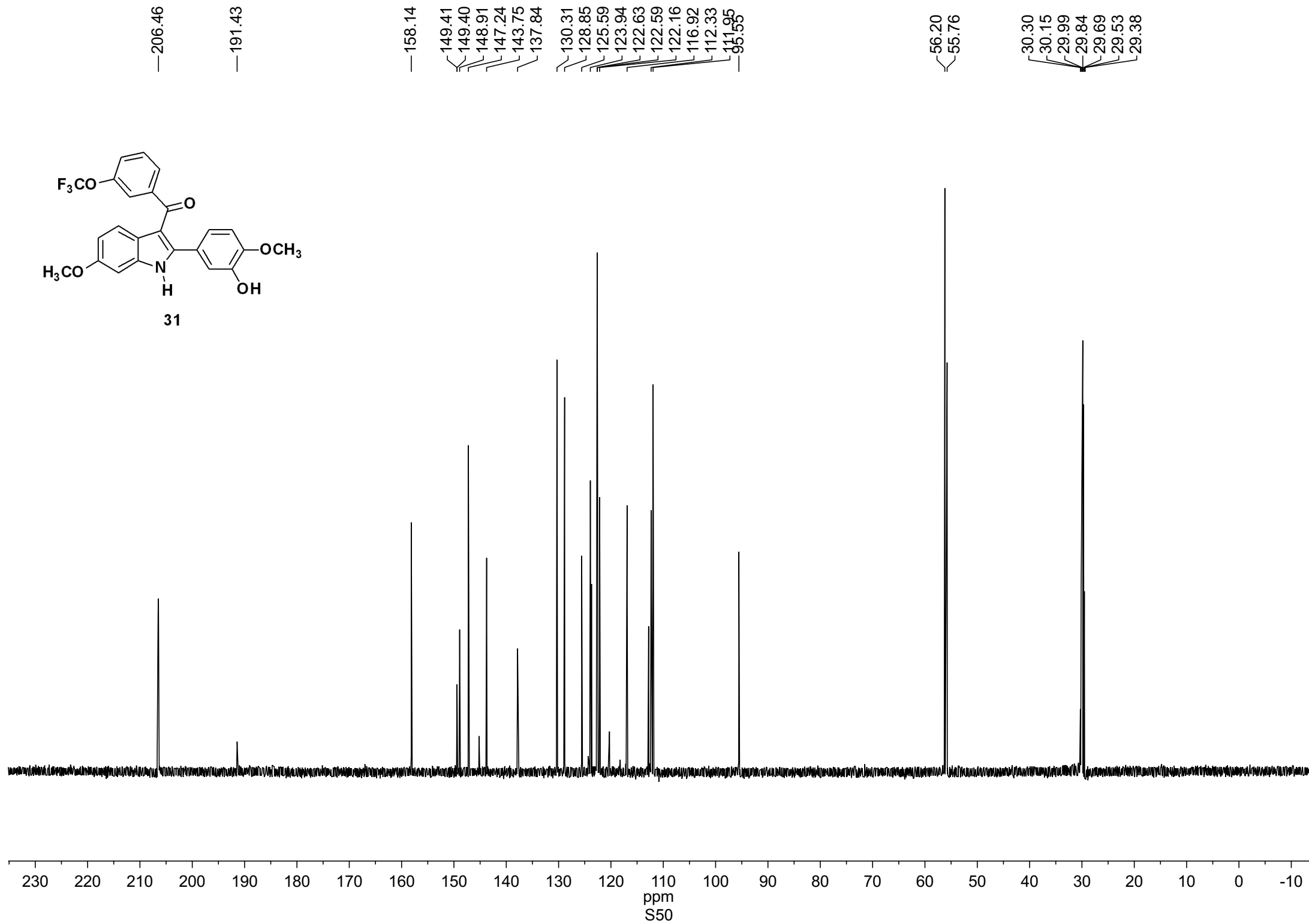
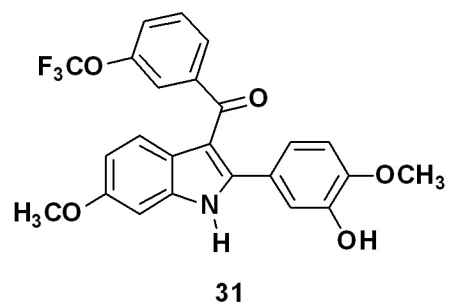


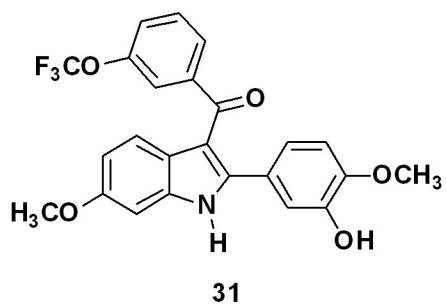
NL:  
7.52E5  
C<sub>25</sub>H<sub>18</sub>O<sub>4</sub>N<sub>1</sub>F<sub>6</sub>  
pa Chrg 1

NL:  
1.05E7  
RH-I-06#14 RT:  
0.14 AV: 1 T:  
FTMS + p ESI  
Full ms  
[200.00-2000.00]

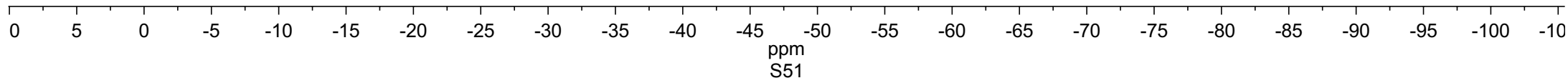








---58.50

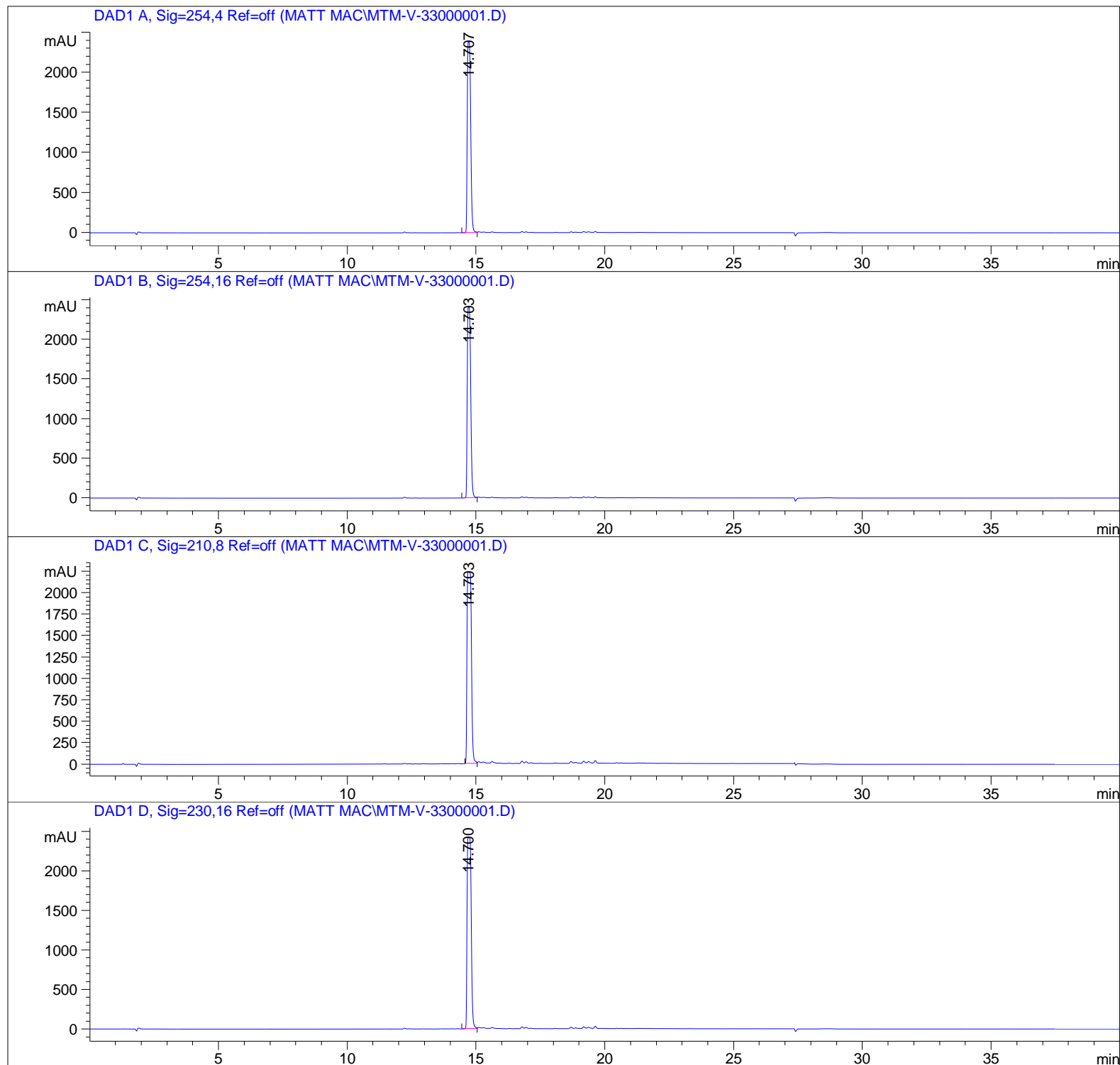


Sample Name: run1

## HPLC traces of compound 31

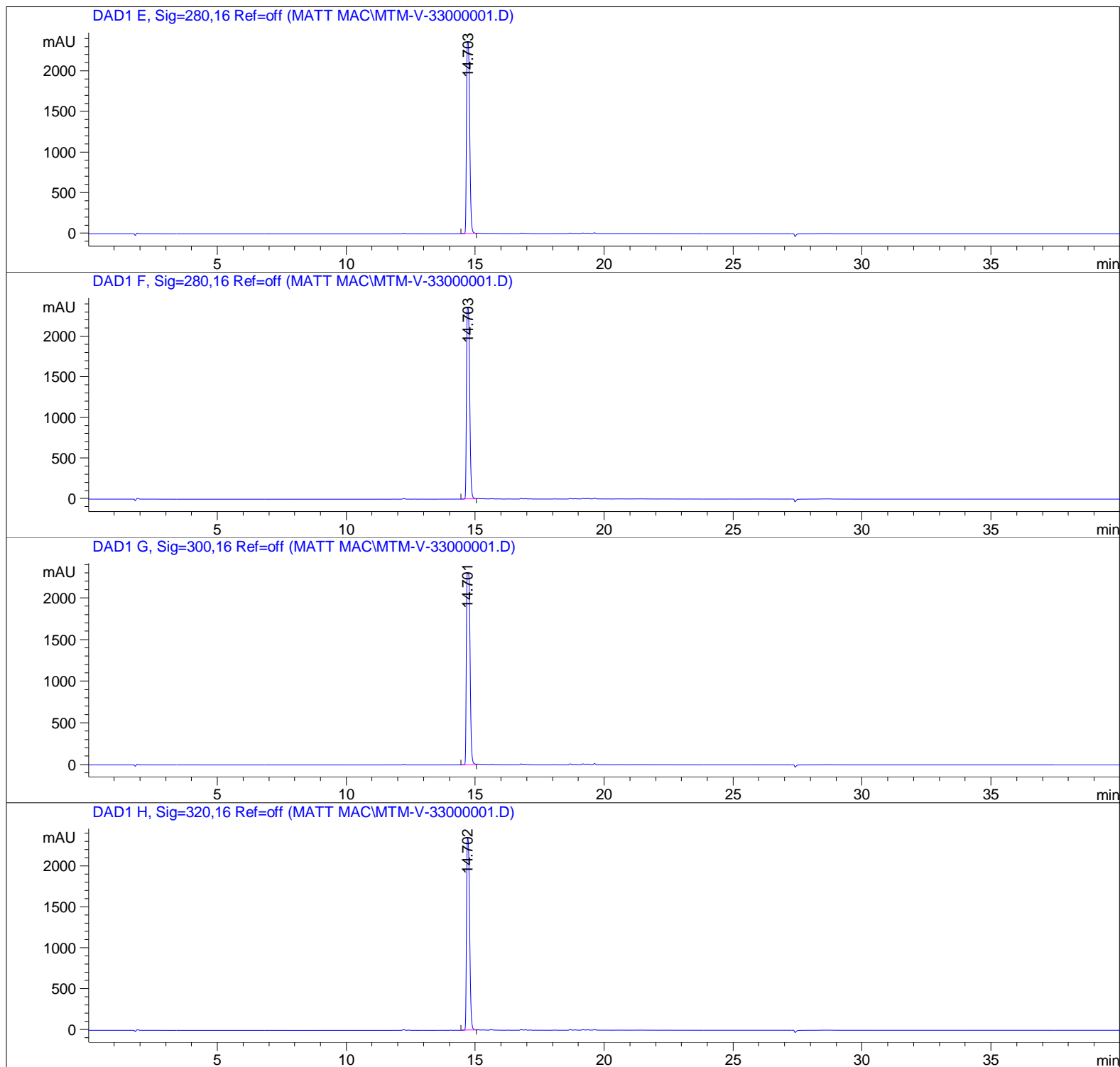
=====

Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/10/2013 10:51:03 AM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/10/2013 10:04:38 AM by Matt Mac  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/10/2013 10:52:42 AM by Matt Mac  
(modified after loading)



Sample Name: run1

## HPLC traces of compound 31

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 31

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.707	BV	0.1464	2.17409e4	2383.37598	100.0000

Totals : 2.17409e4 2383.37598

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.703	BV	0.1489	2.21007e4	2411.10132	100.0000

Totals : 2.21008e4 2411.10132

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.703	BV	0.1598	2.59557e4	2230.39380	100.0000

Totals : 2.59557e4 2230.39380

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.700	BV	0.1769	2.63170e4	2418.76001	100.0000

Totals : 2.63170e4 2418.76001

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.703	BV	0.1372	2.00450e4	2357.87817	100.0000

Totals : 2.00450e4 2357.87817

Sample Name: run1

## HPLC traces of compound 31

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.703	BV	0.1372	2.00450e4	2357.87817	100.0000

Totals : 2.00450e4 2357.87817

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.701	BV	0.1575	2.24037e4	2303.29663	100.0000

Totals : 2.24037e4 2303.29663

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.702	BV	0.1321	1.93282e4	2345.59521	100.0000

Totals : 1.93282e4 2345.59521

=====  
\*\*\* End of Report \*\*\*

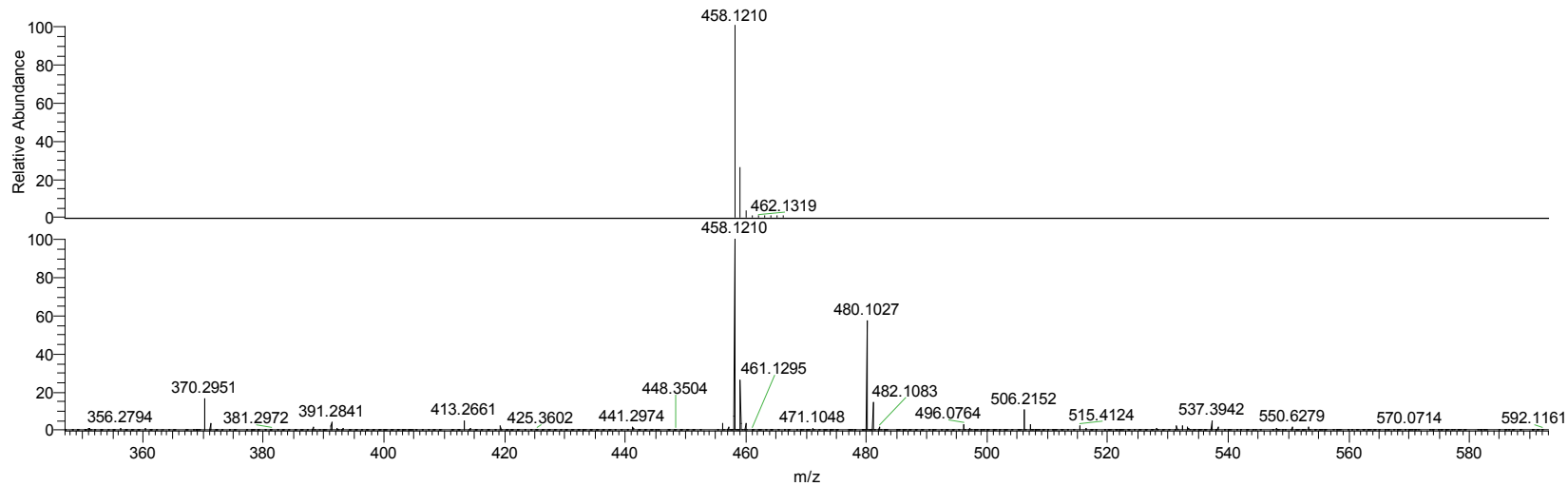
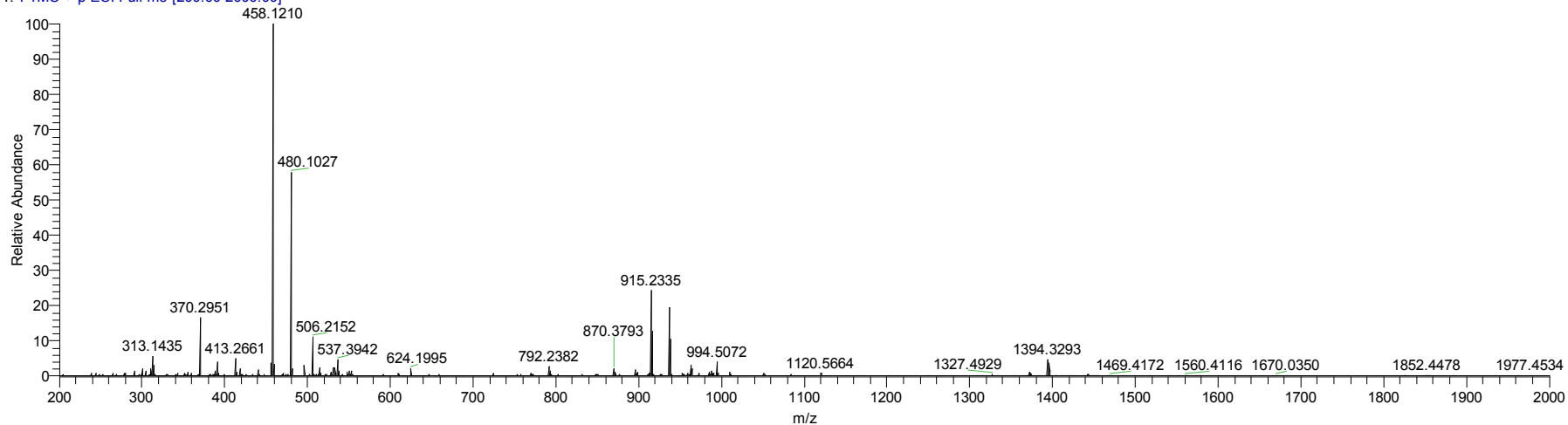
# HRMS of compound 31

C:\Xcalibur\...Matt2-10-2013\MTM-V-33

2/10/2013 12:38:13 PM

MTM-V-33

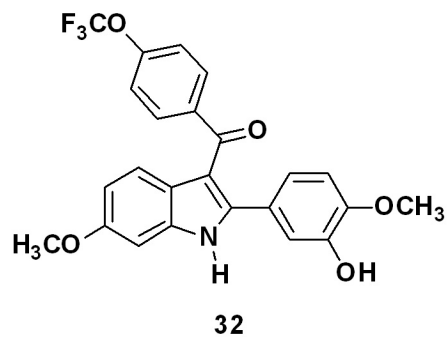
MTM-V-33 #20 RT: 0.17 AV: 1 NL: 1.18E7  
T: FTMS + p ESI Full ms [200.00-2000.00]



NL:  
7.59E5  
C<sub>24</sub>H<sub>19</sub>O<sub>5</sub>NF<sub>3</sub>  
C<sub>24</sub>H<sub>19</sub>O<sub>5</sub>N<sub>1</sub>F<sub>3</sub>  
pa Chrg 1

NL:  
1.18E7  
MTM-V-33#20  
RT: 0.17 AV: 1 T:  
FTMS + p ESI Full  
ms  
[200.00-2000.00]





—10.86

7.92  
7.90  
7.69  
7.66  
7.64  
7.11  
7.09  
7.04  
7.03  
6.90  
6.88  
6.88  
6.86  
6.86  
6.71

3.84  
3.77

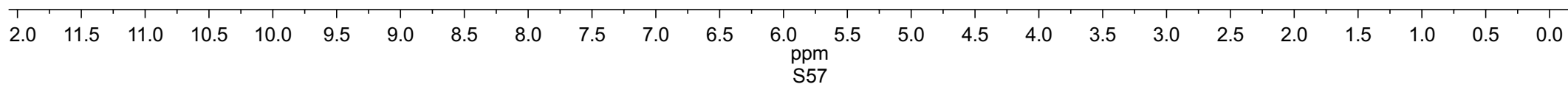
—2.94

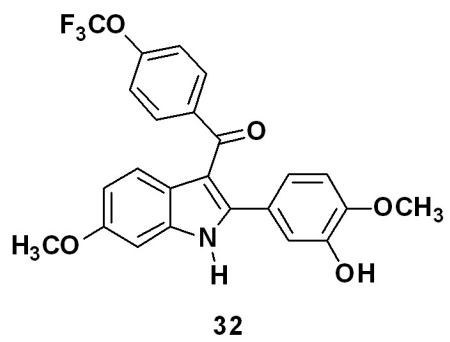
2.06  
2.05  
2.05  
2.05  
2.04

0.90

1.00  
0.97  
1.97  
2.01  
1.00  
0.98  
1.03  
2.01

3.00  
3.01

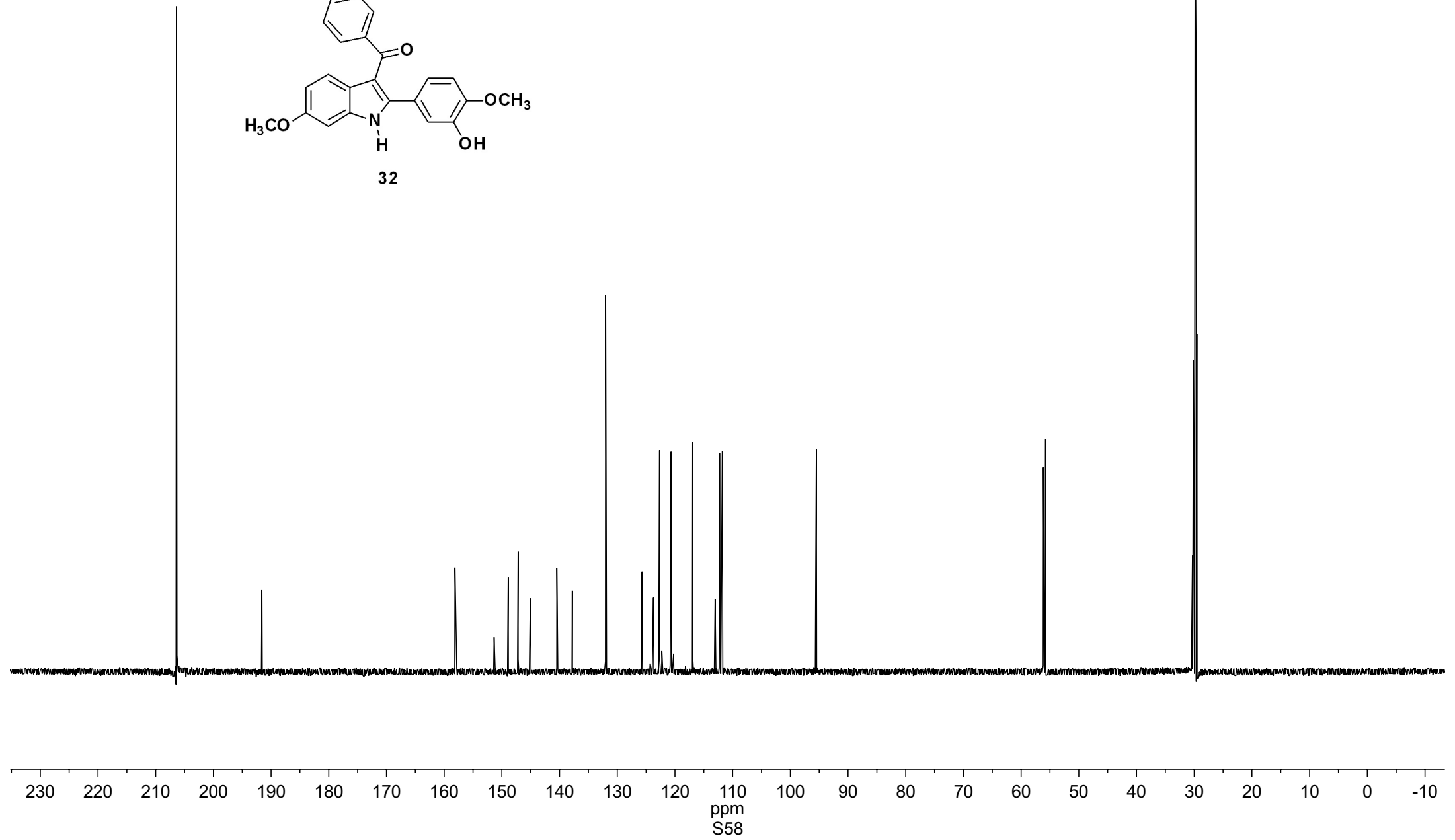


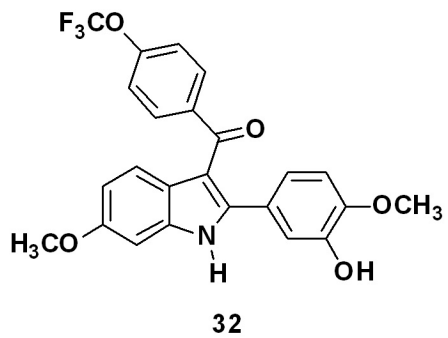


206.40  
191.59  
158.13  
151.36  
151.34  
151.33  
151.32  
148.90  
147.18  
145.07  
140.47  
137.80  
132.01  
125.70  
124.30  
123.73  
122.72  
122.67  
122.27  
120.68  
120.23  
118.19  
116.93  
113.04  
112.26  
111.79  
95.50

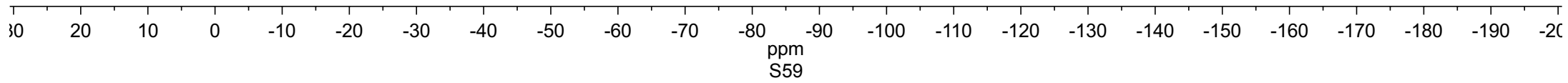
56.14  
55.77

30.30  
30.15  
29.99  
29.84  
29.69  
29.53  
29.38





58.50

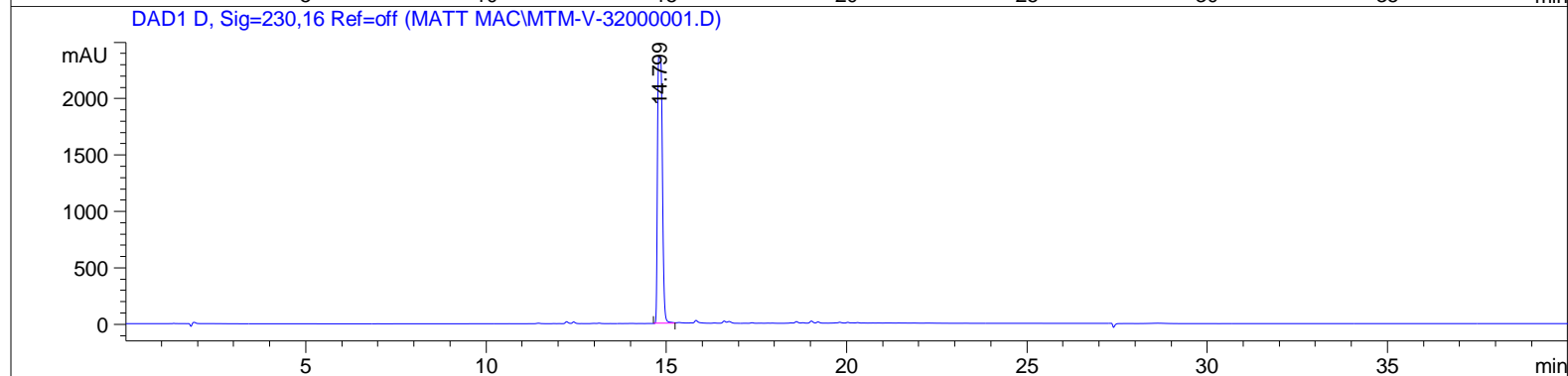
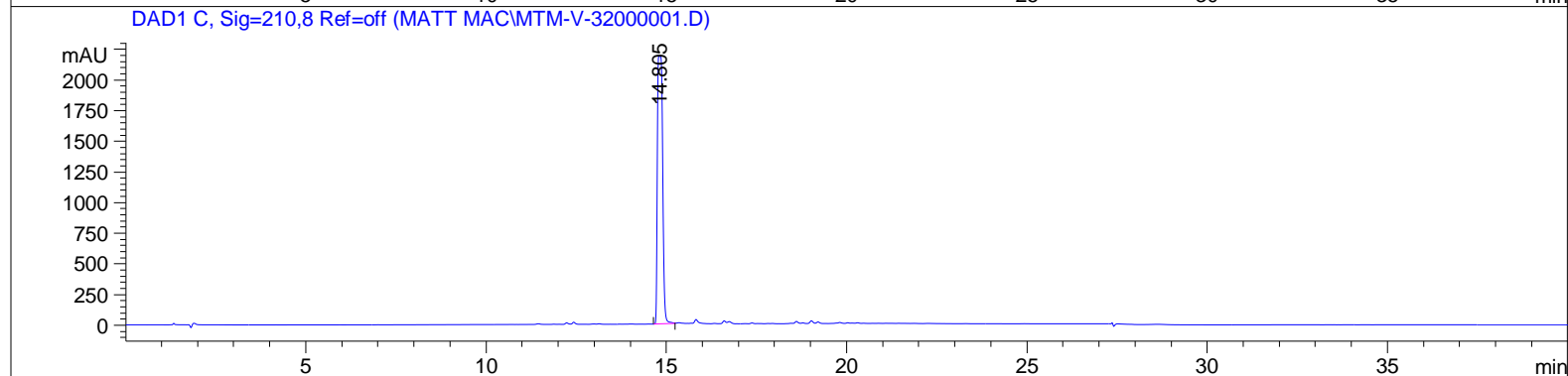
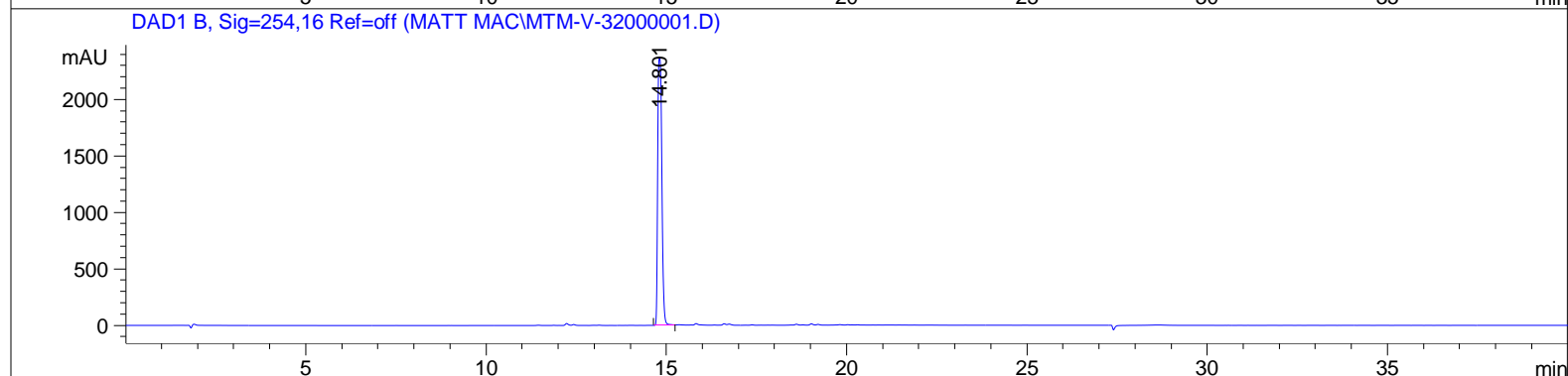
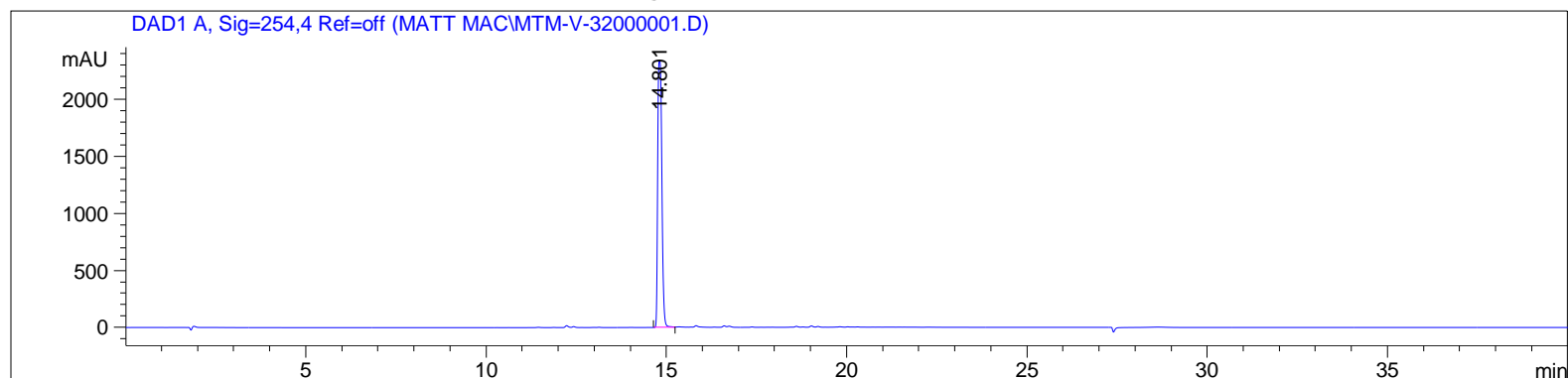


Sample Name: run1

## HPLC traces of compound 32

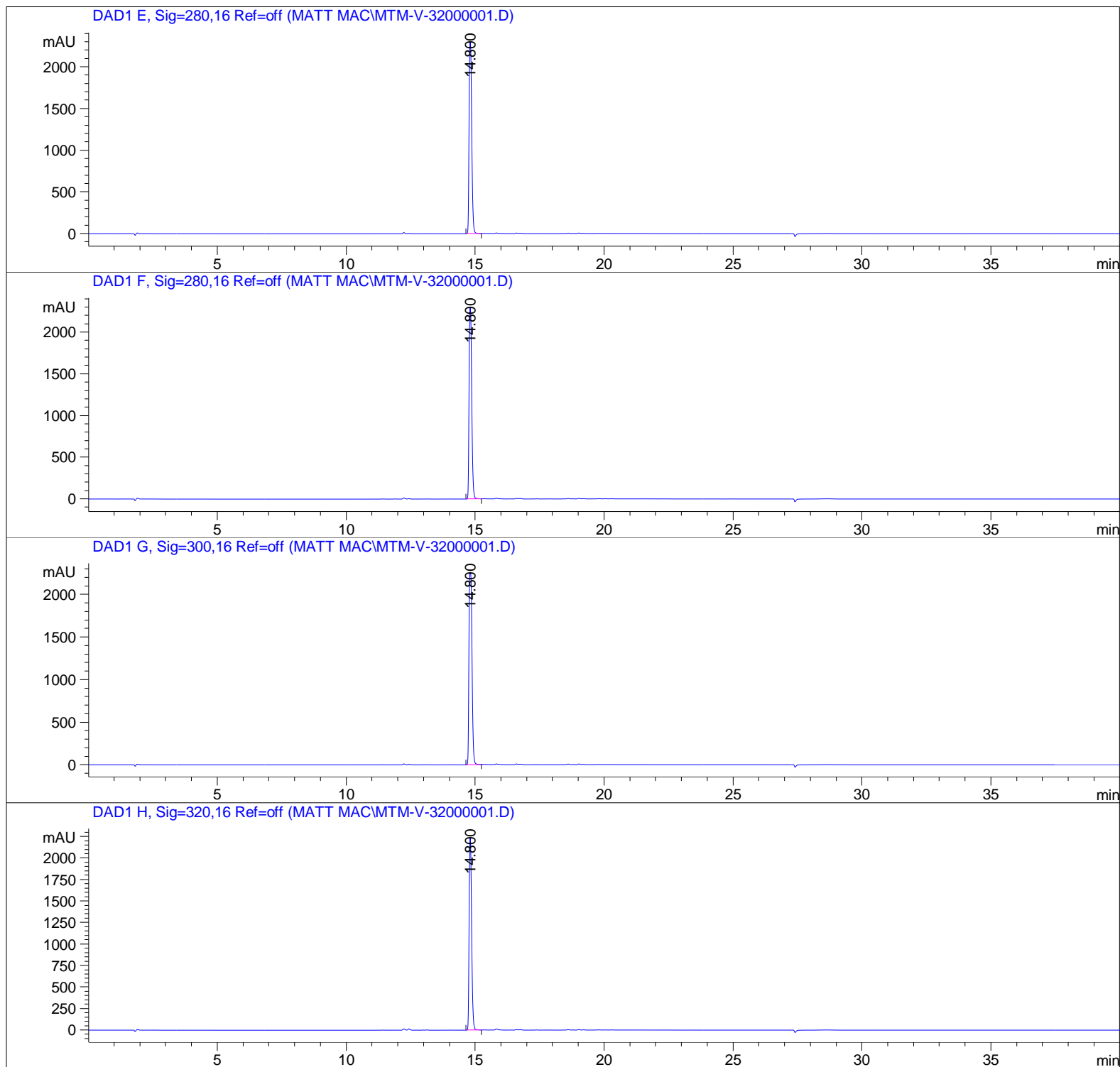
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Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/9/2013 10:48:37 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 10:45:53 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/9/2013 2:04:11 PM by Matt Mac  
(modified after loading)



Sample Name: run1

## HPLC traces of compound 32

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 32

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.801	BV	0.1293	1.86964e4	2338.97241	100.0000

Totals : 1.86964e4 2338.97241

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.801	BV	0.1292	1.88715e4	2362.03735	100.0000

Totals : 1.88715e4 2362.03735

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.805	BV	0.1658	2.20478e4	2183.30298	100.0000

Totals : 2.20478e4 2183.30298

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.799	BV	0.1507	2.20887e4	2369.97437	100.0000

Totals : 2.20887e4 2369.97437

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.800	BV	0.1131	1.63461e4	2295.18311	100.0000

Totals : 1.63461e4 2295.18311

Sample Name: run1

## HPLC traces of compound 32

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.800	BV	0.1131	1.63461e4	2295.18311	100.0000

Totals : 1.63461e4 2295.18311

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.800	BV	0.1317	1.84678e4	2251.13892	100.0000

Totals : 1.84678e4 2251.13892

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.800	BV	0.1063	1.49695e4	2231.31665	100.0000

Totals : 1.49695e4 2231.31665

=====  
\*\*\* End of Report \*\*\*

# HRMS of compound 32

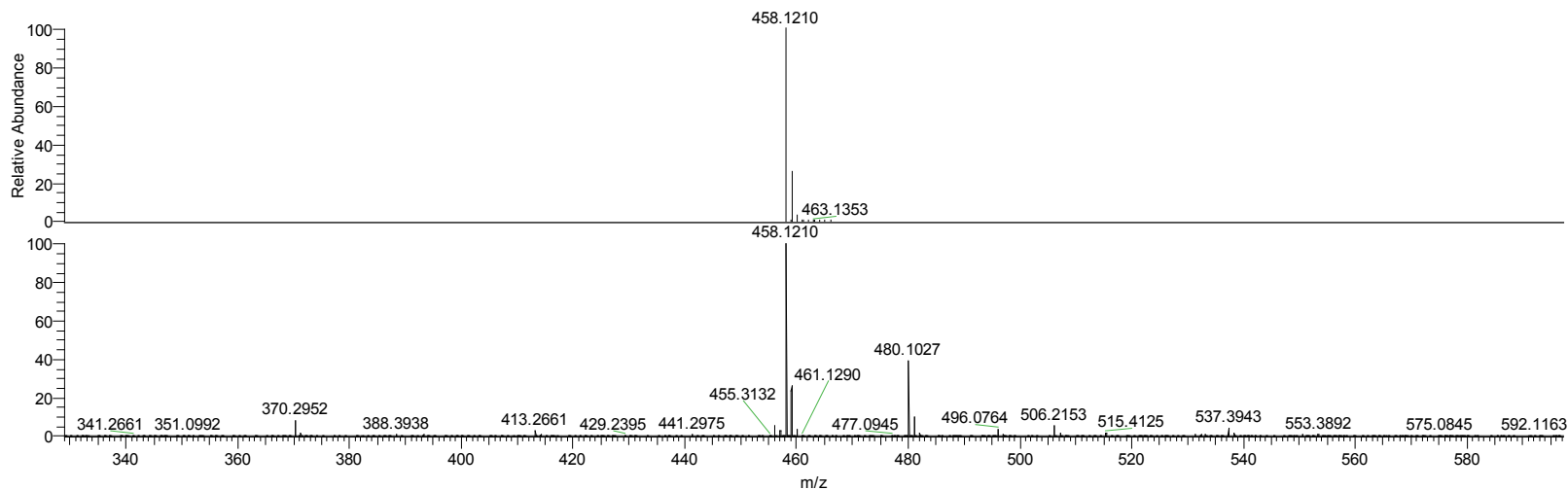
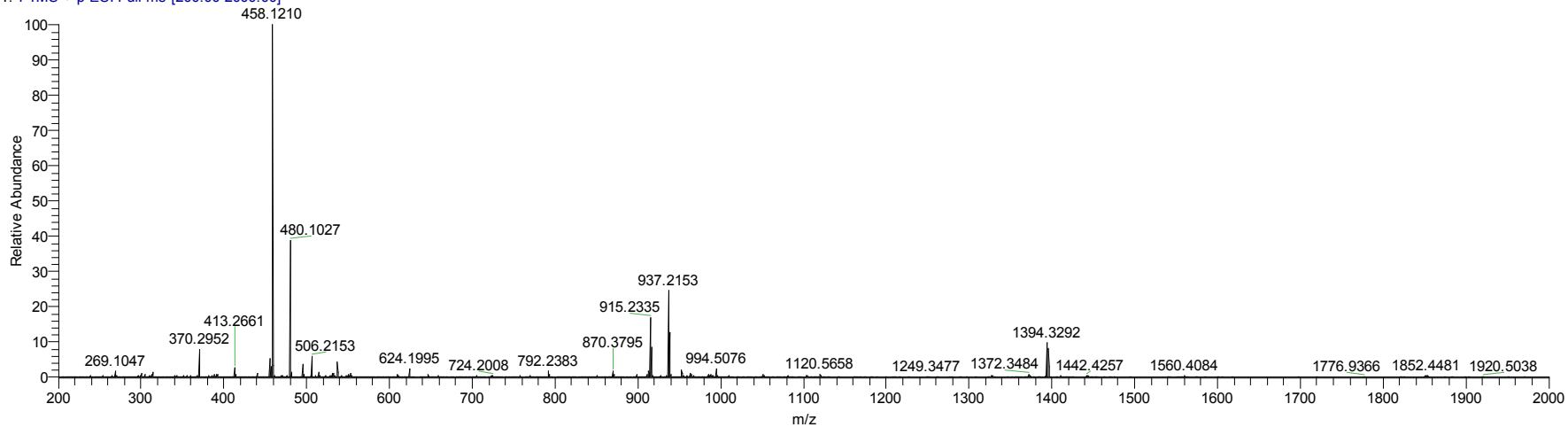
C:\Xcalibur\...Matt\2-10-2013\MTM-V-32

2/10/2013 12:25:45 PM

MTM-V-32

MTM-V-32 #7 RT: 0.05 AV: 1 NL: 2.22E7

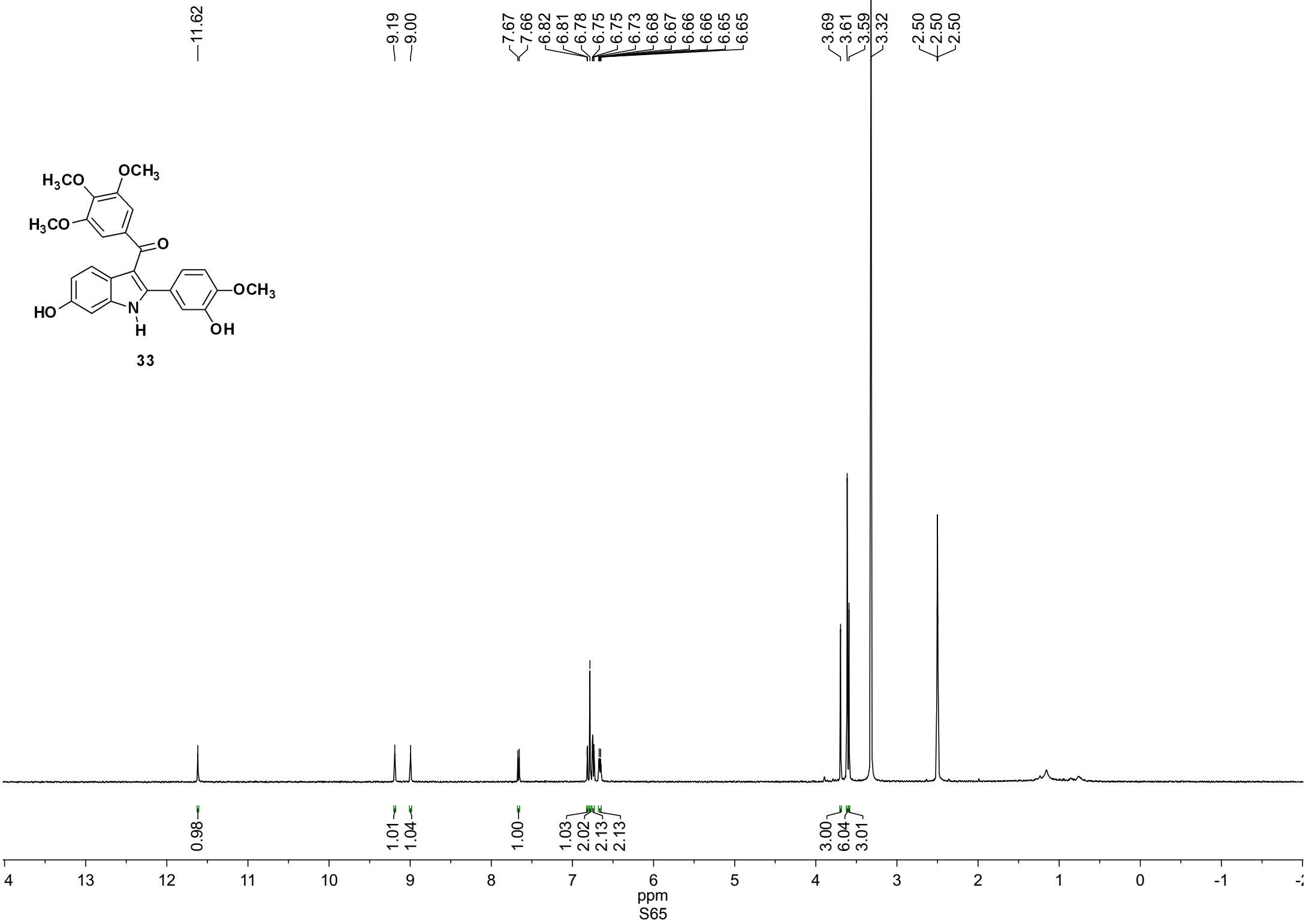
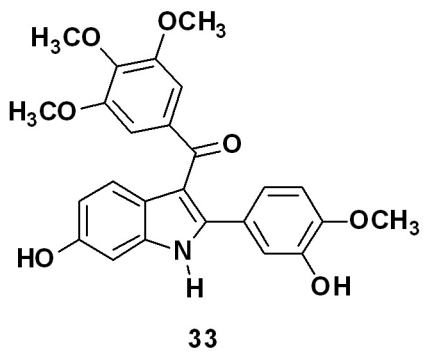
T: FTMS + p ESI Full ms [200.00-2000.00]

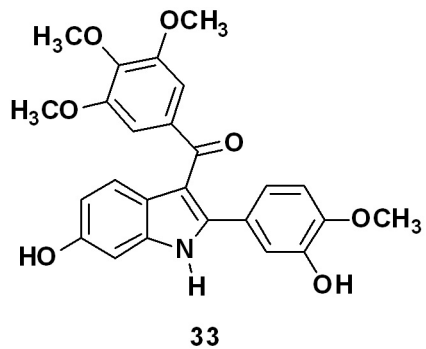


NL:  
7.59E5  
C<sub>24</sub>H<sub>19</sub>O<sub>5</sub>NF<sub>3</sub>  
C<sub>24</sub>H<sub>19</sub>O<sub>5</sub>N<sub>1</sub>F<sub>3</sub>  
pa Chrg 1

NL:  
2.22E7  
MTM-V-32#7 RT:  
0.05 AV: 1 T:  
FTMS + p ESI  
Full ms  
[200.00-2000.00]



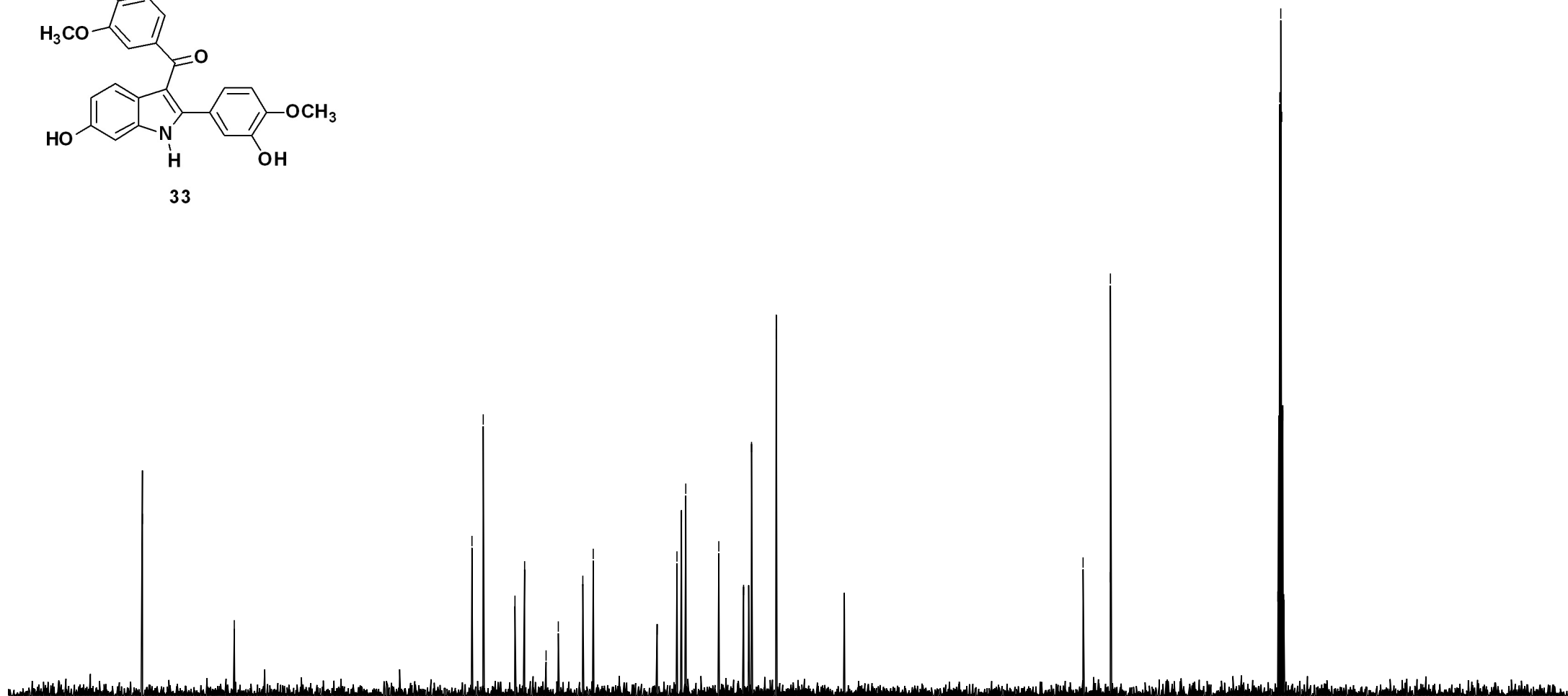




155.17  
 153.42  
 148.50  
 147.00  
 143.68  
 141.78  
 137.98  
 136.36  
 126.46  
 123.38  
 122.69  
 122.01  
 116.89  
 113.05  
 112.26  
 111.82  
 107.99  
 97.43

60.41  
 56.18  
 56.17

30.21  
 30.06  
 29.91  
 29.89  
 29.75  
 29.74  
 29.60  
 29.59  
 29.45  
 29.43  
 29.29



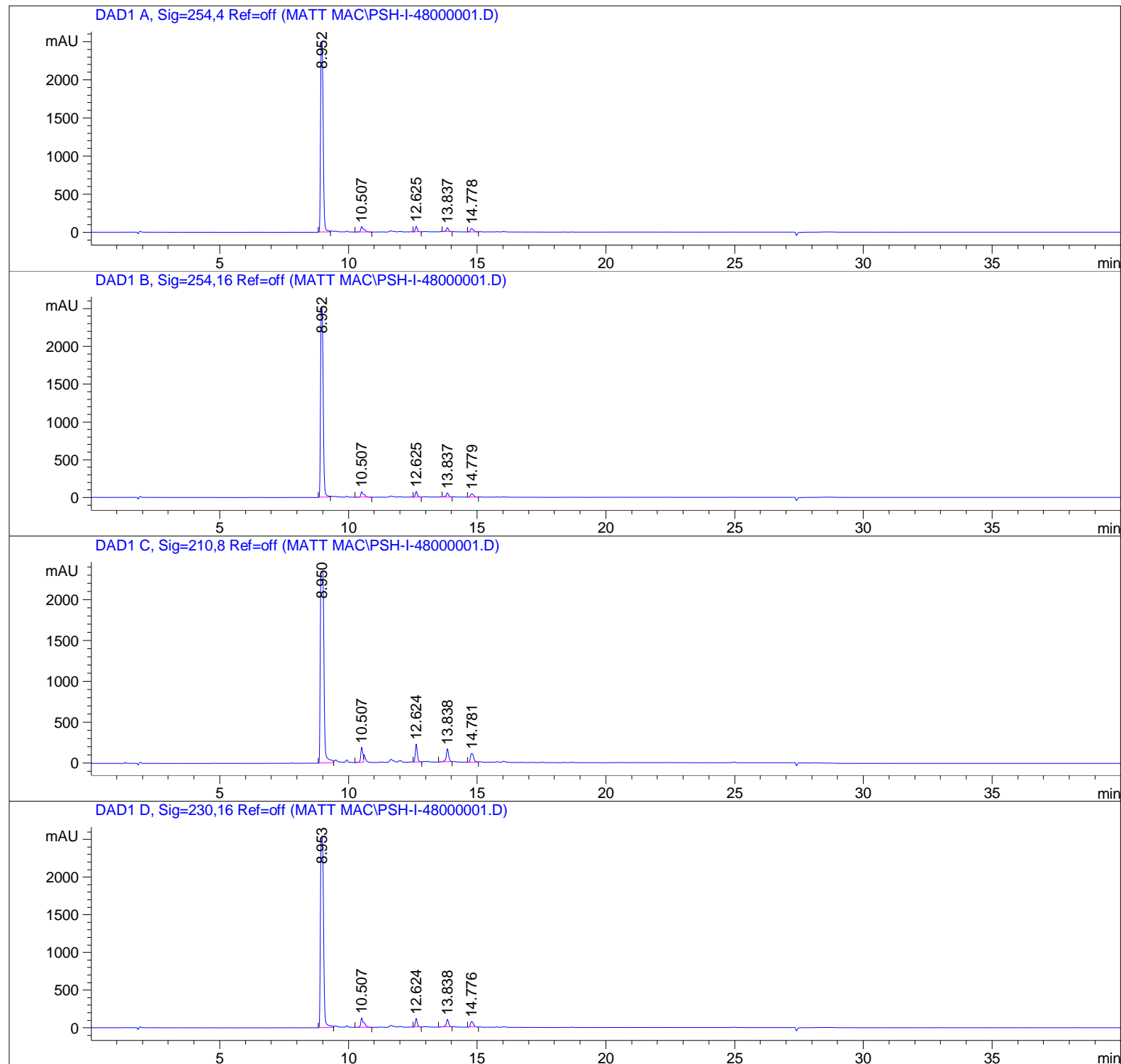
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

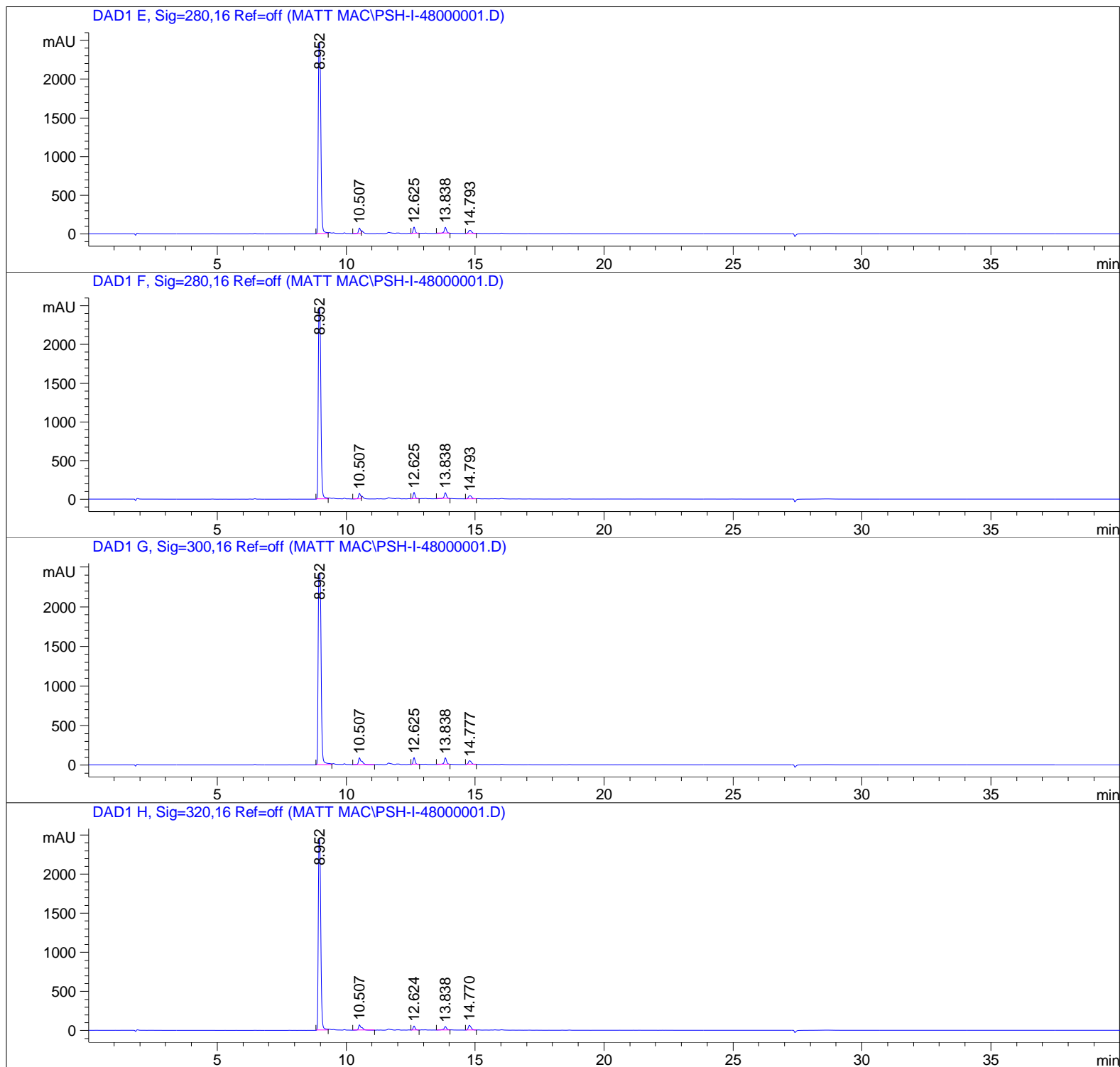
ppm  
 S66

Sample Name: run1

## HPLC traces of compound 33

=====  
Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/8/2013 9:52:08 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/8/2013 9:30:46 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/3/2013 5:04:04 PM by Laxman



HPLC traces of compound **33**=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 33

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.952	BV	0.1133	1.74400e4	2503.49414	90.6932
2	10.507	BB	0.1183	610.17493	70.97384	3.1731
3	12.625	VV	0.0842	406.46713	73.85258	2.1138
4	13.837	VV	0.1047	393.10352	54.14516	2.0443
5	14.778	BV	0.1371	379.91687	43.85746	1.9757

Totals :                                   1.92296e4   2746.32318

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.952	BV	0.1130	1.75295e4	2525.12695	90.7013
2	10.507	BB	0.1182	618.83783	72.06956	3.2020
3	12.625	VV	0.0841	405.30692	73.71142	2.0971
4	13.837	VV	0.1050	394.96179	54.20537	2.0436
5	14.779	BV	0.1377	378.02029	43.34686	1.9560

Totals :                                   1.93266e4   2768.46016

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.950	BV	0.1577	2.28634e4	2345.01953	83.7926
2	10.507	BV	0.0861	1096.52075	187.73811	4.0187
3	12.624	VV	0.0843	1212.12024	219.94164	4.4423
4	13.838	BV	0.1033	1167.94214	163.60349	4.2804
5	14.781	BV	0.1384	945.71265	107.69555	3.4660

Totals :                                   2.72857e4   3023.99831

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.953	BV	0.1354	2.11507e4	2534.16040	87.2935
2	10.507	BB	0.1178	1058.27429	123.76330	4.3677

Sample Name: run1

## HPLC traces of compound 33

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
3	12.624	VV	0.0846	639.06421	115.47739	2.6376
4	13.838	BV	0.1035	740.73499	103.53637	3.0572
5	14.776	BV	0.1350	640.64758	75.48686	2.6441

Totals :                                   2.42294e4  2952.42432

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.952	BV	0.1131	1.71869e4	2472.61279	90.5848
2	10.507	BV	0.0859	419.13235	72.05910	2.2091
3	12.625	VV	0.0840	451.04239	82.25859	2.3773
4	13.838	BV	0.1015	549.10632	78.58857	2.8941
5	14.793	BV	0.1445	367.09229	40.21583	1.9348

Totals :                                   1.89733e4  2745.73488

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.952	BV	0.1131	1.71869e4	2472.61279	90.5848
2	10.507	BV	0.0859	419.13235	72.05910	2.2091
3	12.625	VV	0.0840	451.04239	82.25859	2.3773
4	13.838	BV	0.1015	549.10632	78.58857	2.8941
5	14.793	BV	0.1445	367.09229	40.21583	1.9348

Totals :                                   1.89733e4  2745.73488

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.952	BV	0.1265	1.91870e4	2420.31030	89.6657
2	10.507	BB	0.1181	743.72498	86.64207	3.4756
3	12.625	VB	0.0835	472.35669	86.76642	2.2074
4	13.838	VV	0.1002	582.41565	84.67338	2.7218
5	14.777	BV	0.1360	412.87323	48.15561	1.9295

Totals :                                   2.13983e4  2726.54778

Sample Name: run1

## HPLC traces of compound 33

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.952	BV	0.1054	1.62748e4	2453.87549	90.6305
2	10.507	BB	0.1190	586.09778	67.68012	3.2638
3	12.624	VV	0.0850	289.21191	51.90499	1.6106
4	13.838	BV	0.1074	337.07236	44.99344	1.8771
5	14.770	BV	0.1219	470.12784	61.00558	2.6180

Totals :                                   1.79573e4  2679.45962

=====  
\*\*\* End of Report \*\*\*

# HRMS of compound 33

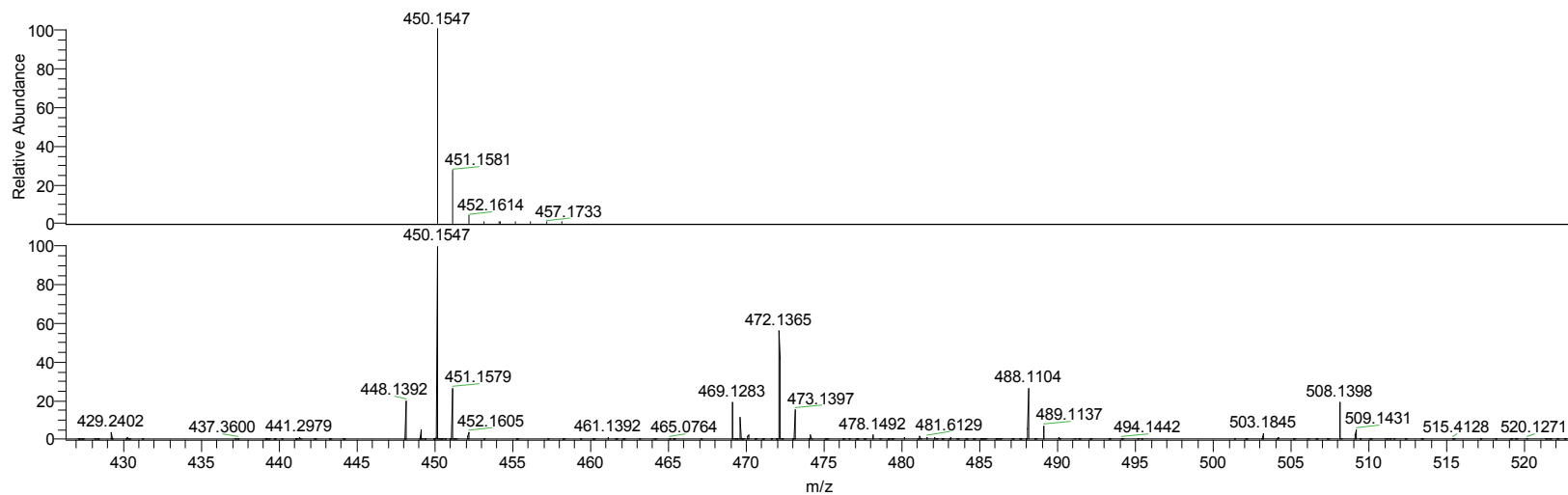
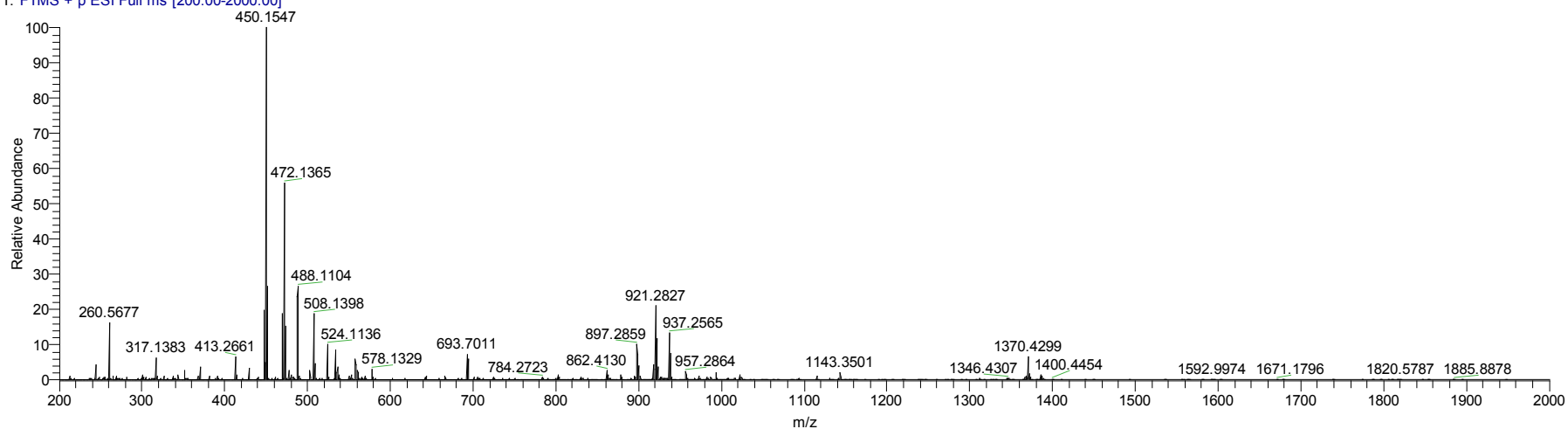
C:\Xcalibur\...Matt\2-10-2013\PSH-I48

2/10/2013 8:21:48 PM

PSH-I48

PSH-I48 #20 RT: 0.16 AV: 1 NL: 7.60E7

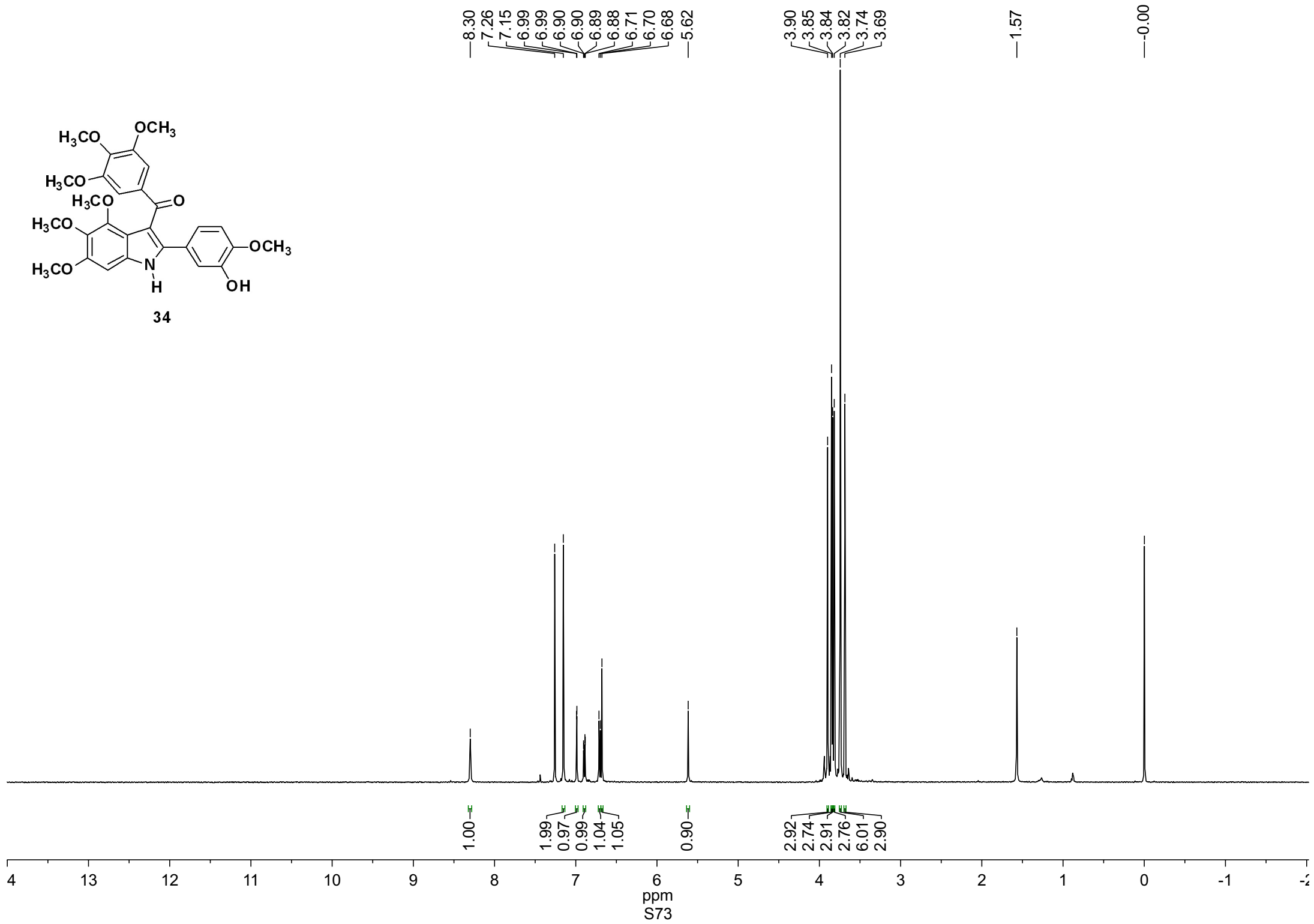
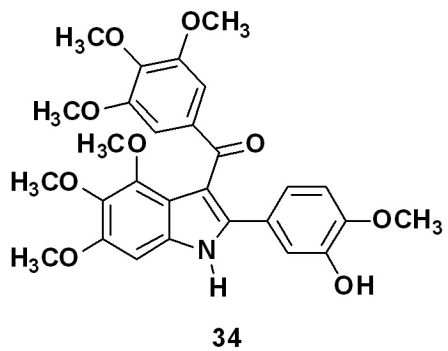
T: FTMS + p ESI Full ms [200.00-2000.00]

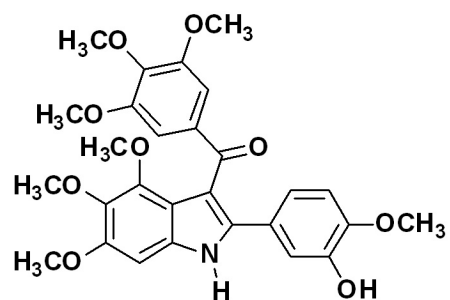


NL:  
7.46E5  
C<sub>25</sub>H<sub>24</sub>O<sub>7</sub>N:  
C<sub>25</sub>H<sub>24</sub>O<sub>7</sub>N<sub>1</sub>  
pa Chrg 1

NL:  
7.60E7  
PSH-I48#20 RT:  
0.16 AV: 1 T:  
FTMS + p ESI Full  
ms  
[200.00-2000.00]







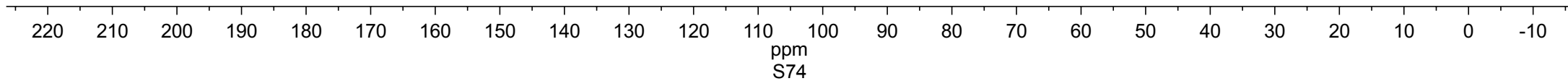
— 193.44

152.83  
152.16  
146.84  
146.48  
145.84  
142.11  
137.80  
137.04  
134.57  
132.36  
125.14  
120.48  
116.56  
113.68  
112.59  
110.94  
107.50

— 89.73

77.41  
77.46  
76.91

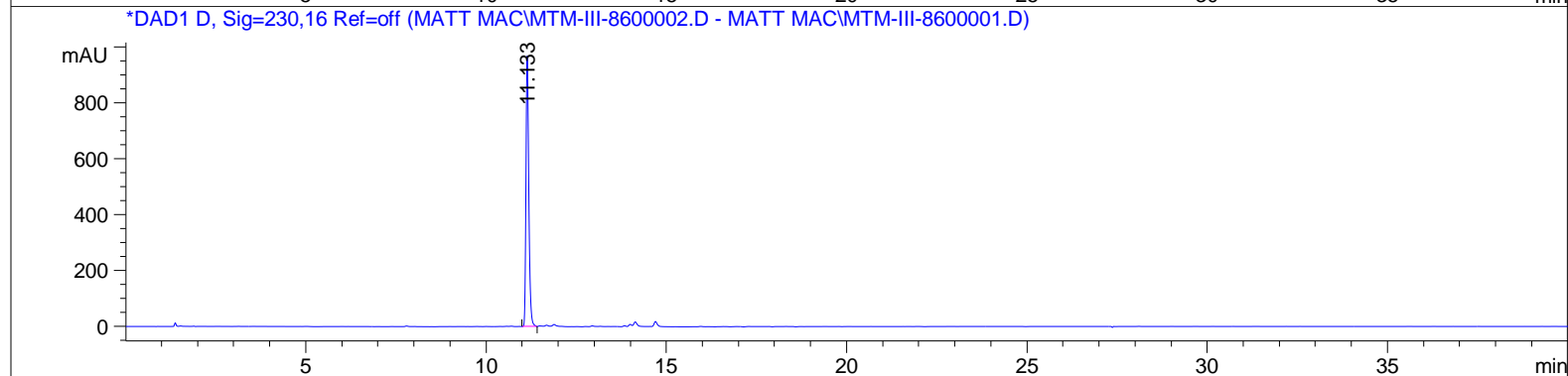
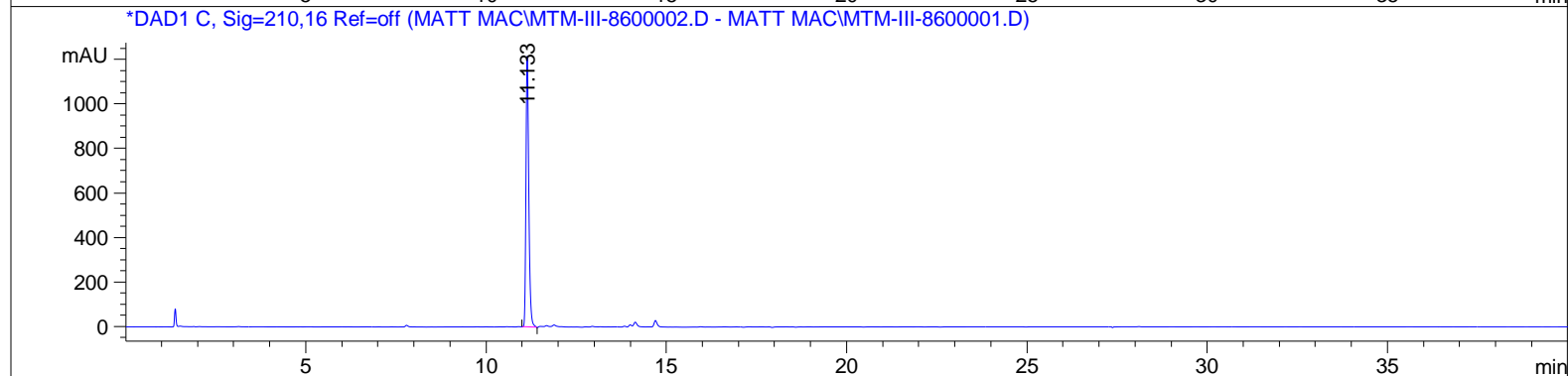
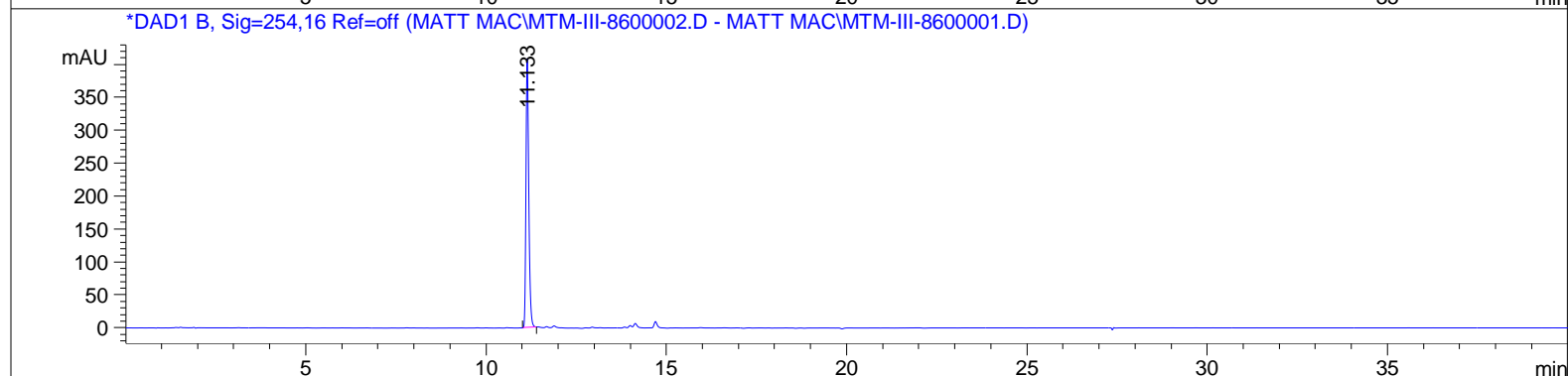
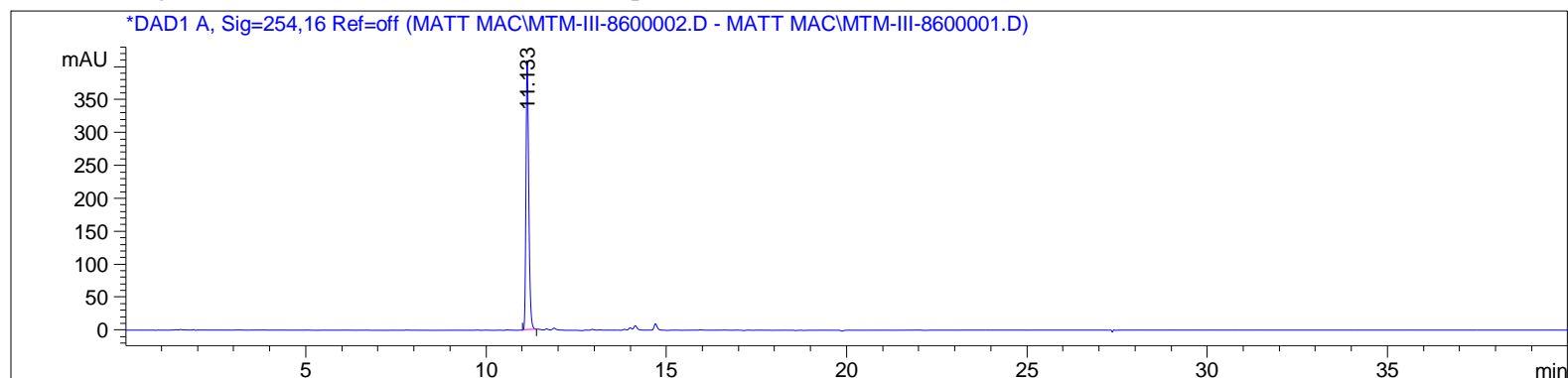
61.37  
61.00  
60.78  
56.40  
56.33  
56.07



Sample Name: run1

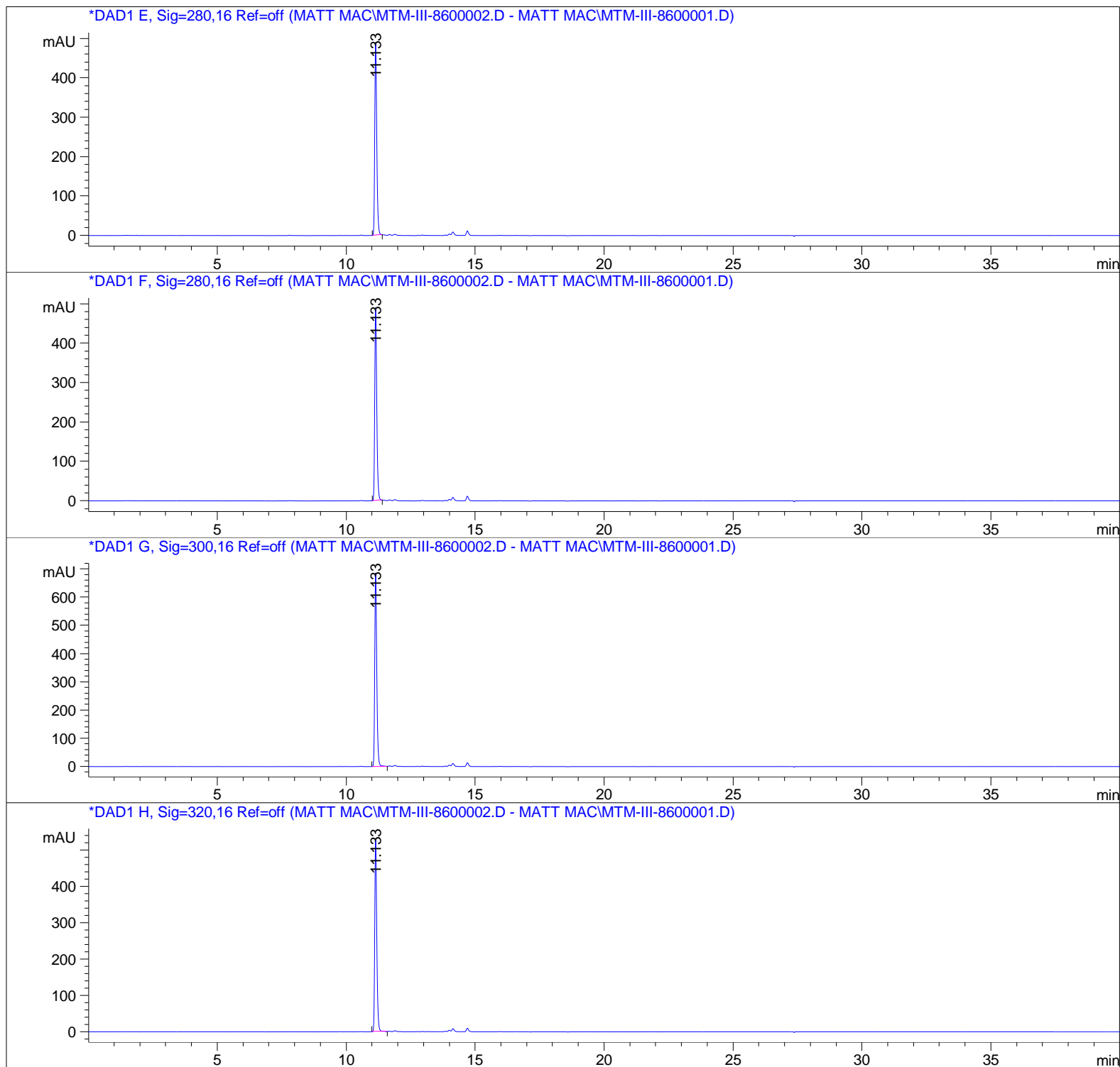
HPLC traces of compound **34**

=====  
Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/7/2013 4:14:42 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/7/2013 4:13:16 PM by Matt Mac  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/3/2013 5:04:04 PM by Laxman



Sample Name: run1

## HPLC traces of compound 34

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

HPLC traces of compound 34

Signal 1: DAD1 A, Sig=254,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BB	0.0810	2210.16919	409.56378	100.0000

Totals : 2210.16919 409.56378

Signal 2: DAD1 B, Sig=254,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BB	0.0810	2210.16919	409.56378	100.0000

Totals : 2210.16919 409.56378

Signal 3: DAD1 C, Sig=210,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	VB	0.0817	6658.21045	1218.85291	100.0000

Totals : 6658.21045 1218.85291

Signal 4: DAD1 D, Sig=230,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BB	0.0815	5278.77148	970.38177	100.0000

Totals : 5278.77148 970.38177

Sample Name: run1

## HPLC traces of compound 34

Signal 5: DAD1 E, Sig=280,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BB	0.0809	2644.89453	490.63278	100.0000

Totals : 2644.89453 490.63278

Signal 6: DAD1 F, Sig=280,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BB	0.0809	2644.89453	490.63278	100.0000

Totals : 2644.89453 490.63278

Signal 7: DAD1 G, Sig=300,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BV	0.0816	3745.30640	686.99261	100.0000

Totals : 3745.30640 686.99261

Signal 8: DAD1 H, Sig=320,16 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.133	BV	0.0815	2904.22461	533.46991	100.0000

Totals : 2904.22461 533.46991

=====  
\*\*\* End of Report \*\*\*

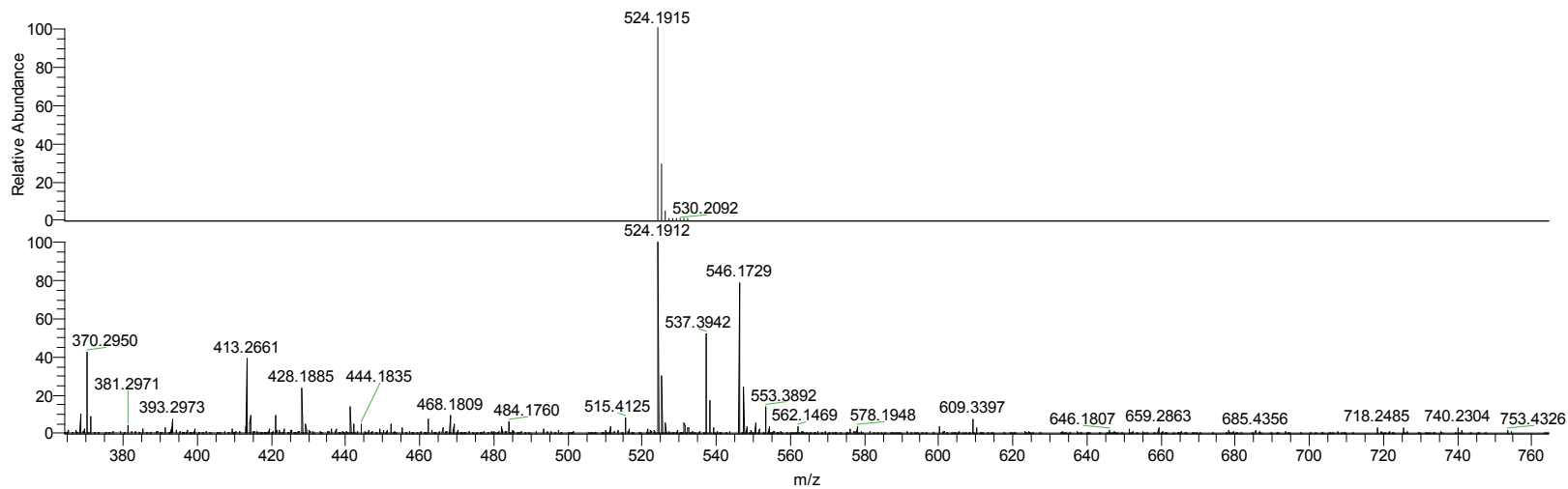
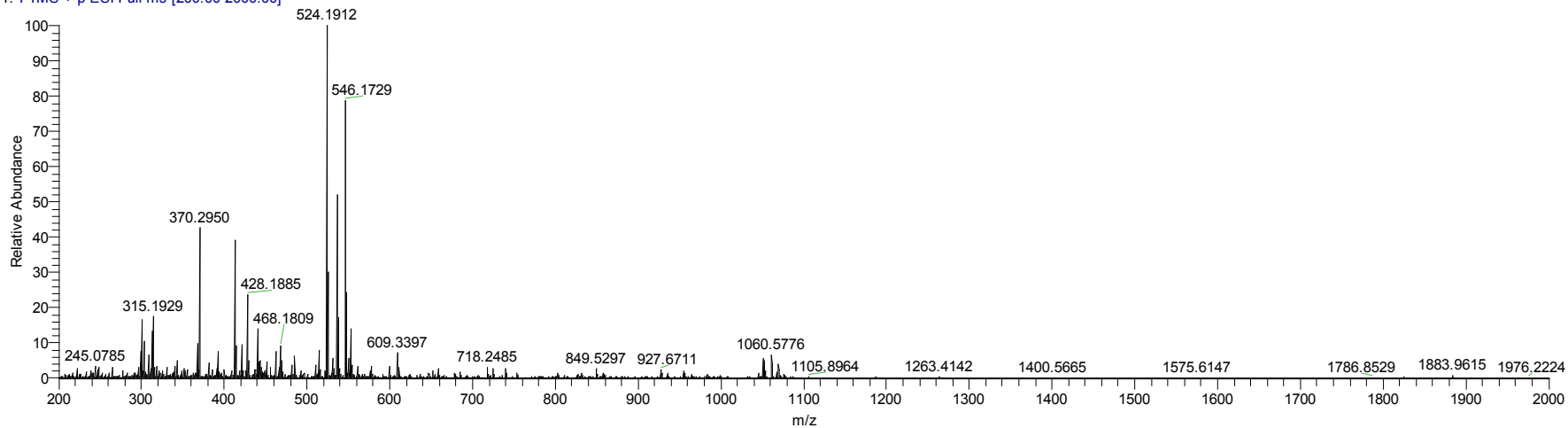
# HRMS of compound 34

C:\Xcalibur\...2-10-2013\MTM-III-86

2/10/2013 4:13:03 PM

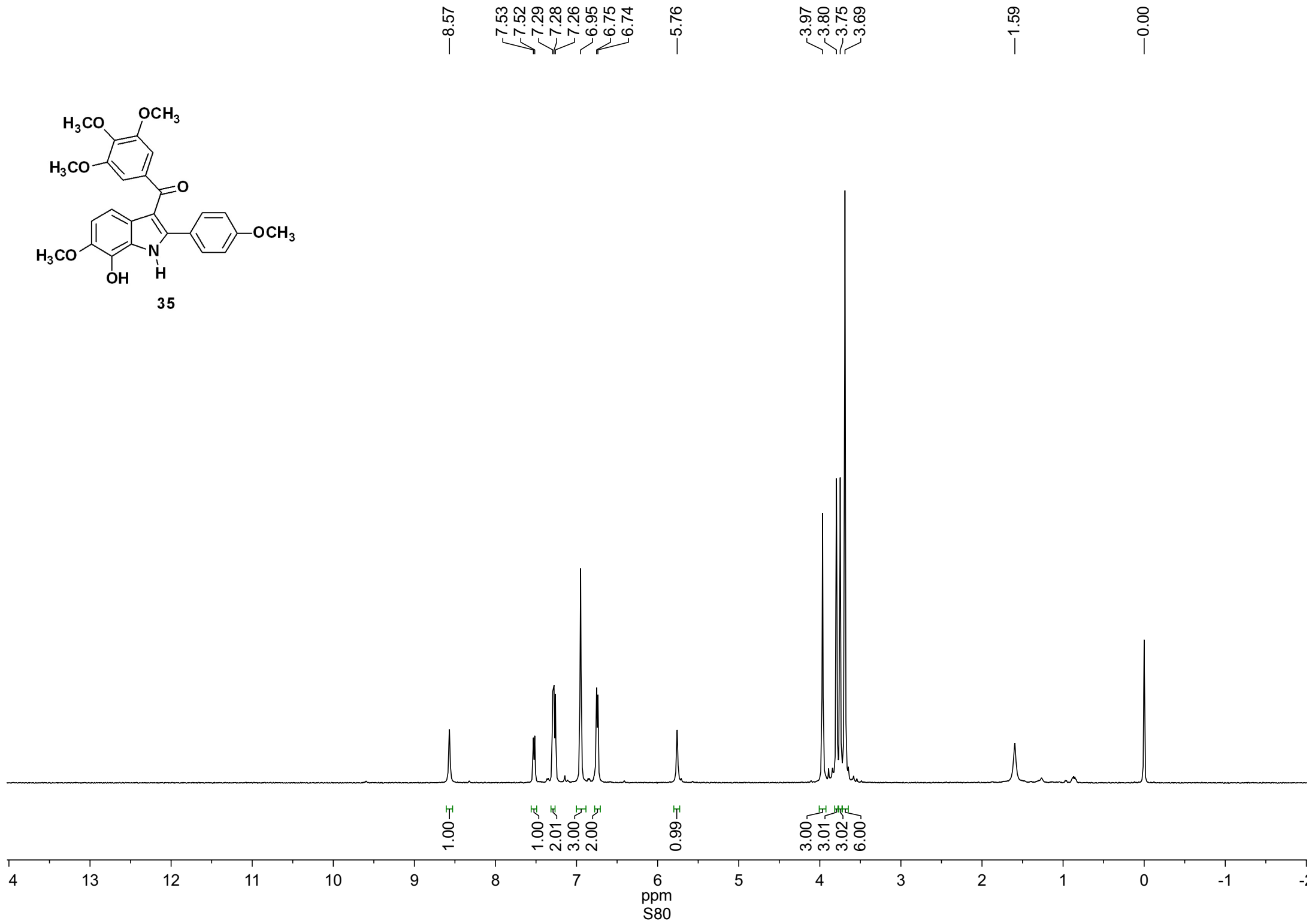
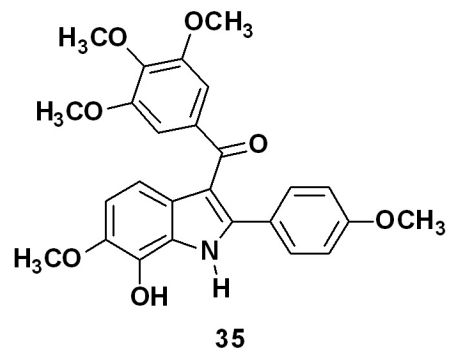
MTM-III-86

MTM-III-86 #20 RT: 0.17 AV: 1 NL: 7.70E6  
T: FTMS + p ESI Full ms [200.00-2000.00]

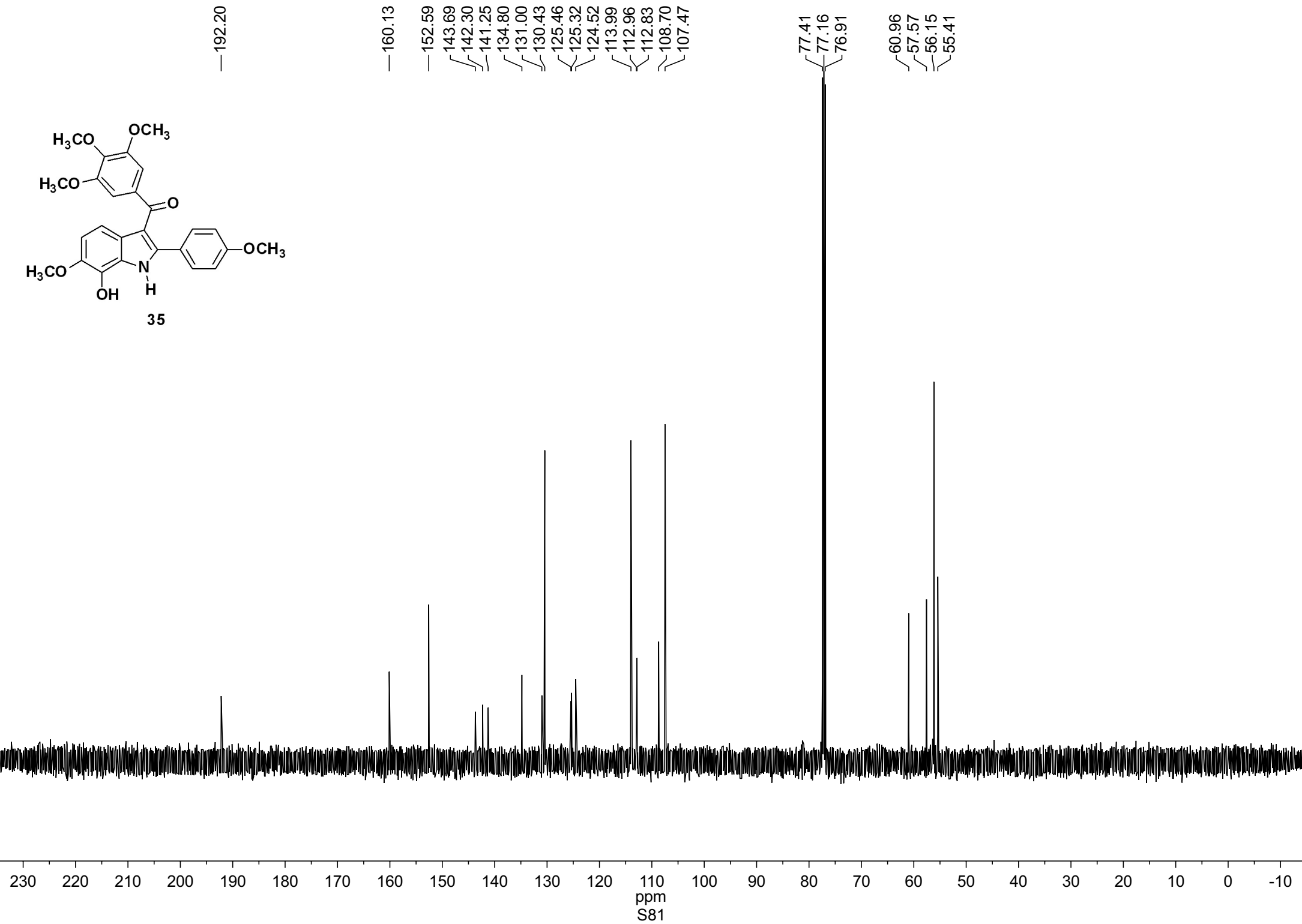
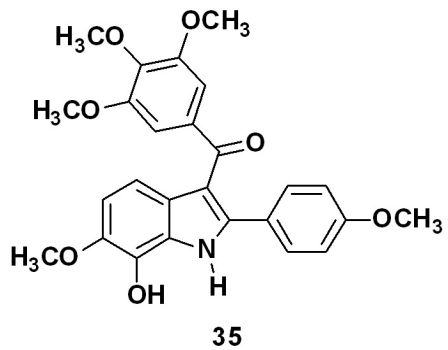


NL:  
7.17E5  
C<sub>27</sub>H<sub>24</sub>O<sub>4</sub>N<sub>8</sub>:  
C<sub>27</sub>H<sub>24</sub>O<sub>4</sub>N<sub>8</sub>  
pa Chrg 1

NL:  
7.70E6  
MTM-III-86#20 RT:  
0.17 AV: 1 T:  
FTMS + p ESI Full  
ms  
[200.00-2000.00]



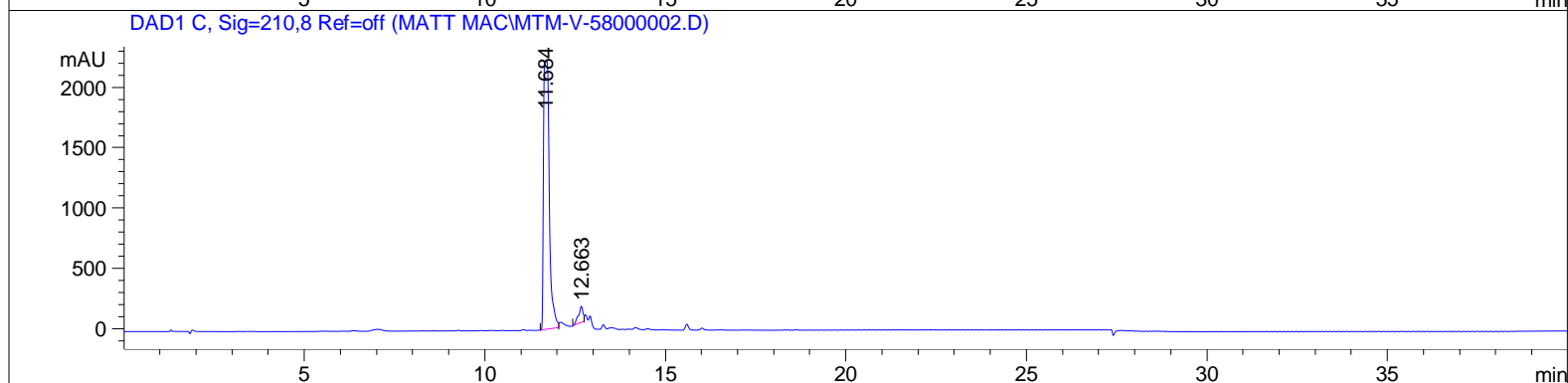
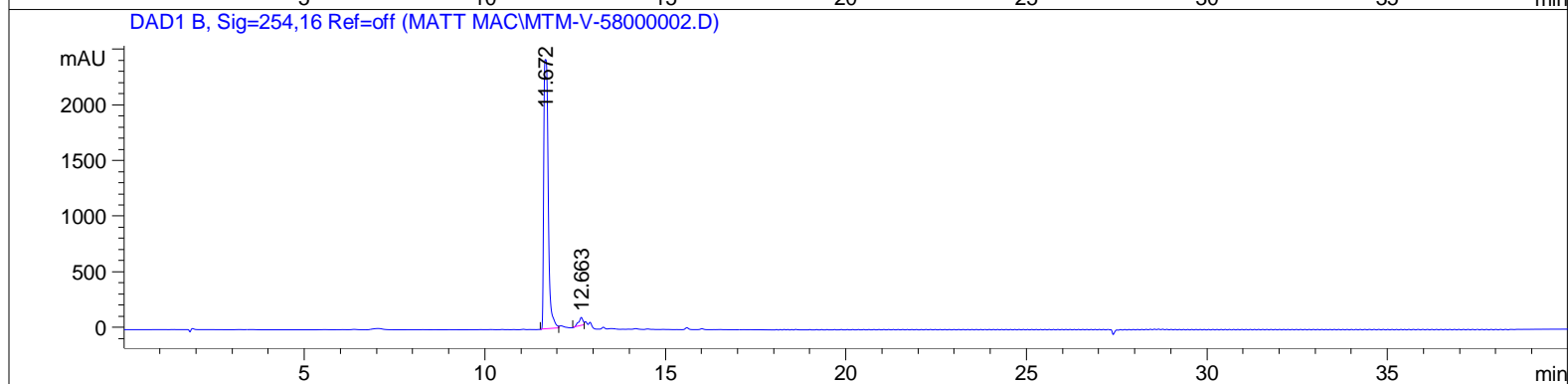
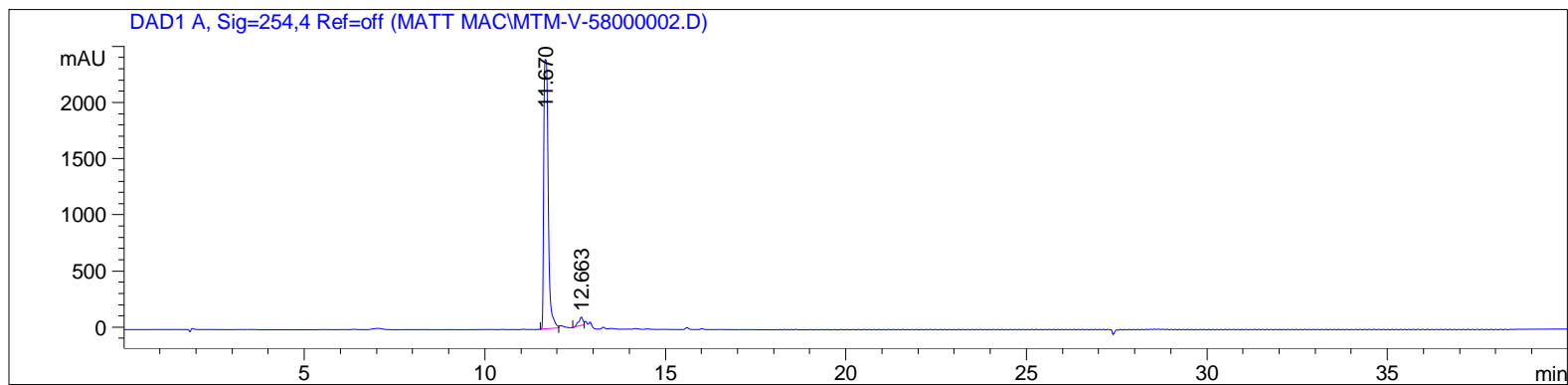




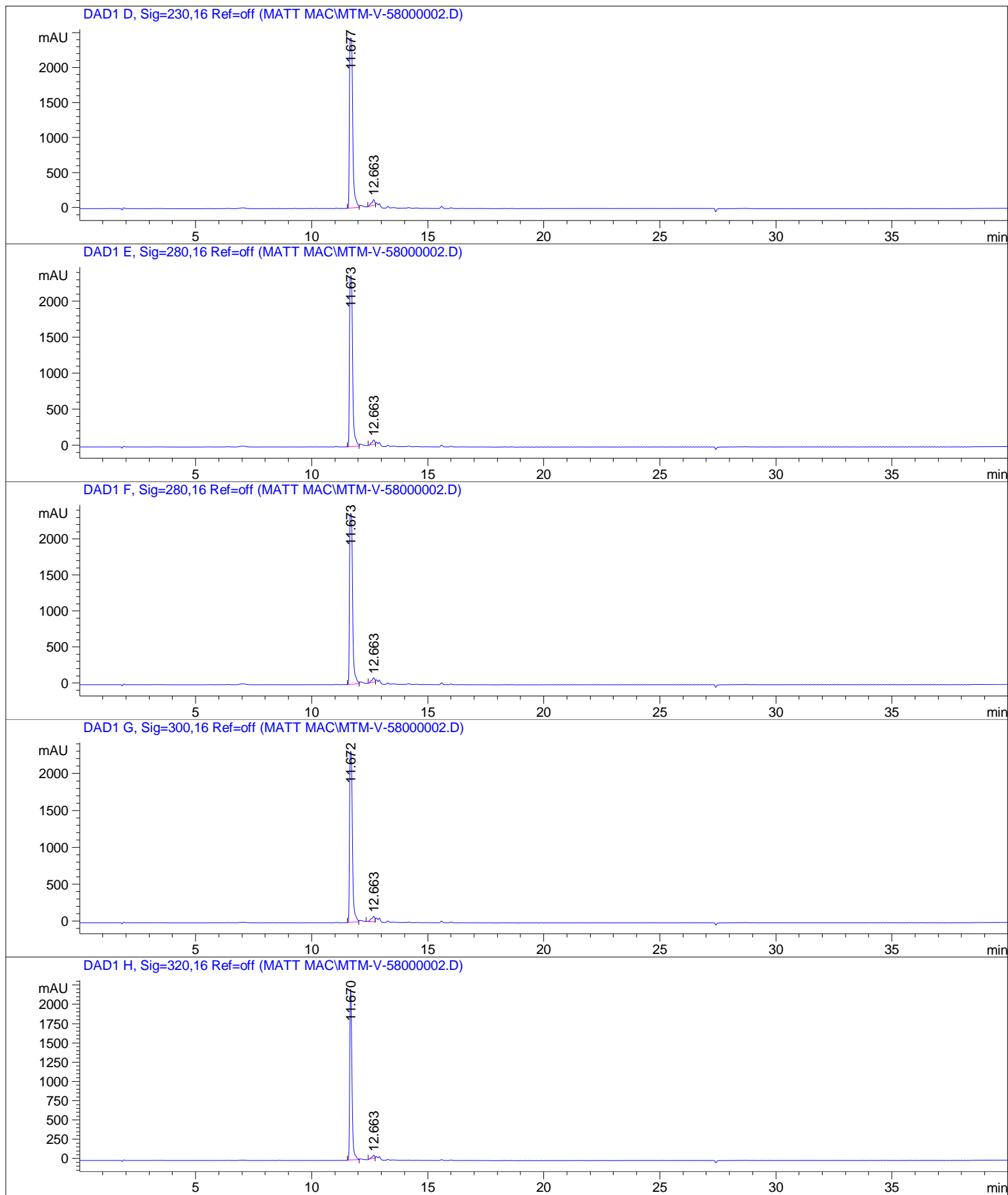
Sample Name: run1

## HPLC traces of compound 35

=====  
Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 1/25/2013 3:29:20 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 1/25/2013 3:22:08 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\DATA\MATT MAC\MTM-V-58000002.D\DA.M (MASTERMETHOD.M)  
Last changed : 1/25/2013 4:52:52 PM by Matt Mac  
Sample Info :



### HPLC traces of compound 35



Sample Name: run1

## HPLC traces of compound 35

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.670	BV	0.1366	2.06994e4	2400.60474	96.8656
2	12.663	BV	0.1233	669.79010	77.10614	3.1344

Totals : 2.13692e4 2477.71088

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.672	BV	0.1390	2.09971e4	2425.36963	96.9310
2	12.663	BV	0.1241	664.80243	75.93778	3.0690

Totals : 2.16619e4 2501.30741

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.684	BV	0.1768	2.49809e4	2228.70850	95.3229
2	12.663	BV	0.1273	1225.71509	135.74158	4.6771

Totals : 2.62066e4 2364.45007

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.677	BV	0.1549	2.35212e4	2429.63184	96.4298
2	12.663	BV	0.1388	870.83435	86.97546	3.5702

Sample Name: run1

## HPLC traces of compound 35

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Totals :				2.43920e4	2516.60730	

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.673	BV	0.1442	2.16120e4	2373.22510	97.4647
2	12.663	BV	0.1249	562.18378	63.75766	2.5353
Totals :				2.21741e4	2436.98276	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.673	BV	0.1442	2.16120e4	2373.22510	97.4647
2	12.663	BV	0.1249	562.18378	63.75766	2.5353
Totals :				2.21741e4	2436.98276	

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.672	BV	0.1341	1.95065e4	2319.21680	96.0807
2	12.663	BV	0.1414	795.70215	76.45817	3.9193
Totals :				2.03022e4	2395.67496	

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.670	BV	0.1026	1.46092e4	2224.54712	97.2378
2	12.663	BV	0.1257	415.00085	45.78540	2.7622
Totals :				1.50242e4	2270.33252	

Sample Name: run1

HPLC traces of compound **35**

=====  
\*\*\* End of Report \*\*\*

# HRMS of compound 35

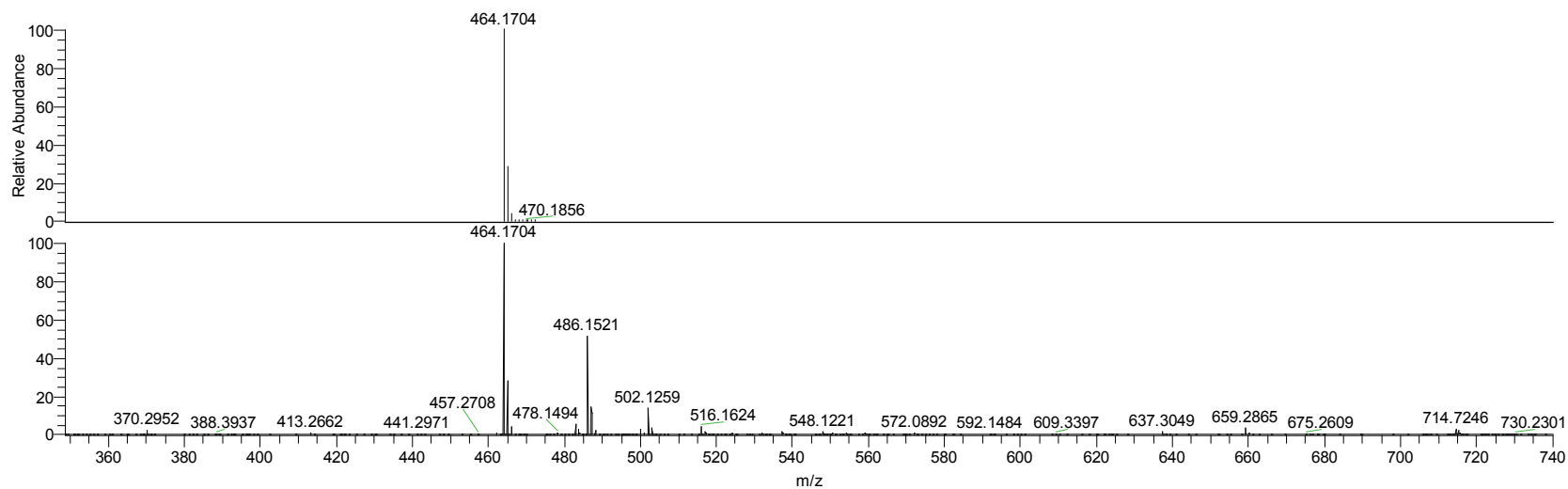
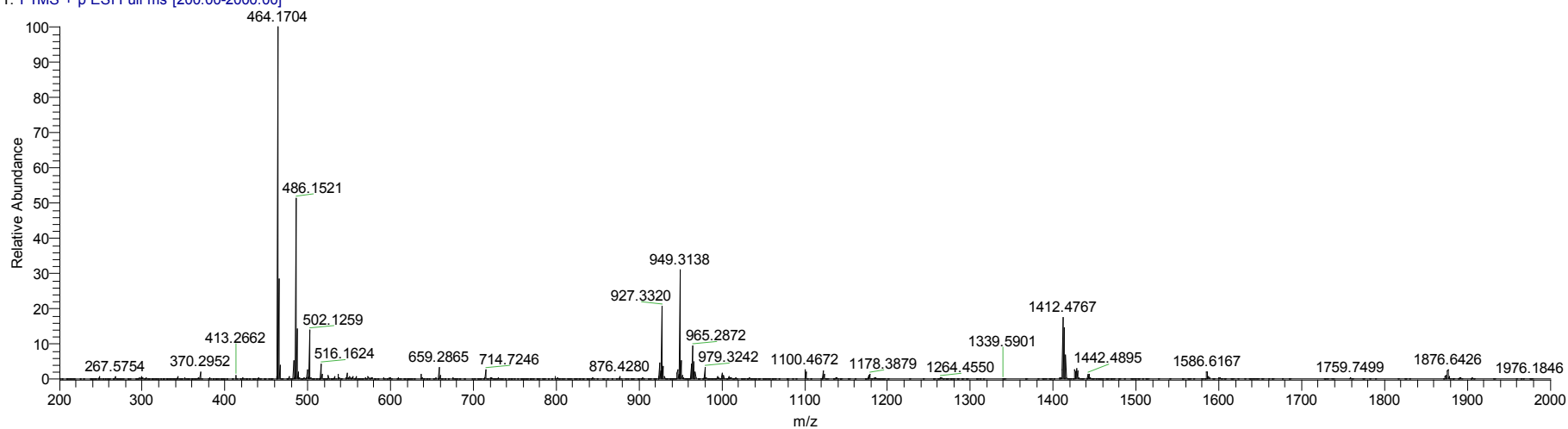
C:\Xcalibur\...Matt2-10-2013\MTM-V-58

2/10/2013 4:22:35 PM

MTM-V-58

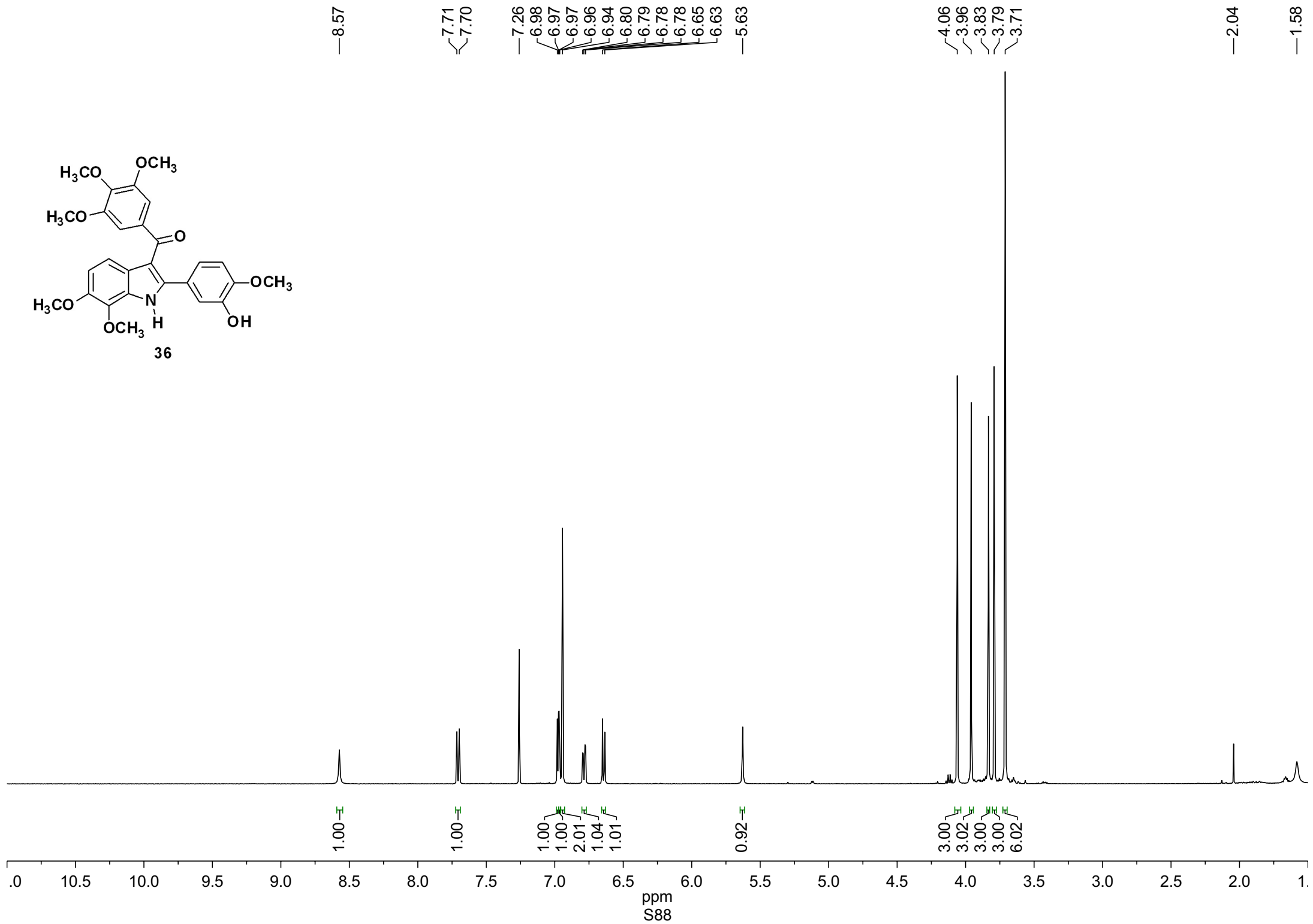
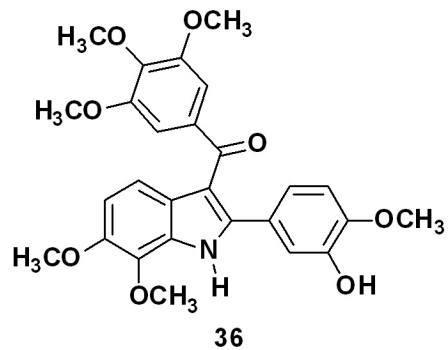
MTM-V-58 #10 RT: 0.08 AV: 1 NL: 1.22E8

T: FTMS + p ESI Full ms [200.00-2000.00]

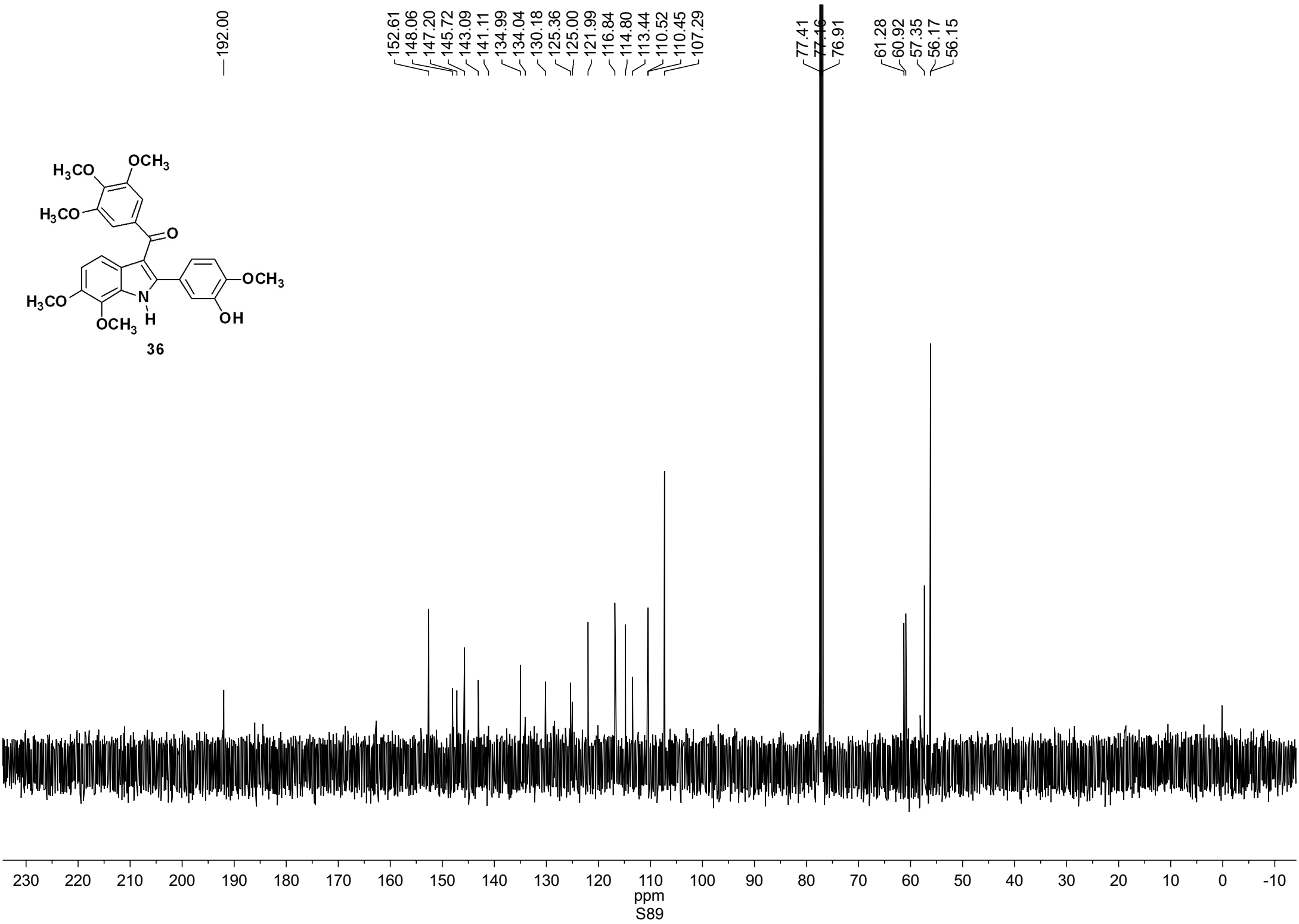
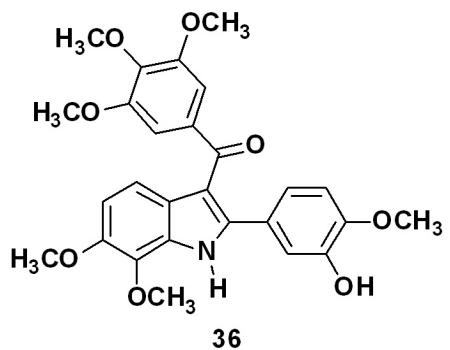


NL:  
7.38E5  
C<sub>26</sub>H<sub>26</sub>O<sub>7</sub>N:  
C<sub>26</sub>H<sub>26</sub>O<sub>7</sub>N<sub>1</sub>  
pa Chrg 1

NL:  
1.22E8  
MTM-V-58#10  
RT: 0.08 AV: 1 T:  
FTMS + p ESI Full  
ms  
[200.00-2000.00]



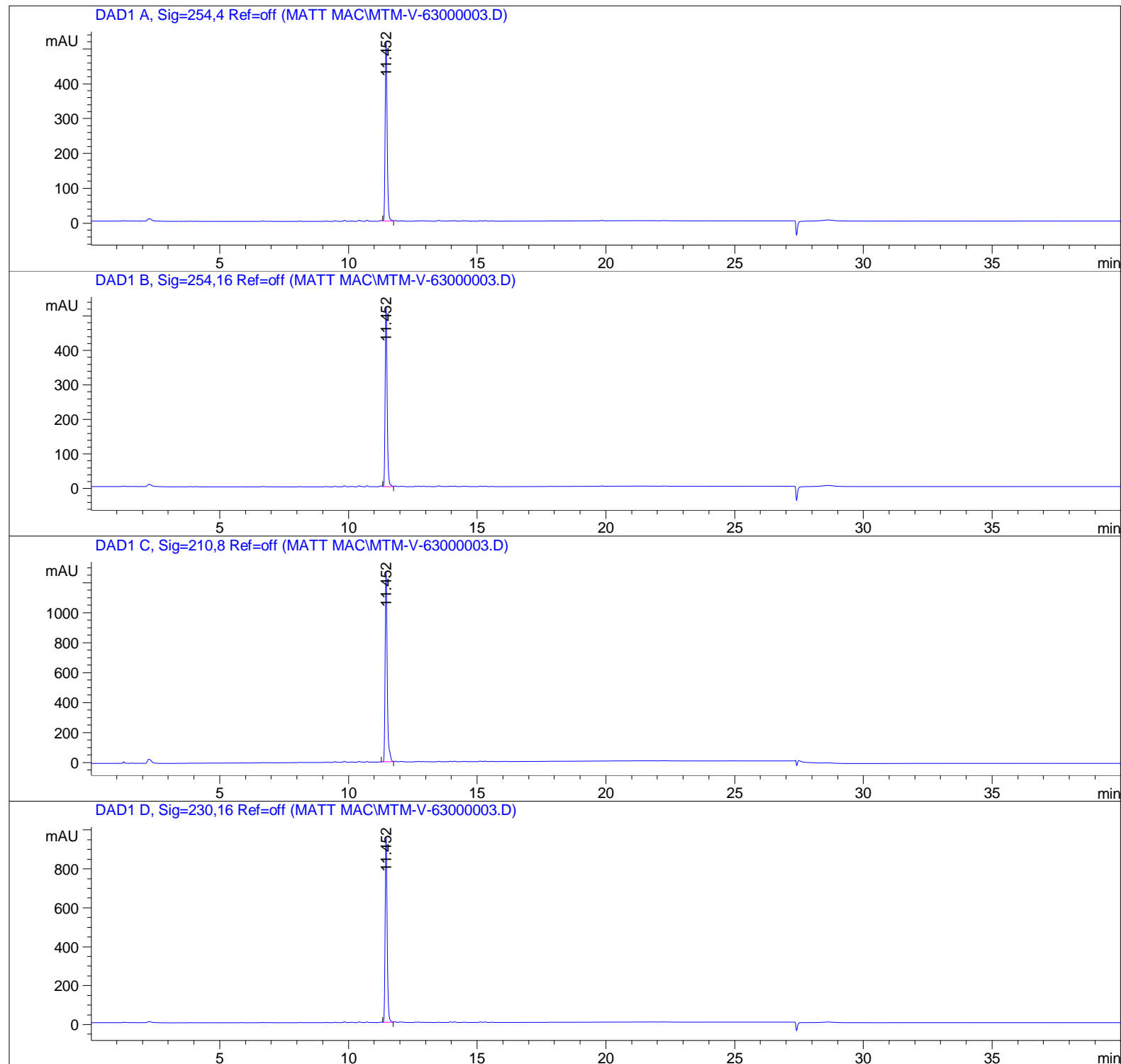




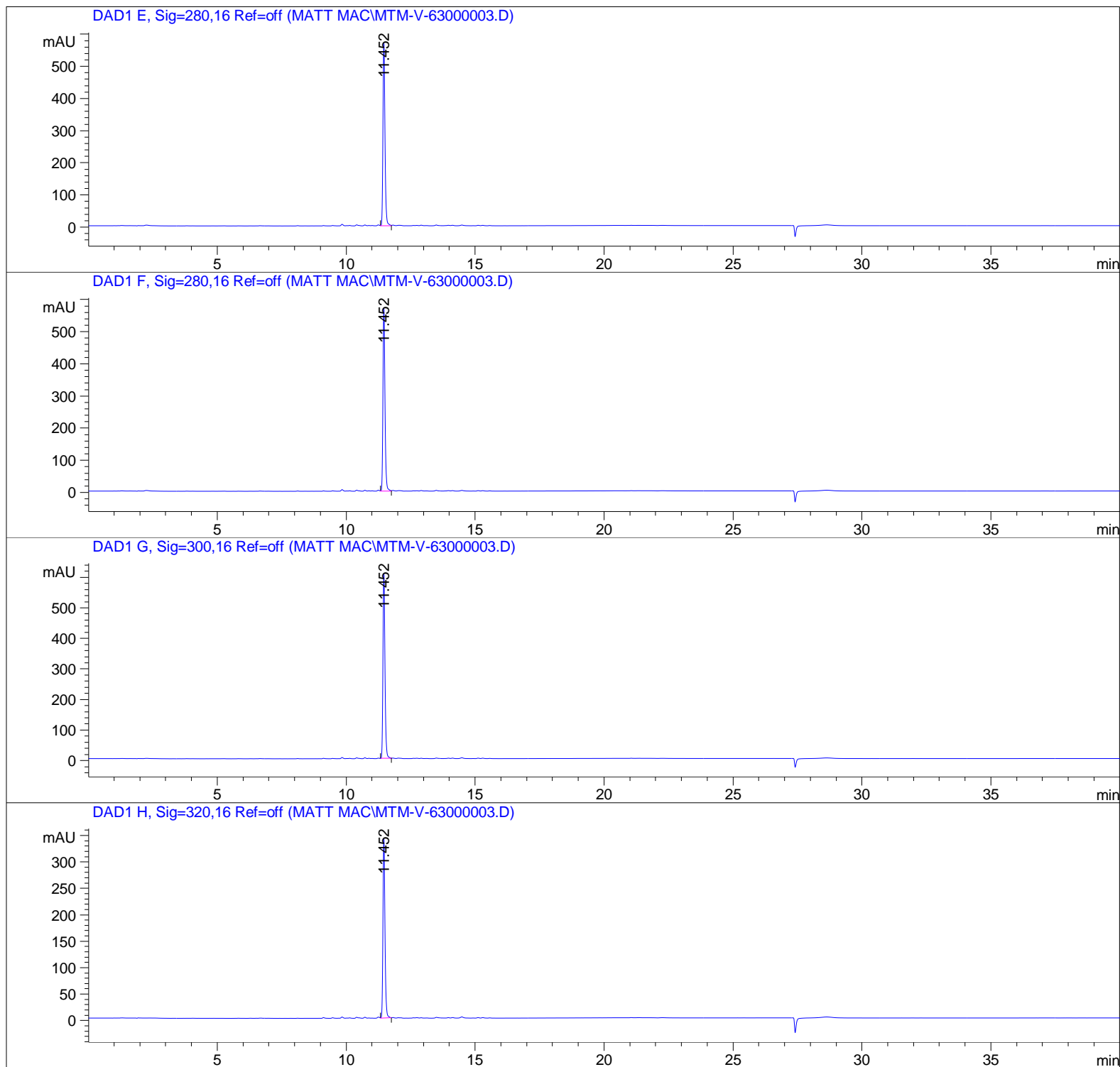
Sample Name: run1

HPLC traces of compound **36**

=====  
Acq. Operator : Matt Mac  
Acq. Instrument : Instrument 1 Location : -  
Injection Date : 3/4/2013 1:27:41 PM  
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M  
Last changed : 3/4/2013 12:54:38 PM by Matt Mac  
Analysis Method : C:\CHEM32\1\DATA\MATT MAC\MTM-V-63000003.D\DA.M (MASTERMETHOD.M)  
Last changed : 3/4/2013 2:17:56 PM by Matt Mac



## HPLC traces of compound 36

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Sample Name: run1

## HPLC traces of compound 36

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0809	2782.00977	516.37561	100.0000

Totals : 2782.00977 516.37561

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0809	2812.19629	521.91907	100.0000

Totals : 2812.19629 521.91907

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	BV	0.0858	7160.16650	1269.44250	100.0000

Totals : 7160.16650 1269.44250

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0813	5182.18311	954.98956	100.0000

Totals : 5182.18311 954.98956

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0809	3076.47729	570.49207	100.0000

Totals : 3076.47729 570.49207

Sample Name: run1

## HPLC traces of compound 36

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0809	3076.47729	570.49207	100.0000

Totals : 3076.47729 570.49207

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0809	3278.34961	607.59808	100.0000

Totals : 3278.34961 607.59808

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.452	VV	0.0808	1831.79126	340.07983	100.0000

Totals : 1831.79126 340.07983

=====  
\*\*\* End of Report \*\*\*

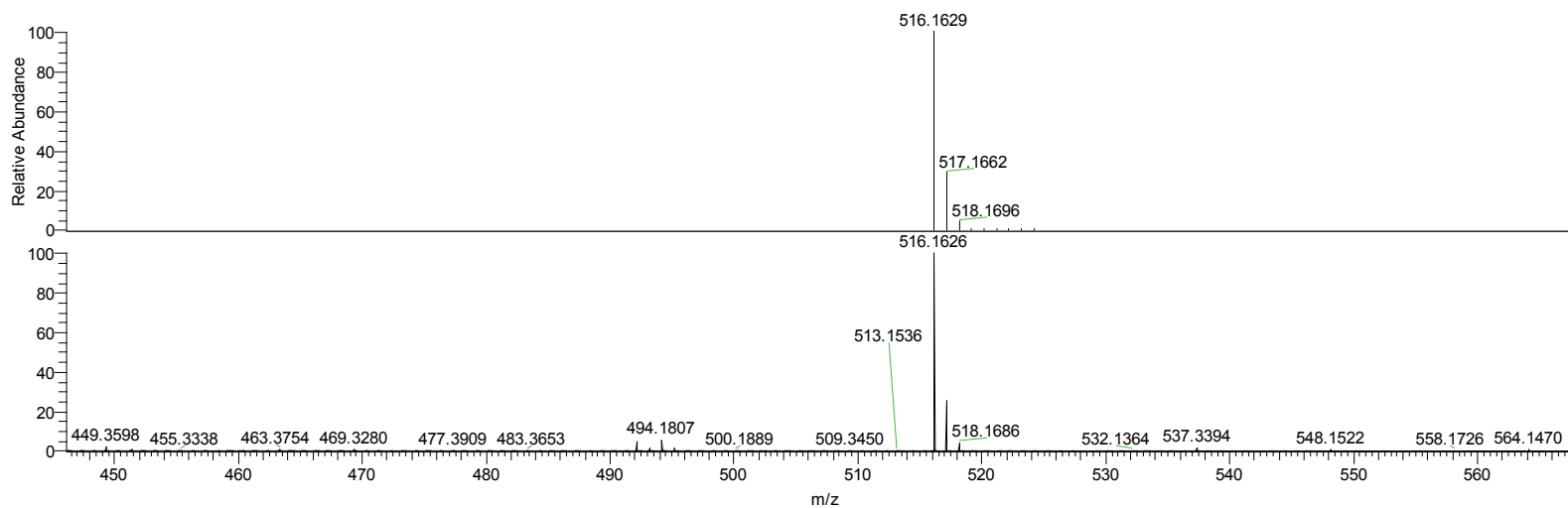
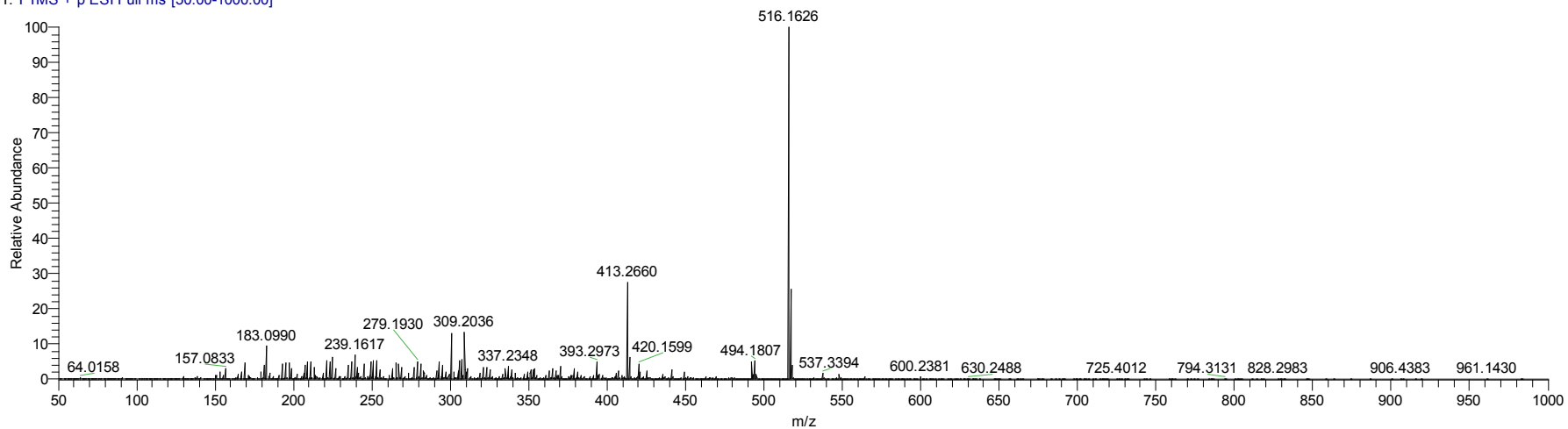
# HRMS of compound 36

C:\Xcalibur\...MTM-V-63\_130310125003

3/10/2013 2:06:26 PM

MTM-V-63

MTM-V-63\_130310125003 #13 RT: 0.10 AV: 1 NL: 8.21E7  
T: FTMS + p ESI Full ms [50.00-1000.00]



NL:  
7.29E5  
C<sub>27</sub>H<sub>27</sub>O<sub>8</sub>N Na:  
C<sub>27</sub>H<sub>27</sub>O<sub>8</sub>N<sub>1</sub>Na<sub>1</sub>  
pa Chrg 1

NL:  
8.21E7  
MTM-V-  
63\_130310125003#13  
RT: 0.10 AV: 1 T:  
FTMS + p ESI Full  
ms [50.00-1000.00]

### X-ray Crystallographic Analysis:

X-ray crystallographic analysis of compound **10**.<sup>S1</sup> Crystallographic data were collected on a crystal of **10** with dimensions 0.27 x 0.15 x 0.13 mm<sup>3</sup>. Data were collected at 110 K on a Bruker X8 Apex using Mo KR radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The structure was solved by direct methods after correction of the data using SADABS. Crystallographic data and refinement details for the complex mentioned herein is found in the Supporting Information (Table S1-S4). The thermal ellipsoid plots at 50% probability for compound **10** is displayed in Figure S1. All data were processed using the Bruker AXS SHELXTL software, version 6.10.

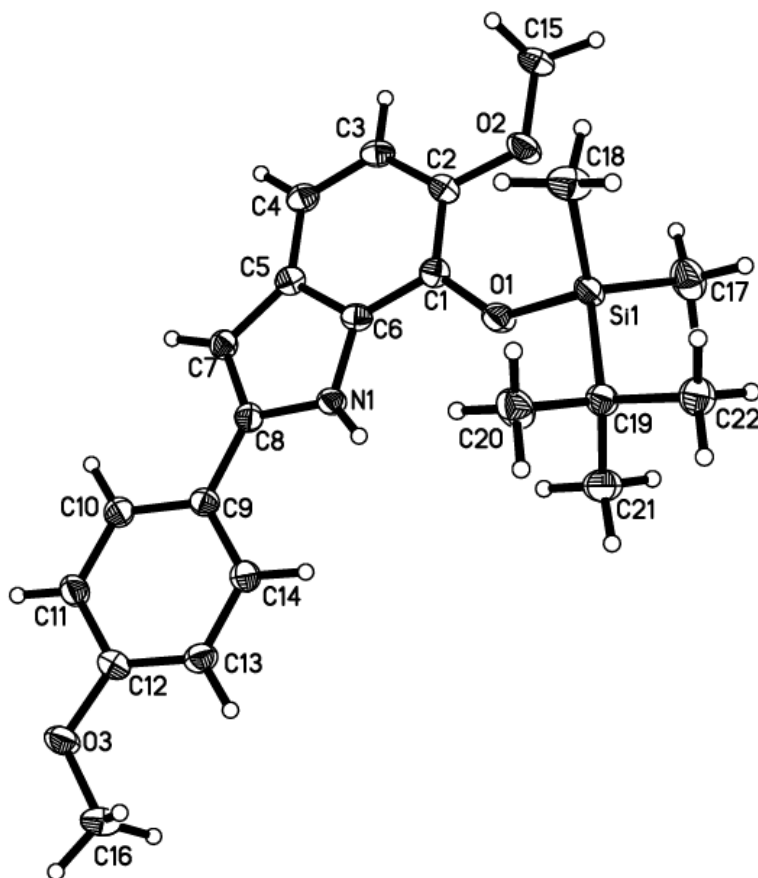


Figure S1. X-ray crystallography of compound **10**.

Table S1. Crystal data and structure refinement for 10.

Identification code	kp50
Empirical formula	C <sub>22</sub> H <sub>29</sub> N O <sub>3</sub> Si
Formula weight	383.55
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.3314(5) Å $\alpha$ = 97.114(2)°. b = 9.6558(5) Å $\beta$ = 94.927(2)°. c = 15.1609(9) Å $\gamma$ = 99.888(2)°.
Volume	1042.84(11) Å <sup>3</sup>
Z	2
Density (calculated)	1.221 Mg/m <sup>3</sup>
Absorption coefficient	0.134 mm <sup>-1</sup>
F(000)	412
Crystal size	0.27 x 0.15 x 0.13 mm <sup>3</sup>
Theta range for data collection	1.36 to 26.37°.
Index ranges	-9<=h<=9, -8<=k<=12, -18<=l<=18
Reflections collected	17172
Independent reflections	4231 [R(int) = 0.0490]
Completeness to theta = 26.37°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9823 and 0.9647
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4231 / 0 / 255
Goodness-of-fit on F <sup>2</sup>	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.1042
R indices (all data)	R1 = 0.0564, wR2 = 0.1142
Largest diff. peak and hole	0.340 and -0.313 e.Å <sup>-3</sup>



Table S2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **10**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Si(1)	4713(1)	9097(1)	1851(1)	21(1)
O(1)	4220(2)	7418(1)	2037(1)	26(1)
O(2)	3856(2)	6872(1)	191(1)	28(1)
O(3)	768(2)	2922(1)	6726(1)	28(1)
N(1)	2658(2)	5171(2)	2980(1)	20(1)
C(1)	3300(2)	6151(2)	1571(1)	20(1)
C(2)	3079(2)	5808(2)	644(1)	21(1)
C(3)	2156(2)	4453(2)	238(1)	23(1)
C(4)	1451(2)	3422(2)	740(1)	23(1)
C(5)	1660(2)	3736(2)	1675(1)	20(1)
C(6)	2594(2)	5099(2)	2067(1)	19(1)
C(7)	1117(2)	2997(2)	2405(1)	20(1)
C(8)	1734(2)	3898(2)	3191(1)	20(1)
C(9)	1561(2)	3677(2)	4120(1)	19(1)
C(10)	443(2)	2452(2)	4313(1)	23(1)
C(11)	226(2)	2227(2)	5182(1)	25(1)
C(12)	1118(2)	3234(2)	5895(1)	22(1)
C(13)	2259(2)	4445(2)	5724(1)	25(1)
C(14)	2468(2)	4661(2)	4844(1)	24(1)
C(15)	3613(3)	6623(2)	-762(1)	27(1)
C(16)	1662(3)	3927(2)	7474(1)	29(1)
C(17)	6965(3)	9383(2)	1362(1)	34(1)
C(18)	2779(3)	9591(2)	1155(1)	33(1)
C(19)	4968(2)	10083(2)	3024(1)	23(1)
C(20)	3072(3)	9877(2)	3394(1)	31(1)
C(21)	6344(3)	9509(2)	3636(1)	32(1)
C(22)	5653(3)	11685(2)	3021(1)	28(1)

Table S3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **10**.

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Si(1)-O(1)	1.6635(12)
Si(1)-C(18)	1.8580(19)
Si(1)-C(17)	1.860(2)
Si(1)-C(19)	1.8879(18)
O(1)-C(1)	1.367(2)
O(2)-C(2)	1.375(2)
O(2)-C(15)	1.426(2)
O(3)-C(12)	1.367(2)
O(3)-C(16)	1.428(2)
N(1)-C(6)	1.374(2)
N(1)-C(8)	1.386(2)
C(1)-C(2)	1.393(2)
C(1)-C(6)	1.393(2)
C(2)-C(3)	1.404(2)
C(3)-C(4)	1.384(2)
C(4)-C(5)	1.403(2)
C(5)-C(6)	1.407(2)
C(5)-C(7)	1.437(2)
C(7)-C(8)	1.377(2)
C(8)-C(9)	1.464(2)
C(9)-C(14)	1.396(2)
C(9)-C(10)	1.396(2)
C(10)-C(11)	1.379(2)
C(11)-C(12)	1.394(2)
C(12)-C(13)	1.382(2)
C(13)-C(14)	1.392(2)
C(19)-C(21)	1.532(2)
C(19)-C(20)	1.534(2)
C(19)-C(22)	1.543(2)
O(1)-Si(1)-C(18)	111.85(8)
O(1)-Si(1)-C(17)	108.82(8)
C(18)-Si(1)-C(17)	113.09(9)
O(1)-Si(1)-C(19)	101.50(7)

C(18)-Si(1)-C(19)	110.31(8)
C(17)-Si(1)-C(19)	110.67(9)
C(1)-O(1)-Si(1)	136.84(11)
C(2)-O(2)-C(15)	118.03(14)
C(12)-O(3)-C(16)	117.14(14)
C(6)-N(1)-C(8)	109.35(14)
O(1)-C(1)-C(2)	125.36(15)
O(1)-C(1)-C(6)	117.24(15)
C(2)-C(1)-C(6)	117.35(15)
O(2)-C(2)-C(1)	114.75(15)
O(2)-C(2)-C(3)	124.85(15)
C(1)-C(2)-C(3)	120.38(16)
C(4)-C(3)-C(2)	121.61(16)
C(3)-C(4)-C(5)	119.27(16)
C(4)-C(5)-C(6)	118.14(16)
C(4)-C(5)-C(7)	135.97(16)
C(6)-C(5)-C(7)	105.88(14)
N(1)-C(6)-C(1)	128.28(15)
N(1)-C(6)-C(5)	108.47(15)
C(1)-C(6)-C(5)	123.25(15)
C(8)-C(7)-C(5)	108.16(15)
C(7)-C(8)-N(1)	108.11(14)
C(7)-C(8)-C(9)	130.51(15)
N(1)-C(8)-C(9)	121.37(15)
C(14)-C(9)-C(10)	117.27(16)
C(14)-C(9)-C(8)	122.51(15)
C(10)-C(9)-C(8)	120.22(15)
C(11)-C(10)-C(9)	121.54(16)
C(10)-C(11)-C(12)	120.31(16)
O(3)-C(12)-C(13)	125.15(16)
O(3)-C(12)-C(11)	115.49(15)
C(13)-C(12)-C(11)	119.35(16)
C(12)-C(13)-C(14)	119.81(16)
C(13)-C(14)-C(9)	121.69(16)
C(21)-C(19)-C(20)	108.49(15)
C(21)-C(19)-C(22)	109.60(15)

C(20)-C(19)-C(22)	108.58(14)
C(21)-C(19)-Si(1)	110.38(12)
C(20)-C(19)-Si(1)	109.42(12)
C(22)-C(19)-Si(1)	110.33(12)

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Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **10**. The anisotropic displacement factor exponent takes the form:  $-2p^2[ h^2 a^2 U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
Si(1)	27(1)	19(1)	17(1)	4(1)	5(1)	3(1)
O(1)	41(1)	18(1)	16(1)	1(1)	1(1)	-1(1)
O(2)	43(1)	25(1)	16(1)	4(1)	6(1)	1(1)
O(3)	38(1)	27(1)	16(1)	2(1)	5(1)	2(1)
N(1)	26(1)	17(1)	16(1)	1(1)	1(1)	1(1)
C(1)	22(1)	18(1)	20(1)	1(1)	2(1)	4(1)
C(2)	24(1)	22(1)	18(1)	4(1)	4(1)	6(1)
C(3)	26(1)	26(1)	16(1)	-1(1)	0(1)	7(1)
C(4)	25(1)	23(1)	20(1)	-2(1)	0(1)	4(1)
C(5)	21(1)	20(1)	20(1)	1(1)	2(1)	5(1)
C(6)	21(1)	21(1)	17(1)	2(1)	2(1)	7(1)
C(7)	22(1)	18(1)	21(1)	2(1)	2(1)	2(1)
C(8)	18(1)	19(1)	22(1)	5(1)	2(1)	4(1)
C(9)	20(1)	20(1)	20(1)	4(1)	1(1)	5(1)
C(10)	26(1)	21(1)	21(1)	0(1)	3(1)	0(1)
C(11)	29(1)	22(1)	22(1)	4(1)	6(1)	0(1)
C(12)	25(1)	24(1)	19(1)	5(1)	5(1)	8(1)
C(13)	28(1)	24(1)	20(1)	0(1)	-1(1)	2(1)
C(14)	28(1)	20(1)	23(1)	5(1)	0(1)	0(1)
C(15)	34(1)	32(1)	15(1)	6(1)	4(1)	8(1)
C(16)	37(1)	33(1)	17(1)	1(1)	1(1)	8(1)
C(17)	39(1)	33(1)	33(1)	6(1)	15(1)	4(1)
C(18)	42(1)	33(1)	23(1)	3(1)	0(1)	11(1)
C(19)	28(1)	19(1)	20(1)	3(1)	2(1)	2(1)
C(20)	39(1)	31(1)	24(1)	2(1)	12(1)	4(1)
C(21)	44(1)	24(1)	24(1)	4(1)	-5(1)	3(1)
C(22)	34(1)	20(1)	28(1)	3(1)	2(1)	4(1)

S1. Crystallographic data for structure **10** (deposition number CCDC 935741) reported in this paper have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-(0) 1223-336033 or e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)).