Supporting Information

A versatile approach to oligostilbenoid natural products – synthesis of permethylated analogues of viniferifuran, malibatol A, and shoreaphenol

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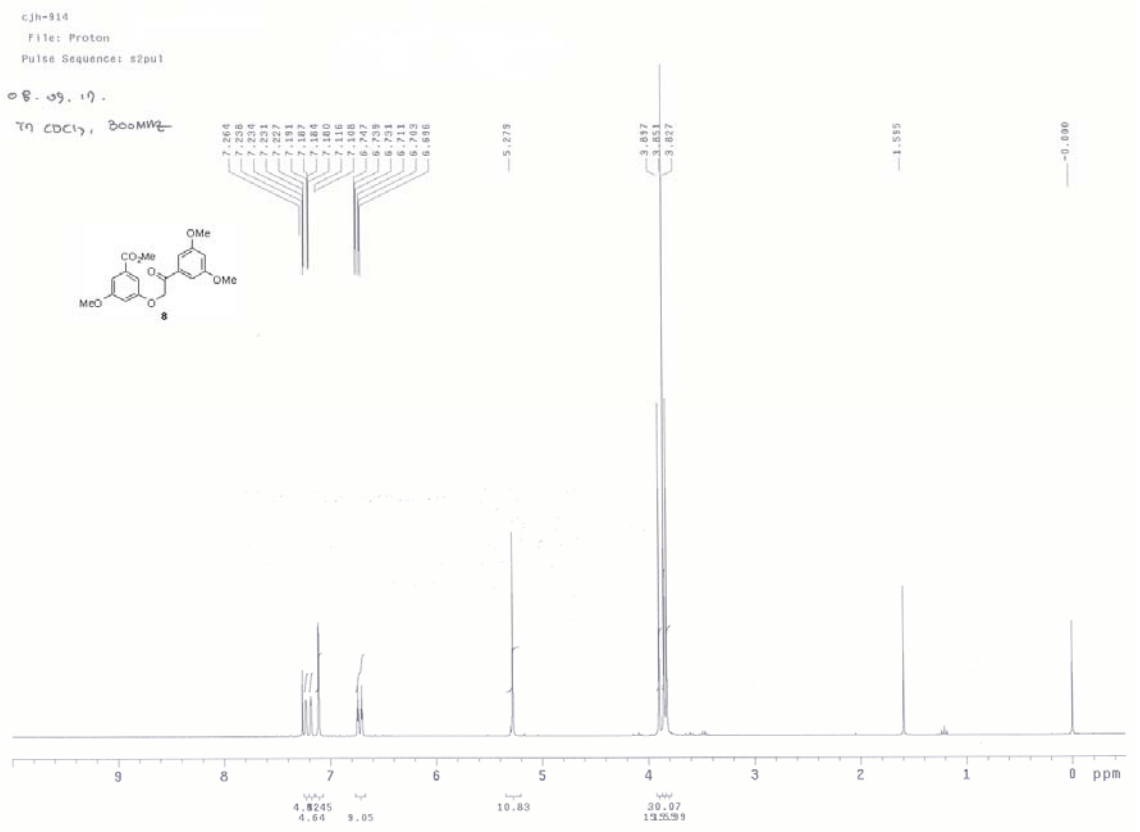
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7.191
7.187
7.184
7.180
7.116
7.108
6.747
6.738
6.731
6.711
6.703
6.696
5.279
3.847
3.831
3.827
1.595
0.000
OMe
CO2Me
OMe
MeO
O
8
9
8
7
6
5
4
3
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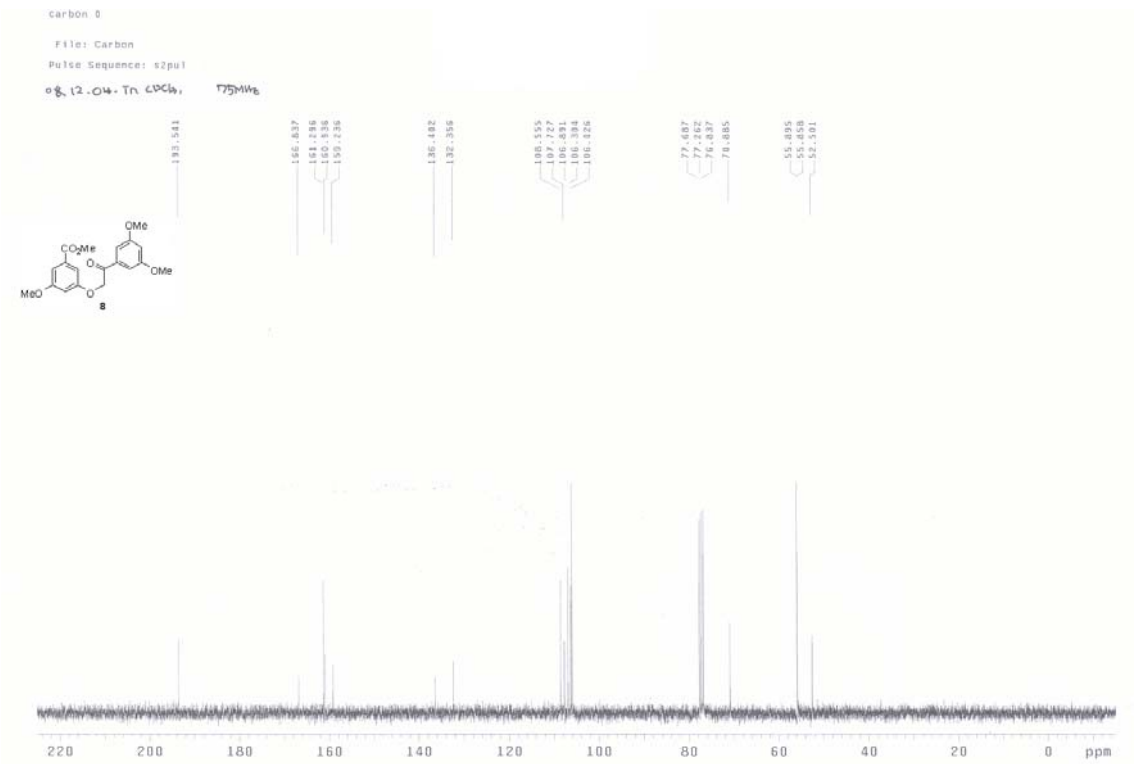
4.82
4.64
45
3.05
10.83
30.07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166.837
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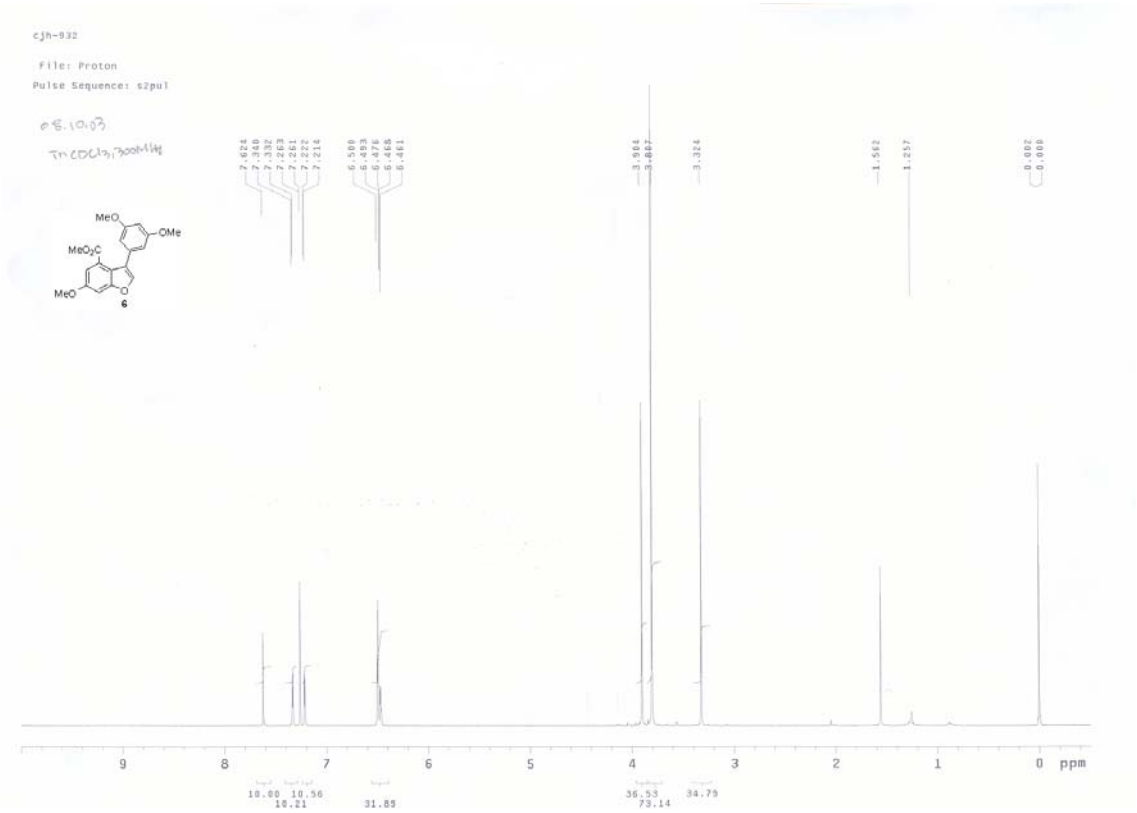
160.938
159.256
136.482
132.356
108.555
107.727
106.891
106.304
106.026
77.407
77.202
76.837
76.885
55.895
55.458
52.591
OMe
CO2Me
OMe
MeO
8
220
200
180
160
140
120
100
80
60
40
20
0 ppm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OMe
MeO2C
MeO
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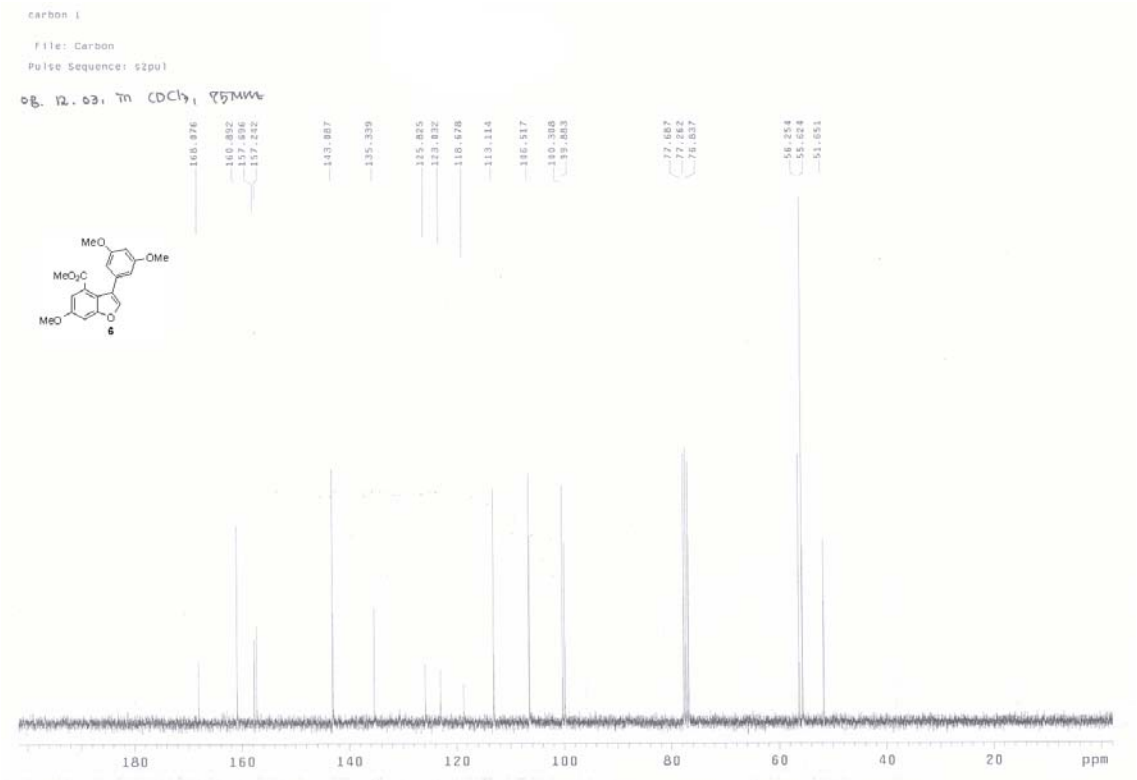
9
8
7
6
5
4
3
2
1
0 ppm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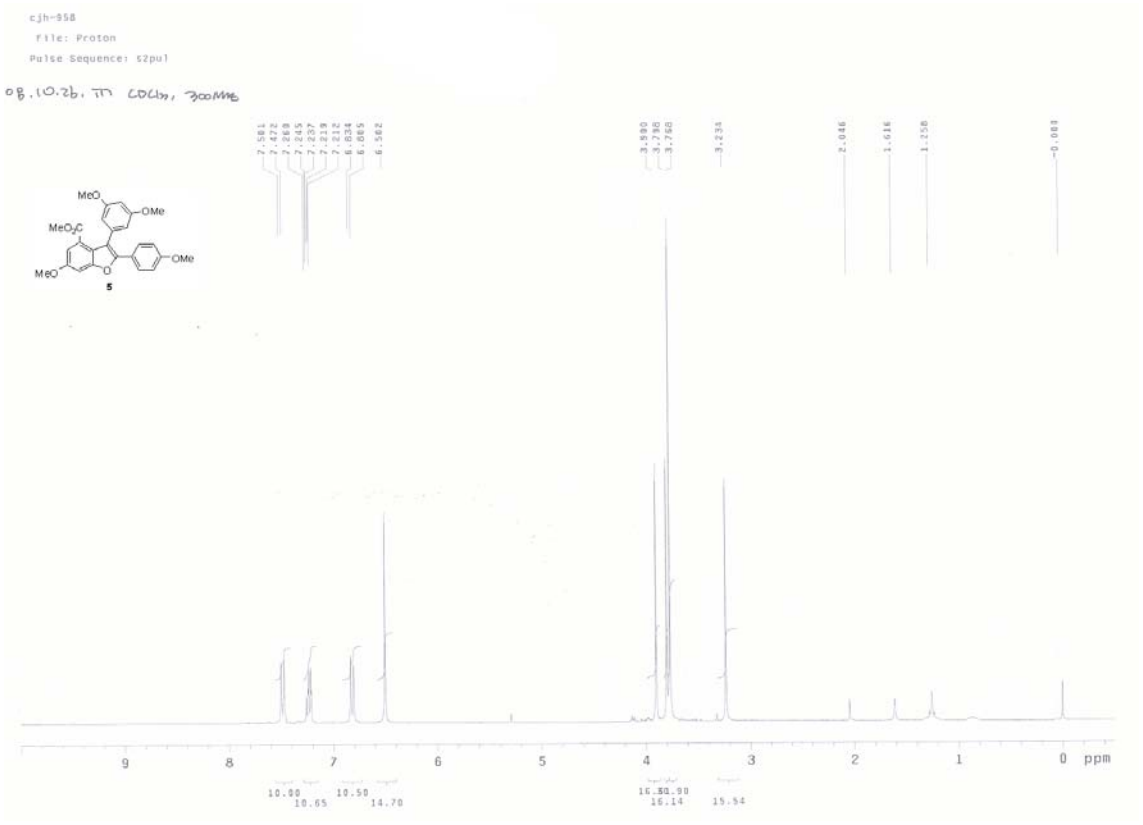
OMe
MeO2C
MeO
6
180
160
140
120
100
80
60
40
20
ppm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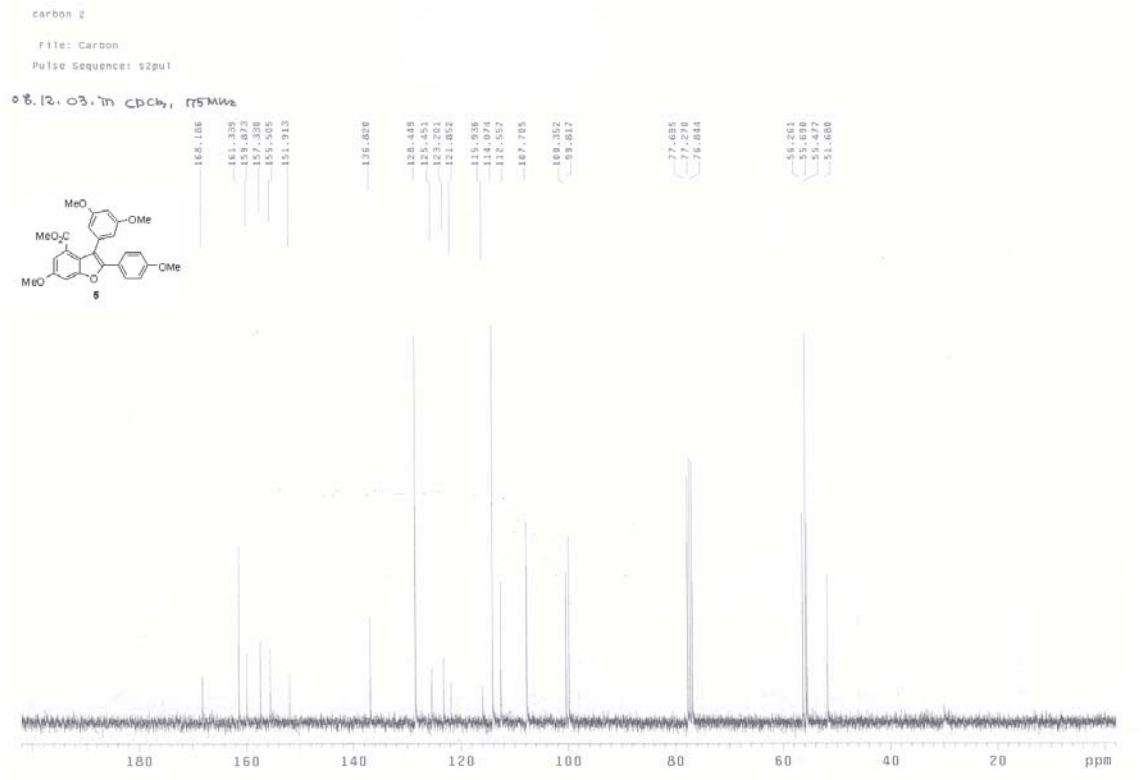
OMe
MeO2C
OMe
MeO
5
7.581
7.472
7.269
7.245
7.237
7.219
7.212
6.834
6.865
6.562
3.590
3.780
3.760
3.234
2.046
1.616
1.258
0.069
9
8
7
6
5
4
3
2
1
0 ppm
10.00
10.65
10.50
14.70
16.30
16.14
15.90
15.54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Pulse Sequence: s2pul
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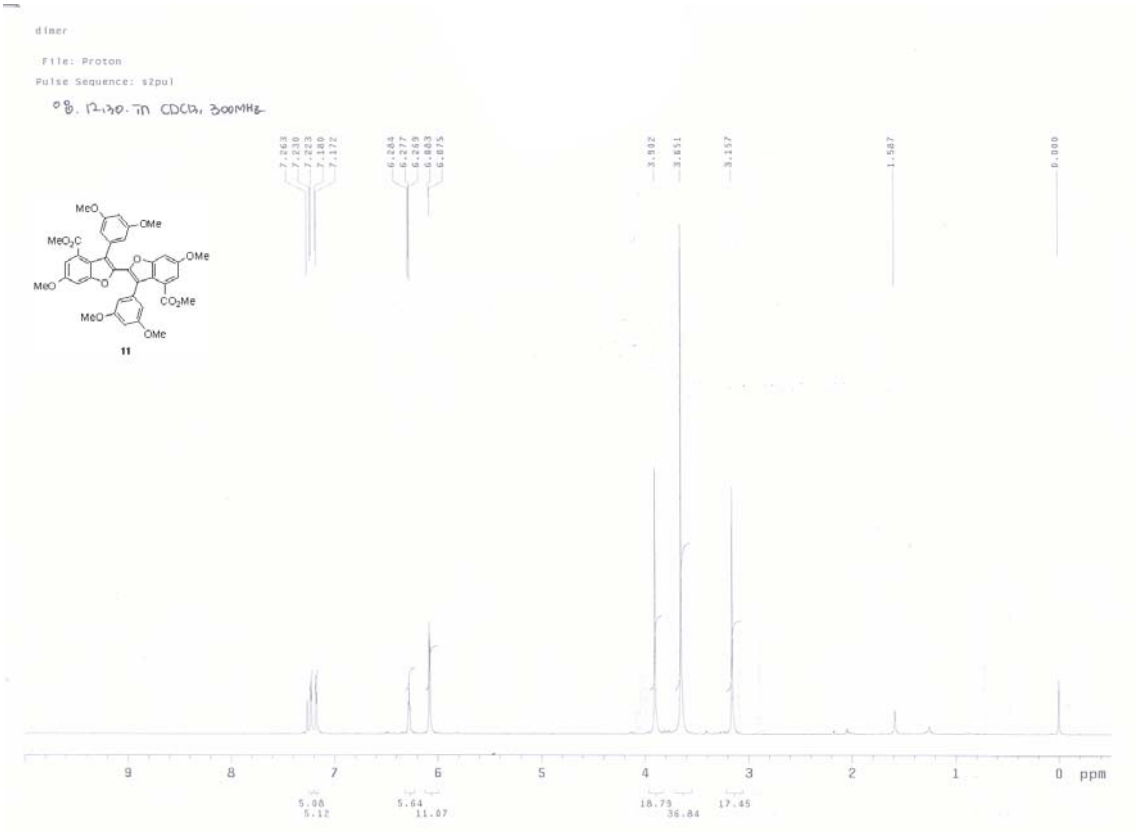
MeO
OMe
MeO2C
OMe
MeO
5
168.186
161.339
159.873
157.338
155.505
151.913
136.828
128.449
125.451
123.201
121.652
115.936
114.074
112.557
107.705
100.352
59.817
77.695
77.270
76.844
56.261
55.698
55.477
51.608
180
160
140
120
100
80
60
40
20
ppm


dimer
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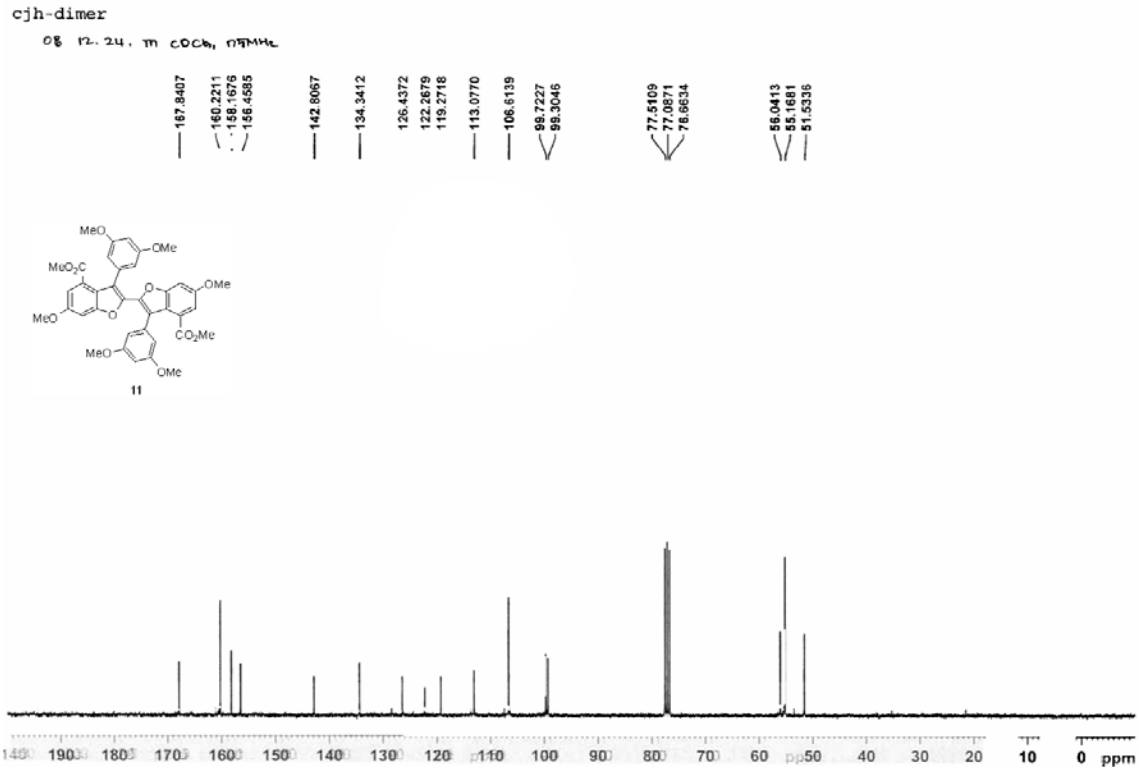
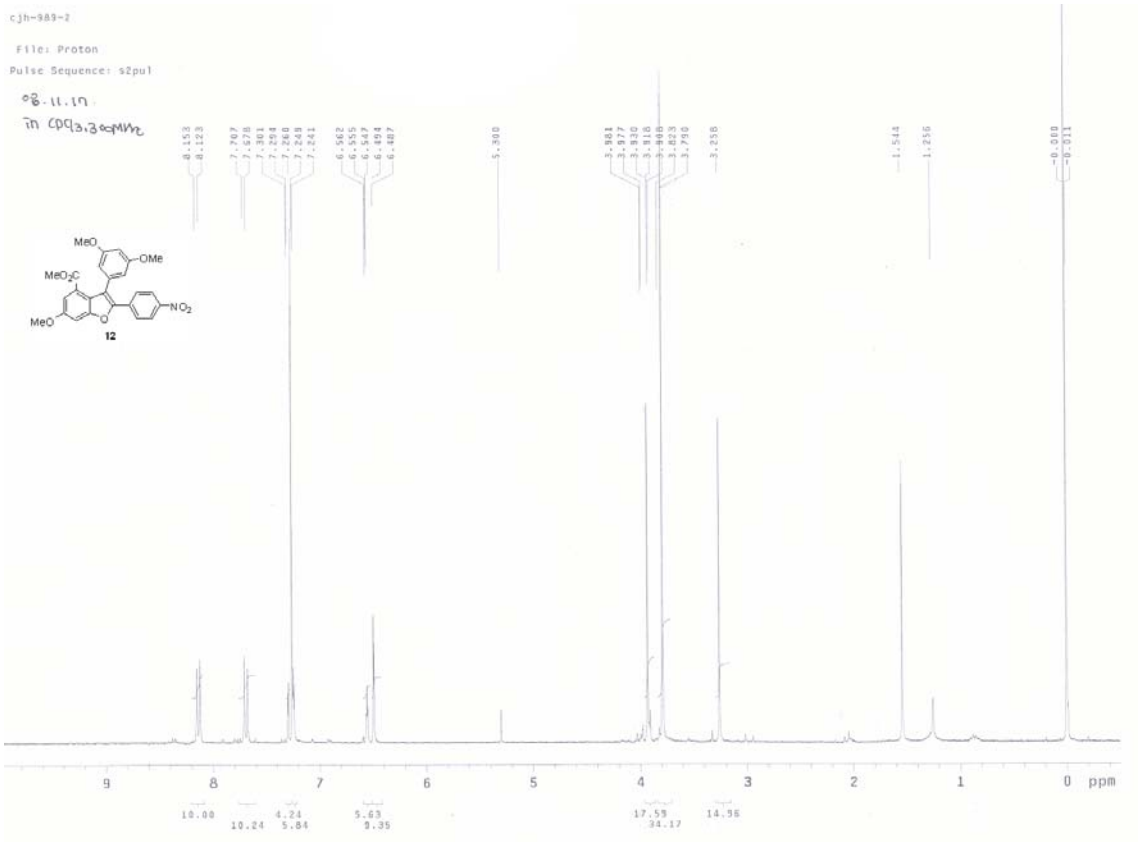
7.263
7.230
7.223
7.180
7.172
6.284
6.277
6.269
6.483
6.475
3.902
3.651
3.157
1.587
0.000
MeO
OMe
MeO2C
OMe
MeO
CO2Me
MeO
OMe
11
9
8
7
6
5
4
3
2
1
0 ppm
5.08
5.12
5.64
11.07
18.79
36.84
17.45


cjh-dimer
08 12.24. in CDCl3, 75MHz
167.8407
160.2211
158.1676
156.4585
142.8067
134.3412
126.4372
122.2679
119.2718
113.0770
106.6139
99.7227
99.3046
77.5109
77.0871
76.6634
56.0413
55.1681
51.5336
MeO
OMe
MeO2C
OMe
MeO
CO2Me
MeO
OMe
11
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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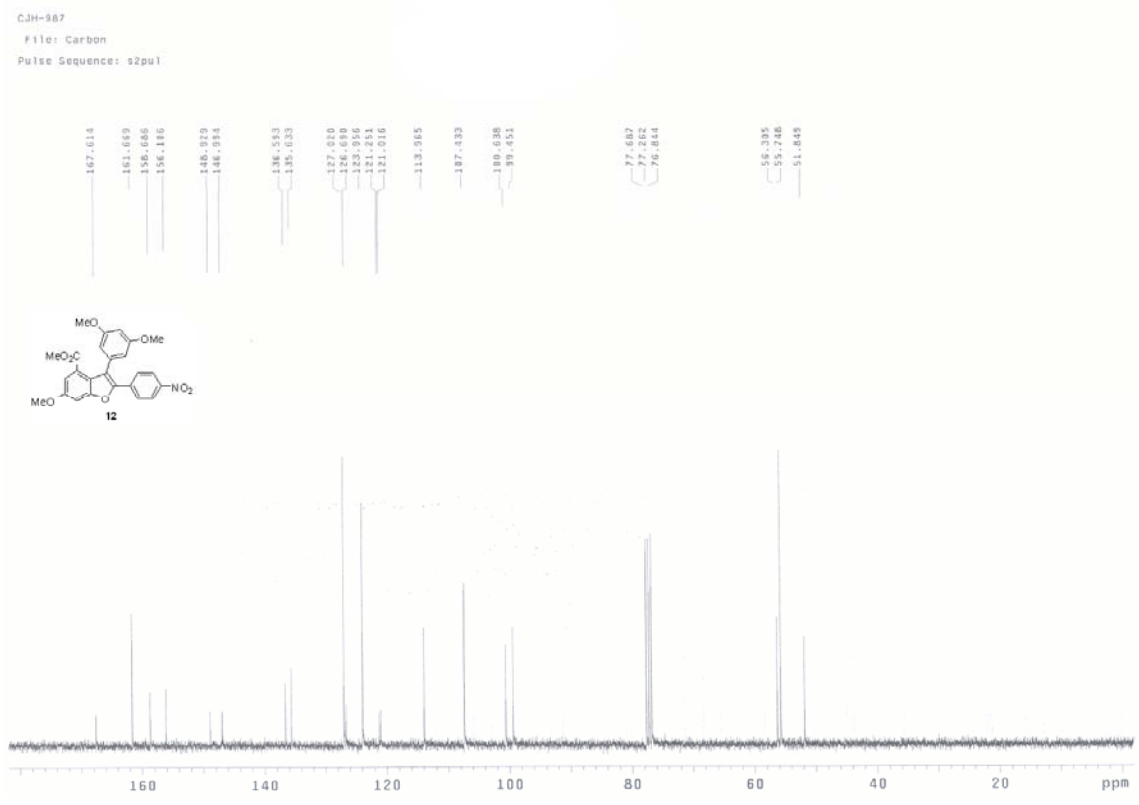
File: Proton
Pulse Sequence: s2pul
08.11.17
in CDCl3, 300MHz
MeO
OMe
MeO2C
NO2
MeO
12
8.153
8.123
7.707
7.678
7.301
7.294
7.260
7.248
7.241
6.562
6.555
6.543
6.494
6.487
5.300
3.981
3.977
3.930
3.916
3.846
3.835
3.790
3.258
1.544
1.256
0.000
-0.011
9
8
7
6
5
4
3
2
1
0 ppm
10.00
10.24
4.24
5.84
5.63
9.35
17.55
34.17
14.56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Pulse Sequence: s2pul
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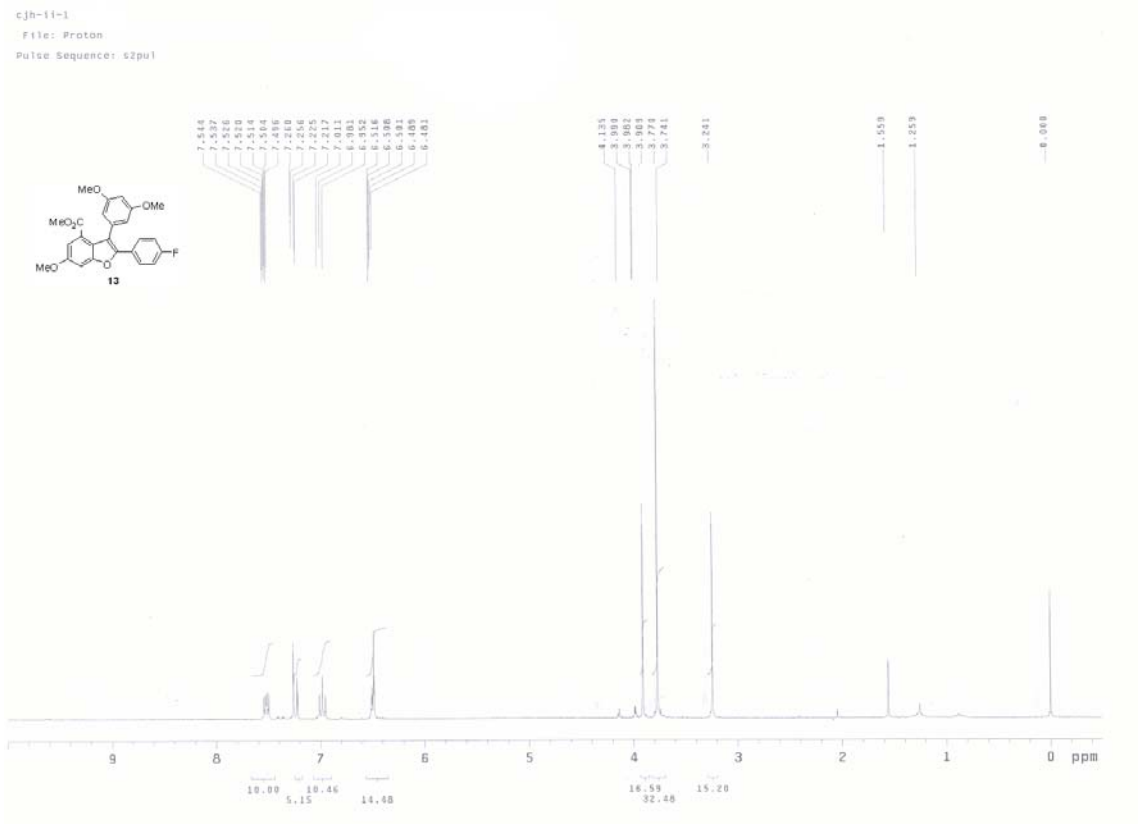
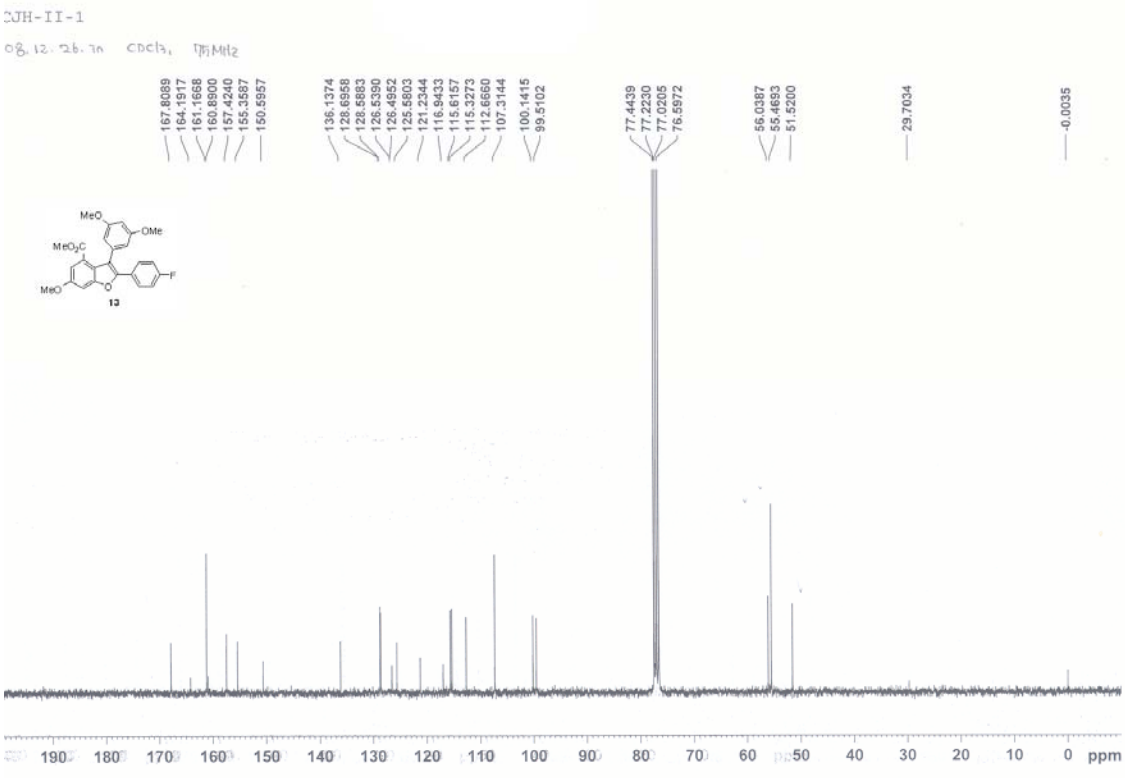
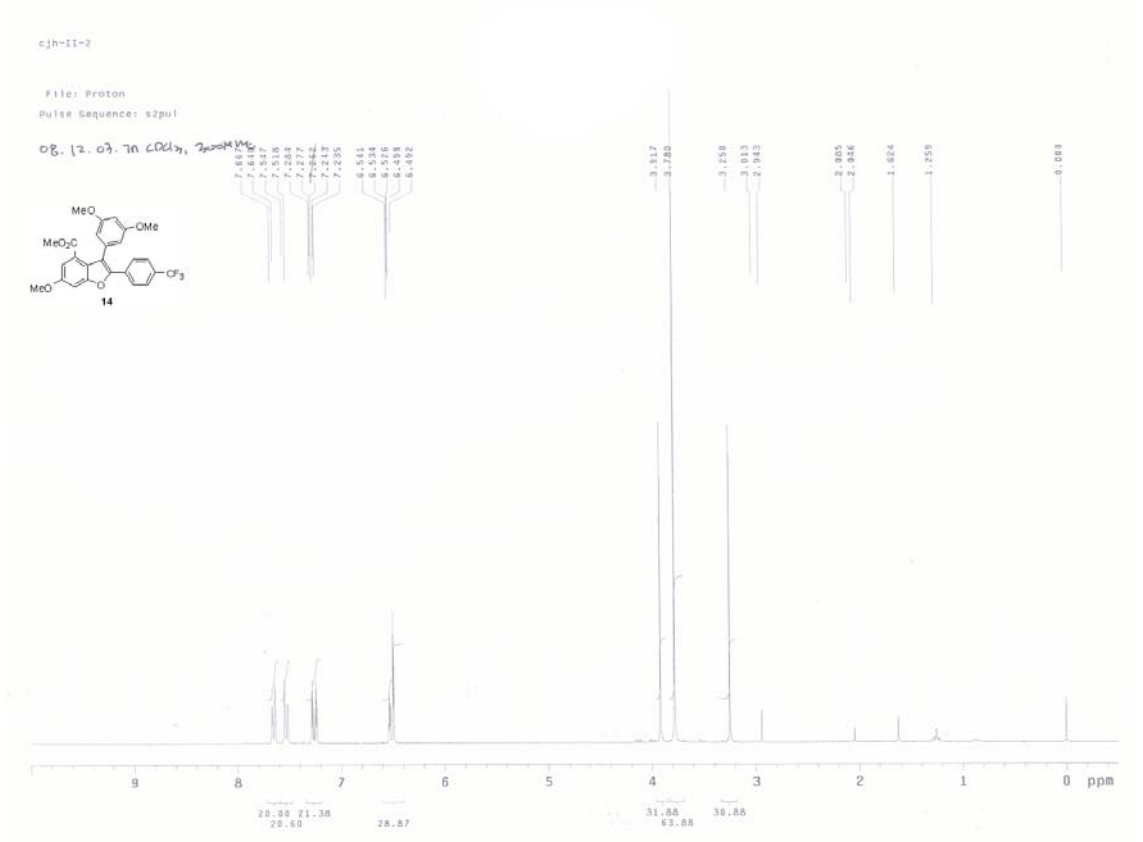
161.649
158.686
156.186
148.929
146.994
138.593
135.033
127.020
126.690
123.956
121.251
121.016
113.965
107.433
100.638
99.451
77.682
77.262
76.844
56.395
55.748
51.845
MeO
OMe
MeO2C
NO2
MeO
12
160
140
120
100
80
60
40
20
ppm


cjh-ii-1
File: Proton
Pulse Sequence: s2pul
MeO
OMe
MeO2C
F
MeO
13
ppm


CJH-II-1
CDCl3
TMS
MeO
OMe
MeO2C
F
MeO
13
ppm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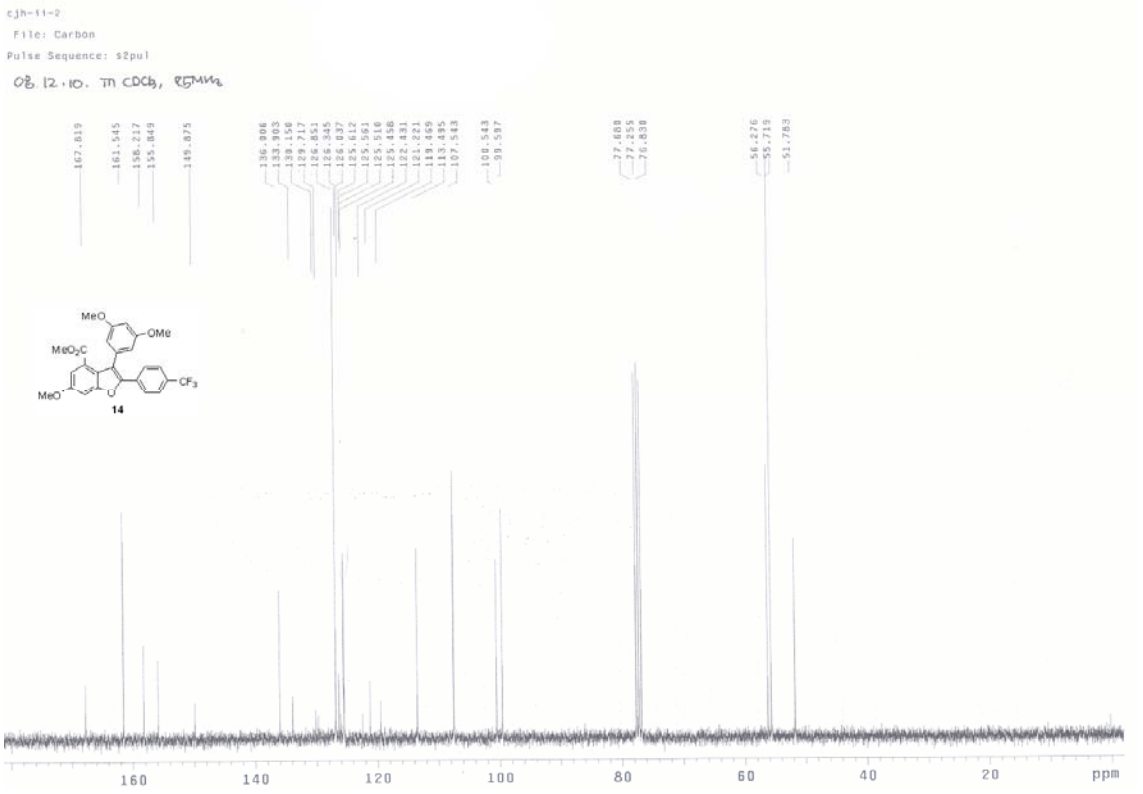
Pulse Sequence: s2pul
08.12.03. In CDCl3, 300MHz
MeO
OMe
MeO2C
CF3
MeO
14
ppm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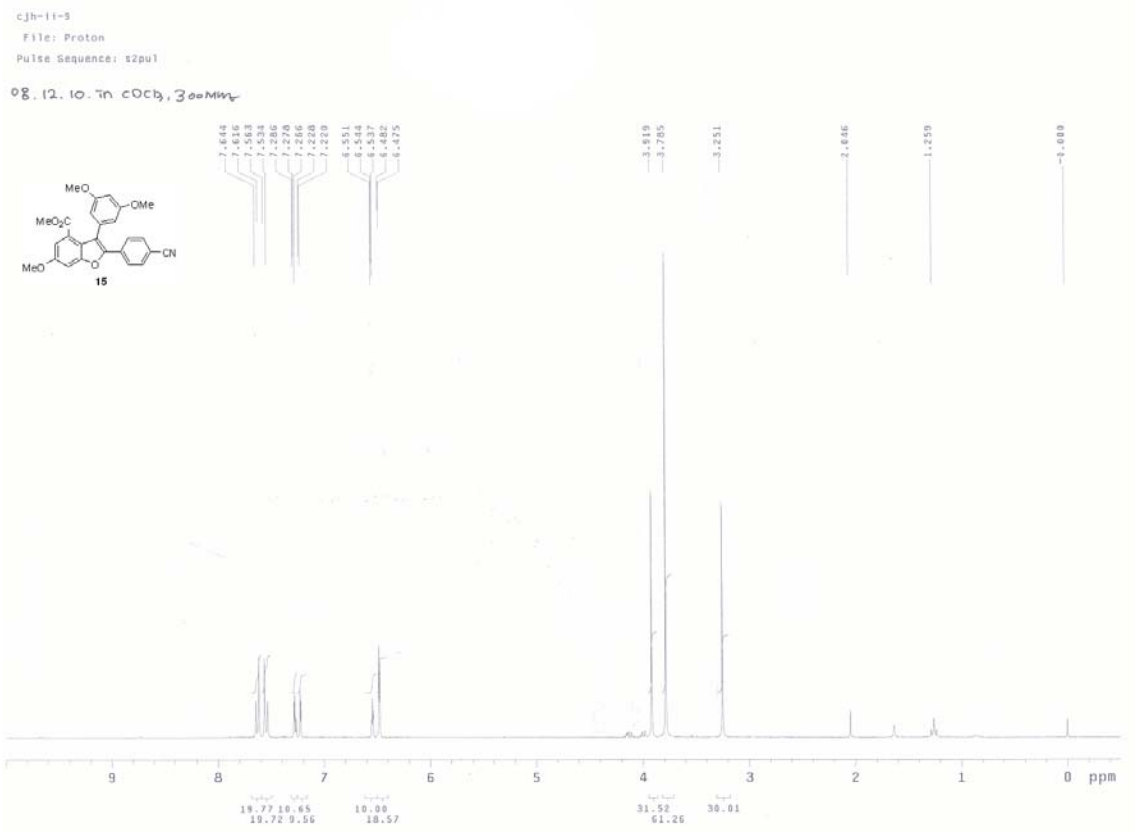
08.12.10. In CDCl3, RT
MeO
OMe
MeO2C
CF3
MeO
14
ppm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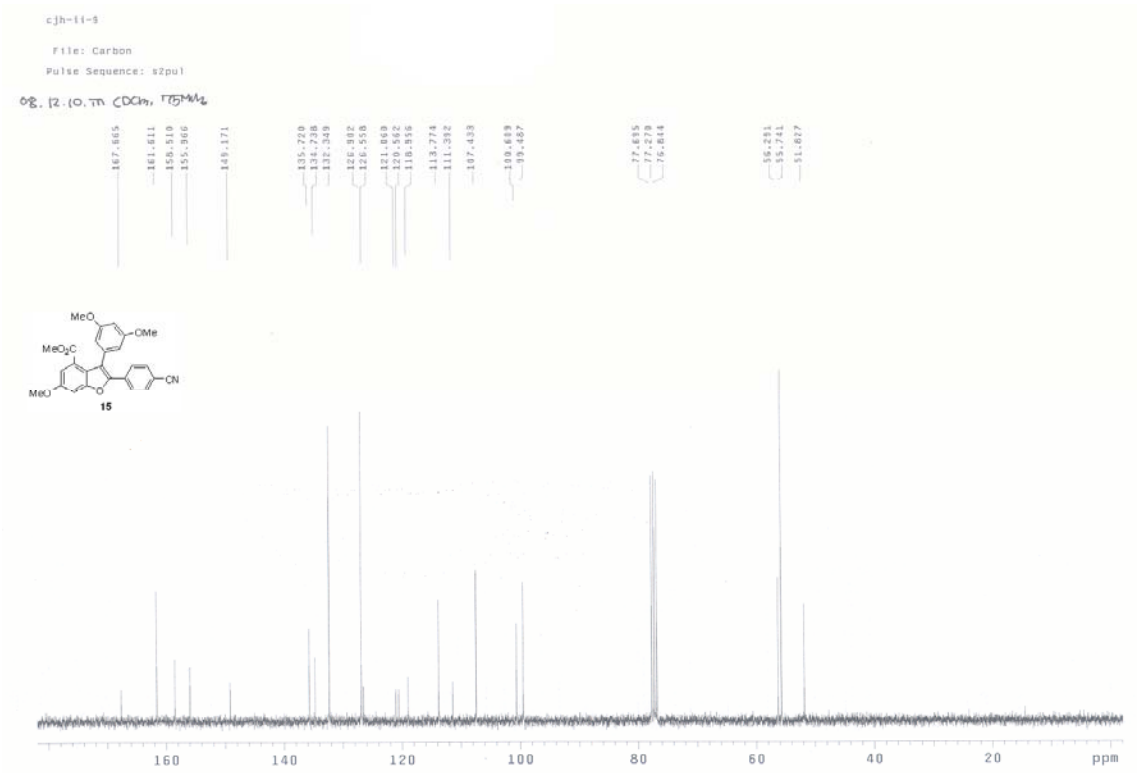
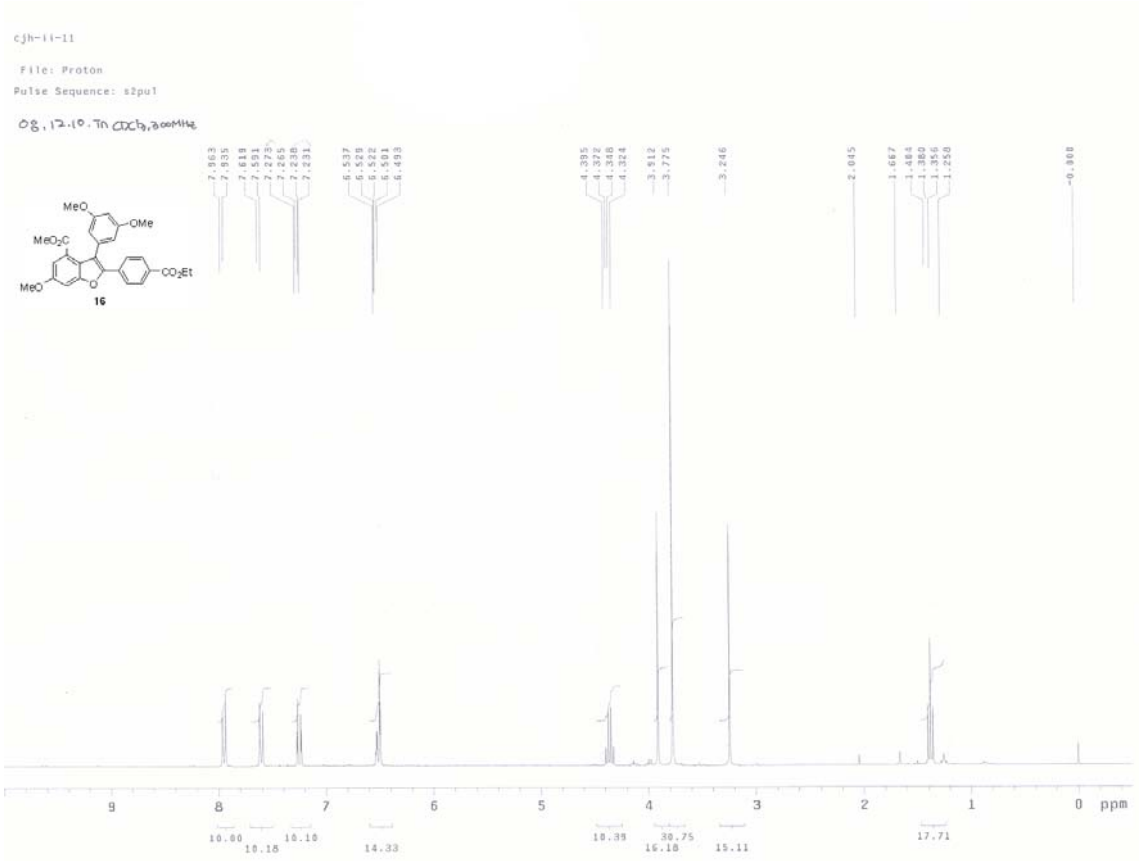
Pulse Sequence: s2pul
08.12.10.1H CDCl3, 300MHz
MeO
OMe
MeO2C
CN
MeO
15
7.644
7.616
7.563
7.534
7.286
7.276
7.266
7.220
6.551
6.544
6.537
6.482
6.475
3.819
3.785
3.251
2.046
1.259
1.000
9
8
7
6
5
4
3
2
1
0 ppm
19.77 10.65
19.72 9.56
10.00
18.57
31.52
61.26
30.01


cjh-ii-5
File: Carbon
Pulse Sequence: s2pul
08.12.10.1H CDCl3, 75MHz
167.865
161.611
150.510
155.966
149.171
135.720
134.238
132.349
126.902
126.558
121.869
120.582
110.956
113.774
111.382
107.433
100.689
99.487
77.655
77.279
76.844
56.291
55.741
51.827
MeO
OMe
MeO2C
CN
MeO
15
160
140
120
100
80
60
40
20
ppm


cjh-ii-11
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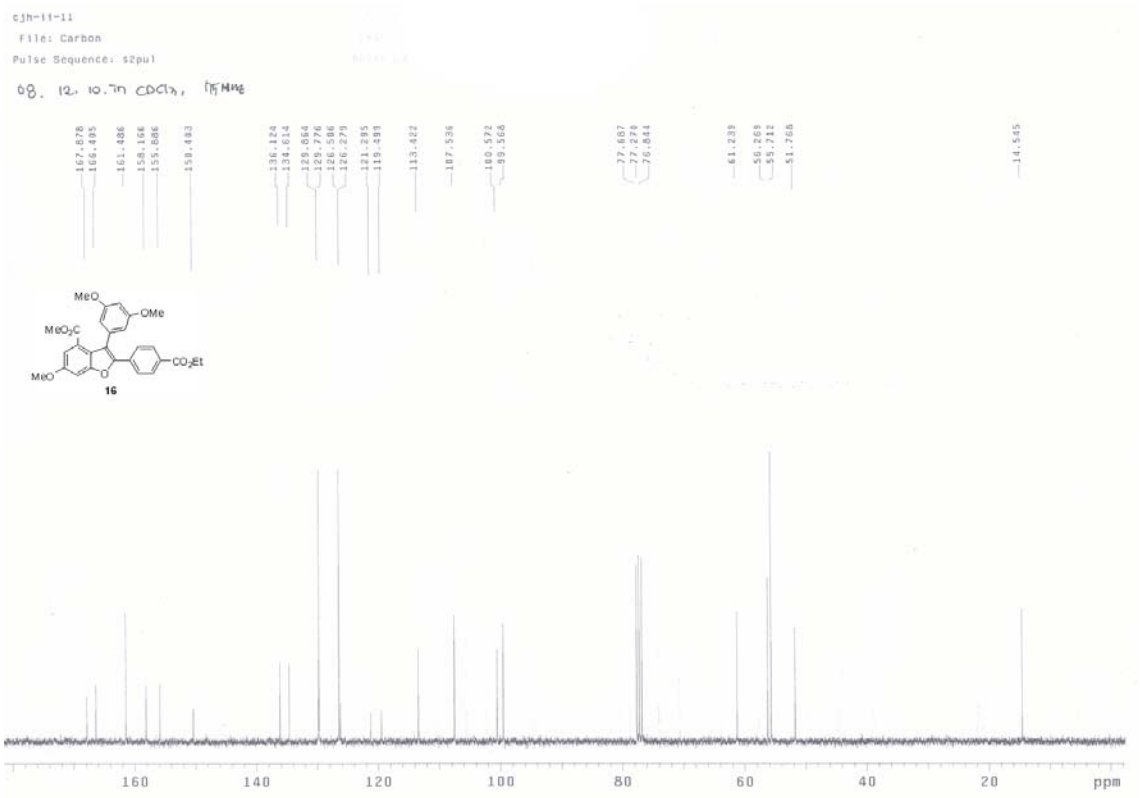
08.12.10.Th CDCl3,300MHz
MeO
OMe
MeO2C
CO2Et
MeO
O
16
7.863
7.835
7.619
7.591
7.275
7.265
7.238
7.231
6.537
6.528
6.522
6.501
6.493
4.395
4.372
4.348
4.324
3.912
3.775
3.246
2.045
1.667
1.484
1.380
1.356
1.250
-0.000
9
8
7
6
5
4
3
2
1
0 ppm
10.00
10.15
10.10
14.33
10.39
30.75
16.18
15.11
17.71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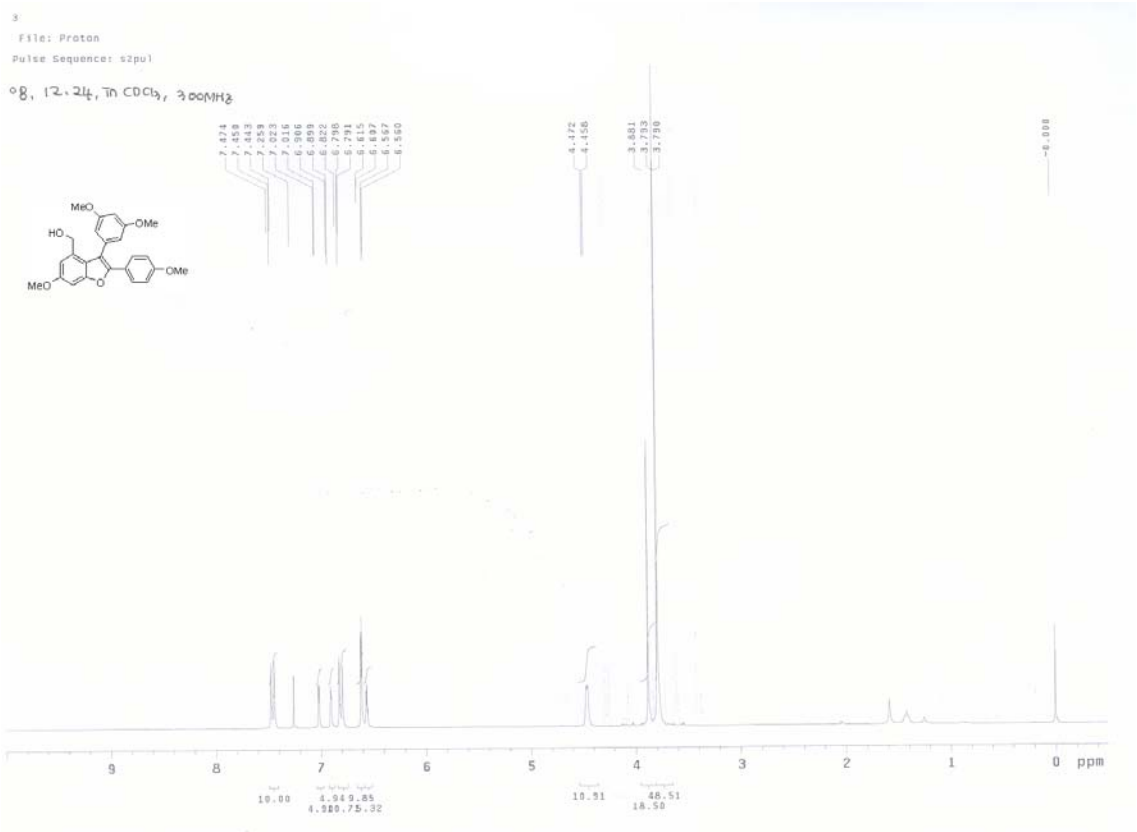
167.678
166.495
161.486
158.166
155.086
150.483
136.124
134.614
129.864
129.776
126.596
126.279
121.295
119.493
113.422
107.536
100.572
99.568
77.067
77.270
76.844
61.239
56.269
55.712
51.768
14.545
MeO
OMe
MeO2C
CO2Et
MeO
O
16
160
140
120
100
80
60
40
20
ppm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Pulse Sequence: s2pul
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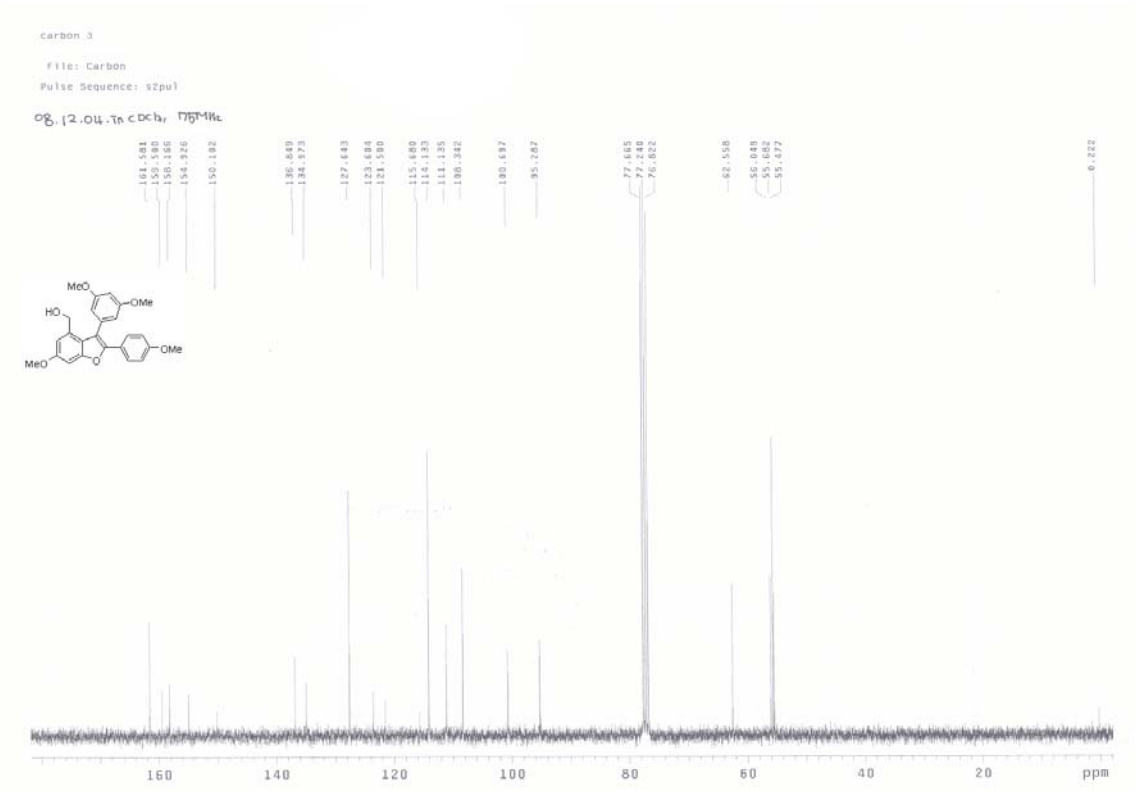
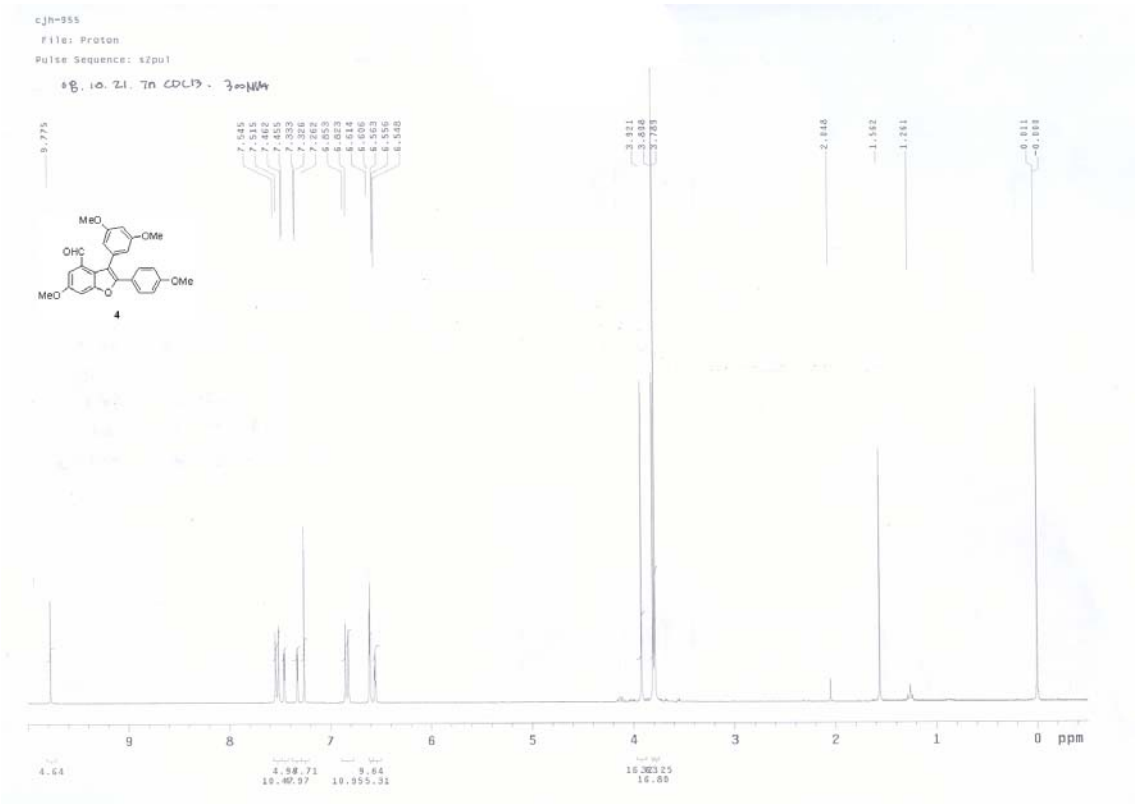
MeO
OMe
HO
OMe
MeO
7.474
7.458
7.443
7.259
7.023
7.016
6.906
6.899
6.822
6.798
6.791
6.615
6.607
6.567
6.560
4.172
4.156
3.881
3.793
3.790
0.000
9
8
7
6
5
4
3
2
1
0 ppm
10.00
4.94
9.85
4.92
10.75
5.32
10.51
48.51
18.50


carbon 3
File: Carbon
Pulse Sequence: s2pul
08. 12. 04. in CDCl3, 75MHz
MeO
OMe
HO
OMe
MeO
161.581
159.500
158.186
154.926
150.102
136.849
136.973
127.643
123.684
121.500
115.689
114.133
111.135
100.342
100.697
95.282
77.665
77.240
76.822
62.558
56.048
55.682
55.477
0.222
160
140
120
100
80
60
40
20
ppm


cjh-955
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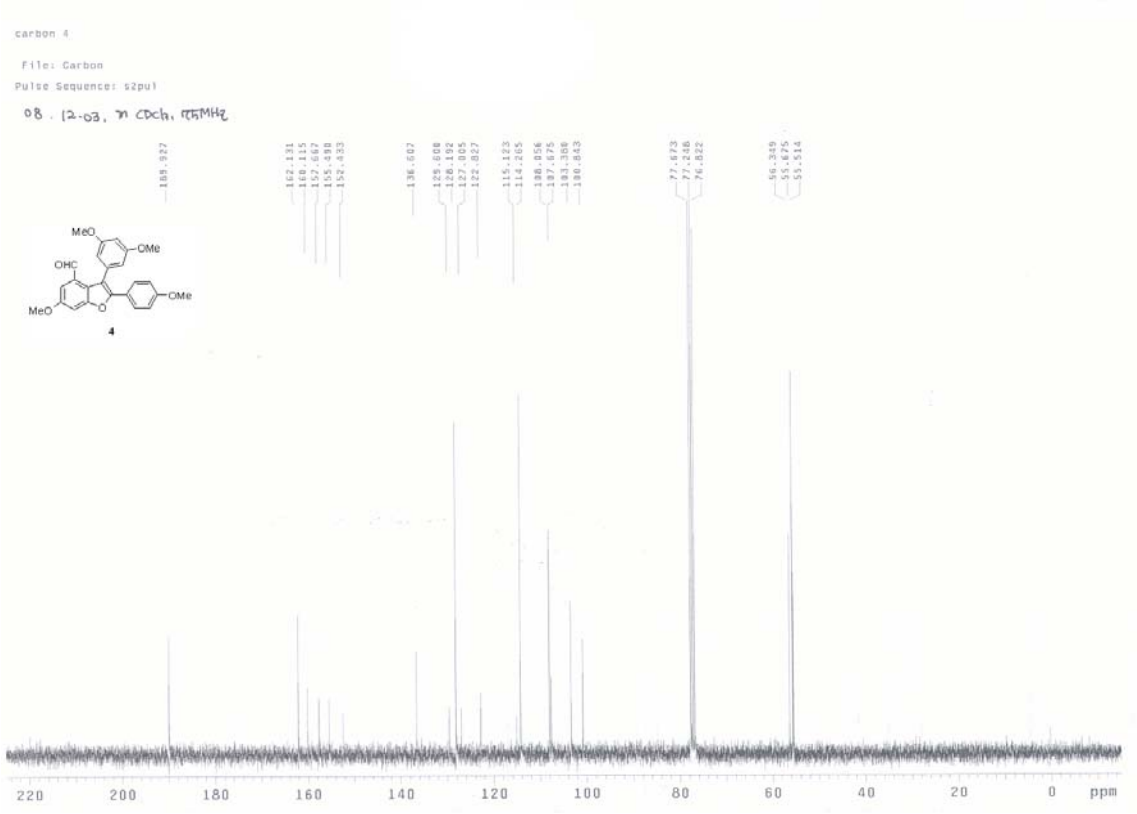
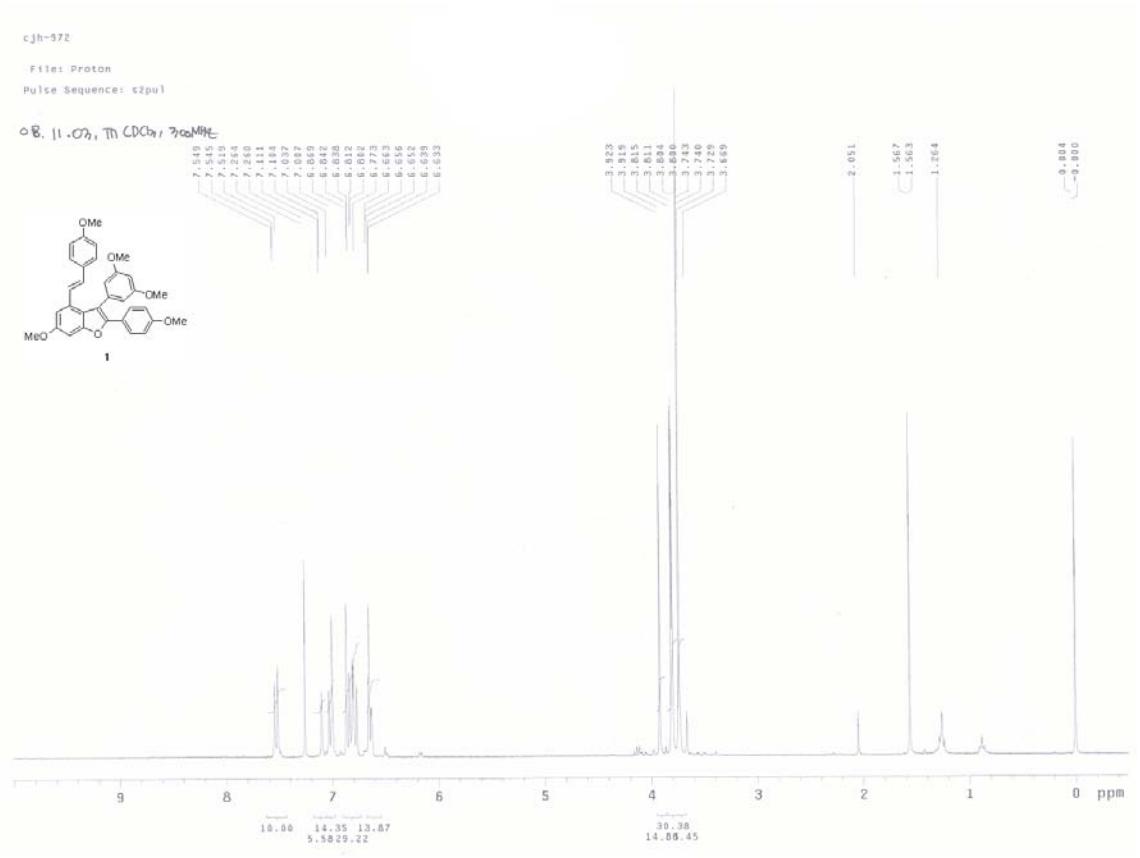
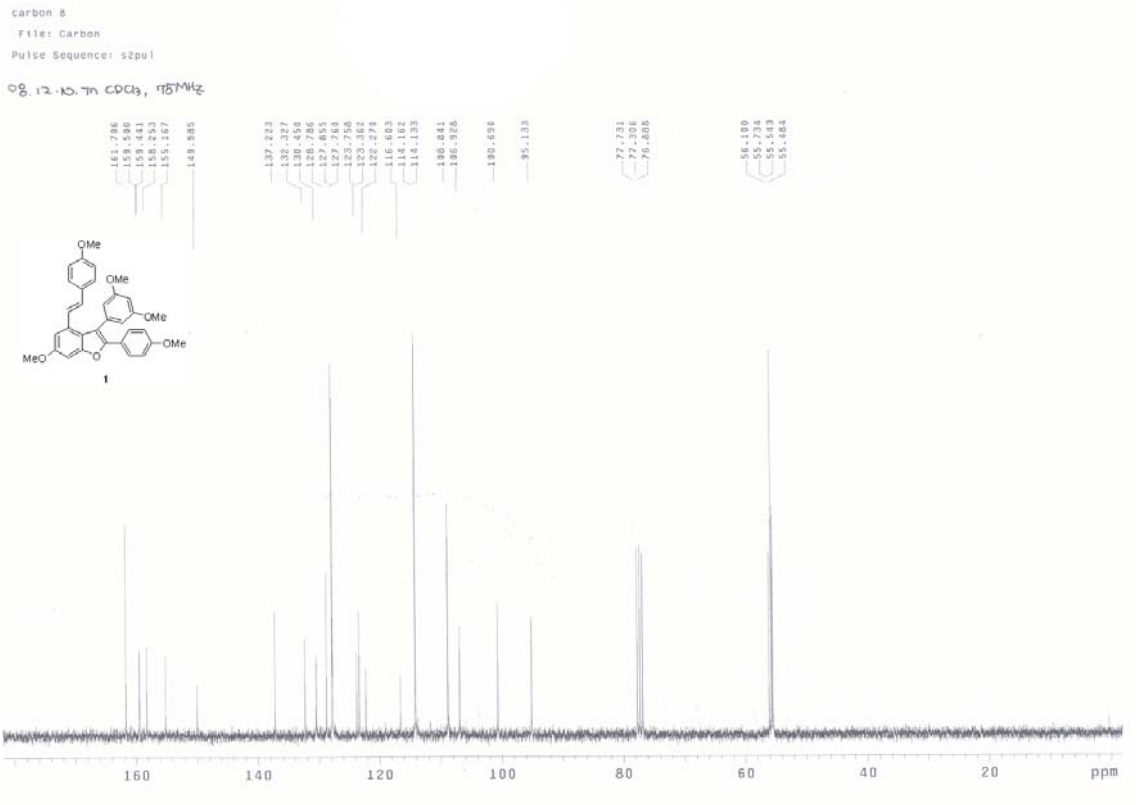
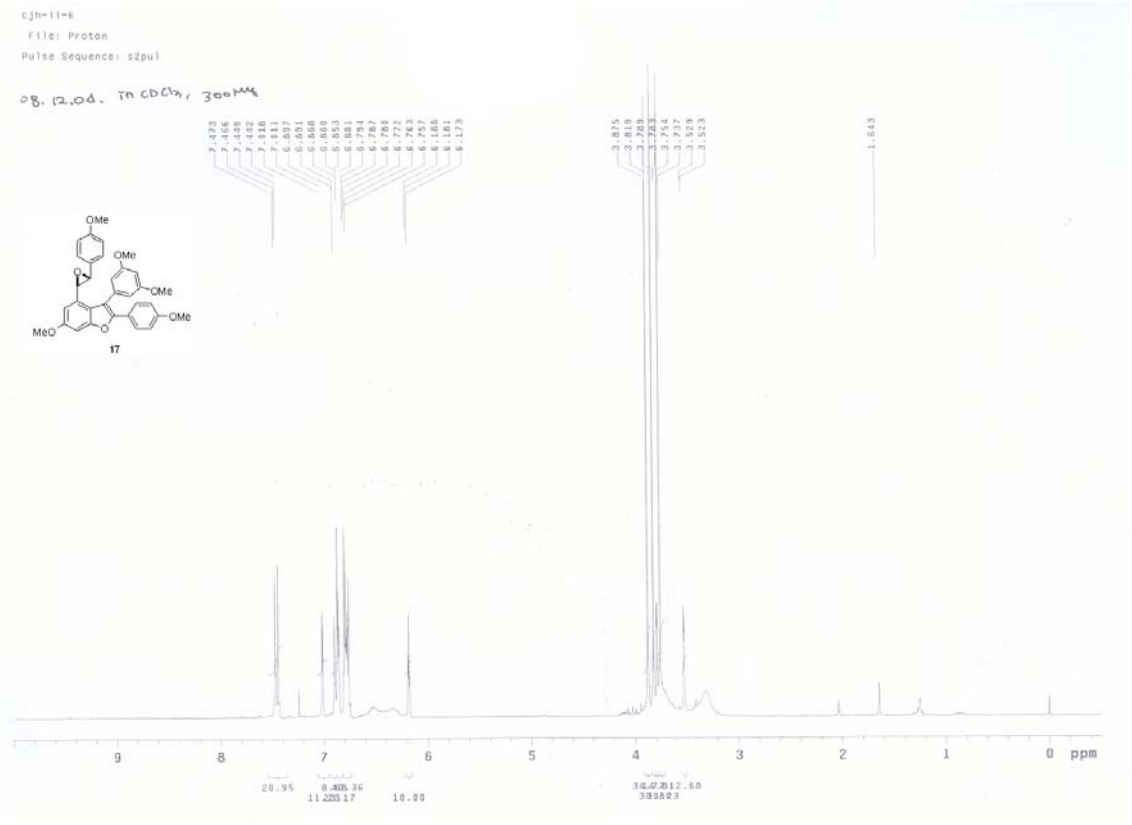
Pulse Sequence: s2pul
08. 10. 21. in CDCl3. 300MHz
9.775
7.545
7.515
7.492
7.455
7.333
7.326
7.262
6.853
6.823
6.614
6.606
6.563
6.556
6.548
3.821
3.804
3.789
2.848
1.562
1.261
0.011
-0.068
MeO
OMe
OHC
OMe
MeO
O
4
9
8
7
6
5
4
3
2
1
0 ppm
4.64
4.98.71
10.40.97
9.64
10.955.31
16.383.25
16.88


carbon 4
File: Carbon
Pulse Sequence: s2pul
08. 12-03, in CDCl3, 75MHz
189.927
162.131
160.115
157.667
155.498
152.433
136.607
129.608
126.192
127.005
122.827
115.123
114.265
100.056
97.675
93.368
80.843
77.673
77.256
76.822
56.349
55.675
55.514
MeO
OMe
OHC
OMe
MeO
O
4
220
200
180
160
140
120
100
80
60
40
20
0 ppm


cjh-572
File: Proton
Pulse Sequence: s2pul
08. 11. 07, in CDCl3, 700MHz
OMe
OMe
OMe
MeO
OMe
1
7.549
7.545
7.515
7.264
7.260
7.111
7.104
7.037
7.097
6.669
6.642
6.638
6.612
6.612
6.773
6.663
6.656
6.652
6.639
6.633
3.823
3.819
3.815
3.811
3.804
3.686
3.743
3.740
3.729
3.669
2.051
1.567
1.563
1.264
0.884
0.880
9
8
7
6
5
4
3
2
1
0
ppm
10.00
14.35
13.87
5.58
29.22
30.38
14.88.45


carbon 8
File: Carbon
Pulse Sequence: s2pul
08. 12. 10. in CDCl3, 175MHz
OMe
OMe
OMe
MeO
OMe
1
161.706
159.590
158.841
158.253
155.167
149.985
137.223
132.327
130.458
128.786
127.651
127.260
123.760
123.360
122.274
116.603
114.162
114.133
100.841
100.326
100.698
95.133
77.731
77.306
76.880
56.100
55.734
55.543
55.484
160
140
120
100
80
60
40
20
ppm


cjh-ii-6
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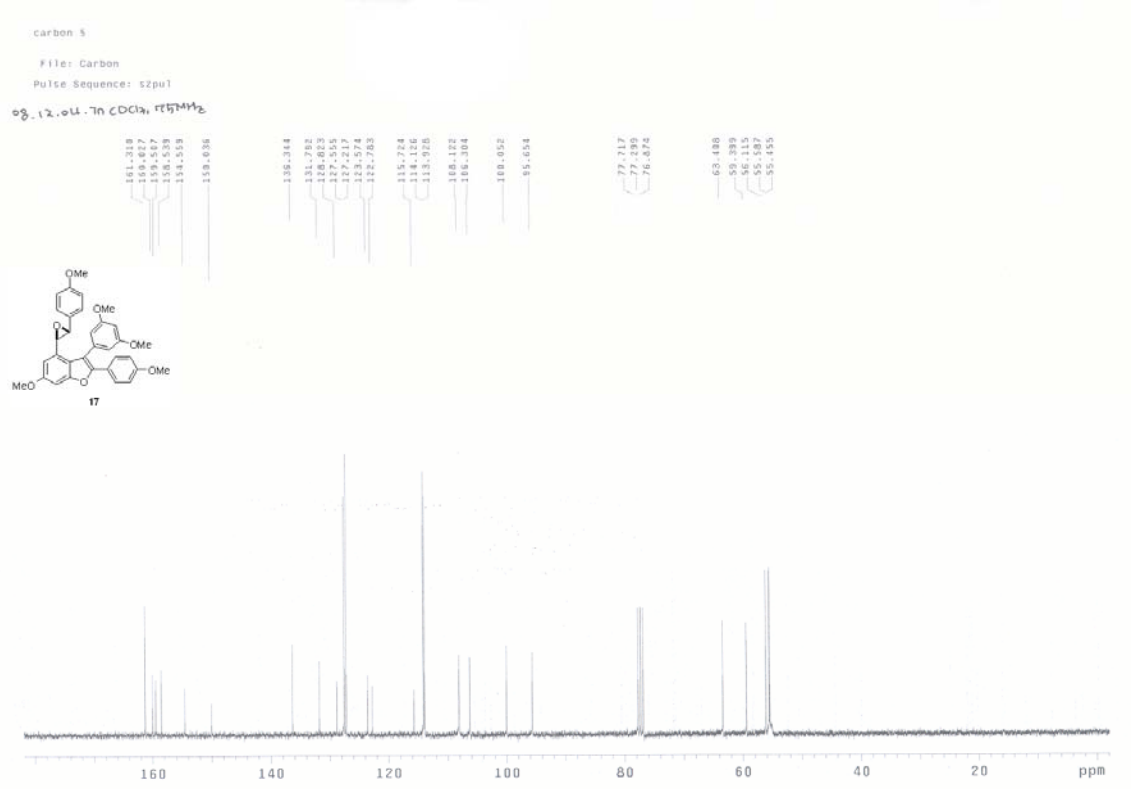
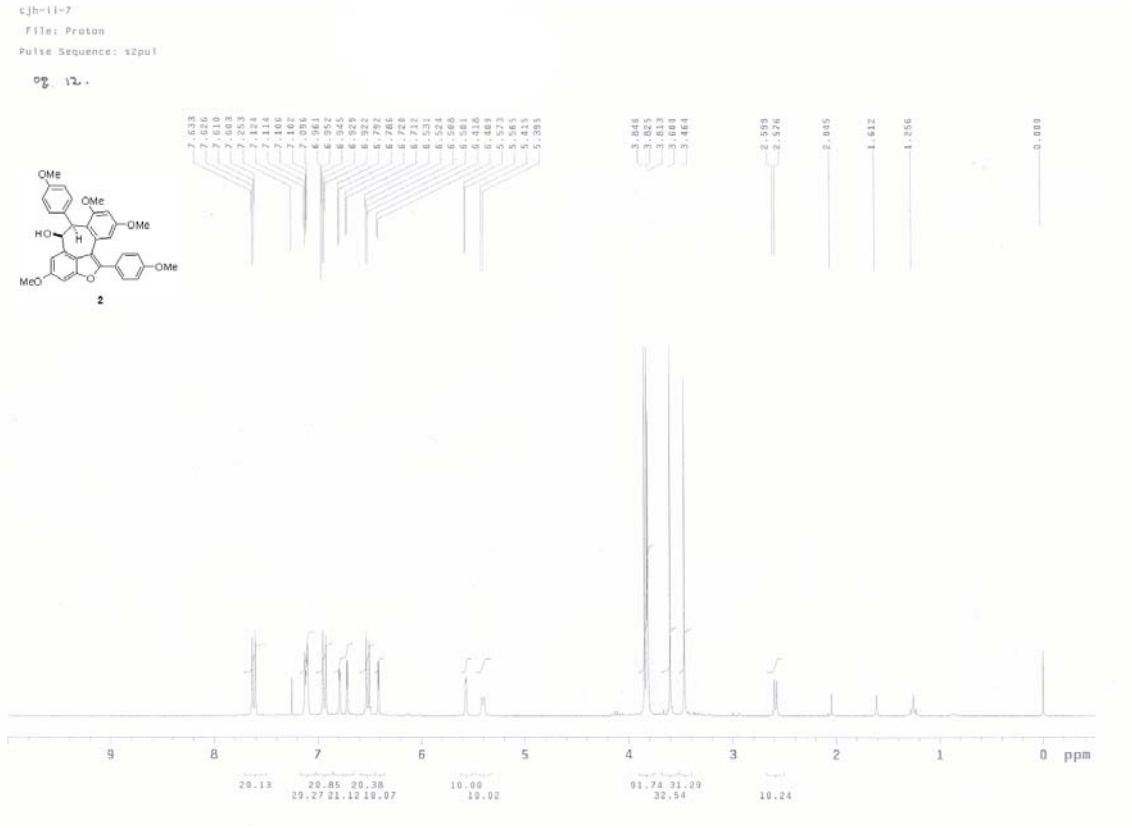
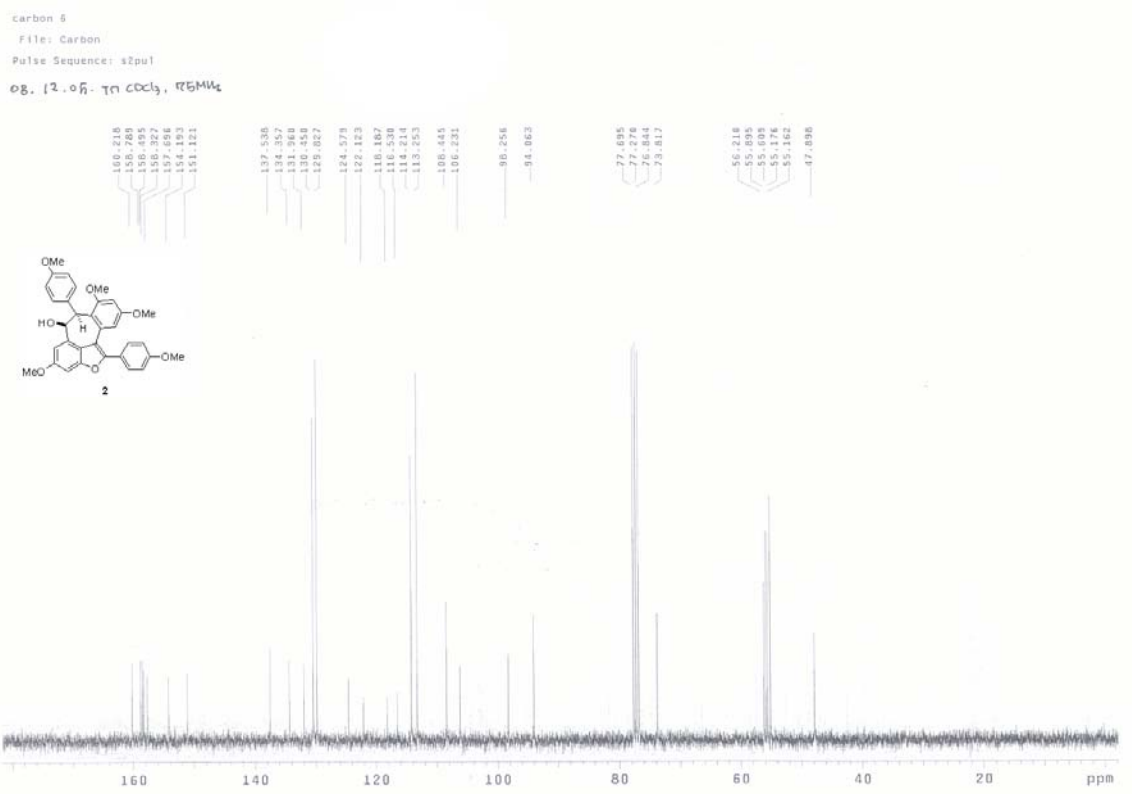
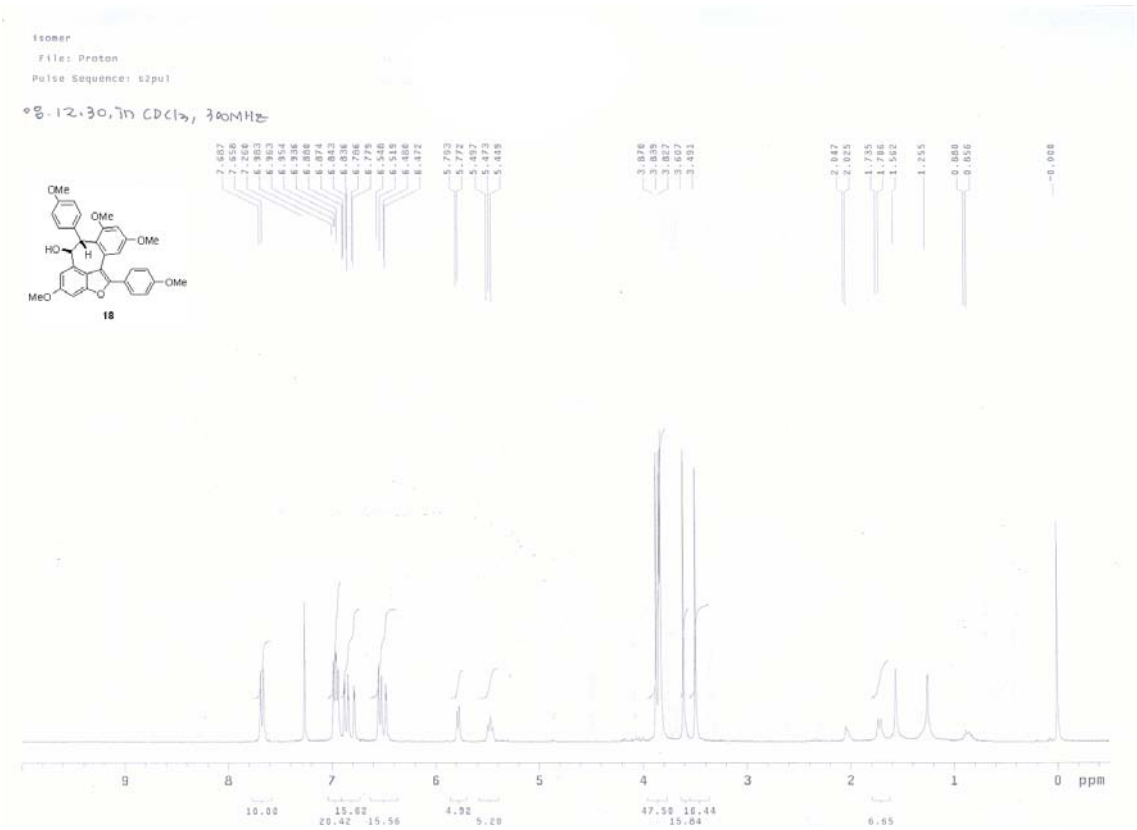
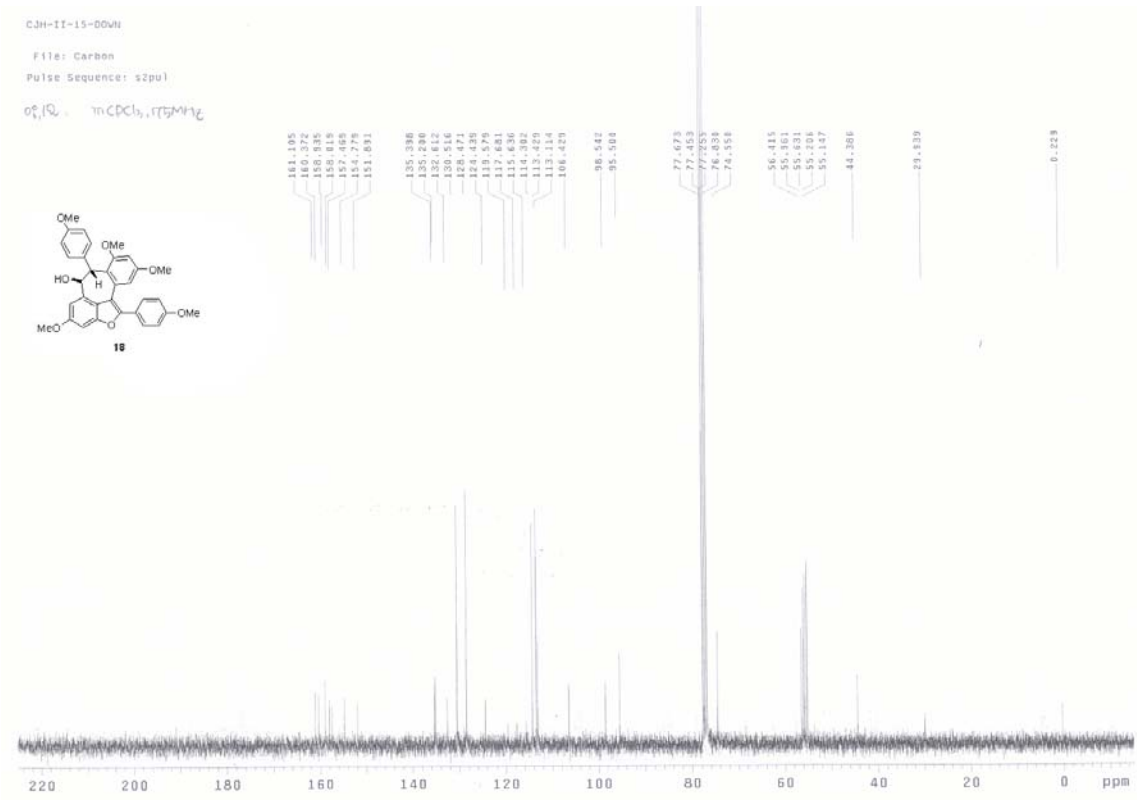
Pulse Sequence: s2pul
08.12.04. In CDCl3, 300MHz
OMe
OMe
OMe
OMe
MeO
17
7.473
7.466
7.449
7.442
7.016
6.811
6.637
6.631
6.868
6.869
6.853
6.801
6.794
6.787
6.780
6.772
6.763
6.757
6.186
6.181
6.173
3.875
3.819
3.789
3.783
3.764
3.737
3.529
3.523
1.643
9
8
7
6
5
4
3
2
1
0 ppm
20.95
10.00

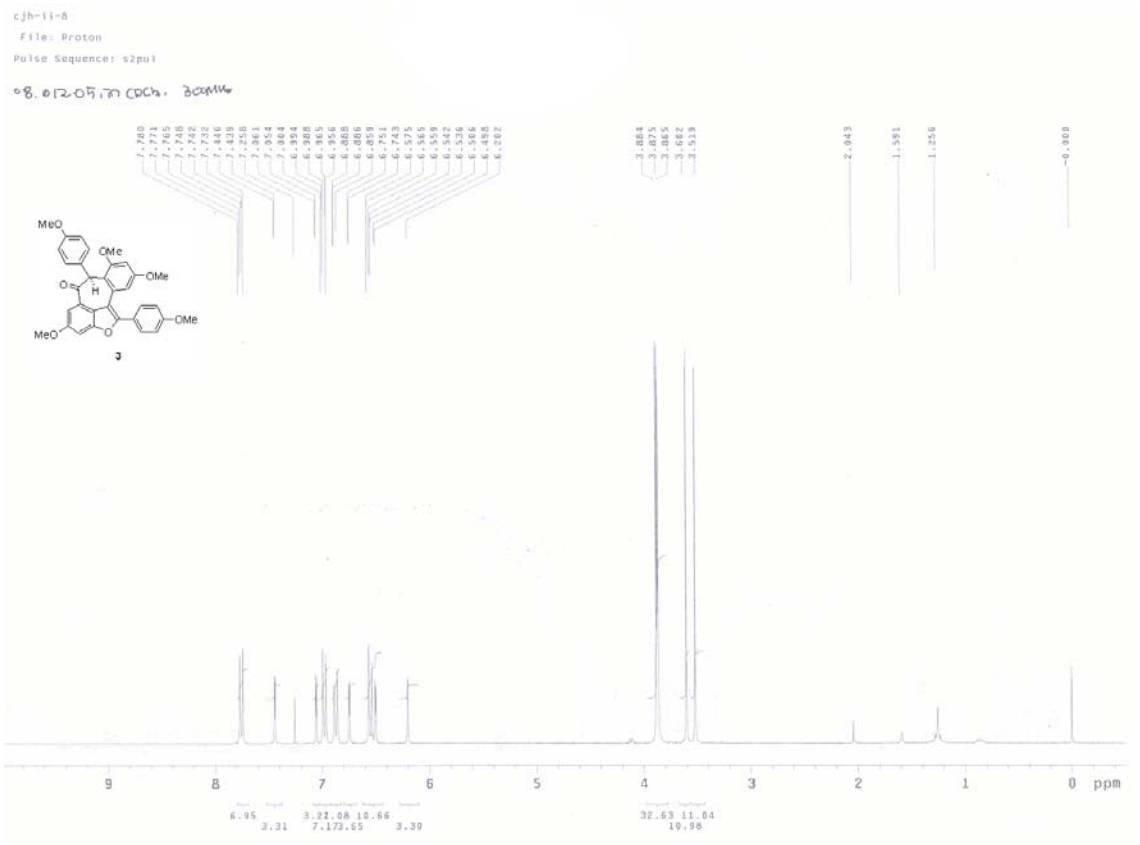

carbon 5
File: Carbon
Pulse Sequence: s2pul
08.12.04. In CDCl3, 75MHz
OMe
OMe
OMe
OMe
MeO
17
161.318
160.027
159.567
158.539
154.559
150.036
136.344
131.782
128.823
127.555
127.217
123.774
122.765
115.724
114.725
113.926
108.122
106.304
100.052
95.654
77.717
77.299
76.874
63.486
59.399
56.115
55.587
55.455
160
140
120
100
80
60
40
20
ppm

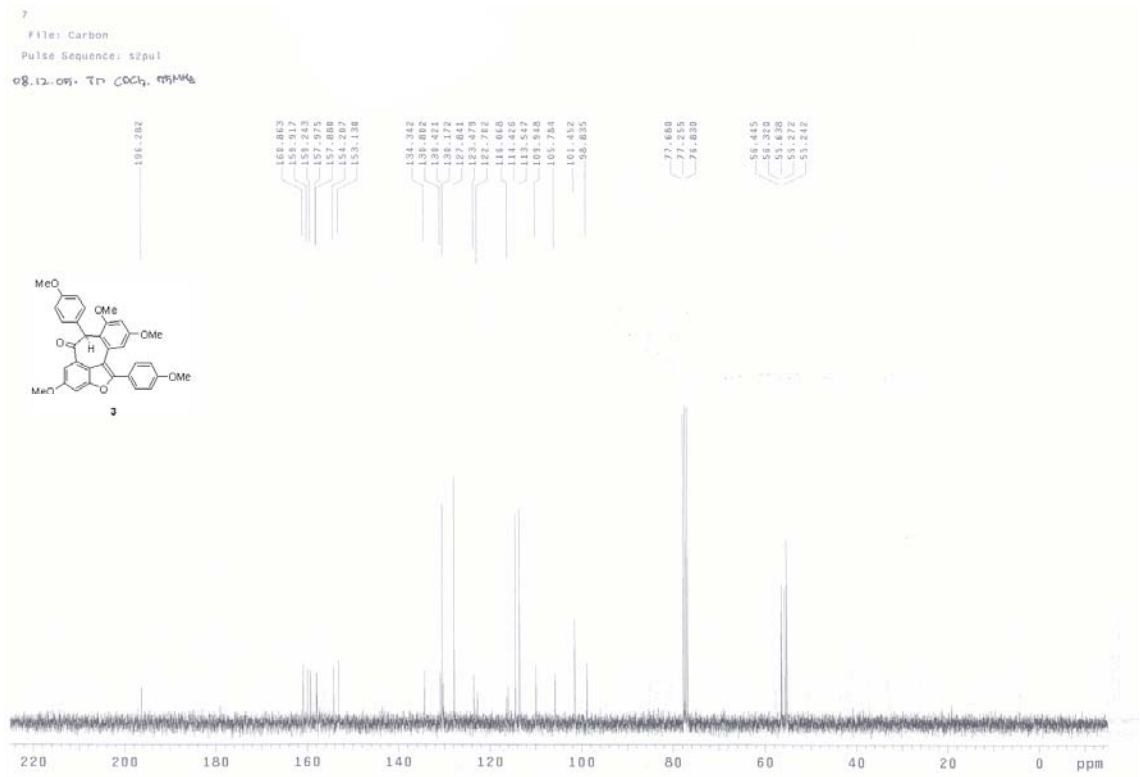

cjh-ii-7
File: Proton
Pulse Sequence: s2pul
OMe
OMe
OMe
HO
H
MeO
OMe
2
ppm


carbon 6
File: Carbon
Pulse Sequence: s2pul
OMe
OMe
OMe
HO
H
MeO
OMe
2
ppm


Isomer
File: Proton
Pulse Sequence: s2pul
18
9 8 7 6 5 4 3 2 1 0 ppm


CJH-II-15-DOWN
File: Carbon
Pulse Sequence: s2pul
18
220 200 180 160 140 120 100 80 60 40 20 0 ppm


cjh-ii-8
File: Proton
Pulse Sequence: s2pul
MeO
OMe
OMe
OMe
MeO
3
ppm


File: Carbon
Pulse Sequence: s2pul
MeO
OMe
OMe
OMe
MeO
3
ppm

Comparison of spectral data of 1~3 with those of the same compounds derived from the natural products

300 MHz ^{1}H NMR ($CDCl_3$) of synthetic **1**	600 MHz ^{1}H NMR ($CDCl_3$) of **1** derived from the natural product
7.53 (2H, d, 9.0)	7.52 (2H, d, 9.2)
7.11 (1H, d, 2.1)	7.09 (1H, d, 2.2)
7.01 (2H, s)	7.01 (2H, d, 8.8)
7.04 (1H, s)	6.99 (1H, d, 2.2)
6.87 (2H, s)	6.87 (1H, d, 16.1) 6.84 (1H, d, 16.1)
6.82 (2H, d, 8.7)	6.81 (2H, d, 9.2)
6.78 (2H, d, 8.7)	6.77 (2H, d, 8.8)
6.65 (2H, s)	6.65 (2H, d, 2.2)
6.63 (1H, t, 2.1)	6.62 (1H, t, 2.2)
3.92 (3H, s)	3.90 (3H, s)
3.82 (3H, s)	3.79 (3H, s)
3.80 (3H, s)	3.78 (3H, s)
3.74 (6H, s)	3.73 (6H, s)

700 MHz ^{1}H NMR ($CDCl_3$) of synthetic **1**	600 MHz ^{1}H NMR ($CDCl_3$) of **1** derived from the natural product
7.52 (2H, d, 8.9)	7.52 (2H, d, 9.2)
7.10 (1H, d, 2.1)	7.09 (1H, d, 2.2)
7.01 (2H, d, 8.7)	7.01 (2H, d, 8.8)
6.99 (1H, d, 2.1)	6.99 (1H, d, 2.2)
6.87 (1H, d, 16.3)	6.87 (1H, d, 16.1)
6.84 (1H, d, 16.3)	6.84 (1H, d, 16.1)
6.81 (2H, d, 8.9)	6.81 (2H, d, 9.2)
6.77 (2H, d, 8.7)	6.77 (2H, d, 8.8)
6.65 (2H, d, 2.3)	6.65 (2H, d, 2.2)
6.63 (1H, t, 2.3)	6.62 (1H, t, 2.2)
3.91 (3H, s)	3.90 (3H, s)
3.79 (3H, s)	3.79 (3H, s)
3.78 (3H, s)	3.78 (3H, s)
3.74 (6H, s)	3.73 (6H, s)

75 MHz ^{13}C NMR ($CDCl_3$) of synthetic **1**	150 MHz ^{13}C NMR ($CDCl_3$) of **1** derived from the natural product
161.7	161.4
159.5	159.2
159.4	159.1
158.3	158.0
155.2	154.9
150.0	149.7
137.2	136.9
132.3	132.0
130.5	130.1
128.8	128.5
127.9	127.6
127.8	127.5
123.8	123.5
123.4	123.1
122.3	122.0

116.6	116.3
114.2	113.9
114.1	113.8
108.8	108.5
106.9	106.6
100.7	100.4
95.1	94.8
56.1	55.8
55.7	55.4
55.5	55.3
55.4	55.2

300 MHz ^{1}H NMR ($CDCl_3$) of synthetic **2**	300 MHz ^{1}H NMR ($CDCl_3$) of **2** derived from the natural product
7.62 (2H, d, 9.0)	7.61 (2H, d, 8.8)
7.12~7.10 (3H, m)	7.12 (1H, d, 2.0) 7.11 (2H, d, 8.6)
6.94 (2H, d, 9.0)	6.93 (2H, d, 8.8)

6.79 (1H, d, 2.4)	6.78 (1H, d, 2.0)
6.72 (1H, d, 2.4)	6.71 (1H, d, 2.0)
6.52 (2H, d, 9.0)	6.51 (2H, d, 8.6)
6.41 (1H, d, 2.7)	6.41 (1H, d, 2.4)
5.57 (1H, d, 2.4)	5.57 (1H, br d)
5.40 (1H, d, 6.0)	5.40 (1H, br d)
3.85 (3H, s)	3.84 (3H, s)
3.83 (3H, s)	3.82 (3H, s)
3.81 (3H, s)	3.81 (3H, s)
3.60 (3H, s)	3.60 (3H, s)
3.46 (3H, s)	3.46 (3H, s)
2.59 (1H, d, 6.9)	4.89 (1H, br s)

75 MHz ^{13}C NMR ($CDCl_3$) of synthetic **2**	75 MHz ^{13}C NMR ($CDCl_3$) of **2** derived from the natural product
160.2	160.0
158.8	158.5
158.5	158.2

158.3	158.1
157.7	157.4
154.2	153.9
151.1	150.8
137.5	137.2
134.4	134.1
132.0	131.7
130.5	130.2
129.8	129.5
124.6	124.3
122.1	121.9
118.2	117.9
116.5	116.3
114.2	113.9
113.3	113.0
108.4	108.2
106.2	106.0
98.3	98.0

94.1	93.8
73.8	73.5
56.2	55.6
55.9	55.1
55.6	54.9
55.2	54.9
55.1	54.9
47.9	47.6

300 MHz ^{1}H NMR ($CDCl_3$) of synthetic **3**	300 MHz ^{1}H NMR ($CDCl_3$) of **3** derived from the natural product
7.77 (2H, d, 9.0)	7.75 (2H, d, 8.8)
7.44 (1H, d, 2.1)	7.44 (1H, d, 2.1)
7.06 (1H, d, 2.1)	7.05 (1H, d, 2.1)
6.98 (2H, d, 8.7)	6.97 (2H, d, 8.8)
6.87 (2H, d, 8.7)	6.87 (2H, dd, 1.3, 8.3)
6.75 (1H, d, 2.1)	6.75 (1H, d, 2.6)
6.55 (2H, d, 8.7)	6.55 (2H, d, 8.3)

6.50 (1H, d, 2.4)	6.50 (1H, d, 2.6)
6.20 (1H, s)	6.20 (1H, br s)
3.89 (3H, s)	3.89 (3H, s)
3.88 (3H, s)	3.86 (3H, s)
3.87 (3H, s)	3.85 (3H, s)
3.61 (3H, s)	3.60 (3H, s)
3.52 (3H, s)	3.52 (3H, s)

75 MHz ^{13}C NMR ($CDCl_3$) of synthetic **3**	75 MHz ^{13}C NMR ($CDCl_3$) of **3** derived from the natural product
196.3	196.0
160.9	160.6
159.9	159.7
159.2	159.0
158.0	157.7
157.9	157.6
154.2	154.0
153.1	152.9

134.3	134.1
130.8	130.5
130.4	130.2
130.2	129.9
127.8	127.6
123.5	123.2
122.7	122.4
116.5	116.2
116.1	115.8
114.4	114.2
113.5	113.3
109.9	109.7
105.8	105.5
101.5	101.2
98.8	98.6
56.4	56.2
56.3	56.1
55.6	55.4

55.3	55.0 (3C)
55.2	

Crystallographic details for 5 and 11

Crystal data and structure refinement for 3,4-diarylbenzofuran **(5)**

Identification code	3,4-diarylbenzofuran **(5)**	
Empirical formula	C26 H24 O7	
Formula weight	448.45	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.6796(1) Å	= 81.579(1)°.
	b = 8.7072(1) Å	= 78.919(1)°.
	c = 17.3304(2) Å	= 87.911(1)°.
Volume	1124.94(2) $Å^3$	
Z	2	
Density (calculated)	1.324 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	
F(000)	472	
Crystal size	0.42 x 0.38 x 0.21 mm^3	
Theta range for data collection	1.21 to 28.35°.	
Index ranges	-10<=h<=10, -11<=k<=11, -22<=l<=22	
Reflections collected	20569	
Independent reflections	5535 [R(int) = 0.0211]	
Completeness to theta = 28.35°	98.6 %	
Absorption correction	None	
Max. and min. transmission	0.9801 and 0.9607	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5535 / 0 / 298	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.1164	
R indices (all data)	R1 = 0.0615, wR2 = 0.1284	
Largest diff. peak and hole	0.161 and -0.229 $e.Å^{-3}$	

Crystal data and structure refinement for Benzofuran dimer **(11)**

Identification code	benzofuran dimer **(11)**	
Empirical formula	C38 H34 O12	
Formula weight	682.65	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.5867(1) Å	= 79.655(1)°.
	b = 7.9569(1) Å	= 81.410(1)°.
	c = 14.3677(2) Å	= 81.762(1)°.
Volume	837.59(2) $Å^3$	
Z	1	
Density (calculated)	1.353 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	358	
Crystal size	0.29 x 0.21 x 0.07 mm^3	
Theta range for data collection	1.45 to 28.30°.	
Index ranges	-10<=h<=8, -10<=k<=10, -19<=l<=19	
Reflections collected	15109	
Independent reflections	4103 [R(int) = 0.0269]	
Completeness to theta = 28.30°	98.5 %	
Absorption correction	None	
Max. and min. transmission	0.9929 and 0.9712	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4103 / 0 / 227	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.1011	
R indices (all data)	R1 = 0.0679, wR2 = 0.1141	
Extinction coefficient	0.019(3)	
Largest diff. peak and hole	0.202 and -0.144 $e.Å^{-3}$	