Supporting Information

Synthesis of Benzofused Cyclobutaoxepanones via Intramolecular Annulation of *o*-Cinnamyl Chalcones

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Taiwan

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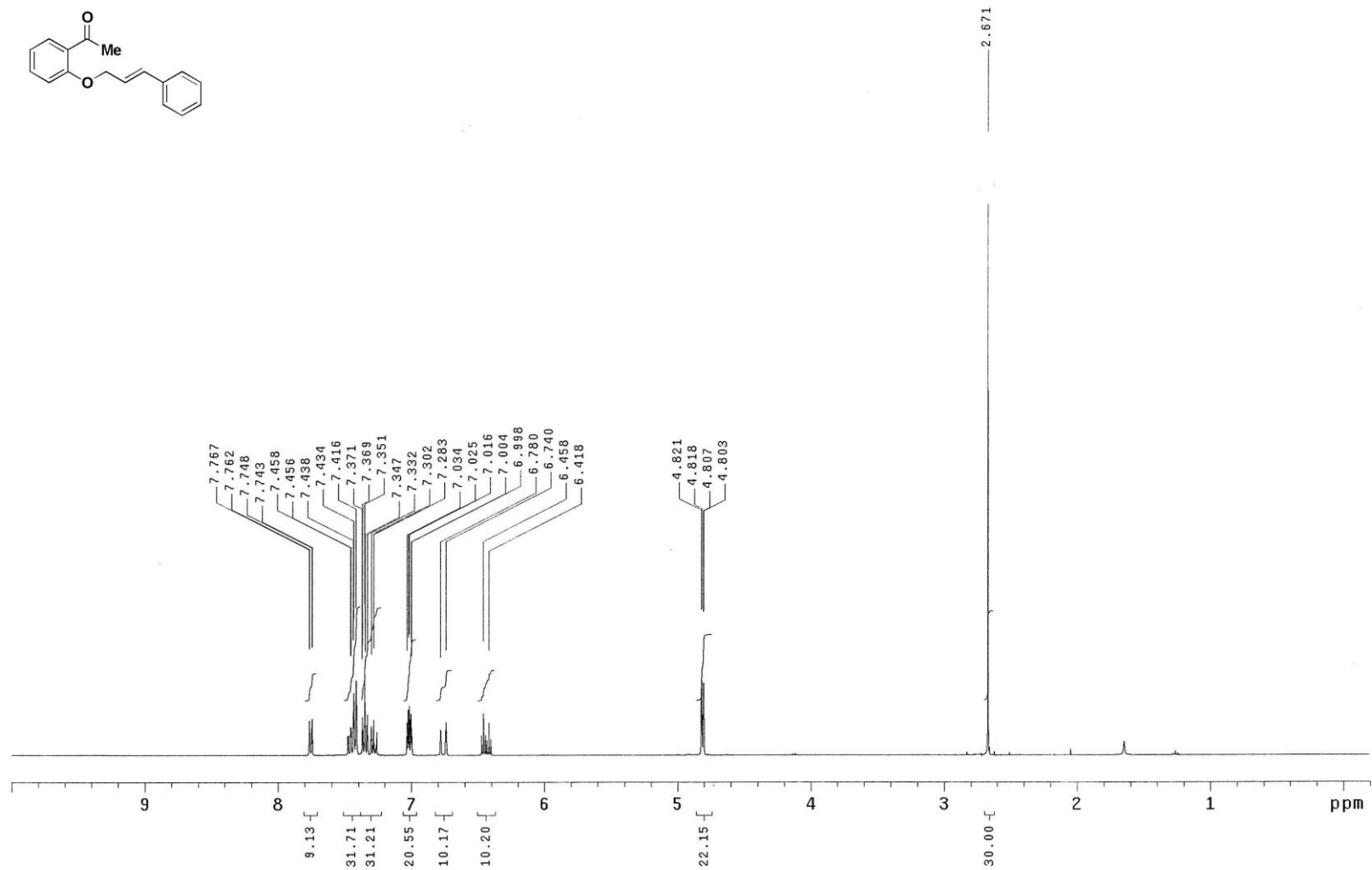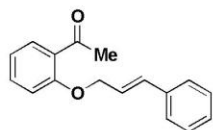# Compound 4a (^{1}H-NMR spectral data)

SS1060309

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 10 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.767
7.762
7.748
7.743
7.458
7.456
7.438
7.434
7.416
7.371
7.369
7.351
7.347
7.332
7.302
7.283
7.034
7.025
7.016
7.004
6.998
6.780
6.740
6.458
6.418

4.821
4.818
4.807
4.803

2.671

9   8   7   6   5   4   3   2   1   ppm

9.13

31.71
31.21

20.55

10.17

10.20

22.15

30.00

Compound 4a (^{13}C-NMR spectral data)

SS1060309
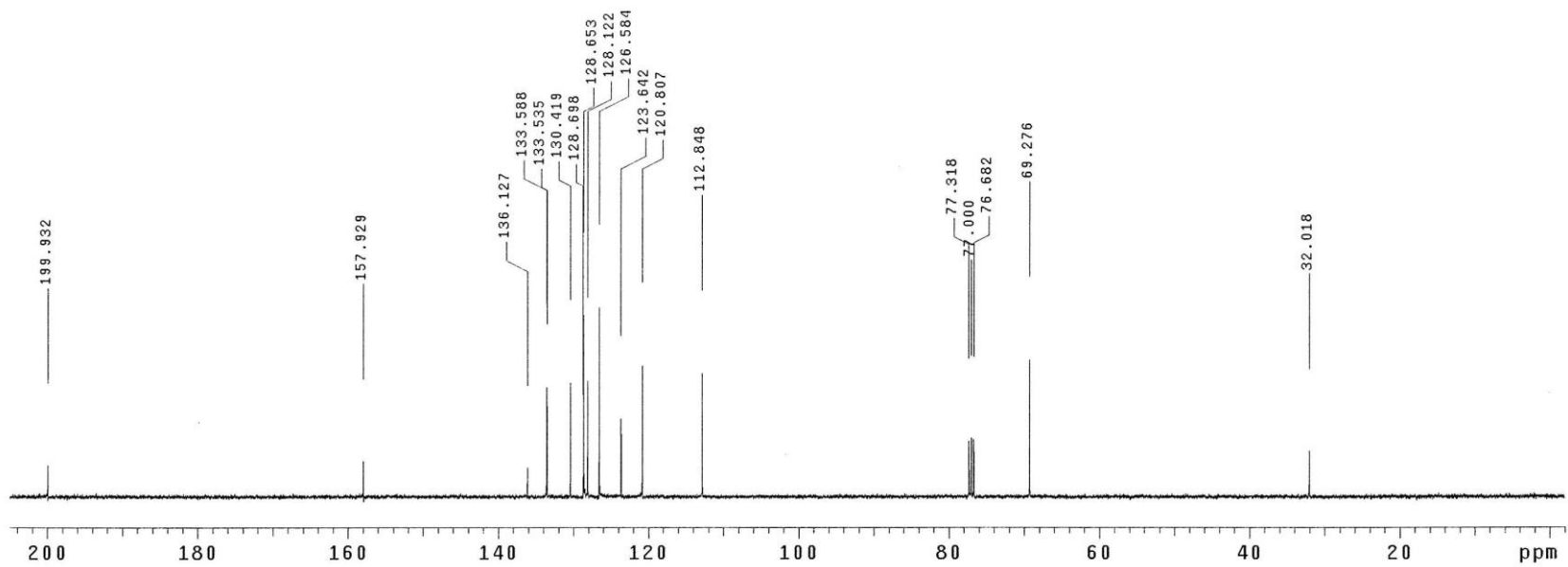
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 10 2017
Solvent: CDCl3
Ambient temperature
Total 1024 repetitions

199.932
157.929
136.127
133.588
133.535
130.419
128.698
128.653
128.122
126.584
123.642
120.807
112.848
77.318
77.000
76.682
69.276
32.018

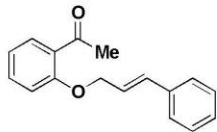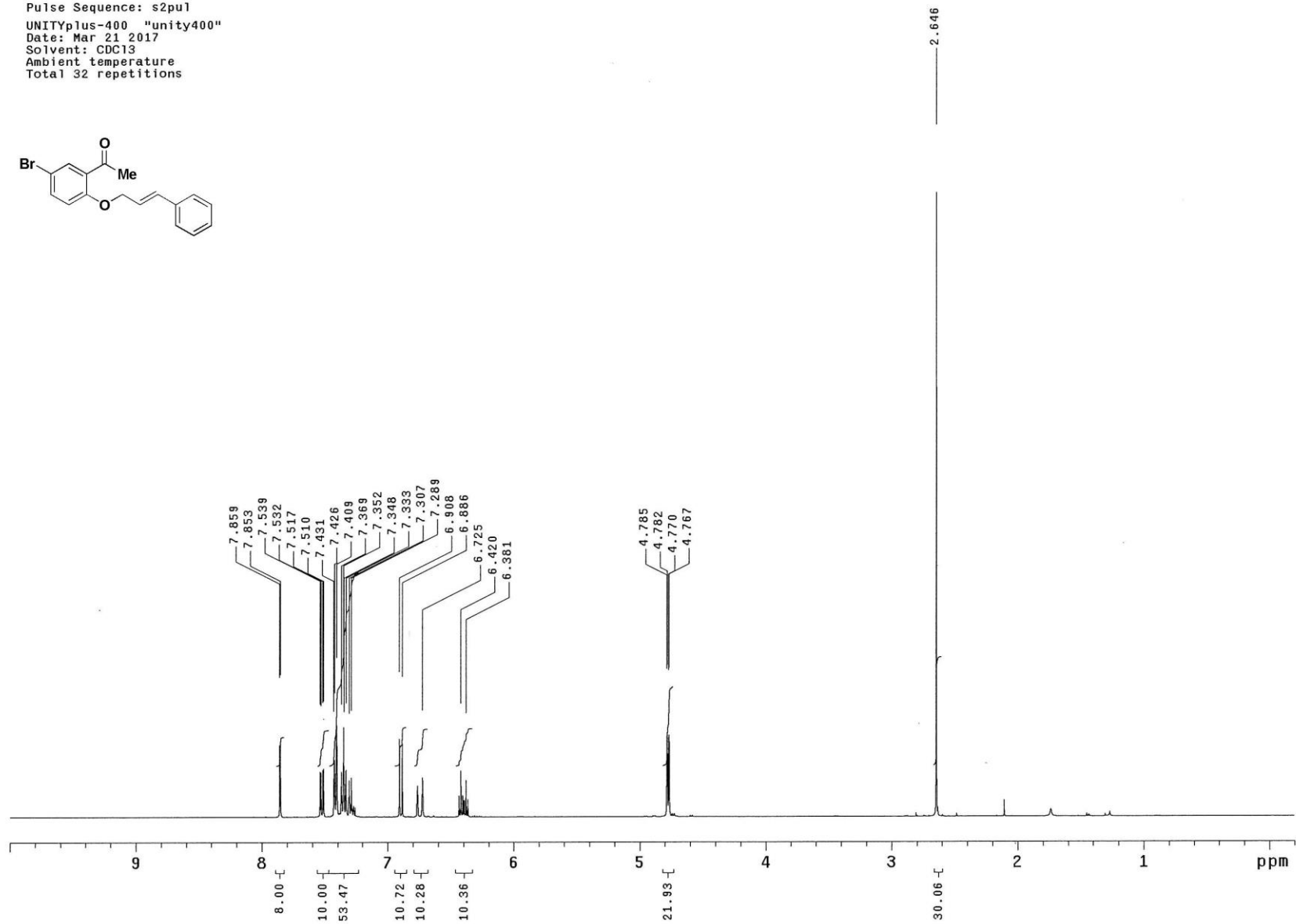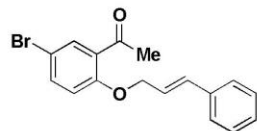200 180 160 140 120 100 80 60 40 20 ppm

Compound 4b (¹H-NMR spectral data)

SS1060320

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 21 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.859
7.853
7.539
7.532
7.517
7.510
7.431
7.426
7.409
7.369
7.352
7.348
7.333
7.307
7.289
6.908
6.886
6.725
6.420
6.381

4.785
4.782
4.770
4.767

2.646

9	8	7	6	5	4	3	2	1	ppm

8.00
10.00
53.47
10.72
10.28
10.36
21.93
30.06

Compound 4b (^{13}C-NMR spectral data)

SS1060320

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: Mar 21 2017
Solvent: CDC13
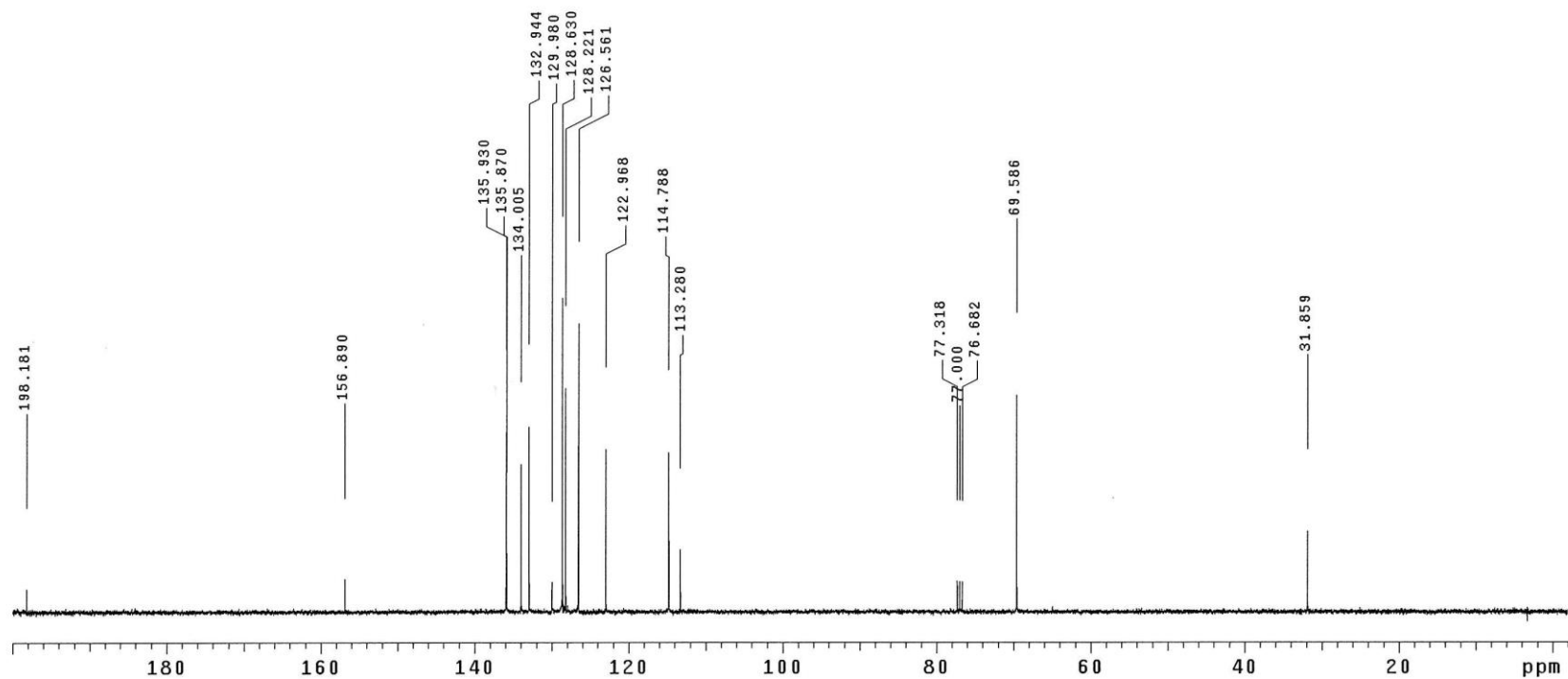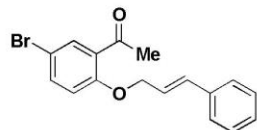Ambient temperature
Total 240 repetitions

Peaks: 198.181, 156.890, 135.930, 135.870, 134.005, 132.944, 129.980, 128.630, 128.221, 126.561, 122.968, 114.788, 113.280, 77.318, 77.000, 76.682, 69.586, 31.859

Compound 4c (^{1}H-NMR spectral data)

MC1080416
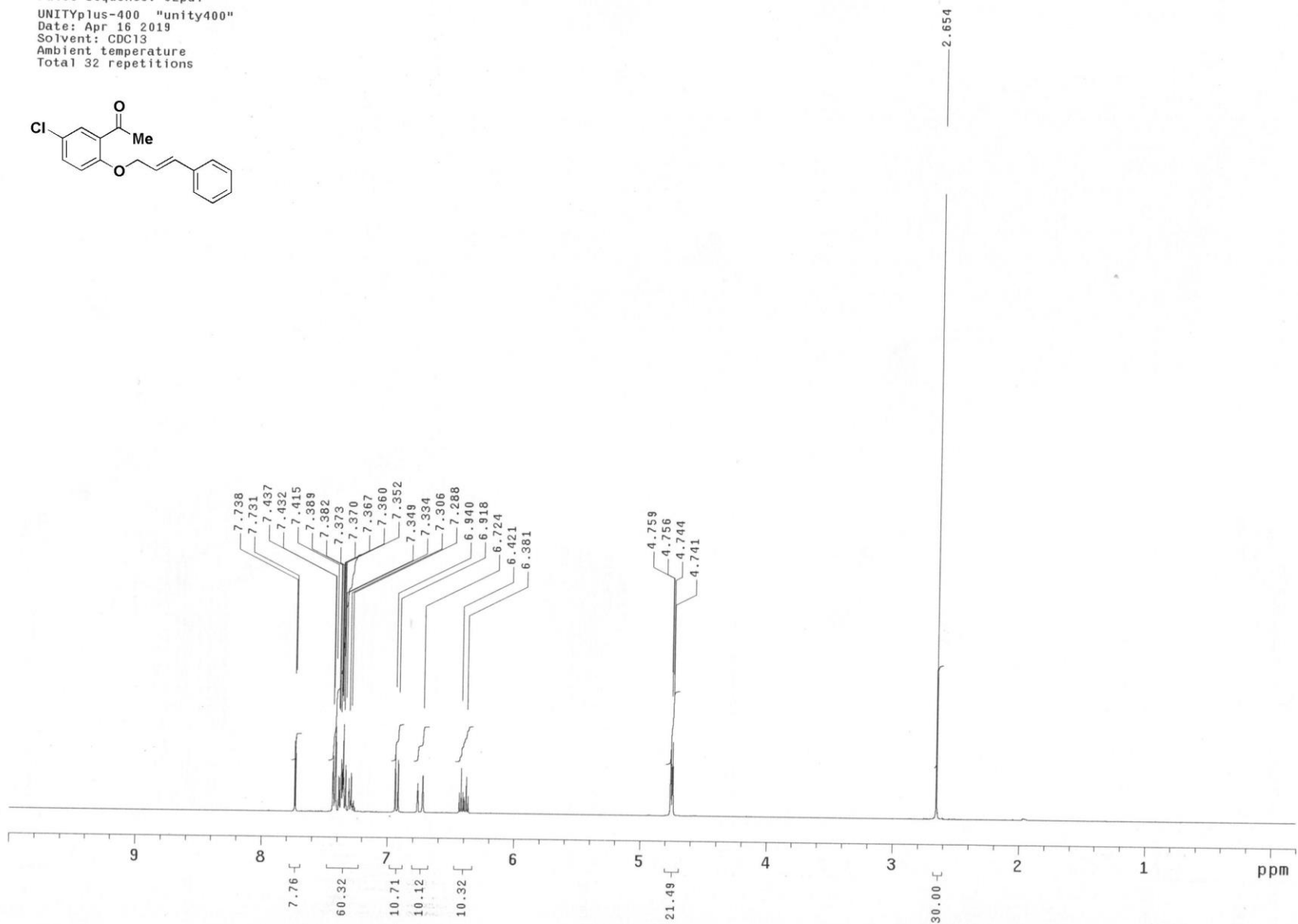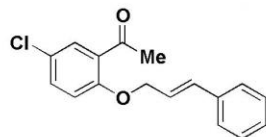
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 16 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

2.654

7.738
7.731
7.437
7.432
7.415
7.389
7.382
7.373
7.370
7.367
7.360
7.352
7.349
7.334
7.306
7.288
6.940
6.918
6.724
6.421
6.381

4.759
4.756
4.744
4.741

9   8   7   6   5   4   3   2   1   ppm

7.76
60.32
10.71
10.12
10.32
21.49
30.00

Compound 4c (^{13}C-NMR spectral data)

MC1080416

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 16 2019
Solvent: CDC13
Ambient temperature
Total 320 repetitions

198.006

156.329

135.786
133.815
132.906
129.851
129.350

128.509
128.077
126.455

125.879
122.915

114.281

77.318
77.000
76.682

69.503

31.775

180   160   140   120   100   80   60   40   20   ppm
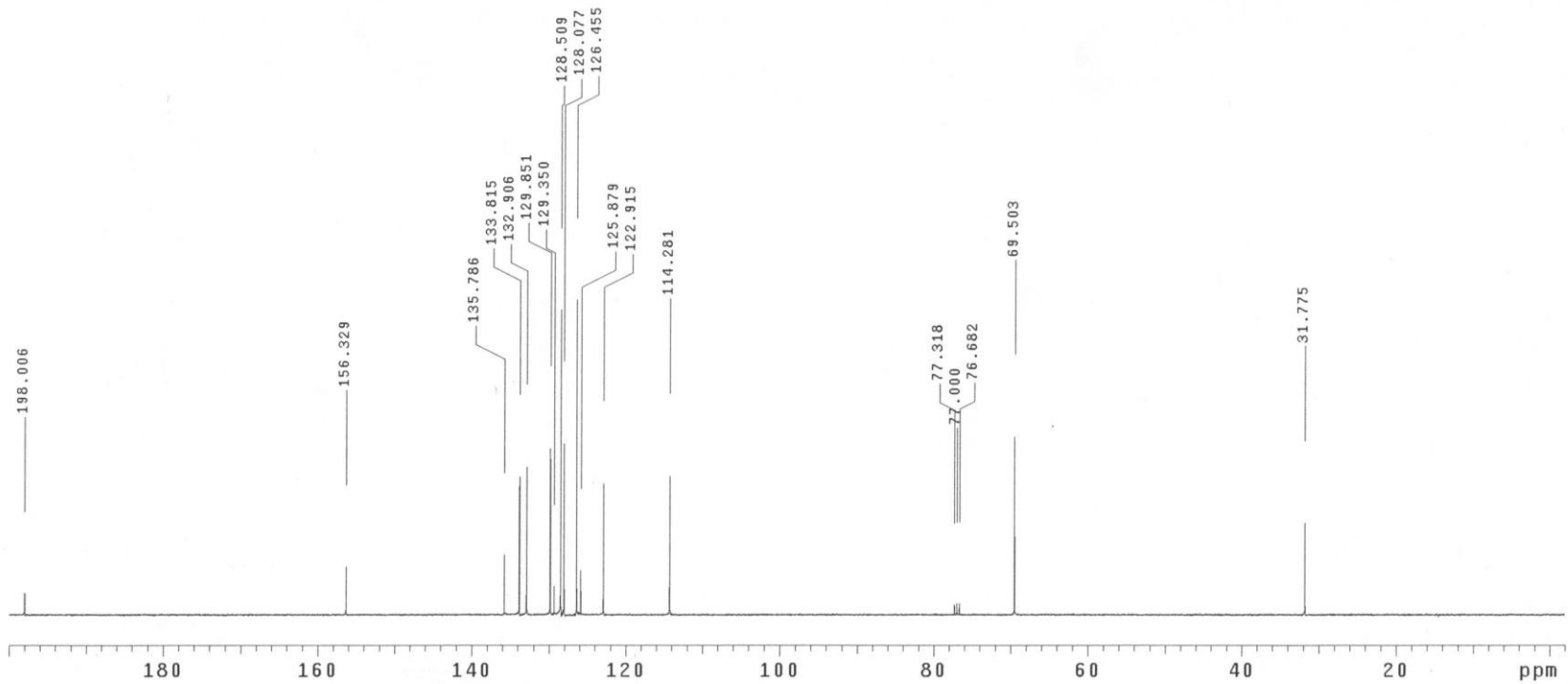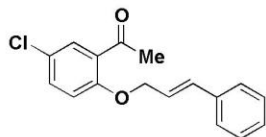
Compound 4d (¹H-NMR spectral data)

MC1080123

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 23 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Peaks: 7.432, 7.415, 7.373, 7.355, 7.336, 7.291, 6.436, 4.787, 4.784, 4.773, 4.769, 2.669

Integrations: 74.78, 10.61, 11.38, 12.15, 11.86, 23.61, 30.00
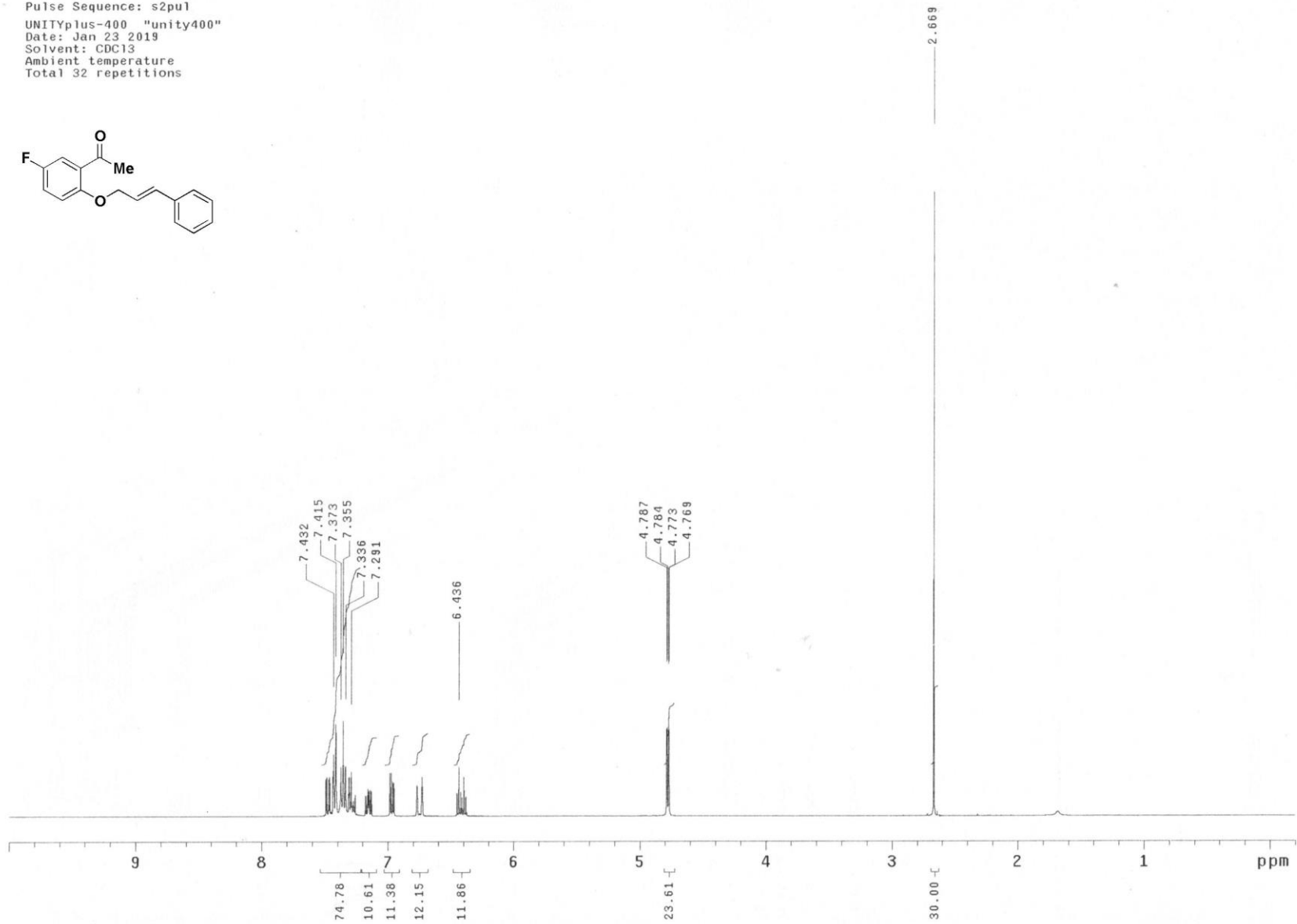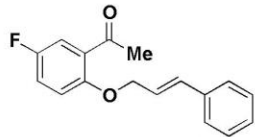
Compound 4d (^{13}C-NMR spectral data)

MC1080123

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 23 2019
Solvent: CDCl3
Ambient temperature
Total 1072 repetitions

157.982
155.594
154.176

135.968
133.830

128.661
128.206
126.606
126.576
123.332
120.080
119.845
116.653

116.418
114.425
114.356

77.318
77.000
76.682

69.981

31.912

180   160   140   120   100   80   60   40   20   ppm
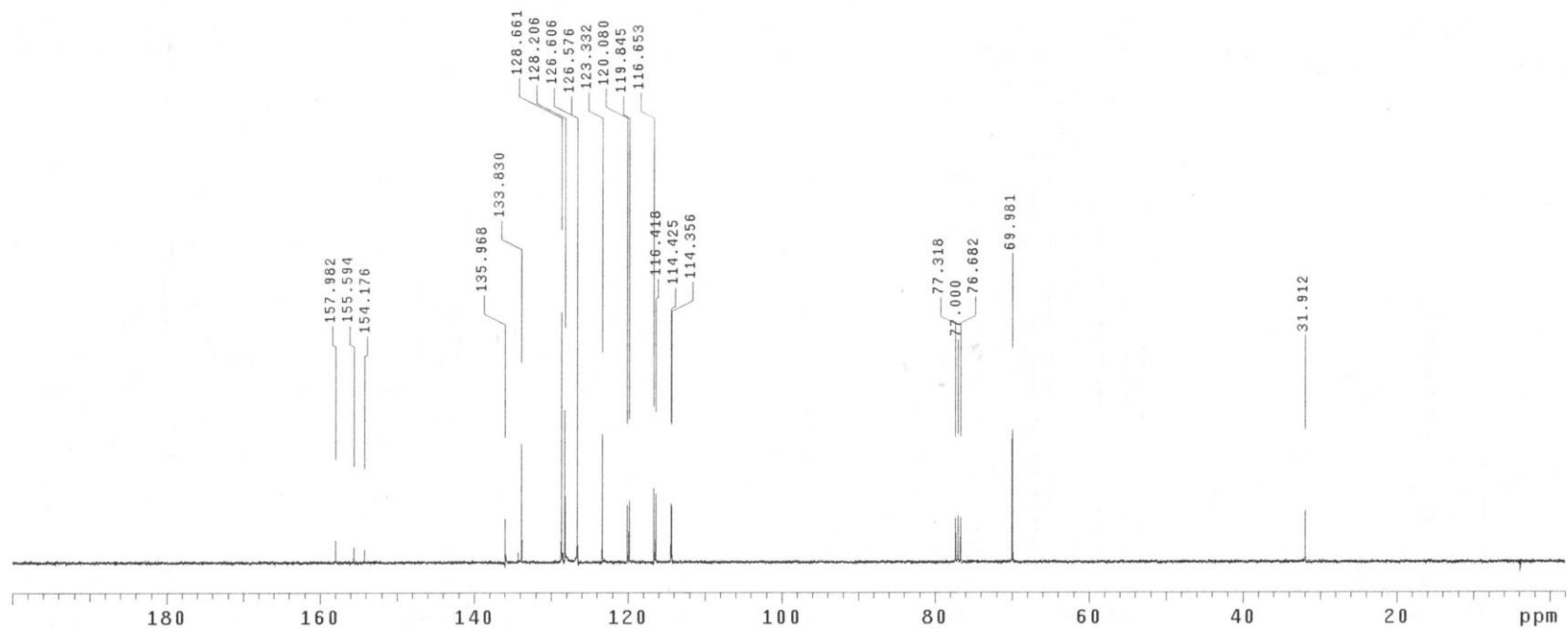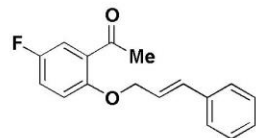
Compound 4e (^{1}H-NMR spectral data)

MC1080103

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 7 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.555
7.549
7.426
7.409
7.363
7.346
7.326
7.260
6.921
6.900
6.447

4.786
4.783
4.771
4.768

2.660

2.306

1.643

8.80
64.60
10.68
10.14
10.47
22.20
30.00
31.87

9   8   7   6   5   4   3   2   1   ppm
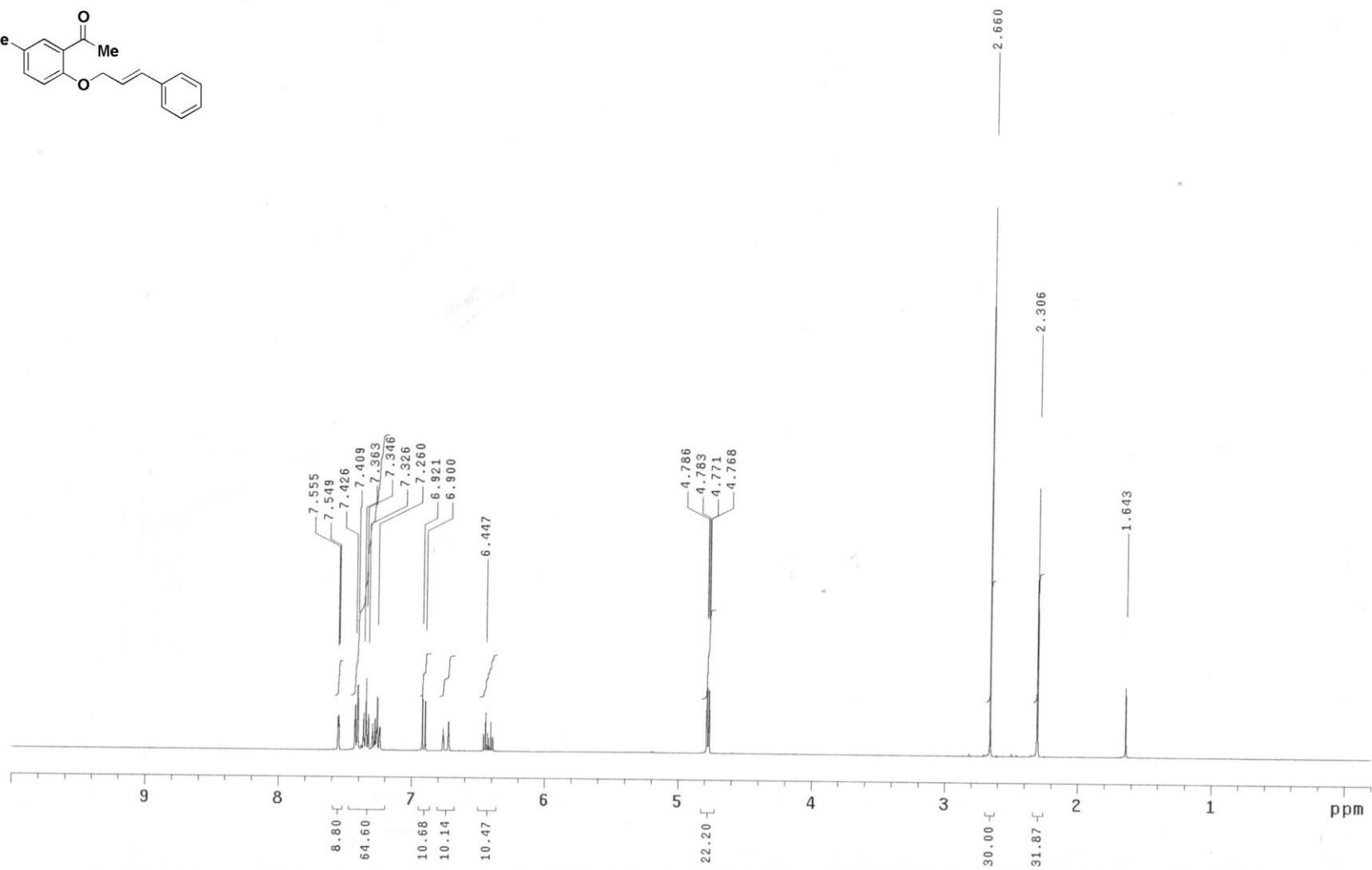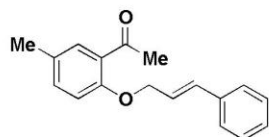
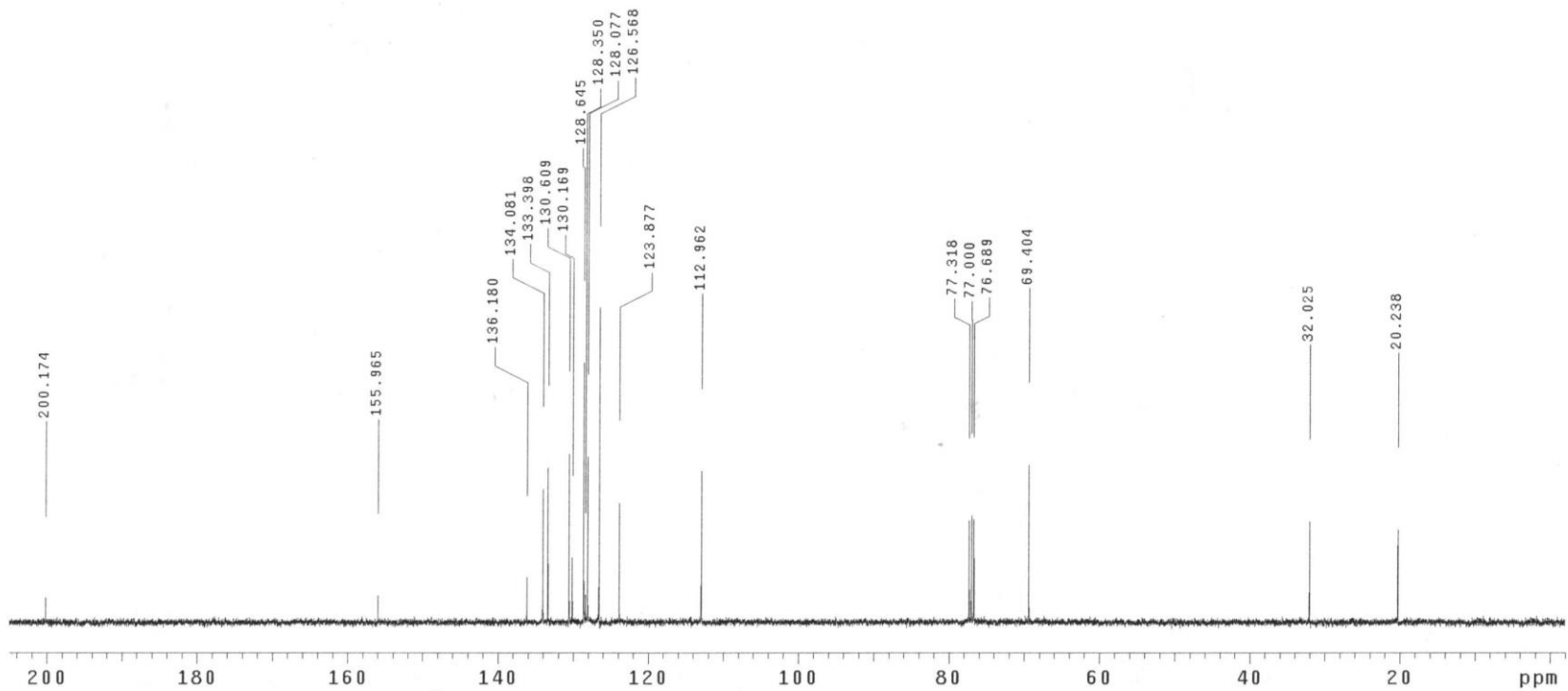# Compound 4e (^{13}C-NMR spectral data)

MC1080103

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 7 2019
Solvent: CDCl3
Ambient temperature
Total 816 repetitions

200.174
155.965
136.180
134.081
133.398
130.609
130.169
128.645
128.350
128.077
126.568
123.877
112.962
77.318
77.000
76.689
69.404
32.025
20.238

200   180   160   140   120   100   80   60   40   20   ppm
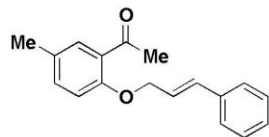
Compound 4f (¹H-NMR spectral data)

MC1080124

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 29 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.874
7.852
7.435
7.417
7.352
6.551
6.529
6.511
6.505
6.454
4.786
4.783
4.771
4.768
3.846
2.634

9.19
21.75
34.83
10.30
31.92
21.73
31.72
30.00

9 8 7 6 5 4 3 2 1 ppm

Compound 4f (¹³C-NMR spectral data)

MC1080124

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 29 2019
Solvent: CDCl3
Ambient temperature
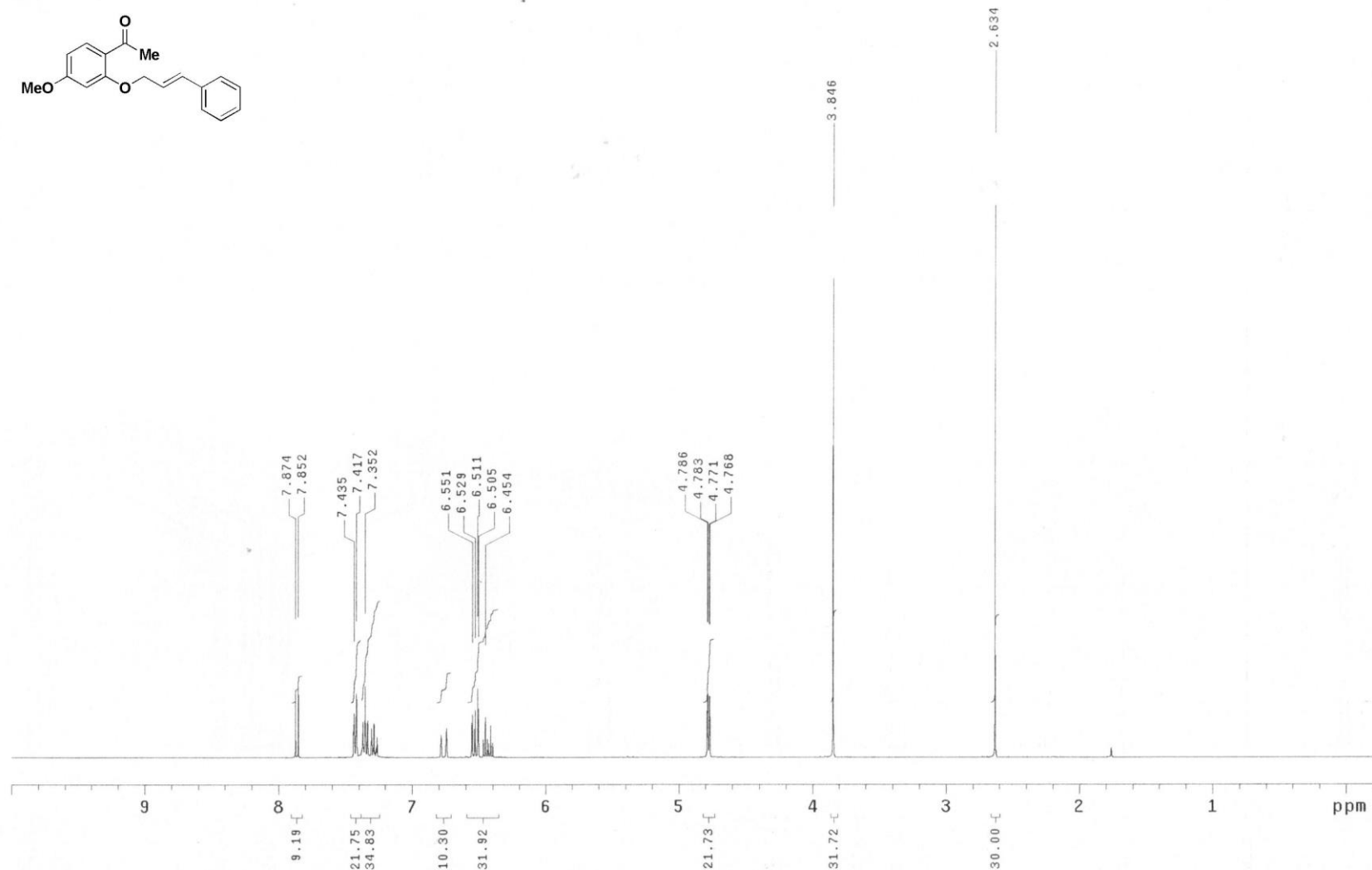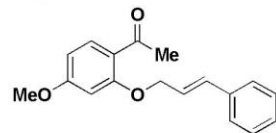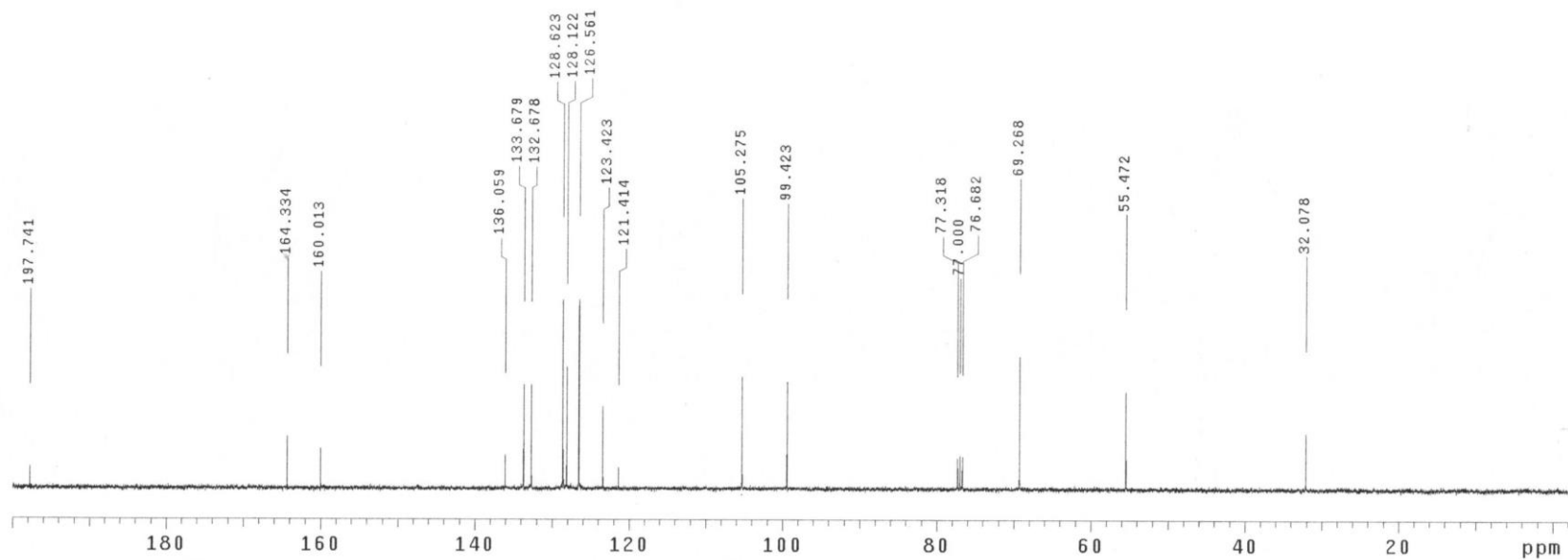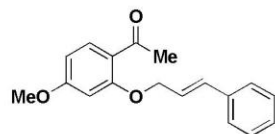Total 272 repetitions

Compound 4g (^{1}H-NMR spectral data)

MC1071224

Pulse Sequence: s2pul
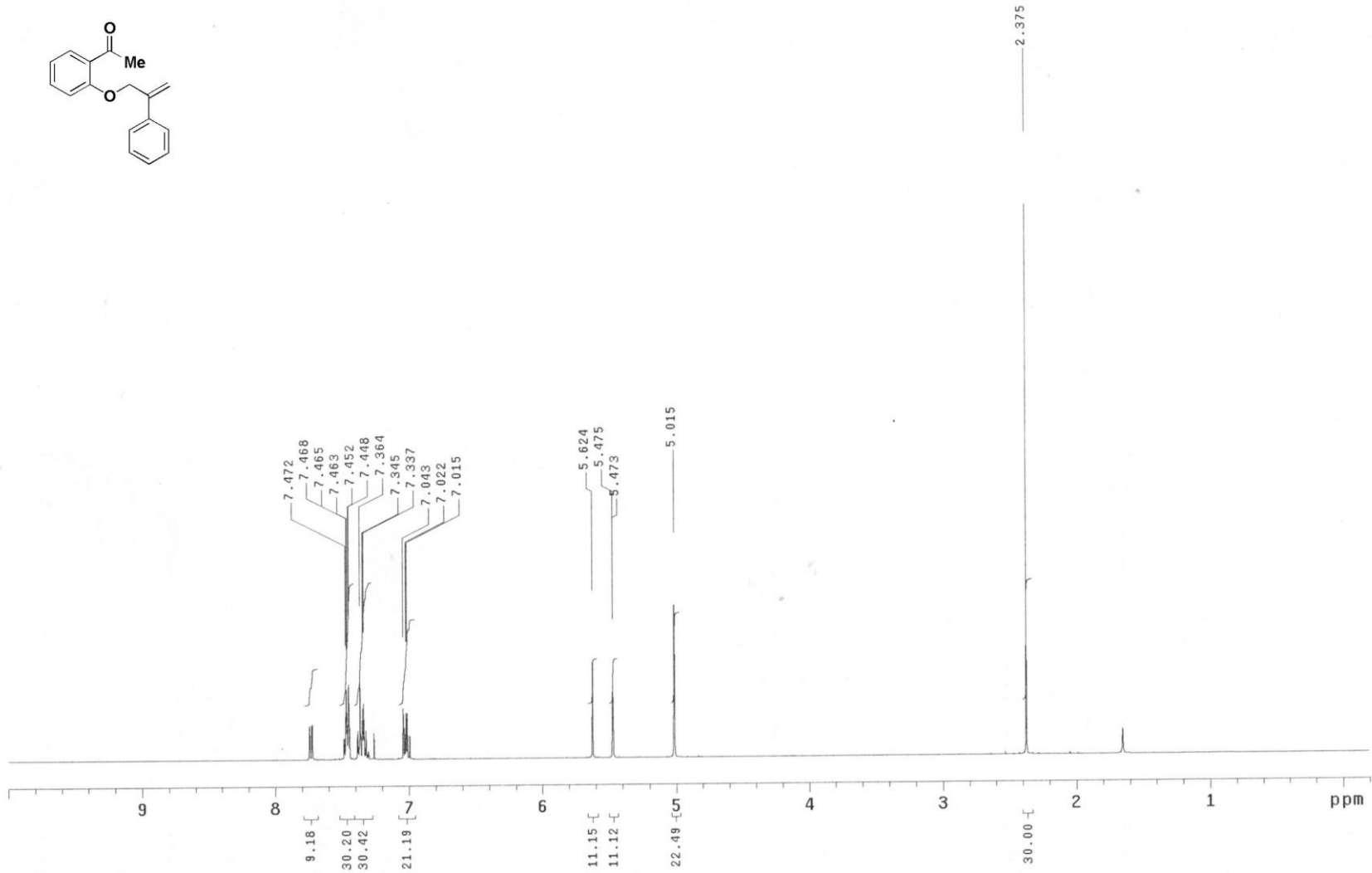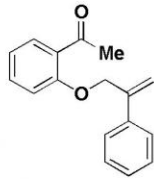UNITYplus-400 "unity400"
Date: Dec 24 2018
Solvent: CDC13
Ambient temperature
Total 32 repetitions

Compound 4g (^{13}C-NMR spectral data)

MC1071224

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 24 2018
Solvent: CDC13
Ambient temperature
Total 2272 repetitions

199.886
157.838
142.904
138.121
133.542
130.465
128.532
128.175
126.083
120.860
115.668
112.620
77.318
77.000
76.682
70.526
31.715

200   180   160   140   120   100   80   60   40   20   ppm

Compound 4h (^{1}H-NMR spectral data)

MC1080429

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2019
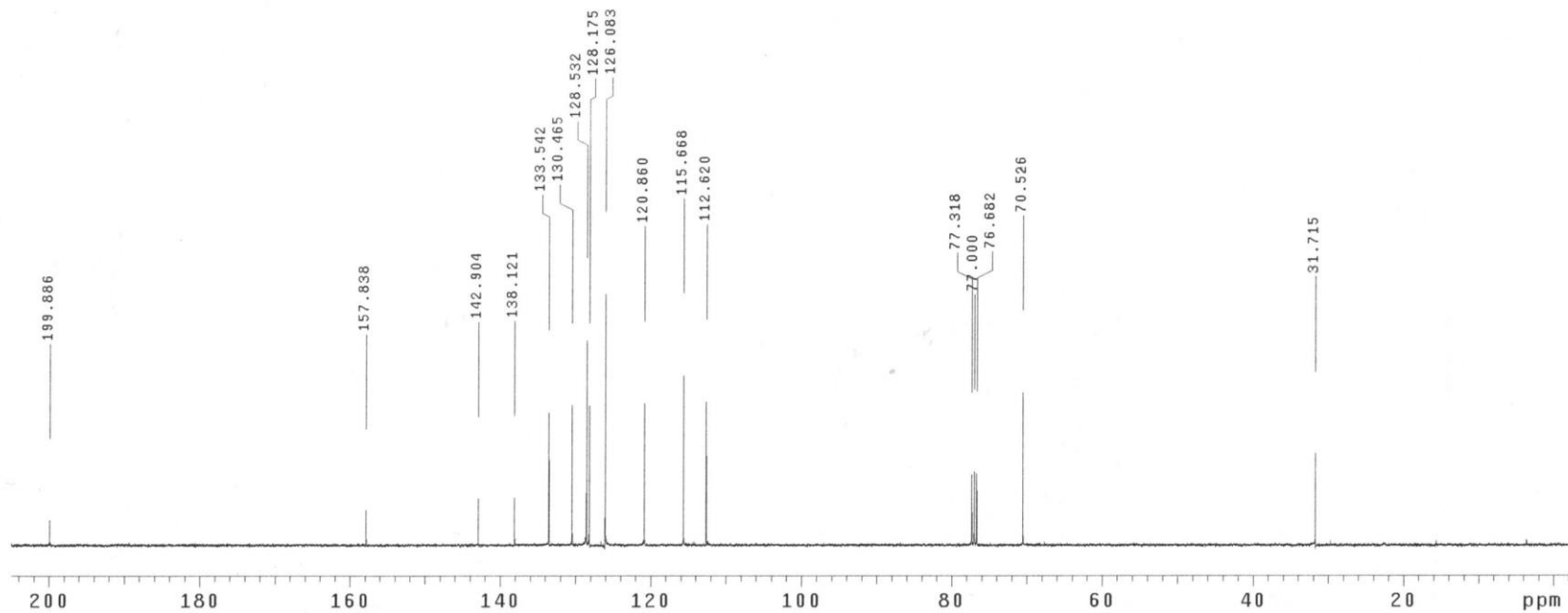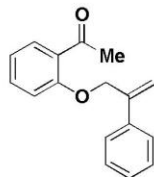Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.599
7.594
7.579
7.575
7.237
7.235
6.807
6.804
6.786
6.775
6.767
6.753
5.588
4.362
4.359
4.345
2.464
2.458
1.604
1.601
1.588
1.585

10.56
12.14
23.68
9.16
12.93
20.00
35.07
34.58

9   8   7   6   5   4   3   2   1   ppm
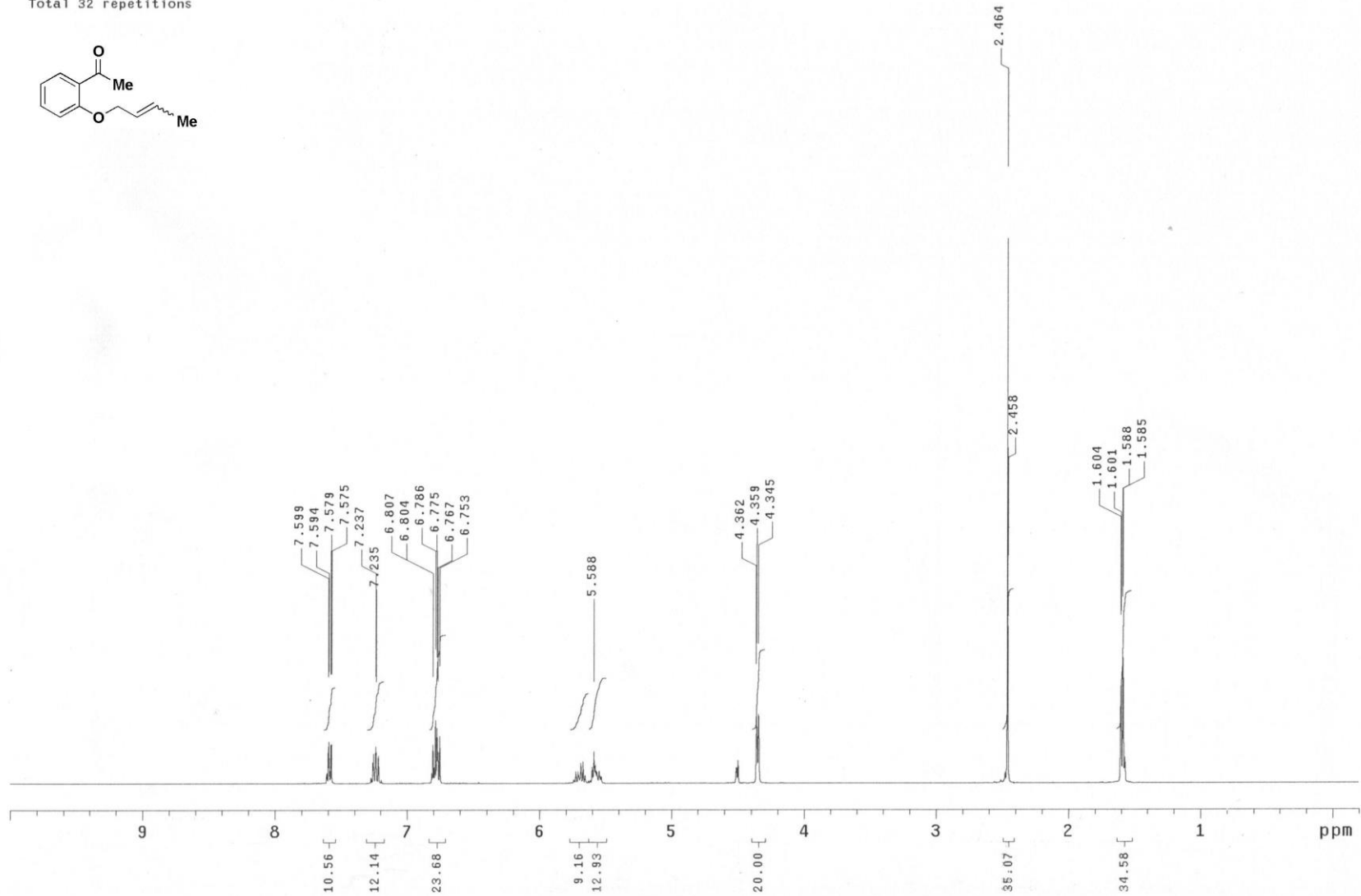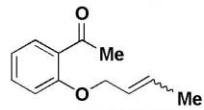
Compound 4h (^{13}C-NMR spectral data)

MC1080429

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2019
Solvent: CDCl3
Ambient temperature
Total 128 repetitions

198.764
157.633
133.057
133.012
129.995
129.752
129.699
128.380
127.827
125.045
124.484
119.928
119.867
112.332
112.188
68.631
63.643
31.434
31.396
17.228

180   160   140   120   100   80   60   40   20   ppm
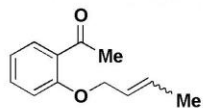
Compound 4i (^{1}H-NMR spectral data)

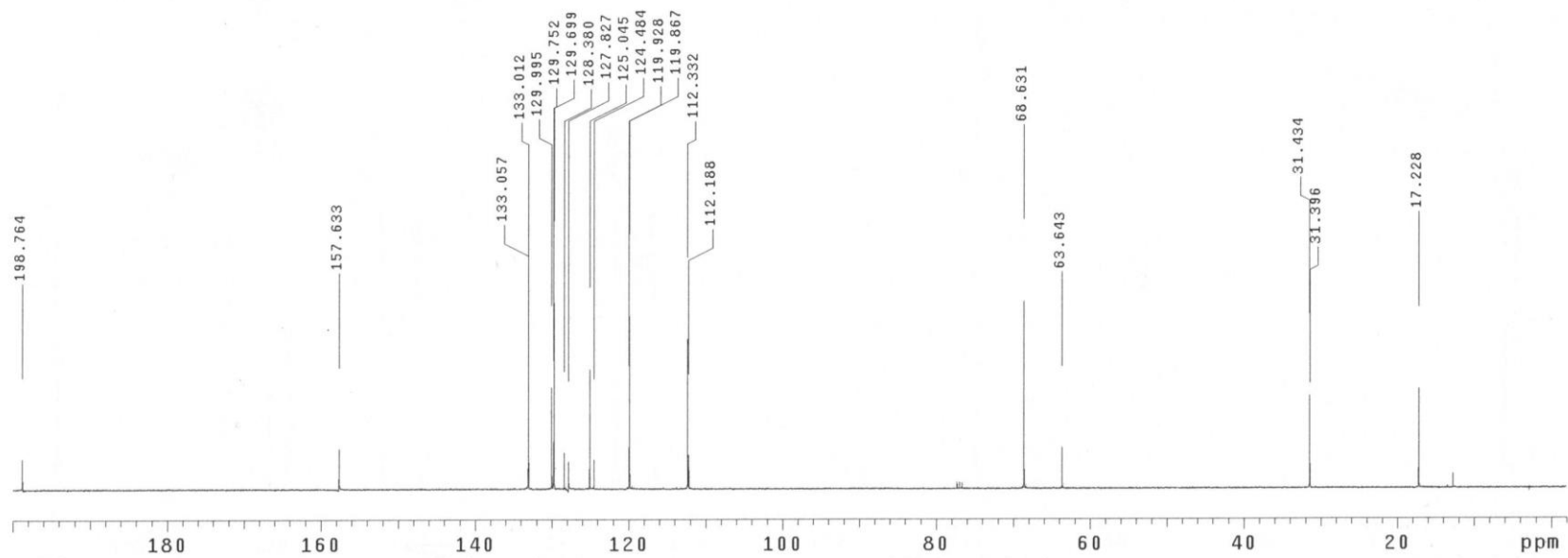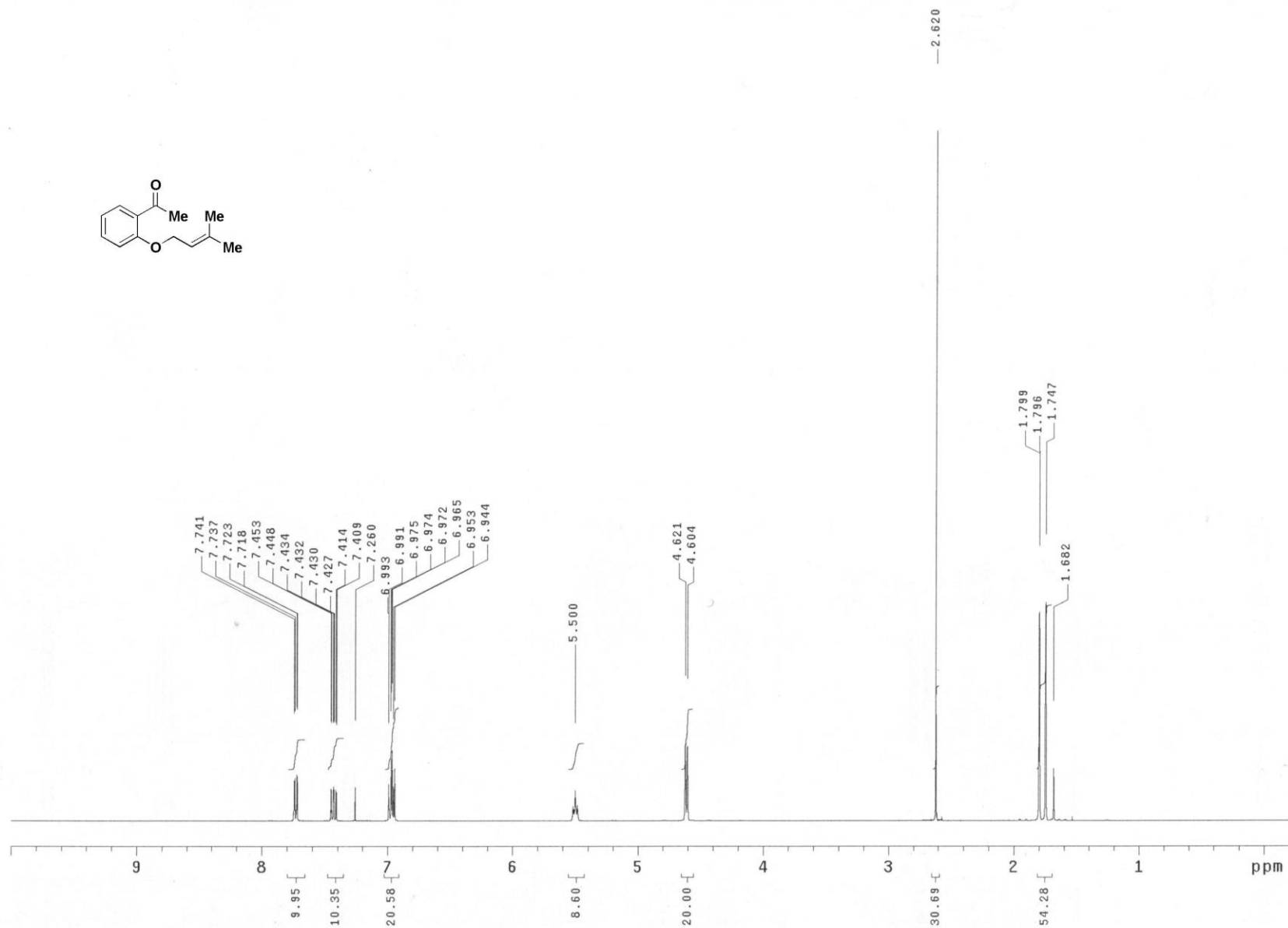# Compound 4i (^{13}C-NMR spectral data)

MCXK2CO3

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 18 2019
Solvent: CDC13
Ambient temperature
Total 2256 repetitions

200.076
158.300
138.250
133.489
130.336
128.577
120.398
119.155
112.727
77.311
77.000
76.682
65.349
31.972
25.703
18.214

200   180   160   140   120   100   80   60   40   20   ppm
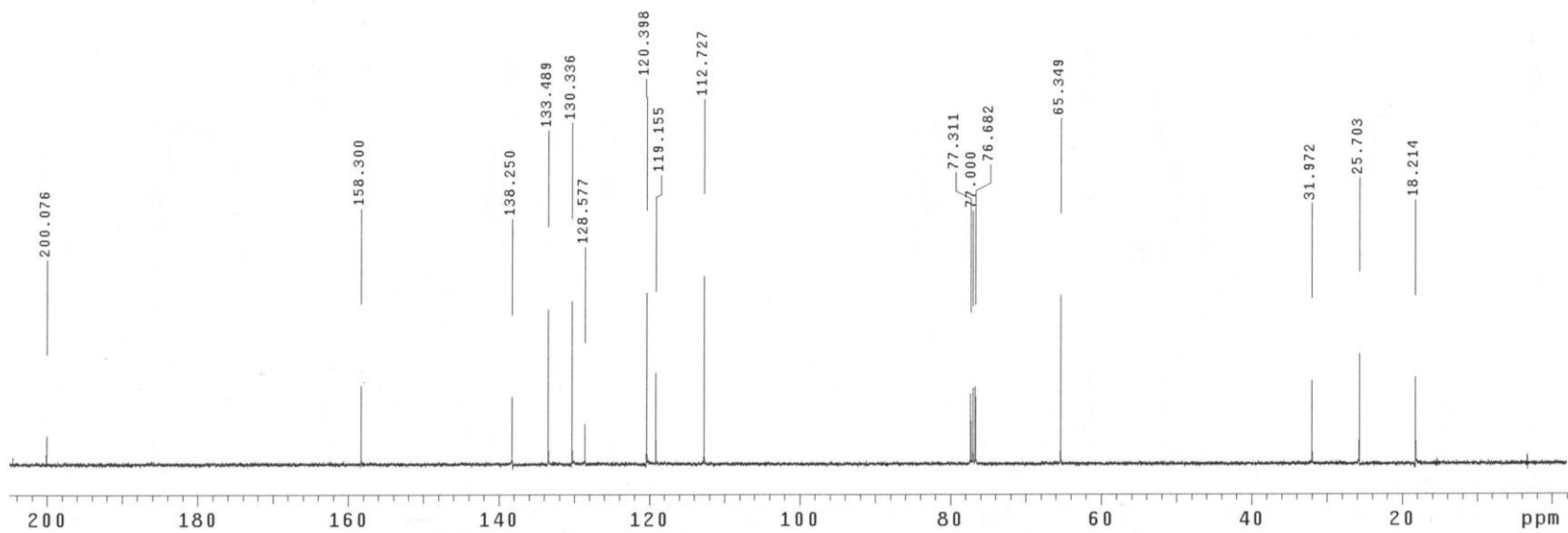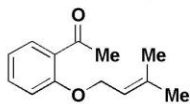
Compound 4j (^{1}H-NMR spectral data)

MCNBsCin

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 15 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.623
7.621
7.604
7.600
7.588
7.479
7.459
7.360
7.260
7.244
7.227
6.375
2.630

9 8 7 6 5 4 3 2 1 ppm

41.77
26.01
81.56
10.32
11.34
10.95
21.45
30.00
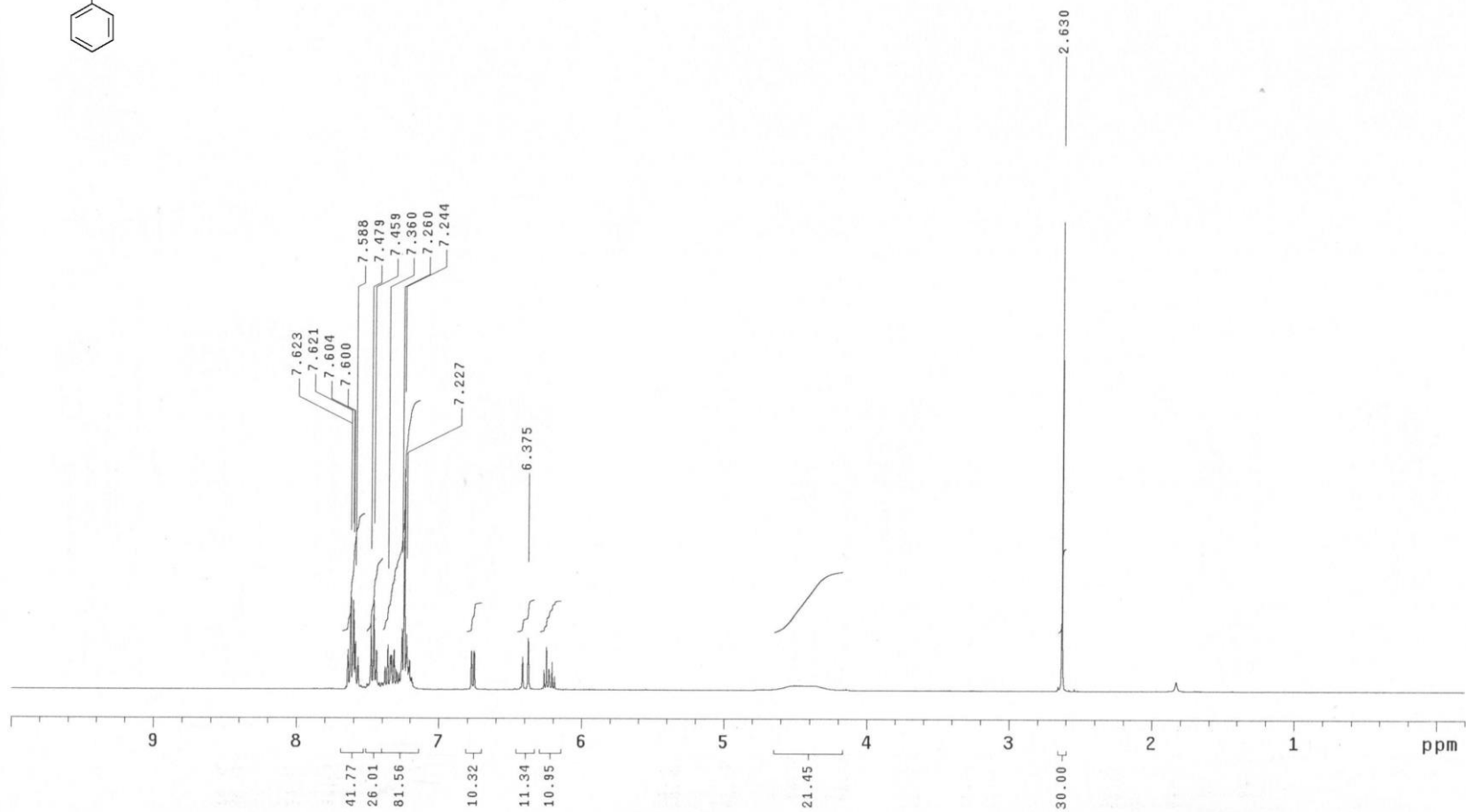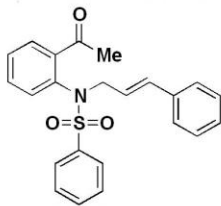
Compound 4j (^{13}C-NMR spectral data)

MCNBsCin

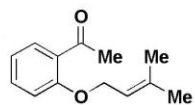Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 15 2019
Solvent: CDCl3
Ambient temperature
Total 480 repetitions

200.424
141.517
138.106
136.203
136.021
134.642
132.822
131.101
129.047
128.949
128.797
128.433
128.274
127.857
127.743
126.349
123.286
77.318
77.000
76.682
54.153
30.077

200   180   160   140   120   100   80   60   40   20   ppm
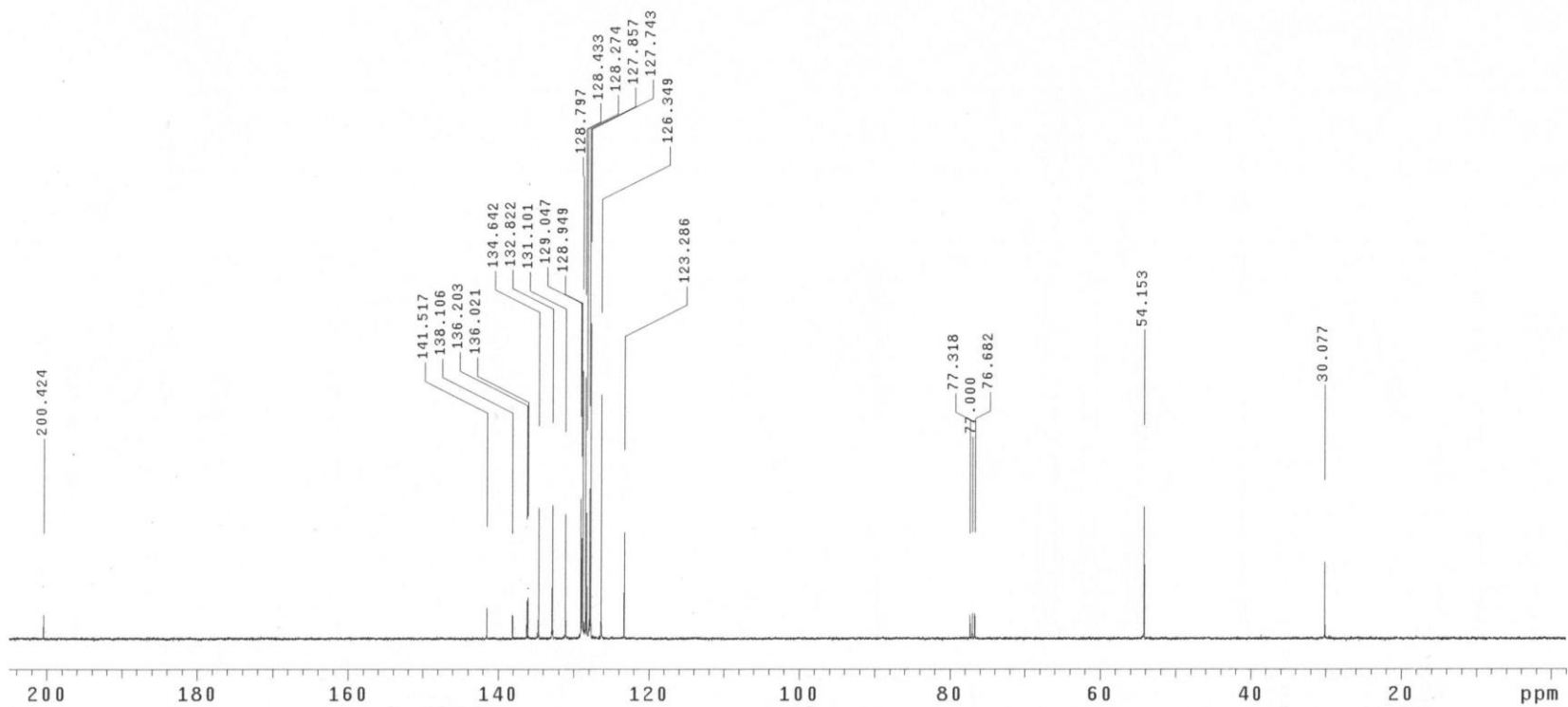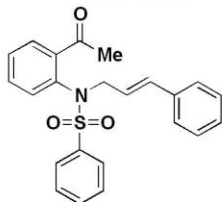
Compound 4k (^{1}H-NMR spectral data)

MC1080502

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 3 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

10.601

7.896
7.891
7.876
7.871
7.540
7.537
7.447
7.443

7.425
7.373
7.355
7.351
7.335
7.305
7.287
7.037
7.017

6.747
6.442
6.403

4.797
4.793
4.783
4.779

8.00

8.79
10.31
20.89
30.68

20.00

9.93

10.23

21.47

10   9   8   7   6   5   4   3   2   1   ppm

Compound 4k (^{13}C-NMR spectral data)

MC1080502

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 3 2019
Solvent: CDC13
Ambient temperature
Total 80 repetitions

189.516
160.786
135.915
135.733
133.262
128.494
128.221
127.963
126.432
124.886
123.233
120.686
112.749
77.318
77.000
76.682
68.874

180   160   140   120   100   80   60   40   20   ppm

Compound 5a (^{1}H-NMR spectral data)

MC1071214

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 14 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.715
7.710
7.696
7.691
7.649
7.610
7.447
7.438
7.436
7.433
7.408
7.220
7.217
7.208
7.204
7.200
7.193
7.138
7.133
7.117
7.112
7.058
7.042
7.039
7.008
6.988
6.729
6.689
6.654
6.633
6.385
6.345
4.744
4.740
4.730
4.727
3.816
3.711

20.05
20.77
51.55
11.25
31.58
20.22
10.29
20.15
29.95
30.00

9 8 7 6 5 4 3 2 1 ppm

Compound 5a (^{13}C-NMR spectral data)

MC1071214

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 14 2018
Solvent: CDC13
Ambient temperature
Total 576 repetitions

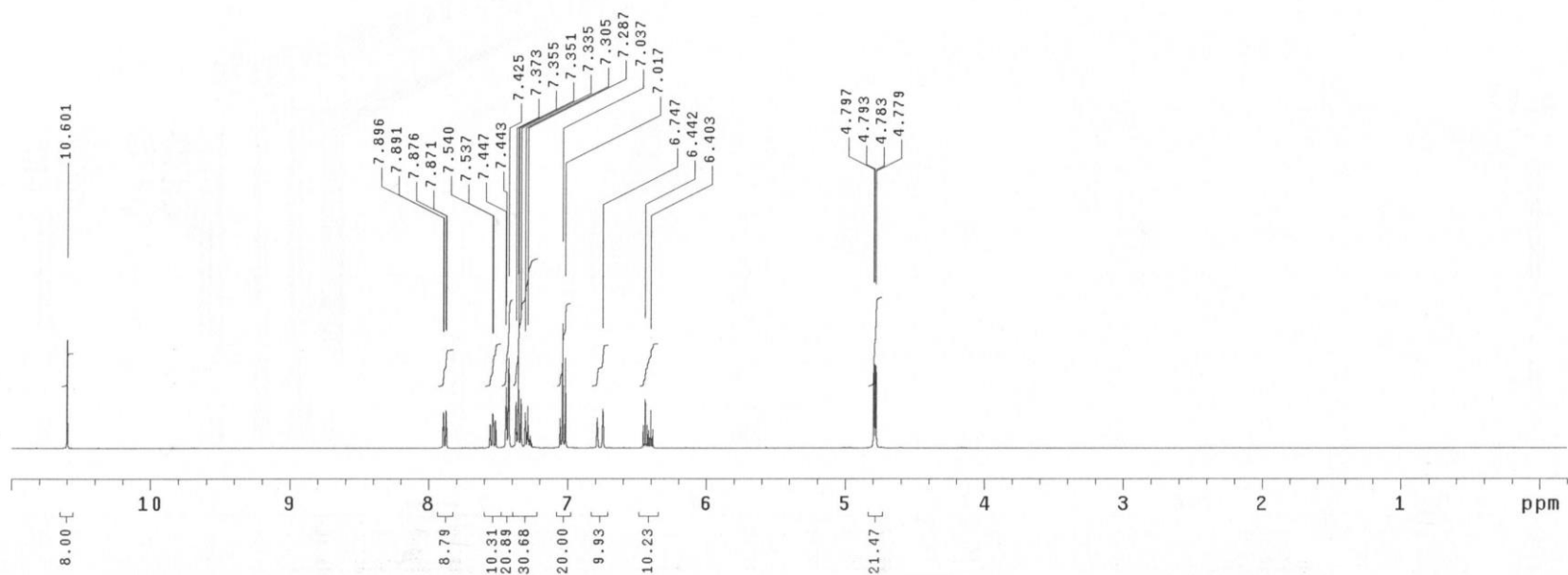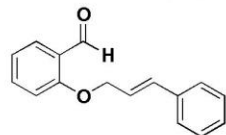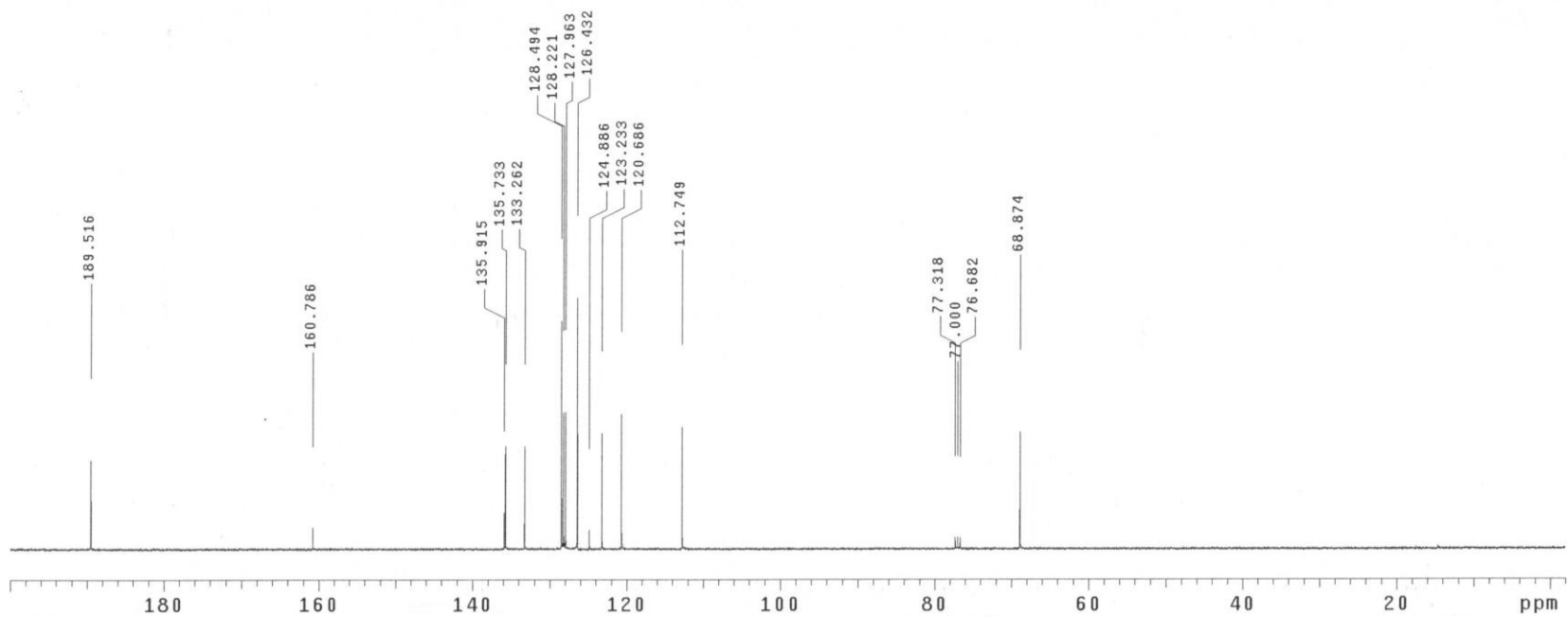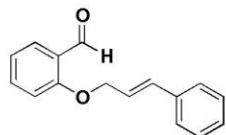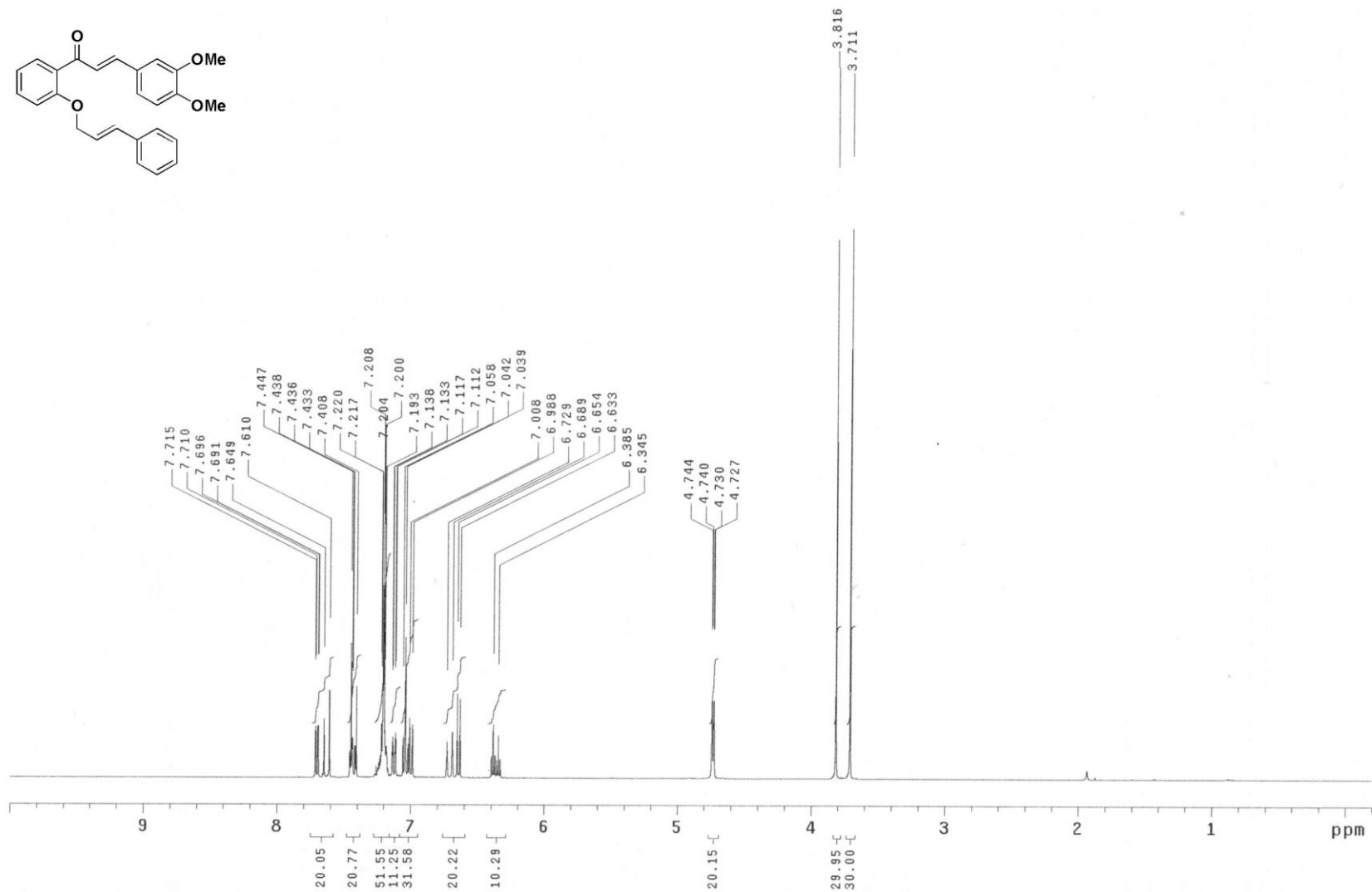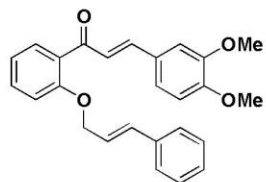# Compound 5b (^{1}H-NMR spectral data)

MC1080114

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 14 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

3.820
3.709

7.210
7.200
7.125

7.777
7.771
7.621
7.582
7.491
7.485
7.367
7.328

7.121
7.104
7.100
7.020
7.017

6.884
6.862
6.668
6.644
6.624

4.708
4.696

8.26
10.36
10.00
13.47
52.26
11.25
10.55
10.56
21.34
10.81
20.14
30.00
30.58

9   8   7   6   5   4   3   2   1   ppm

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Compound 5b (^{13}C-NMR spectral data)

MC1080114

Pulse Sequence: s2pul

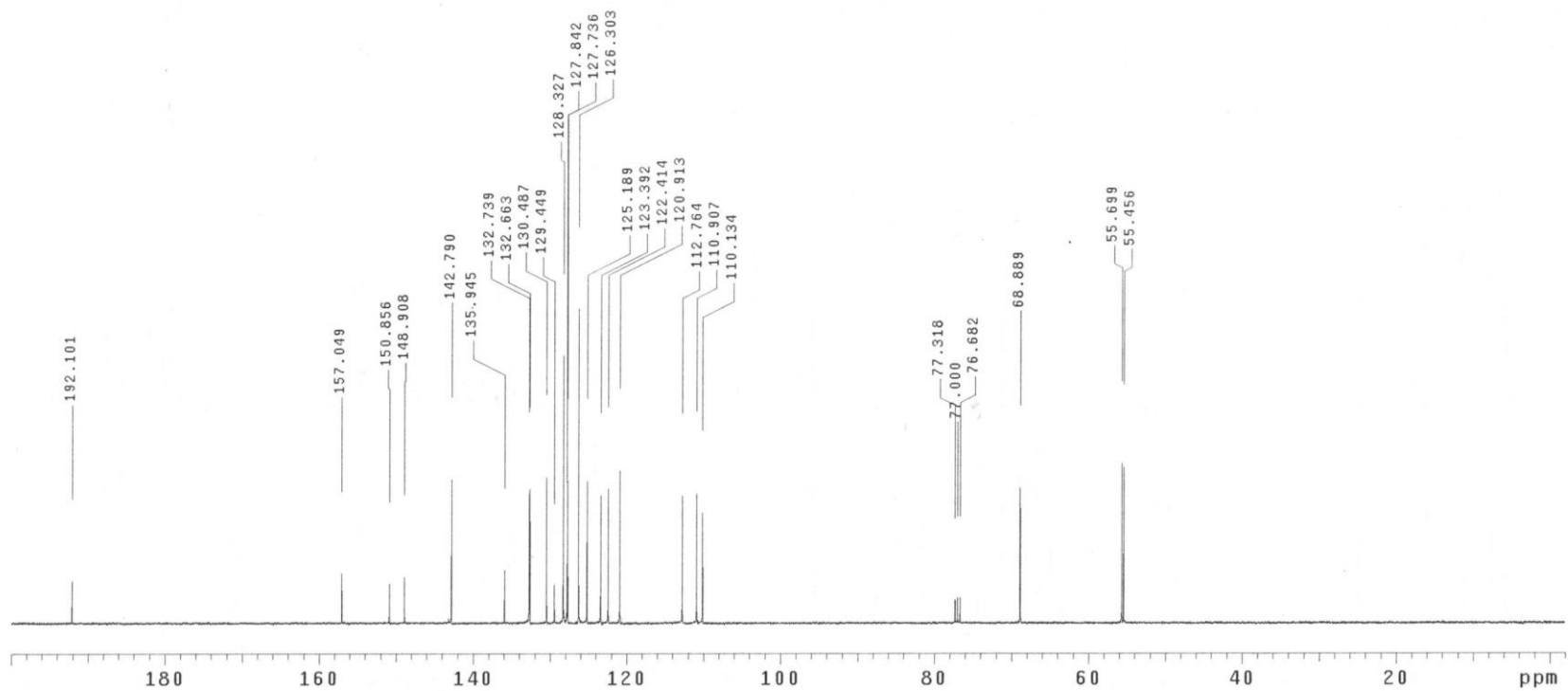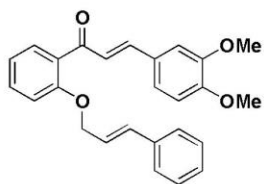UNITYplus-400 "unity400"
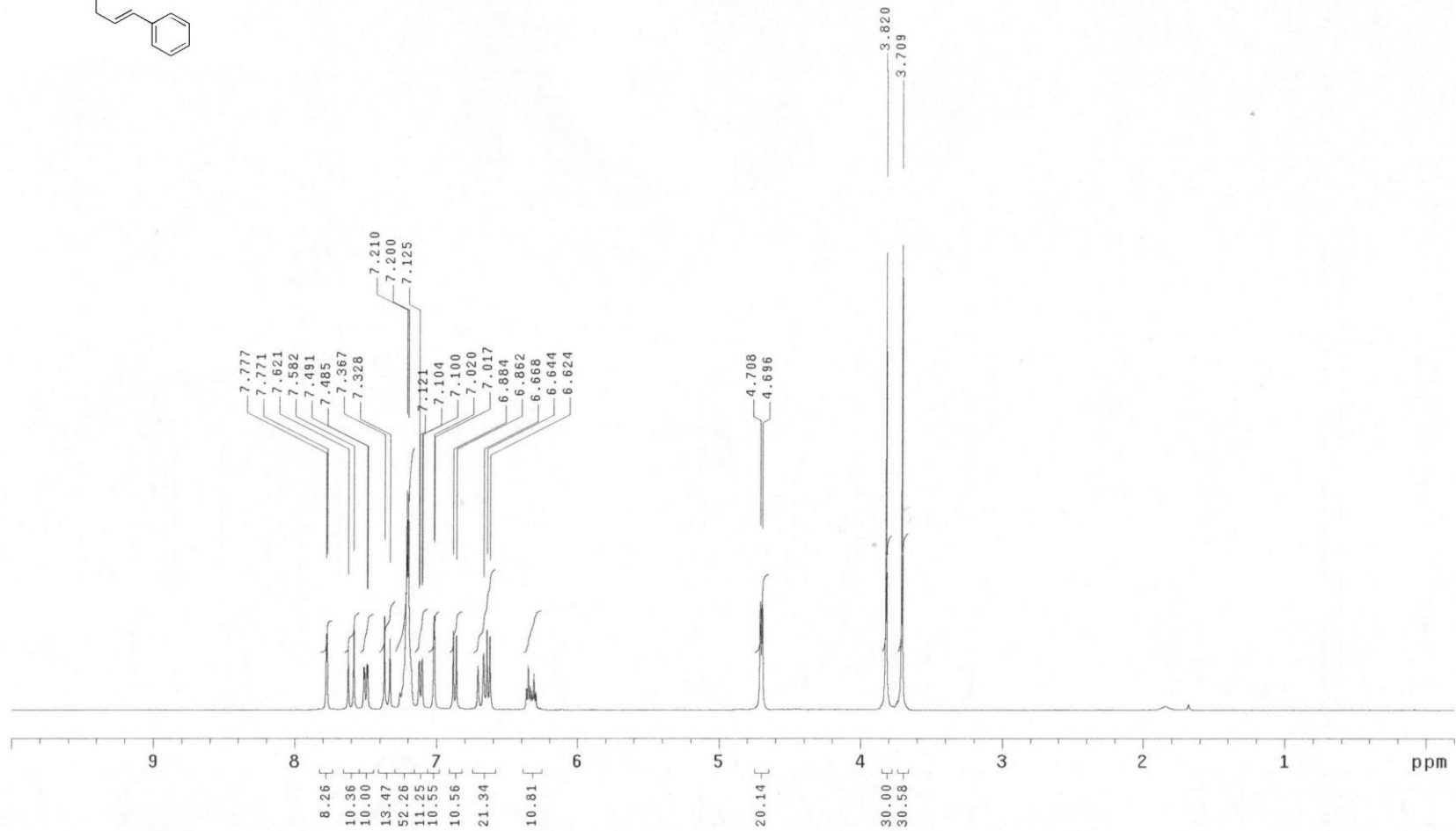Date: Jan 14 2019
Solvent: CDCl3
Ambient temperature
Total 256 repetitions
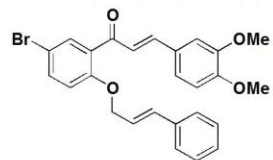
Compound 5c (^{1}H-NMR spectral data)

MCaldolCl

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 16 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.651
7.644
7.633
7.594
7.373
7.333
7.260
7.256
7.243
7.236
7.052
7.047
6.988
6.966
6.698
6.677
4.772
4.768
4.757
4.754
3.859
3.750
1.627

17.44
19.80
49.88
10.48
10.36
19.66
9.95
20.31
30.17
30.00

9   8   7   6   5   4   3   2   1   ppm

Compound 5c (^{13}C-NMR spectral data)

MCaldolC1

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
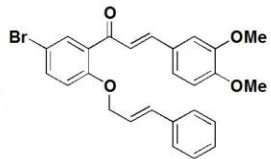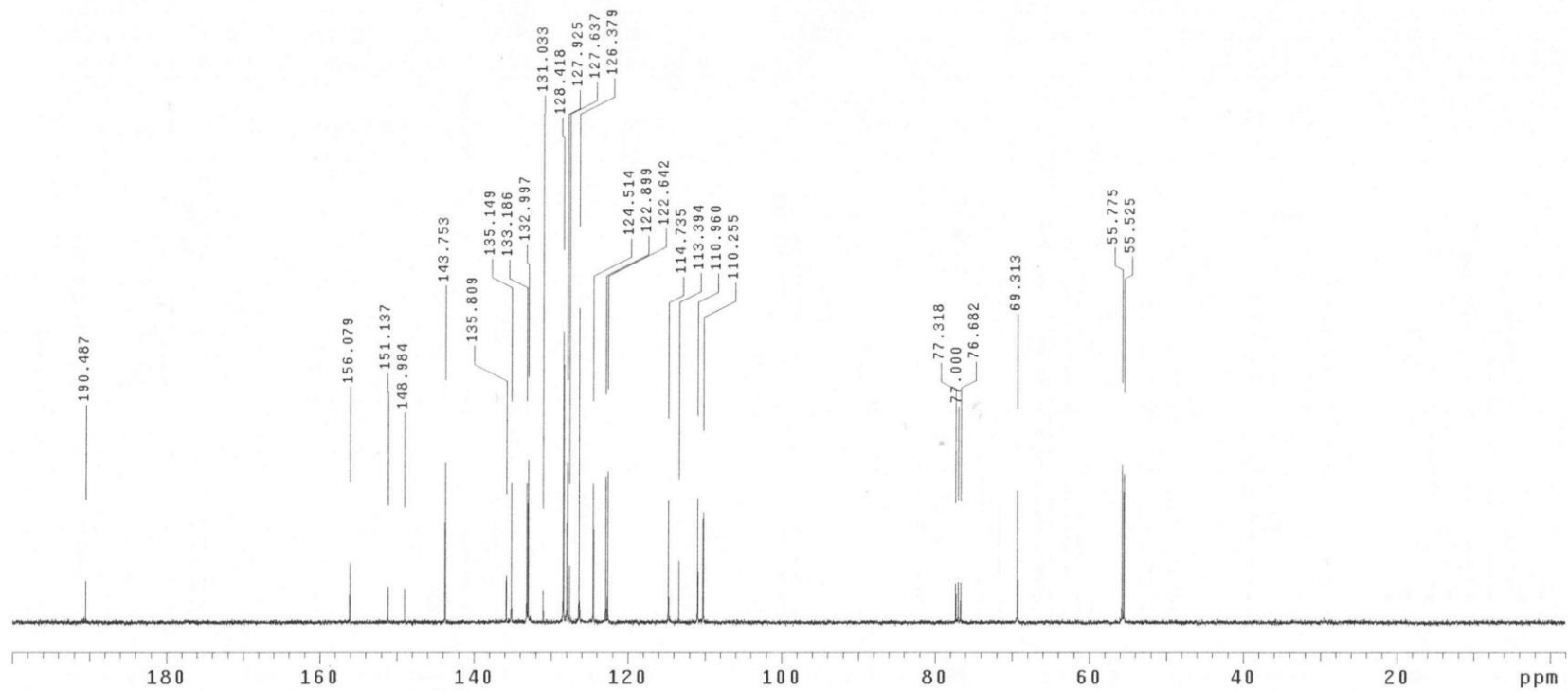Date: May 16 2019
Solvent: CDC13
Ambient temperature
Total 4368 repetitions

190.949
155.670
151.281
149.143
144.011
135.961
133.323
132.276
130.904
130.245
128.554
128.069
127.796
126.500
126.386
124.688
123.104
122.801
114.500
111.066
110.331
77.318
77.000
76.682
69.602
55.919
55.684

180   160   140   120   100   80   60   40   20   ppm

Compound 5d (^{1}H-NMR spectral data)

MC1080129

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 31 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

3.860
3.748

7.651
7.612
7.426
7.387
7.260
7.256
7.244
7.237
7.165
7.160
7.146
7.057
7.052
6.694
6.673
6.400
4.762
4.758
4.748
4.744
1.606

9.70
20.00
50.81
20.21
21.70
20.01
10.13
20.56
30.78
30.50

9   8   7   6   5   4   3   2   1   ppm

Compound 5d (^{13}C-NMR spectral data)

MC1080129

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 31 2019
Solvent: CDCl3
Ambient temperature
Total 5248 repetitions

Compound 5e (¹H-NMR spectral data)

MC1080118

Pulse Sequence: s2pul
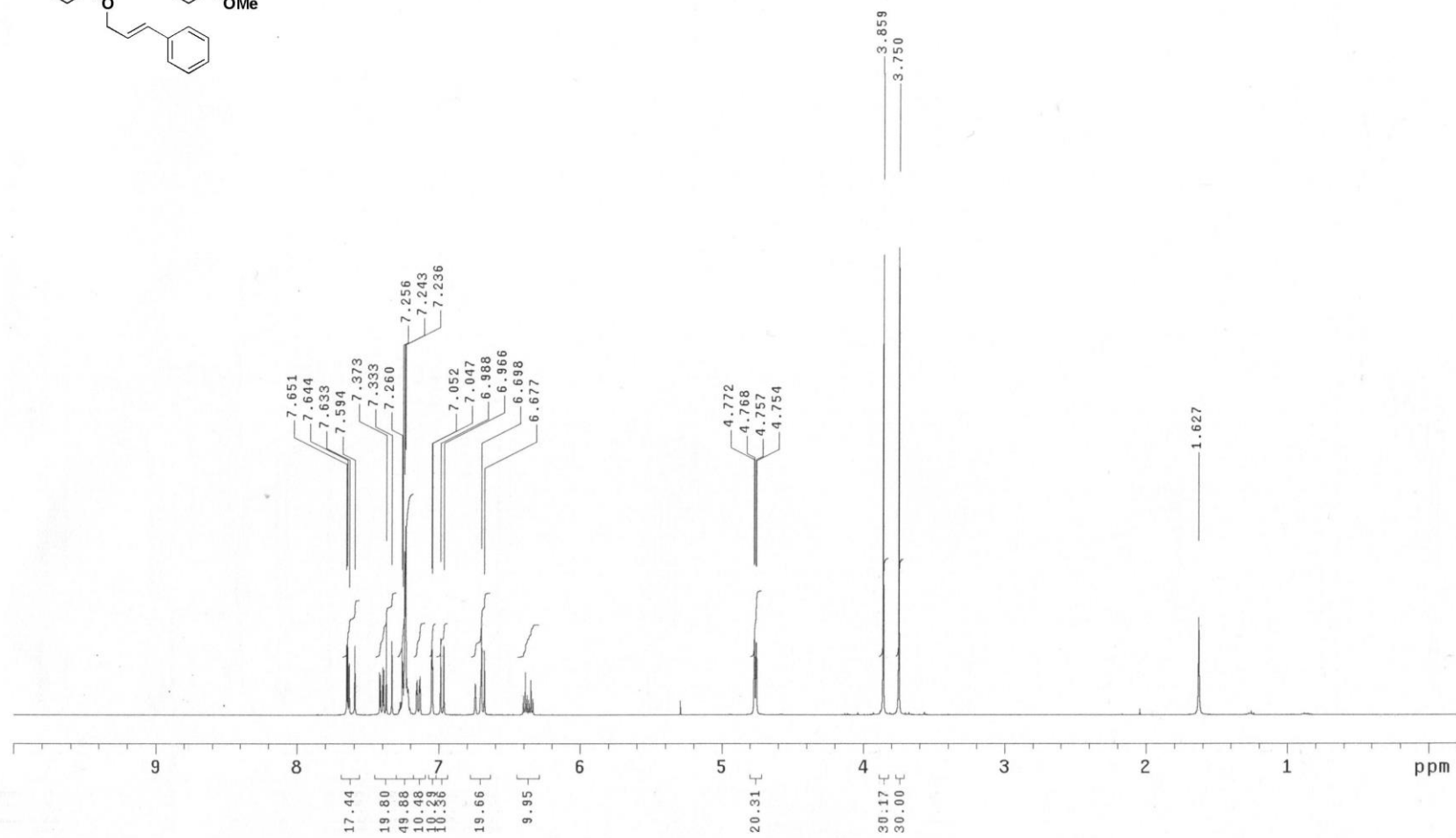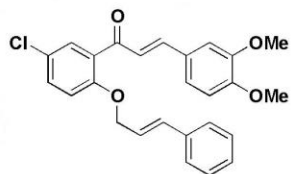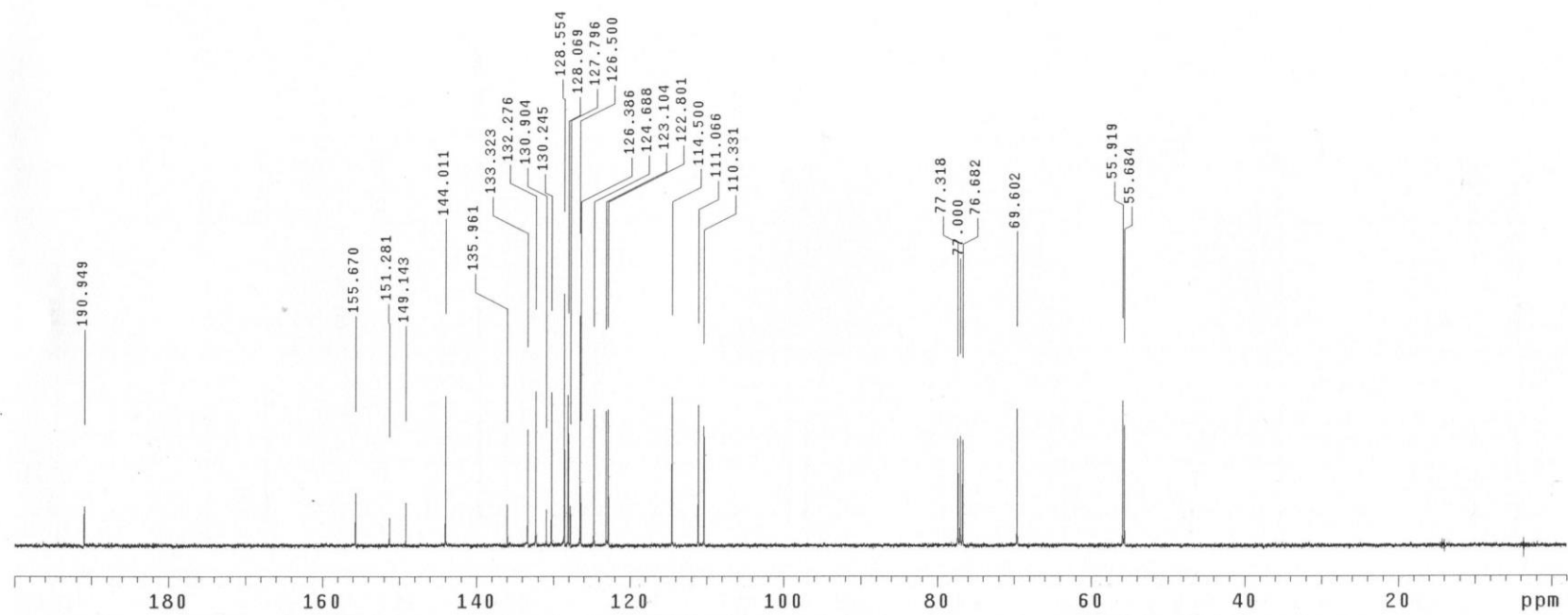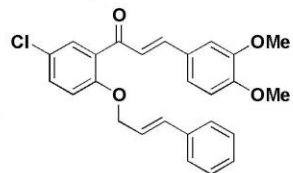
UNITYplus-400 "unity400"
Date: Jan 22 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 5e (^{13}C-NMR spectral data)

MC1080118

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
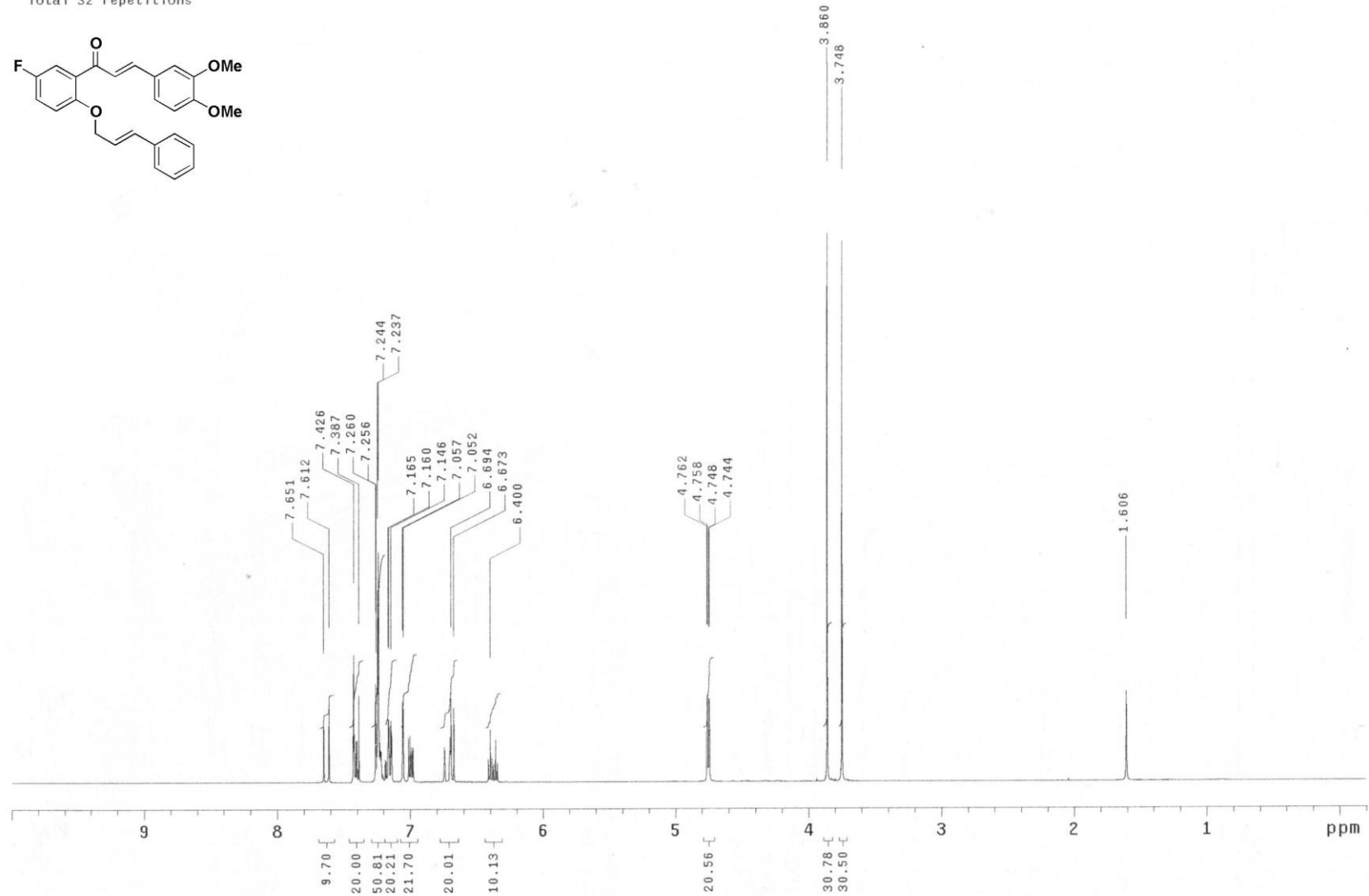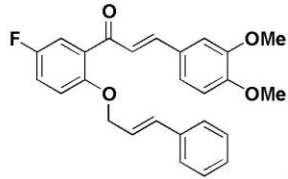Date: Jan 22 2019
Solvent: CDCl3
Ambient temperature
Total 944 repetitions

192.442
155.169
150.924
149.014
142.806
136.112
133.345
132.671
130.874
130.487
129.373
128.441
128.031
127.819
126.394
125.356
123.726
122.520
113.075
110.975
110.202
77.318
77.000
76.682
69.260
55.828
55.578
20.276

180   160   140   120   100   80   60   40   20   ppm

Compound 5f (¹H-NMR spectral data)

Compound 5f (^{13}C-NMR spectral data)

MC1080211

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 12 2019
Solvent: CDCl3
Ambient temperature
Total 256 repetitions
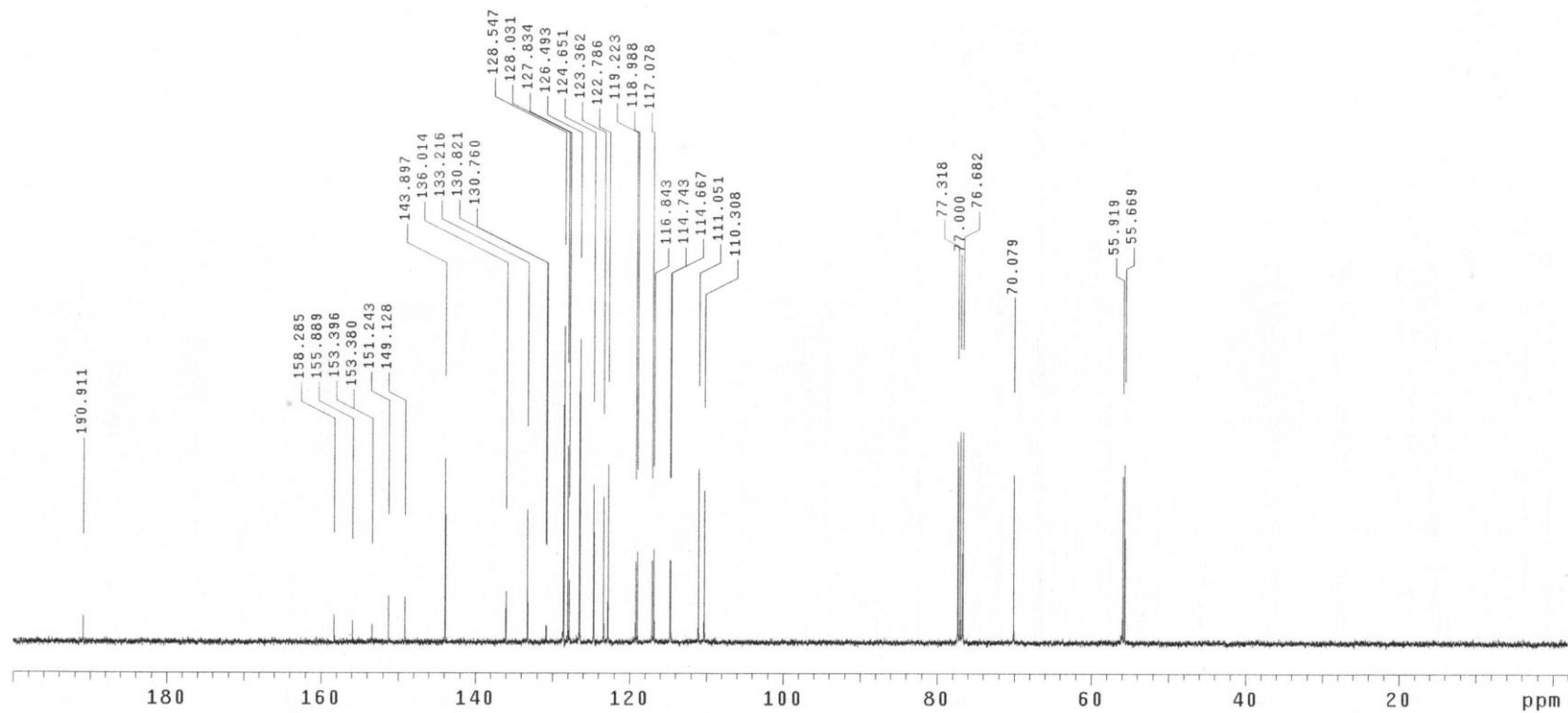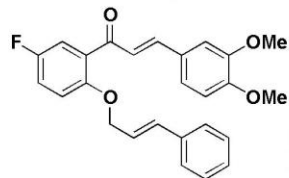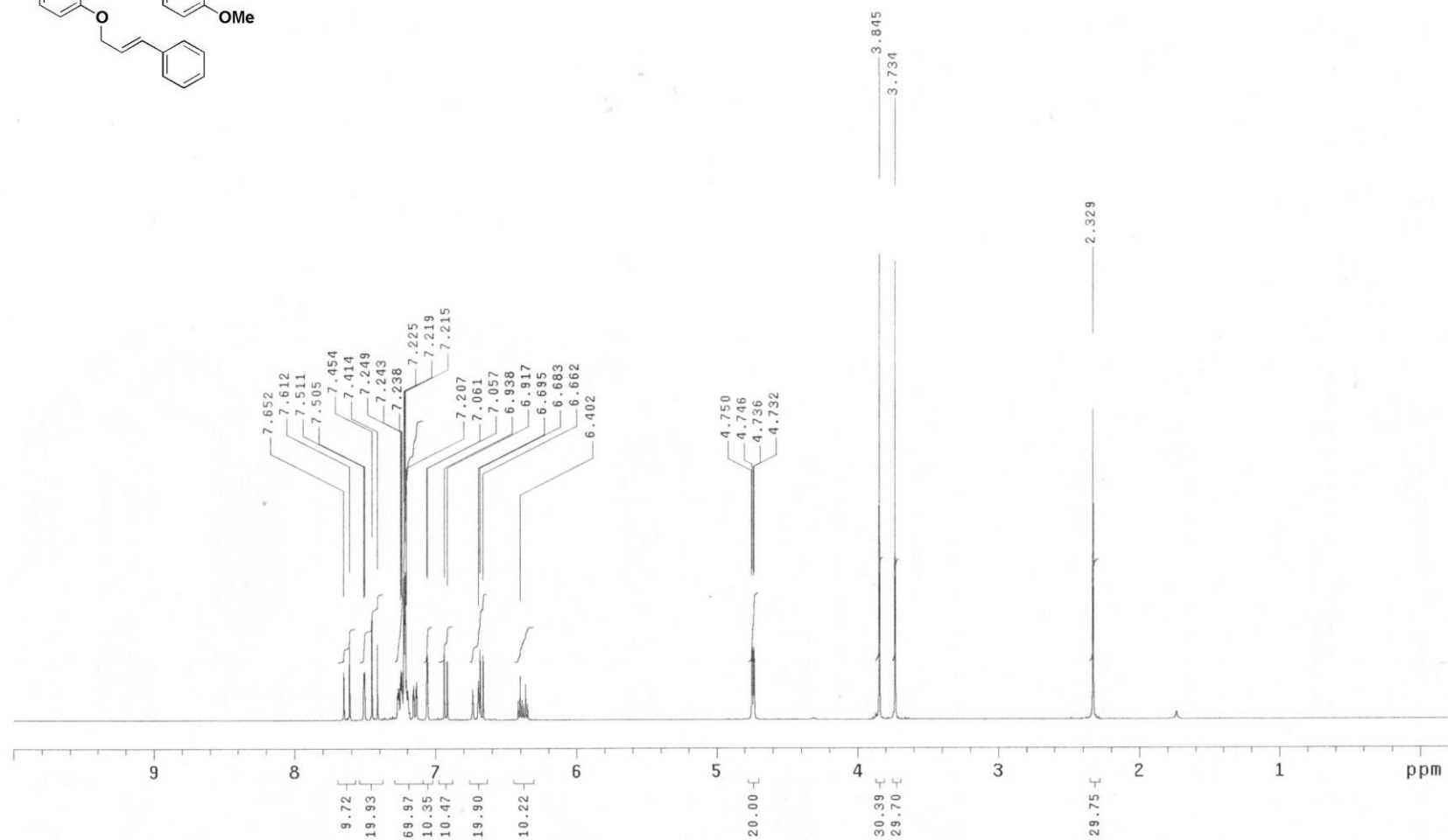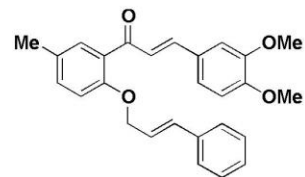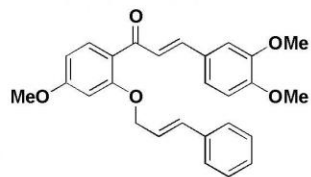
Compound 5g (^{1}H-NMR spectral data)

MC1080213

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 14 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.588
7.408
7.369
7.221
7.212
7.045
7.025
7.001
6.675
6.656
5.851
4.722
4.719
4.709
4.706

9   8   7   6   5   4   3   2   1   ppm

9.72
10.06
21.43
50.62
41.25
19.54
10.31
20.00
20.34

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Compound 5g (^{13}C-NMR spectral data)

191.896
157.102
149.348
148.097
142.192
135.961
132.807
132.602
130.472
129.358
129.282
128.236
127.561
126.288
125.348
124.597
123.324
120.868
112.780
108.292
106.503
101.242
68.798

180 160 140 120 100 80 60 40 20 ppm
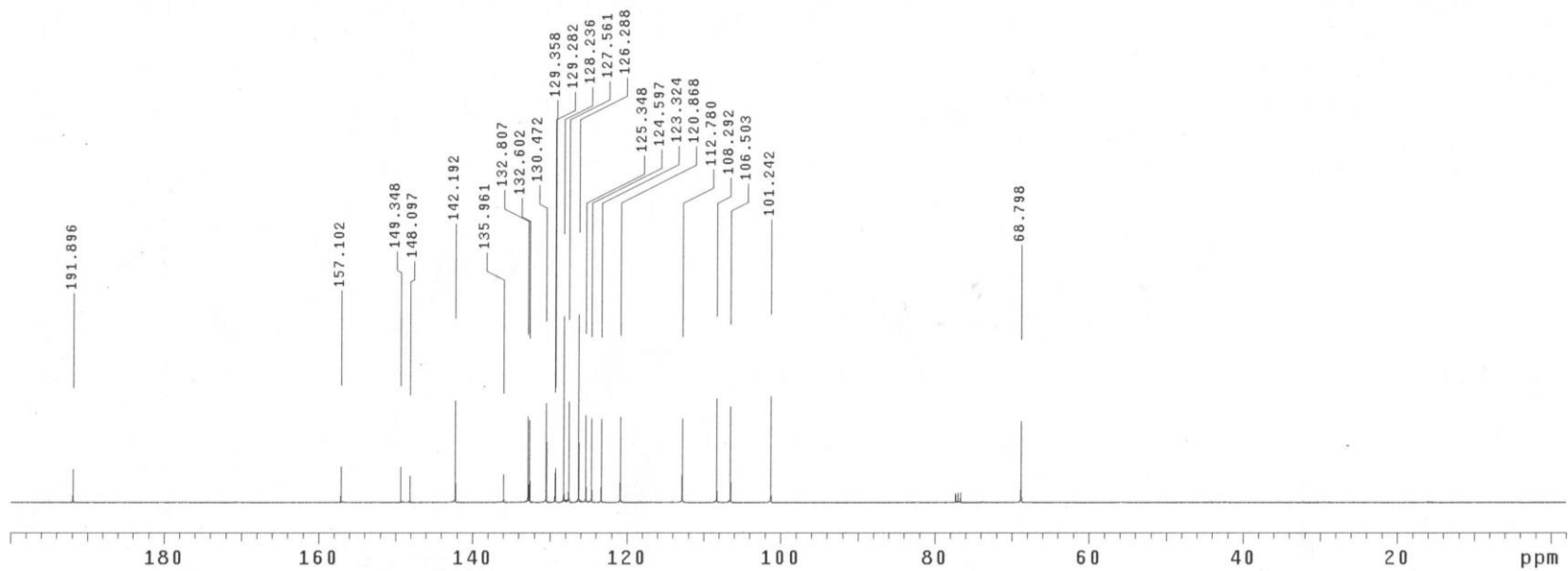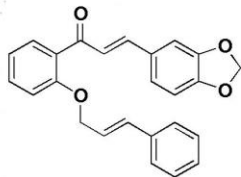
Compound 5h (^{1}H-NMR spectral data)

MC1080214
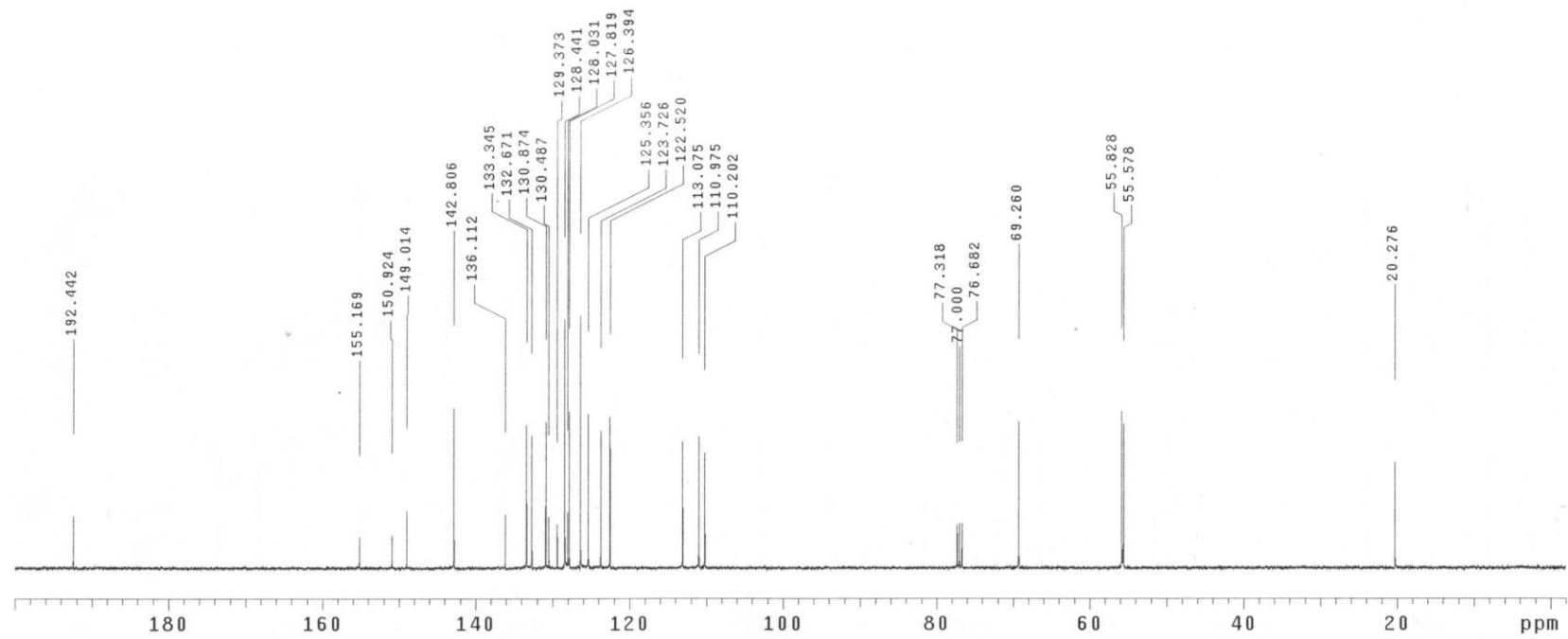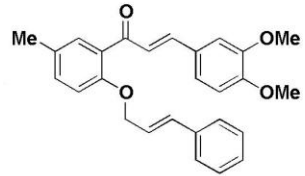
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 15 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.737

3.846

7.572
7.428
7.389
7.221
7.214

7.199
7.194
7.071
7.055
6.797

4.804
4.800
4.790
4.786

19.40
20.83
49.50
20.49
30.38
10.00
20.40
29.39
58.38
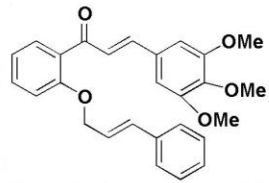
Compound 5h (^{13}C-NMR spectral data)

MC1080214

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 15 2019
Solvent: CDCl3
Ambient temperature
Total 816 repetitions

192.541
157.095
153.342
143.003
140.069
136.036
132.913
132.496
130.601
130.503
129.654
128.517
127.940
126.553
126.326
123.453
121.141
112.924
105.457
77.318
77.000
76.682
69.018
60.892
55.911

180   160   140   120   100   80   60   40   20   ppm

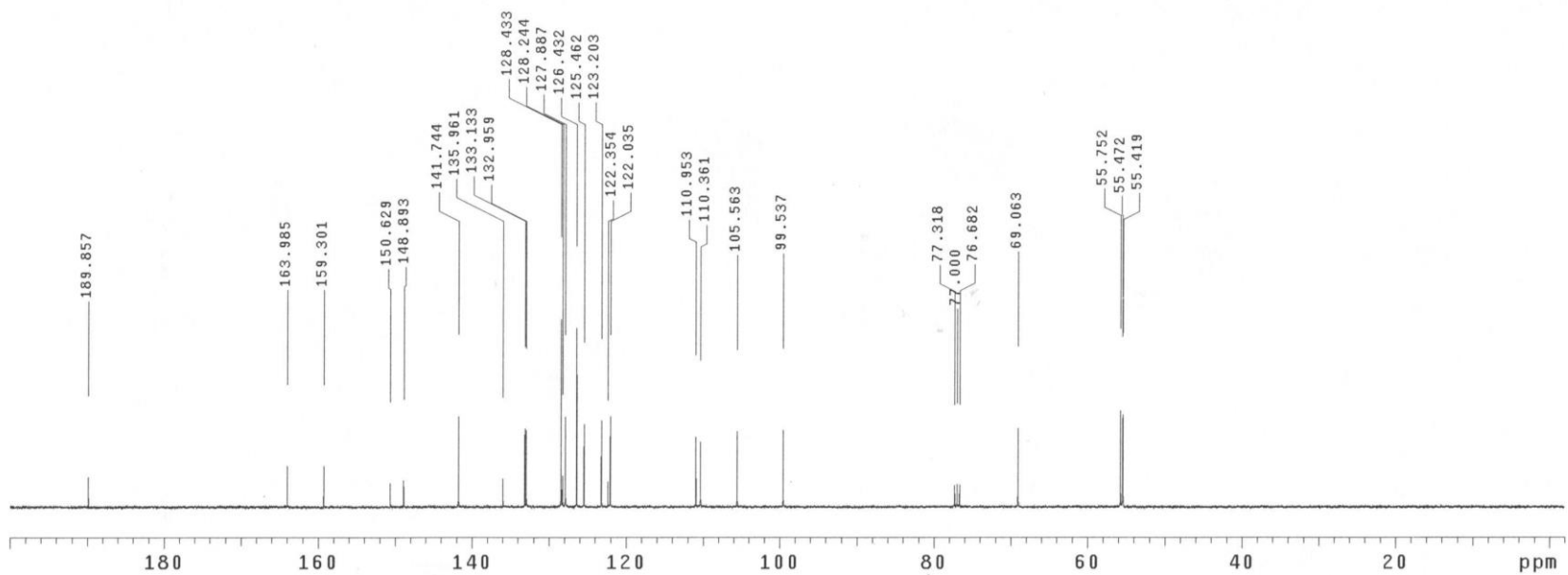# Compound 5i (^{1}H-NMR spectral data)

MC10Me

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 15 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.668
7.591
7.552
7.242
7.239
7.234
7.174
7.155
4.764
4.761
4.751
4.747
3.704

20.09
10.32
10.70
103.59
10.00
10.30
10.56
21.11
30.00

9 8 7 6 5 4 3 2 1 ppm

Compound 5i (^{13}C-NMR spectral data)

MC10Me

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
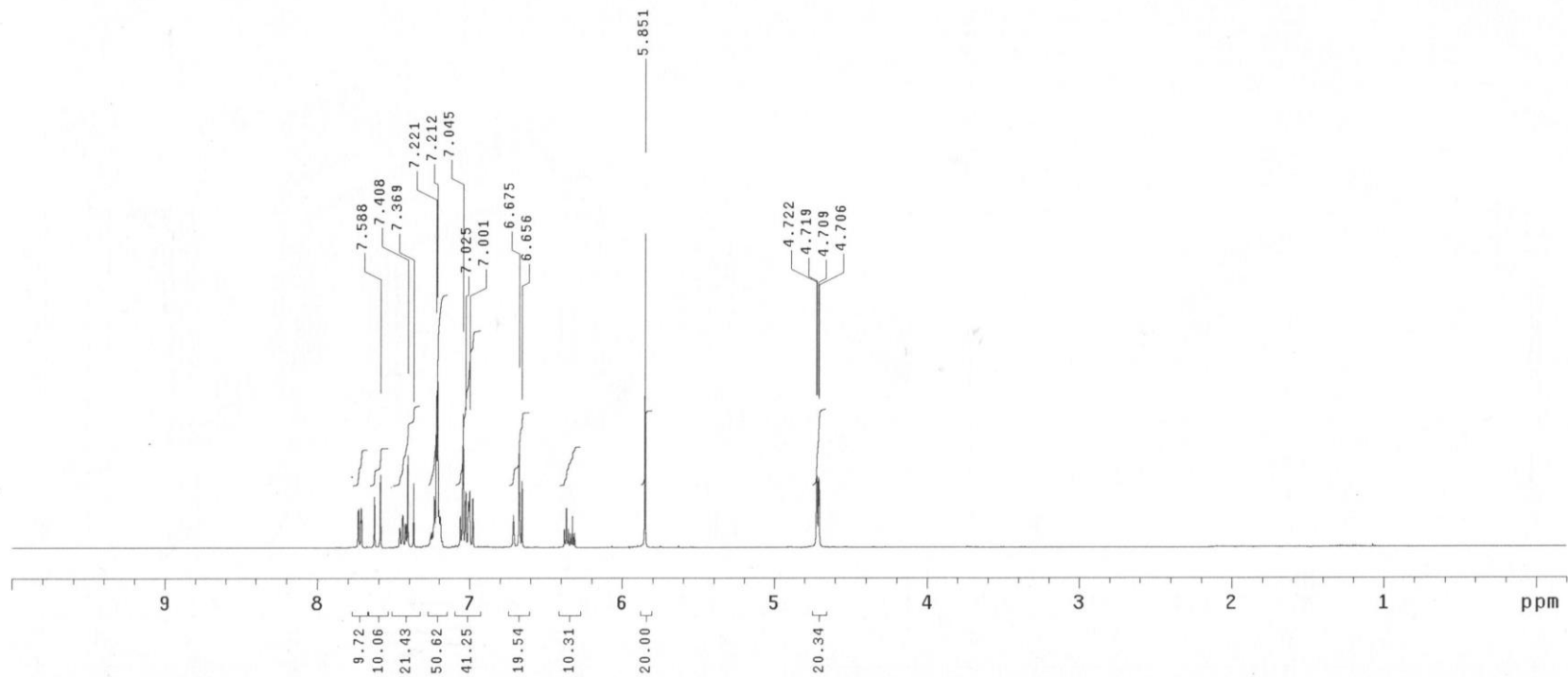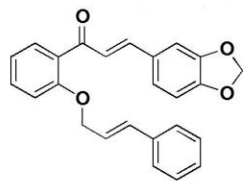Date: Feb 15 2019
Solvent: CDC13
Ambient temperature
Total 128 repetitions

192.131

159.702
157.231

142.351
136.286
135.961
133.027
132.762
130.586
129.692
129.222
128.335
127.713
127.387
126.341
123.324
120.944
120.739
115.872
113.174
112.802

68.919

54.933

180   160   140   120   100   80   60   40   20   ppm

Compound 5j (^{1}H-NMR spectral data)

MC4-OMe

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 27 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.643
7.508
7.488
7.486
7.449
7.260
7.259
7.064
6.743
6.722
4.784
4.780
4.770
4.766
3.764

19.50 40.79 49.09 20.61 29.18 10.00 20.75 30.19

9 8 7 6 5 4 3 2 1 ppm
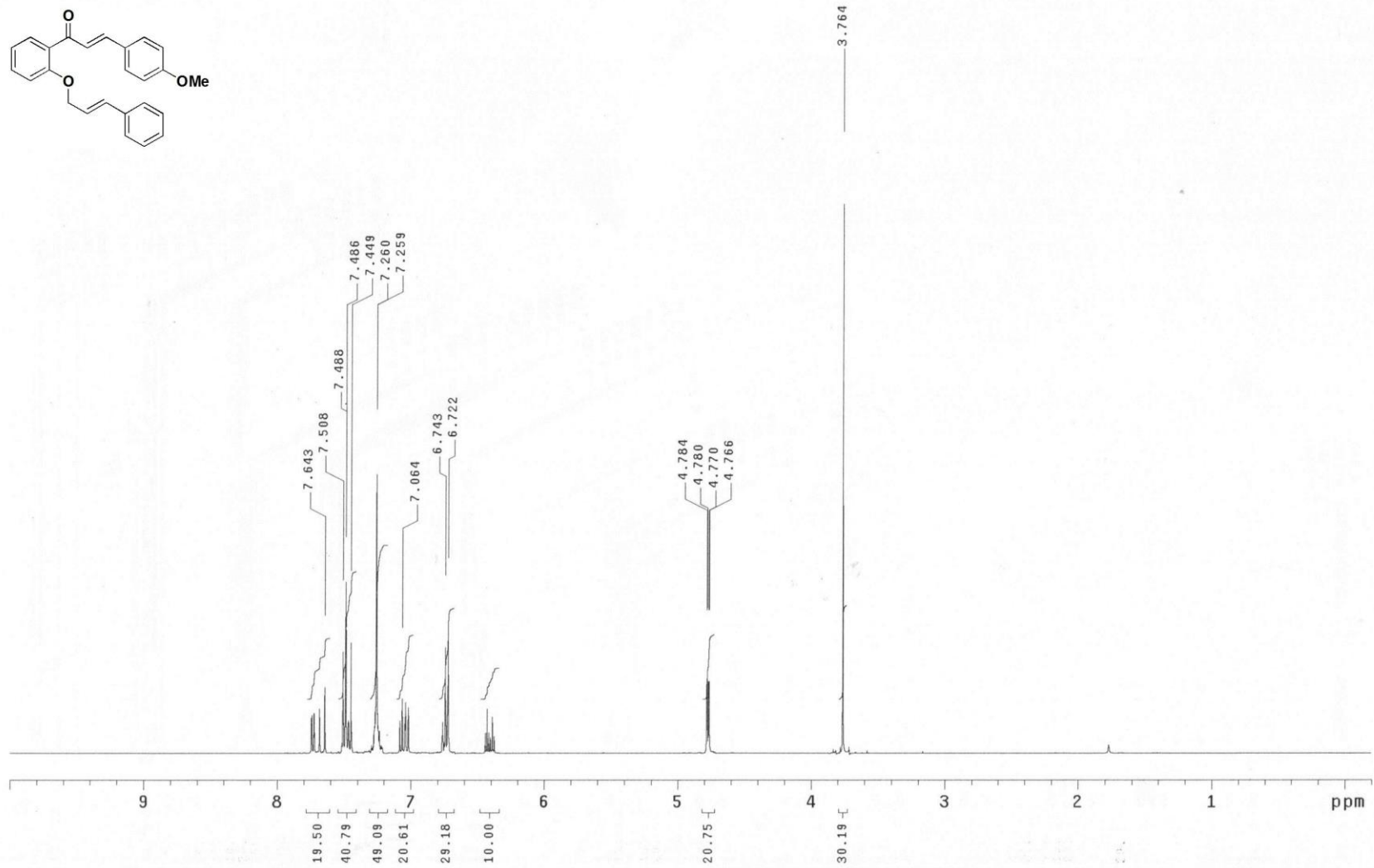
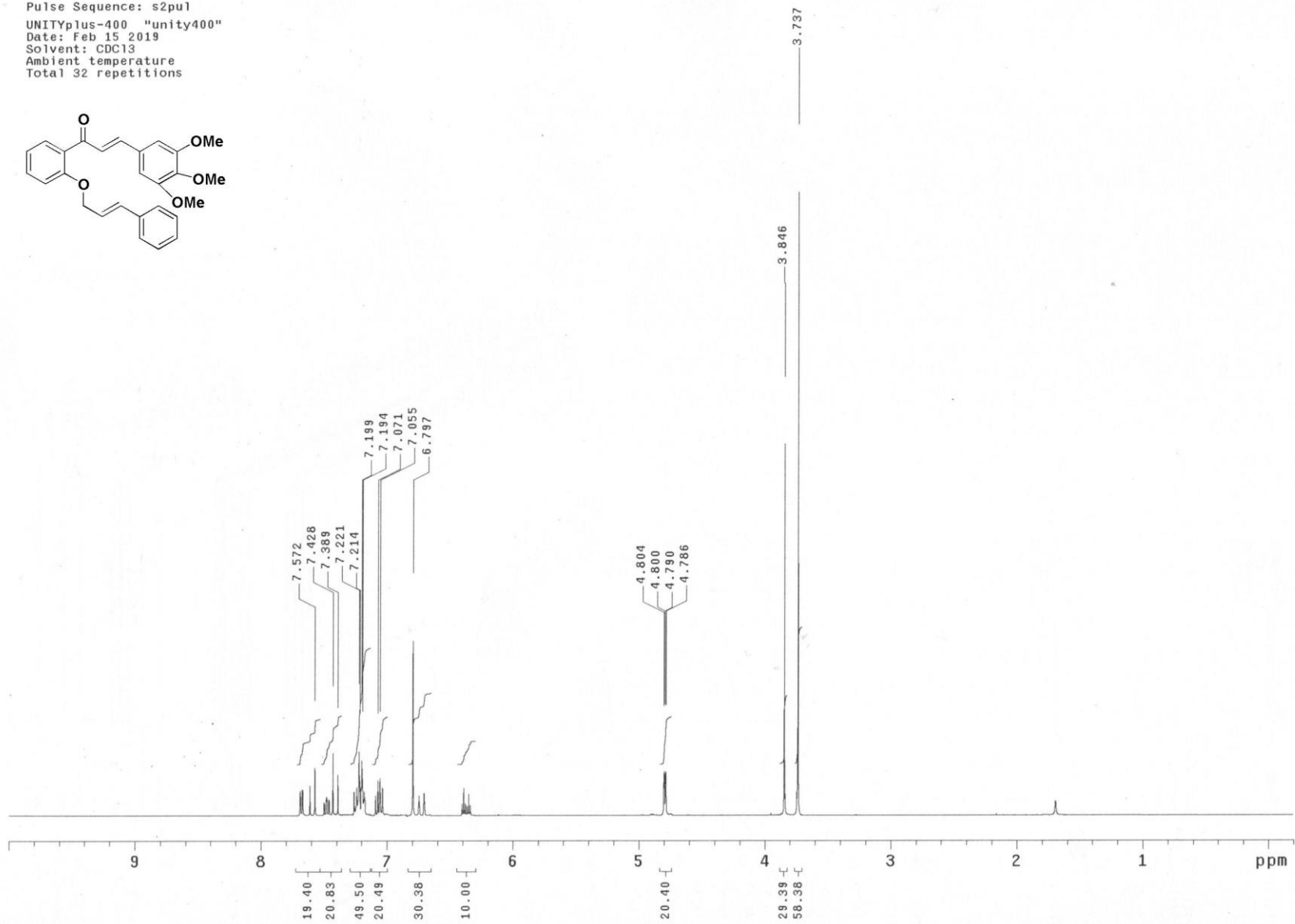# Compound 5j (^{13}C-NMR spectral data)

MC4-OMe

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 27 2019
Solvent: CDCl3
Ambient temperature
Total 816 repetitions

192.207
161.264
157.269
142.586
136.127
133.103
132.837
130.662
129.995
129.585
128.456
127.834
127.751
126.508
125.105
123.582
121.035
114.243
112.939
77.318
77.000
76.682
69.101
55.237

180 160 140 120 100 80 60 40 20 ppm

Compound 5k (^{1}H-NMR spectral data)

MC2,3,4-3OMe

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: Feb 25 2019
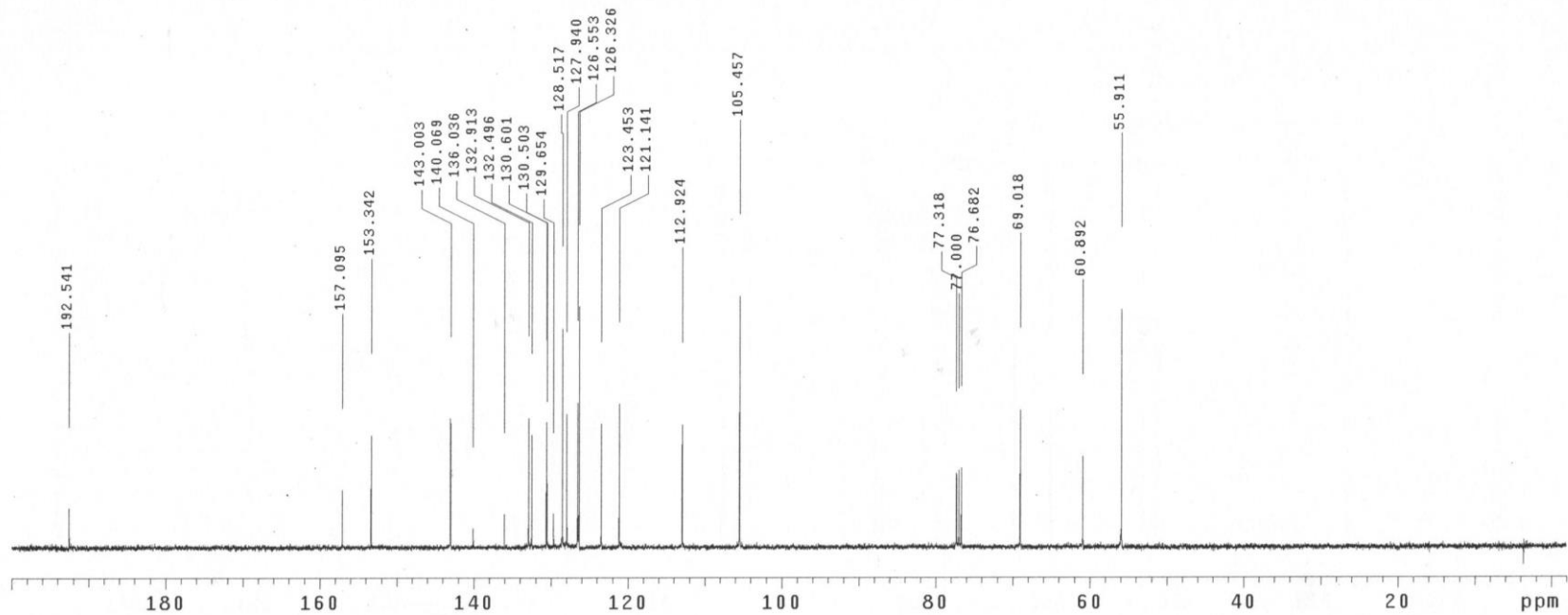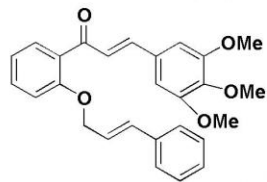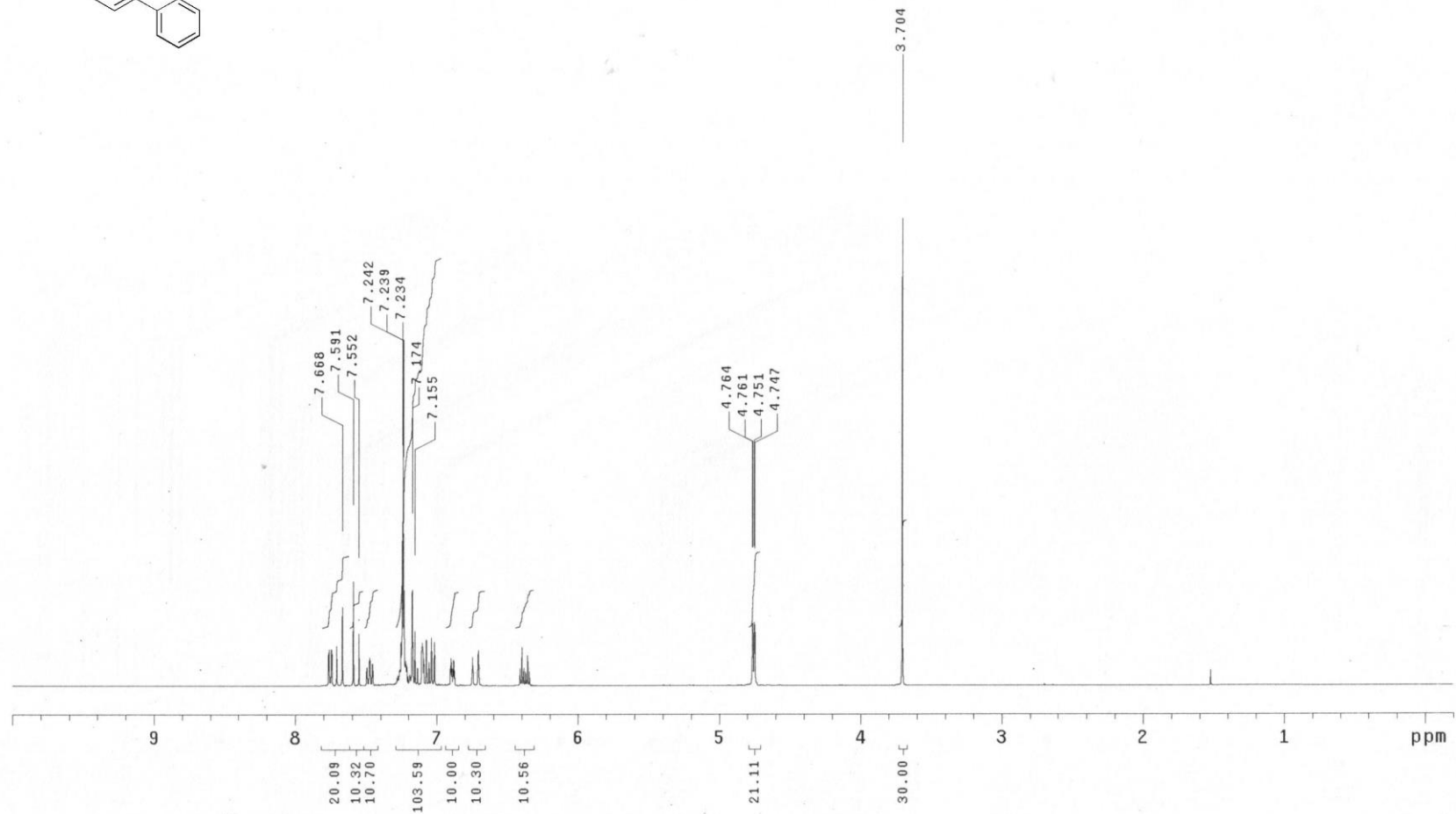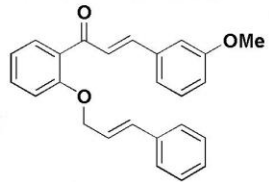Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Peak labels: 7.959, 7.919, 7.739, 7.735, 7.721, 7.716, 7.562, 7.522, 7.296, 7.274, 7.255, 7.253, 7.245, 7.232, 7.044, 7.043, 7.016, 6.995, 6.708, 6.419, 6.338, 6.316, 4.755, 4.752, 4.741, 4.738, 3.874, 3.823, 3.769

Integration: 9.11, 9.40, 9.95, 10.56, 60.52, 20.51, 9.95, 20.41, 20.00, 90.36

X-axis: 9, 8, 7, 6, 5, 4, 3, 2, 1, ppm
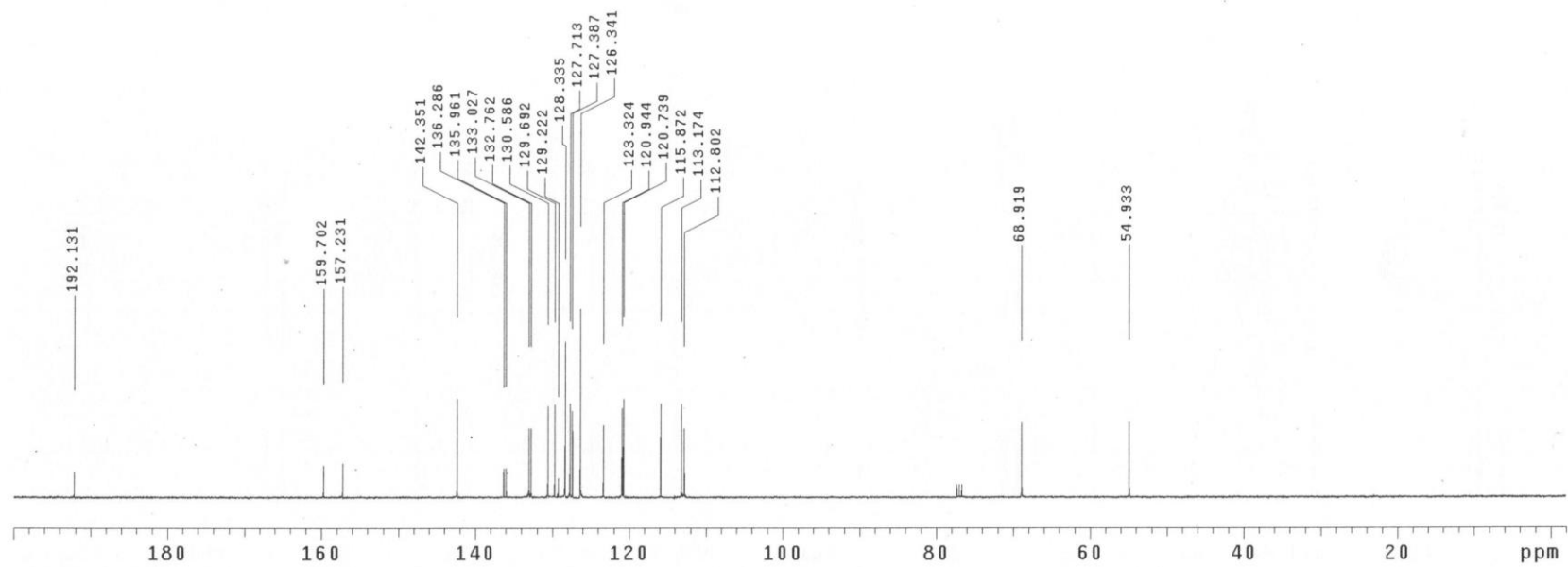
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Compound 5k (^{13}C-NMR spectral data)

MC2,3,4-3OMe
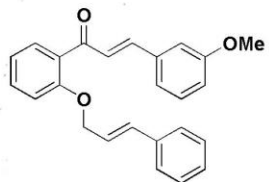
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 25 2019
Solvent: CDCl3
Ambient temperature
Total 480 repetitions

192.283

157.216
155.306
153.456

142.139
137.492
136.135
132.928
132.777
130.624
129.555
128.357
127.705
126.447
126.189
123.597
122.899
122.013
120.936
112.802
107.488

77.326
77.000
76.689
68.995
61.384
60.679
55.820

Compound 5l (^{1}H-NMR spectral data)

MC1080304

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 4 2019
Solvent: CDCl3
Ambient temperature
Total 80 repetitions

MC1080304

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 4 2019
Solvent: CDC13
Ambient temperature
Total 28592 repetitions

77.318
77.205
77.000
76.682

129.222
128.562
127.903
126.538

133.125
132.997
131.367
130.783
129.578

123.741
122.361
121.110
120.913
116.456
113.060

157.375
155.427

138.629
136.249

193.977

69.276

200   180   160   140   120   100   80   60   40   20   ppm

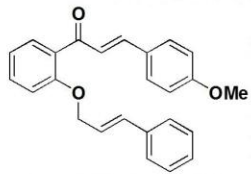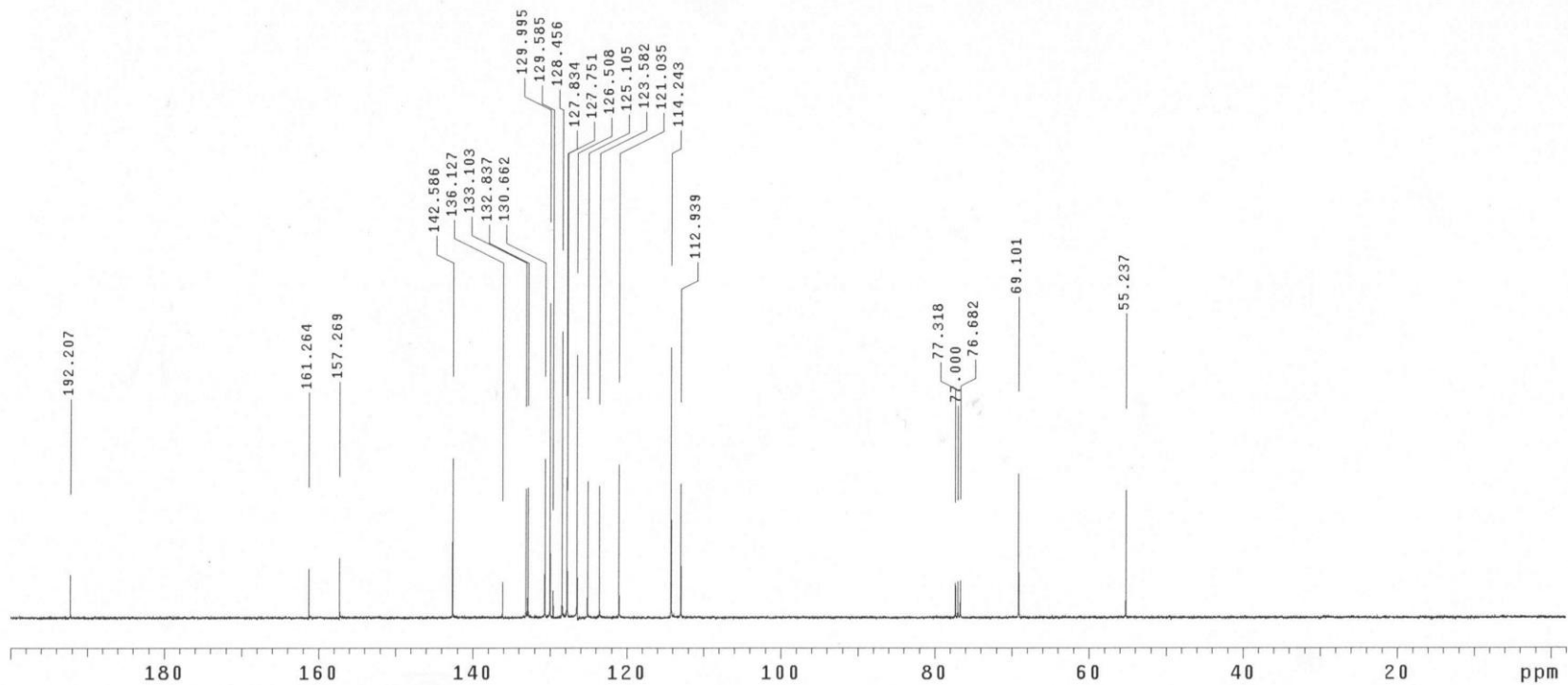# Compound 5m (¹H-NMR spectral data)

MC24MeO2

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 12 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

Compound 5m (^{13}C-NMR spectral data)
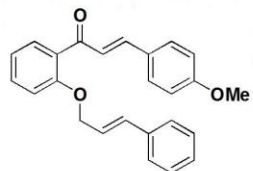
MC24MeO2

Pulse Sequence: s2pul

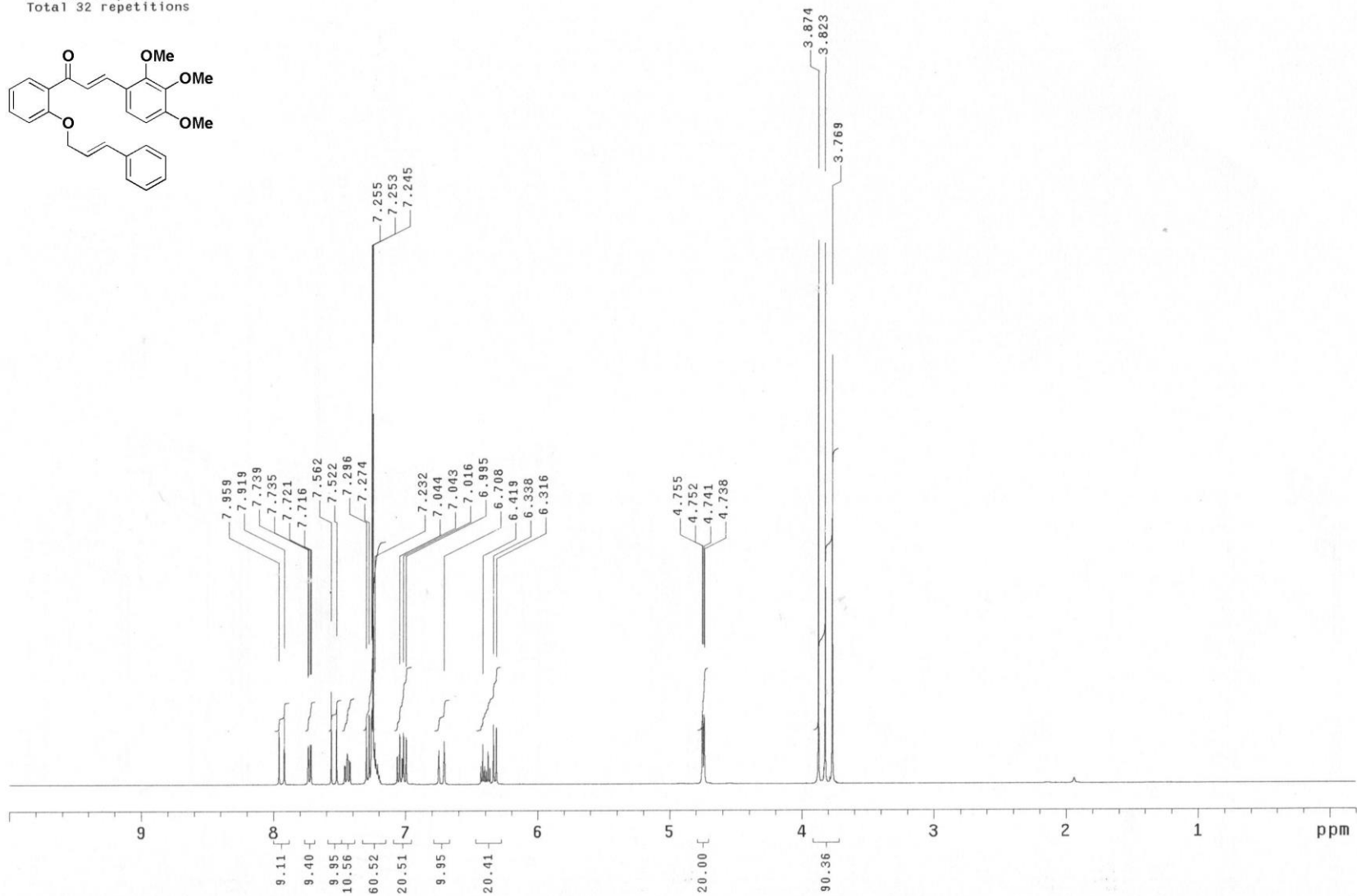UNITYplus-400 "unity400"
Date: Mar 12 2019
Solvent: CDC13
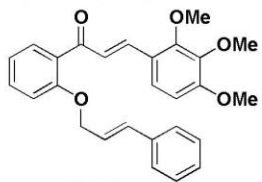Ambient temperature
Total 224 repetitions

192.882

162.674
160.013
157.057

138.326
136.196
132.625
132.466
130.510
130.101

129.972
128.373
127.668
126.432

125.280
123.680
120.906
117.078
112.863

105.123

98.263

77.318
77.000
76.682

68.965

55.290
55.267

180   160   140   120   100   80   60   40   20   ppm
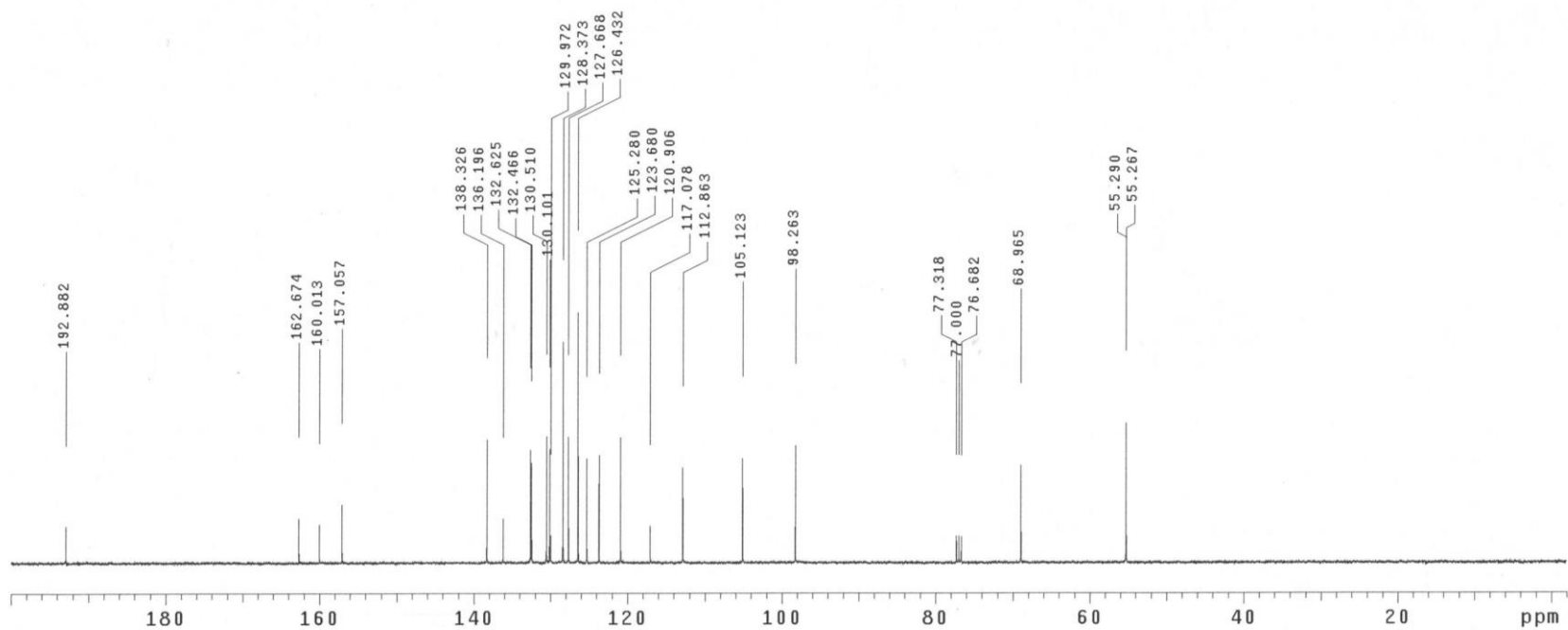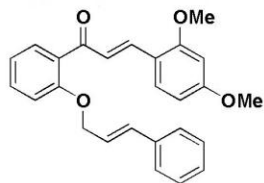
Compound 5n (^{1}H-NMR spectral data)

MC4NO2Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2019
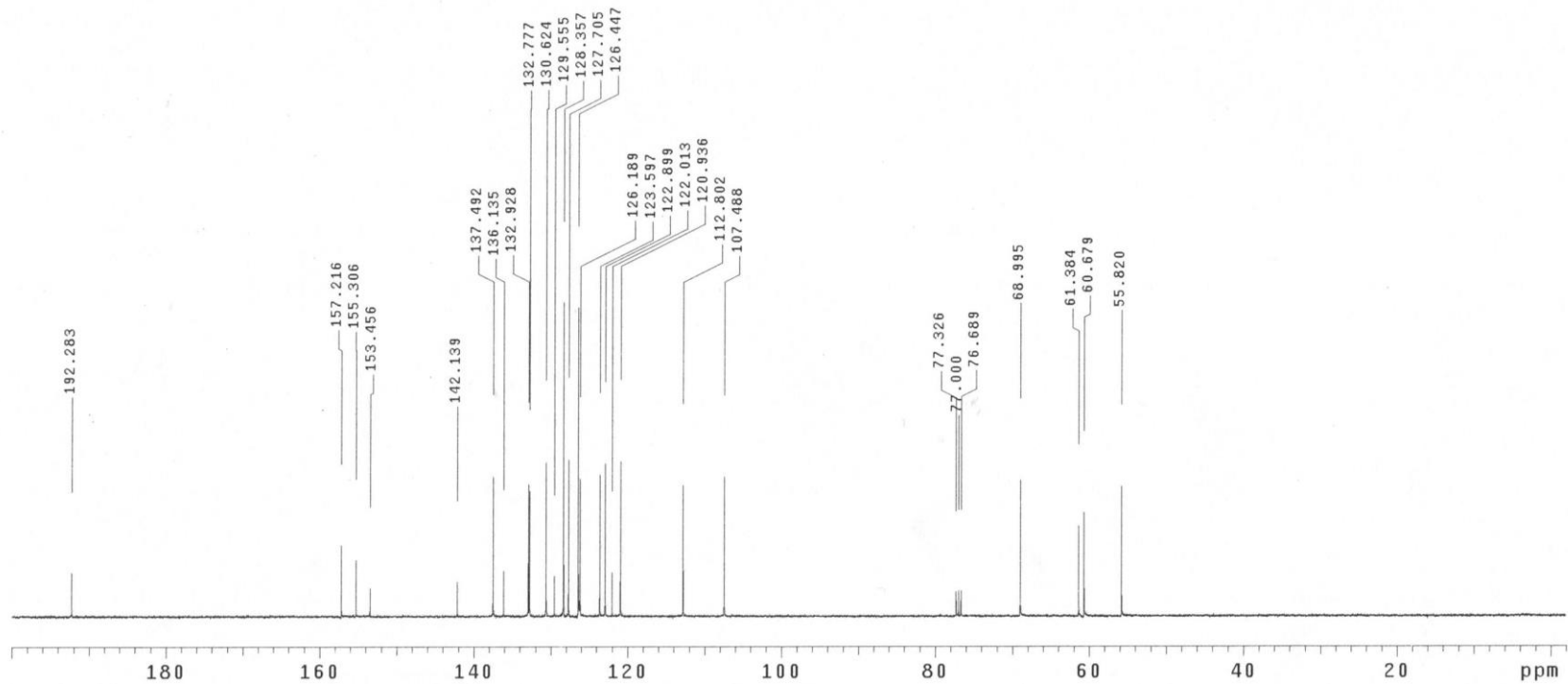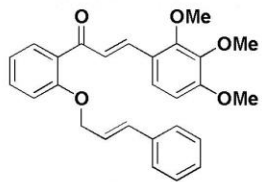Solvent: CDC13
Ambient temperature
Total 32 repetitions

Peaks: 7.931, 7.909, 7.751, 7.711, 7.667, 7.618, 7.596, 7.288, 7.281, 7.276, 7.275, 7.260, 7.092, 7.090, 7.073, 7.053, 6.445, 4.815, 4.811, 4.800, 4.796

Integrals: 18.99, 9.59, 17.81, 23.82, 11.10, 52.61, 22.05, 10.00, 10.43, 21.46
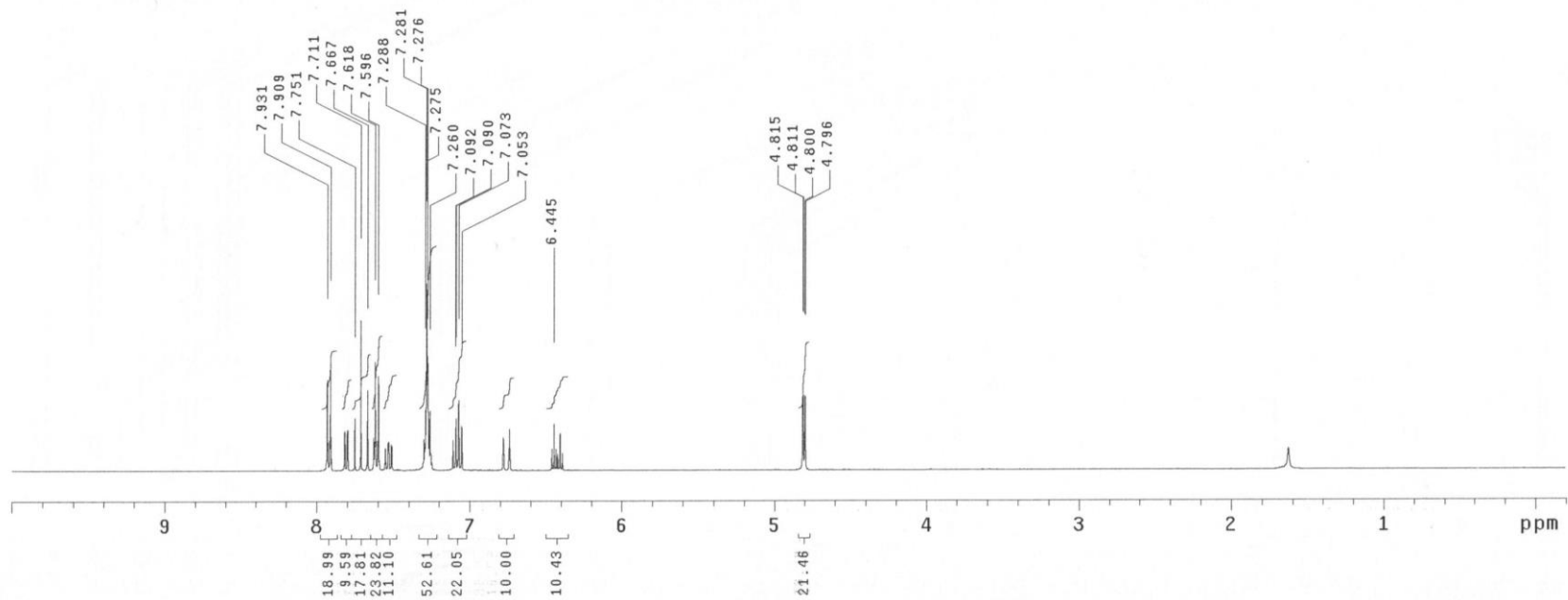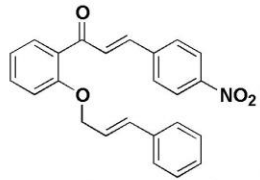
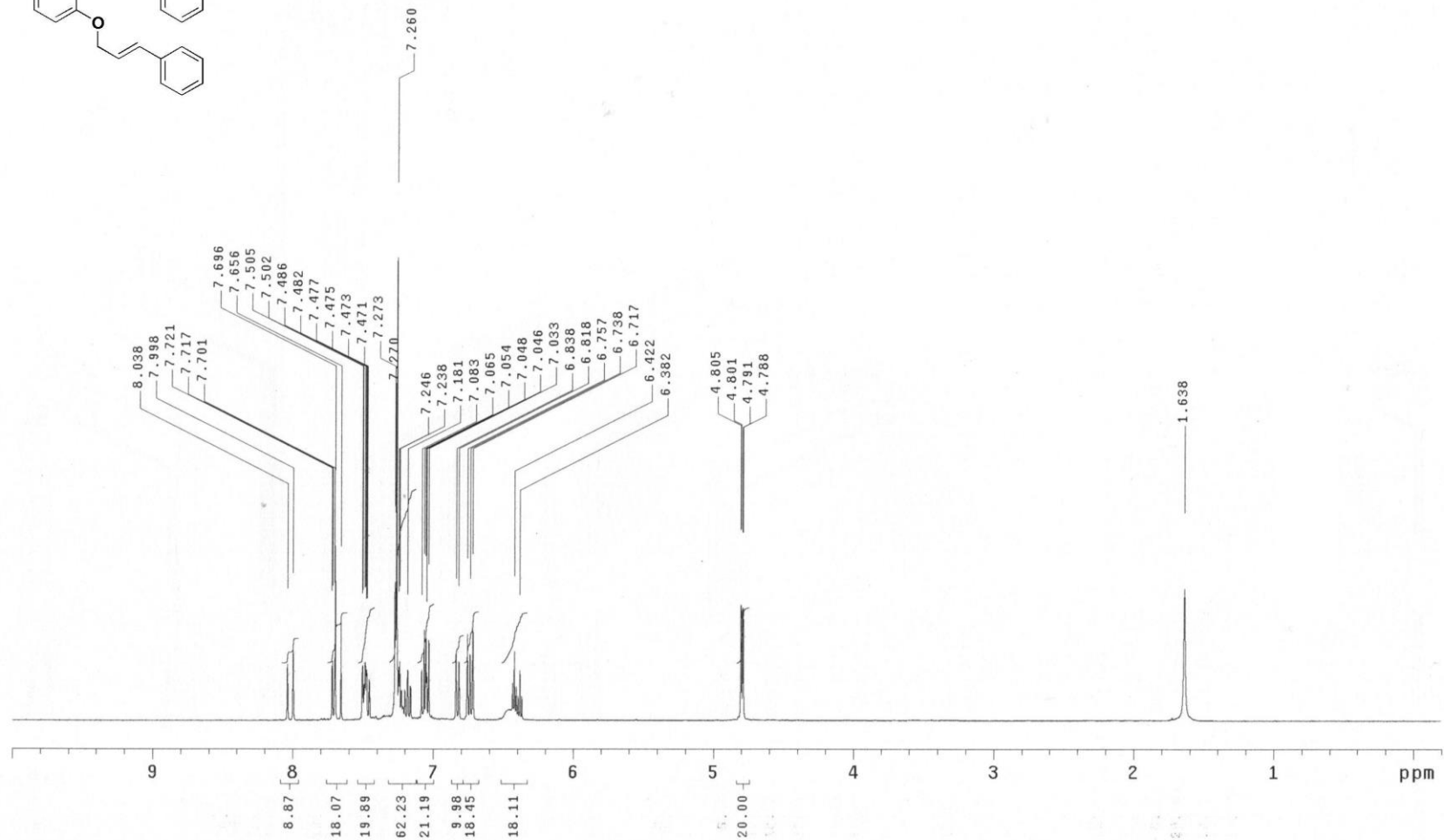# Compound 5n (¹³C-NMR spectral data)

MC4NO2Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2019
Solvent: CDCl3
Ambient temperature
Total 2048 repetitions

190.957
157.929
148.104
141.449
138.515
135.809
134.232
134.043
131.185
131.117
128.691
128.592
128.456
126.440
123.999
123.112
121.323
112.931
77.318
77.000
76.682
69.321

180   160   140   120   100   80   60   40   20   ppm
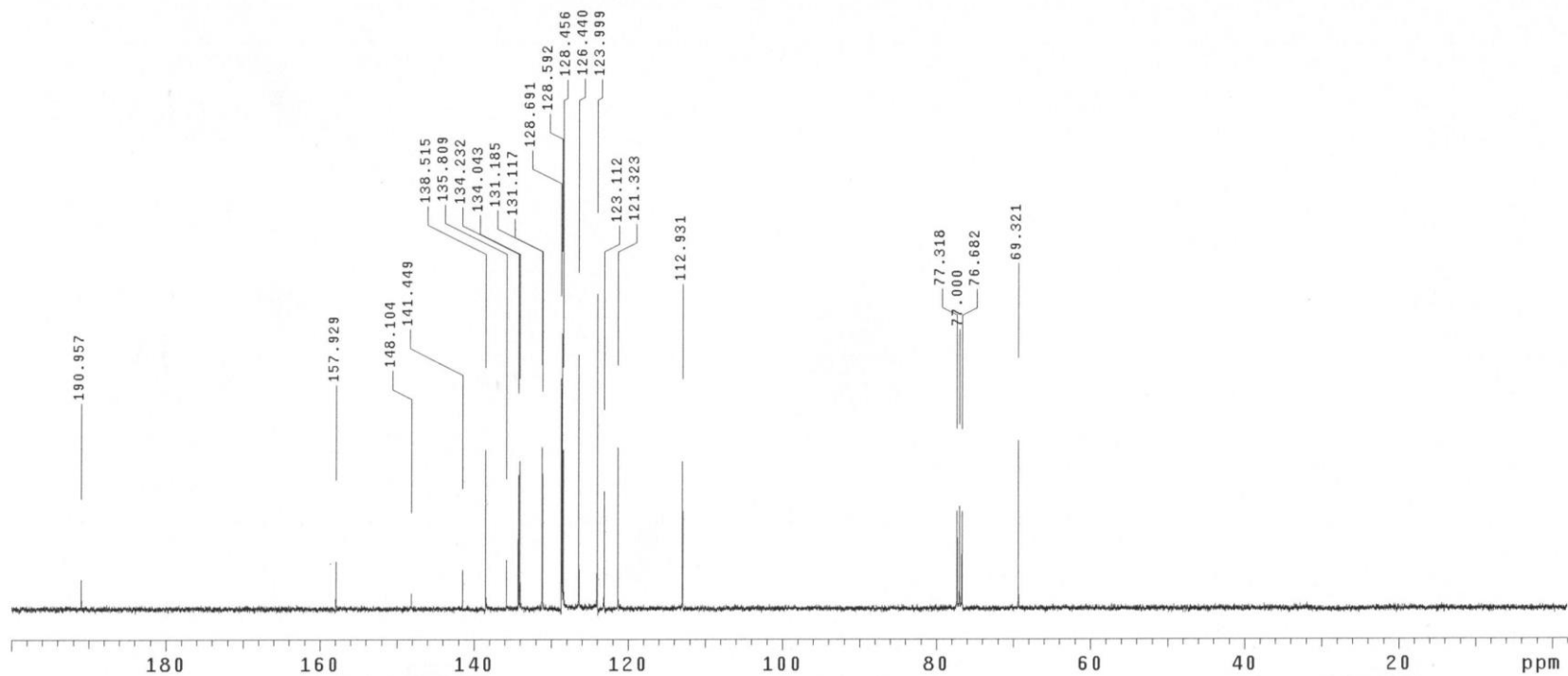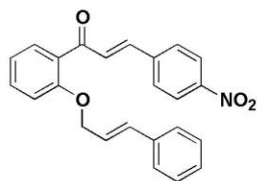
Compound 5o (¹H-NMR spectral data)

MC4PhAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
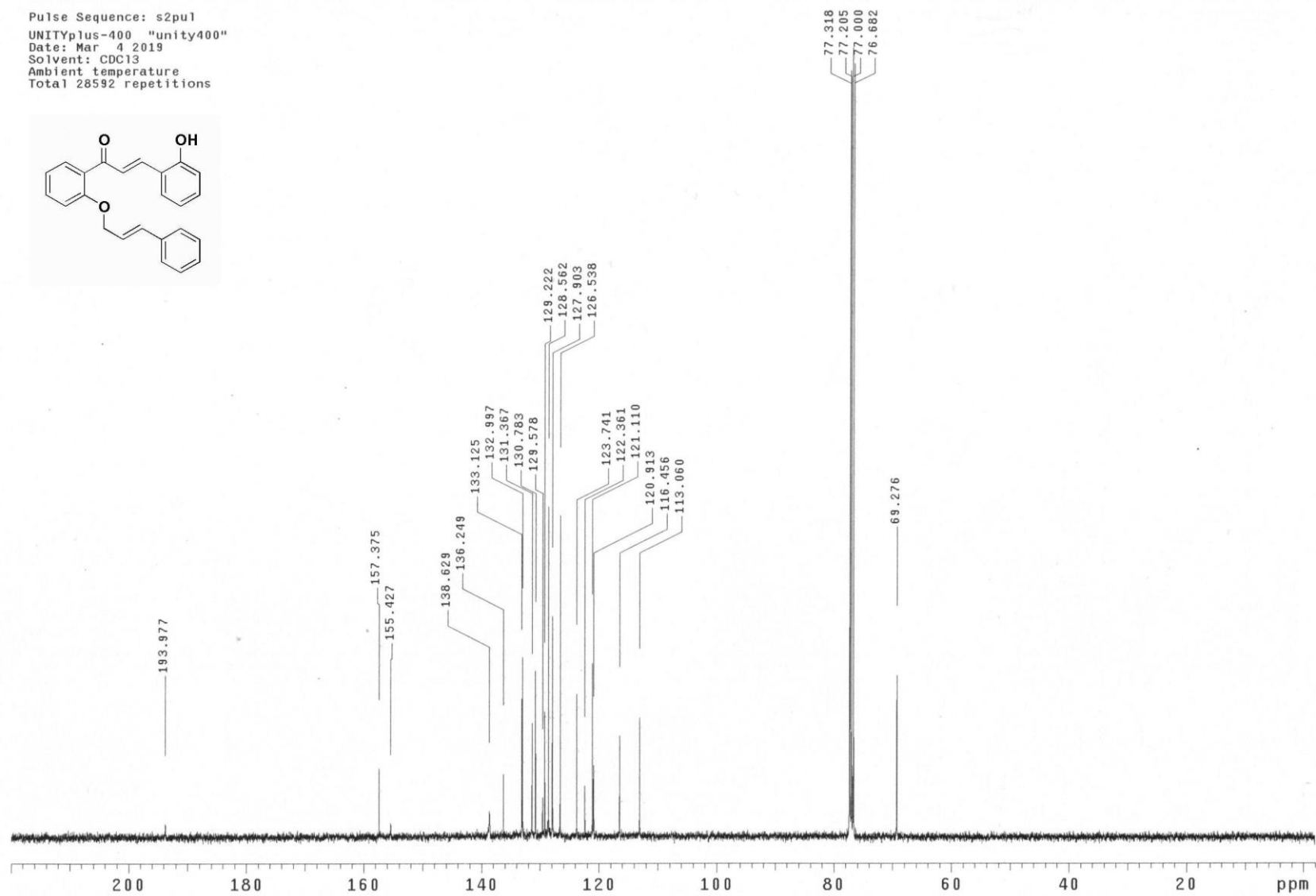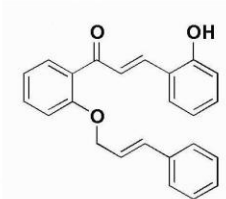Date: Apr 8 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.738
7.677
7.642
7.637
7.621
7.566
7.547
7.545
7.482
7.463
7.442
7.271
7.266
7.263
7.260
7.254
7.251
7.233
7.098
7.069
4.813
4.810
4.799
4.795

9   8   7   6   5   4   3   2   1   ppm

19.85
119.52
51.13
23.28
10.00
10.43
20.87
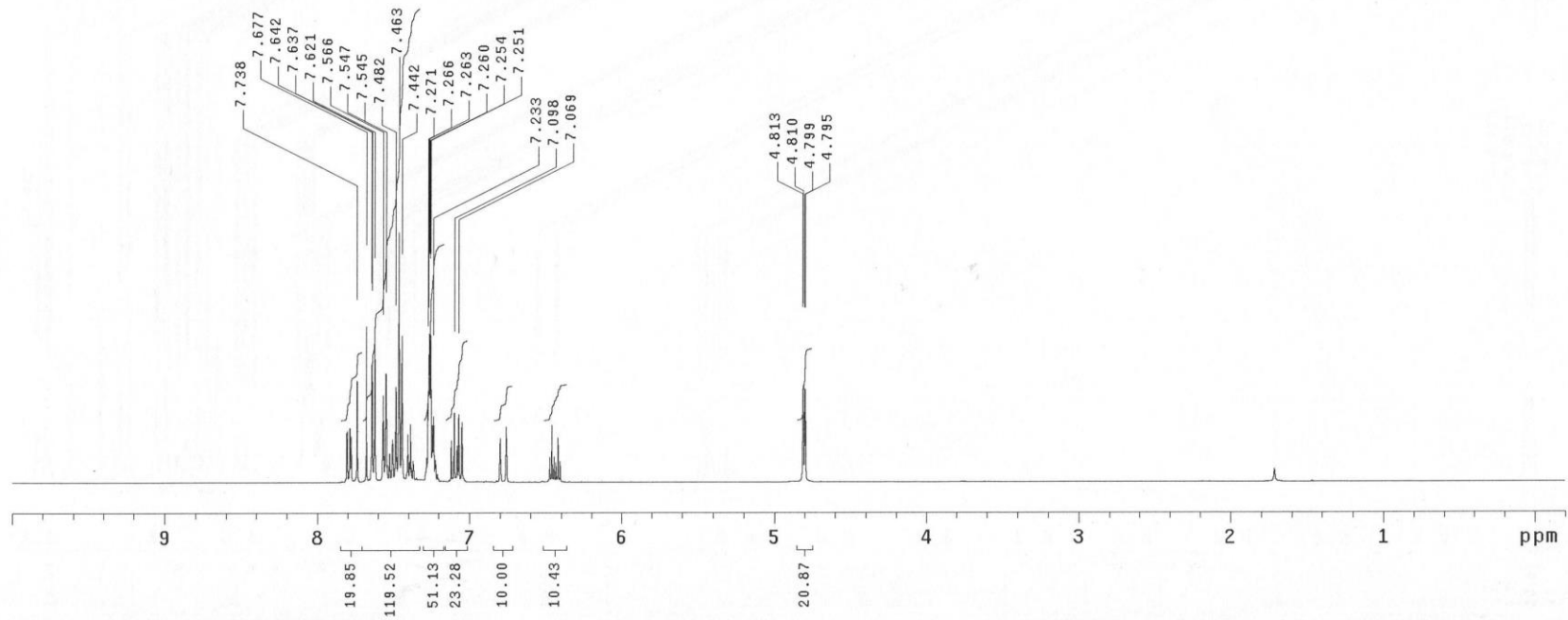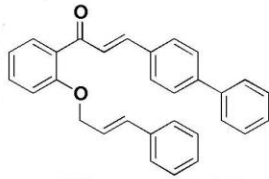
Compound 5o (^{13}C-NMR spectral data)

MC4PhAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 8 2019
Solvent: CDC13
Ambient temperature
Total 656 repetitions

192.003

157.474

142.677
141.979
140.062
136.089
134.065
133.285
133.171
130.844
129.328

128.805
128.767
128.501
127.903
127.683
127.387
127.160
126.902
126.523

123.476
121.110
112.931

77.318
77.000
76.682

69.139

180   160   140   120   100   80   60   40   20   ppm
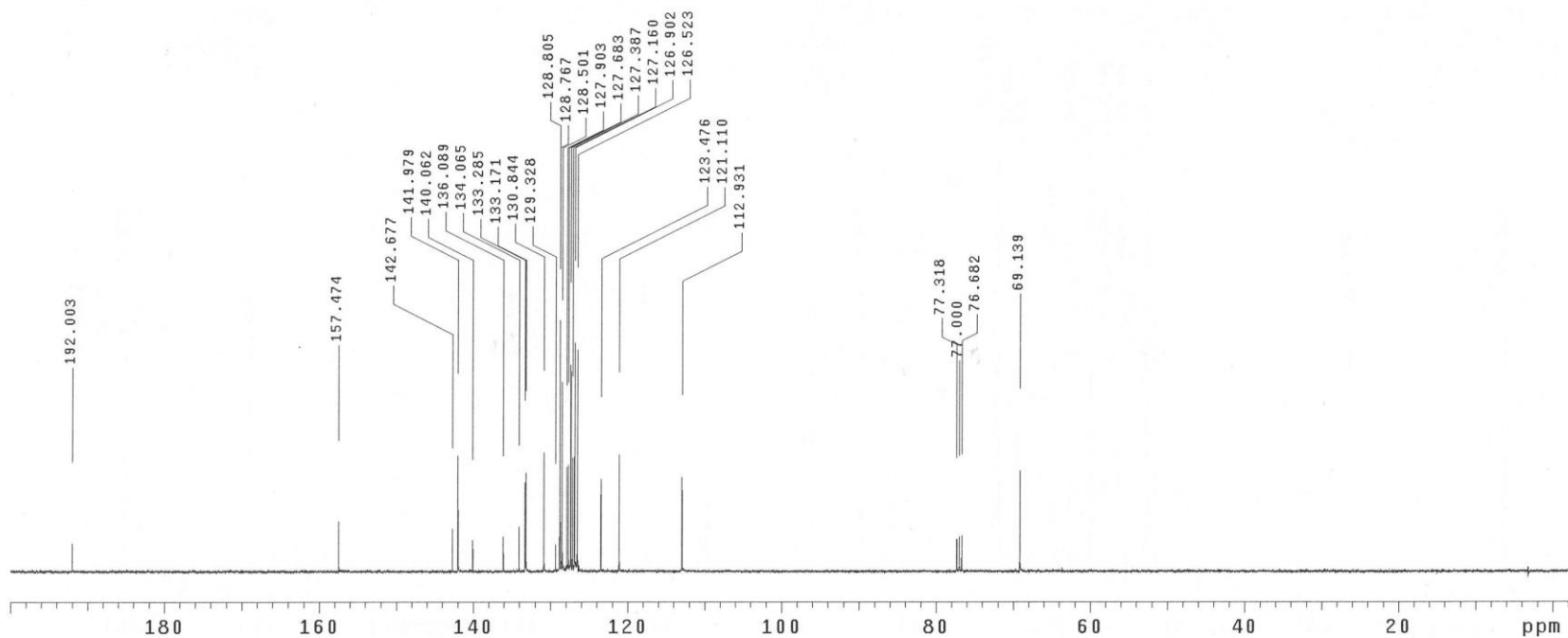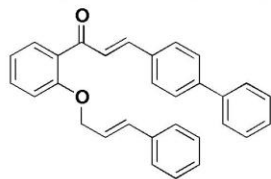
Compound 5p (¹H-NMR spectral data)

MC,3,4-2Cl-Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 25 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.601
7.596

7.540
7.331
7.326
7.272
7.268
7.265

7.260
7.250
7.244
7.195
7.174
7.075
7.059

4.805
4.801
4.791
4.787

8.77
9.18
28.97
14.02
57.62
21.47
10.42
10.00
20.13

9   8   7   6   5   4   3   2   1   ppm
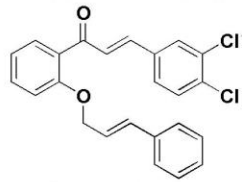
Compound 5p (^{13}C-NMR spectral data)

MC,3,4-2Cl-Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 25 2019
Solvent: CDC13
Ambient temperature
Total 1024 repetitions

191.555

157.603

139.258
135.945
135.278
133.785
133.588
133.558

133.110
130.935
130.791
129.934
128.949
128.888
128.585
128.138
126.917
126.455

123.248
121.247
112.992

77.318
77.000
76.682

69.245

180	160	140	120	100	80	60	40	20	ppm

Compound 5q (^{1}H-NMR spectral data)

MCNAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 23 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.957
7.836
7.768
7.765
7.752
7.710
7.670
7.608
7.502
7.500
7.484
7.479
7.195
7.191
7.177
7.155
7.141
7.096
7.094
7.070
4.812
4.809
4.798
4.794

9   8   7   6   5   4   3   2   1   ppm

10.61
11.21
49.08
10.84
30.59
67.19
9.36
9.89
20.00

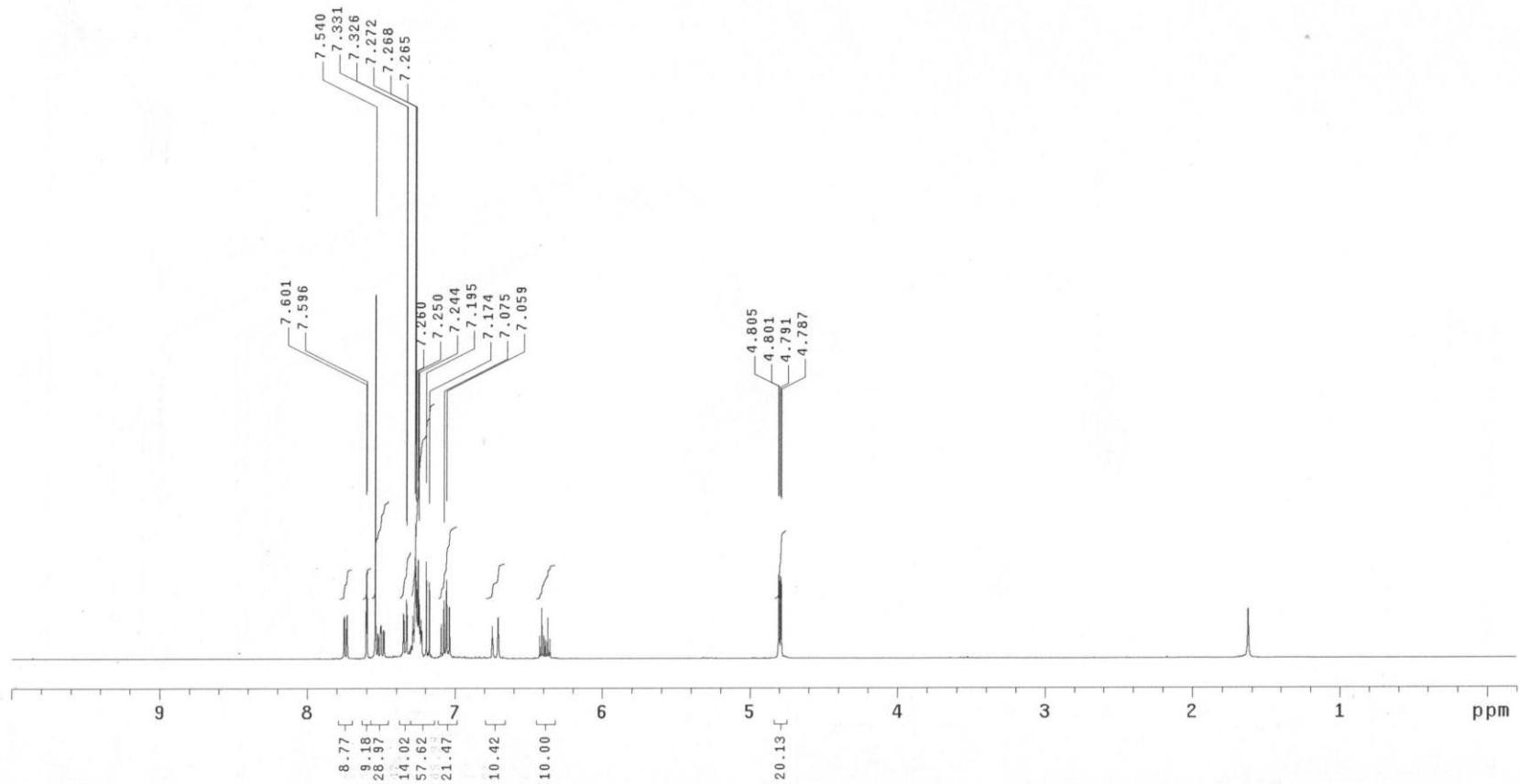# Compound 5q (^{13}C-NMR spectral data)

MCNAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 23 2019
Solvent: CDCl3
Ambient temperature
Total 576 repetitions

192.276
157.428
142.722
136.052
134.156
133.300
133.201
133.133
132.671
130.813
130.321
129.441
128.653
128.509
128.448
127.857
127.675
127.546
127.046
126.530
126.470
123.658
123.491
121.141
112.977
77.318
77.000
76.682
69.200

Compound 5r (^{1}H-NMR spectral data)

MC20 Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
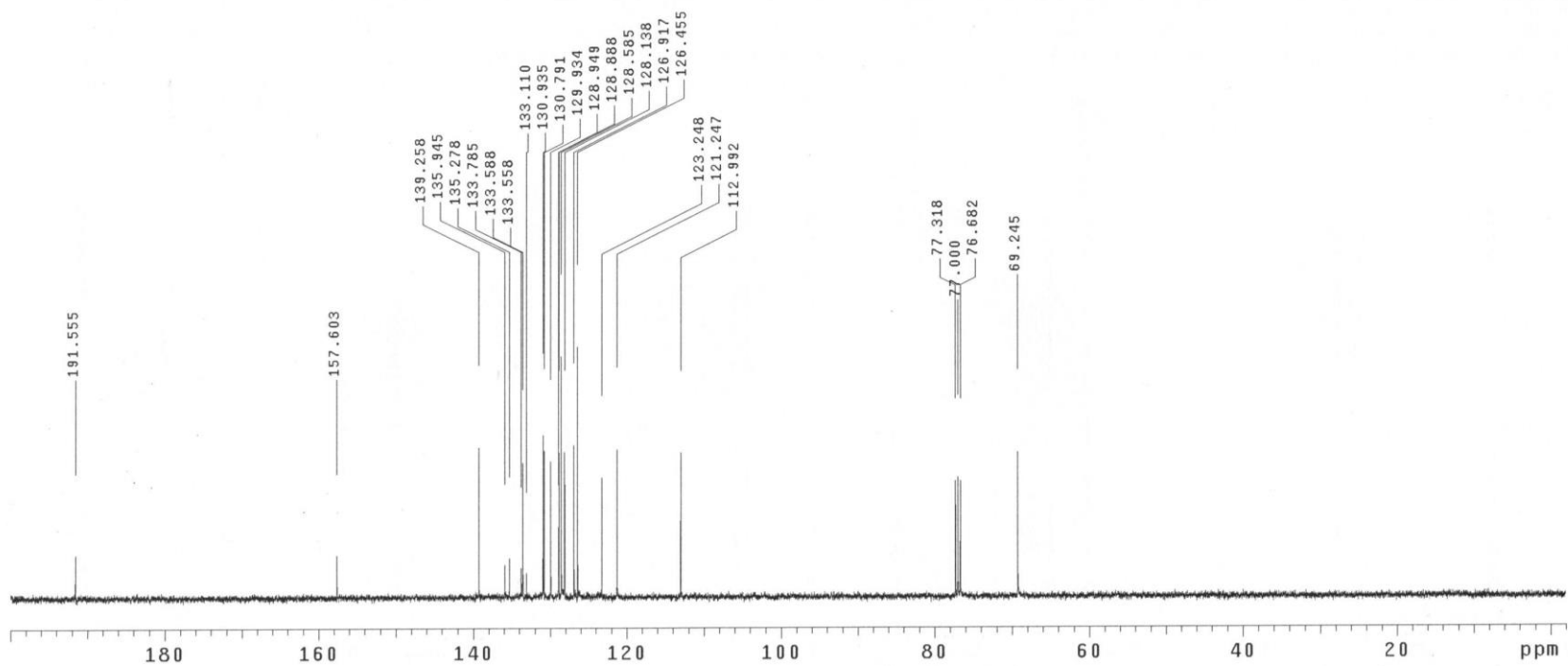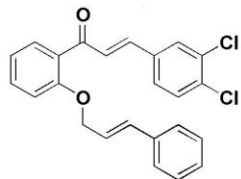Date: Apr 18 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.756
7.752
7.738
7.733
7.515
7.512
7.295
7.294
7.290
7.287
7.283
7.275
7.054
7.051
7.018
6.998
6.747
6.644
6.642
6.635
6.424
6.420
6.416
6.411
4.766
4.753

9.00
16.85
10.85
56.21
20.12
9.46
9.03
18.48
20.00

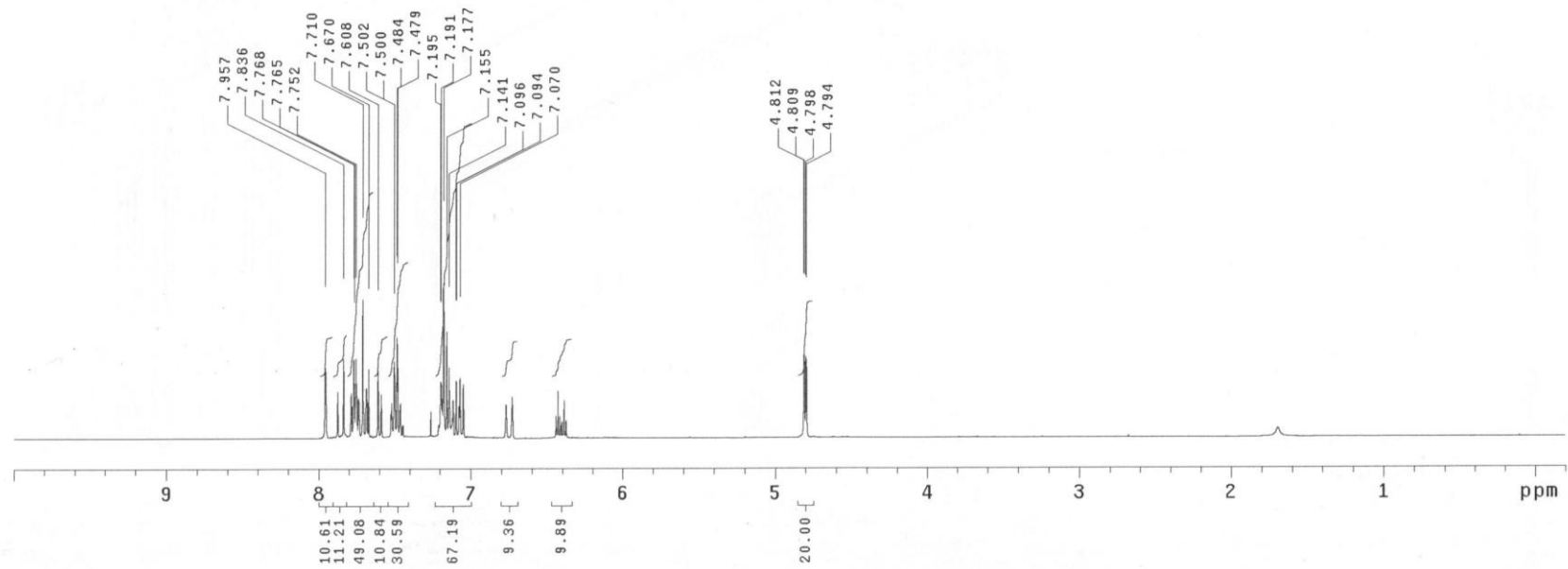# Compound 5r (^{13}C-NMR spectral data)

MC20 Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 18 2019
Solvent: CDC13
Ambient temperature
Total 752 repetitions

Peak labels: 191.578, 157.262, 151.531, 144.549, 136.173, 132.936, 132.519, 130.503, 129.206, 128.698, 128.327, 127.614, 126.295, 124.681, 123.460, 120.860, 115.418, 112.886, 112.264, 68.889

x-axis: 180 160 140 120 100 80 60 40 20 ppm
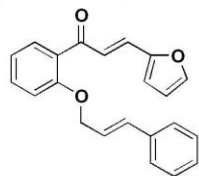
Compound 5s (^{1}H-NMR spectral data)

MC2Saldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2019
Solvent: CDCl3
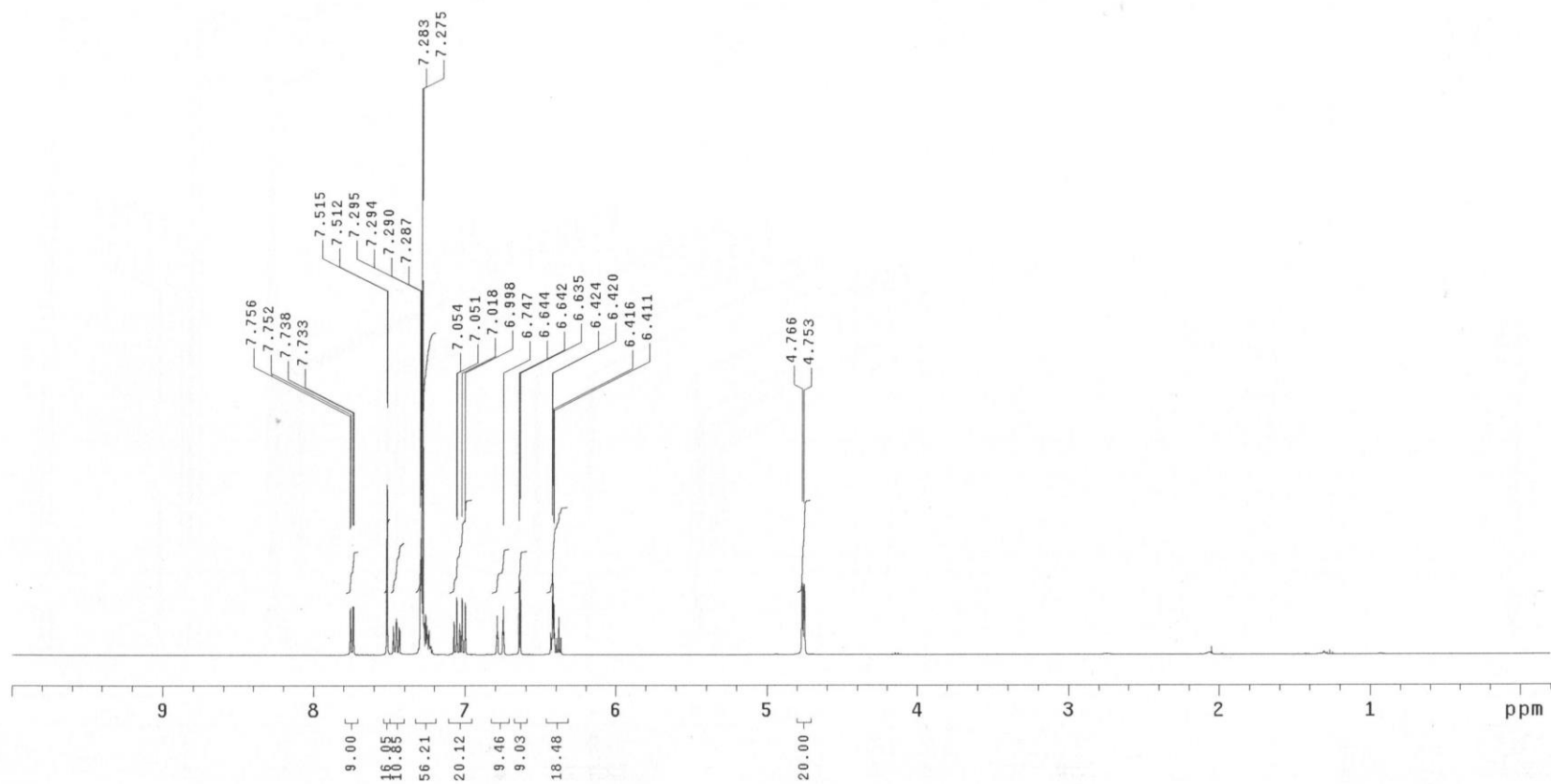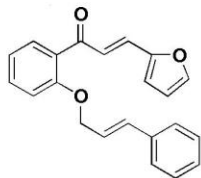Ambient temperature
Total 32 repetitions

7.276
7.267

7.287
7.285

7.847
7.808
7.749
7.744
7.729
7.725
7.475
7.474
7.433
7.394

7.265
7.258
7.252
7.250
7.083
7.065
7.043
7.022
7.012
7.003
7.000
6.991
6.775
6.735
6.442
6.402

4.796
4.792
4.782
4.778

9.19
9.30

20.36

68.46

31.19

10.00

10.27

21.12

9   8   7   6   5   4   3   2   1   ppm

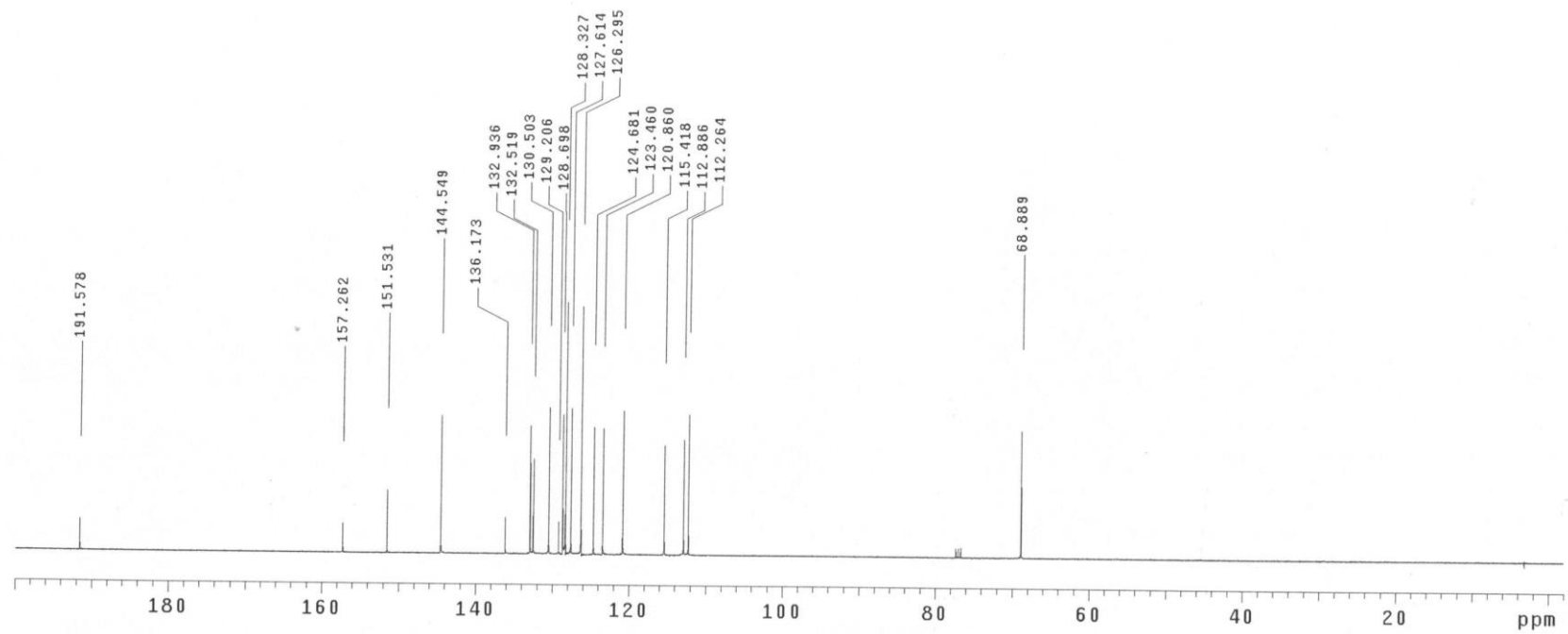# Compound 5s (^{13}C-NMR spectral data)

MC2Saldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2019
Solvent: CDC13
Ambient temperature
Total 256 repetitions

191.555

157.345

140.569
136.188
134.968
133.072
133.019
131.321
130.677

129.222
128.410
128.274
128.092
127.781
126.493

126.250
123.529
121.020
112.886

77.318
77.000
76.689

69.094

180   160   140   120   100   80   60   40   20   ppm

Compound 5t (^{1}H-NMR spectral data)

MC2-FAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
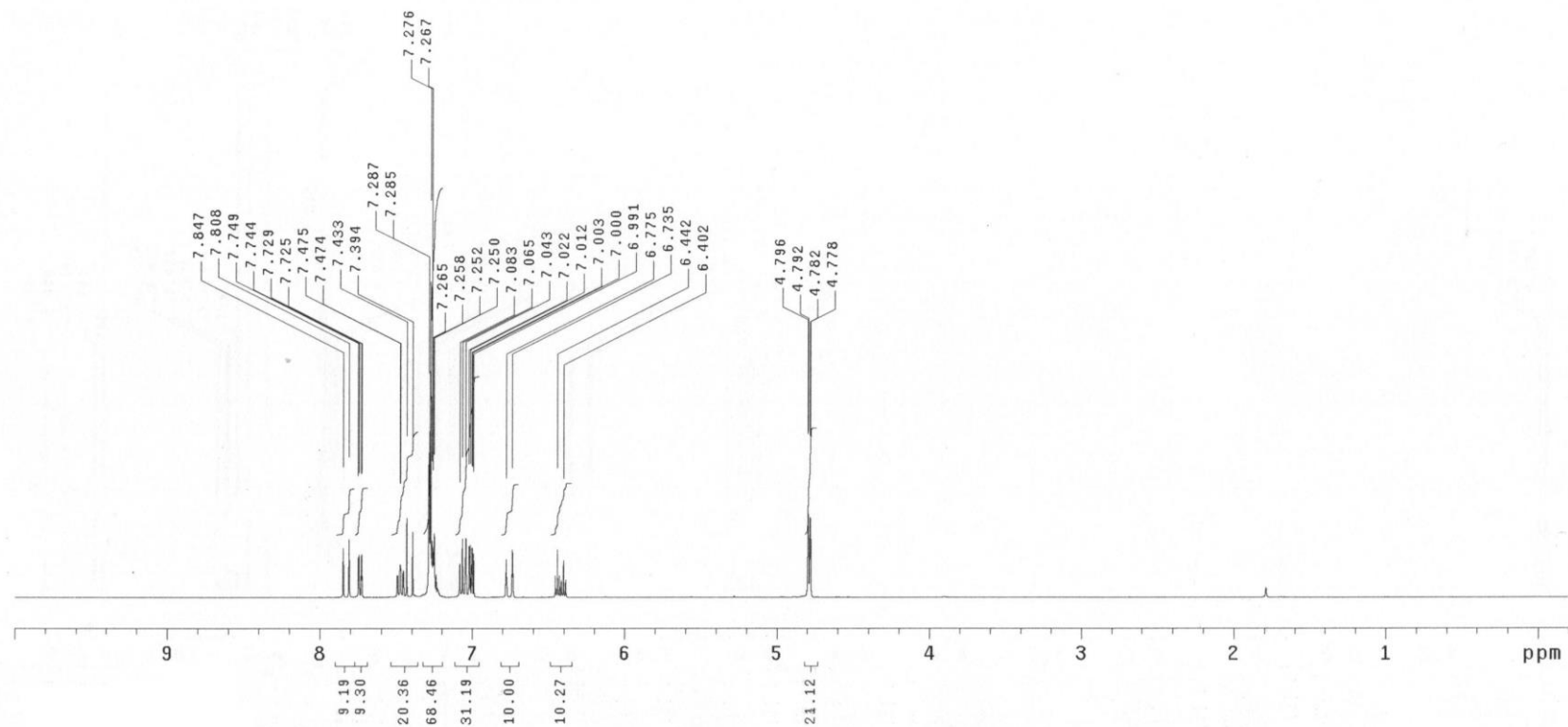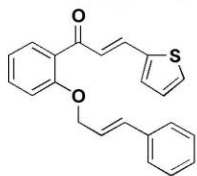Date: Mar 28 2019
Solvent: CDCl3
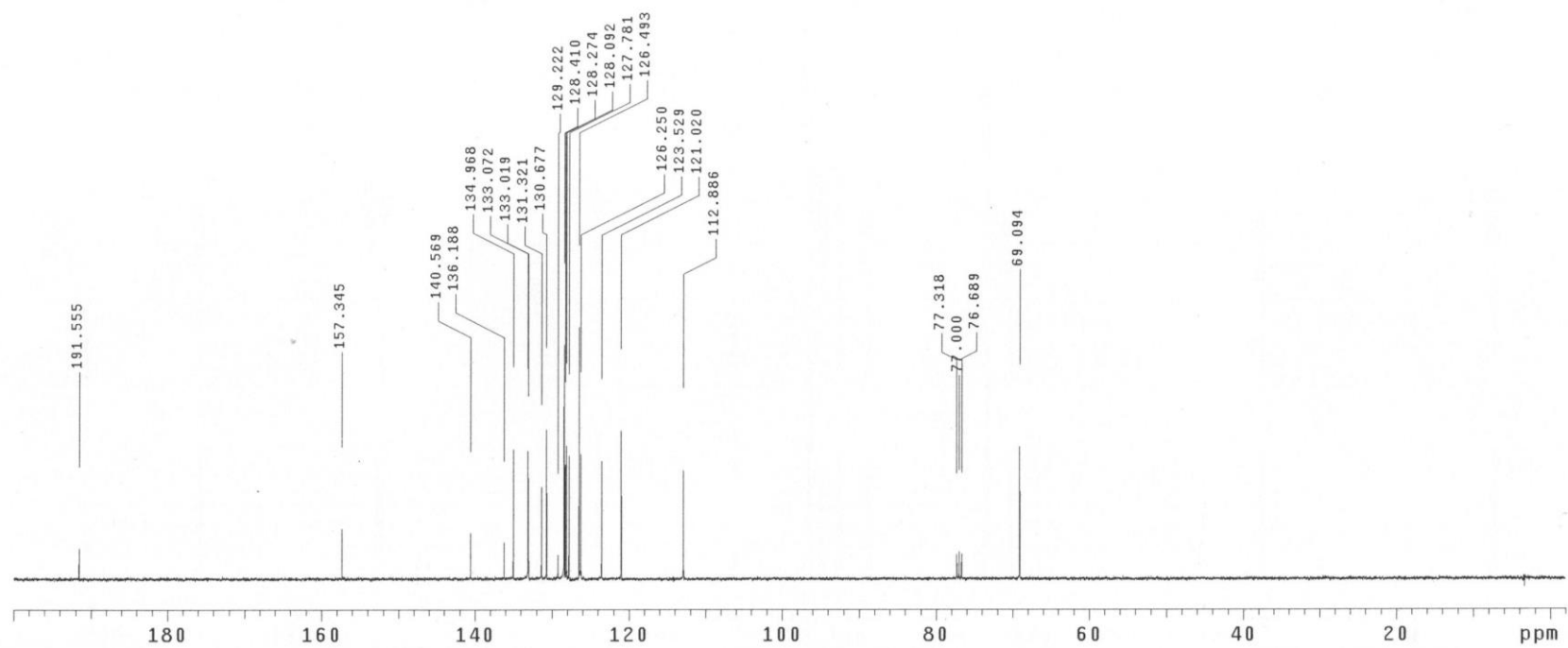Ambient temperature
Total 32 repetitions

Peaks: 7.917, 7.877, 7.813, 7.809, 7.794, 7.790, 7.736, 7.696, 7.552, 7.548, 7.470, 7.469, 7.273, 7.269, 7.261, 7.251, 7.246, 7.080, 7.063, 7.062, 7.020, 6.999, 6.908, 6.907, 6.745, 6.705, 6.410, 6.371, 4.739, 4.736, 4.725, 4.722

Integrations: 9.67, 9.78, 10.00, 10.56, 10.58, 60.73, 30.84, 10.32, 10.02, 10.38, 20.83

ppm scale: 9 8 7 6 5 4 3 2 1

S-62
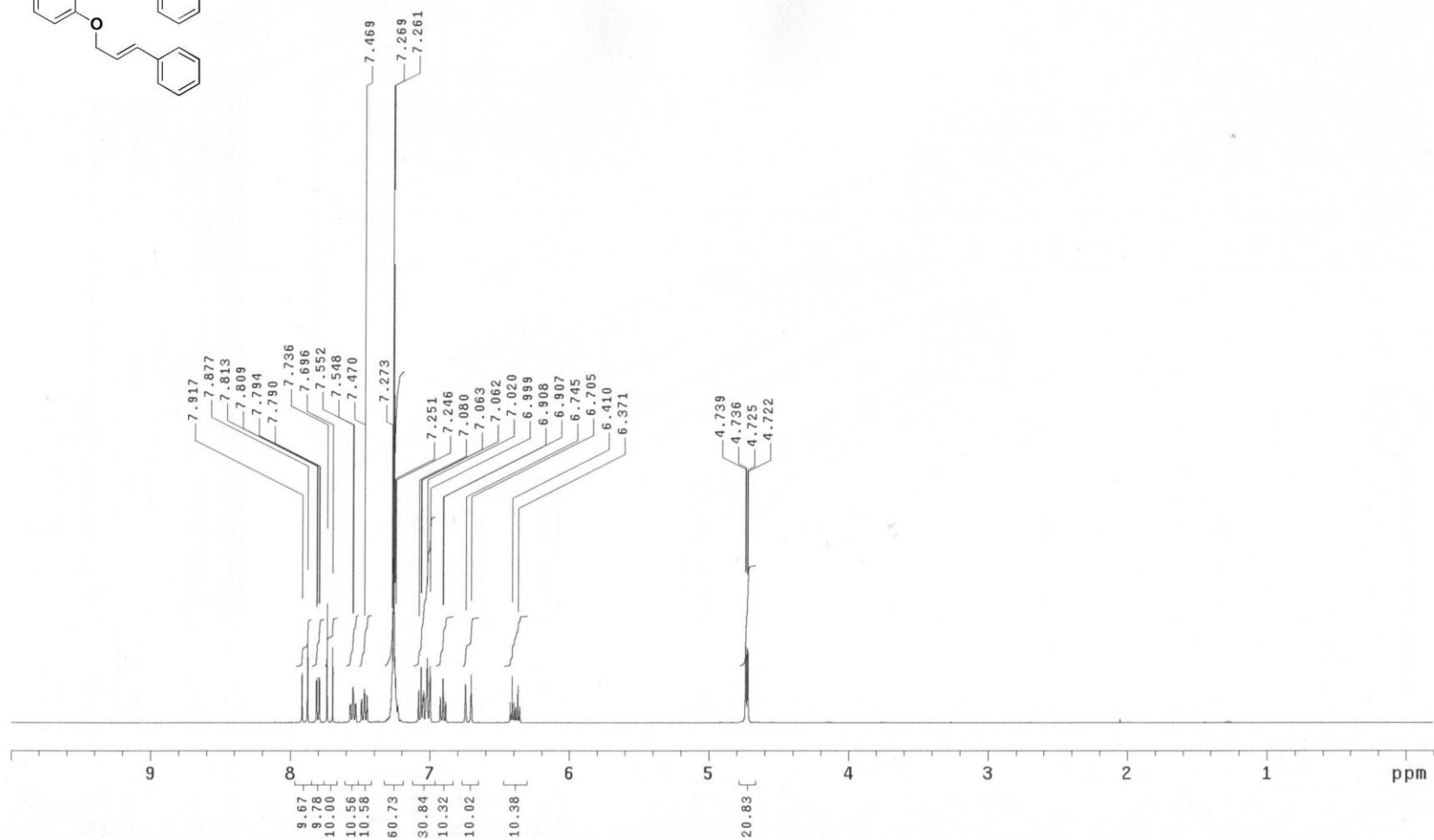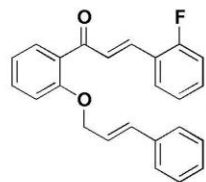
Compound 5t (^{13}C-NMR spectral data)

MC2-FAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 28 2019
Solvent: CDCl3
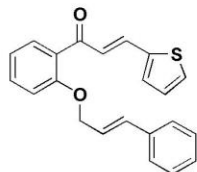Ambient temperature
Total 352 repetitions

191.639
162.553
160.028
157.368
135.915
134.391
134.361
133.209
132.989
131.268
131.185
130.647
129.229
129.168
128.805
128.782
128.752
127.675
126.273
124.218
124.188
123.233
122.968
122.854
120.845
115.910
115.690
112.719
77.318
77.000
76.682
68.889
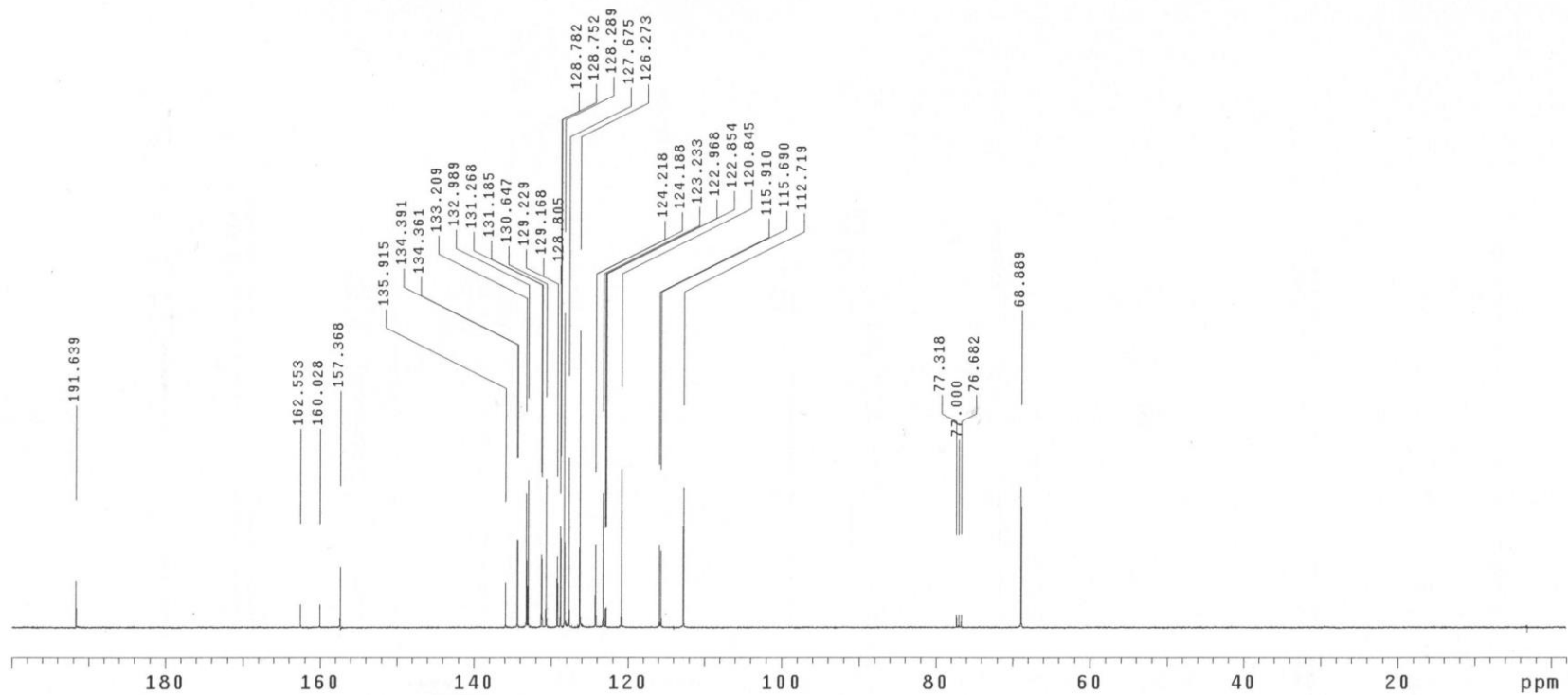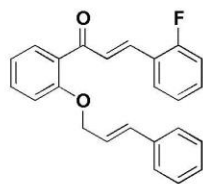
Compound 5u (¹H-NMR spectral data)

MC3NAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 23 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.732
8.727
8.488
8.484
8.476
8.472
7.748
7.743
7.728
7.724
7.625
7.623
7.250
7.238
7.234
7.227
7.224
7.066
7.050
7.048
7.031
7.029
7.010
6.687
6.386
6.346
4.769
4.766
4.755
4.752

9 8 7 6 5 4 3 2 1 ppm

10.00
9.61
20.41
20.00
11.11
52.65
32.63
10.42
10.86
21.97

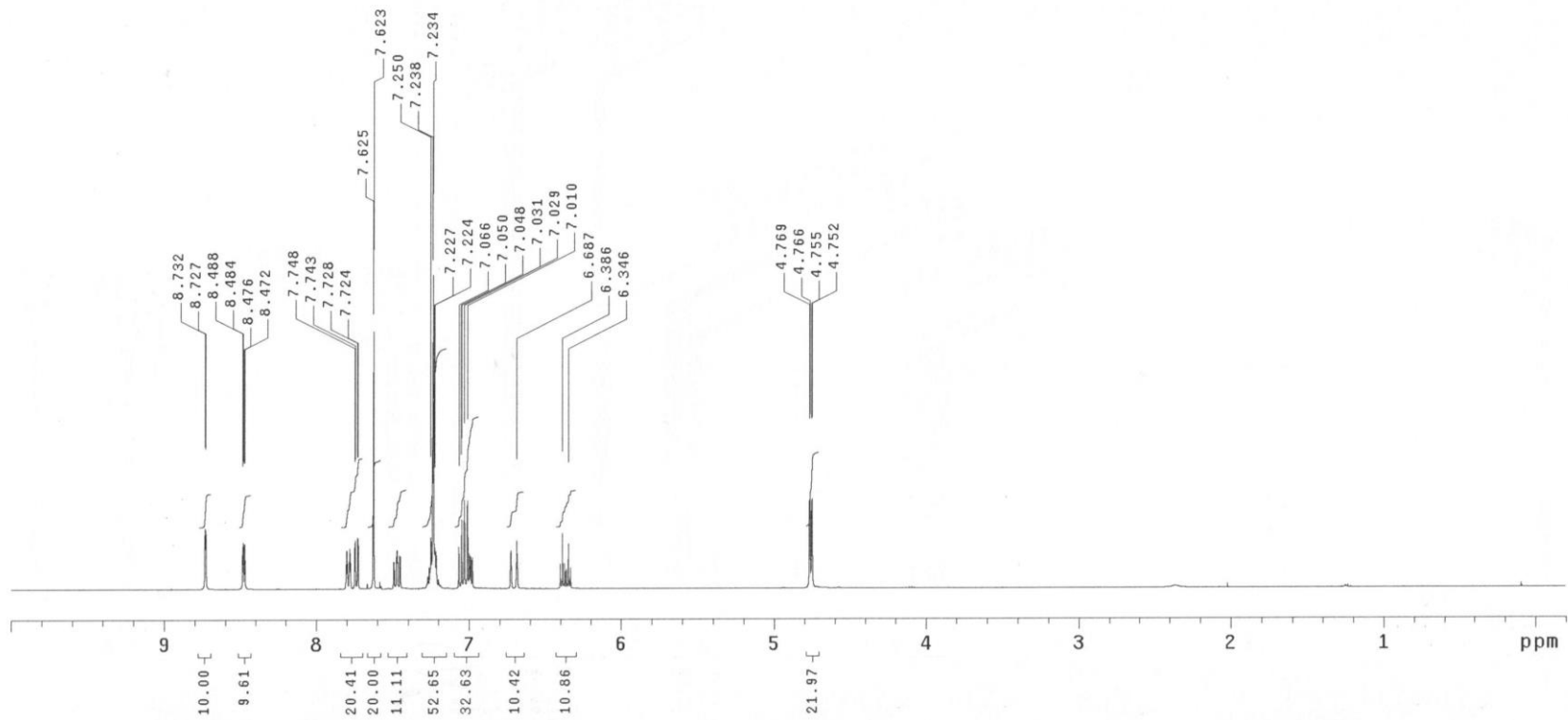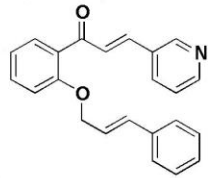# Compound 5u (^{13}C-NMR spectral data)

MC3NAldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
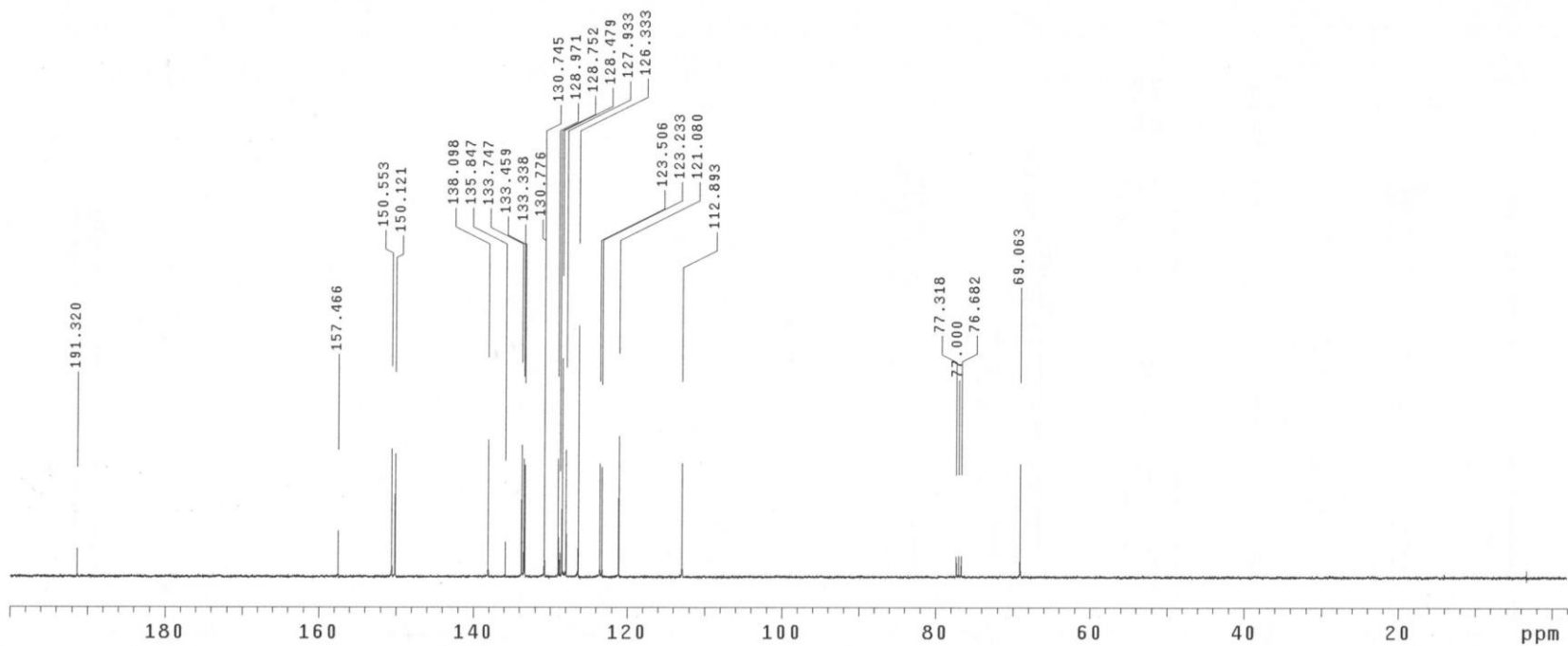Date: Apr 23 2019
Solvent: CDCl3
Ambient temperature
Total 240 repetitions

191.320

157.466

150.553
150.121

138.098
135.847
133.747
133.459
133.338
130.776

130.745
128.971
128.752
128.479
127.933
126.333

123.506
123.233
121.080
112.893

77.318
77.000
76.682

69.063

180   160   140   120   100   80   60   40   20   ppm

Compound 5v (^{1}H-NMR spectral data)

MC3,4-2OMe Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
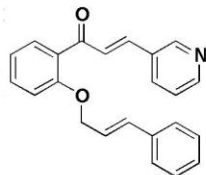Date: Apr 18 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

3.852
3.791

7.651
7.636
7.631
7.559
7.519
7.391
7.386
7.371
7.367
7.290
7.251
7.238
7.228
7.220
7.040
7.023
7.019
7.008
6.998
6.993
6.794
6.772

5.511
5.473
5.470

4.924

9.76
10.17
30.79
33.33
40.68
10.33

20.34

20.28

31.42
30.06

9   8   7   6   5   4   3   2   1   ppm
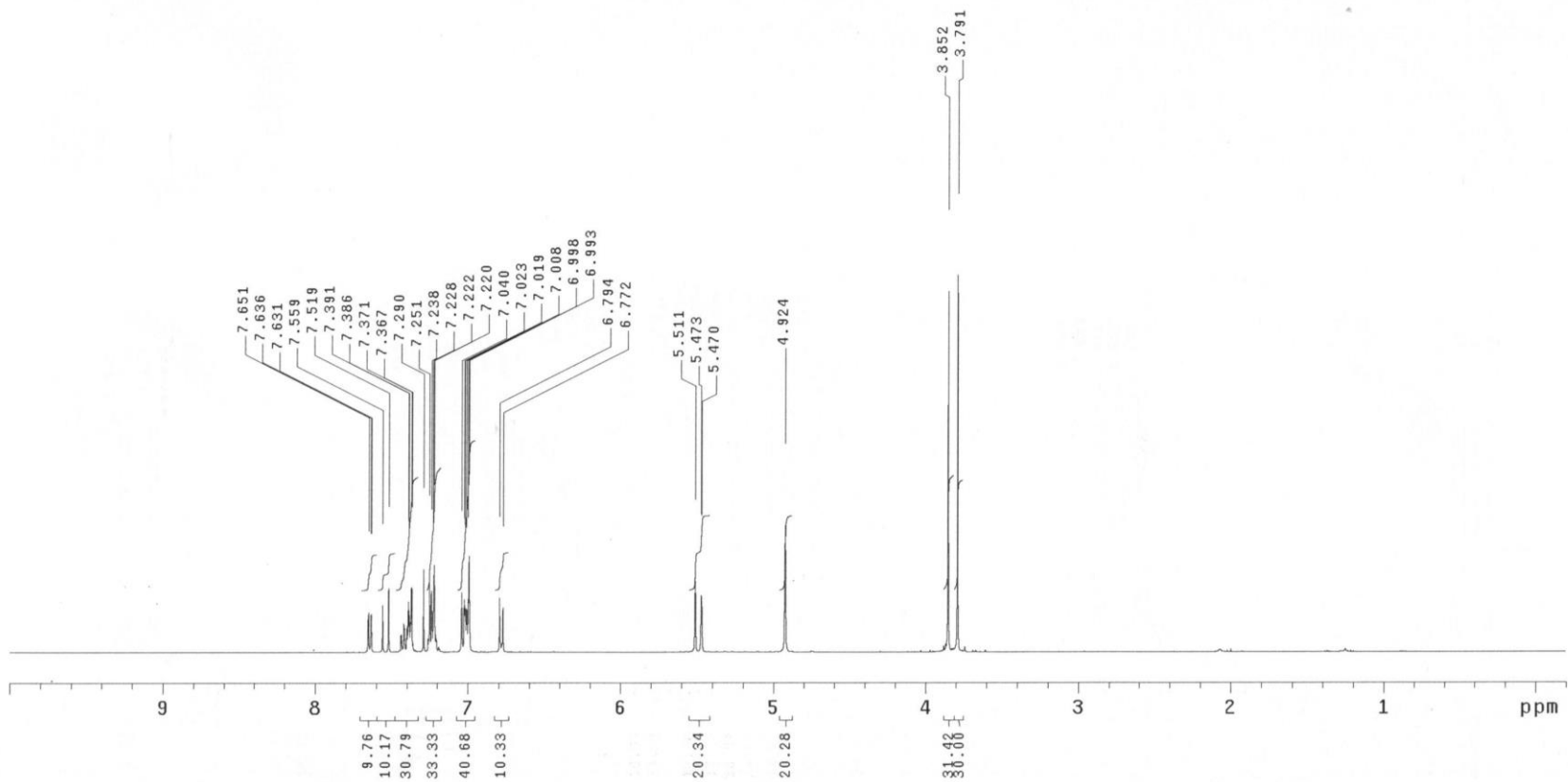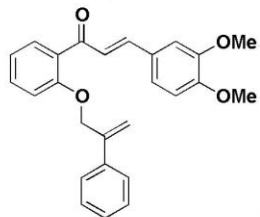
Compound 5v (^{13}C-NMR spectral data)

MC3,4-2OMe Aldol

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Apr 18 2019
Solvent: CDCl3
Ambient temperature
Total 720 repetitions

192.215
156.716
150.818
148.764
142.927
142.336
137.750
132.451
130.215
129.631
128.198
127.766
127.698
125.568
124.848
122.710
120.906
114.432
112.772
110.763
109.899
70.011
55.616
55.479

180 160 140 120 100 80 60 40 20 ppm

Compound 5w (^{1}H-NMR spectral data)

MC4-NO2Aldol

Pulse Sequence: s2pul

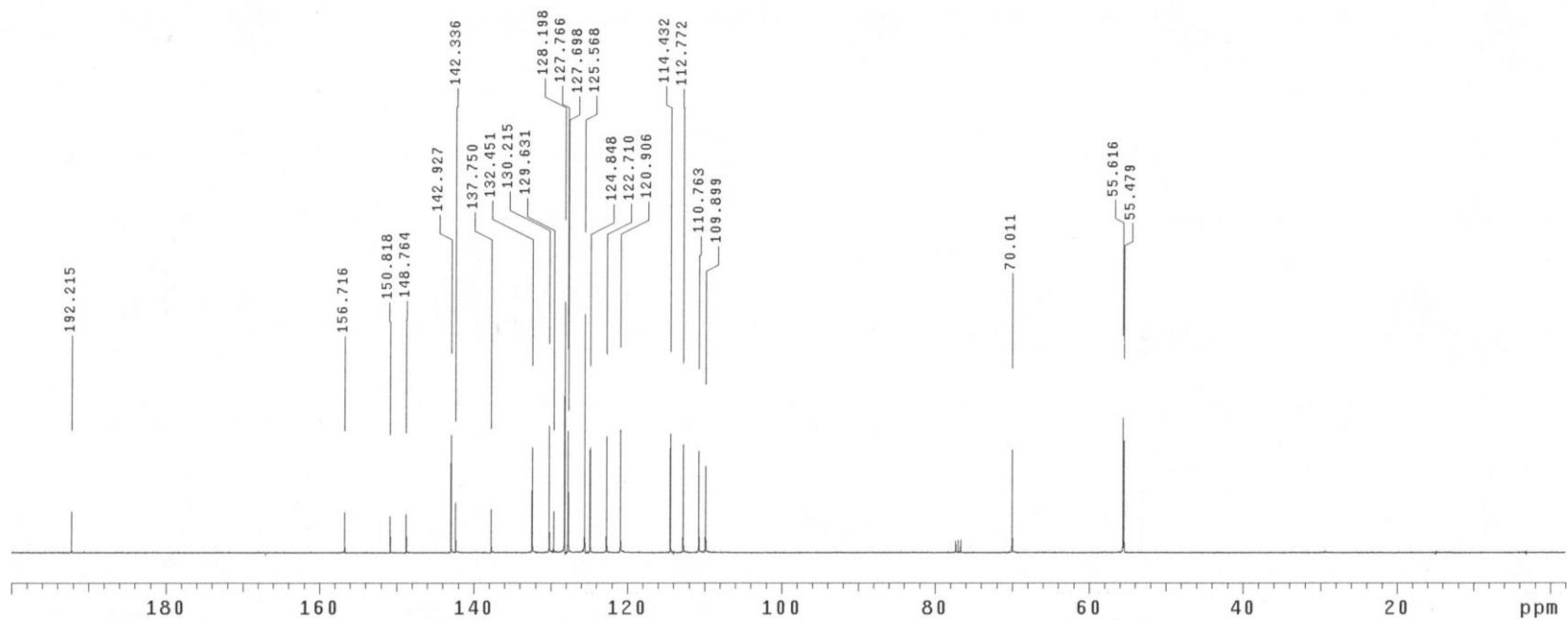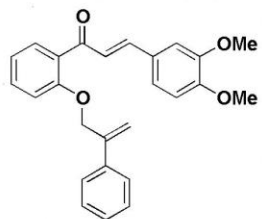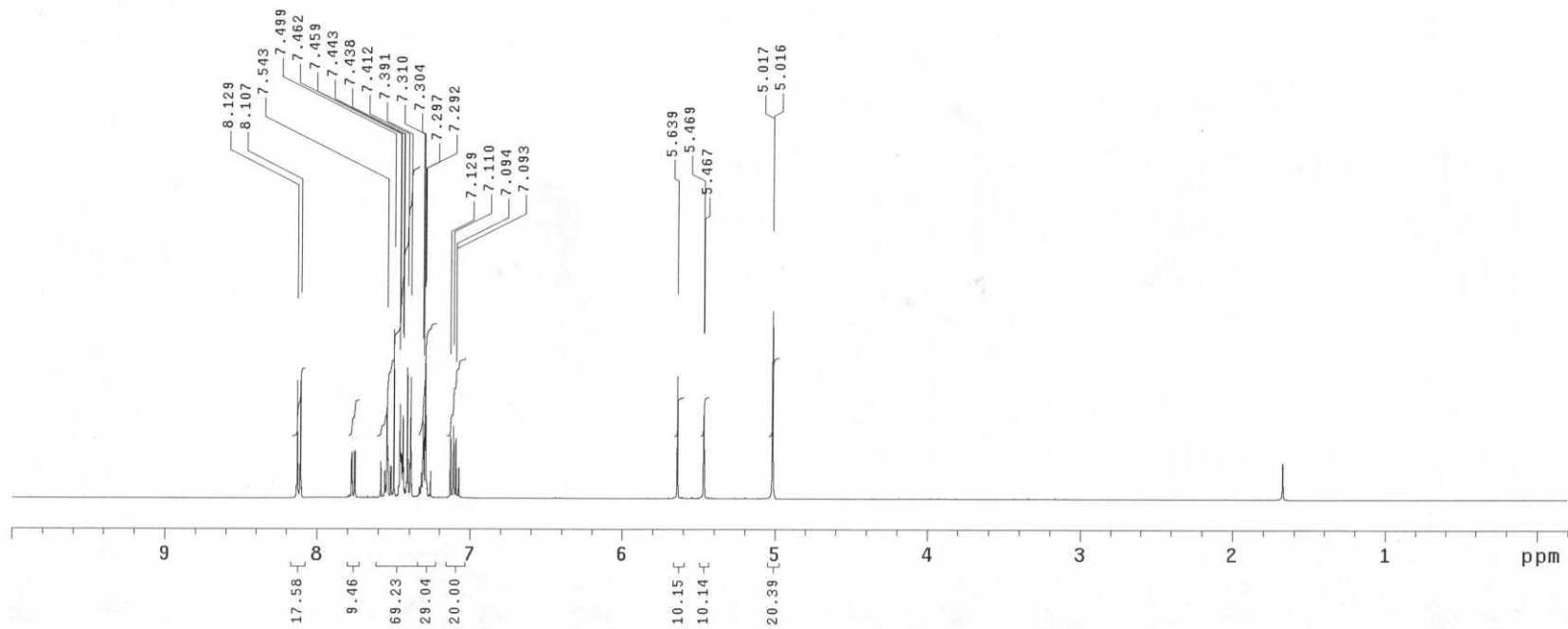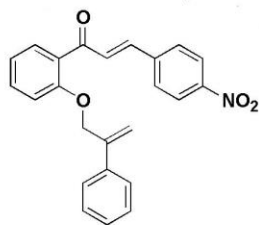UNITYplus-400 "unity400"
Date: Apr 8 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

Compound 5w (^{13}C-NMR spectral data)

MC4-NO2Aldol

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 8 2019
Solvent: CDCl3
Ambient temperature
Total 512 repetitions

191.085

157.618

148.066

142.176
141.373

138.796
137.515
133.884
131.162
130.525

128.714
128.600
128.251
125.727
123.877

121.376

115.933
112.780

77.318
77.000
76.682

70.625

180   160   140   120   100   80   60   40   20   ppm

Compound 5x (^{1}H-NMR spectral data)

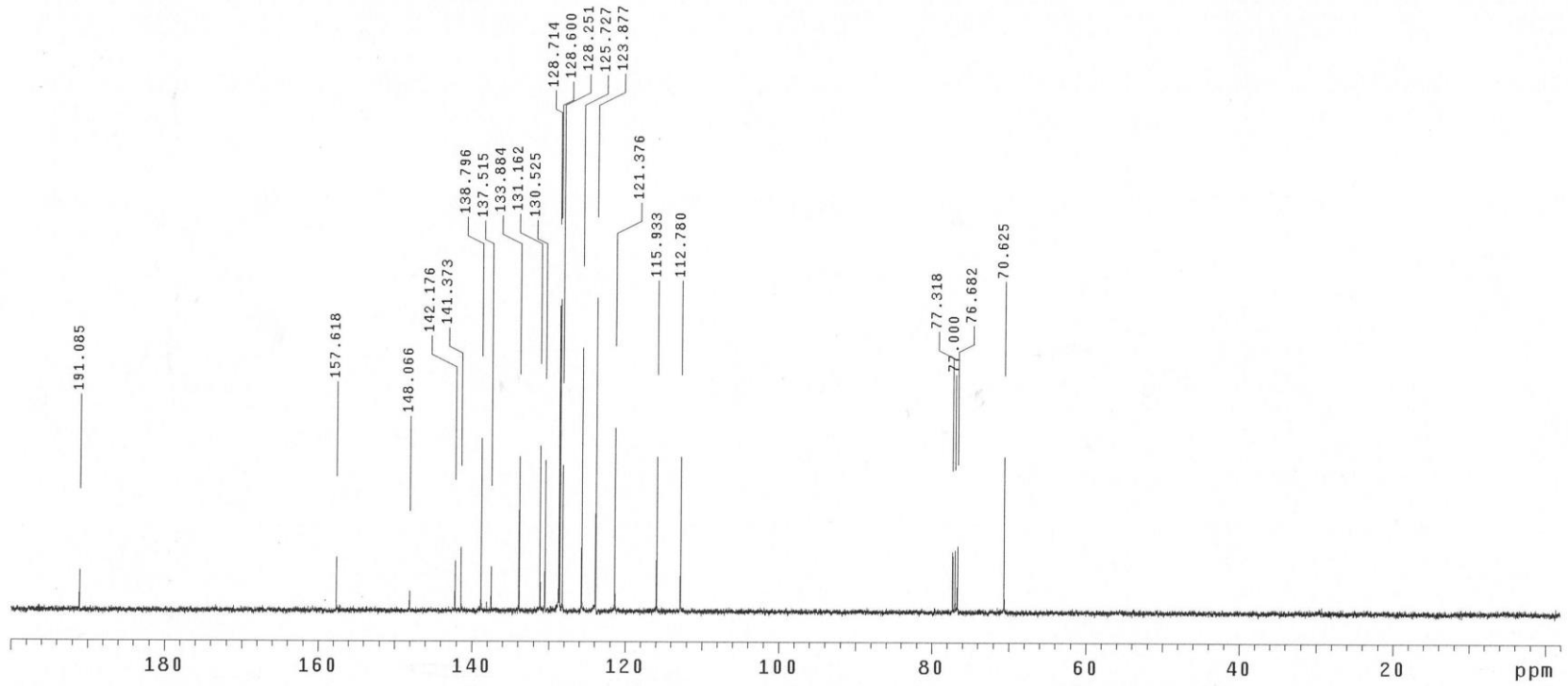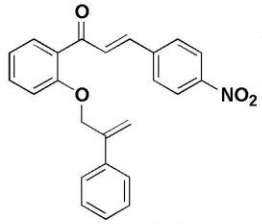MC1080423

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 23 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 5x (^{13}C-NMR spectral data)

MC1080423

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
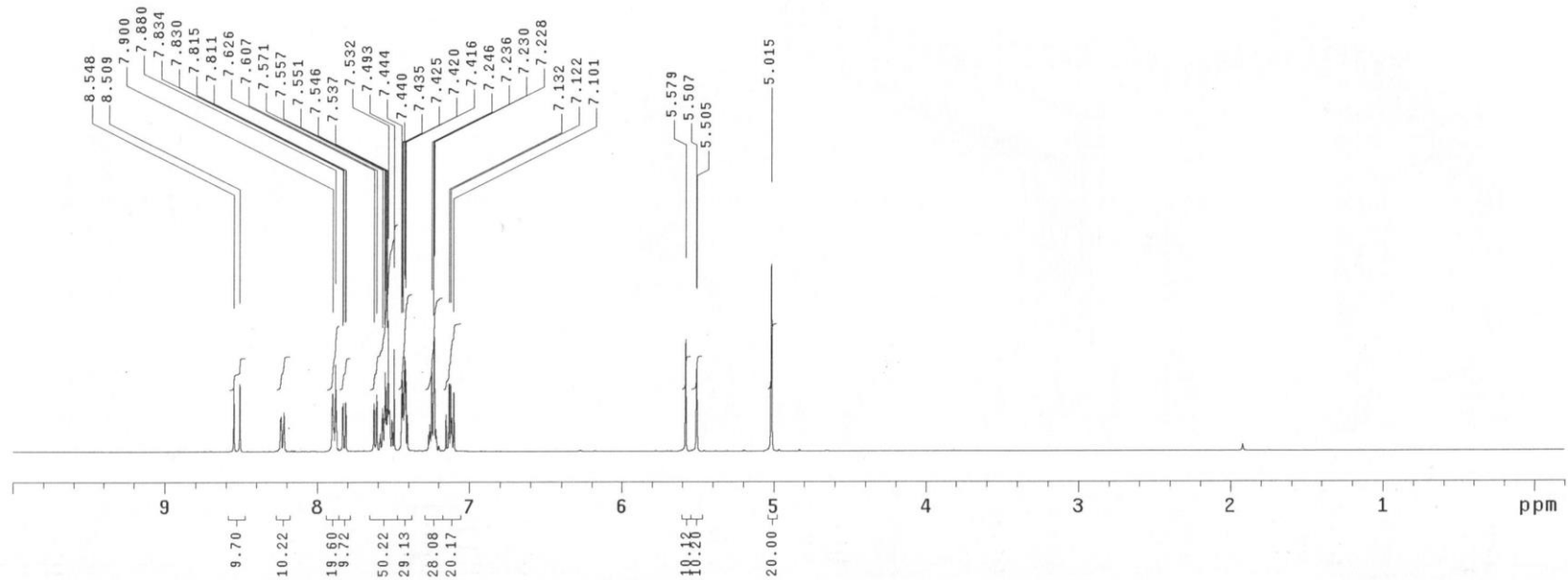Date: Apr 23 2019
Solvent: CDCl3
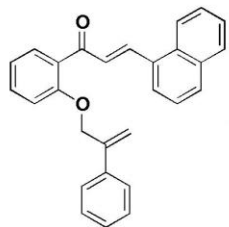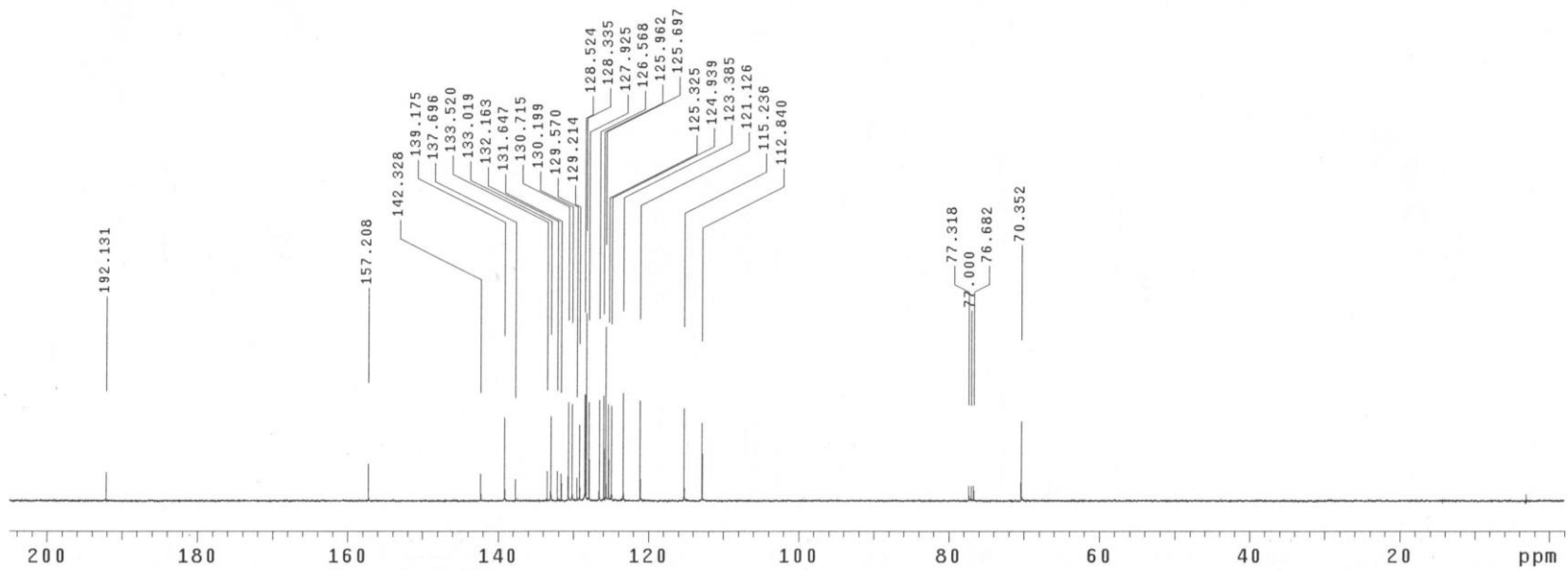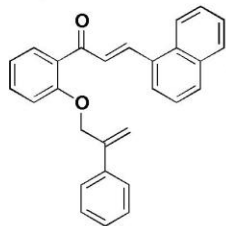Ambient temperature
Total 176 repetitions

192.131

157.208

142.328
139.175
137.696
133.520
133.019
132.163
131.647
130.715
130.199
129.570
129.214

128.524
128.335
127.925
126.568
125.962
125.697
125.325
124.939
123.385
121.126
115.236
112.840

77.318
77.000
76.682
70.352

200   180   160   140   120   100   80   60   40   20   ppm

Compound 5y (^{1}H-NMR spectral data)

MC1080415
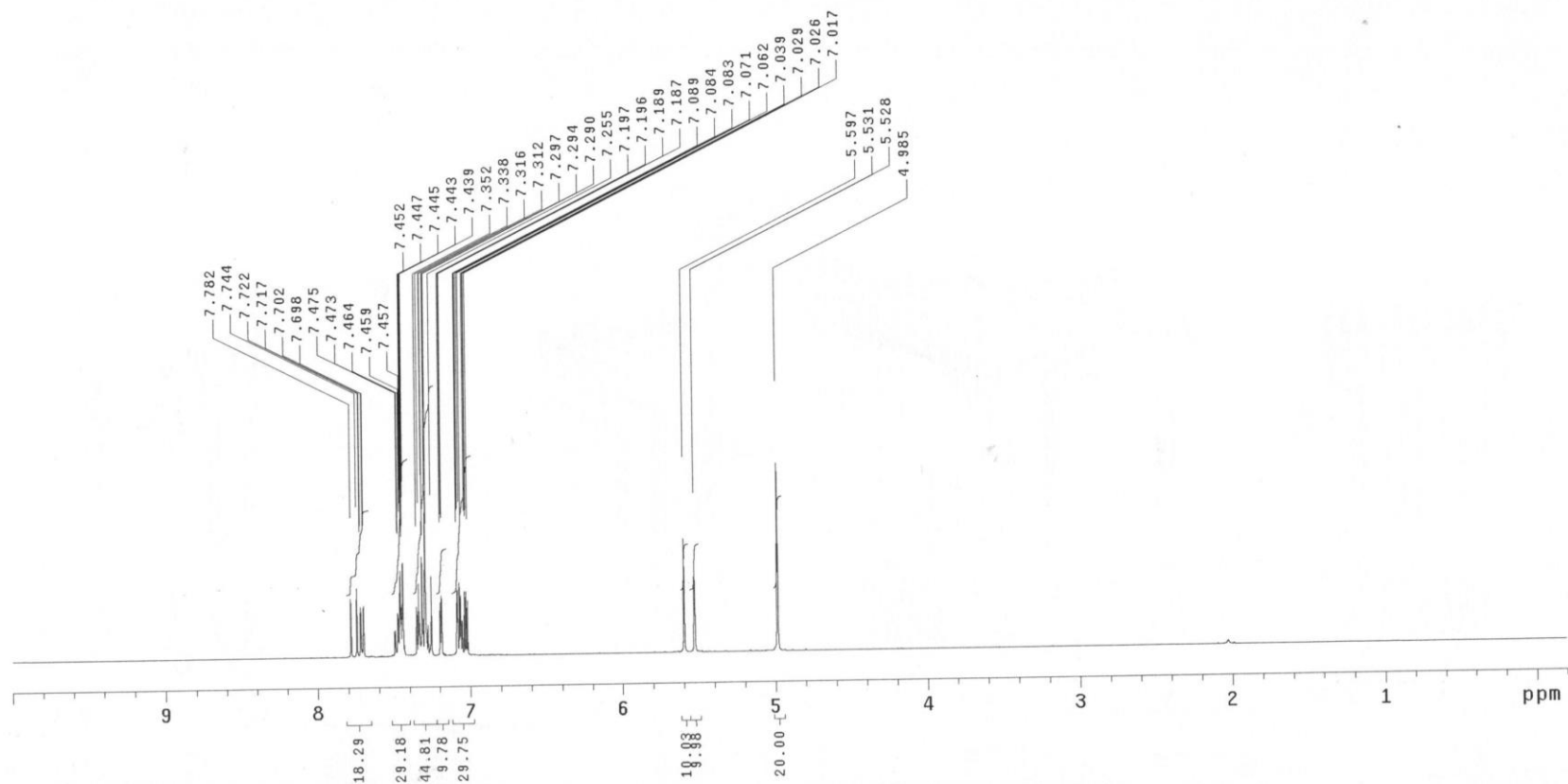
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 15 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.782
7.744
7.722
7.717
7.702
7.698
7.475
7.473
7.464
7.459
7.457

7.452
7.447
7.445
7.443
7.439
7.352
7.338
7.316
7.312
7.297
7.294
7.290
7.255
7.197
7.196
7.189
7.187
7.089
7.084
7.083
7.071
7.062
7.039
7.029
7.026
7.017

5.597
5.531
5.528

4.985

18.29
29.18
44.81
9.78
29.75

19.03
9.98

20.00

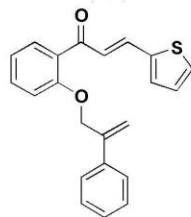9   8   7   6   5   4   3   2   1   ppm

Compound 5y (¹³C-NMR spectral data)

MC1080415

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 15 2019
Solvent: CDCl3
Ambient temperature
Total 752 repetitions

Peaks: 191.646, 156.989, 142.207, 140.304, 137.848, 135.104, 132.792, 131.109, 130.427, 129.343, 128.357, 128.304, 127.956, 127.857, 125.772, 125.719, 120.997, 114.781, 112.878, 70.132

ppm axis: 180 160 140 120 100 80 60 40 20 ppm
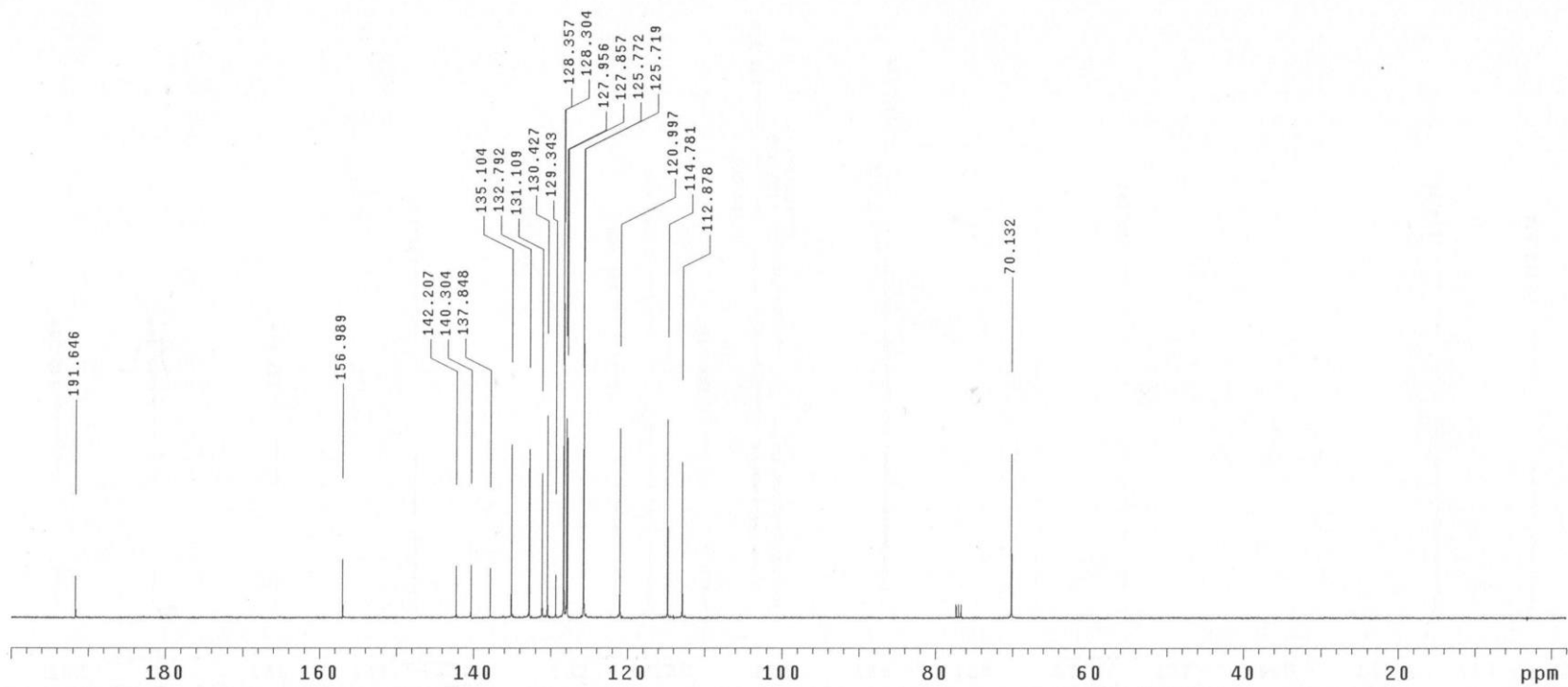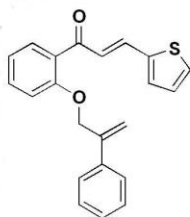
Compound 5z (¹H-NMR spectral data)

MCCr2OMe

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 16 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.887

7.579
7.540
7.343
7.304
7.090
7.004
7.002
6.965
6.944
6.856
6.836

4.536
4.533
4.530
4.521
4.519

1.653
1.649
1.637
1.633

9   8   7   6   5   4   3   2   1   ppm

22.76 25.04 25.19 24.75 12.32   8.95 12.30   20.00   72.44   27.99
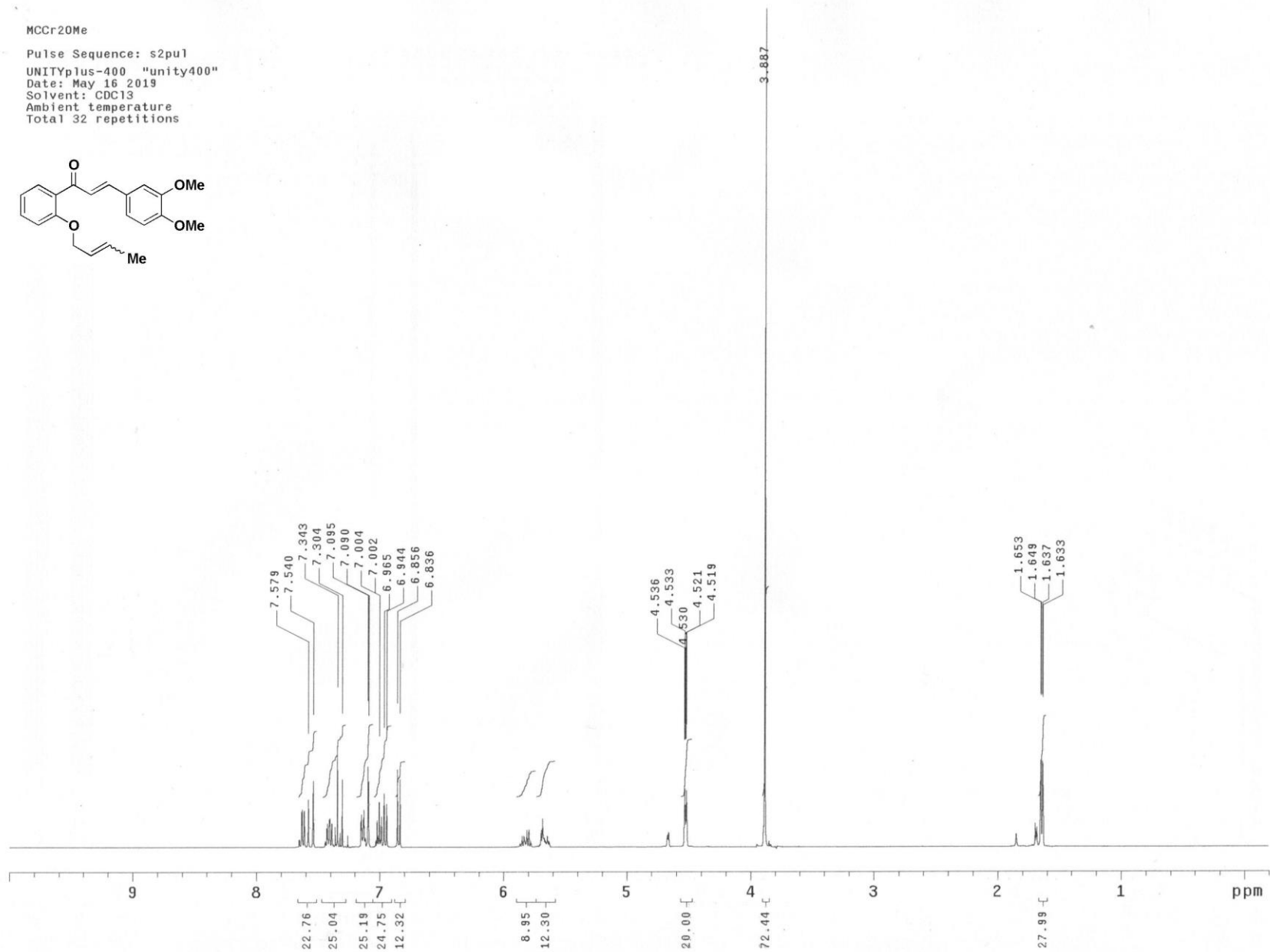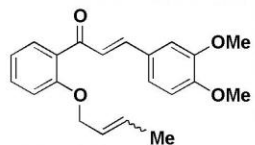
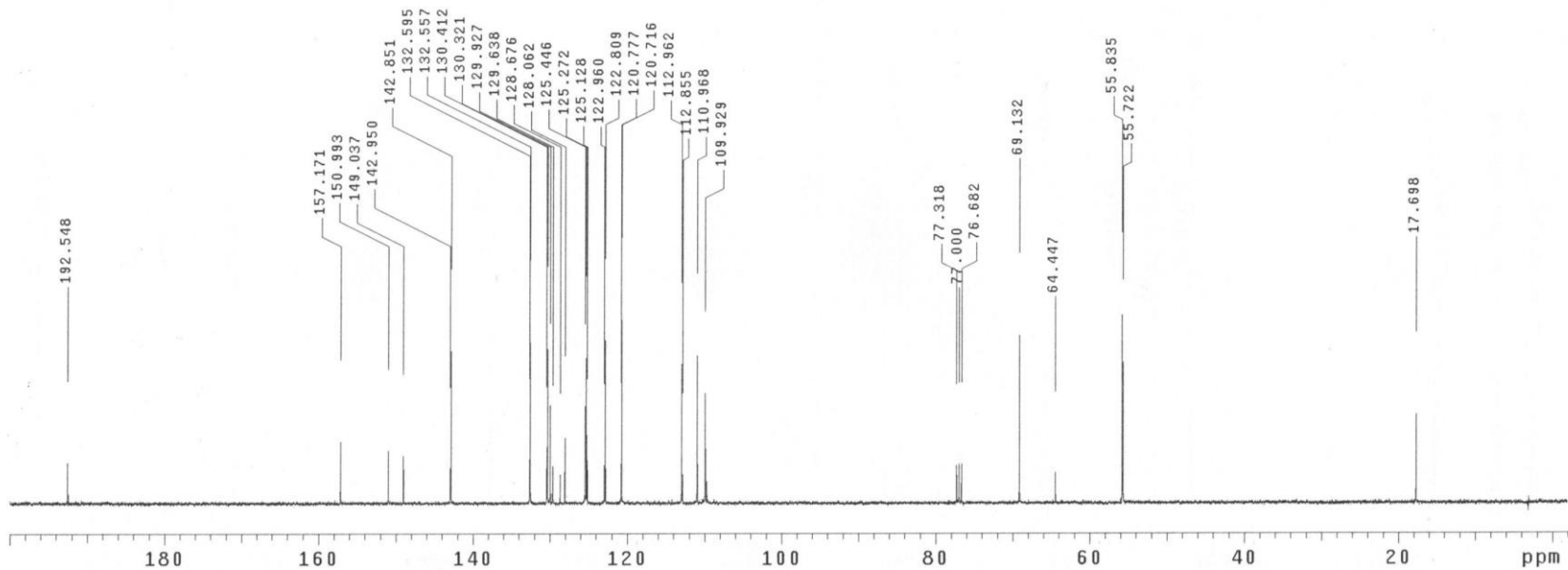# Compound 5z (^{13}C-NMR spectral data)

MCCr2OMe

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 16 2019
Solvent: CDCl3
Ambient temperature
Total 544 repetitions

192.548

157.171
150.993
149.037
142.950
142.851
132.595
132.557
130.412
130.321
129.927
129.638
128.676
128.062
125.446
125.272
125.128
122.960
122.809
120.777
120.716
112.962
112.855
110.968
109.929

77.318
77.000
76.682
69.132
64.447
55.835
55.722
17.698

180	160	140	120	100	80	60	40	20	ppm
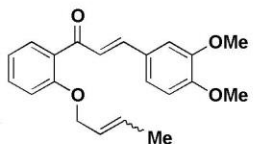
Compound 5aa (¹H-NMR spectral data)

MC1NACr

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
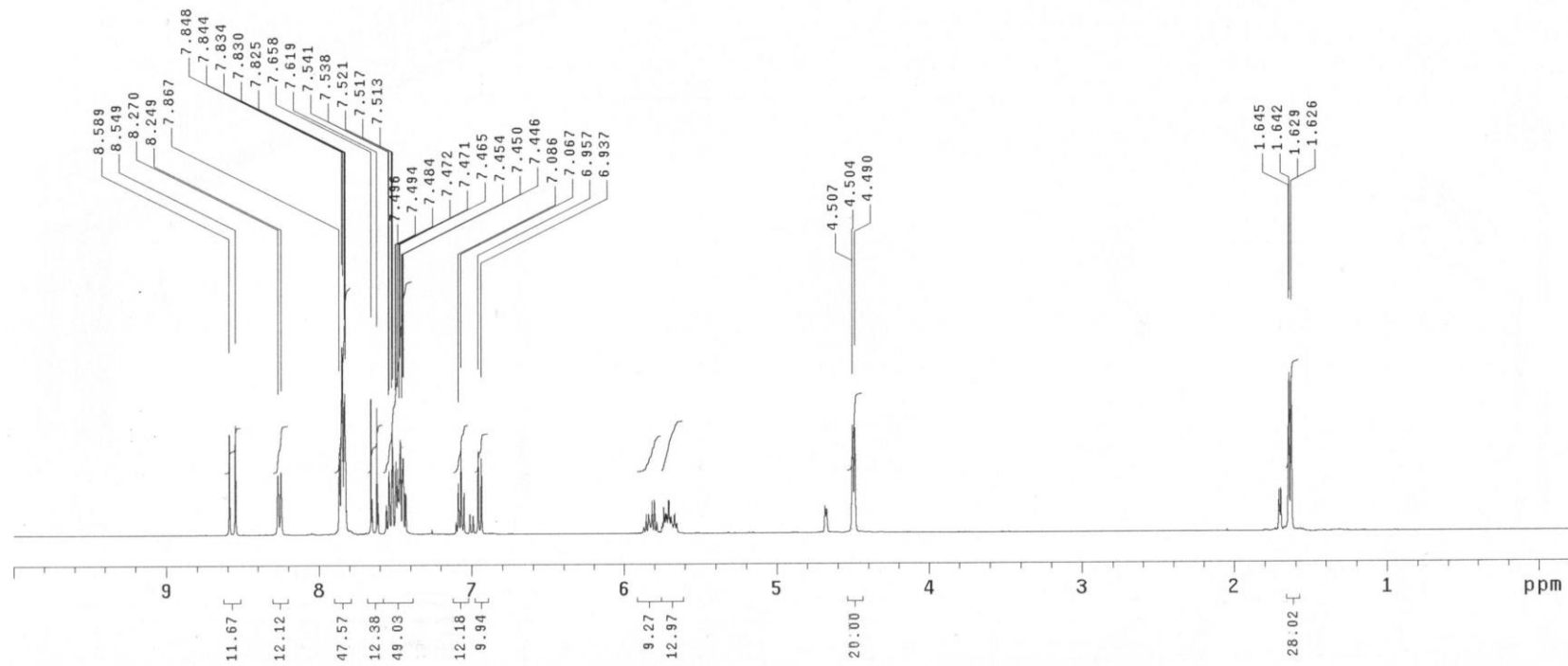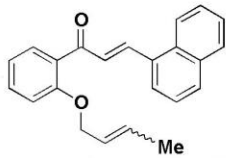Date: May 10 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.589
8.549
8.270
8.249
7.867
7.848
7.844
7.834
7.830
7.825
7.658
7.619
7.541
7.538
7.521
7.517
7.513
7.496
7.494
7.484
7.472
7.471
7.465
7.454
7.450
7.446
7.086
7.067
6.957
6.937
4.507
4.504
4.490
1.645
1.642
1.629
1.626

9   8   7   6   5   4   3   2   1   ppm

11.67
12.12
47.57
12.38
49.03
12.18
9.94
9.27
12.97
20.00
28.02

S-76

Compound 5aa (^{13}C-NMR spectral data)
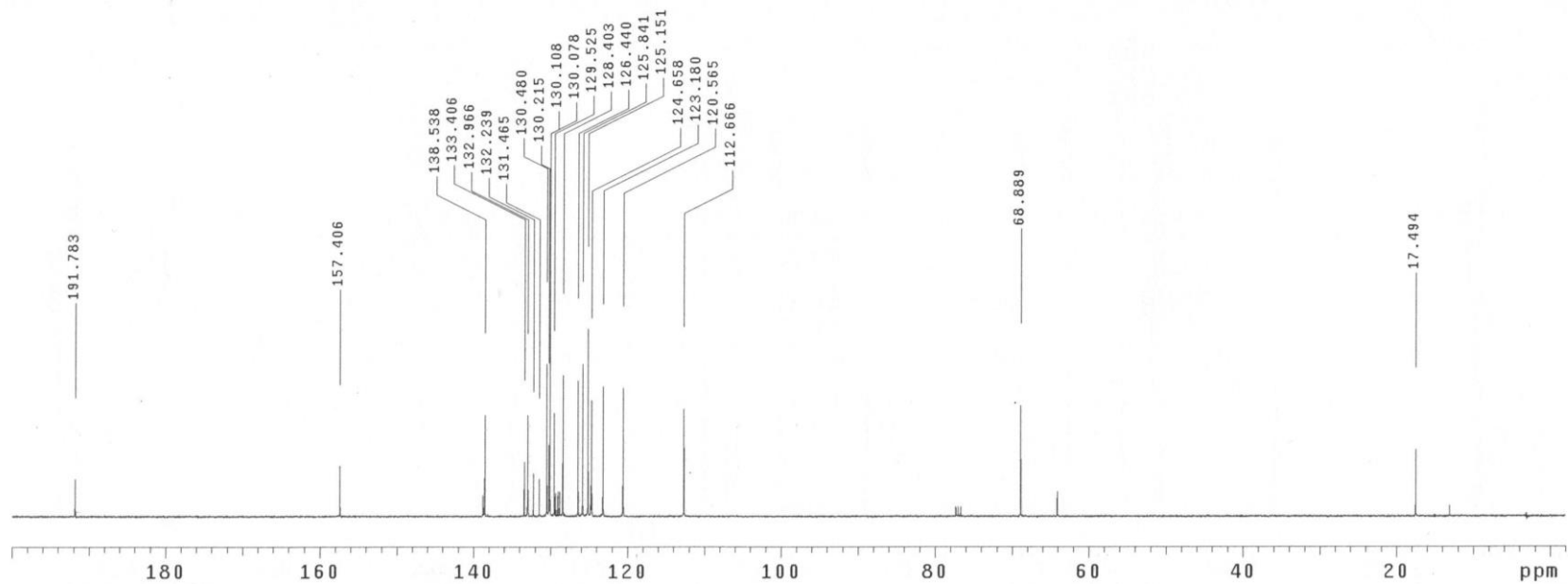
MC1NACr

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 10 2019
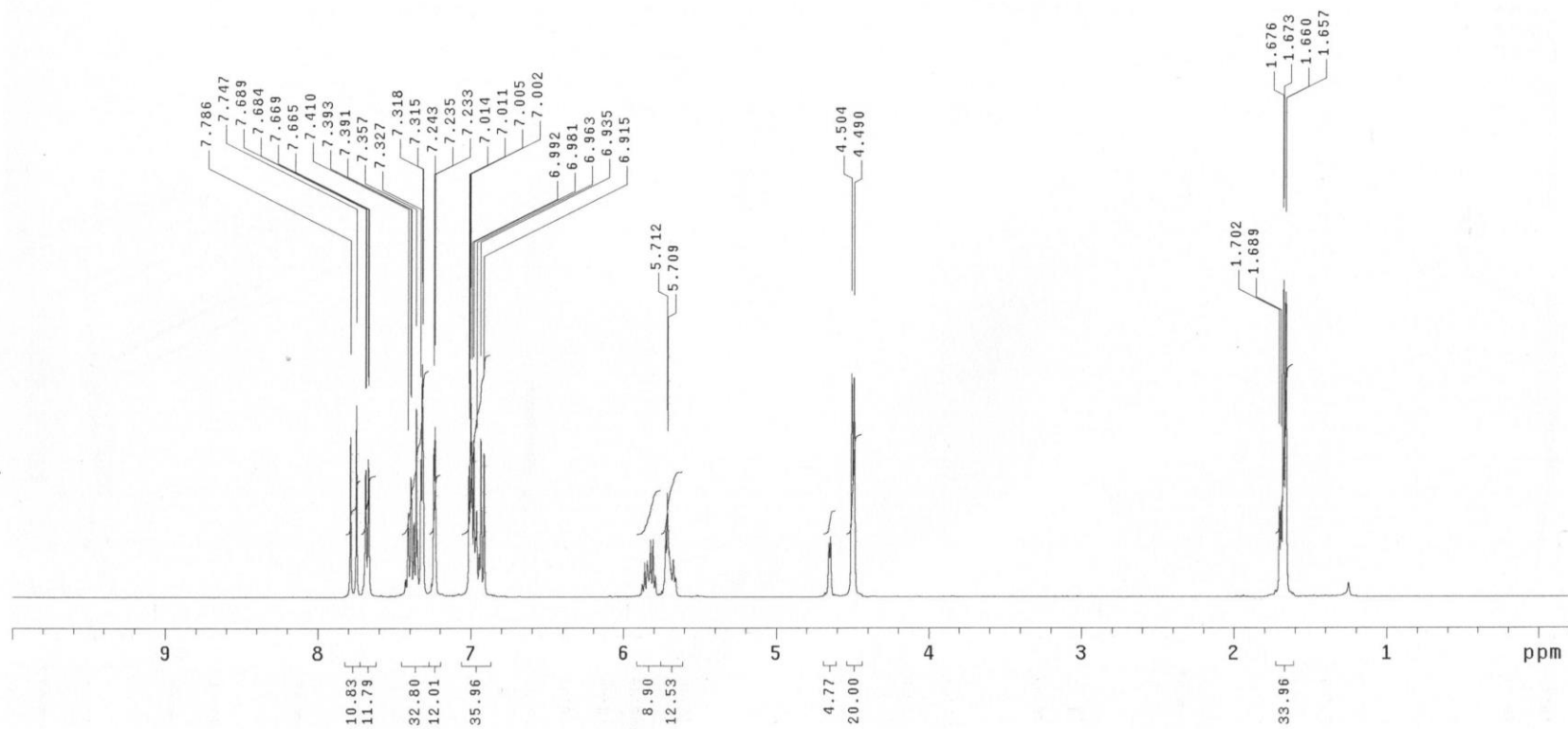Solvent: CDCl3
Ambient temperature
Total 128 repetitions

191.783
157.406
138.538
133.406
132.966
132.239
131.465
130.480
130.215
130.108
130.078
129.525
128.403
126.440
125.841
125.151
124.658
123.180
120.565
112.666
68.889
17.494

180   160   140   120   100   80   60   40   20   ppm
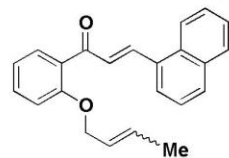
Compound 5ab (¹H-NMR spectral data)

MCCrS

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
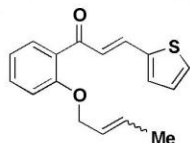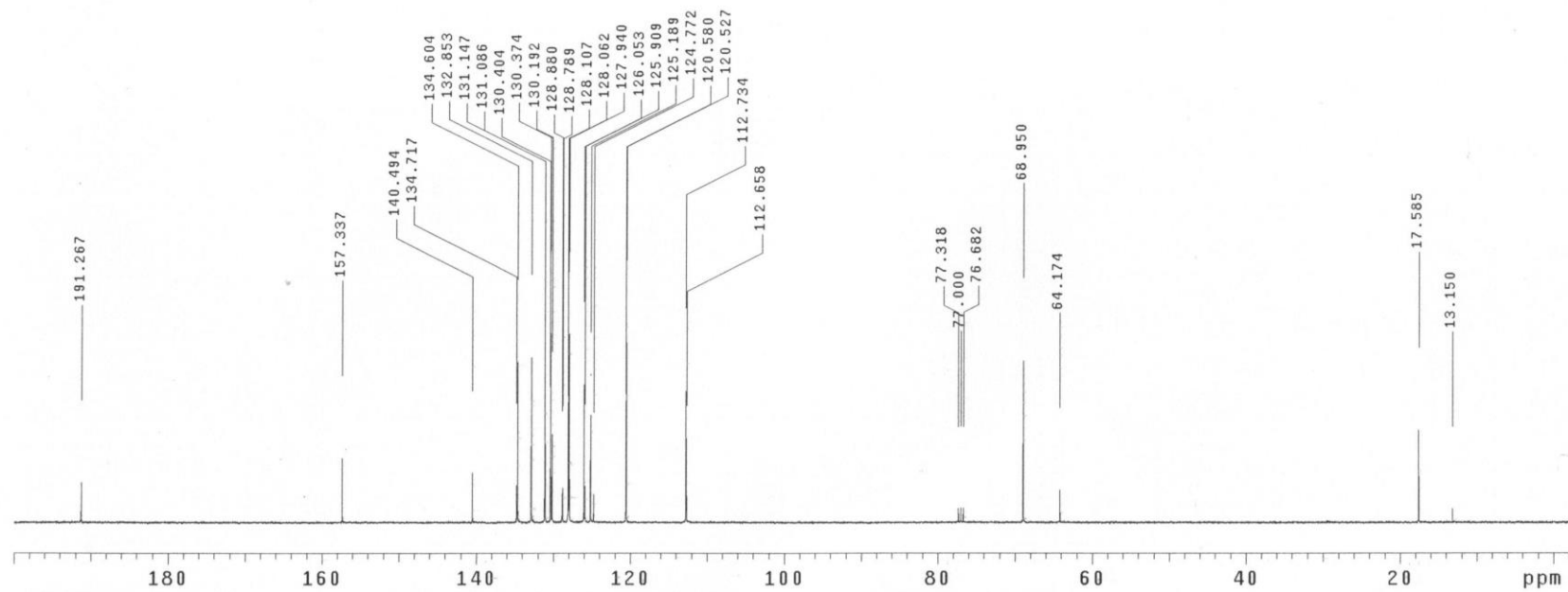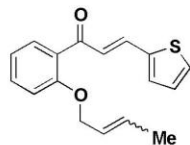Date: May 20 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Peaks (ppm): 7.786, 7.747, 7.689, 7.684, 7.669, 7.665, 7.410, 7.393, 7.391, 7.357, 7.327, 7.318, 7.315, 7.243, 7.235, 7.233, 7.014, 7.011, 7.005, 7.002, 6.992, 6.981, 6.963, 6.935, 6.915, 5.712, 5.709, 4.504, 4.490, 1.702, 1.689, 1.676, 1.673, 1.660, 1.657

Integrations: 10.83, 11.79, 32.80, 12.01, 35.96, 8.90, 12.53, 4.77, 20.00, 33.96

Compound 5ab (¹³C-NMR spectral data)

MCCrS
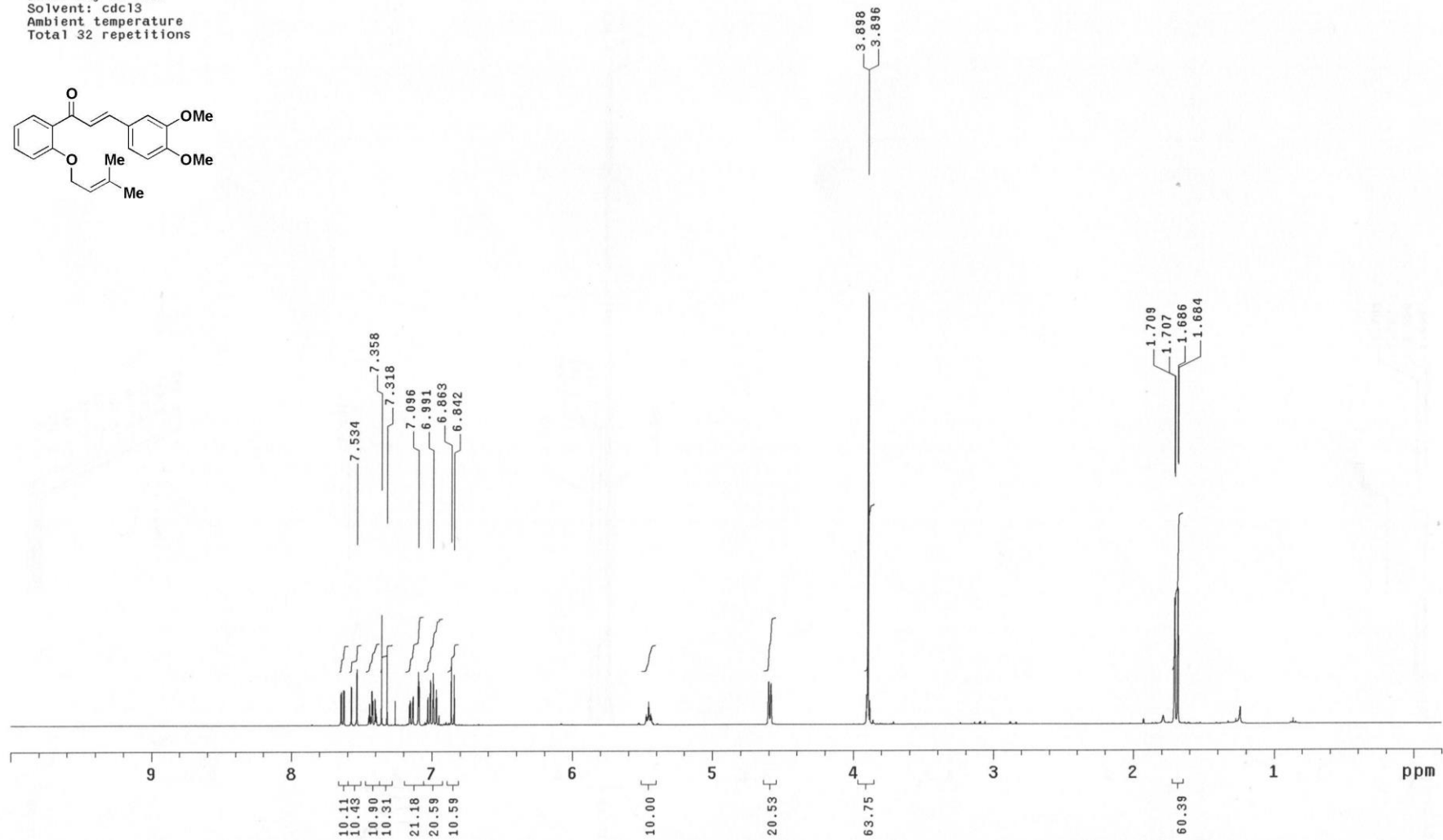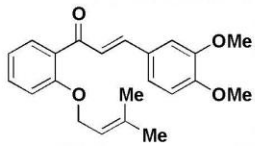
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 20 2019
Solvent: CDCl3
Ambient temperature
Total 224 repetitions

191.267
157.337
140.494
134.717
134.604
132.853
131.147
131.086
130.404
130.374
130.192
128.880
128.789
128.107
128.062
127.940
126.053
125.909
125.189
124.772
120.580
120.527
112.734
112.658
77.318
77.000
76.682
68.950
64.174
17.585
13.150

180   160   140   120   100   80   60   40   20   ppm

Compound 5ac (^{1}H-NMR spectral data)

MCprenyl

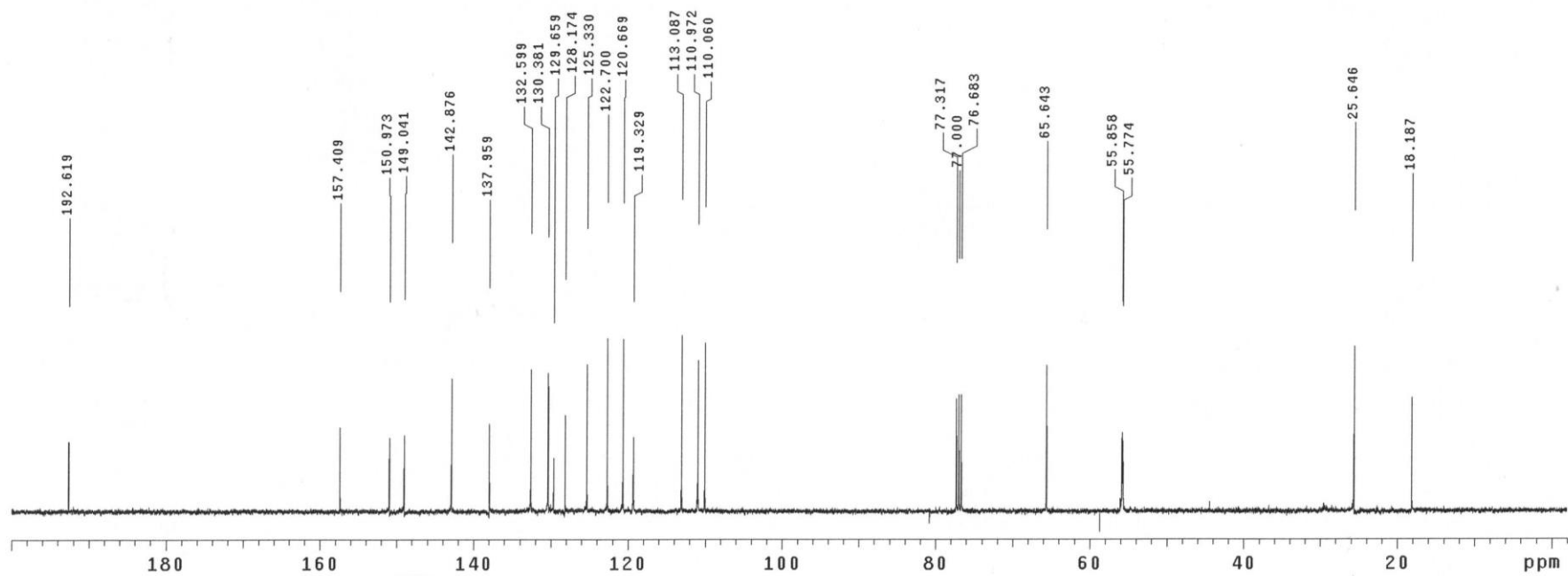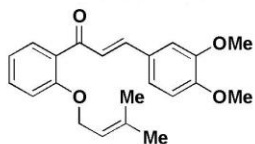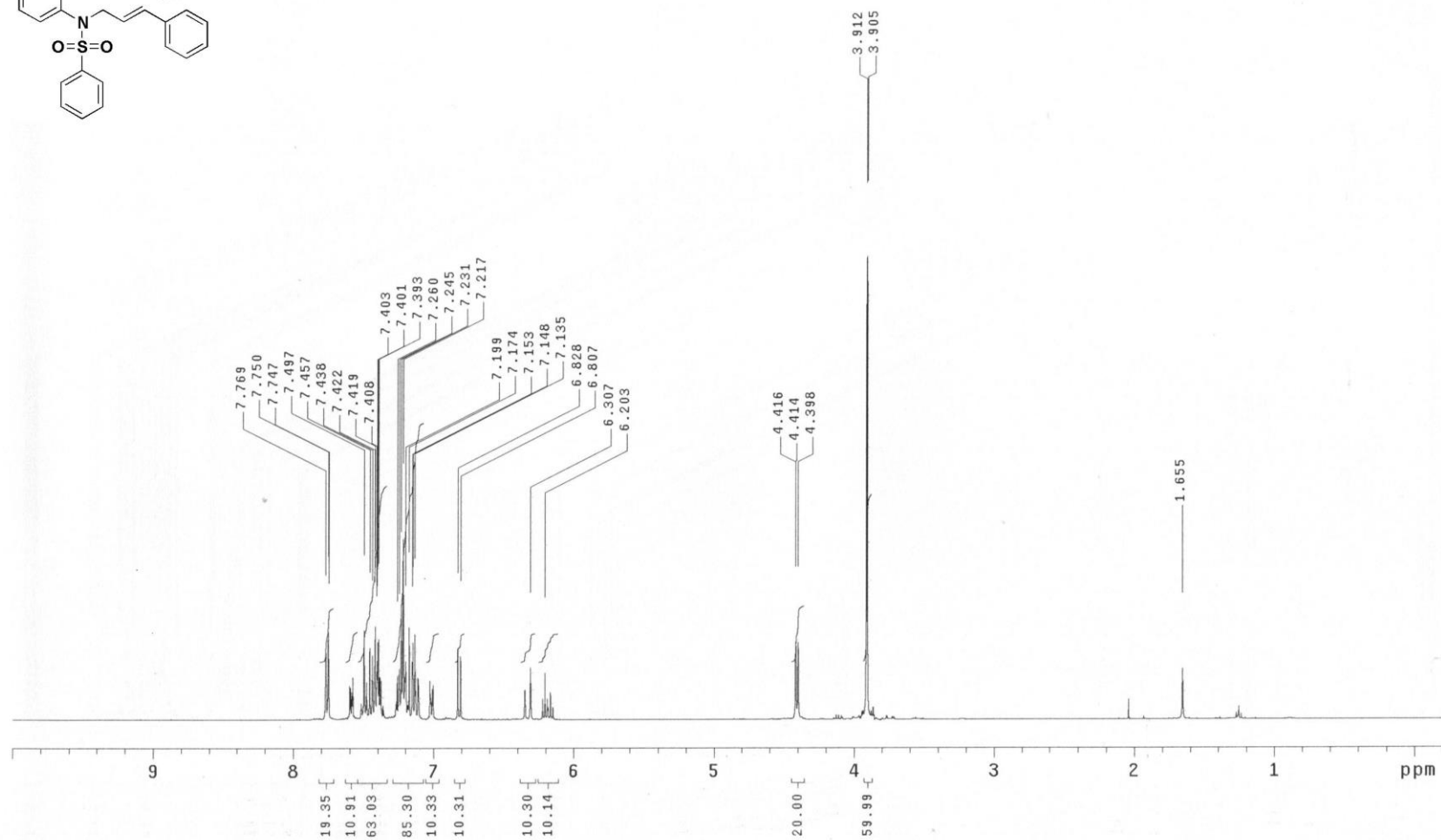Pulse Sequence: s2pul

Mercury-400BB "MerPlus400"
Date: May 22 2019
Solvent: cdcl3
Ambient temperature
Total 32 repetitions

3.898
3.896

7.534
7.358
7.318
7.096
6.991
6.863
6.842

1.709
1.707
1.686
1.684

10.11
10.43
10.90
10.31
21.18
20.59
10.59

10.00

20.53

63.75

60.39

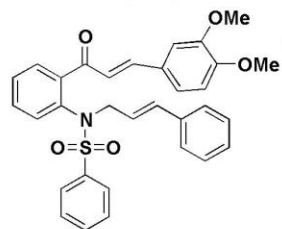9   8   7   6   5   4   3   2   1   ppm

Compound 5ac (^{13}C-NMR spectral data)

MCprenyl

Pulse Sequence: s2pul

Mercury-400BB "MerPlus400"
Date: May 22 2019
Solvent: cdcl3
Ambient temperature
Total 256 repetitions

192.619
157.409
150.973
149.041
142.876
137.959
132.599
130.381
129.659
128.174
125.330
122.700
120.669
119.329
113.087
110.972
110.060
77.317
77.000
76.683
65.643
55.858
55.774
25.646
18.187

180 160 140 120 100 80 60 40 20 ppm

Compound 5ad (^{1}H-NMR spectral data)

MC1080610
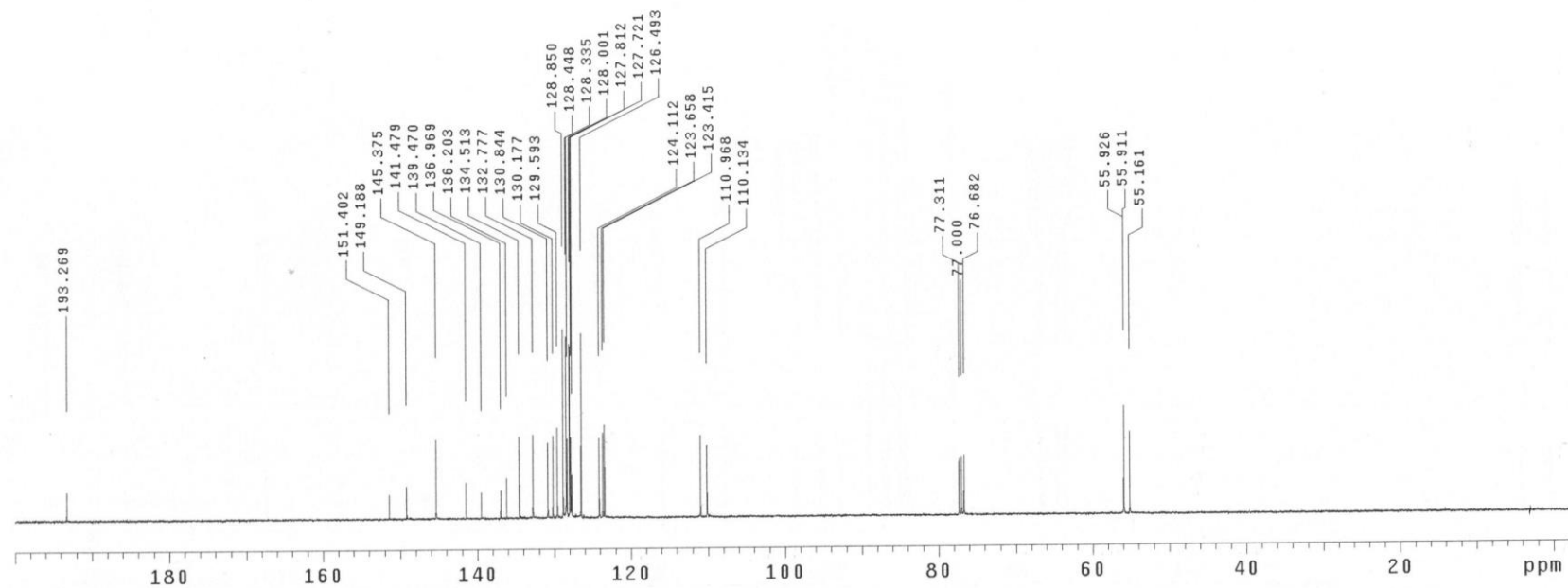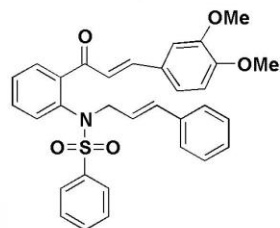
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 10 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.769
7.750
7.747
7.497
7.457
7.438
7.422
7.419
7.408
7.403
7.401
7.393
7.260
7.245
7.231
7.217
7.199
7.174
7.153
7.148
7.135
6.828
6.807
6.307
6.203
4.416
4.414
4.398
3.912
3.905
1.655

19.35 10.91 63.03   85.30 10.33 10.31   10.30 10.14   20.00 59.99

ppm 9 8 7 6 5 4 3 2 1

S-82

Compound 5ad (^{13}C-NMR spectral data)

Compound 5ae (^{1}H-NMR spectral data)

MC1080430

Pulse Sequence: s2pul

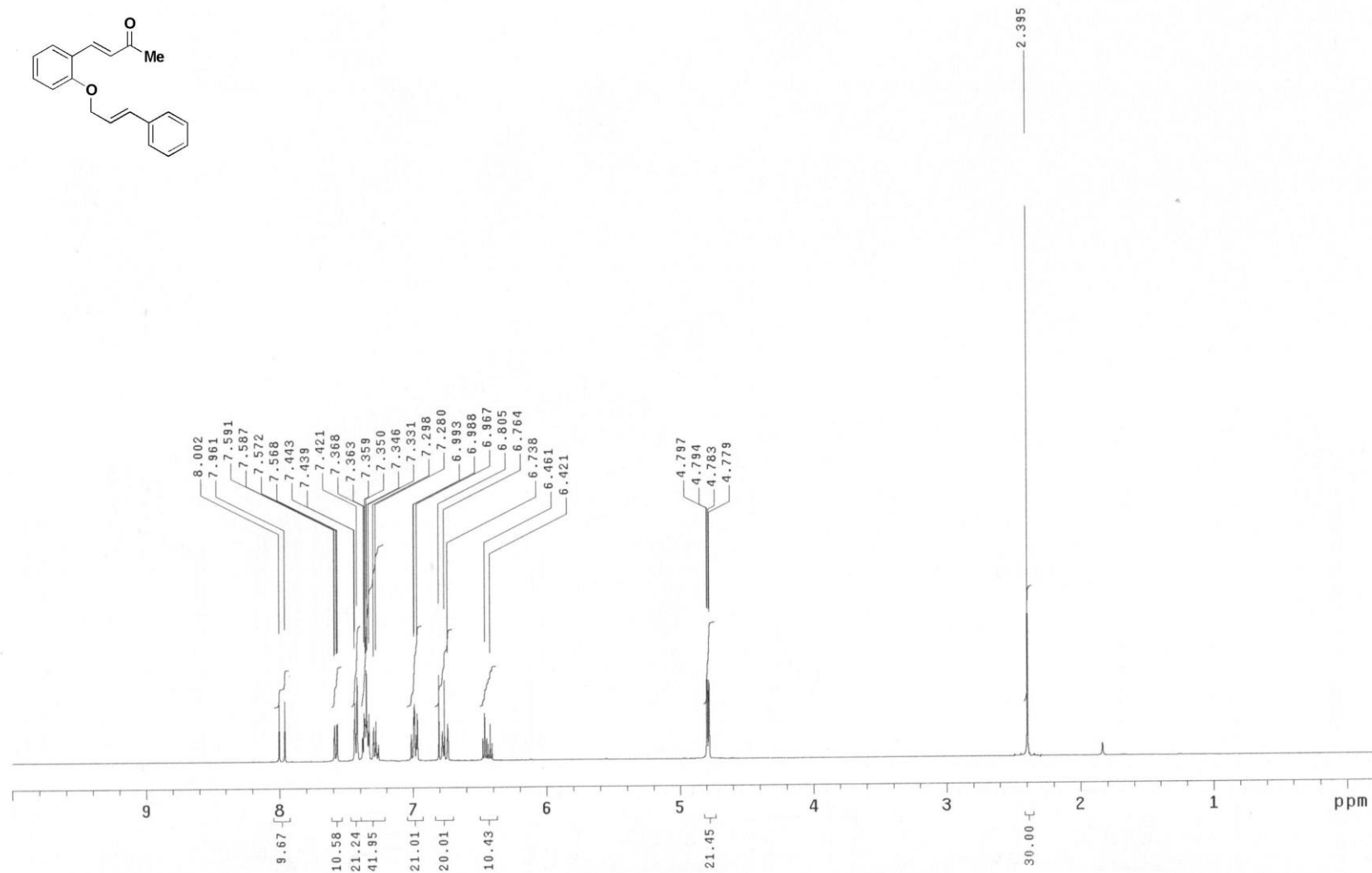UNITYplus-400 "unity400"
Date: May 2 2019
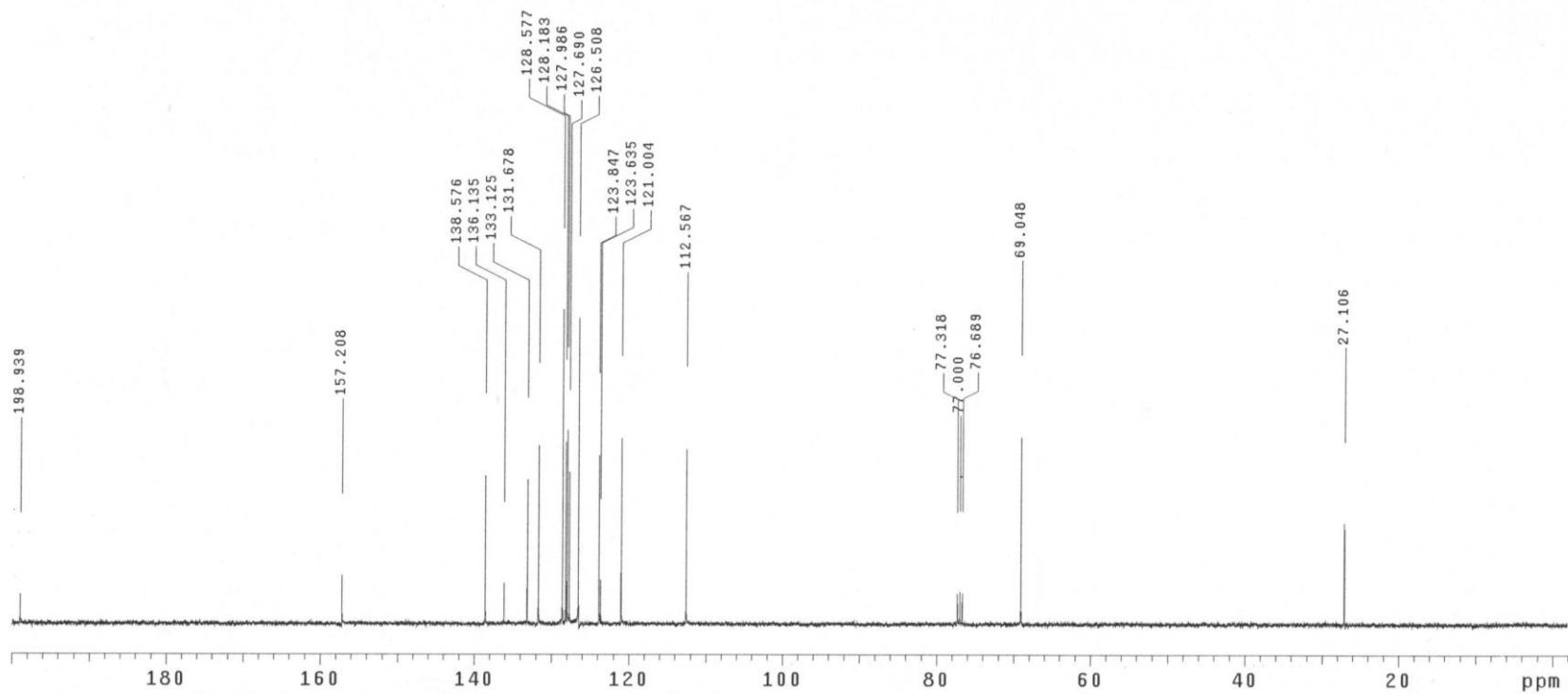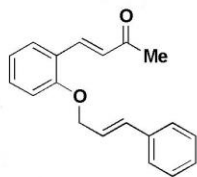Solvent: CDC13
Ambient temperature
Total 32 repetitions

2.395

8.002
7.961
7.591
7.587
7.572
7.568
7.443
7.439
7.421
7.368
7.363
7.359
7.350
7.346
7.331
7.298
7.280
6.993
6.988
6.967
6.805
6.764
6.738
6.461
6.421

4.797
4.794
4.783
4.779

9.67
10.58
21.24
41.95
21.01
20.01
10.43
21.45
30.00

9 8 7 6 5 4 3 2 1 ppm

MC1080430

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2019
Solvent: CDC13
Ambient temperature
Total 256 repetitions

198.939

157.208

138.576
136.135
133.125
131.678

128.577
128.183
127.986
127.690
126.508

123.847
123.635
121.004

112.567

77.318
77.000
76.689

69.048

27.106

180 160 140 120 100 80 60 40 20 ppm
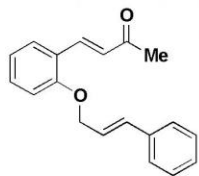
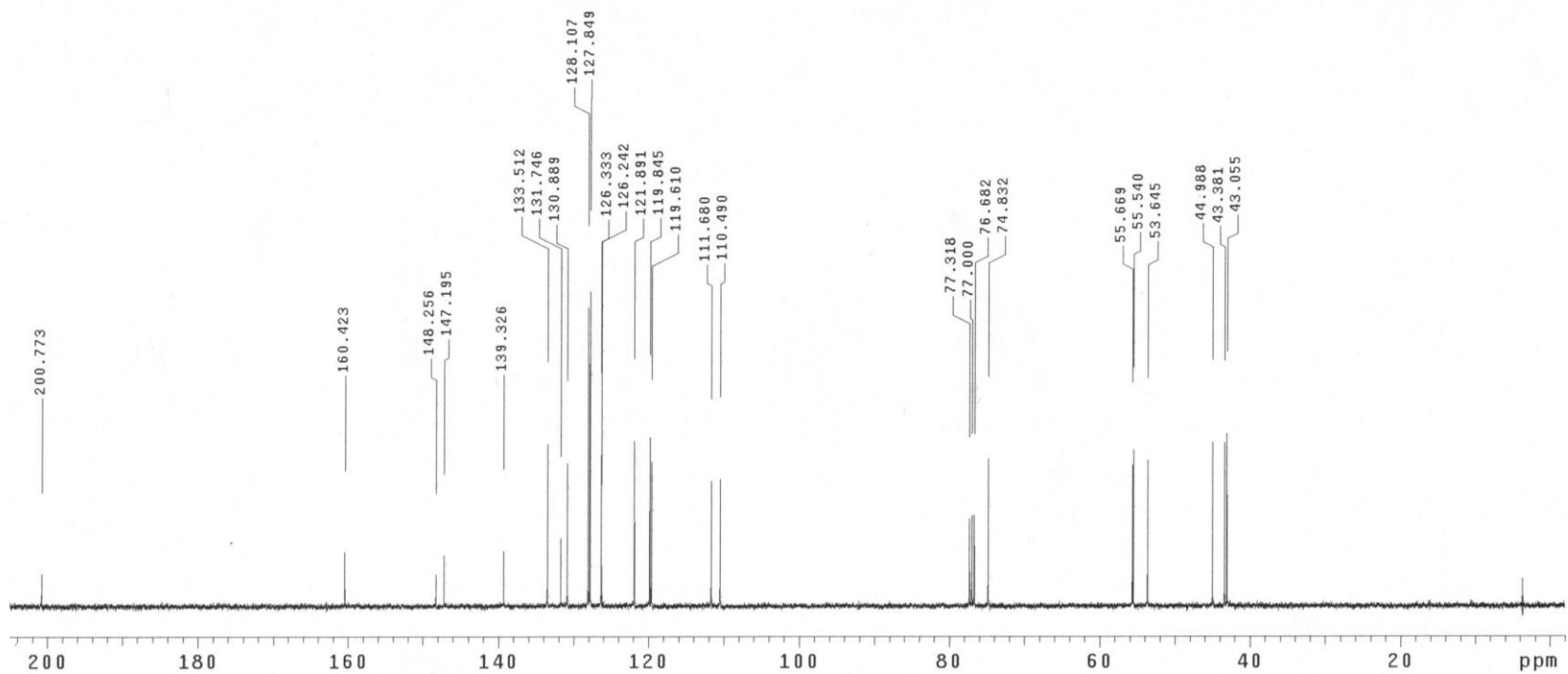# Compound 6a (¹H-NMR spectral data)

MC1080218

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 14 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.757
3.578

7.767
7.763
7.748
7.744
7.432
7.431
7.260
7.149
7.146
7.131
7.098
7.085
7.079
7.067
7.065
7.062
7.005
7.002
6.984
6.622
6.609
6.605
6.305
6.301
4.524
4.514
4.493
4.484
4.342
4.320
3.958
1.611

8.94
9.87
67.73
20.13
9.88
20.21
10.35
20.56
30.27
10.90
30.00
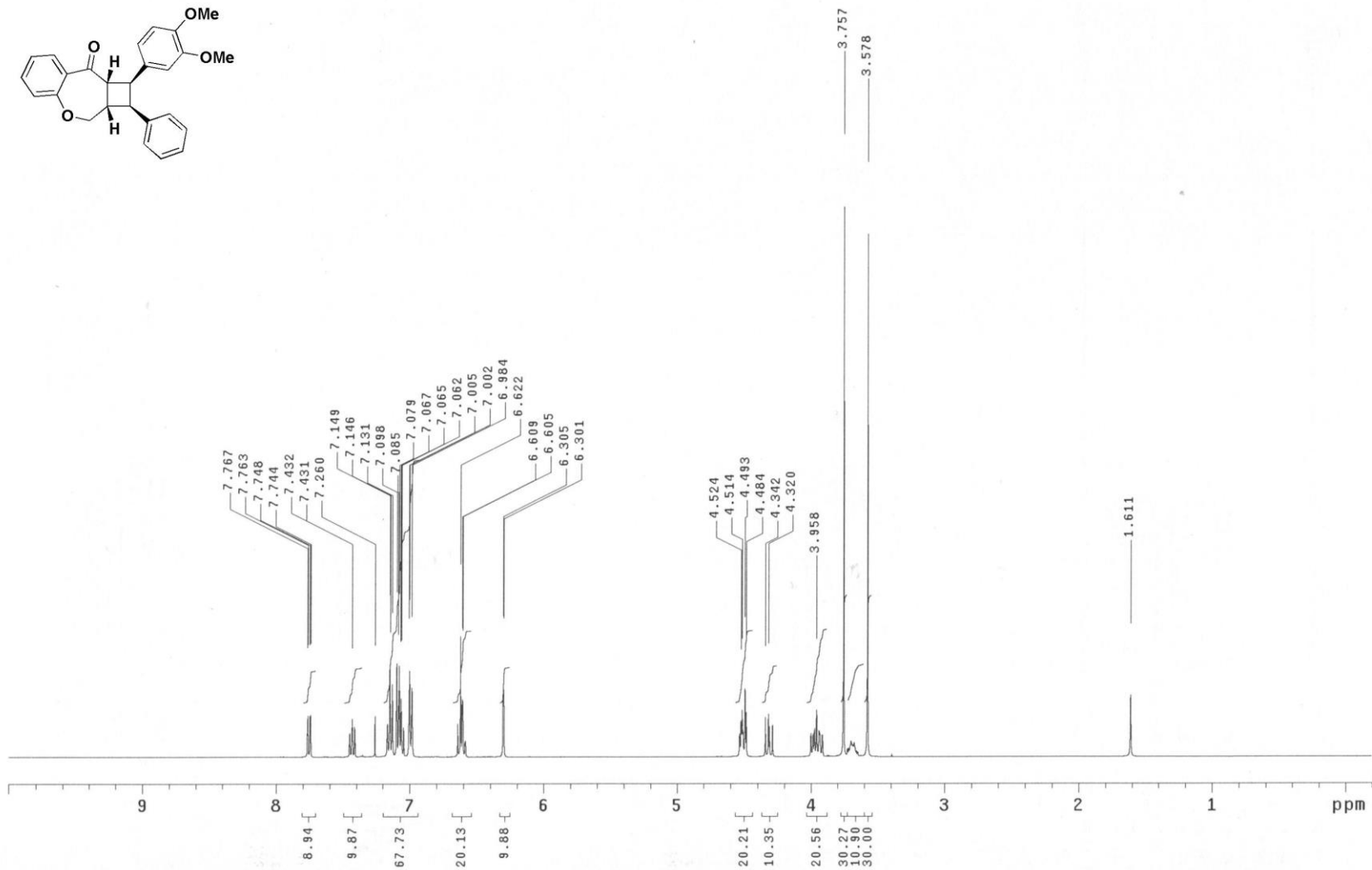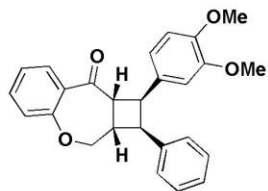
Compound 6a (^{13}C-NMR spectral data)

MC1080218

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 14 2019
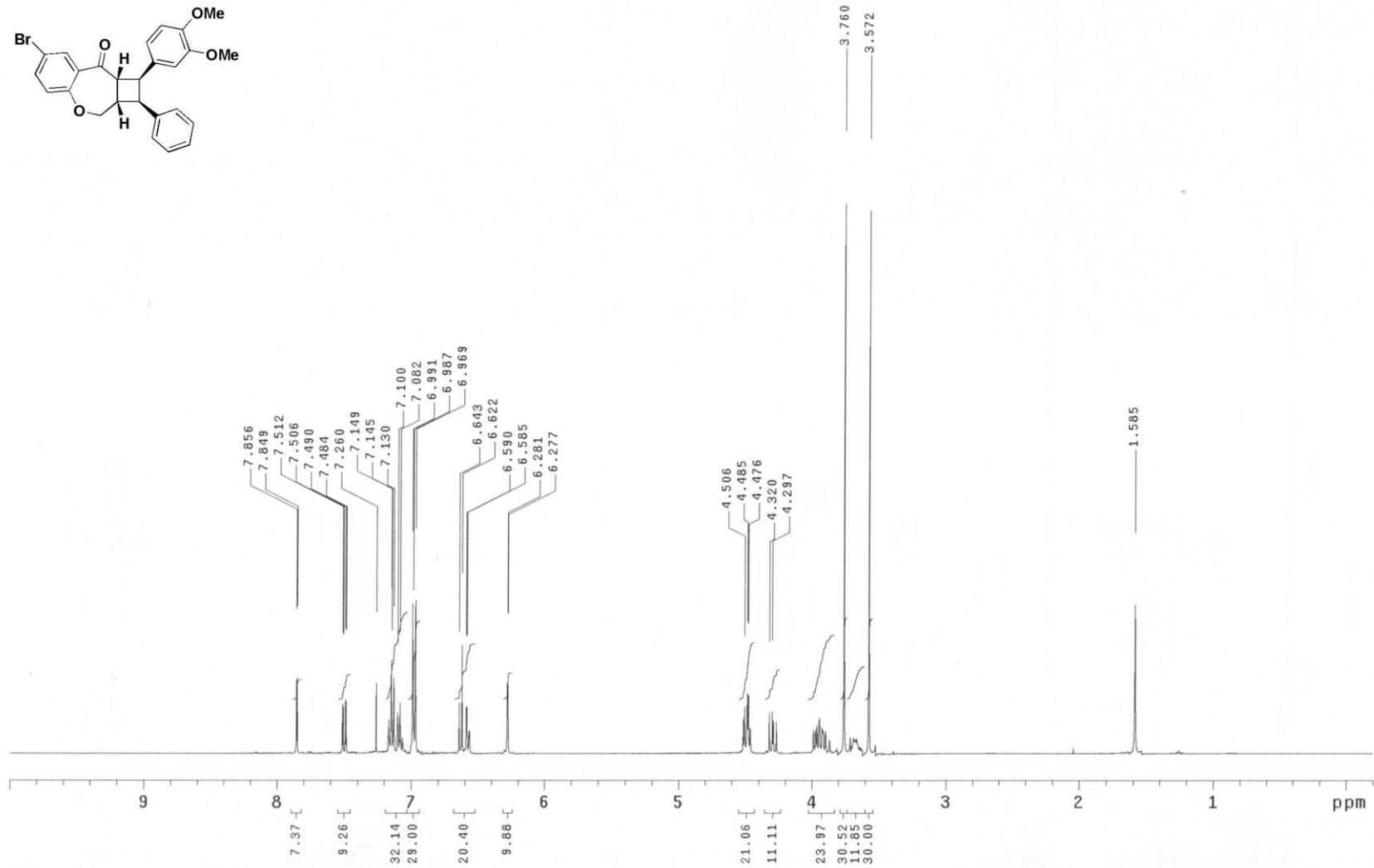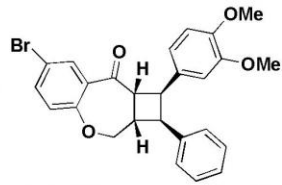Solvent: CDCl3
Ambient temperature
Total 1600 repetitions

200.773
160.423
148.256
147.195
139.326
133.512
131.746
130.889
128.107
127.849
126.333
126.242
121.891
119.845
119.610
111.680
110.490
77.318
77.000
76.682
74.832
55.669
55.540
53.645
44.988
43.381
43.055

200   180   160   140   120   100   80   60   40   20   ppm
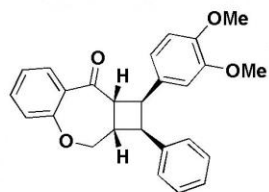
Compound 6b (^{1}H-NMR spectral data)
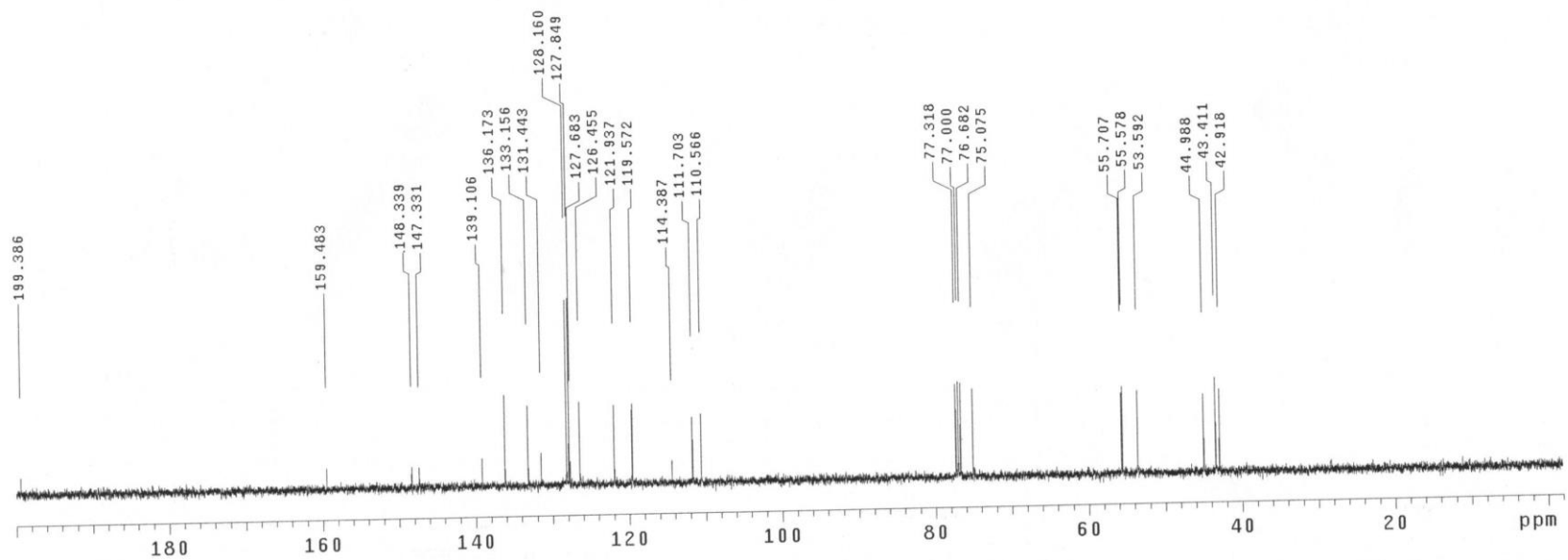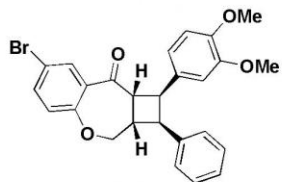

MC1080322

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

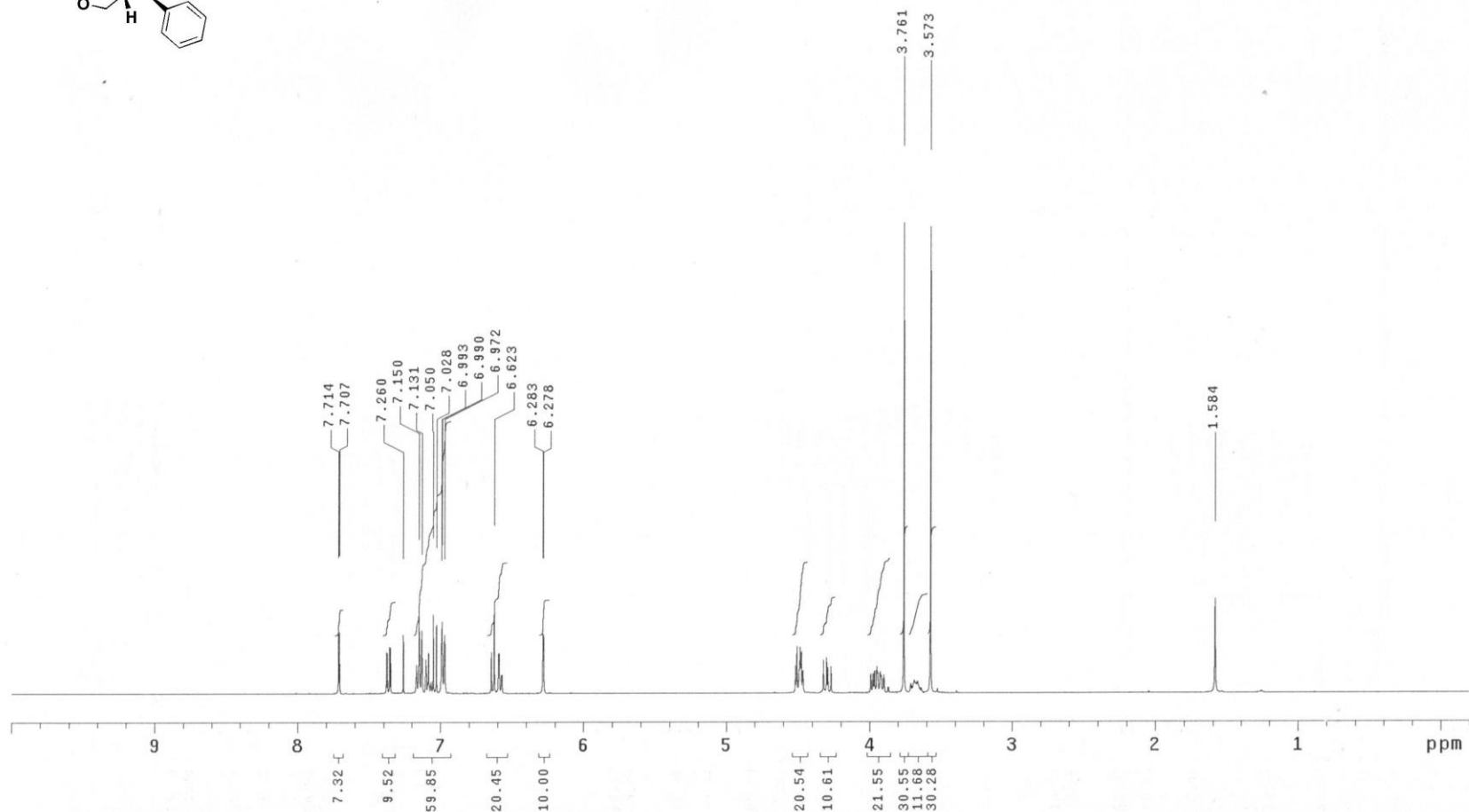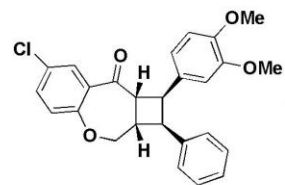# Compound 6b (^{13}C-NMR spectral data)

MC1080322

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2019
Solvent: CDC13
Ambient temperature
Total 576 repetitions

199.386
159.483
148.339
147.331
139.106
136.173
133.156
131.443
128.160
127.849
127.683
126.455
121.937
119.572
114.387
111.703
110.566
77.318
77.000
76.682
75.075
55.707
55.578
53.592
44.988
43.411
42.918

Compound 6c (^{1}H-NMR spectral data)

MC1080613

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 13 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.714
7.707
7.260
7.150
7.131
7.050
7.028
6.993
6.990
6.972
6.623
6.283
6.278
3.761
3.573
1.584

7.32
9.52
59.85
20.45
10.00
20.54
10.61
21.55
30.55
11.68
30.28

Compound 6c (^{13}C-NMR spectral data)
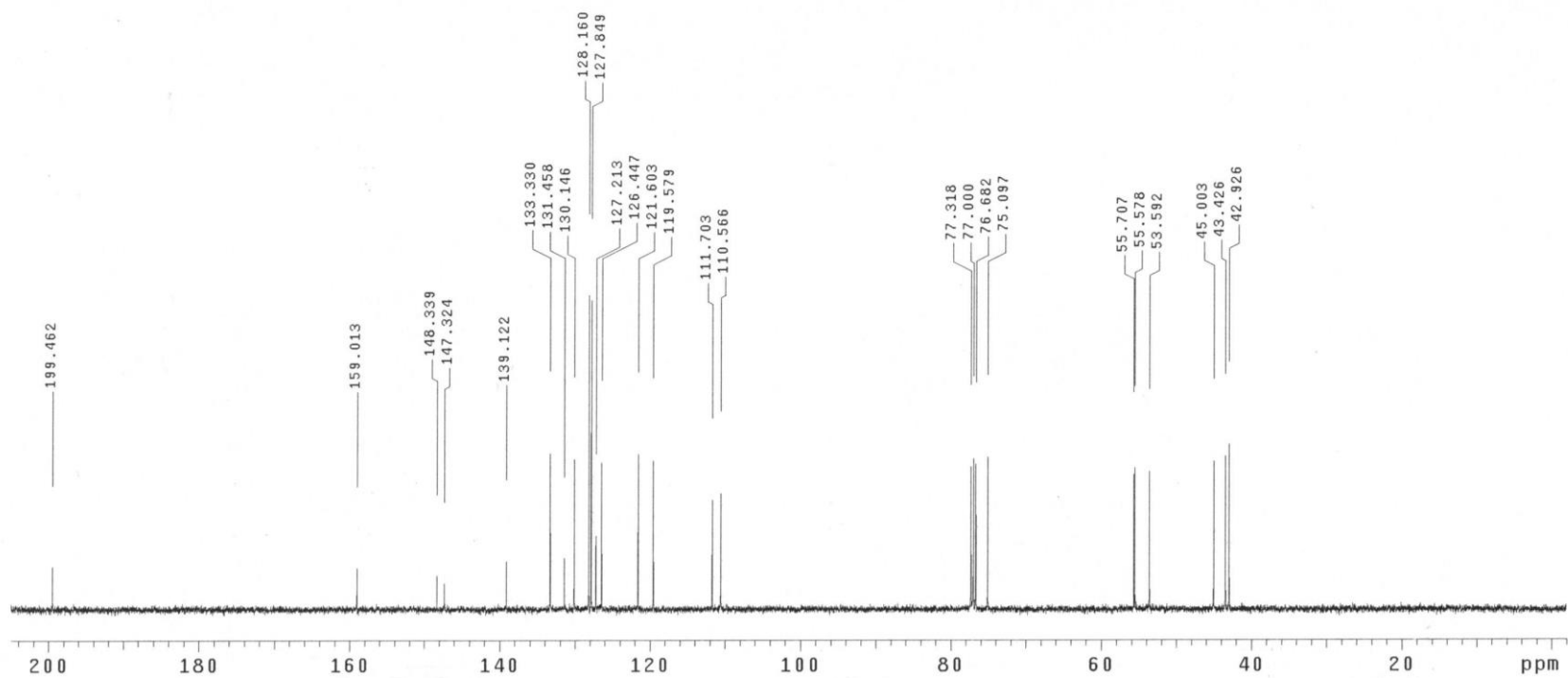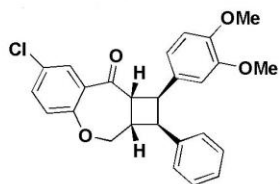
Compound 6d (^{1}H-NMR spectral data)

MC1080403

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: Apr 8 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.755
3.574

7.151
7.147
7.143
7.135
7.132
7.125
7.080
7.067
7.003
6.999
6.982
6.642
6.621
6.598
6.594
6.293
6.288

4.493
4.484
4.463
4.453
4.324
4.303

1.622

8.56
47.91
20.09
20.00
9.87
20.13
10.61
20.79
30.17
10.63
30.09
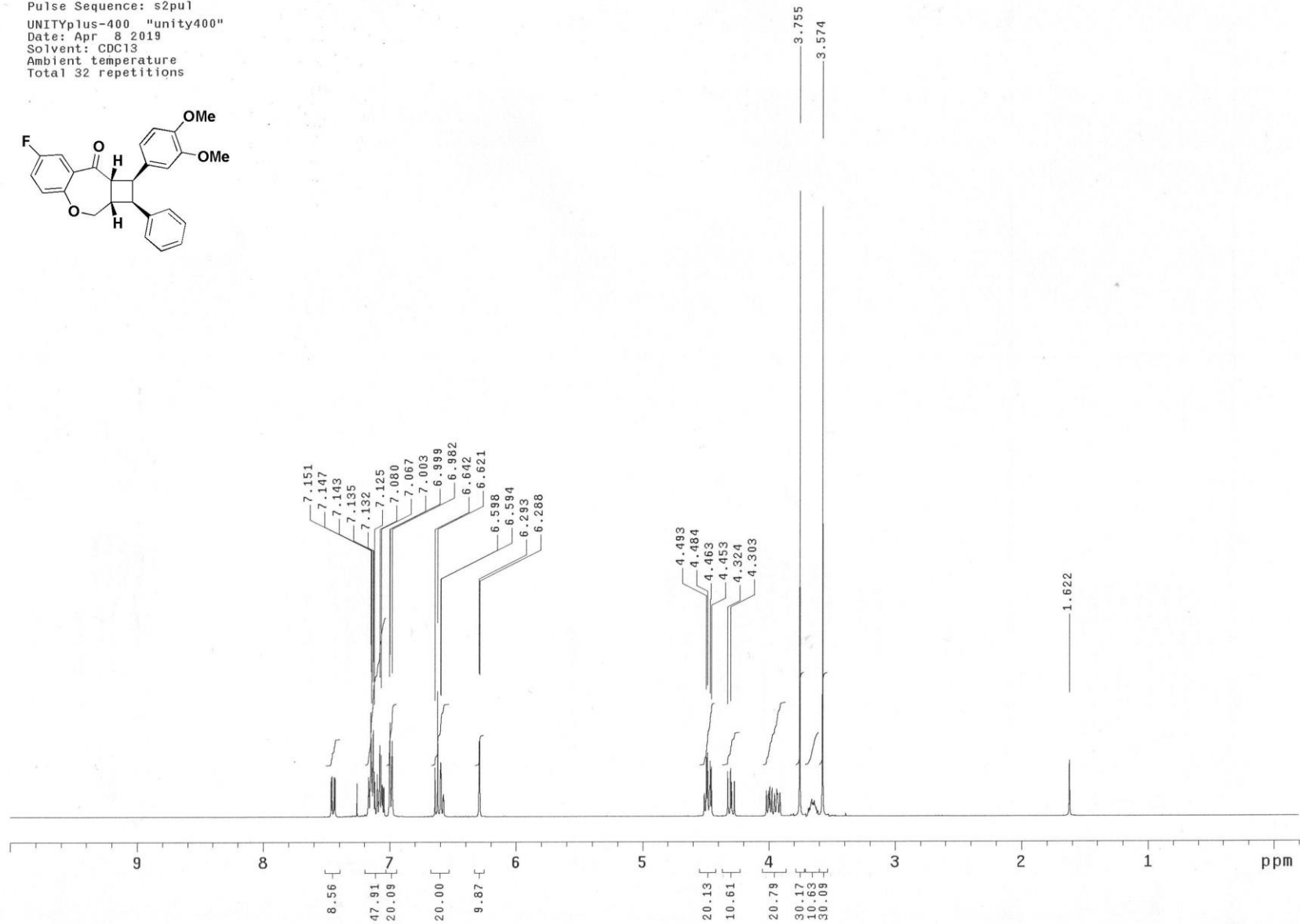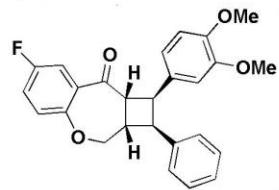
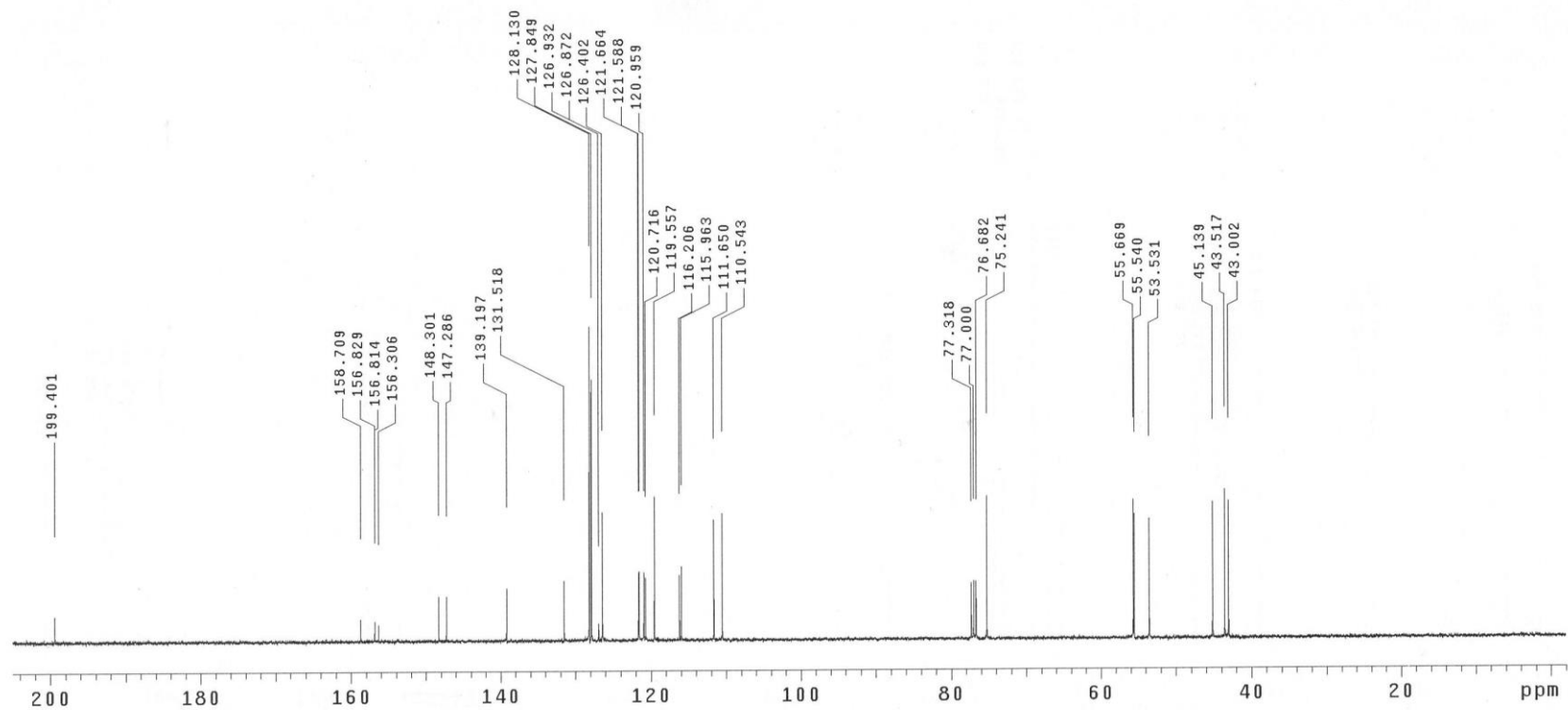# Compound 6d (^{13}C-NMR spectral data)

MC1080403

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 8 2019
Solvent: CDC13
Ambient temperature
Total 1408 repetitions

199.401
158.709
156.829
156.814
156.306
148.301
147.286
139.197
131.518
128.130
127.849
126.932
126.872
126.402
121.664
121.588
120.959
120.716
119.557
116.206
115.963
111.650
110.543
77.318
77.000
76.682
75.241
55.669
55.540
53.531
45.139
43.517
43.002

200 180 160 140 120 100 80 60 40 20 ppm
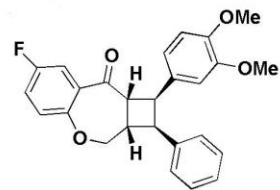
Compound 6e (¹H-NMR spectral data)

Compound 6e (^{13}C-NMR spectral data)

200.948
158.535
148.294
147.217
139.478
134.490
131.867
131.382
130.669
128.122
127.918
126.333
119.761
119.617
111.696
110.543
77.318
77.000
76.682
74.840
55.707
55.570
53.728
45.132
43.487
43.153
20.291

Compound 6f (¹H-NMR spectral data)

MC1080314

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
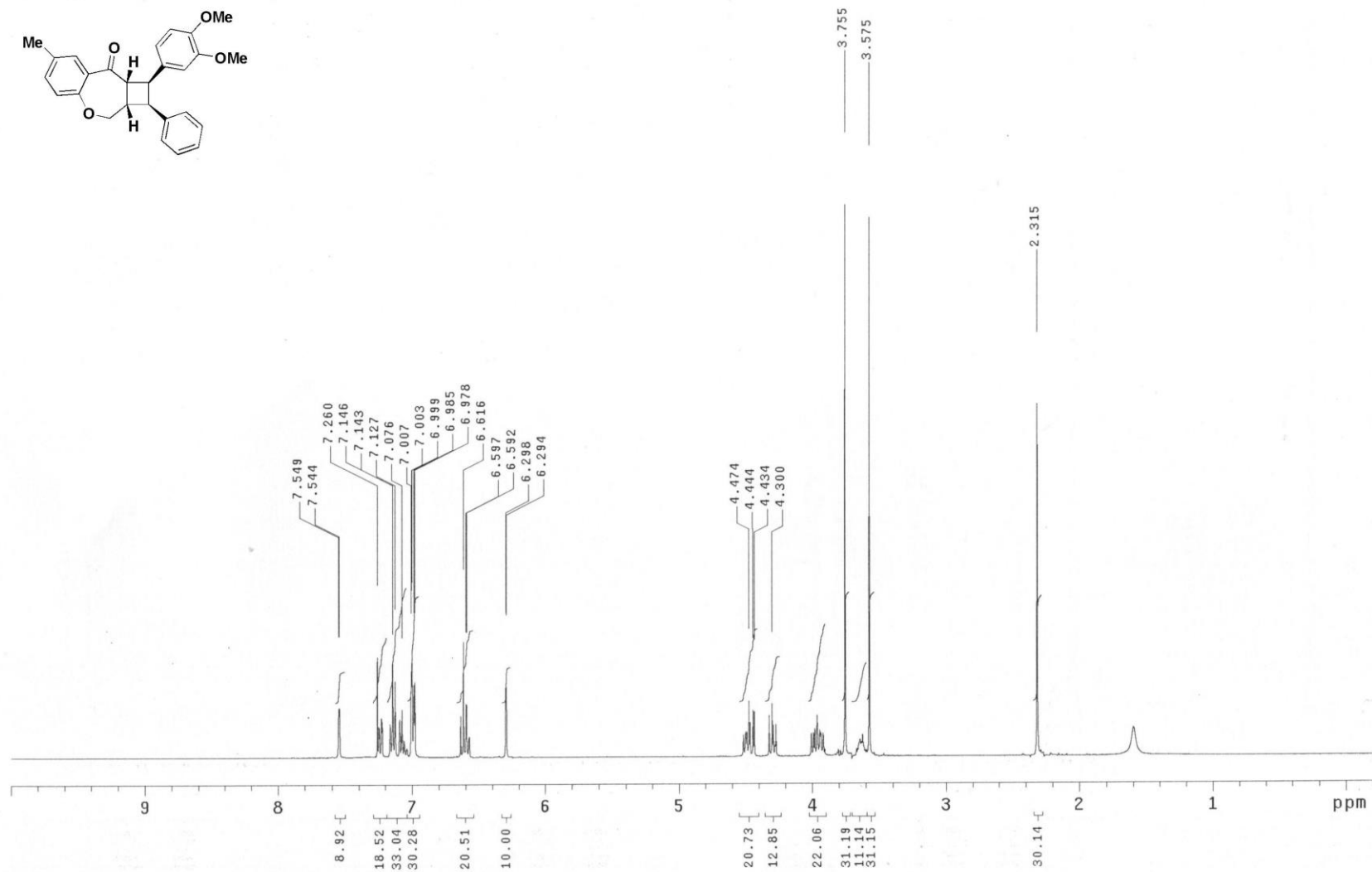Date: Apr 29 2019
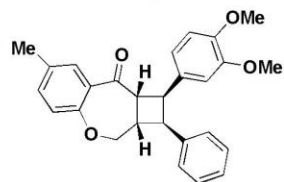Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.788
7.766
7.146
7.143
7.127
7.074
7.014
7.011
6.993
6.654
6.647
6.631
6.625
6.610
6.598
6.594
6.571
6.565
6.296
6.292

4.461
4.452
4.377
4.357

3.949

3.840
3.748
3.572

1.654

9.21
29.66
19.92
38.97
9.80
20.02
10.47
21.02
32.00
30.00
40.57

Compound 6f (^{13}C-NMR spectral data)

MC1080314

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2019
Solvent: CDC13
Ambient temperature
Total 480 repetitions

Compound 6g (^{1}H-NMR spectral data)
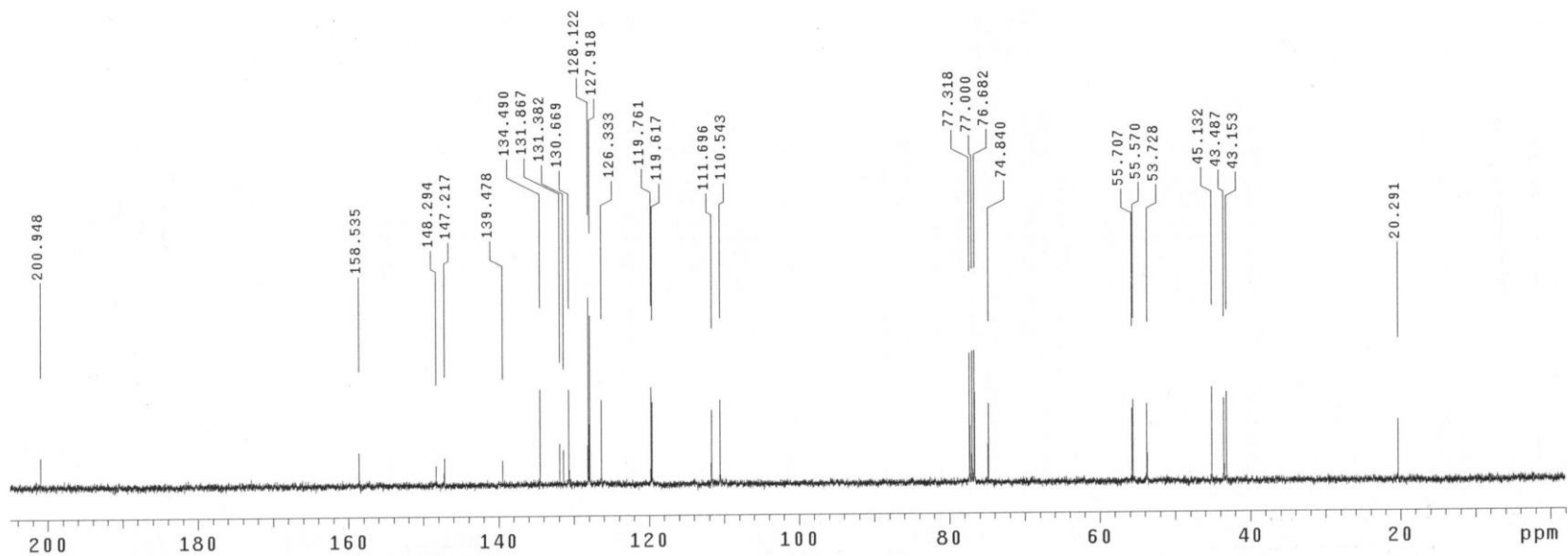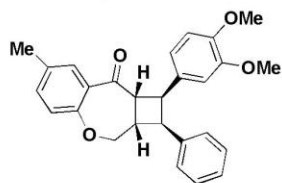

MC1080513

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 15 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
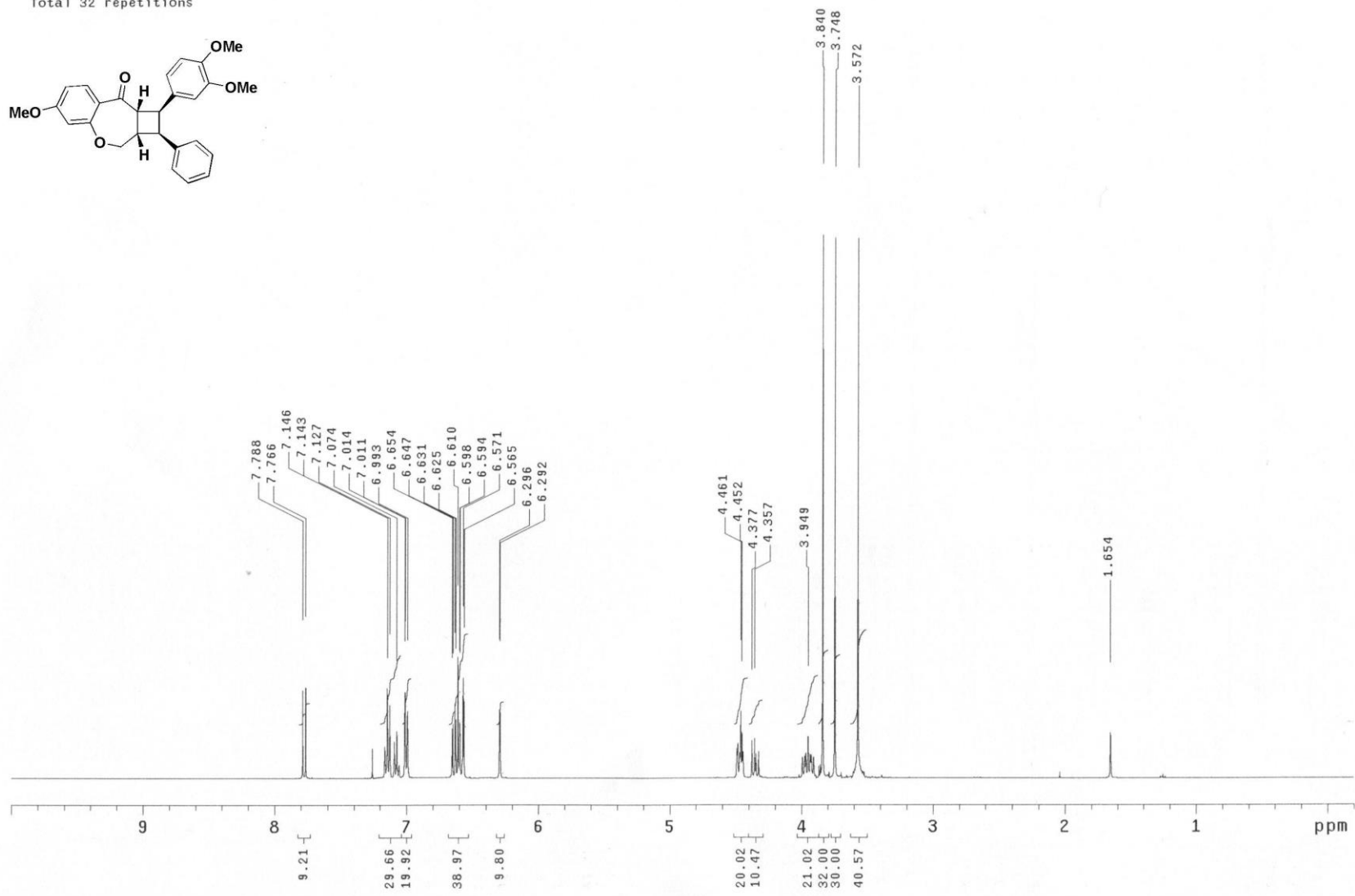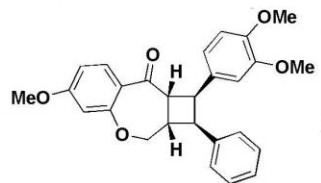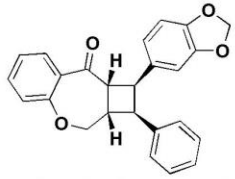
Compound 6g (¹³C-NMR spectral data)

Compound 6h (^{1}H-NMR spectral data)

MC1080426

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 28 2019
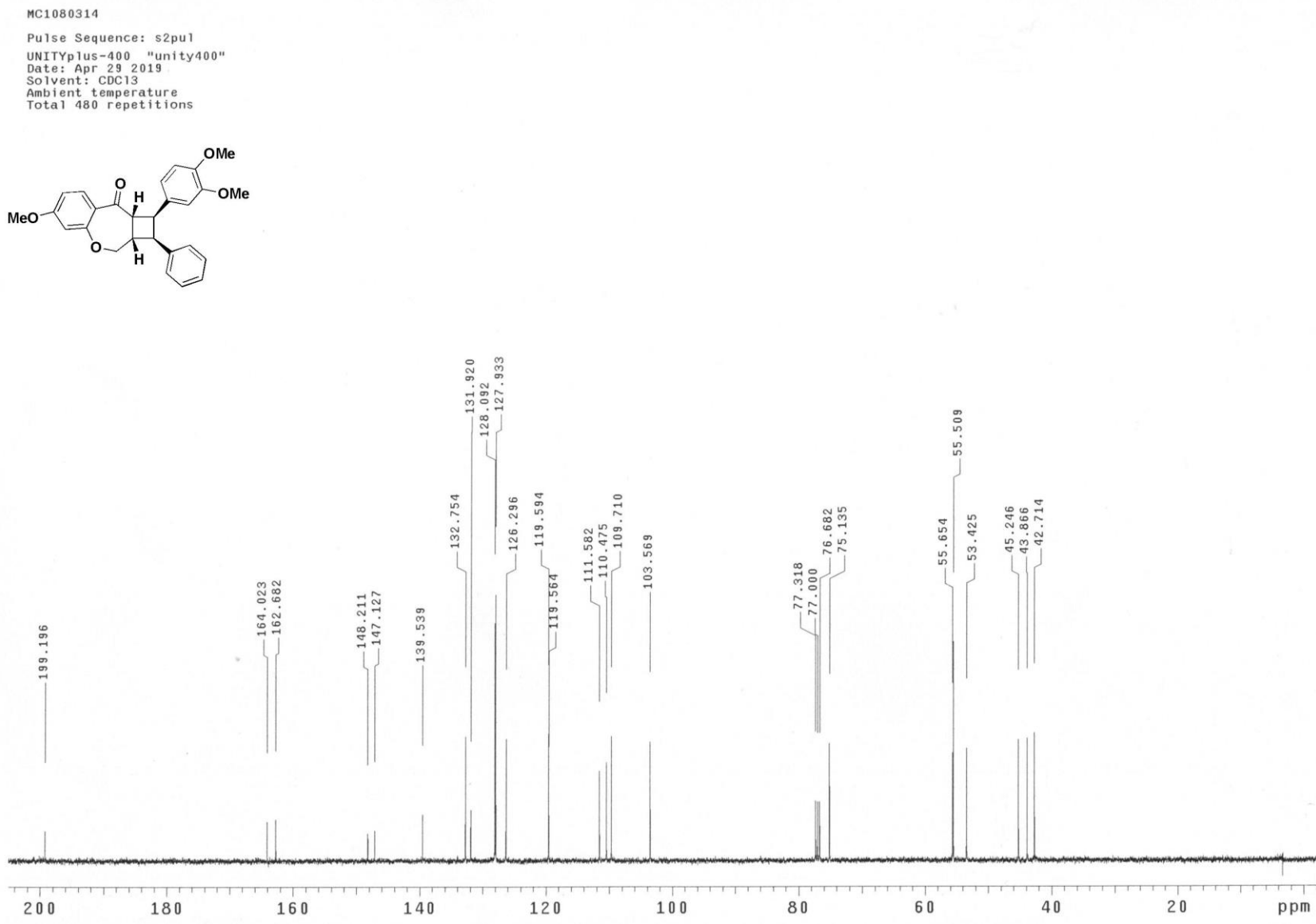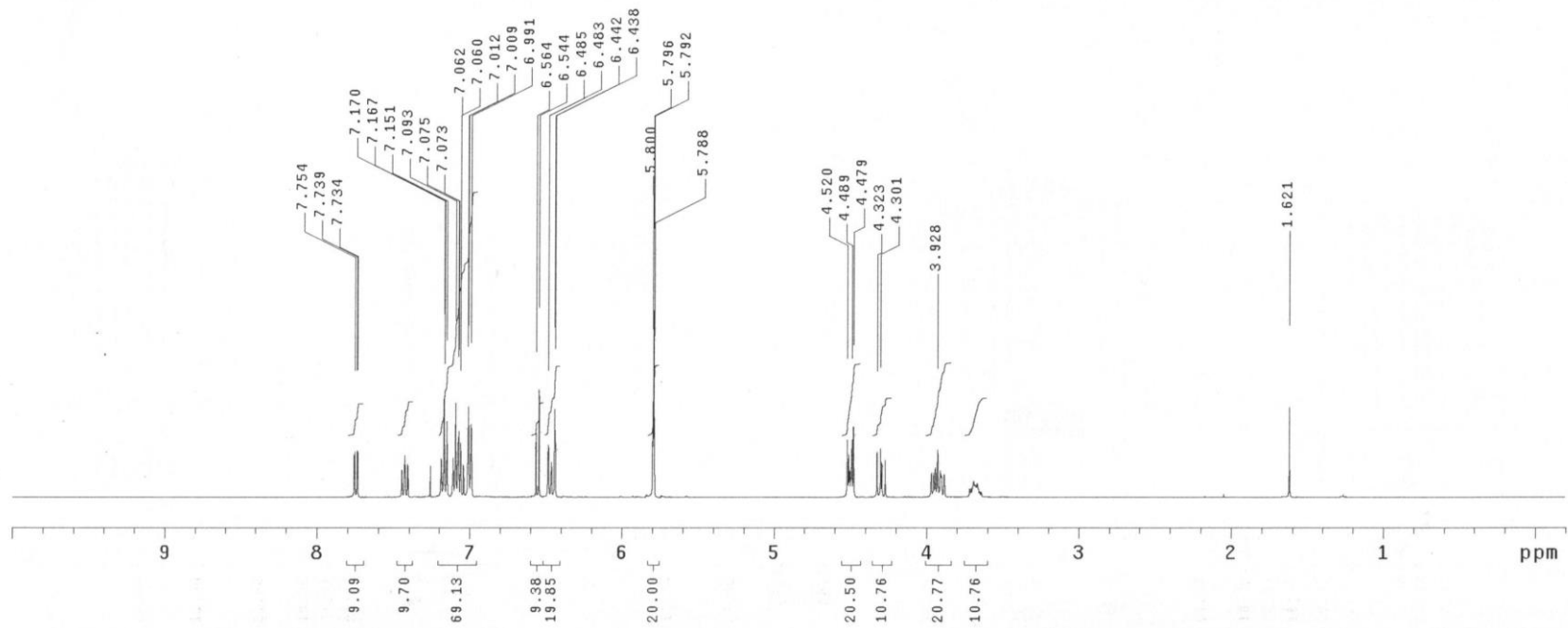Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.165
7.146
7.101
7.099
7.098
7.078
7.077
7.018
7.014
6.997
6.118
4.492
4.482
3.704
3.619

9.21
9.85
70.01
20.00
20.45
10.83
20.94
100.88

9   8   7   6   5   4   3   2   1   ppm

Compound 6h (^{13}C-NMR spectral data)

MC1080426

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 28 2019
Solvent: CDCl3
Ambient temperature
Total 176 repetitions

200.599
160.407
152.592
139.235
134.854
133.565
130.889
128.100
127.774
126.386
126.106
121.891
119.860
105.267
77.318
77.000
76.682
74.749
60.702
55.889
53.683
44.904
43.904
42.926

200 180 160 140 120 100 80 60 40 20 ppm

Compound 6i (^{1}H-NMR spectral data)

MC1080627

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 27 2019
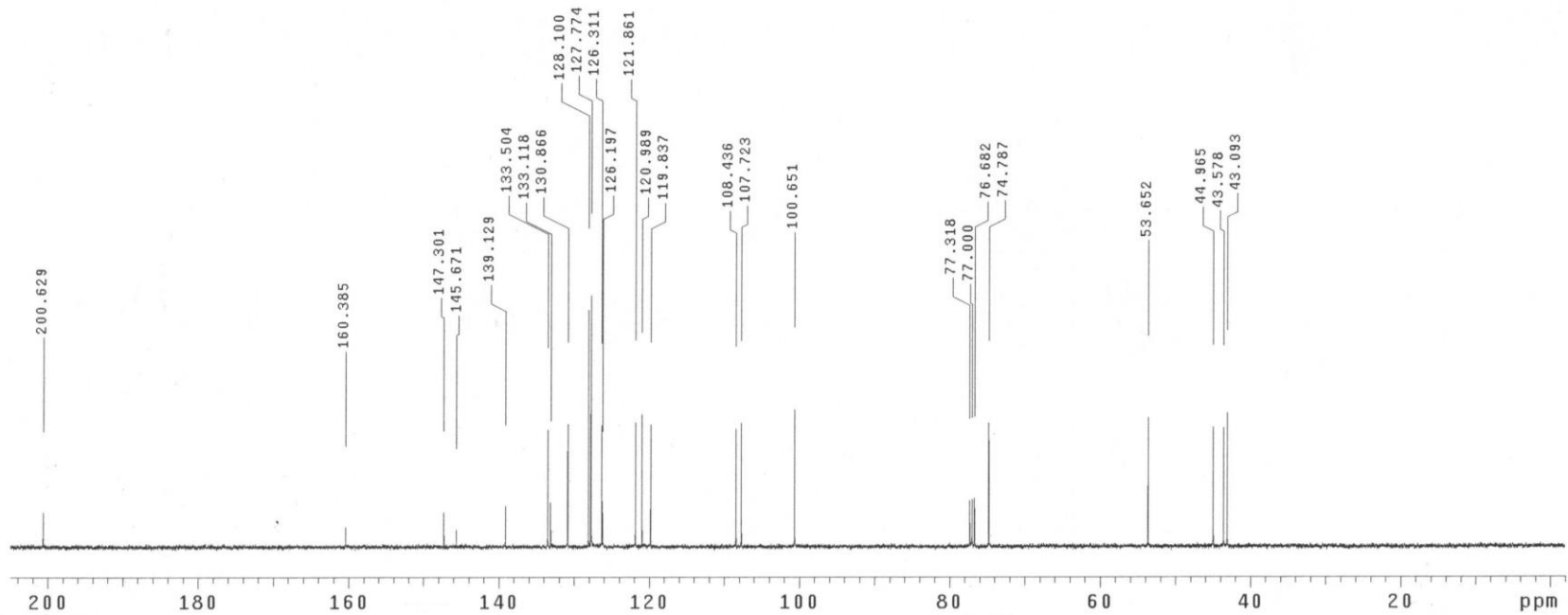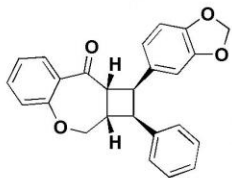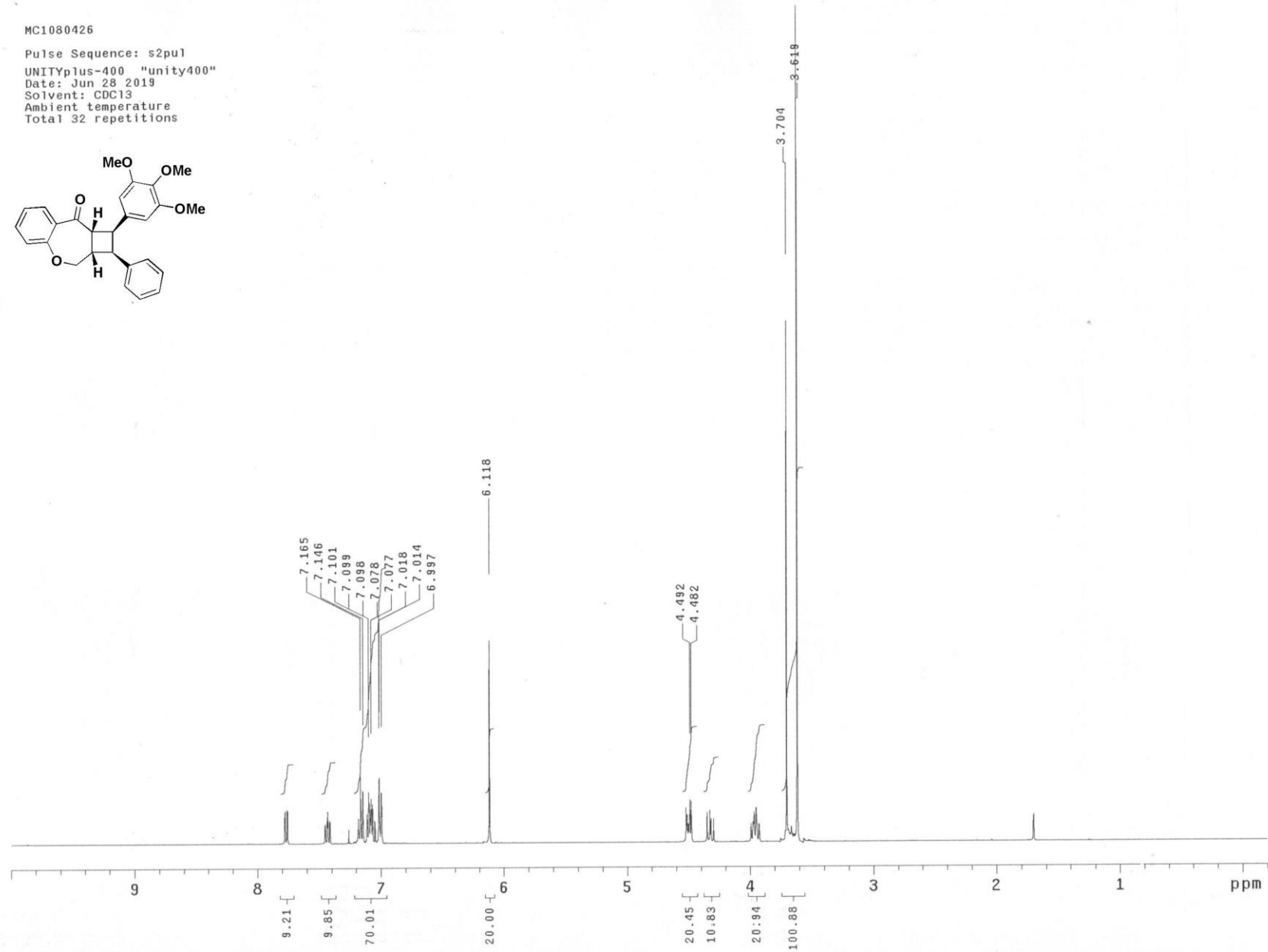Solvent: CDCl3
Ambient temperature
Total 32 repetitions

MeO

3.604

7.767
7.763
7.748
7.743
7.430

7.150
7.147
7.131
7.104
7.102
7.101
7.096
7.085
7.082
7.081

7.080
7.078
7.068
7.066
7.065
7.063
7.033
7.013
7.010
6.993

6.608
6.588
6.586
6.480
6.476

4.521
4.500
4.491
4.337
4.314

1.616

9.32
10.15
81.53
20.00
10.14
21.36
11.11
21.33
11.56
30.83

9 8 7 6 5 4 3 2 1 ppm

Compound 6i (^{13}C-NMR spectral data)
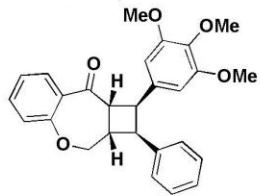
MC1080627

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 27 2019
Solvent: CDC13
Ambient temperature
Total 528 repetitions
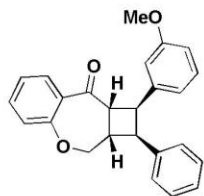
Compound 6j (^{1}H-NMR spectral data)

MC1080629

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 27 2019
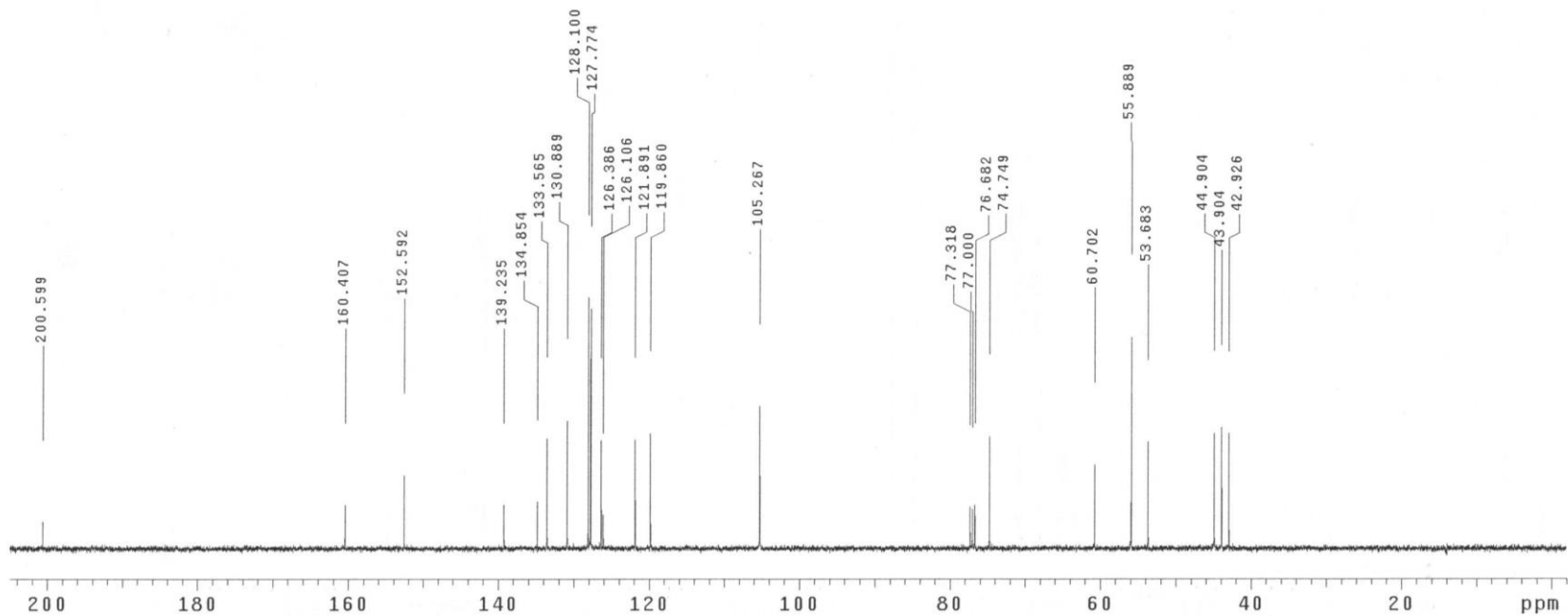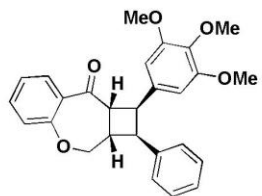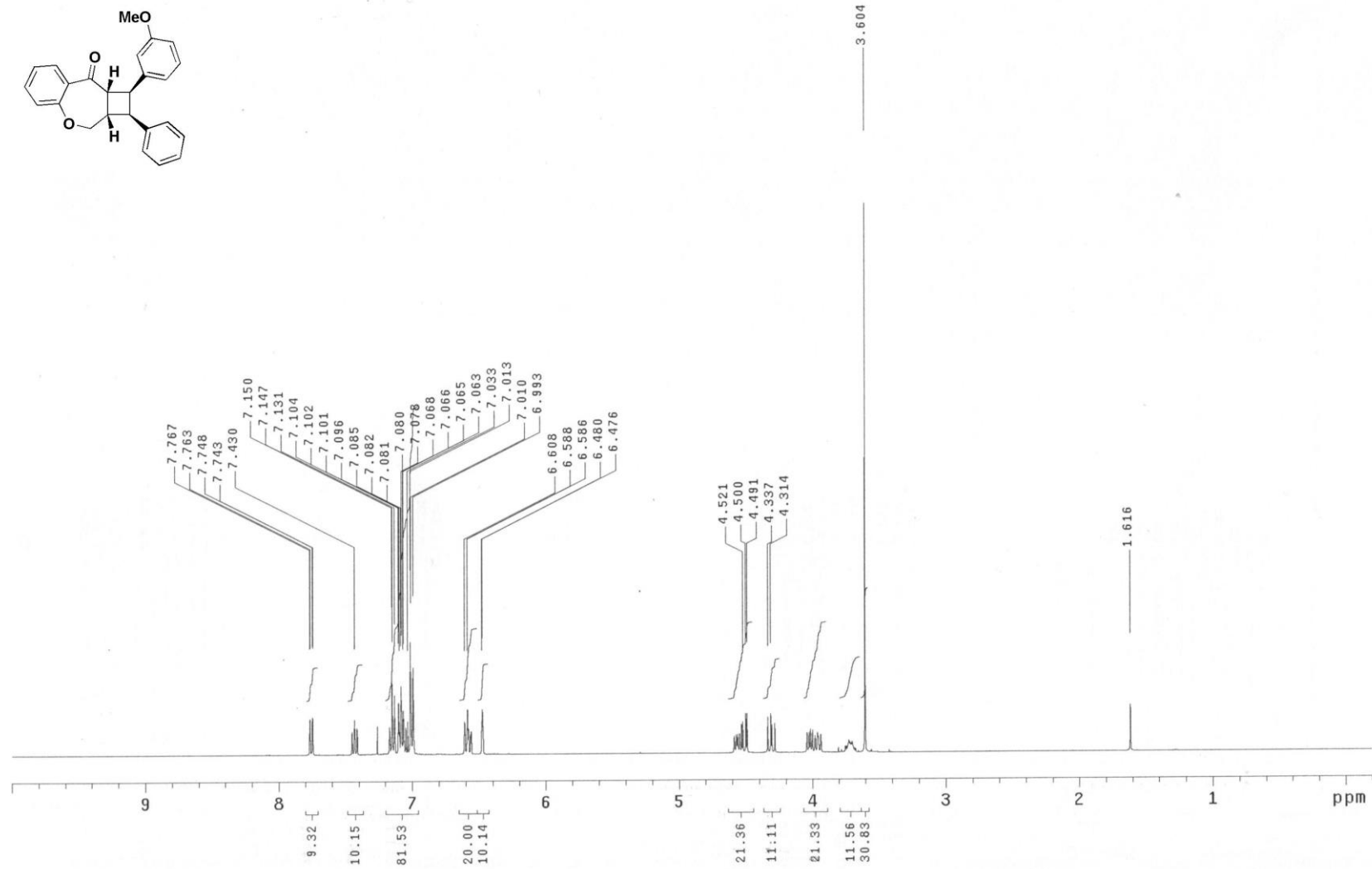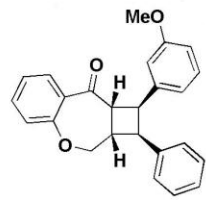Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Peaks: 7.142, 7.123, 7.077, 7.076, 6.987, 6.984, 6.967, 6.898, 6.876, 6.641, 6.619, 3.679, 1.599

Compound 6j (^{13}C-NMR spectral data)

MC1080629

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 27 2019
Solvent: CDC13
Ambient temperature
Total 1120 repetitions

200.788
160.430
157.800
139.311
133.451
131.276
130.859
128.949
128.039
127.827
126.326
126.212
121.853
119.822
113.371
77.318
77.000
76.682
74.870
55.070
53.667
44.995
43.191
43.070

200   180   160   140   120   100   80   60   40   20   ppm

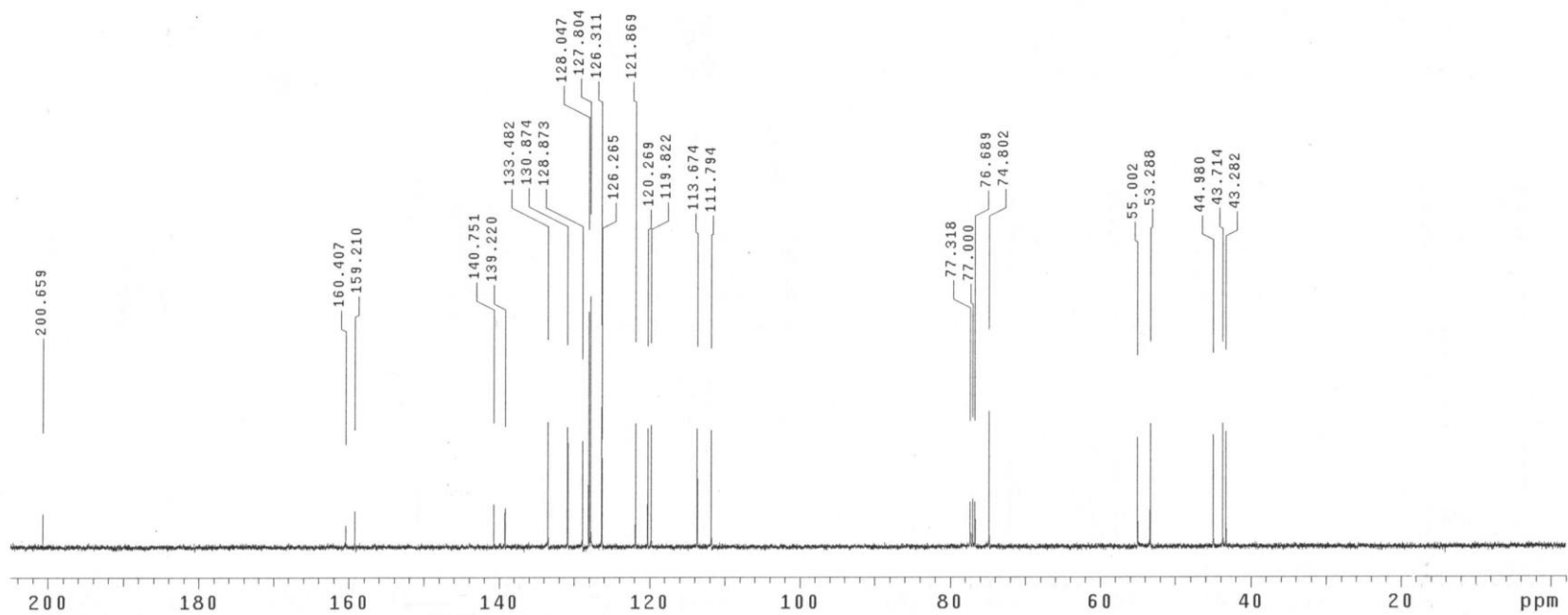# Compound 6k (¹H-NMR spectral data)

MC1080616

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 17 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.102
7.099
7.084
7.082
7.081
7.049
7.047
7.022
7.018
6.472
6.450
3.741
3.640
3.584

9.39
10.50
70.36
10.66
10.00
9.95
10.32
14.45
11.70
18.63
31.66
31.57

Compound 6k (^{13}C-NMR spectral data)

MC1080616

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
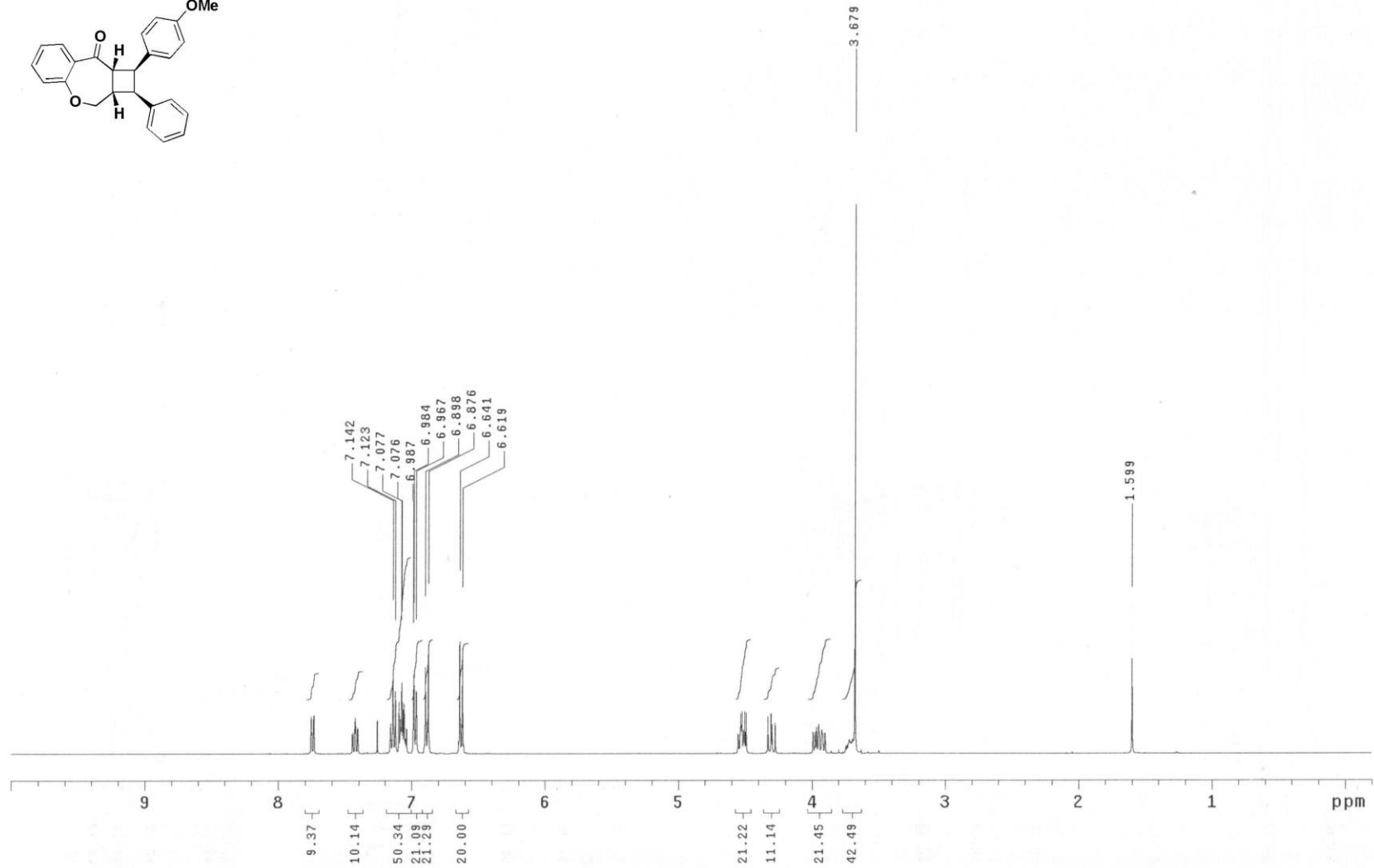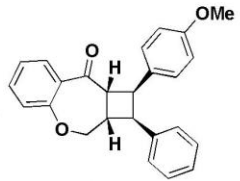Date: Jun 17 2019
Solvent: CDCl3
Ambient temperature
Total 544 repetitions

200.932
160.286
152.228
151.455
141.578
139.728
133.376
130.866
127.834
127.622
126.212
126.015
124.893
121.671
121.603
119.799
106.094
77.318
77.000
76.682
74.673
60.285
60.225
55.737
52.151
44.995
43.404
39.014

200   180   160   140   120   100   80   60   40   20   ppm

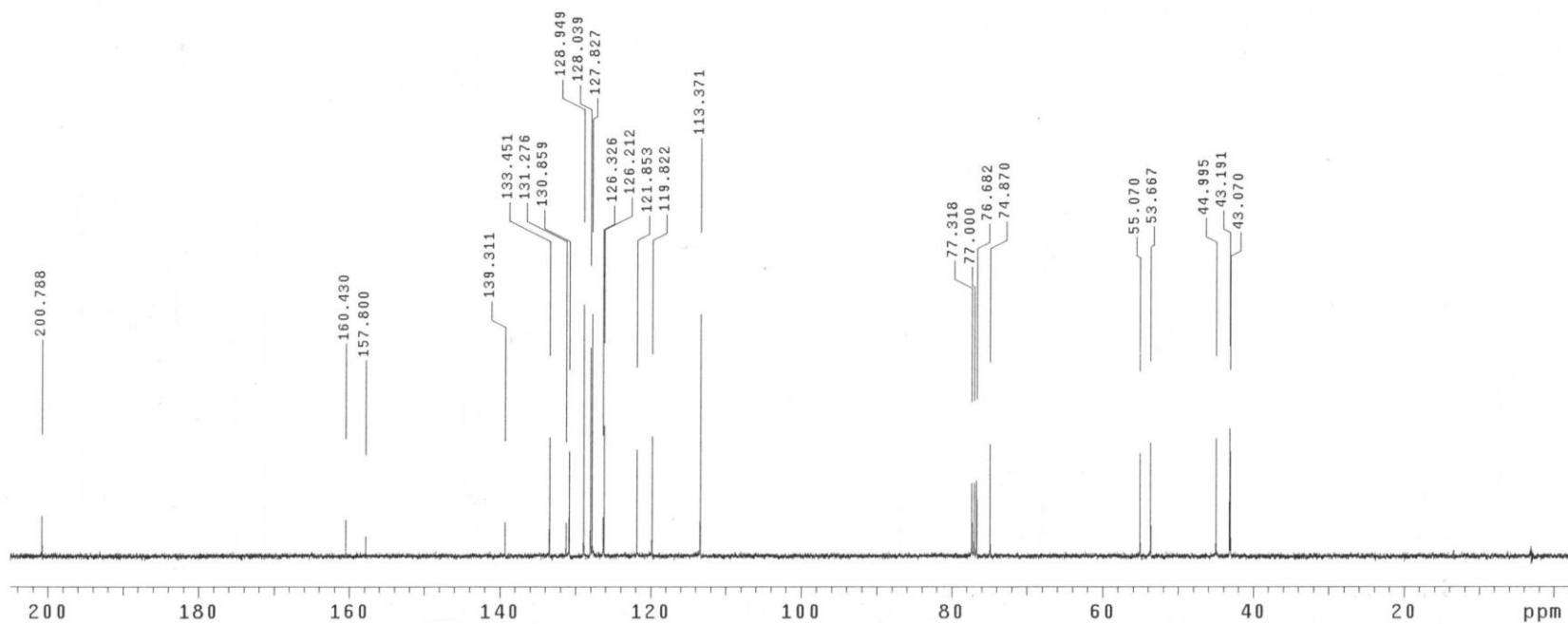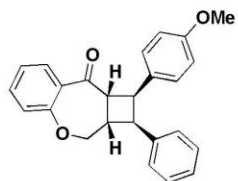# Compound 6l (^{1}H-NMR spectral data)

MC1080516

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 27 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions
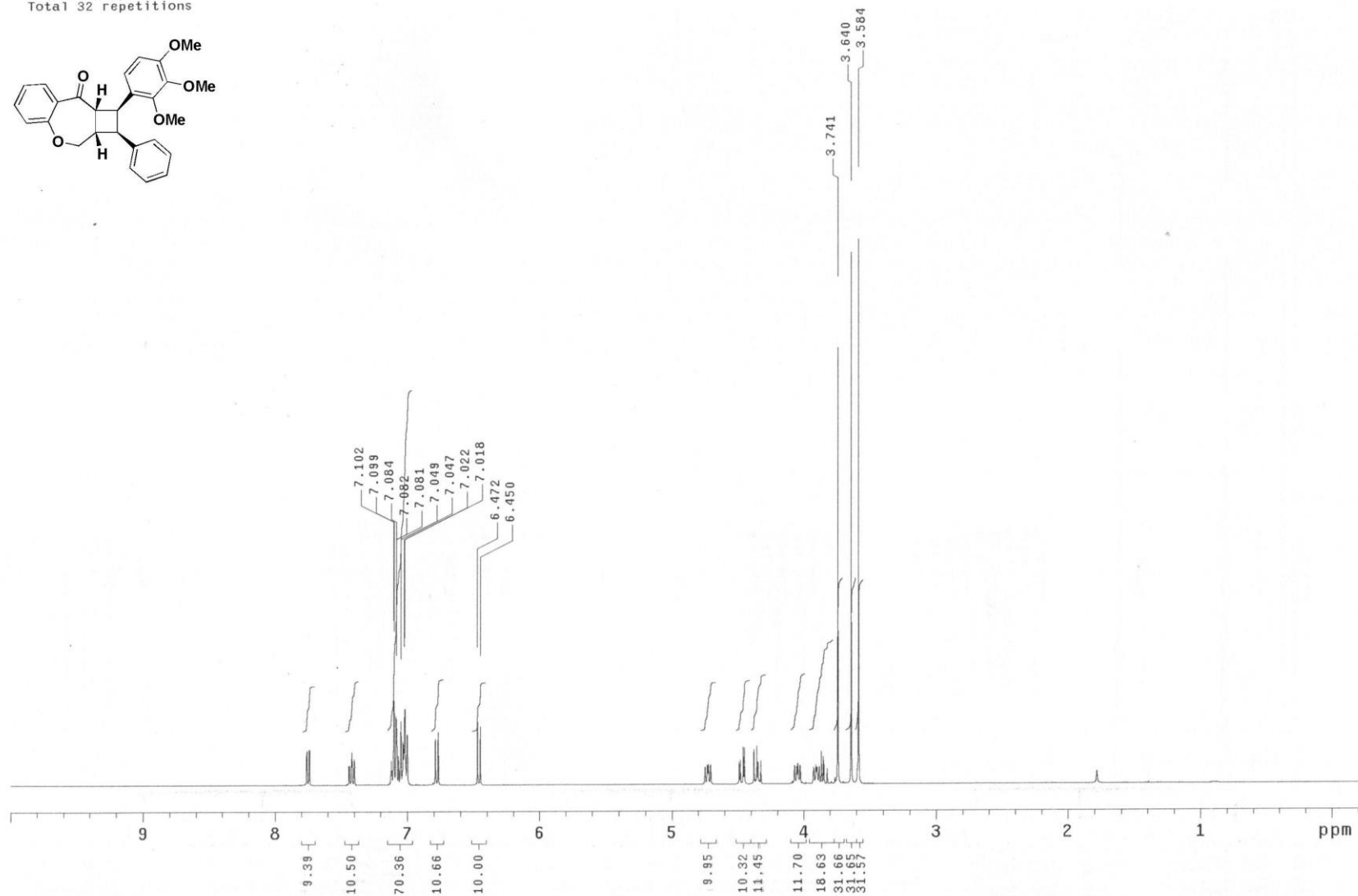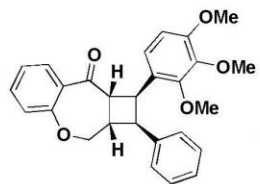
Compound 6I (^{13}C-NMR spectral data)

MC1080516

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: May 27 2019
Solvent: CDC13
Ambient temperature
Total 9808 repetitions

202.767
159.718
155.063
140.888
136.499
130.025
128.744
128.698
128.577
127.107
126.561
126.477
126.174
124.992
124.711
119.867
117.608
77.318
77.000
76.682
73.604
53.523
45.700
43.206
40.288

200   180   160   140   120   100   80   60   40   20   ppm

Compound 6m (^{1}H-NMR spectral data)

MC1080506

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 7 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.686
3.450

7.749
7.745
7.261
7.103
7.100
7.093
7.089
7.082
7.079
7.074
7.071
7.068
7.051
7.050
7.048
7.025
7.018
7.001
6.997
6.980
6.315
6.080
6.074
4.421
4.418
4.410
4.400
1.597

9.08
10.28
80.36
10.31
10.39
10.00
20.77
13.52
12.25
31.01
42.12

Compound 6m (^{13}C-NMR spectral data)

MC1080506

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 7 2019
Solvent: CDC13
Ambient temperature
Total 2064 repetitions

Compound 6n (¹H-NMR spectral data)

MC1080604

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 14 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6n (^{13}C-NMR spectral data)
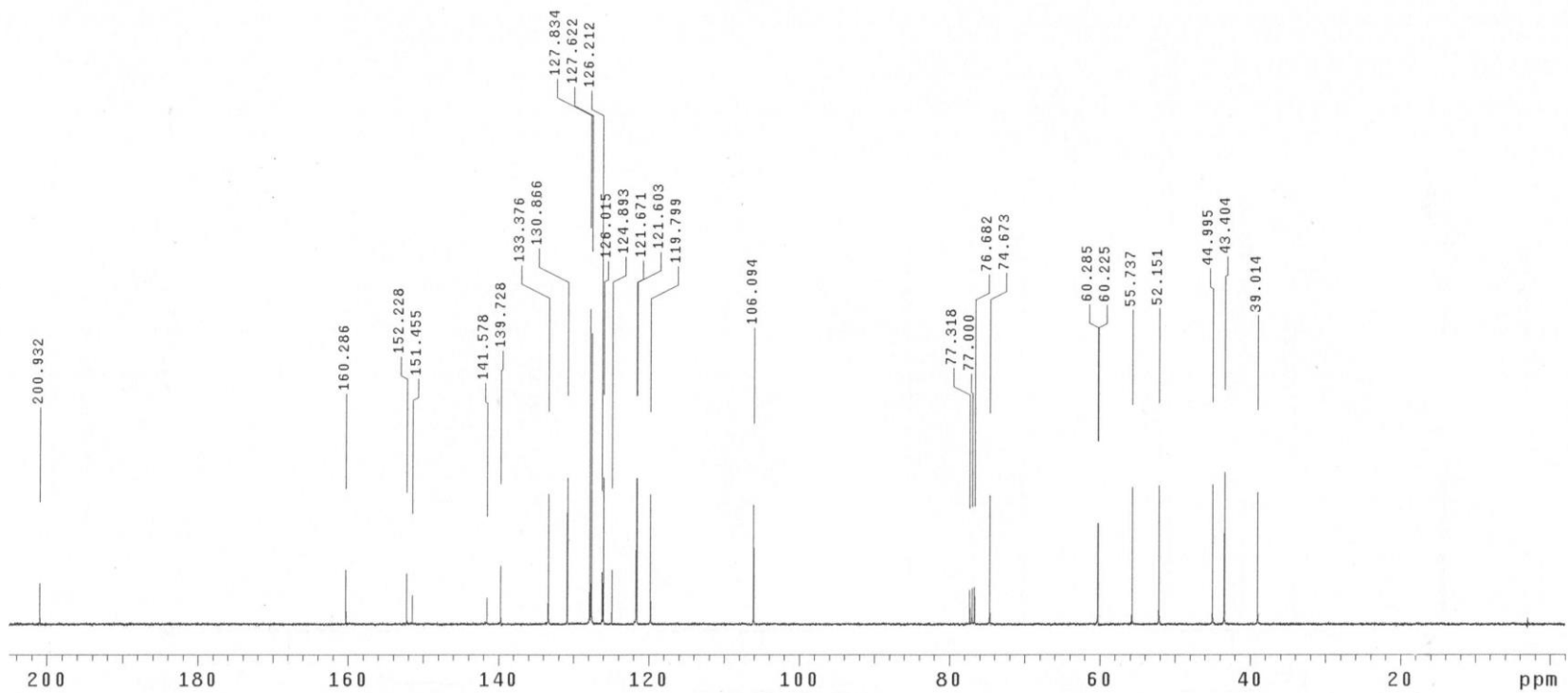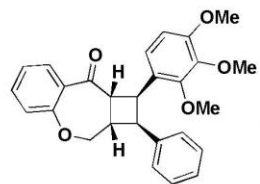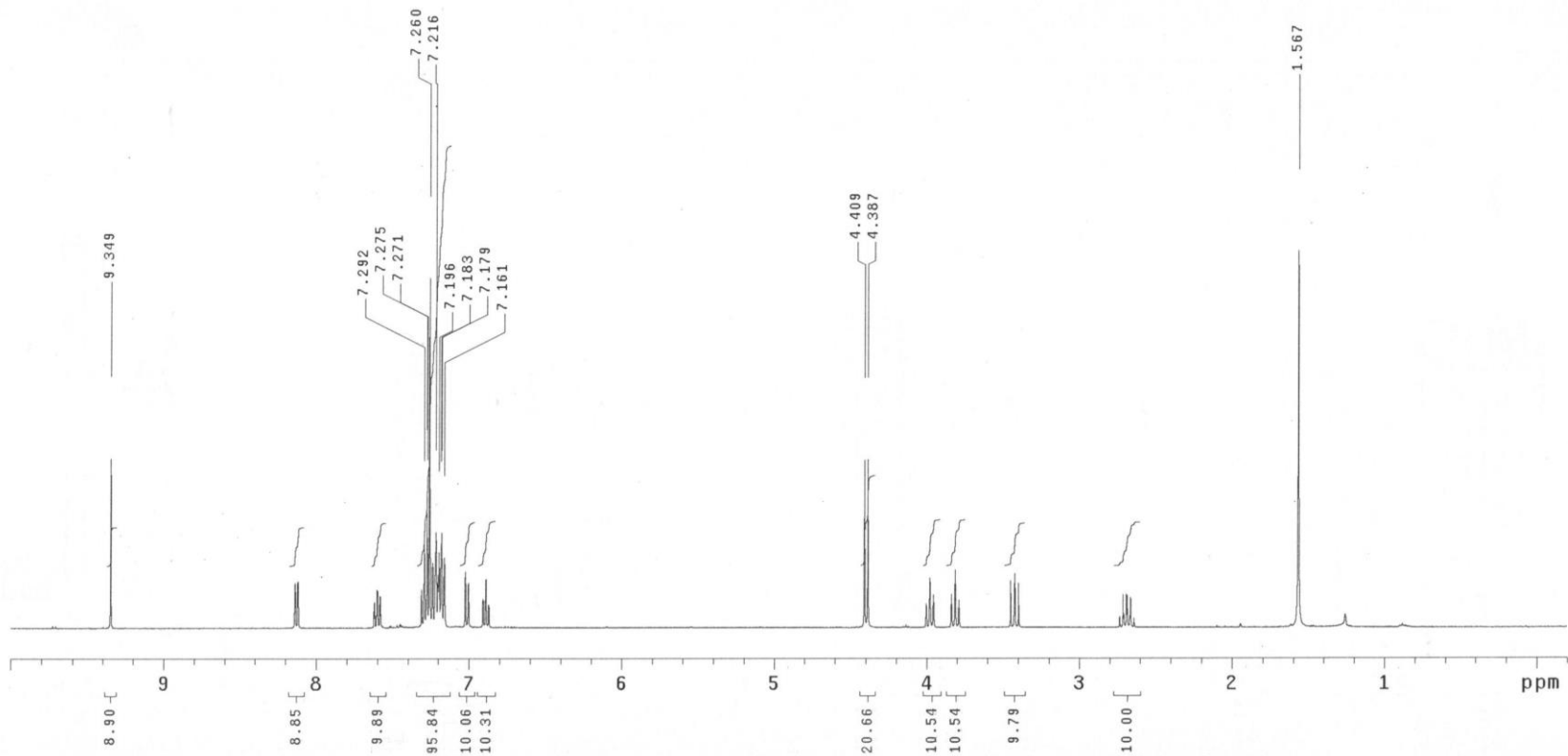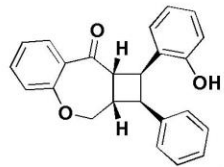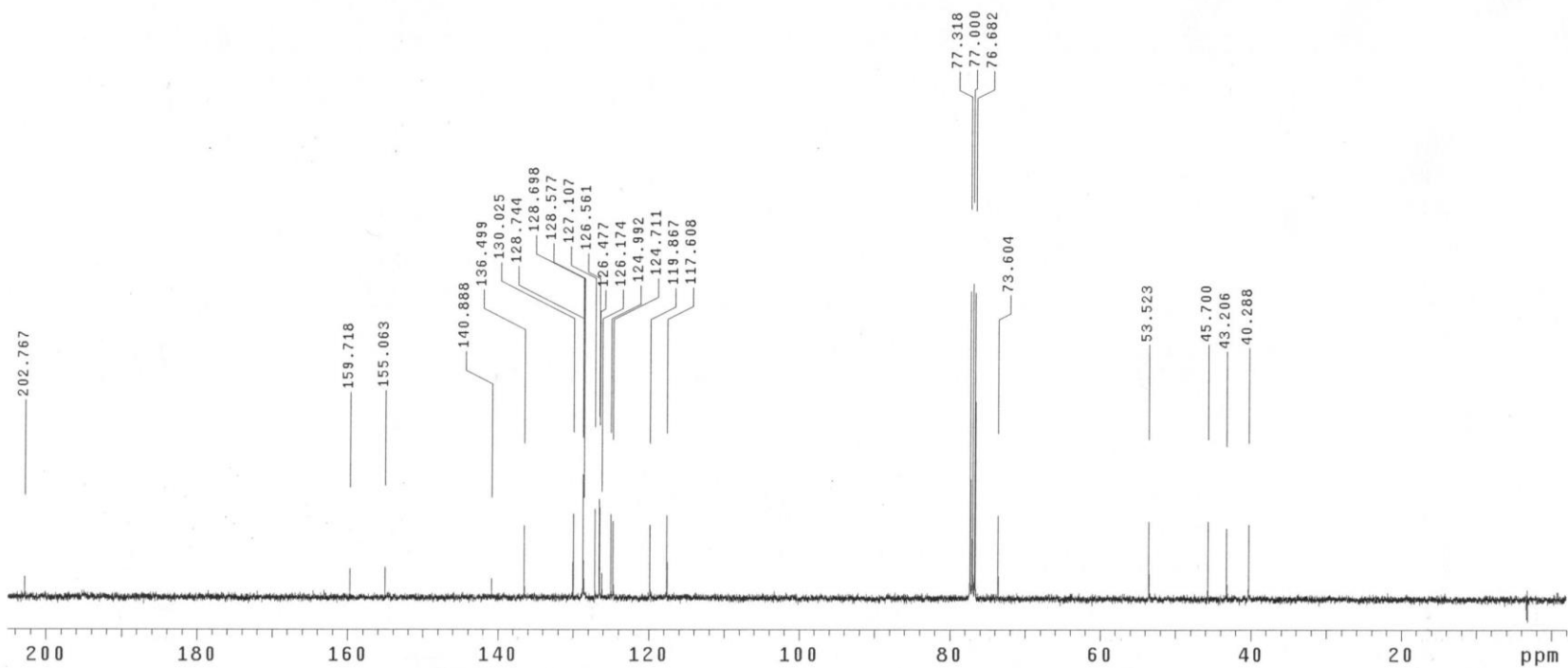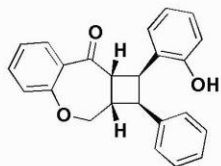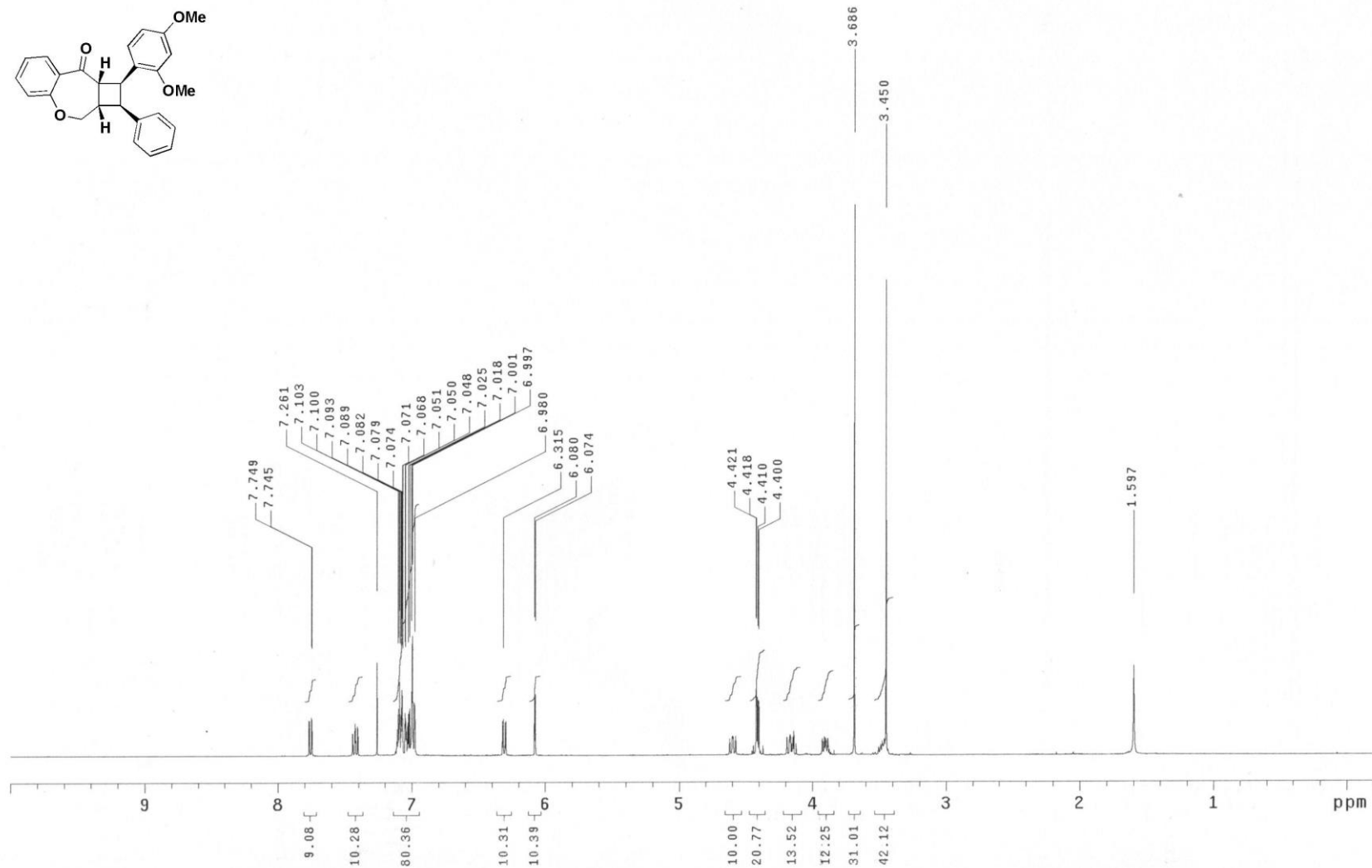
MC1080604

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 14 2019
Solvent: CDC13
Ambient temperature
Total 400 repetitions

Peaks: 199.977, 160.453, 147.164, 146.171, 138.257, 133.861, 130.942, 128.668, 128.403, 127.652, 126.856, 125.841, 123.112, 122.050, 120.011, 77.318, 77.000, 76.682, 74.597, 52.879, 45.086, 43.798, 43.009

Compound 6o (^{1}H-NMR spectral data)

MC1080430

Pulse Sequence: s2pul

Mercury-400BB "MerPlus400"
Date: May 22 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
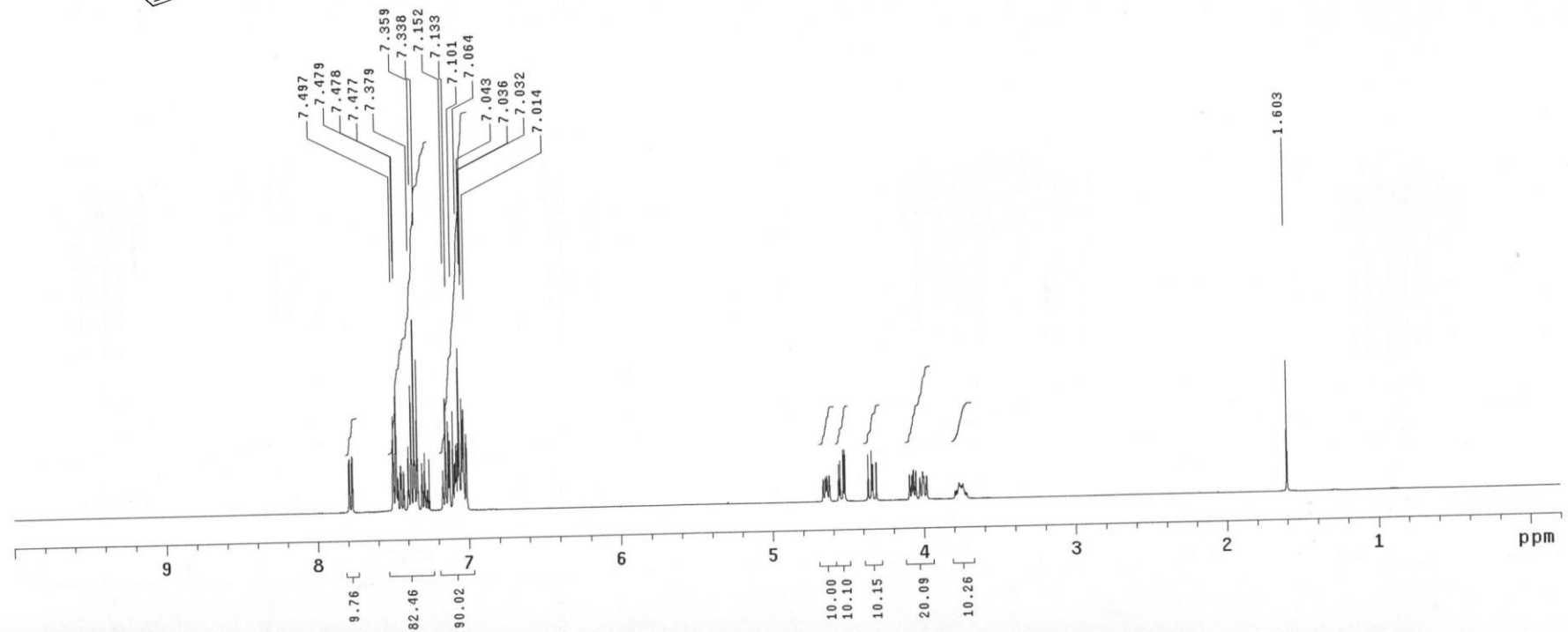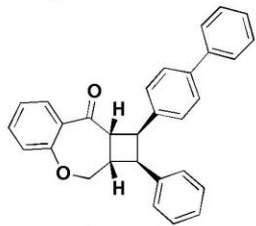
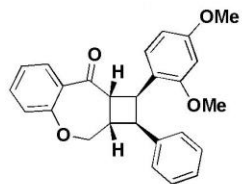# Compound 6o (^{13}C-NMR spectral data)

MC1080430

Pulse Sequence: s2pul

Mercury-400BB "MerPlus400"
Date: May 22 2019
Solvent: cdcl3
Ambient temperature
Total 400 repetitions

200.700
160.429
140.654
139.157
138.707
138.310
133.511
130.881
128.606
128.354
128.090
127.823
127.014
126.800
126.548
126.327
126.250
121.887
119.841
77.317
77.000
76.683
74.835
53.366
45.020
43.470
43.329
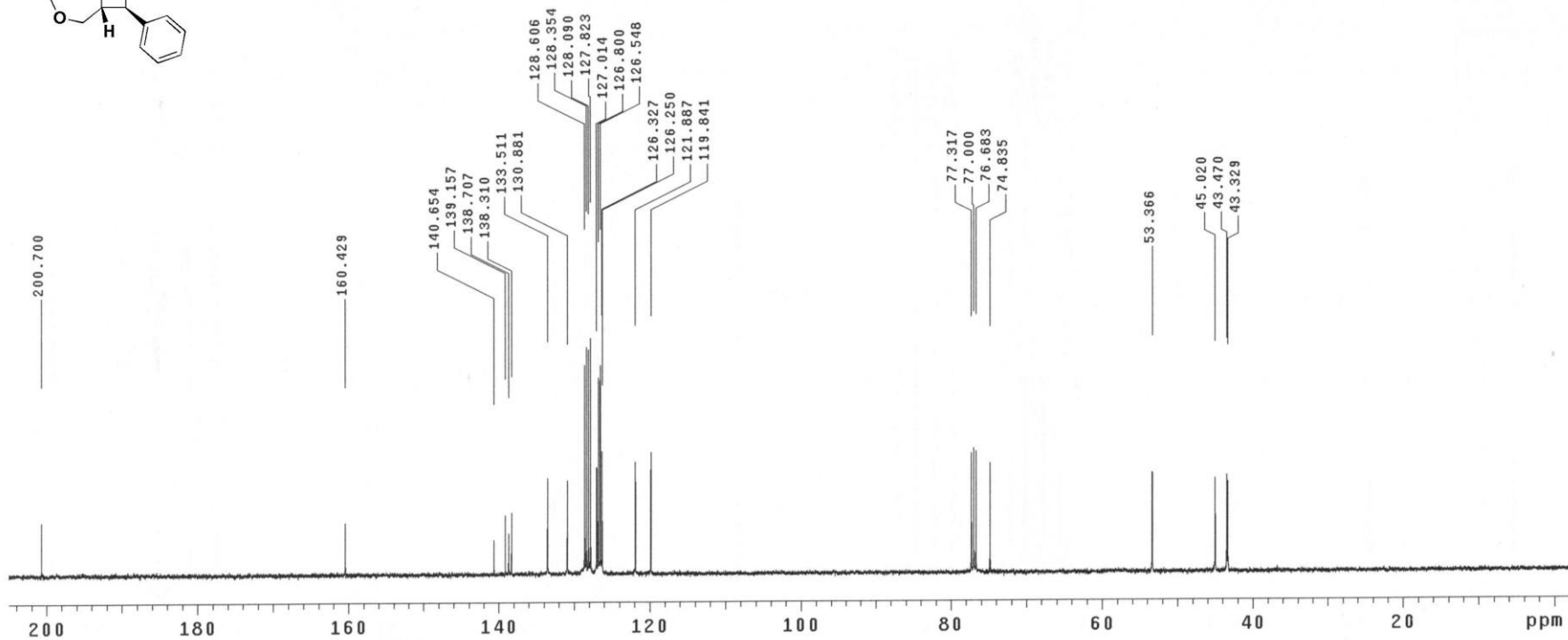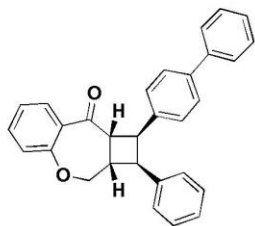
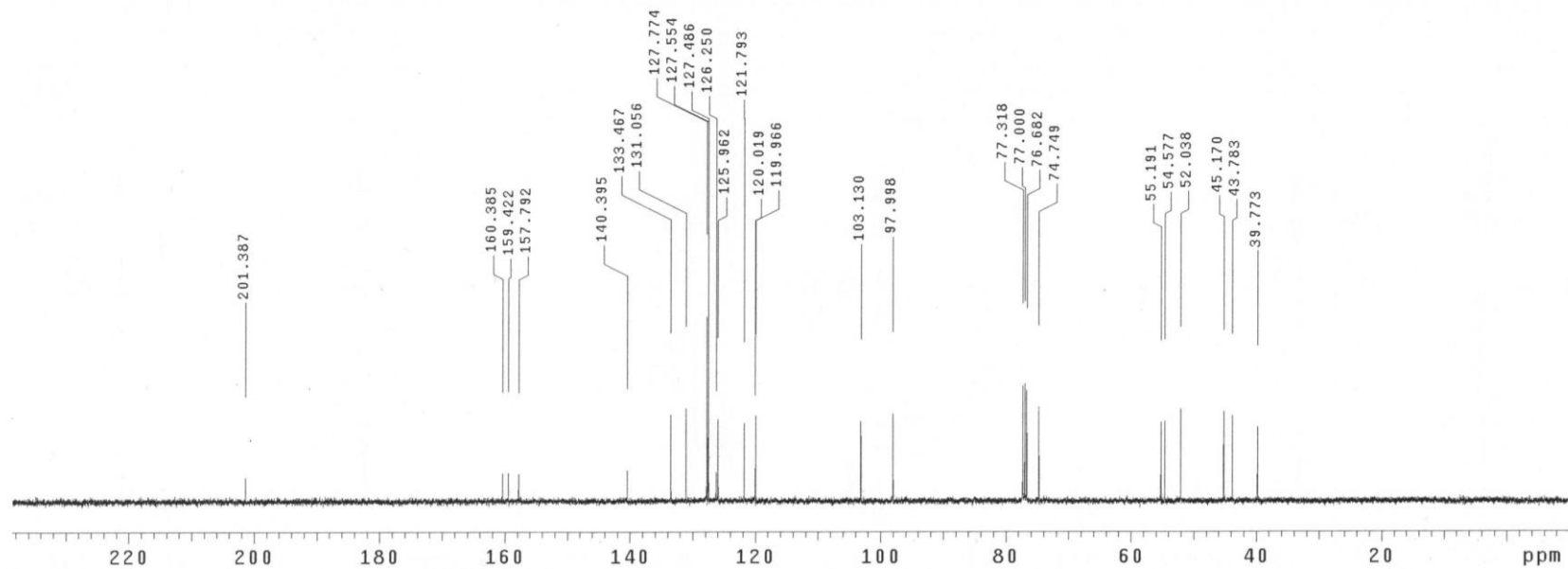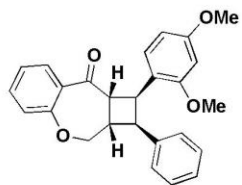# Compound 6p (¹H-NMR spectral data)

MC10806C12

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 11 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
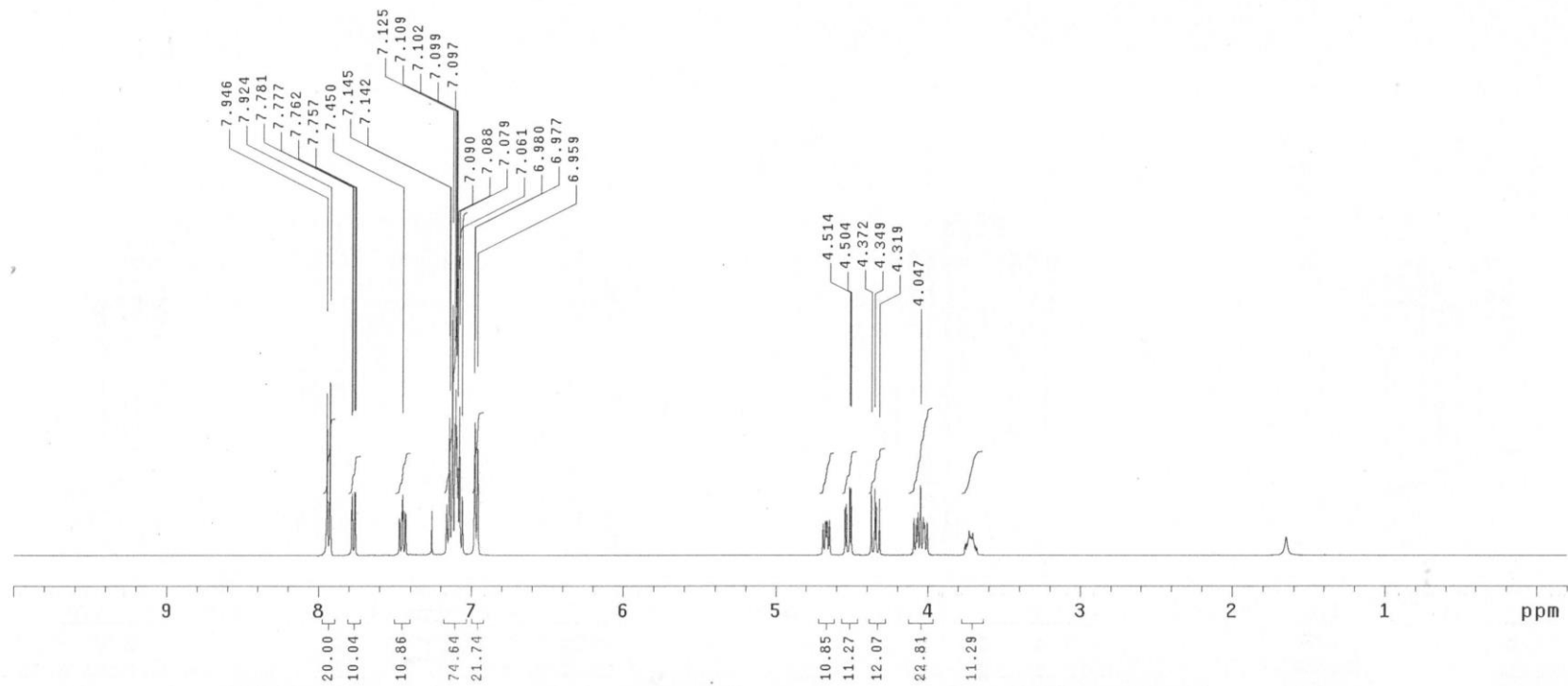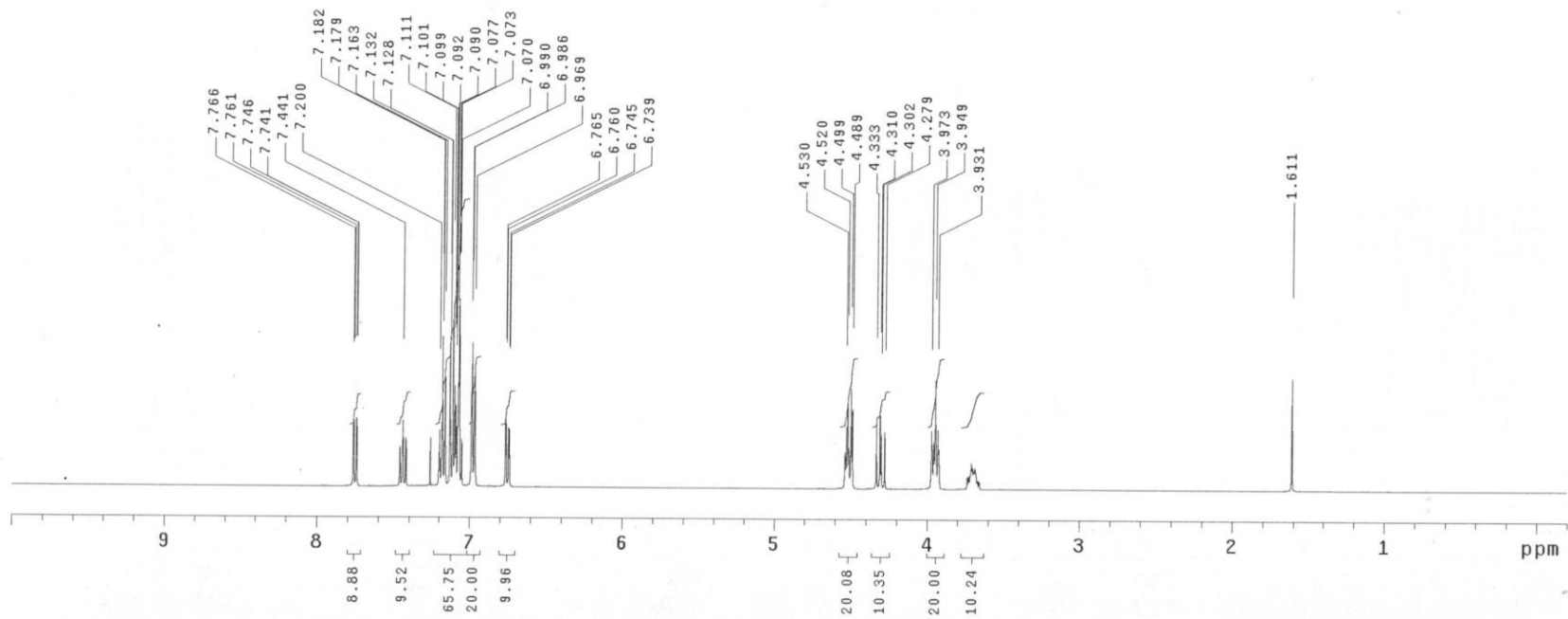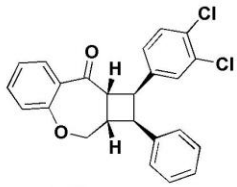
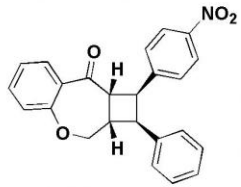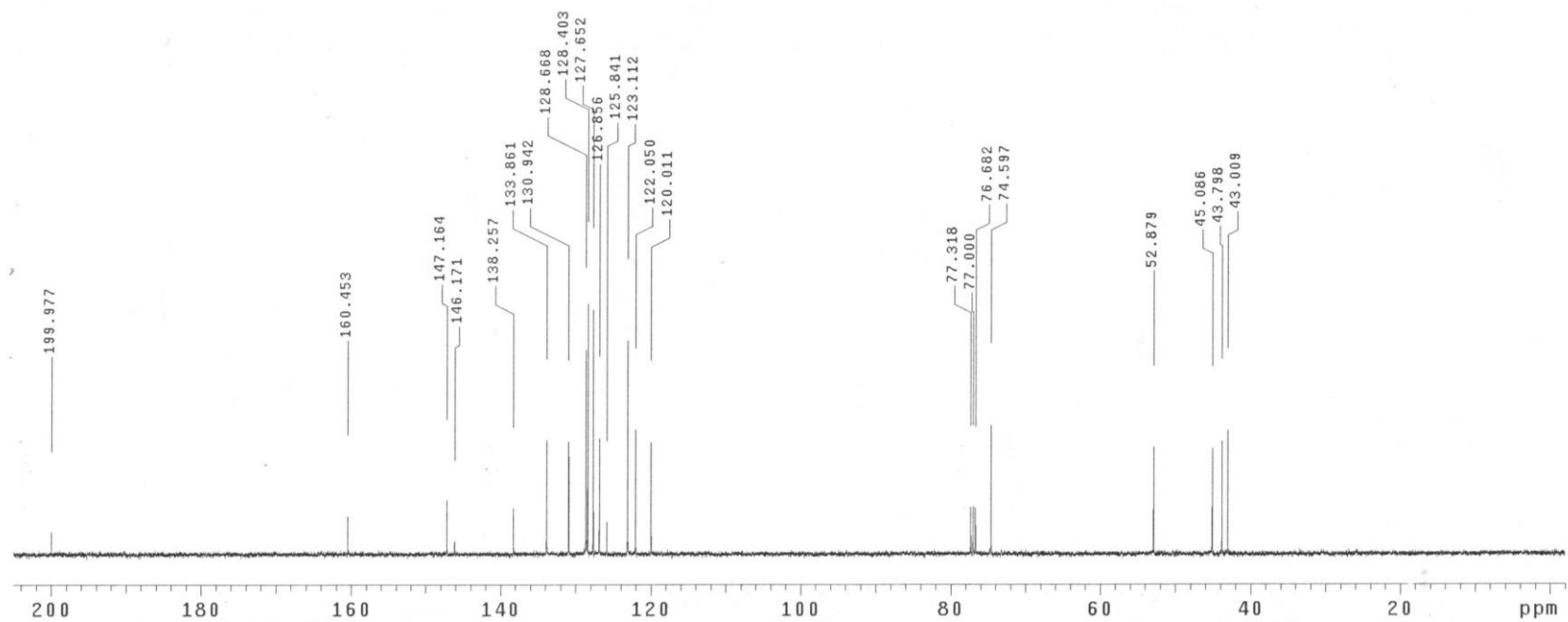# Compound 6p (^{13}C-NMR spectral data)

MC10806C12

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jul 11 2019
Solvent: CDC13
Ambient temperature
Total 576 repetitions

Peaks labeled: 200.136, 160.415, 139.629, 138.364, 133.739, 131.943, 130.912, 130.010, 129.828, 129.782, 128.357, 127.713, 127.417, 126.750, 125.970, 121.990, 119.936, 77.318, 77.000, 76.689, 74.650, 53.061, 44.829, 43.032, 42.896

Compound 6q (¹H-NMR spectral data)

MC1080515

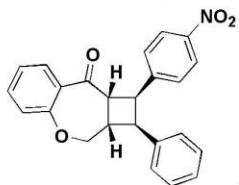Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 20 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.813
7.809
7.793
7.789
7.718
7.699
7.659
7.658
7.561
7.518
7.497
7.453
7.408
7.405
7.389
7.385
7.381
7.362
7.142
7.140
7.121
7.119
7.105
7.103
7.084
7.066
7.034
7.016
6.996
6.992
6.975
6.971

4.542
4.532
4.393
4.370

1.616

9.59
19.39
49.24
75.97
9.73
10.11
10.29
10.16
10.00
10.03

9 8 7 6 5 4 3 2 1 ppm
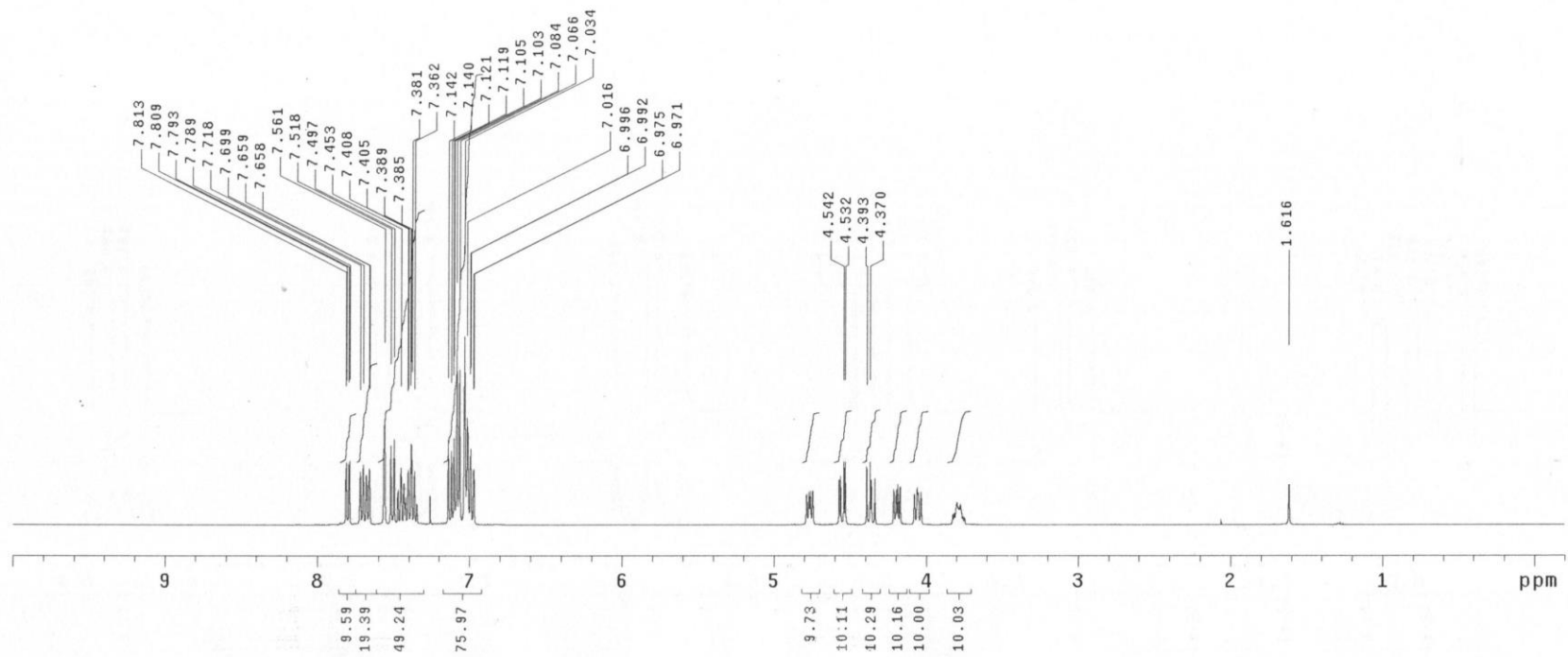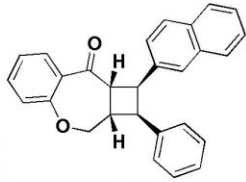
Compound 6q (^{13}C-NMR spectral data)

MC1080515

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: May 20 2019
Solvent: CDC13
Ambient temperature
Total 1104 repetitions

200.720
160.460
139.159
136.840
133.527
133.118
131.867
130.920
128.069
127.804
127.577
127.402
126.690
126.311
126.273
125.985
125.742
125.295
121.899
119.860
77.318
77.000
76.689
74.840
53.258
45.041
43.851
43.487

200   180   160   140   120   100   80   60   40   20   ppm

Compound 6r (^{1}H-NMR spectral data)

MC1080508

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 9 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.726
7.724
7.721
7.707
7.705
7.702
7.701
7.419
7.417
7.414
7.401
7.396
7.221

7.204
7.200
7.185
7.159
7.141
7.123
7.120
7.118
7.116
7.080
7.078
7.077
7.069
7.065
7.064
7.058

7.054
7.047
7.039

6.125
6.121
6.118
6.117
6.113
6.112
5.956
5.954
5.949
5.947

4.587
4.576
4.557
4.547
4.148
4.120
4.090
3.933
3.923
3.776

1.624

9   8   7   6   5   4   3   2   1   ppm

9.30   10.28   78.69   8.86 9.29   20.65   11.01 11.01 10.00 10.77

Compound 6r (^{13}C-NMR spectral data)

199.780
160.483
153.312
141.487
138.849
133.338
130.556
128.009
127.175
126.500
126.424
121.709
119.678
109.990
107.291
77.318
77.000
76.682
74.946
52.106
44.647
43.222
37.476

200 180 160 140 120 100 80 60 40 20 ppm

Compound 6s (^{1}H-NMR spectral data)

MC1080520

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 21 2019
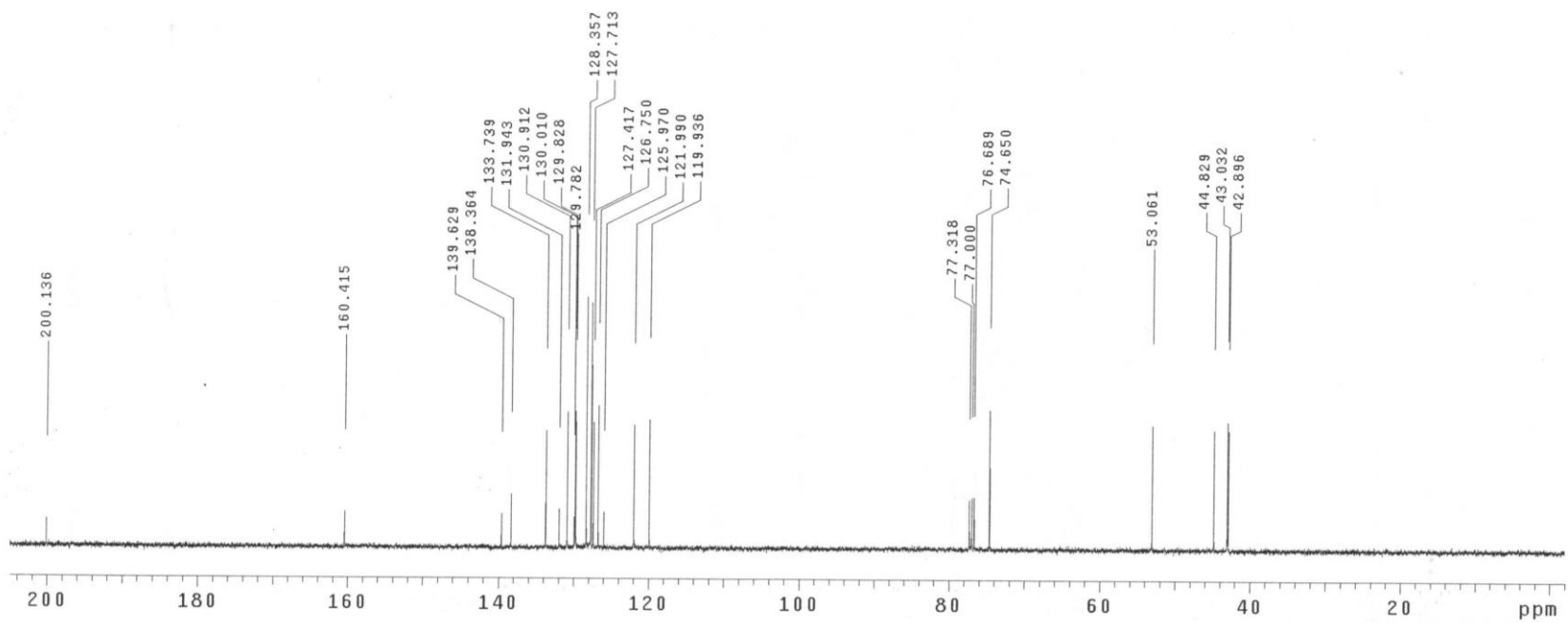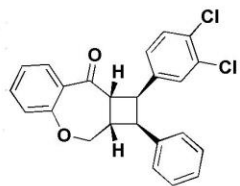Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.764
7.760
7.745
7.740
7.440
7.438
7.204
7.200
7.185
7.159
7.142
7.108
7.106
7.098
7.088
7.086
7.080
7.078
7.076
7.072
7.068
7.061
7.058
7.051
6.985
6.982
6.973
6.969
6.776
6.768
6.764
6.755
6.673
6.670
6.668
6.661

3.923
3.919
3.914
3.907
3.893

8.95 9.92 67.75 8.07 9.03 9.22   9.36 10.28 10.45 30.00

9   8   7   6   5   4   3   2   1   ppm

S-122
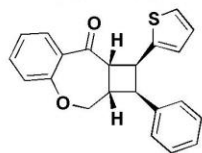
Compound 6s (^{13}C-NMR spectral data)

Mc1080520
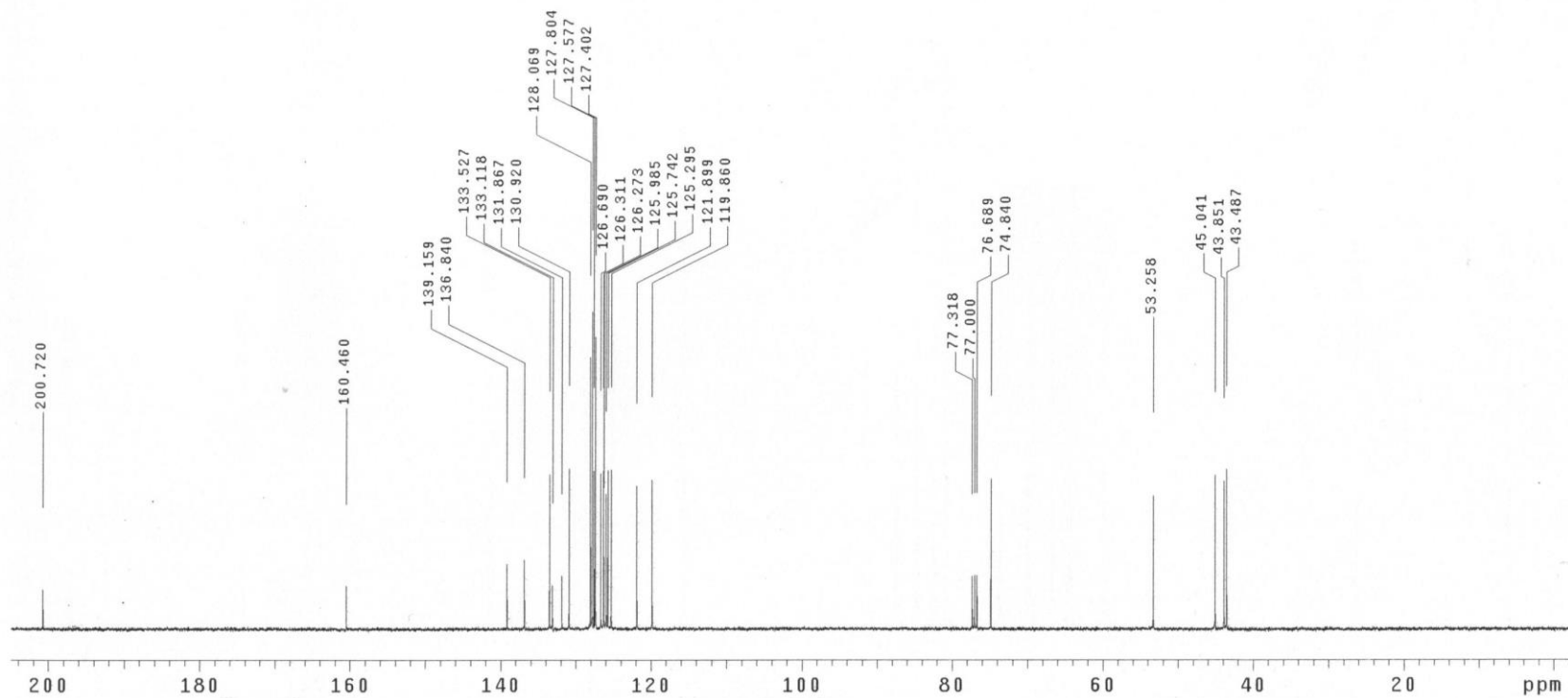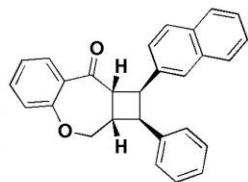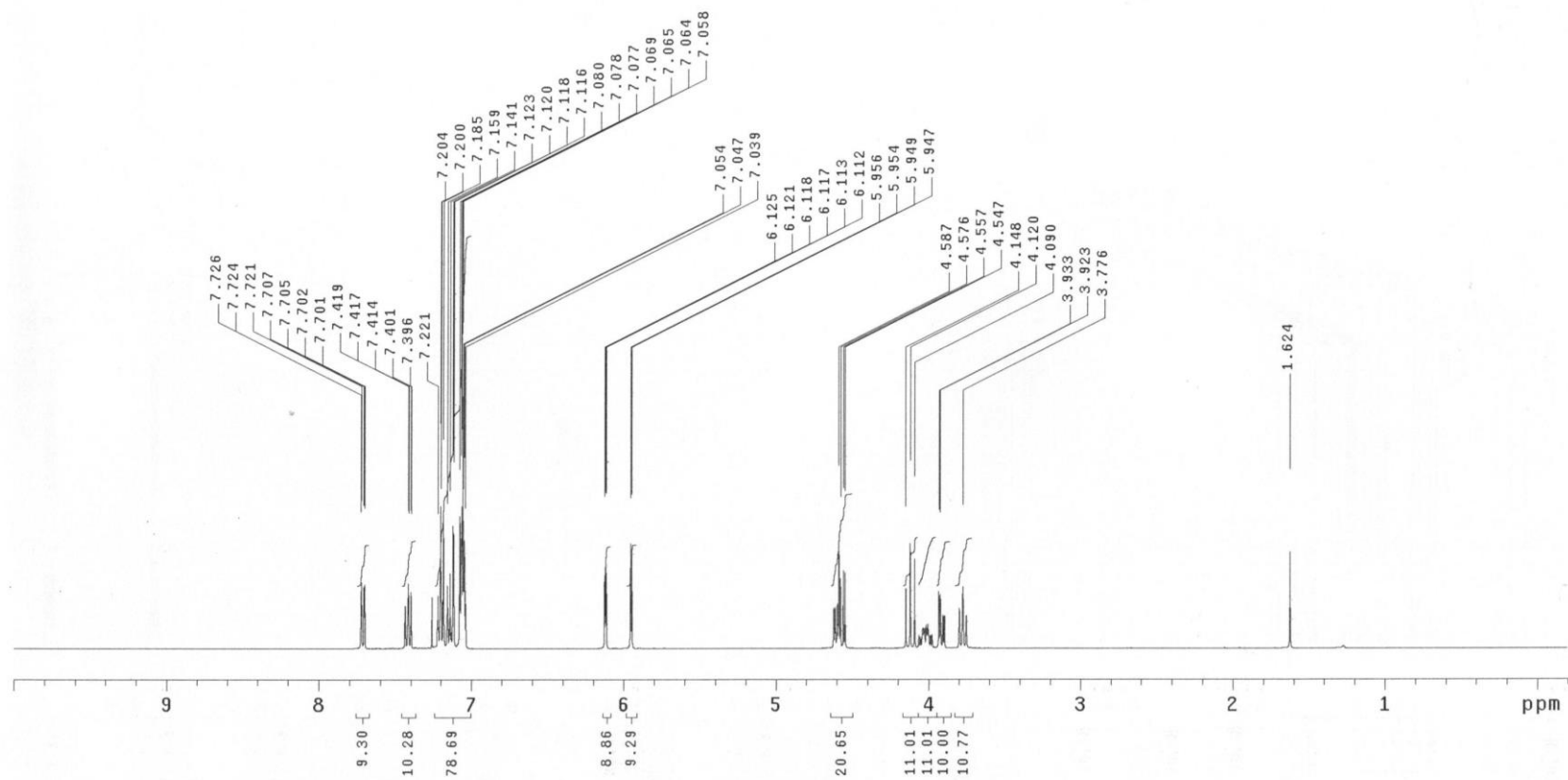
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 21 2019
Solvent: CDCl3
Ambient temperature
Total 304 repetitions

Peaks: 199.659, 160.453, 142.722, 138.386, 133.451, 130.692, 128.024, 127.599, 126.568, 126.402, 126.250, 124.999, 123.946, 121.846, 119.761, 77.318, 77.000, 76.682, 74.794, 55.161, 45.374, 42.577, 39.492

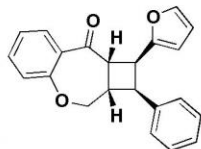200 180 160 140 120 100 80 60 40 20 ppm

Compound 6t (¹H-NMR spectral data)

MC1080521
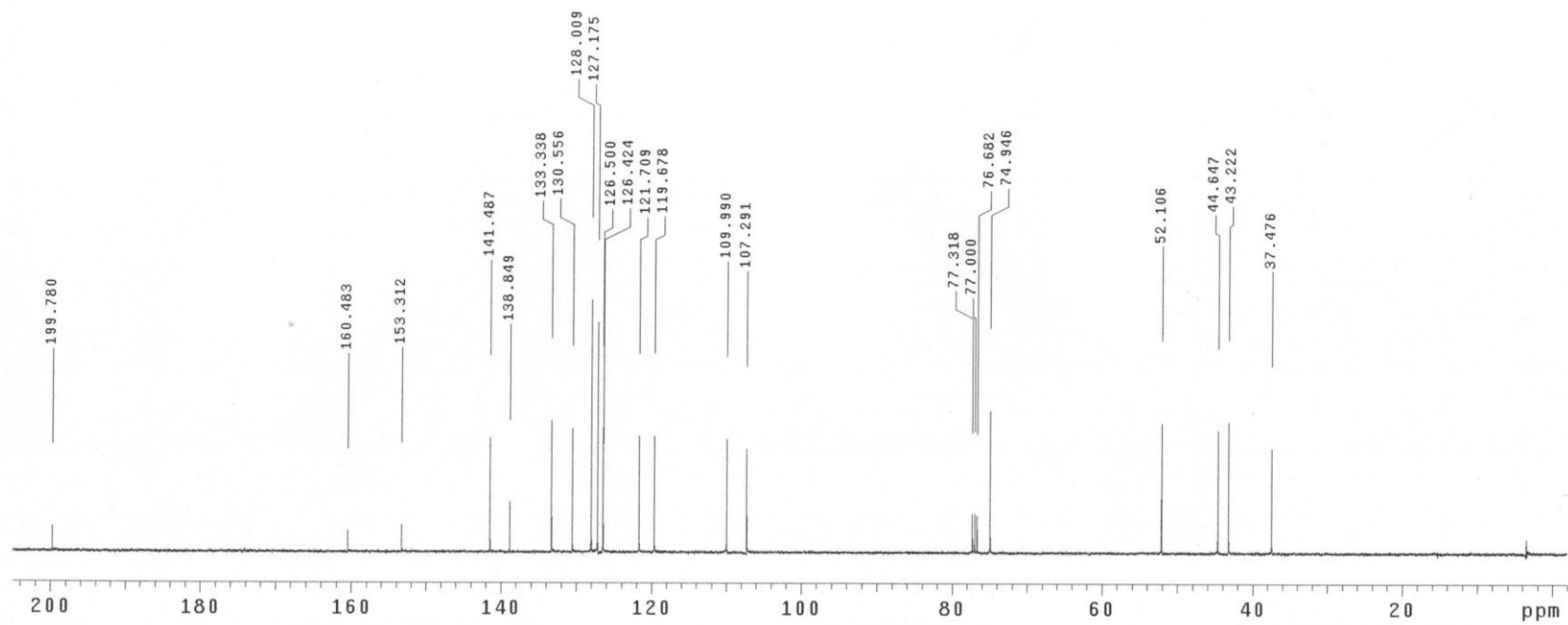
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 21 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.780
7.776
7.761
7.756
7.446
7.145
7.142
7.122
7.105
7.101
7.091
7.071
7.055
7.051
7.034
6.959
6.944
6.941
4.480
4.471
4.414
4.392
1.625

8.94
10.17
97.10
9.00
9.44
10.30
10.42
10.45
10.41
10.06

9   8   7   6   5   4   3   2   1   ppm
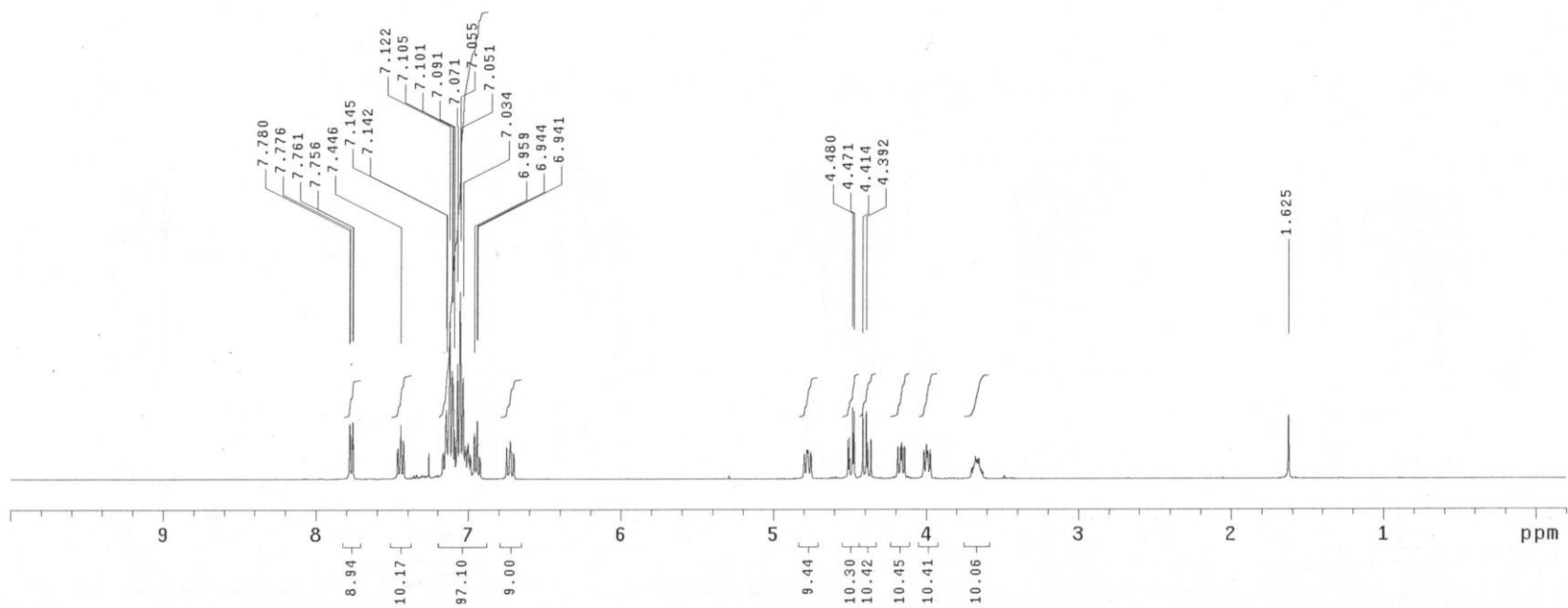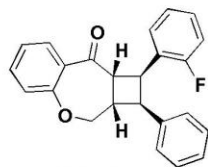
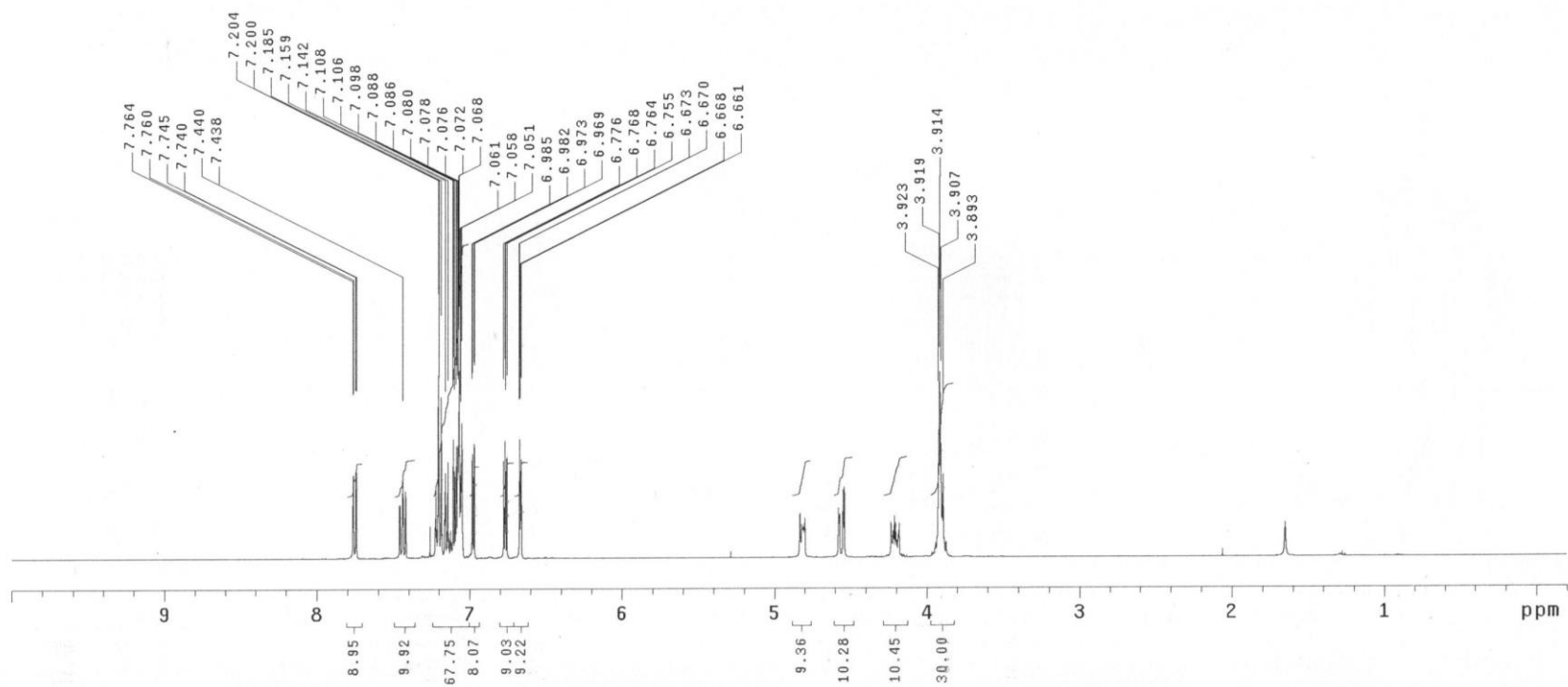# Compound 6t (^{13}C-NMR spectral data)

MC1080521

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 21 2019
Solvent: CDC13
Ambient temperature
Total 1344 repetitions

200.546
161.742
160.385
159.301
139.114
133.641
130.980
128.251
128.206
128.024
127.940
127.910
127.614
126.424
126.371
126.273
126.053
123.582
123.551
121.884
119.981
114.917
114.697
77.318
77.000
76.682
74.627
51.606
44.851
43.153
38.779

S-125
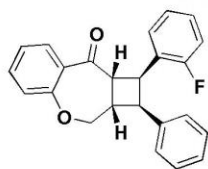
Compound 6u (^{1}H-NMR spectral data)

MC1080606

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
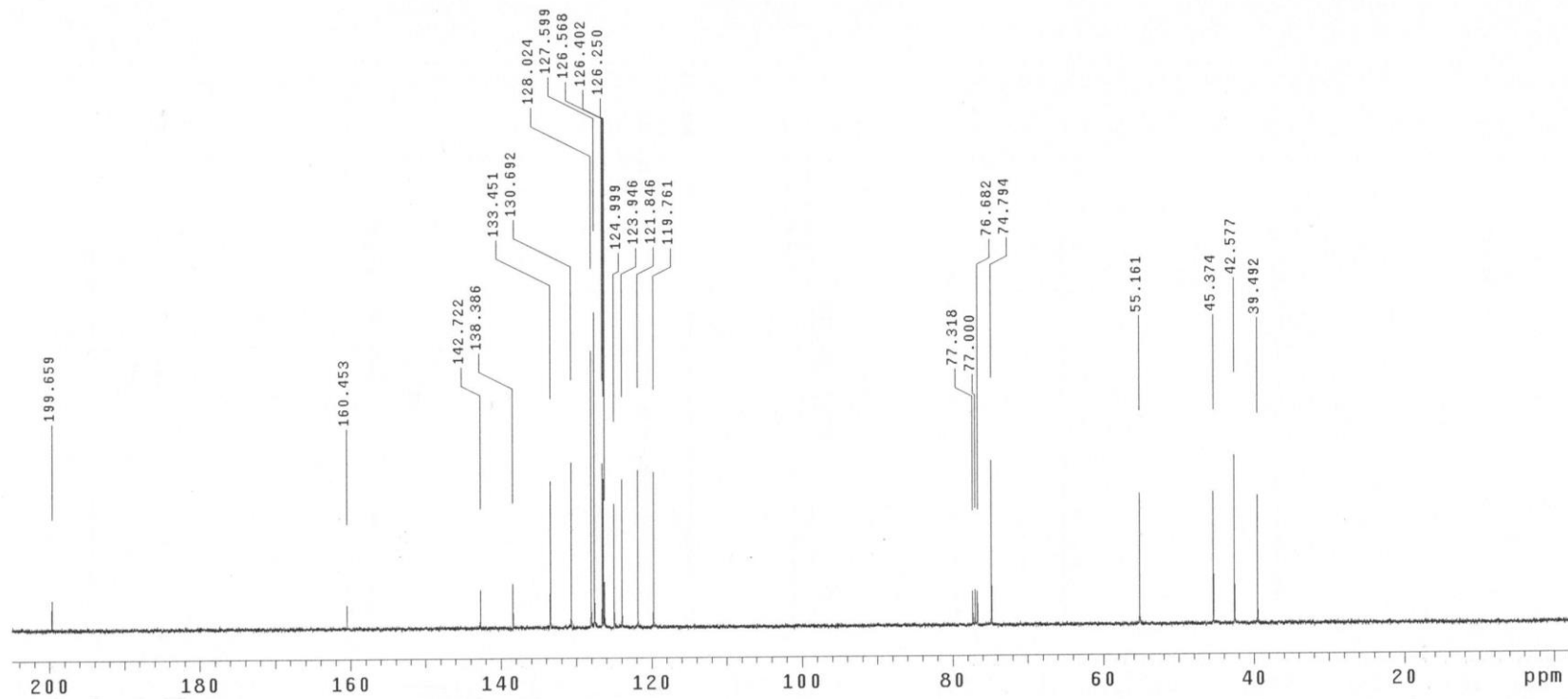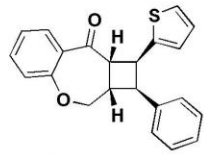Date: Jun 6 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.276
8.270
8.263
8.259
8.251
8.247
7.755
7.750
7.735
7.731
7.435
7.233
7.156
7.138
7.135
7.119
7.101
7.099
7.081
7.078
7.066
7.064
7.061
7.046
6.967
6.948

4.557
4.547
4.527
4.517
4.329
4.305
4.275
4.010
3.986
3.968

17.68
8.69
9.27
10.84
46.01
28.25

19.44
10.00
19.28
9.97

9   8   7   6   5   4   3   2   1   ppm

S-126

Compound 6u (^{13}C-NMR spectral data)

MC1080606

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 6 2019
Solvent: CDCl3
Ambient temperature
Total 816 repetitions

200.061
160.377
149.552
147.490
138.242
135.195
134.619
133.664
130.836
128.327
127.652
126.614
126.030
122.748
121.929
119.875
77.318
77.000
76.689
74.665
52.591
44.685
42.812
41.440

200   180   160   140   120   100   80   60   40   20   ppm
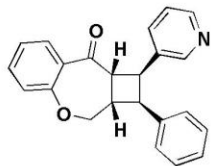
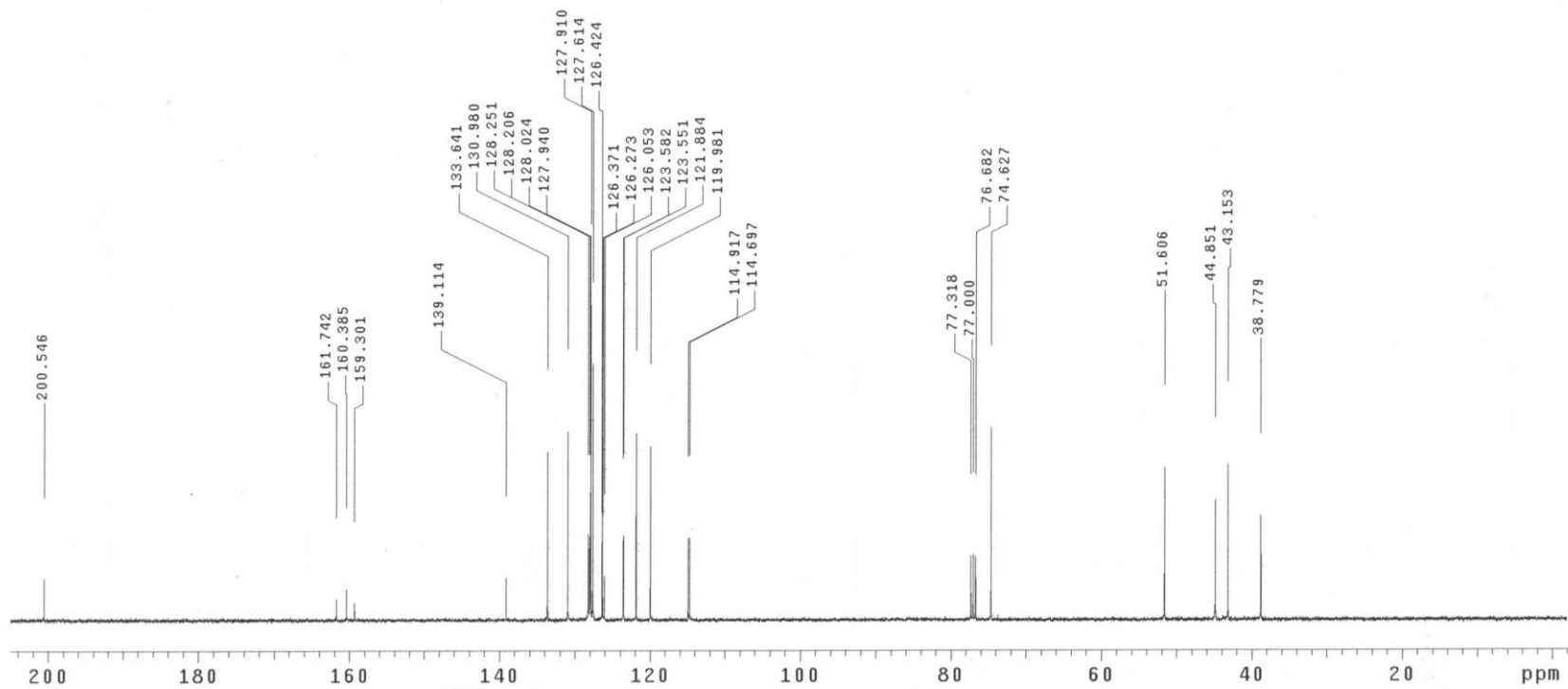# Compound 6ac (^{1}H-NMR spectral data)

MC1080624

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 25 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Peaks: 7.771, 7.766, 7.751, 7.747, 7.403, 7.260, 7.055, 7.037, 7.035, 7.034, 7.020, 6.813, 6.793, 6.717, 6.712, 6.636, 6.631, 4.530, 4.514, 4.338, 4.331, 3.972, 3.949, 3.859, 3.844, 3.801, 3.777, 1.611, 1.351, 0.871

Integrals: 8.72, 9.89, 19.49, 11.27, 10.92, 19.93, 10.33, 10.16, 13.04, 75.18, 9.66, 30.00, 31.10

ppm axis: 9, 8, 7, 6, 5, 4, 3, 2, 1, ppm

S-128

Compound 6ac (^{13}C-NMR spectral data)

MC1080624

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
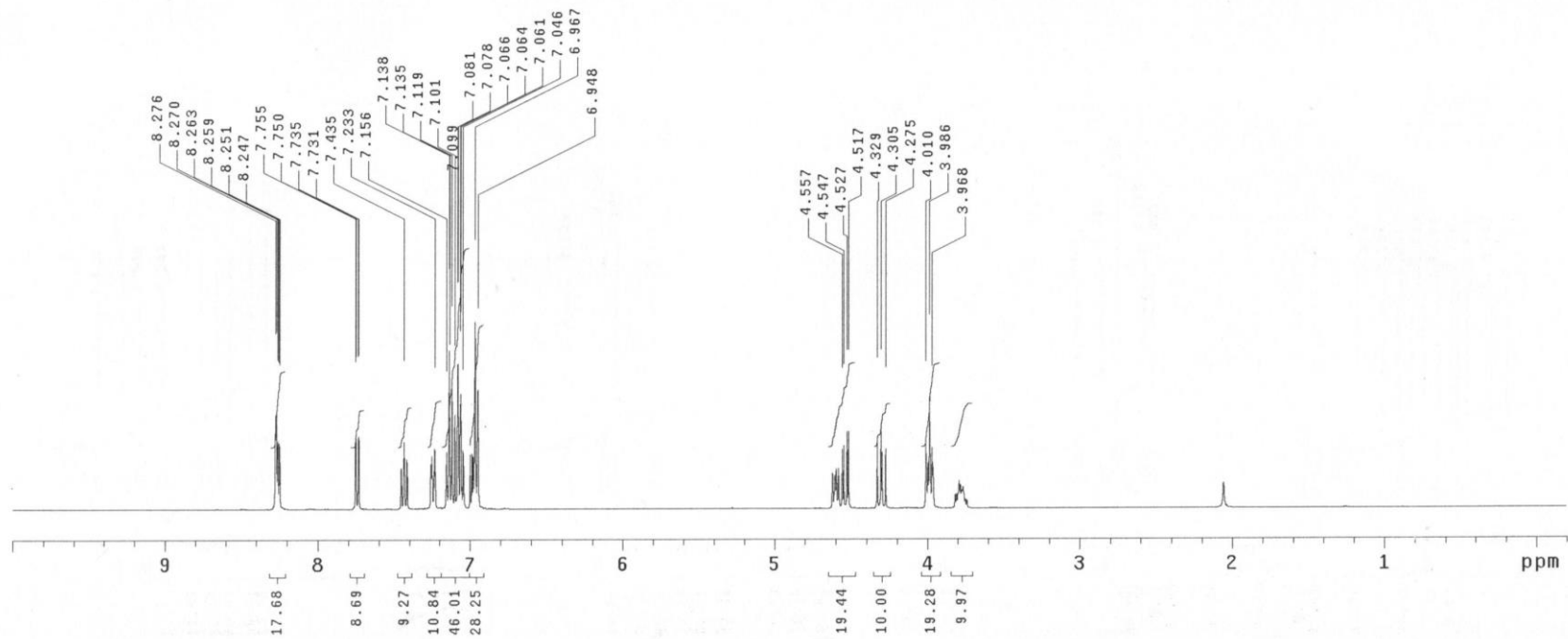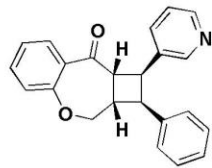Date: Jun 25 2019
Solvent: CDCl3
Ambient temperature
Total 2240 repetitions

201.660
160.150
148.688
147.612
133.694
132.337
131.215
125.856
121.778
120.269
118.996
111.013
110.687
77.311
77.000
76.682
72.384
55.866
55.835
50.802
50.620
46.830
40.030
25.408
24.452

200 180 160 140 120 100 80 60 40 20 ppm
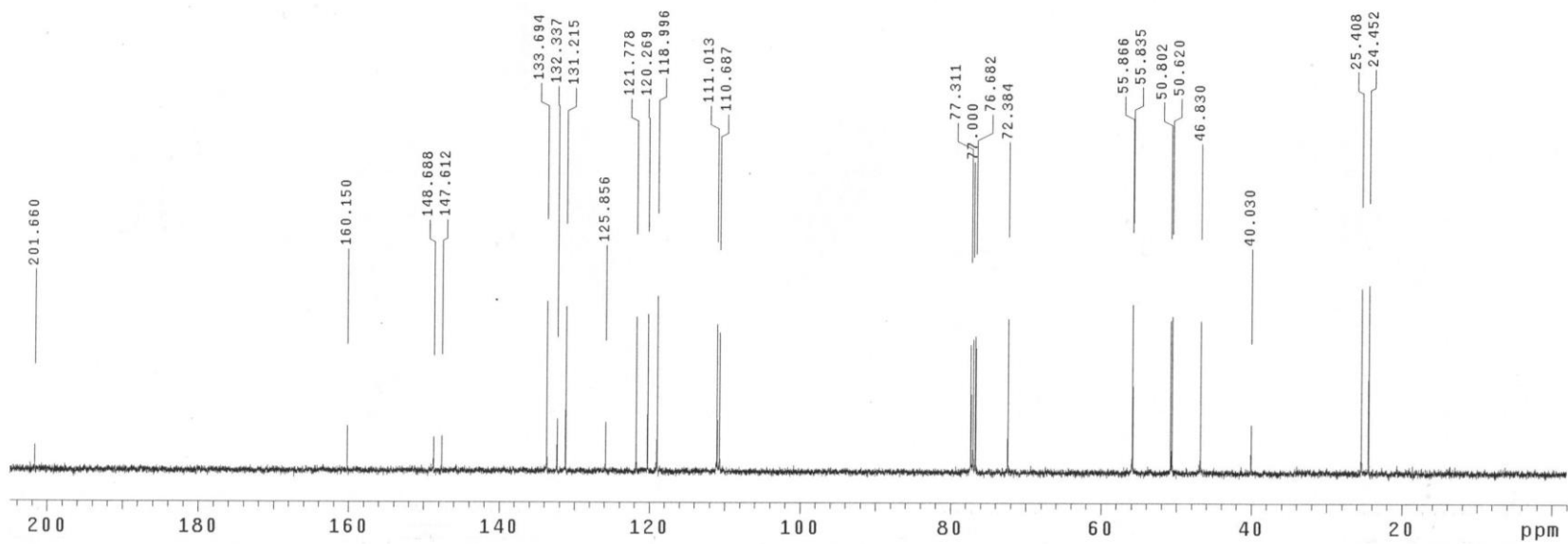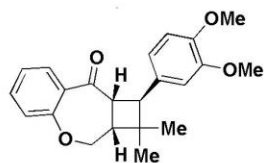
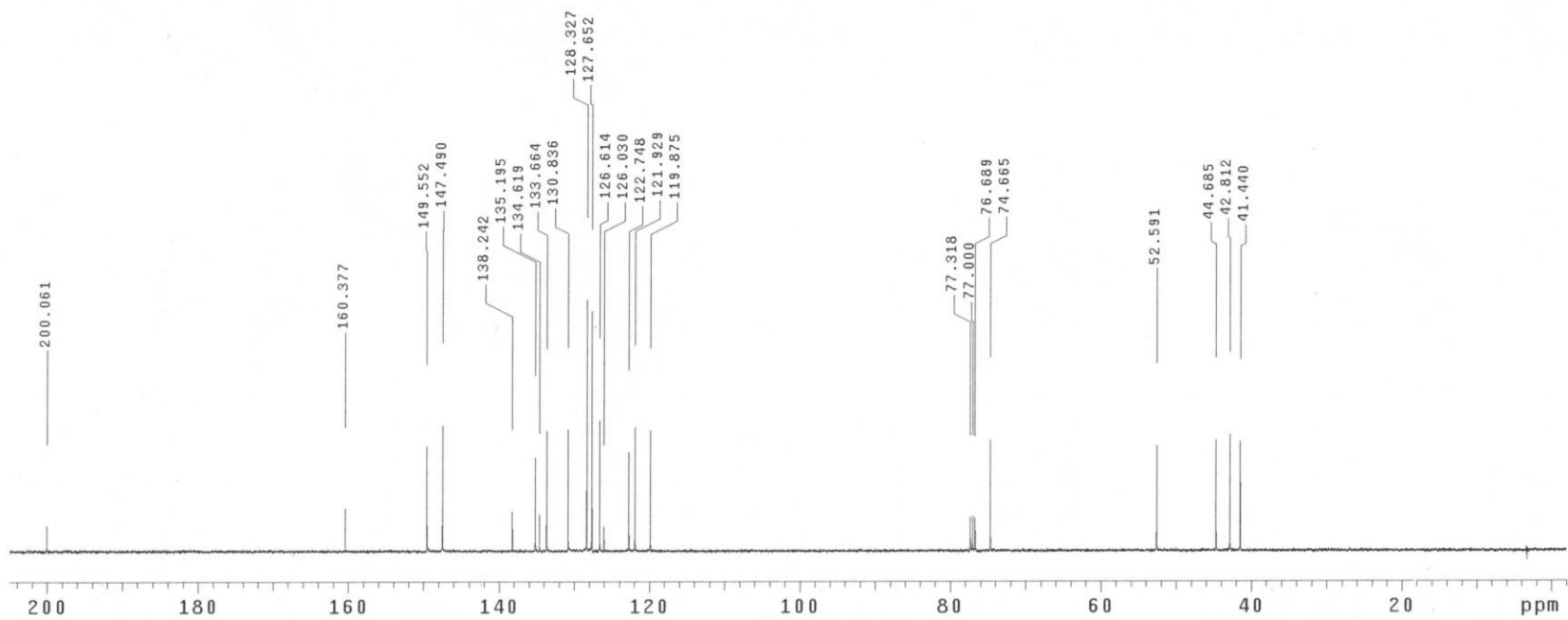# Compound 6ad (^{1}H-NMR spectral data)

MC10806NBS

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
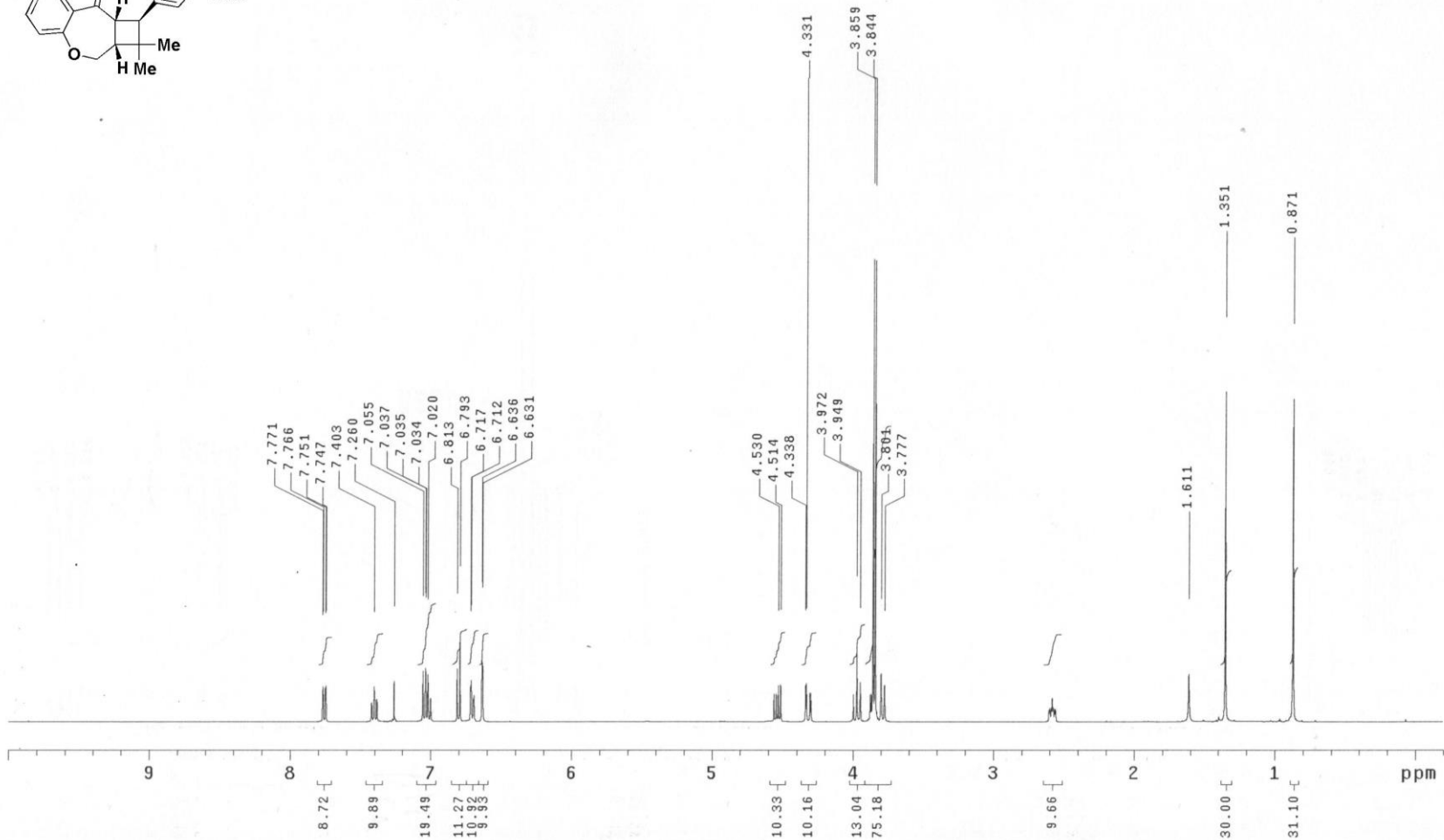Date: Jun 27 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Peaks: 7.813, 7.810, 7.794, 7.791, 7.504, 7.487, 7.484, 7.466, 7.151, 7.132, 6.922, 6.904, 6.646, 6.626, 6.257, 6.252, 3.797, 3.559

Integrals (from left): 37.96, 11.24, 30.80, 12.58, 32.29, 20.57, 10.14, 10.12, 9.73, 10.10, 10.13, 10.25, 30.00, 11.95, 30.07, 10.99, 9.90

Compound 6ad (^{13}C-NMR spectral data)

MC10806NBS

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
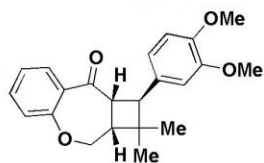Date: Jun 27 2019
Solvent: CDCl3
Ambient temperature
Total 928 repetitions

199.651
148.324
147.392
140.948
140.713
138.591
133.072
132.784
132.542
131.230
130.965
129.388
128.084
127.402
126.690
126.349
126.182
125.628
119.359
112.984
110.437
77.318
77.000
76.682
55.972
55.729
55.691
55.545
51.545
46.026
42.623
41.986

Compound 7a (^{1}H-NMR spectral data)

MC0218DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 20 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

Peaks: 7.351, 7.333, 7.314, 7.271, 7.260, 7.254, 6.870, 6.701, 6.675, 6.613, 6.609, 4.447, 4.102, 4.078, 3.824, 3.719

Integrations: 69.32, 10.08, 10.14, 20.46, 9.78, 20.52, 10.43, 22.28, 30.87, 30.00, 10.26

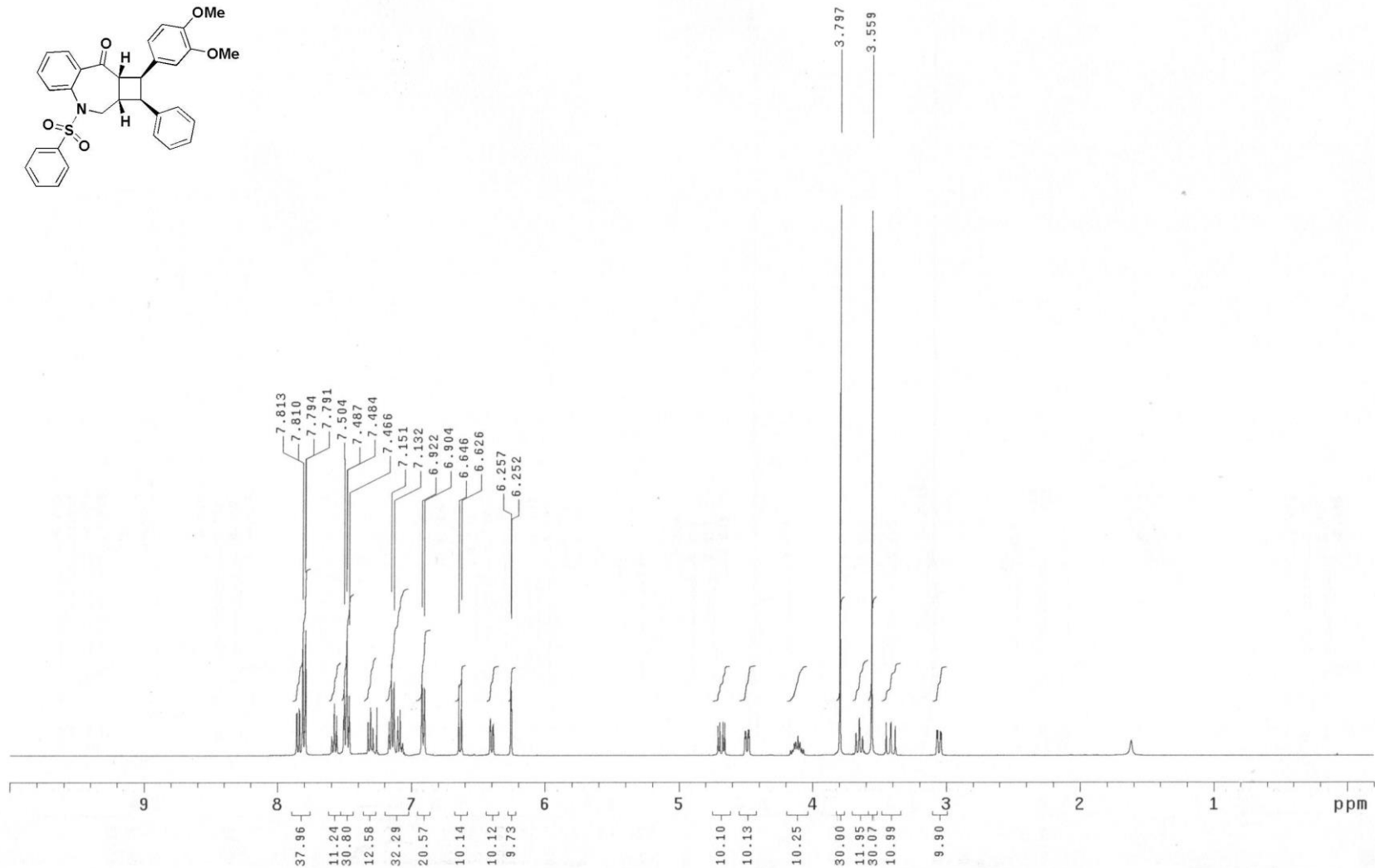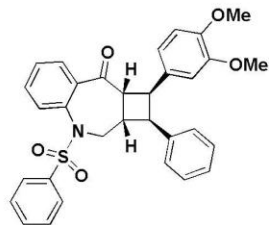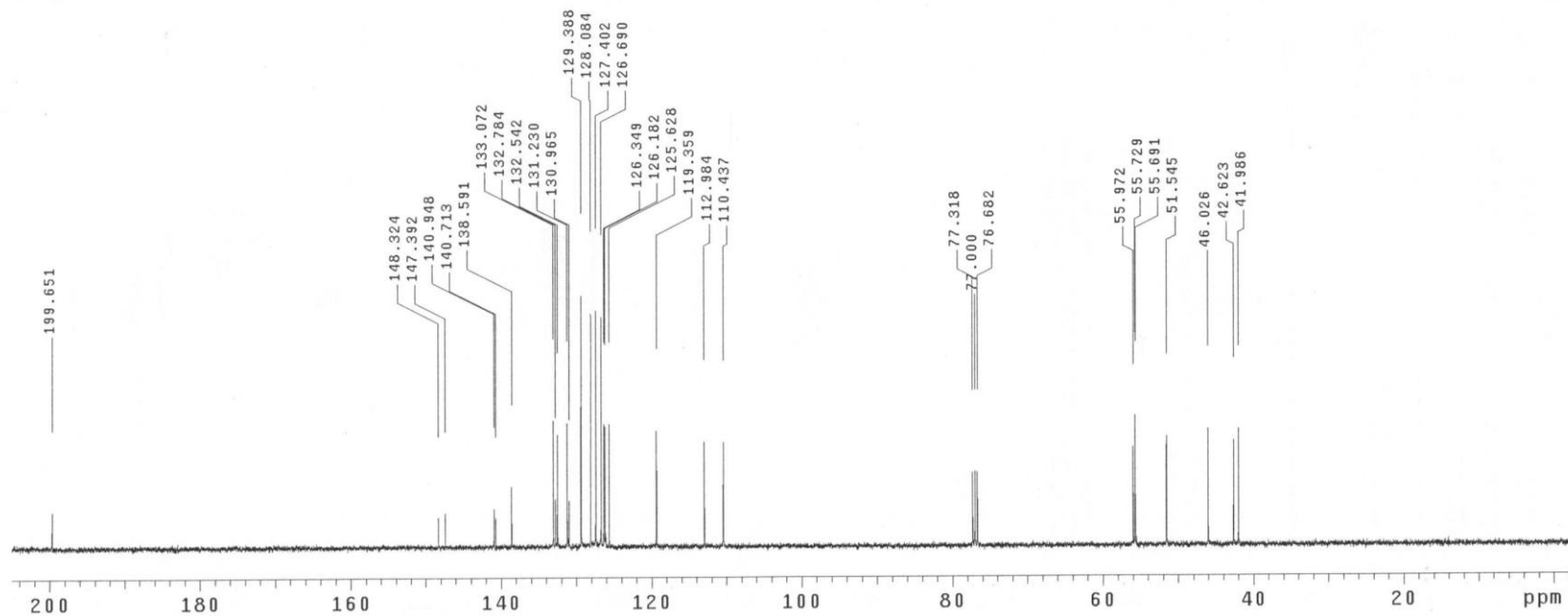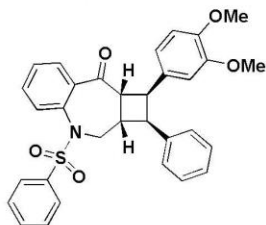# Compound 7a (¹³C-NMR spectral data)

MC0218DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
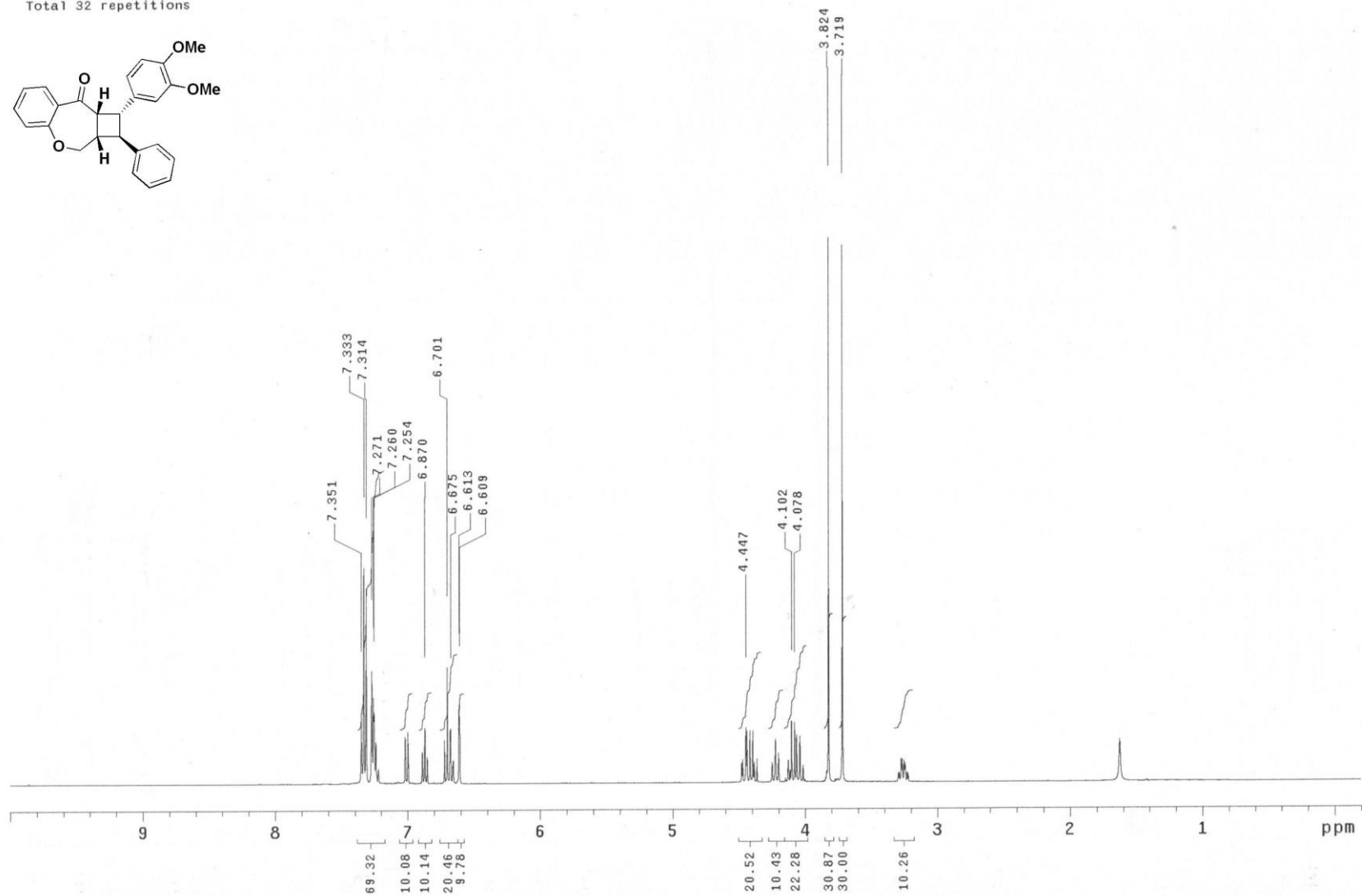Date: Feb 20 2019
Solvent: CDCl3
Ambient temperature
Total 1232 repetitions

Compound 7d (¹H-NMR spectral data)

MC0403DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 9 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.833
3.753

7.337
7.319
7.271
7.266
7.263
7.252
7.051
7.049
6.711
6.638
6.633

4.425
4.109
4.085

1.579

9   8   7   6   5   4   3   2   1   ppm

20.07
32.44

28.28

30.15

20.99
10.58
20.92

30.49
30.00

10.14

MC0403DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
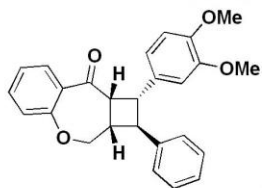Date: Apr 9 2019
Solvent: CDC13
Ambient temperature
Total 3360 repetitions

199.522
158.376
155.980
155.283
148.620
147.642
142.260
131.427
128.721
128.229
128.168
126.864
126.379
121.323
121.247
120.678
120.443
119.231
116.350
116.107
110.809
110.634
77.318
77.000
76.682
72.687
55.835
55.714
54.160
46.512
43.055
42.297

200   180   160   140   120   100   80   60   40   20   ppm
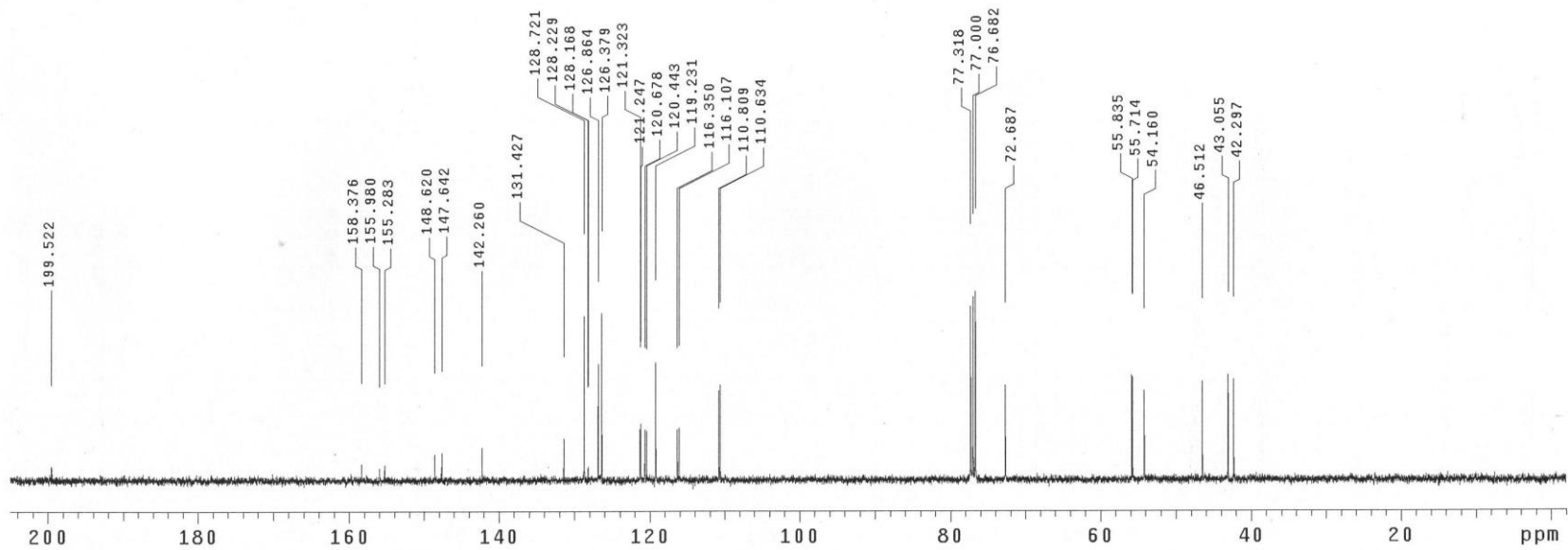
Compound 7e (¹H-NMR spectral data)

MC0319DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 20 2019
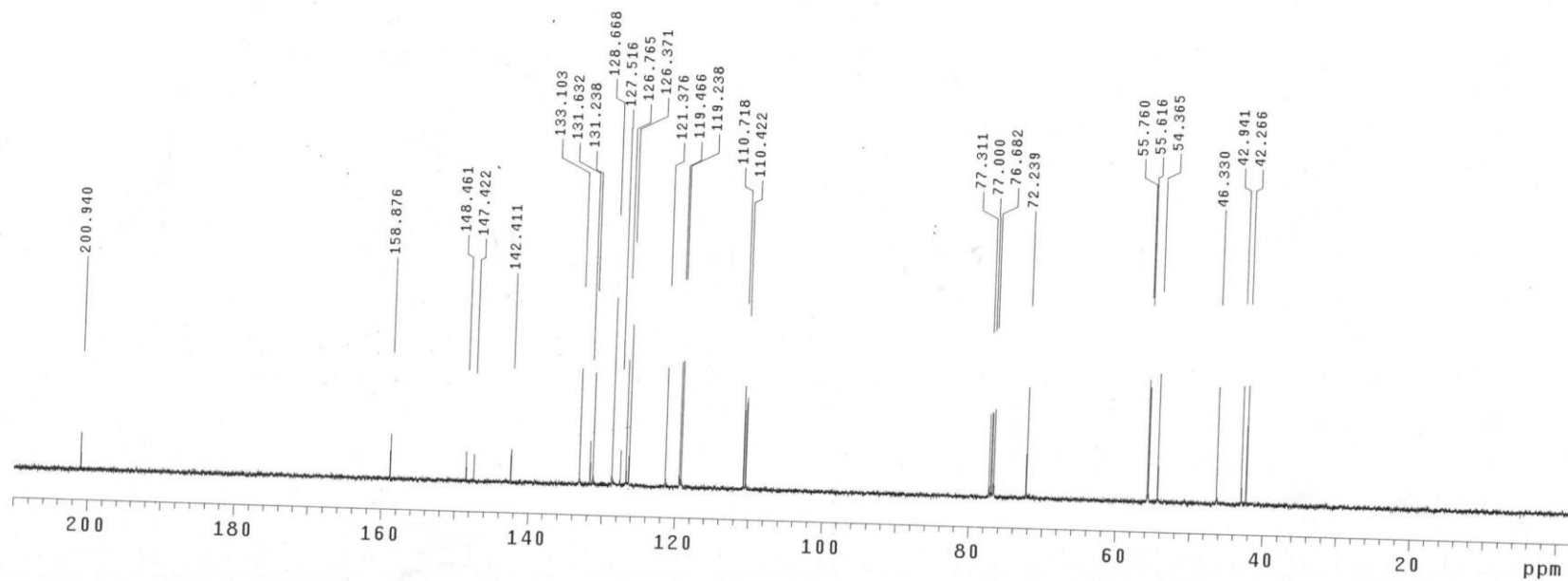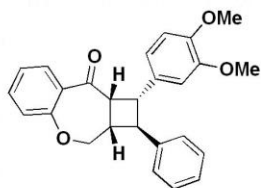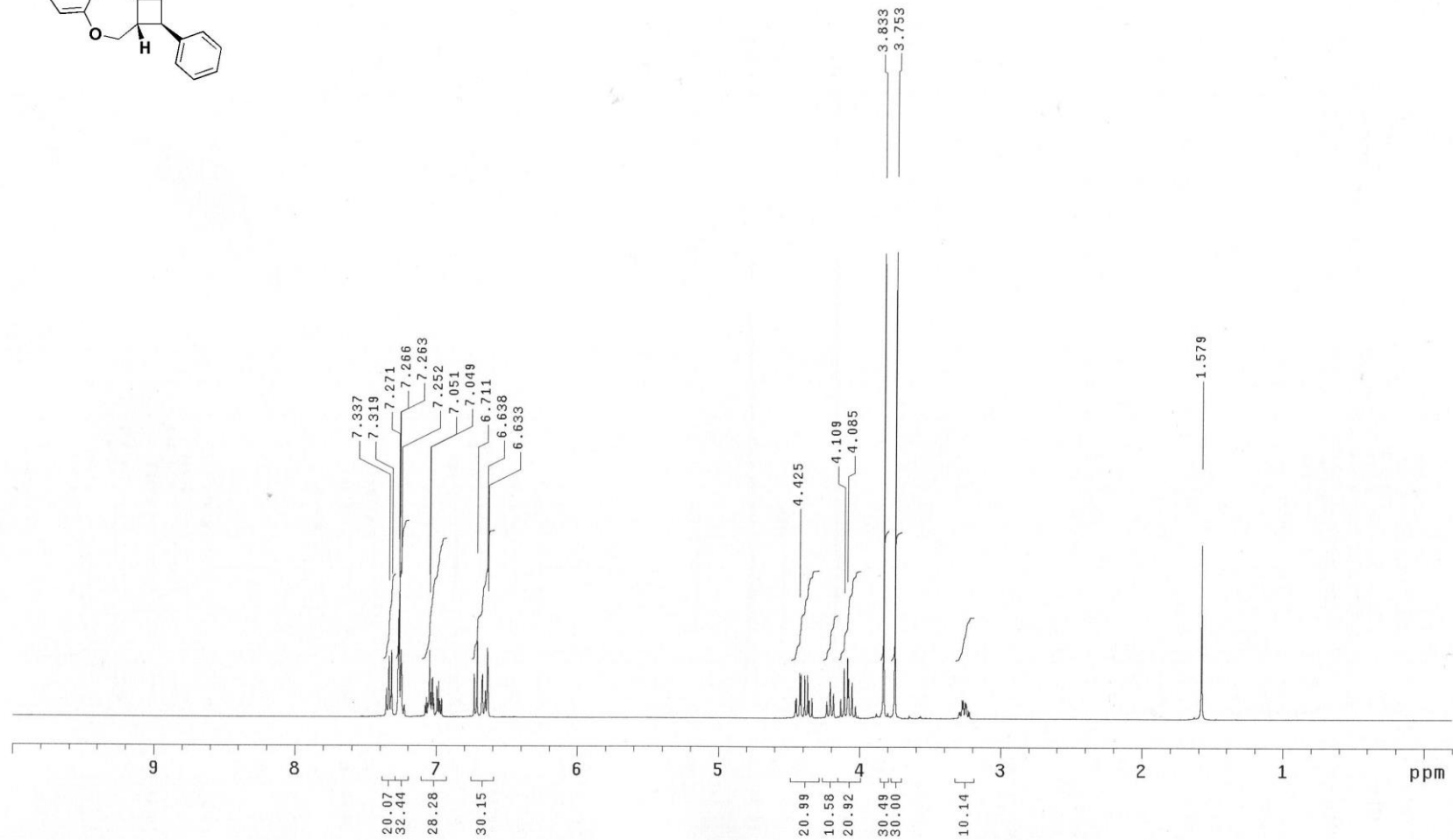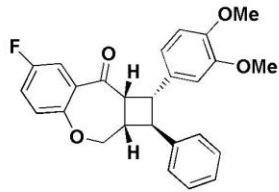Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.327
7.309
7.265
7.260
7.247
7.093
7.089
7.088
7.087
6.914
6.893
6.720
6.699
6.670
6.665
6.607
6.602

4.410
4.402
4.385
4.365
4.222
4.081
4.058
4.053
4.029
3.826
3.713

2.178

1.596

51.21
18.95
9.57
30.65

21.23
10.73
21.32
30.81
30.85
10.37

30.00

ppm 9 8 7 6 5 4 3 2 1

S-136

Compound 7e (^{13}C-NMR spectral data)

MC0319DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 20 2019
Solvent: CDCl3
Ambient temperature
Total 1600 repetitions

201.213
156.913
148.491
147.460
142.540
134.088
131.738
130.957
130.753
128.661
127.235
126.743
126.379
119.359
110.680
110.475
77.318
77.000
76.682
72.164
55.782
55.578
54.463
46.474
42.926
42.236
20.086

200   180   160   140   120   100   80   60   40   20   ppm

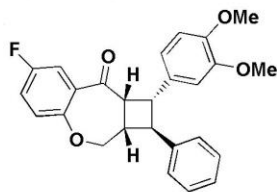# Compound 7f (^{1}H-NMR spectral data)
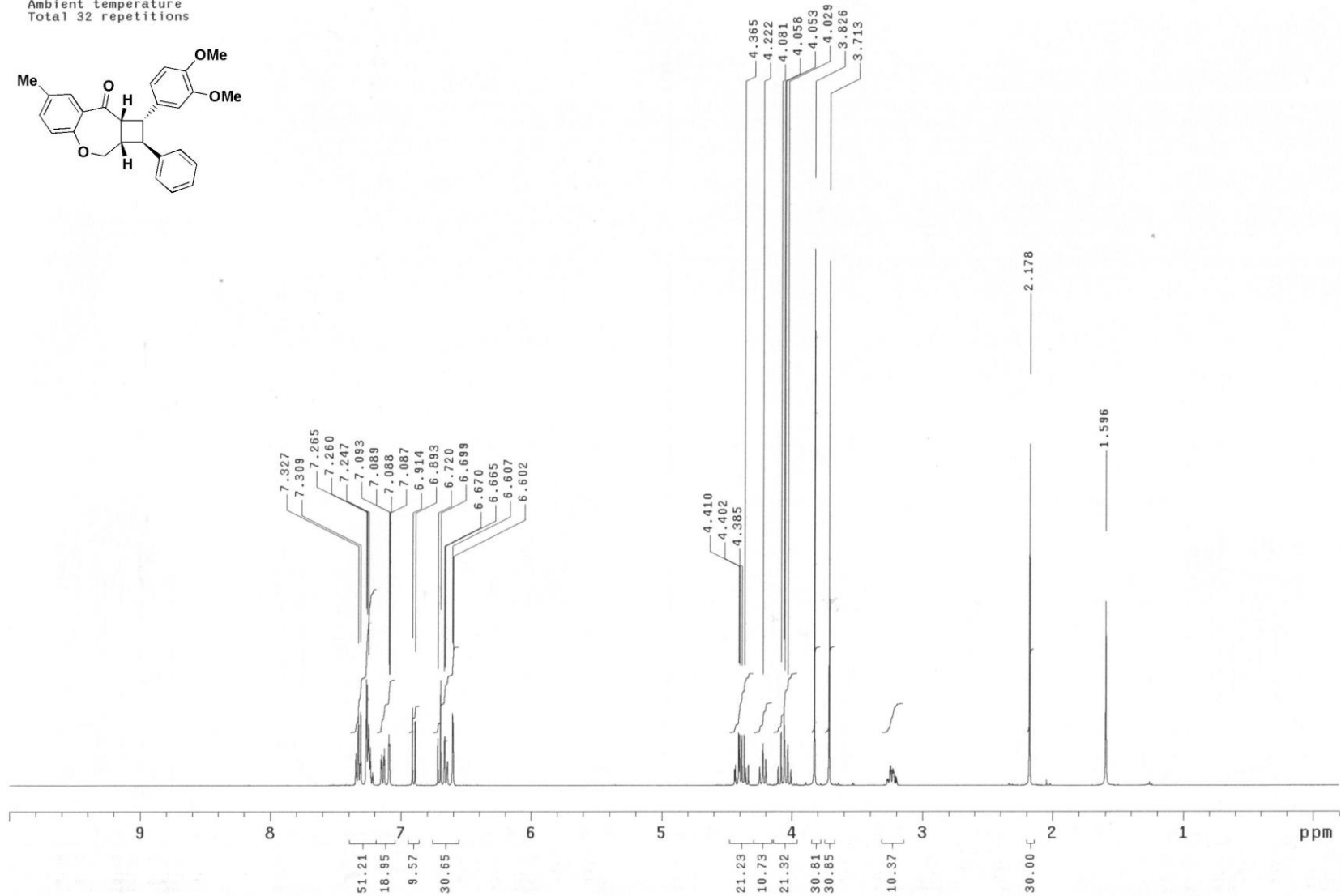
MC0314DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 15 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 7f (^{13}C-NMR spectral data)

MC0314DN

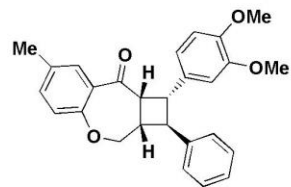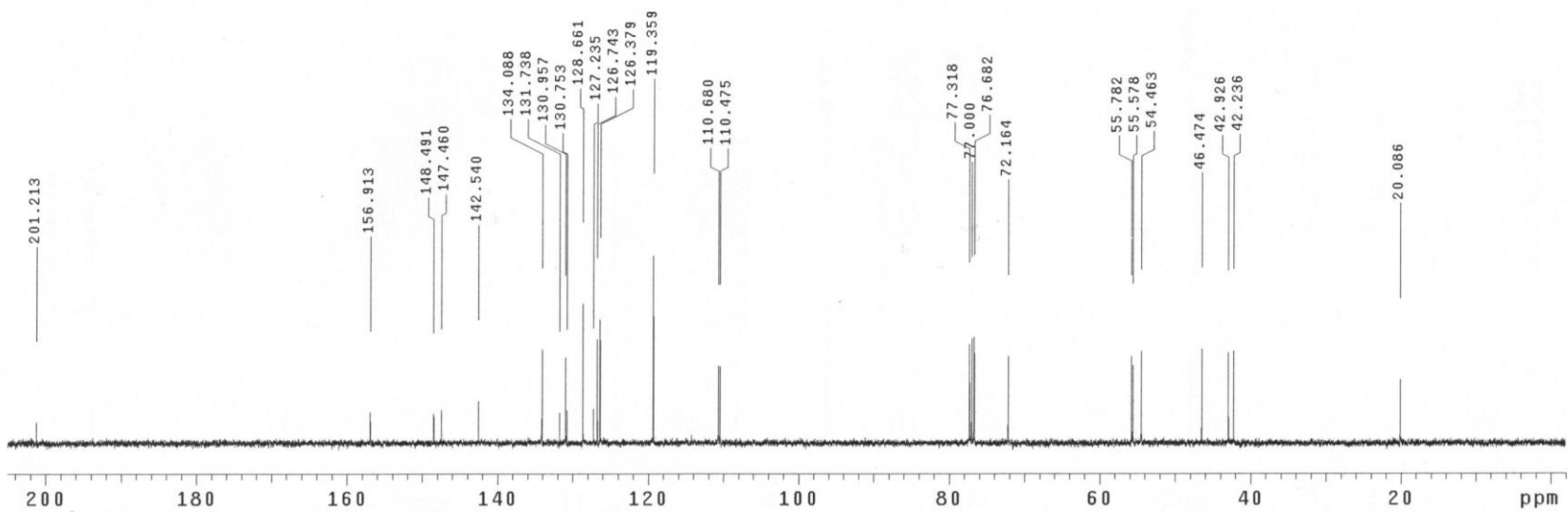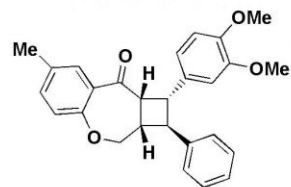Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 15 2019
Solvent: CDC13
Ambient temperature
Total 1152 repetitions
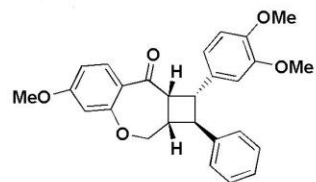
Compound 7h (^{1}H-NMR spectral data)

MC0426DN

Pulse Sequence: s2pul
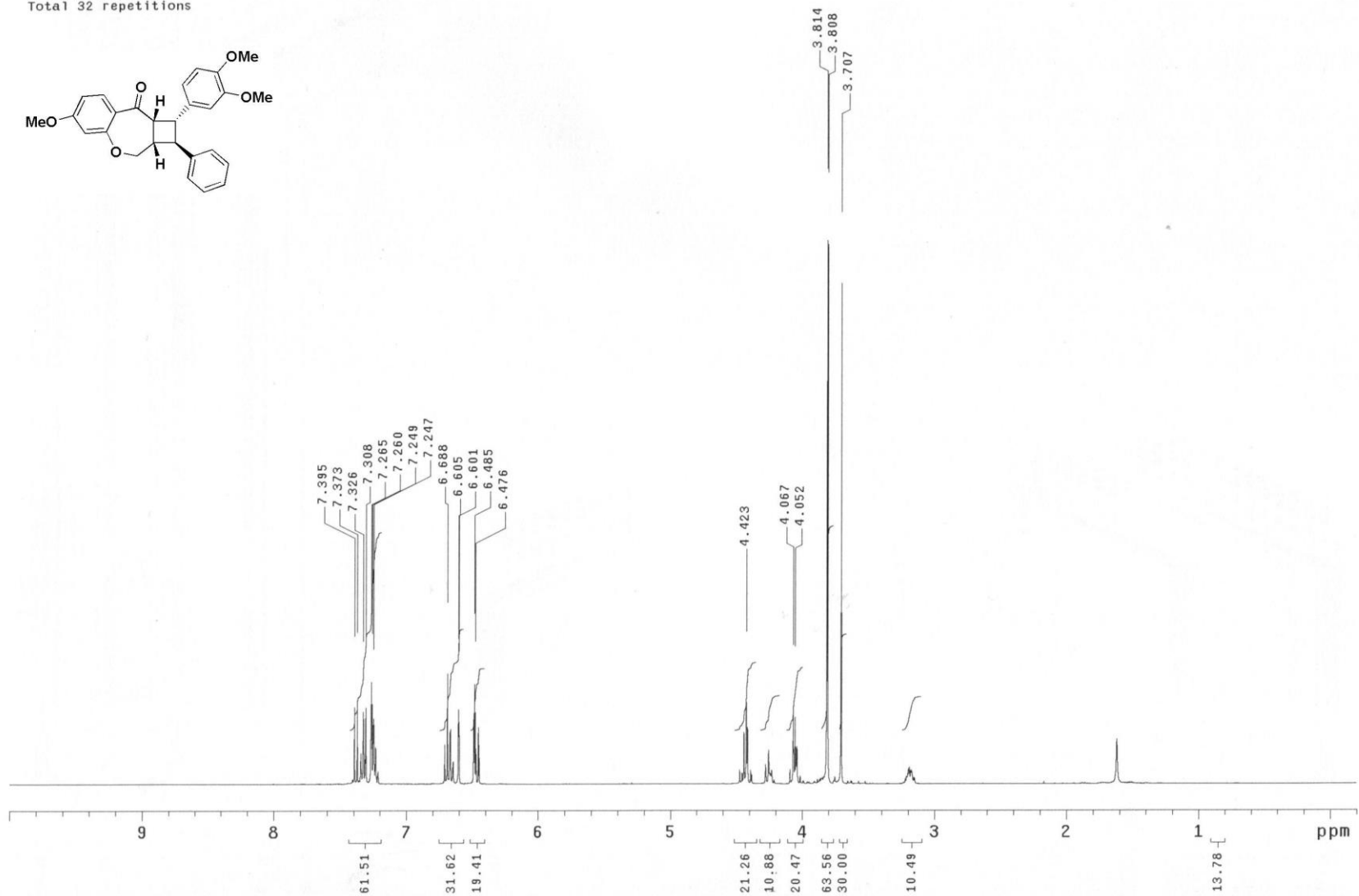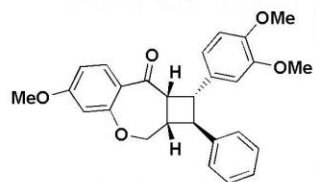
UNITYplus-400 "unity400"
Date: Apr 26 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

7.350
7.348
7.345
7.329
7.282
7.261

6.268

4.425

3.782

3.686

1.625

69.24
9.86
10.00
19.63
21.22
10.66
20.89
28.63
58.14
10.24

Compound 7h (^{13}C-NMR spectral data)

MC0426DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 26 2019
Solvent: CDCl3
Ambient temperature
Total 2016 repetitions

201.107
158.581
152.804
142.548
136.370
134.778
133.141
131.344
128.729
127.539
126.819
126.326
121.353
119.405
104.108
77.318
77.000
76.682
71.823
60.755
55.889
54.850
46.656
42.236
41.789

200 180 160 140 120 100 80 60 40 20 ppm

Compound 7j (^{1}H-NMR spectral data)

7.346
7.341
7.331
7.326
7.322
7.307
7.265
7.260
7.246
7.075
7.054
7.006
6.784
6.762

4.062
4.040

3.768

1.578

35.62
30.19
19.26
9.24
10.10
18.10

10.00
10.22
29.24
28.48
9.78

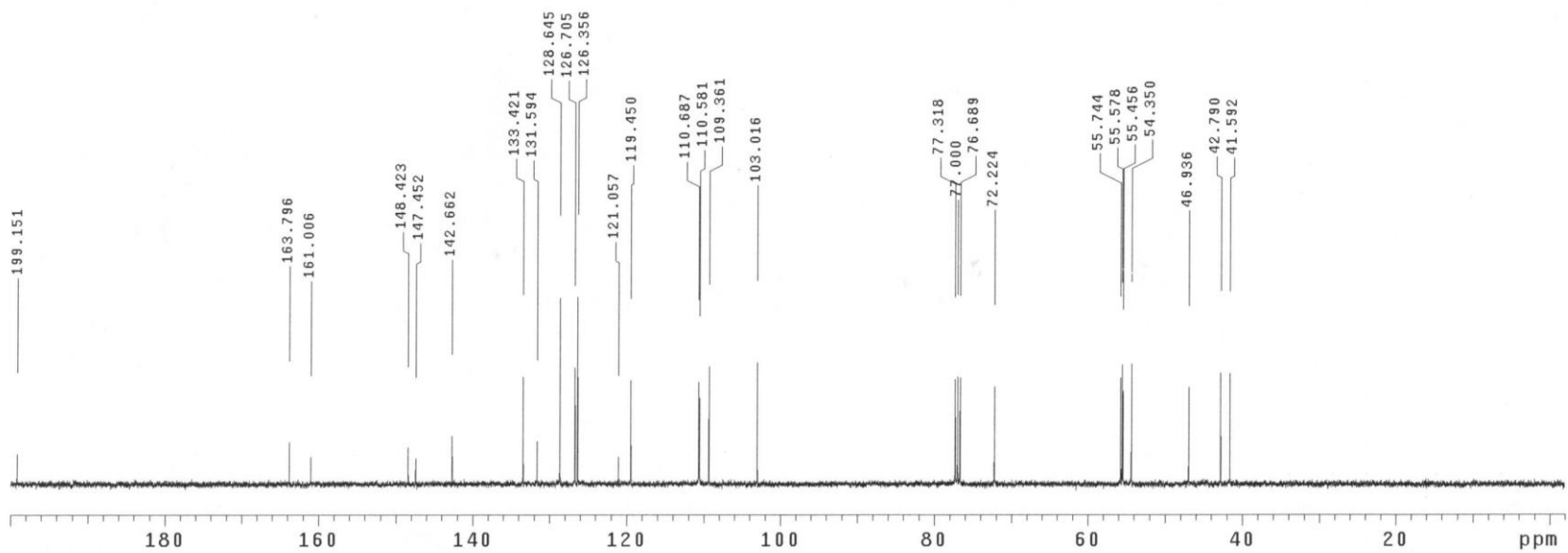# Compound 7j (^{13}C-NMR spectral data)

MC0627DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 27 2019
Solvent: CDC13
Ambient temperature
Total 2144 repetitions

200.902
159.088
158.004
142.252
133.012
131.215
131.041
128.676
128.168
127.554
126.803
126.462
121.376
119.405
113.424
77.318
77.000
76.689
72.641
55.168
53.857
45.928
43.495
42.888

200   180   160   140   120   100   80   60   40   20   ppm

Compound 7m (¹H-NMR spectral data)

MC0506DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
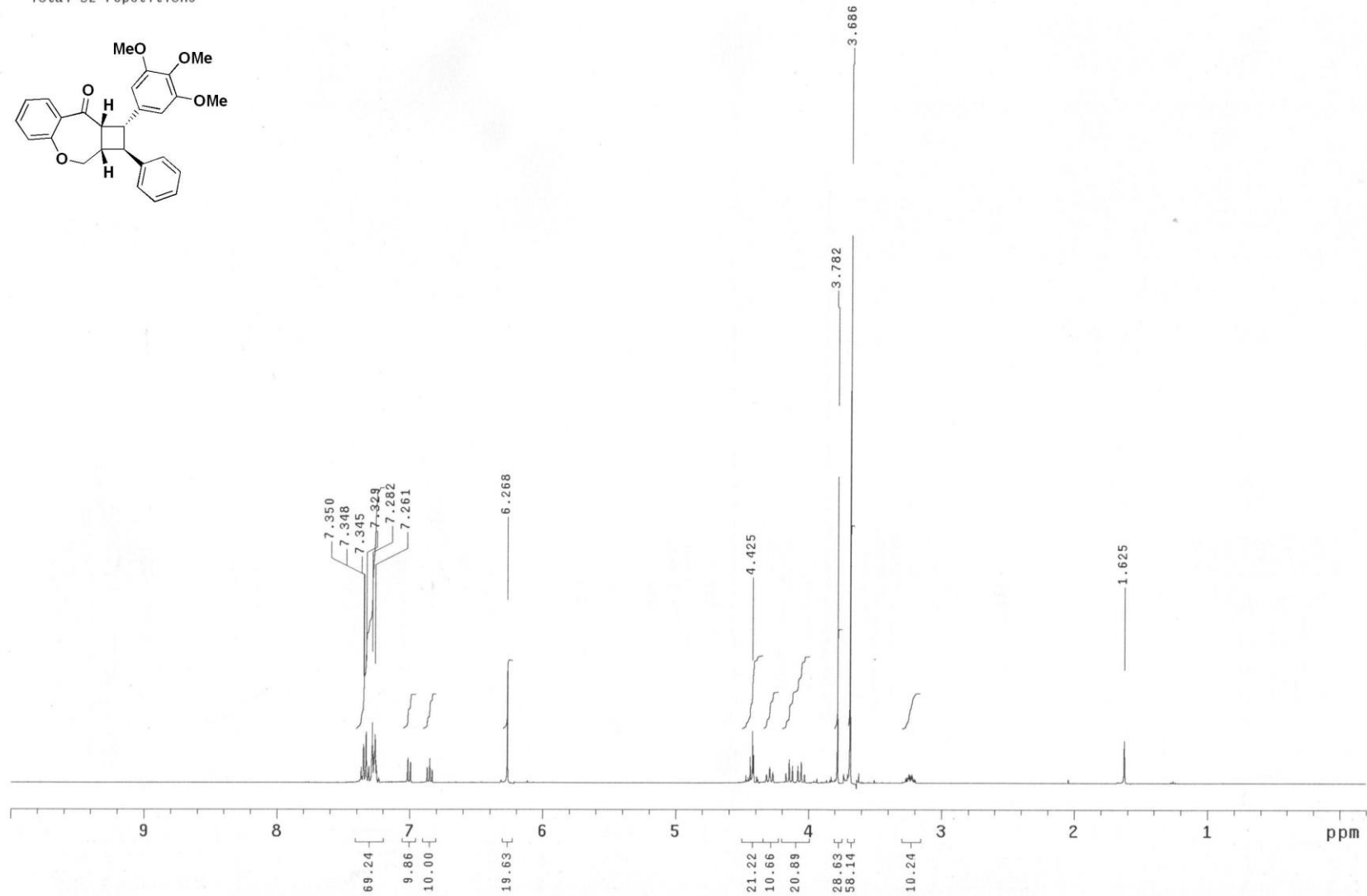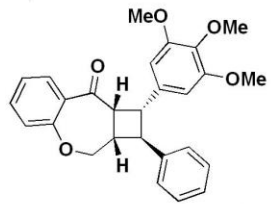Date: May 7 2019
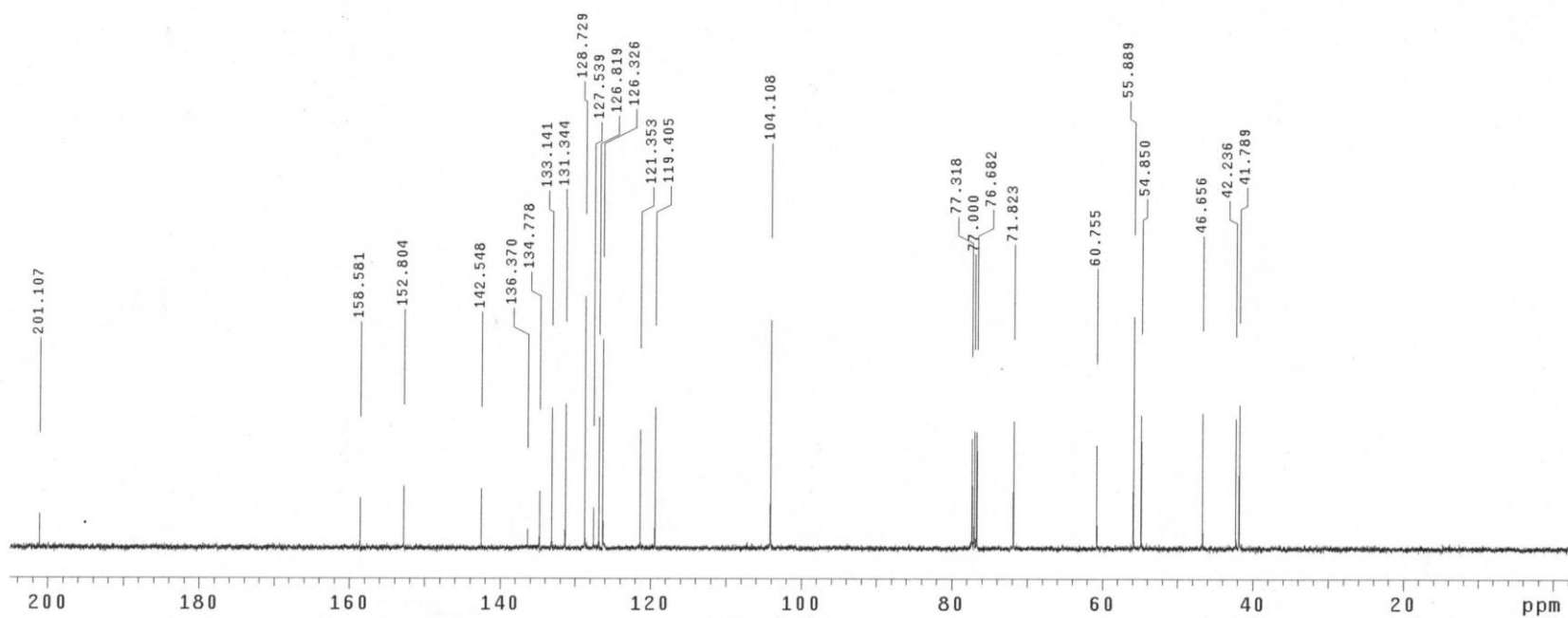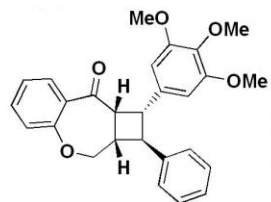Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.374
7.354
7.336
7.331
7.318
7.314
7.298
7.293
7.276
7.005
6.989
6.984
6.969
6.967
6.902
6.417
6.411
6.382
6.361
4.531
4.238
4.067
4.054
4.049
3.782
3.735
1.608

65.91
19.02
9.77
18.83
10.00
10.19
29.66
59.37
10.03

9   8   7   6   5   4   3   2   1   ppm
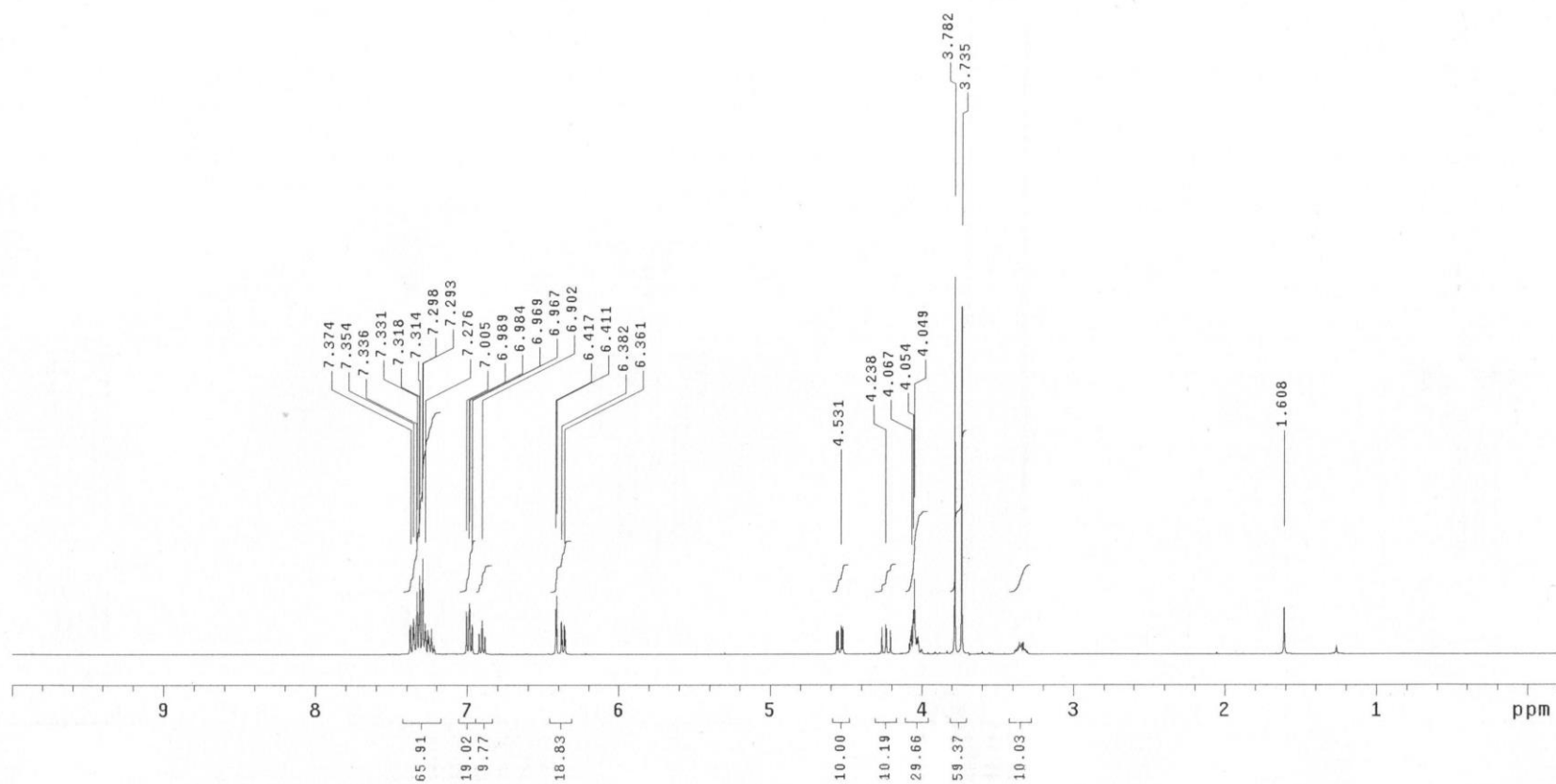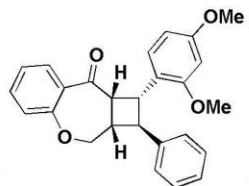
Compound 7m (^{13}C-NMR spectral data)

Peaks (ppm): 200.667, 159.392, 159.354, 158.103, 142.336, 132.542, 130.442, 128.623, 127.743, 126.947, 126.697, 126.629, 121.277, 120.724, 119.246, 103.357, 98.013, 77.318, 77.000, 76.682, 73.407, 55.244, 55.100, 52.818, 44.419, 43.108, 41.637

Compound 7o (¹H-NMR spectral data)

MC0430DN

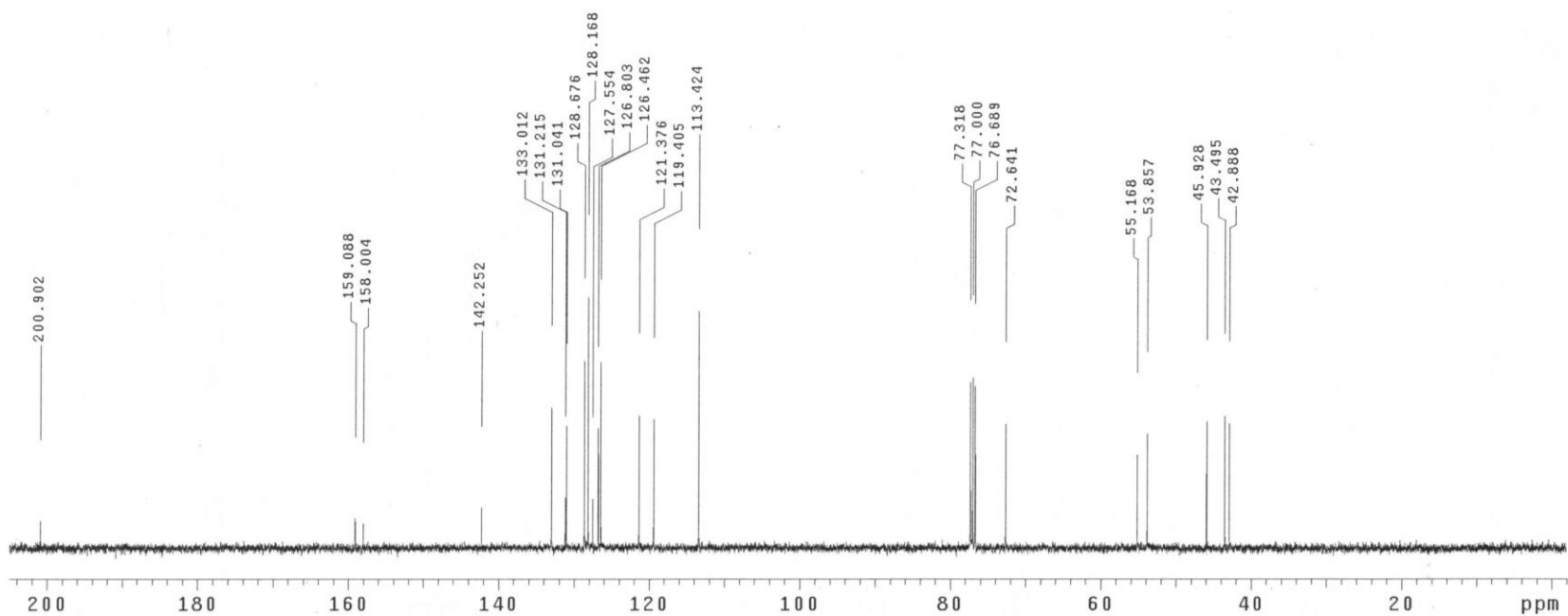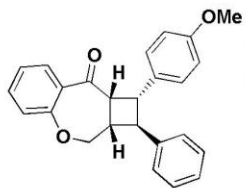Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 31 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.580
7.562
7.479
7.458
7.421
7.352
7.350
7.333
7.320
7.318
7.314
7.309
7.260
7.230
7.209

4.152
4.136

1.569

20.59
139.32
9.61
9.78

10.08
10.48
30.00

9.98

Compound 7o (^{13}C-NMR spectral data)

MC0430DN

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: May 31 2019
Solvent: CDCl3
Ambient temperature
Total 10016 repetitions

200.773
159.119
142.101
141.024
139.000
138.462
132.997
130.920
128.744
128.638
127.478
127.440
126.993
126.902
126.682
126.515
121.383
119.352
77.318
77.000
76.682
72.702
53.834
45.973
43.366
43.199

200   180   160   140   120   100   80   60   40   20   ppm

Compound 7q (¹H-NMR spectral data)

MC0515DN

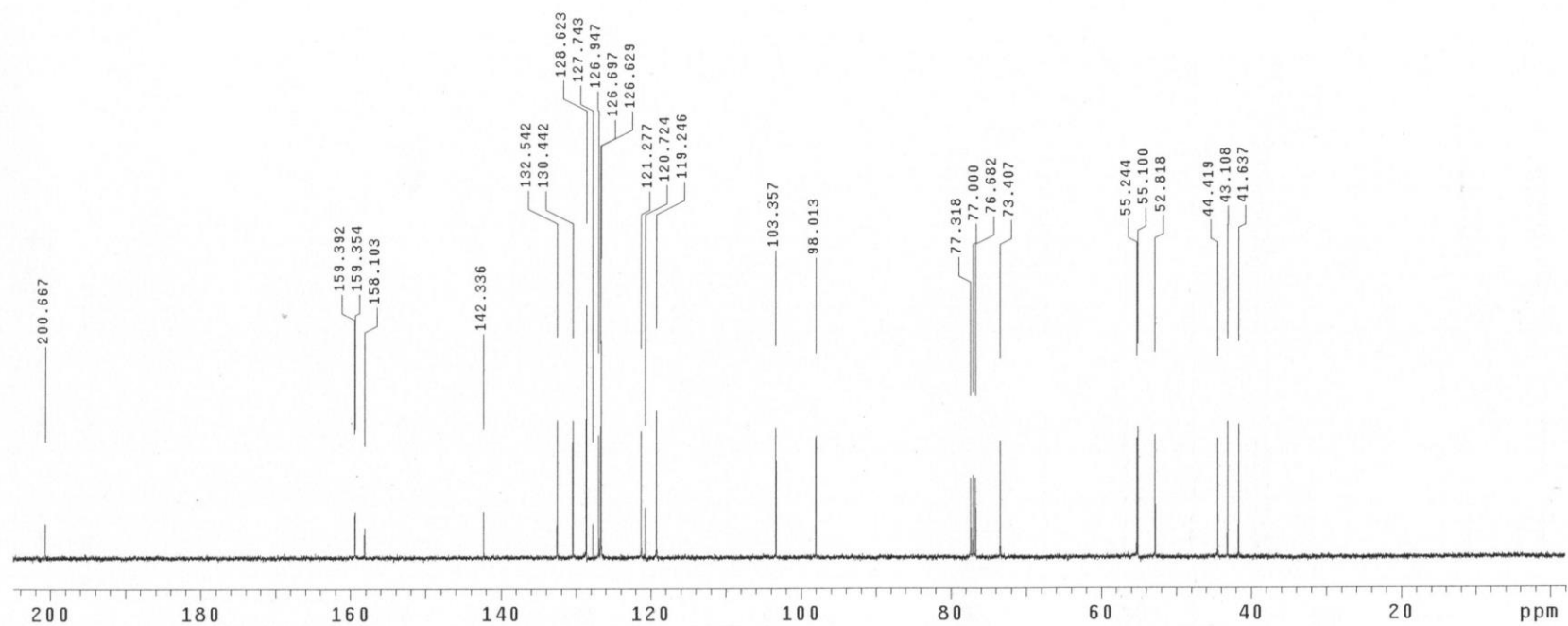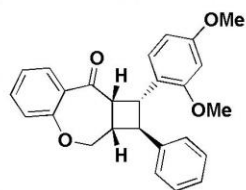Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: May 20 2019
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

7.414
7.406
7.399
7.390
7.340
7.324
7.318
7.316
7.313
7.295
7.260
7.258
7.252

4.203
4.180

1.575

21.37 10.65 10.98 100.30 9.25 10.07   10.22 40.81   10.00

9   8   7   6   5   4   3   2   1   ppm

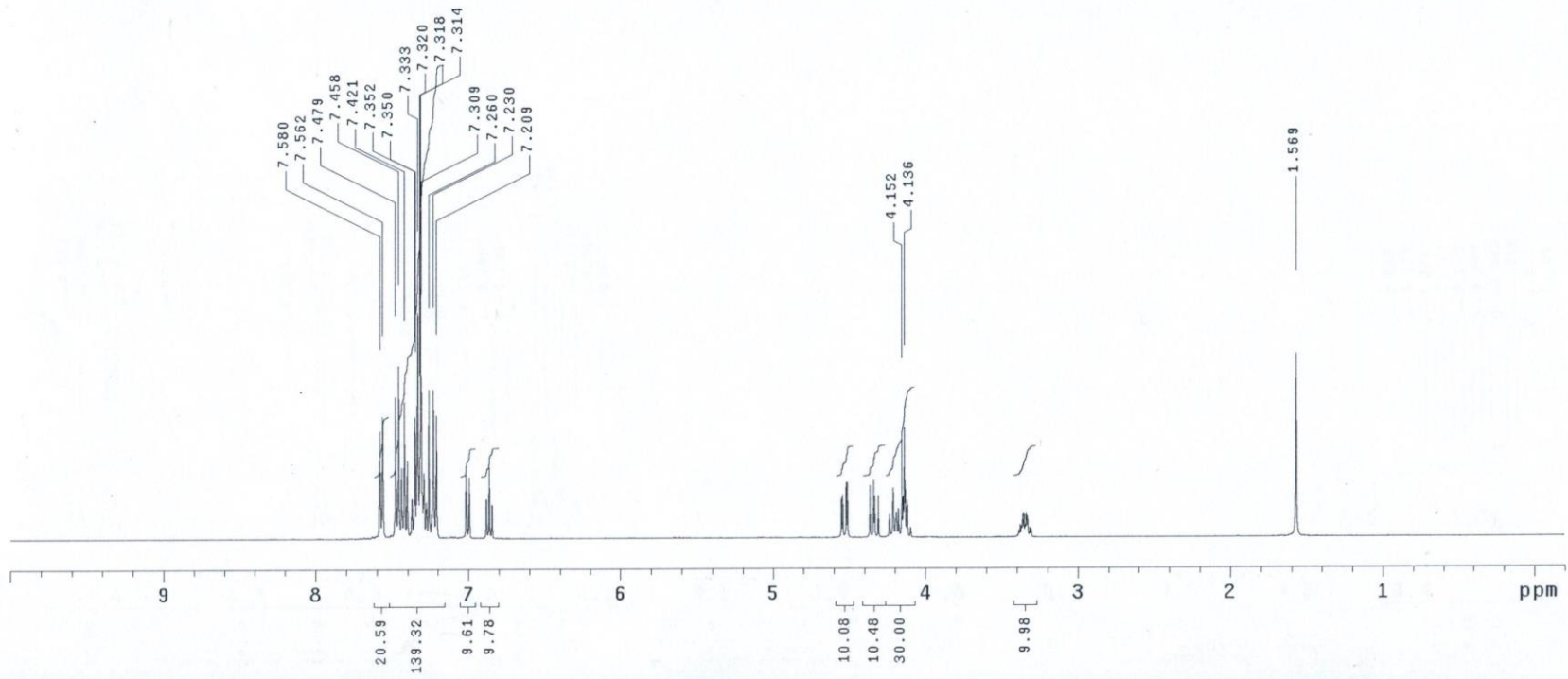# Compound 7q (^{13}C-NMR spectral data)

MC0515DN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 20 2019
Solvent: CDCl3
Ambient temperature
Total 6016 repetitions

200.561
159.210
142.192
136.961
133.247
133.004
132.170
130.882
128.752
127.668
127.599
127.455
126.879
126.462
126.015
125.803
125.325
125.121
121.368
119.352
77.318
77.000
76.682
72.861
53.781
46.421
43.381
43.244

200 180 160 140 120 100 80 60 40 20 ppm

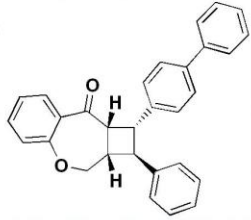# Compound 8 (^{1}H-NMR spectral data)

MCMe2324

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 10 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
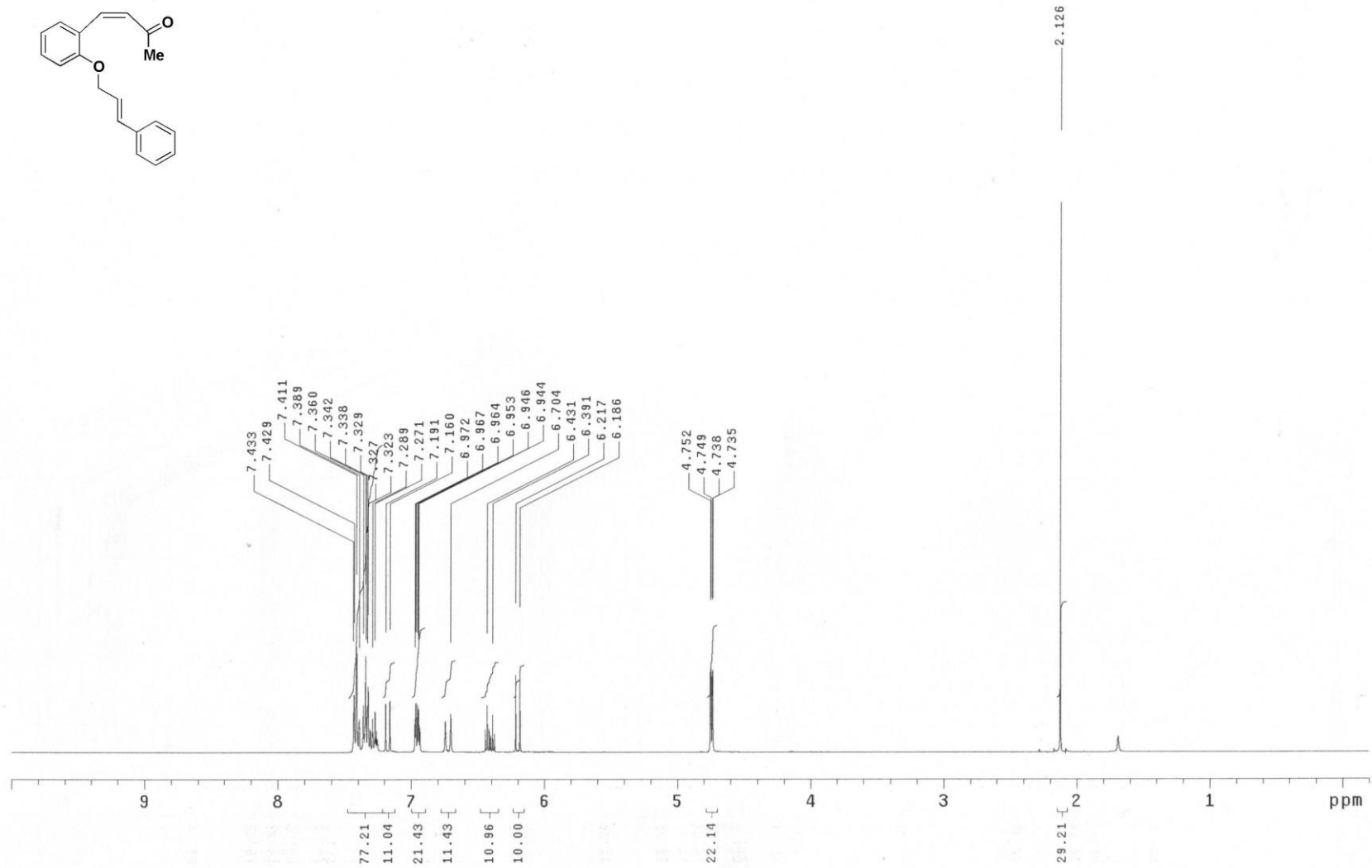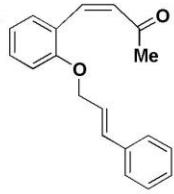
Compound 8 (^{13}C-NMR spectral data)

MCMe2324

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 10 2019
Solvent: CDCl3
Ambient temperature
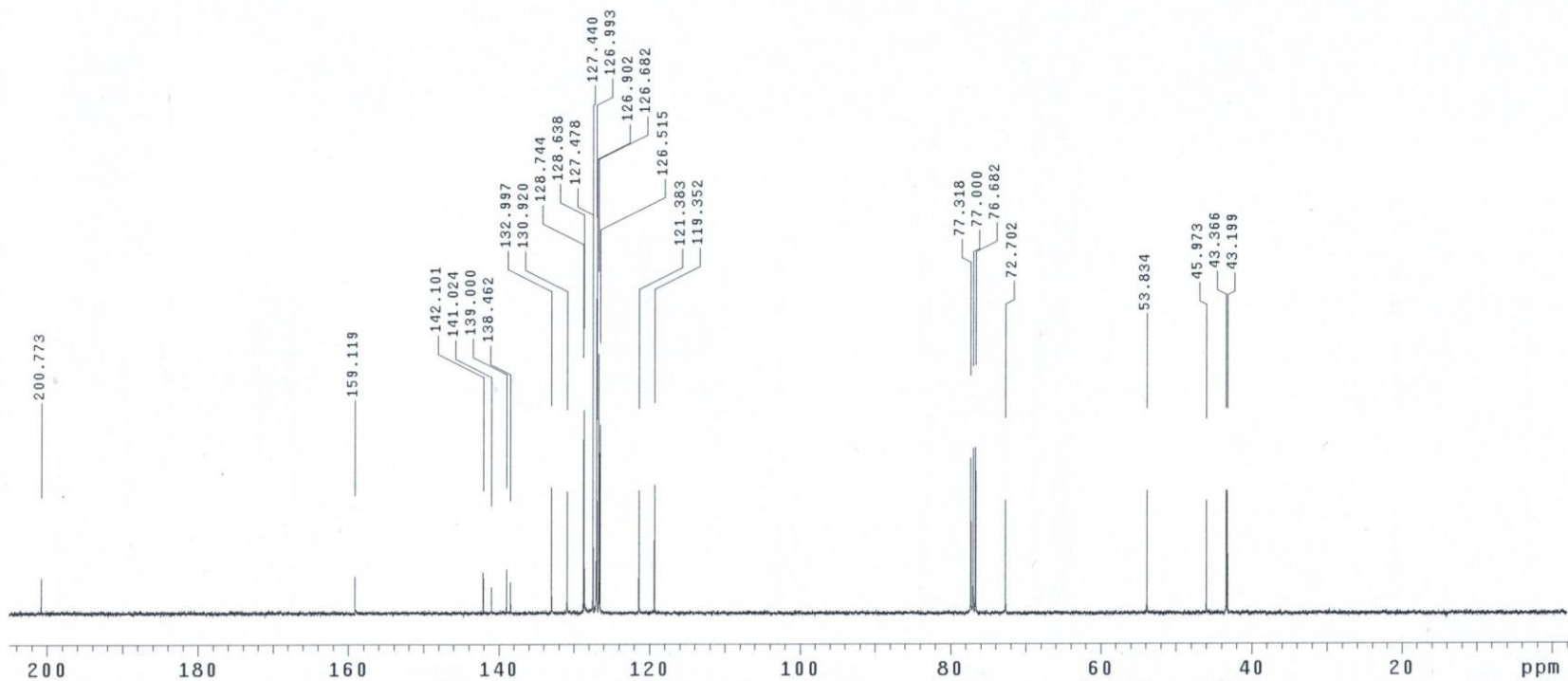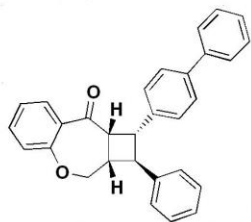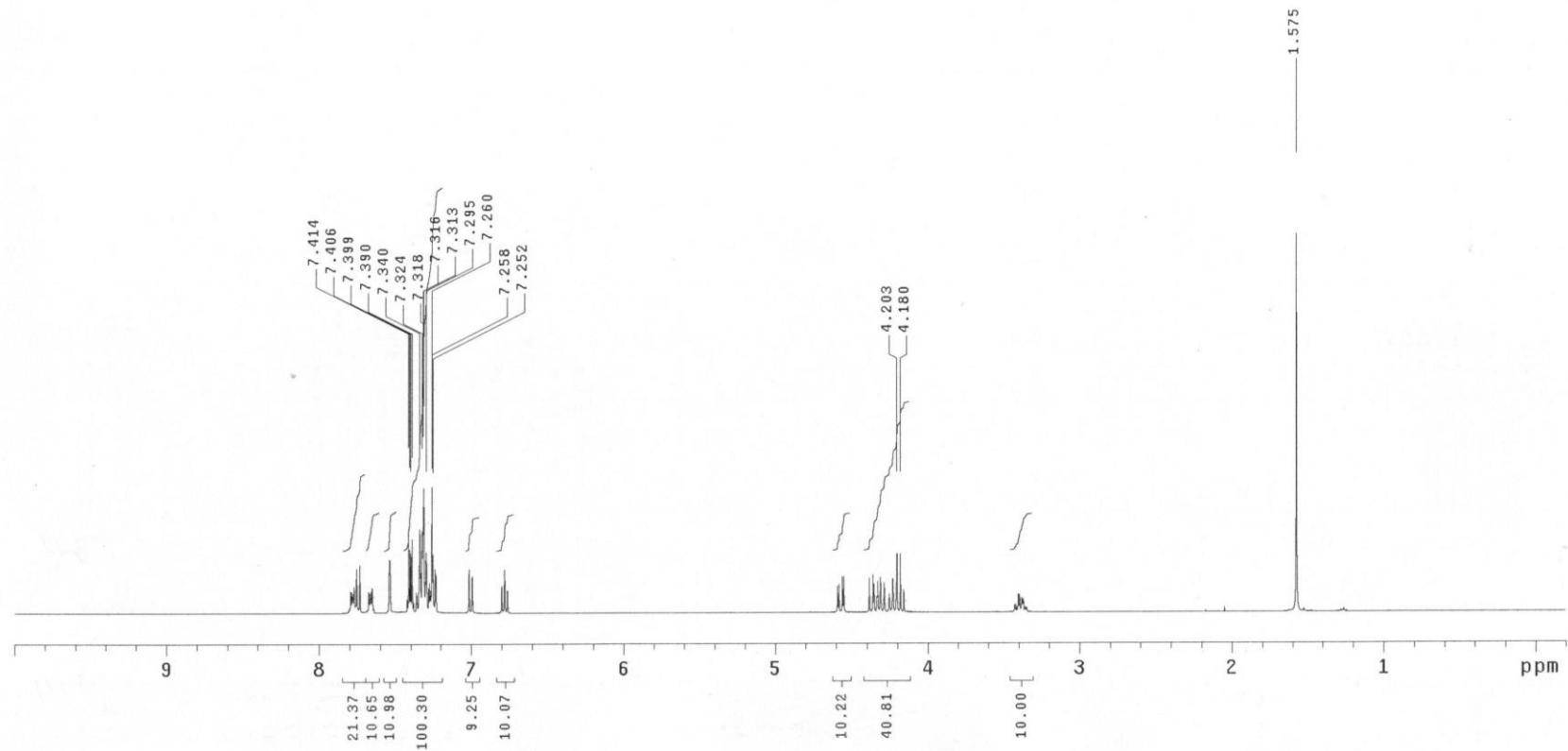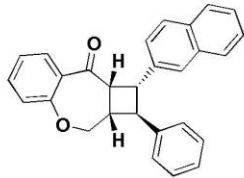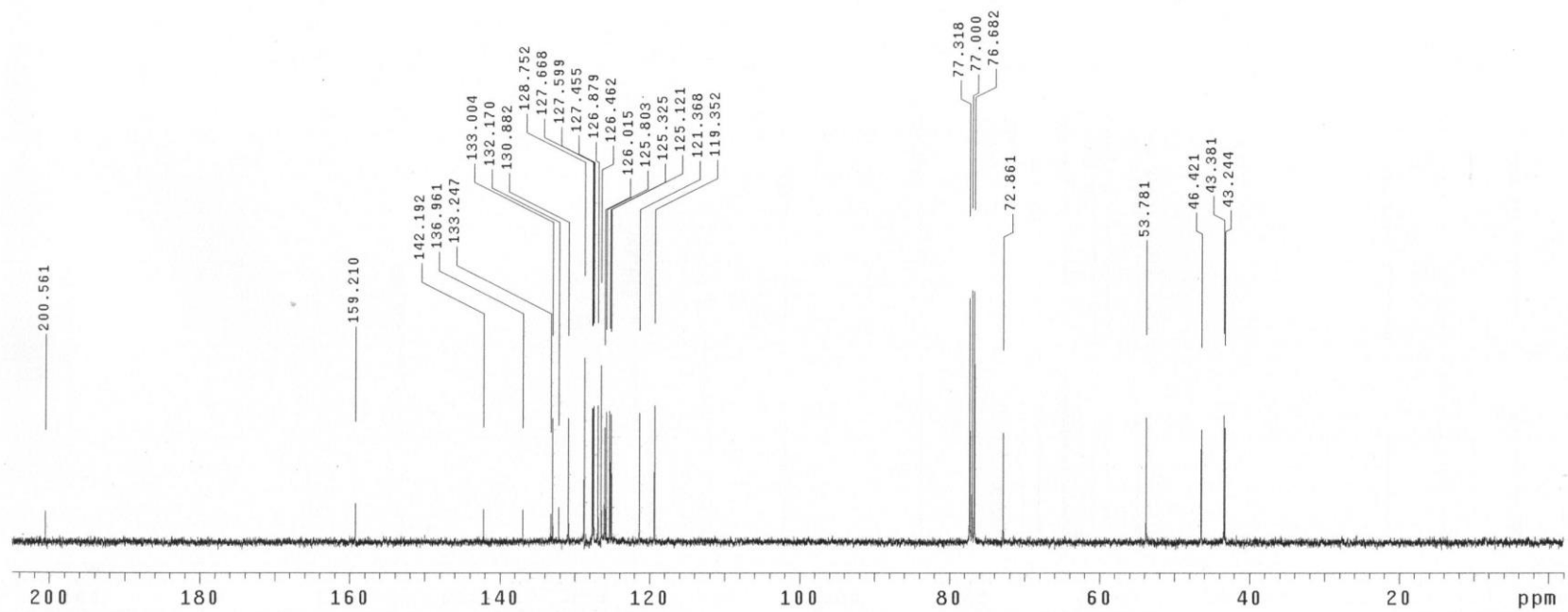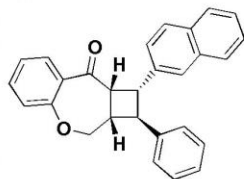Total 2832 repetitions

201.160
156.117
136.279
136.211
133.050
130.889
130.510
129.616
128.585
127.948
126.530
124.977
124.127
120.504
111.991
77.318
77.000
76.682
69.010
30.342

200   180   160   140   120   100   80   60   40   20   ppm
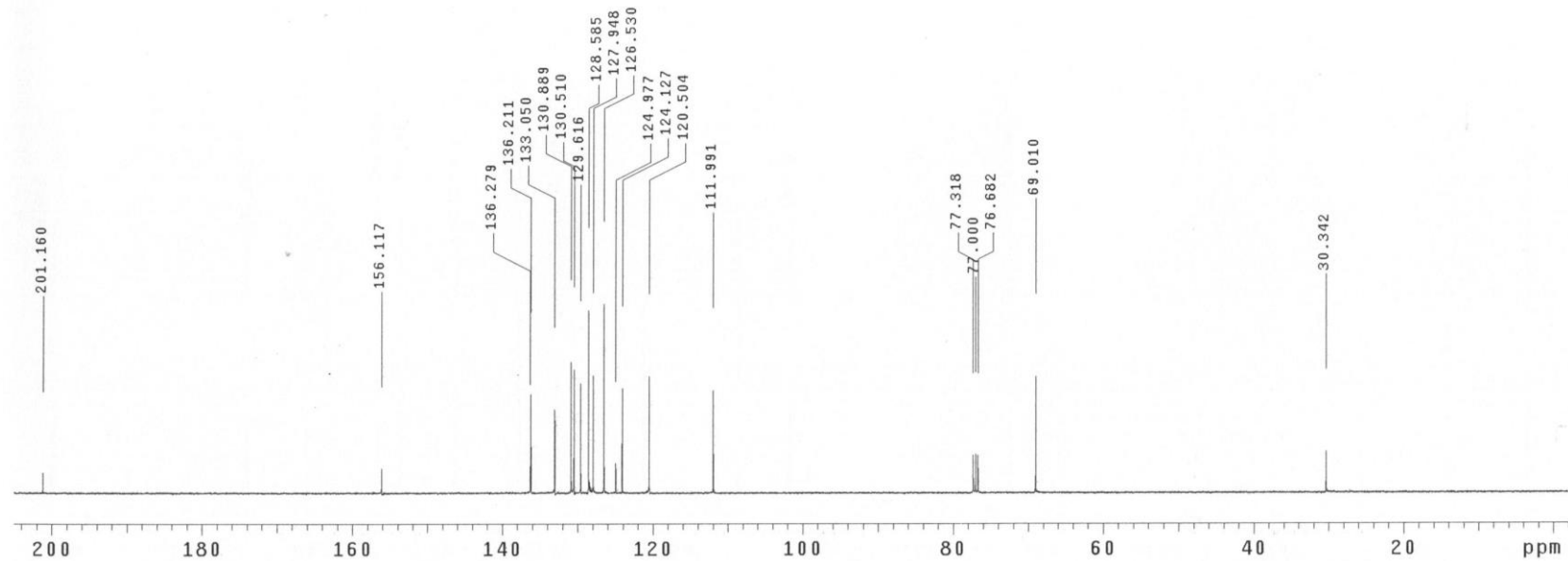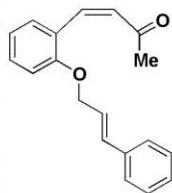
X-ray crystal data of compound 6a (CCDC 1943157)
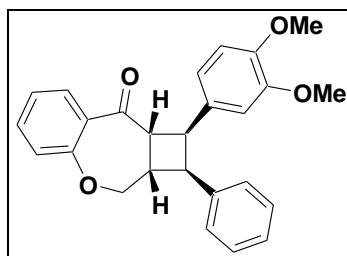
Sample preparation : A solution of compound **6a** (30 mg) in CH_2Cl_2 (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.

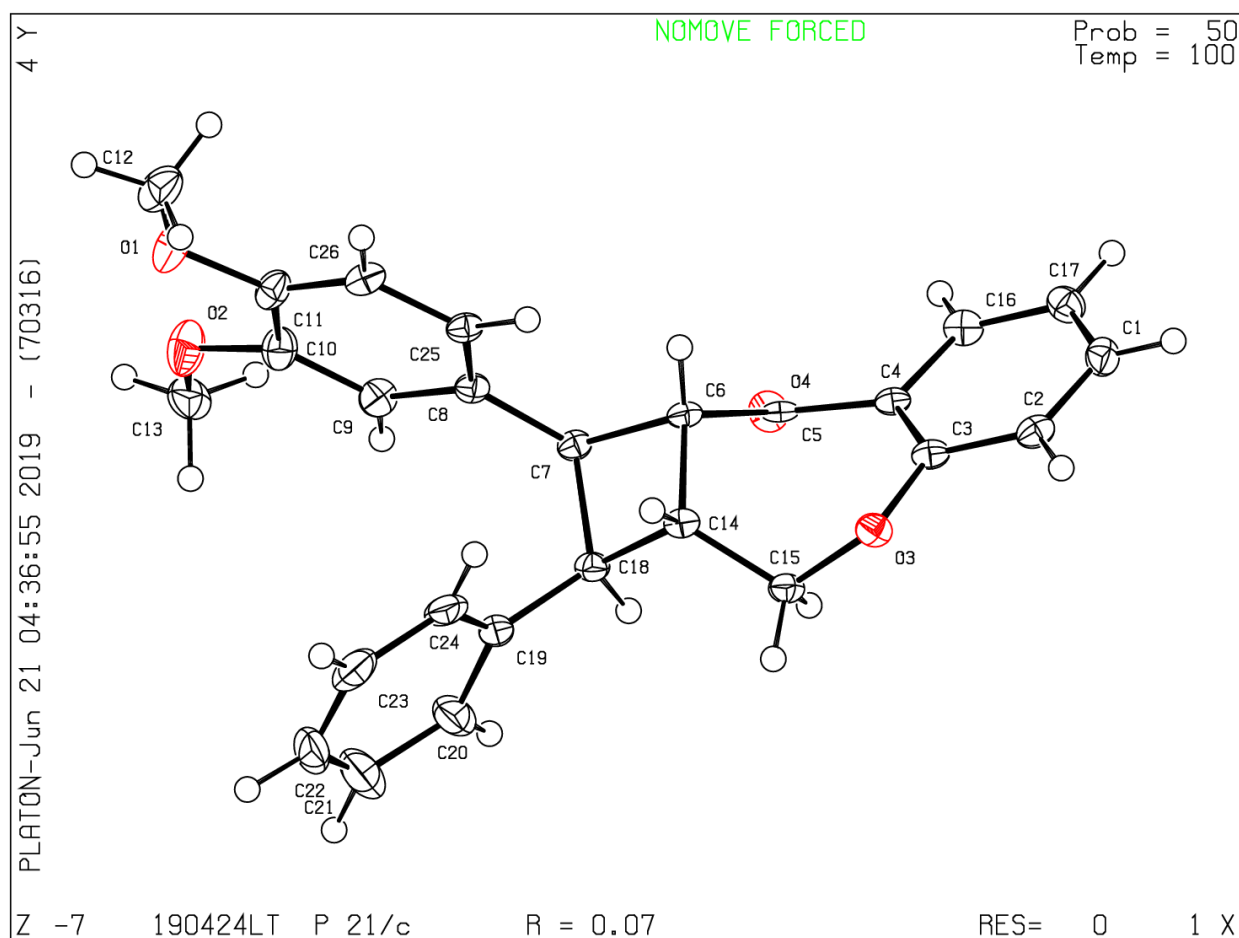|	
Identification code	190424LT
Empirical formula	C26 H24 O4
Formula weight	400.45
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 17.962(3) Å α = 90°.
	b = 10.2398(15) Å β = 93.763(6)°.
	c = 11.0654(16) Å γ = 90°.
Volume	2030.8(5) Å^3
Z	4
Density (calculated)	1.310 Mg/m^3
Absorption coefficient	0.087 mm^{-1}
F(000)	848
Crystal size	0.27 x 0.25 x 0.25 mm^3
Theta range for data collection	2.273 to 26.665°.
Index ranges	-22<=h<=22, -12<=k<=12, -13<=l<=13
Reflections collected	28293
Independent reflections	4214 [R(int) = 0.0777]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.4629
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4214 / 0 / 273
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)]	R1 = 0.0733, wR2 = 0.2118
R indices (all data)	R1 = 0.0878, wR2 = 0.2262
Extinction coefficient	n/a
Largest diff. peak and hole	0.694 and -0.430 e.Å^{-3}

X-ray crystal data of compound 6d (CCDC 1943158)
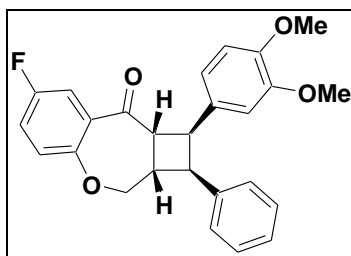

Sample preparation : A solution of compound **6d** (30 mg) in CH$_2$Cl$_2$ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.
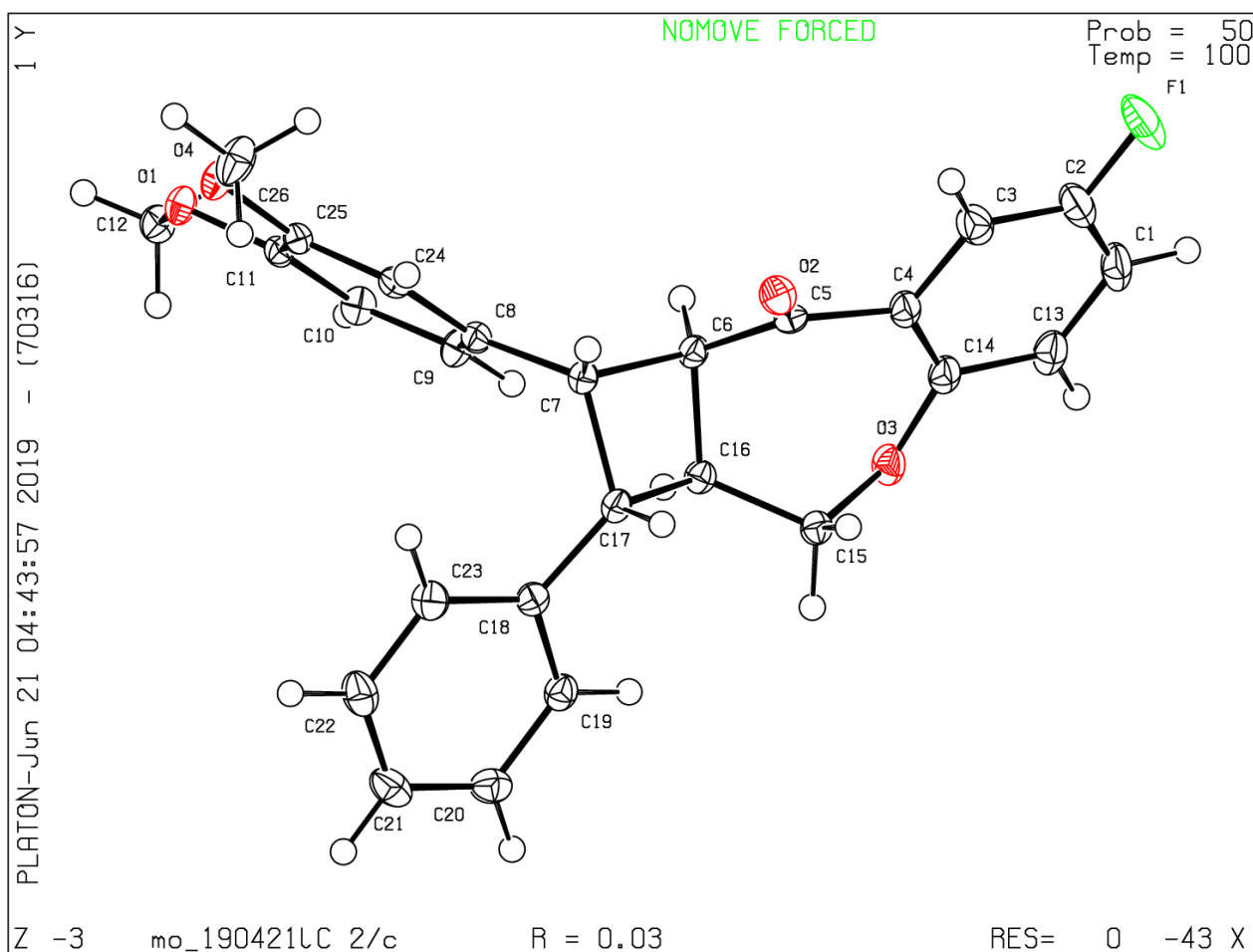
Identification code	mo_190421lt_0m
Empirical formula	C26 H23 F O4
Formula weight	418.44
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 27.5645(11) Å α = 90°.
	b = 7.0521(3) Å β = 114.5740(10)°.
	c = 22.8442(10) Å γ = 90°.
Volume	4038.4(3) Å^3
Z	8
Density (calculated)	1.376 Mg/m^3
Absorption coefficient	0.098 mm^{-1}
F(000)	1760
Crystal size	0.25 x 0.20 x 0.20 mm^3
Theta range for data collection	1.625 to 26.487°.
Index ranges	-34<=h<=34, -8<=k<=8, -28<=l<=28
Reflections collected	34057
Independent reflections	4175 [R(int) = 0.0291]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.7264
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4175 / 0 / 282
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0835
R indices (all data)	R1 = 0.0412, wR2 = 0.0881
Extinction coefficient	n/a
Largest diff. peak and hole	0.296 and -0.208 e.Å^{-3}

X-ray crystal data of compound 7a (CCDC 1943159)
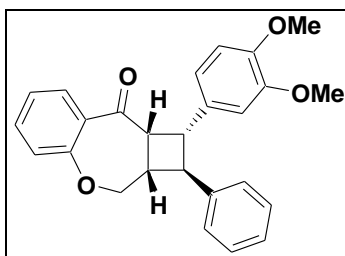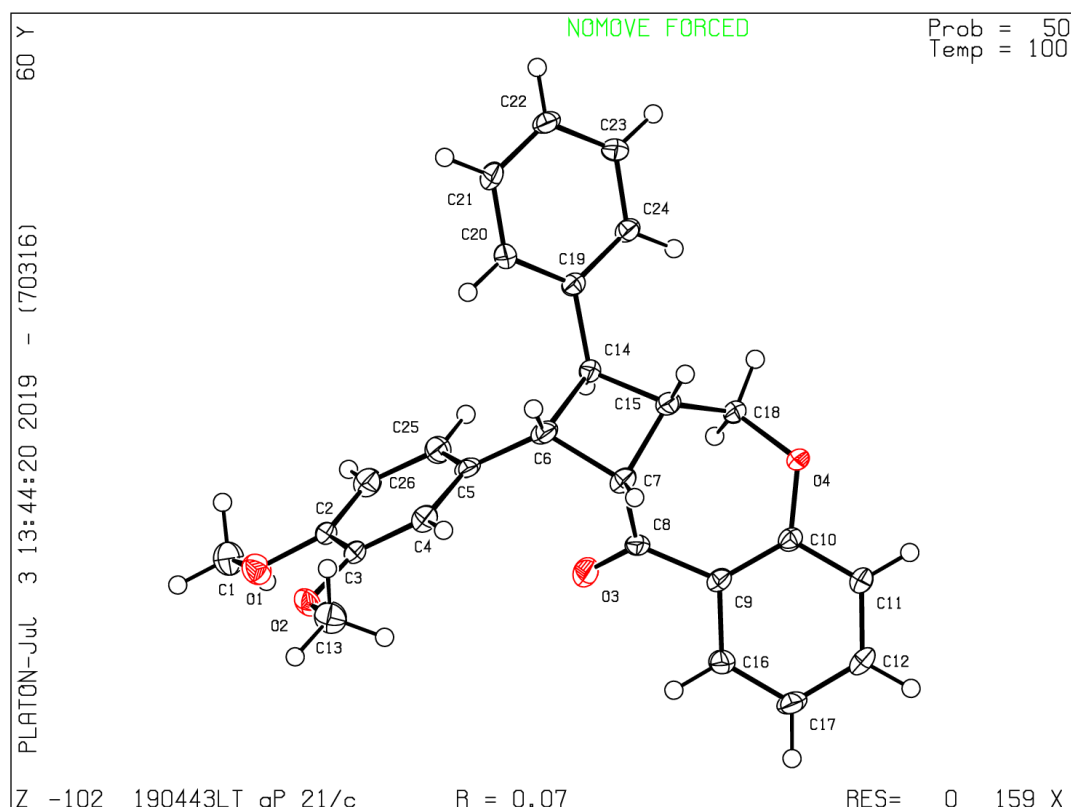

Sample preparation : A solution of compound **7a** (30 mg) in CH_2Cl_2 (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.
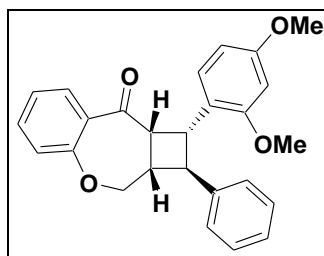
Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.
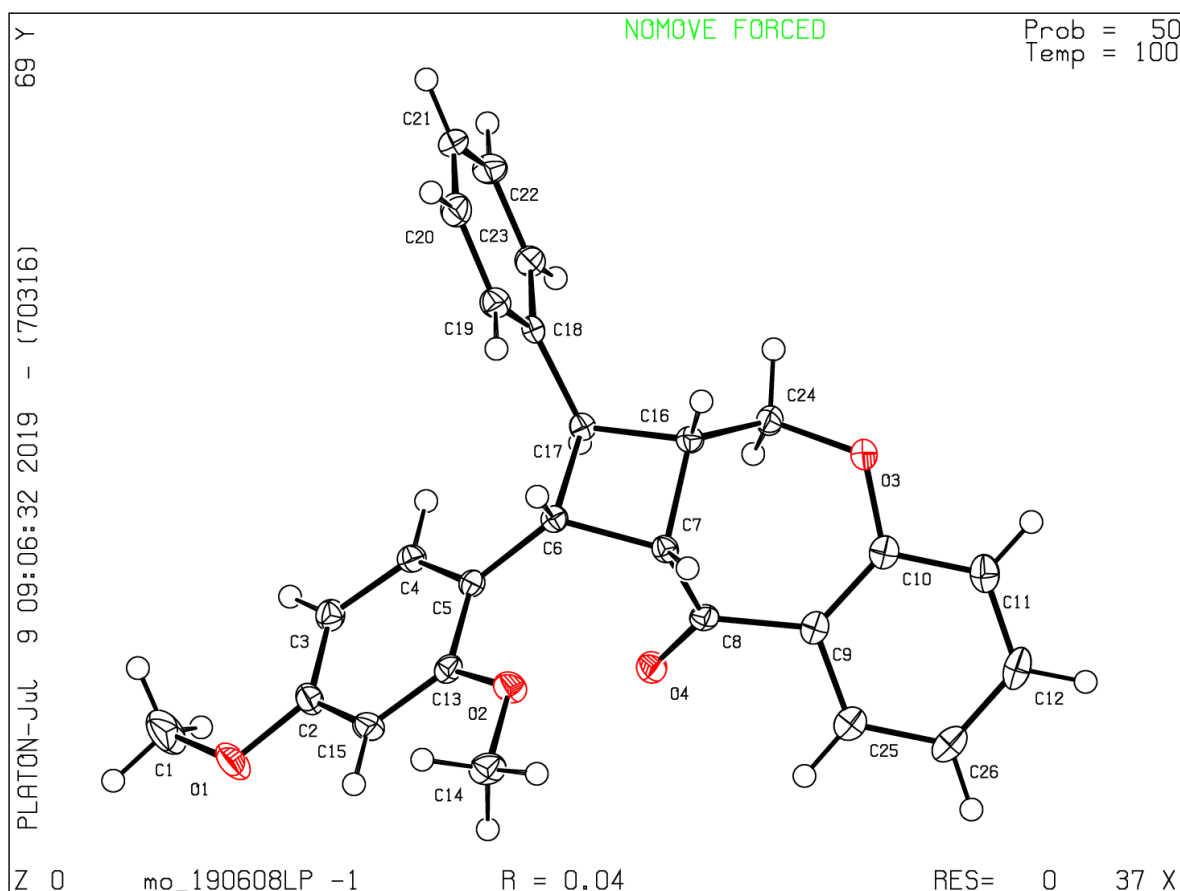
Identification code	190443LT_a
Empirical formula	C26 H24 O4
Formula weight	400.45
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 13.8730(7) Å $\quad$ α = 90°.
	b = 22.7202(12) Å $\quad$ β = 98.843(2)°.
	c = 6.3384(3) Å $\quad$ γ = 90°.
Volume	1974.10(17) Å^3
Z	4
Density (calculated)	1.347 Mg/m^3
Absorption coefficient	0.090 mm^{-1}
F(000)	848
Crystal size	0.14 x 0.12 x 0.04 mm^3
Theta range for data collection	1.485 to 26.410°.
Index ranges	-15<=h<=17, -17<=k<=28, -7<=l<=7
Reflections collected	14699
Independent reflections	4040 [R(int) = 0.0306]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6781
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4040 / 0 / 273
Goodness-of-fit on F^2	1.131
Final R indices [I>2sigma(I)]	R1 = 0.0716, wR2 = 0.1719
R indices (all data)	R1 = 0.0849, wR2 = 0.1787
Extinction coefficient	n/a
Largest diff. peak and hole	0.711 and -0.293 e.Å^{-3}

X-ray crystal data of compound 7m (CCDC 1943160)

Sample preparation : A solution of compound **7m** (30 mg) in CH_2Cl_2 (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.

Identification code	mo_190608LT_0m
Empirical formula	C26 H24 O4
Formula weight	400.45
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.4174(5) Å $\quad$ α = 92.823(2)°.
	b = 10.5047(5) Å $\quad$ β = 108.693(2)°.
	c = 11.7070(6) Å $\quad$ γ = 109.839(2)°.
Volume	1015.58(9) Å^3
Z	2
Density (calculated)	1.310 Mg/m^3
Absorption coefficient	0.087 mm^{-1}
F(000)	424
Crystal size	0.30 x 0.28 x 0.27 mm^3
Theta range for data collection	1.866 to 26.432°.
Index ranges	-11<=h<=11, -13<=k<=13, -14<=l<=14
Reflections collected	23935
Independent reflections	4180 [R(int) = 0.0254]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.7241
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4180 / 0 / 273
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.0856
R indices (all data)	R1 = 0.0443, wR2 = 0.0909
Extinction coefficient	n/a
Largest diff. peak and hole	0.268 and -0.254 e.Å^{-3}