Supporting Information

A Novel One-pot Synthesis of Flavones

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807, Taiwan
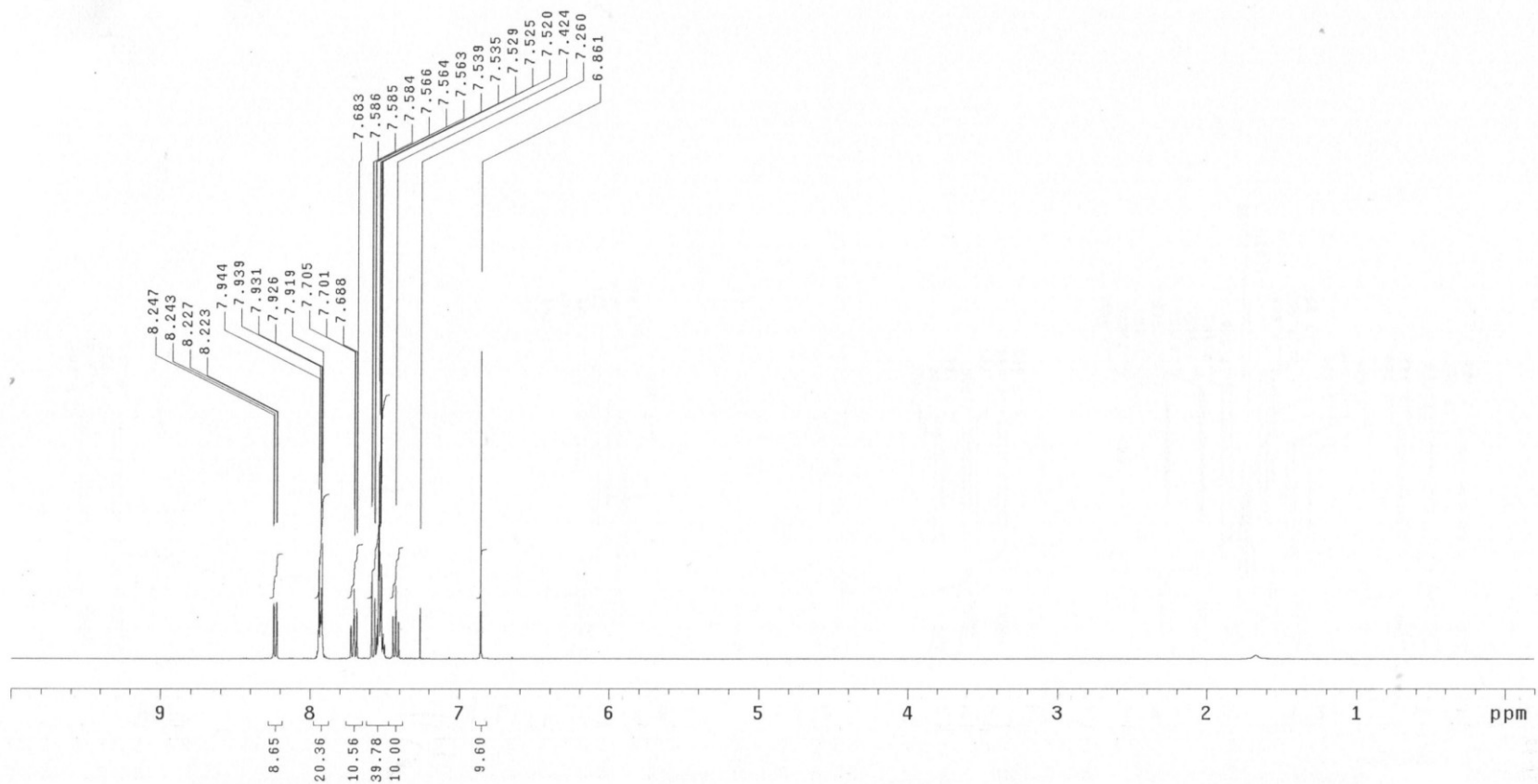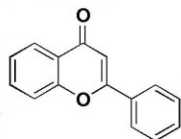
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Compound 4a (^{1}H-NMR spectral data)

MC0701

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.247
8.243
8.227
8.223
7.944
7.939
7.931
7.926
7.919
7.705
7.701
7.688
7.683
7.586
7.585
7.584
7.566
7.564
7.563
7.539
7.535
7.529
7.525
7.520
7.424
7.260
6.861

8.65
20.36
10.56
39.78
10.00
9.60

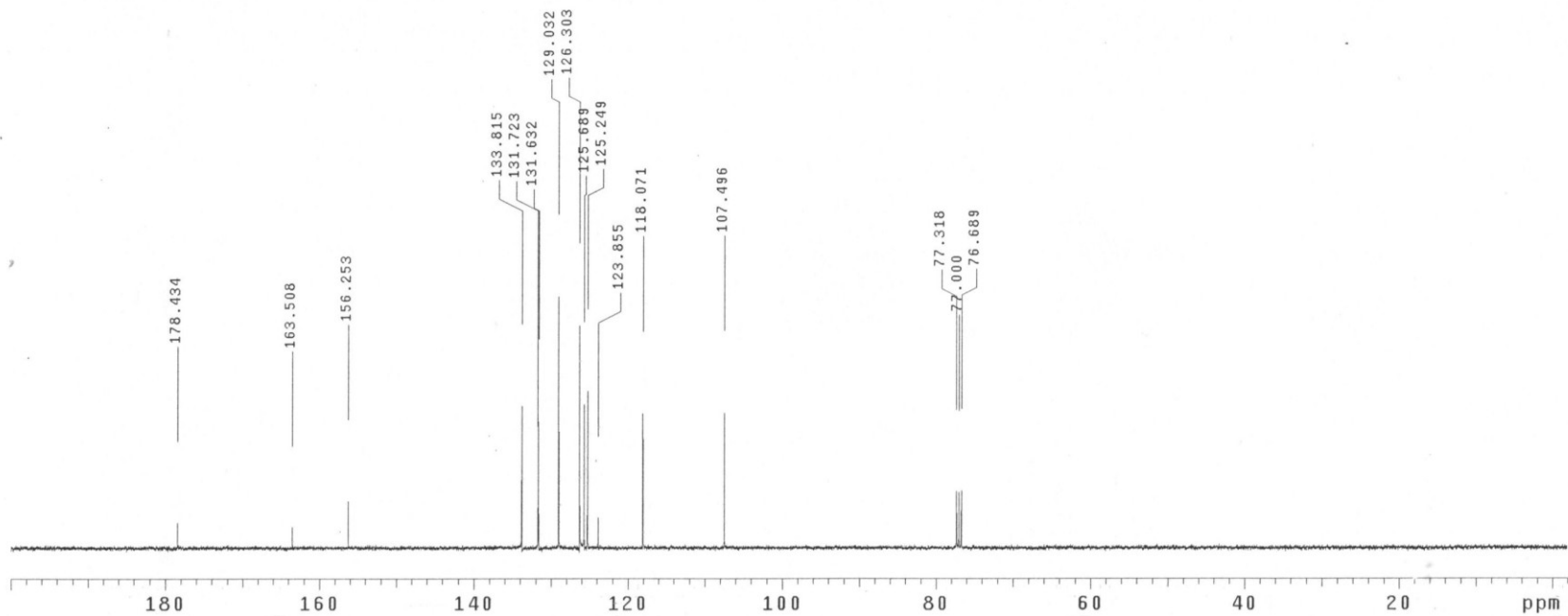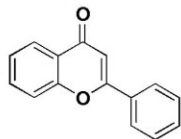9   8   7   6   5   4   3   2   1   ppm

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

MC0701

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 1264 repetitions

178.434
163.508
156.253
133.815
131.723
131.632
129.032
126.303
125.689
125.249
123.855
118.071
107.496
77.318
77.000
76.689

180   160   140   120   100   80   60   40   20   ppm

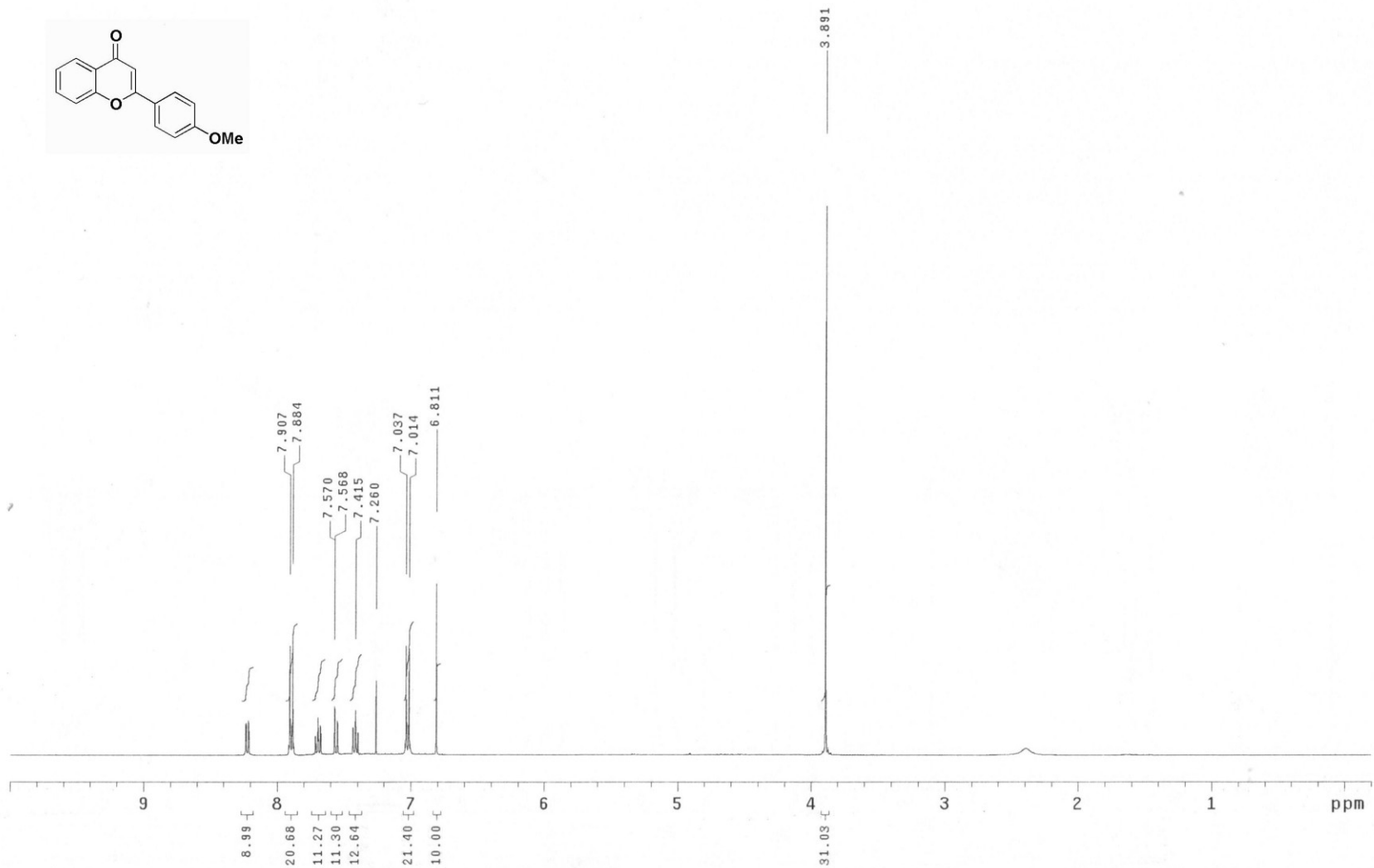# Compound 4b (^{1}H-NMR spectral data)

MC0730

Pulse Sequence: s2pul

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

3.891

7.907
7.884
7.570
7.568
7.415
7.260
7.037
7.014
6.811

8.99 20.68 11.27 11.30 12.64 21.40 10.00 31.03

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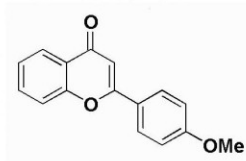
Compound 4b (^{13}C-NMR spectral data)

MC0730

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
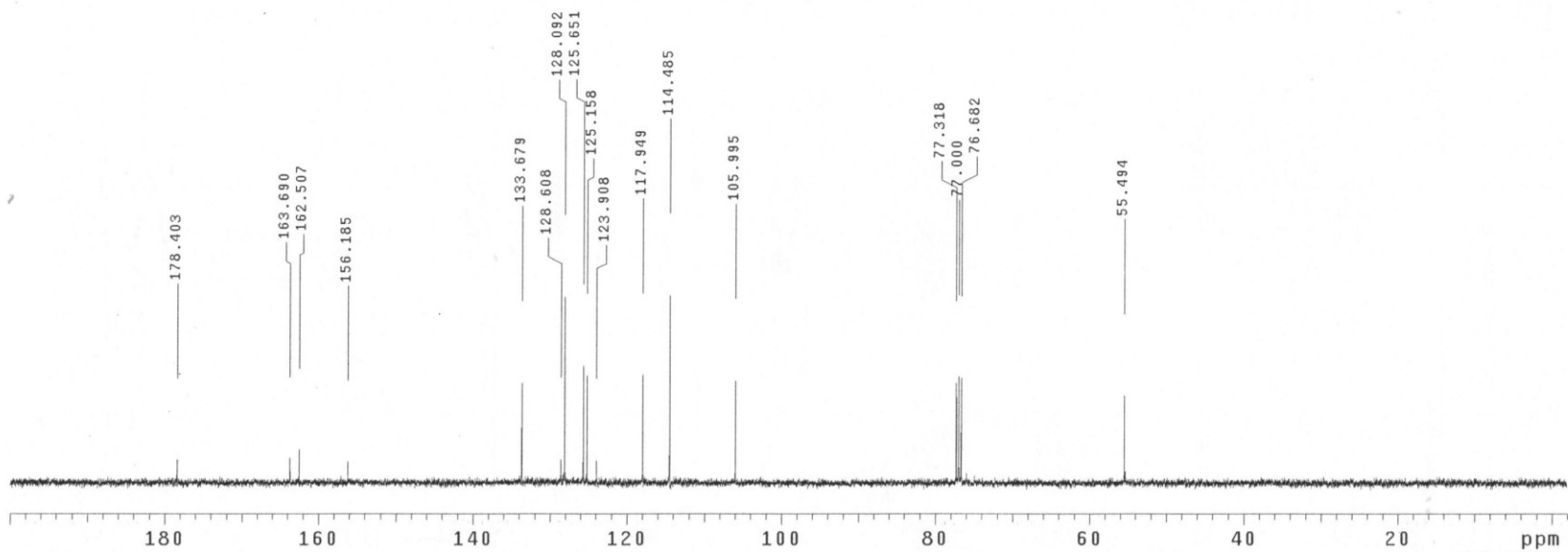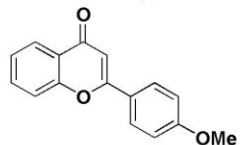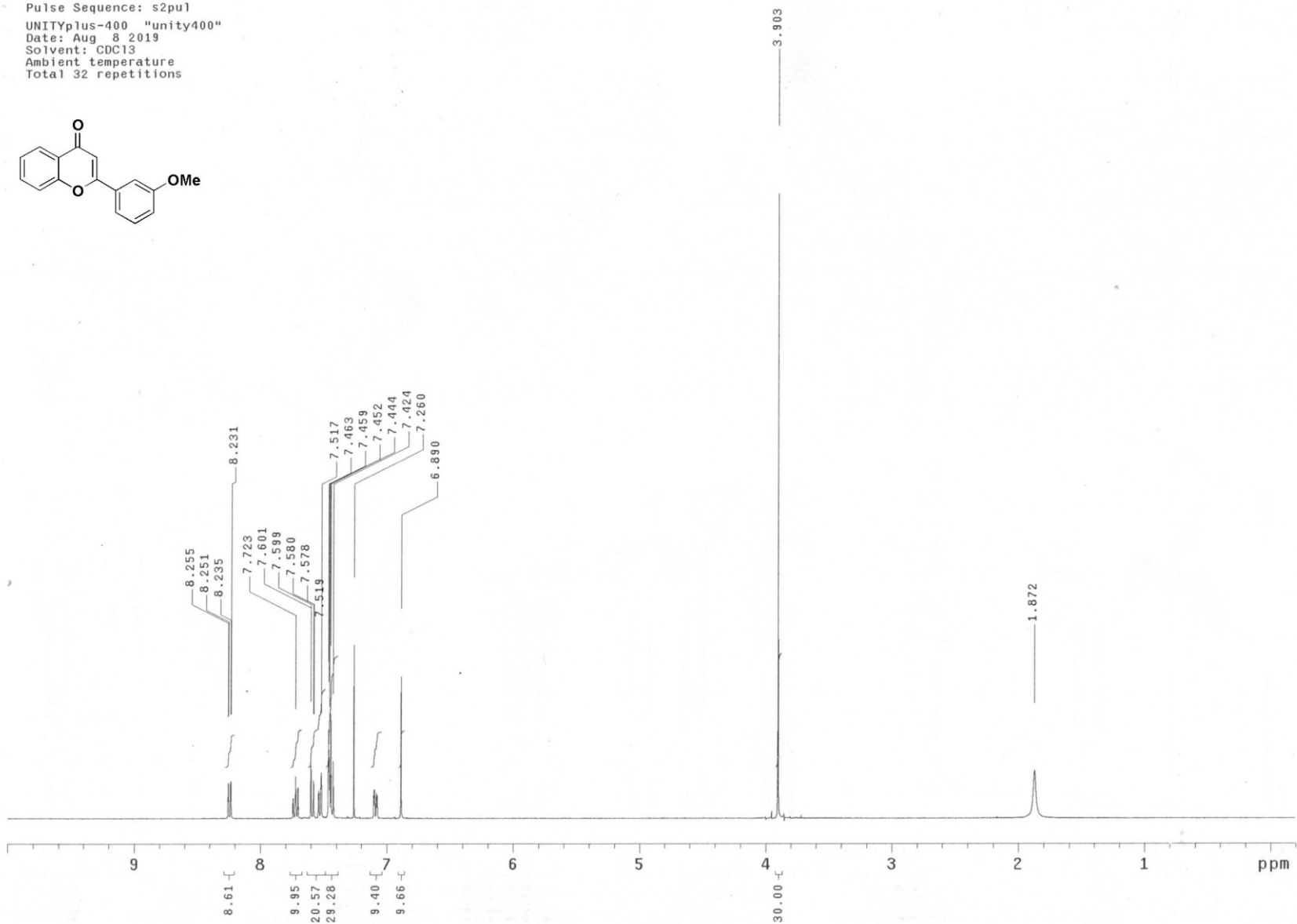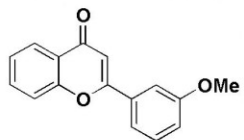Date: Jul 31 2019
Solvent: CDCl3
Ambient temperature
Total 1024 repetitions

178.403
163.690
162.507
156.185
133.679
128.608
128.092
125.651
125.158
123.908
117.949
114.485
105.995
77.318
77.000
76.682
55.494

180   160   140   120   100   80   60   40   20   ppm

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

MC0807

Pulse Sequence: s2pul

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

3.903

8.255
8.251
8.235
8.231

7.723
7.601
7.599
7.580
7.578
7.519
7.517
7.463
7.459
7.452
7.444
7.424
7.260
6.890

1.872

8.61

9.95
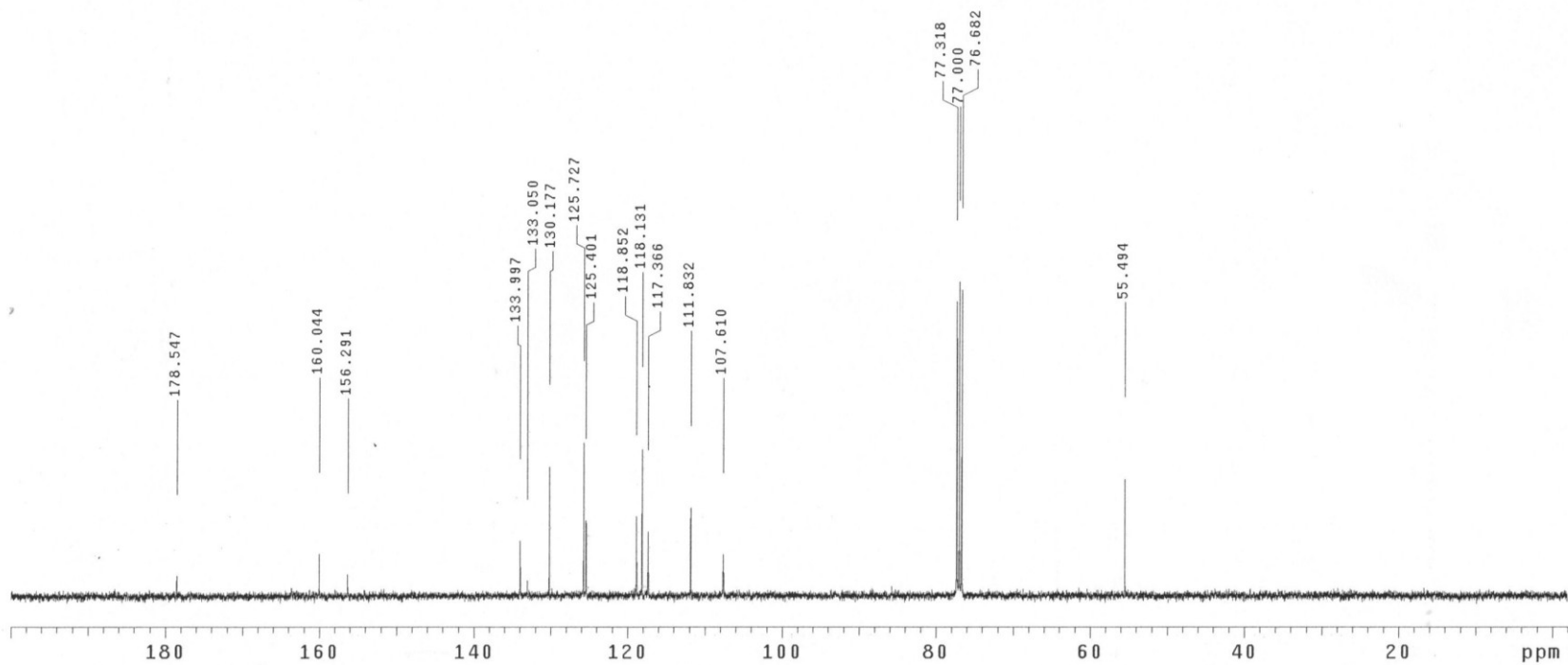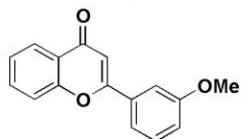20.57
29.28

9.40
9.66

30.00

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

MC0807

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 8 2019
Solvent: CDCl3
Ambient temperature
Total 8032 repetitions

178.547
160.044
156.291
133.997
133.050
130.177
125.727
125.401
118.852
118.131
117.366
111.832
107.610
77.318
77.000
76.682
55.494

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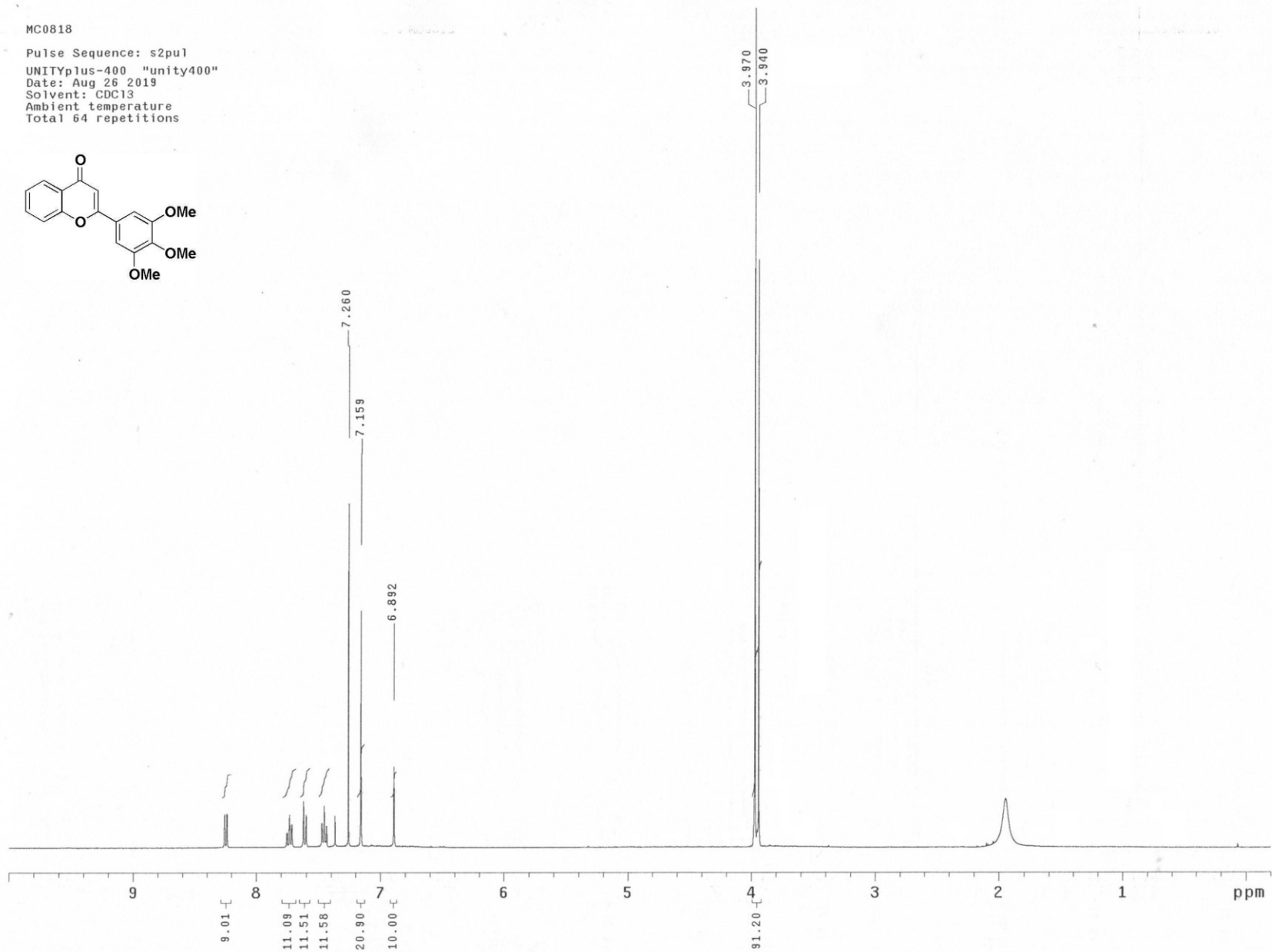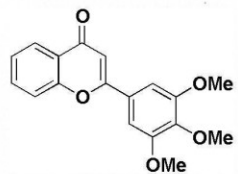

MC0818

Pulse Sequence: s2pul

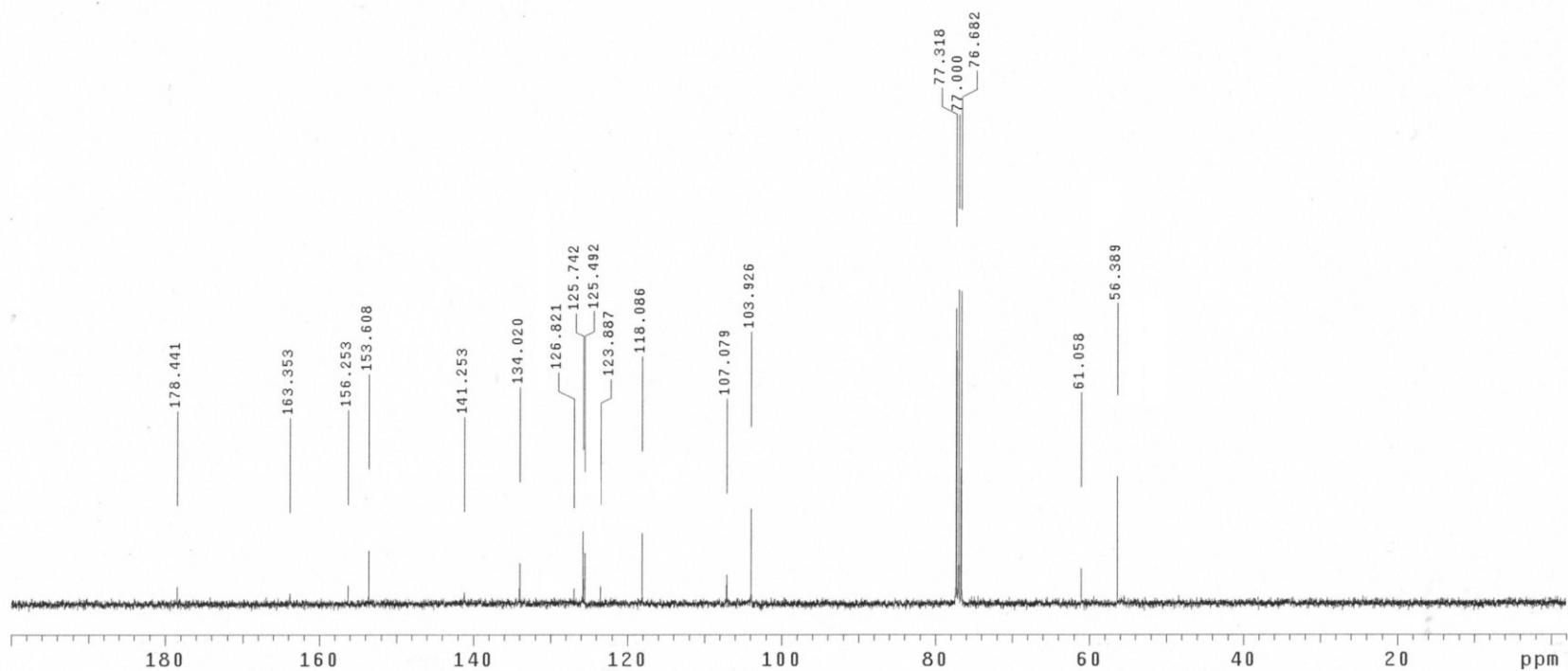UNITYplus-400 "unity400"
Date: Aug 26 2019
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

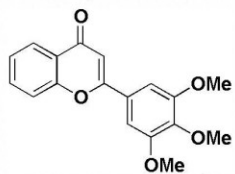# Compound 4d (^{13}C-NMR spectral data)

MC0818

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 26 2019
Solvent: CDC13
Ambient temperature
Total 7200 repetitions

178.441
163.353
156.253
153.608
141.253
134.020
126.821
125.742
125.492
123.887
118.086
107.079
103.926
77.318
77.000
76.682
61.058
56.389

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

MC0813

Pulse Sequence: s2pul

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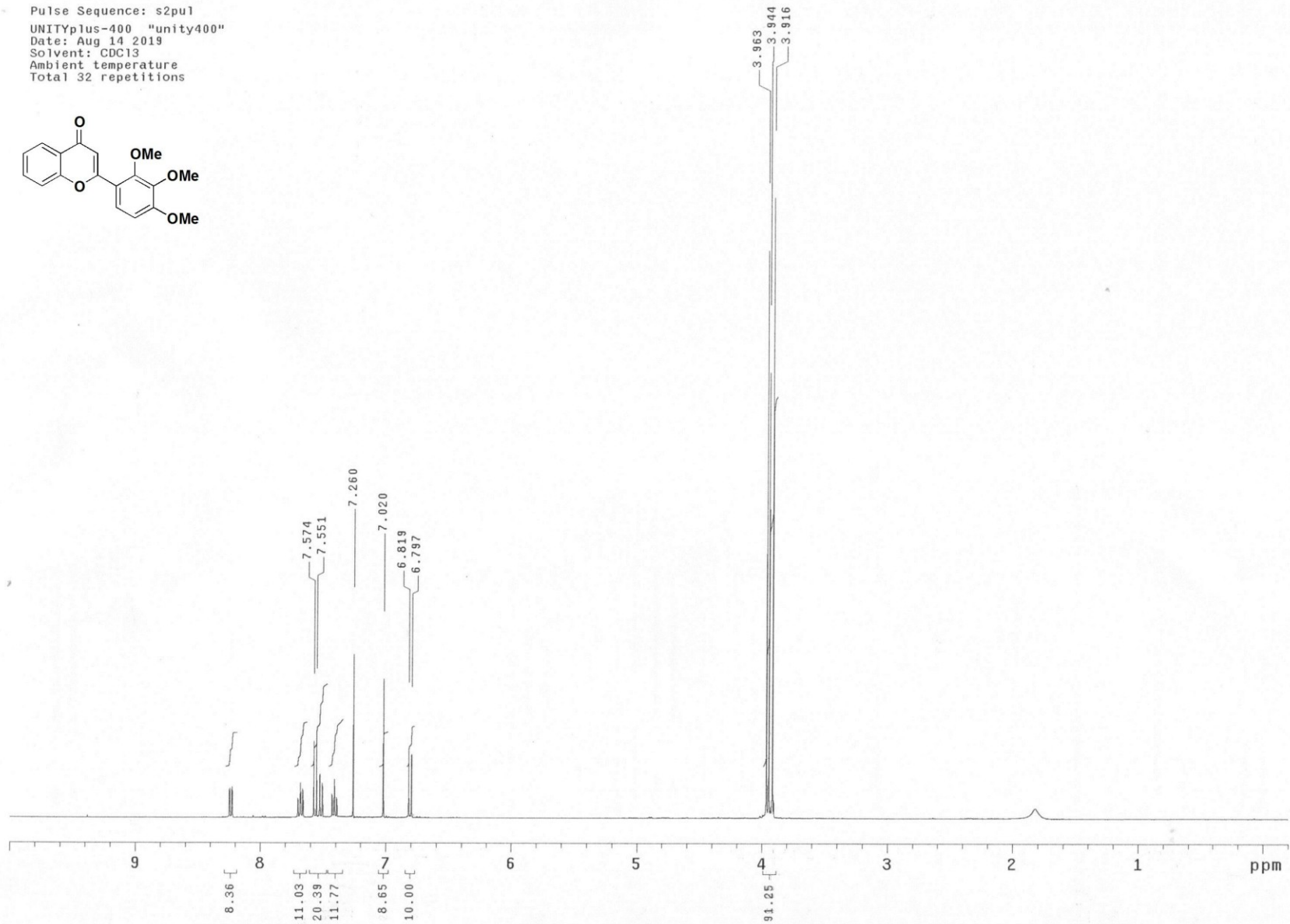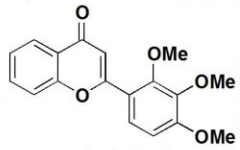Date: Aug 14 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.963
3.944
3.916

7.574
7.551
7.260
7.020
6.819
6.797

9 8 7 6 5 4 3 2 1 ppm

8.36
11.03
20.39
11.77
8.65
10.00
91.25

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

MC0813
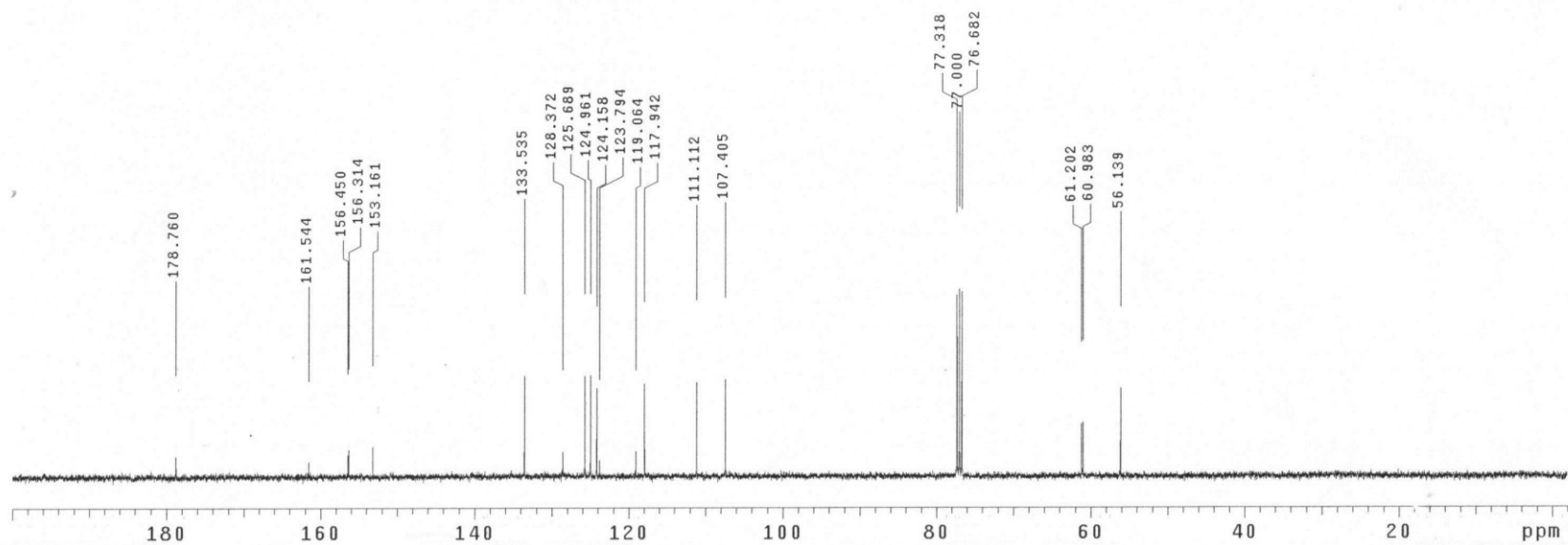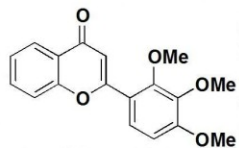
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 14 2019
Solvent: CDCl3
Ambient temperature
Total 4608 repetitions

178.760
161.544
156.450
156.314
153.161
133.535
128.372
125.689
124.961
124.158
123.794
119.064
117.942
111.112
107.405
77.318
77.000
76.682
61.202
60.983
56.139

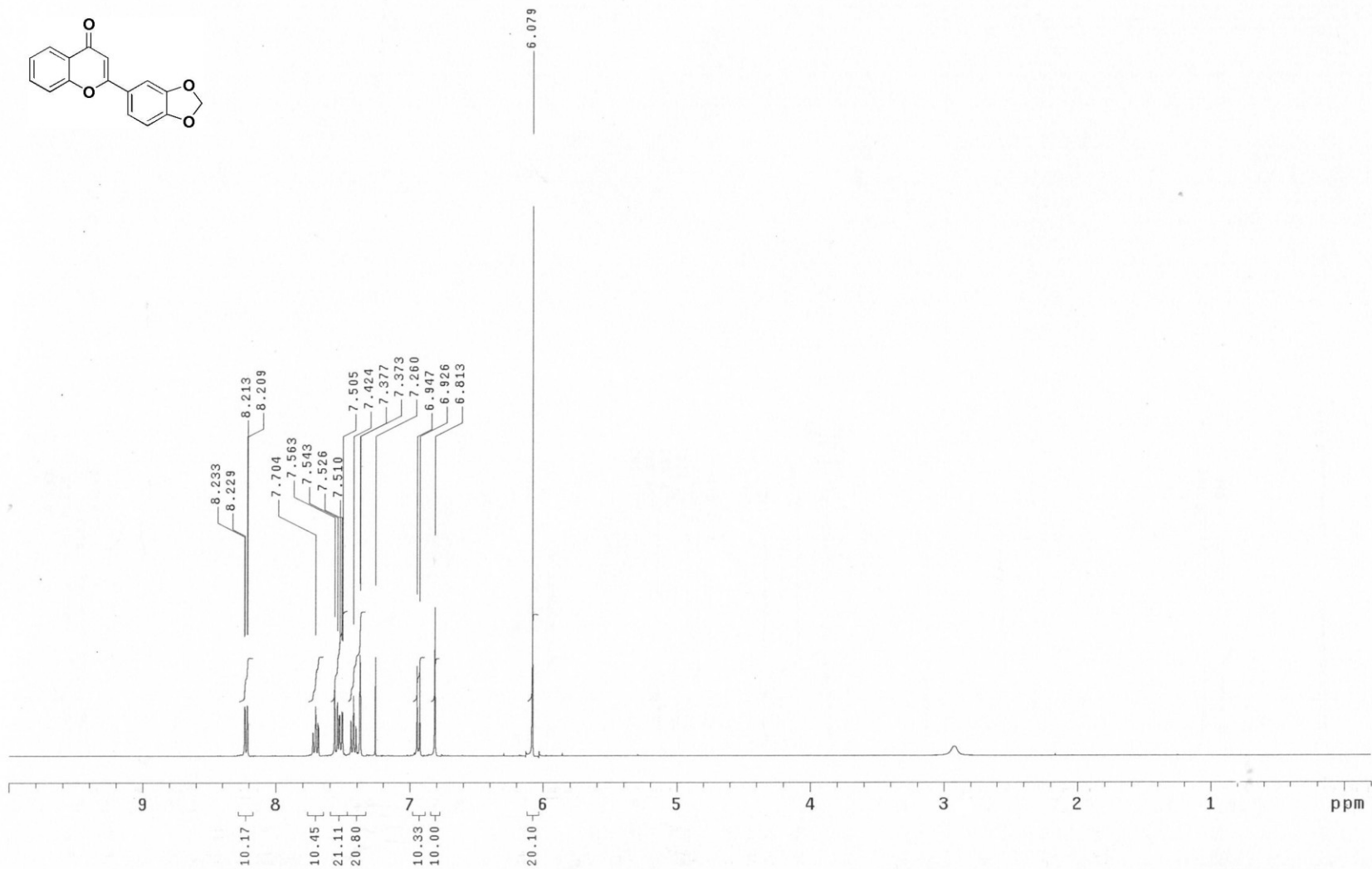# Compound 4f (^{1}H-NMR spectral data)

MC0822

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 22 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.233
8.229
8.213
8.209
7.704
7.563
7.543
7.526
7.510
7.505
7.424
7.377
7.373
7.260
6.947
6.926
6.813
6.079

10.17
10.45
21.11
20.80
10.33
10.00
20.10
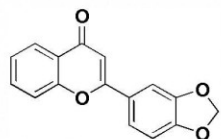
Compound 4f (^{13}C-NMR spectral data)

MC0822

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
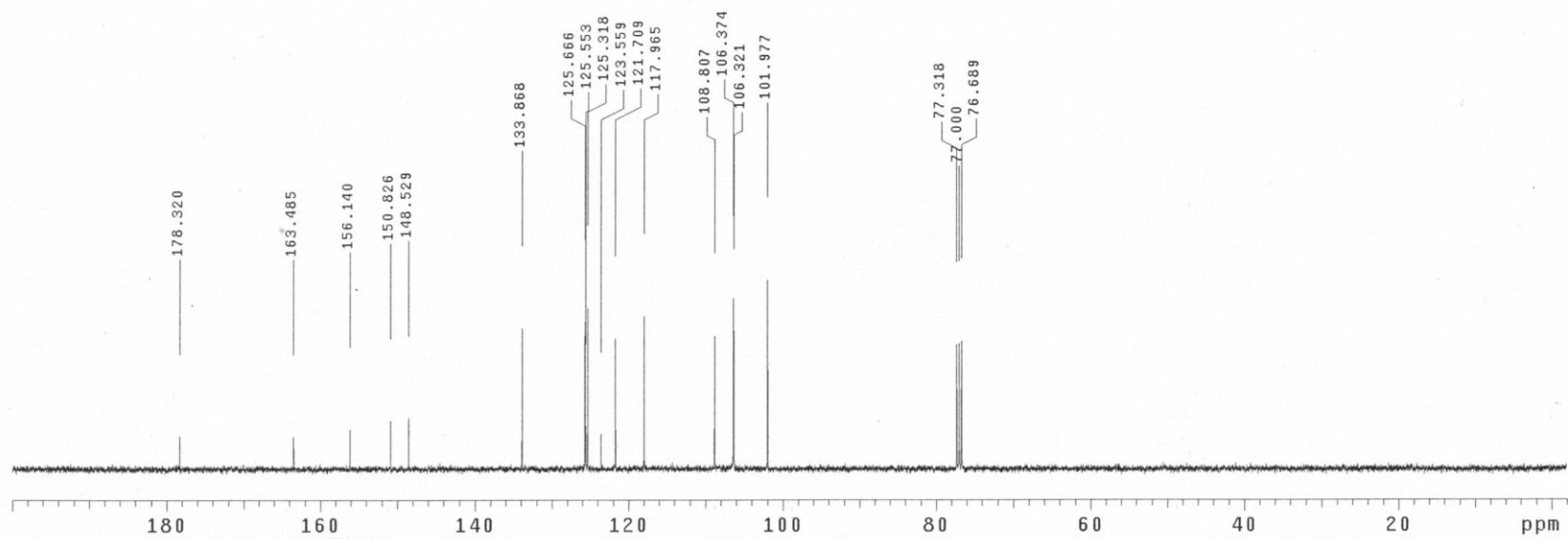Date: Aug 22 2019
Solvent: CDC13
Ambient temperature
Total 2272 repetitions

178.320
163.485
156.140
150.826
148.529
133.868
125.666
125.553
125.318
123.559
121.709
117.965
108.807
106.374
106.321
101.977
77.318
77.000
76.689

180   160   140   120   100   80   60   40   20   ppm

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

MC0821

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
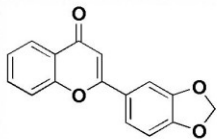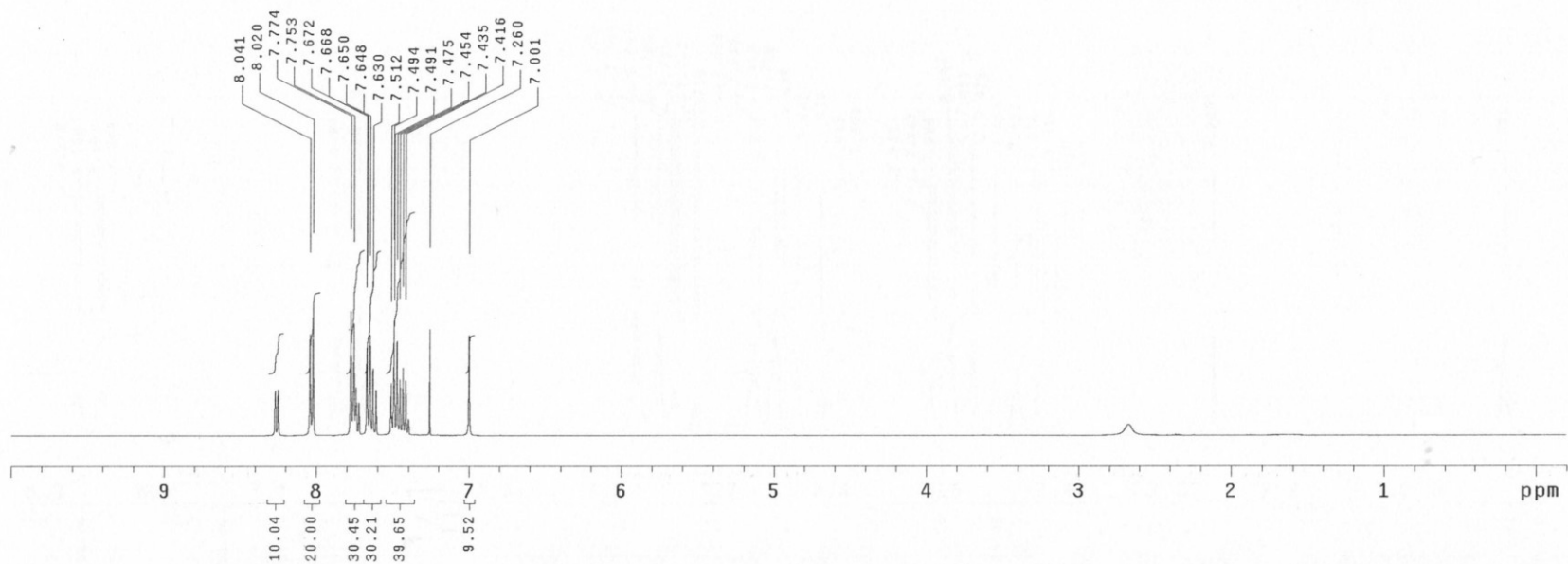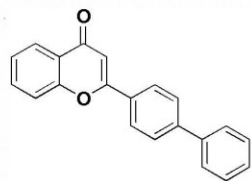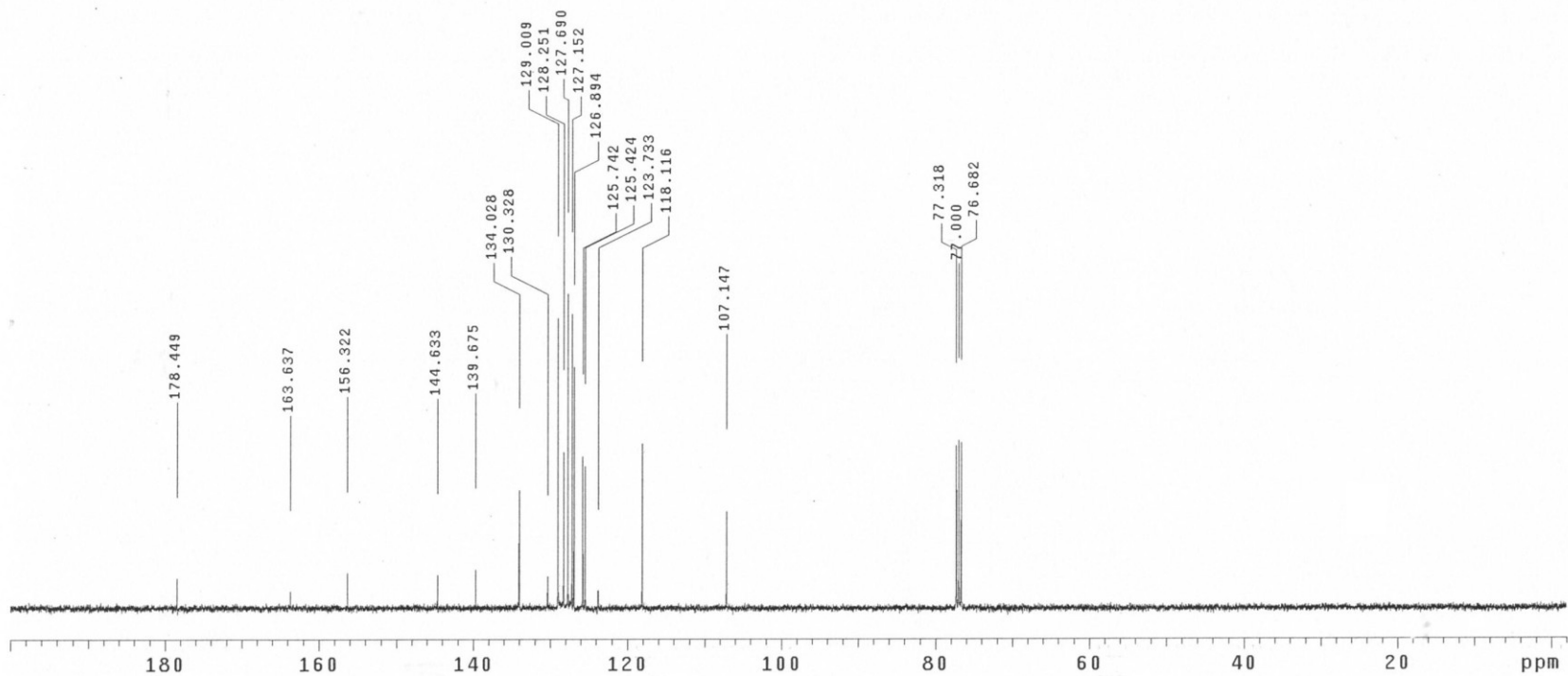Date: Aug 22 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

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

MC0821

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 22 2019
Solvent: CDC13
Ambient temperature
Total 3728 repetitions

Peaks: 178.449, 163.637, 156.322, 144.633, 139.675, 134.028, 130.328, 129.009, 128.251, 127.690, 127.152, 126.894, 125.742, 125.424, 123.733, 118.116, 107.147, 77.318, 77.000, 76.682

Compound 4h (¹H-NMR spectral data)

MC0726

Pulse Sequence: s2pul

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

3.990
3.970

8.246
8.242
8.226
8.222

7.704
7.701
7.598
7.592
7.577
7.571
7.445
7.427
7.425
7.407
7.401
7.260
7.006
6.985
6.823

9   8   7   6   5   4   3   2   1   ppm

8.56
10.50
20.57
21.83
10.87
9.49
60.00

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

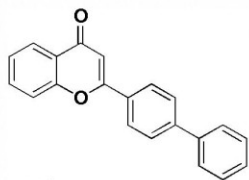MC0726

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jul 29 2019
Solvent: CDCl3
Ambient temperature
Total 4752 repetitions

Compound 4i (¹H-NMR spectral data)

MC0801

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 5 2019
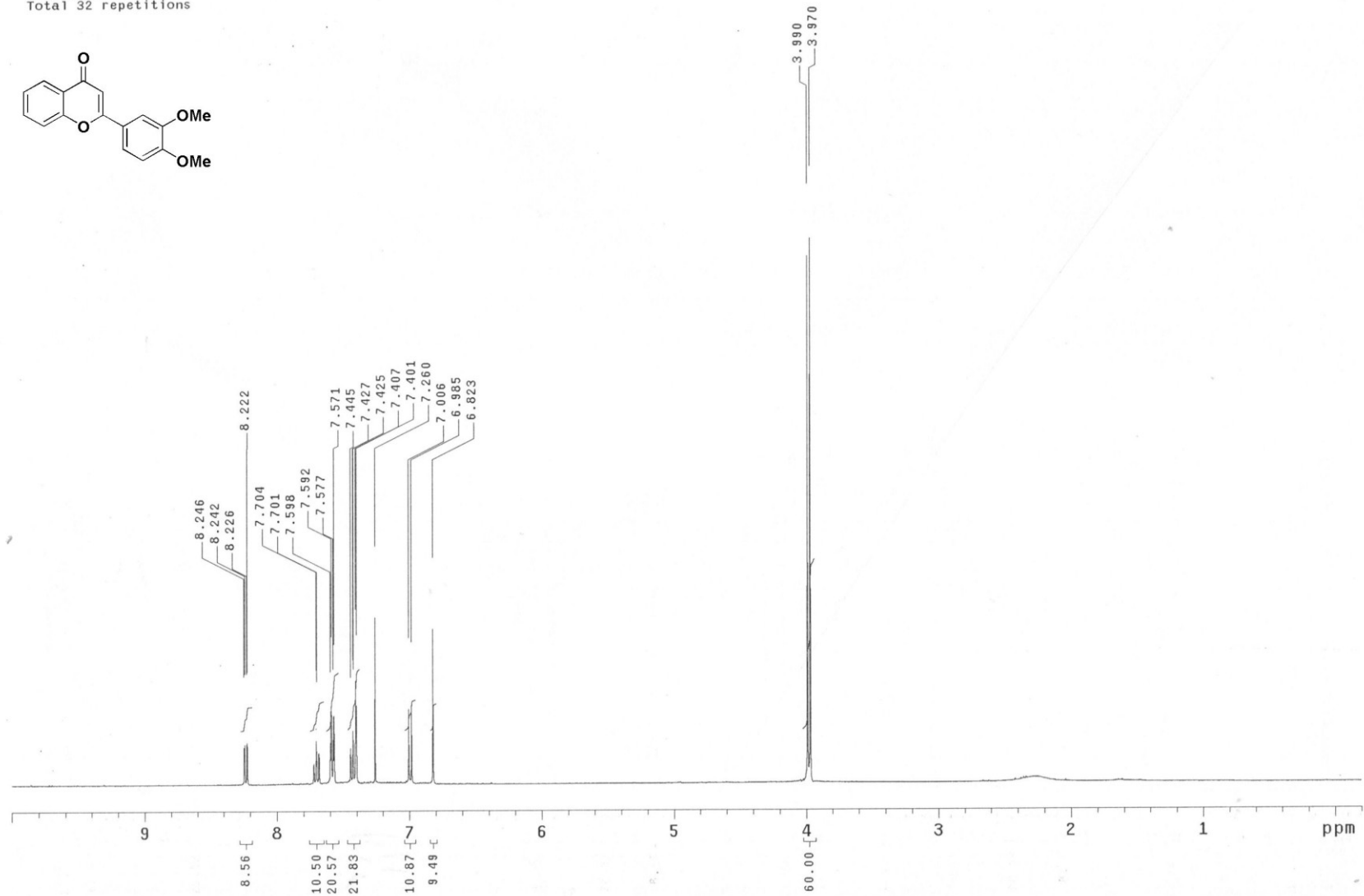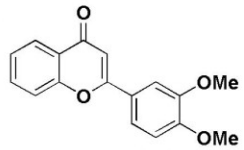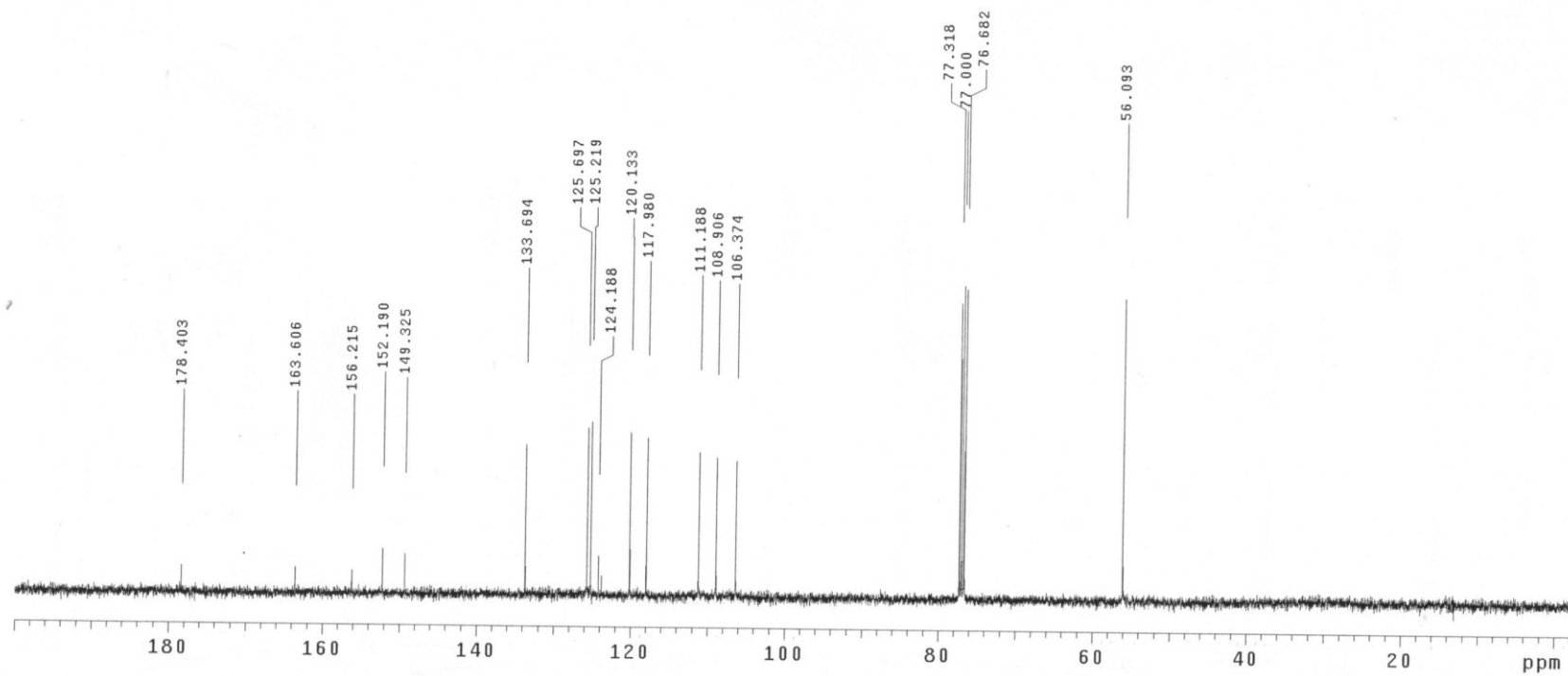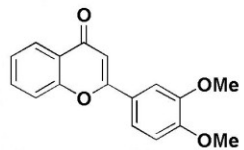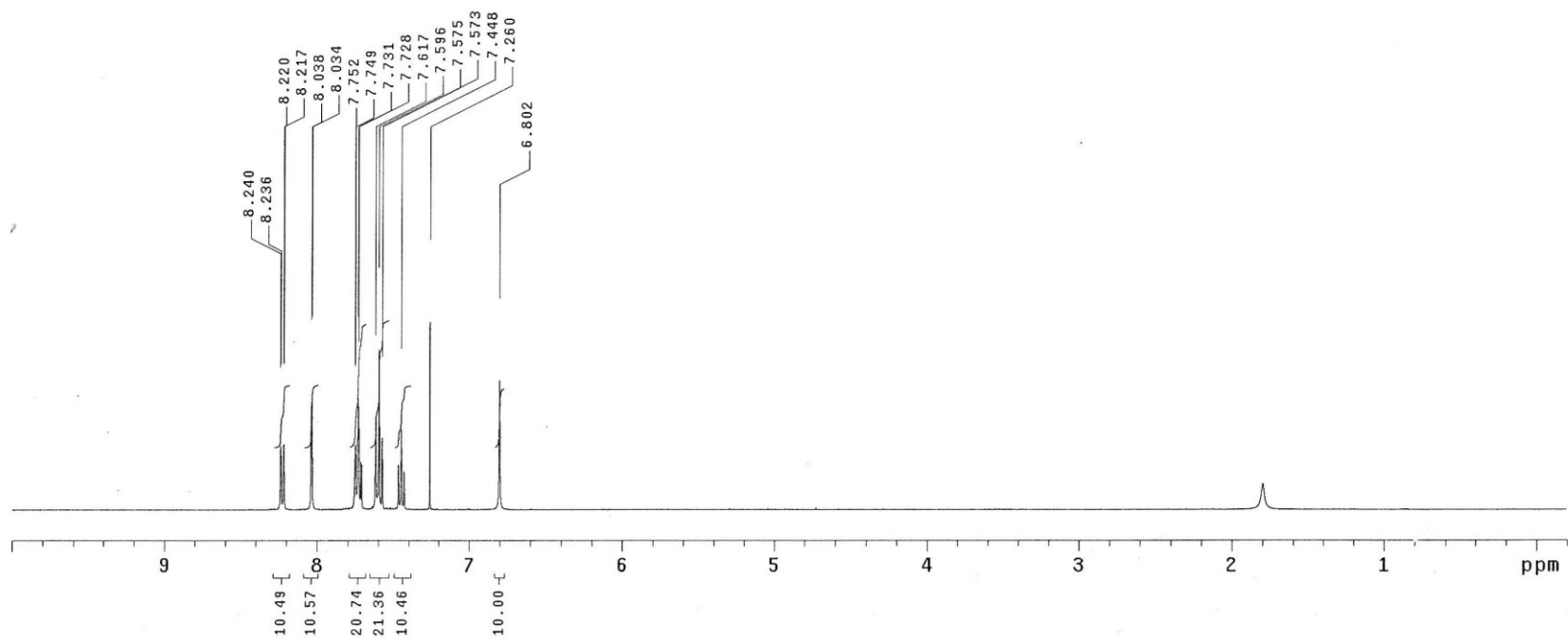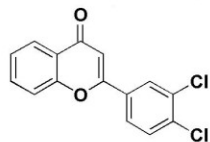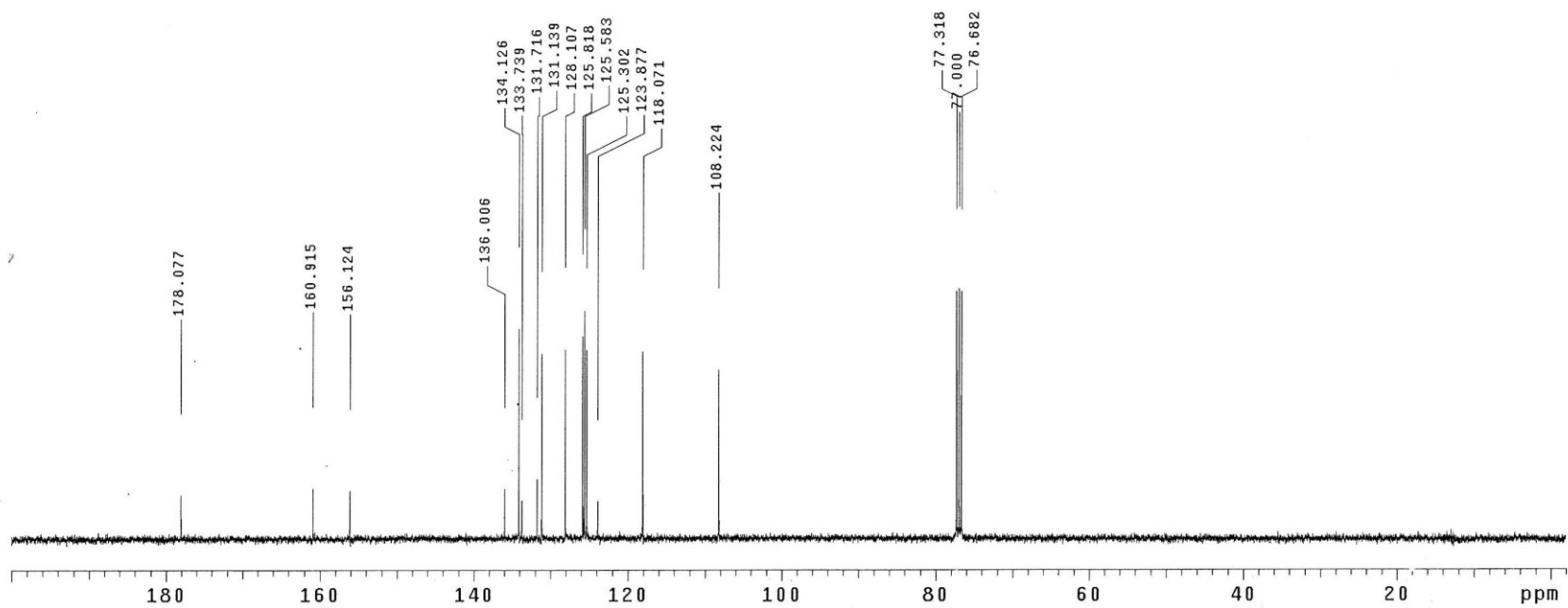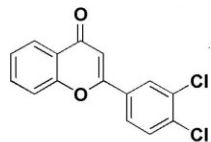Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.240
8.236
8.220
8.217
8.038
8.034
7.752
7.749
7.731
7.728
7.617
7.596
7.575
7.573
7.448
7.260
6.802

10.49
10.57
20.74
21.36
10.46
10.00

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

MC0801

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 5 2019
Solvent: CDCl3
Ambient temperature
Total 6576 repetitions

178.077
160.915
156.124
136.006
134.126
133.739
131.716
131.139
128.107
125.818
125.583
125.302
123.877
118.071
108.224
77.318
77.000
76.682

180   160   140   120   100   80   60   40   20   ppm

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

MC0716

Pulse Sequence: s2pul

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

3.901

7.927
7.922
7.909
7.903
7.590
7.582
7.527
7.523
7.517
7.508
7.495
7.307
7.299
7.284
7.276
6.867

9   8   7   6   5   4   3   2   1   ppm

20.00
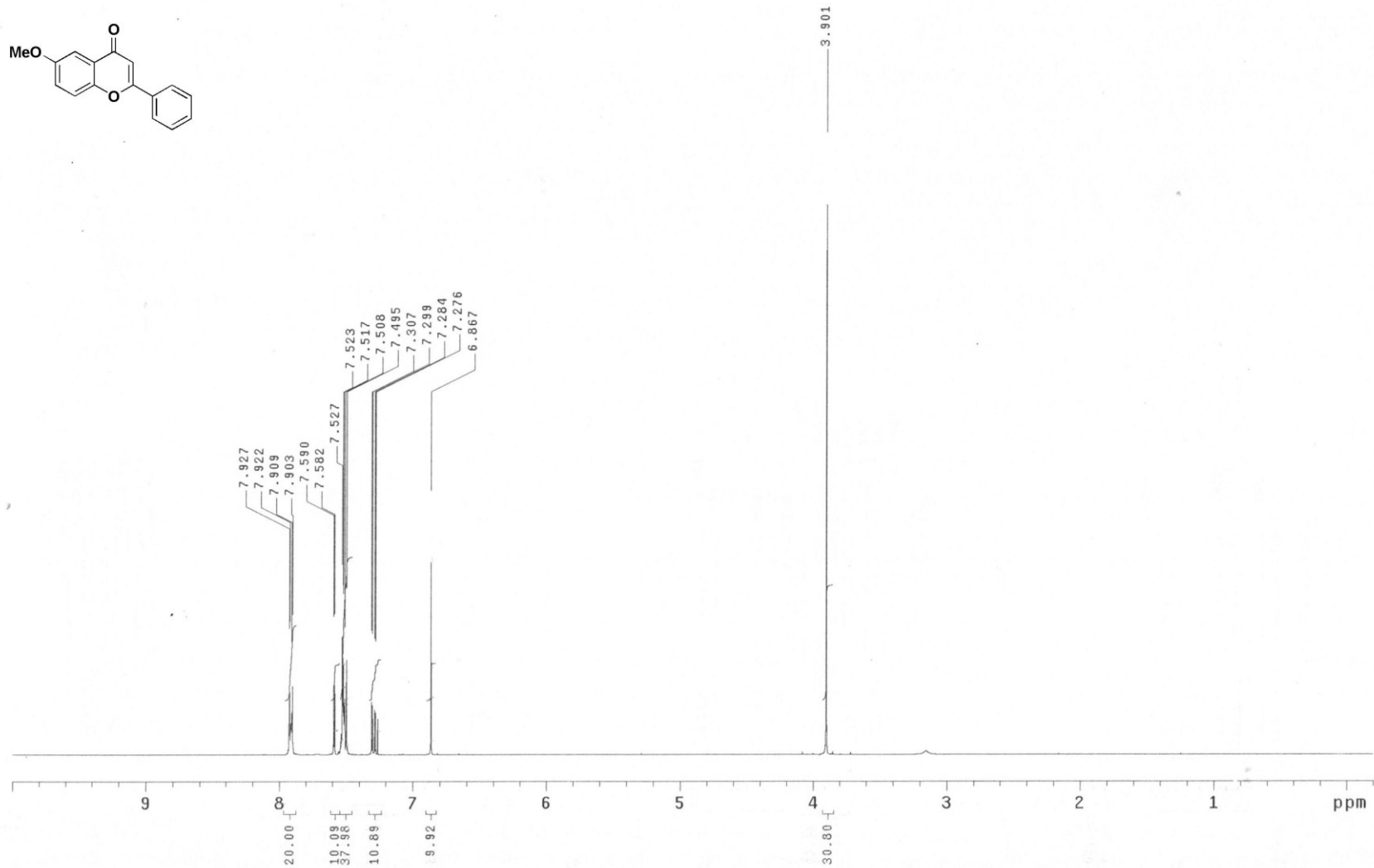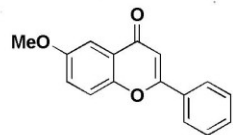10.09
37.98
10.89
9.92
30.80

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

MC0716

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 21 2019
Solvent: CDC13
Ambient temperature
Total 656 repetitions

MeO

178.252
163.341
157.034
151.091
131.753
131.556
129.009
126.250
124.362
123.938
119.488
106.655
104.760
77.318
77.000
76.682
55.911

180   160   140   120   100   80   60   40   20   ppm

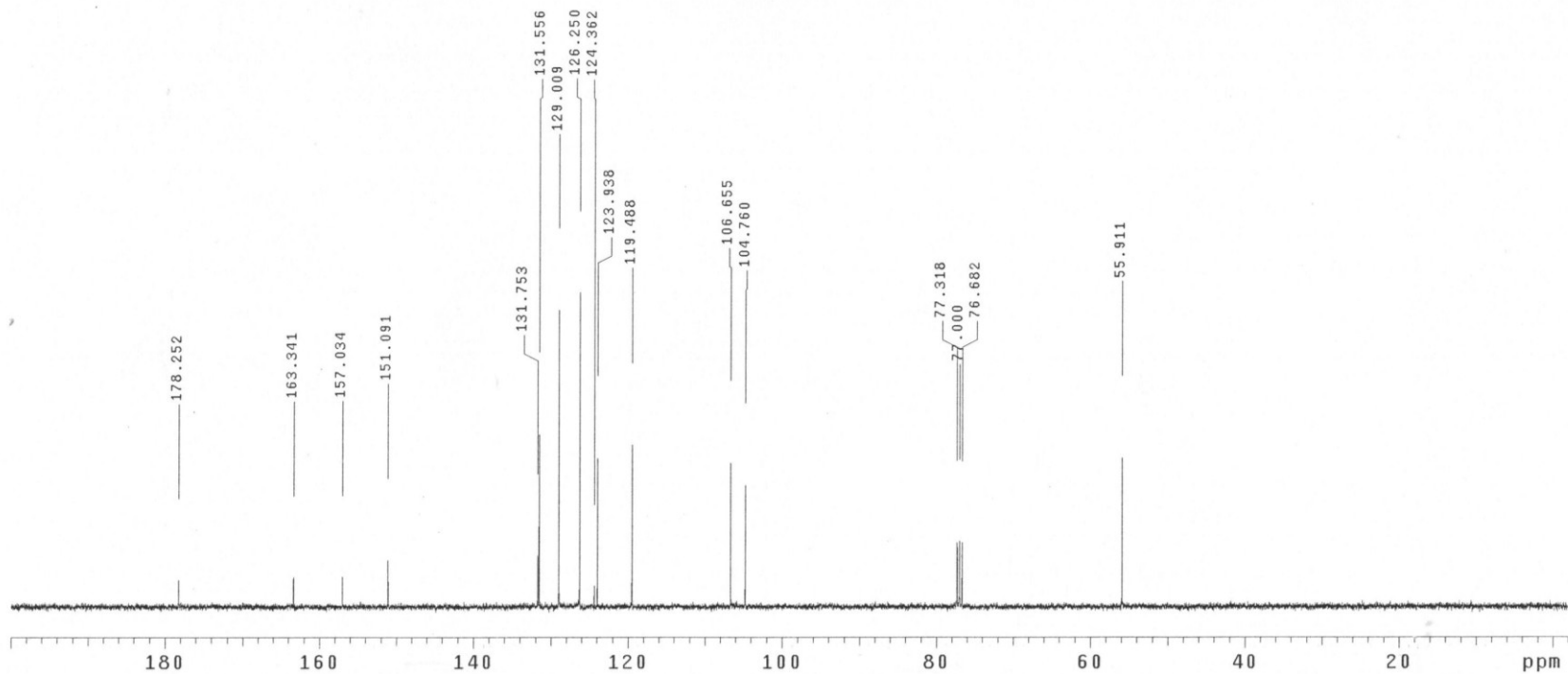# Compound 4k (¹H-NMR spectral data)

MC0717

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

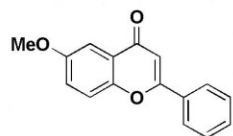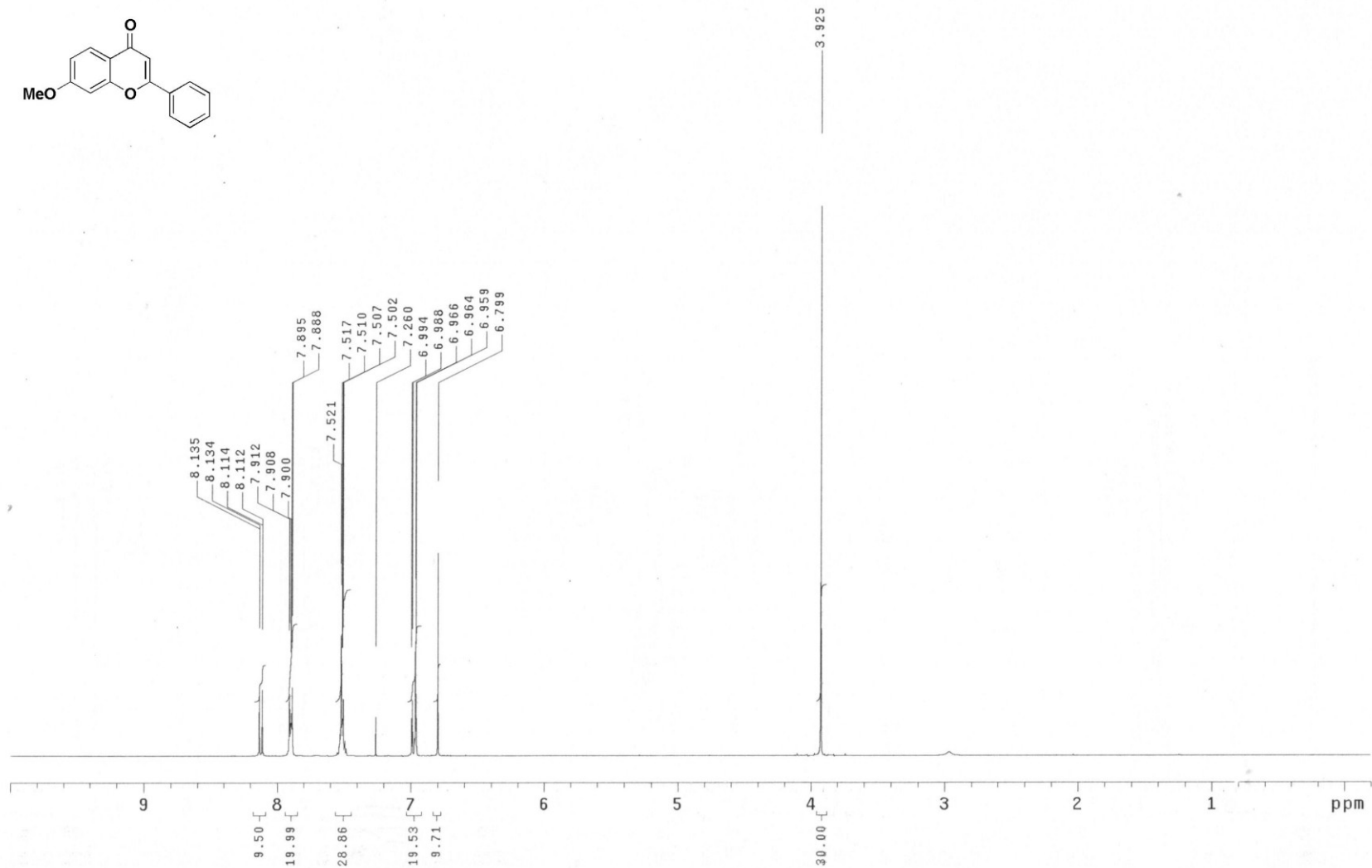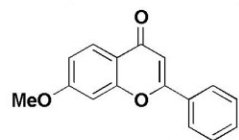# Compound 4k (^{13}C-NMR spectral data)

MC0717

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 656 repetitions

177.812
164.266
163.182
158.012
131.738
131.465
128.987
127.008
126.167
117.631
114.516
107.329
100.370
77.318
77.000
76.682
55.835

180   160   140   120   100   80   60   40   20   ppm

S-23

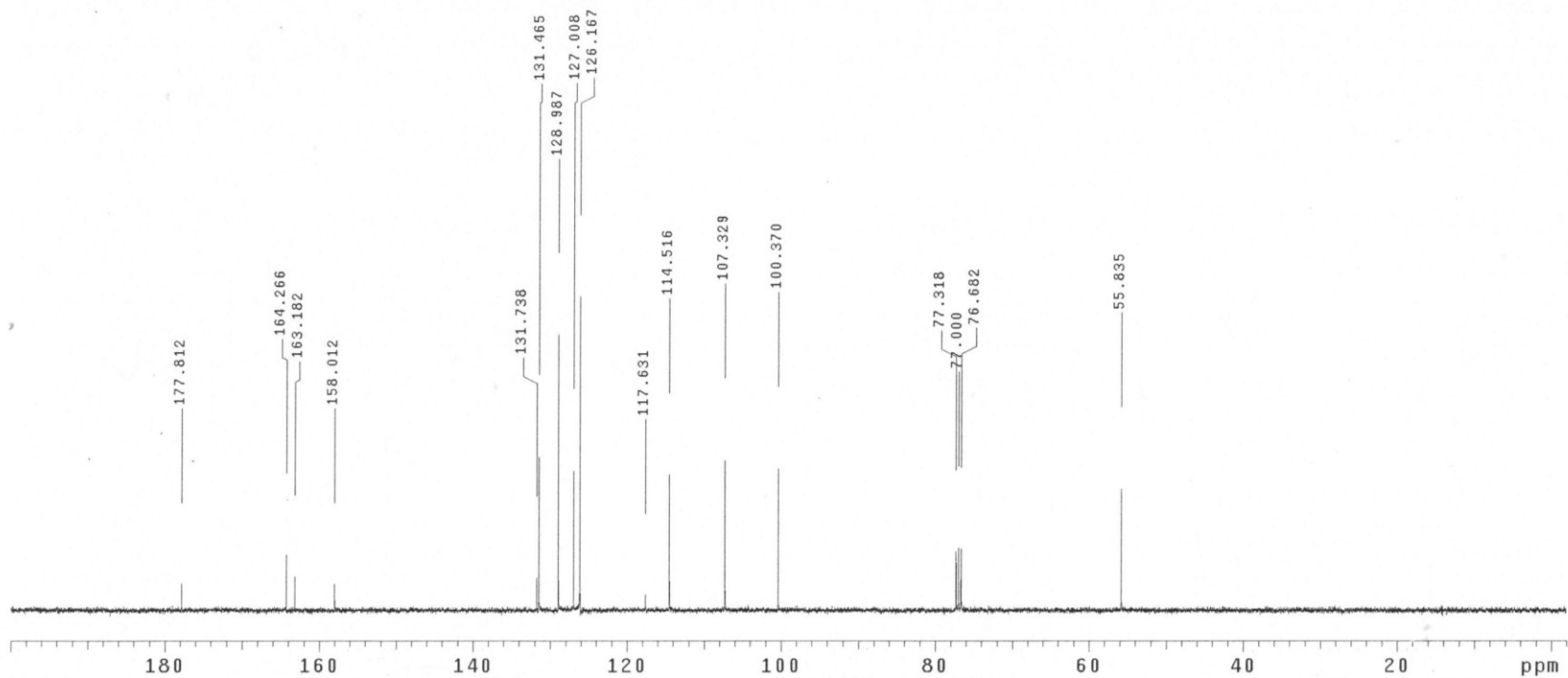# Compound 4I (^{1}H-NMR spectral data)

MC0720

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

3.862

7.869
7.866
7.850
7.845
7.519
7.517
7.516
7.497

6.633
6.475
6.469
6.349
6.343

20.00
30.34
9.68
9.08
8.49
31.74

9   8   7   6   5   4   3   2   1   ppm

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

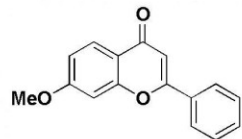MC0720

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
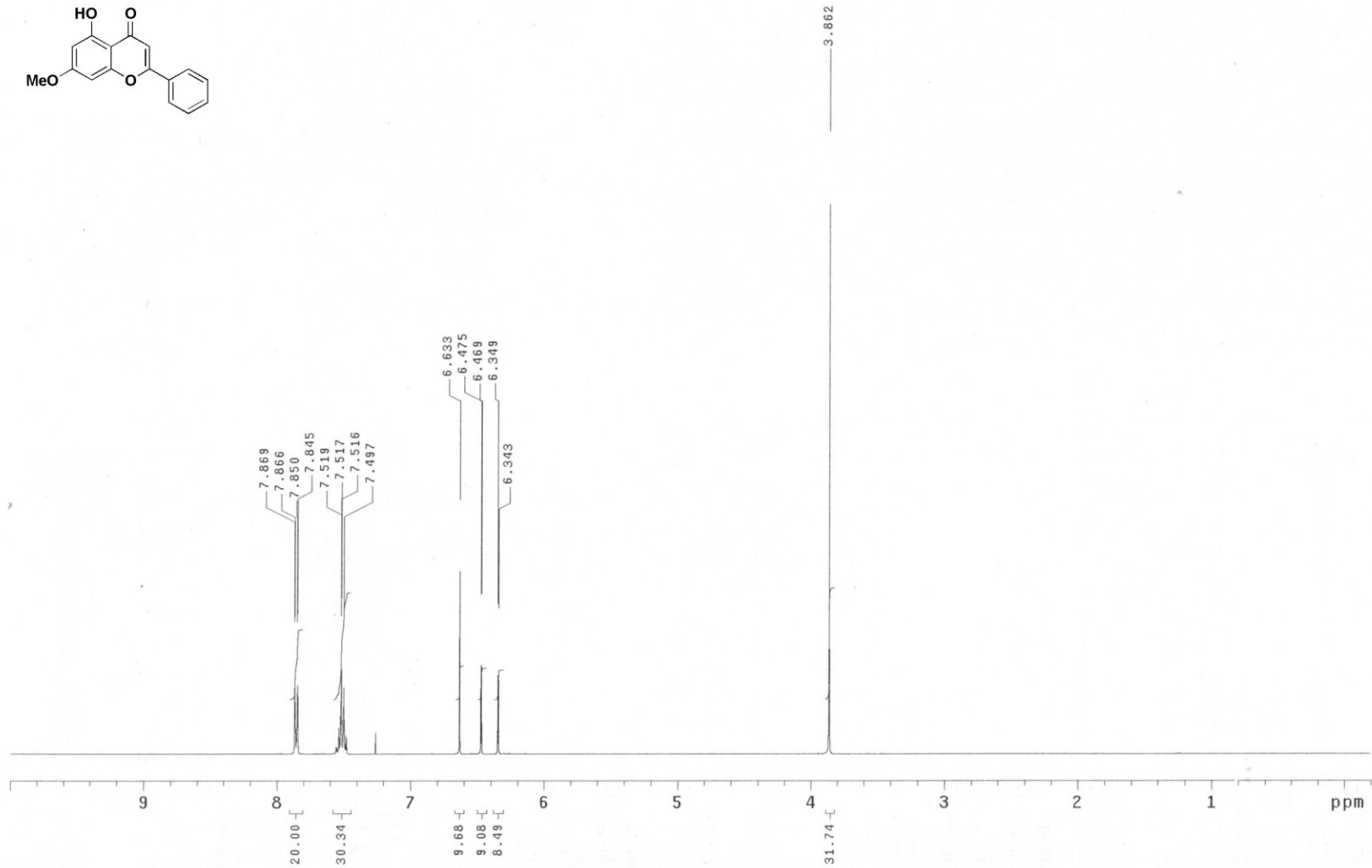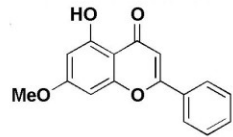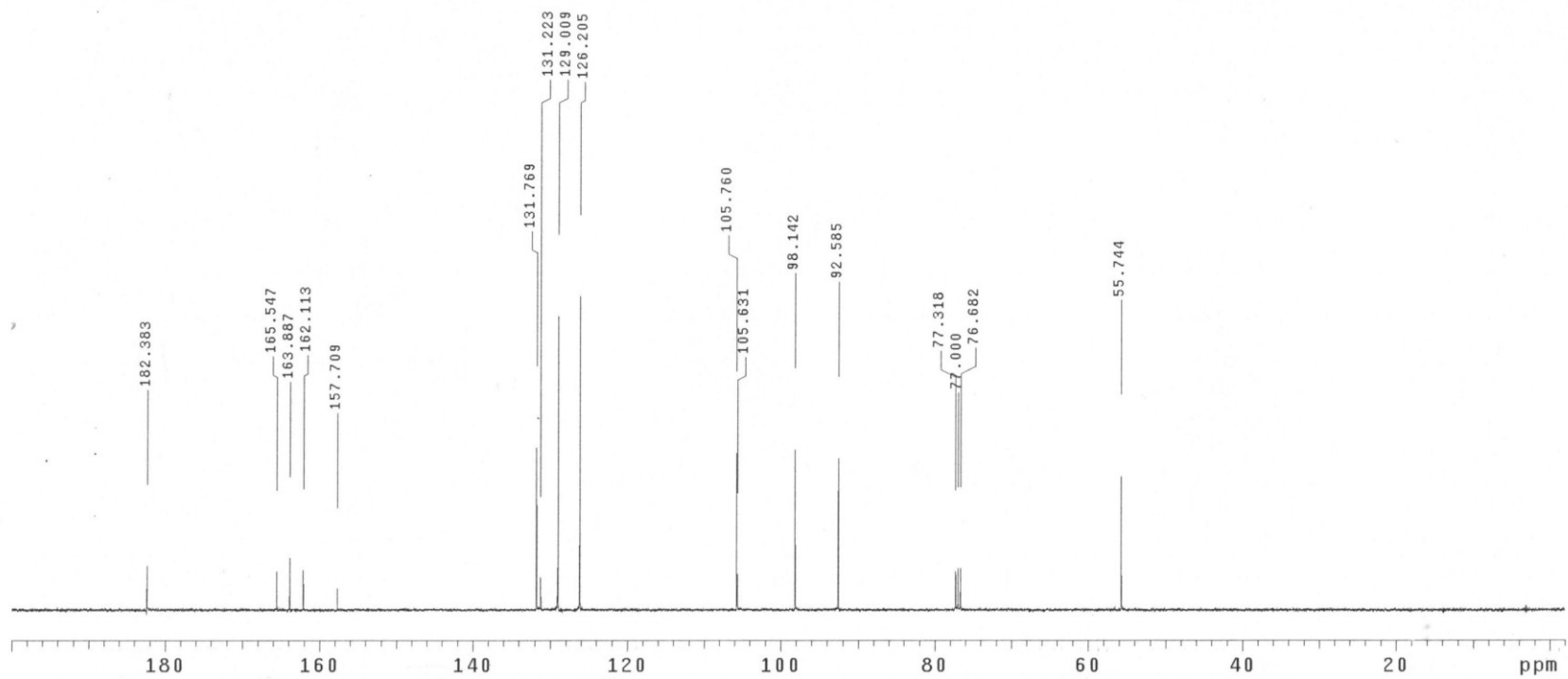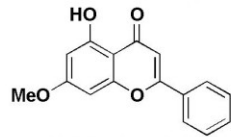Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 1248 repetitions

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

MC0722

Pulse Sequence: s2pul

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

7.869
7.864
7.856
7.853
7.845
7.495
7.490
7.481
7.477
7.260
6.666
6.564
6.558
6.366
6.361
3.945
3.902
1.847

22.54
33.52
9.95
10.00
10.94
61.02

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

MC0722

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 21 2019
Solvent: CDCl3
Ambient temperature
Total 1600 repetitions

177.600
164.038
160.877
160.627
159.884
131.496
131.139
128.888
125.901
109.255
109.005
96.156
92.798
77.318
77.000
76.682
56.381
55.722

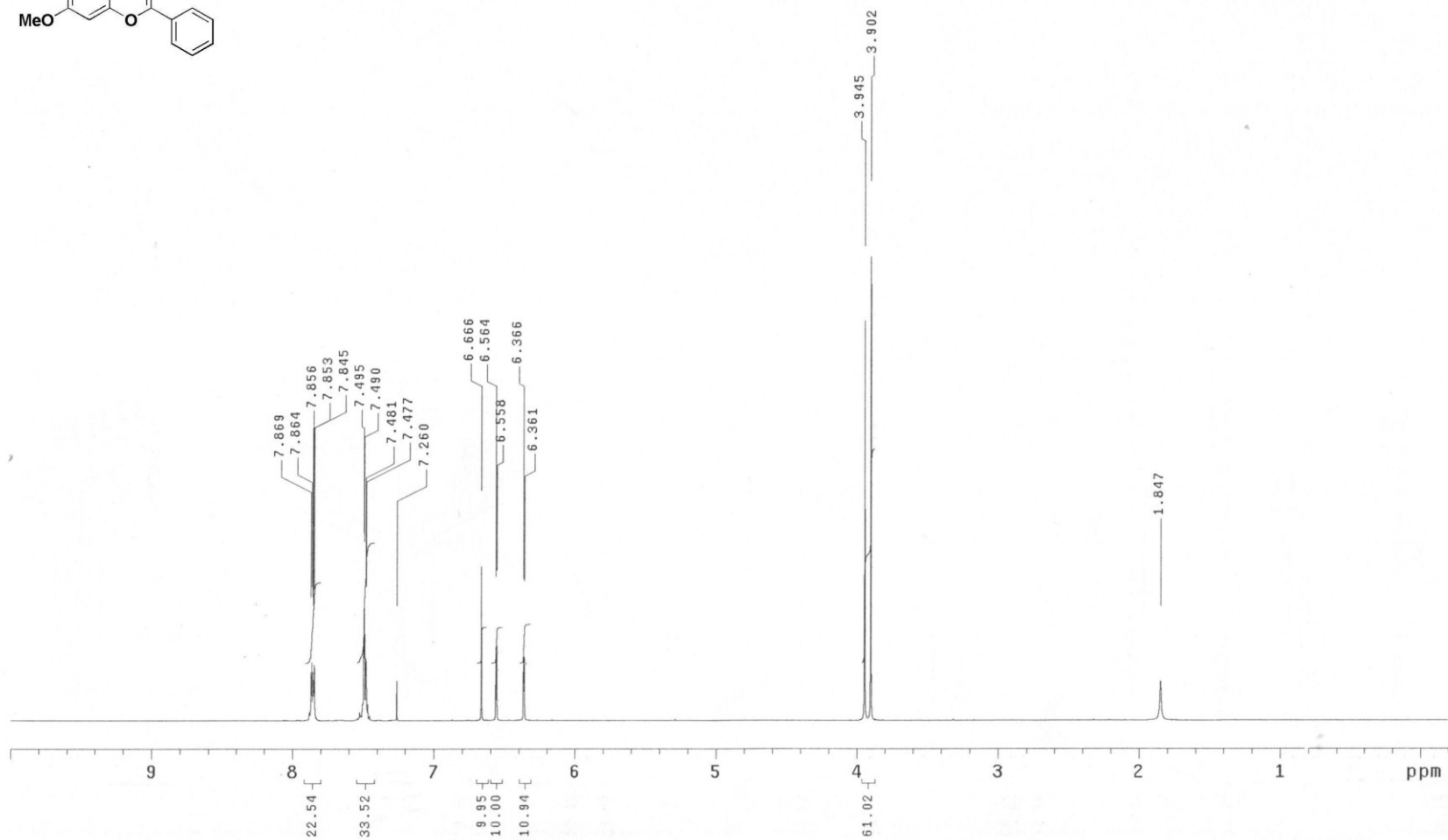# Compound 4n (^{1}H-NMR spectral data)

MC0806

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 12 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.399
8.394
8.382
8.376
8.255
8.252
8.251
8.235
8.231
8.126
8.121
8.108
8.103
7.761
7.757
7.754
7.740
7.736
7.620
7.618
7.617
7.599
7.597
7.596
7.491
7.488
7.473
7.471
7.469
7.260
6.916

18.32
8.74
20.28
10.45
10.00
10.36
9.63

9   8   7   6   5   4   3   2   1   ppm

S-28

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

MC0806

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 12 2019
Solvent: CDCl3
Ambient temperature
Total 2384 repetitions

Compound 4o (^{1}H-NMR spectral data)
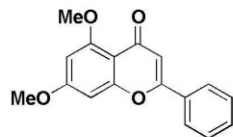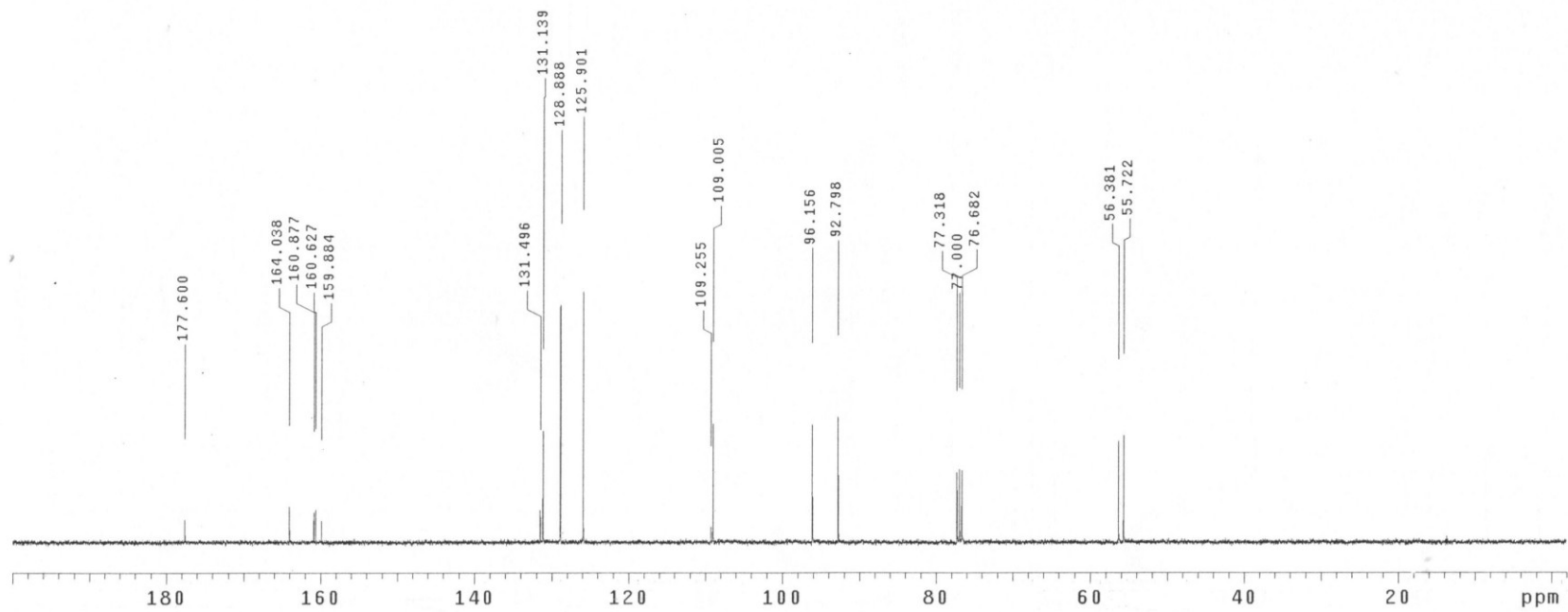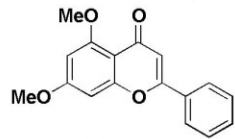
MC0811

Pulse Sequence: s2pul
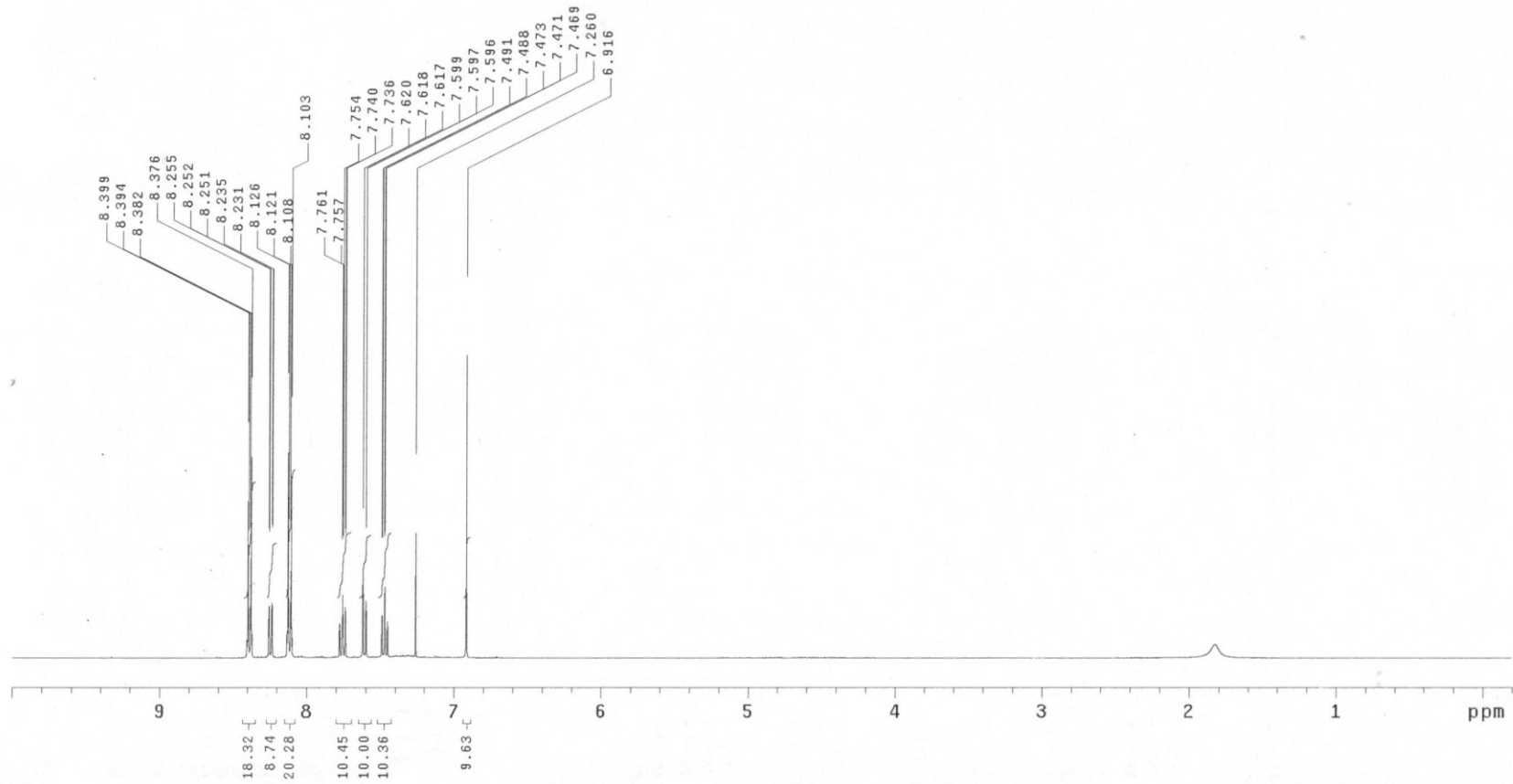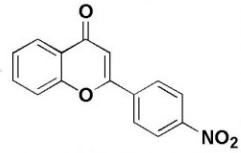
UNITYplus-400 "unity400"
Date: Aug 21 2019
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

8.521
8.287
8.283
8.267
8.263
7.998
7.976
7.965
7.960
7.757
7.753
7.739
7.735
7.684

7.682
7.663
7.619
7.612
7.604
7.594
7.588
7.486
7.468
7.465
7.463
7.260

7.066

1.884

10.00
8.96
43.02
11.62
31.91
11.17
10.55

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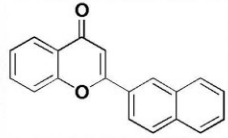
Compound 4o (^{13}C-NMR spectral data)

MC0811

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
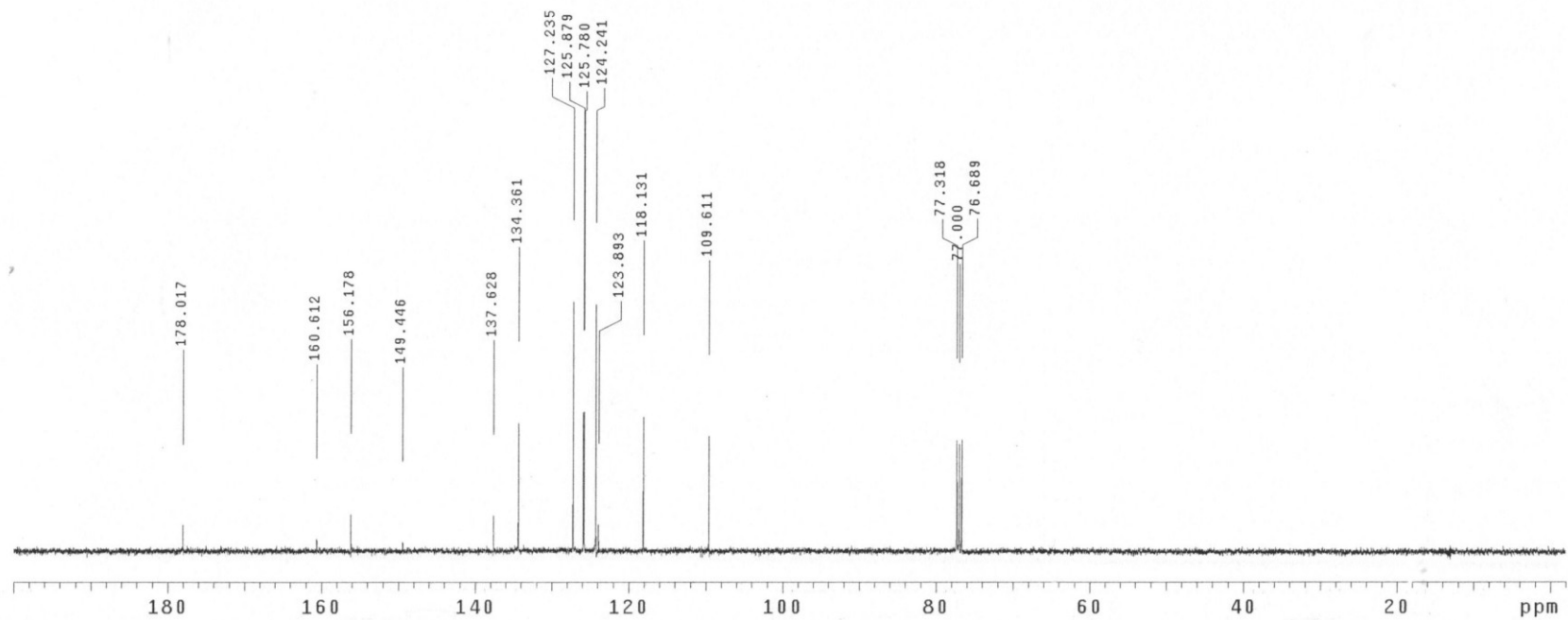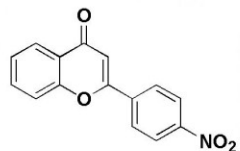Date: Aug 21 2019
Solvent: CDC13
Ambient temperature
Total 31488 repetitions

178.517
163.743
156.413
134.755
133.990
132.921
129.108
129.009
128.843
128.130
127.857
127.129
125.788
125.393
122.558
118.147
107.723
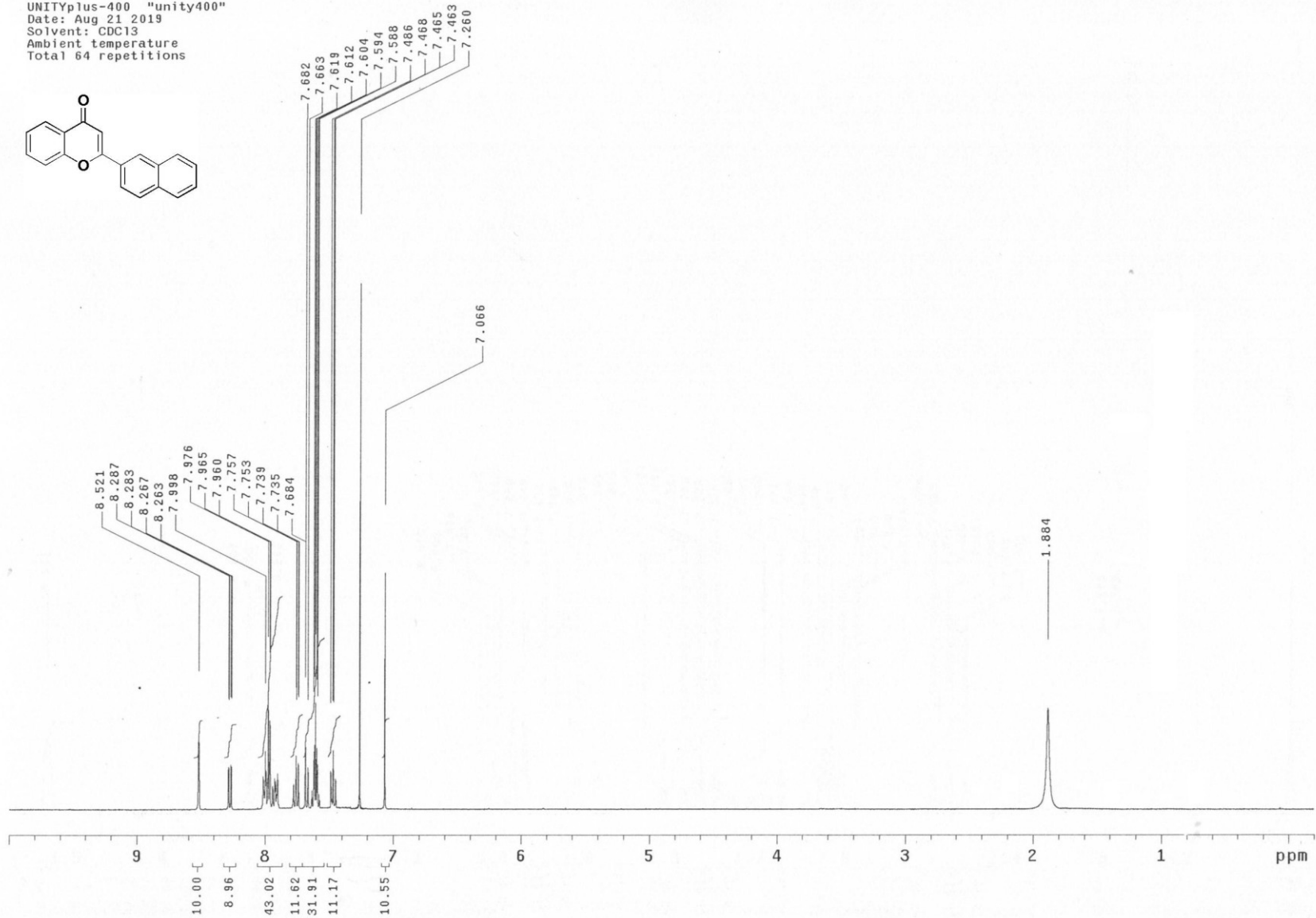77.318
77.205
77.000
76.682

MC0820F

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 22 2019
Solvent: CDC13
Ambient temperature
Total 160 repetitions

7.565
7.546
7.545
7.544
7.440
7.332
7.330
7.260

6.959

8.257
8.253
8.237
8.233
7.943
7.938
7.715
7.567
7.566

1.700

9   8   7   6   5   4   3   2   1   ppm

10.00
11.37
12.32
24.06
13.83
14.14
34.51
10.78

Compound 4p (¹³C-NMR spectral data)

MC0820F

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
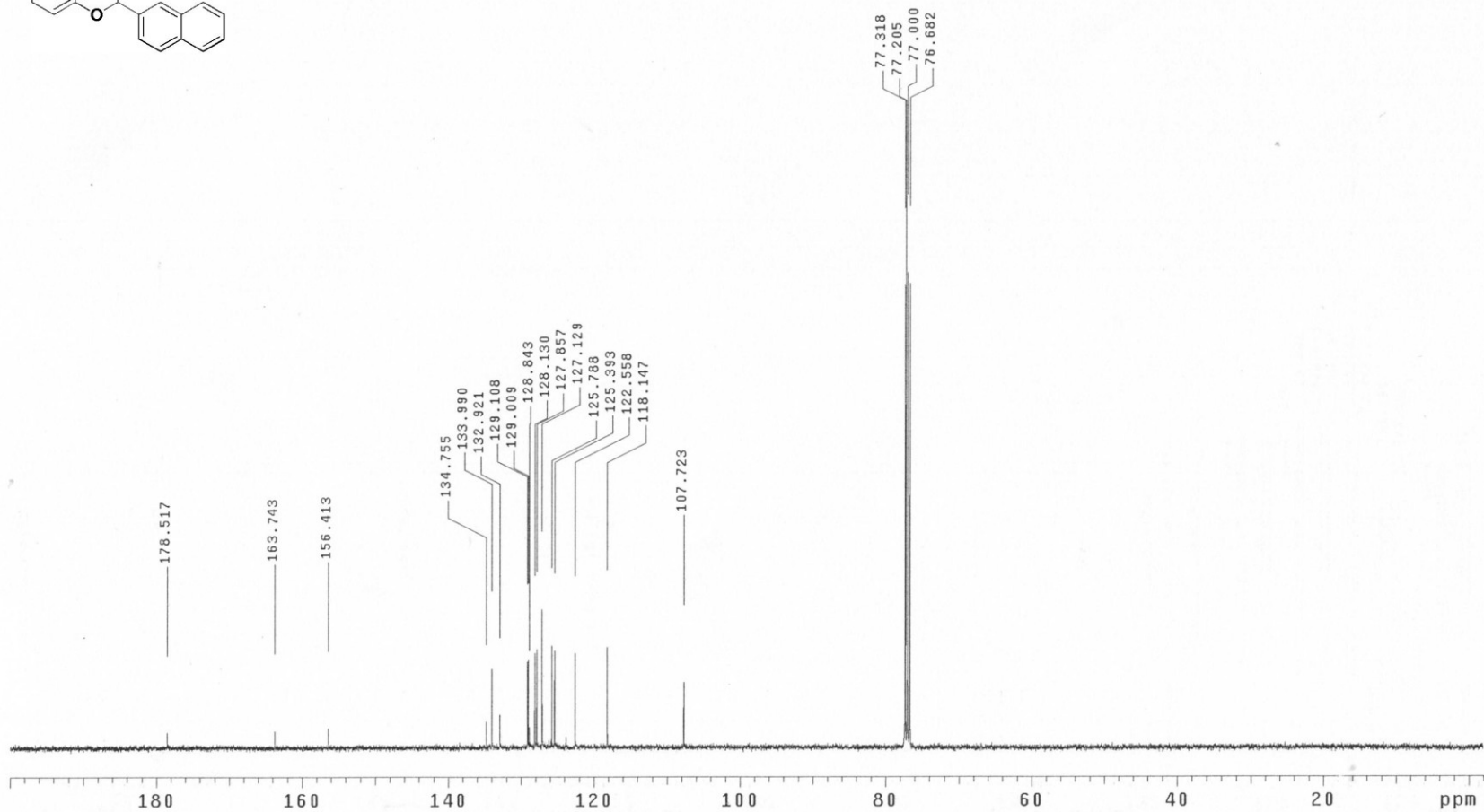Date: Aug 22 2019
Solvent: CDCl3
Ambient temperature
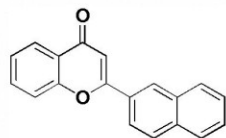File: U0223-10
Total 32000 repetitions

178.464

161.833
159.293
158.891
156.382

133.914
132.959
132.868
129.078
125.772
125.325
124.651
124.613
123.809
118.071
117.108
116.881
112.446
112.340
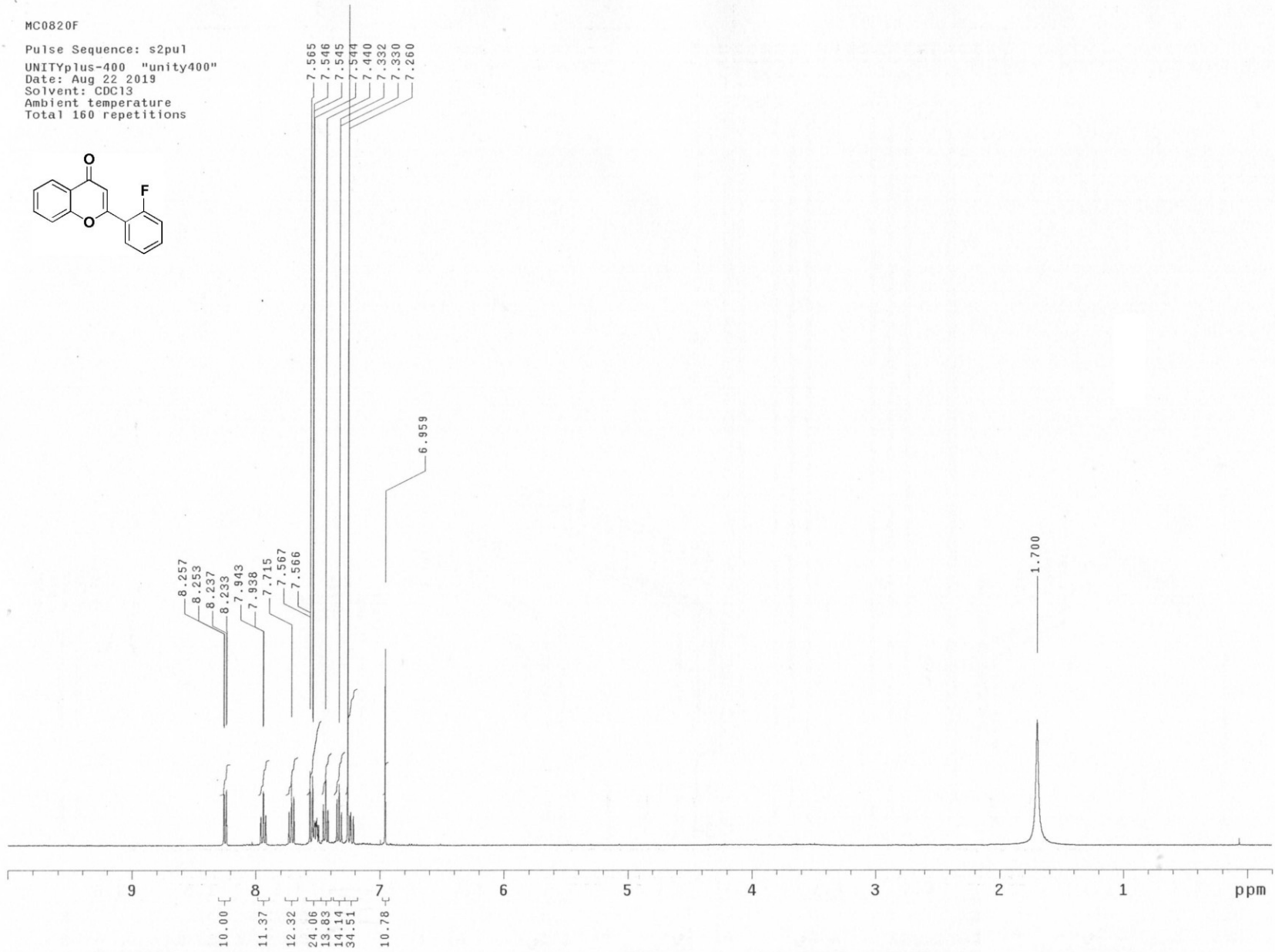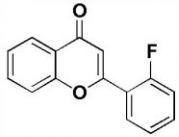
77.318
77.205
77.000
76.682

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

MC0828
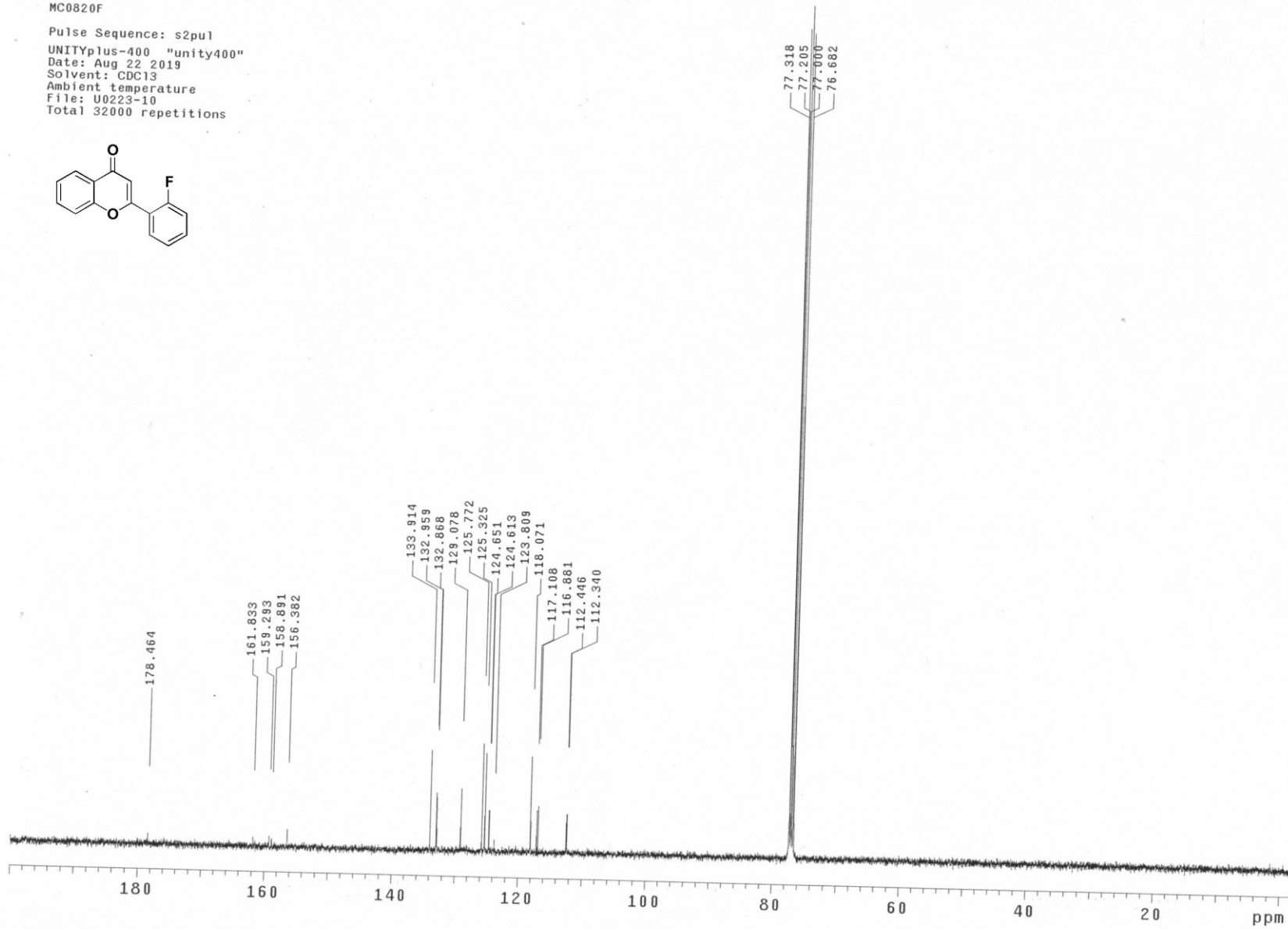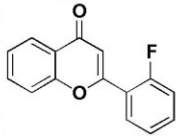
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 29 2019
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

7.513
7.494
7.493
7.491
7.429
7.427
7.411
7.409
7.407
7.260

7.150
7.142
6.758

8.229
8.224
8.209
8.204
7.686
7.681
7.678
7.665
7.660
7.637
7.635
7.632
7.631
7.515
7.514

6.624
6.619
6.615
6.611

9.22
22.51
12.63
12.89
10.00
8.40
9.07
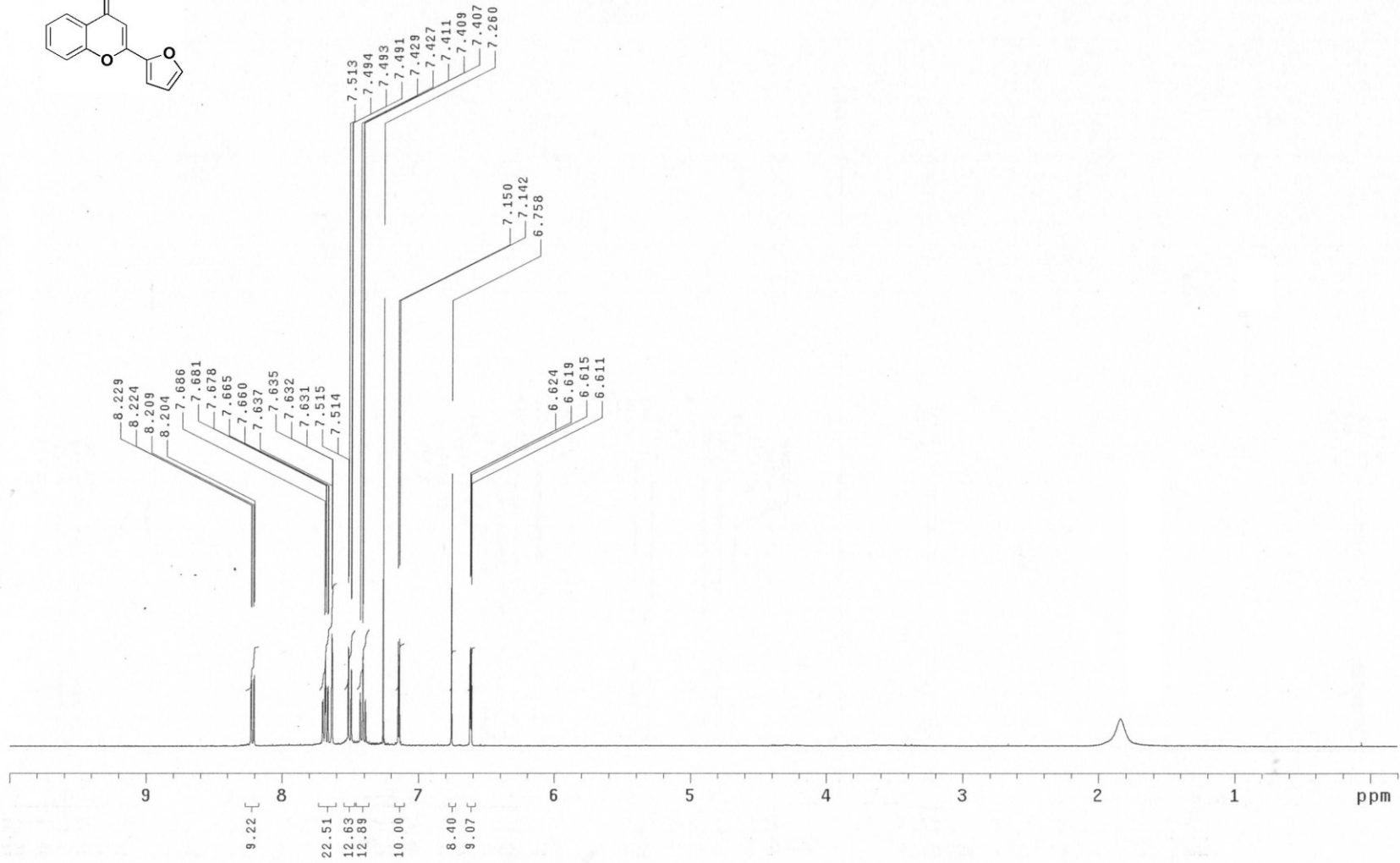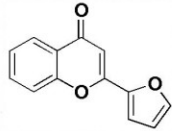
Compound 4q (^{13}C-NMR spectral data)

MC0828

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 29 2019
Solvent: CDCl3
Ambient temperature
Total 30640 repetitions

177.865

155.821
155.230

146.399
145.823

133.755

125.788
125.219
124.128

117.874

113.090
112.522

105.495

77.318
77.205
77.000
76.682

180   160   140   120   100   80   60   40   20   ppm

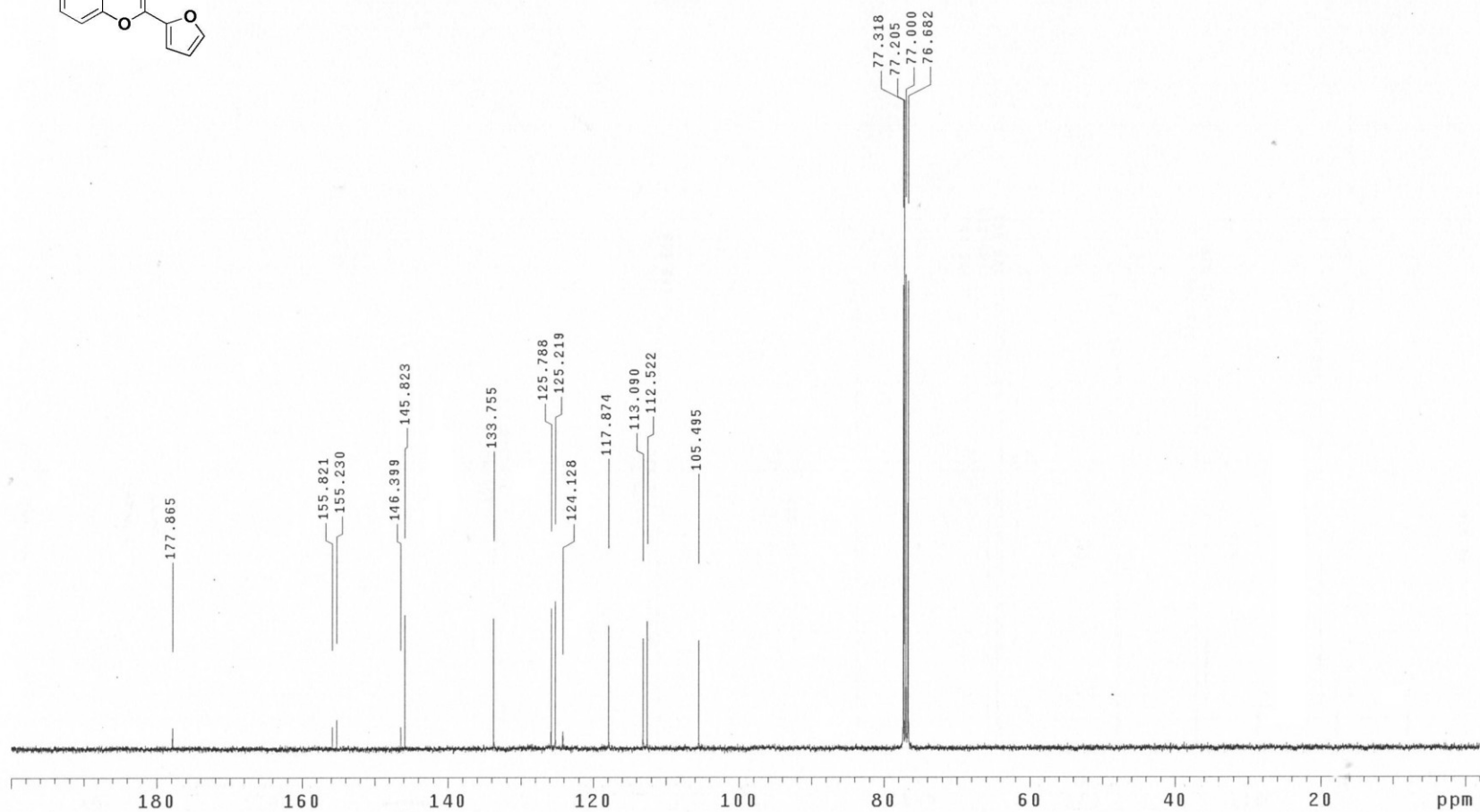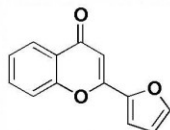# Compound 4r (^{1}H-NMR spectral data)

MC0812S

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 80 repetitions

8.221
8.206
8.202
7.742
7.739
7.733
7.730
7.691
7.592
7.589
7.580
7.577
7.547
7.546
7.526
7.524
7.417
7.415
7.260
7.204
7.194
7.191
7.182
6.715

10.00
23.50
23.86
13.67
12.39
9.79

9   8   7   6   5   4   3   2   1   ppm

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

177.933
159.066
155.935
135.172
133.755
130.260
128.494
128.456
125.704
125.272
123.983
117.927
106.207
77.318
77.205
77.000
76.682

180   160   140   120   100   80   60   40   20   ppm

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

MC0827

Pulse Sequence: s2pul

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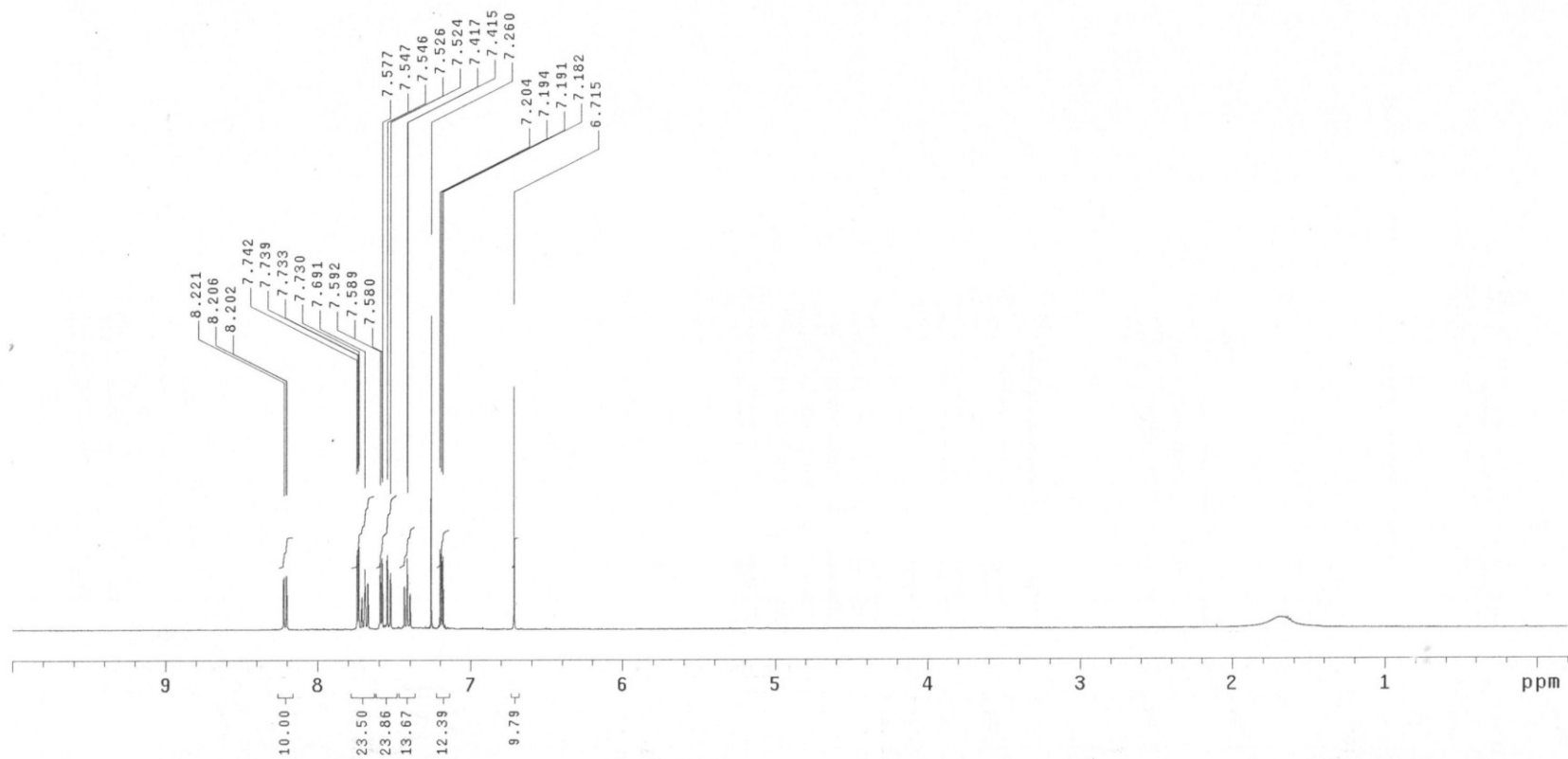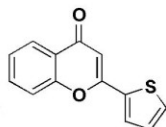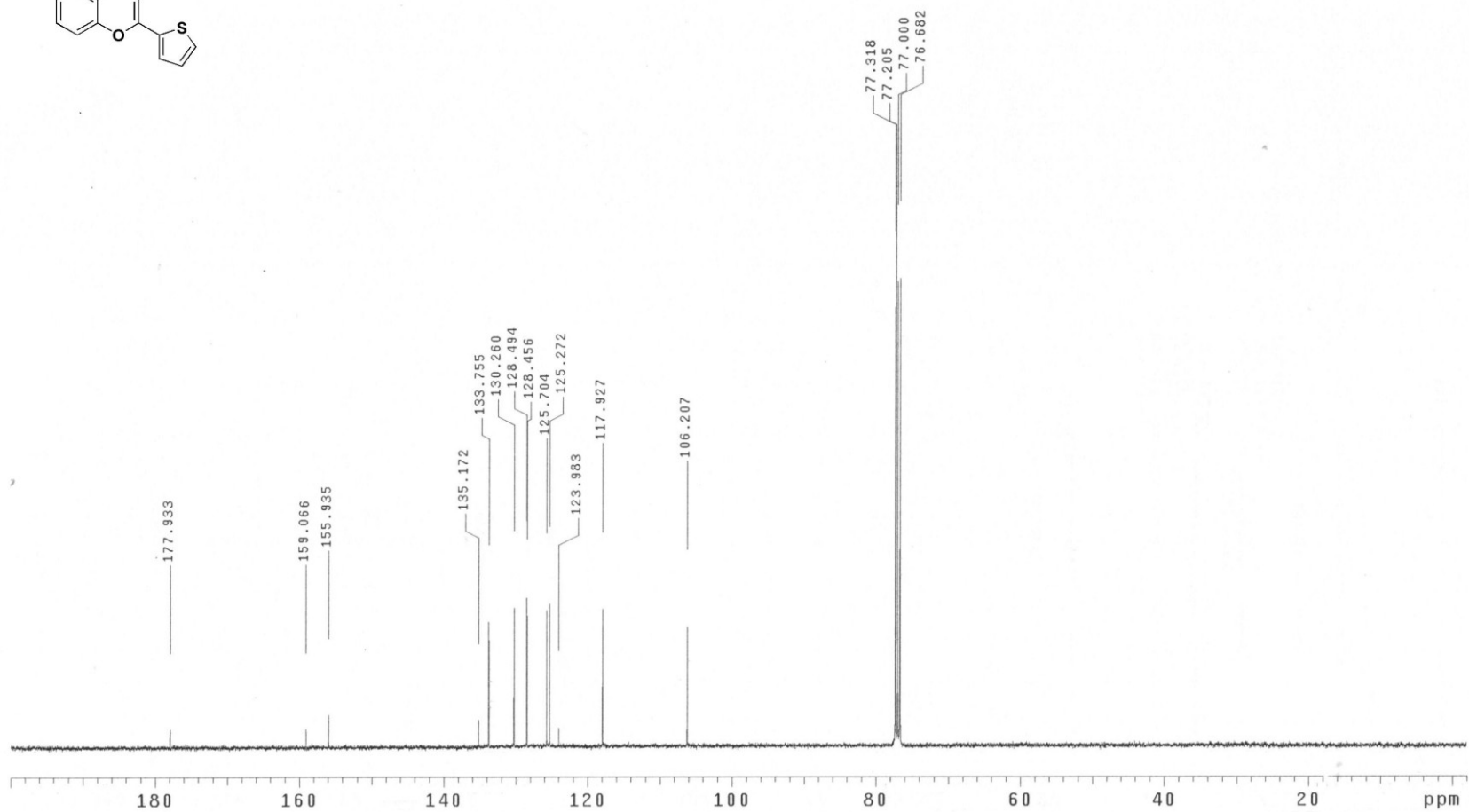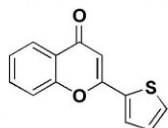Date: Aug 29 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.335
8.331
8.315
8.311
8.050
8.029
7.948
7.776
7.735
7.613
7.595
7.587
7.579
7.571
7.561
7.540
7.539
7.486
7.260
6.732
1.778

10.52
10.79
10.34
10.05
21.75
52.69
10.00

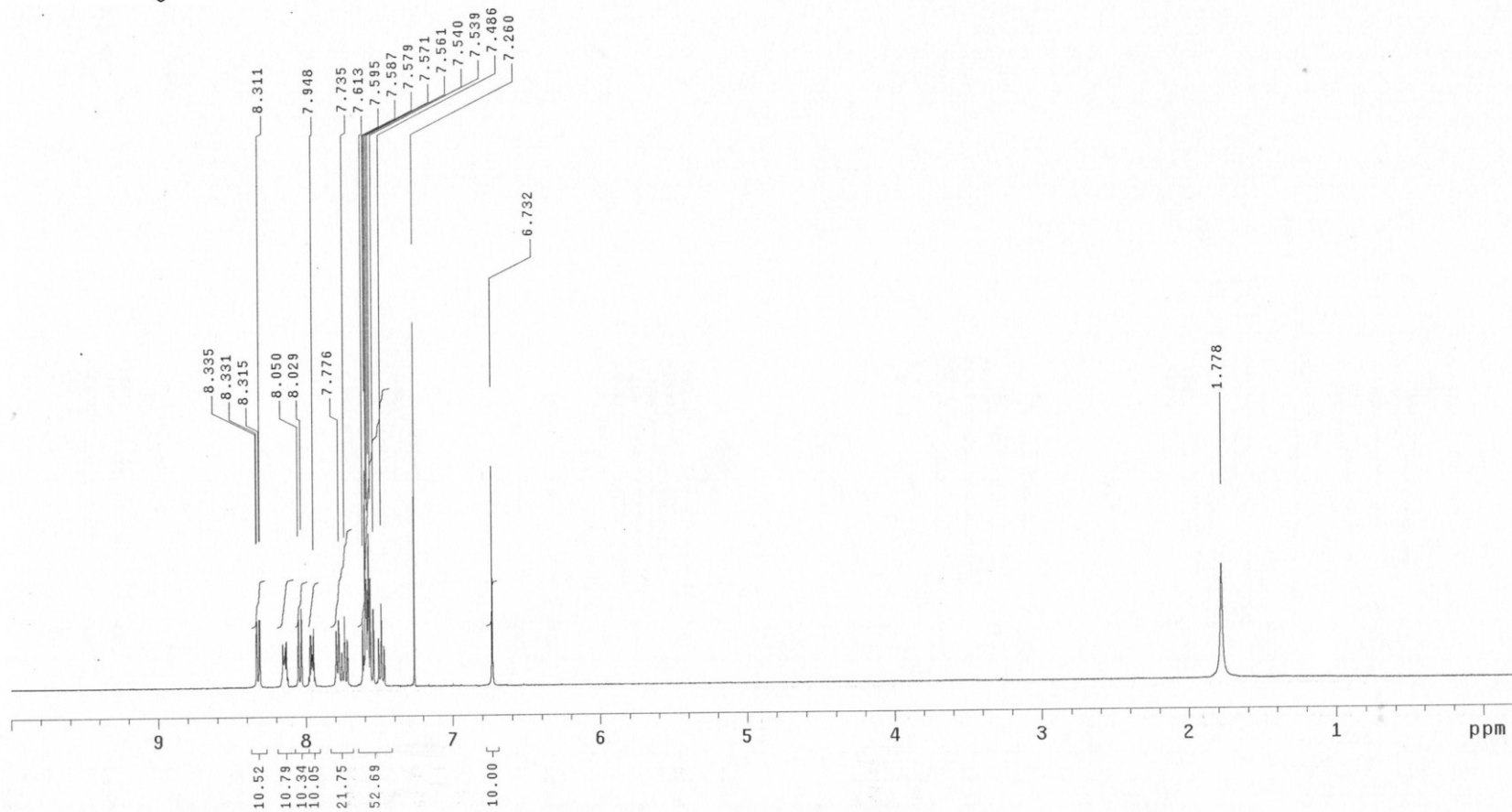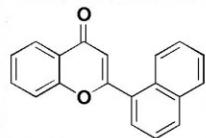# Compound 4s (^{13}C-NMR spectral data)

MC0827

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 29 2019
Solvent: CDCl3
Ambient temperature
Total 3584 repetitions

178.335
165.615
156.761
133.952
133.755
131.564
130.616
130.397
128.744
128.016
127.470
126.599
125.886
125.431
125.075
124.870
123.961
118.260
113.015
77.318
77.000
76.689

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

MC0819

Pulse Sequence: s2pul

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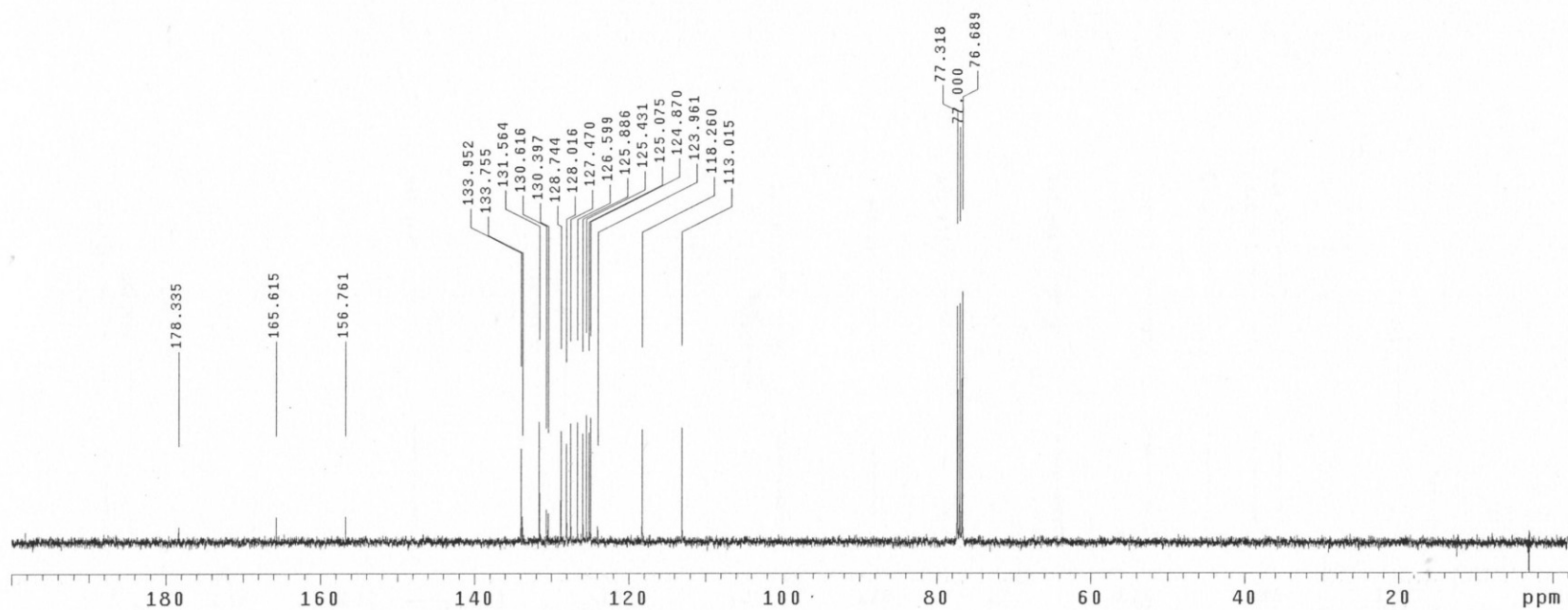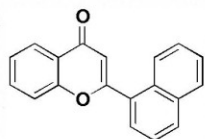Total 32 repetitions

7.869
7.862
7.849
7.841
7.576
7.566
7.554
7.375
7.260
6.998
6.978
6.808

3.967
3.983

10.00 20.13 20.76 10.09 9.49   60.15   6.71

9   8   7   6   5   4   3   2   1   ppm

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

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

MC0814
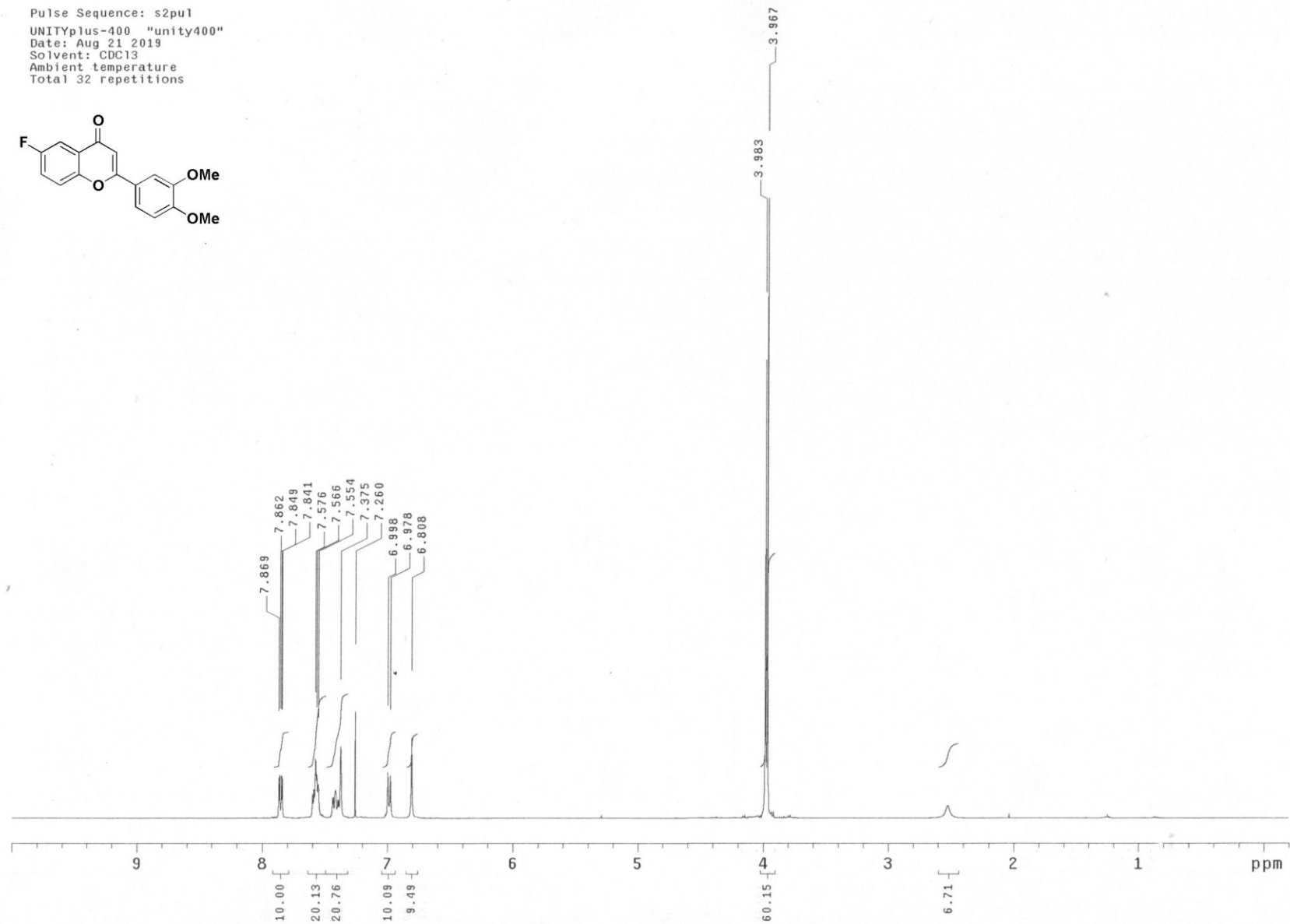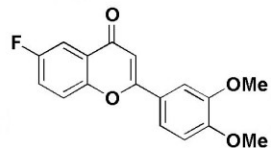
Pulse Sequence: s2pul

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

3.986
3.973

7.546
7.524
7.523
7.375
7.370
7.260

7.005
6.984
6.780

8.196
8.190

7.629
7.622
7.553

7.01

9.56
20.00
10.71

10.44
9.70

61.07

9   8   7   6   5   4   3   2   1   ppm

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

MC0814

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 15 2019
Solvent: CDC13
Ambient temperature
Total 11536 repetitions
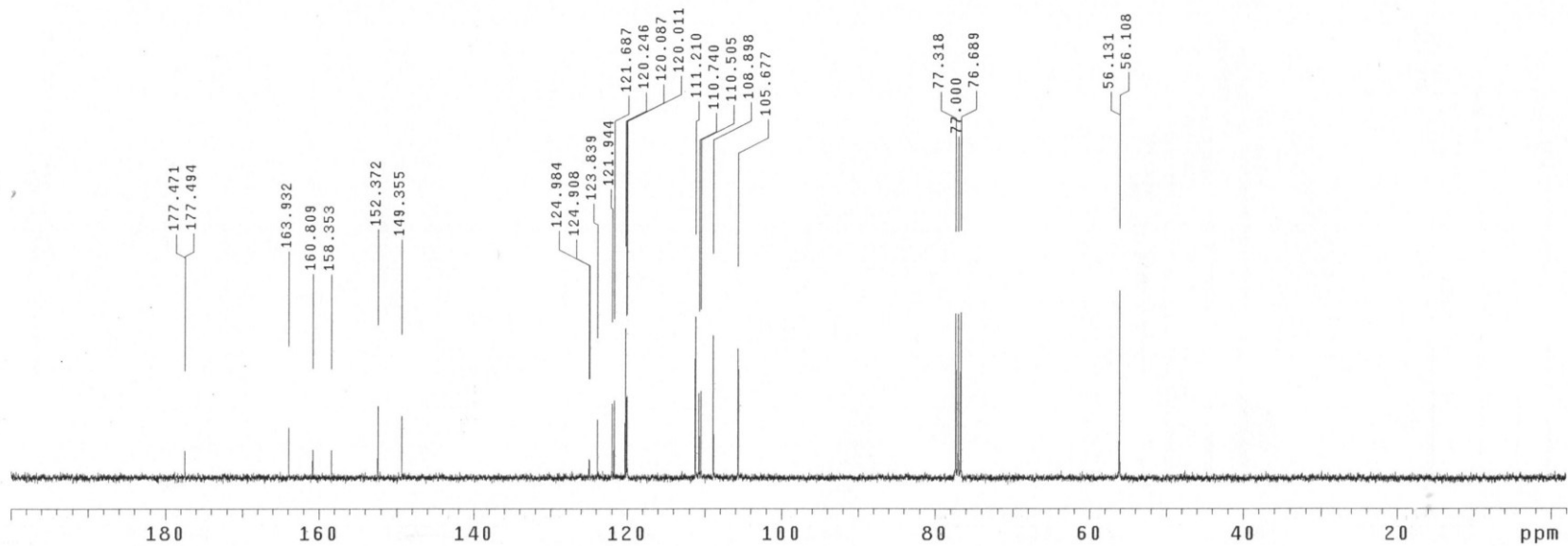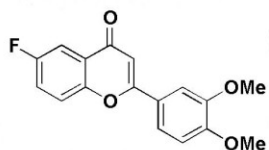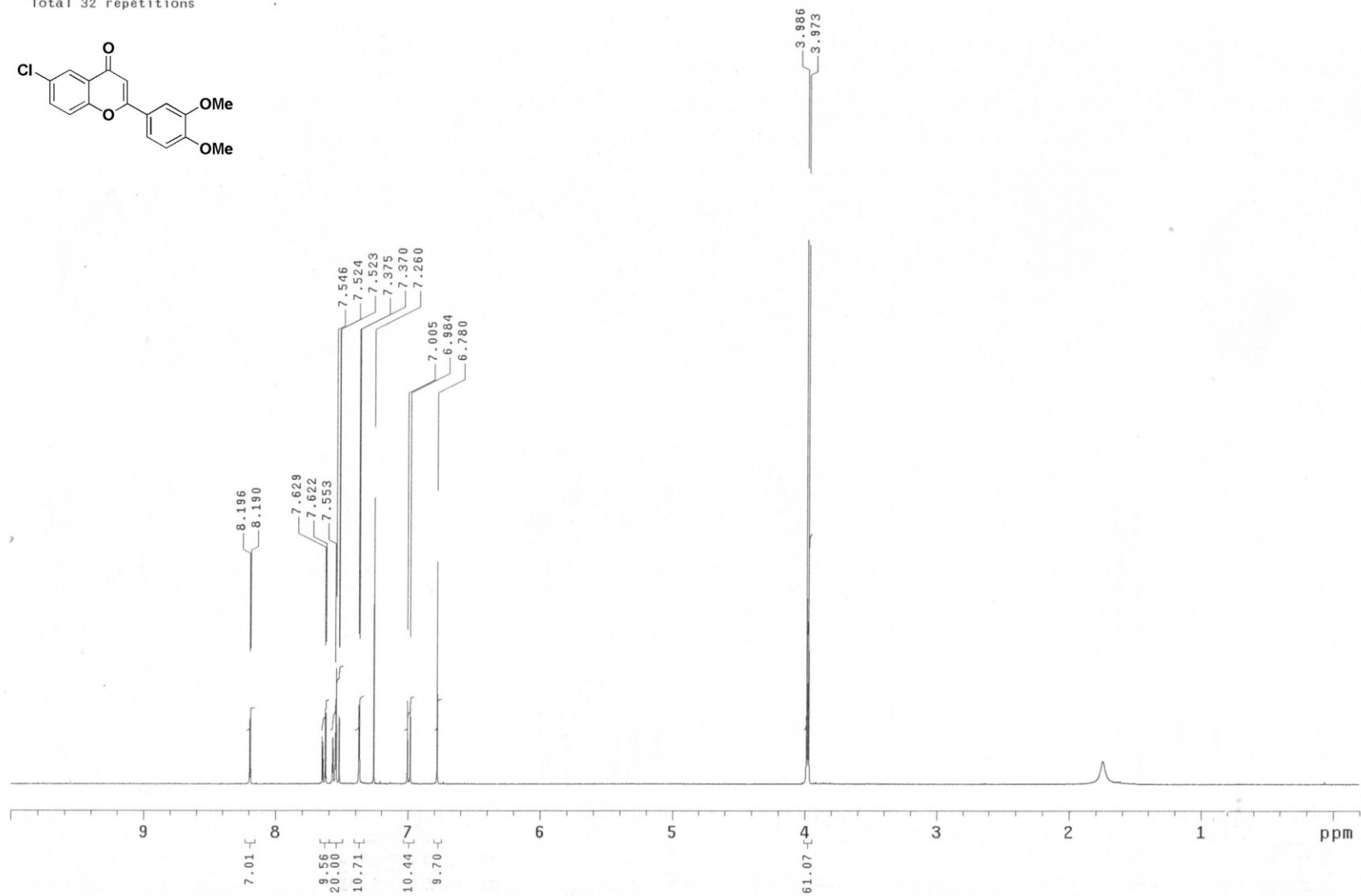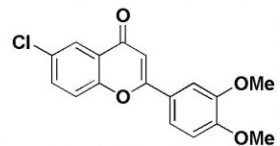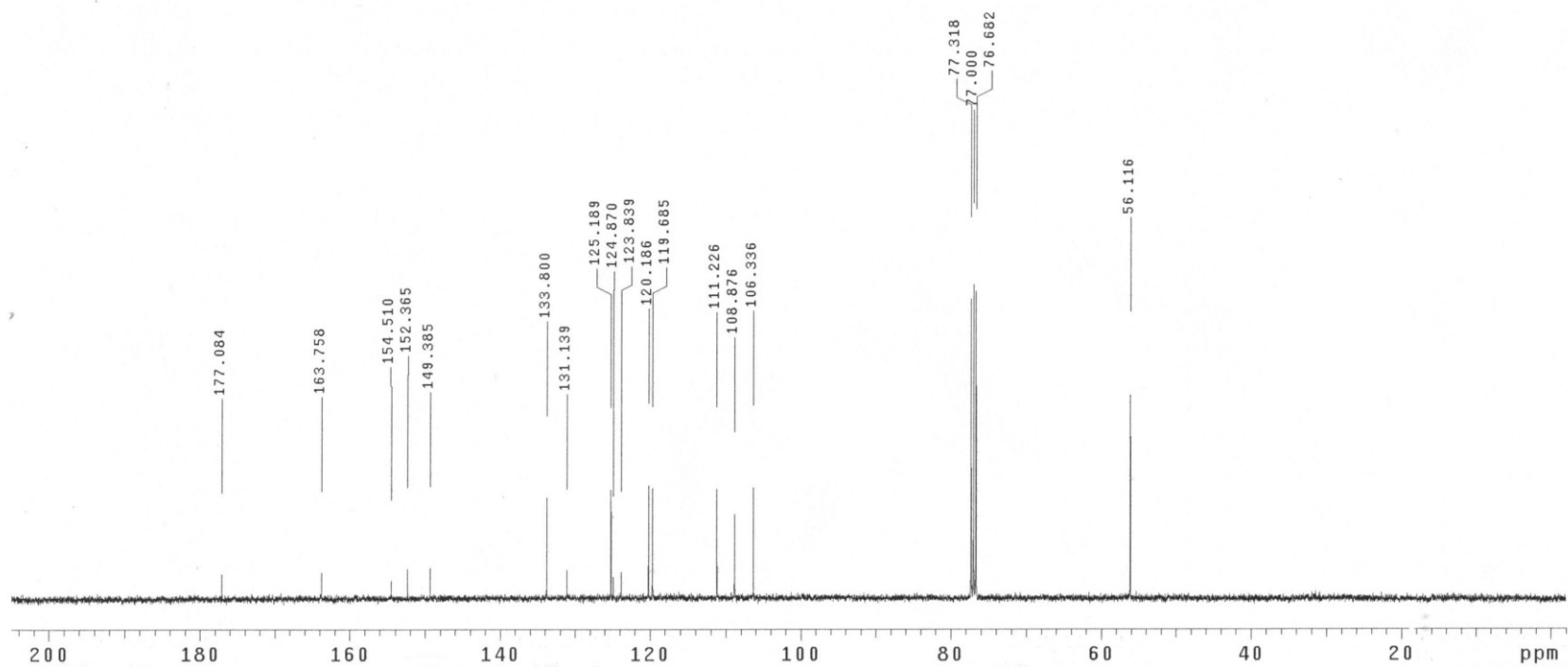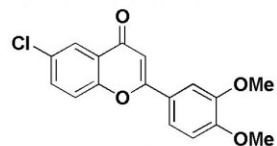
Compound 4v (^{1}H-NMR spectral data)

MC0826

Pulse Sequence: s2pul

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

8.342
8.336
7.784
7.778
7.762
7.755
7.479
7.457
7.364
7.359
7.260
6.995
6.974
6.810
3.980
3.966
2.065

9.46
10.19
10.79
10.40
10.25
10.34
10.00
61.23
14.03
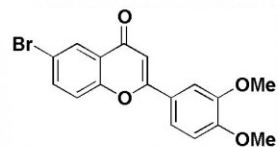
Compound 4v (^{13}C-NMR spectral data)

MC0826

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 27 2019
Solvent: CDCl3
Ambient temperature
Total 2048 repetitions

176.902
163.894
154.927
152.456
149.370
136.635
128.327
125.052
123.688
120.292
119.920
118.654
111.210
108.868
106.245
77.318
77.000
76.682
56.108

180   160   140   120   100   80   60   40   20   ppm

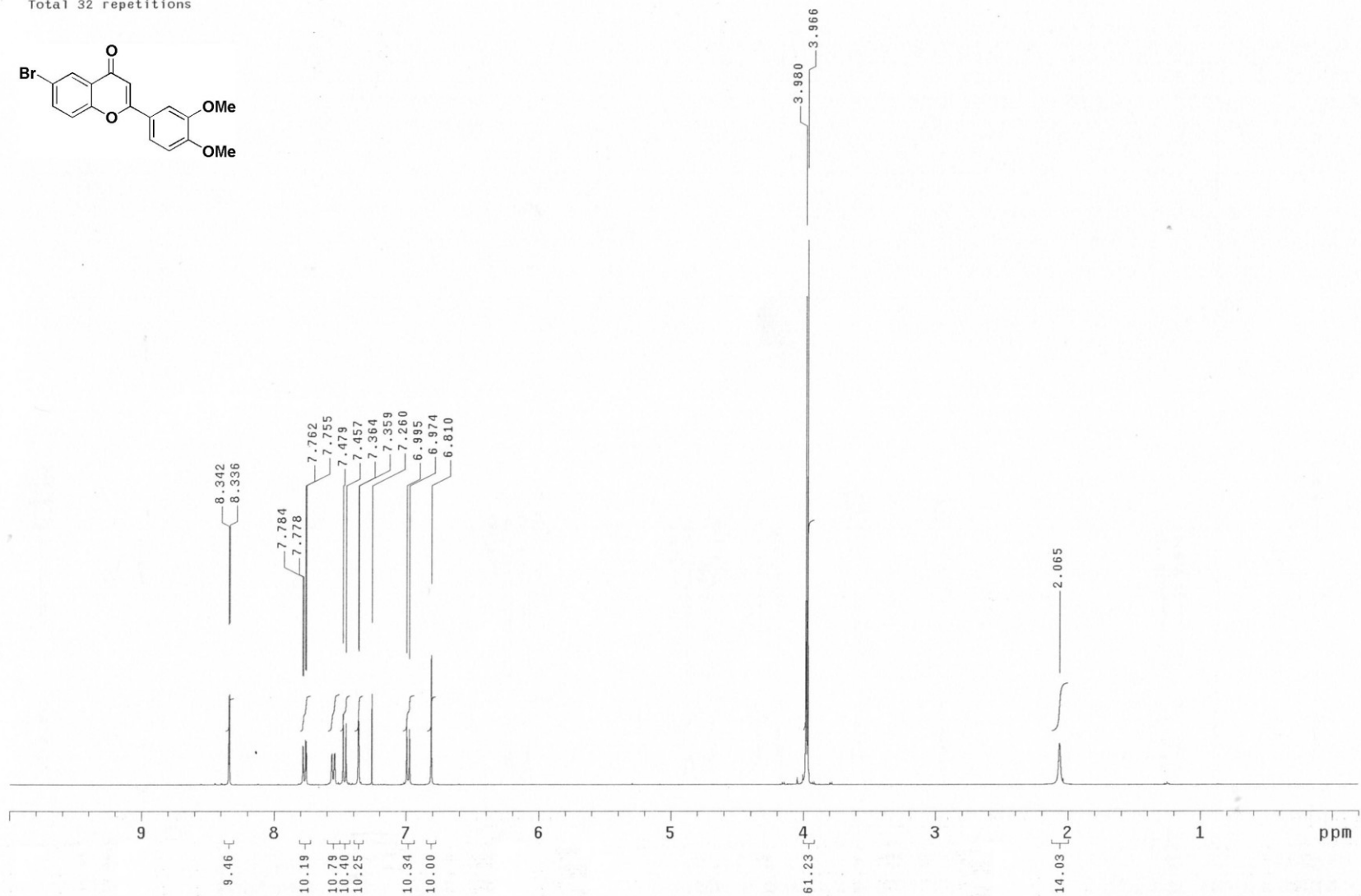# Compound 4w (^{1}H-NMR spectral data)

MC0823

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
Date: Aug 27 2019
Solvent: CDCl3
Ambient temperature
Total 112 repetitions

7.260

3.982

2.498

1.984

8.046

7.569
7.439

9   8   7   6   5   4   3   2   1   ppm

10.06

30.77
10.27

10.02
10.28

60.98

30.70

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

MC0823

Pulse Sequence: s2pul

UNITYplus-400   "unity400"
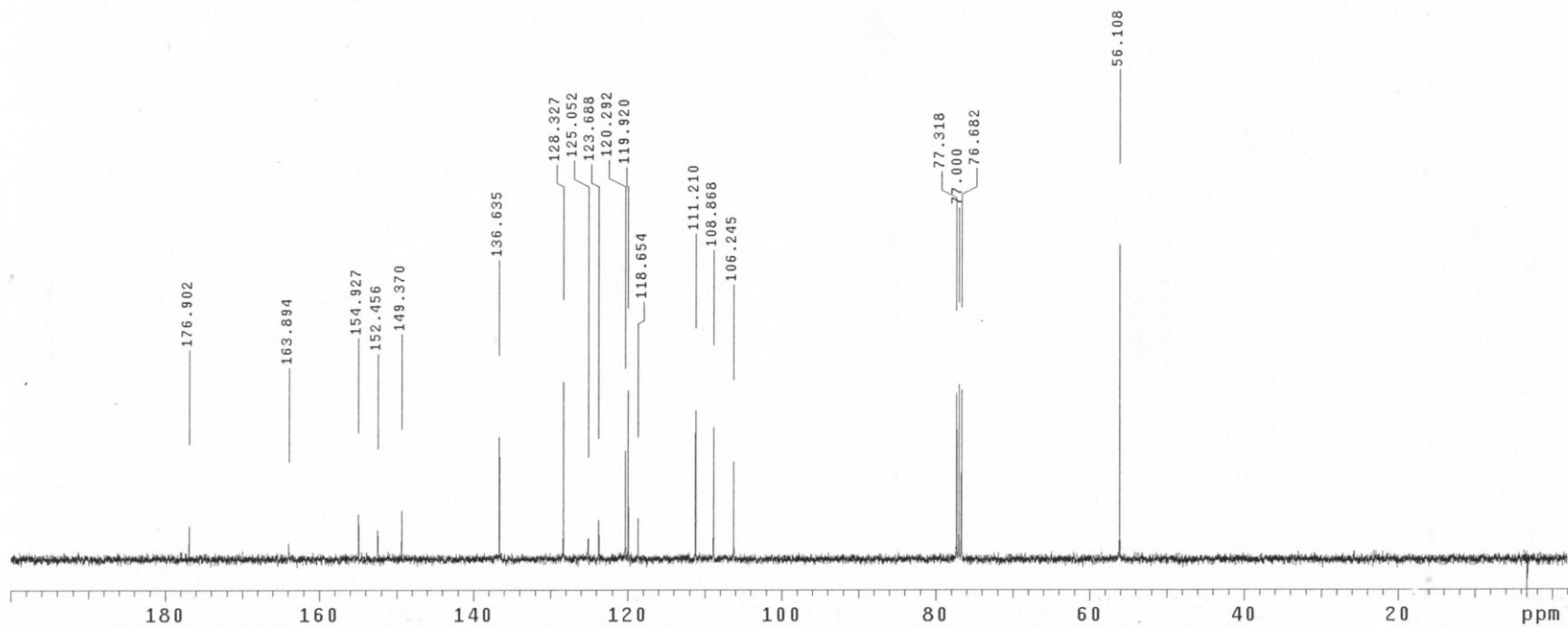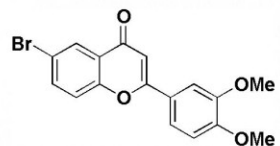Date: Aug 27 2019
Solvent: CDCl3
Ambient temperature
Total 32000 repetitions

178.358
164.751
154.624
152.691
149.408
135.650
125.583
125.007
123.809
123.112
120.815
117.866
117.639
111.286
109.118
77.318
77.197
77.000
76.682
56.260
56.192
21.026

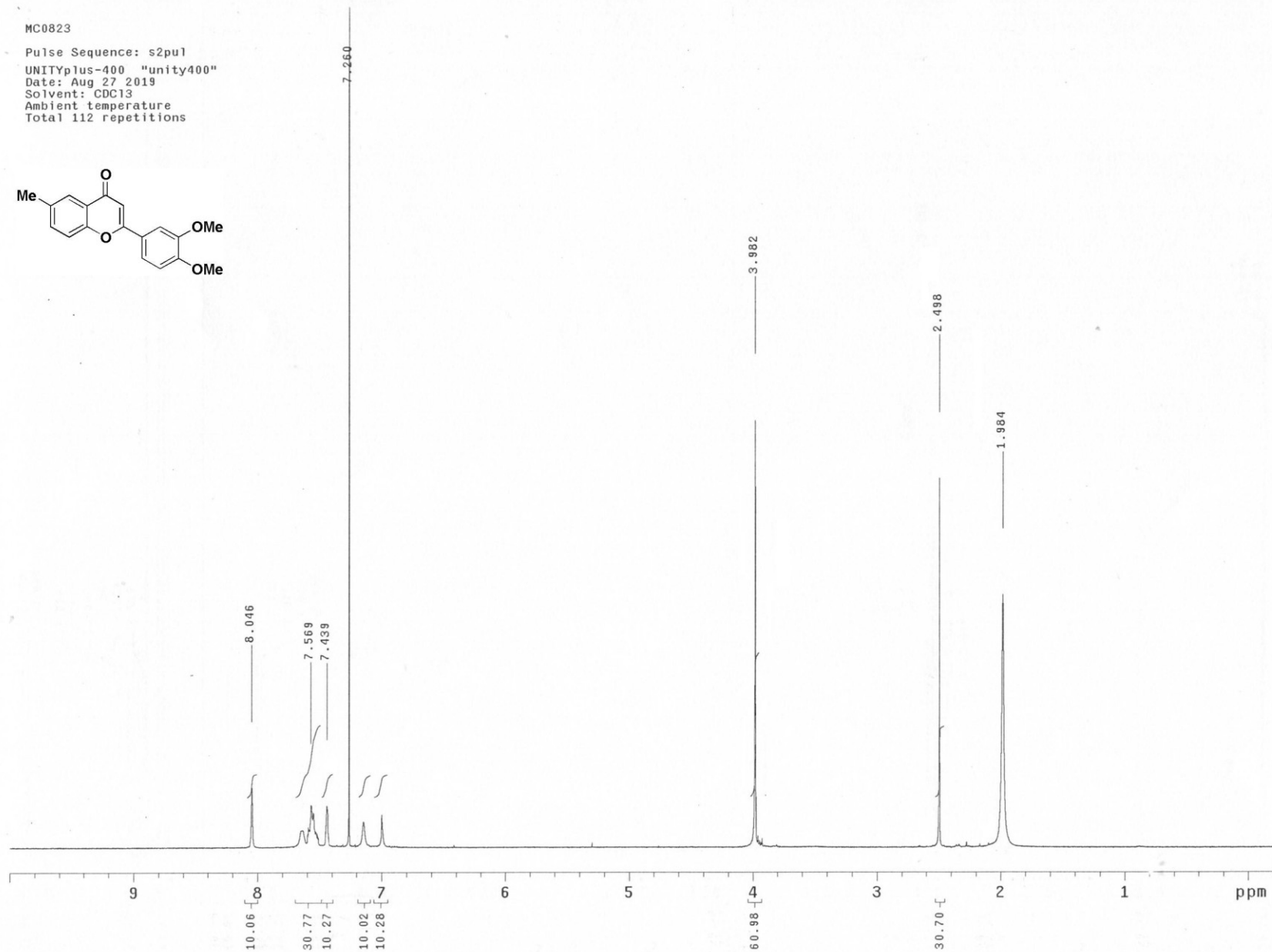180   160   140   120   100   80   60   40   20   ppm

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

MC0815

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDC13
Ambient temperature
Total 32 repetitions

Peaks: 8.146, 8.124, 7.385, 7.380, 7.260, 6.993, 6.894, 3.988, 3.967, 3.950

Integrations: 10.00, 11.14, 10.17, 32.01, 11.81, 92.51

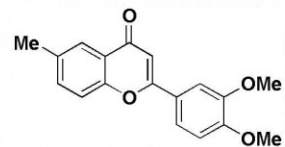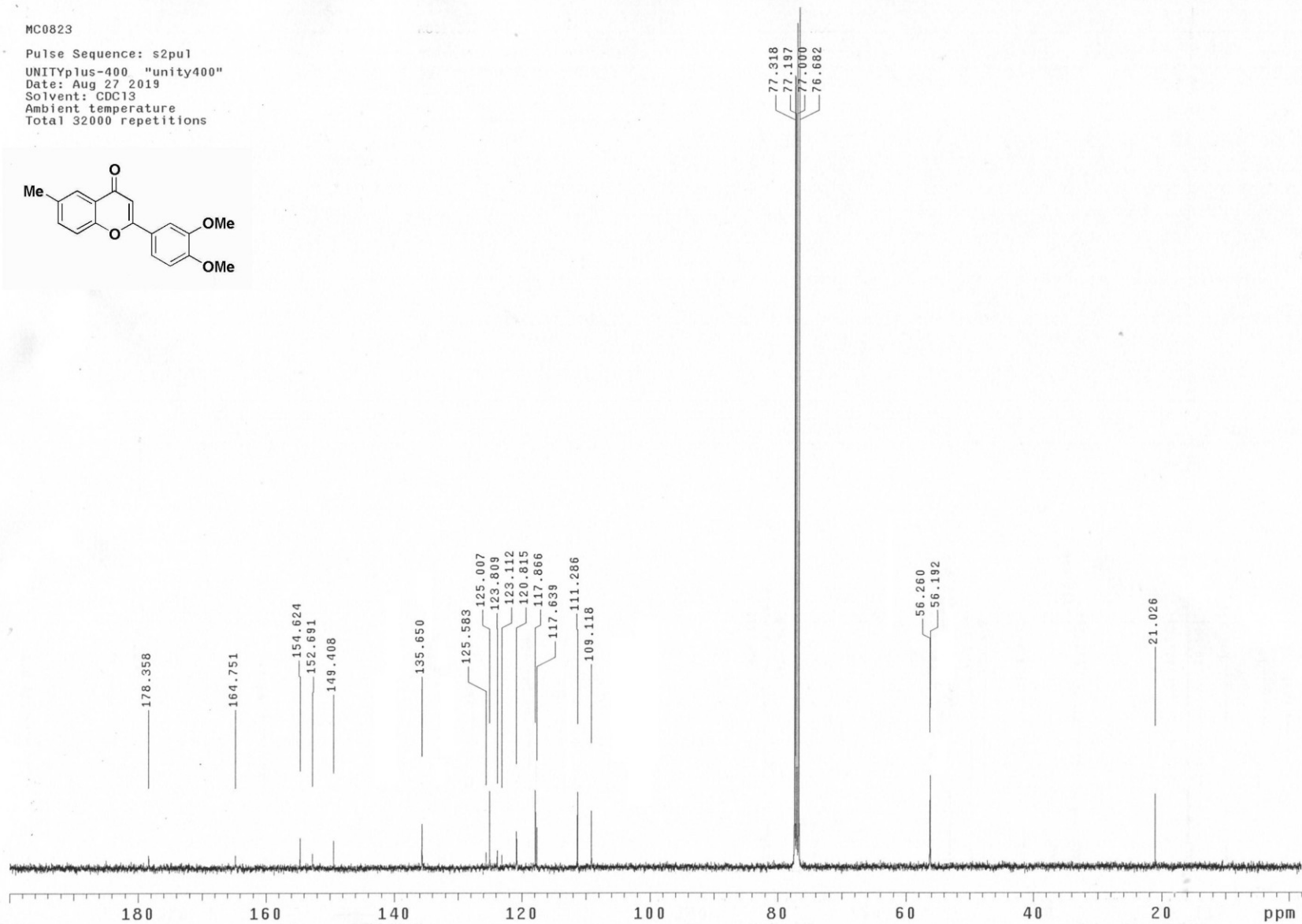# Compound 4x (^{13}C-NMR spectral data)

MC0815

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 19 2019
Solvent: CDCl3
Ambient temperature
Total 4464 repetitions
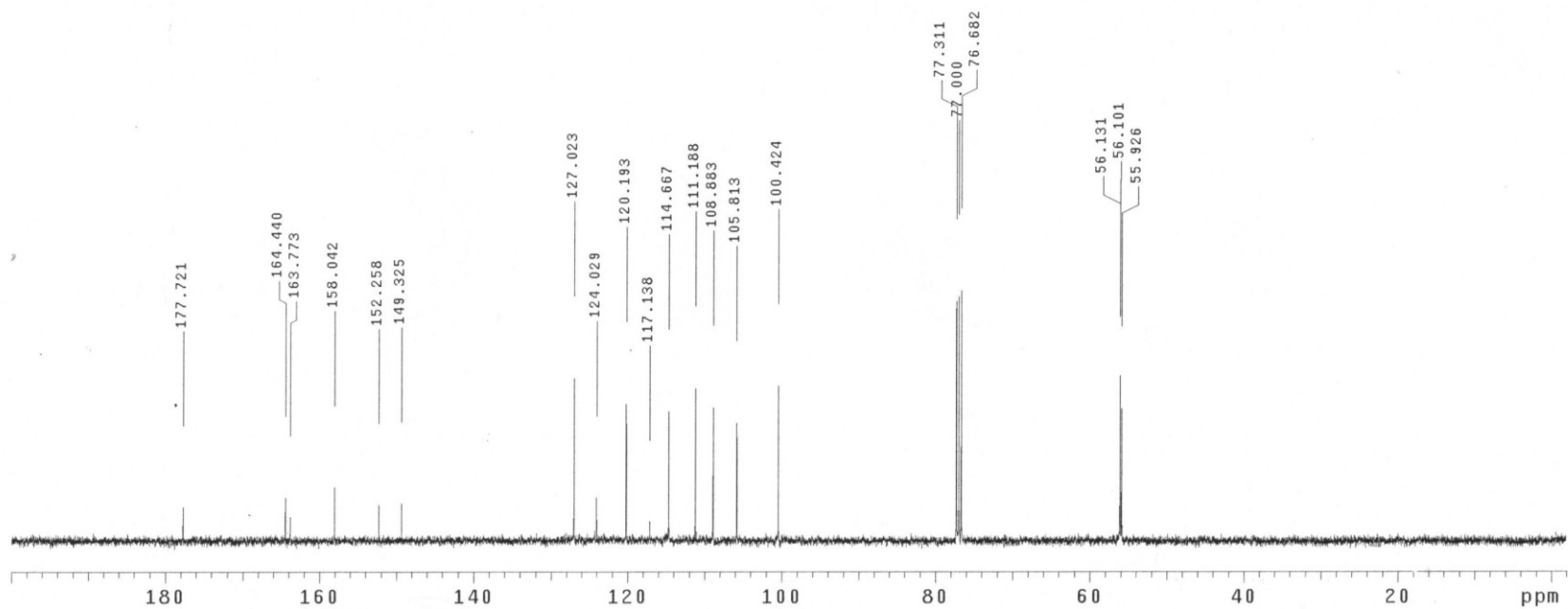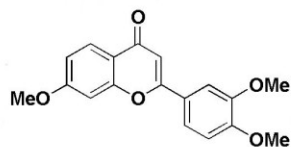
Compound 4y (^{1}H-NMR spectral data)
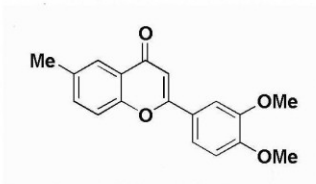
MC0310

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 10 2021
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

4.051

8.014
8.009
7.994
7.989
7.812
7.789
7.542
7.540
7.533
7.523
7.260
7.068
7.045
6.959

20.30
10.09
30.86
11.04
10.00
32.15

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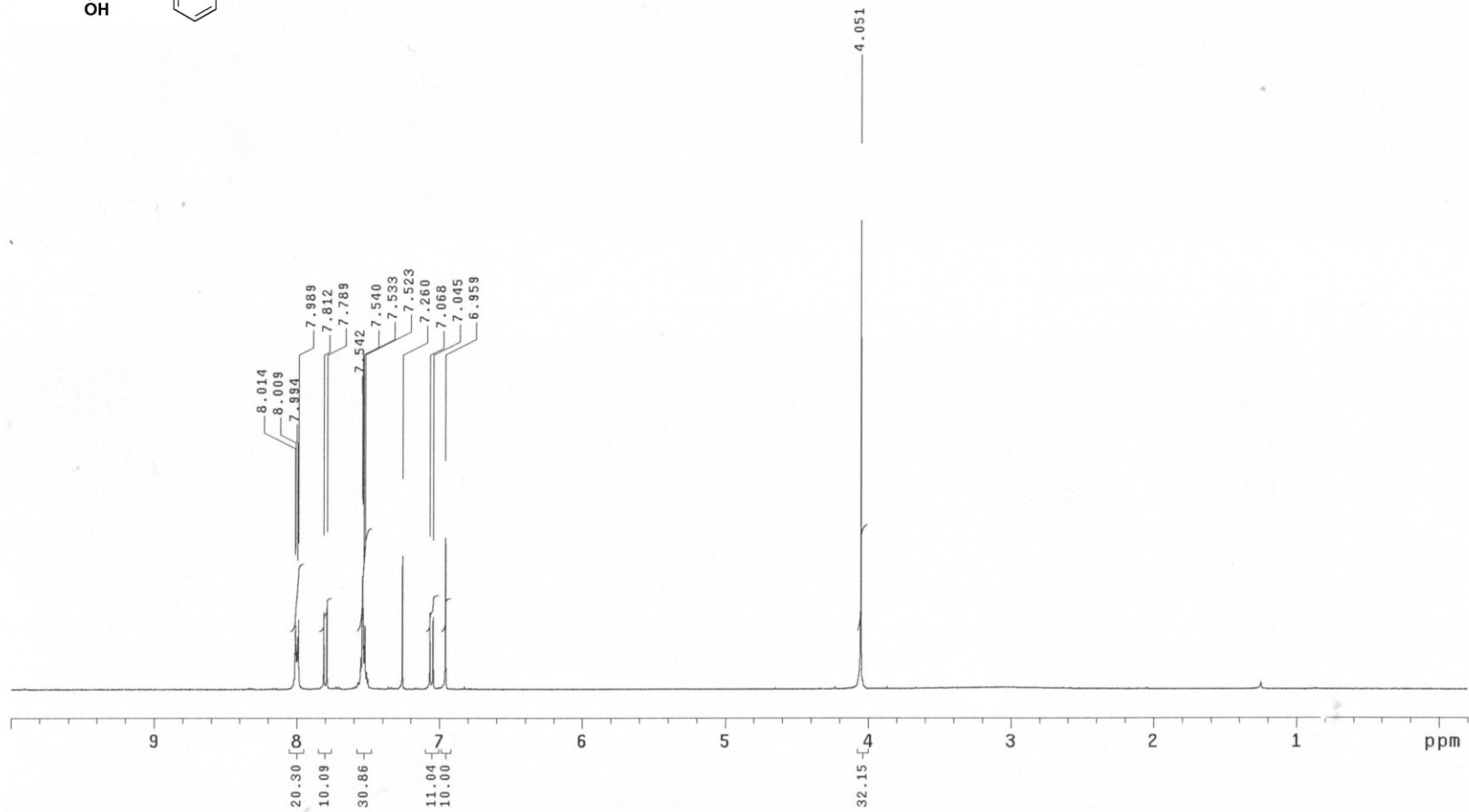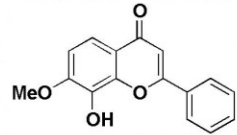
Compound 4y (^{13}C-NMR spectral data)

MC0310

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
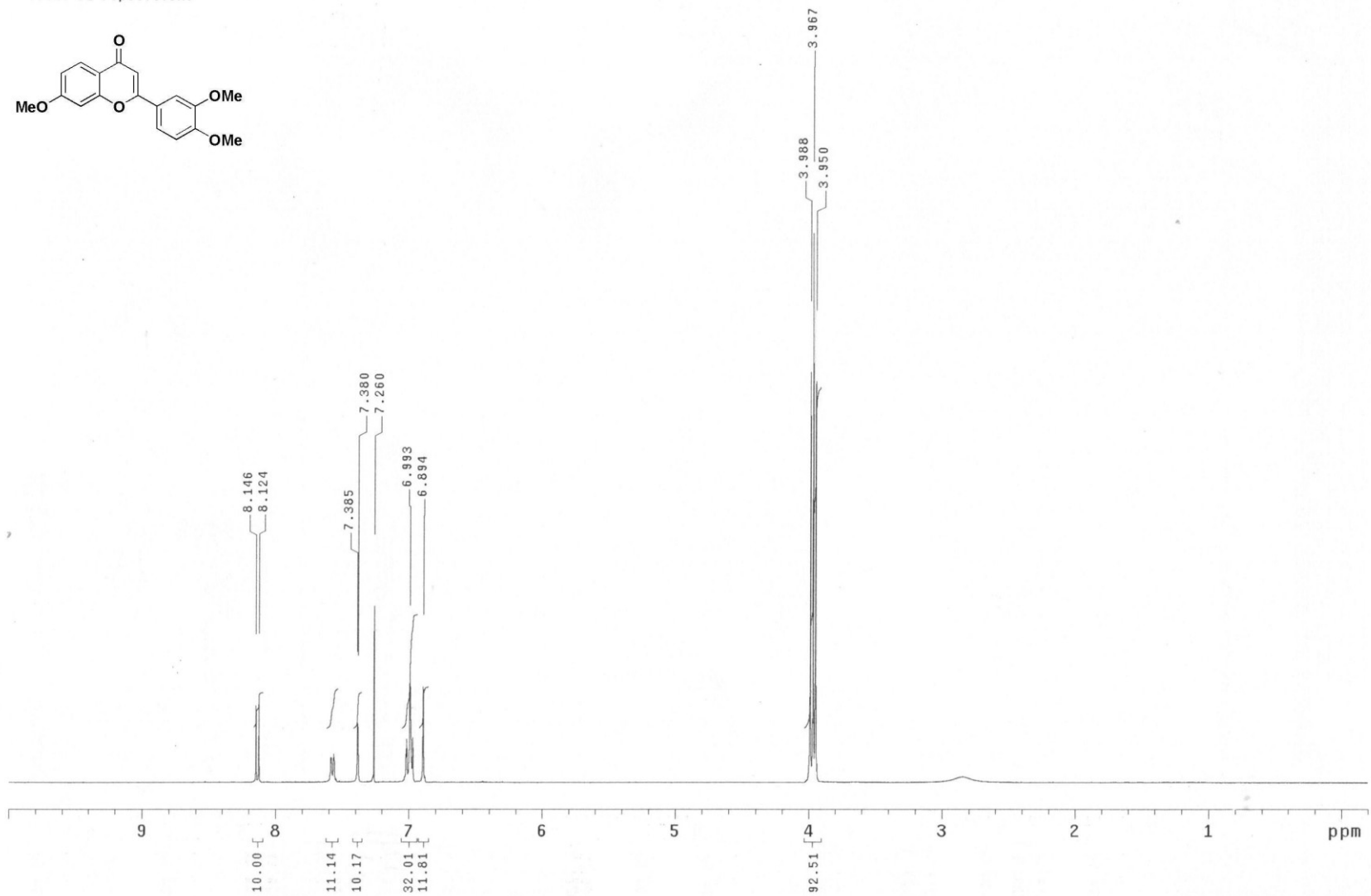Date: Mar 10 2021
Solvent: CDCl3
Ambient temperature
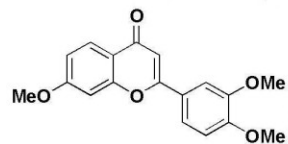Total 40080 repetitions

77.318
77.205
77.000
76.682

129.055
126.402
131.594
116.539
108.648
106.708
134.035
150.030
144.913
178.252
56.669

180   160   140   120   100   80   60   40   20   ppm
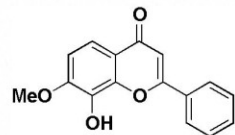
Compound 3q (^{1}H-NMR spectral data)

MC0805

Pulse Sequence: s2pul

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

12.894

7.933
7.928
7.912
7.908
7.701
7.664
7.576
7.562
7.560
7.559
7.557
7.539
7.538
7.511
7.507
7.493
7.489
7.486
7.472
7.468
7.260
7.029
7.027
7.026
7.008
7.006
6.958
6.955
6.940
6.937
6.935
6.920
6.916
6.776
6.768
6.547
6.543
6.539
6.534

12.57
10.13
32.55
21.29
10.45
10.00

8.48

12 11 10 9 8 7 6 5 4 3 2 1 ppm

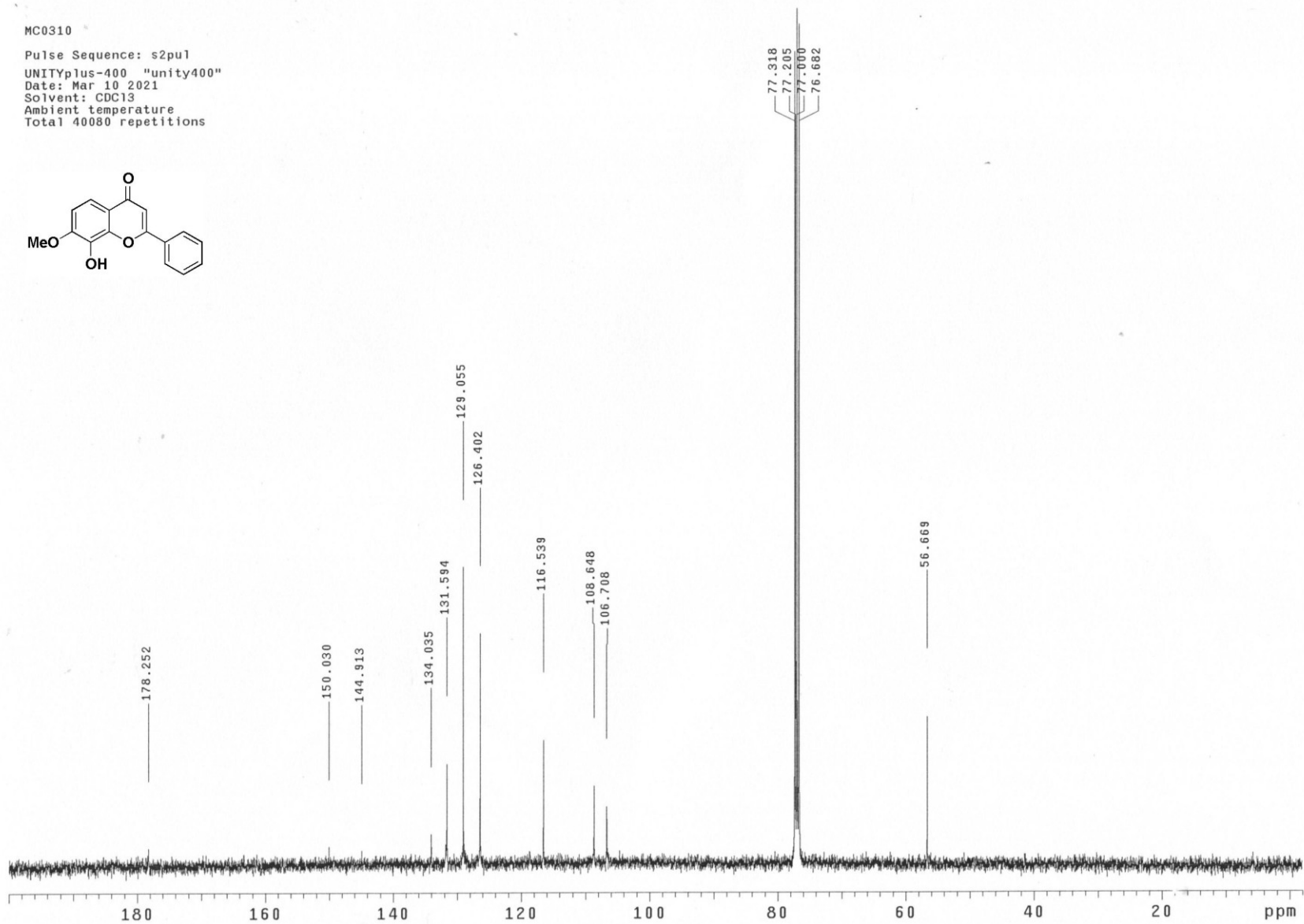# Compound 3q (^{13}C-NMR spectral data)

MC0805

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 7 2019
Solvent: CDCl3
Ambient temperature
Total 1120 repetitions

Peaks (ppm): 193.314, 163.531, 151.523, 145.391, 136.279, 131.101, 129.616, 120.034, 118.821, 118.526, 117.616, 117.100, 112.871, 77.318, 77.000, 76.682

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

YE0810

Pulse Sequence: s2pul

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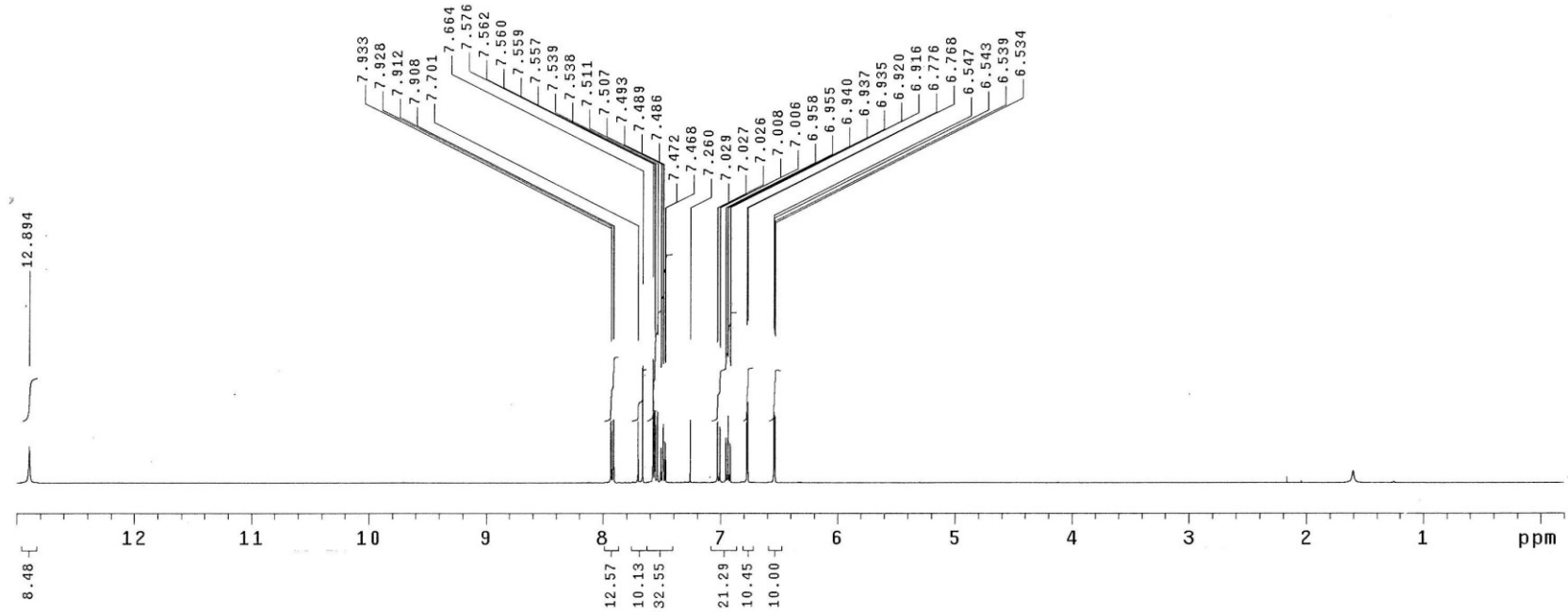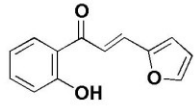Date: Aug 9 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.958
7.953
7.938
7.933
7.519
7.517
7.515
7.512
7.511
7.506
7.499
7.494
7.489
7.487
7.467
7.464
7.446
7.427
7.411
7.393
7.081
7.077
7.074
7.063
7.055
7.053

3.135
3.102
3.093
3.060
2.926
2.919
2.884
2.877

9.34
61.88
20.00
10.05
11.72
11.74

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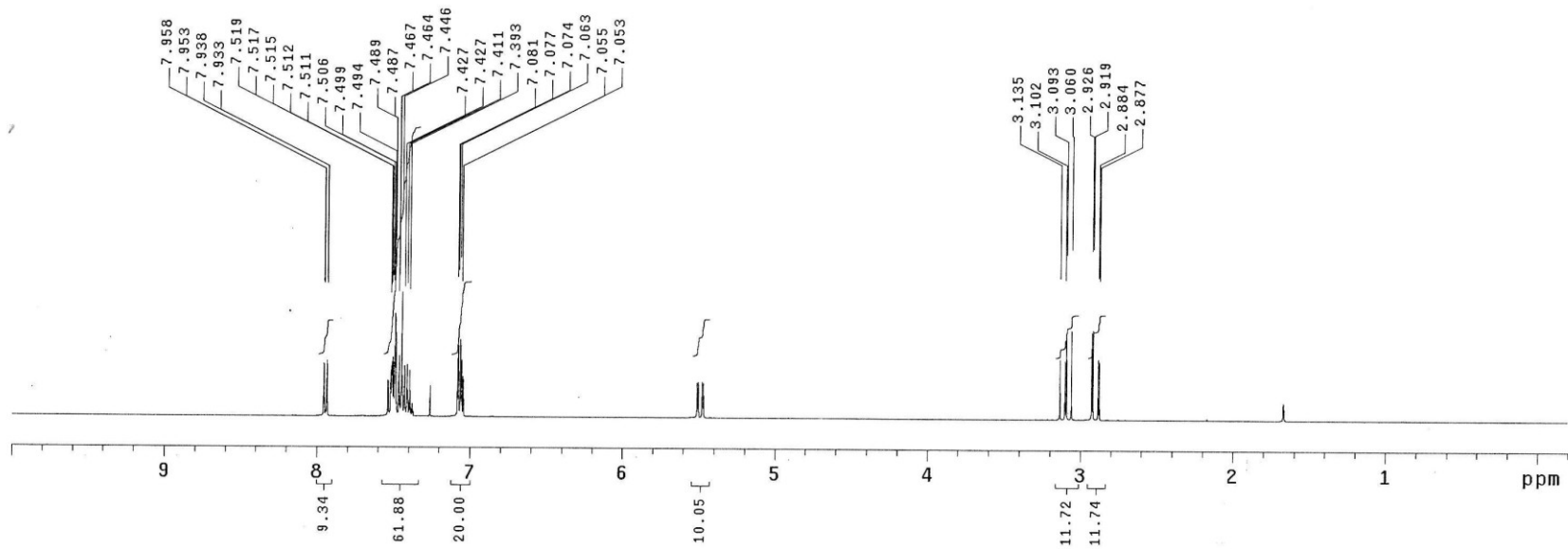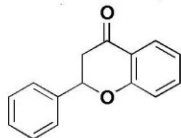
Compound 5a (^{13}C-NMR spectral data)

YE0810
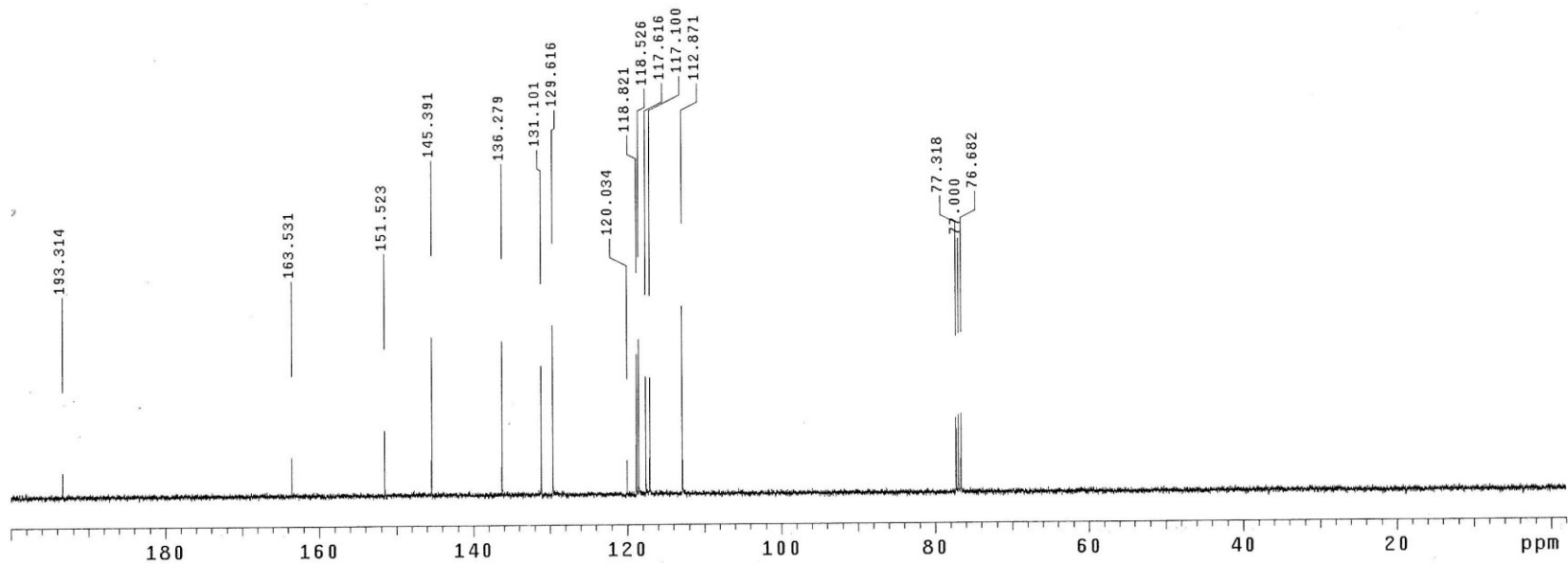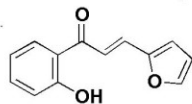
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Aug 9 2019
Solvent: CDC13
Ambient temperature
Total 640 repetitions

191.912

161.529

138.712
136.158

128.820
128.736
127.023
126.114

121.580
120.913
118.101

79.562
77.318
77.000
76.682

44.639

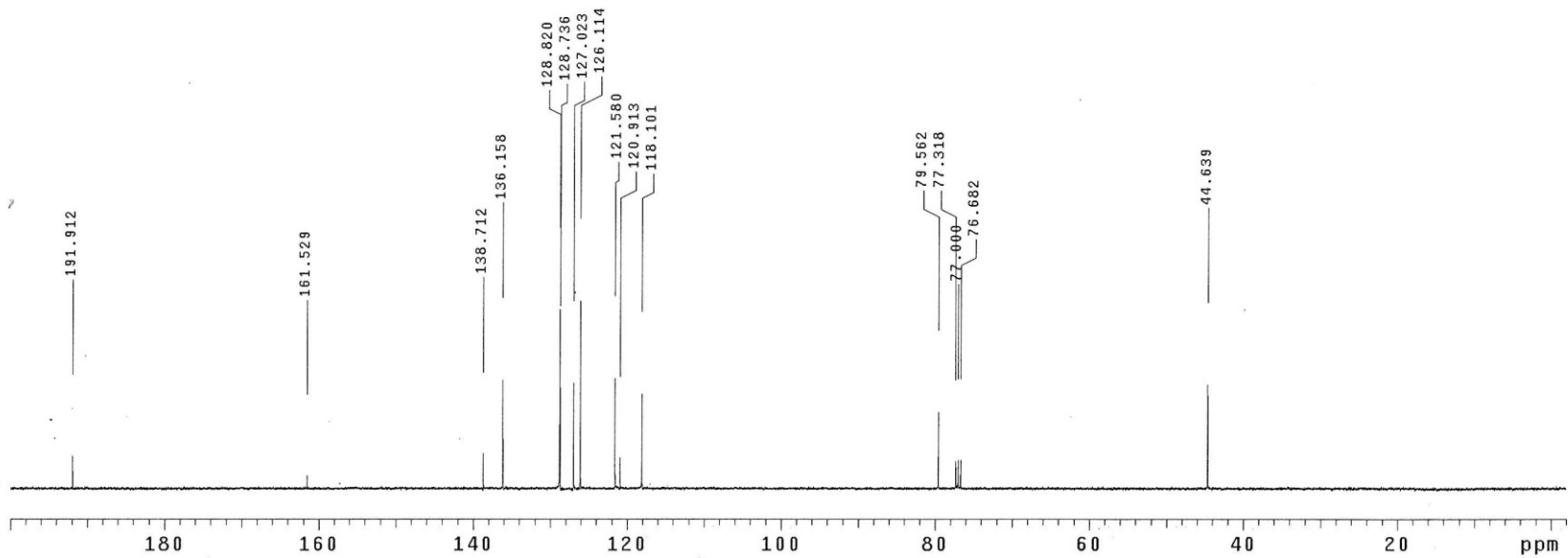180 160 140 120 100 80 60 40 20 ppm
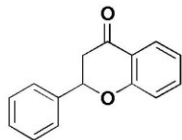
Compound 6a (^{1}H-NMR spectral data)

MC918

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 19 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

8.185
8.181
8.165
8.160
7.632
7.420
7.400
7.398
7.369
7.260
6.171
2.382

9.21
10.05
20.16
9.98
32.23

9 8 7 6 5 4 3 2 1 ppm

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

MC918

Pulse Sequence: s2pul
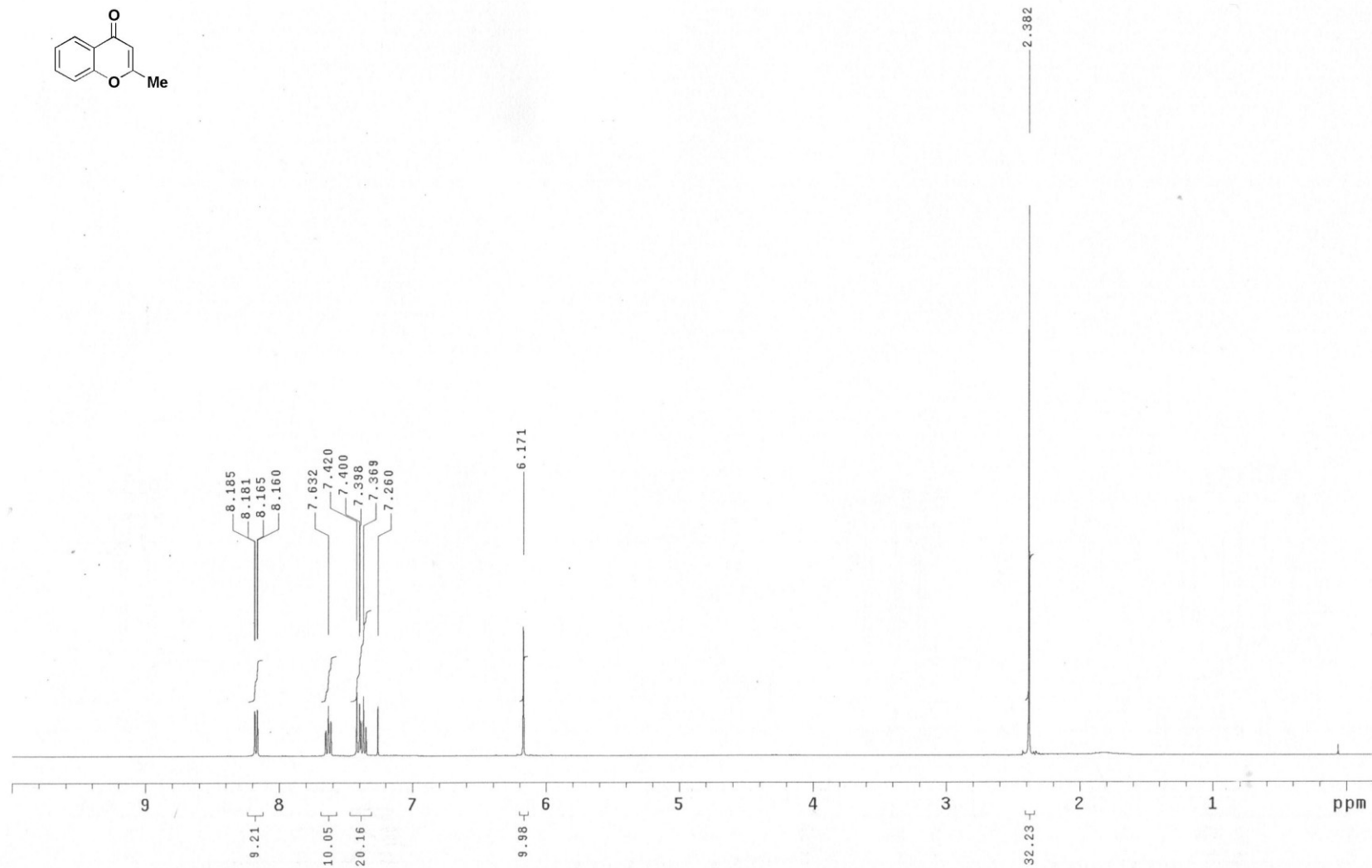
UNITYplus-400 "unity400"
Date: Sep 19 2019
Solvent: CDC13
Ambient temperature
Total 2240 repetitions

178.237
166.161
156.473
133.414
125.644
124.901
123.584
117.752
110.559
77.318
77.000
76.682
20.571

180 160 140 120 100 80 60 40 20 ppm
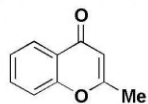
Compound 7a (^{1}H-NMR spectral data)

MC732

Pulse Sequence: s2pul

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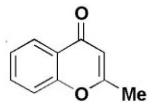Date: Sep 6 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

7.873
7.868
7.853
7.849
7.436
7.435
6.981
6.979
6.977
6.947
6.946
6.926
6.925
6.923

4.517
4.501
4.485

2.793
2.778
2.776
2.761

9.46
10.20
20.00
24.09
24.31

9   8   7   6   5   4   3   2   1   ppm

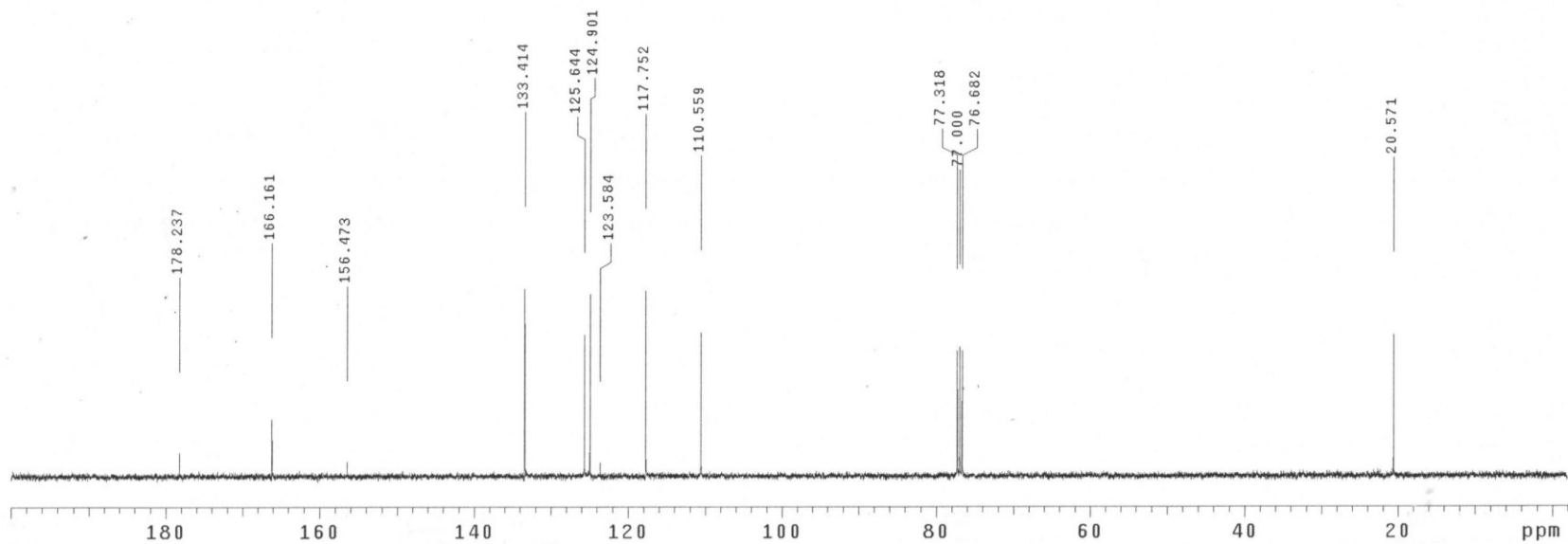# Compound 7a (^{13}C-NMR spectral data)

MC732

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
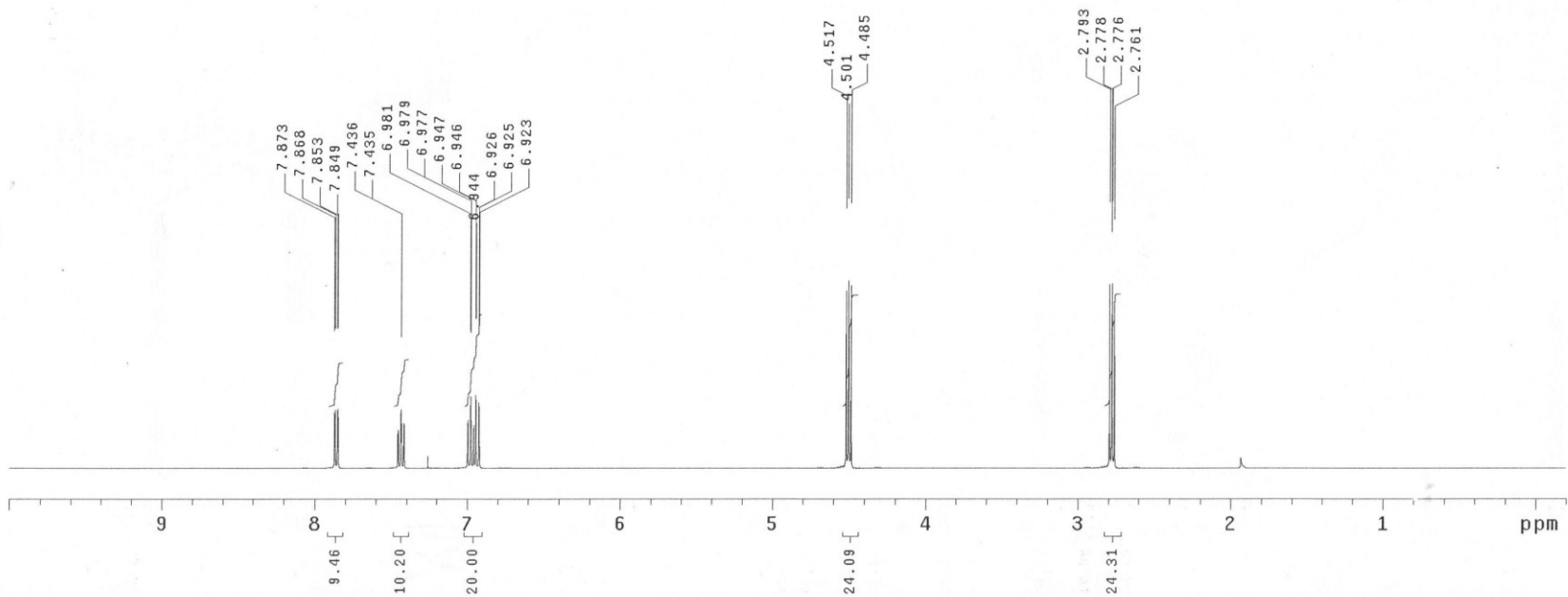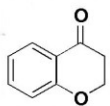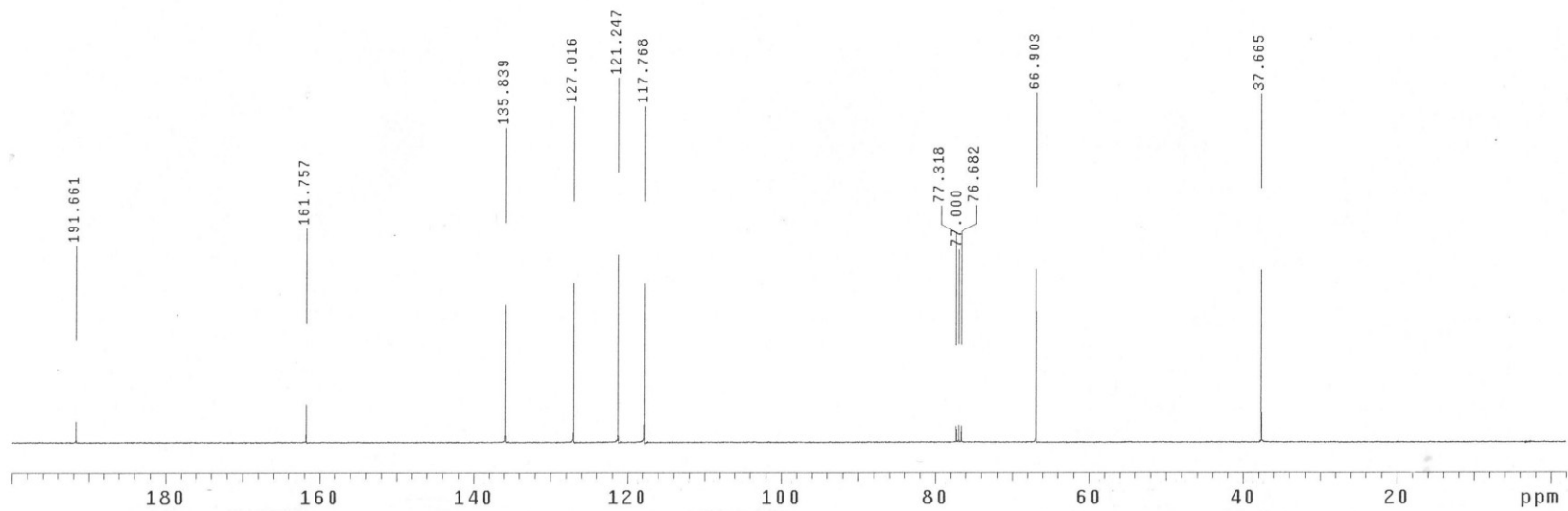Date: Sep 6 2019
Solvent: CDCl3
Ambient temperature
Total 2944 repetitions

191.661

161.757

135.839

127.016

121.247

117.768

77.318
77.000
76.682

66.903

37.665

180 160 140 120 100 80 60 40 20 ppm
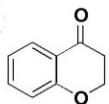
X-ray crystal data of compound 4t (CCDC 1957347)
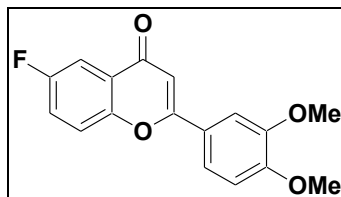
Sample preparation : A solution of compound **4t** (30 mg) in CH_2Cl_2 (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.
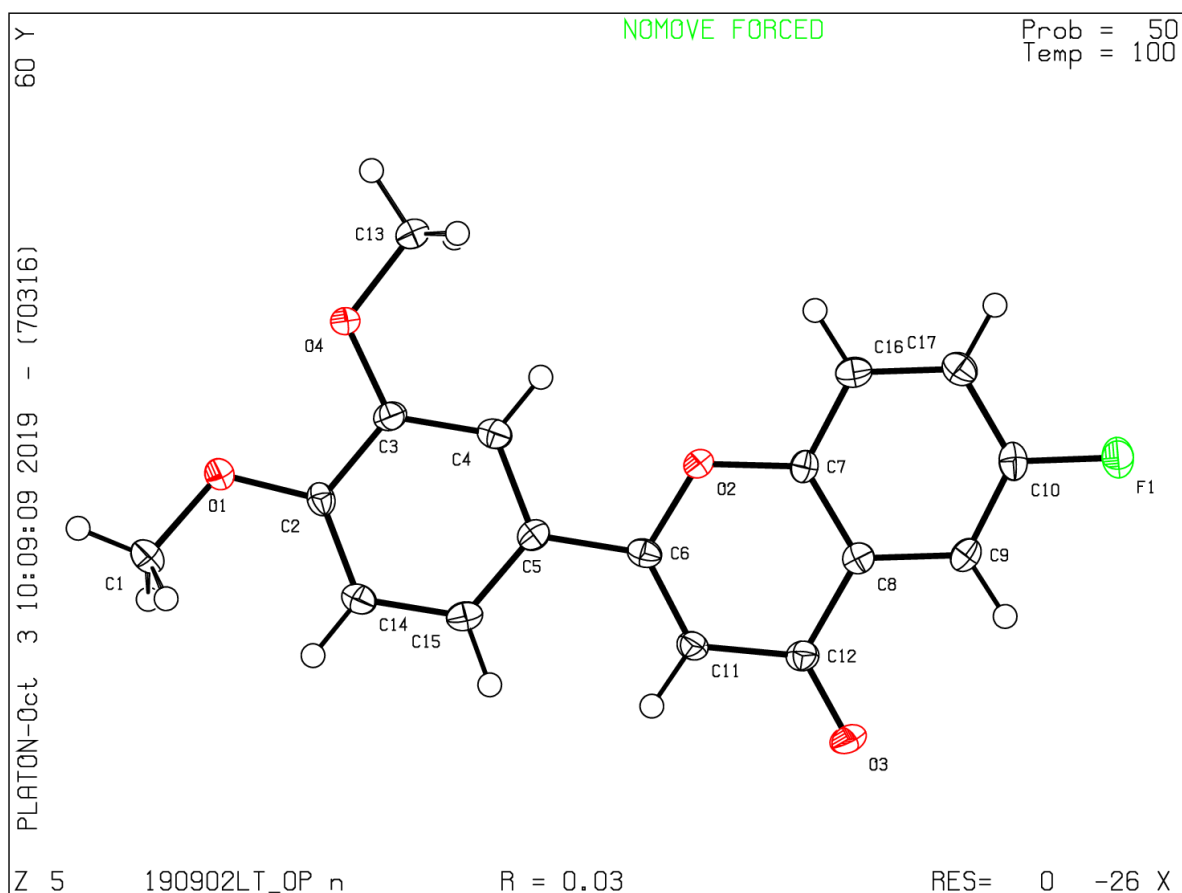
Empirical formula	C17 H13 F O4
Formula weight	300.27
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	Pn
Unit cell dimensions	a = 4.0051(3) Å $\alpha = 90°$.
	b = 10.1298(8) Å $\beta = 92.222(3)°$.
	c = 16.3327(12) Å $\gamma = 90°$.
Volume	662.13(9) Å^3
Z	2
Density (calculated)	1.506 Mg/m^3
Absorption coefficient	0.116 mm^{-1}
F(000)	312
Crystal size	0.10 x 0.08 x 0.01 mm^3
Theta range for data collection	2.010 to 26.380°.
Index ranges	-4<=h<=5, -12<=k<=12, -20<=l<=13
Reflections collected	3830
Independent reflections	1987 [R(int) = 0.0207]
Completeness to theta = 25.242°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6849
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1987 / 2 / 201
Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0799
R indices (all data)	R1 = 0.0307, wR2 = 0.0827
Absolute structure parameter	0.3(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.207 and -0.209 e.Å^{-3}