

Supporting Information
One-pot two-step synthesis of 3-iodo-4-aryloxy coumarins and their Pd/C-catalyzed annulation to coumestans

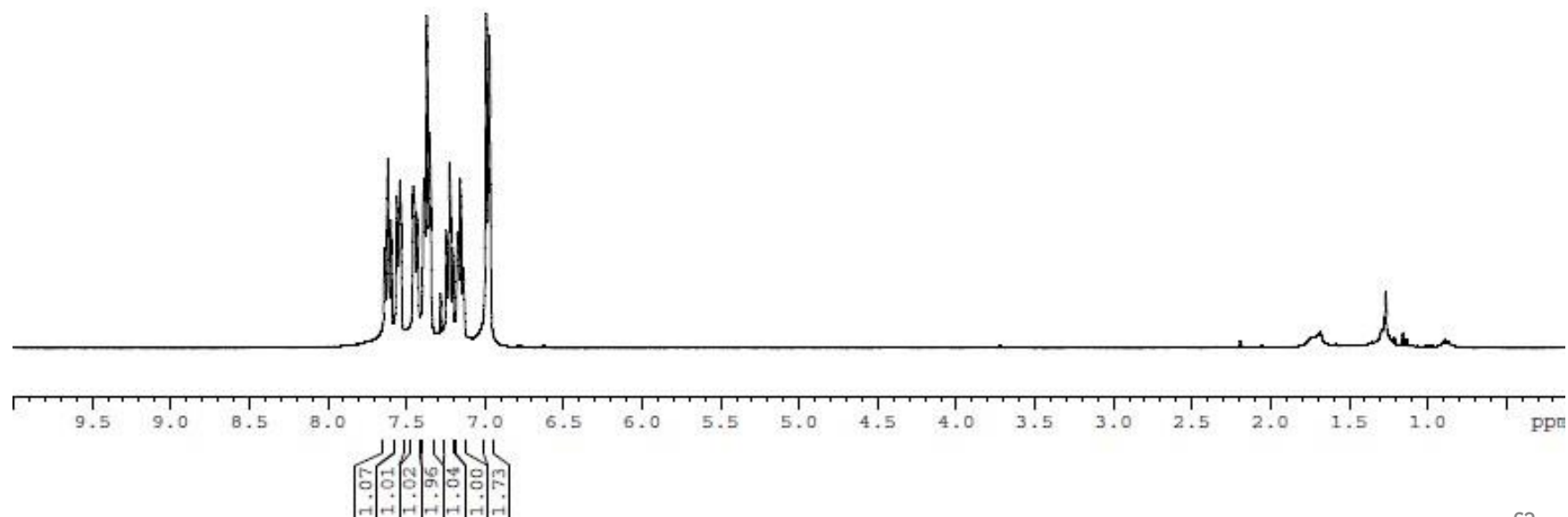
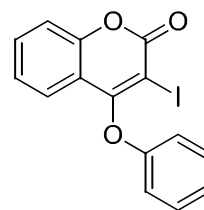
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Email: npanda@nitrkl.ac.in; niranjana.panda@gmail.com

¹H of 3-iodo-4-phenoxy-2H-chromen-2-one (3aa)

¹H of NP-IM-595 16.4.2015



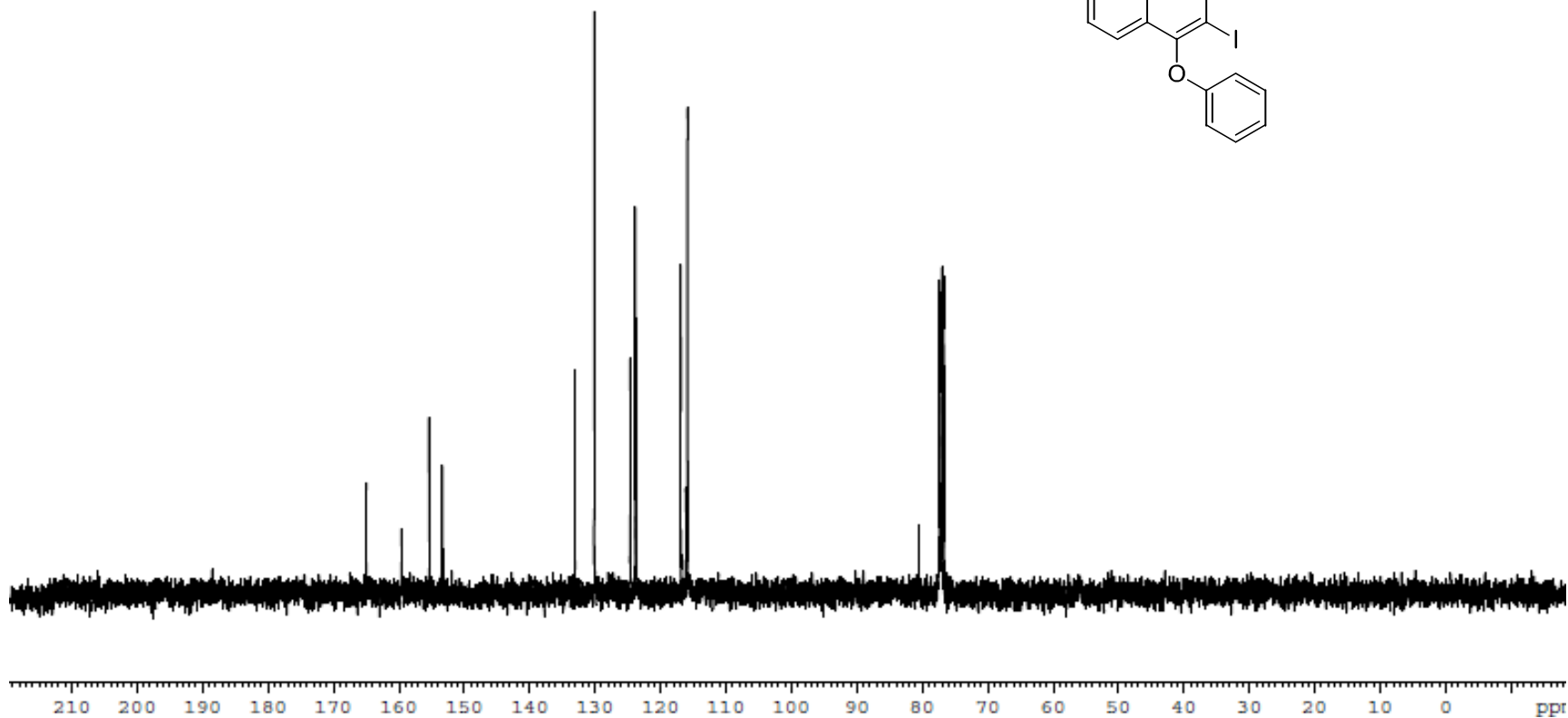
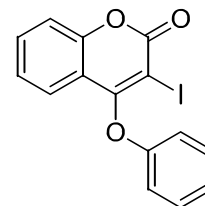
^{13}C of 3-iodo-4-phenoxy-2H-chromen-2-one (3aa)

^{13}C of NP-IM-595 16.4.2015

164.99
159.60
155.40
153.32

133.10
130.15
124.66
123.86
123.76
116.88
116.19
115.89

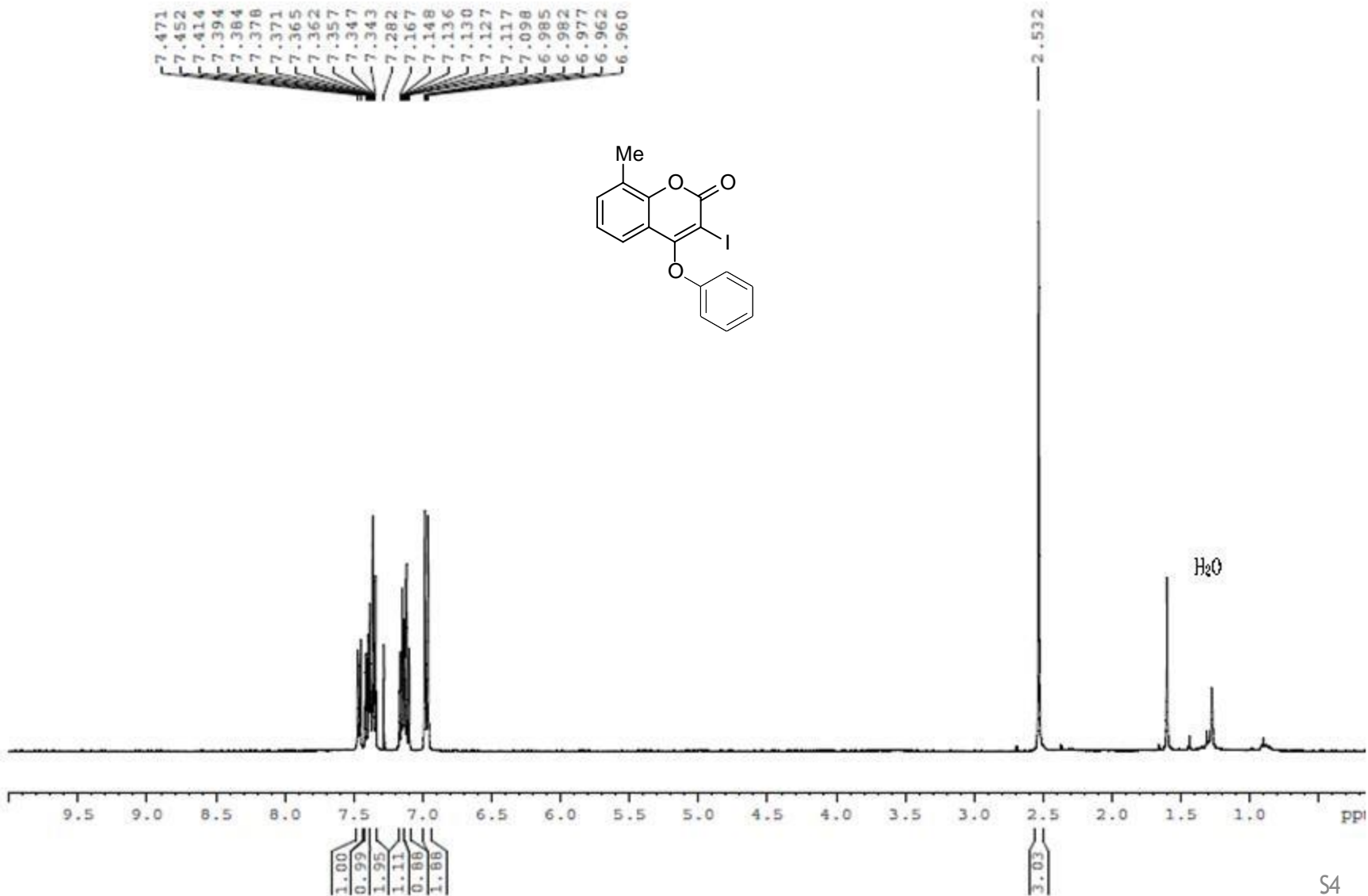
80.54
77.35
77.03
76.71



¹H of 3-iodo-8-methyl-4-phenoxy-2H-chromen-2-one (3ab)

NP-IM-974

1H



¹³C of 3-iodo-8-methyl-4-phenoxy-2H-chromen-2-one (3ab)

NP-IM-974

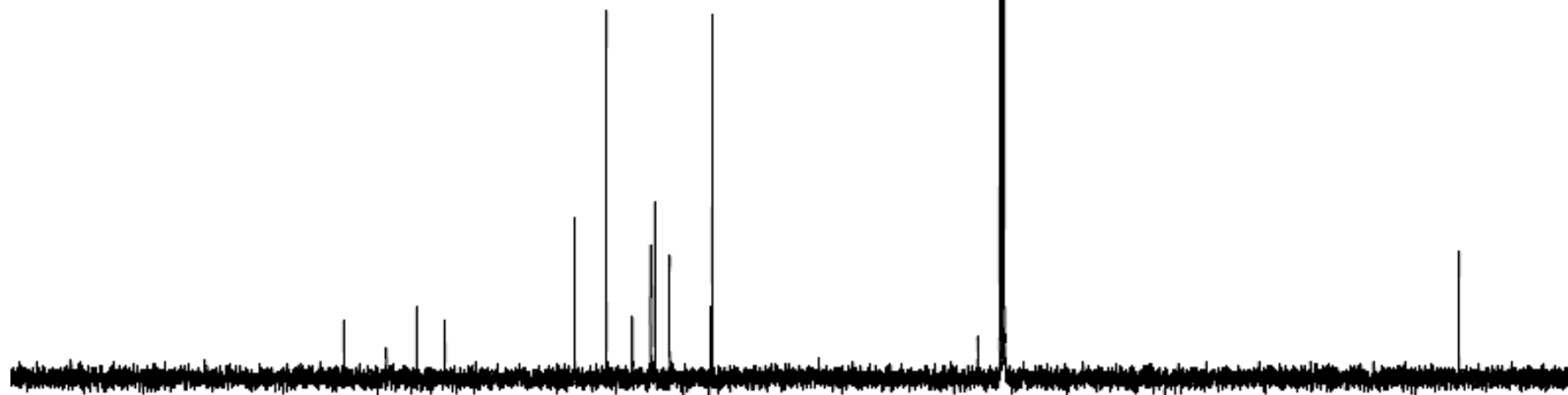
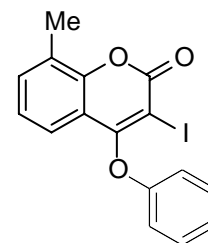
¹³C

165.36
159.65
155.62
151.81

134.39
130.13
126.60
124.21
123.65
121.60
116.16
115.91

80.33
77.34
77.02
76.70

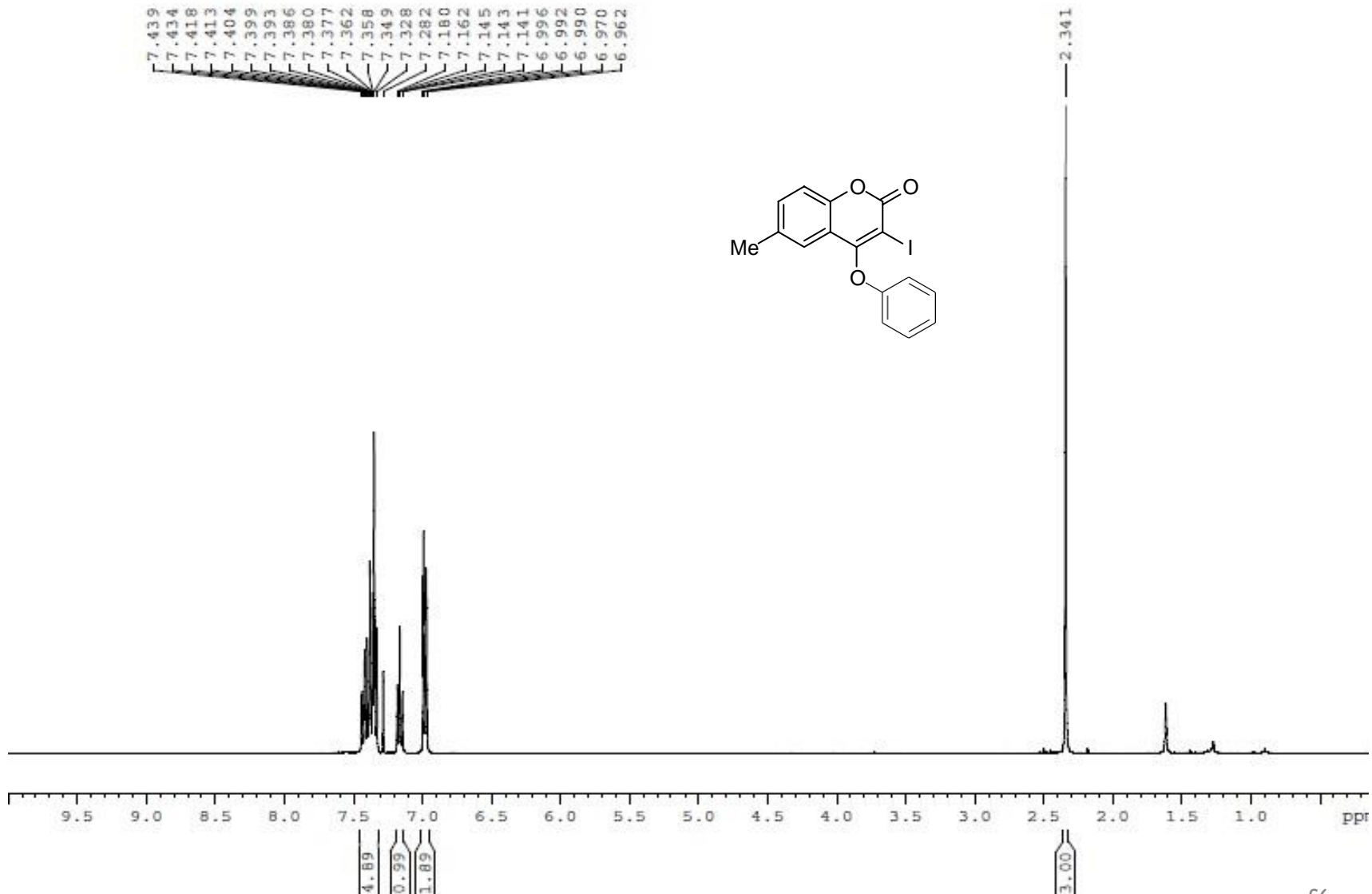
15.72



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

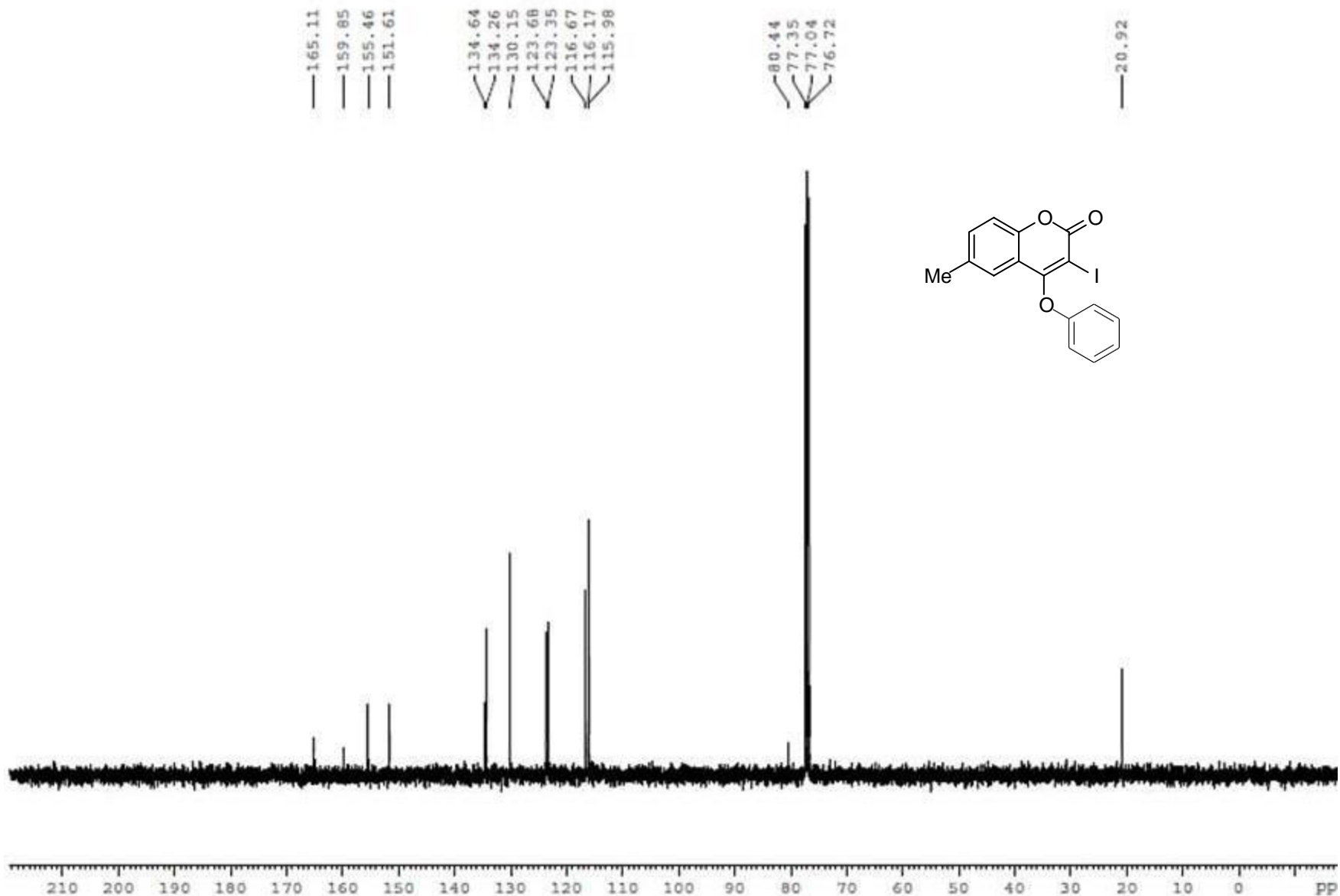
¹H of 3-iodo-6-methyl-4-phenoxy-2H-chromen-2-one (3ac)

¹H of NP-IM-4-Me H.C-O-Ar 27.5.2016



¹³C of 3-iodo-6-methyl-4-phenoxy-2H-chromen-2-one (3ac)

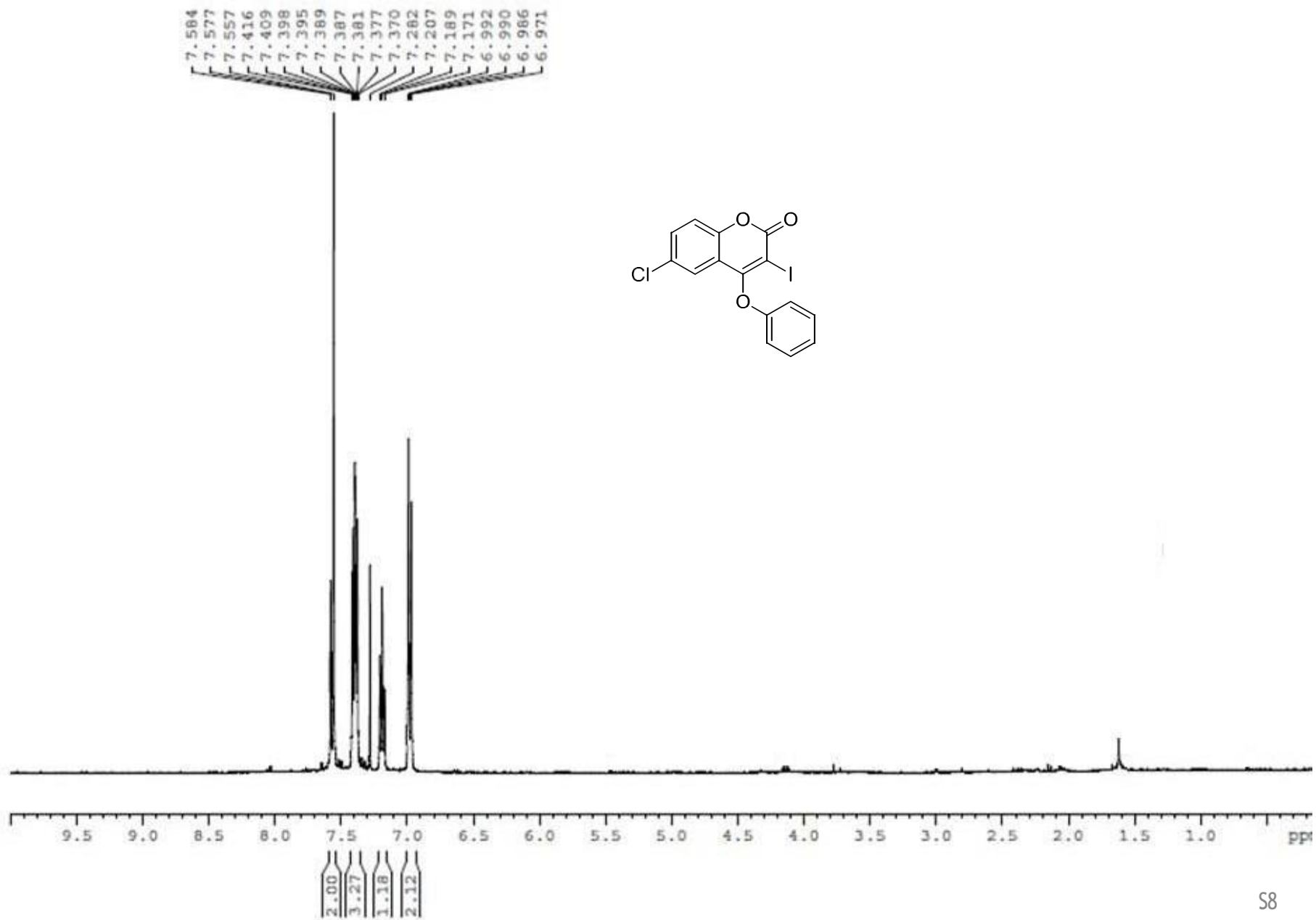
13C of NP-IM-4-Me HC O-Ar 27.5.2016



¹H of 6-chloro-3-iodo-4-phenoxy-2H-chromen-2-one (3ad)

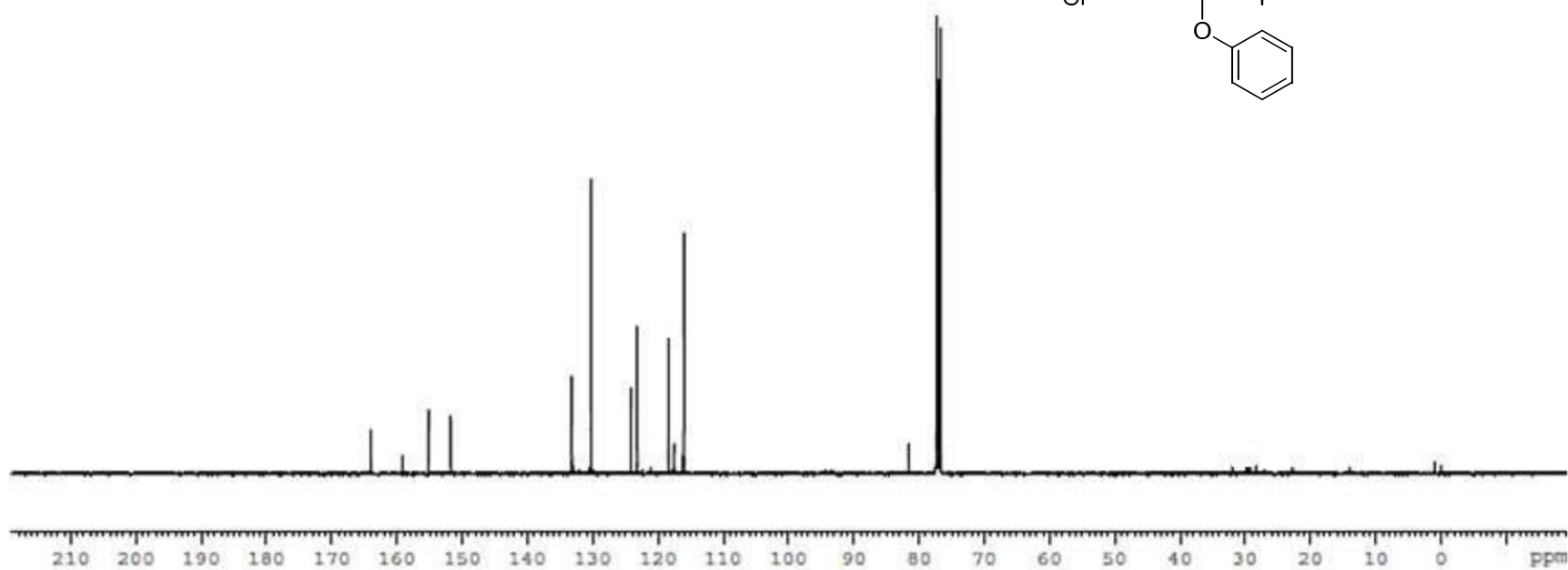
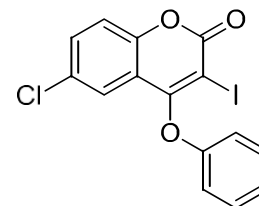
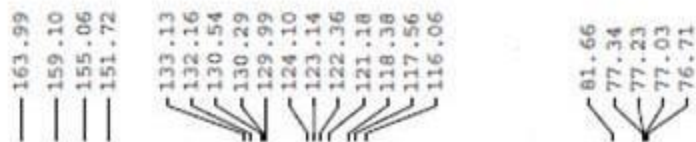
NP-IM-977

1H



¹³C of 6-chloro-3-iodo-4-phenoxy-2H-chromen-2-one (3ad)

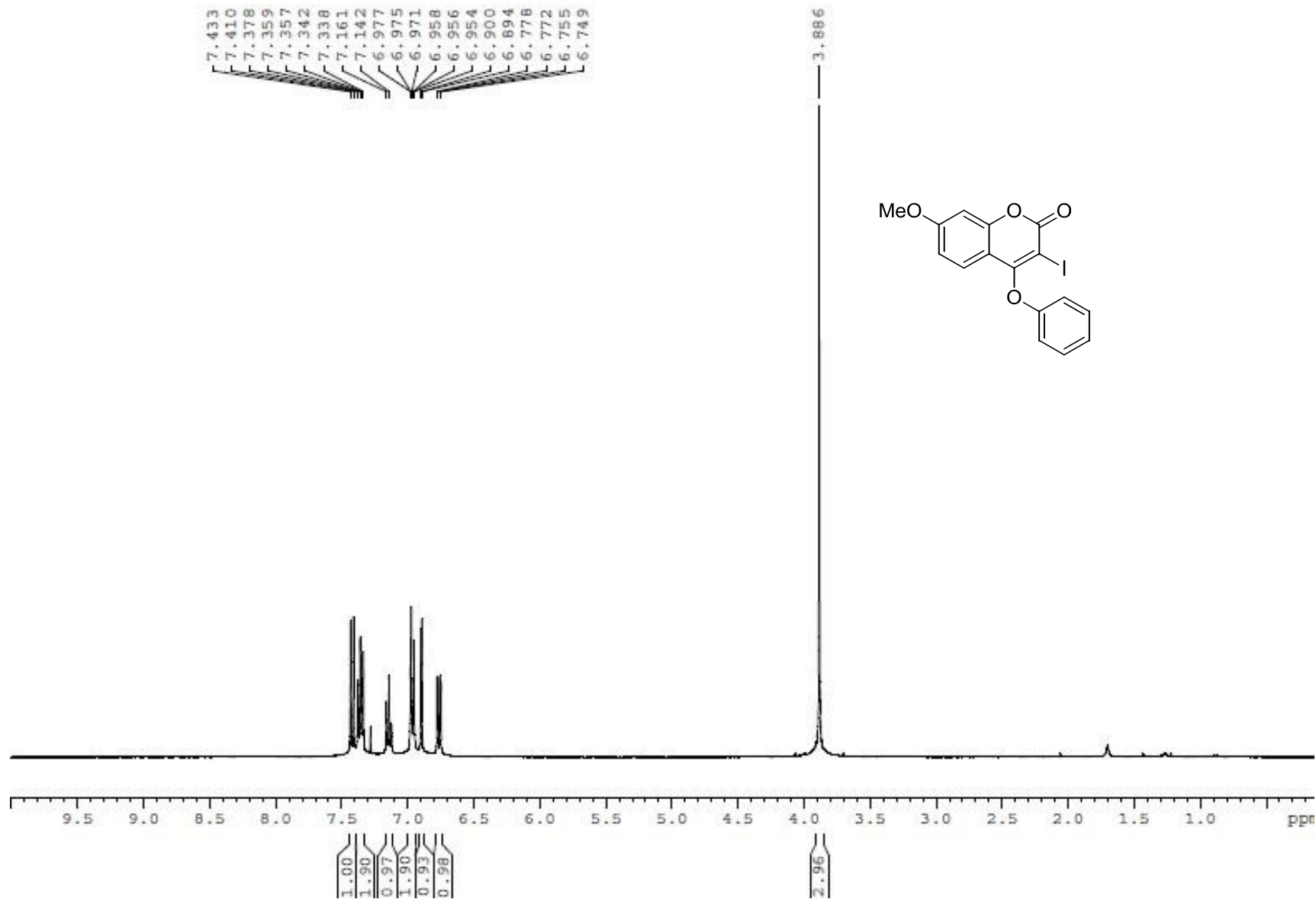
NP-IM-977 13C



¹H of 3-iodo-7-methoxy-4-phenoxy-2H-chromen-2-one (3ae)

¹H of NP-IM-1298

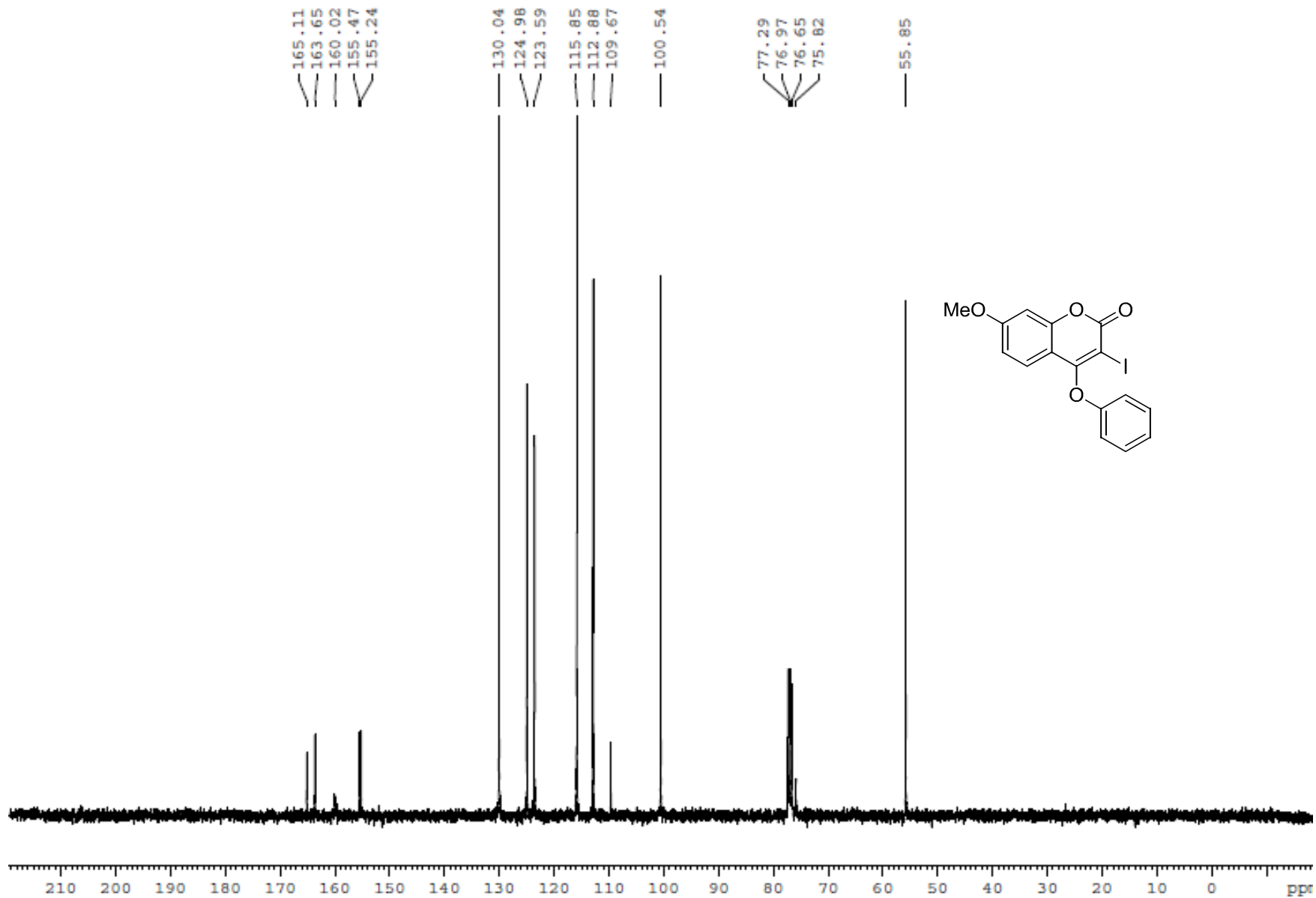
18.1.2017



¹³C of 3-iodo-7-methoxy-4-phenoxy-2H-chromen-2-one (3ae)

¹³C of NP-IM-1298

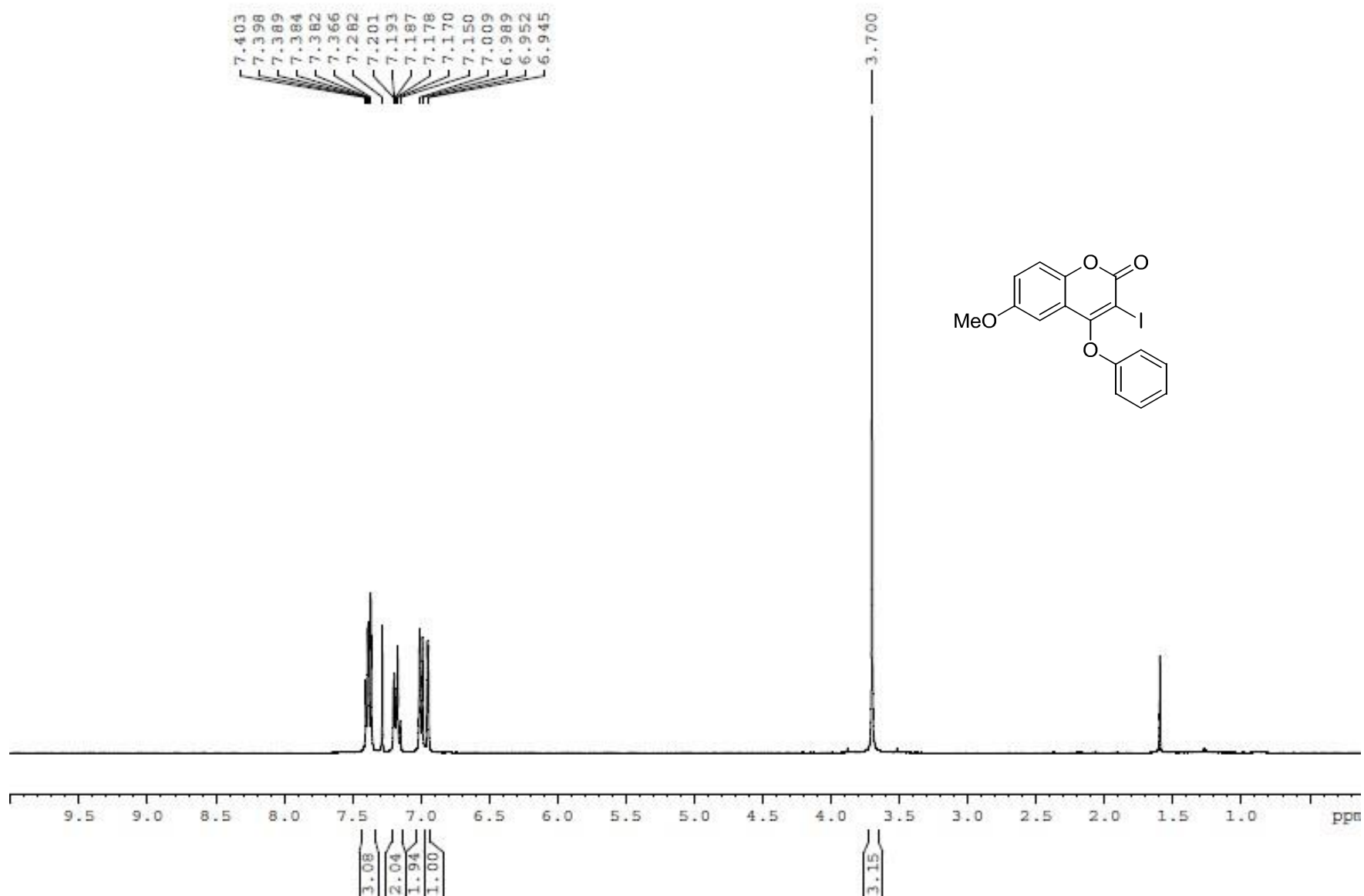
18.1.2017



¹H of 3-iodo-6-methoxy-4-phenoxy-2H-chromen-2-one (3af)

¹H of NP-Im-1254

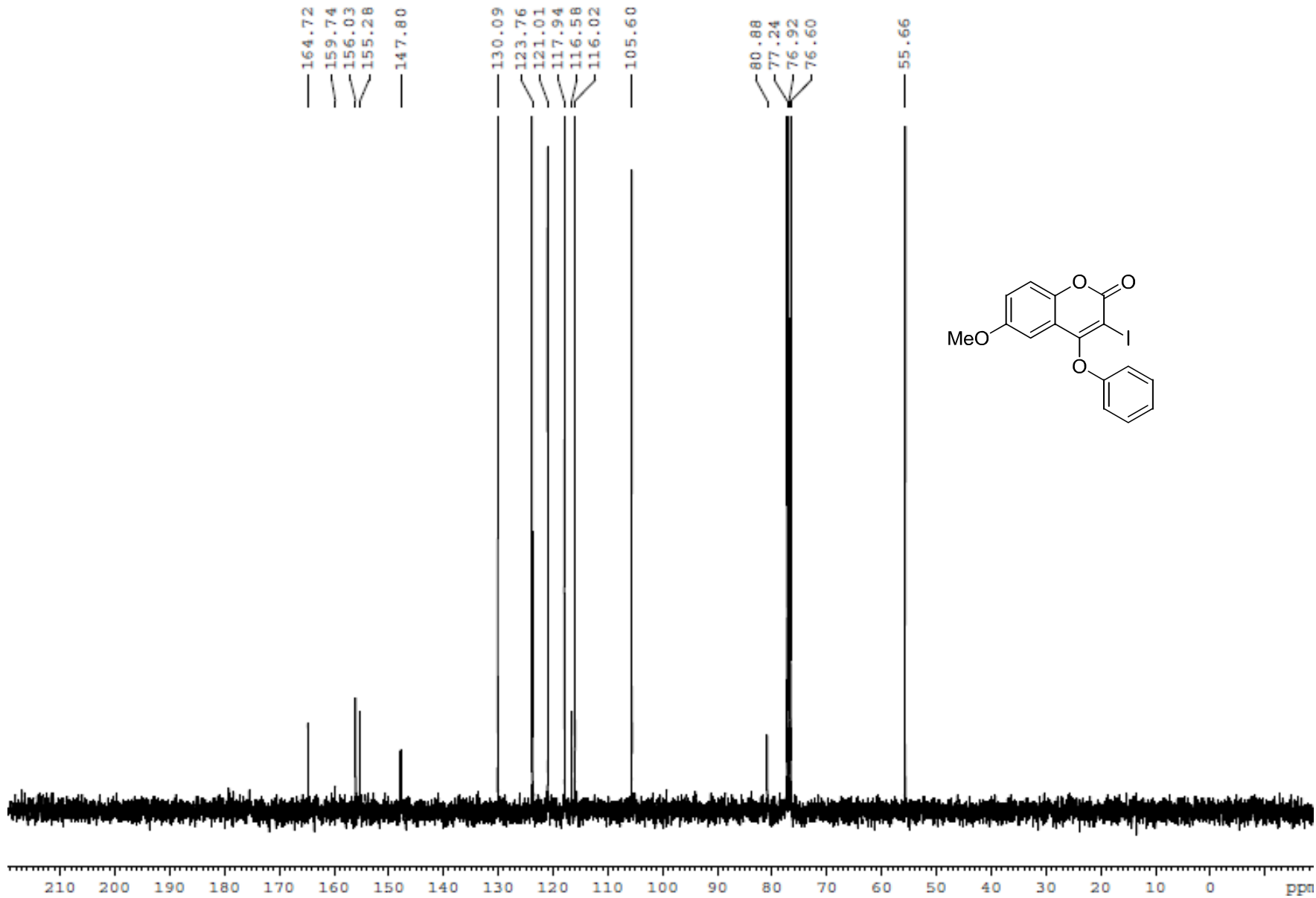
24.1.2017



13C of 3-iodo-6-methoxy-4-phenoxy-2H-chromen-2-one (3af)

13C of NP-IM-1254

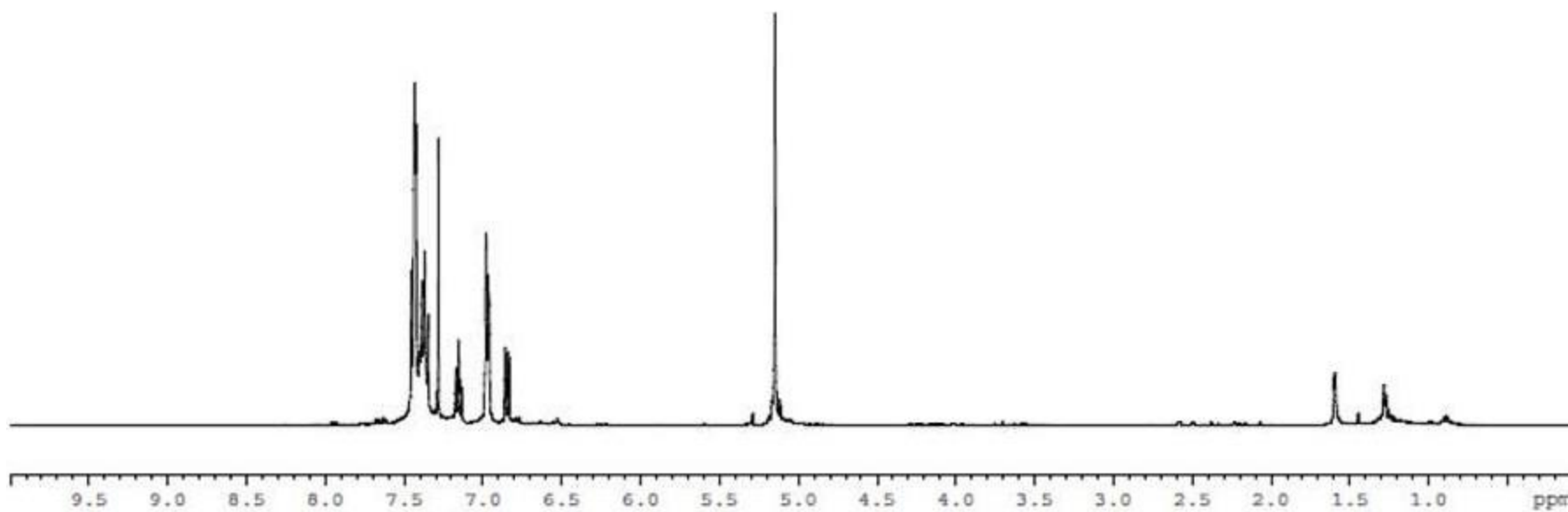
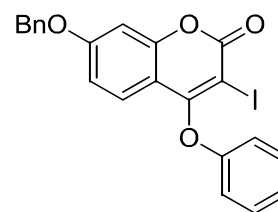
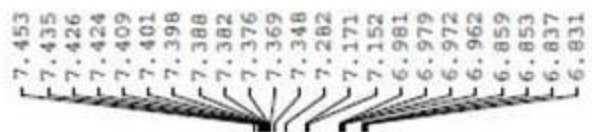
31.1.2017



¹H of 7-(benzyloxy)-3-iodo-4-phenoxy-2H-chromen-2-one (3ag)

¹H of NP-Im-1261 (A)

24.1.2017



¹³C of 7-(benzyloxy)-3-iodo-4-phenoxy-2H-chromen-2-one (3ag)

¹³C of NP-IM-1261(A)

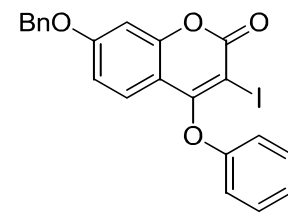
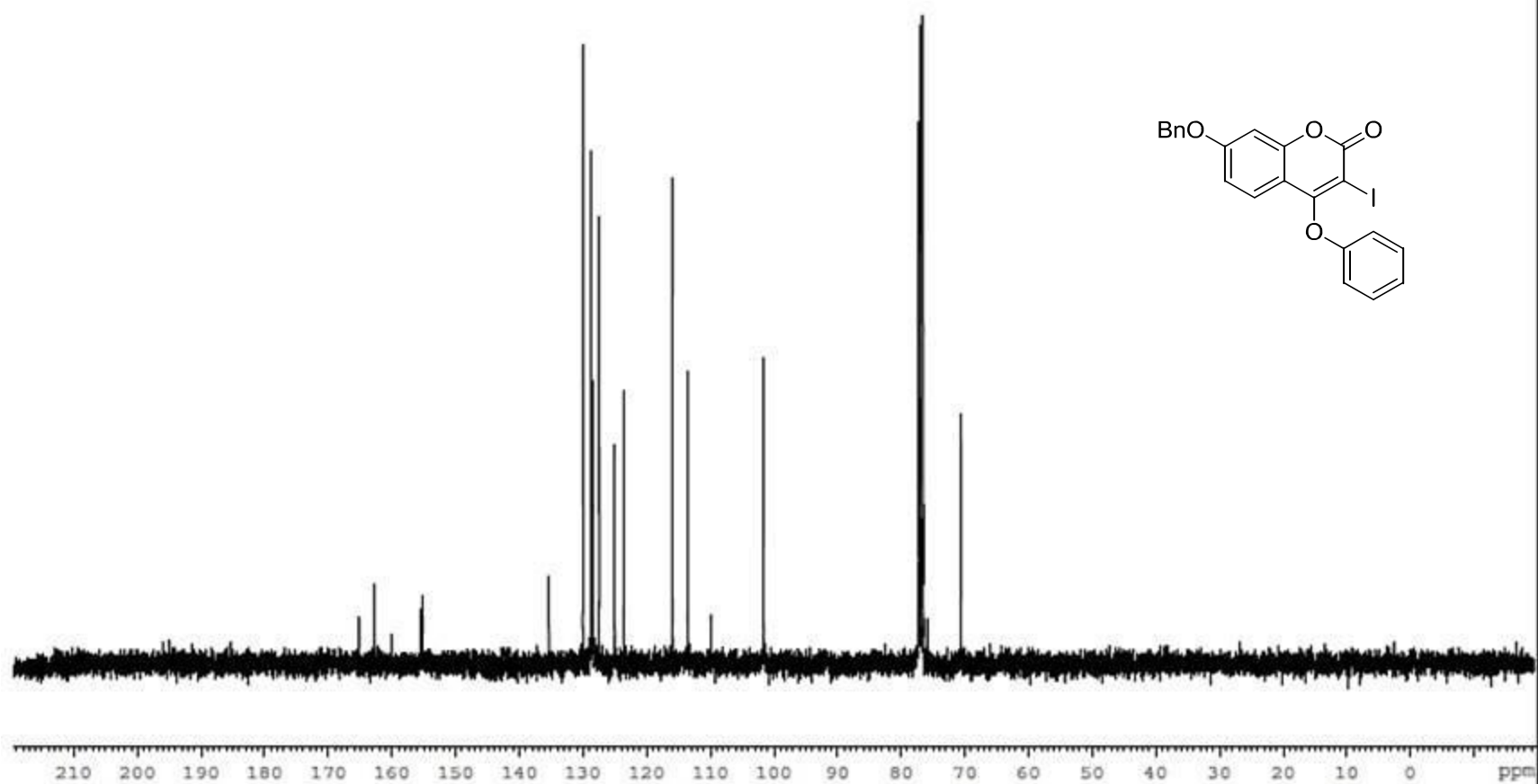
31.1.2017

165.08
162.68
159.99
155.46
155.15

135.32
130.03
128.70
128.41
127.42
124.99
123.58
115.87
113.52

101.58

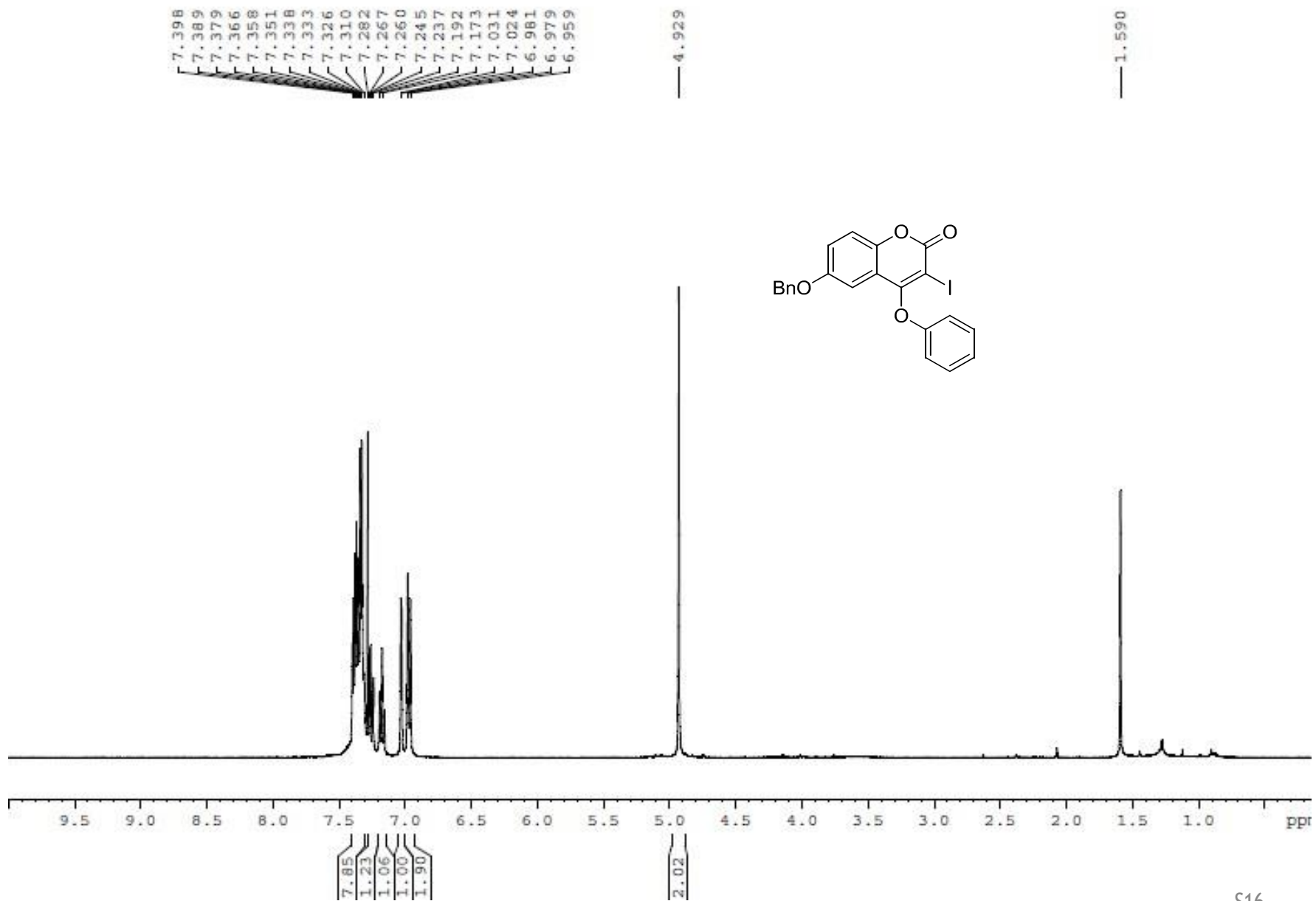
77.22
76.90
76.59
75.93
70.58



¹H of 6-(benzyloxy)-3-iodo-4-phenoxy-2H-chromen-2-one (3ah)

¹H of NP-Im-1262

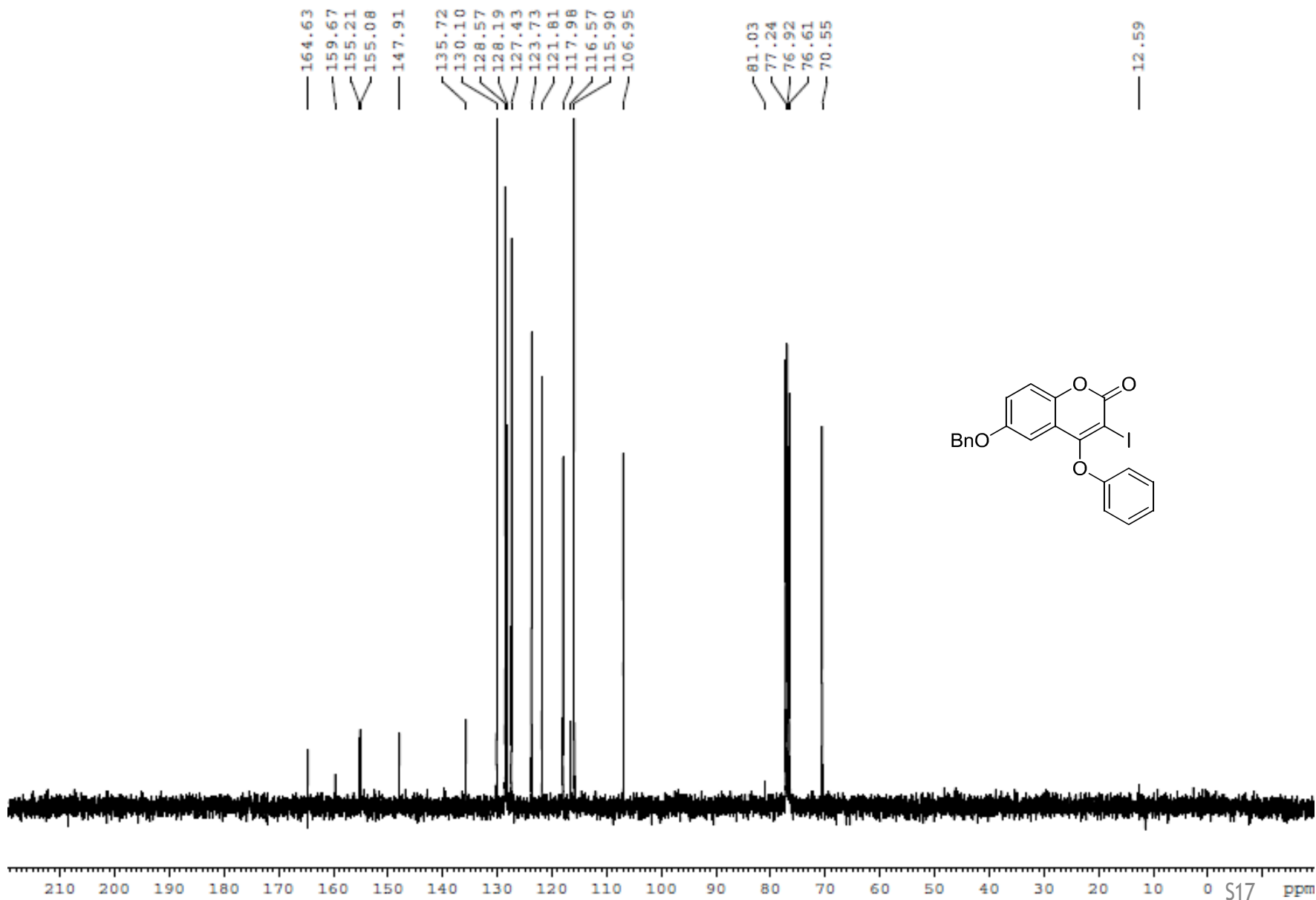
24.1.2017



¹³C of 6-(benzyloxy)-3-iodo-4-phenoxy-2H-chromen-2-one (3ah)

¹³C of NP-IM-1262

31.1.2017



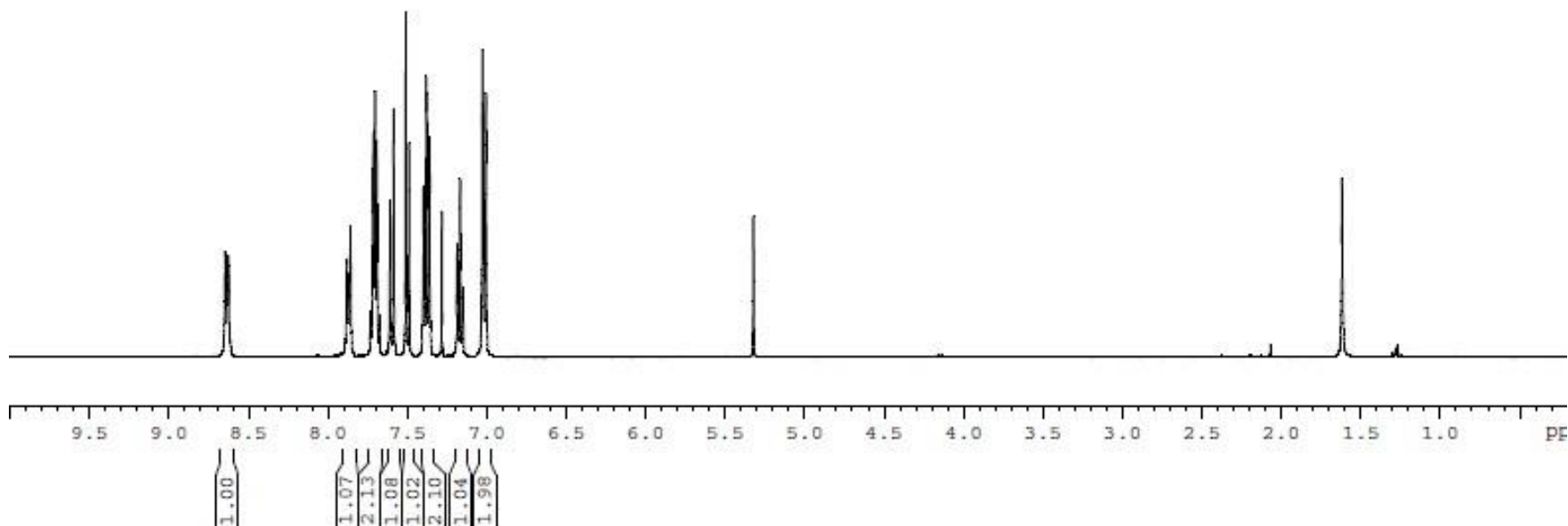
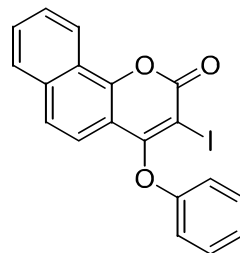
¹H of 3-iodo-4-phenoxy-2H-benzo[h]chromen-2-one (3ai)

¹H of NP-IM-1156

02.12.2016

8.647
8.633
8.623
7.880
7.874
7.871
7.860
7.857
7.728
7.716
7.712
7.703
7.693
7.689
7.676
7.608
7.586
7.510
7.488
7.399
7.394
7.380
7.378
7.363
7.359
7.353
7.282
7.186
7.167
7.149
7.027
7.025
7.005
6.997
5.321

1.617

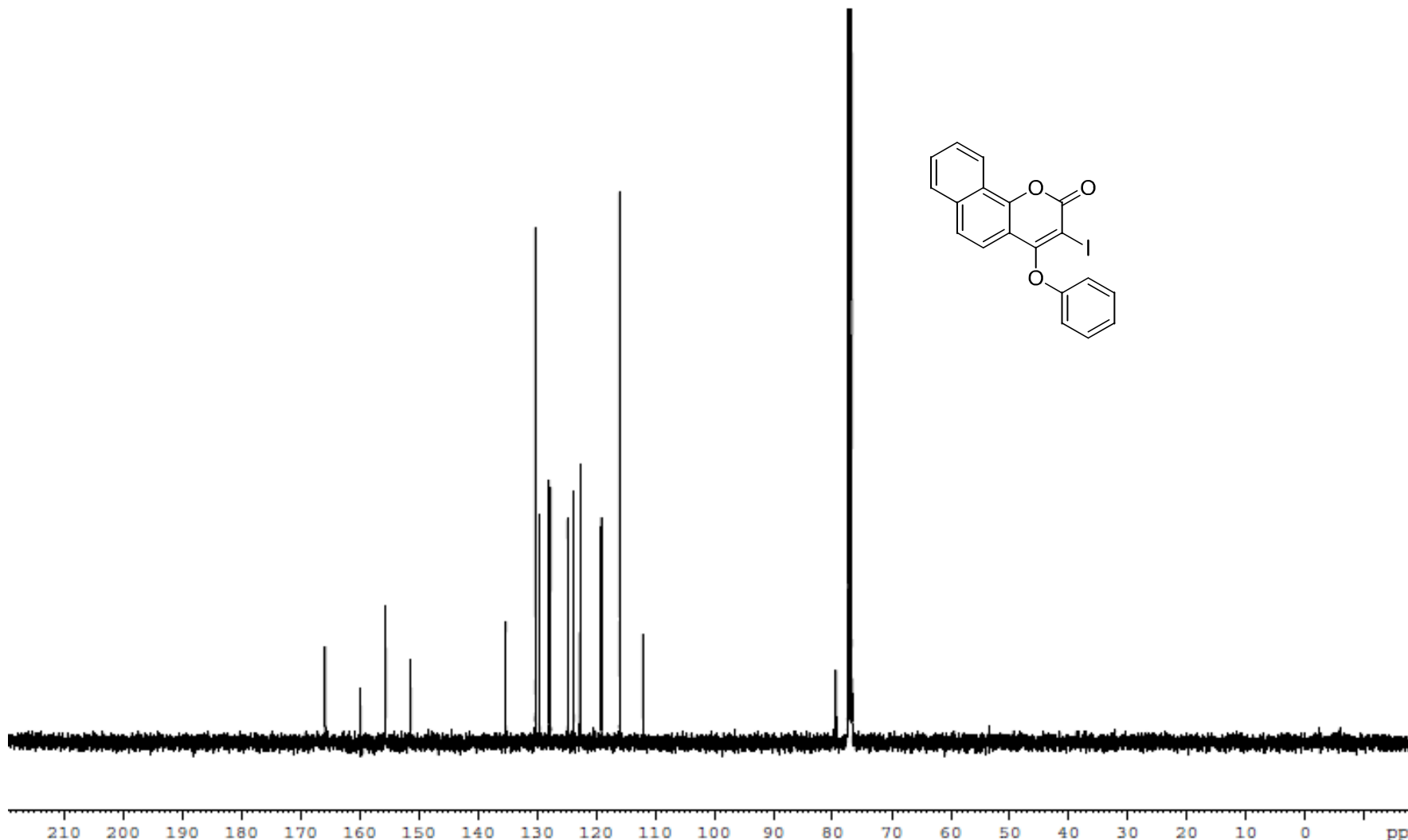


¹³C of 3-iodo-4-phenoxy-2H-benzo[h]chromen-2-one (3ai)

¹³C of NP-IM-1156

05.12.2016

165.79
159.84
155.60
151.36
135.28
130.23
129.53
127.95
127.65
124.75
123.78
122.70
122.60
119.08
115.98
112.01
79.42
77.37
77.05
76.73

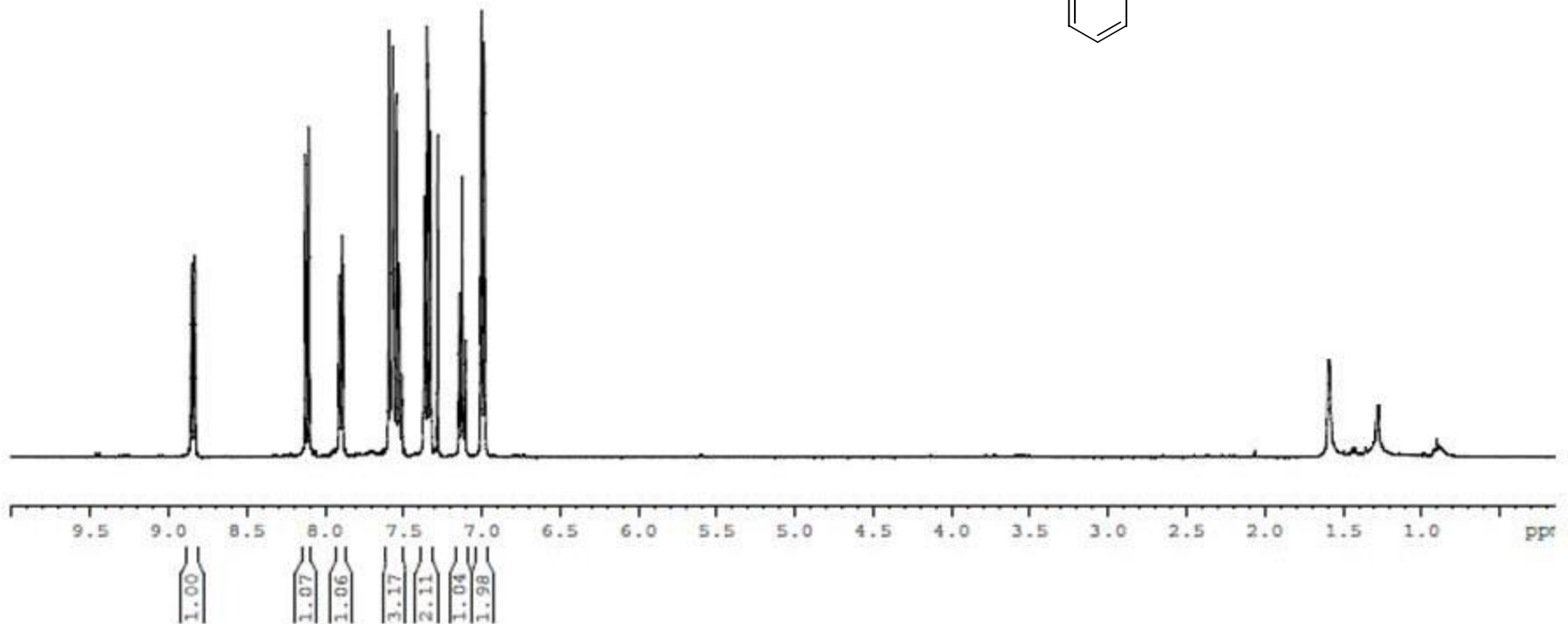
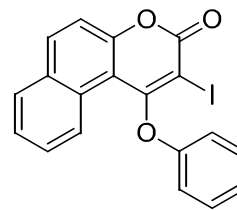


¹H of 2-iodo-1-phenoxy-3H-benzo[*f*]chromen-3-one (3aj)

¹H of NP-IM-1013

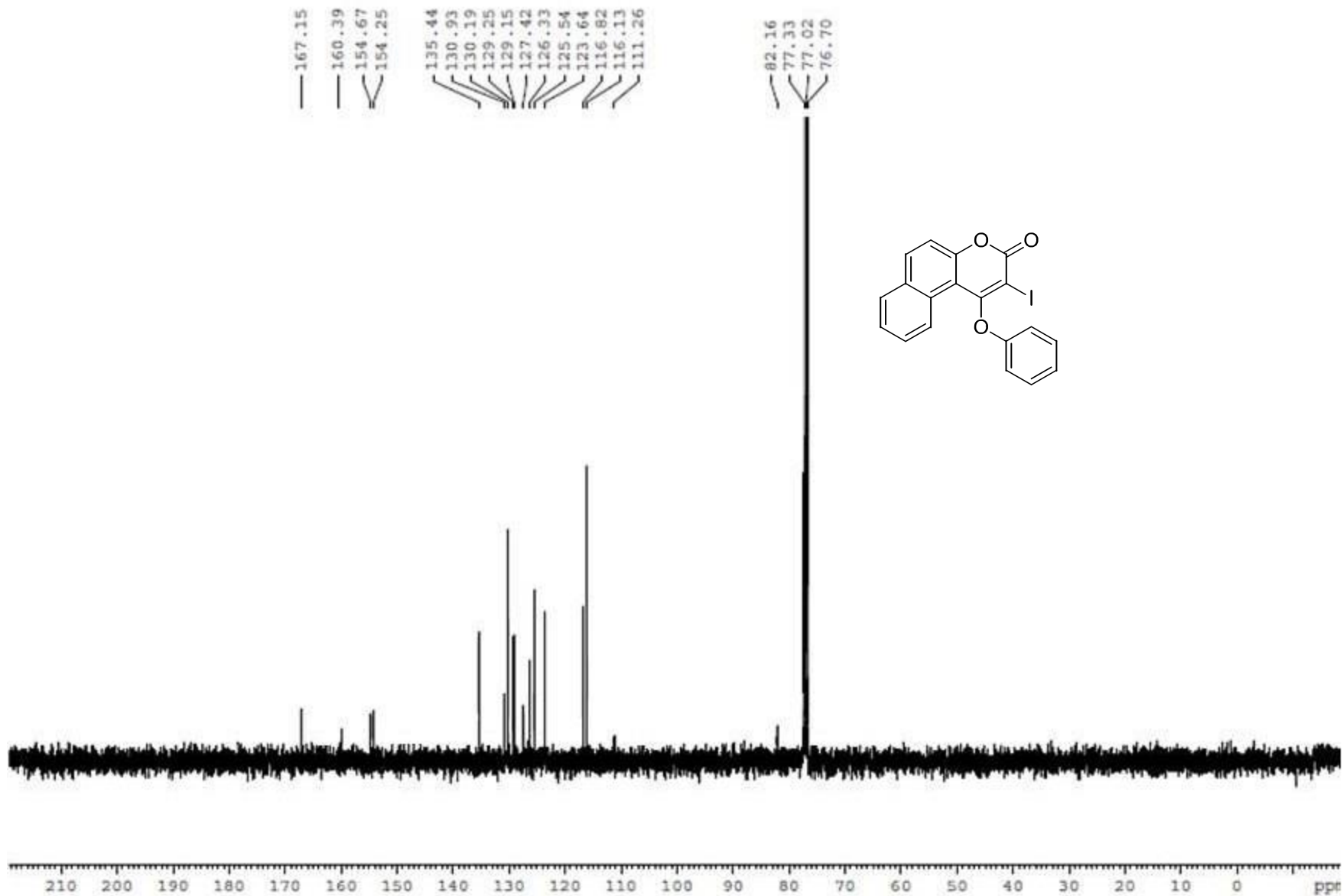
15.6.2016

8.852
8.831
8.126
8.104
7.911
7.892
7.887
7.594
7.585
7.580
7.571
7.567
7.563
7.548
7.543
7.528
7.525
7.511
7.508
7.367
7.363
7.349
7.347
7.327
7.321
7.282
7.143
7.124
7.106
7.003
6.984



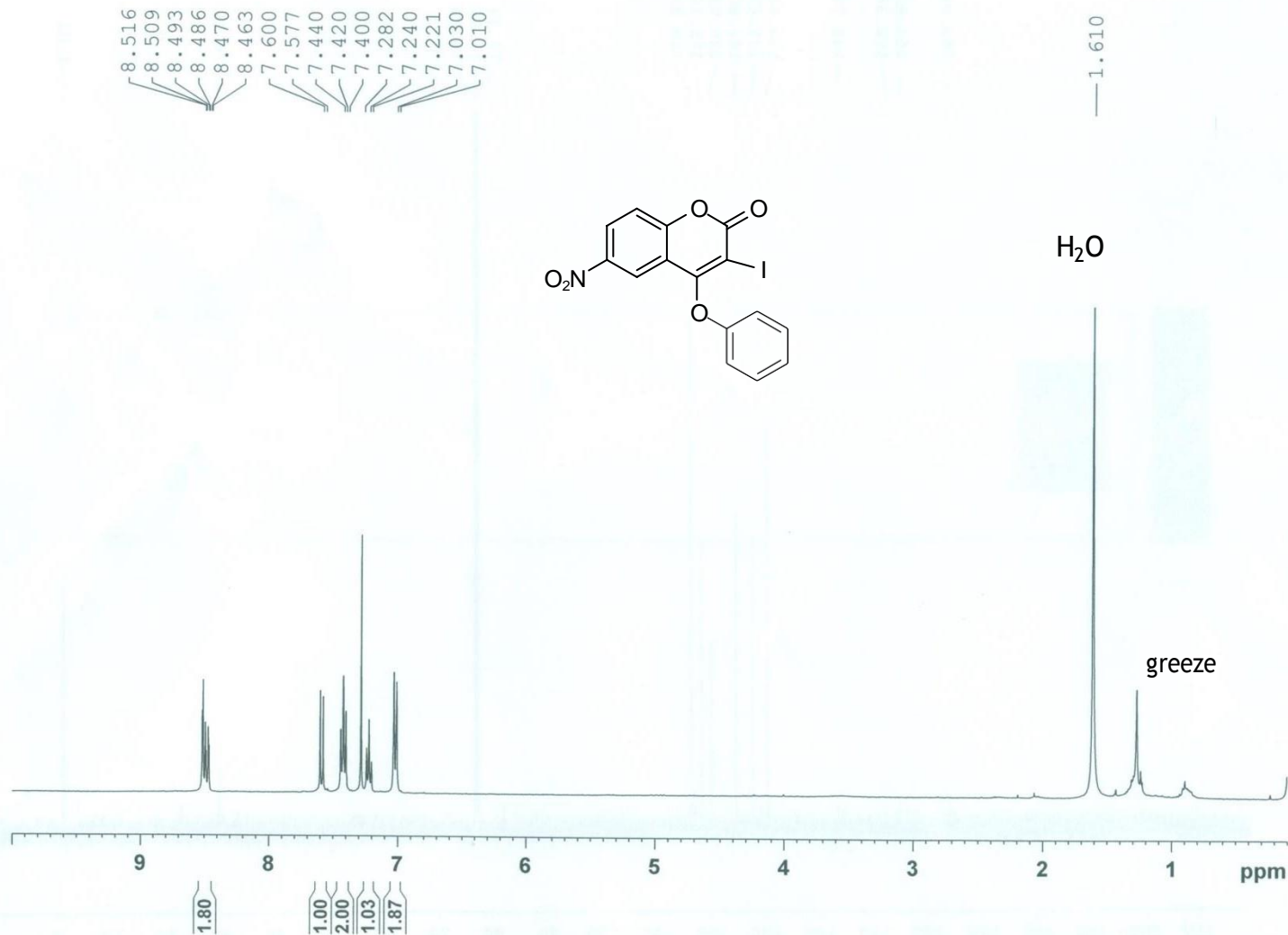
¹³C of 2-iodo-1-phenoxy-3H-benzo[*f*]chromen-3-one (3aj)

¹³C of NP-IM-1013



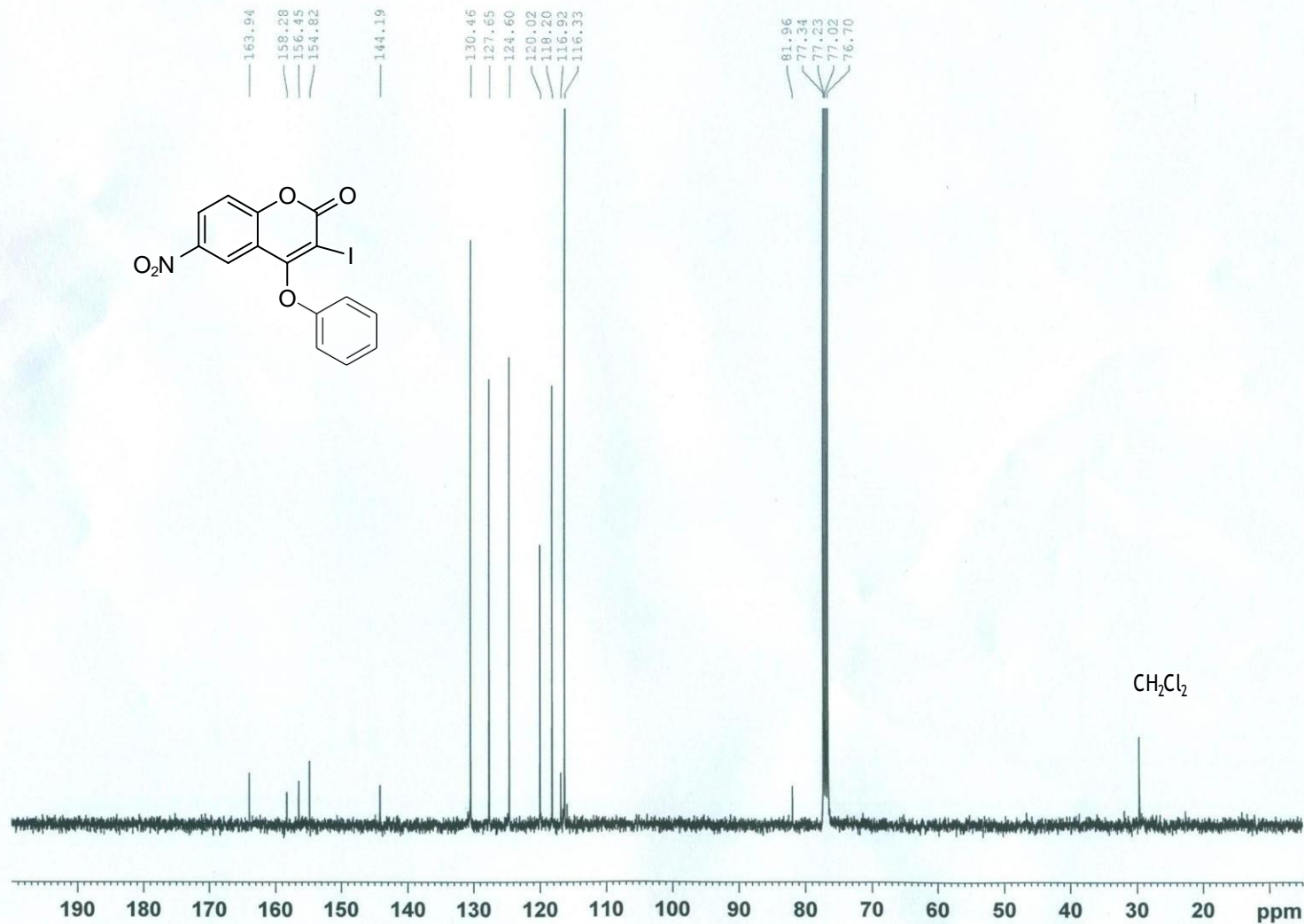
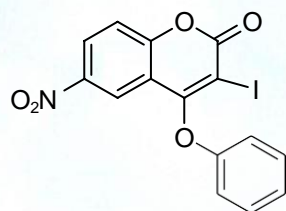
¹H of 3-iodo-6-nitro-4-phenoxy-2H-chromen-2-one (3ak)

¹H of NP-IM-3AL 25.8.2017



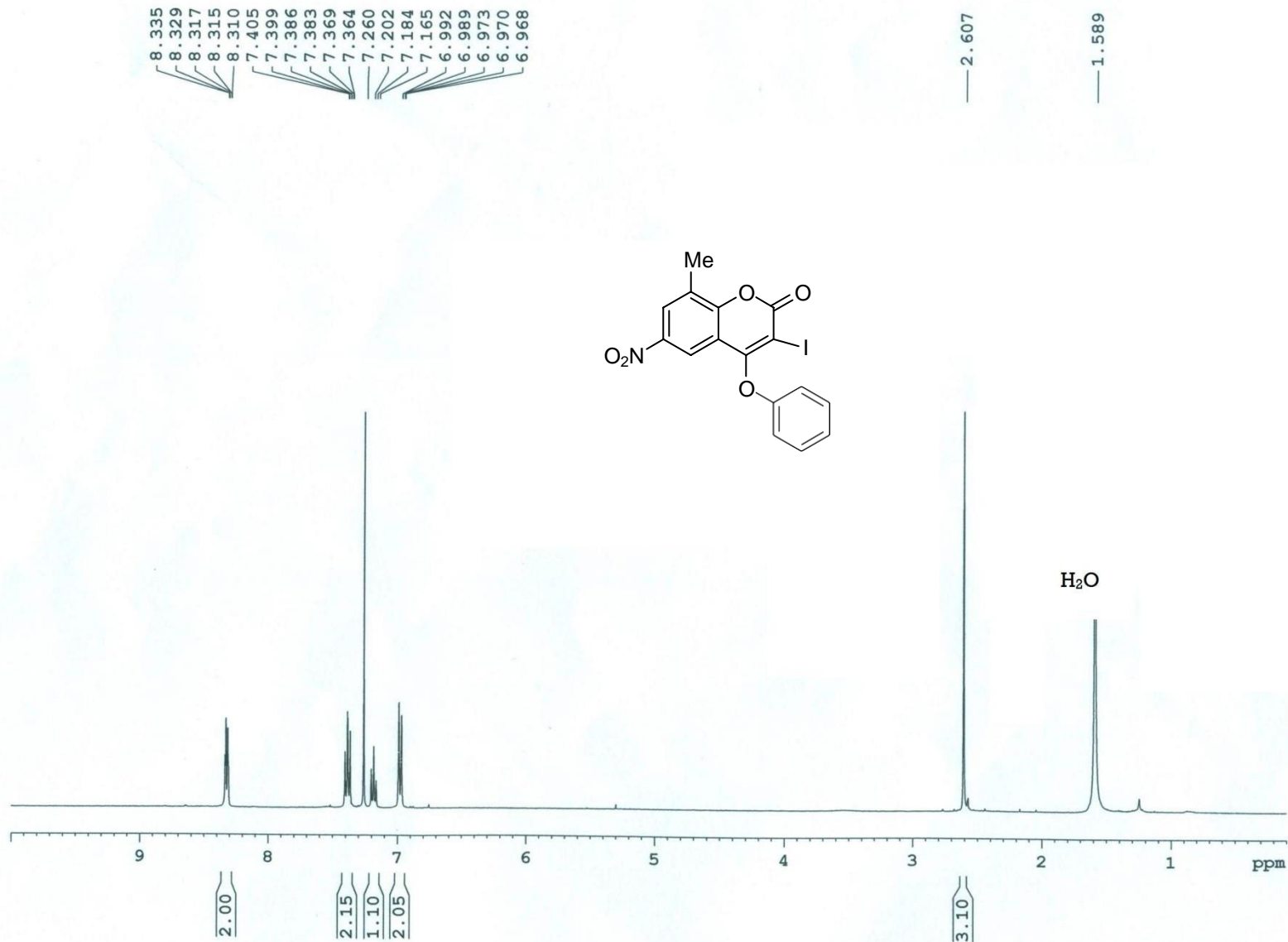
¹H of 3-iodo-6-nitro-4-phenoxy-2H-chromen-2-one (3ak)

13C of NP-IM-3AL 25.8.2017



¹H of 3-iodo-8-methyl-6-nitro-4-phenoxy-2H-chromen-2-one (3al)

¹H of NP-IM-3AM



¹³C of 3-iodo-8-methyl-6-nitro-4-phenoxy-2H-chromen-2-one (3al)

¹³C of NP-IM-O-C-N 04.01.2017

— 164.36
— 158.38
— 154.96

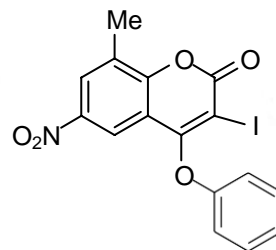
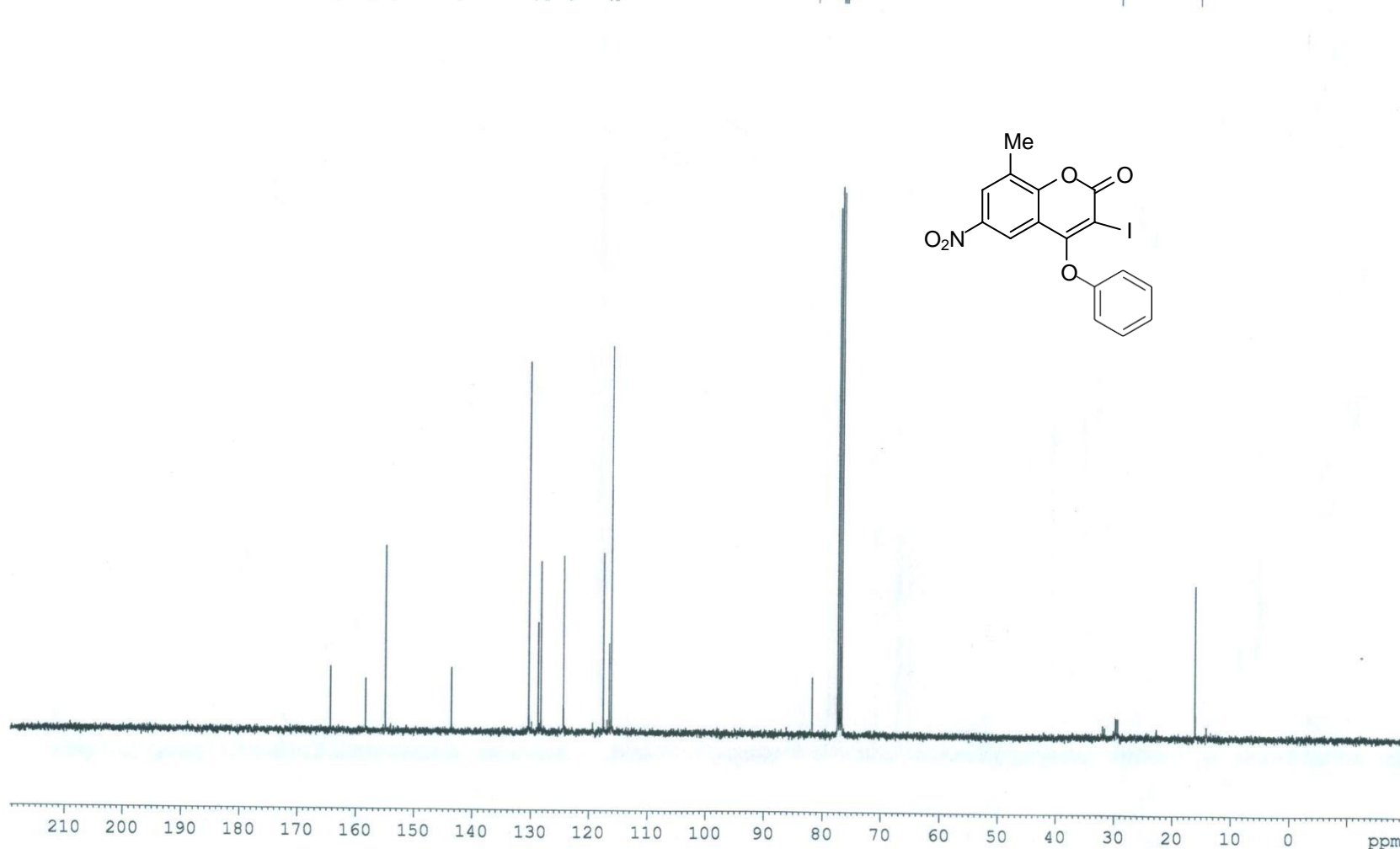
— 143.59

130.42
128.81
128.35
124.44
117.58
116.61
116.25

81.79
77.40
77.08
76.76

— 29.72

— 16.08

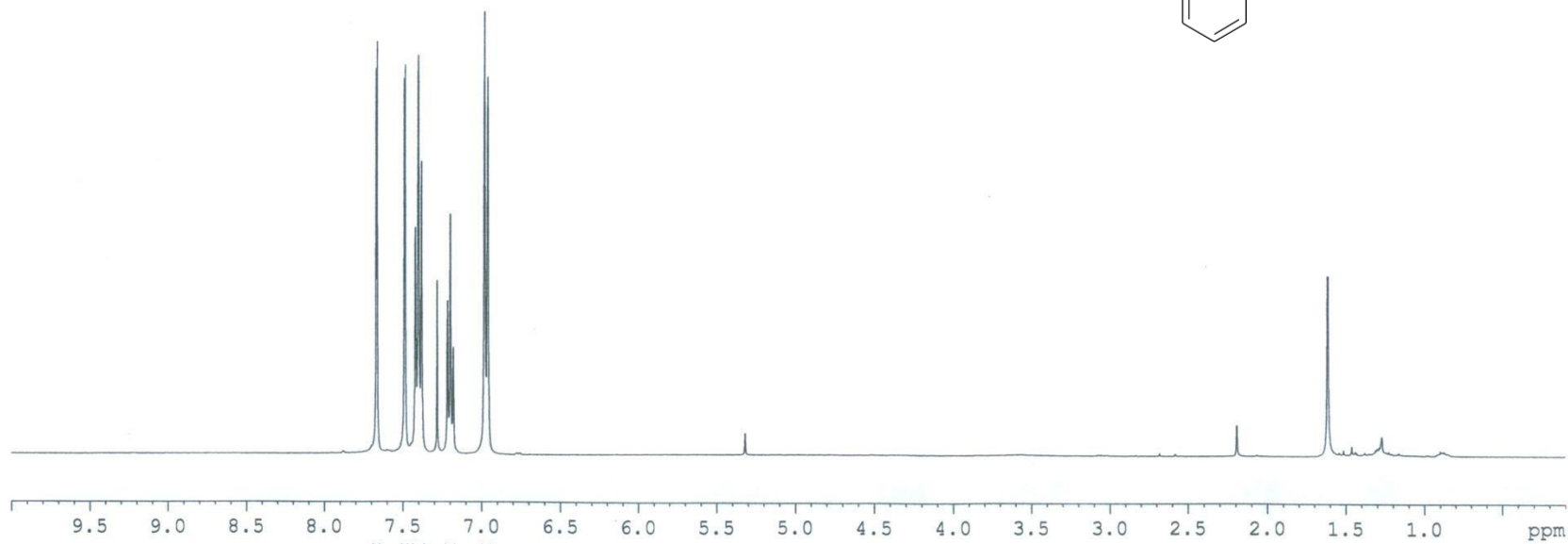
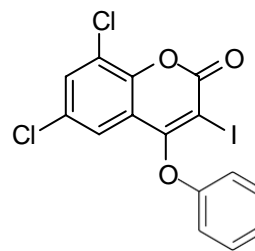


¹H NMR 6,8-dichloro-3-iodo-4-phenoxy-2H-chromen-2-one (3am)

¹H of NP-IM-dichloro-O-Ar

3.2.2017

7.668
7.662
7.490
7.484
7.421
7.416
7.402
7.381
7.282
7.216
7.198
7.179
6.981
6.979
6.959



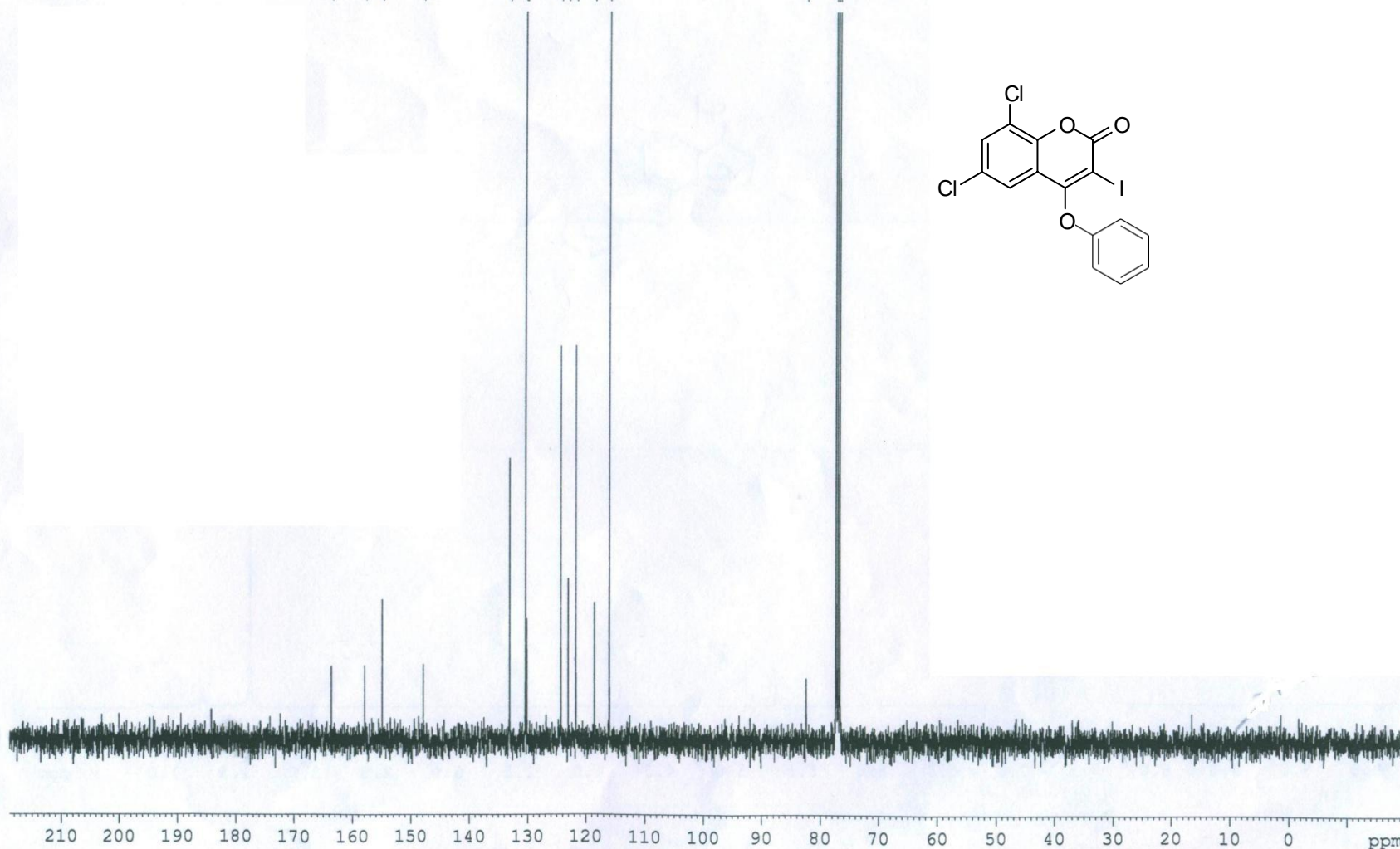
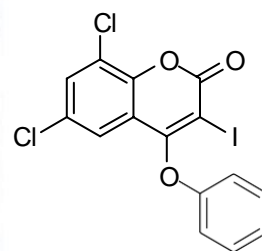
1.00
1.01
2.30
1.12
2.16

¹³C NMR of 6,8-dichloro-3-iodo-4-phenoxy-2H-chromen-2-one (3am)

NP-IM-dicholoro -o-Ar13c

3.2.2017

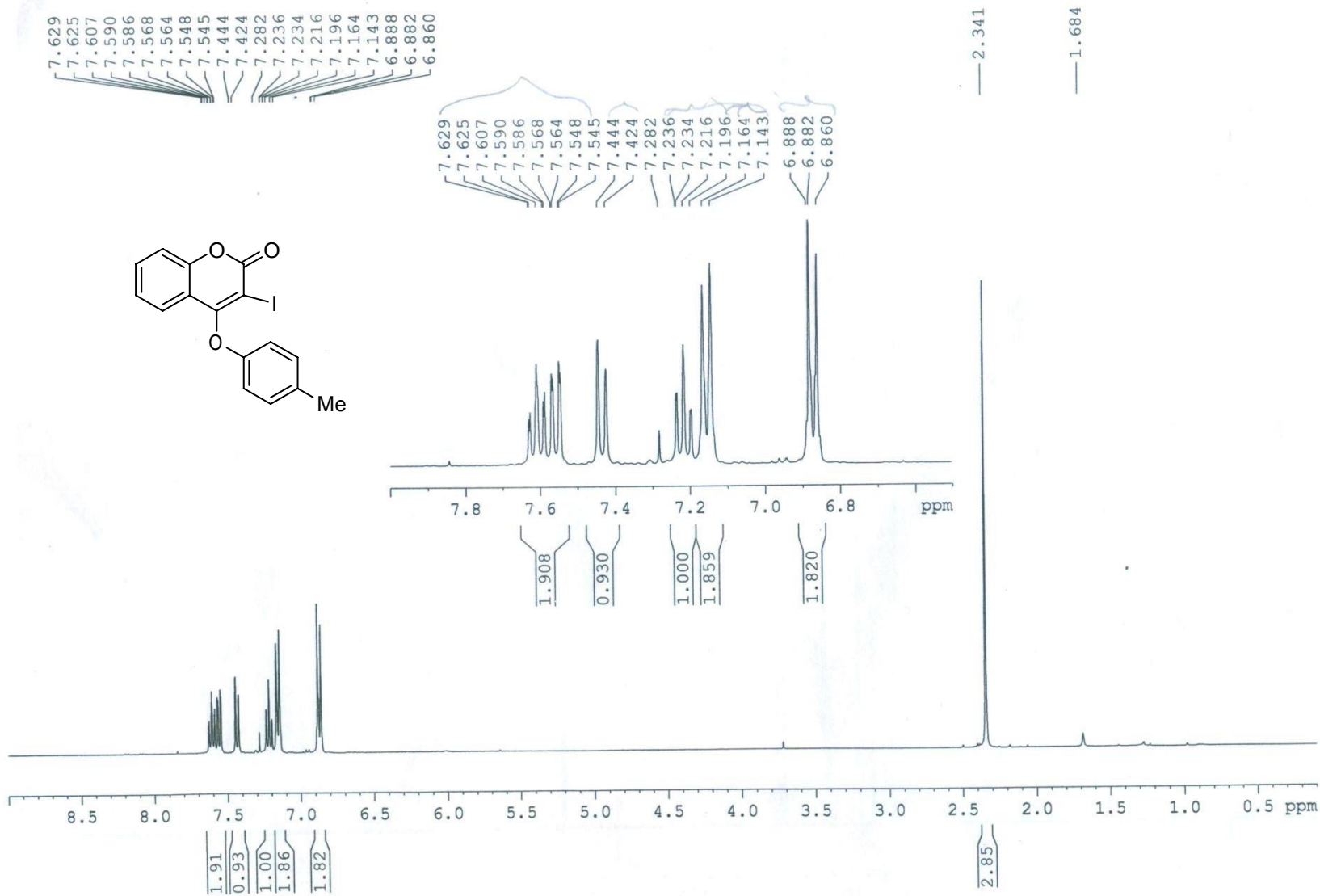
163.60
157.92
154.92
147.84
133.09
130.36
130.14
124.27
123.03
121.70
118.54
116.03
82.41
77.36
77.04
76.72



¹H of 4-(p-toloxoy)-3-iodo-2H-chromen-2-one (3ba)

¹H of NP-IM-1296

27.2.2017



¹³C of 4-(p-tolyloxy)-3-iodo-2H-chromen-2-one (3ba)

¹³C of NP-IM-1296

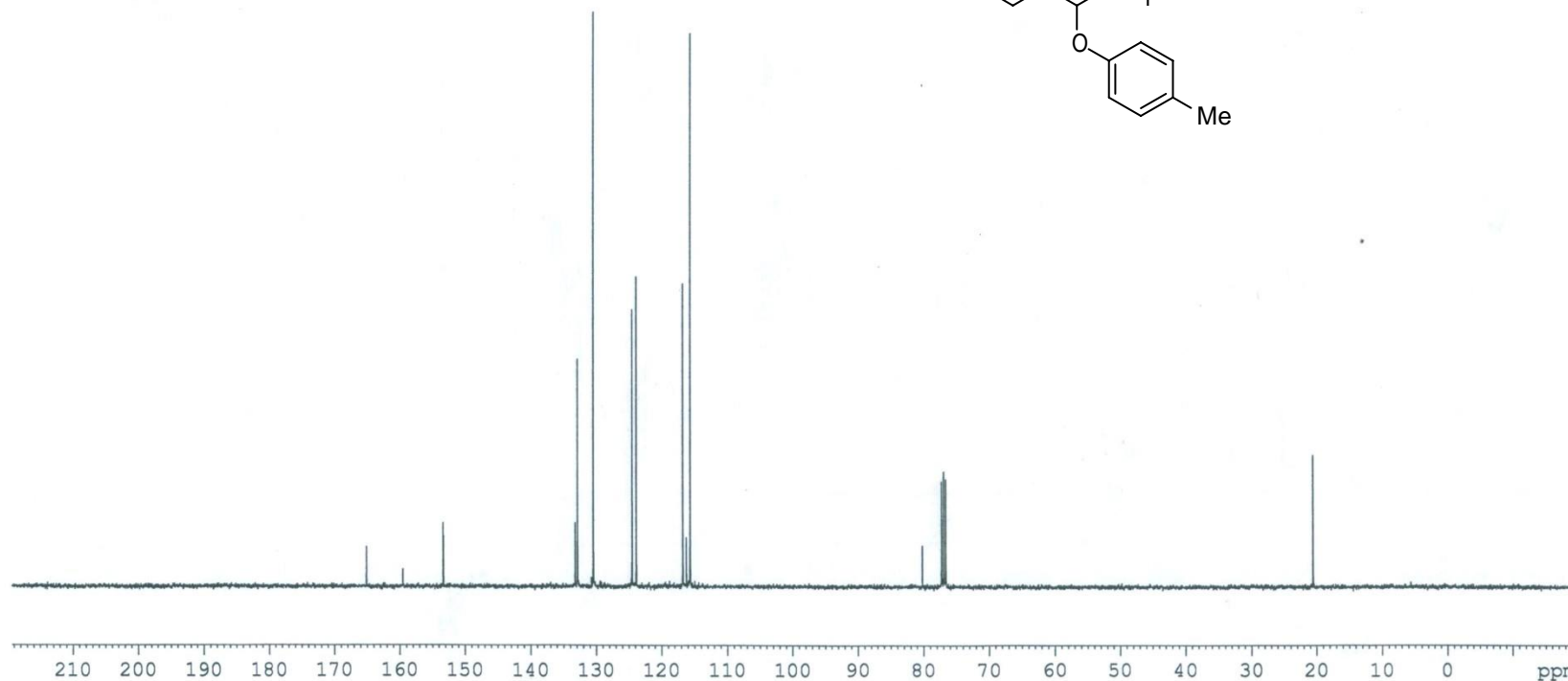
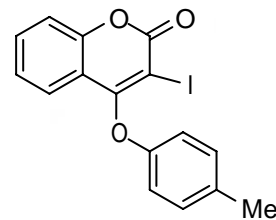
27.2.2017

— 165.11
— 159.54
— 153.37
— 153.30

— 133.26
— 132.90
— 130.48
— 124.50
— 123.86
— 116.77
— 116.25
— 115.66

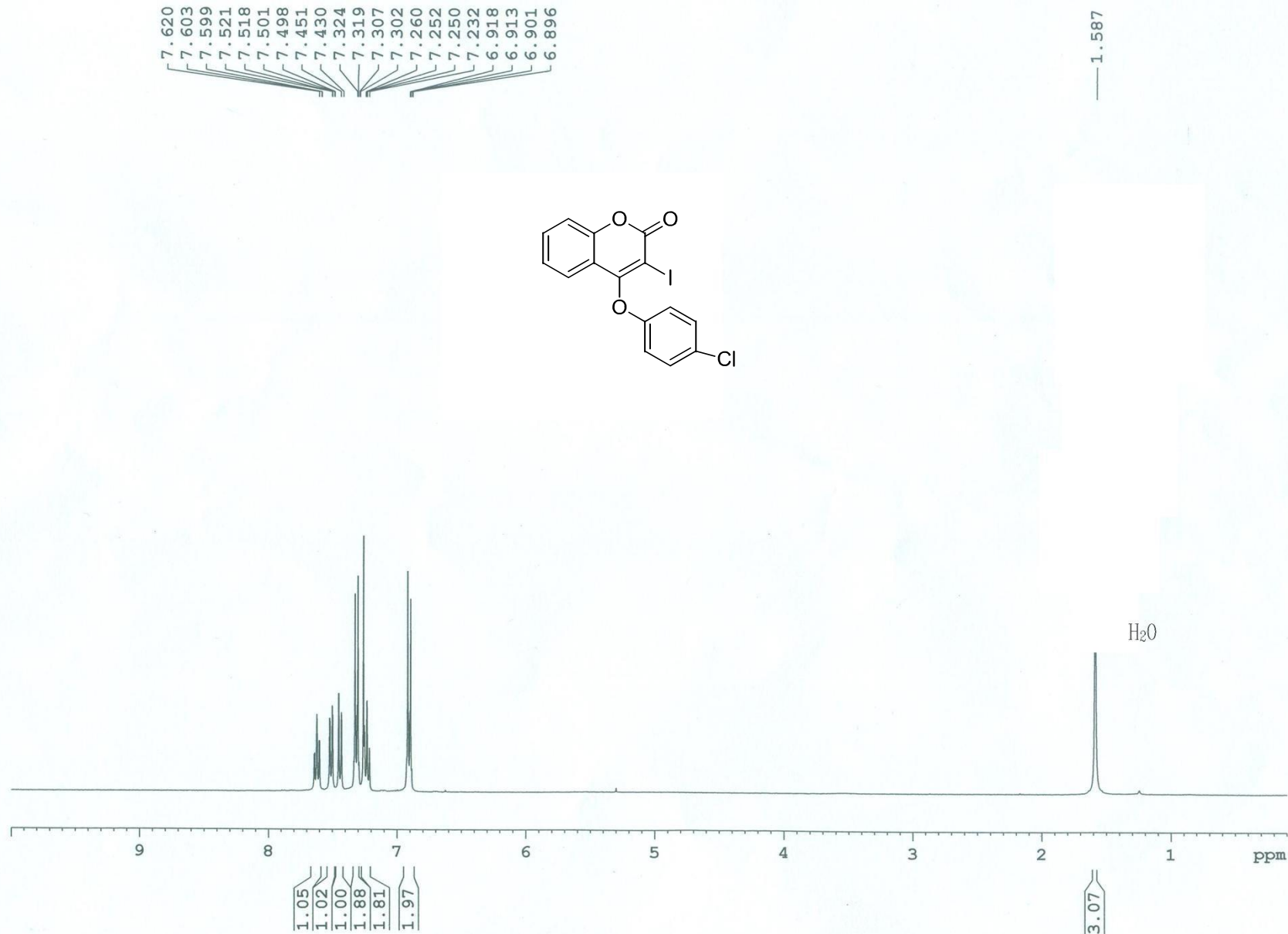
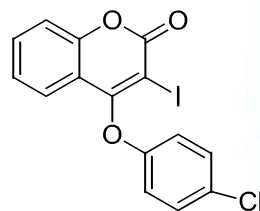
— 80.19
— 77.27
— 76.95
— 76.63

— 20.54



¹H of 4-(4-chlorophenoxy)-3-iodo-2H-chromen-2-one (3ca)

¹H of NP-IM-3CA



¹³C of 4-(4-chlorophenoxy)-3-iodo-2H-chromen-2-one (3ca)

¹³C of NP-IM-1316

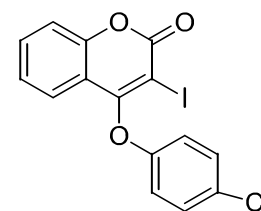
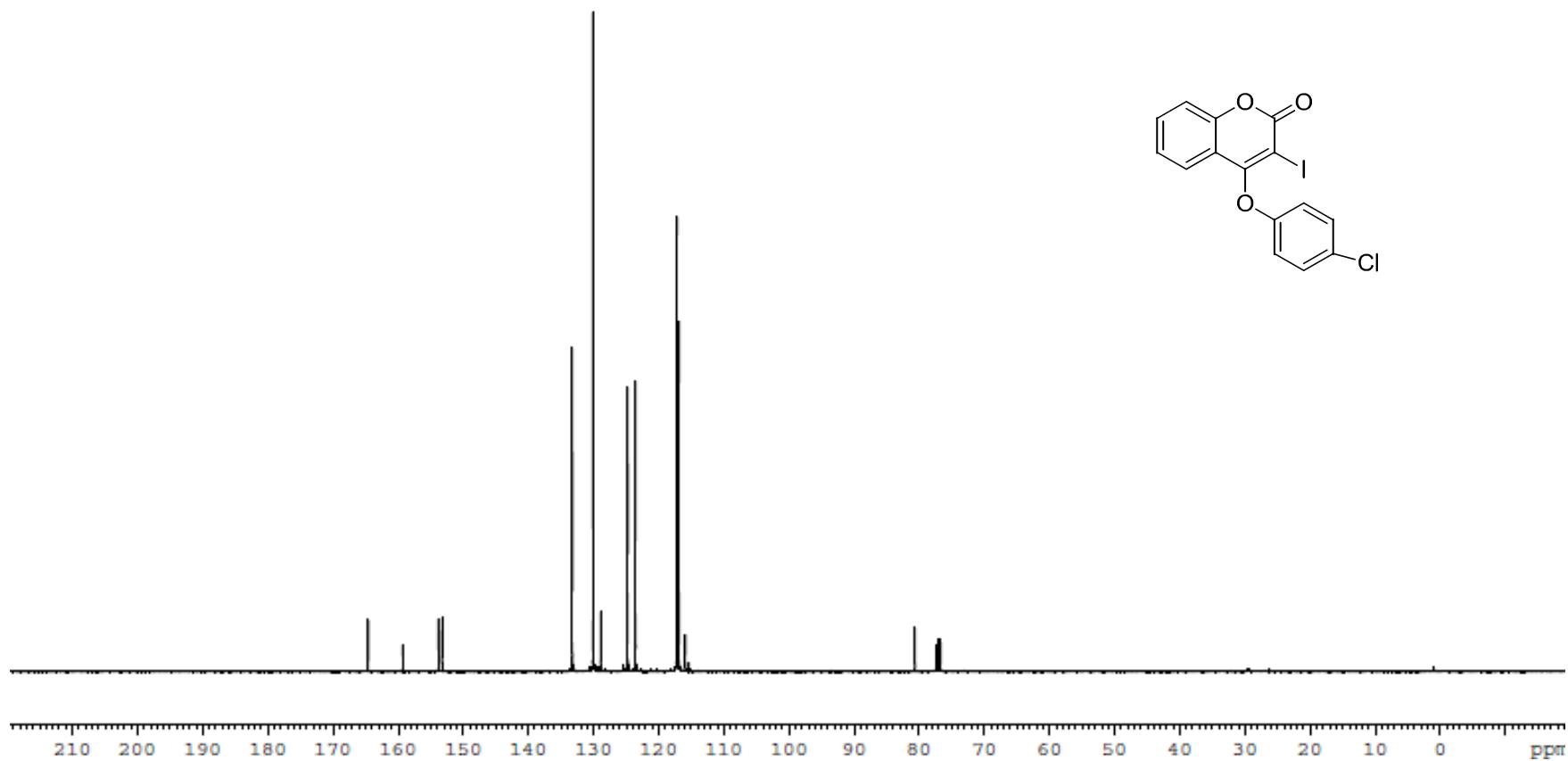
22.3.2017

164.57
159.27
153.80
153.24
133.25
130.07
128.85
124.73
123.56
117.21
116.89
115.89
115.32

80.65
77.38
77.06
76.75

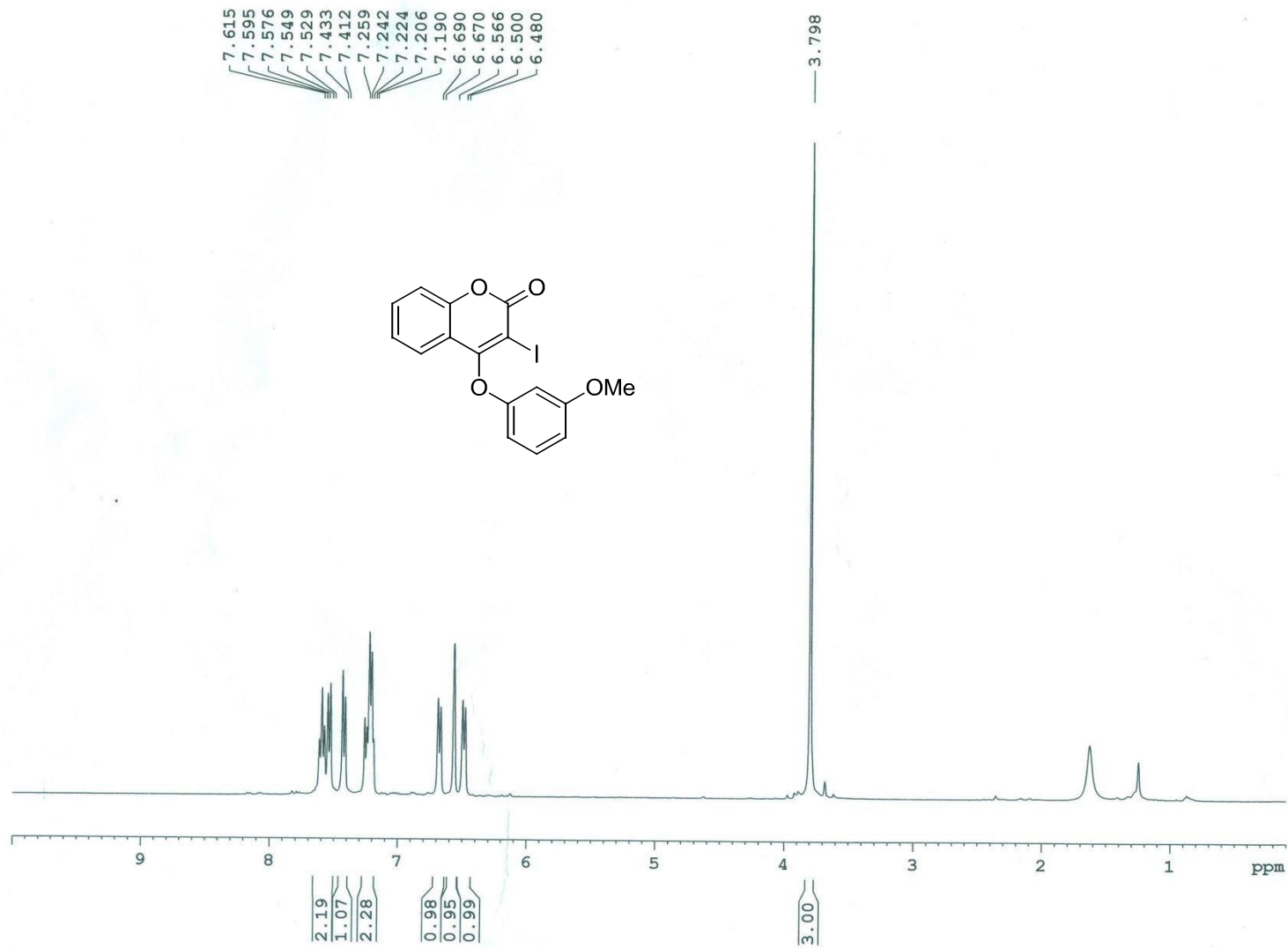
29.59

0.95



¹H of 3-iodo-4-(3-methoxyphenoxy)-2H-chromen-2-one (3da)

¹H of NP-IM-3EA



¹³C of 3-iodo-4-(3-methoxyphenoxy)-2H-chromen-2-one (3da)

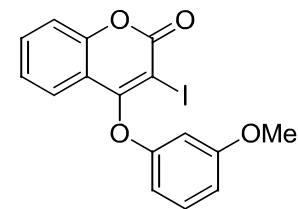
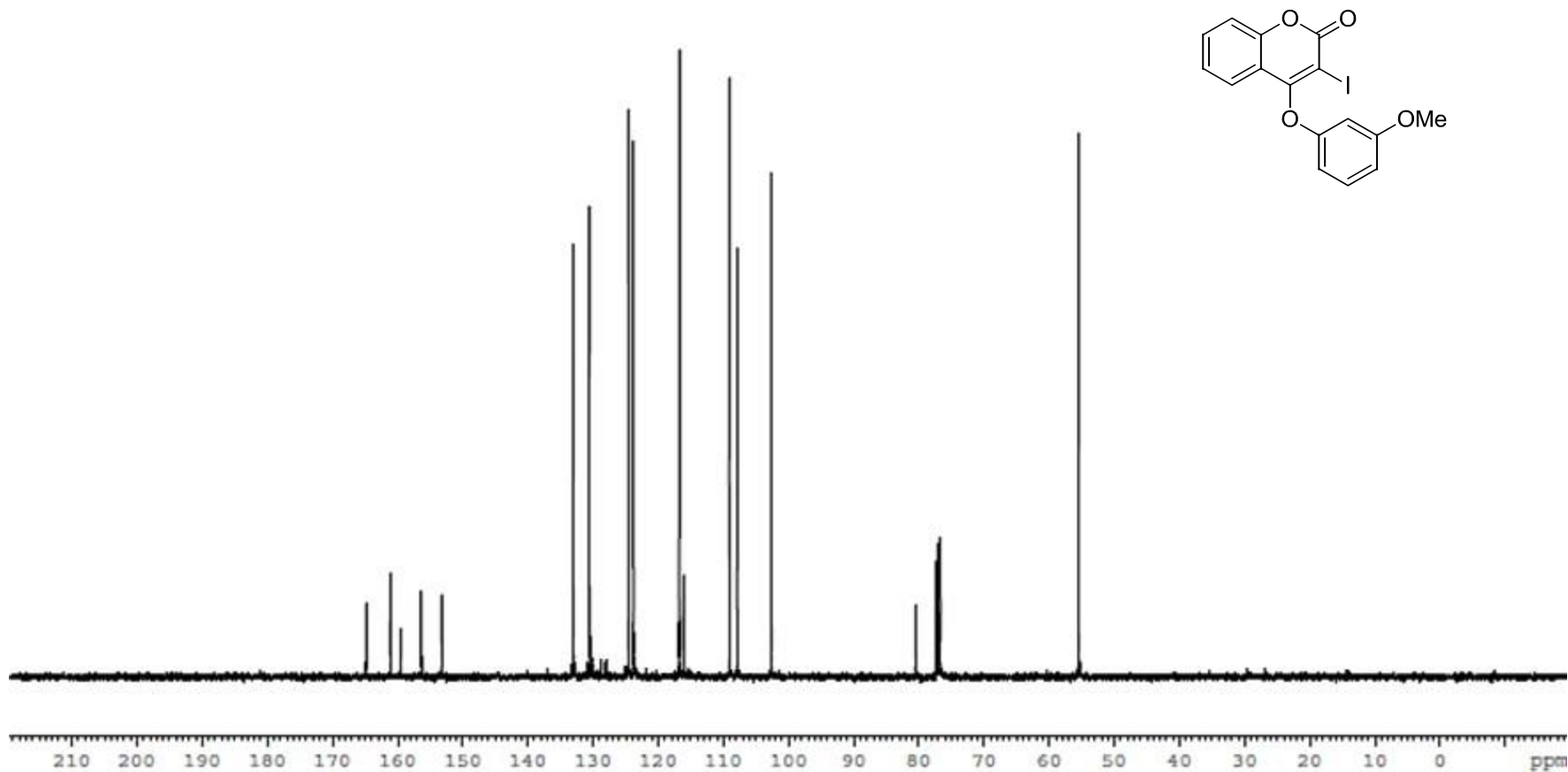
¹³C of NP-IM-1299 27.2.2017

164.82
161.14
159.44
156.32
153.26

132.99
130.48
124.58
123.77
116.77
116.12
109.07
107.87
102.61

80.52
77.31
76.99
76.67

55.43



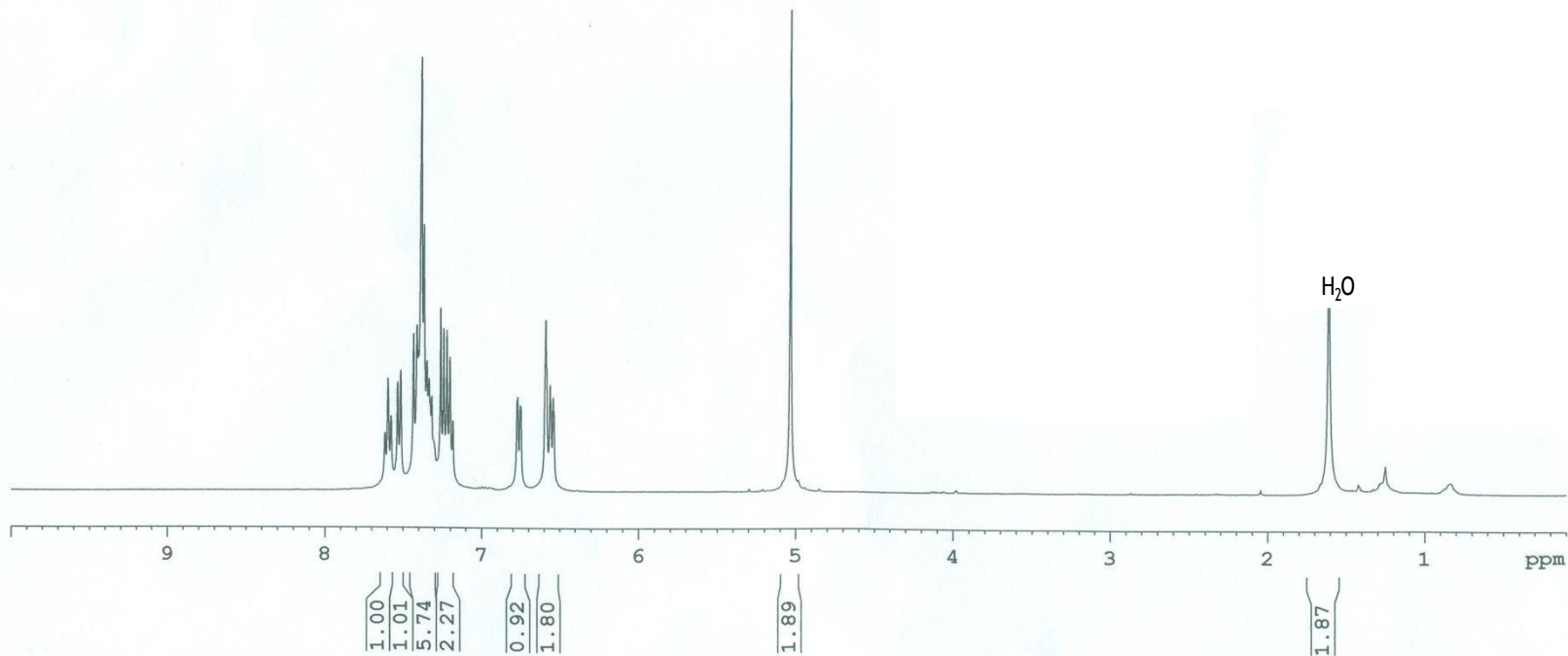
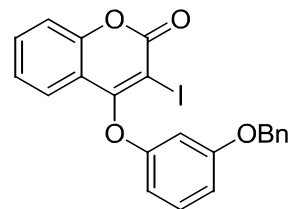
¹H of 4-(3-(benzyloxy)phenoxy)-3-iodo-2H-chromen-2-one (3ea)

¹H of NP-IM-3FA

7.614
7.596
7.577
7.535
7.515
7.433
7.411
7.402
7.383
7.367
7.348
7.333
7.327
7.317
7.260
7.241
7.221
7.202
7.183
6.773
6.769
6.753
6.749
6.590
6.563
6.543

5.035

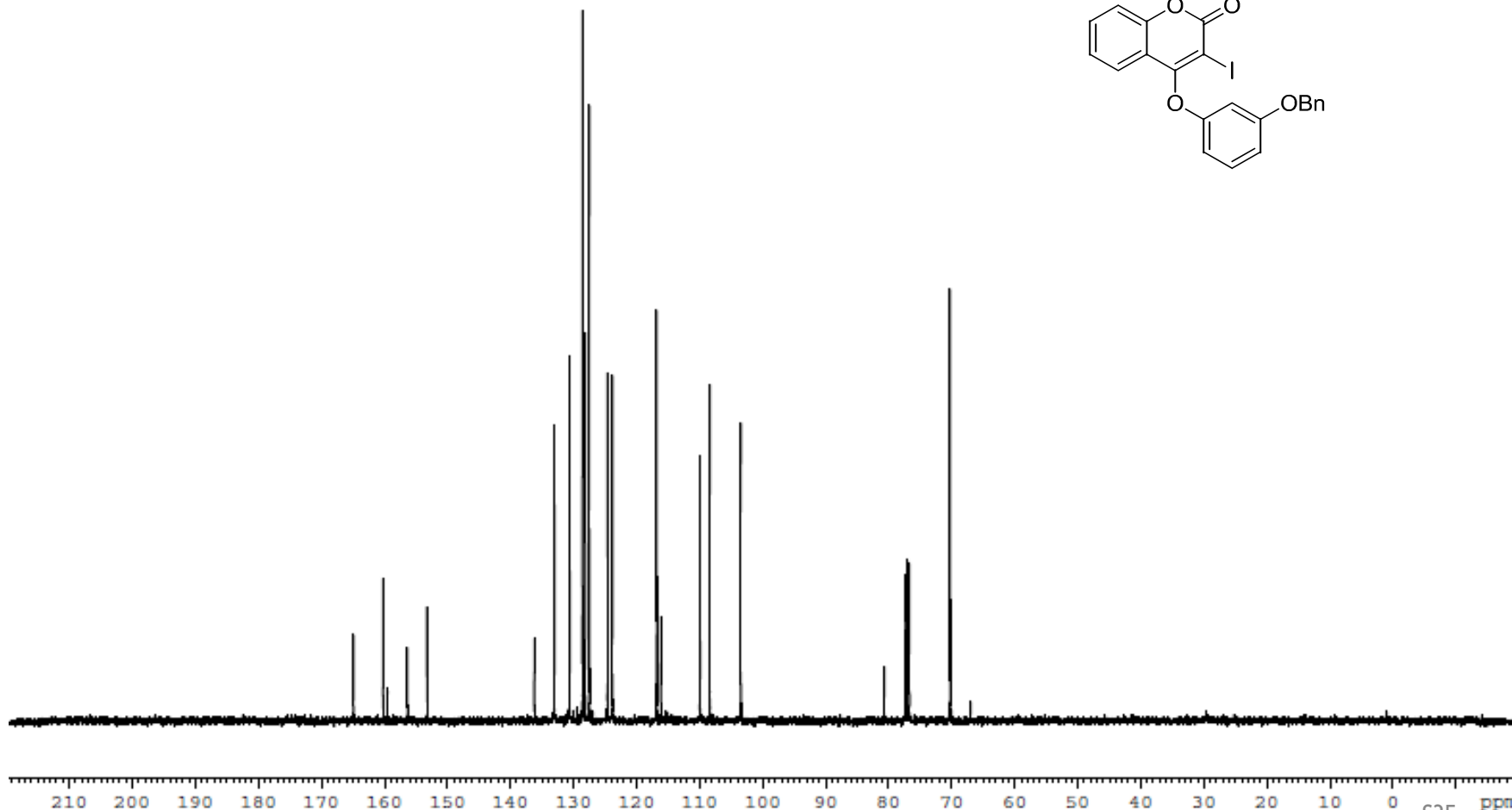
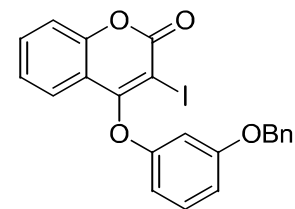
1.609



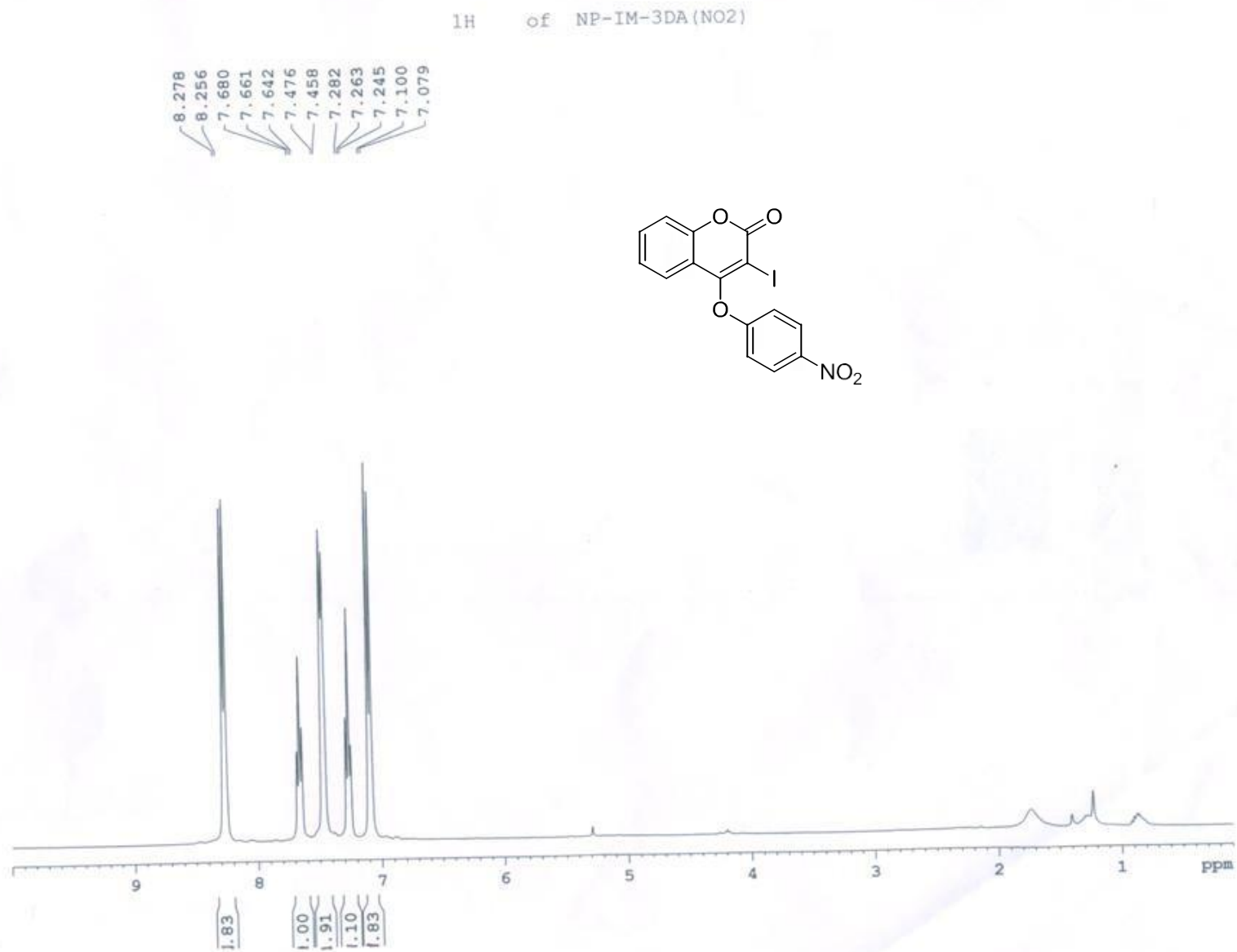
¹³C of 4-(3-(benzyloxy)phenoxy)-3-iodo-2H-chromen-2-one (3ea)

¹³C of NP-IM-1300 27.2.2017

164.85
160.21
159.49
156.33
153.26
136.20
133.03
130.60
128.57
128.10
127.46
124.62
123.79
116.80
116.12
109.92
108.36
103.43
80.67
77.33
77.01
76.69
70.23



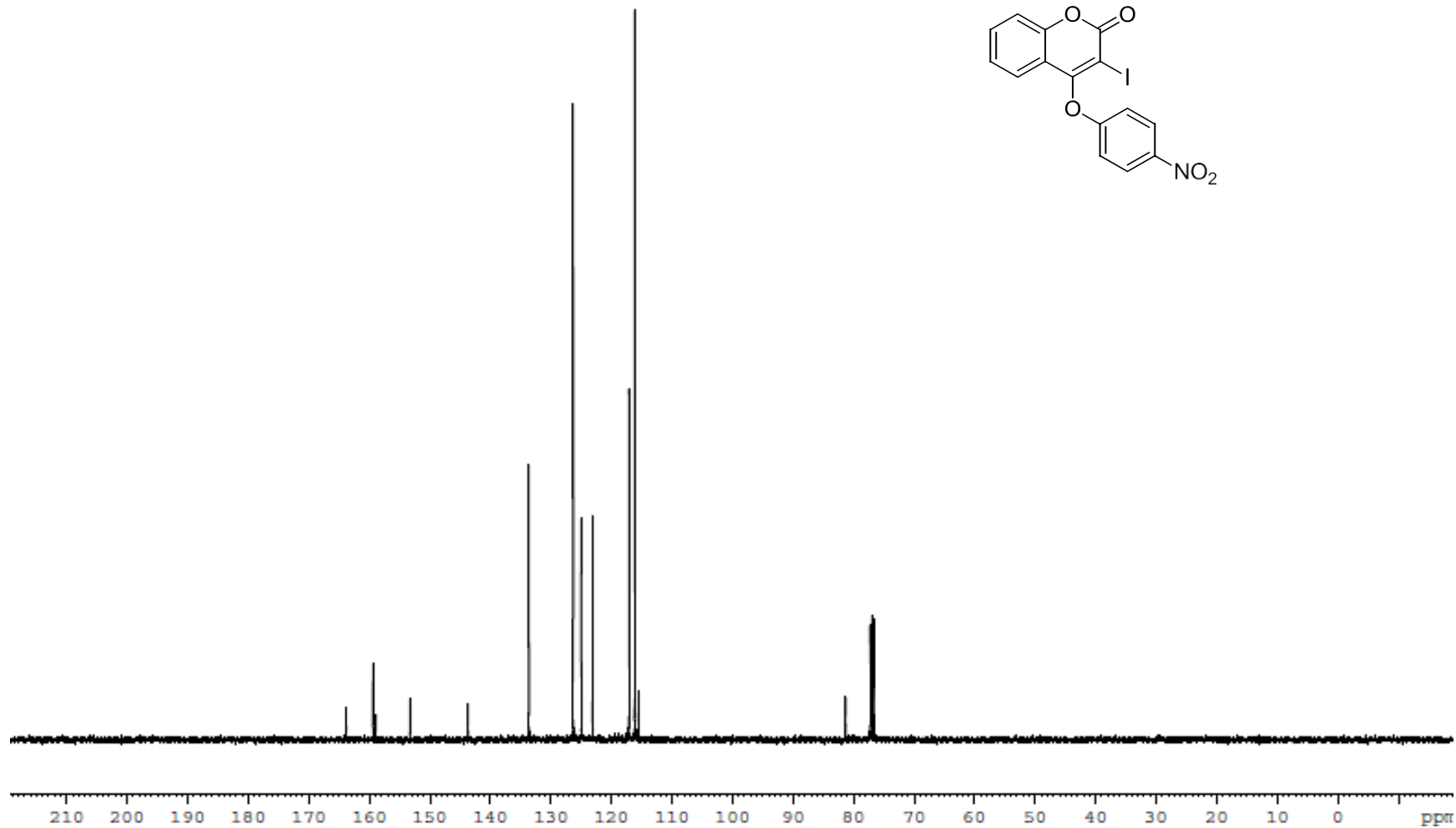
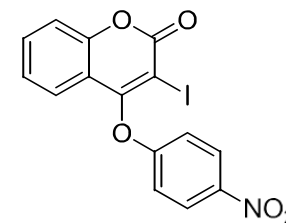
¹H of 3-iodo-4-(4-nitrophenoxy)-2H-chromen-2-one (3fa)



¹³C of 3-iodo-4-(4-nitrophenoxy)-2H-chromen-2-one (3fa)

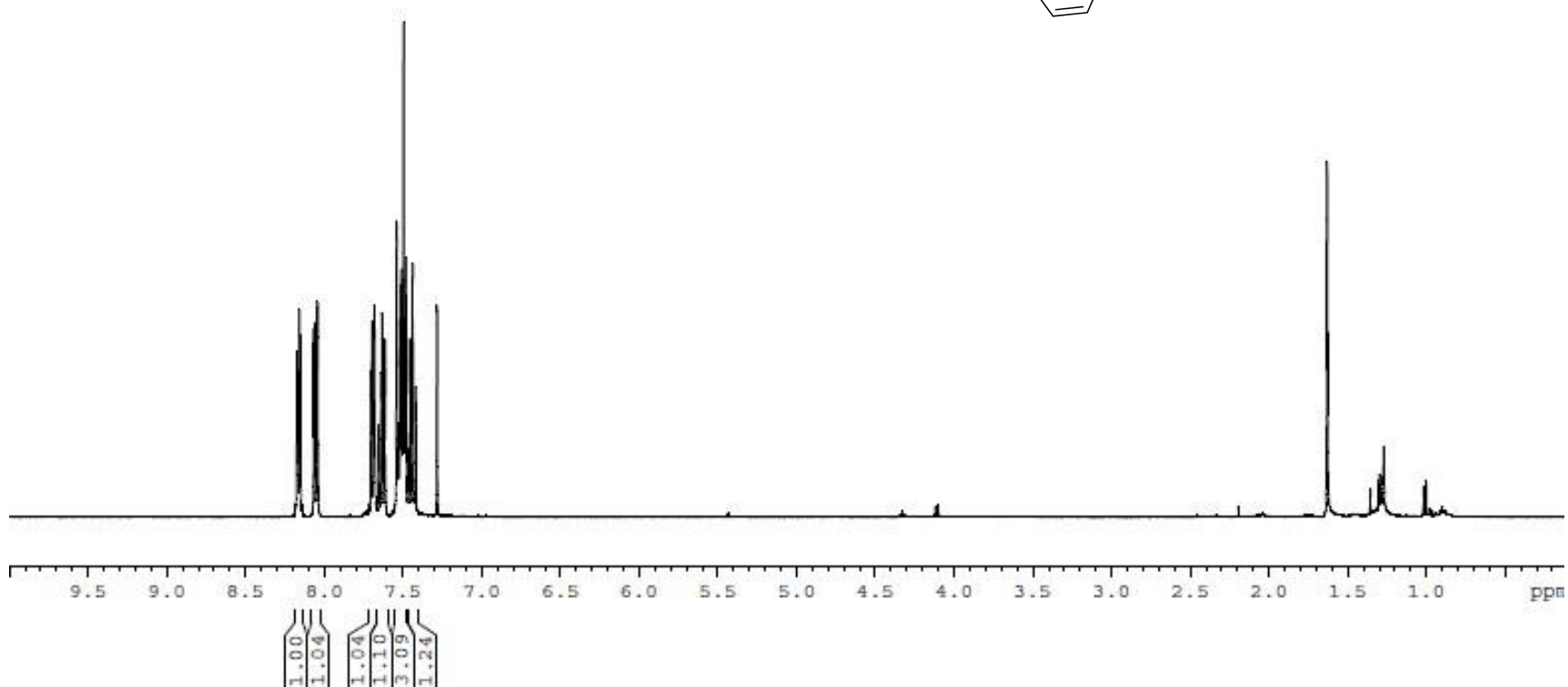
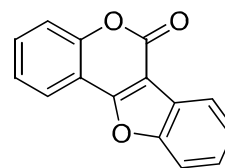
¹³C of NP-IM-1297 27.2.2017

163.84
159.40
158.91
153.27
143.69
133.64
126.33
124.98
123.11
117.11
116.18
115.51
81.28
77.27
76.95
76.63



¹H of 6H-benzofuro[3,2-c]chromen-6-one (4aa)

¹H of NP-IM-599 22.4.2015



¹³C of 6H-benzofuro[3,2-c]chromen-6-one (4aa)

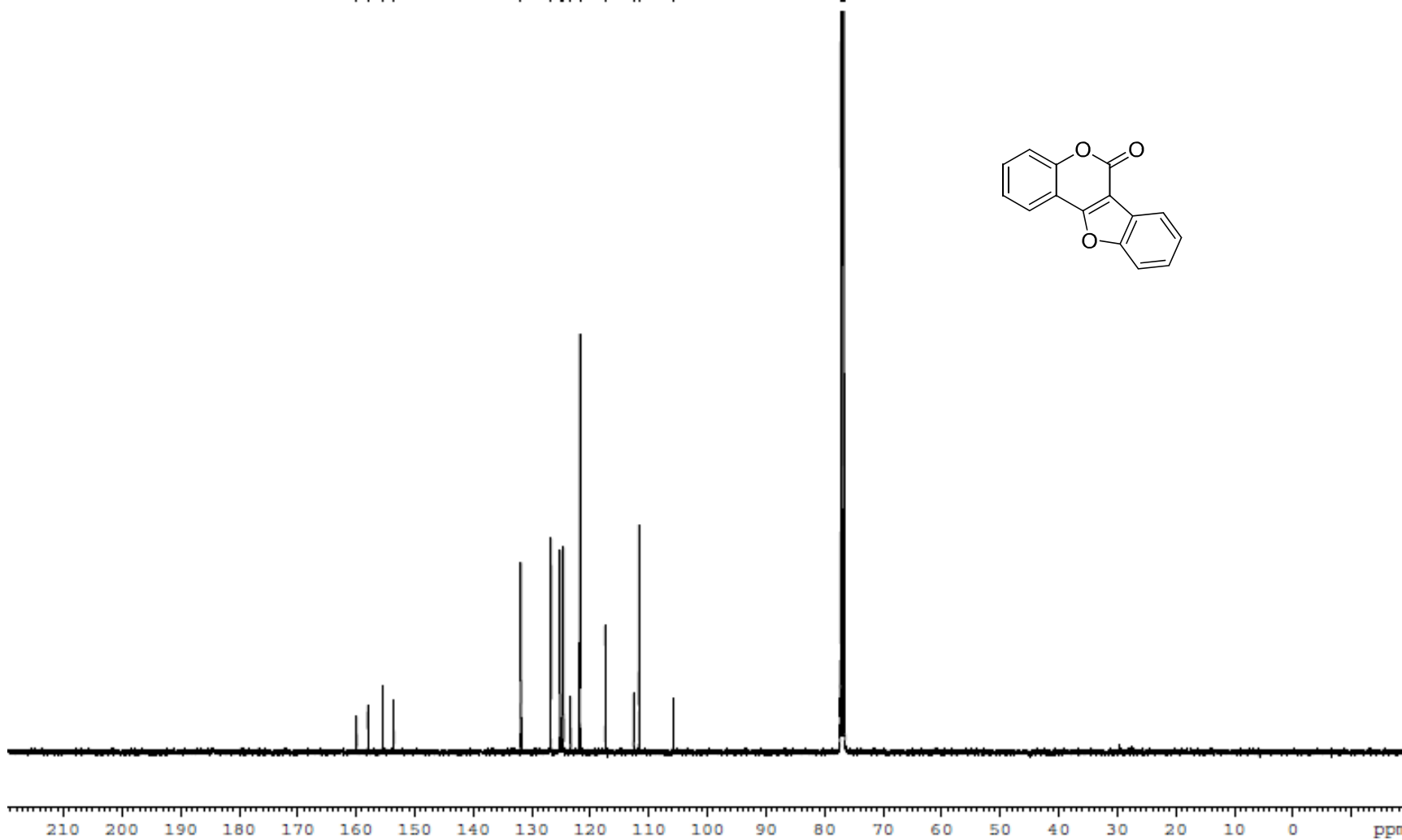
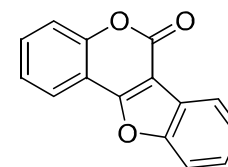
¹³C of NP-IM-599

22.4.2015

159.94
158.02
155.46
153.61

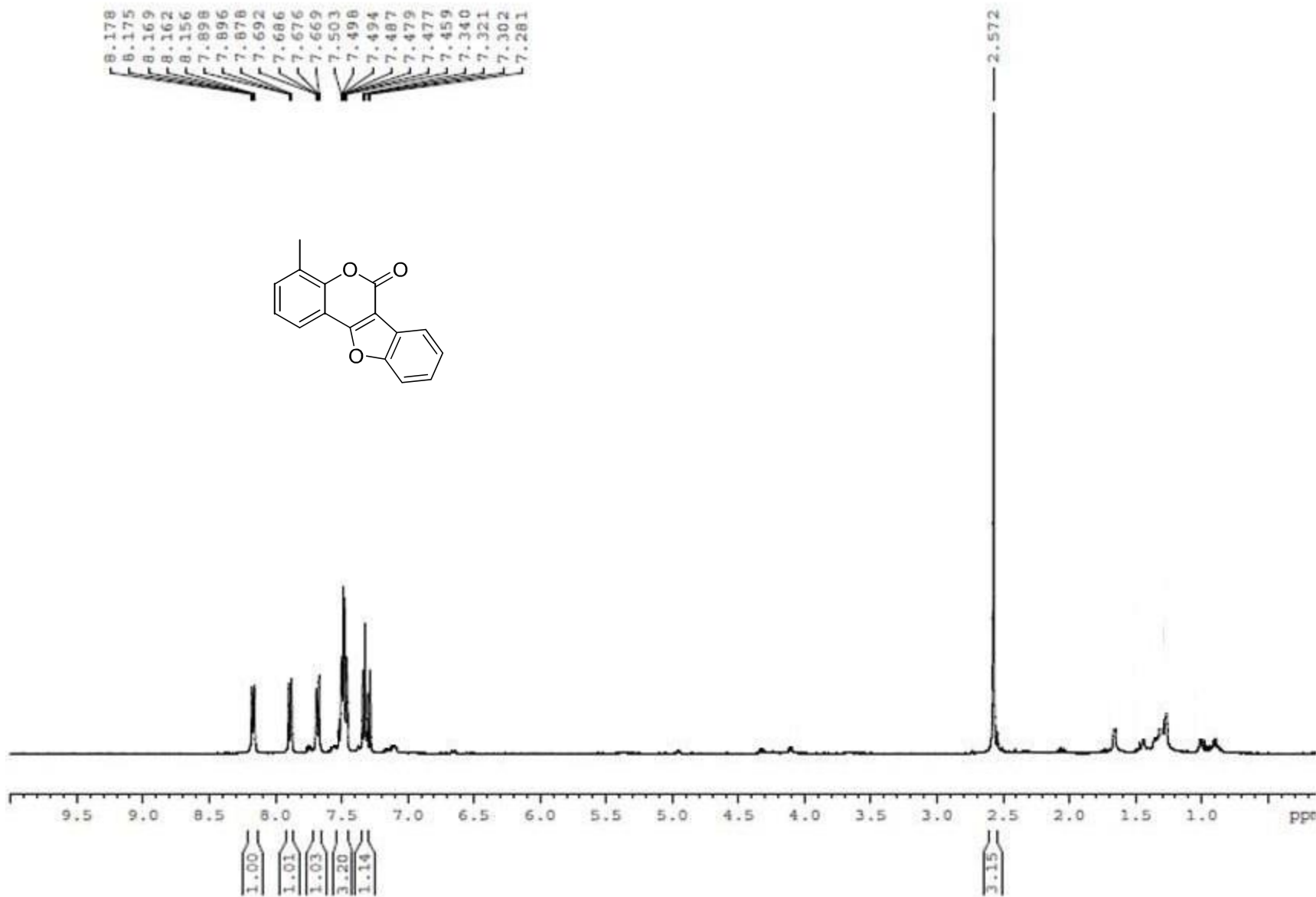
131.87
126.71
125.16
124.59
123.37
121.81
117.44
112.58
111.69
105.83

77.28
77.16
76.96
76.64



¹H of methyl-6H-benzofuro[3,2-c]chromen-6-one (4ab)

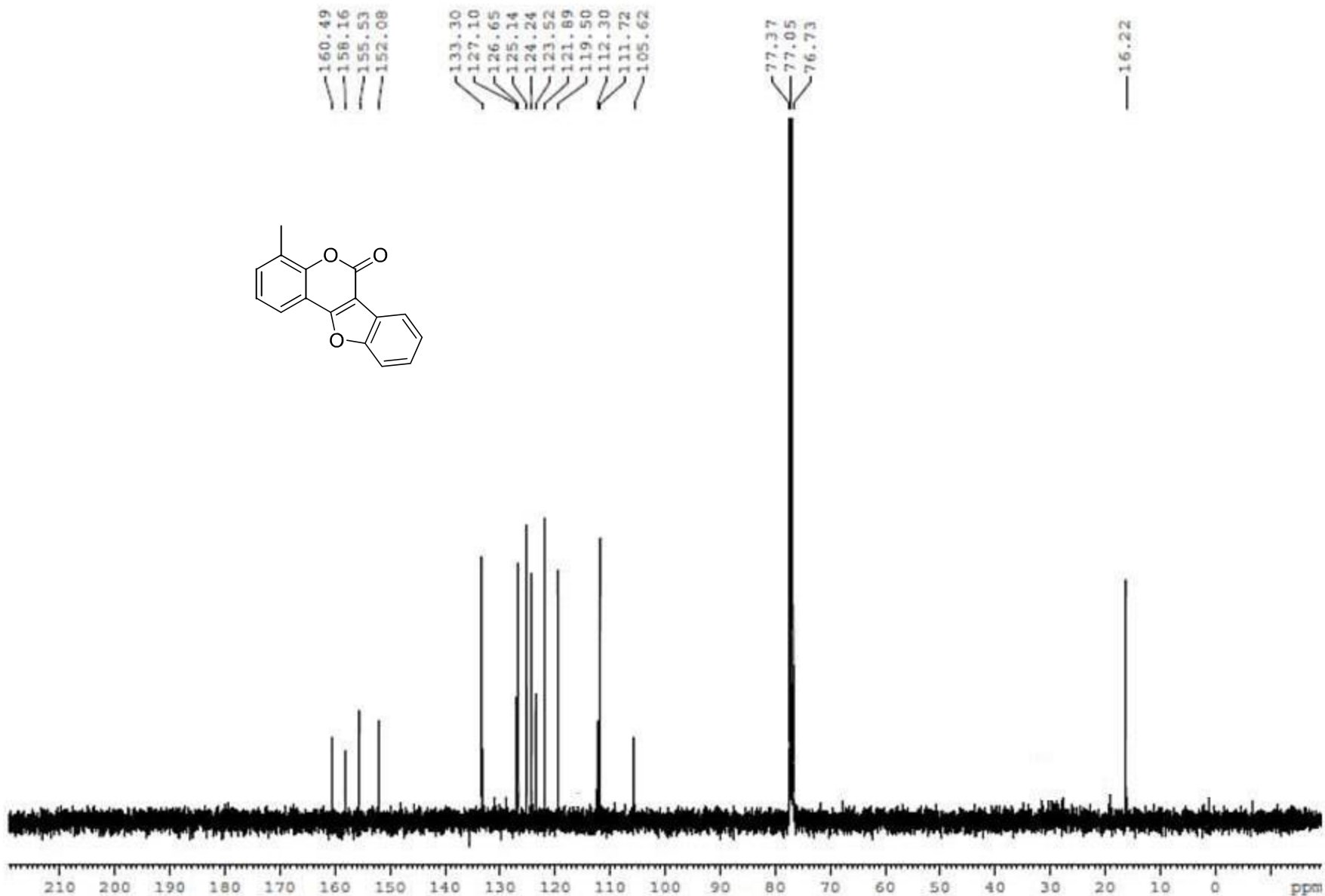
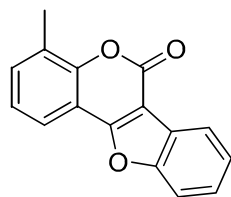
¹H of NP-IM-1205 14.12.2016



¹³C of methyl-6H-benzofuro[3,2-c]chromen-6-one (4ab)

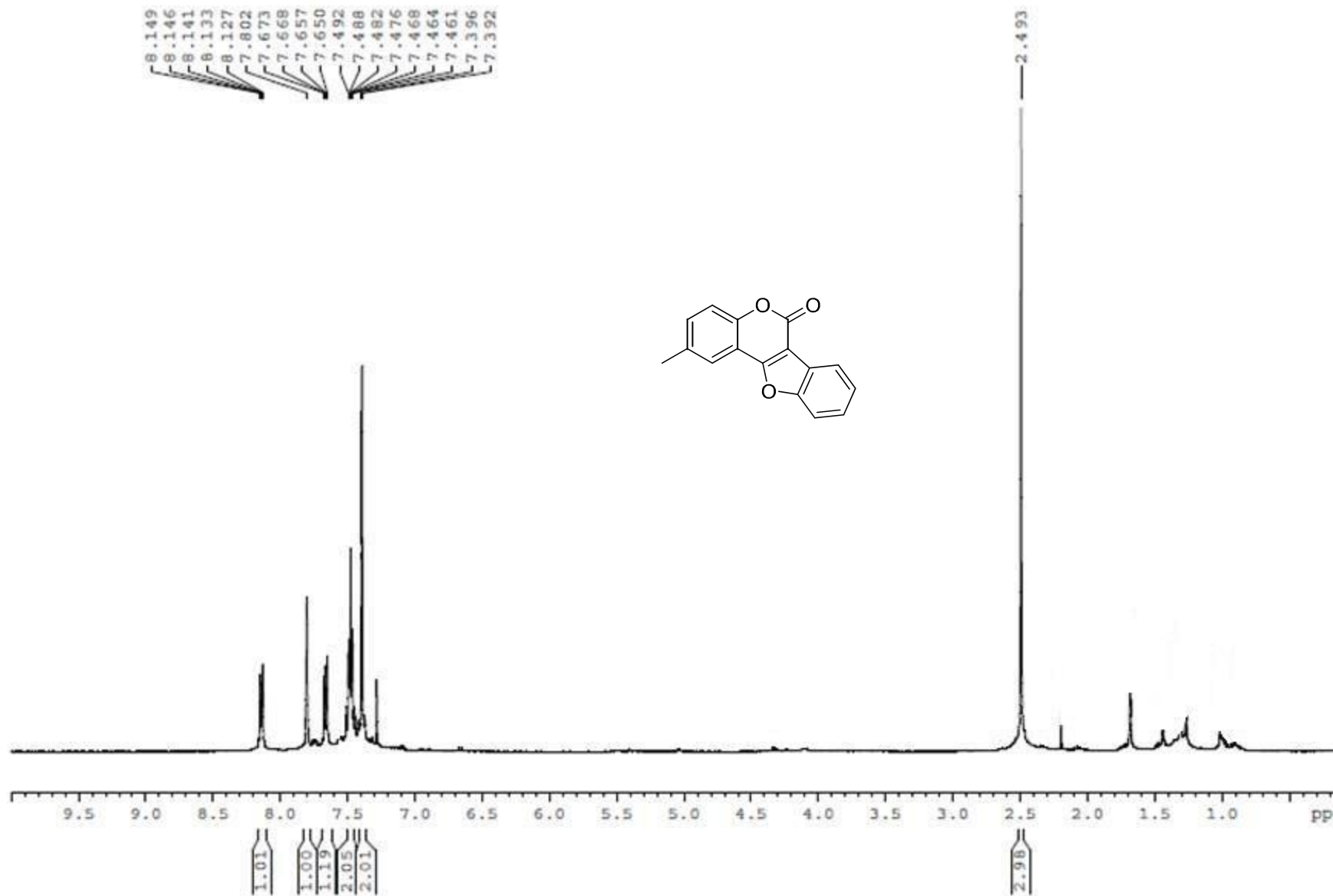
¹³C of NP-IM-1205

14.12.2016



¹H of 2-methyl-6H-benzofuro[3,2-c]chromen-6-one (4ac)

¹H of NP-IM-1206 14.12.2016



¹³C of 2-methyl-6H-benzofuro[3,2-c]chromen-6-one (4ac)

¹³C of NP-IM-1206

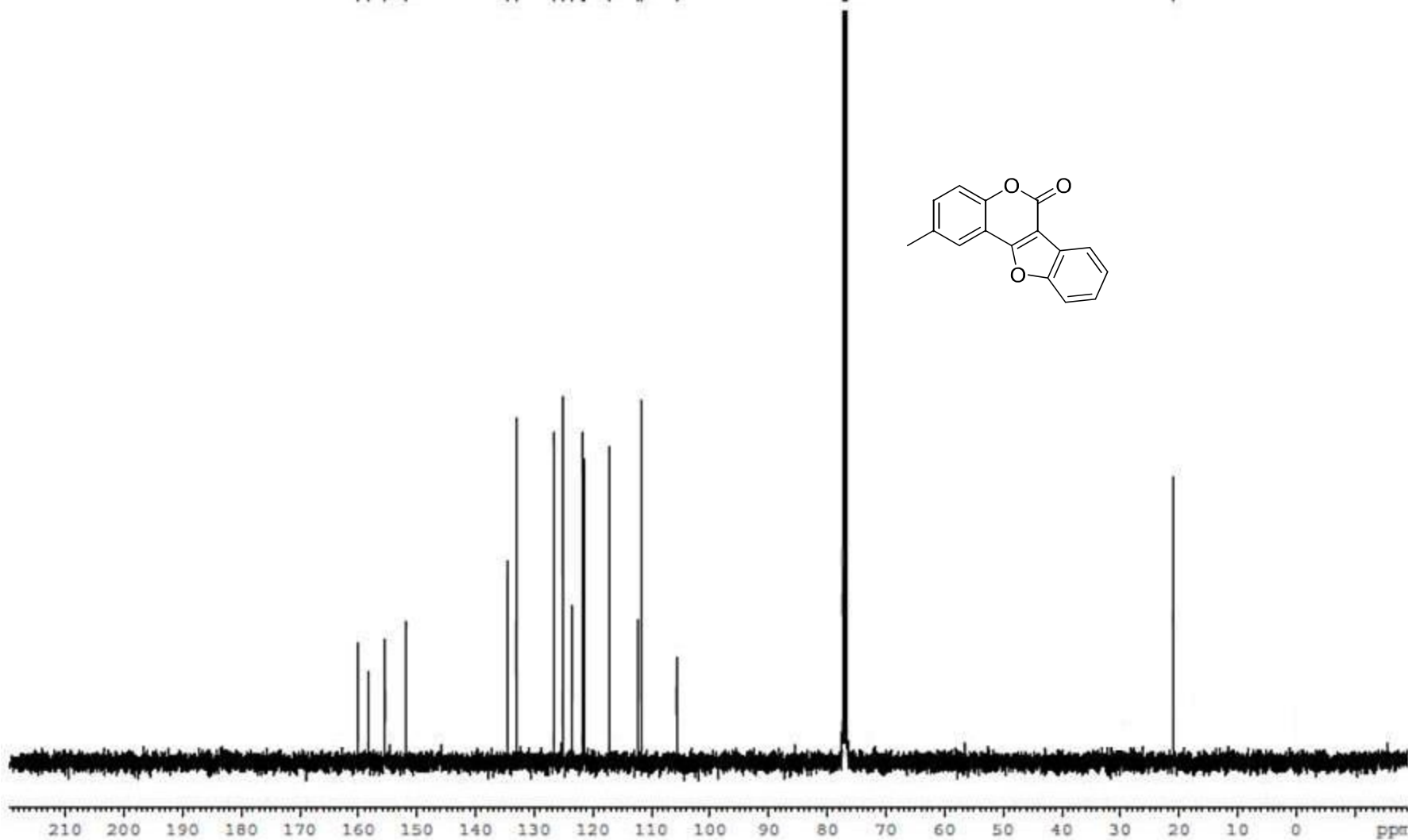
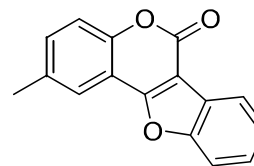
14.12.2016

160.05
158.32
155.45
151.86

134.58
133.04
126.66
125.17
123.51
121.82
121.51
117.20
112.24
111.70
105.73

77.37
77.06
76.74

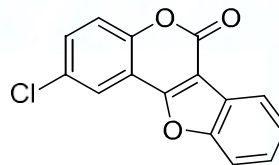
20.99



¹H of 2-chloro-6H-benzofuro[3,2-c]chromen-6-one (4ad)

¹H of NP-IM-4AD

8.165
8.147
8.028
7.701
7.681
7.573
7.550
7.528
7.509
7.491
7.473
7.451
7.258



1.583
H₂O



1.00
0.95
1.05
4.06

6.32

¹³C of 2-chloro-6H-benzofuro[3,2-c]chromen-6-one (4ad)

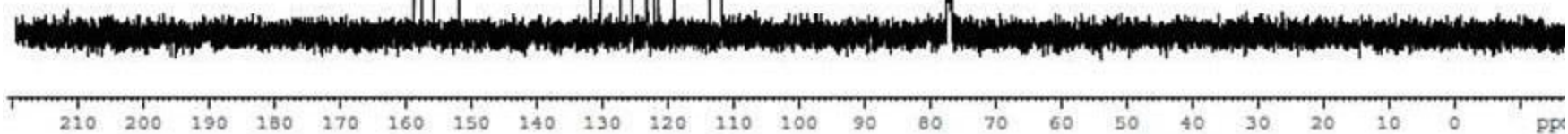
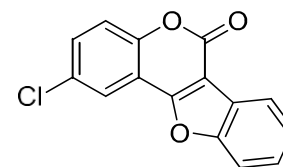
¹³C of NP-IM-1207

15.12.2016

158.67
157.52
155.67
151.95

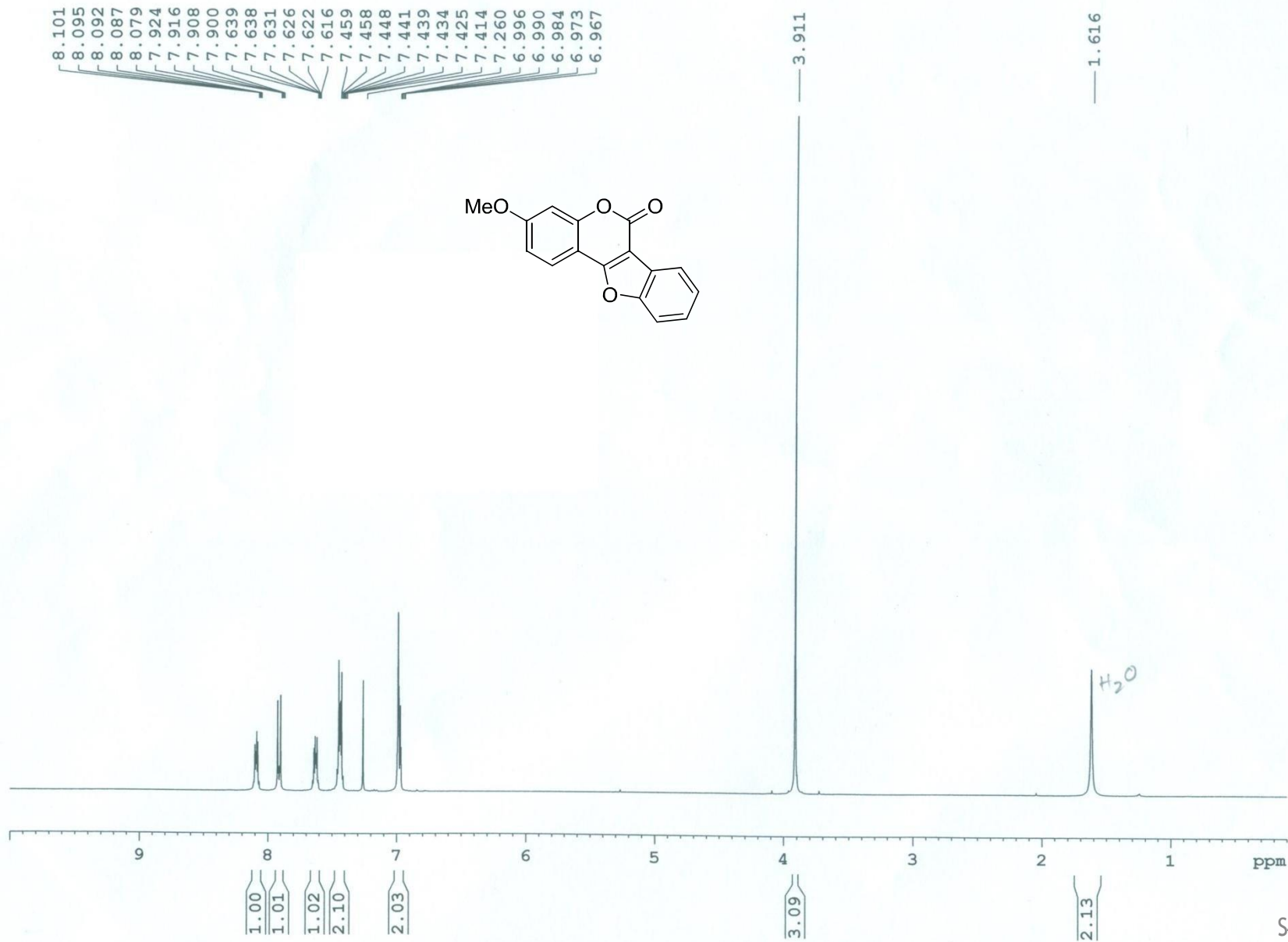
131.90
130.28
127.27
125.48
123.18
122.03
121.38
118.98
113.74
111.90

77.35
77.03
76.71



¹H of 3-methoxy-6H-benzofuro[3,2-c]chromen-6-one (4ae)

¹H of NP-IM-4AE



¹³C of 3-methoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (4ae)

¹³C of NP-IM-1274

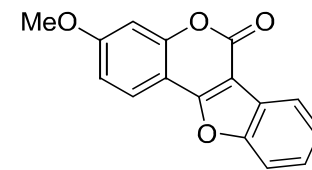
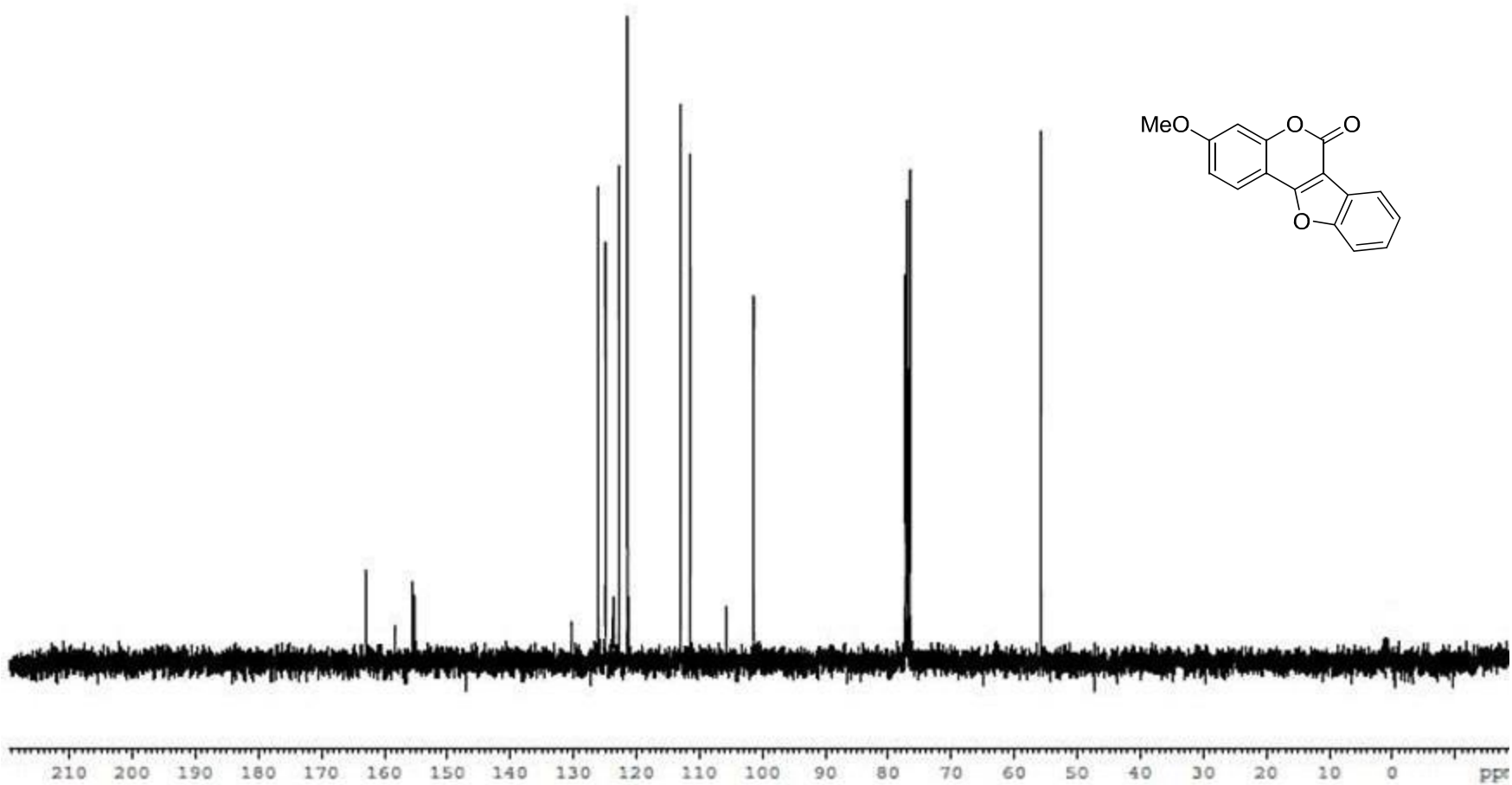
31.1.2017

162.92
158.25
155.49
155.12

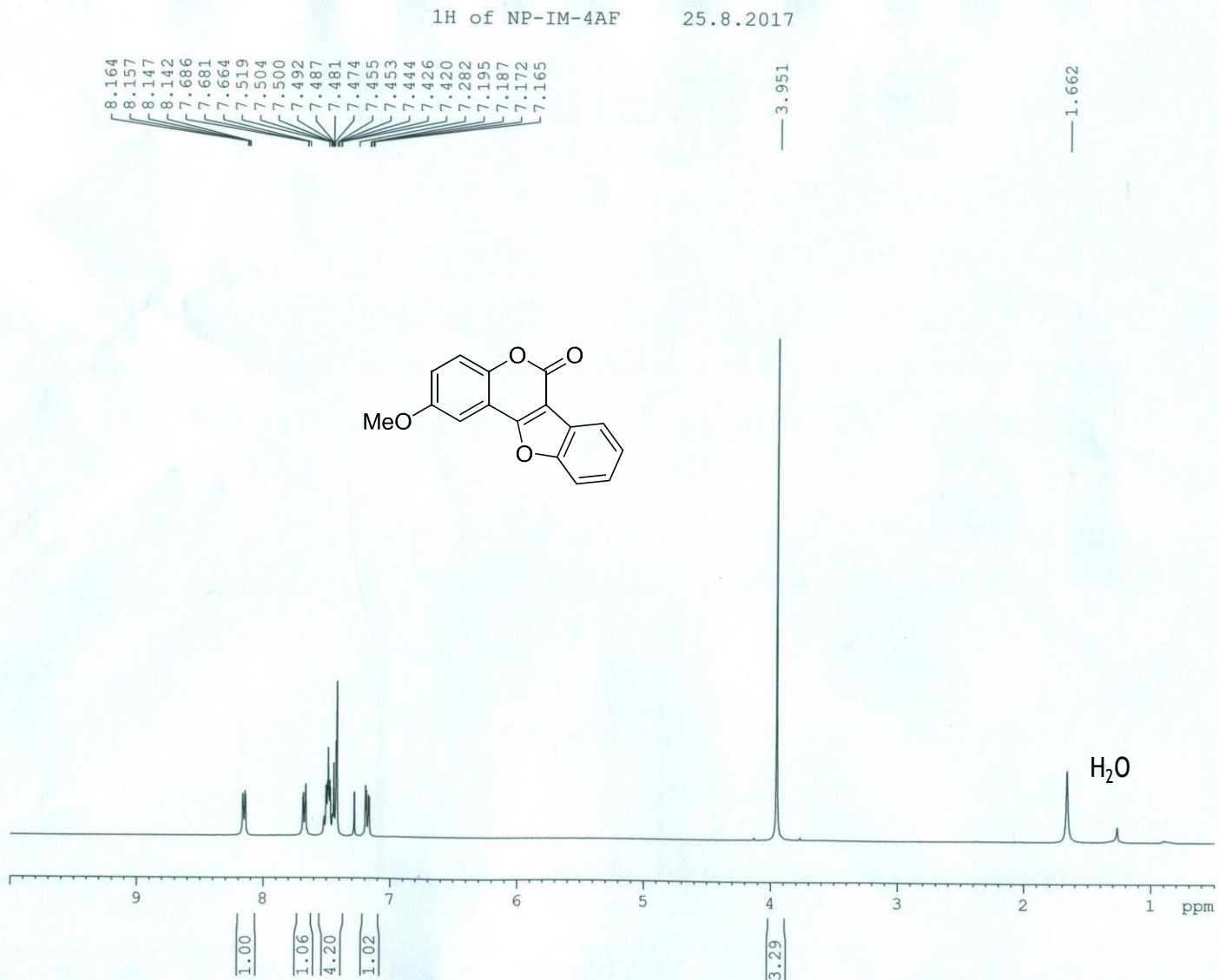
130.24
126.03
124.96
123.51
122.75
121.38
121.23
112.98
111.42
105.74
101.31

77.24
76.92
76.60

55.73



¹H of 2-methoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (4af)



¹³C of 2-methoxy-6H-benzofuro[3,2-c]chromen-6-one (4af)

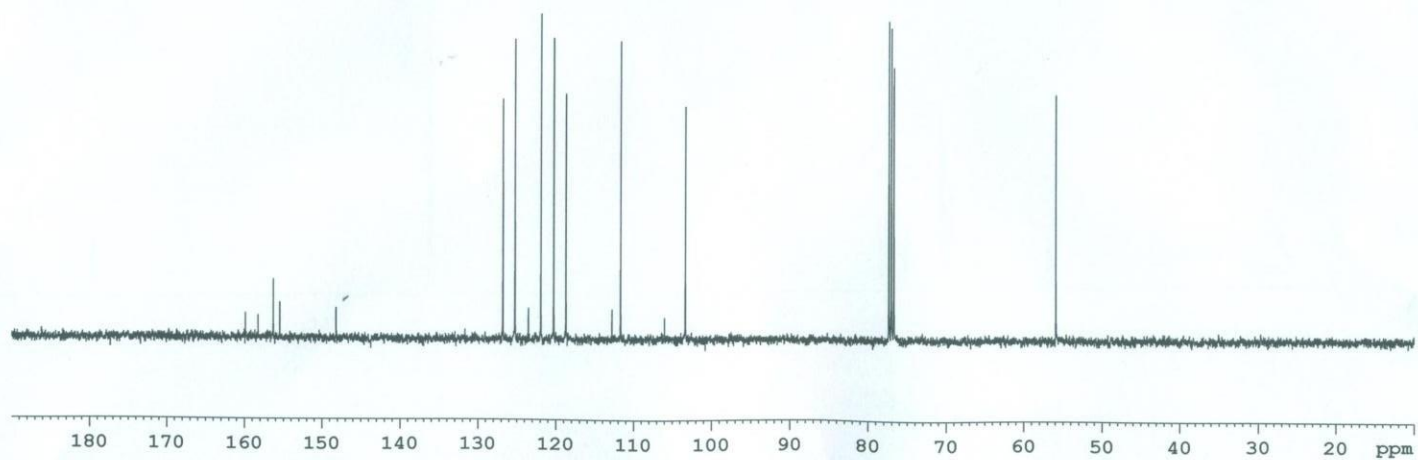
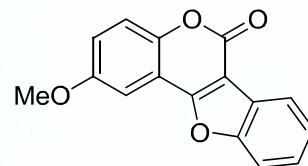
¹³C of NP-IM-4AF 25.8.2017

159.89
158.27
156.32
155.47
— 148.20

126.79
125.23
123.50
121.92
120.29
118.72
112.79
111.70
— 106.00
— 103.34

77.36
77.04
76.72

— 55.95

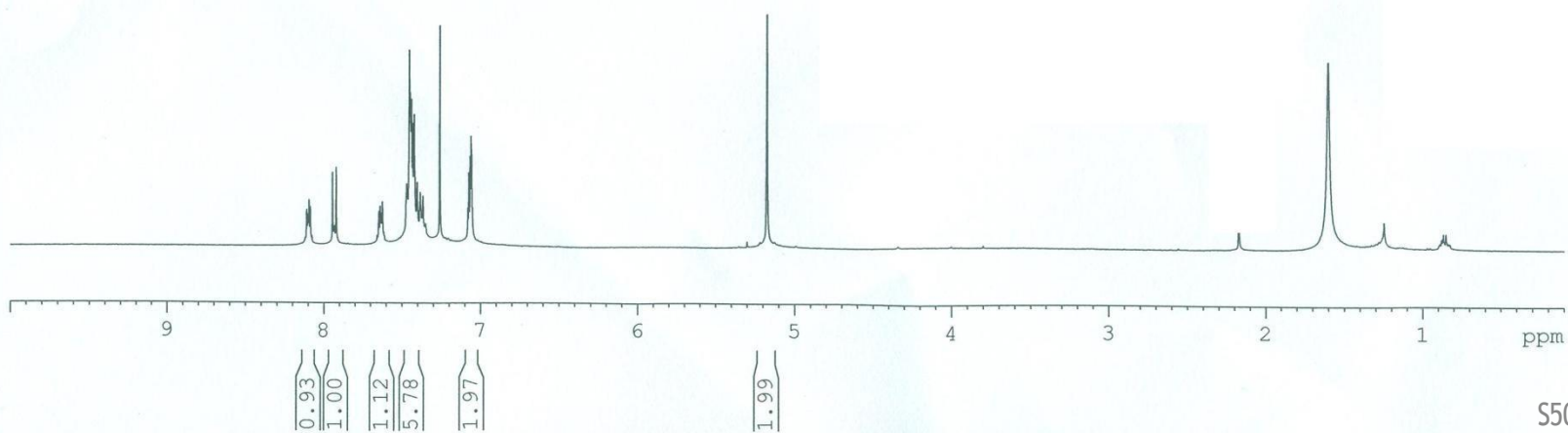
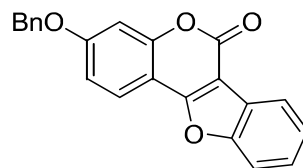


¹H of 3-(benzyloxy)-6H-benzofuro[3,2-c]chromen-6-one (4ag)

¹H of NP-IM-4AG 29.8.2017

8.109
8.095
8.086
7.944
7.921
7.647
7.639
7.631
7.625
7.470
7.455
7.450
7.446
7.441
7.432
7.423
7.404
7.389
7.385
7.380
7.367
7.260
7.081
7.075
7.067
7.062
7.058
7.052
— 5.174

— 1.604



¹³C of 3-(benzyloxy)-6H-benzofuro[3,2-c]chromen-6-one (4ag)

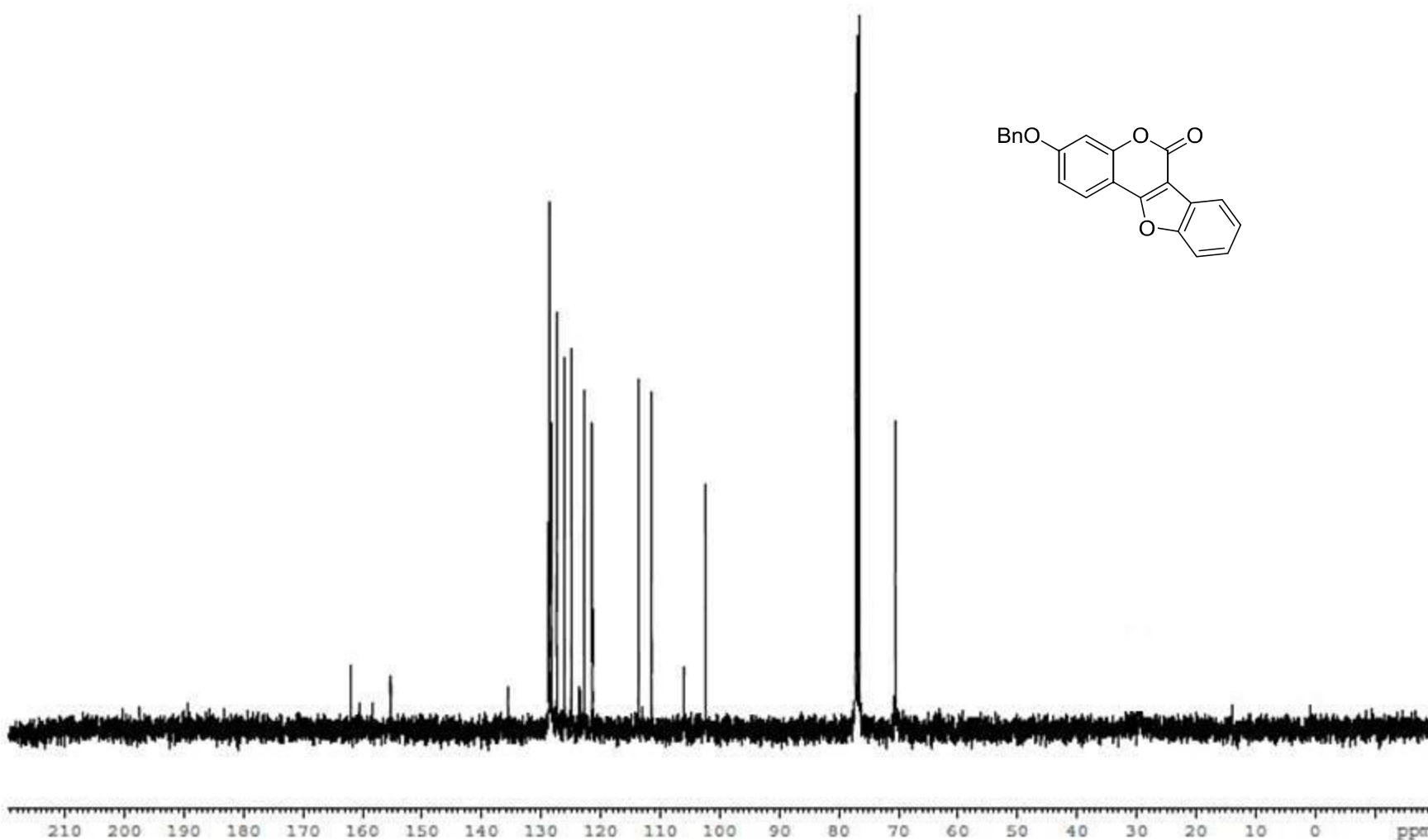
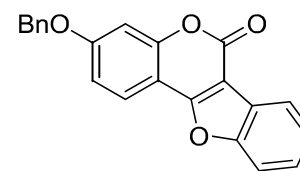
¹³C of NP-IM-1264

31.1.2017

161.99
160.52
158.23
155.42
155.18

135.58
128.67
128.31
127.41
126.05
124.97
123.56
122.78
121.42
113.62
113.00
111.42
106.00
102.44

77.21
76.89
76.57
70.51



¹H of 2-(benzyloxy)-6H-benzofuro[3,2-c]chromen-6-one (4ah)

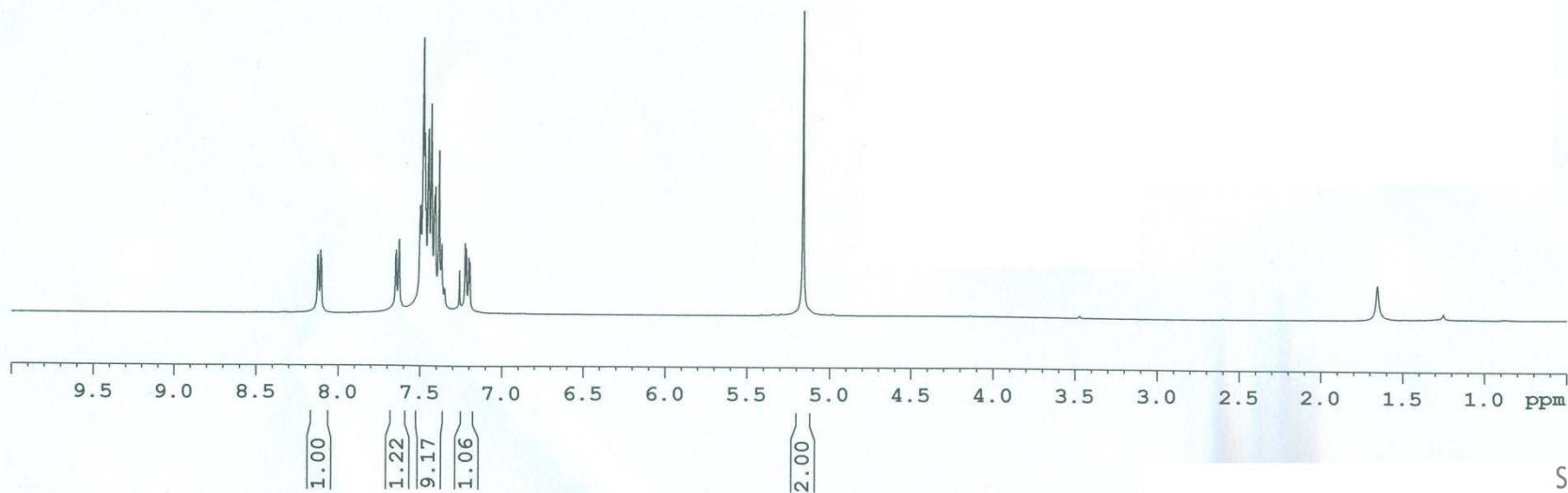
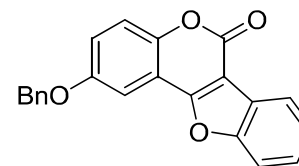
¹H of NP-IM-4AH

29.8.2017

8.125
8.119
8.108
8.103
7.648
7.645
7.627
7.498
7.480
7.472
7.465
7.449
7.432
7.412
7.407
7.384
7.375
7.369
7.351
7.259
7.226
7.218
7.203
7.196

— 5.163

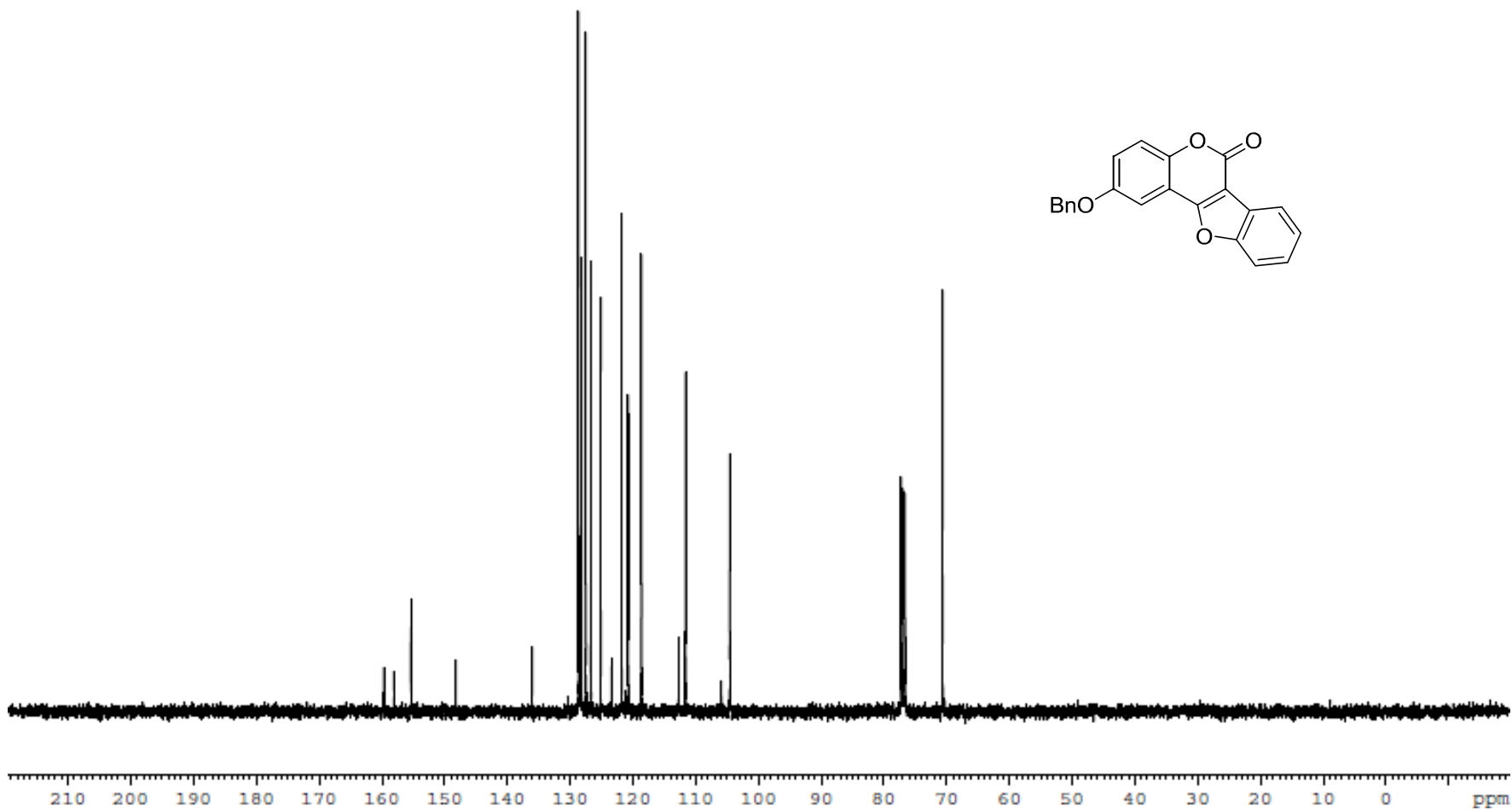
— 1.657



¹³C of 2-(benzyloxy)-6H-benzofuro[3,2-c]chromen-6-one(4ah)

¹³C of NP-IM-P-OBncypdt 22.3.2017

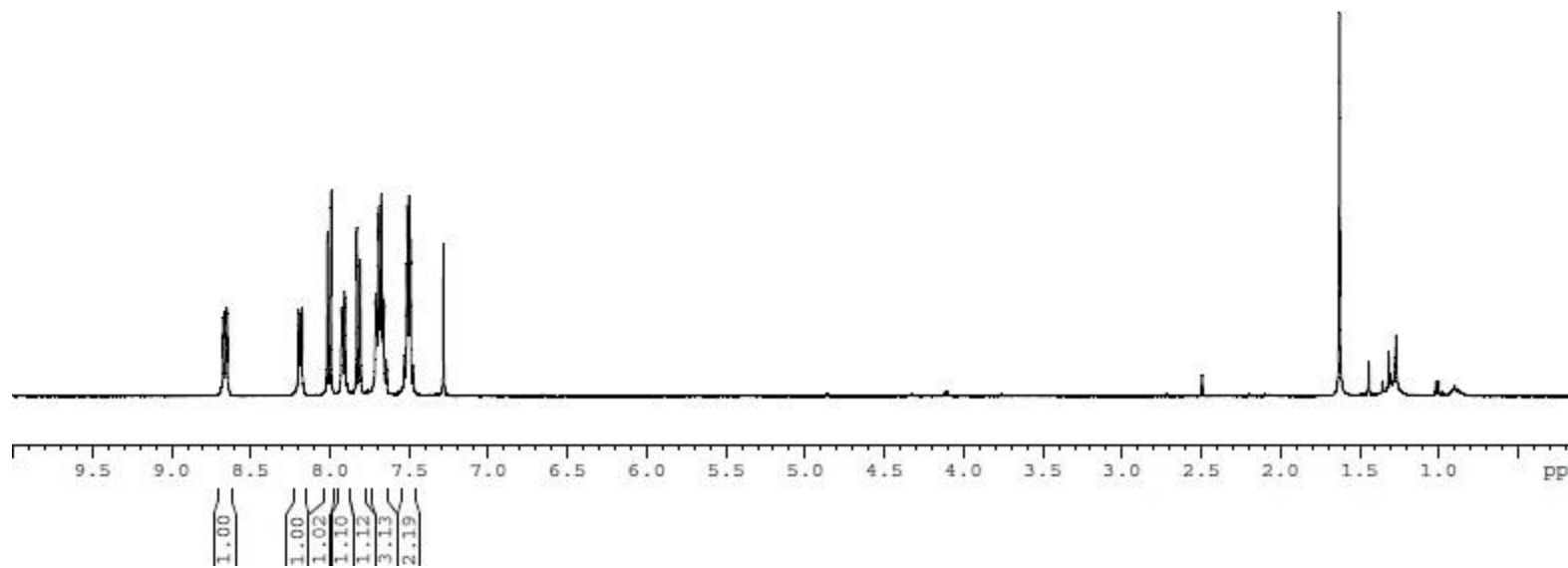
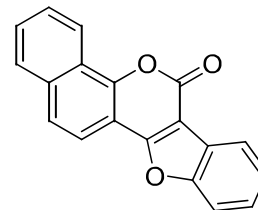
159.67
158.08
155.34
155.30
148.18
136.05
128.64
128.22
127.49
126.67
125.10
123.36
121.78
120.73
118.62
112.70
111.59
105.88
104.54
77.26
76.94
76.62
70.62



¹H of 8H-benzo[h]benzofuro[3,2-c]chromen-8-one (4ai)

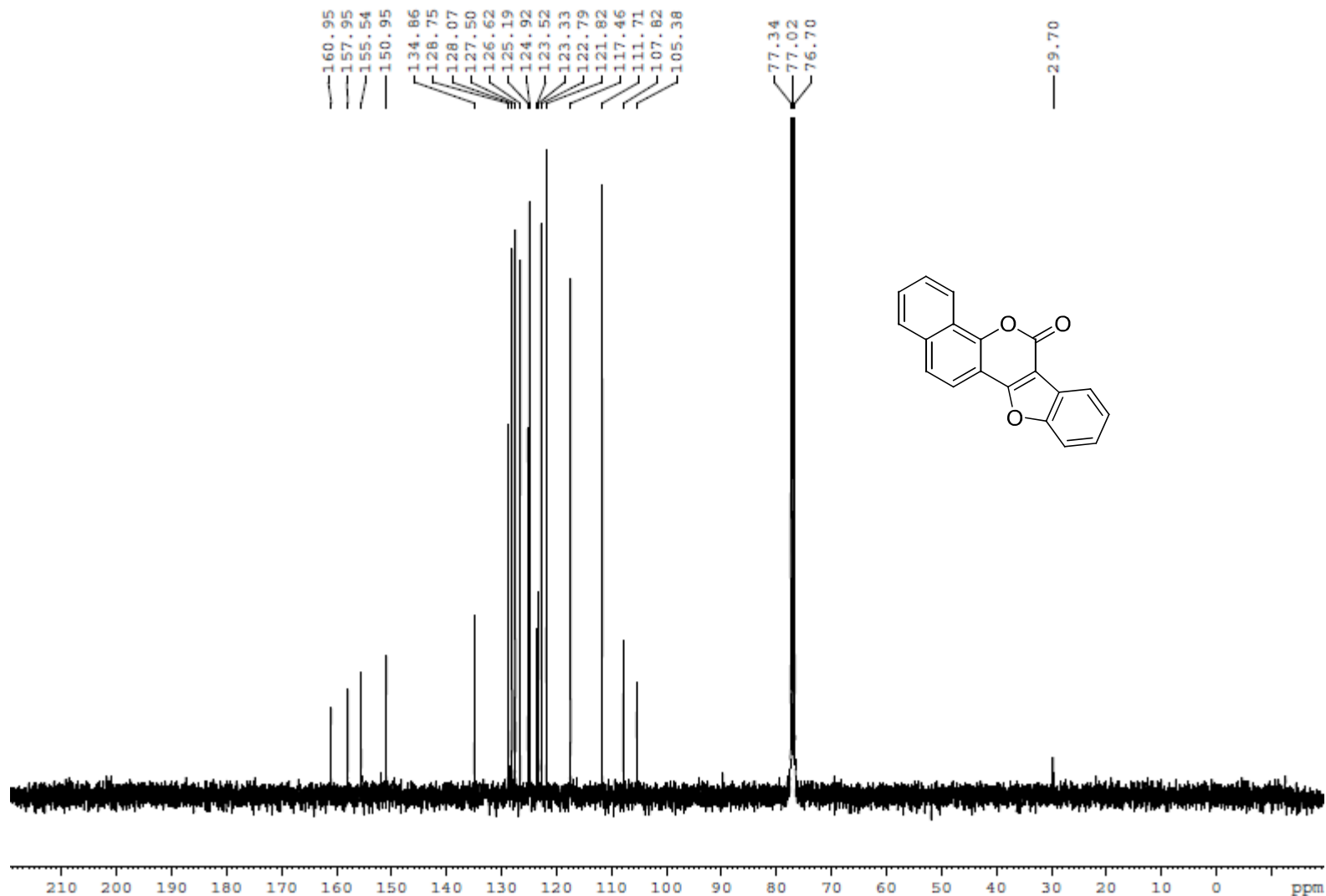
¹H of NP-IM-1203 15.12.2016

8.649
8.197
8.192
8.184
8.181
8.174
8.014
7.993
7.926
7.919
7.908
7.903
7.829
7.807
7.712
7.706
7.700
7.692
7.689
7.680
7.675
7.668
7.661
7.657
7.644
7.527
7.514
7.510
7.501
7.491
7.474
7.282



¹³C of 8H-benzo[h]benzofuro[3,2-c]chromen-8-one (4ai)

NP-IM-1213-1-naph 13c 7.2.2017

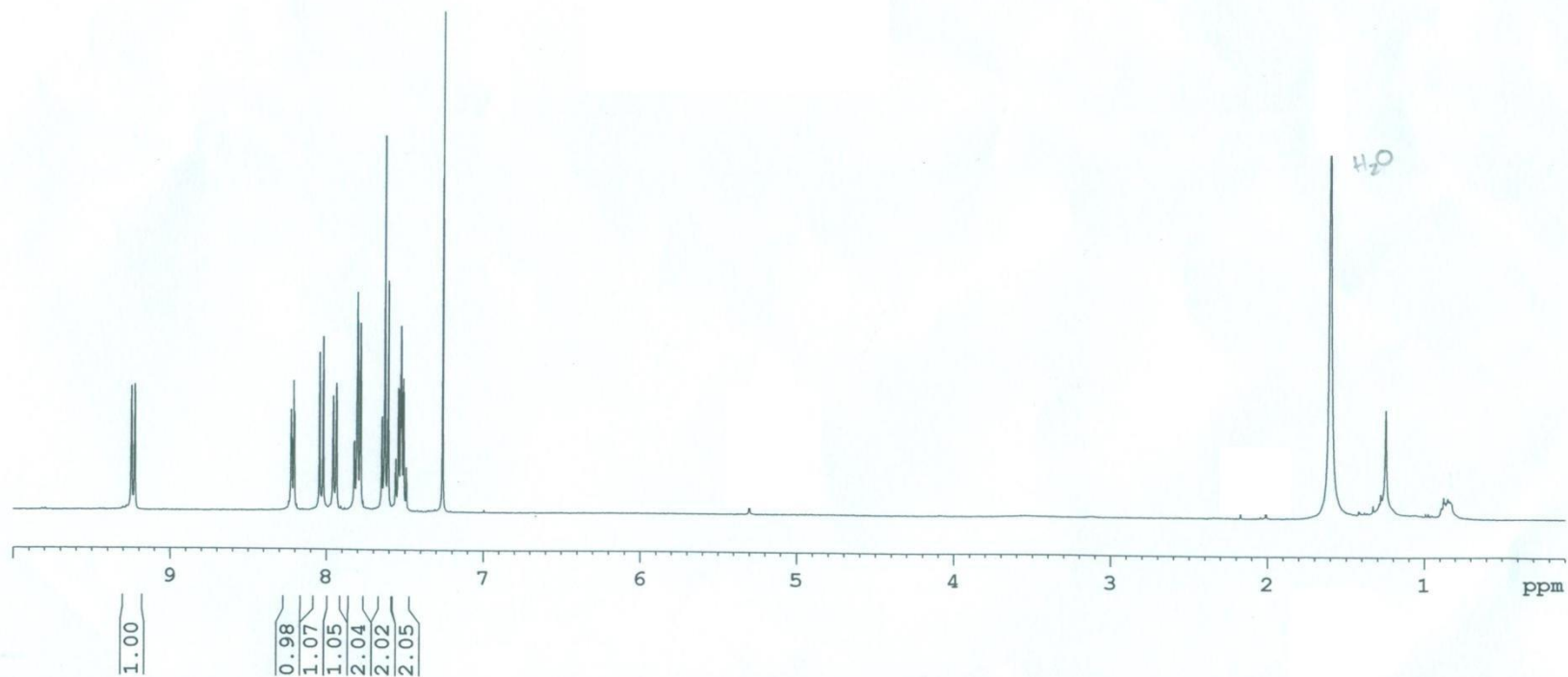
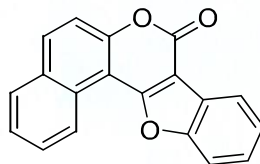


¹H of 8H-benzo[*f*]benzofuro[3,2-*c*]chromen-8-one (4aj)

¹H of NP-IM-4AK

8.226
8.224
8.220
8.210
8.205
8.043
8.021
7.957
7.936
7.821
7.803
7.799
7.786
7.782
7.648
7.645
7.628
7.610
7.605
7.543
7.539
7.529
7.525
7.524
7.519
7.510
7.507
7.260

—1.601

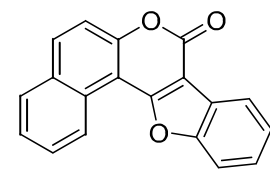
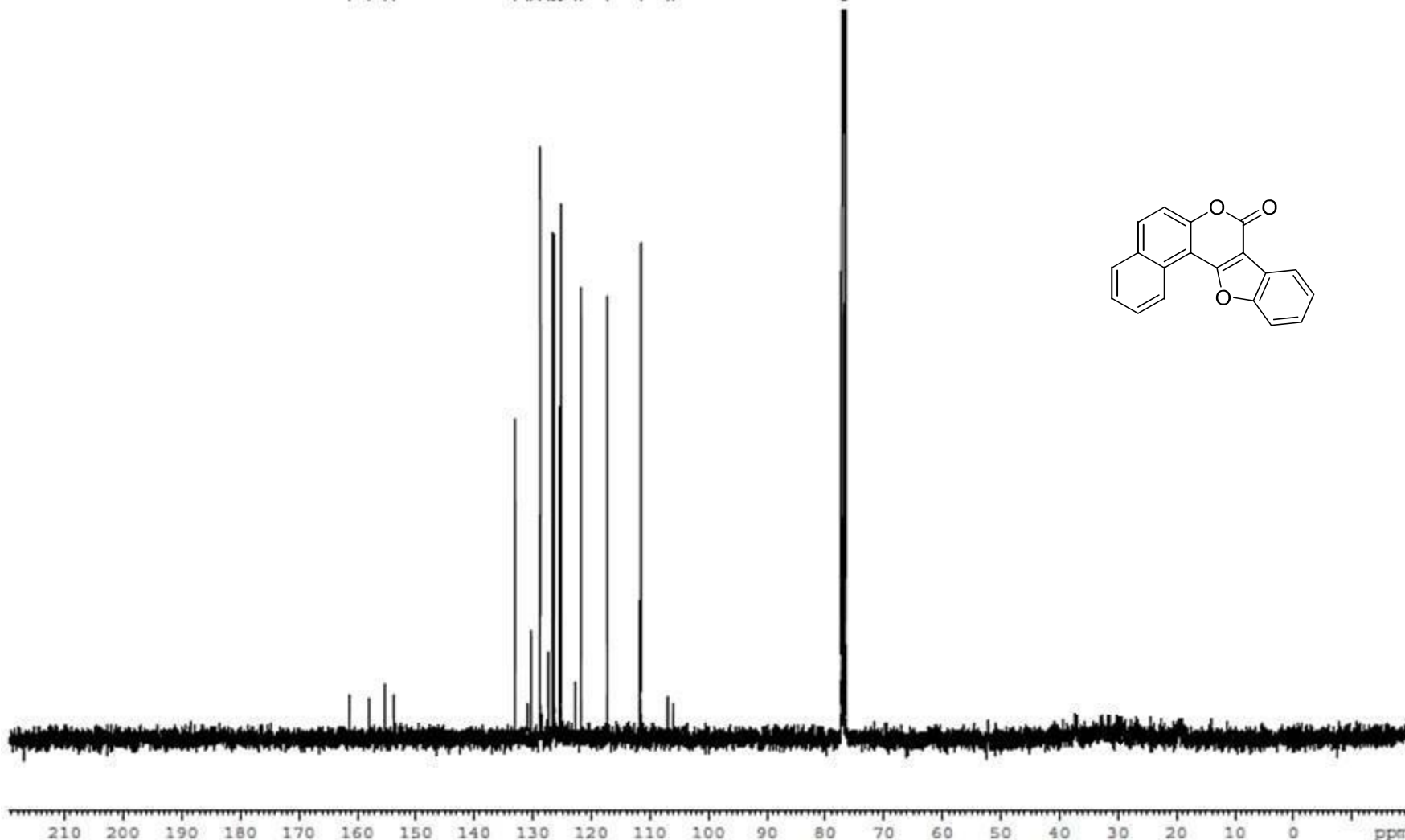


¹³C of 8H-benzo[f]benzofuro[3,2-c]chromen-8-one (4aj)

¹³C of NP-IM-1213(R)

7.2.2017

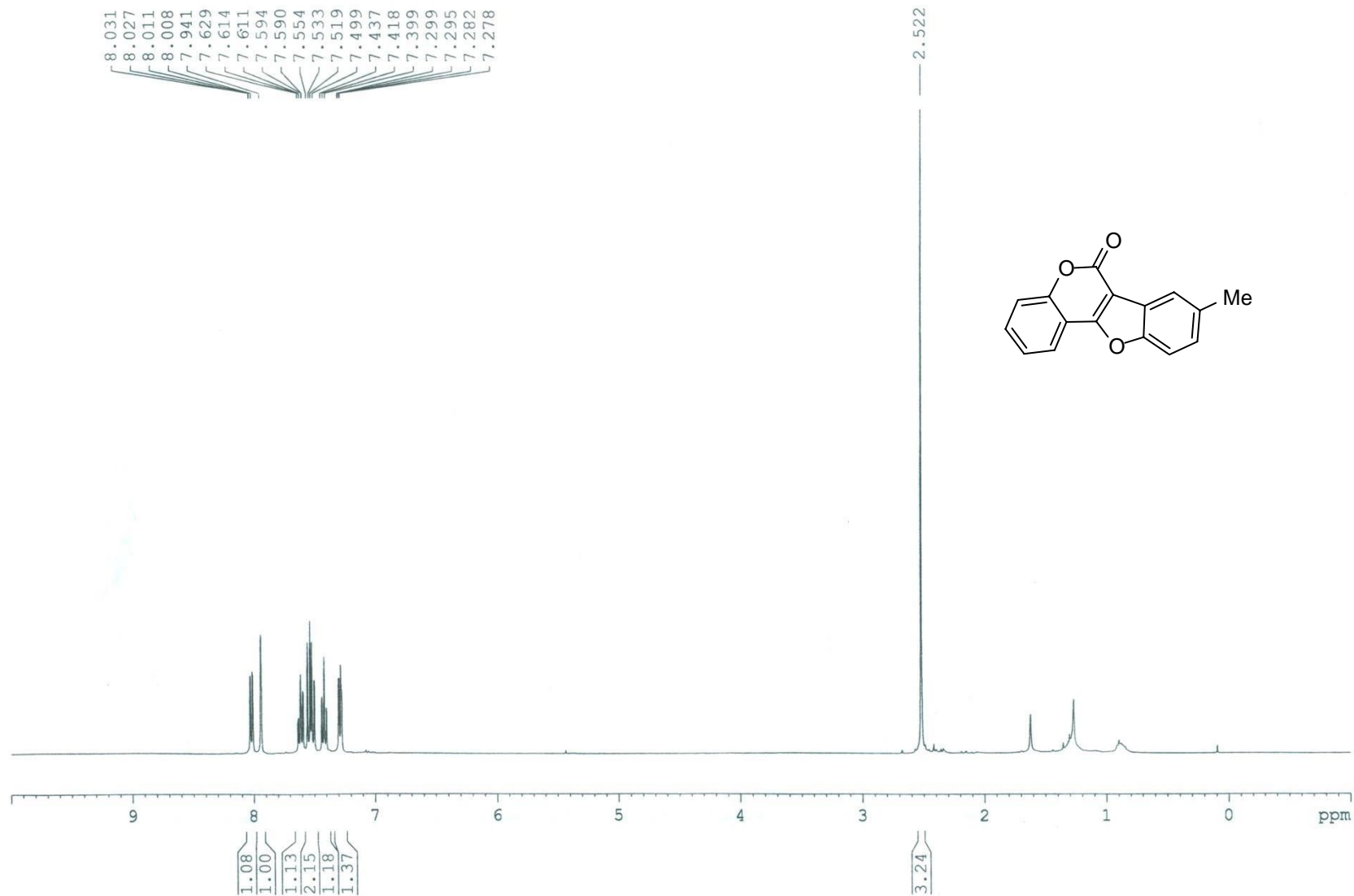
161.29
157.95
155.36
153.79
133.02
130.79
130.28
128.70
127.42
126.63
126.28
125.42
125.23
122.78
121.75
117.30
111.60
107.03
106.03
77.21
76.89
76.58



¹H of 8-methyl-6H-benzofuro[3,2-c]chromen-6-one (4ba)

¹H of NP-IM-1325

29.3.2017



¹³C of 8-methyl-6H-benzofuro[3,2-c]chromen-6-one (4ba)

13C of NP-IM-1325 29.3.2017

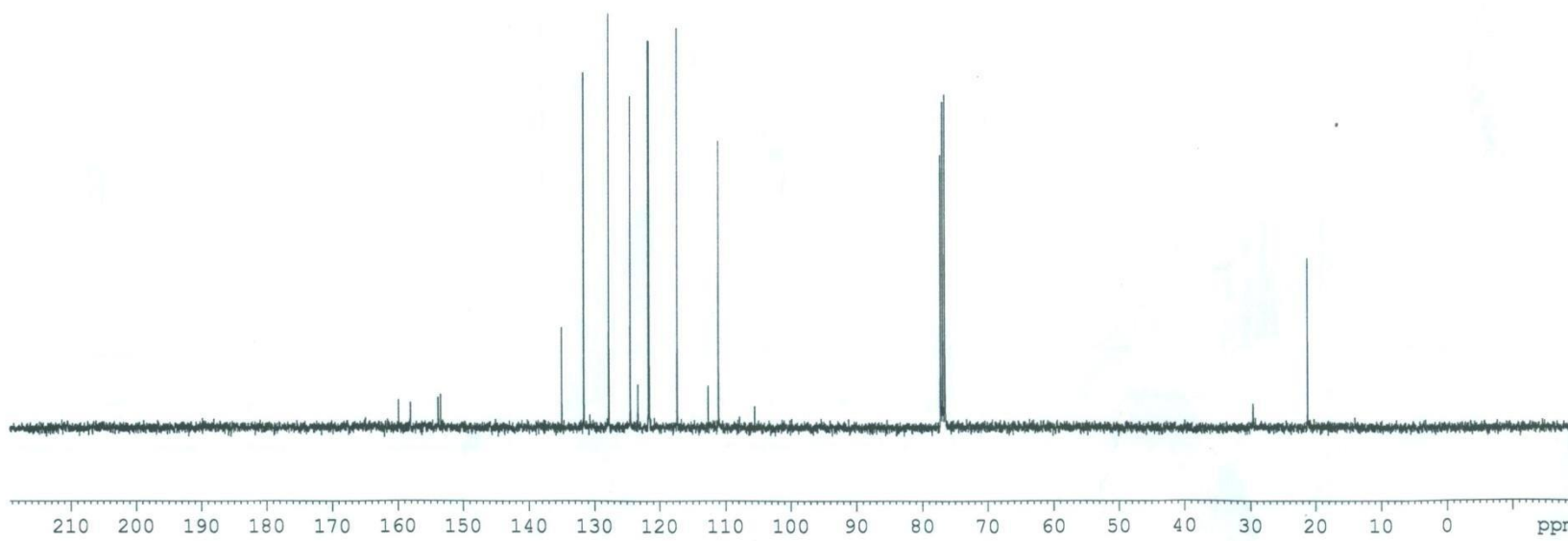
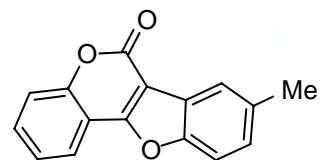
159.92
158.08
153.87
153.48

135.03
131.63
127.80
124.47
123.31
121.69
121.56
117.34
112.65
111.07
105.56

77.22
76.90
76.59

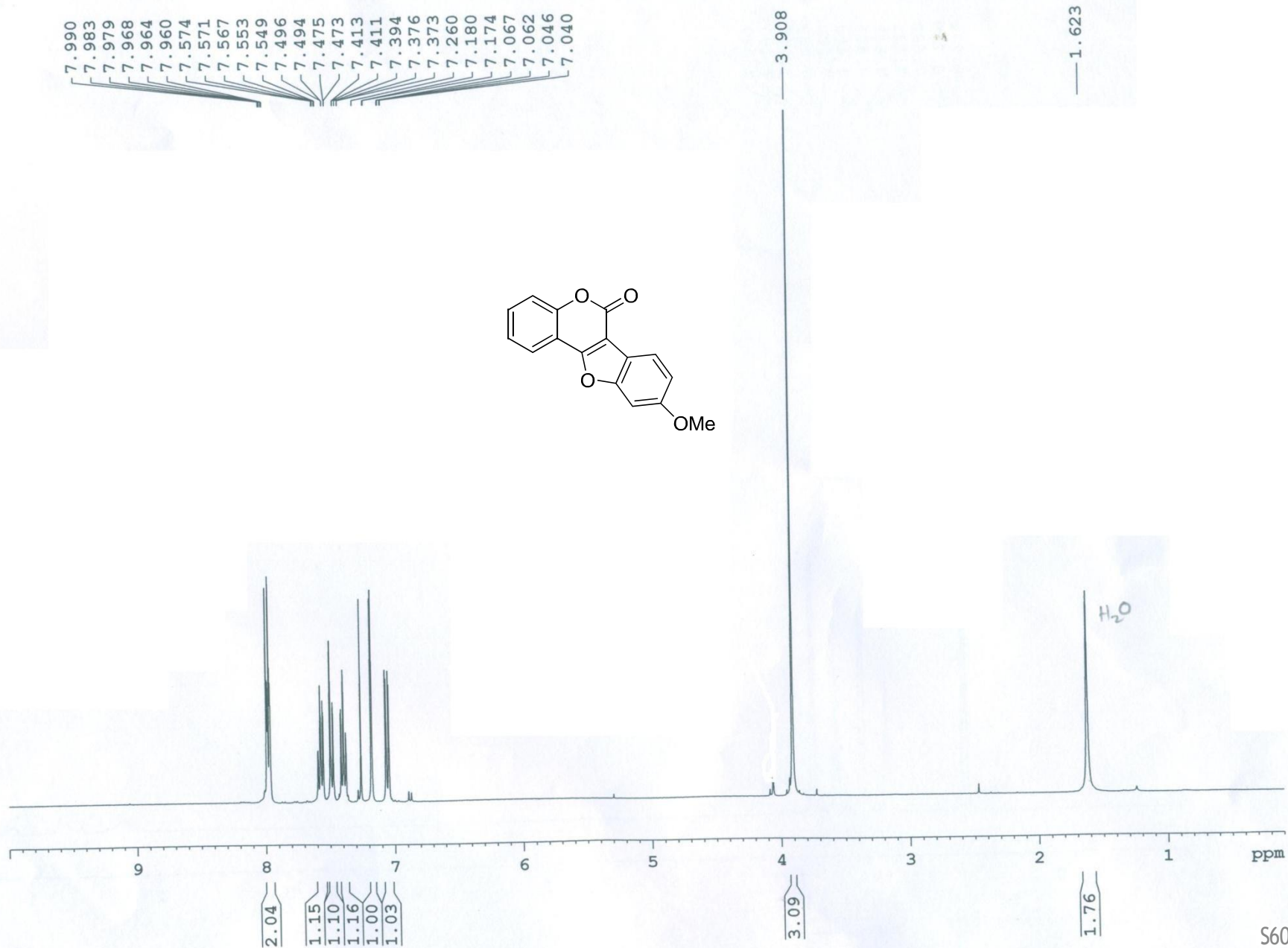
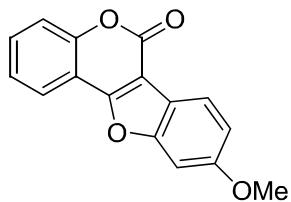
29.59

21.22



¹H of 9-methoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (4da)

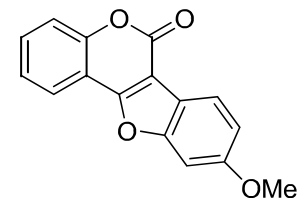
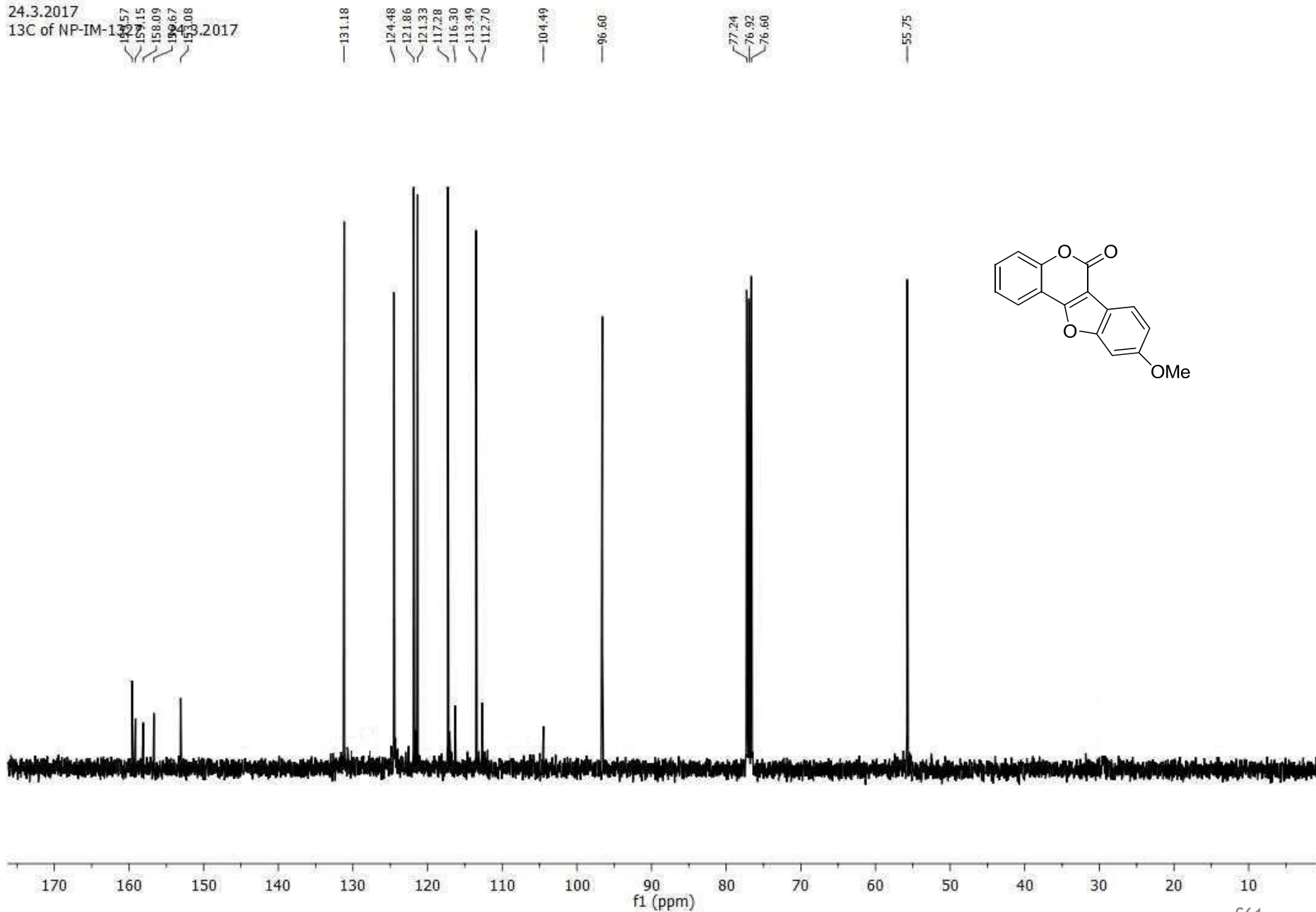
1H of NP-IM-4DA



¹³C of 9-methoxy-6H-benzofuro[3,2-c]chromen-6-one (4da)

24.3.2017

13C of NP-IM-132



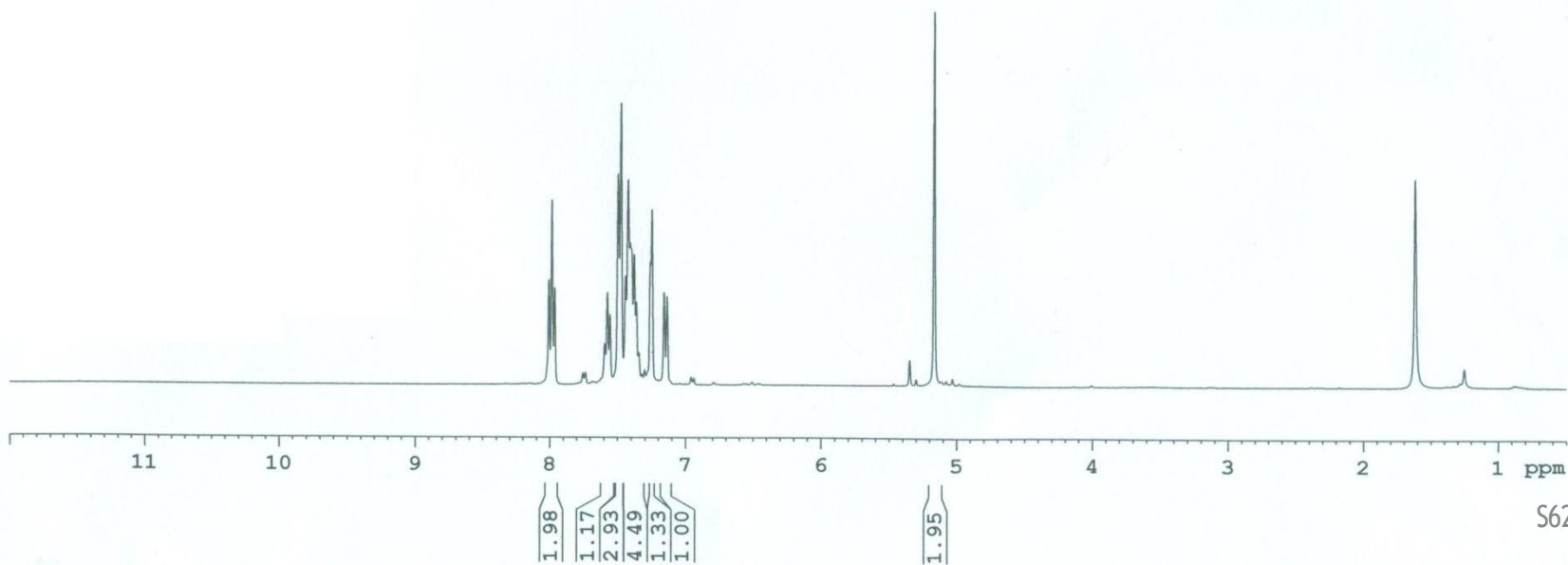
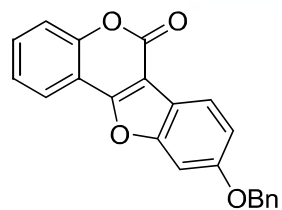
¹H of 9-(benzyloxy)-6*H*-benzofuro[3,2-*c*]chromen-6-one (4ea)

¹H of NP-IM-4EA

8.006
7.984
7.963
7.592
7.572
7.554
7.494
7.474
7.440
7.422
7.406
7.377
7.361
7.342
7.258
7.247
7.157
7.135

— 5.163

— 1.615

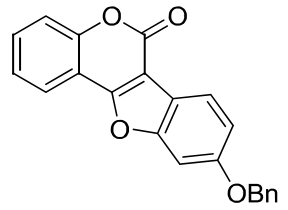
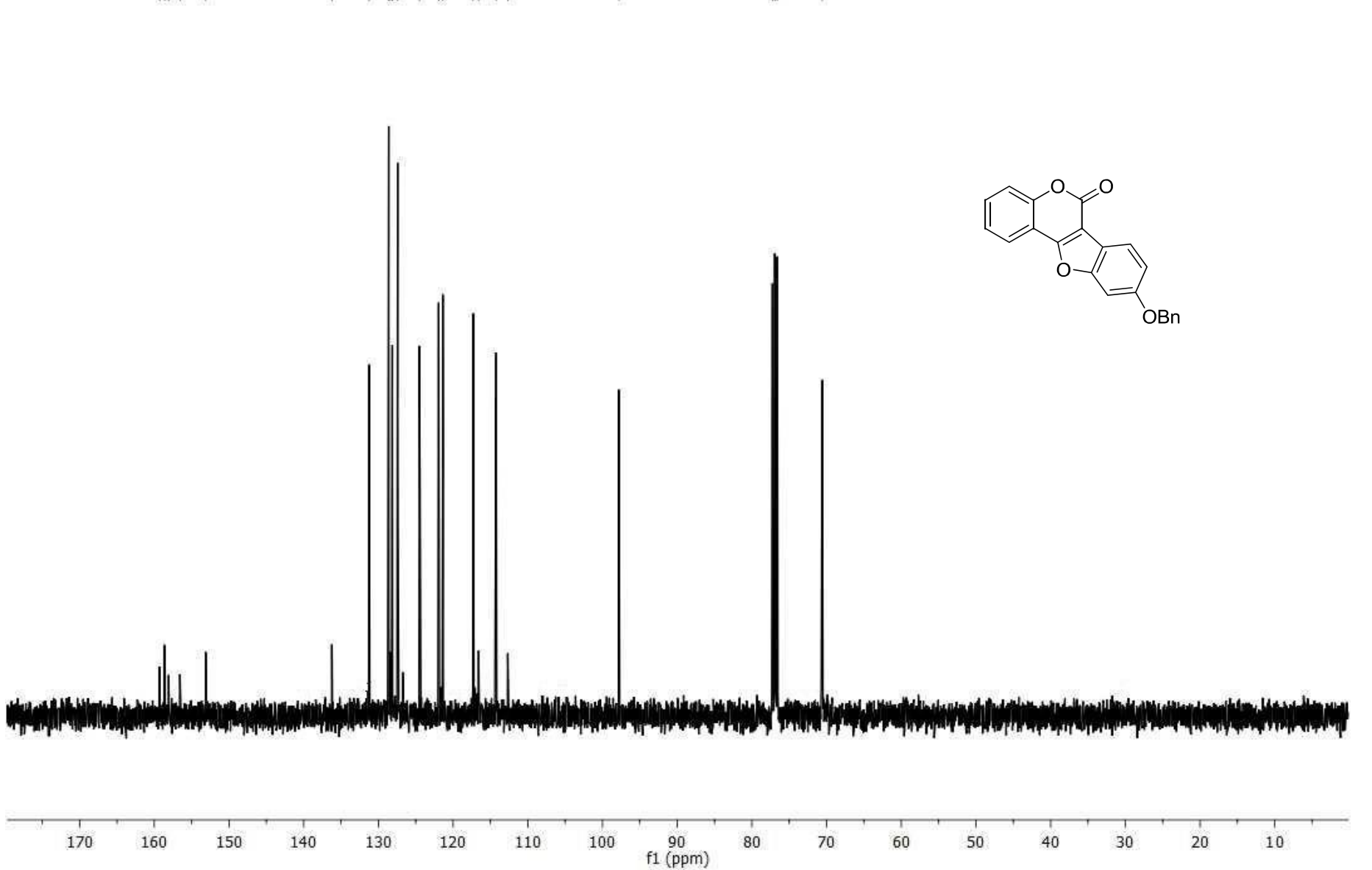


¹³C of 9-(benzyloxy)-6H-benzofuro[3,2-c]chromen-6-one (4da)

24.3.2017

13 C of NP-IM-132

24.3.2017

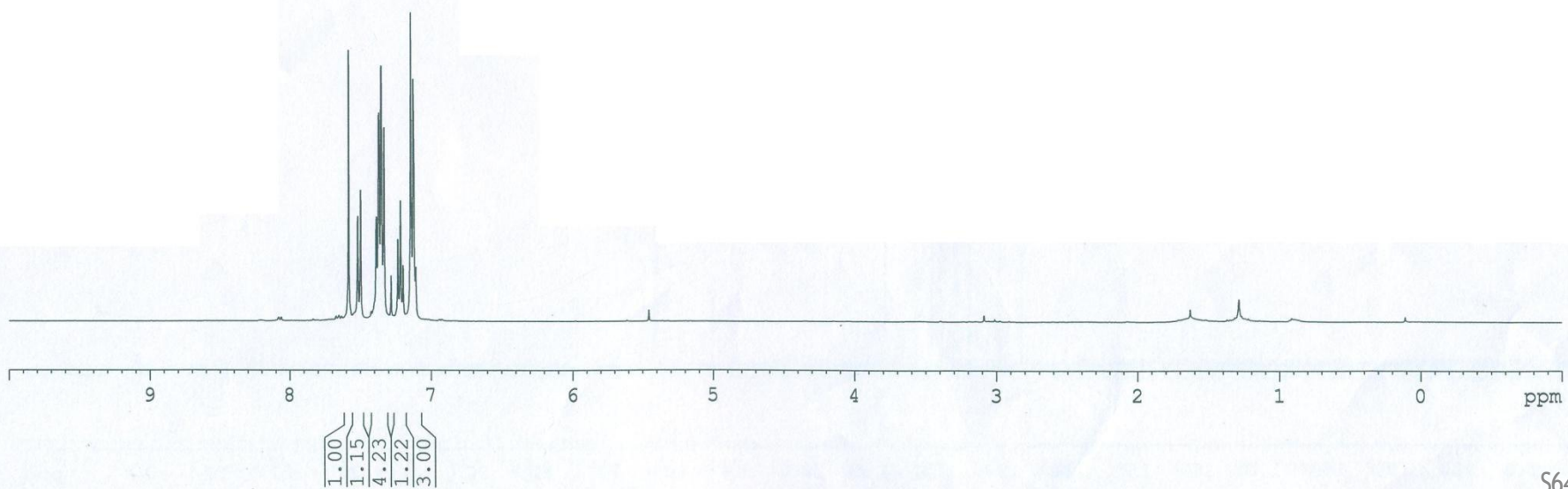
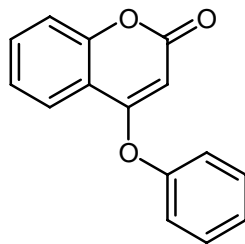


¹H NMR of 4-phenoxy-2H-chromen-2-one (5aa)

¹H of NP-IM-1027

15.6.2016

7.582
7.517
7.497
7.386
7.370
7.368
7.352
7.332
7.282
7.234
7.215
7.197
7.143
7.125
7.107



¹³C NMR of 4-phenoxy-2H-chromen-2-one (5aa)

¹³C of NP-IM-1027

— 157.63
— 154.05

— 139.87
— 132.97
— 129.66
— 124.98
— 123.10
— 122.62
— 122.04
— 119.28
— 116.73
— 112.10

— 77.35
— 77.03
— 76.71

