Supporting Information for

Efficient synthesis of novel pyrrolo[2,3-c]pyridone derivatives using Ugi four-component reaction followed by condensation reaction

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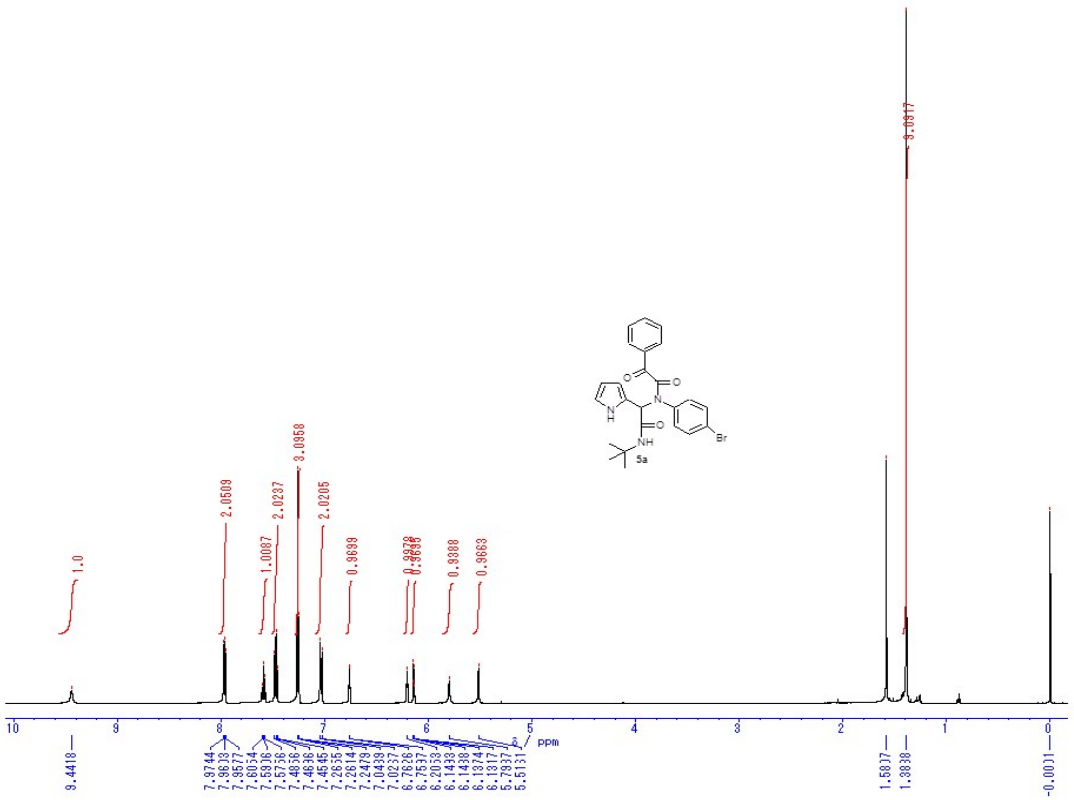
Experimental procedure for the PTSA promoted sequential one pot of synthesis pyrrolo[2,3-c]pyridone (6a):

Pyrrole-2-carbaldehyde (1 mmol), 4-bromo aniline (1 mmol), phenylglyoxylic acid (1.2 mmol) and *t*-butyl isocyanide (1 mmol) were taken in 3 mL methanol. This mixture was stirred at room temperature for 60 min and PTSA (50 mol%) was added to the same reaction mixture and heated at 50^{o}C for 2h. The volatiles were removed under reduced pressure and product 6a was purified by flash column chromatography in 70% yield.

Table 1. Crystal data and structure refinement for **6g**

CCDC number	1484244
Empirical formula	$2C_{25}H_{24}BrN_3O_3 \cdot 2H2O$
Formula weight	1024.80
Temperature	90K
Wavelength	0.71073A
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a= 17.720 (4) alpha=90 deg. b= 9.681(2) beta= 107.915(2) deg. c = 27.874(6) gamma=90 deg.
Volume	4549.9 (18) $Å^3$
Z	4
Absorption correction	Semiemperical from equivalents
Goodness of fit	1.13
Theta range for data collection	1.22 to 25.01 deg.
Refinement method	Full-matrix least sqares
Crystal size	0.40 × 0.15 × 0.15 mm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5a
Br
ppm
9.4418
7.9744
7.9638
7.9577
7.6054
7.5936
7.5756
7.4856
7.4636
7.4545
7.2655
7.2614
7.2479
7.0439
7.0237
6.7626
6.7537
6.2033
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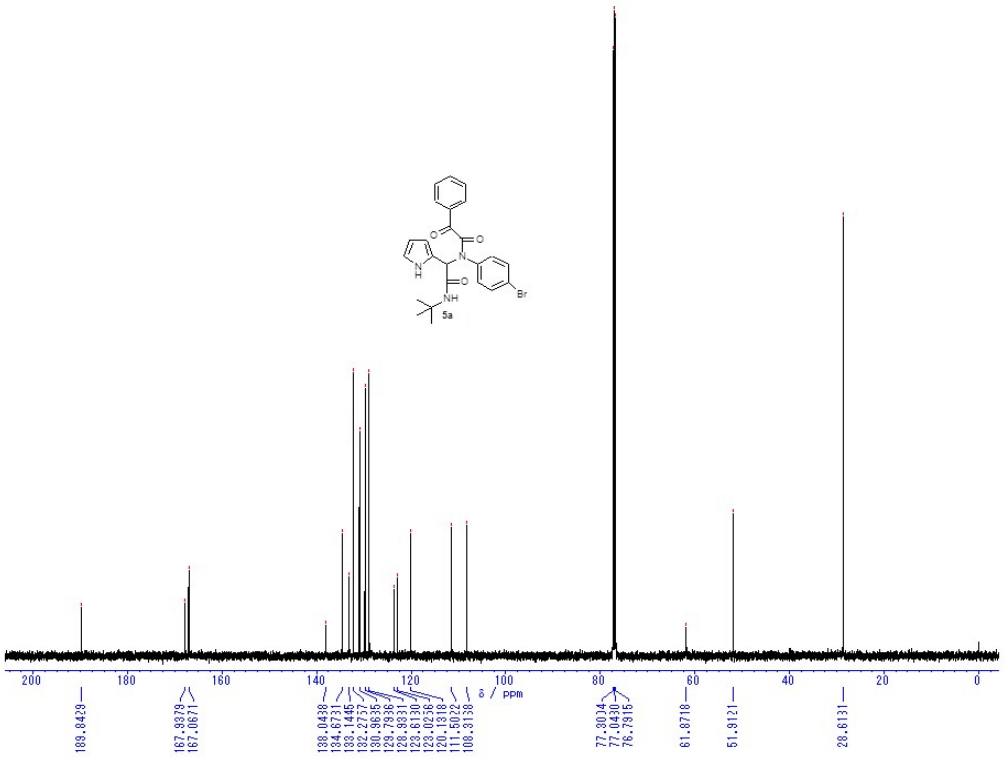
6.1438
6.1374
6.1317
5.7937
5.5131
1.5837
1.3838
-0.0031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200
180
160
140
120
100
80
60
40
20
0
δ / ppm
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167.0671
138.0438
134.6731
133.1445
132.2757
130.9635
129.7936
128.8831
123.6130
123.0256
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111.5022
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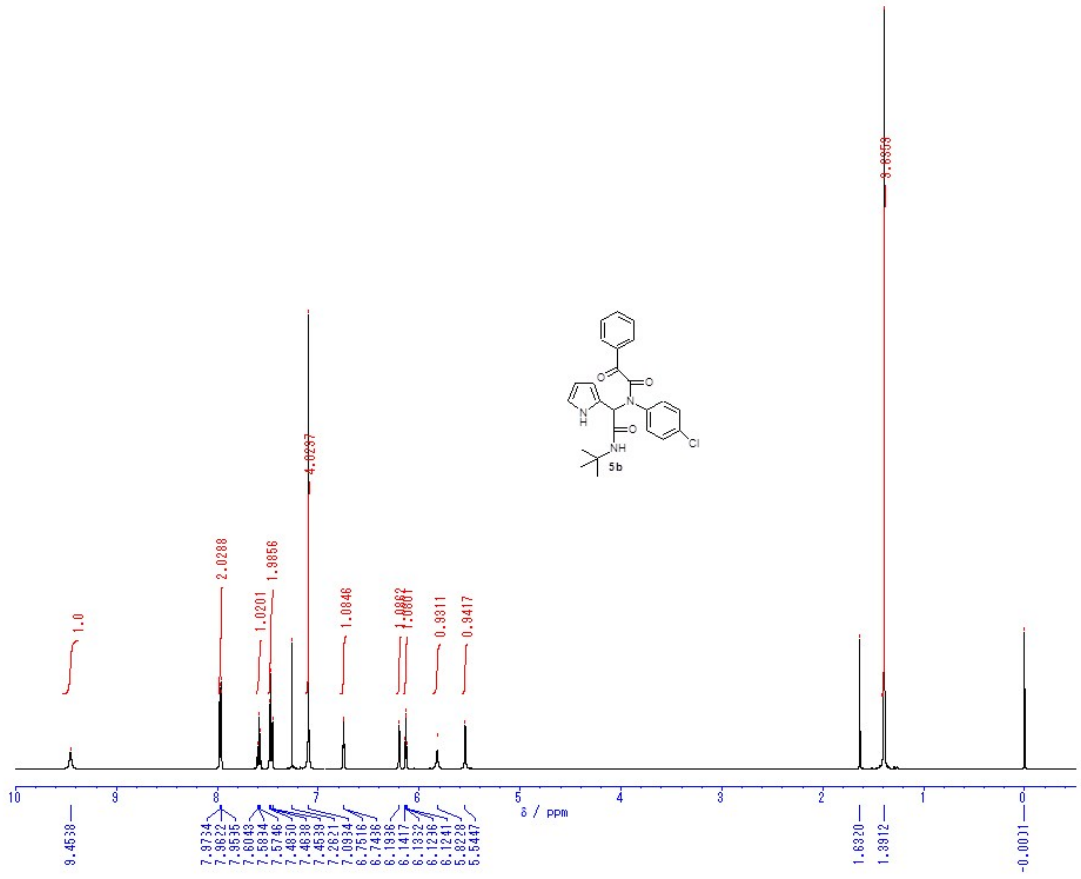
76.7916
61.8718
51.9121
28.6131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1.0201
4.0237
1.0846
0.9311
0.9417
8.8858
δ / ppm
9.4538
7.8734
7.8622
7.8535
7.6043
7.5834
7.5746
7.4650
7.4638
7.4539
7.2621
7.0934
6.7516
6.7438
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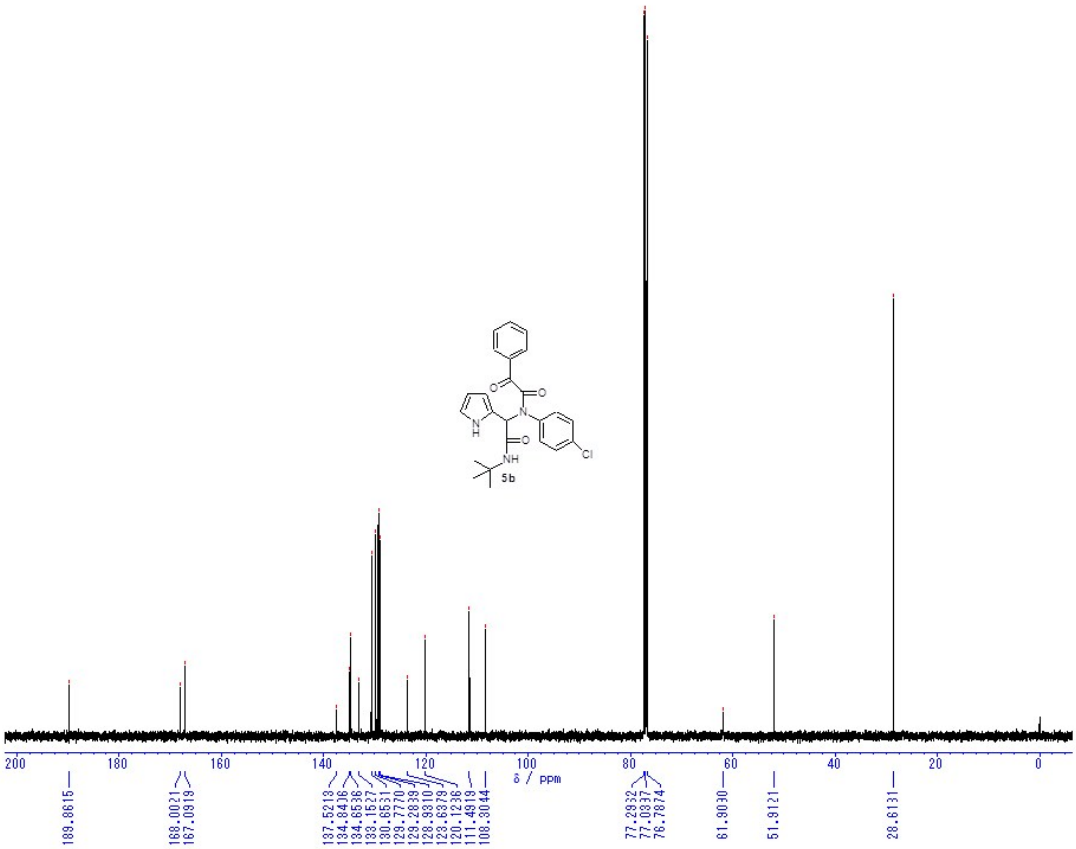
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O
N
Cl
O
NH
5b
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
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168.0021
167.0819
137.5218
134.8436
134.6536
133.1527
130.8531
129.7770
129.2839
128.3810
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77.0837
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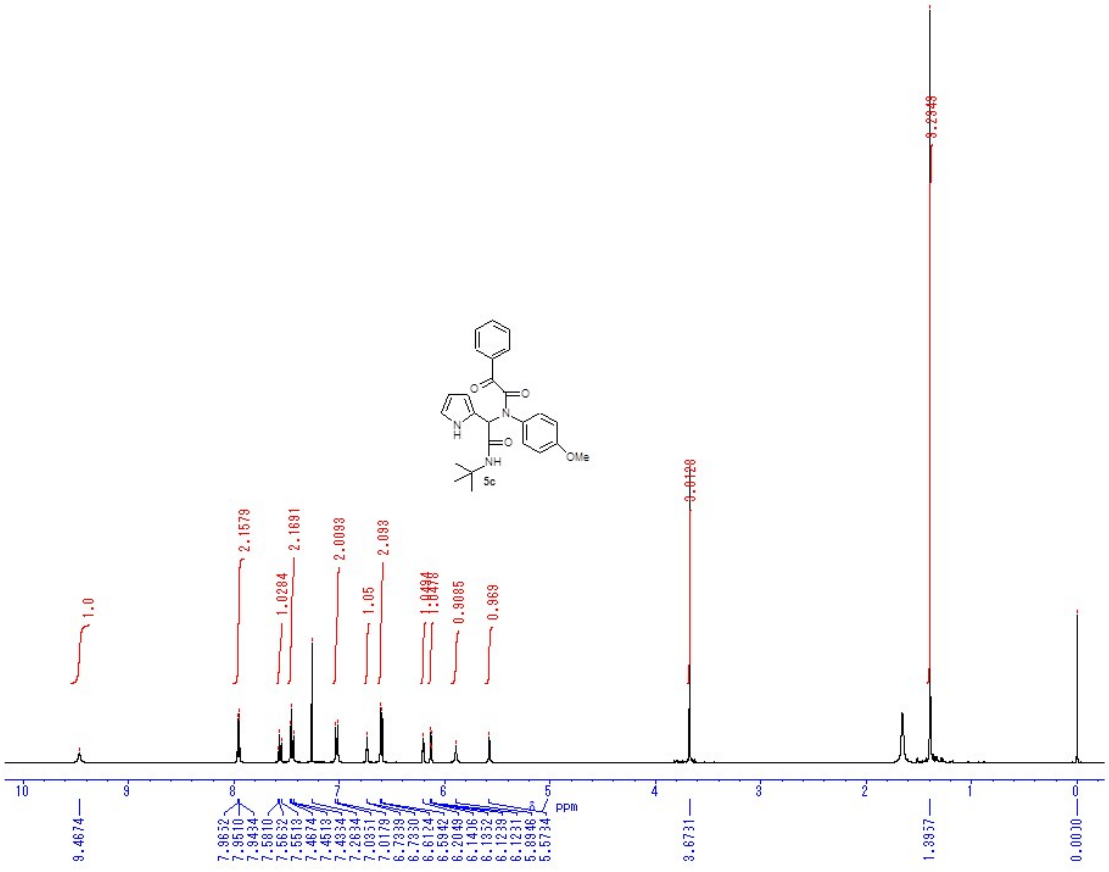
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5c
OMe
ppm
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7.3852
7.3610
7.8434
7.6010
7.6632
7.5513
7.4674
7.4613
7.4334
7.2634
7.0351
7.0179
6.7839
6.7330
6.6124
6.5842
6.2049
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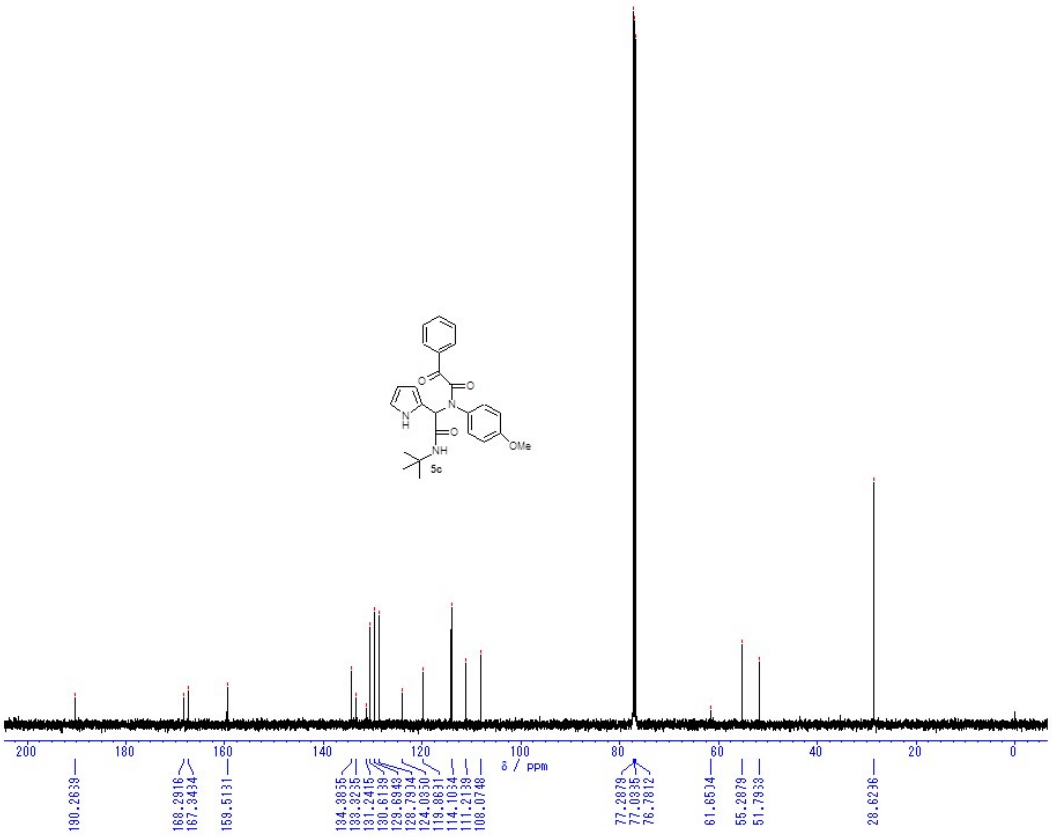
O
O
N
H
O
NH
OMe
5c
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180
160
140
120
100
80
60
40
20
0
δ / ppm
190.2638
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167.3434
159.5131
134.3856
133.3235
131.2415
130.6139
129.6948
128.7934
124.0350
119.8631
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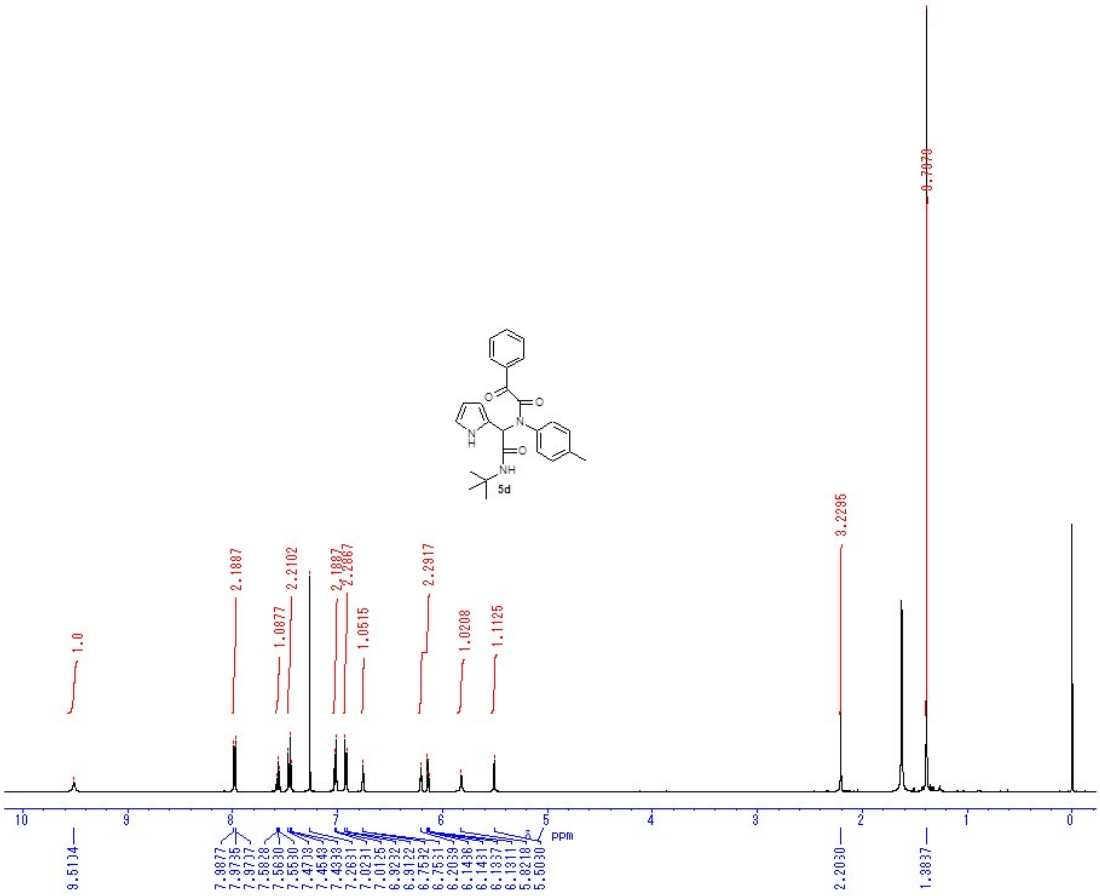
28.6236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3.2295
9.0970
5d
10
9
8
7
6
5
4
3
2
1
0
PPM
9.5134
7.9877
7.9735
7.9737
7.5828
7.5630
7.5530
7.4733
7.4543
7.4339
7.2831
7.1031
7.0125
6.8232
6.8122
6.7932
6.7551
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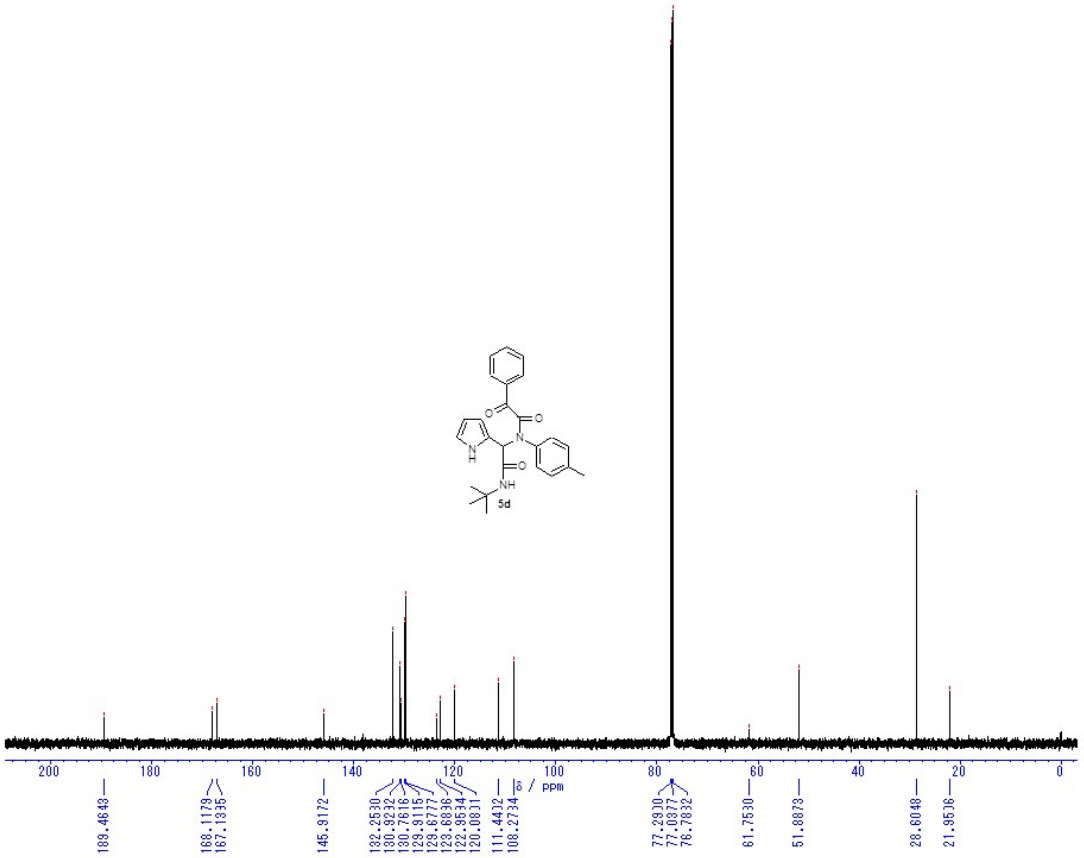
6.1337
6.1311
5.8218
5.5030
2.2030
1.3837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180
160
140
120
100
80
60
40
20
0
δ / ppm
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145.8172
132.2530
130.9232
130.7616
129.9115
129.6777
123.6836
122.9534
120.0831
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77.0377
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61.7530
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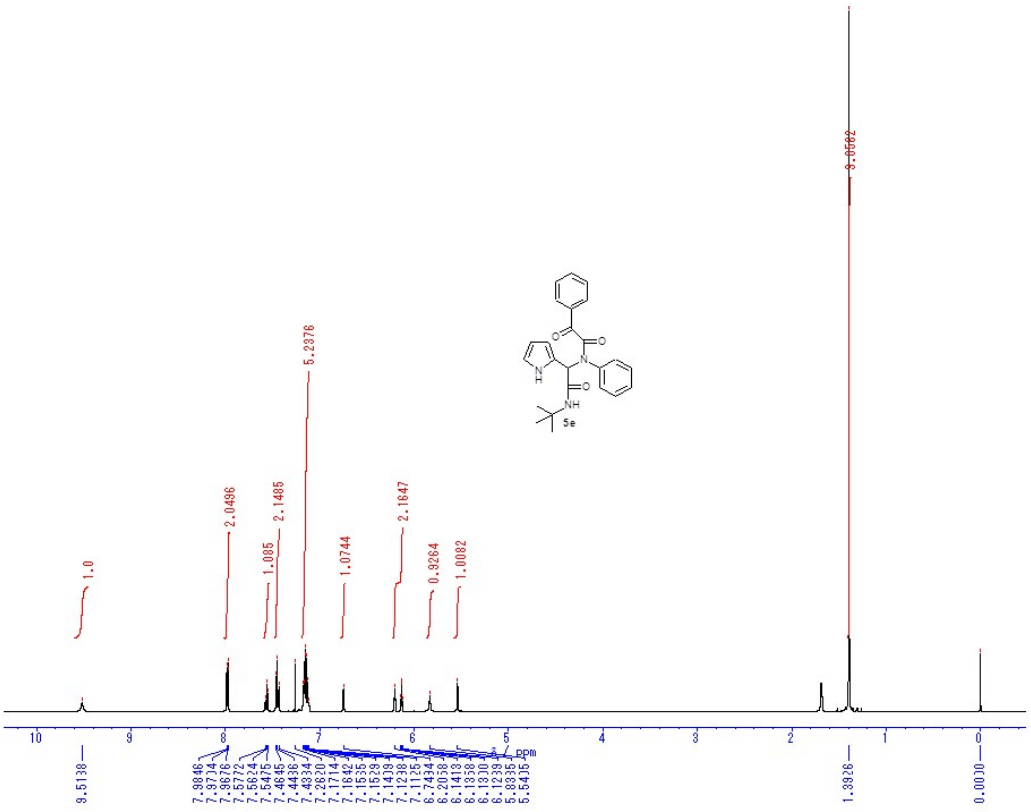
21.9536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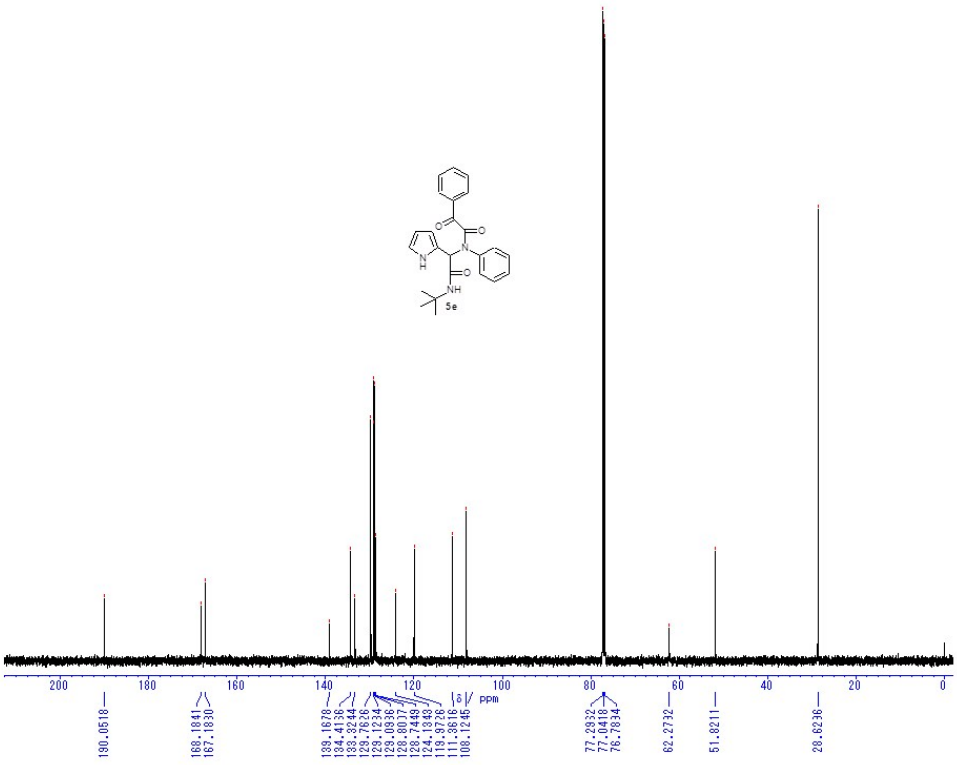
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180
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140
120
100
80
60
40
20
0
δ / ppm
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139.1678
134.4136
133.3244
129.3676
129.1234
129.0936
128.8037
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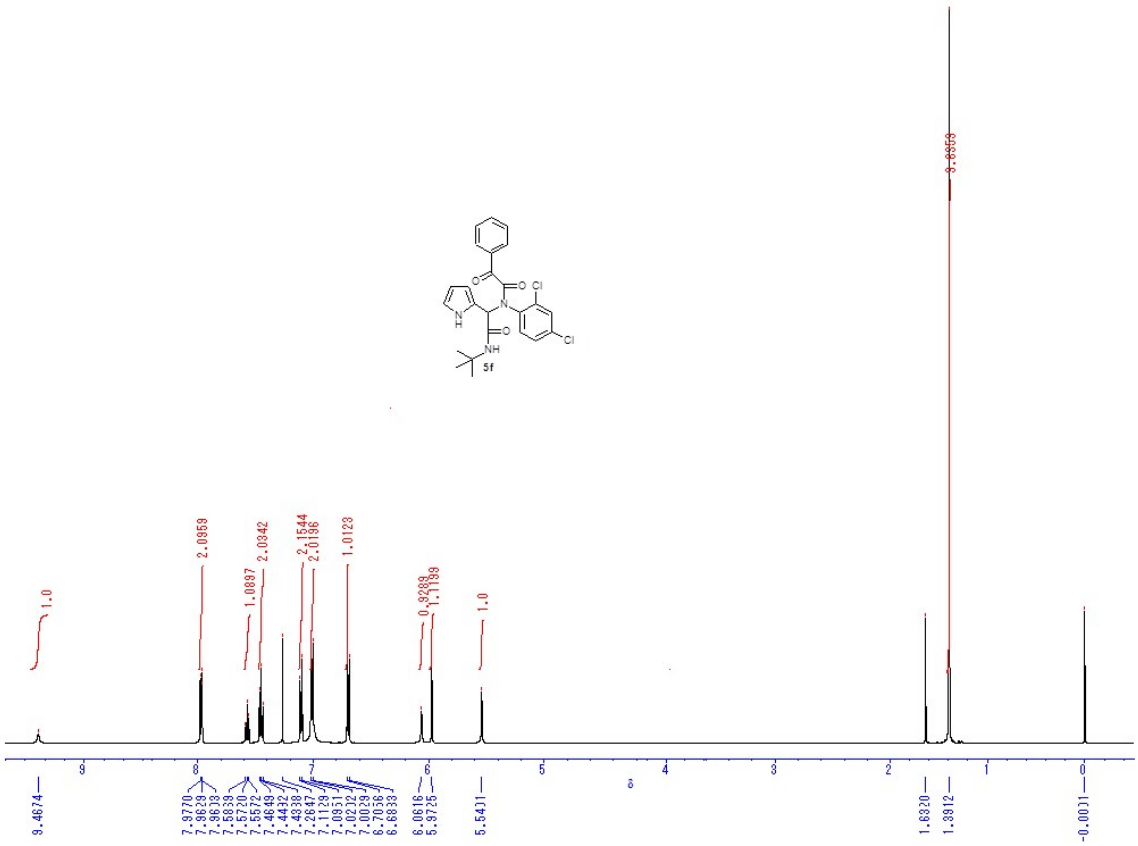
51.8211
28.8236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3.6859
9.4674
7.9770
7.9629
7.9613
7.5839
7.5720
7.5572
7.4649
7.4432
7.4338
7.2647
7.1129
7.0931
7.0232
7.0029
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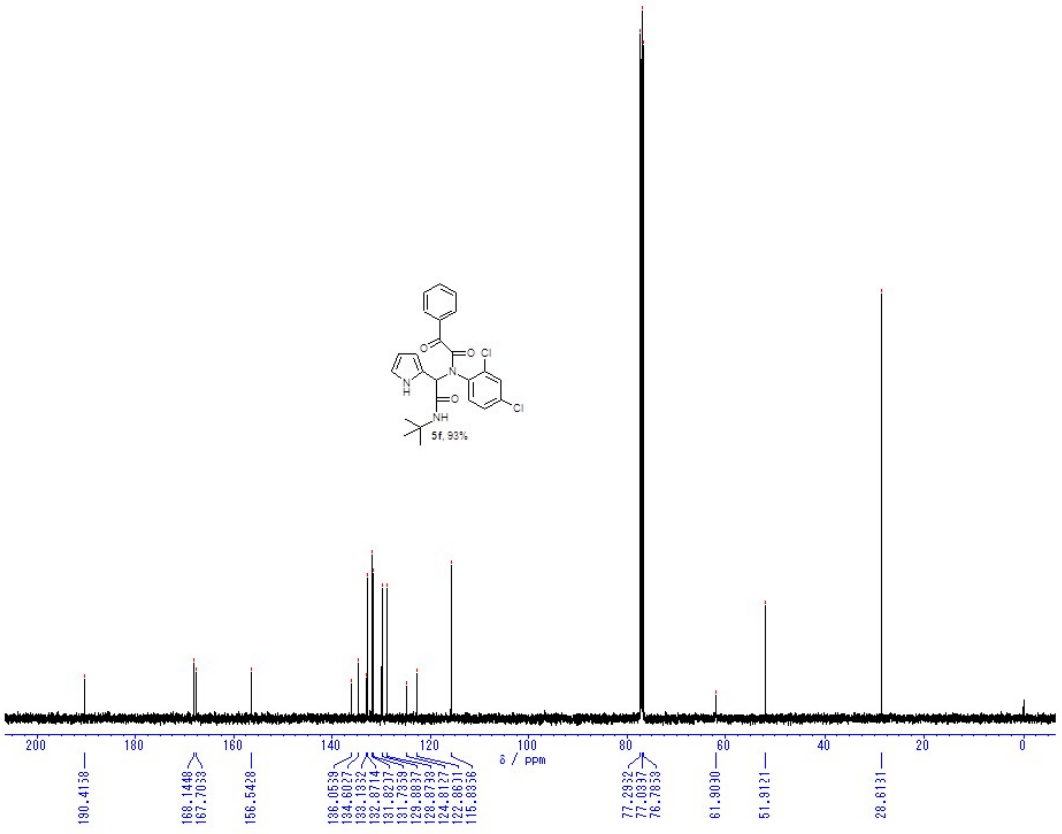
δ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200
180
160
140
120
100
80
60
40
20
0
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136.0539
134.6027
133.1832
132.8714
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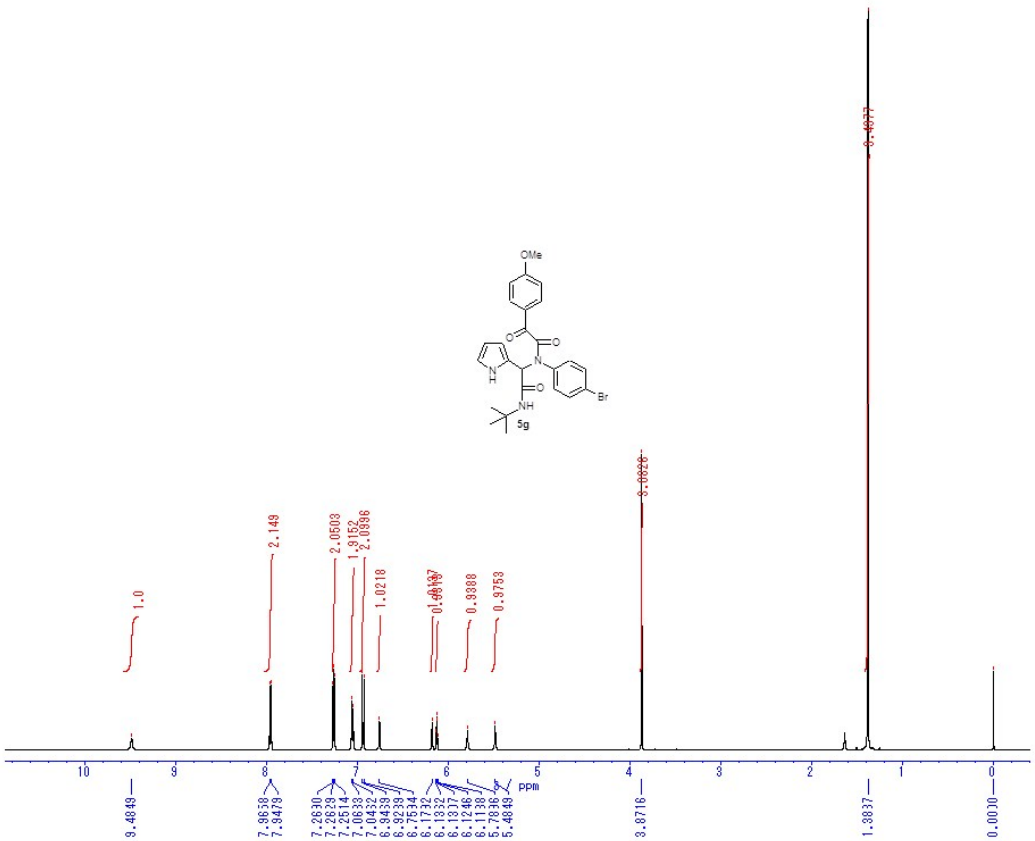
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N
H
O
NH
Br
tBu
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0.9388
0.9753
3.8716
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7.9479
7.2630
7.2629
7.2514
7.0633
7.0432
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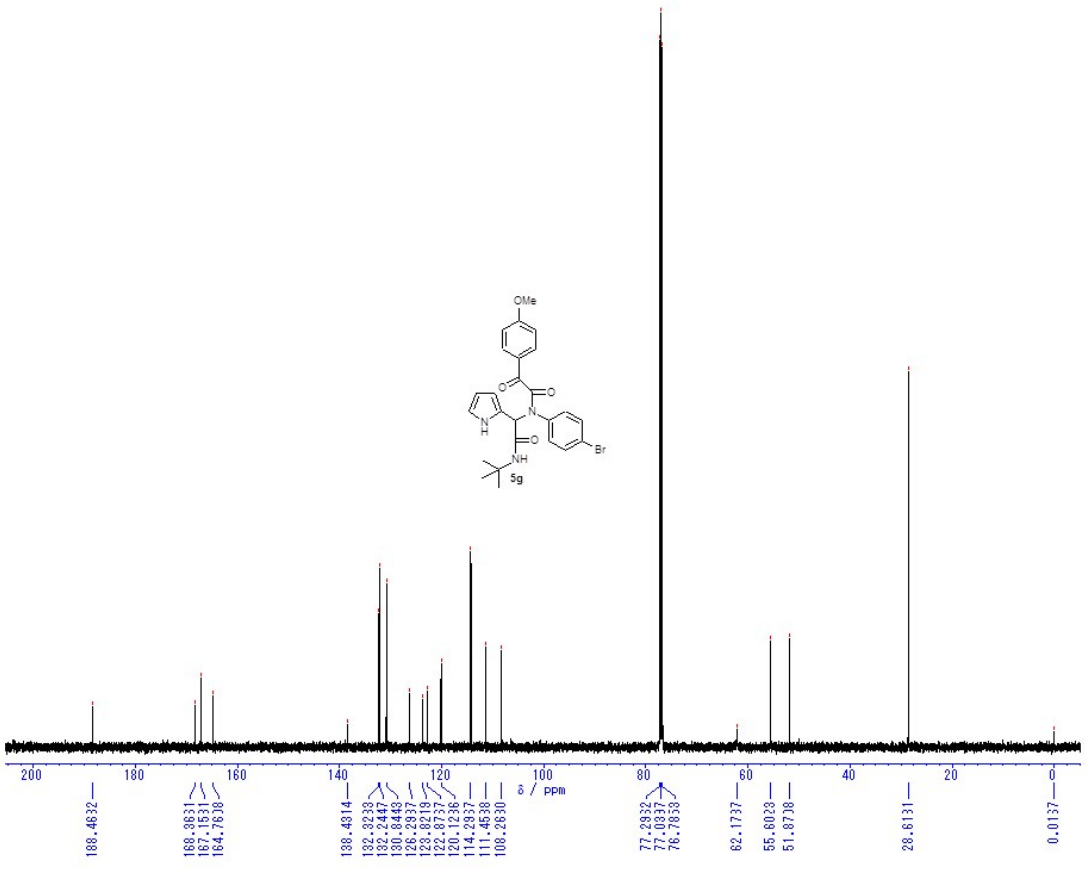
ppm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O
O
N
H
O
NH
Br
5g
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.4632
168.3631
167.1531
164.7638
138.4314
132.3238
132.2447
130.8448
126.2937
123.8219
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114.2937
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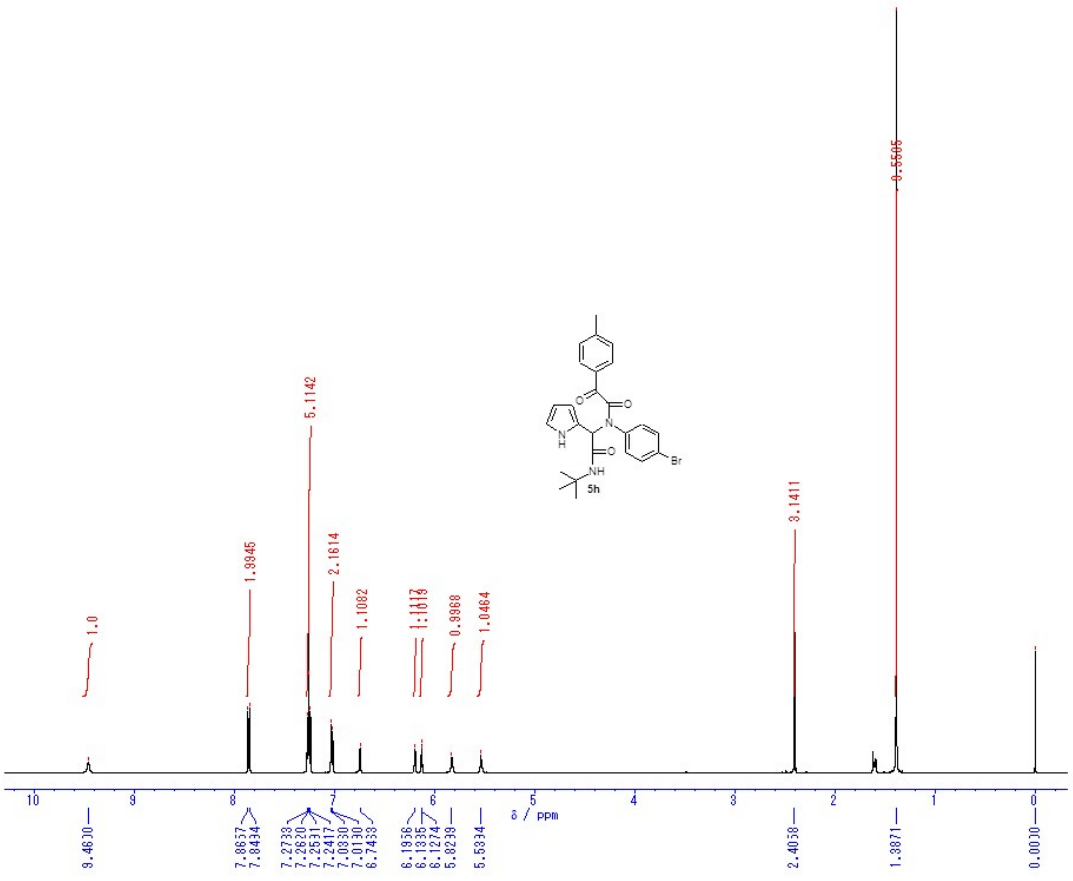
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1.1018
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1.0464
3.1411
6.5505
O
O
N
H
O
NH
Br
5h
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.4630
7.8857
7.8434
7.2733
7.2620
7.2531
7.2417
7.0330
7.0130
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5.5334
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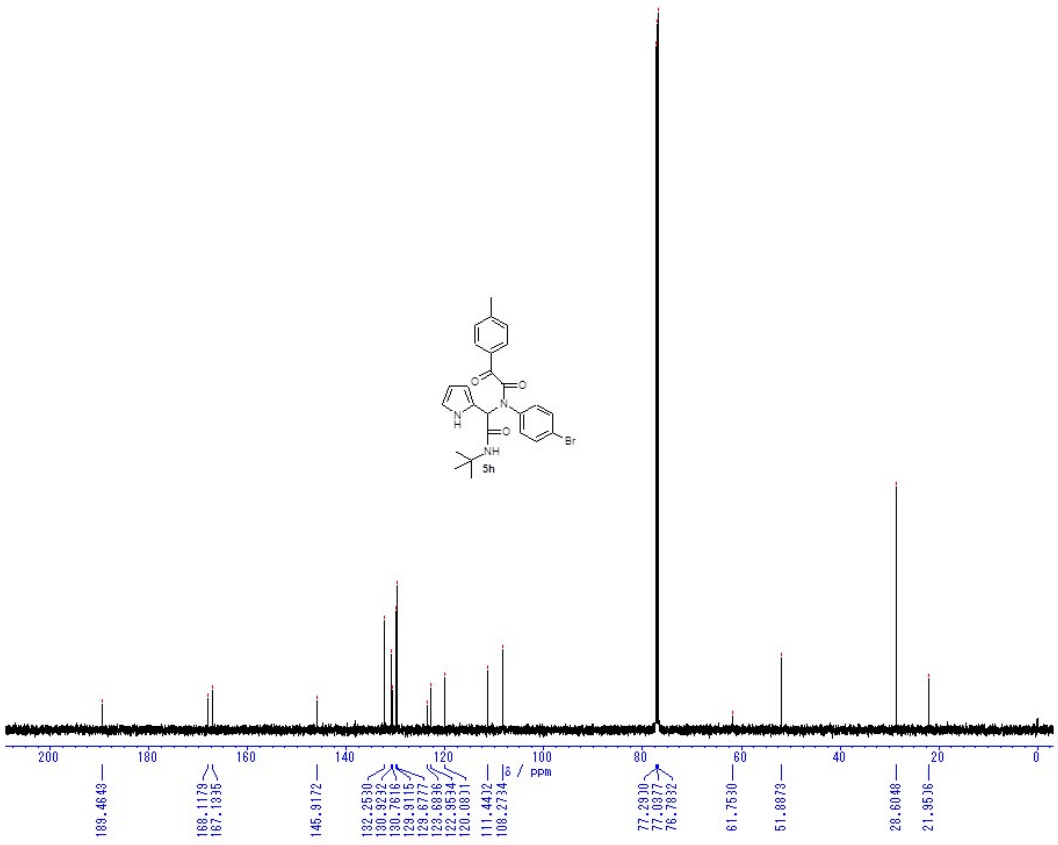
O
O
O
N
H
O
NH
Br
5h
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
189.4643
168.1178
167.1335
145.9172
132.2530
130.8232
130.7616
129.9115
129.6777
123.6836
122.9534
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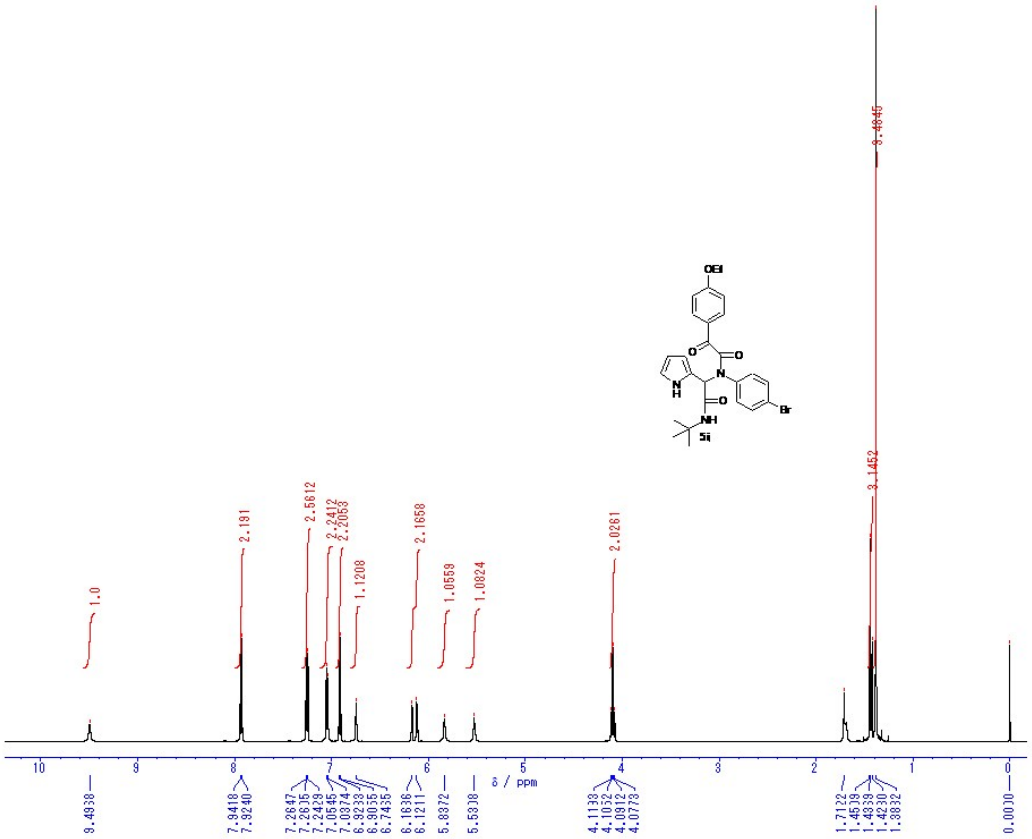
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O
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H
N
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NH
Si
Br
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1.1208
2.1658
1.0559
1.0824
2.0261
3.1452
3.4645
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.4938
7.9418
7.9240
7.2647
7.2635
7.2429
7.0545
7.0374
6.9233
6.9036
6.7436
6.1836
6.1211
5.8372
5.5338
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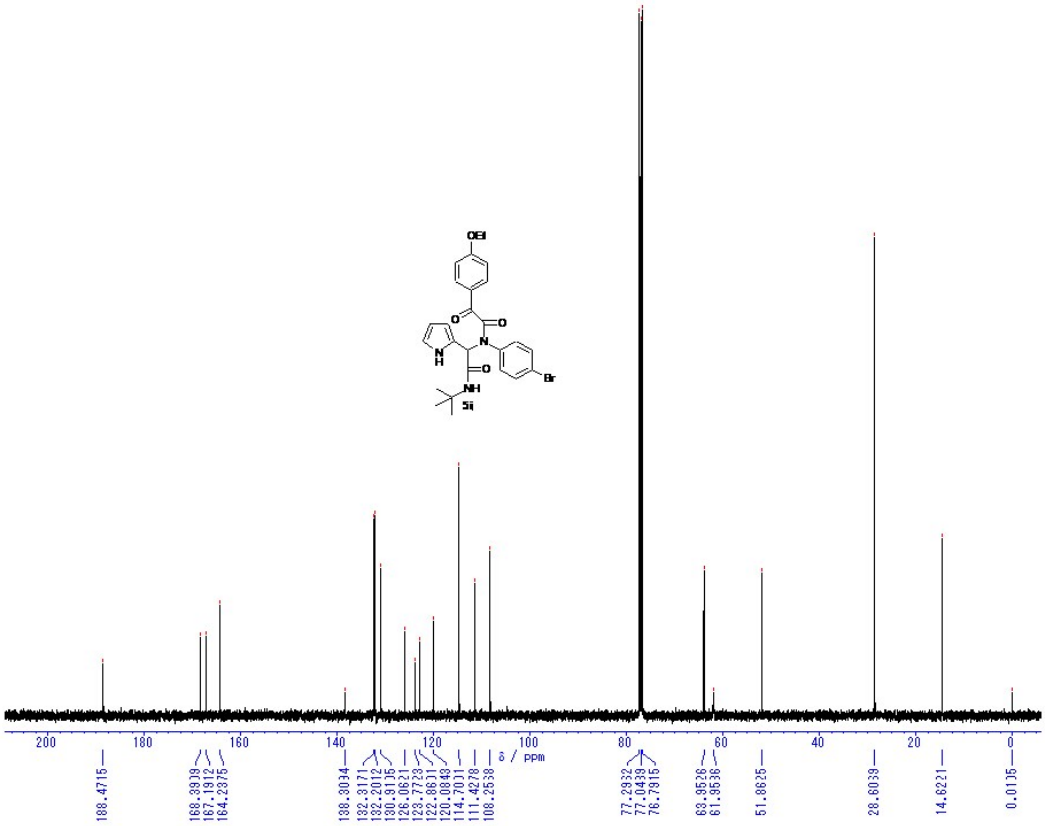
OH
O
O
N
H
N
O
NH
Br
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.4715
168.3939
167.1912
164.2376
138.3034
132.3171
132.2012
130.9135
126.0621
123.7723
122.8631
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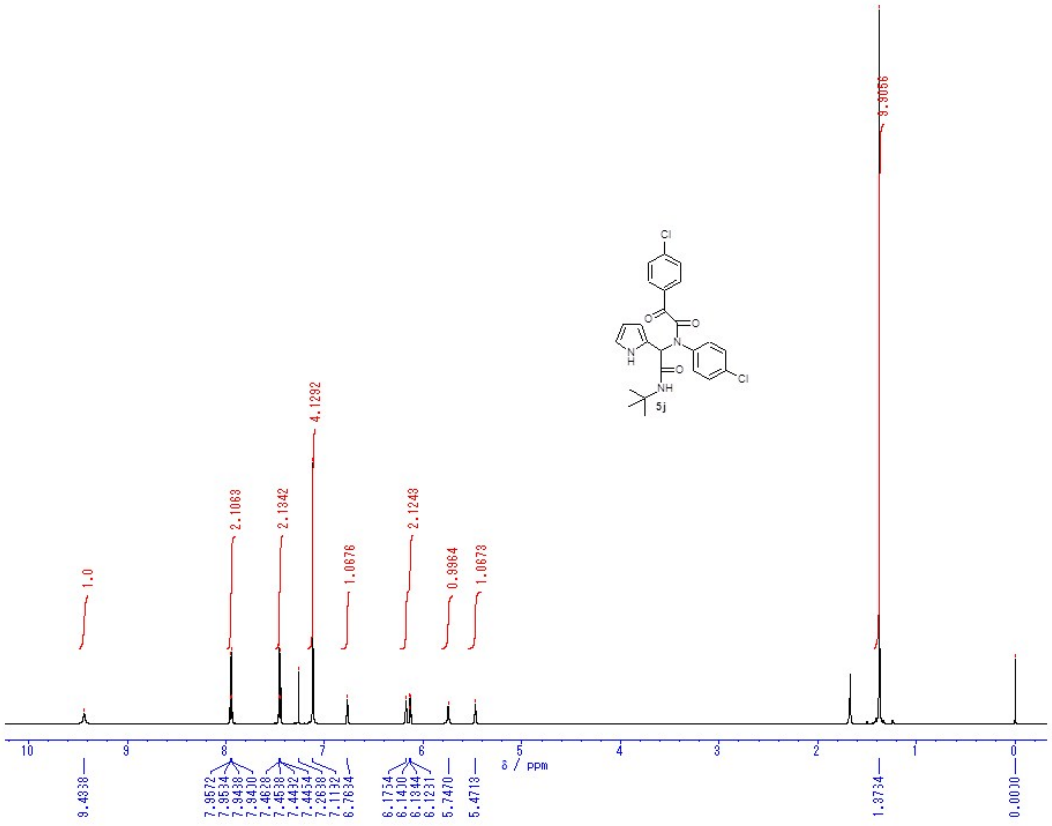
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O
N
H
O
NH
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Cl
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2.1243
1.0676
0.9984
1.0673
1.0
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.4838
7.9572
7.9534
7.8438
7.8410
7.4628
7.4598
7.4432
7.4434
7.2638
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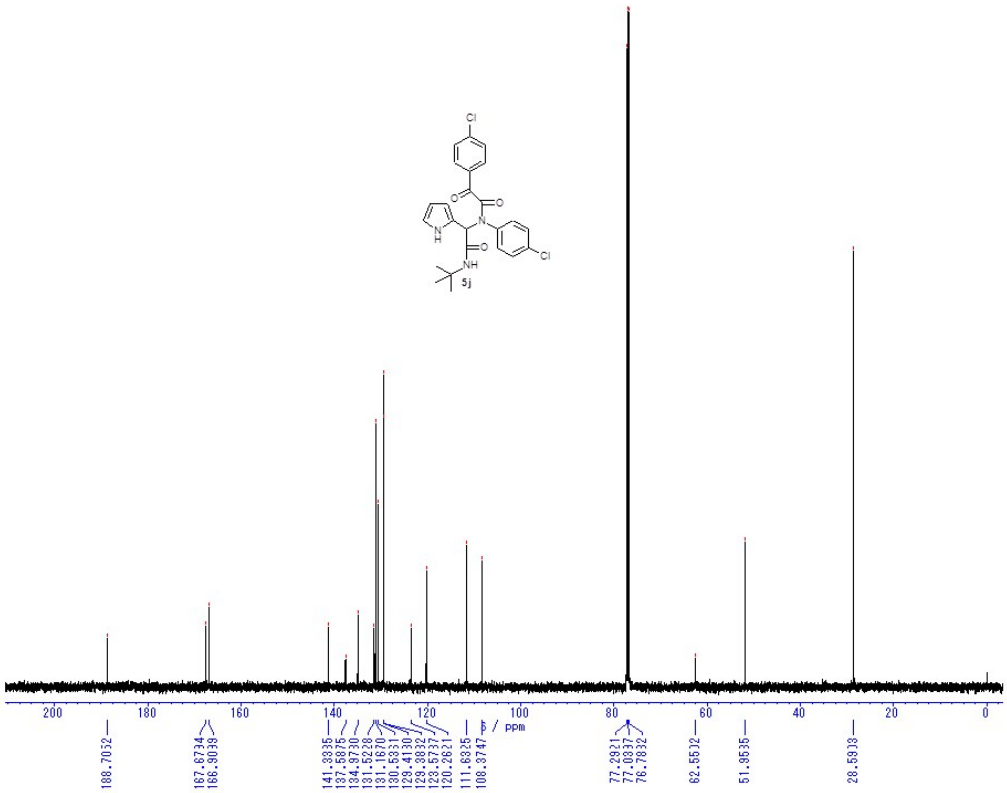
Cl
O
O
N
O
NH
Cl
5j
200
180
160
140
120
100
80
60
40
20
0
f1 / ppm
188.7032
167.6734
166.3039
141.3335
137.5875
134.9730
131.5238
131.1330
130.5331
129.4130
129.3832
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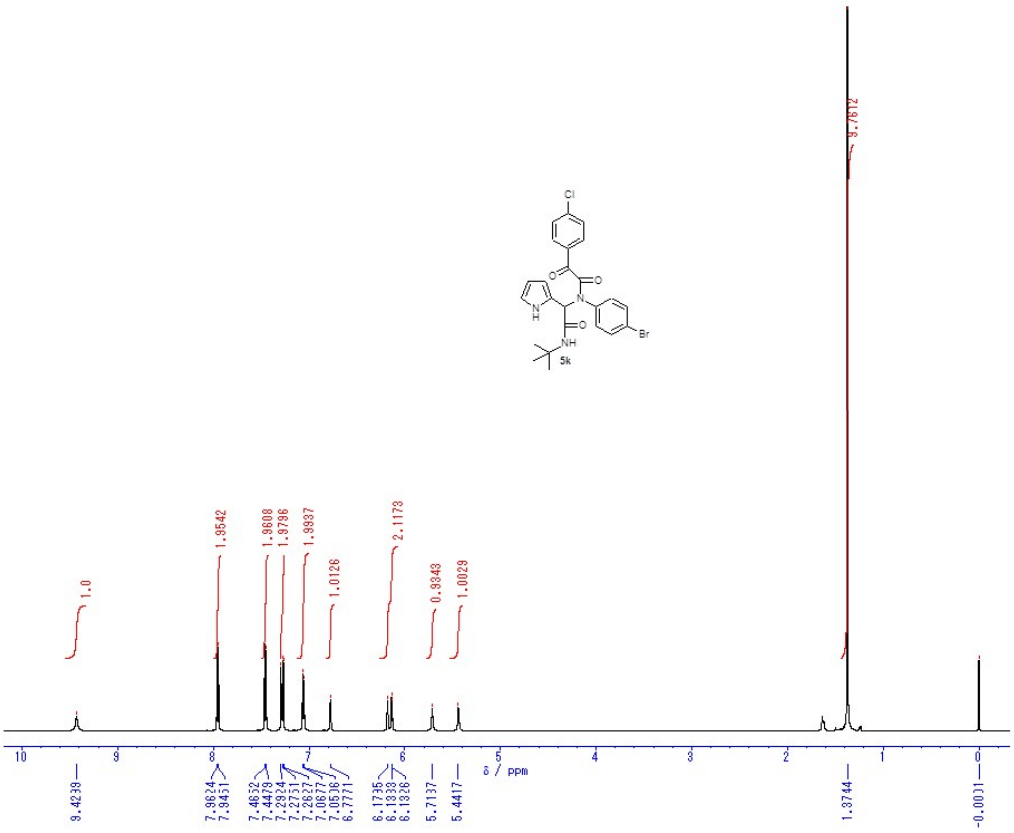
76.7832
62.5532
51.9535
28.5938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O
N
H
O
NH
Br
tBu
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1.0
1.8542
1.9808
1.9796
1.9837
1.0126
2.1178
0.8348
1.0029
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
9.4239
7.9824
7.9451
7.4632
7.4478
7.4324
7.2827
7.0677
7.0536
6.7771
6.1735
6.1333
6.1338
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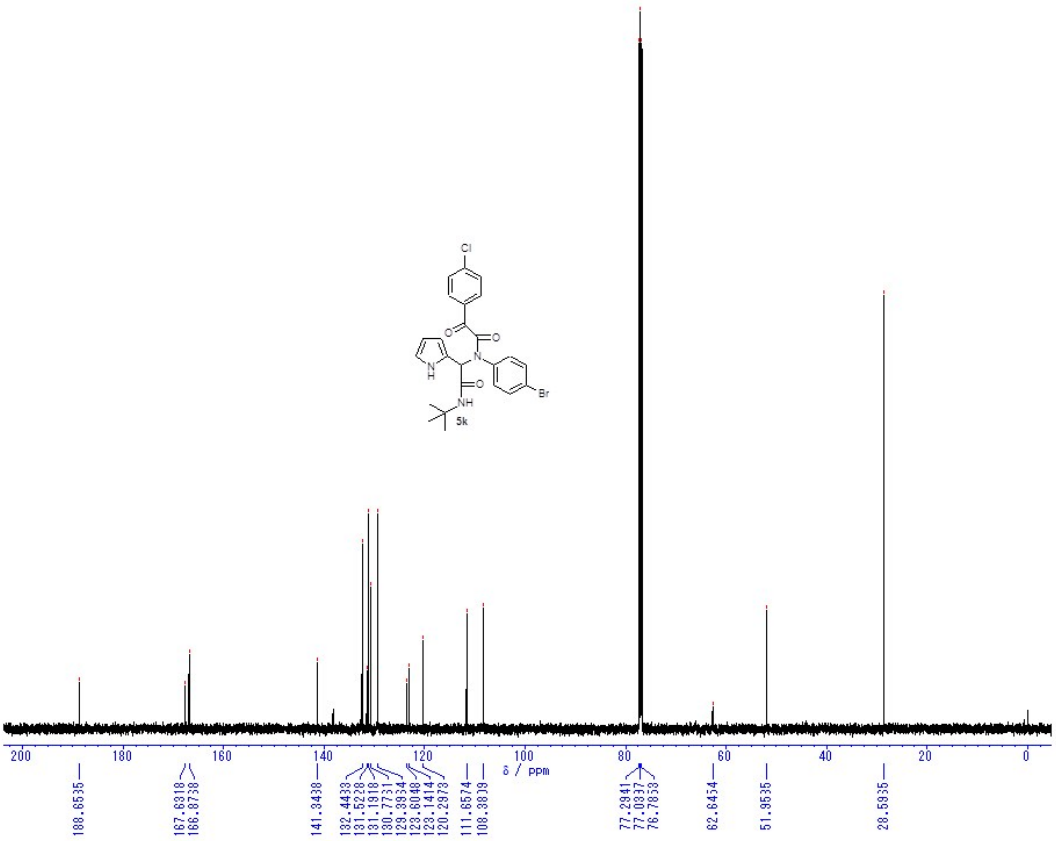
5.4417
1.3744
-0.0031

Star


Cl
O
O
N
H
O
NH
Br
5k
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.6535
167.6318
166.8738
141.3438
132.4433
131.5228
131.1918
130.7731
129.3934
123.6048
123.1414
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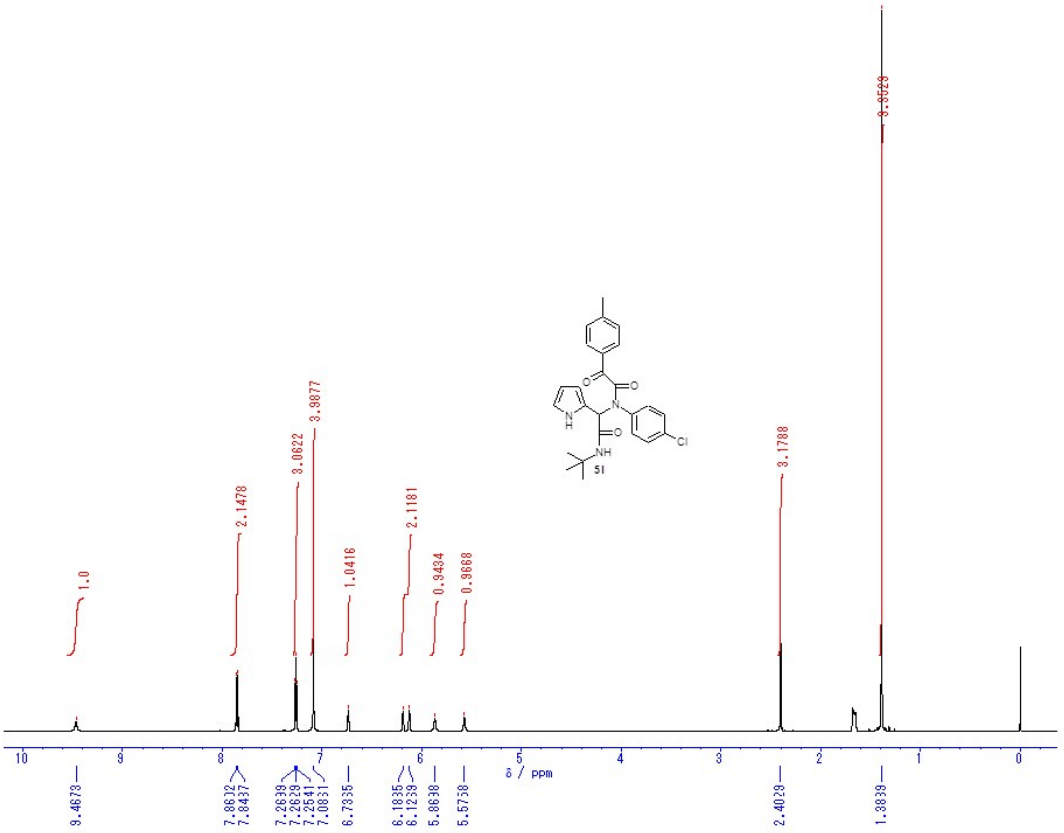
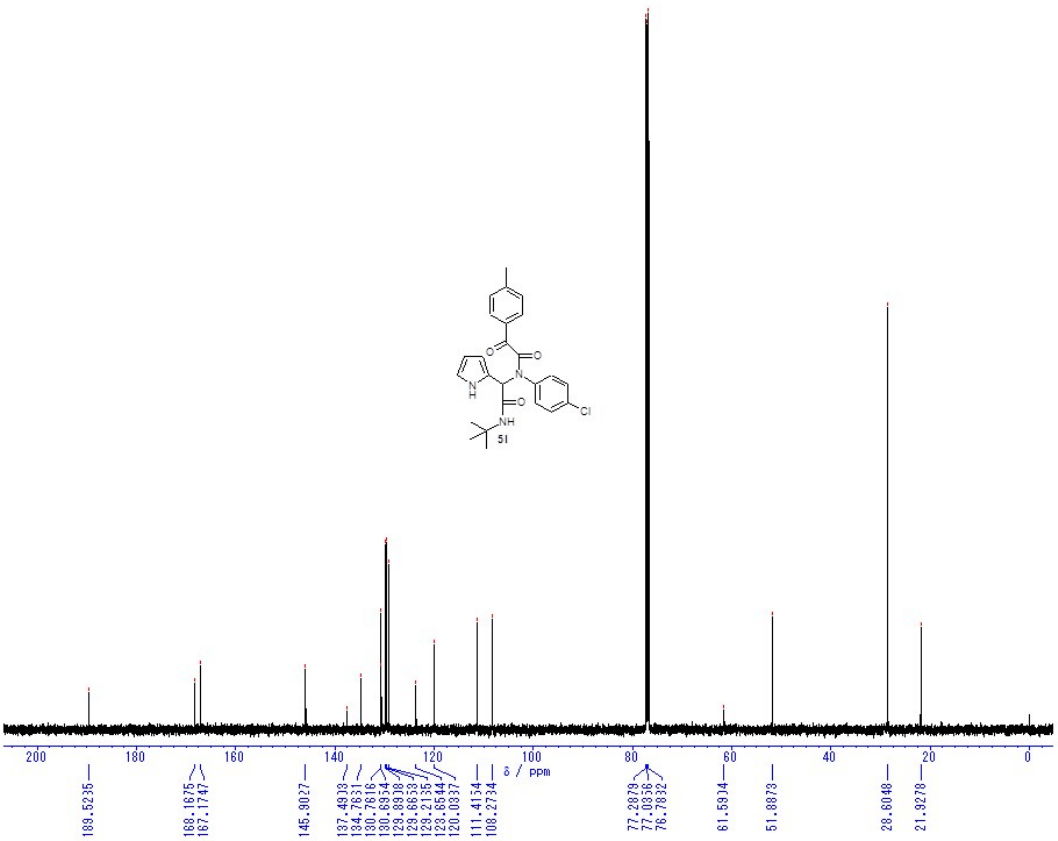
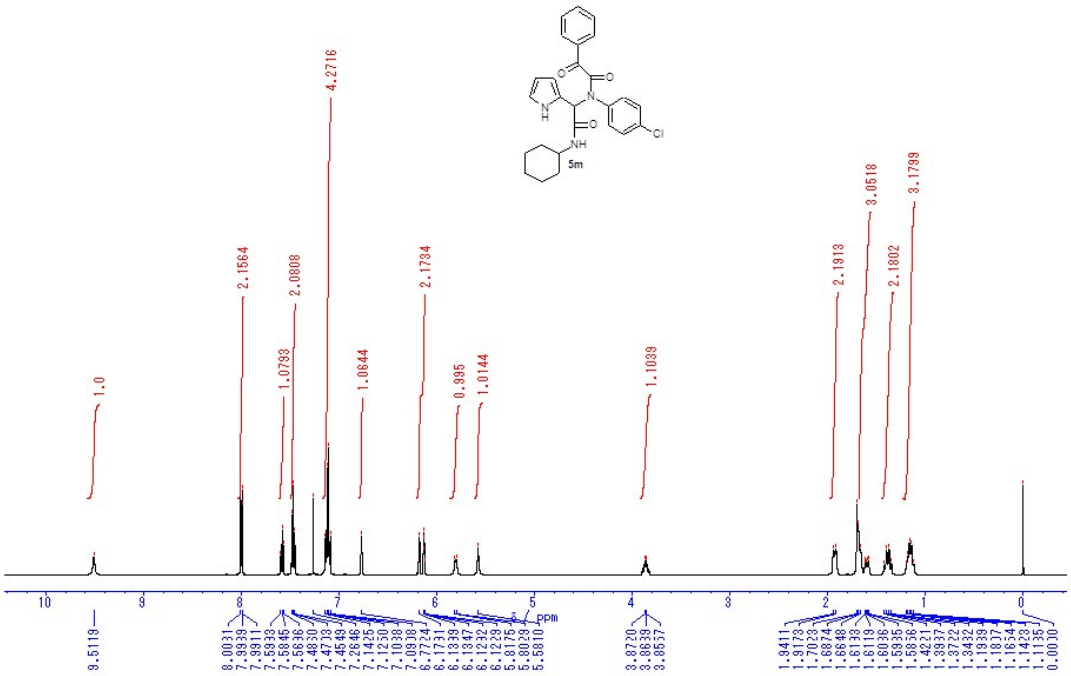
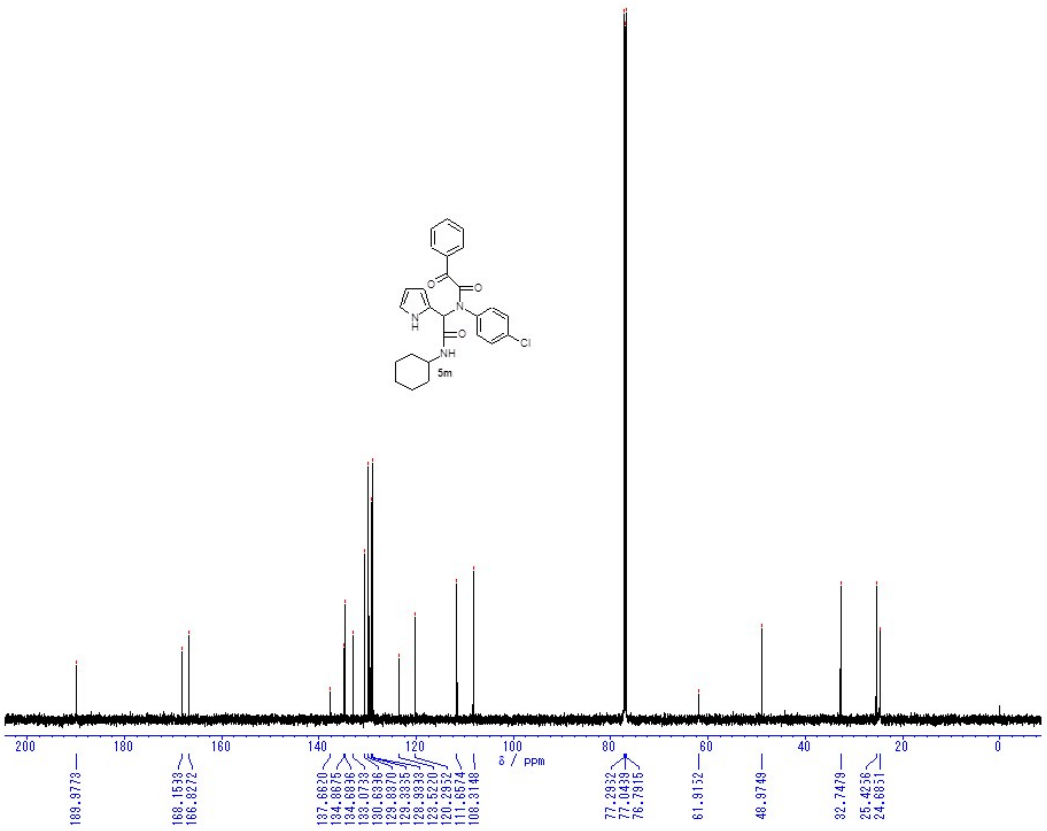
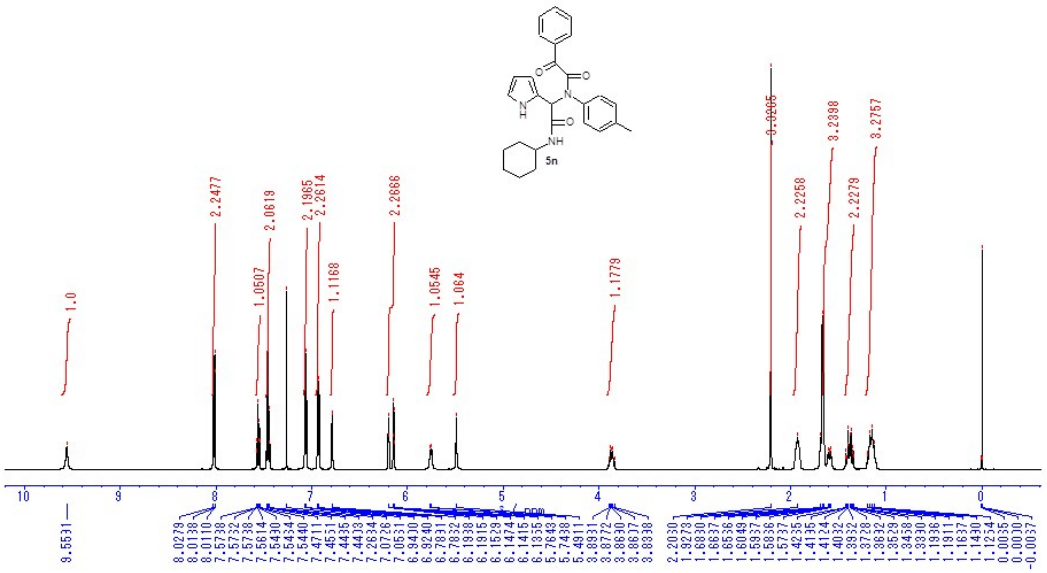
108.3839
77.2941
77.0837
76.7833
62.6454
51.9535
28.5935

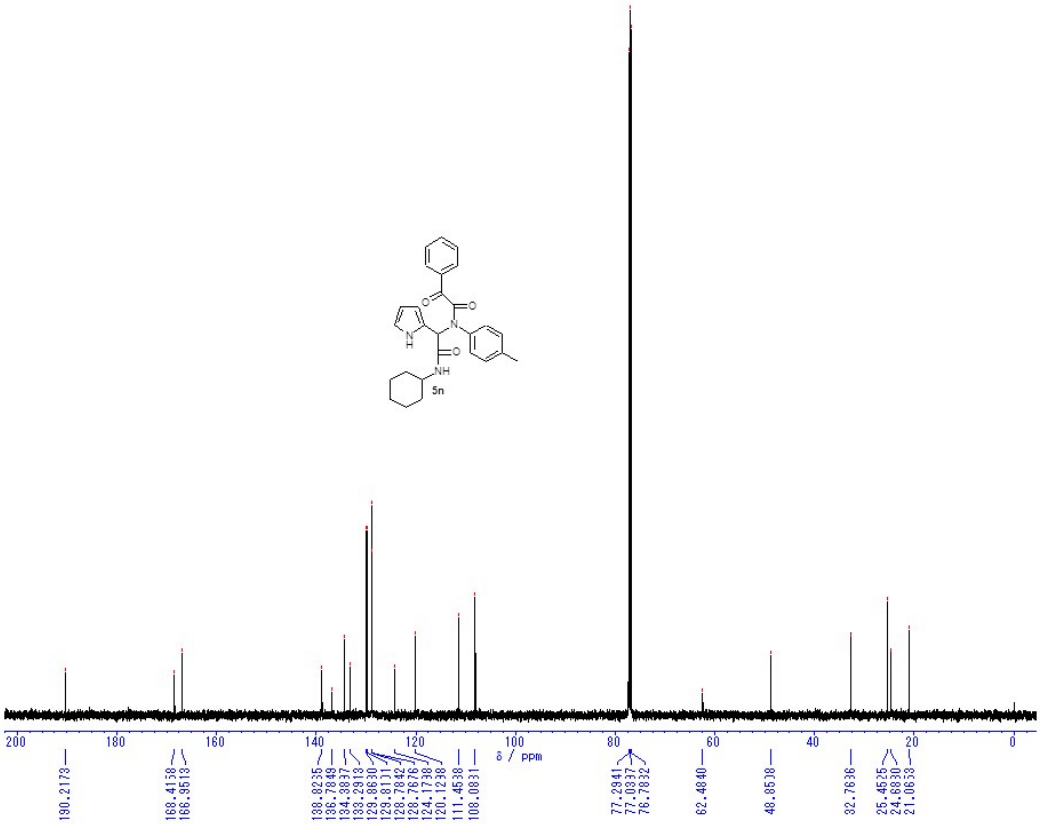

1.0
2.1478
3.0622
3.0877
1.0416
2.1181
0.9434
0.9668
3.1788
9.0629
δ / ppm
9.4673
7.8812
7.8437
7.2639
7.2629
7.2541
7.0831
6.7935
6.1835
6.1239
5.8638
5.5738
2.4029
1.3839

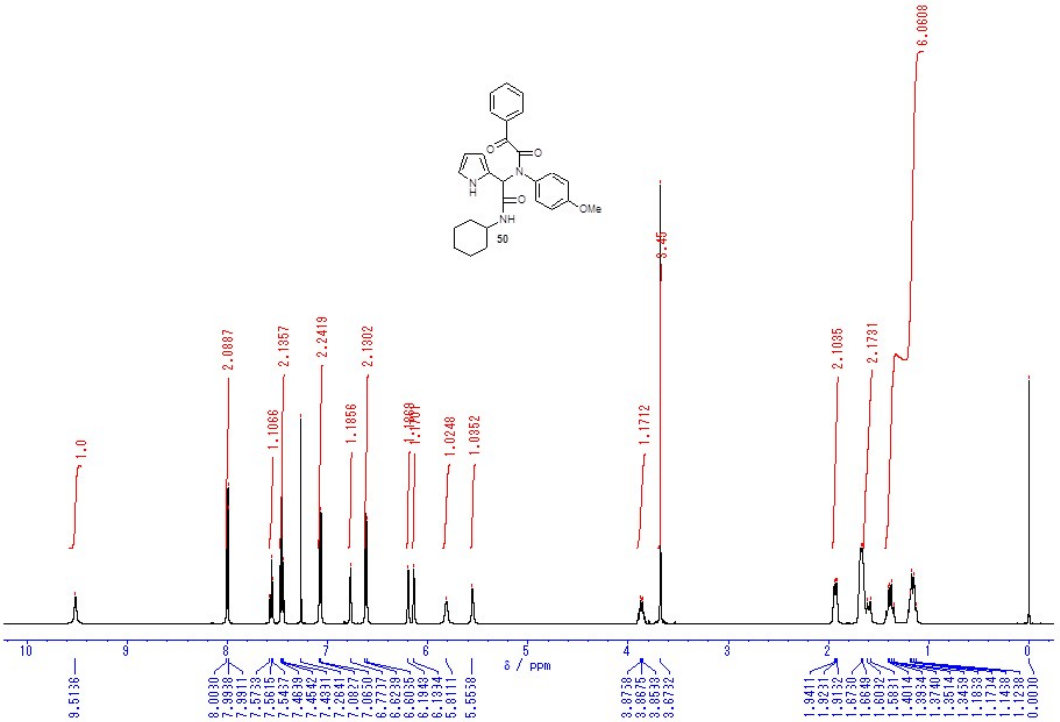

200
180
160
140
120
100
80
60
40
20
0
δ / ppm
183.5235
168.1675
167.1747
145.9027
137.4938
134.7631
130.7616
130.6954
129.8938
129.6653
129.2135
123.6544
120.0337
111.4154
108.2734
77.2879
77.0336
76.7832
61.5914
51.8873
28.6048
21.8278

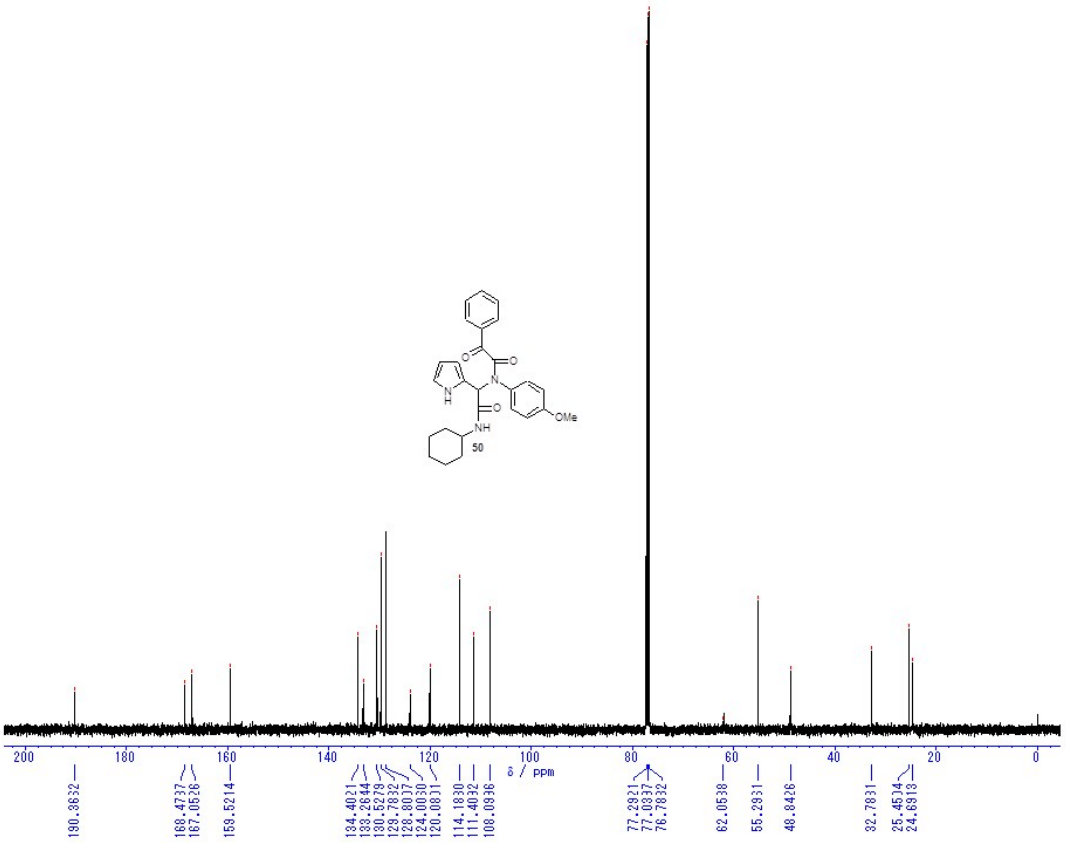

5m
1.0
2.1564
2.0808
1.0793
4.2716
1.0644
2.1784
0.995
1.0144
1.1039
2.1913
3.0518
2.1802
3.1799
ppm

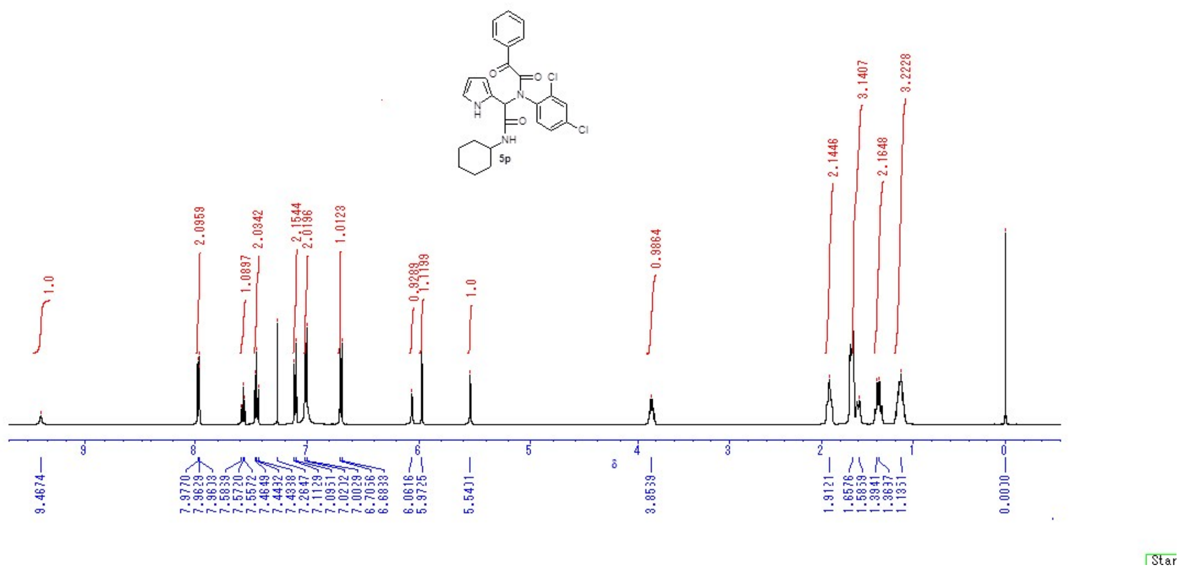

5m
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
189.9773
168.1538
166.8272
137.6820
134.8875
134.6938
130.0338
129.8370
129.8335
128.9333
123.5220
120.2952
111.6574
108.3148
77.2932
77.0439
76.7915
61.9152
48.9749
32.7479
25.4256
24.6851

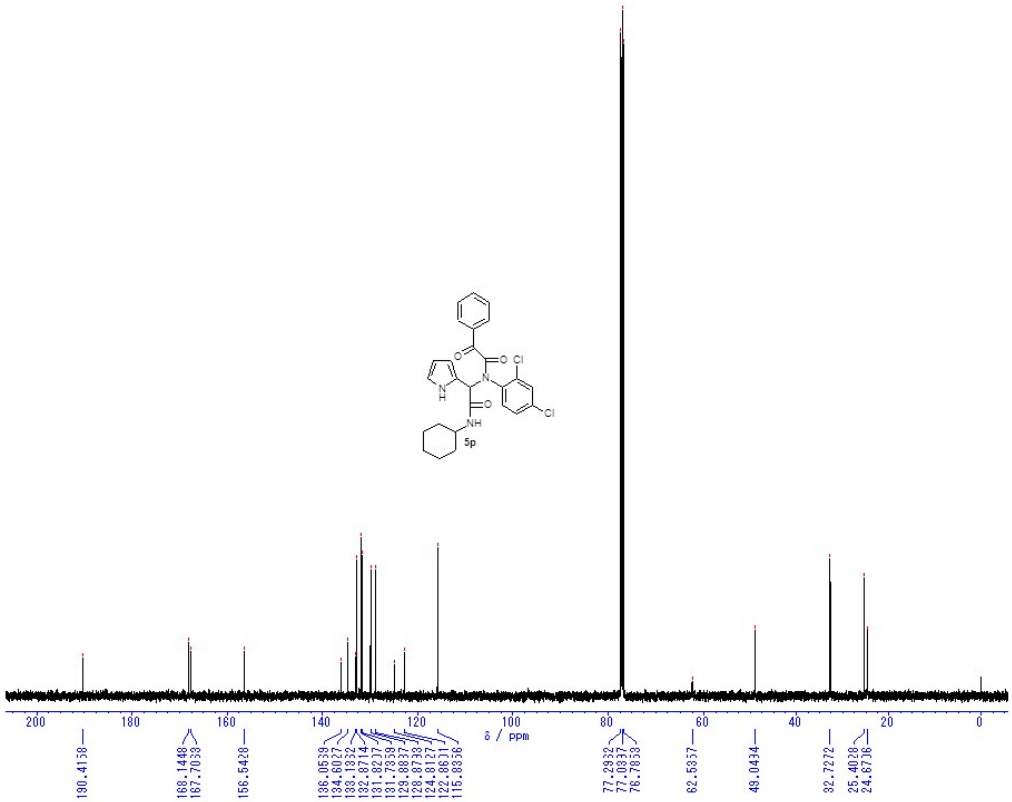

5n
1.0
2.2477
2.0613
1.0507
2.1965
2.2614
1.1168
2.2666
1.0545
1.064
1.1779
3.0205
2.2258
3.2398
2.2279
3.2757
ppm

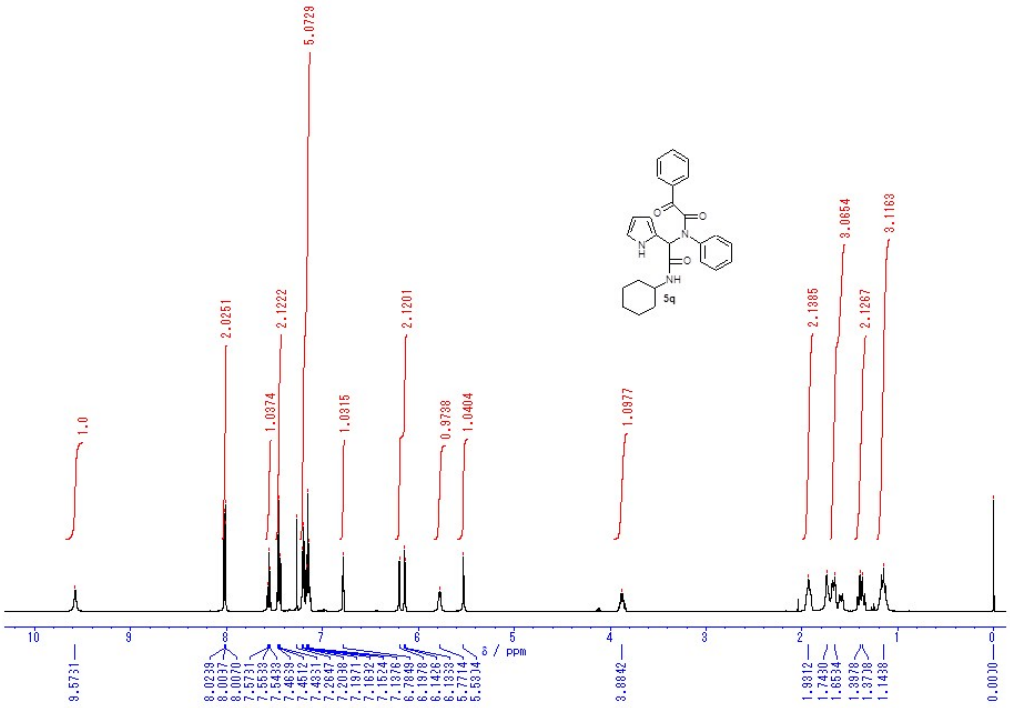

5n
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
190.2178
168.4158
166.9618
138.8235
136.7849
134.3837
133.2913
129.8630
129.8111
128.7842
128.7676
124.1738
120.1238
111.4538
108.0831
77.2941
77.0831
76.7832
62.4840
48.8538
32.7636
25.4525
24.6838
21.0853

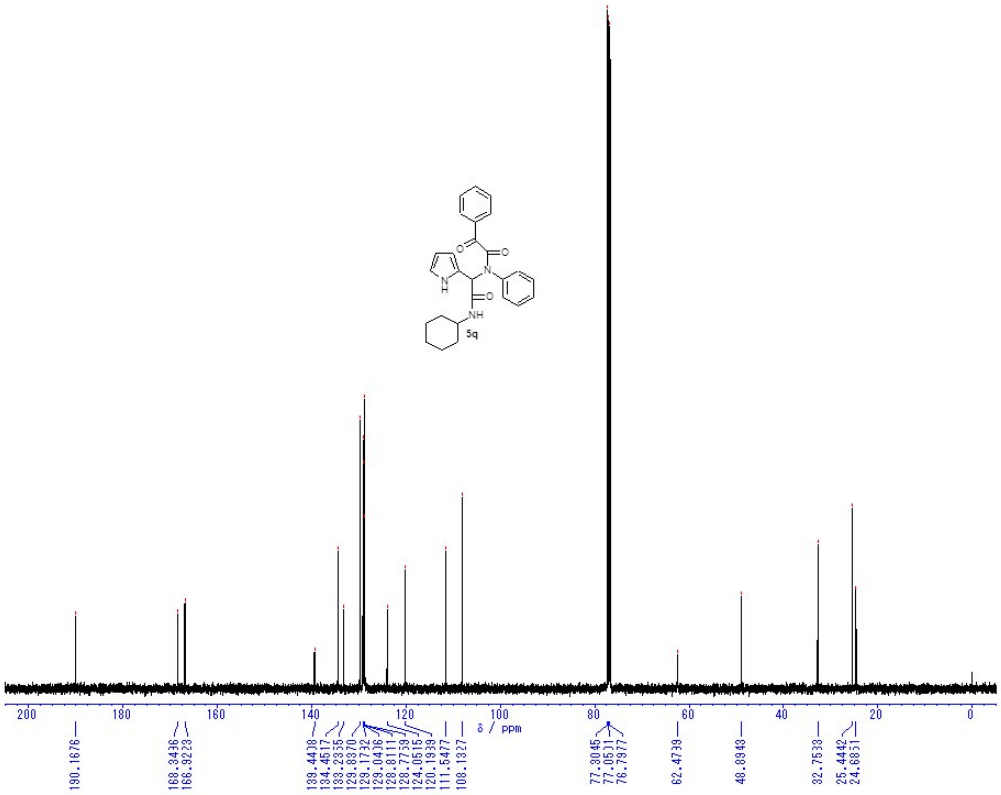

50
OMe
NH
1.0
2.0887
1.1066
2.1357
2.2419
1.1856
2.1302
1.0248
1.0352
1.1712
3.46
2.1035
2.1731
6.0808
δ / ppm

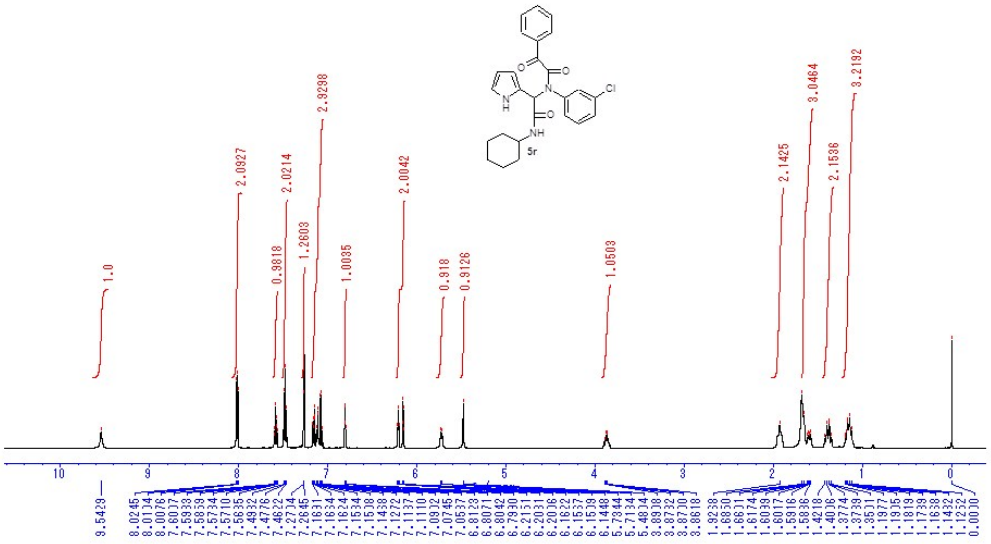

O
O
N
H
O
NH
OMe
50
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
190.3632
168.4737
167.0526
158.5214
134.4021
133.2644
130.5279
129.7832
128.8037
124.0030
120.0831
114.1830
111.4032
108.0396
77.2921
77.0337
76.7832
62.0538
55.2831
48.8426
32.7831
25.4514
24.6918

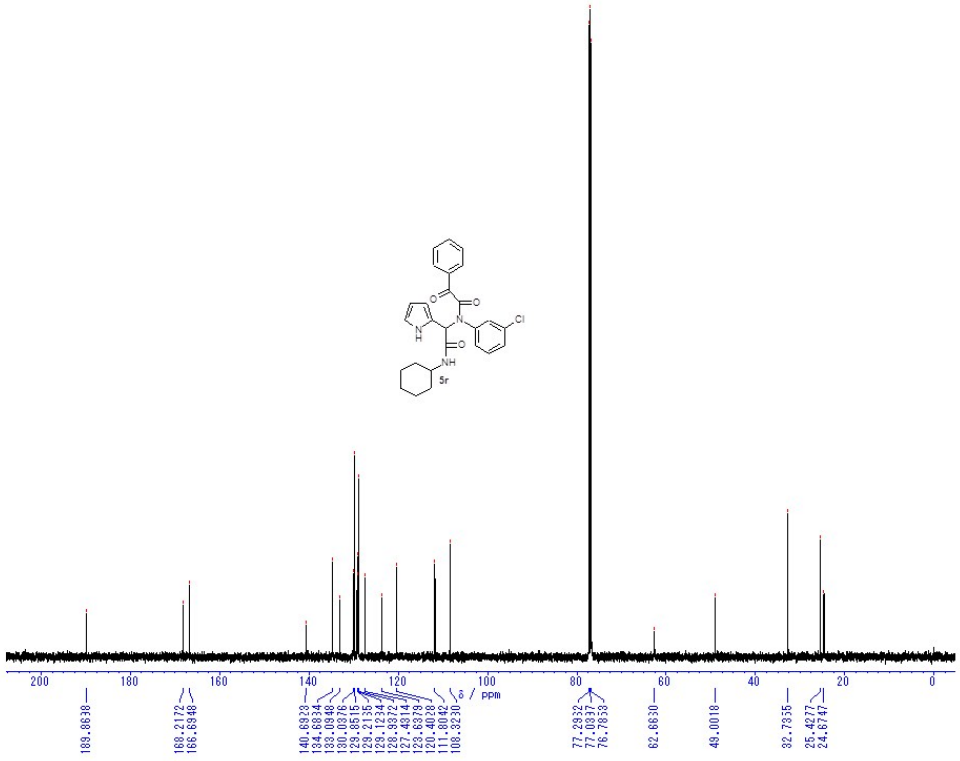


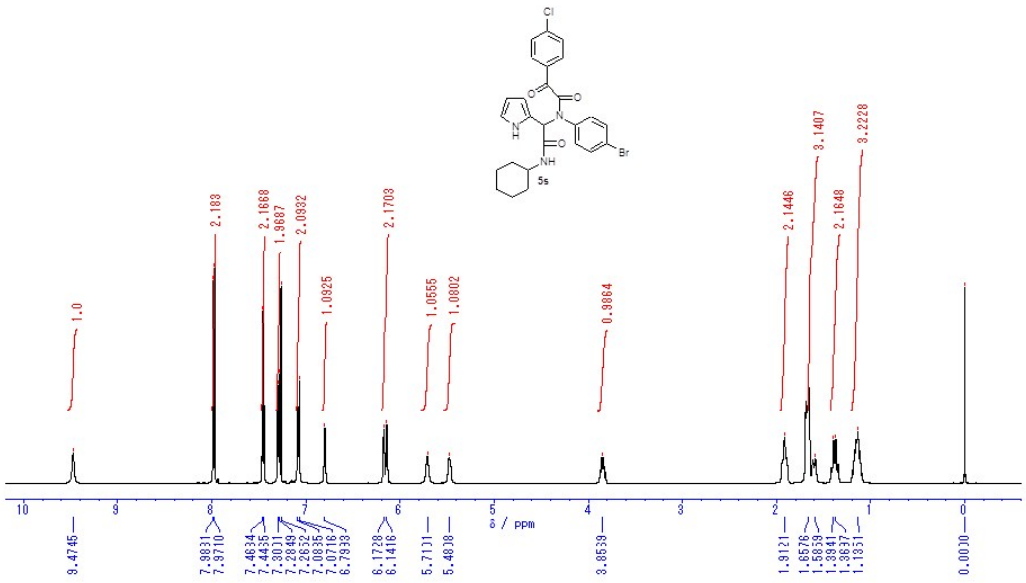

O
O
Cl
N
H
O
Cl
NH
5p
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
190.4158
168.1448
167.7033
158.6428
136.0539
134.6972
134.1952
132.8714
131.8217
131.7359
129.8837
128.8738
124.8127
122.8631
115.8836
77.2932
77.0337
76.7833
62.5837
49.0434
32.7272
25.4028
24.6738

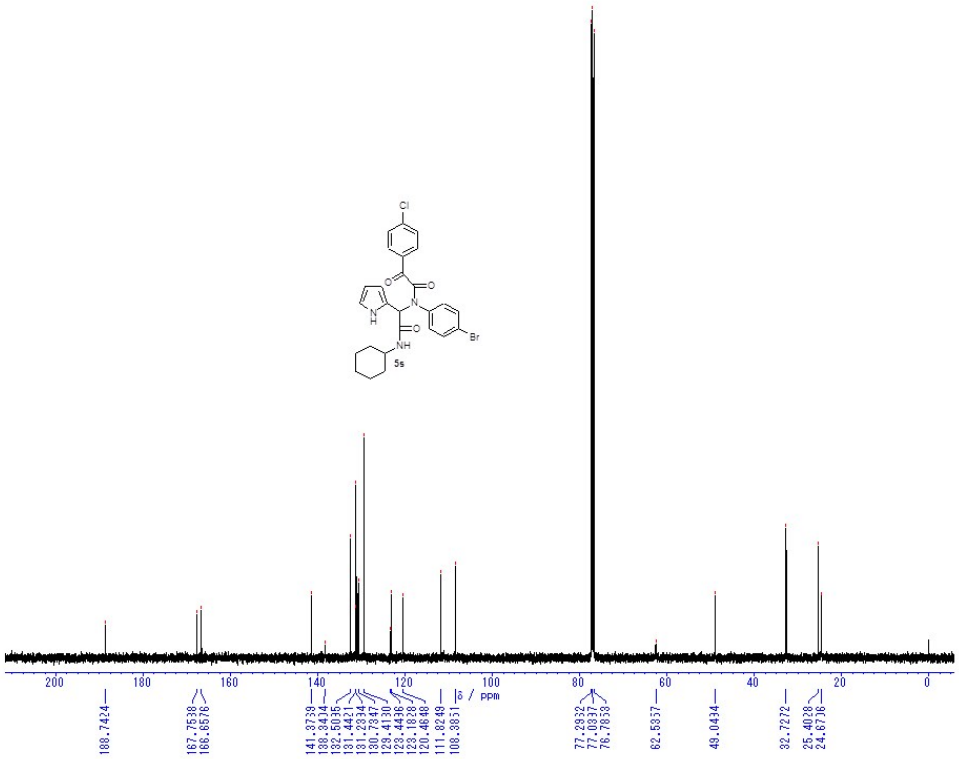

5.0729
2.0251
2.1222
2.1201
3.0654
3.1163
2.1385
2.1267
1.0374
1.0815
1.0377
1.0
0.9738
1.0404
5q
δ / ppm

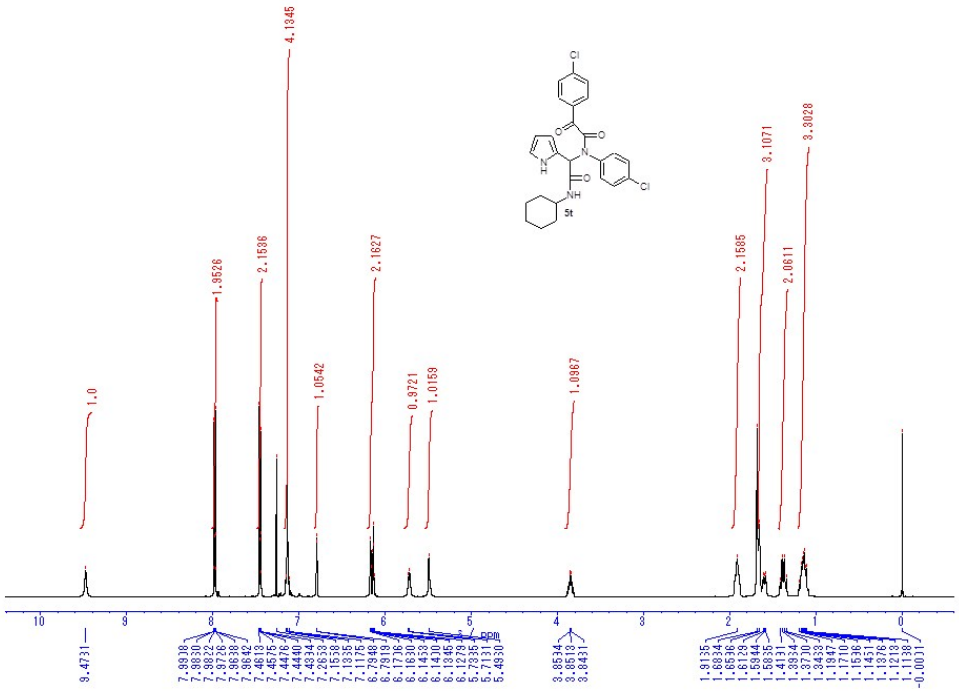

5q
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
190.1676
168.3436
168.9223
139.4438
134.4617
133.2335
129.6870
129.1732
129.0436
128.8111
128.7759
124.0515
120.1939
111.5477
108.1327
77.3045
77.0531
76.7977
62.4739
48.8943
32.7638
25.4442
24.6831

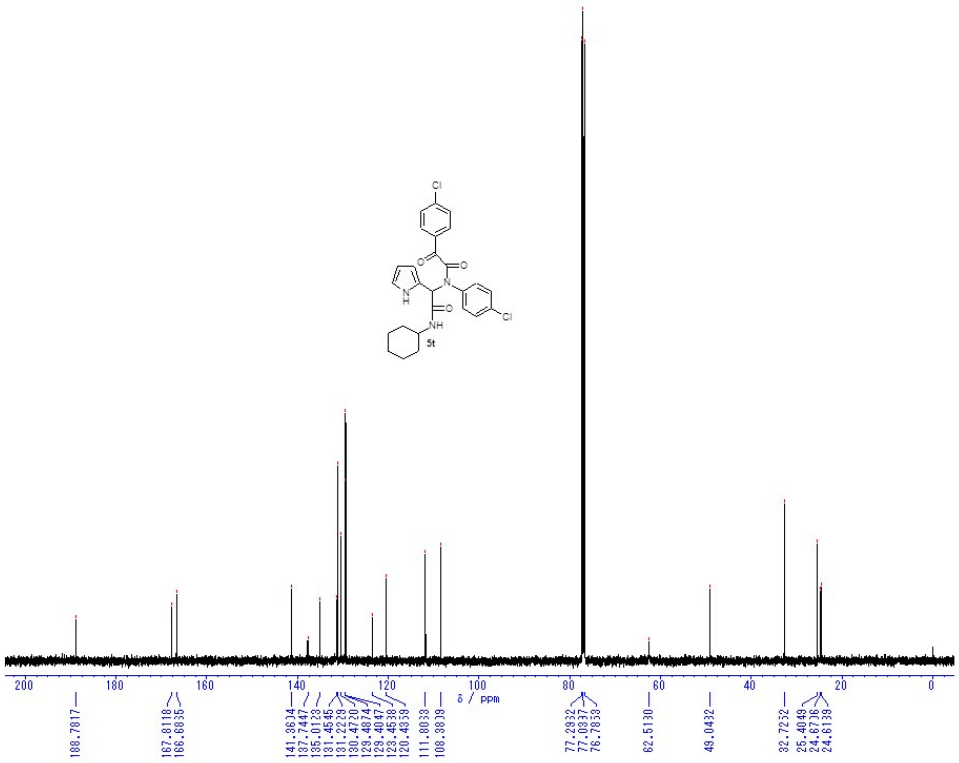

1.0
2.0827
0.9818
2.0214
1.2603
2.9298
1.0035
2.0042
0.918
0.9126
1.0503
2.1425
3.0464
2.1536
3.2192
5r

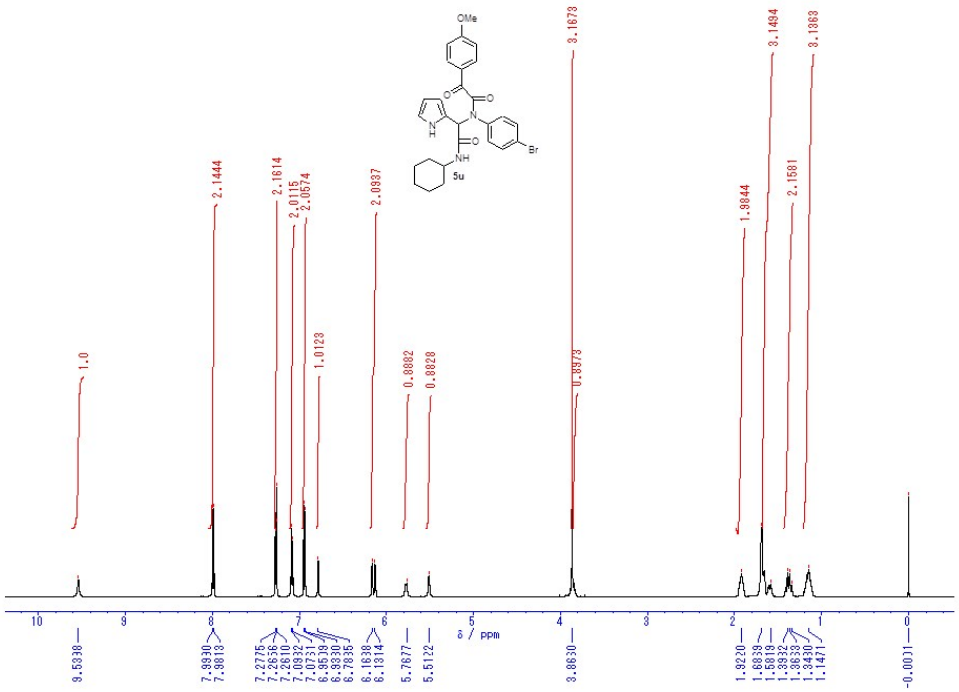

5r
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
189.0838
168.2172
166.6948
140.6323
134.6834
133.0948
130.0376
129.8515
129.2135
129.1234
128.3872
127.4814
123.6379
120.4028
111.8042
108.3230
77.2832
77.0837
76.7833
62.6630
49.0018
32.7335
25.4277
24.6747


Cl
O
O
N
Br
H
O
NH
5s
1.0
2.183
2.1688
1.9687
2.0932
1.0325
2.1703
1.0555
1.0802
0.9864
2.1446
3.1407
2.1648
3.2228
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
8.4745
7.9831
7.9710
7.4634
7.4435
7.3011
7.2849
7.2652
7.0835
7.0716
6.7938
6.1728
6.1418
5.7131
5.4838
3.8539
1.9121
1.6576
1.5839
1.3841
1.3637
1.1931
0.0030


Cl
O
O
N
Br
H
O
NH
5s
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.7424
167.7538
166.6576
141.3739
138.0434
132.4435
131.2354
130.7347
123.4130
123.4436
123.1828
120.4648
111.8249
108.3851
77.2932
77.0337
76.7833
62.5337
49.0434
32.7272
25.4028
24.6736


4.1345
1.9526
2.1538
2.1827
1.0542
0.3721
1.0159
1.0867
2.1585
3.1071
2.0811
3.3028
1.0
9.4731
7.0938
7.0893
7.0882
7.0716
7.0638
7.0642
7.0613
7.0575
7.0440
7.0434
7.0253
7.0158
7.0135
7.0175
6.7948
6.7919
6.7736
6.7630
6.7433
6.7400
6.7245
6.7235
5.7335
5.7131
5.4930
3.8534
3.8513
3.8431
1.9135
1.6834
1.6576
1.6139
1.5944
1.5835
1.4131
1.3834
1.3770
1.3433
1.1947
1.1710
1.1536
1.1431
1.1218
1.1138
-0.0031
ppm


Cl
O
O
N
H
O
NH
5t
Cl
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.7817
167.8118
166.6835
141.3614
137.7447
135.0128
131.4545
131.2238
130.4720
129.4814
129.4037
128.4558
120.4938
111.8033
108.3839
77.2832
77.0337
76.7838
62.5130
49.0432
32.7232
25.4049
24.6776
24.6139


OMe
O
O
N
Br
H
O
NH
5u
1.0
2.1444
2.1614
2.0115
2.0574
1.0123
2.0937
0.8882
0.8828
3.1673
0.8873
1.9844
3.1494
2.1581
3.1363
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
8.5338
7.8930
7.8818
7.2775
7.2636
7.2610
7.0932
7.0731
6.9539
6.9330
6.7835
6.1638
6.1314
5.7677
5.5122
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1.6838
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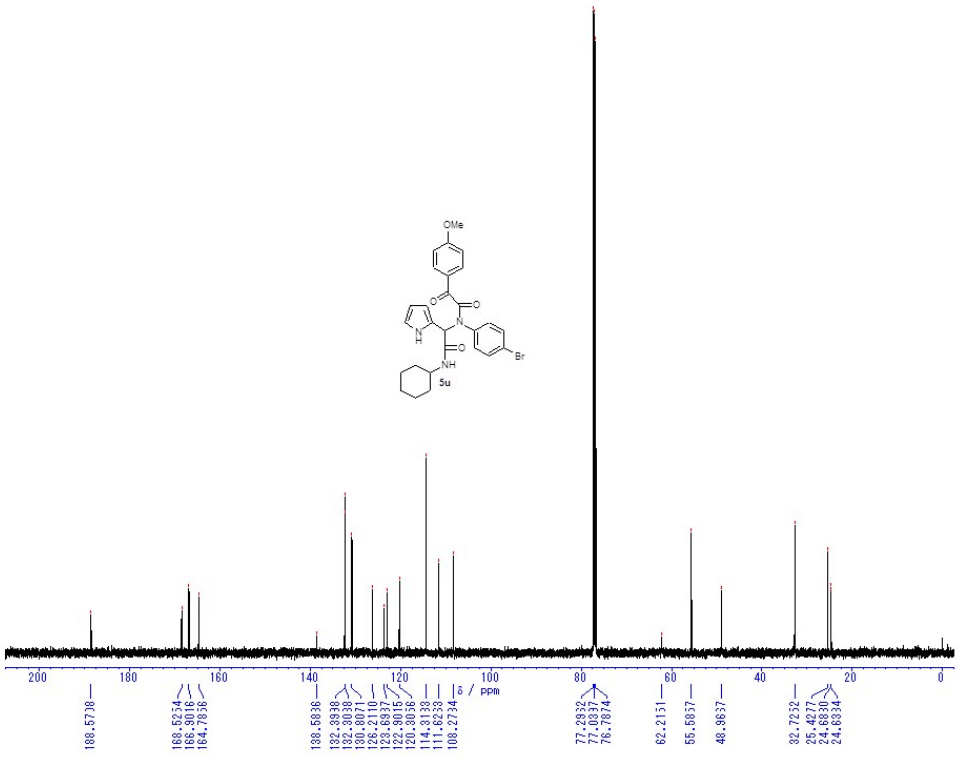
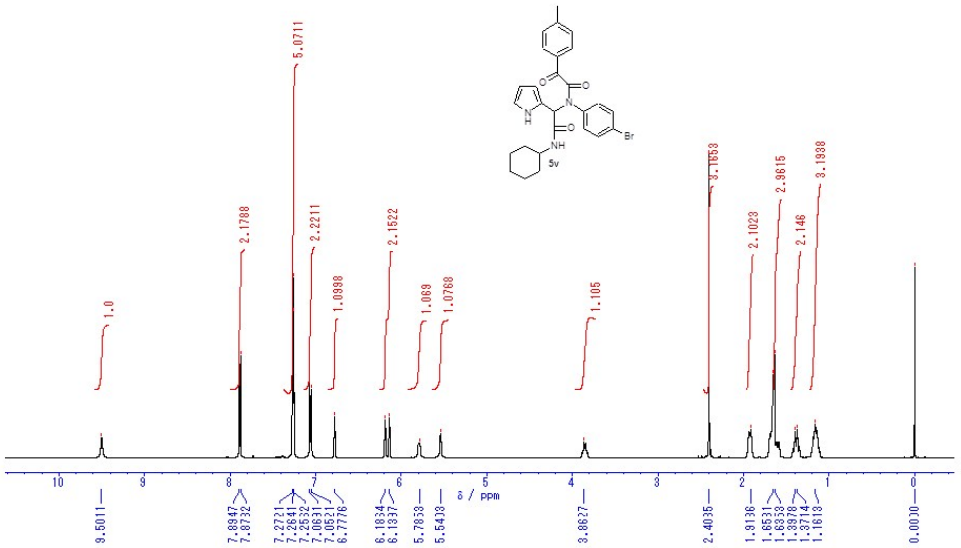
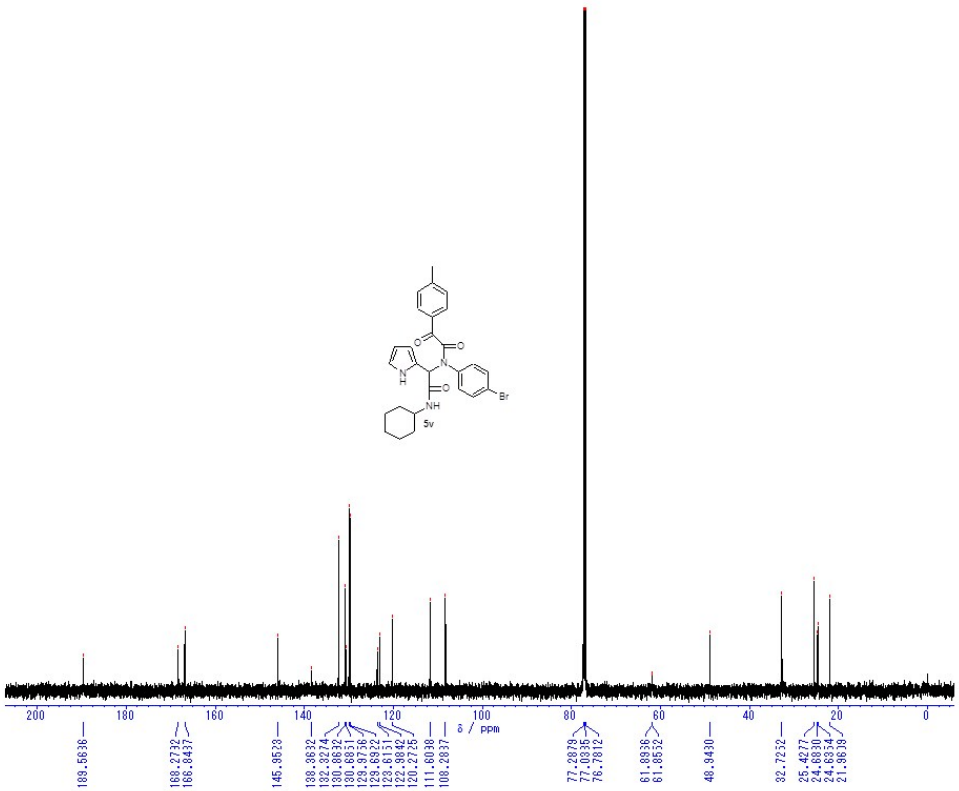
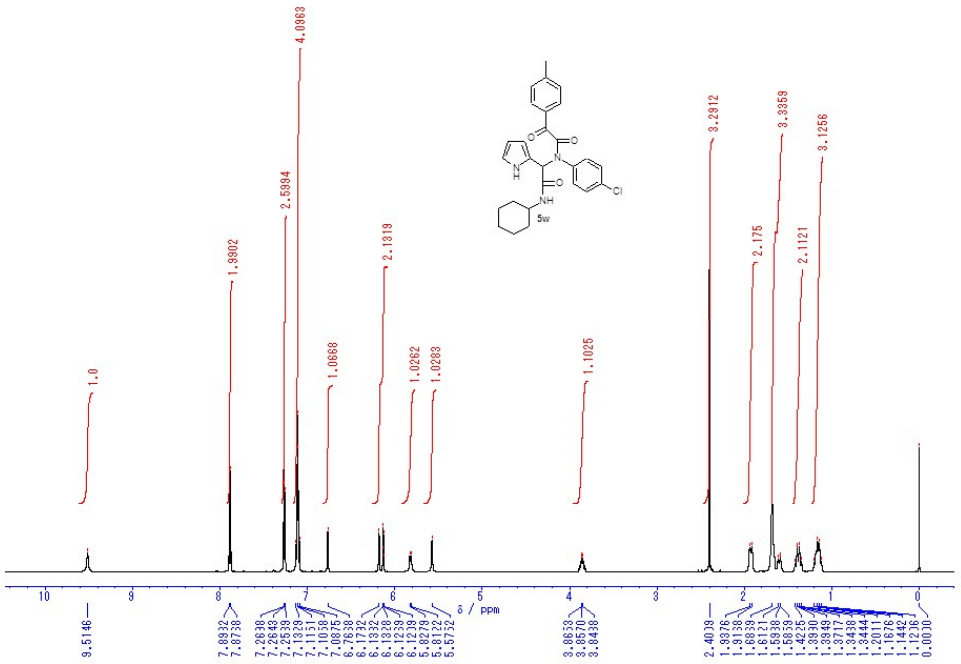
1.3839
1.3633
1.3430
1.1471
-0.0031

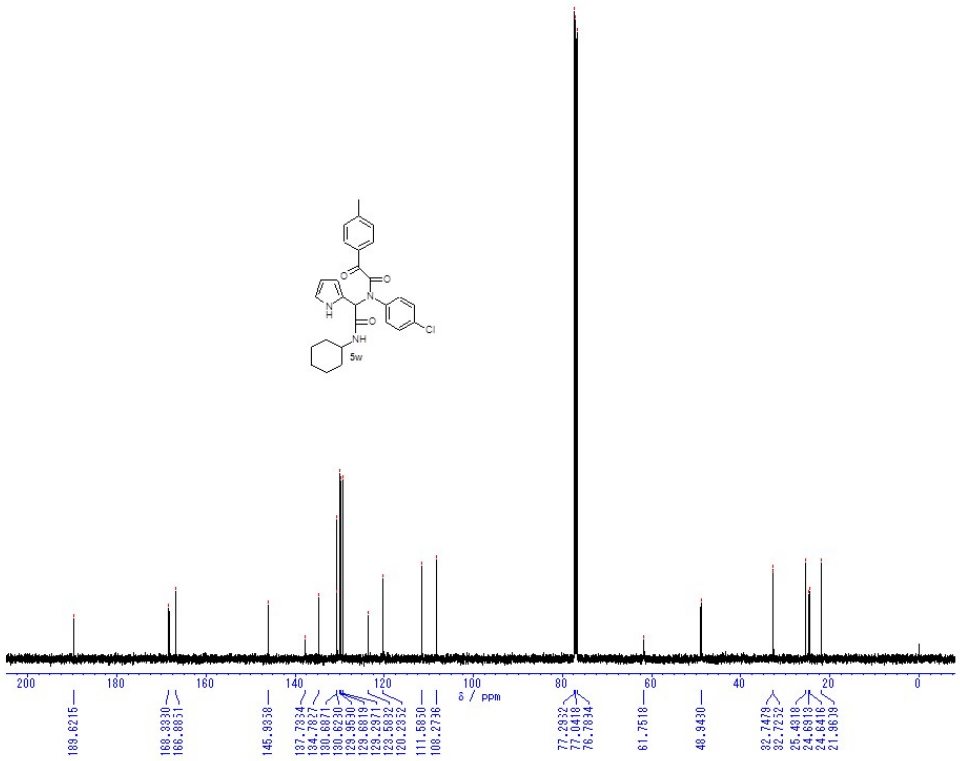
Star

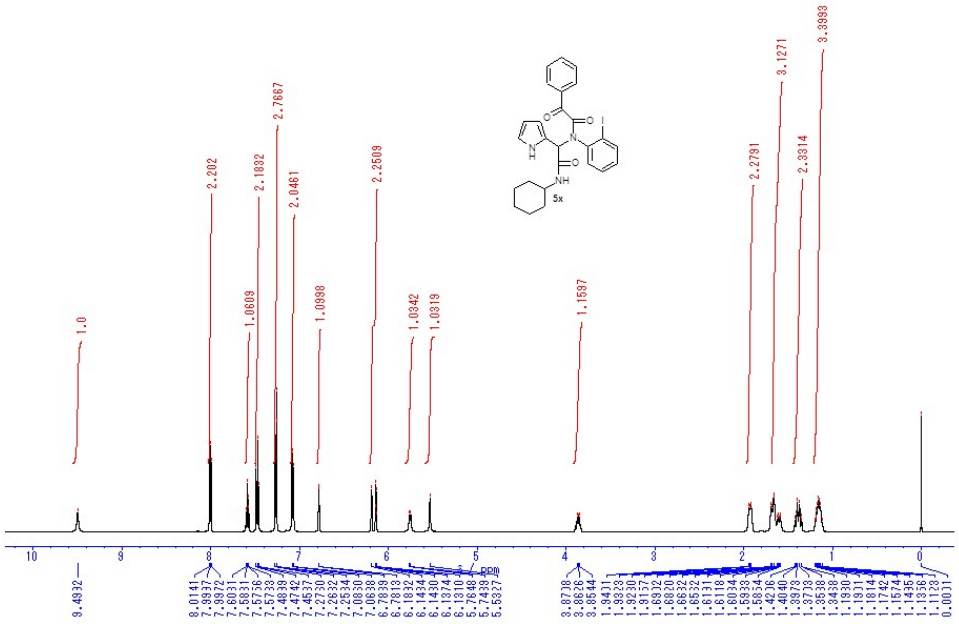

OMe
O
O
O
N
Br
H
N
O
NH
5u
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.5738
168.5254
166.3016
164.7836
138.5836
132.3938
132.3038
130.8071
126.2110
123.6837
122.9015
120.3036
114.3133
111.6233
108.2734
77.2932
77.0837
76.7874
62.2151
55.5857
48.3637
32.7252
25.4277
24.6830
24.6834

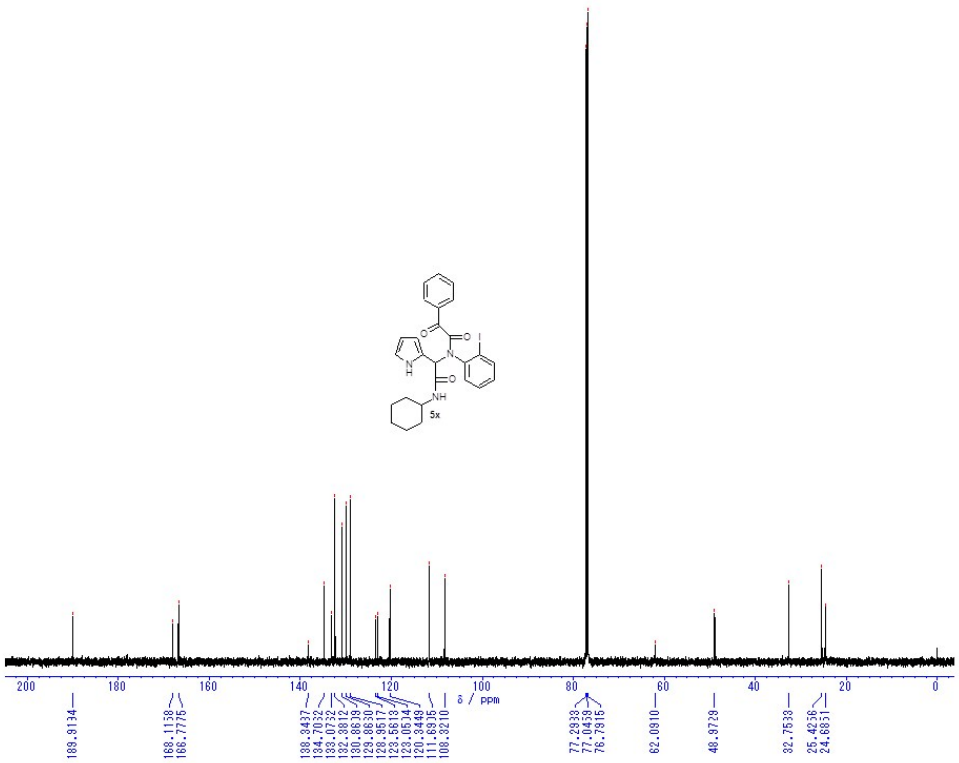

5v
Br
1.0
2.1788
5.0711
2.2211
1.0988
2.1522
1.069
1.0768
1.105
3.1653
2.1023
2.3815
2.146
3.1938
δ / ppm

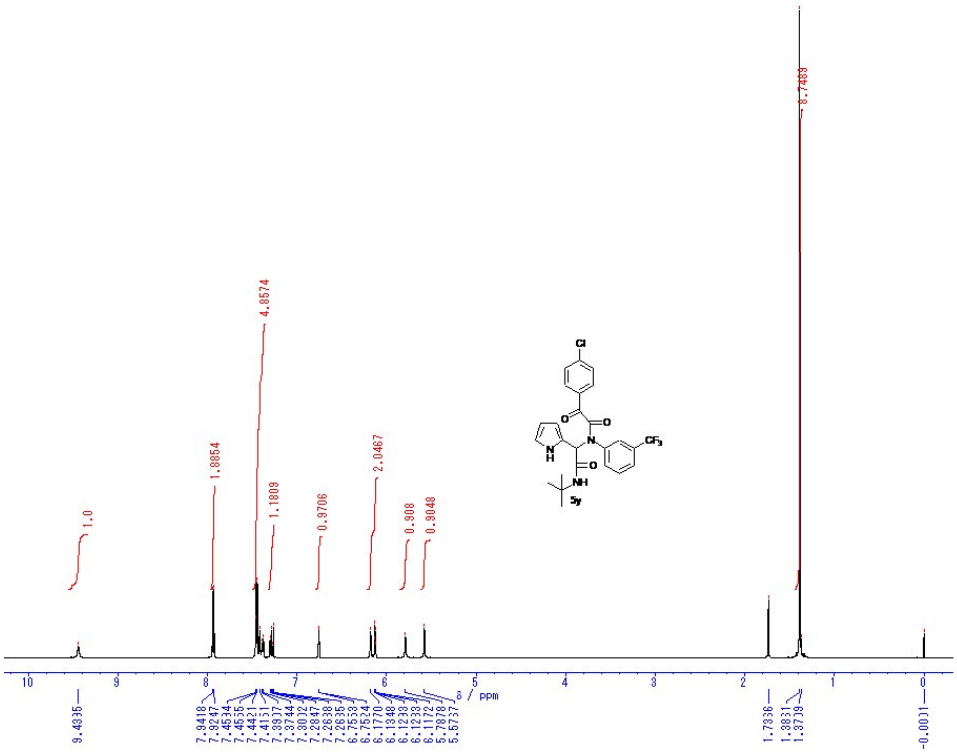

5v
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
189.5636
168.2732
166.8437
145.9523
138.3832
132.3274
130.0831
129.9736
129.6922
123.6151
122.9842
120.2725
111.6038
108.2837
77.2879
77.0835
76.7812
61.8836
61.6532
46.9430
32.7252
25.4277
24.6830
24.6334
21.9639

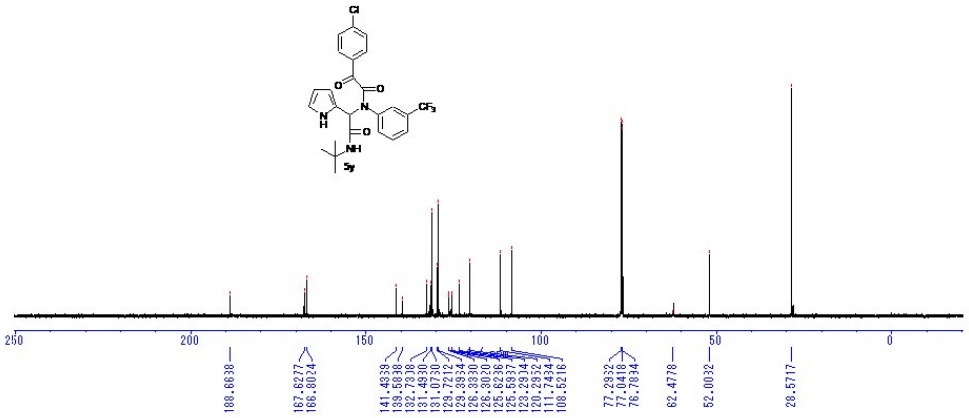

4.0863
2.5394
1.3902
2.1319
1.0668
1.0262
1.0283
1.1025
3.2912
3.3359
3.1258
2.175
2.1121
1.0
5w
δ / PPm

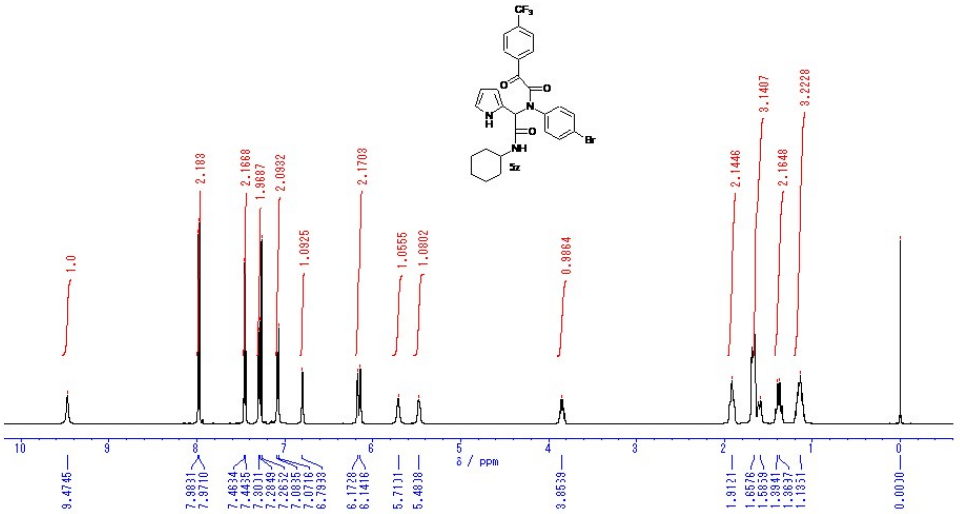

5w
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
189.6215
168.3330
166.8831
145.9338
137.7334
134.7827
130.6871
130.6230
129.4559
129.4019
129.2911
123.5832
120.2332
111.5630
108.2736
77.2832
77.0418
76.7934
61.7518
48.9430
32.7478
32.7232
25.4318
24.6918
24.6418
21.9639

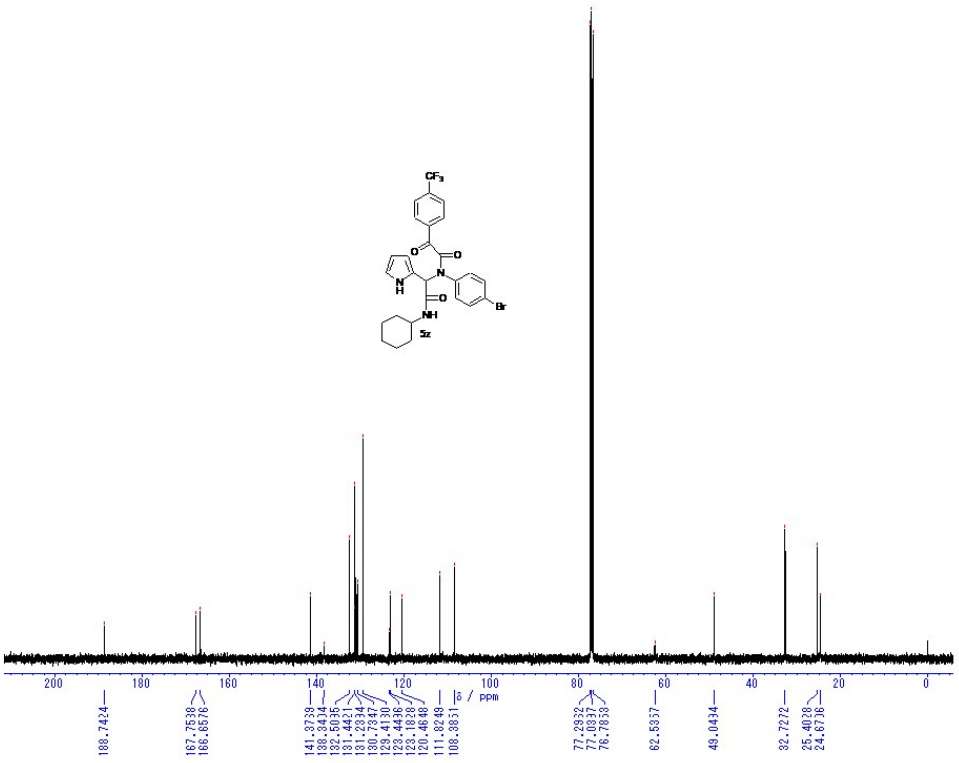

1.0
2.202
1.0609
2.1832
2.7687
2.0461
1.0388
2.2589
1.0342
1.0319
1.1597
2.2791
3.1271
2.3814
3.3933
5x
PPM

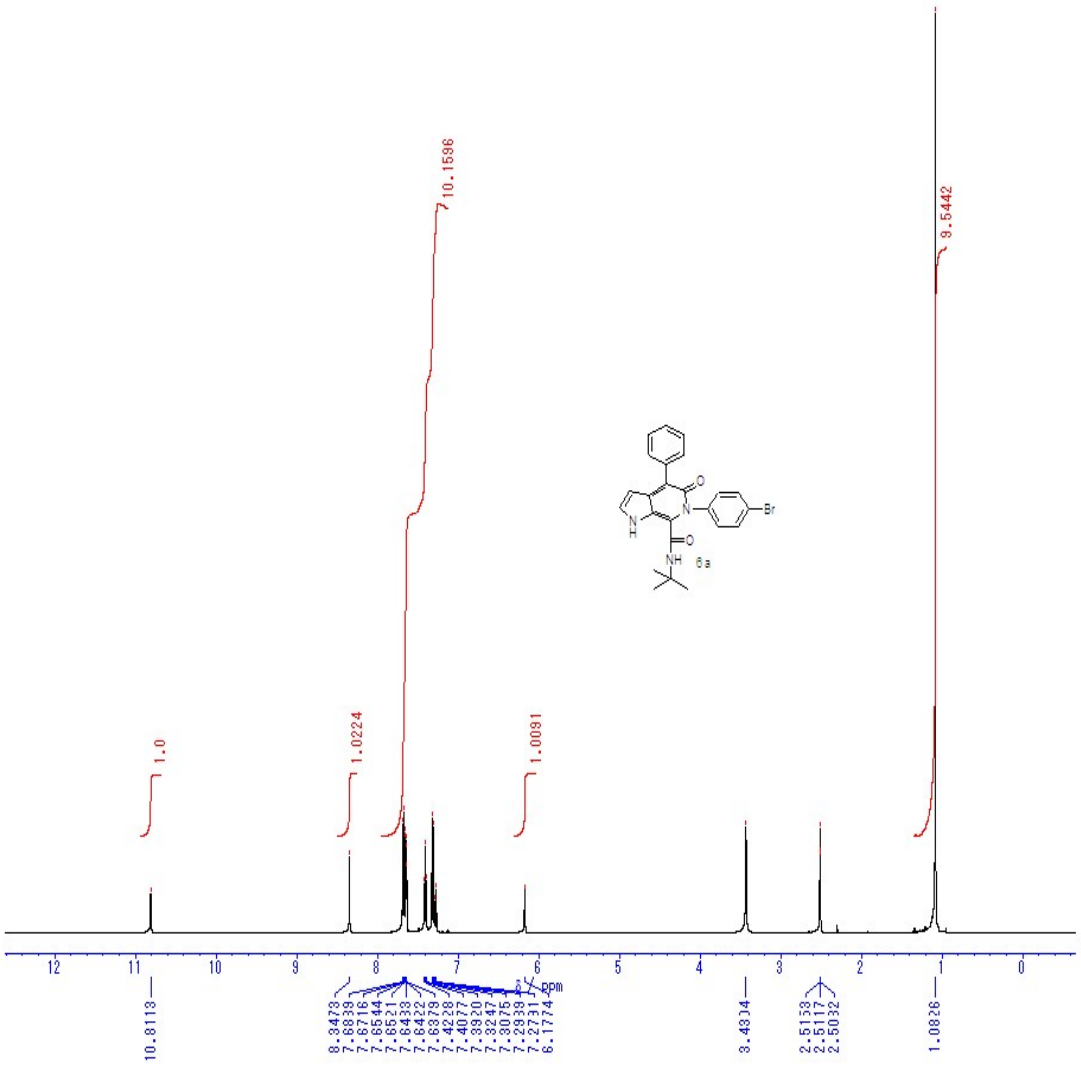

O
O
I
N
H
O
NH
5x
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
189.3134
168.1158
166.7778
138.3437
134.7032
133.0732
132.3812
130.8639
129.8630
128.9517
123.5613
123.0154
121.3448
111.6935
108.3210
77.2933
77.0433
76.7916
62.0910
40.9728
32.7538
25.4256
24.8831

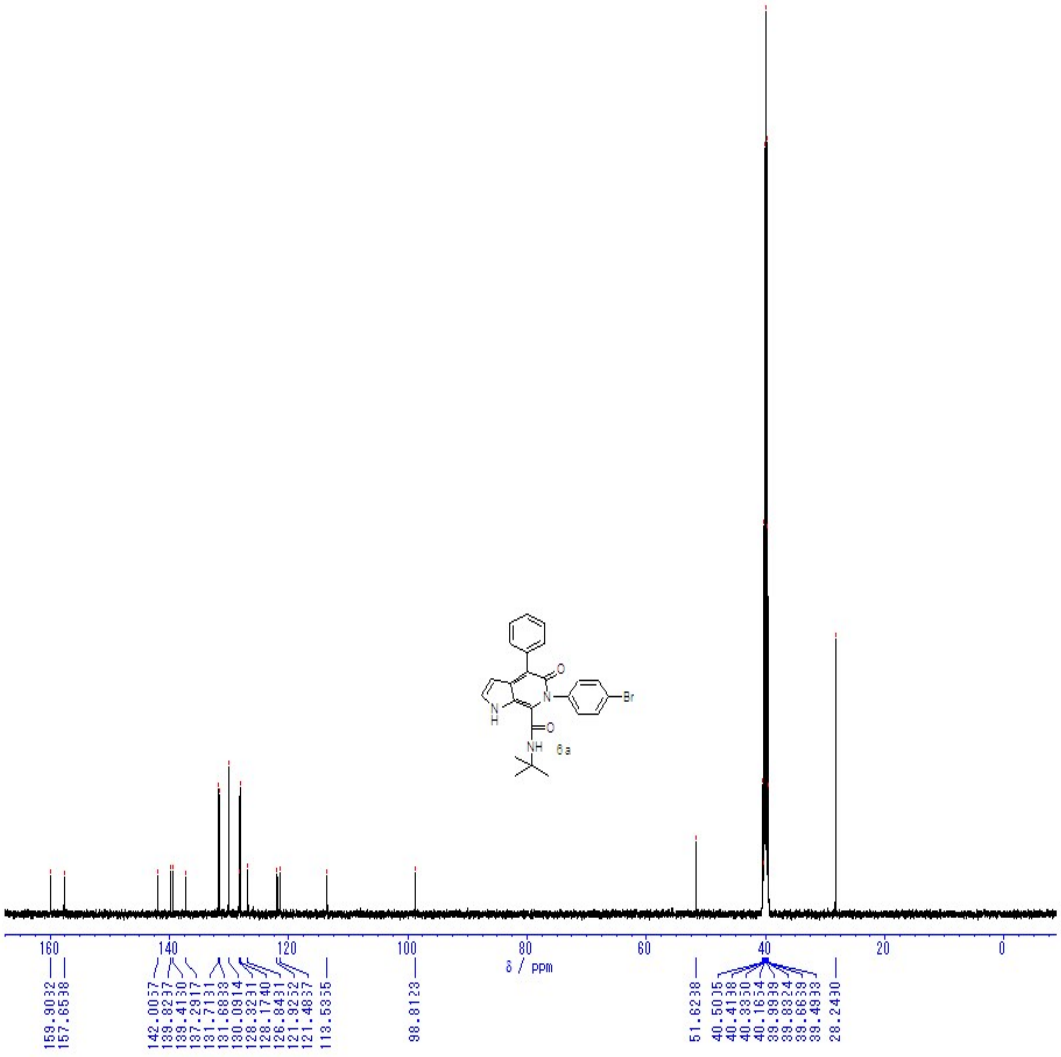

1.0
1.8864
4.8574
1.1808
0.9706
2.0467
0.908
0.9048
8.7483
Cl
O
O
N
H
O
NH
tBu
CF3
ppm


Cl
O
O
N
H
N
O
CF3
NH
Sy
250
200
150
100
50
0
188.6638
167.6277
166.0024
141.4338
139.5838
132.7338
131.4930
131.0730
129.7212
128.9834
128.3330
126.3010
125.6236
125.5937
123.2934
120.2932
111.7434
108.6216
77.2932
77.0418
76.7834
62.4778
52.0032
28.5717


CF3
O
O
N
O
NH
Br
5z
1.0
2.183
2.1668
1.9887
2.0932
1.0325
2.1703
1.0555
1.0802
0.9864
2.1446
3.1407
2.1648
3.2228
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
3.4745
7.9831
7.9710
7.4634
7.4435
7.4011
7.2849
7.2632
7.0837
7.0716
6.7938
6.1728
6.1416
5.7131
5.4838
3.8539
1.9121
1.6576
1.6839
1.3941
1.3837
1.1031
0.0030


CF3
O
O
N
H
O
Br
NH
Xz
200
180
160
140
120
100
80
60
40
20
0
δ / ppm
188.7424
167.7538
166.6578
141.3739
138.3414
132.5035
131.4421
131.2334
130.7347
129.4130
123.4436
123.1828
120.4648
111.8248
108.3831
77.2832
77.0307
76.7838
62.5357
49.0434
32.7272
25.4028
24.6736


10.1596
9.5442
1.0
1.0224
1.0091
6a
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
10.8113
8.3473
7.6839
7.6716
7.6544
7.6521
7.6438
7.6422
7.6379
7.4228
7.4077
7.3920
7.3247
7.3075
7.2939
7.2731
6.1774
3.4814
2.5133
2.5117
2.5032
1.0826


Br
O
N
H
O
NH
6a
160
140
120
100
80
60
40
20
0
δ / ppm
159.9032
157.6538
142.0037
139.8237
139.4130
137.2917
131.7131
131.6838
130.0914
128.3231
128.1740
126.8431
121.9252
121.4837
113.5356
98.8123
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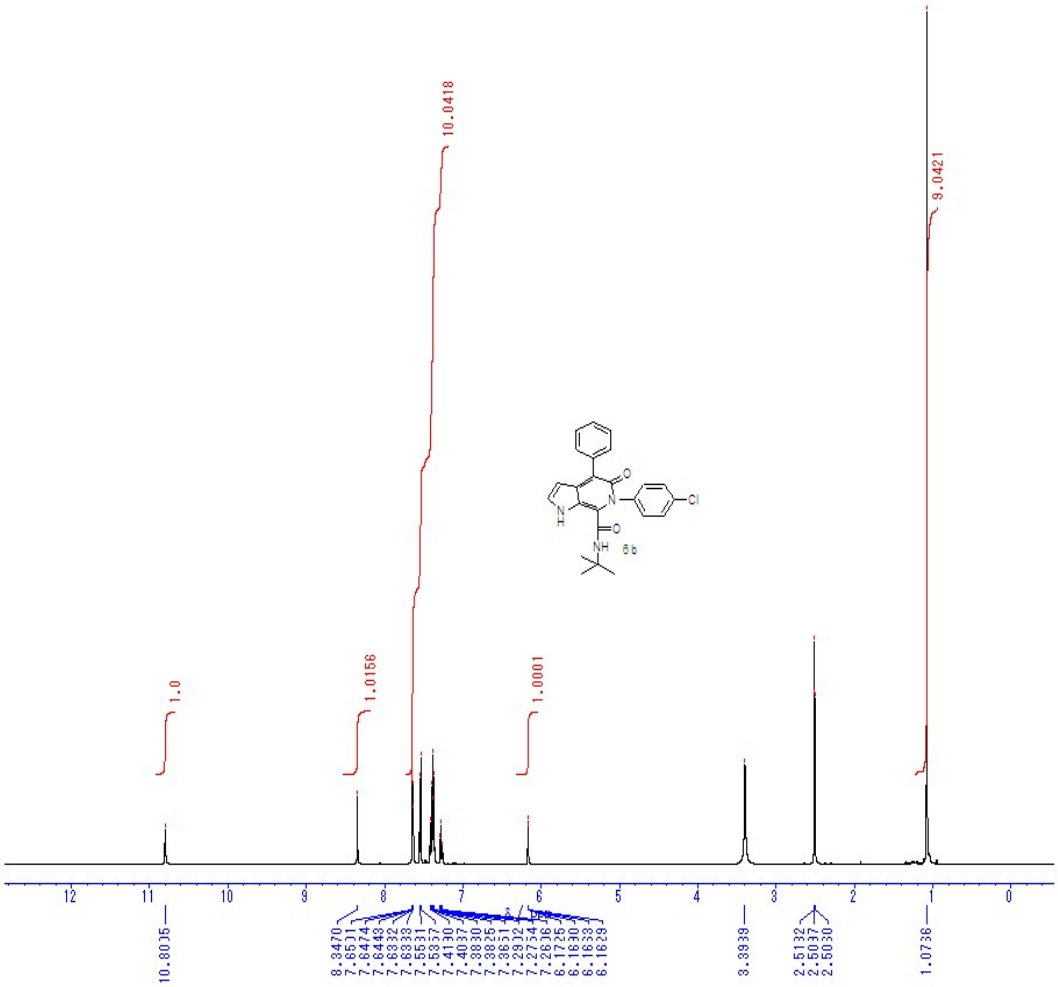
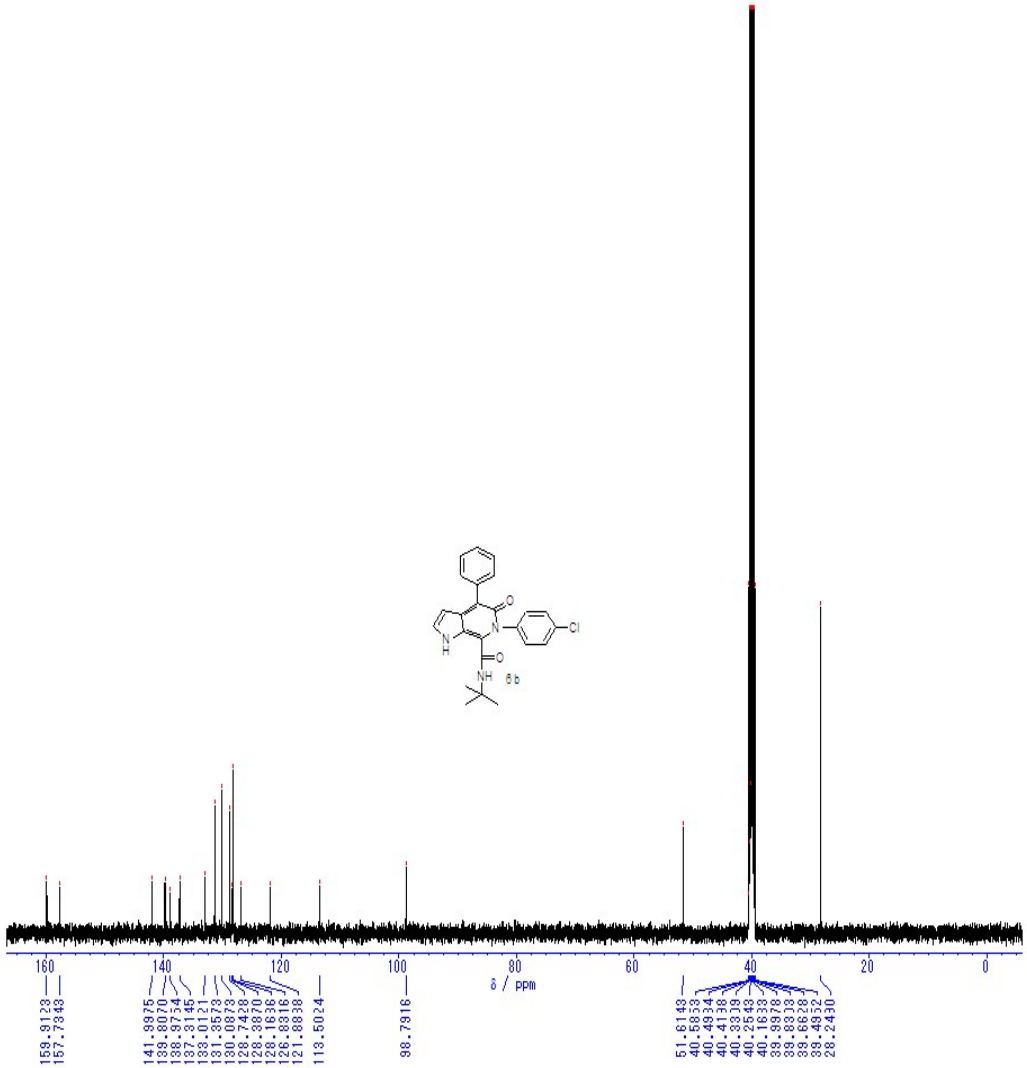
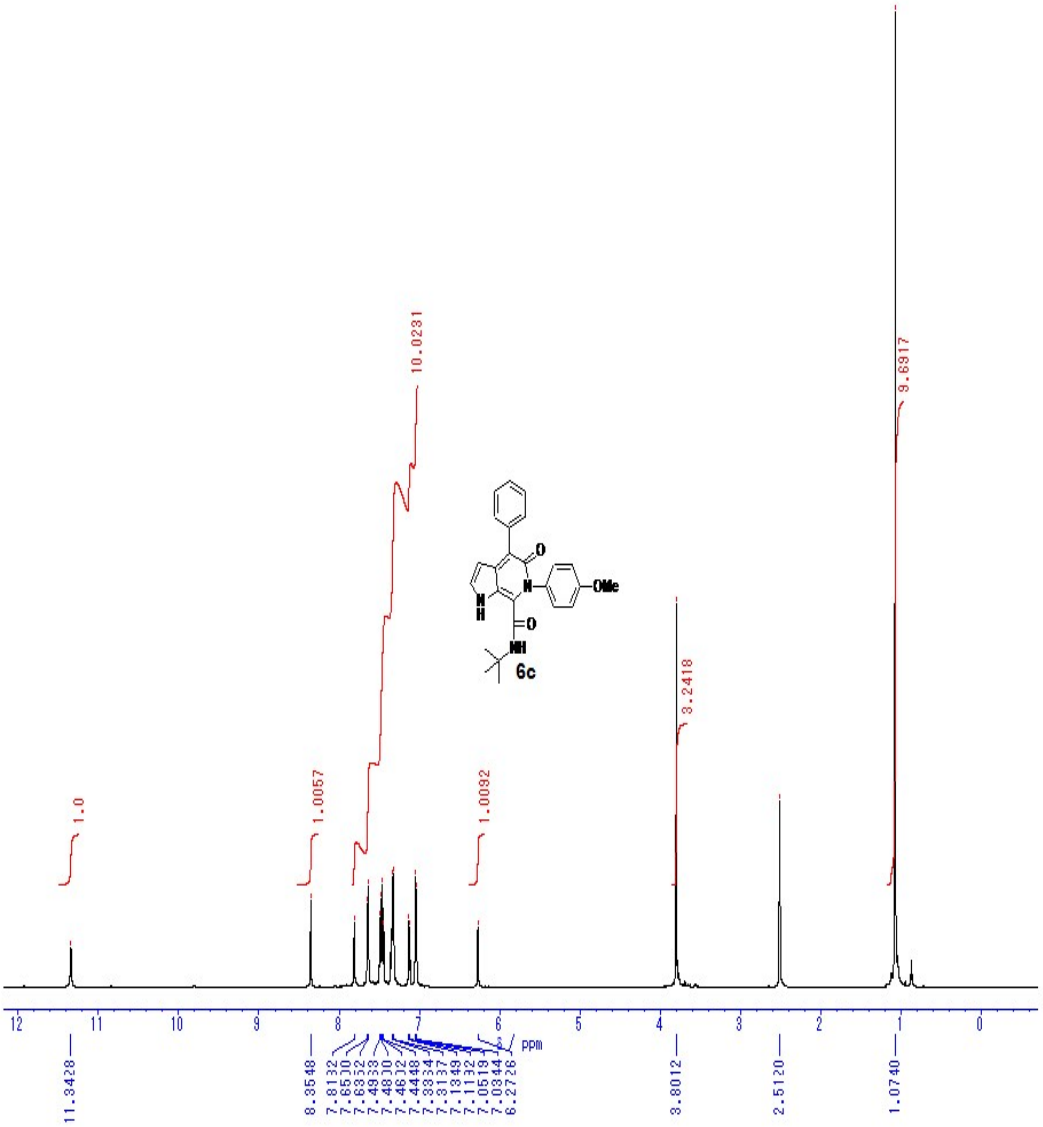
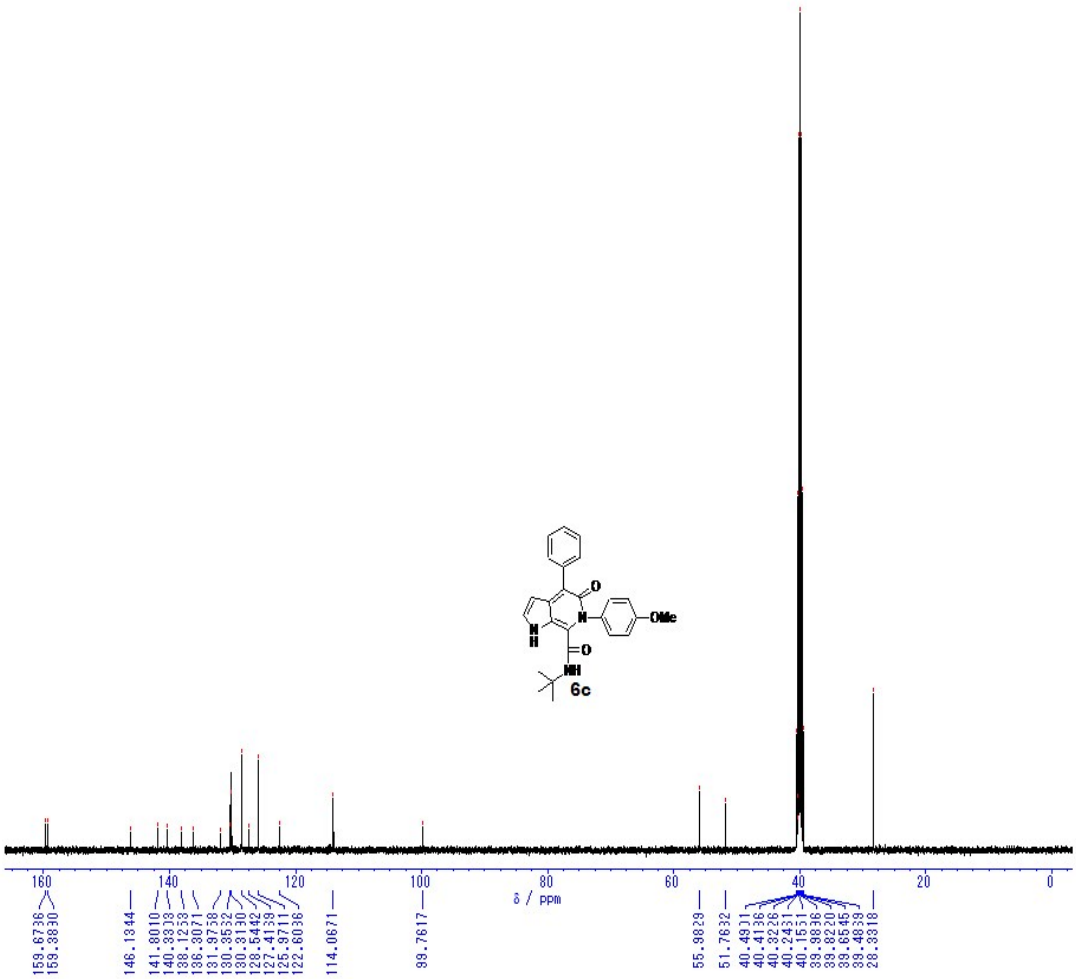
39.9939
39.8324
39.6639
39.4933
28.2430

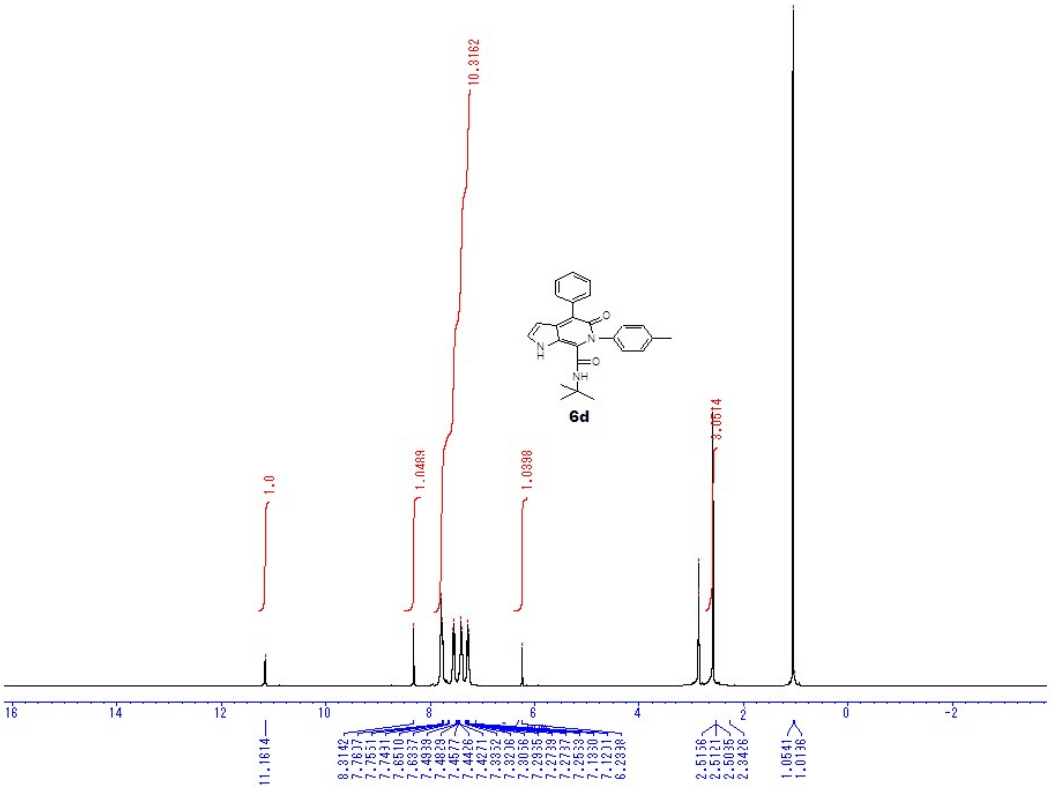

10.0418
9.0421
1.0
1.0156
1.0001
6b
12
11
10
9
8
7
6
5
4
3
2
1
0
10.8035
8.3470
7.6531
7.6474
7.6448
7.6332
7.6338
7.5531
7.5357
7.4130
7.4037
7.3830
7.3825
7.3651
7.2932
7.2734
7.2636
6.1725
6.1630
6.1633
6.1629
3.3939
2.5132
2.5037
2.5030
1.0736


6b
160
140
120
100
80
60
40
20
0
δ / ppm
159.9123
157.7343
141.9975
139.8070
138.9734
137.3145
133.0121
131.3573
130.0873
128.7428
128.3870
128.1636
126.8316
121.8838
113.5024
98.7916
51.6143
40.5853
40.4934
40.4138
40.3339
40.2543
40.1633
39.9978
39.8338
39.6628
39.4932
28.2430

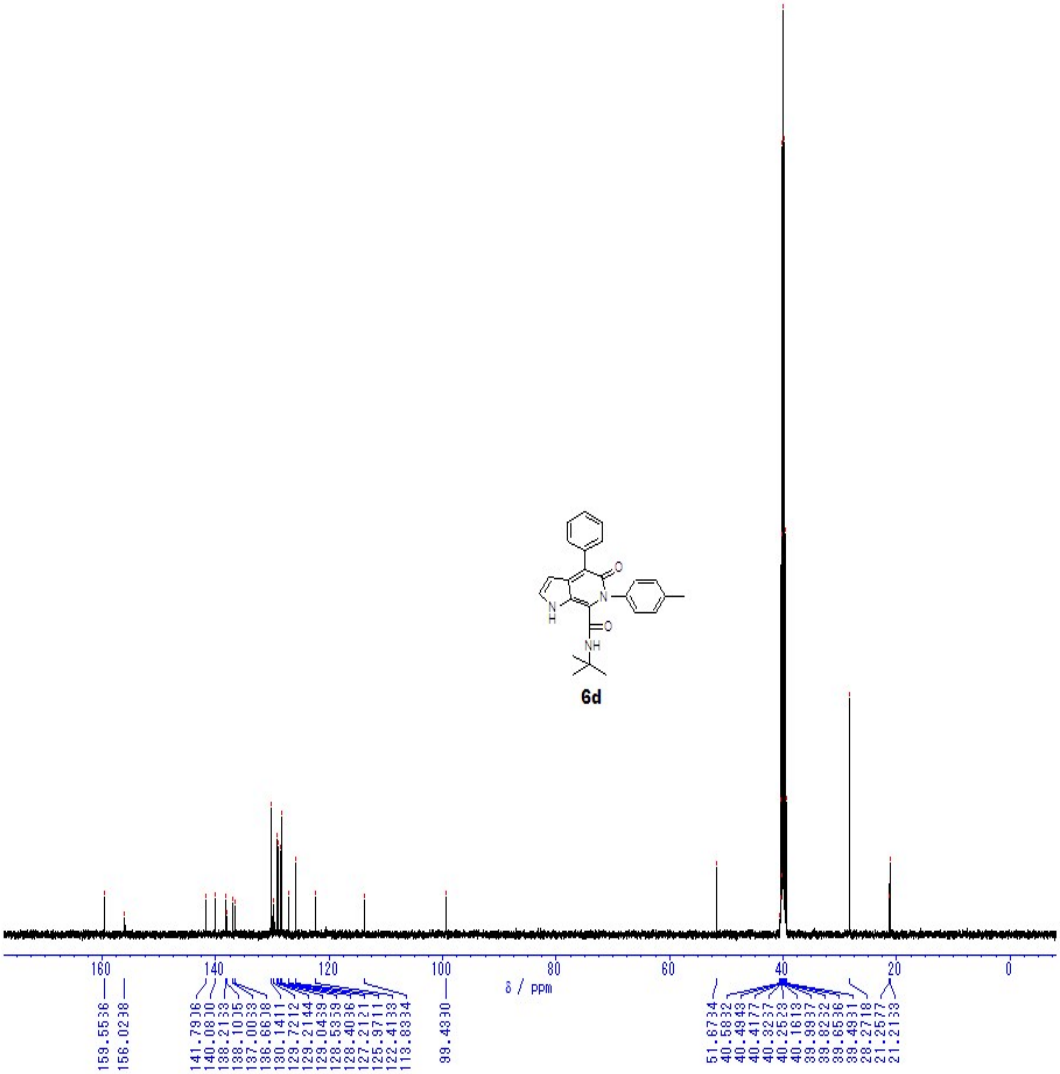

10.0231
9.6317
3.2418
1.0
1.0057
1.0092
OMe
6c
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
11.3428
8.3548
7.8132
7.6530
7.6352
7.4933
7.4830
7.4612
7.4448
7.3334
7.3137
7.1349
7.1132
7.0519
7.0344
6.2726
3.8012
2.5120
1.0740

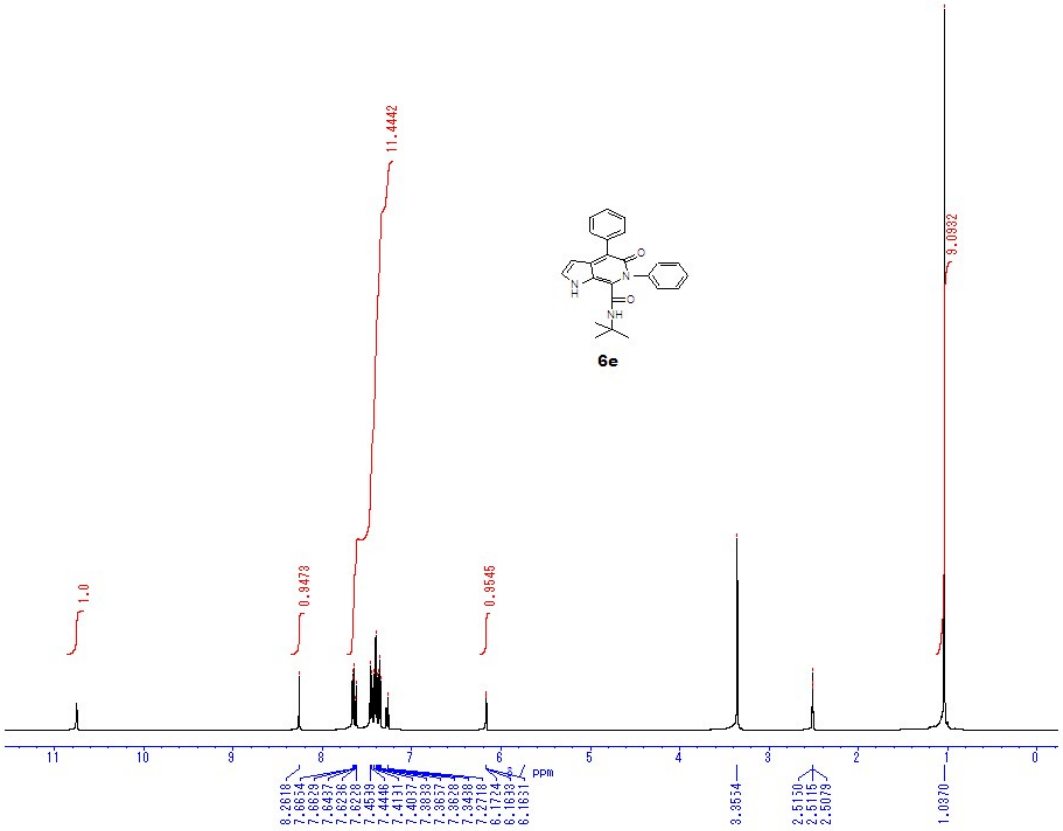
Star


O
N
OMe
H
N
O
NH
6c
160
140
120
100
80
60
40
20
0
δ / ppm
159.6736
159.3830
146.1344
141.8010
140.3313
138.1233
136.3071
131.9758
130.3532
130.3130
128.5442
127.4139
125.9711
122.6036
114.0671
99.7617
55.9829
51.7632
40.4931
40.4136
40.3226
40.2431
40.1531
39.9836
39.8220
39.6545
39.4839
28.3318

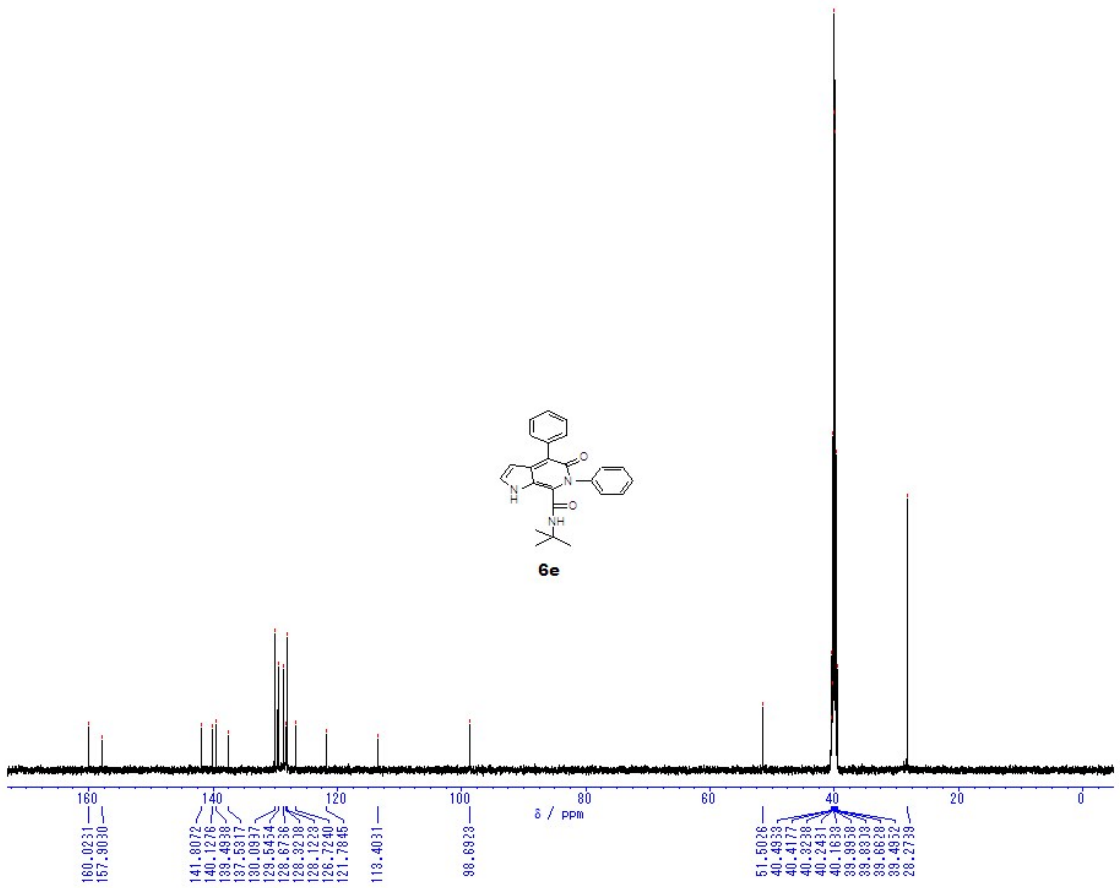

10.3162
1.0
1.0488
1.0398
3.0514
6d
16
14
12
10
8
6
4
2
0
-2
11.1614
8.3142
7.7637
7.7551
7.7431
7.6510
7.6337
7.4939
7.4829
7.4577
7.4426
7.4271
7.3332
7.3216
7.3056
7.2935
7.2739
7.2737
7.2533
7.1330
7.1211
6.2338
2.5136
2.5121
2.5035
2.3426
1.0541
1.0136

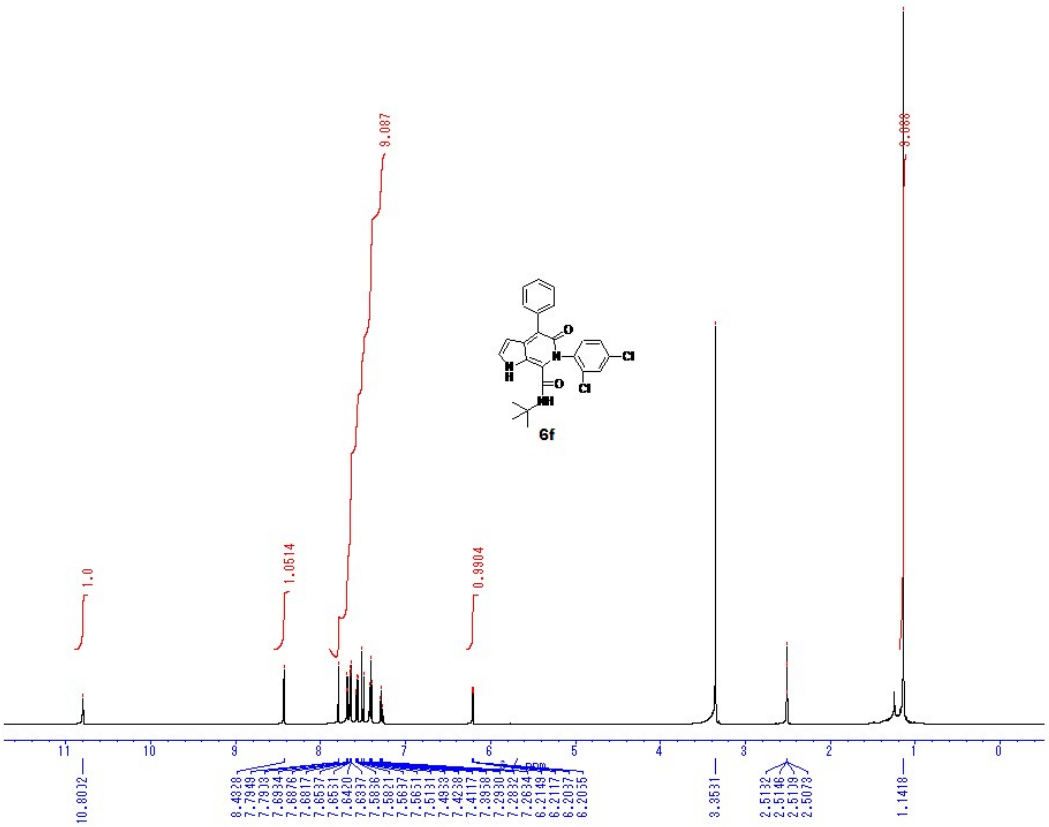
Star

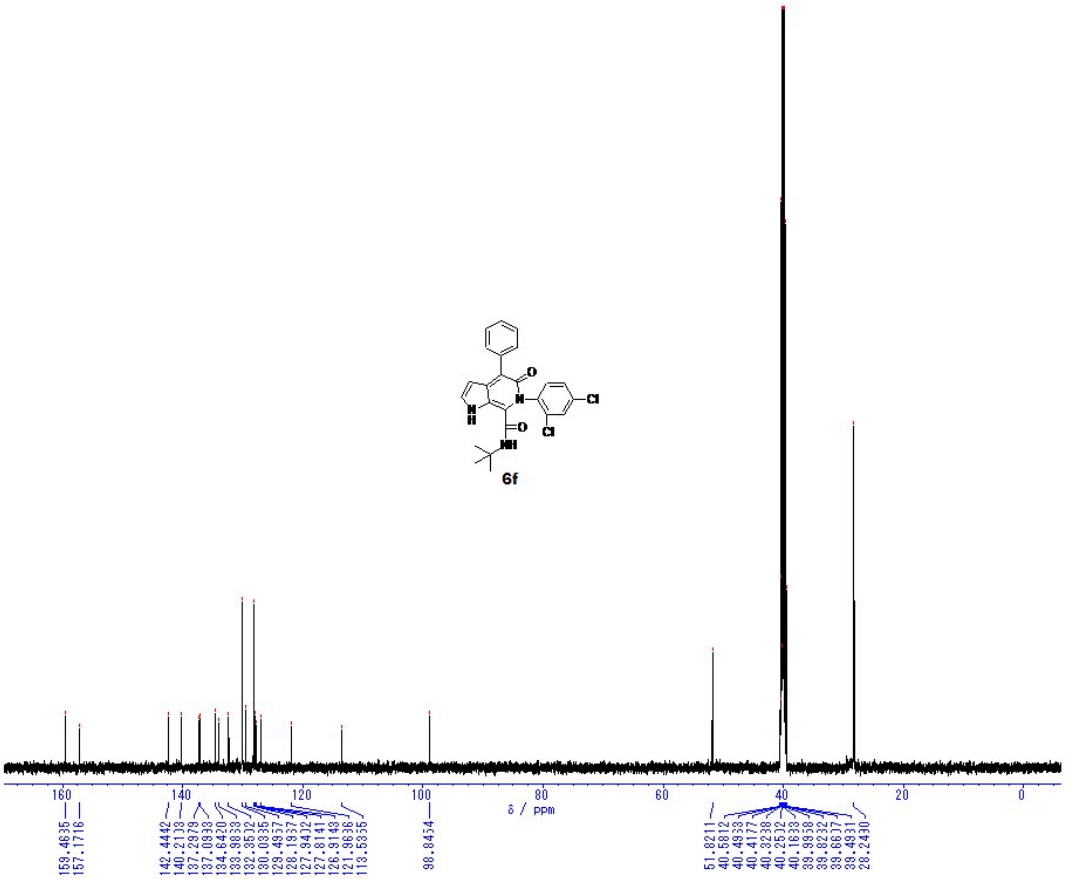

6d
160
140
120
100
80
60
40
20
0
δ / ppm
159.5536
156.0238
141.7916
140.0810
138.2153
138.1015
137.0053
136.6618
130.1411
129.7212
129.2144
129.0459
128.5359
128.4036
127.2121
125.9711
122.4133
113.8334
99.4330
51.6734
40.5832
40.4943
40.4177
40.3237
40.2523
40.1613
39.9937
39.8232
39.6536
39.4931
28.2718
21.2577
21.2133

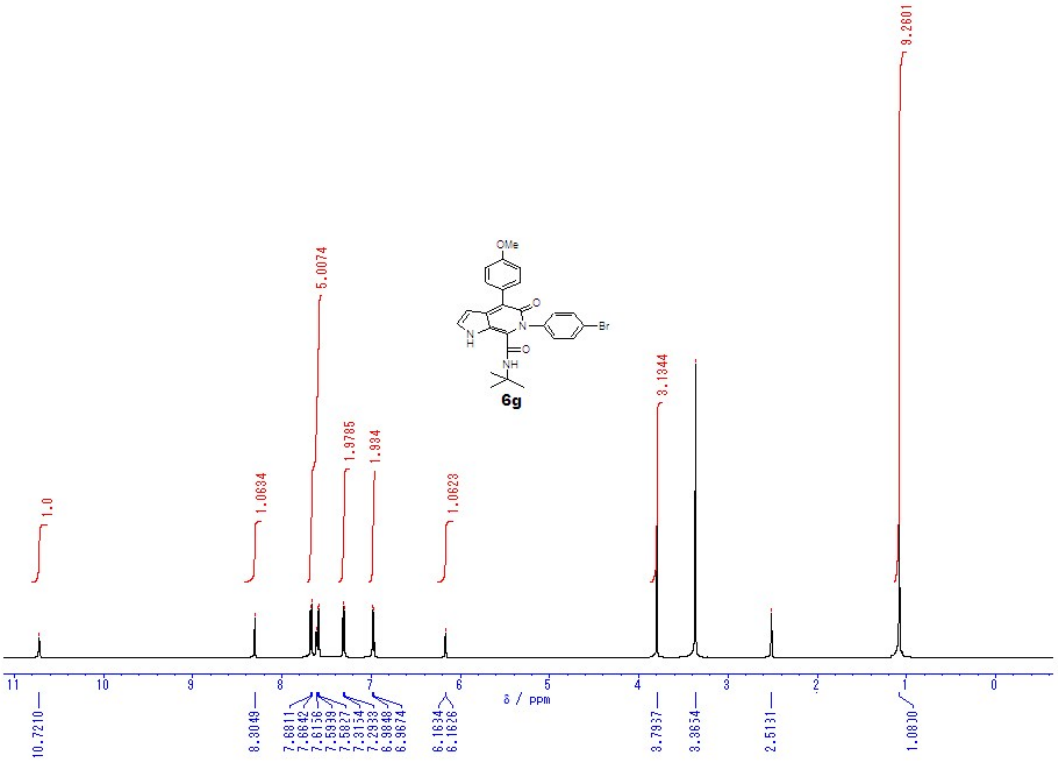

11.4442
9.0932
1.0
0.9473
0.9545
6e
11
10
9
8
7
6
5
4
3
2
1
0
ppm
8.2618
7.6654
7.6629
7.6437
7.6236
7.6228
7.4539
7.4446
7.4131
7.4037
7.3833
7.3657
7.3628
7.3438
7.2718
6.1724
6.1633
6.1631
3.3554
2.5130
2.5115
2.5079
1.0370

Star

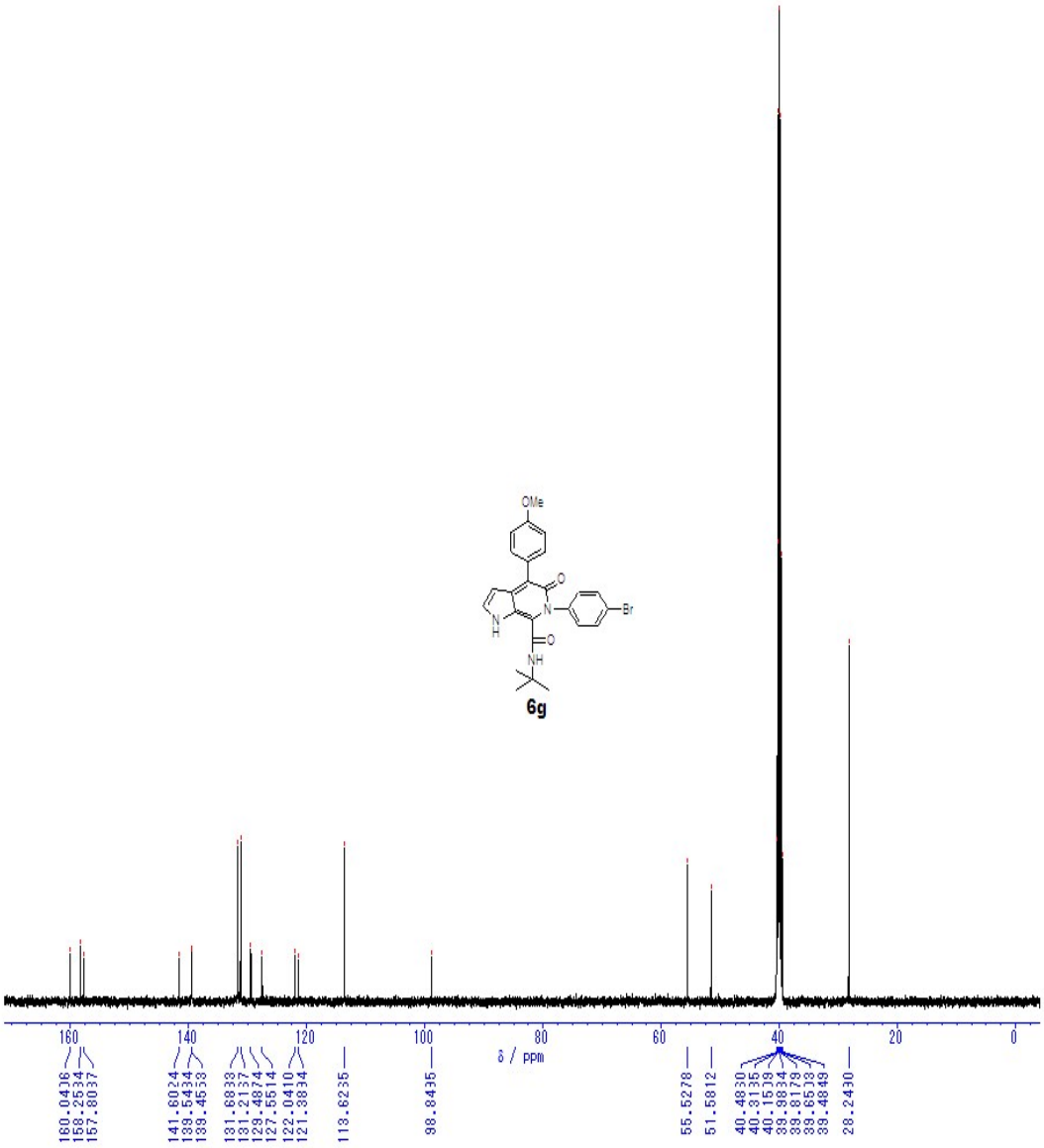

6e
160
140
120
100
80
60
40
20
0
δ / ppm
160.0231
157.9030
141.8072
140.1276
139.4938
137.5317
130.0937
129.5454
128.6736
128.3238
128.1223
126.7240
121.7845
118.4031
98.6923
51.5026
40.4933
40.4177
40.3238
40.2431
40.1633
39.9838
39.8838
39.6628
39.4932
28.2739

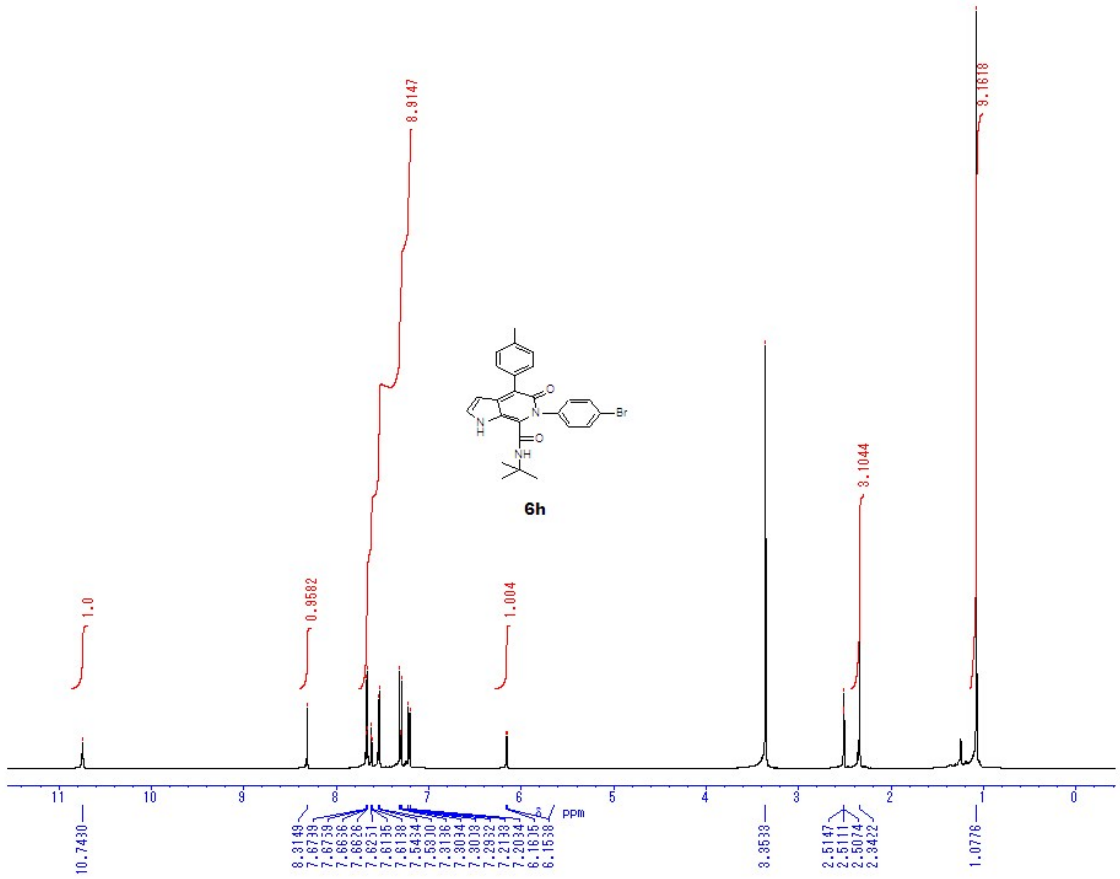

9.087
3.088
1.0
1.0514
0.3904
6f
11
10
9
8
7
6
5
4
3
2
1
0
10.8032
3.3631
2.5132
2.5146
2.5139
2.5073
1.1418

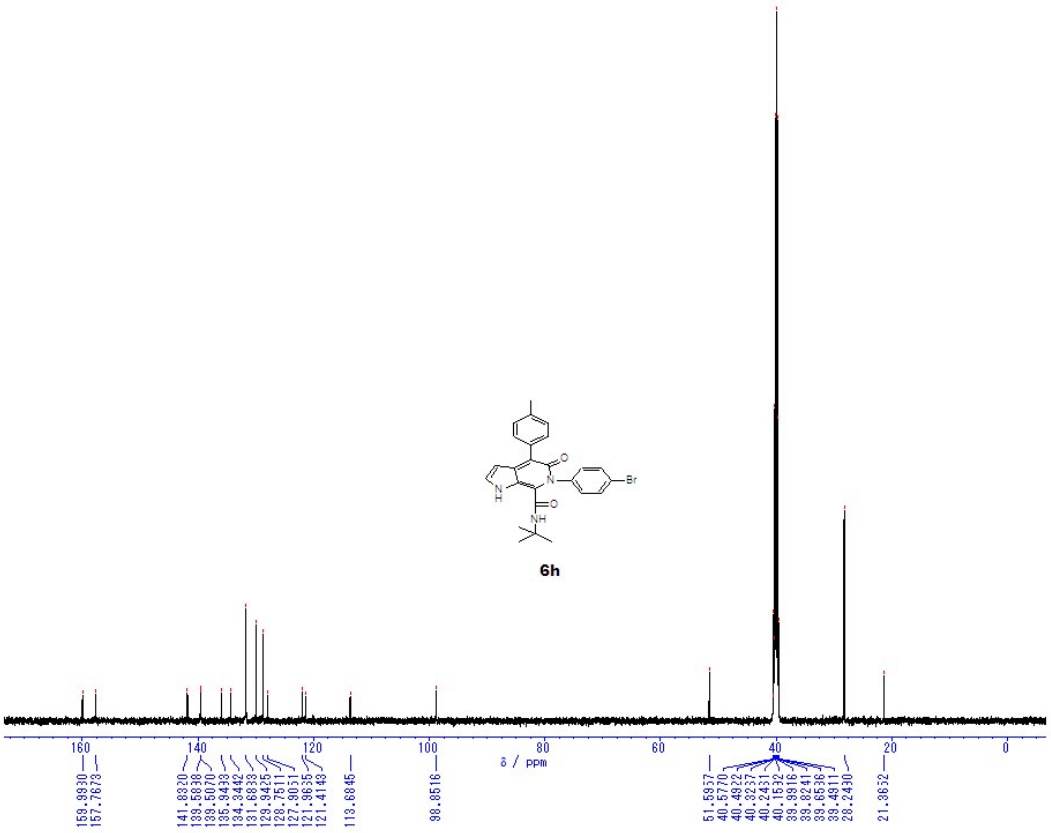

6f
160
140
120
100
80
60
40
20
0
δ / ppm
159.4635
157.1716
142.4442
140.2118
137.2979
137.0938
134.6420
133.9833
132.3532
130.0835
129.4937
128.1937
127.9432
127.8141
126.9148
121.9636
118.6336
98.8454
51.8211
40.8812
40.4933
40.4177
40.2538
40.1532
40.1638
39.9939
39.8232
39.6637
39.4931
28.2490

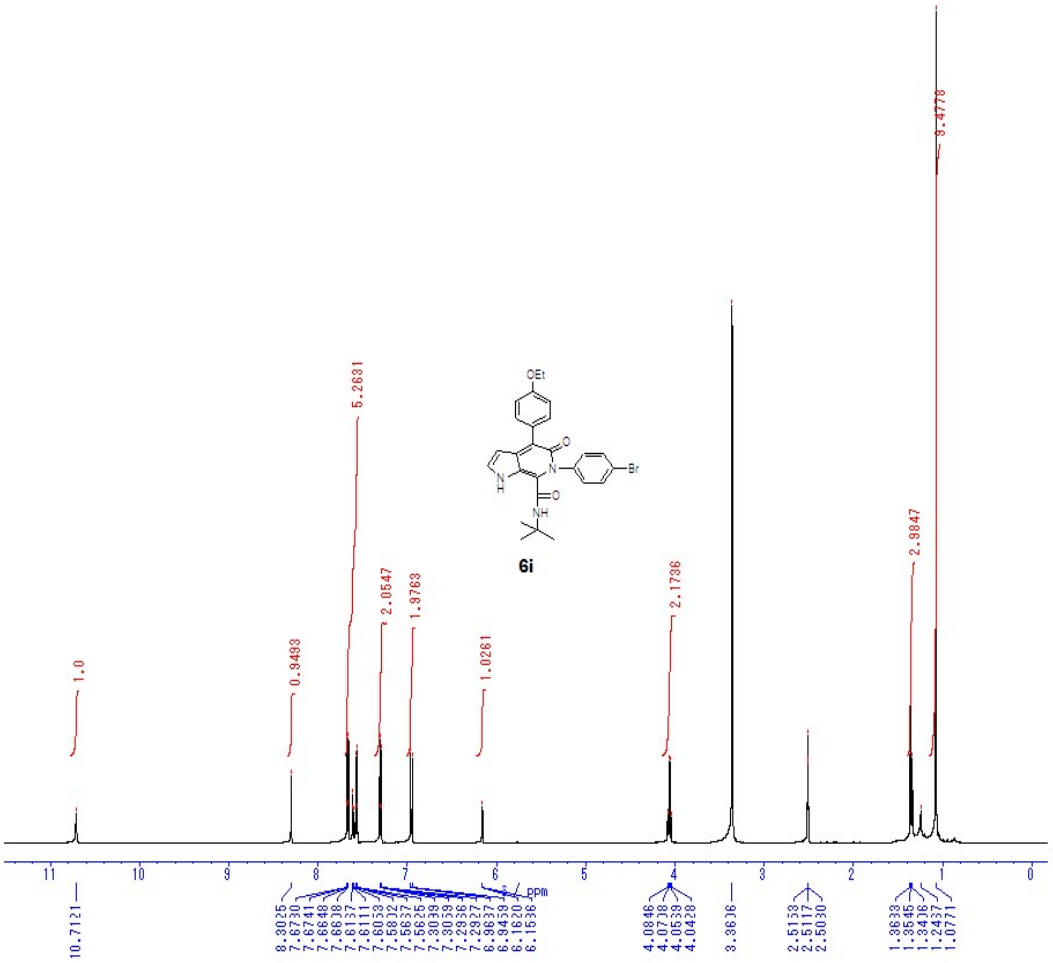

OMe
O
N
Br
H
O
NH
6g
1.0
1.0634
5.0074
1.9785
1.934
1.0623
3.1344
9.2801
11
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
10.7210
8.3049
7.6811
7.6642
7.6156
7.6030
7.5938
7.5827
7.3154
7.2933
6.8848
6.8674
6.1634
6.1626
3.7937
3.3654
2.5131
1.0830

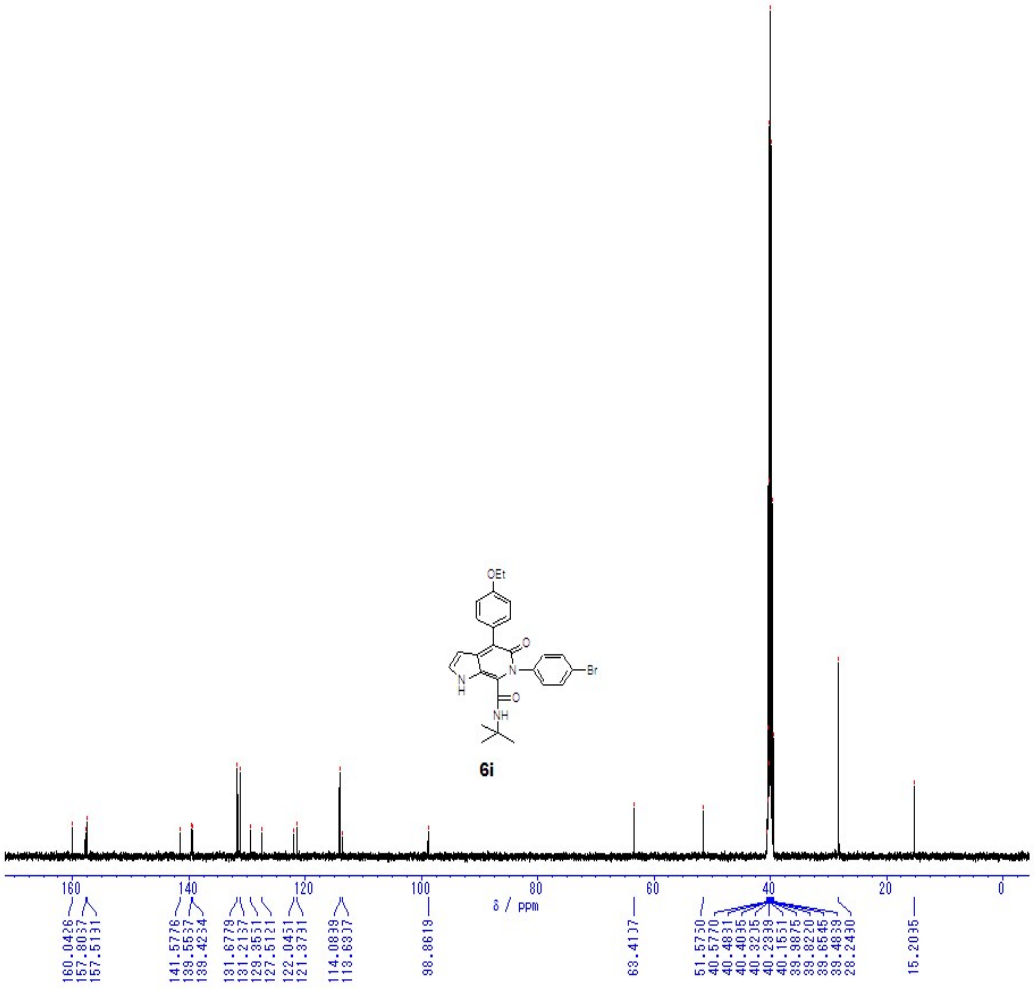
Star

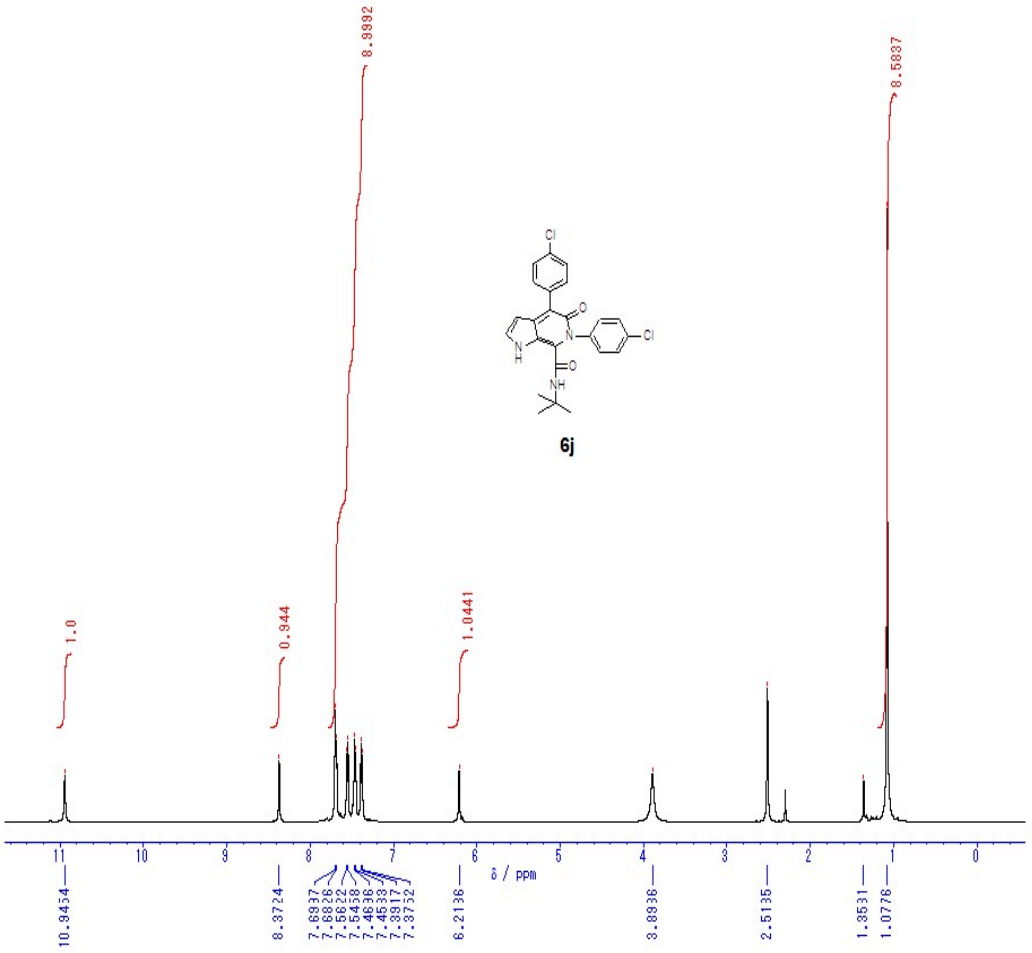

OMe
O
N
Br
H
O
NH
6g
160.0436
158.2534
157.8037
141.6024
139.5434
139.4658
131.6838
131.2137
129.4874
127.5514
122.0410
121.3834
113.6235
98.8435
δ / ppm
55.5278
51.5812
40.4830
40.3135
40.1539
39.9834
39.8179
39.6503
39.4849
28.2430


8.9147
9.1618
9.1044
1.0
0.9582
1.004
6h
ppm
10.7430
8.3149
7.6739
7.6759
7.6636
7.6626
7.6251
7.6135
7.6138
7.5434
7.5310
7.3136
7.3044
7.3013
7.2932
7.2138
7.2034
6.1635
6.1538
3.3533
2.5147
2.5111
2.5074
2.3422
1.0778

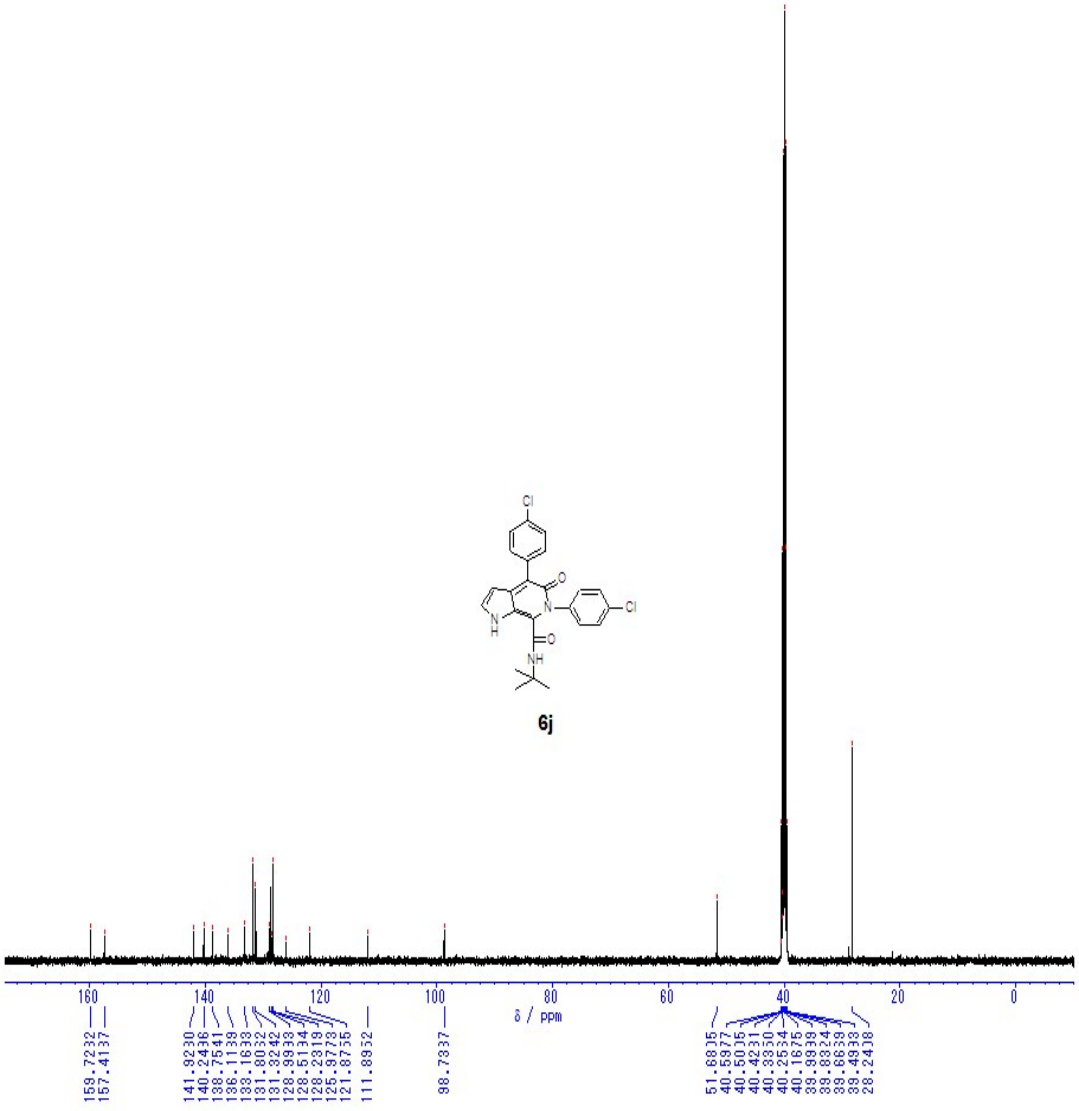

6h
δ / ppm
159.9930
157.7673
141.8320
139.5838
139.5070
135.9433
134.3442
131.6833
129.9425
128.7511
127.9031
121.9635
121.4143
113.6845
98.8516
51.5957
40.5770
40.4922
40.3237
40.2431
40.1532
39.9916
39.8241
39.6536
39.4911
28.2430
21.3632

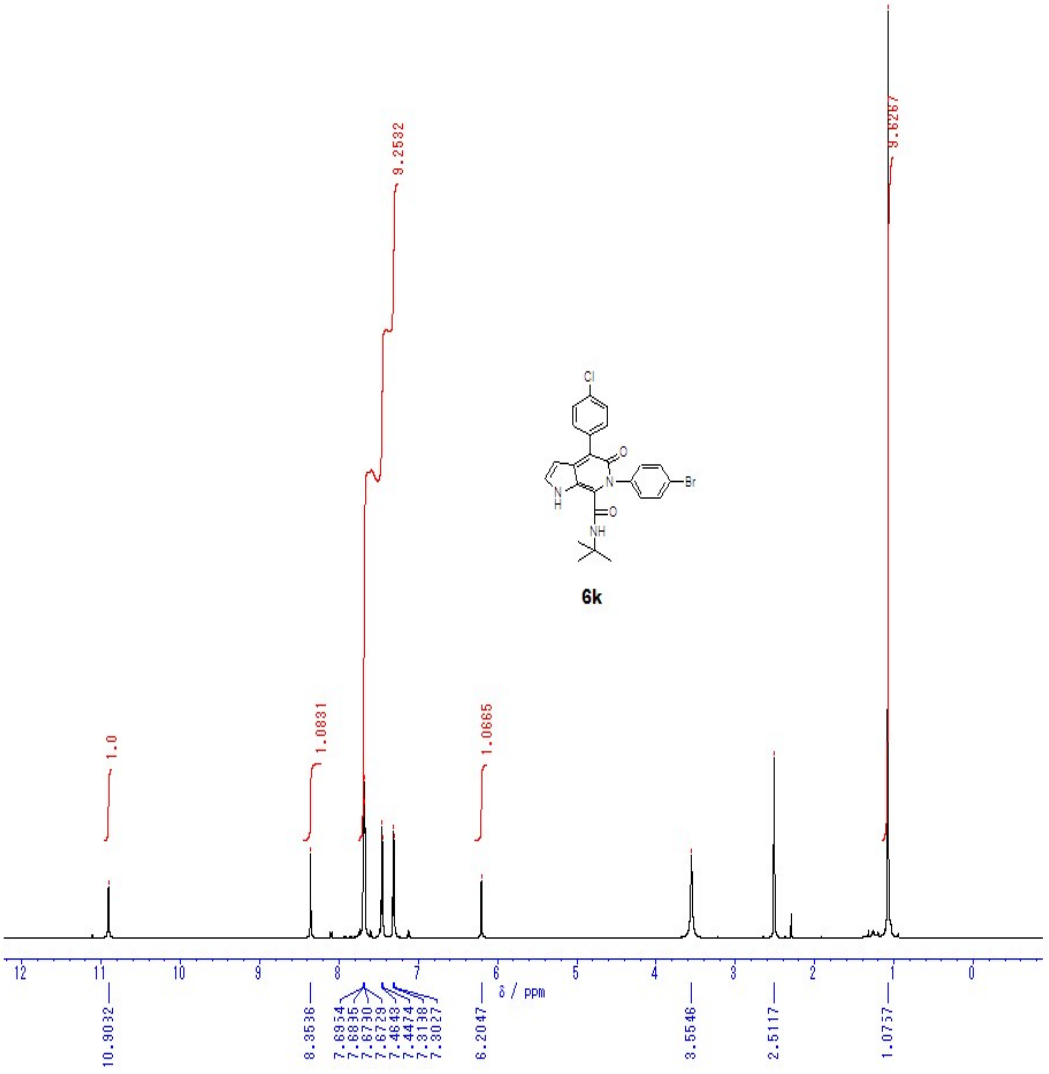

OEt
O
N
Br
H
N
O
NH
6i
1.0
0.9493
5.2631
2.0547
1.9763
1.0261
2.1736
2.9847
8.4778
11
10
9
8
7
6
5
4
3
2
1
0
ppm
10.7121
8.3025
7.6730
7.6741
7.6638
7.6137
7.6111
7.6053
7.5832
7.5657
7.5625
7.3039
7.3039
7.2936
7.2927
6.3637
6.3459
6.1620
6.1536
4.0846
4.0738
4.0539
4.0428
3.3636
2.5153
2.5117
2.5030
1.3633
1.3545
1.3416
1.2457
1.0771


OEt
O
N
Br
NH
O
6i
160
140
120
100
80
60
40
20
0
δ / ppm
160.0428
157.8057
157.6131
141.5776
139.5637
139.4234
131.6779
131.2137
129.3651
127.6121
122.0451
121.3731
114.0839
113.6837
98.8619
63.4137
51.5750
40.5370
40.4831
40.4035
40.2239
40.1631
39.9875
39.8220
39.6545
39.4839
28.2430
15.2036

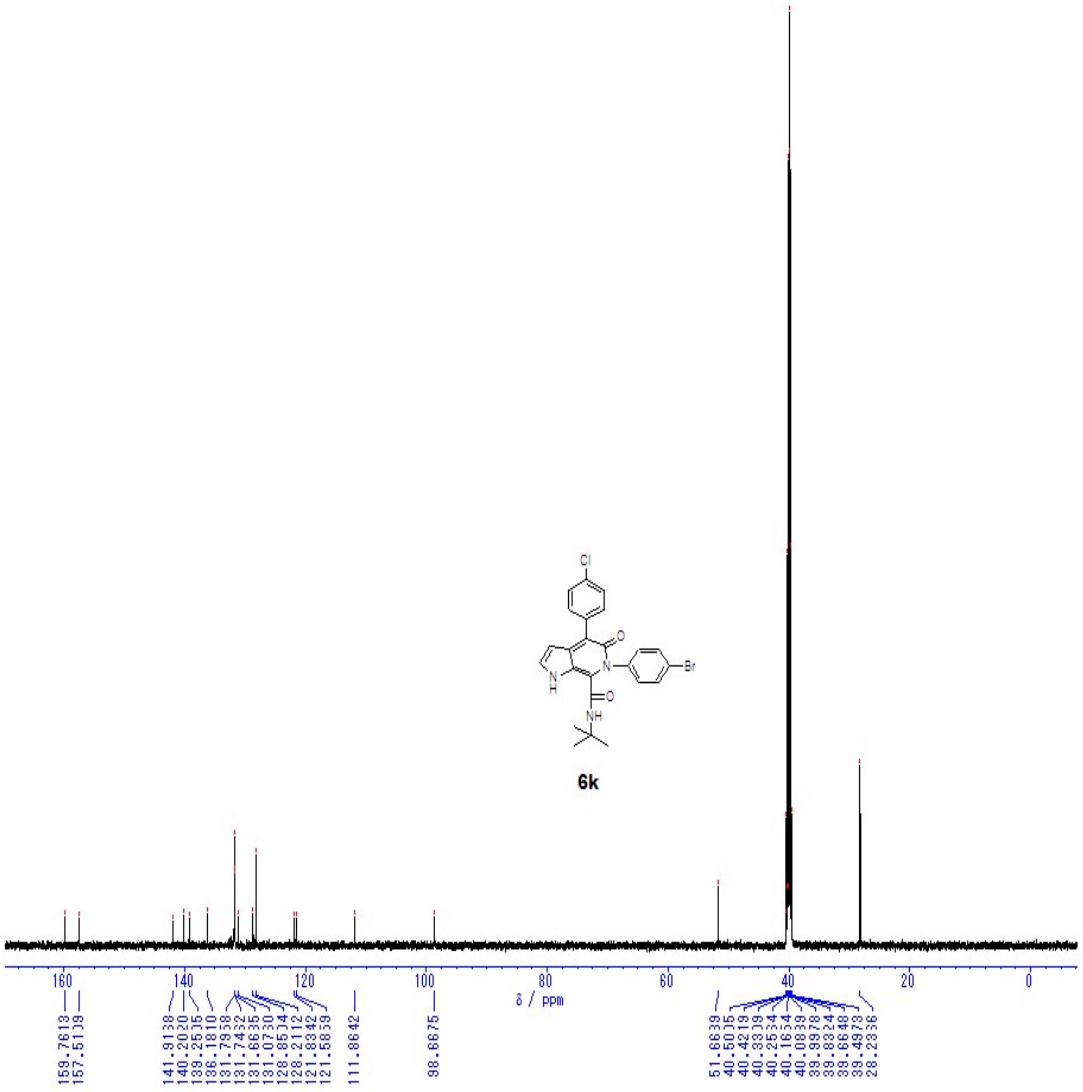

8.9992
8.5837
1.0
0.944
1.0441
Cl
O
N
H
Cl
O
NH
6j
δ / ppm
10.9454
8.3724
7.6937
7.6826
7.5622
7.5438
7.4636
7.4533
7.3817
7.3752
6.2136
3.8936
2.5135
1.3531
1.0776

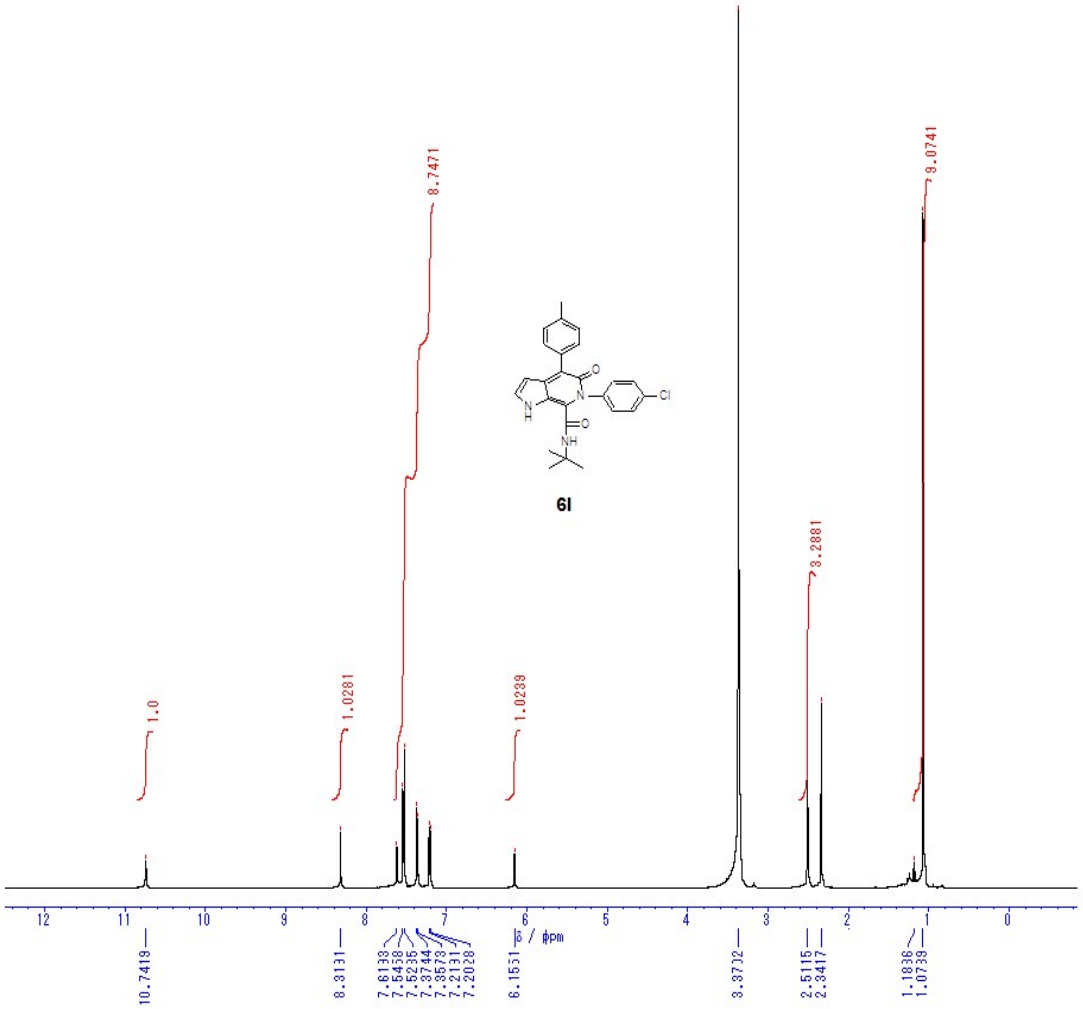
Star


Cl
O
N
Cl
H
O
NH
6j
160
140
120
100
80
60
40
20
0
δ / ppm
159.7232
157.4137
141.8230
140.2436
138.7541
136.1139
133.1633
131.8032
131.3246
128.8933
128.6134
128.2319
125.6778
121.8735
111.8952
98.7337
51.6835
40.5977
40.5035
40.4231
40.3350
40.2534
40.1675
39.9939
39.8324
39.6638
39.4933
28.2438

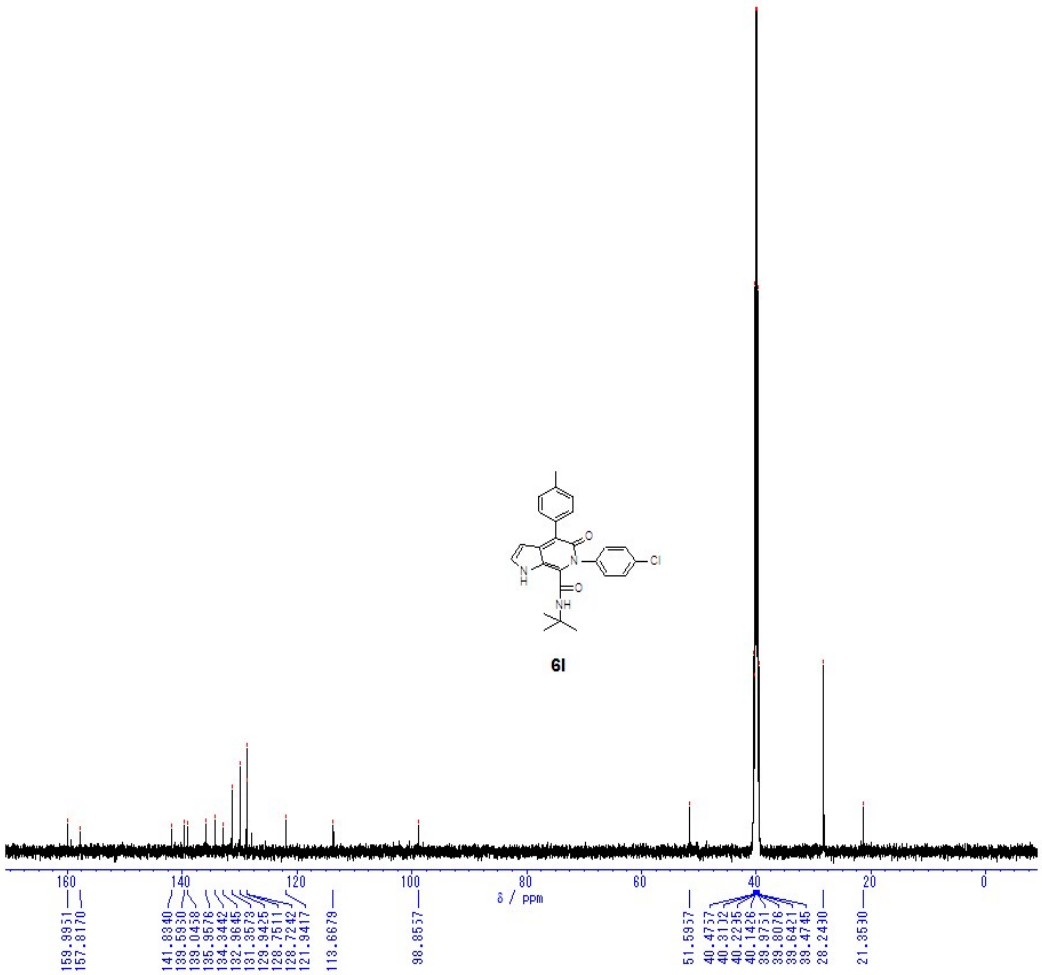

9.2532
9.6287
1.0
1.0831
1.0665
Cl
O
N
Br
H
O
NH
6k
12
11
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
10.3032
8.3536
7.6934
7.6835
7.6730
7.6729
7.4643
7.4474
7.3138
7.3027
6.2047
3.5546
2.5117
1.0757

Star


Cl
O
N
Br
H
O
NH
6k
160
140
120
100
80
60
40
20
0
δ / ppm
159.7613
157.5139
141.9138
140.2020
139.2535
136.1810
131.7958
131.7432
131.6635
131.0730
128.8534
128.2112
121.8342
121.5839
111.8642
98.6675
51.6639
40.5035
40.4218
40.3339
40.2534
40.1654
40.0839
39.9978
39.8324
39.6648
39.4973
28.2336


8.7471
9.0741
8.2881
1.0
1.0281
1.0239
6I
12
11
10
9
8
7
6
5
4
3
2
1
0
δ / ppm
10.7419
8.3131
7.6133
7.5458
7.5235
7.3744
7.3573
7.2131
7.2028
6.1551
3.3732
2.5115
2.3417
1.1836
1.0739

Star


6l
δ / ppm
159.8951
157.8170
141.8340
139.6330
139.0438
135.9578
134.9442
132.8645
131.3573
129.9425
128.7511
128.7242
121.9417
113.6679
98.8557
51.5957
40.4757
40.3112
40.2235
40.1426
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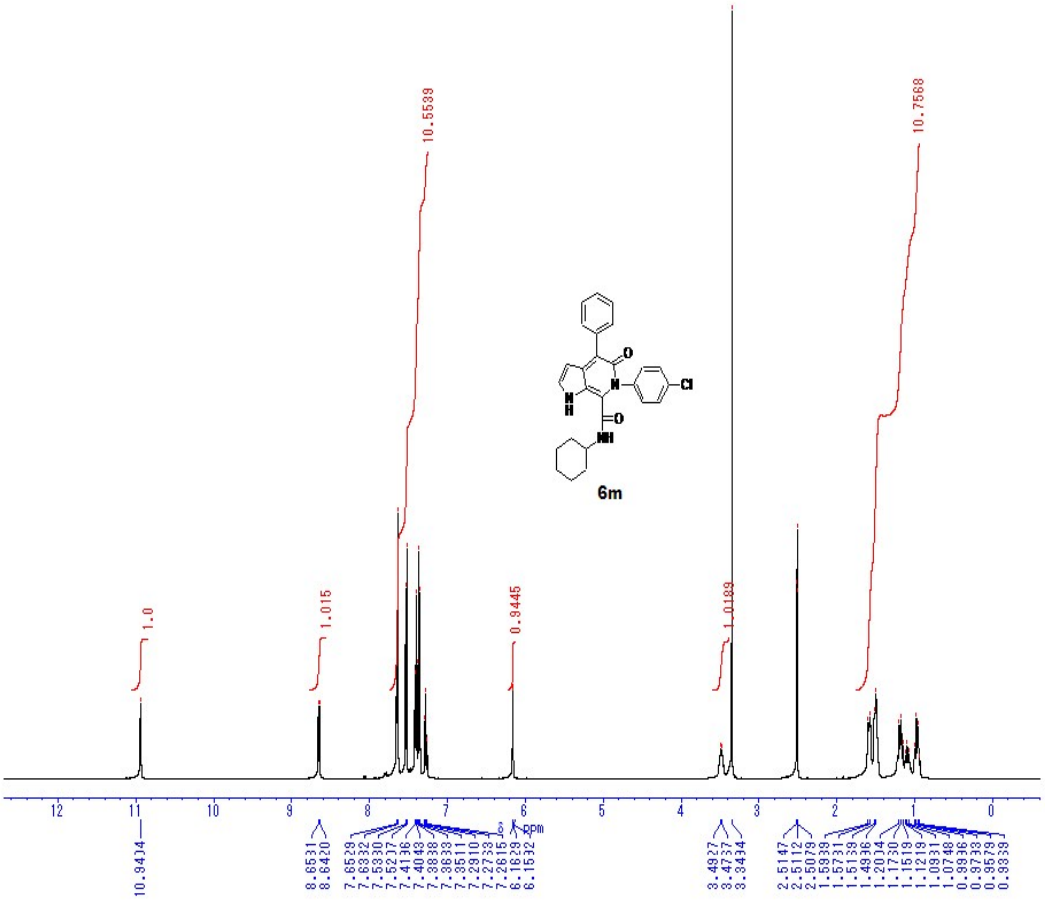
39.8076
39.6421
39.4745
28.2430
21.3530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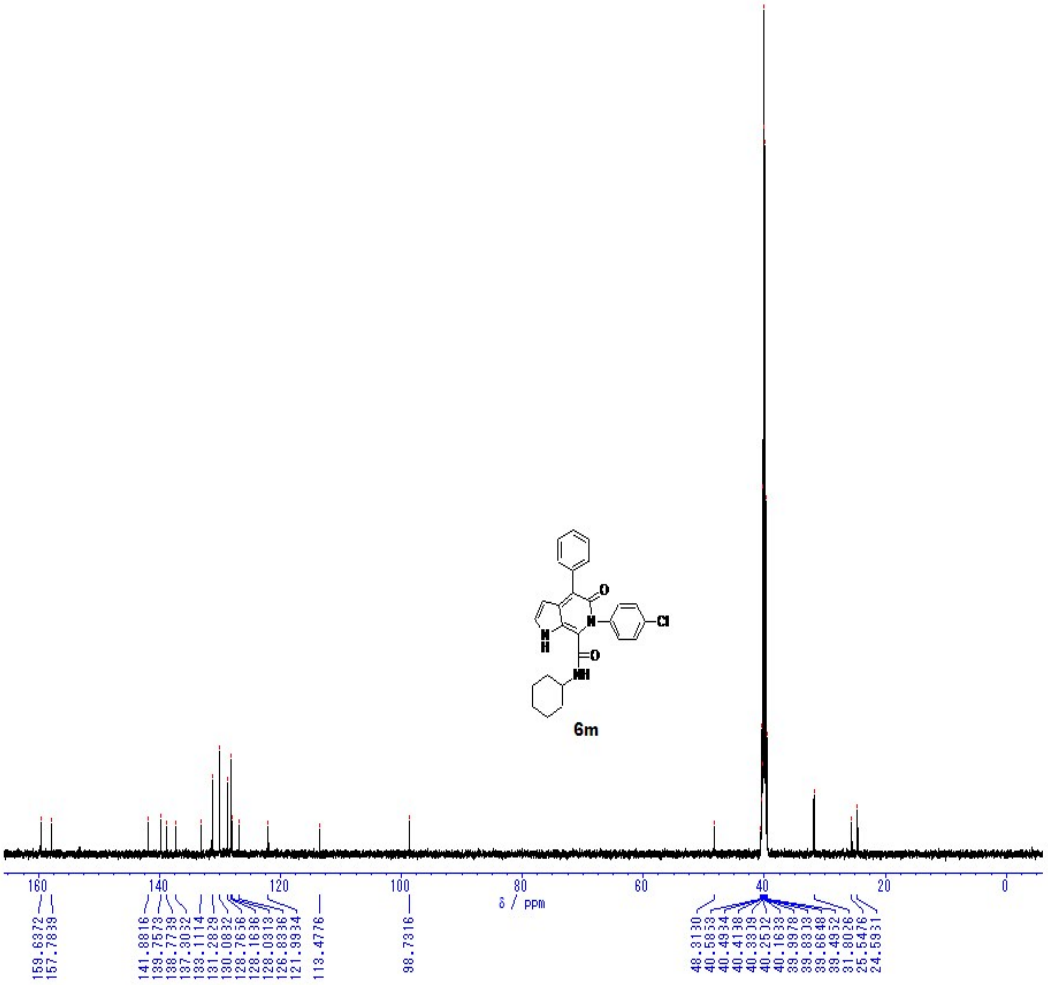
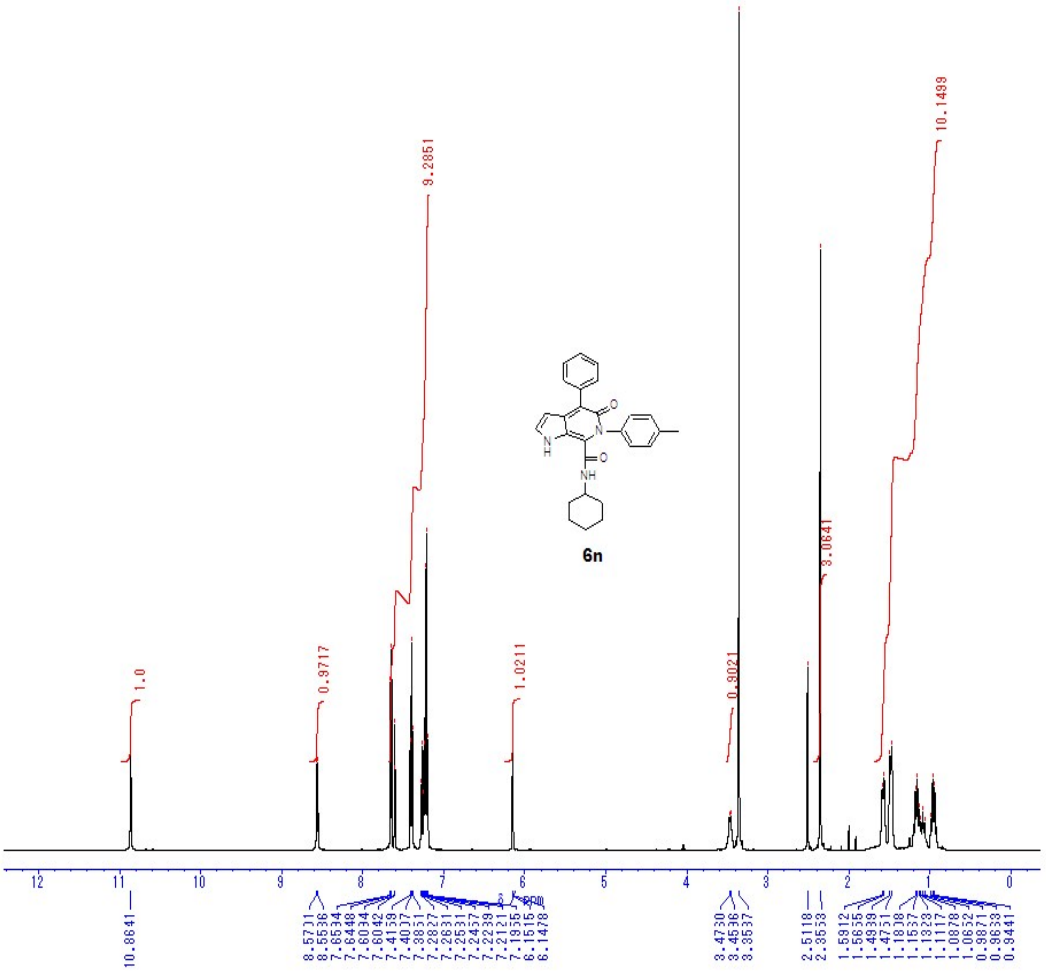
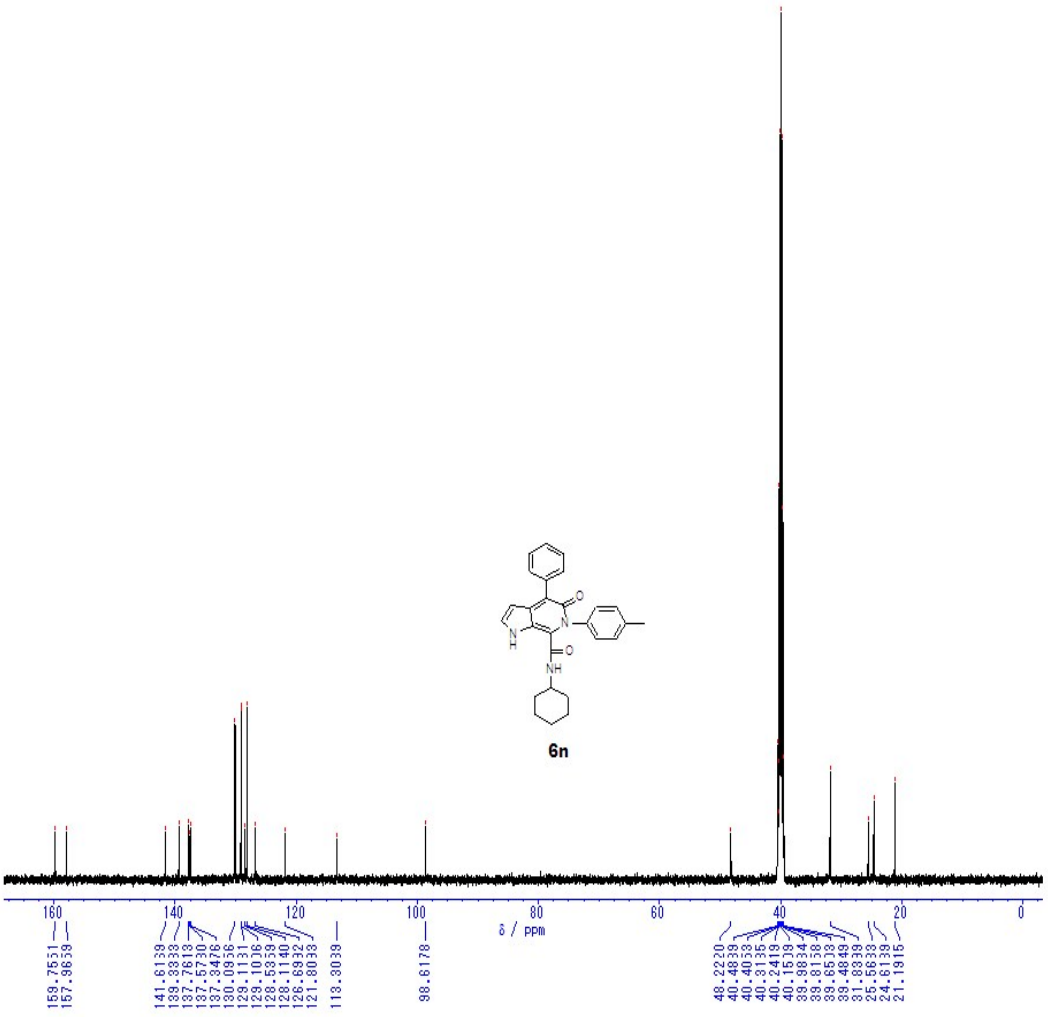
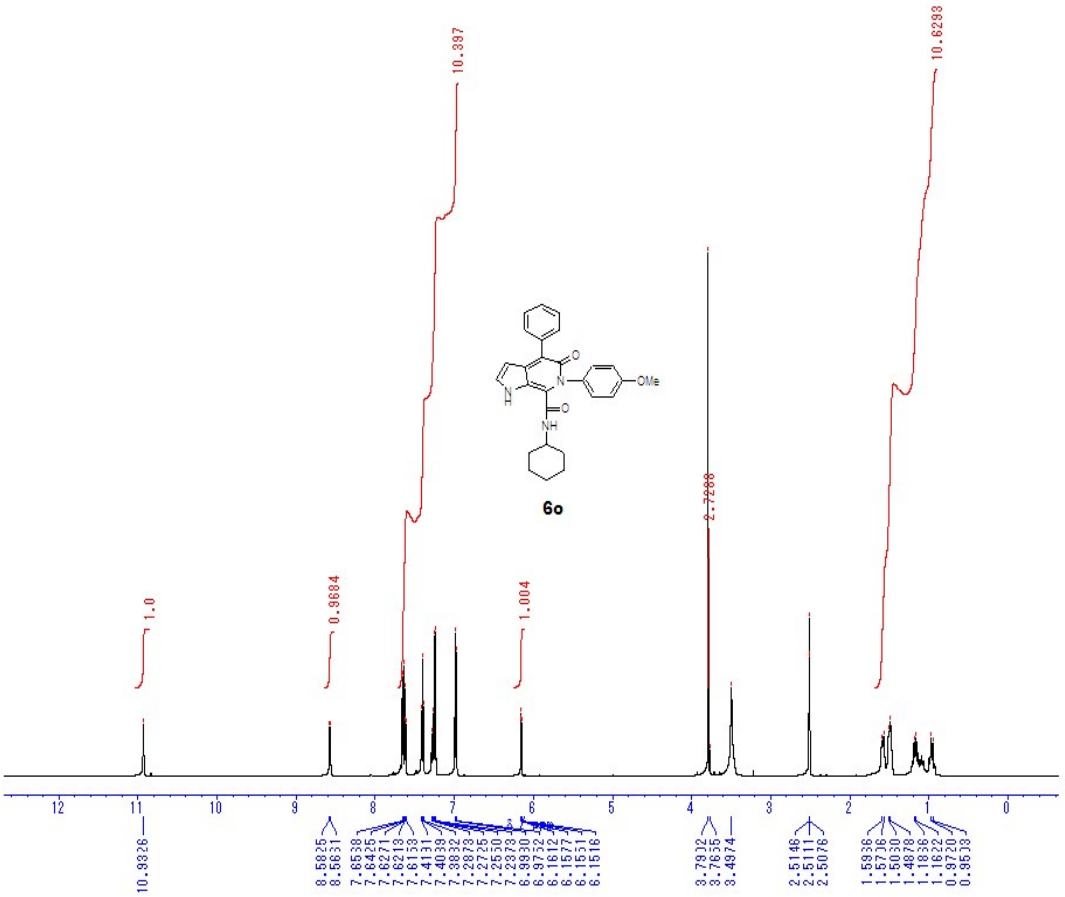
10.7568
1.0
1.015
0.9445
1.0189
6m
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

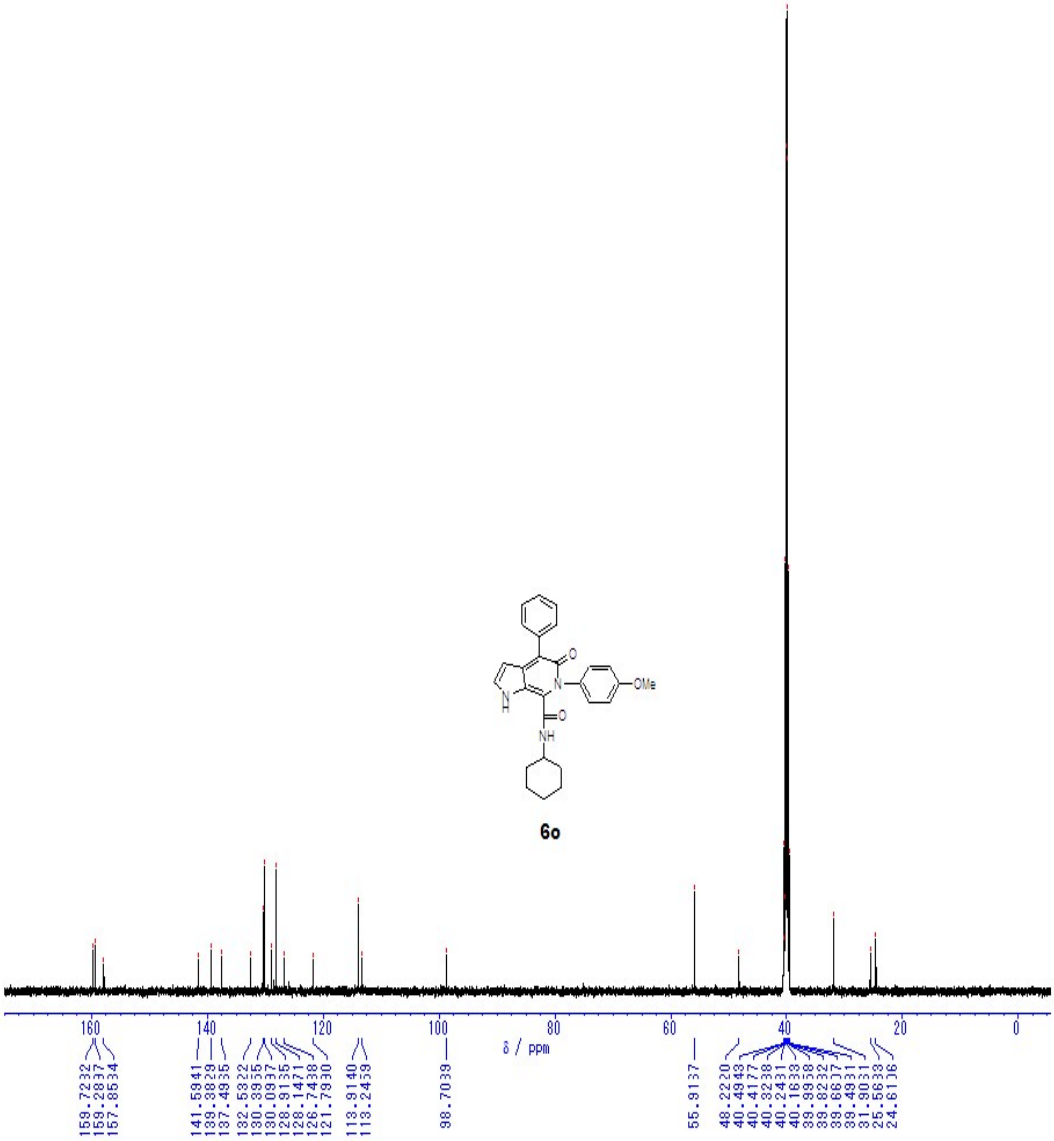

O
N
Cl
H
H
O
NH
6m
160
140
120
100
80
60
40
20
0
δ / ppm
159.6372
157.7833
141.8816
139.7573
138.7738
137.3032
133.1114
131.2829
130.0832
128.7656
128.1636
128.0313
126.8336
121.9934
113.4776
98.7316
48.3130
40.5053
40.4934
40.4138
40.3339
40.2532
40.1833
39.9978
39.8333
39.6648
39.4952
31.8026
25.5476
24.5931

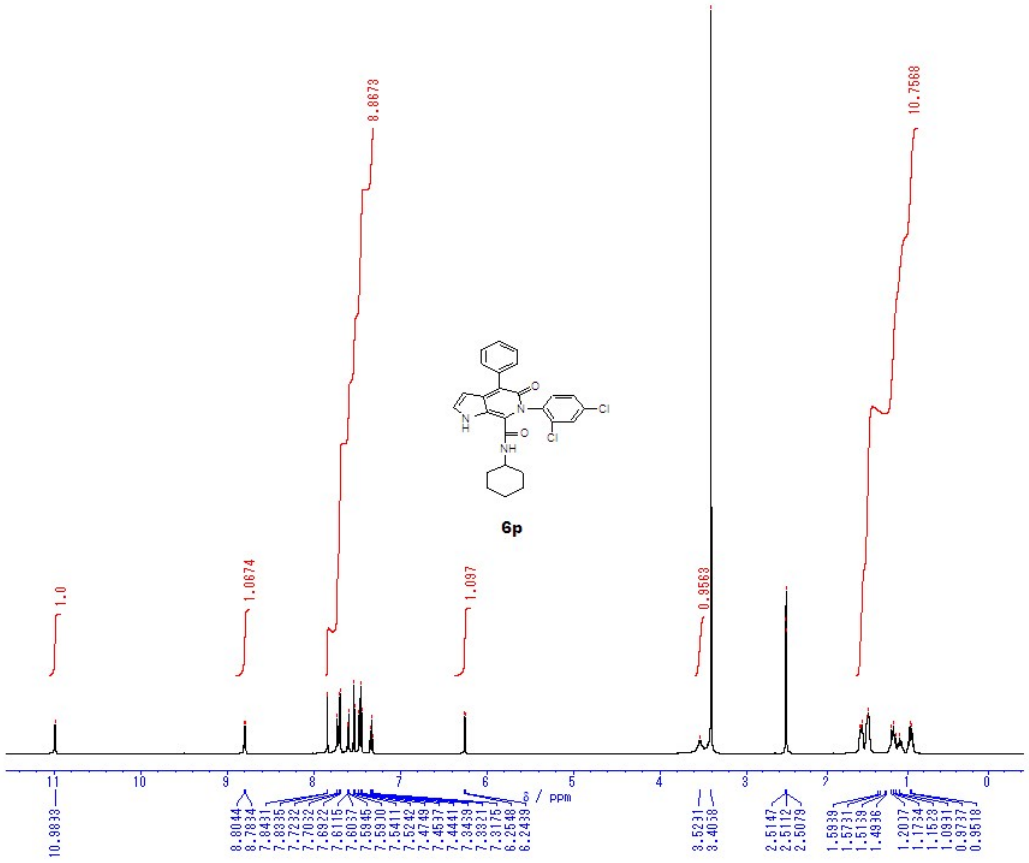

9.2851
10.1499
3.0641
1.0
0.9717
1.0211
0.8021
6n
12
11
10
9
8
7
6
5
4
3
2
1
0
10.8641
8.5731
8.5536
7.6534
7.6448
7.6034
7.6042
7.4159
7.4017
7.3851
7.2827
7.2831
7.2457
7.2239
7.2121
7.1815
6.1516
6.1478
3.4730
3.4536
3.3537
2.5118
2.3653
1.5912
1.5635
1.4939
1.4731
1.1838
1.1537
1.1323
1.1117
1.0878
1.0632
0.9871
0.9633
0.9441

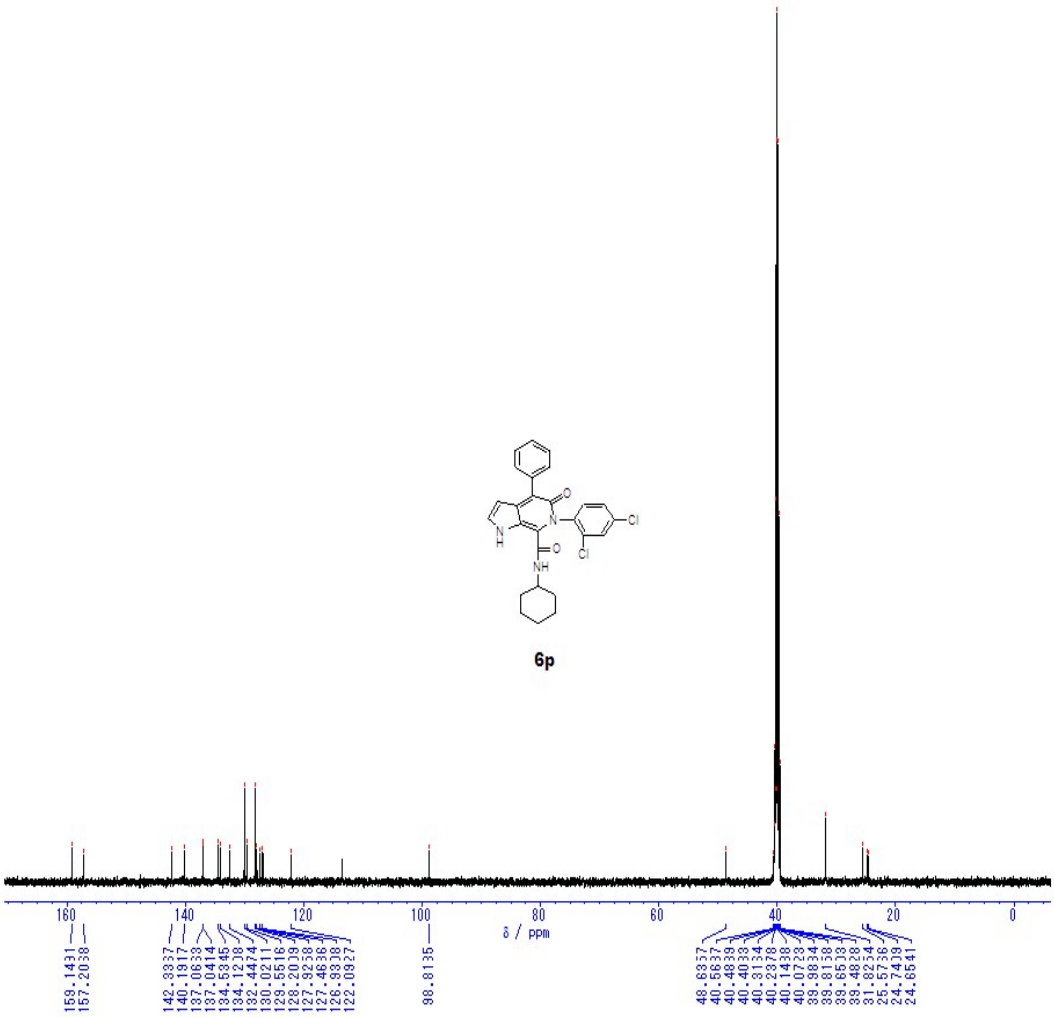
Star

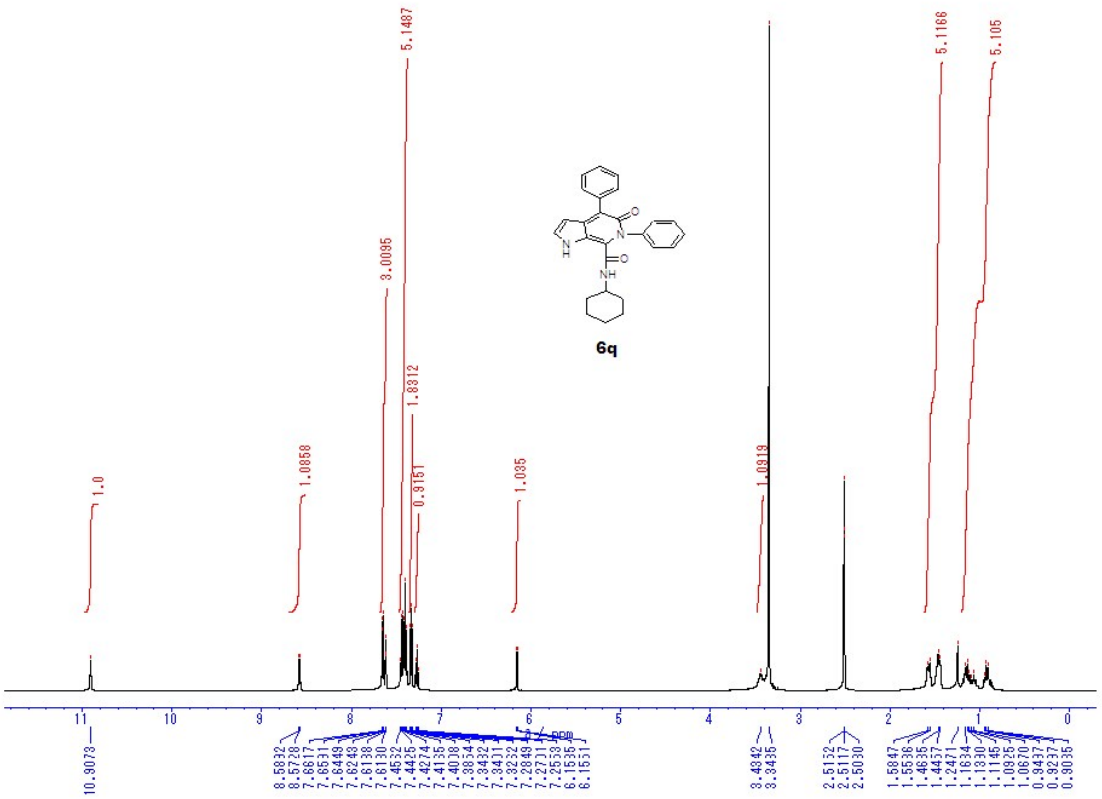

6n
δ / ppm
160
140
120
100
80
60
40
20
0
159.7551
157.8638
141.6139
139.3333
137.7613
137.5730
137.3476
130.0956
129.1131
129.1036
128.5359
128.1140
126.6932
121.8033
113.3039
98.6178
48.2220
40.4839
40.4053
40.3135
40.2419
40.1539
39.9834
39.8158
39.6533
39.4849
31.8339
25.5633
24.6139
21.1915

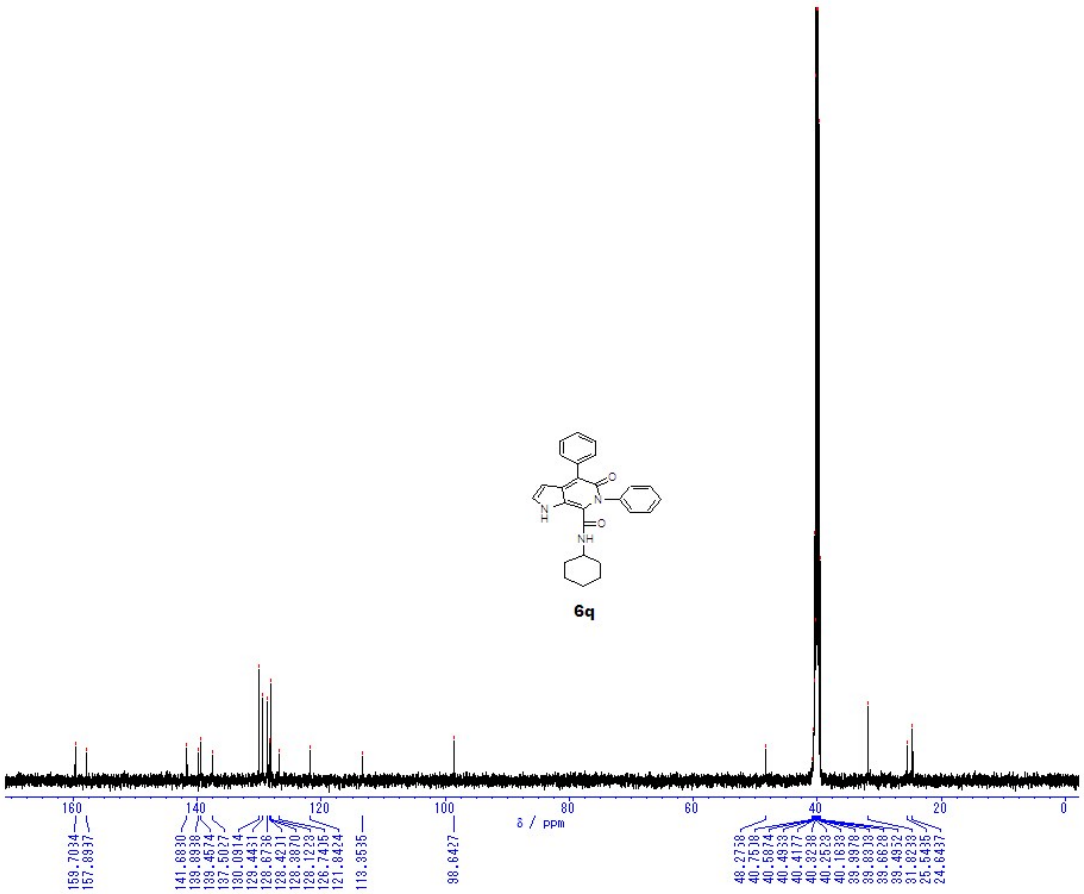

10.387
10.6293
2.7288
1.0
0.9884
1.004
OMe
NH
6o
12
11
10
9
8
7
6
5
4
3
2
1
0
10.9326
8.5825
8.5631
7.6538
7.6425
7.6271
7.6213
7.6158
7.4131
7.4039
7.3832
7.2873
7.2725
7.2550
7.2373
6.9930
6.9752
6.1612
6.1577
6.1551
6.1516
3.7932
3.7635
3.4974
2.5146
2.5111
2.5078
1.5936
1.5736
1.5030
1.4878
1.1836
1.1622
0.9720
0.9533

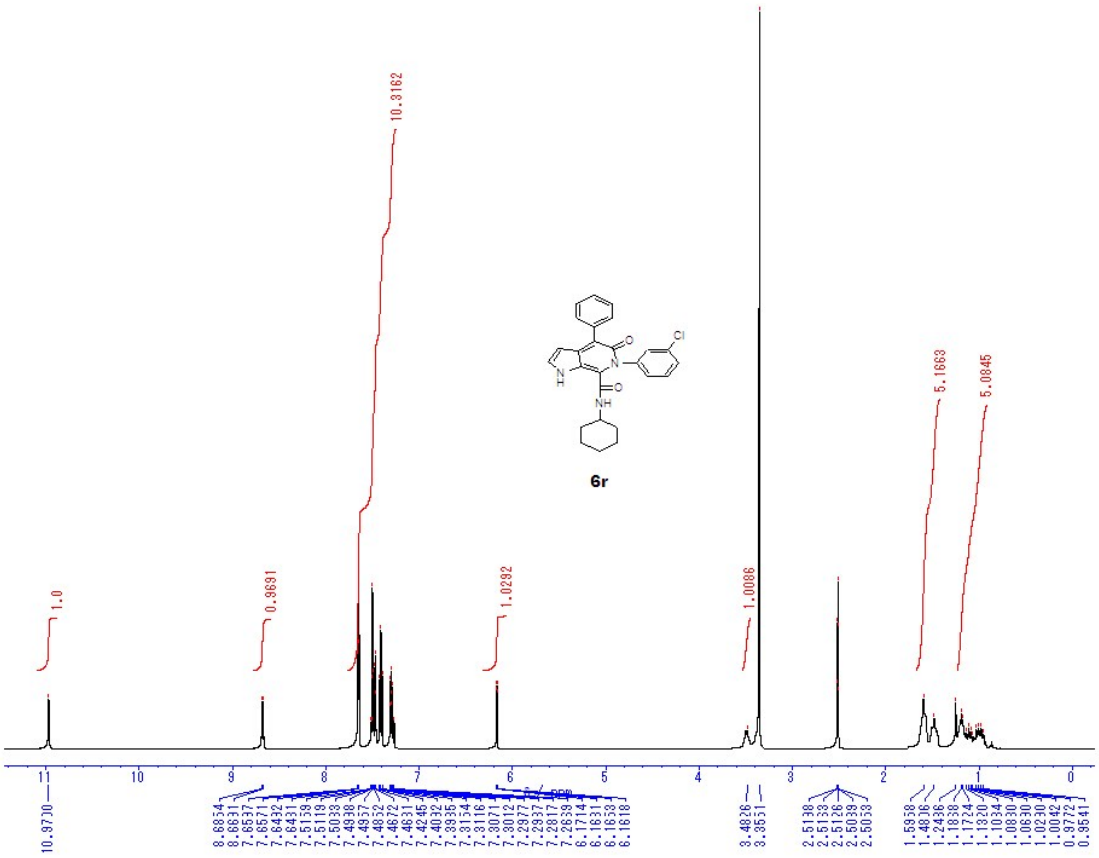

O
N
OMe
H
O
NH
6o
160
140
120
100
80
60
40
20
0
δ / ppm
159.7232
159.2837
157.8534
141.5941
139.3829
137.4935
132.5322
130.3935
130.0937
128.9135
128.1471
126.7438
121.7930
113.9140
113.2459
98.7039
55.9137
48.2220
40.4493
40.4117
40.3238
40.2443
40.1638
39.9833
39.8027
39.6221
31.4931
31.1031
25.5633
24.6136


8.8673
10.7568
1.0
1.0674
1.097
0.9563
6p
ppm


6p
δ / ppm
159.1431
157.2038
142.3337
140.1917
137.0638
137.0414
134.5345
134.1238
132.4474
130.0211
129.5516
128.2039
127.9238
127.4636
126.9398
122.0927
98.8135
48.6337
40.5637
40.4839
40.4033
40.3134
40.2378
40.1438
40.0723
39.9834
39.8158
39.6513
39.4828
31.8234
25.5736
24.7439
24.6541


6q


6q
160
140
120
100
80
60
40
20
0
δ / ppm
159.7034
157.8937
141.6830
139.8938
139.4574
137.5027
130.0914
129.4431
128.6736
128.4211
128.3870
128.1223
126.7435
121.8424
113.3535
98.6427
48.2758
40.7518
40.6874
40.4933
40.4177
40.3238
40.2523
40.1633
39.9978
39.8038
39.6628
39.4932
31.8233
25.5435
24.6437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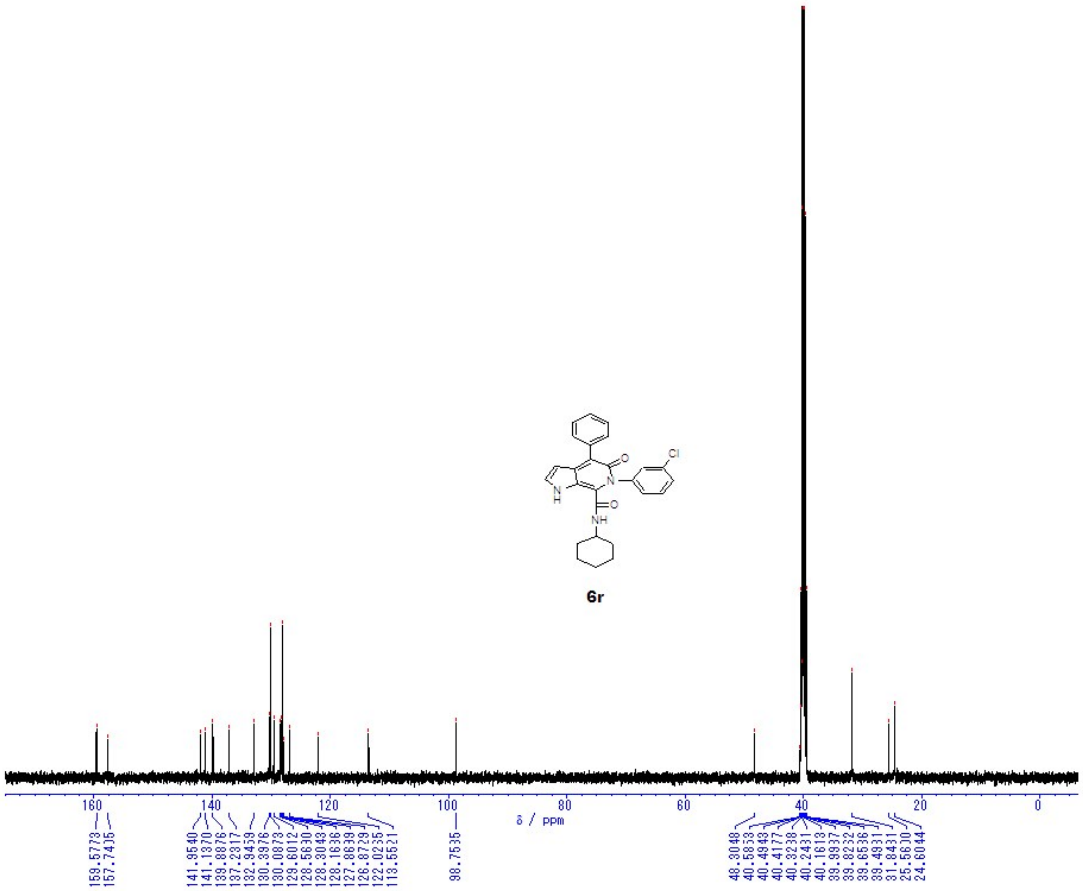
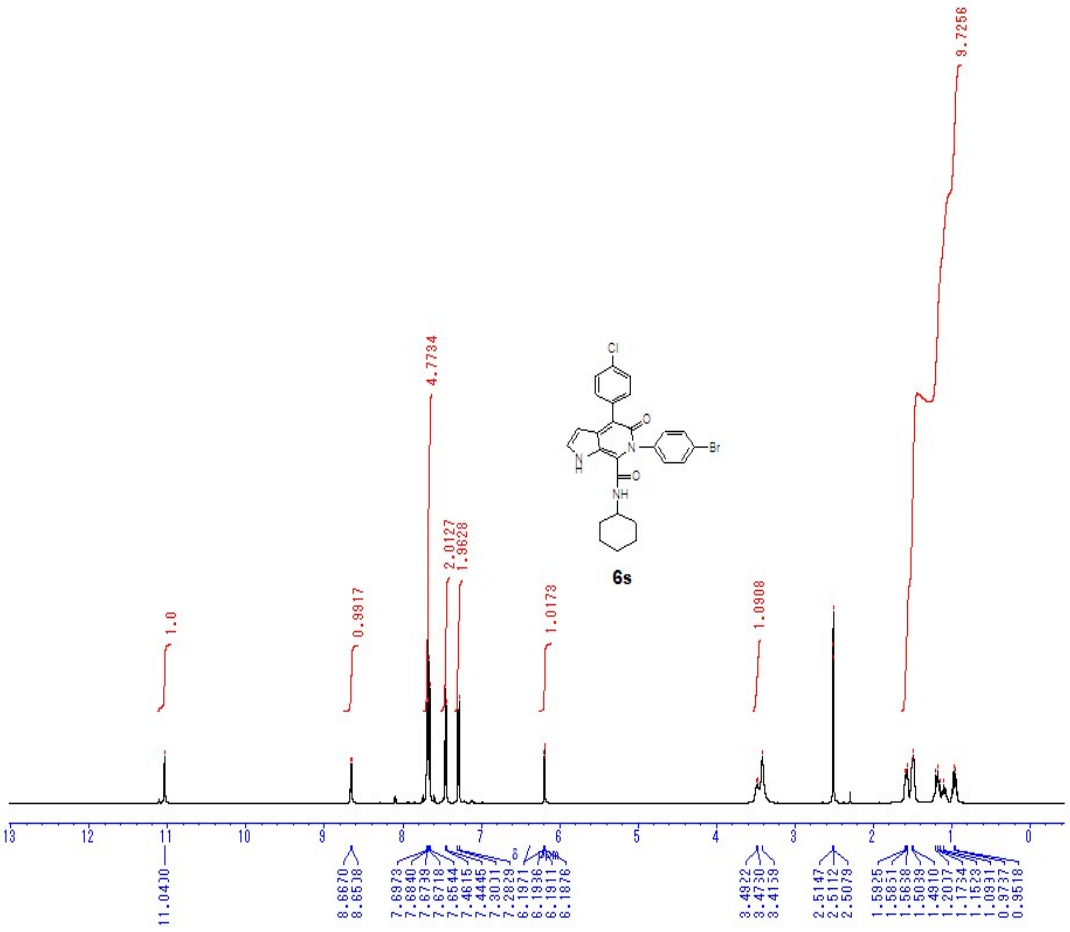
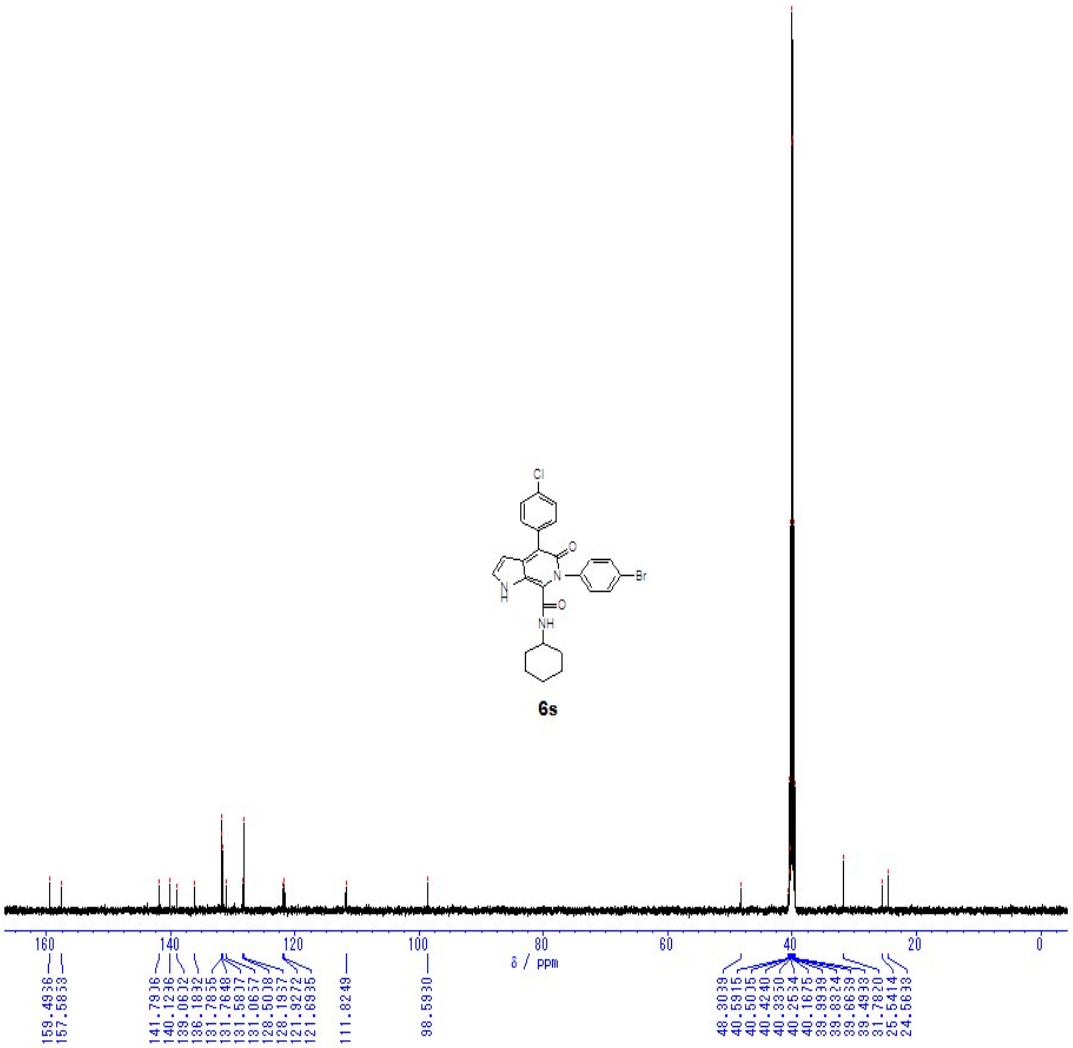
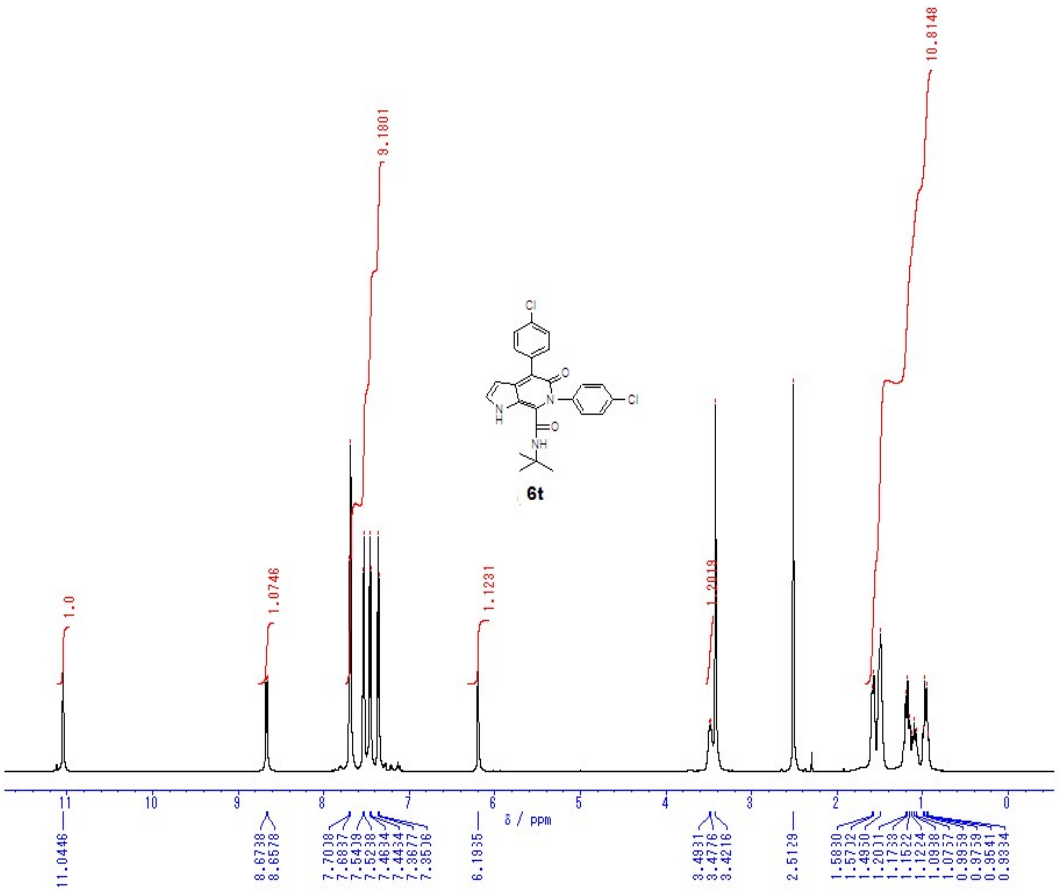
5.1663
5.0845
1.0
0.9691
1.0292
1.0008
6r


Cl
O
N
H
O
NH
6r
160
140
120
100
80
60
40
20
0
δ / ppm
159.5773
157.7435
141.9540
141.1370
139.8876
137.2317
132.9438
130.3876
130.0873
129.6012
128.5630
128.3043
128.1636
127.8639
126.8729
122.0235
118.5521
98.7535
48.3048
40.5833
40.4943
40.4177
40.3238
40.2431
40.1613
39.9937
39.8232
39.6536
39.4831
31.8431
25.6610
24.6044


9.7256
4.7734
2.0127
1.9628
1.0
0.9917
1.0173
1.0908
Cl
Br
O
N
H
NH
6s
13
12
11
10
9
8
7
6
5
4
3
2
1
0
11.0430
8.6670
8.6538
7.6878
7.6840
7.6739
7.6718
7.6644
7.4615
7.4445
7.3011
7.2829
6.1871
6.1836
6.1811
6.1676
3.4922
3.4730
3.4159
2.5147
2.5112
2.5079
1.5925
1.5851
1.5638
1.5039
1.4910
1.2037
1.1734
1.1523
1.0931
0.9737
0.9518


Cl
O
N
Br
H
N
O
NH
6s
160
140
120
100
80
60
40
20
0
δ / ppm
159.4936
157.5833
141.7936
140.1236
139.0632
136.1832
131.7835
131.7648
131.5837
131.0657
128.5038
128.1937
121.8272
121.6935
111.8249
98.5930
48.3039
40.5915
40.5015
40.4240
40.3330
40.2534
40.1675
39.9819
39.8834
39.7833
39.4933
31.7410
25.5414
24.5833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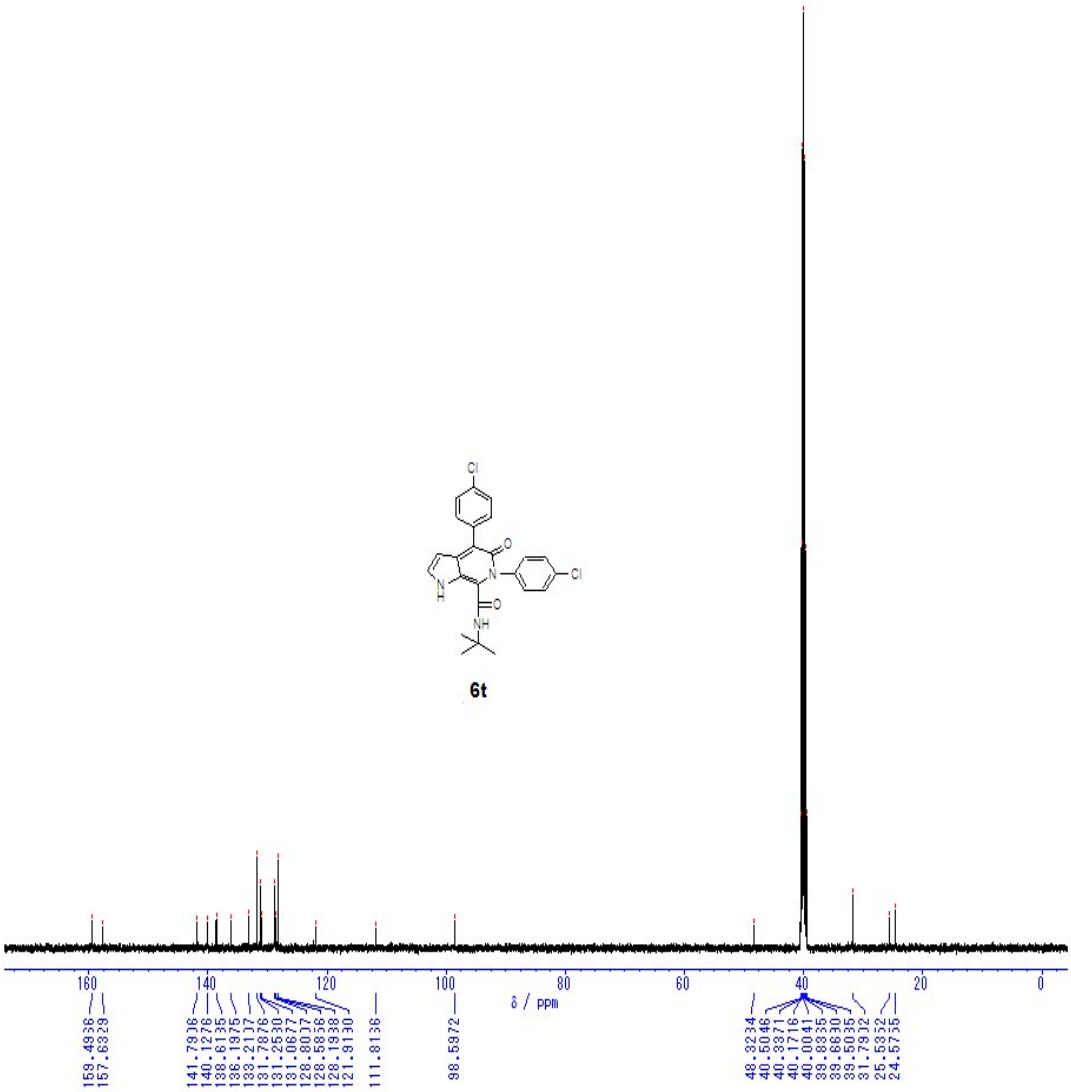
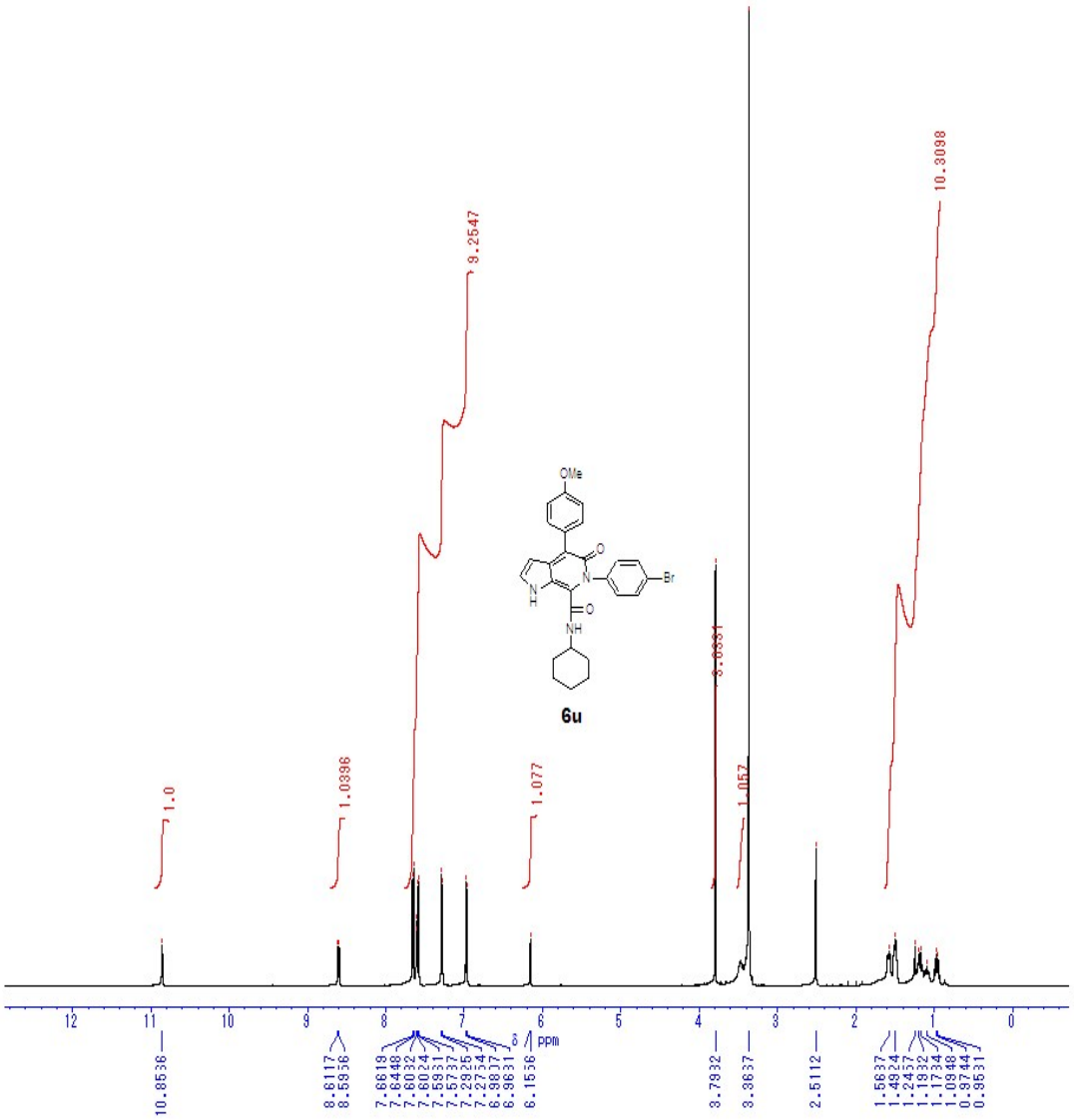
8.1801
1.0
1.0746
1.1231
1.2019
6t
δ / ppm


Cl
O
N
H
Cl
O
NH
6t
160
140
120
100
80
60
40
20
0
δ / ppm
159.4936
157.6329
141.7936
140.1228
138.6135
136.1975
133.2117
131.7878
131.2530
131.0677
128.8037
128.5836
128.1938
121.9130
111.8136
98.5972
48.3234
40.6046
40.3371
40.1716
40.0041
39.8365
39.6690
39.5035
31.7932
25.5332
24.5755


OMe
O
N
Br
H
O
NH
6u
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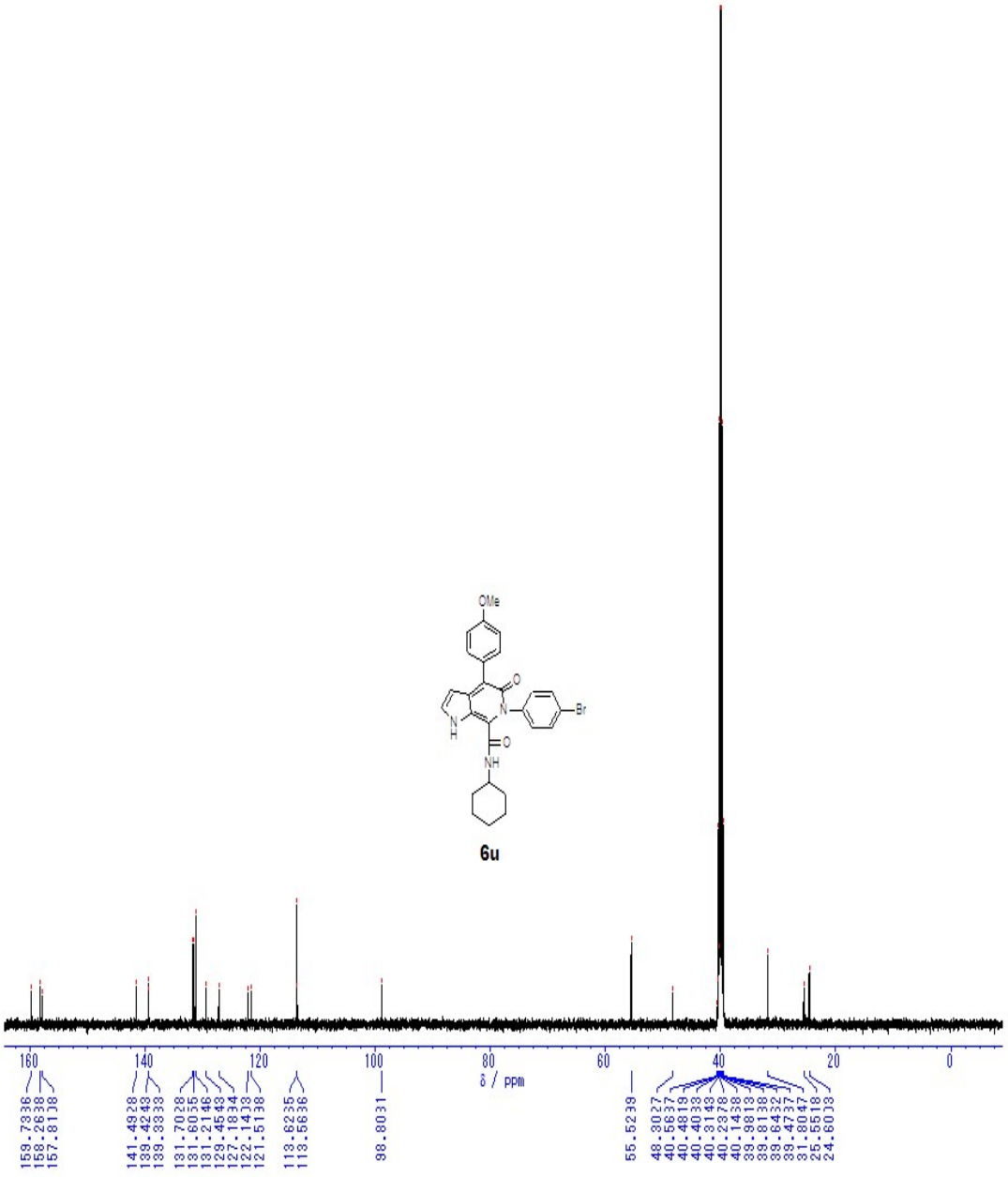
9.2547
3.8831
1.057
1.0396
1.077
1.0
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
10.8536
8.6117
8.5956
7.6819
7.6448
7.6032
7.6024
7.5931
7.5737
7.2925
7.2754
6.9831
6.9831
6.1556
3.7832
3.8837
2.5112
1.5637
1.4824
1.2457
1.1932
1.1734
1.0948
0.9744
0.9631


OMe
O
N
Br
H
O
NH
6u
δ / ppm
159.7336
158.2638
157.8138
141.4928
139.4243
139.3333
131.7028
131.6035
131.2146
129.4543
127.1834
122.1433
121.5138
113.8235
113.5636
98.8031
55.5239
48.8027
40.5637
40.4819
40.4033
40.3143
40.2378
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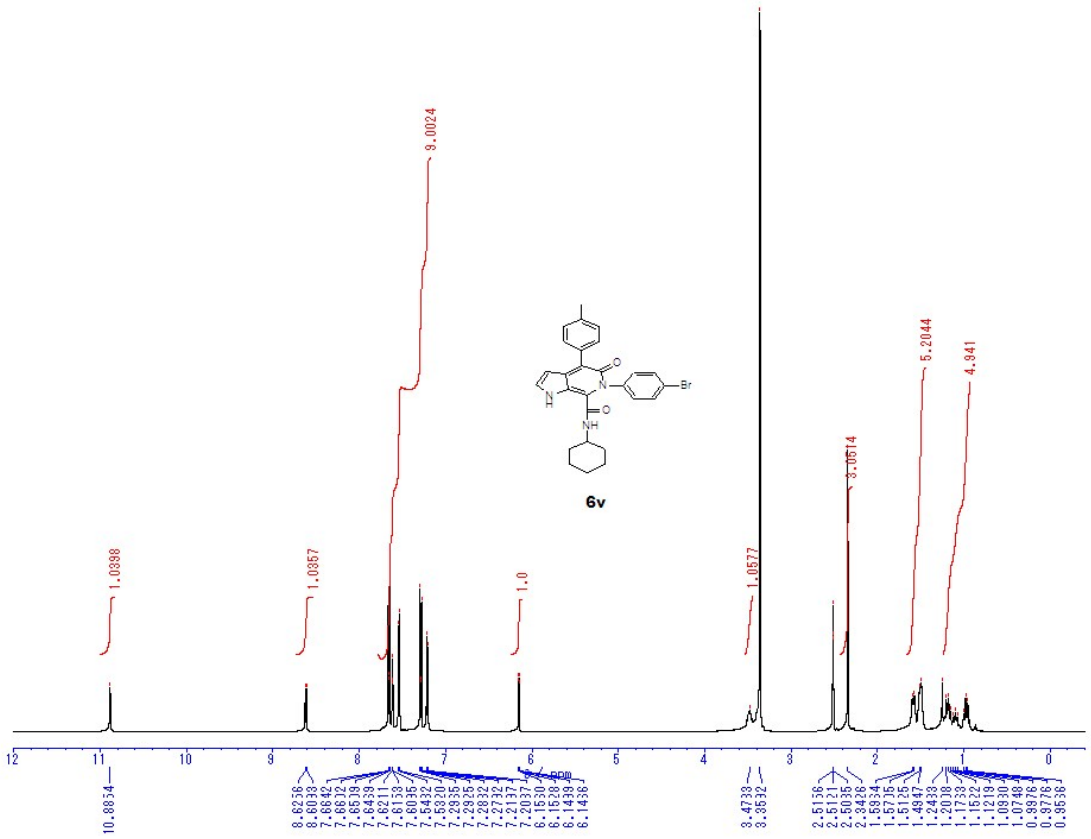
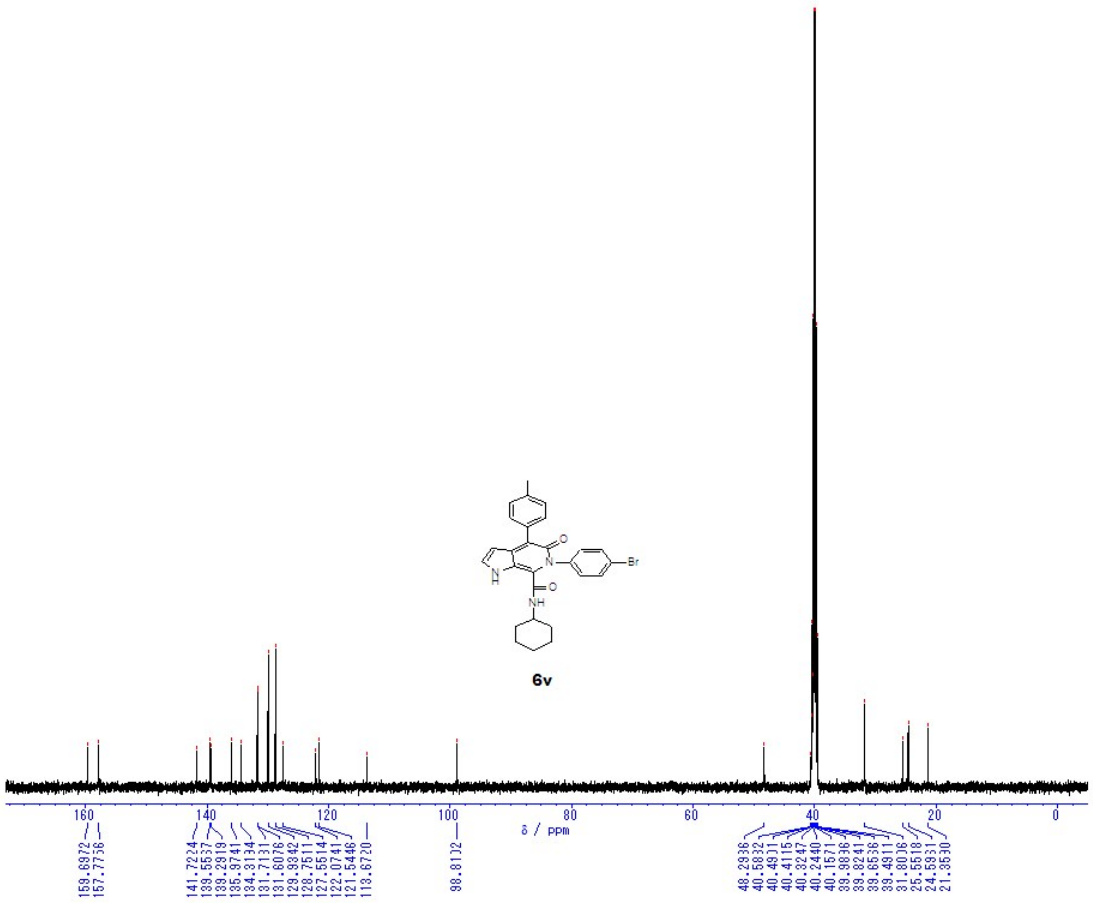
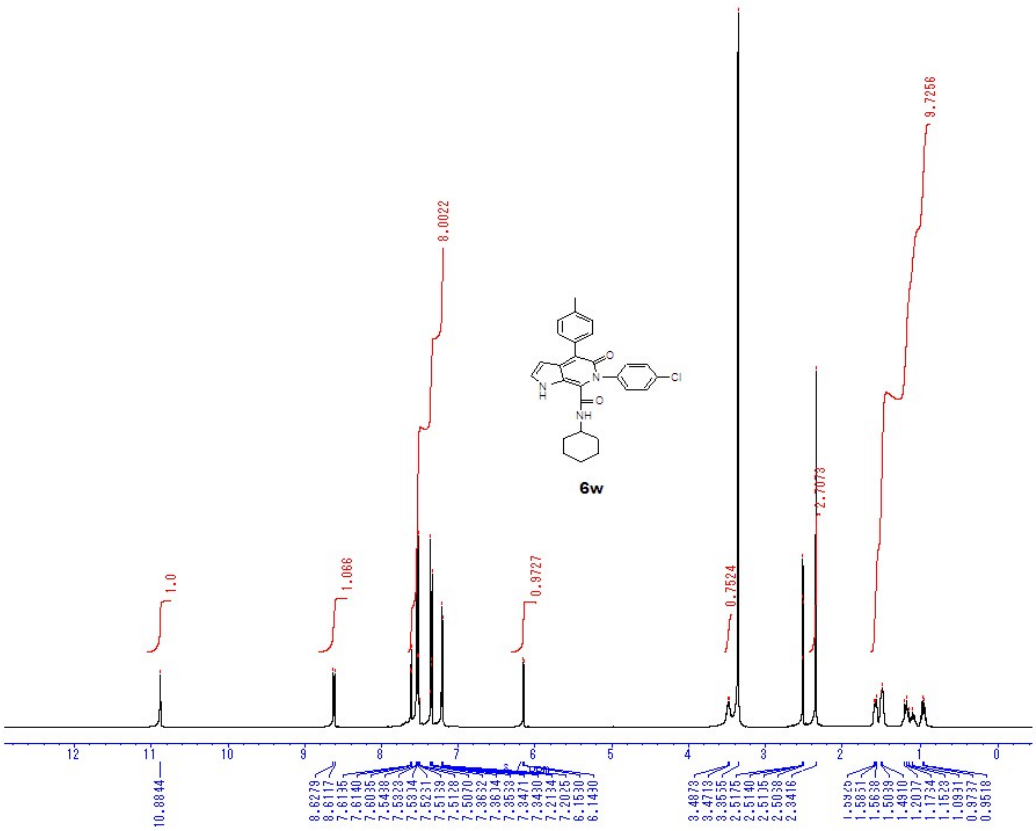
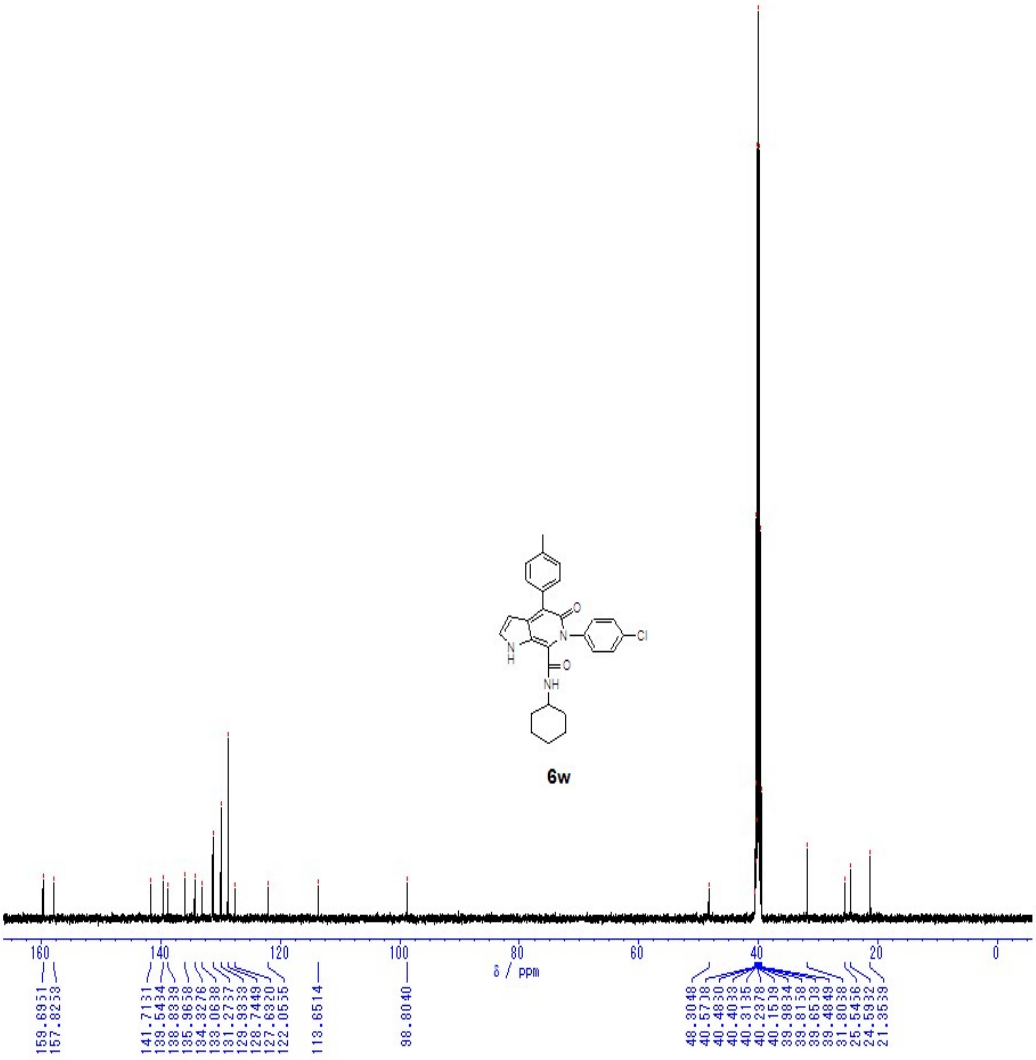
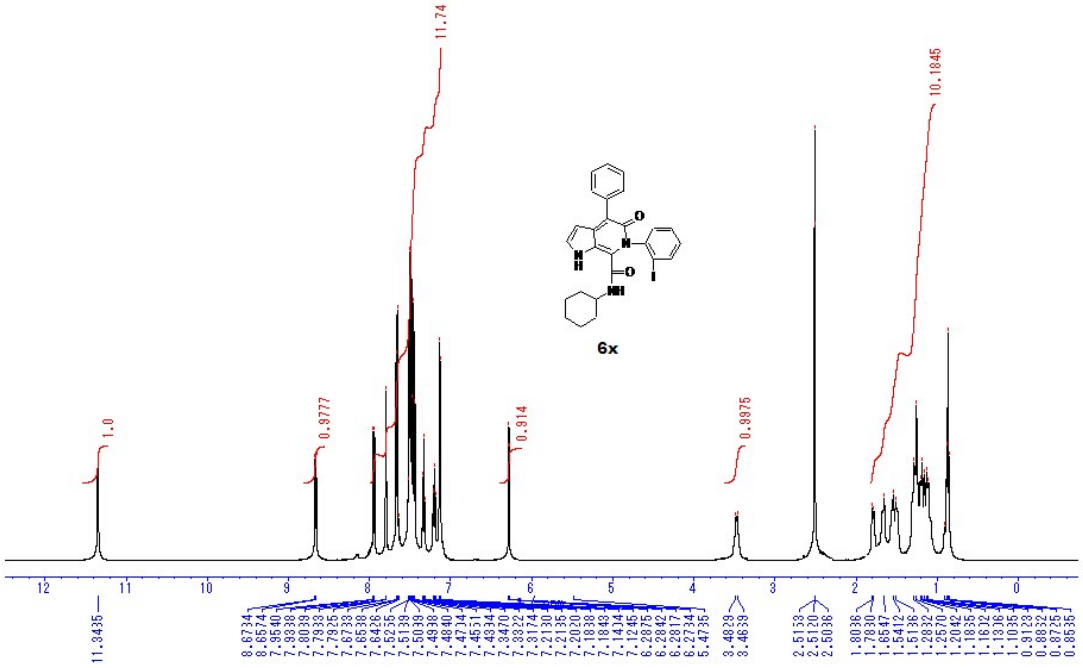
39.6432
39.4737
31.8047
25.5518
24.6033

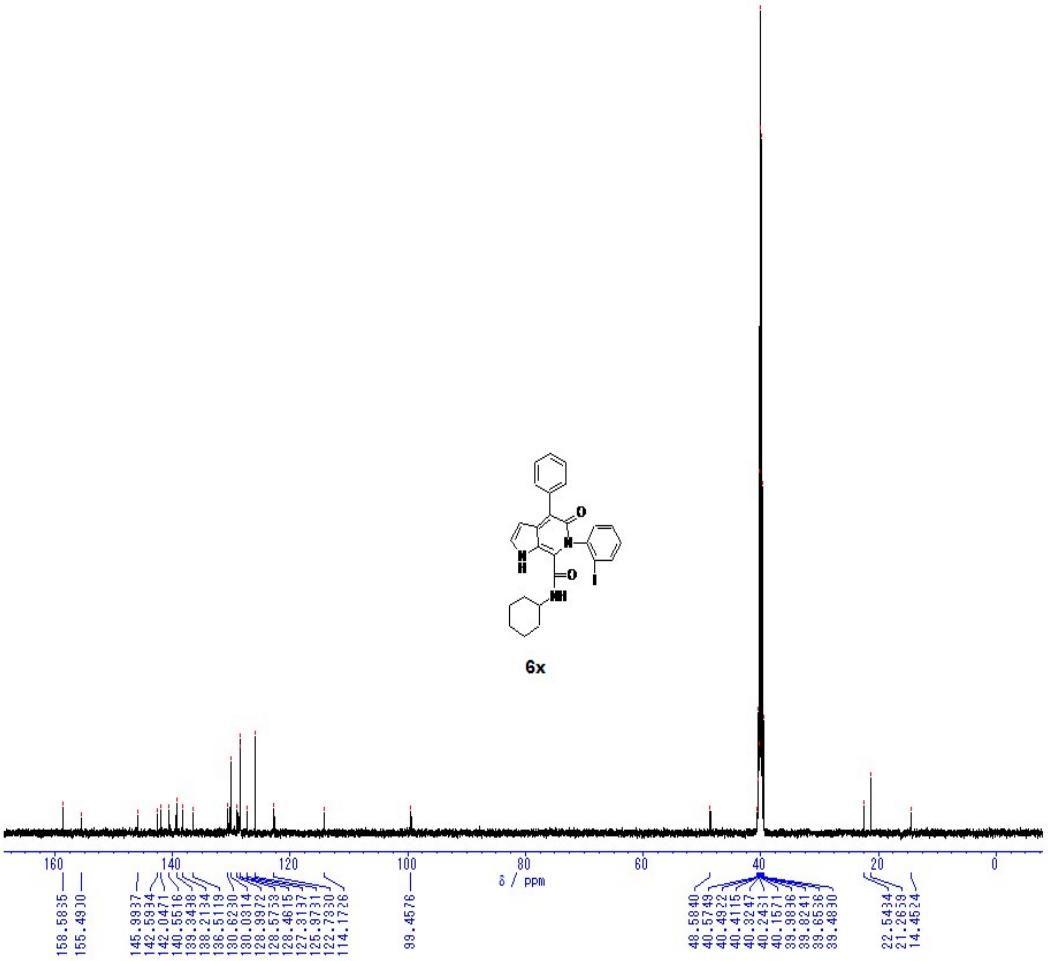

9.0024
5.2044
4.941
3.0614
1.0398
1.0357
1.0
1.0577
6v

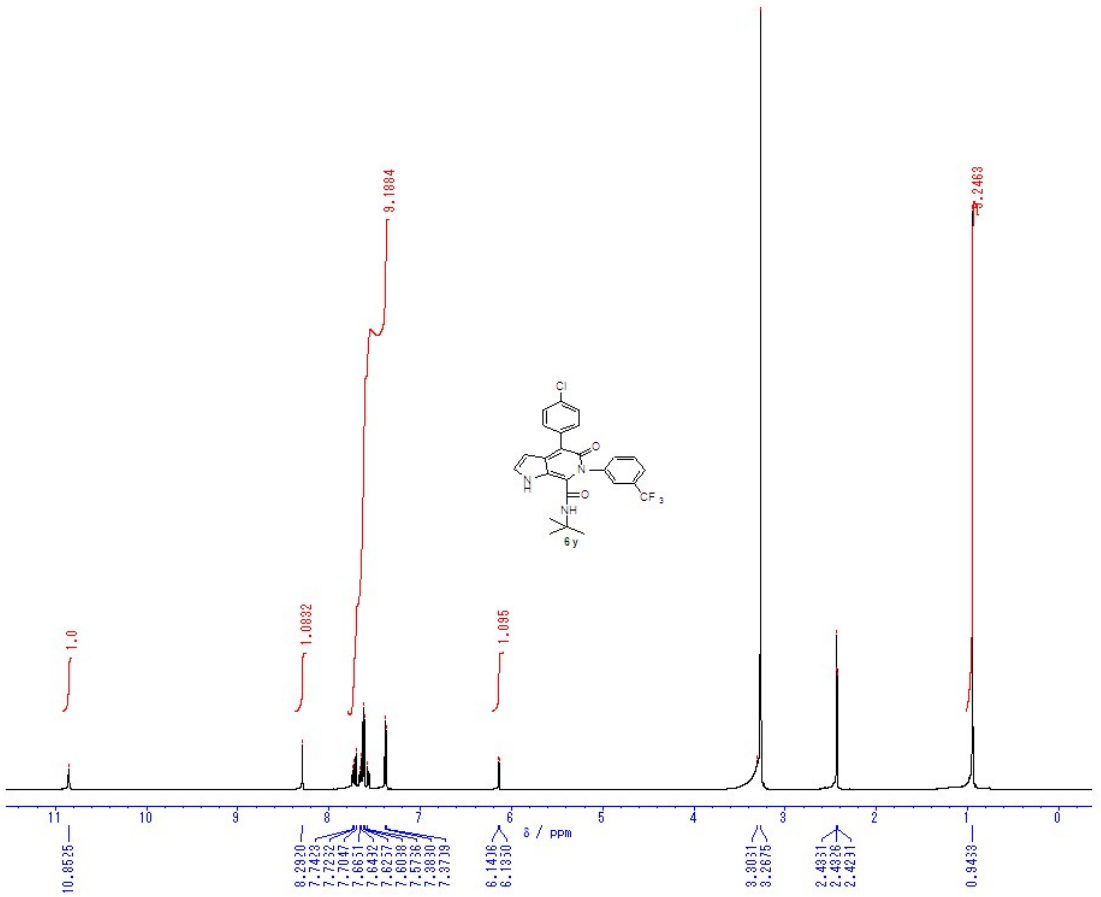

6v
δ / ppm
159.6972
157.7736
141.7224
139.5537
138.2919
135.8741
134.3134
131.7131
131.6076
129.3842
128.7611
127.5514
122.0741
121.5446
113.8720
88.8132
48.2936
40.5832
40.4931
40.4115
40.3247
40.2440
40.1571
39.9836
39.8241
39.6536
39.4911
31.8036
25.5518
24.5931
21.3530

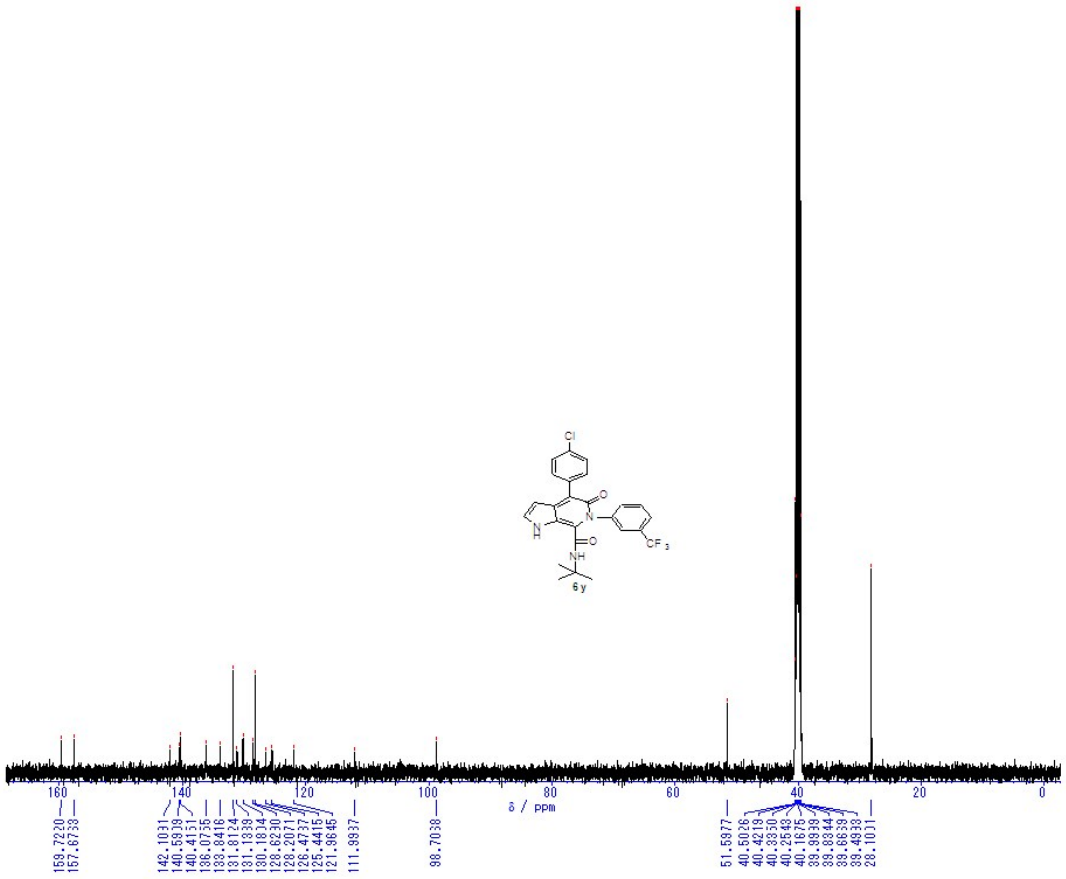

1.0
1.066
8.0022
0.9727
0.7624
12.7073
9.7256
6w


6w
δ / ppm
159.6851
157.8253
141.7131
139.5434
138.8339
135.9658
134.3276
133.0638
131.2737
129.9333
128.7449
127.6320
122.0555
113.6514
98.8040
48.3048
40.5738
40.4830
40.4033
40.3135
40.2378
40.1539
39.9834
39.8158
39.6503
39.4849
31.8038
25.5456
24.5832
21.3539


11.74
10.1845
1.0
0.9777
0.914
0.8975
6x


6x
160
140
120
100
80
60
40
20
0
δ / ppm
158.5835
155.4930
145.9937
142.5934
142.0471
140.5516
139.3498
138.2134
136.5119
130.6230
130.0314
128.9972
128.5758
128.4615
127.3137
125.9731
122.7330
114.1726
98.4576
48.5840
40.5749
40.4922
40.4115
40.3247
40.2431
40.1571
39.9836
39.8241
39.6538
39.4830
22.5434
21.2659
14.4524


1.0
1.0832
9.1884
1.095
3.2463
δ / ppm
10.8626
8.2920
7.7423
7.7232
7.7047
7.6651
7.6432
7.6257
7.6038
7.5736
7.3830
7.3739
6.1436
6.1350
3.8031
3.2675
2.4331
2.4328
2.4231
0.9438


Cl
O
N
H
O
NH
CF3
6y
160
140
120
100
80
60
40
20
0
δ / ppm
159.7220
157.6733
142.1031
140.5938
140.4151
136.0736
133.8416
131.8124
131.1839
130.1834
128.6230
128.2071
126.4737
125.4415
121.9645
111.9937
98.7038
51.5977
40.5026
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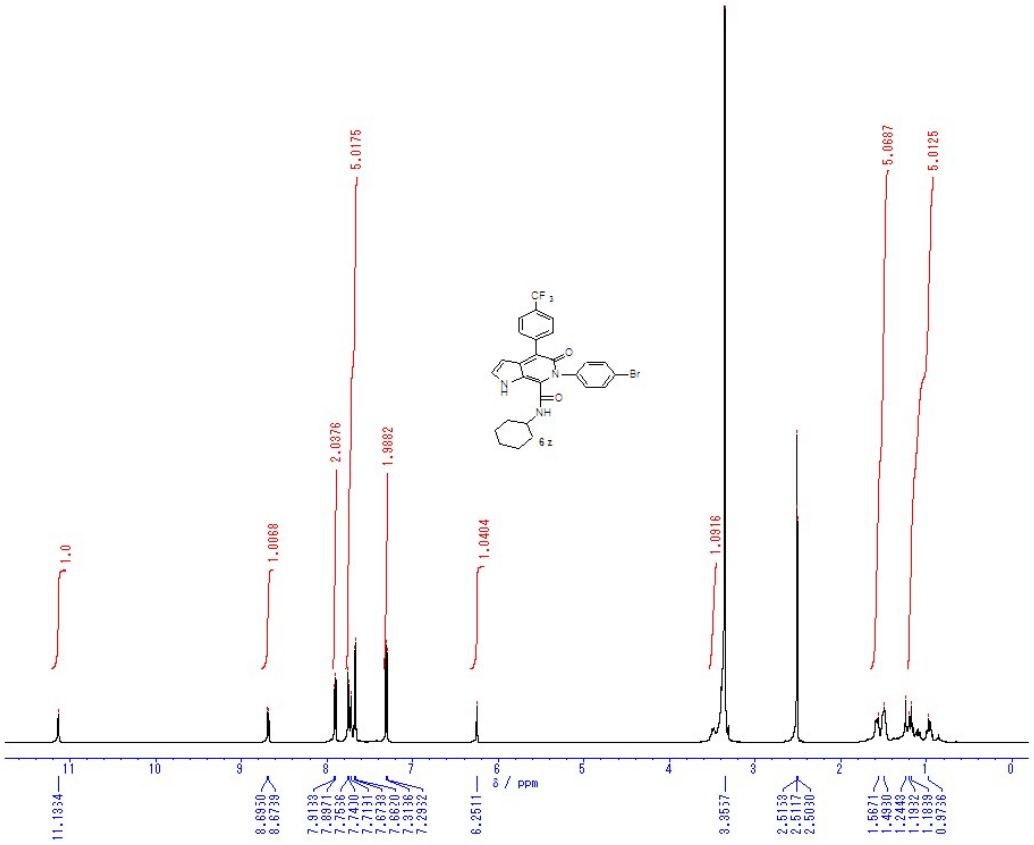
40.3350
40.2543
40.1675
39.9839
39.8344
39.6639
39.4933
28.1031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1.0068
2.0376
5.0175
1.9882
1.0404
1.0916
5.0687
5.0125
δ / ppm
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8.6950
8.6738
7.8133
7.8071
7.7636
7.7430
7.7131
7.6738
7.6620
7.3136
7.2952
6.2511
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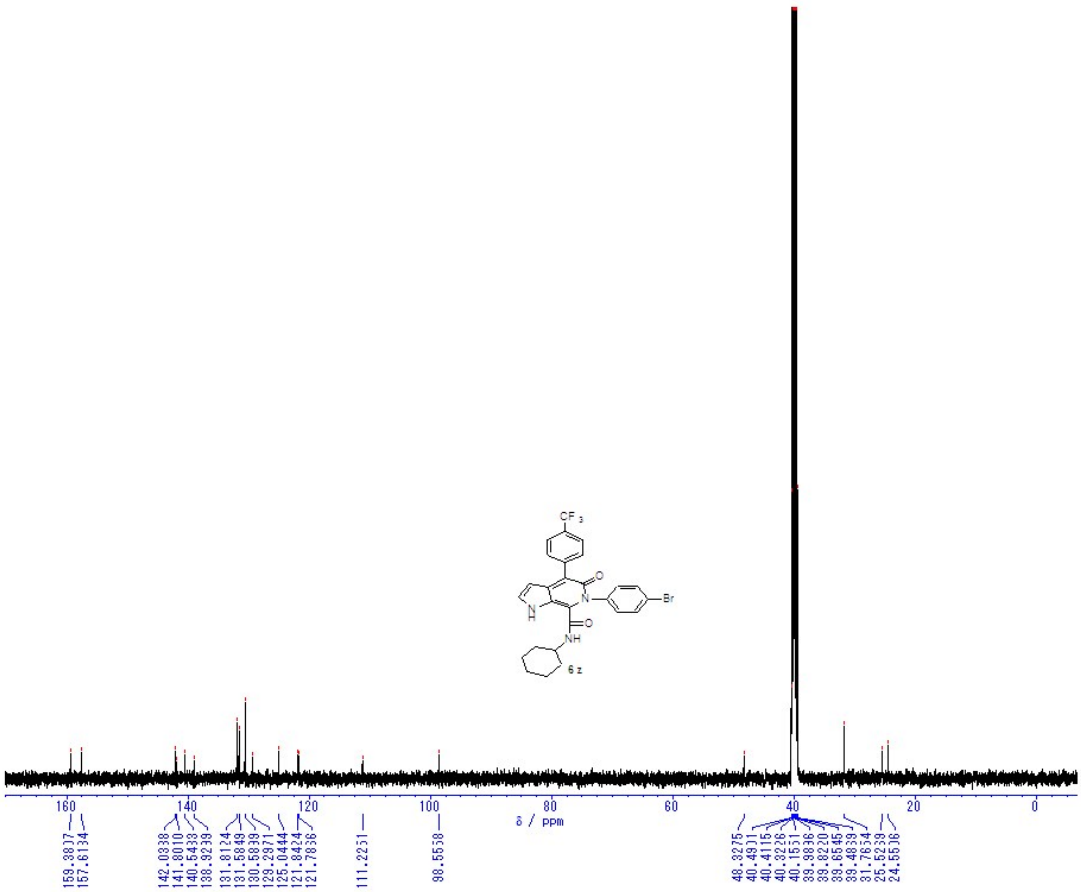
2.5117
2.5030
1.5671
1.4930
1.2448
1.1932
1.1839
0.9736


CF3
O
N
Br
NH
O
6z
160
140
120
100
80
60
40
20
0
δ / ppm
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157.6134
142.0338
141.8010
140.6438
138.3239
131.8124
131.5849
130.5839
129.2971
125.0444
121.8424
121.7836
111.2251
98.5538
48.3275
40.4911
40.4115
40.3218
40.1531
39.9836
39.8210
39.6545
39.4839
31.7634
25.5239
24.5536