Supporting Information for

CoPc-Catalyzed Selective Radical Arylation of Anilines with Arylhydrazines for Synthesis of 2-Aminobiaryls

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General information

All reactions were carried out in air. Solvents were dried by the standard procedures. ^{1}H and ^{13}C NMR spectra were determined in $CDCl_3$ or DMSO-d_6 on a Varian-Inova 300MHz or 400 MHz spectrometer and chemical shifts were reported in ppm from internal TMS(δ). High resolution mass spectra were recorded on a MicroMass-TOF machine (EI). Column chromatography was performed with 300-400 mesh silica gel using flash column techniques. All of the reagents were used directly as obtained commercially unless otherwise noted.

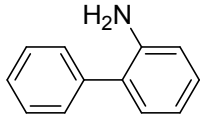
General procedure for reaction between phenylhydrazine and arylamine

To a solution of arylamine (10 mmol) and CoPc (0.1 mmol) in acetonitrile (10 mL), phenylhydrazine (1 mmol) were added. The mixture was heated in an oil bath at 80°C for 24 h. After removal of solvent under reduced pressure, the residue was purified by flash silica gel column chromatography afforded the desired product 2-aminobiaryl.

General procedure for reaction between *p*-anisidine and arylhydrazine

To a solution of *p*-anisidine (10 mmol) and CoPc (0.1 mmol) in acetonitrile (10 mL), arylhydrazine hydrochloride (1 mmol) and triethylamine (3 mmol) were added. The mixture was heated in an oil bath at 80°C for 24 h. After removal of solvent under reduced pressure, the residue was purified by flash silica gel column chromatography afforded the desired product 2-aminobiaryl.

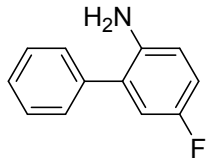
2-Aminobiphenyl (3a)[1]



Brown solid; mp 49-50°C;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.49 (m, 4H), 7.30-7.38 (m, 1H), 7.10-7.20 (m, 2H), 6.76-6.89 (m, 2H), 4.08 (br, s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.0, 139.4, 130.5, 129.1, 128.8, 128.5, 128.0, 127.2, 119.0, 115.9; ESI-MS: Anal. calcd for $C_{12}H_{12}N$ 170.1 [$(M+H)^+$], found 170.1 [$(M+H)^+$].

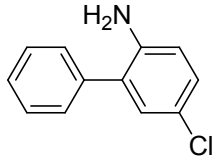
5-Fluorobiphenyl-2-amine (3b)[2]



Brown oil;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.40 (m, 4H), 7.25-7.33 (m, 1H), 6.78-6.87 (m, 2H), 6.73 (dd, J = 5.6, 9.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0 (d, J = 237.9 Hz), 138.2, 137.7, 129.0, 128.9, 127.8, 117.6 (d, J = 7.8 Hz), 116.8 (d, J = 22.5 Hz), 114.9 (d, J = 22.3 Hz). ESI-MS: Anal. Calcd for $C_{12}H_{11}FN$ 188.1 [$(M+H)^+$], found 188.1 [$(M+H)^+$].

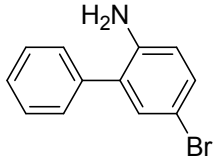
5-Chlorobiphenyl-2-amine (3c)[3]



Brown solid; mp 50-51°C;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.47 (m, 4H), 7.33-7.39 (m, 1H), 7.08-7.14 (m, 2H), 6.74 (d, J = 8.9 Hz, 1H), 4.20 (br, s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 141.1, 137.2, 128.9, 127.9, 127.8, 127.1, 126.6, 122.1, 115.6. ESI-MS: Anal. Calcd for $C_{12}H_{11}ClN$ 204.1 [$(M+H)^+$], found 204.1 [$(M+H)^+$].

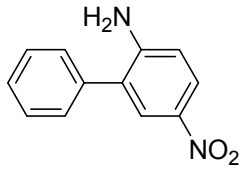
5-Bromobiphenyl-2-amine (3d)[4]



Brown solid; mp 57-58°C;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.52 (m, 5H), 7.18-7.27 (m, 2H), 6.64 (d, J = 8.7 Hz, 1H), 3.63 (br, s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.6, 138.2, 132.8, 131.1, 129.5, 129.0, 128.9, 127.7, 117.1, 110.2. ESI-MS: Anal. Calcd for $C_{12}H_{11}BrN$ 248.0 [$(M+H)^+$], found 248.0 [$(M+H)^+$].

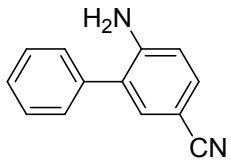
5-Nitrobiphenyl-2-amine (3e)[5]

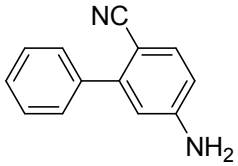


Yellow solid; mp 125-126°C;

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.00-8.11 (m, 2H), 7.46-7.53 (m, 2H), 7.38-7.46 (m, 3H), 6.72 (d, J = 9.1 Hz, 1H), 4.50 (br, s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.8, 139.1, 136.9, 129.3, 128.8, 128.3, 126.6, 126.3, 125.1, 114.0. EI-HRMS: Anal. calcd for $C_{12}H_{11}N_2O_2$ 215.0821 [$(M+H)^+$], found 215.0810 [$(M+H)^+$].

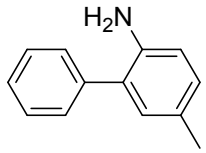
6-Aminobiphenyl-3-carbonitrile (3f) and 5-aminobiphenyl-2-carbonitrile (3f')





^{1}H NMR (300 MHz, $CDCl_3$): δ 7.30-7.60 (m, 13H), 6.69-6.79 (m, 3H), 4.36 (br, s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.7, 147.0, 137.1, 134.4, 133.3, 132.6, 131.9, 129.2, 128.8, 128.2, 127.4, 120.0, 118.7, 118.5, 115.0, 101.0, 100.5. ESI-MS: Anal. Calcd for $C_{13}H_{11}N_2$ 195.1 [$(M+H)^+$], found 195.1 [$(M+H)^+$].

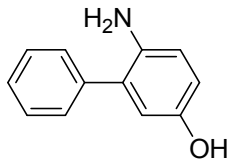
5-Methylbiphenyl-2-amine (3g)[6]



Brown oil;

^{1}H NMR (300 MHz, $CDCl_3$): δ 740-7.46 (m, 4H), 7.30-7.36 (m, 1H), 6.95-7.01 (m, 2H), 6.74 (d, J = 7.9 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.7, 139.3, 131.0, 129.1, 129.0, 128.8, 128.5, 127.2, 116.5, 20.5. ESI-MS: Anal. Calcd for $C_{13}H_{14}N$ 184.1 [$(M+H)^+$], found 184.1 [$(M+H)^+$].

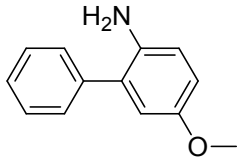
4-Amino-3-phenylphenol (3h)[7]



Brown solid; mp 117-118°C;

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.32-7.42 (m, 4H), 7.25-7.33 (m, 1H), 6.55-6.66 (m, 3H), 4.40 (s, 1H), 3.44(s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): δ 149.4, 140.3, 137.4, 129.1, 129.0, 127.5, 127.1, 117.3, 116.8, 115.7. ESI-MS: Anal. Calcd for $C_{12}H_{12}NO$ 186.1 [$(M+H)^+$], found 186.1 [$(M+H)^+$].

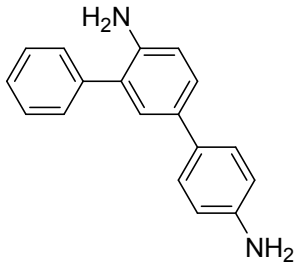
5-Methoxybiphenyl-2-amine (3i)[6]



Brown oil;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.43 (m, 4H), 7.24-7.31 (m, 1H), 6.66-6.80 (m, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.5, 139.1, 135.2, 129.9, 129.1, 128.8, 127.4, 117.9, 115.8, 114.4, 55.8. ESI-MS: Anal. Calcd for $C_{13}H_{14}NO$ 200.1 [$(M+H)^+$], found 200.1 [$(M+H)^+$].

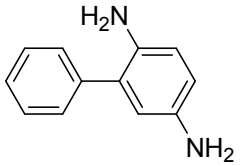
4-Amino-3-phenyl-4'-amino biphenyl (3j)



Brown solid; mp 105-106°C;

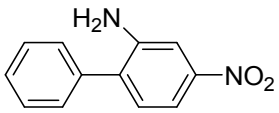
^{1}H NMR (300 MHz, DMSO-d_6): δ 7.42-7.54 (m, 4H), 7.31-7.39 (m, 1H), 7.25 (d, J = 7.9 Hz, 3H), 7.15 (s, 1H), 6.79 (d, J = 8.2 Hz, 1H), 6.59 (d, J = 7.7 Hz, 2H), 5.02 (br, s, 2H), 4.73 (br, s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 147.6, 143.6, 140.3, 130.2, 129.2, 129.1, 128.7, 127.6, 127.2, 126.2, 126.5, 125.9, 116.3, 114.8. EI-HRMS: Anal. calcd for $C_{18}H_{16}N_2$ 260.1313 (M^+), found 260.1319 (M^+).

2,5-Diamobiphenyl (3k)



^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40-7.46 (m, 4H), 7.30-7.36 (m, 1H), 6.64-6.69 (m, 1H), 6.55-6.63 (m, 2H), 3.12 (br, s, 4H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 140.1, 139.3, 135.2, 128.6, 127.3, 126.6, 117.0, 116.5, 115.4. CI-HRMS: Anal. calcd for $C_{12}H_{13}N_2$ 185.1079 [$(M+H)^+$], found 185.1082 [$(M+H)^+$].

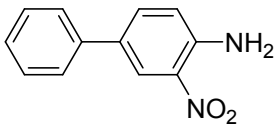
4-Nitrobiphenyl-2-amine (3l)[3]



Yellow solid; mp 70-72°C;

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.63 (d, J = 8.3 Hz, 1H), 7.59 (s, 1H), 7.46-7.52 (m, 2H), 7.38-7.46 (m, 3H), 7.22 (d, J = 8.3 Hz, 1H), 4.09 (br, s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.1, 144.5, 137.4, 133.4, 131.0, 129.2, 128.6, 128.4, 113.1, 109.6. ESI-MS: Anal. Calcd for $C_{12}H_{11}N_2O_2$ 215.1 [$(M+H)^+$], found 215.1 [$(M+H)^+$].

3-Nitrobiphenyl-4-amine (3n)[5]

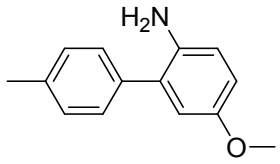


Yellow solid; mp 125-126°C;

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.17 (s, 1H), 8.15 (d, J = 7.2 Hz, 2H), 7.50-7.52 (m, 1H), 7.48 (d, J = 7.2 Hz, 2H),

7.40-7.42 (m, 1H), 6.72 (d, J = 9.1 Hz, 1H), 6.27 (br, s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 142.7, 137.0, 136.4, 132.6, 131.2, 129.4, 129.2, 128.5, 125.7, 116.1. ESI-MS: Anal calcd for $C_{12}H_{11}N_2O_2$ 215.1 [$(M+H)^+$], found 215.1 [$(M+H)^+$].

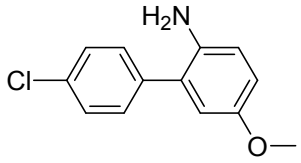
5-Methoxy-4'-methylbiphenyl-2-amine (3o)



Brown oil;

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.35 (d, J = 7.7 Hz, 2H), 7.25 (d, J = 7.3 Hz, 2H), 6.63-6.85 (m, 3H), 3.76 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 137.2, 136.0, 130.3, 129.5, 129.0, 118.2, 115.8, 114.1, 55.8, 21.2. EI-HRMS: Anal. calcd for $C_{14}H_{15}NO$ 213.1154 (M^+), found 213.1155 (M^+).

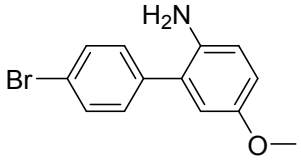
4'-Chloro-5-methoxybiphenyl-2-amine (3q)



Taupe solid; mp 82-83°C;

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34-7.46 (m, 4H), 6.78-6.91 (m, 2H), 6.72 (s, 1H), 5.23 (br, s, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 137.8, 136.4, 133.3, 130.4, 129.0, 127.8, 117.4, 115.7, 114.7, 55.8. EI-HRMS: Anal. calcd for $C_{13}H_{12}ClNO$ 233.0607 (M^+), found 233.0614 (M^+).

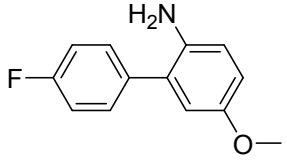
4'-Bromo-5-methoxybiphenyl-2-amine (3r)



Brown oil;

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.52-7.60 (m, 2H), 7.30-7.37 (m, 2H), 6.70-6.82 (m, 2H), 6.65-6.70 (m, 1H), 3.76 (s, 3H), 3.15 (br, s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 138.2, 136.5, 132.4, 131.2, 128.2, 121.9, 117.8, 116.1, 115.2, 56.3; EI-HRMS: Anal. calcd for $C_{13}H_{12}BrNO$ 277.0102 (M^+), found 277.0098 (M^+).

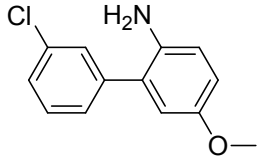
4'-Fluoro-5-methoxybiphenyl-2-amine (3s)



Brown oil;

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34-7.48 (m, 2H), 7.05-7.17 (m, 2H), 6.72-6.82 (m, 2H), 6.70 (s, 1H), 3.77 (s, 3H,); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4, 160.9, 153.1, 136.4, 135.2 (d, J = 3.3 Hz), 130.7 (d, J = 8.0 Hz), 128.2, 117.3, 115.8 (d, J = 3.1 Hz), 115.6, 114.5, 55.8. EI-HRMS: Anal. calcd for $C_{13}H_{12}FNO$ 217.0890 (M^+), found 217.0905 (M^+).

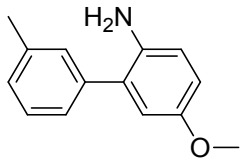
3'-Chloro-5-methoxybiphenyl-2-amine (3v)



Brown oil;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (s, 1H), 7.35-7.40 (m, 2H), 7.30-7.35 (m, 1H), 6.79 (dd, J = 8.7, 2.7 Hz, 1H), 6.72-6.76 (m, 1H), 6.70 (d, J = 2.7 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 141.2, 136.6, 134.6, 130.1, 129.2, 127.5, 127.3, 117.4, 115.5, 115.0, 55.8. ESI-HRMS: Anal. calcd for $C_{13}H_{13}ClNO$ 234.0686 [$(M+H)^+$], found 234.0671 [$(M+H)^+$].

3'-Methyl-5-methoxybiphenyl-2-amine (3w)



Brown oil;

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25 (t, J = 7.5 Hz, 1H), 7.18-7.21 (m, 2H), 7.09 (d, J = 7.6 Hz, 1H), 6.68-6.72 (m, 2H), 6.65-6.67 (m, 1H), 3.70 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.4, 139.1, 138.5, 137.0, 129.8, 128.7, 128.2, 126.1, 117.8, 115.7, 114.3, 55.8, 21.5. EI-HRMS: Anal. calcd for $C_{14}H_{15}NO$ 213.1154 (M^+), found 213.1157 (M^+).

References

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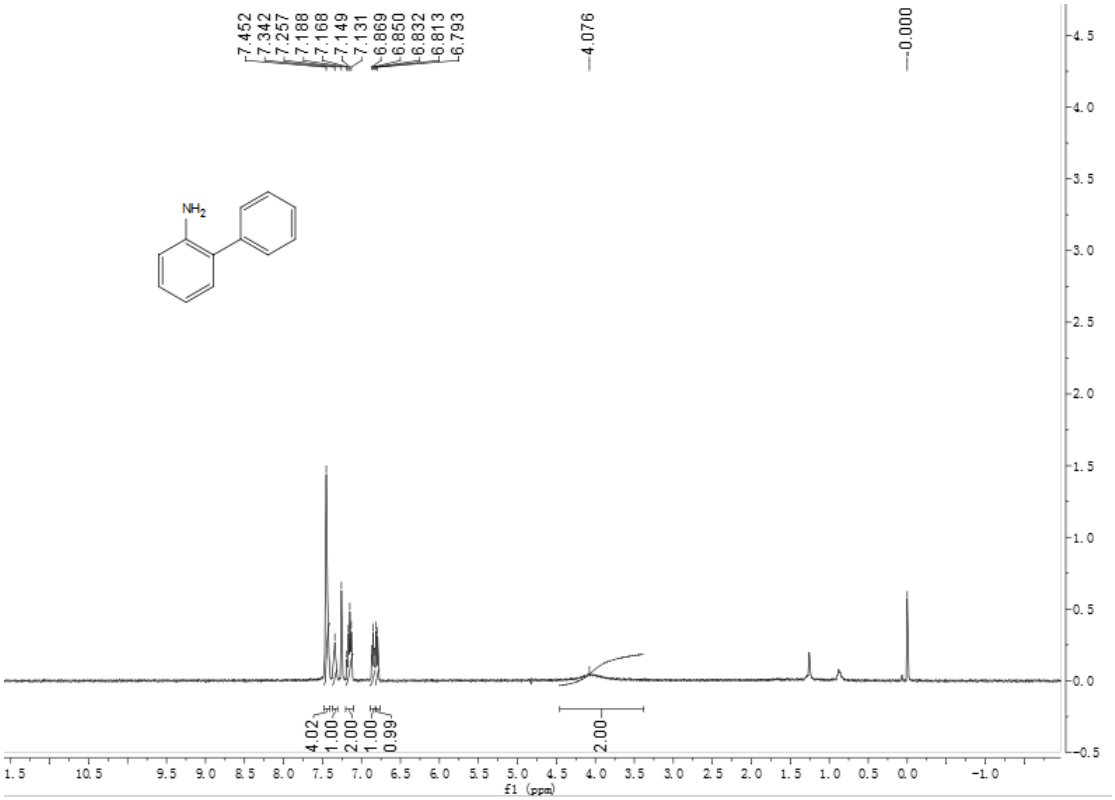
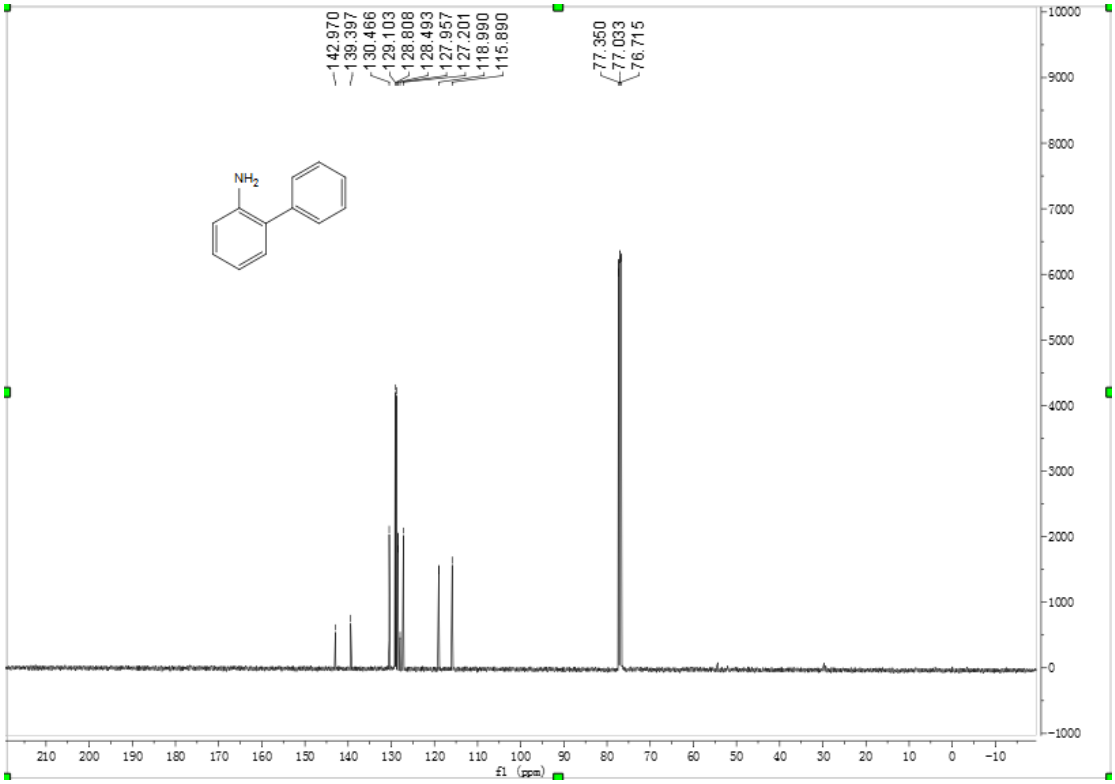
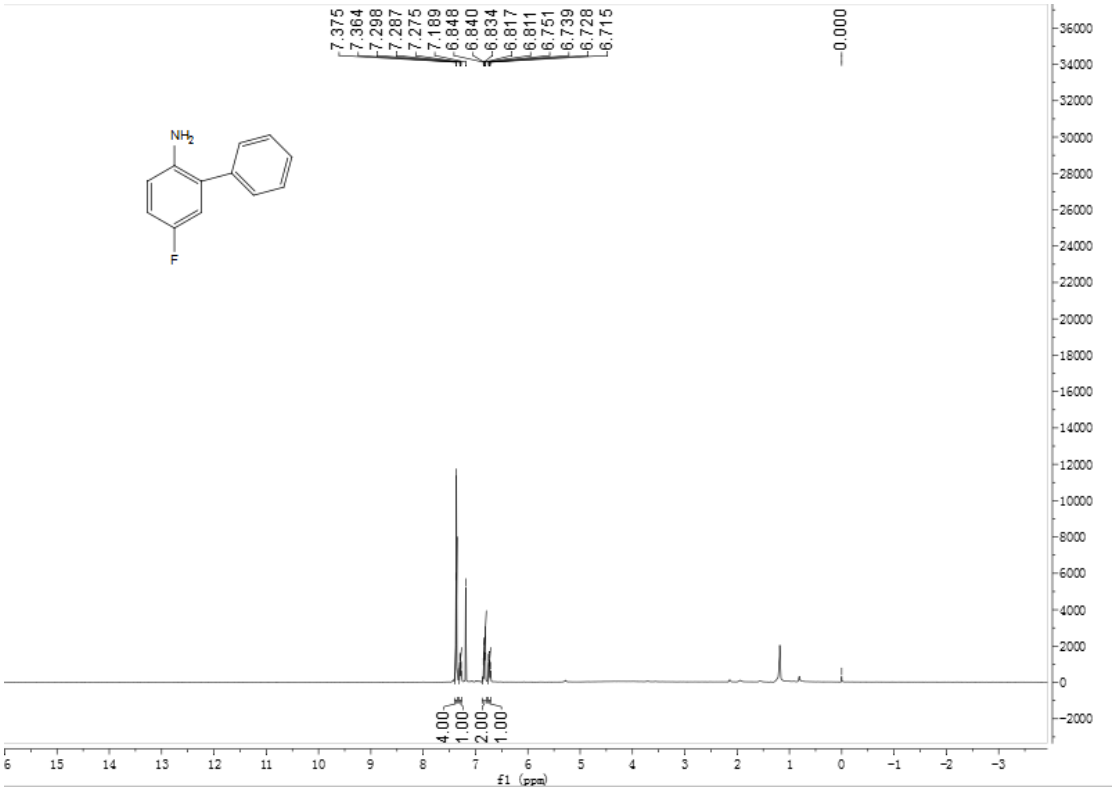
NMR Spectra

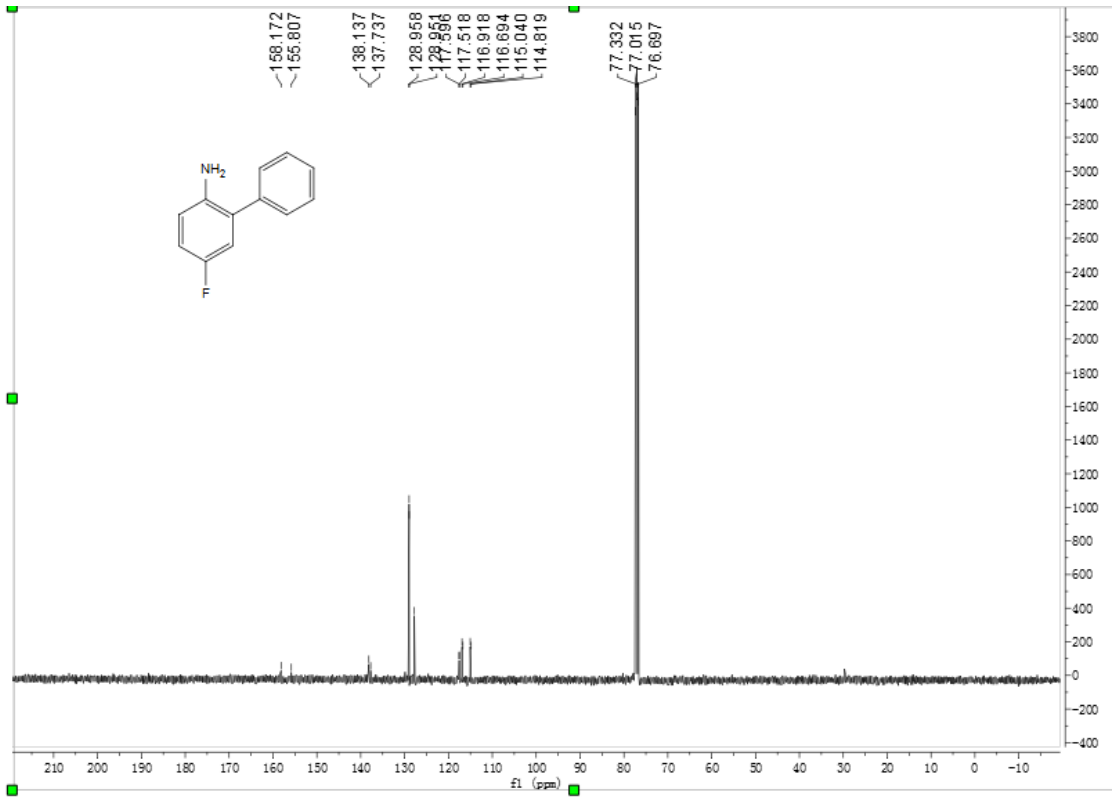
3a



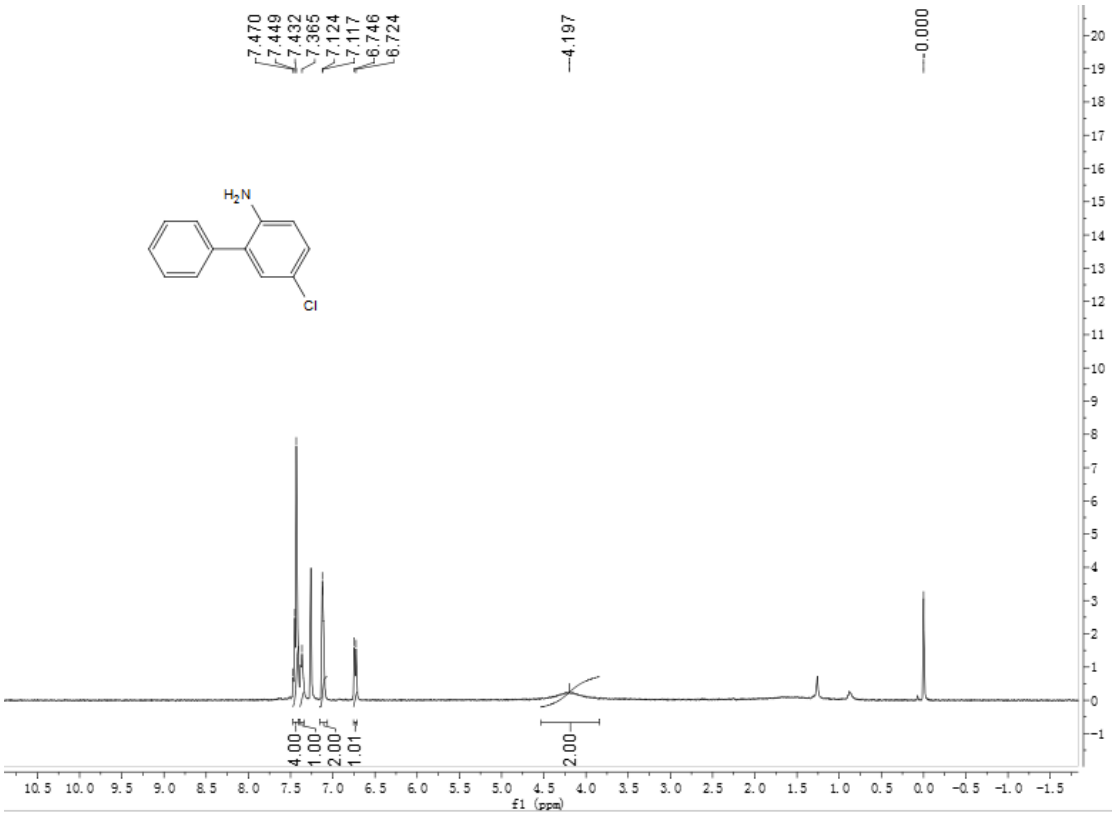


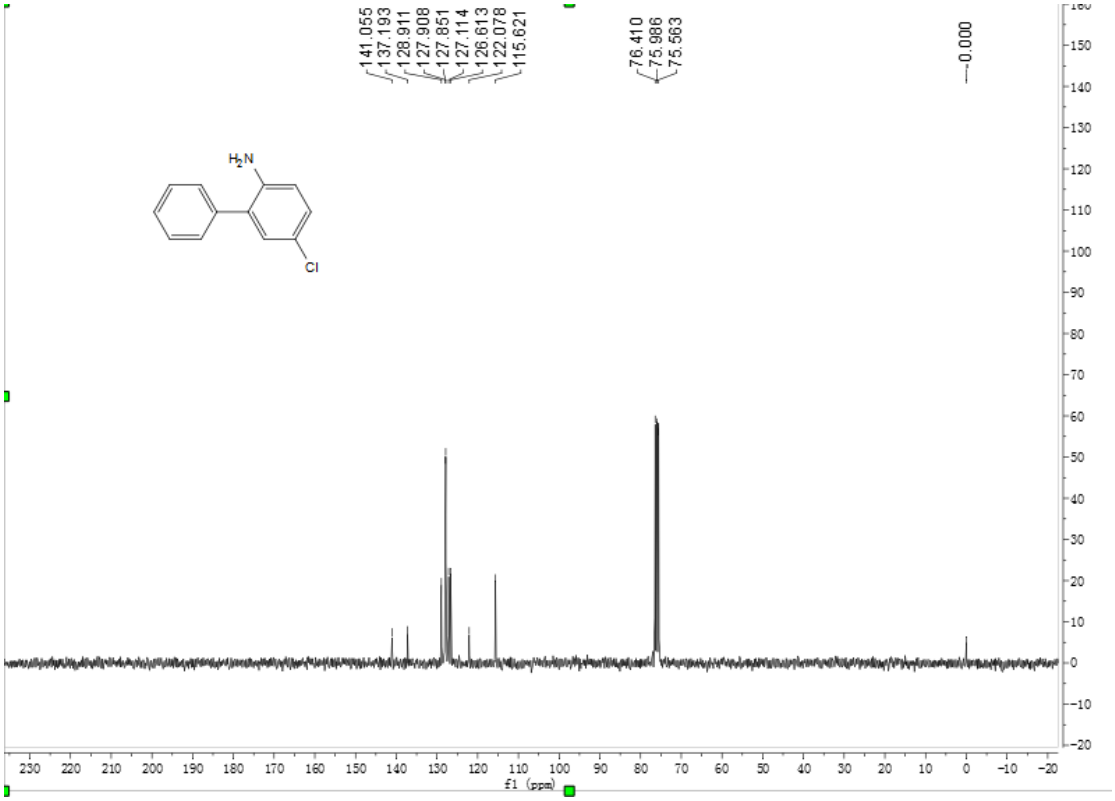
3b


7.375
7.364
7.298
7.287
7.275
7.189
6.848
6.840
6.834
6.817
6.811
6.751
6.739
6.728
6.715
0.000
NH2
F
4.00
1.00
2.00
1.00
f1 (ppm)

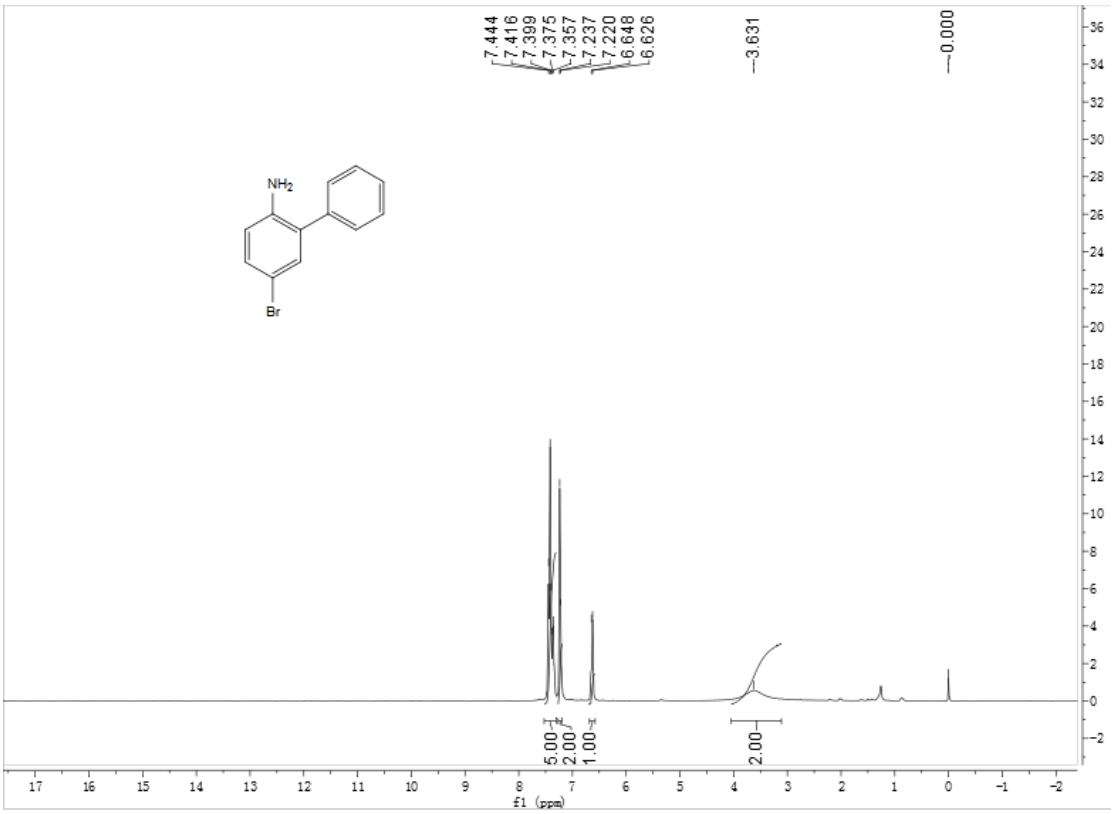

158.172
155.807
138.137
137.737
128.958
128.951
117.596
117.518
116.918
116.694
115.040
114.819
77.332
77.015
76.697
NH2
F
f1 (ppm)

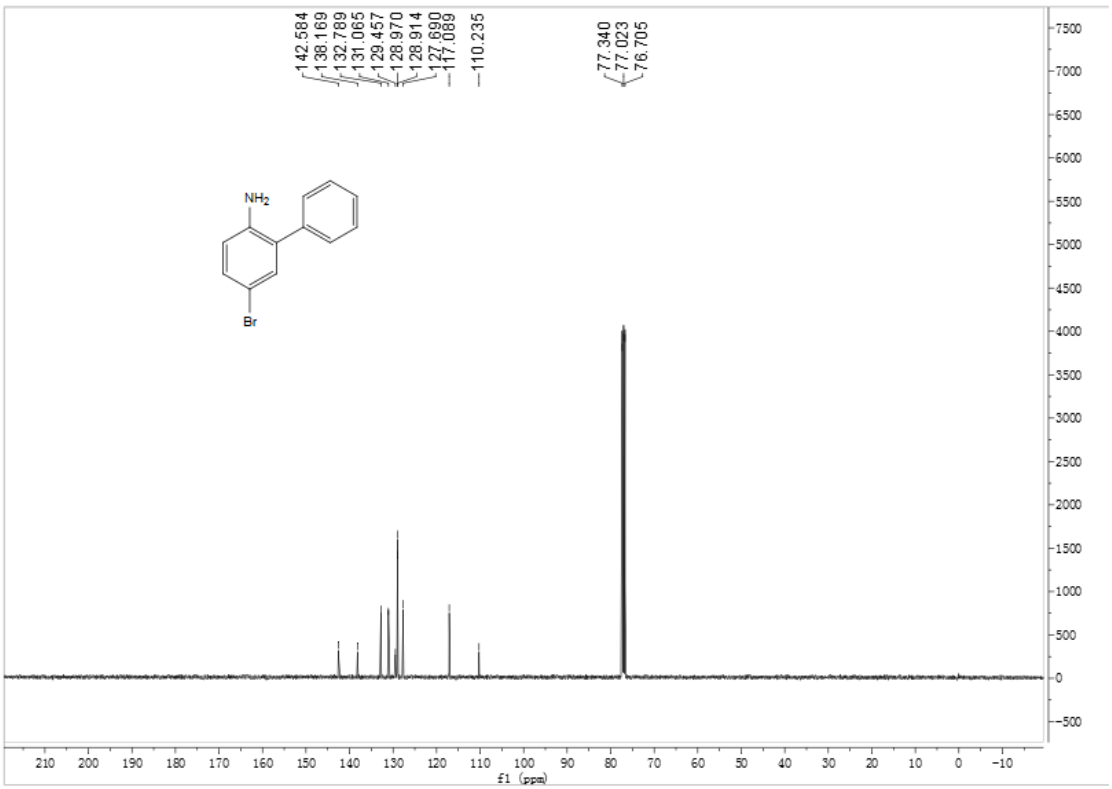
3c


7.470
7.449
7.432
7.365
7.124
7.117
6.746
6.724
4.197
0.000
H_2N
Cl
4.00
1.00
2.00
1.01
2.00
f1 (ppm)

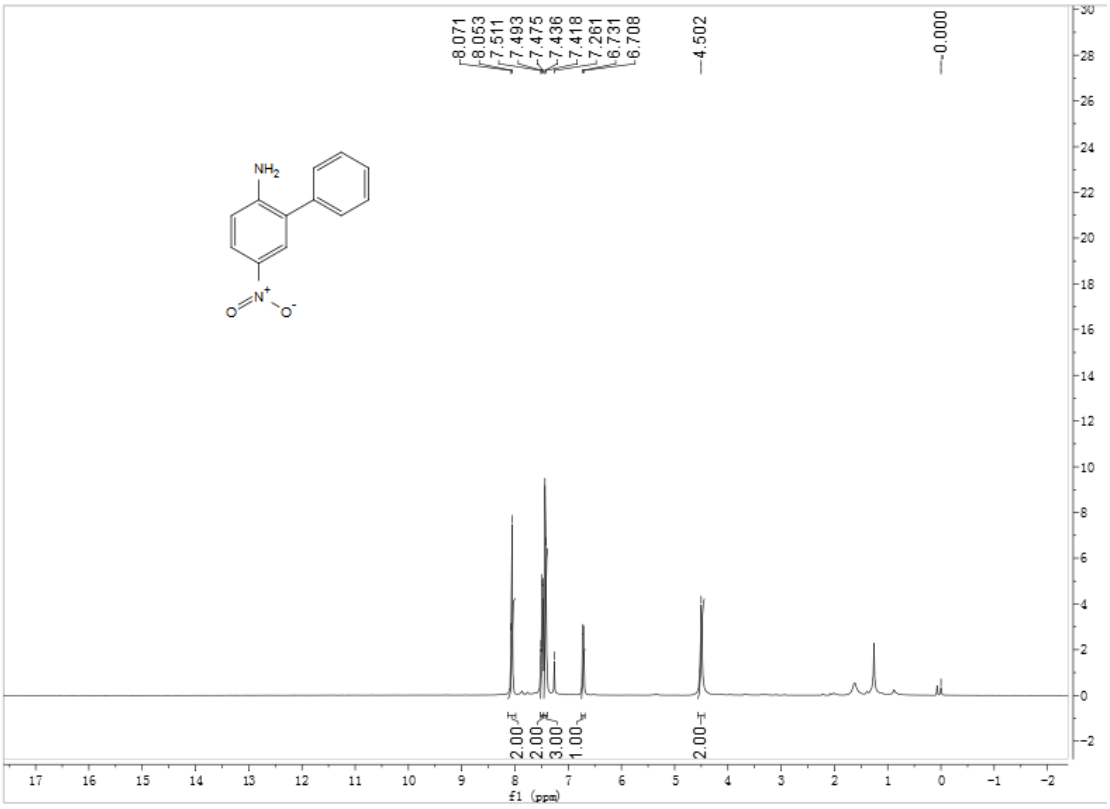

141.055
137.193
128.911
127.908
127.851
127.114
126.613
122.078
115.621
76.410
75.986
75.563
0.000
H_2N
Cl
f1 (ppm)

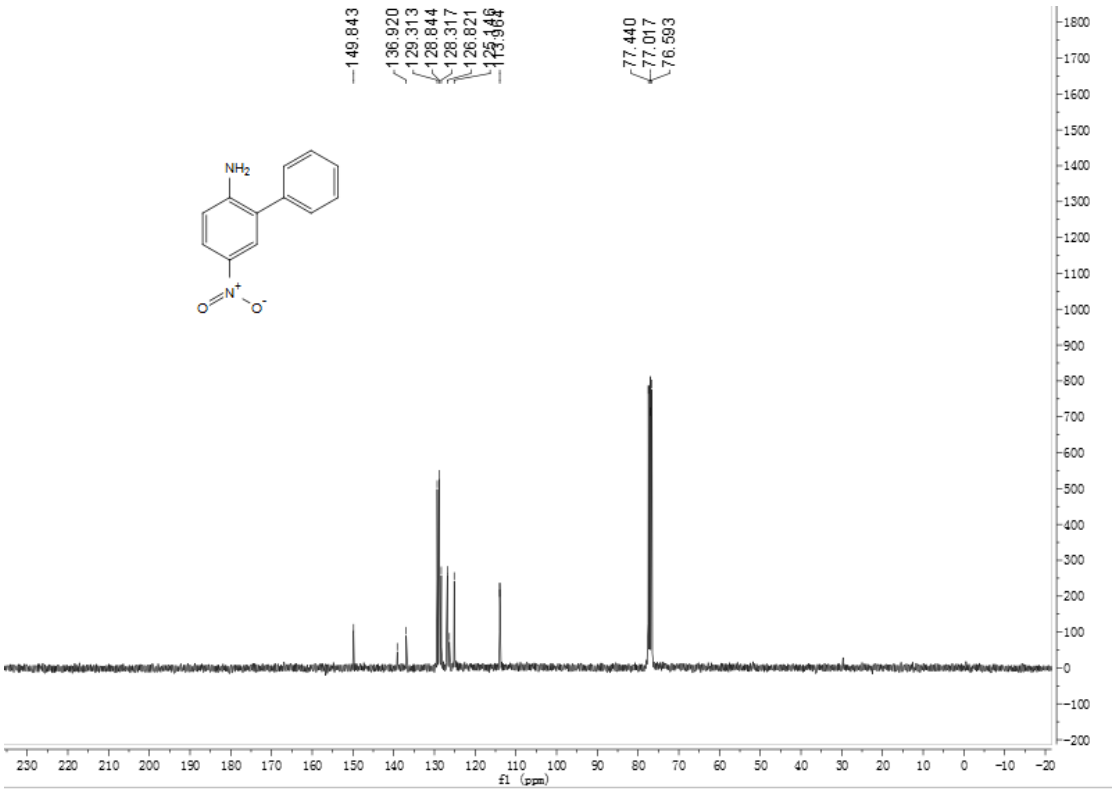
3d


7.444
7.416
7.399
7.375
7.357
7.237
7.220
6.648
6.626
3.631
0.000
NH2
Br
5.00
2.00
1.00
2.00
f1 (ppm)

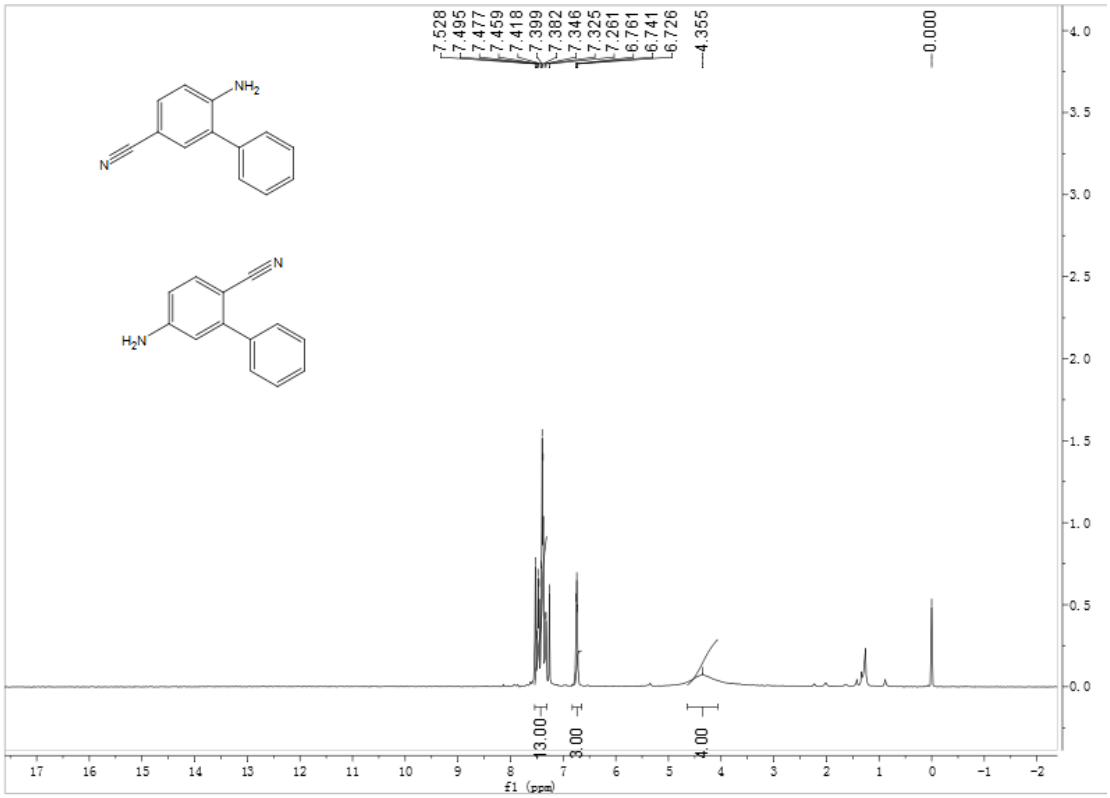

142.584
138.169
132.789
131.065
129.457
128.970
128.914
127.690
117.089
110.235
77.340
77.023
76.705
NH2
Br
f1 (ppm)

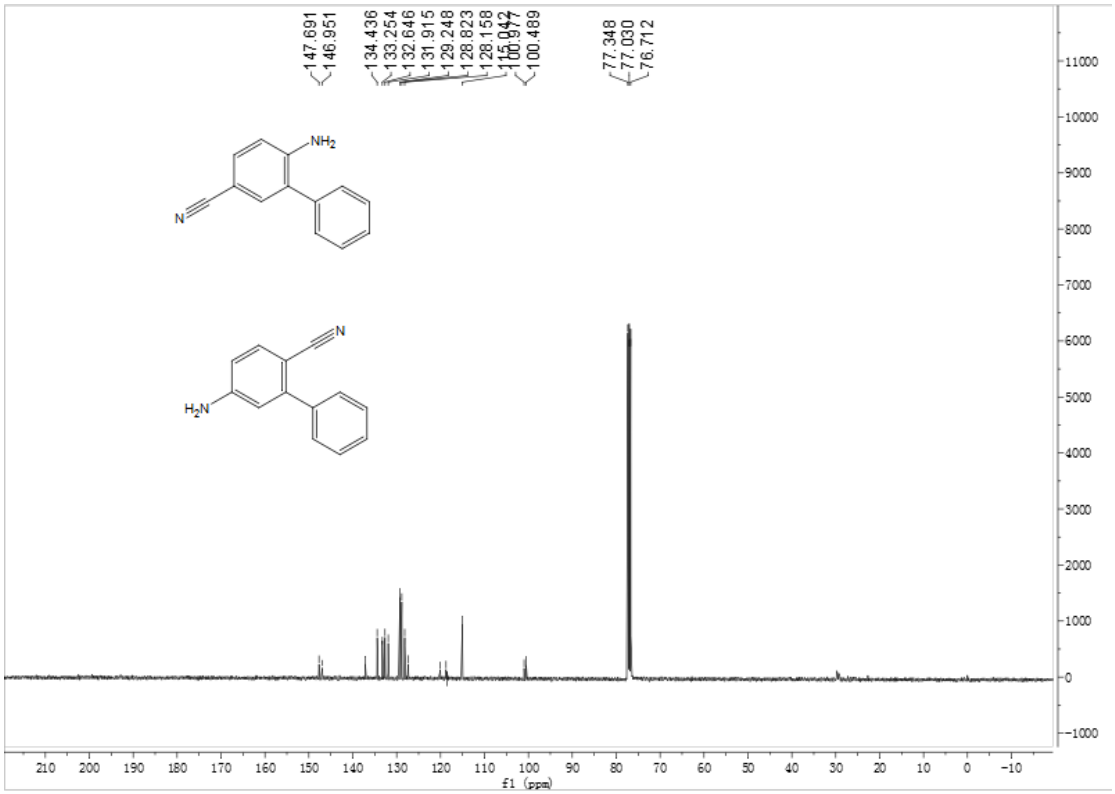
3e


8.071
8.053
7.511
7.493
7.475
7.436
7.418
7.261
6.731
6.708
4.502
0.000
NH2
O
N+
O-
2.00
2.00
3.00
1.00
2.00
f1 (ppm)

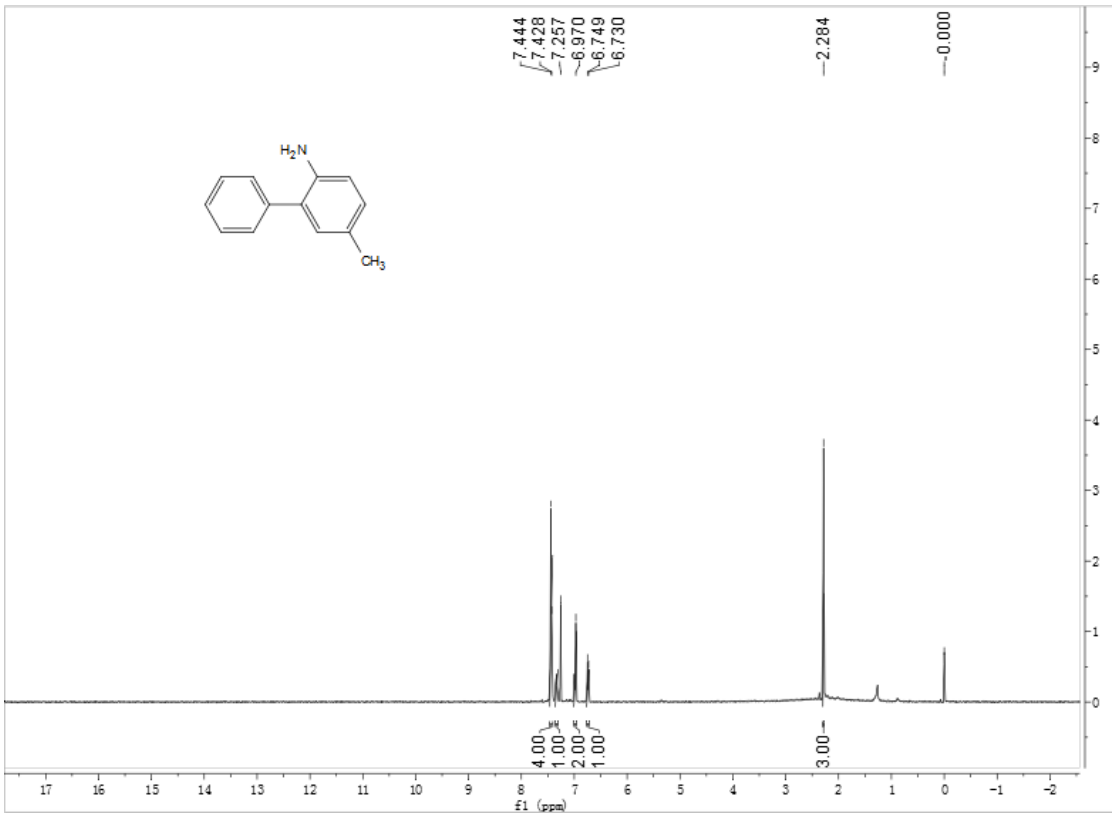

149.843
136.920
129.313
128.844
128.317
126.821
125.146
113.984
77.440
77.017
76.593
NH2
O
N+
O-
f1 (ppm)

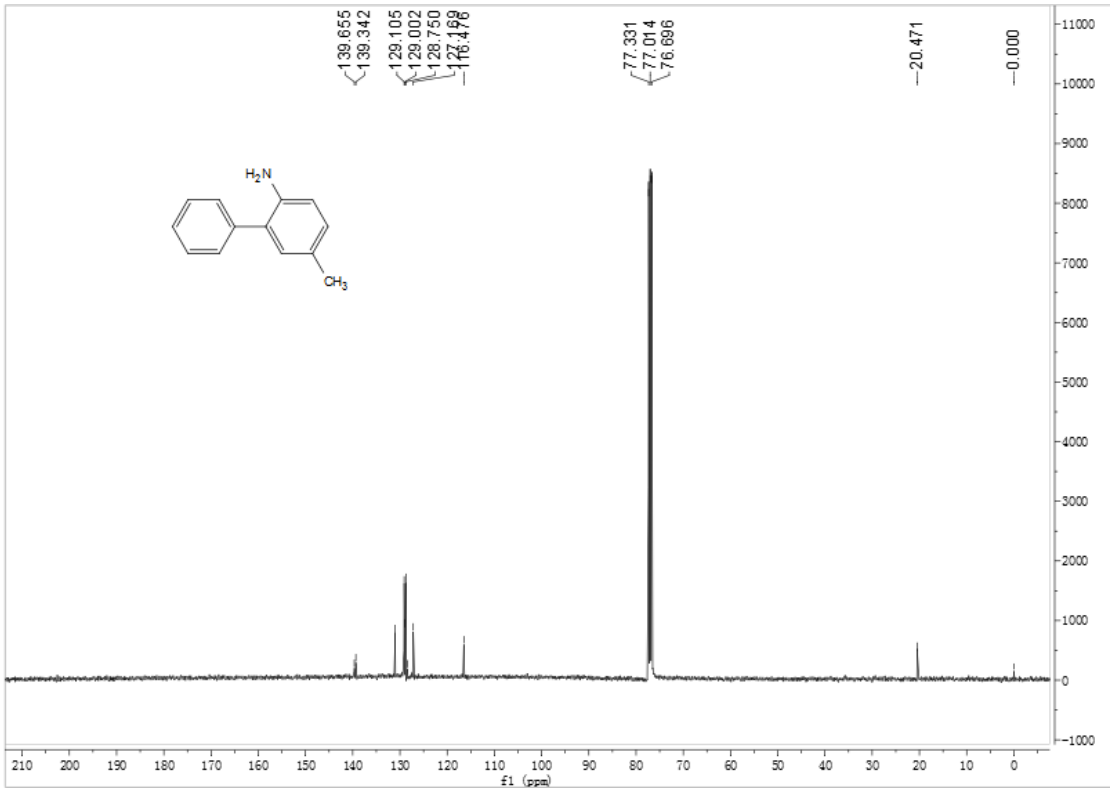
3f and 3f'


7.528
7.495
7.477
7.459
7.418
7.399
7.382
7.346
7.325
7.261
6.761
6.741
6.726
4.355
0.000
NH2
N
H2N
N
13.00
3.00
4.00
f1 (ppm)

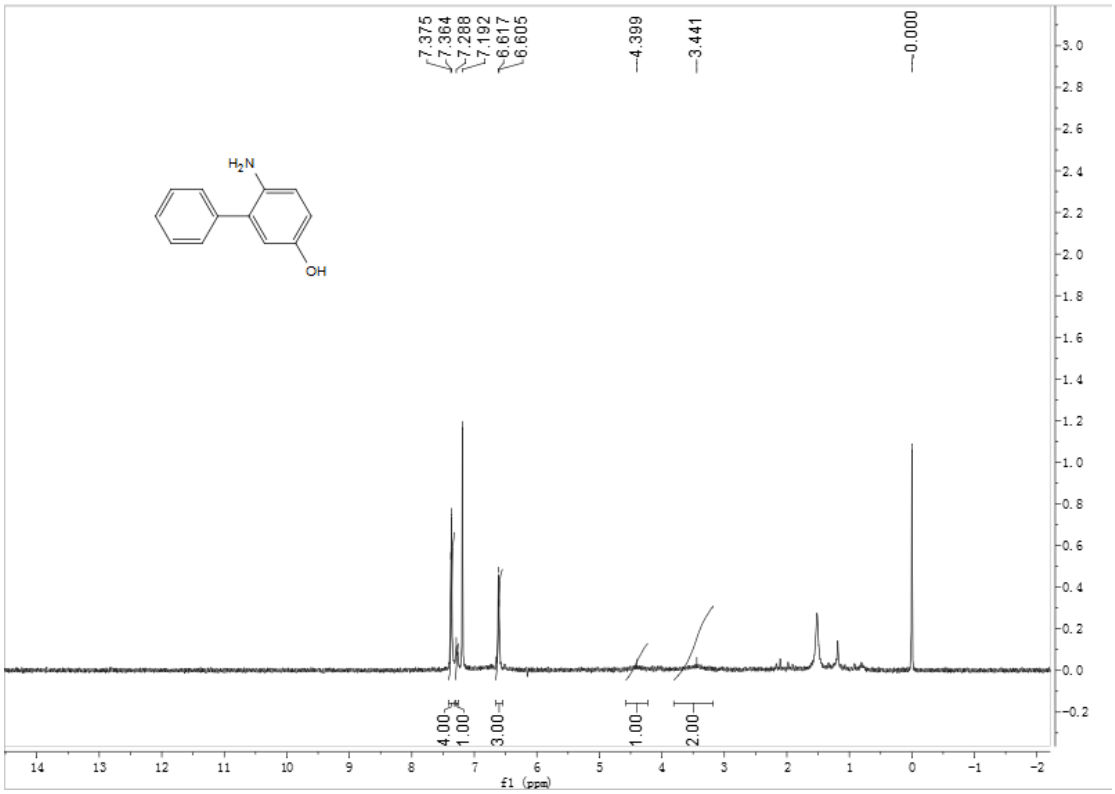

147.691
146.951
134.436
133.254
132.646
131.915
129.248
128.823
128.158
115.042
100.489
77.348
77.030
76.712
NH2
N
H2N
N
f1 (ppm)

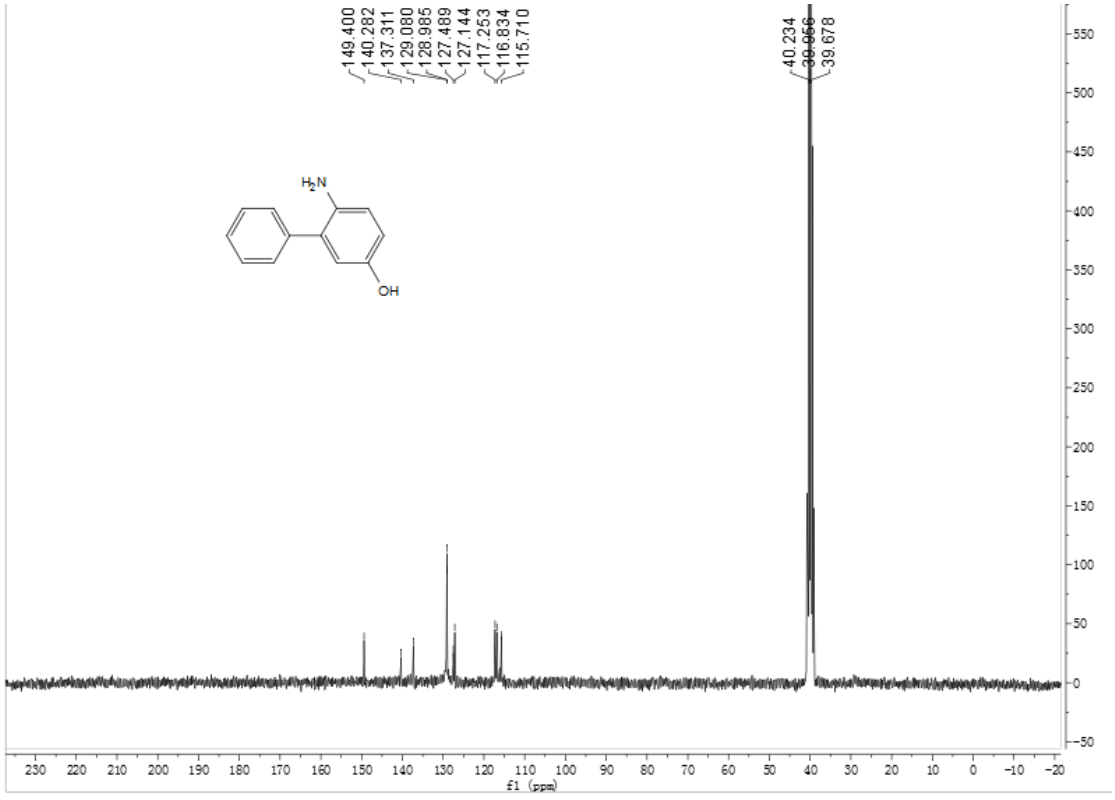
3g


7.444
7.428
7.257
6.970
6.749
6.730
2.284
0.000
4.00
1.00
2.00
1.00
3.00
f1 (ppm)

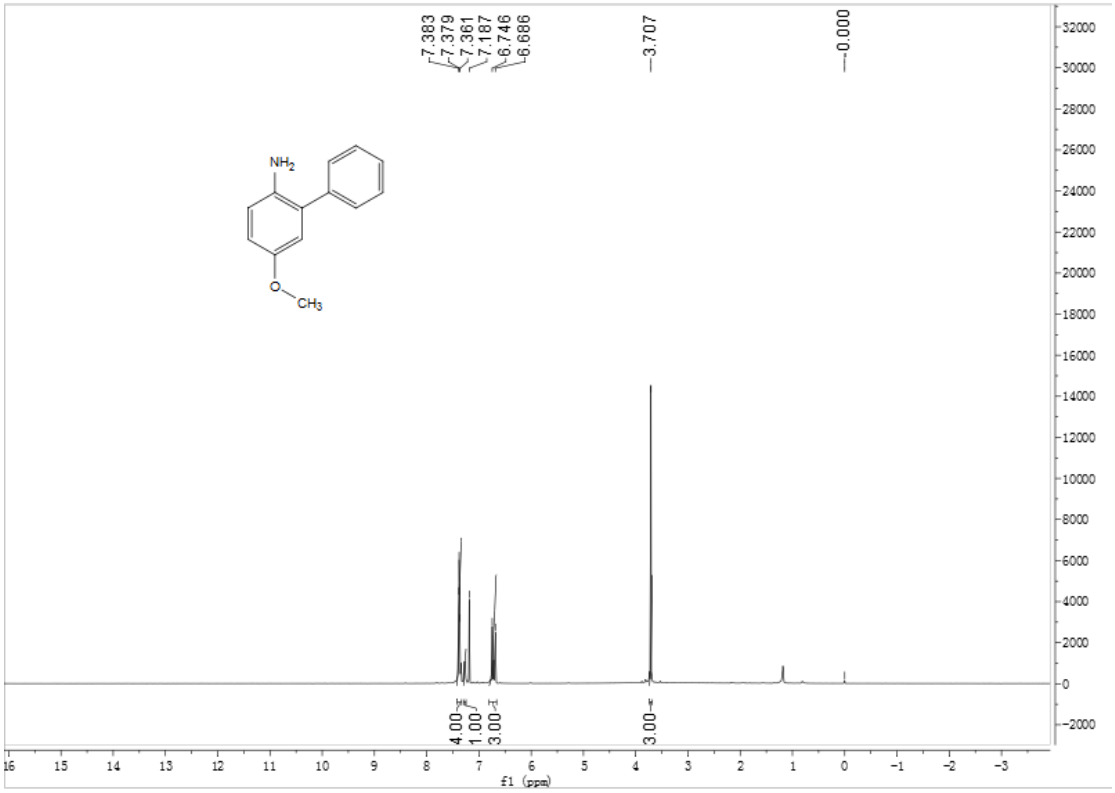

139.655
139.342
129.105
129.002
128.750
77.331
77.014
76.696
20.471
0.000
f1 (ppm)

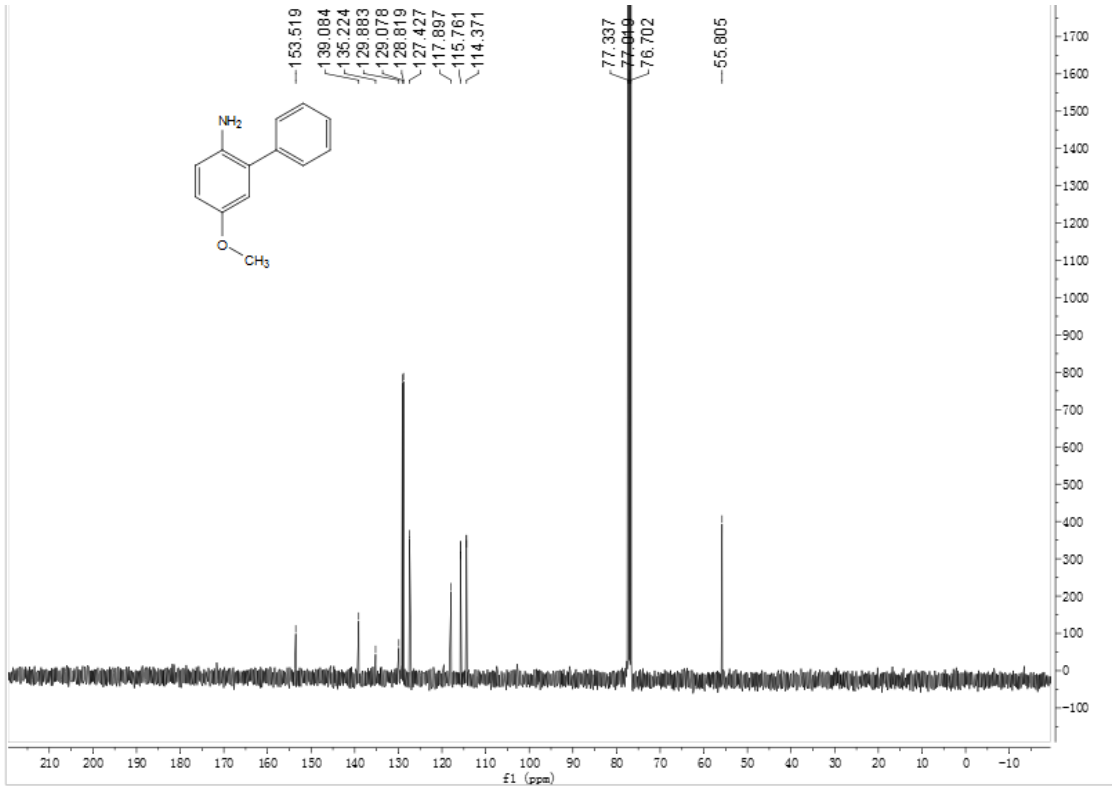
3h


7.375
7.364
7.288
7.192
6.617
6.605
4.399
3.441
0.000
4.00
1.00
3.00
1.00
2.00
f1 (ppm)

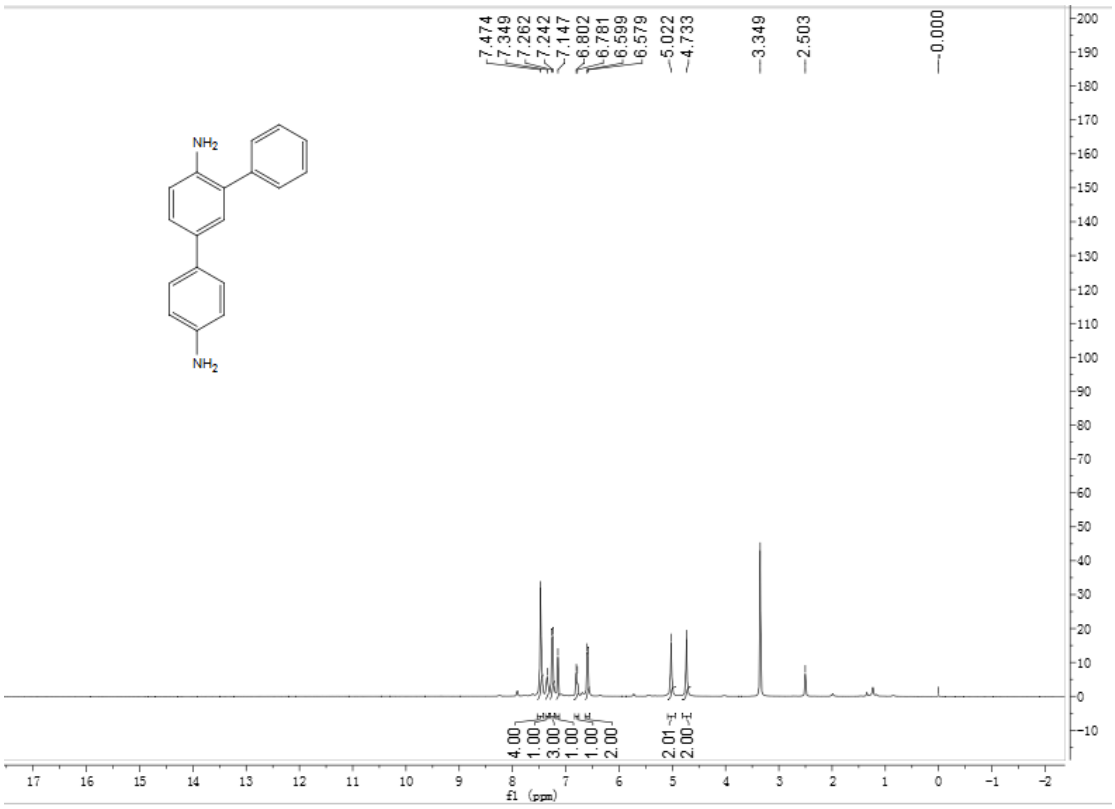

149.400
140.282
137.311
129.080
128.985
127.489
127.144
117.253
116.834
115.710
40.234
39.678
f1 (ppm)

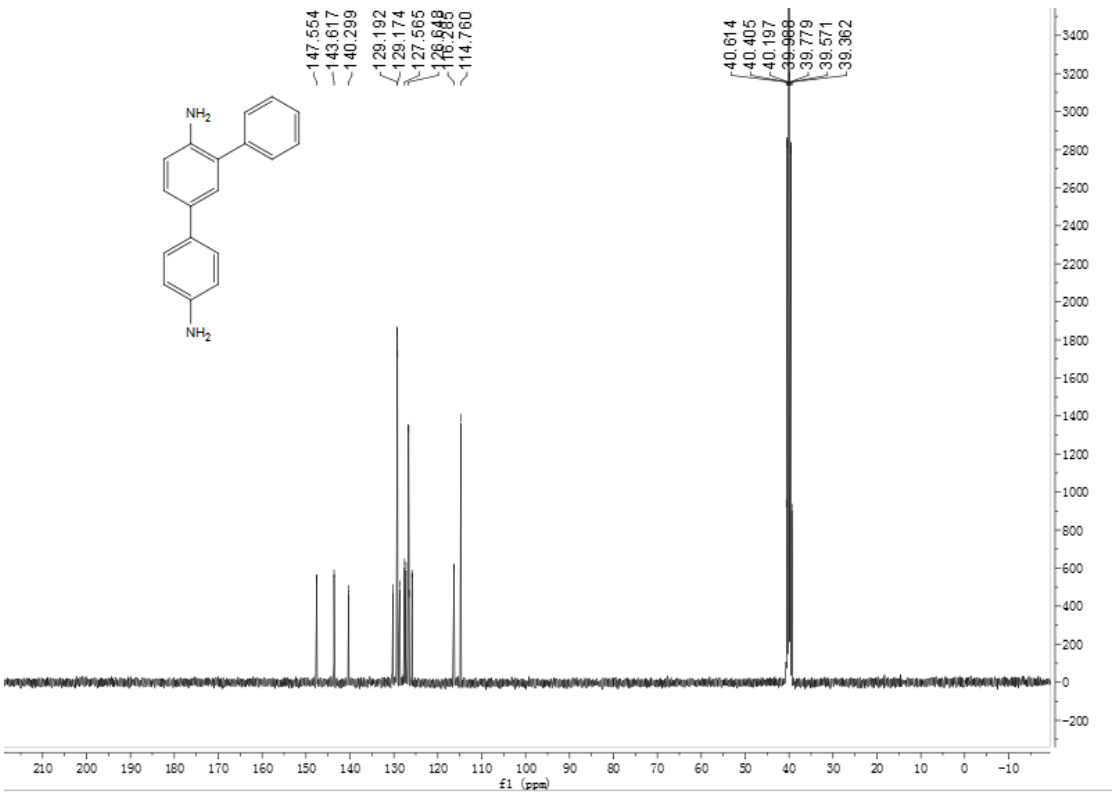
3i


7.383
7.379
7.361
7.187
6.746
6.686
3.707
0.000
NH2
O
CH3
4.00
1.00
3.00
3.00
f1 (ppm)

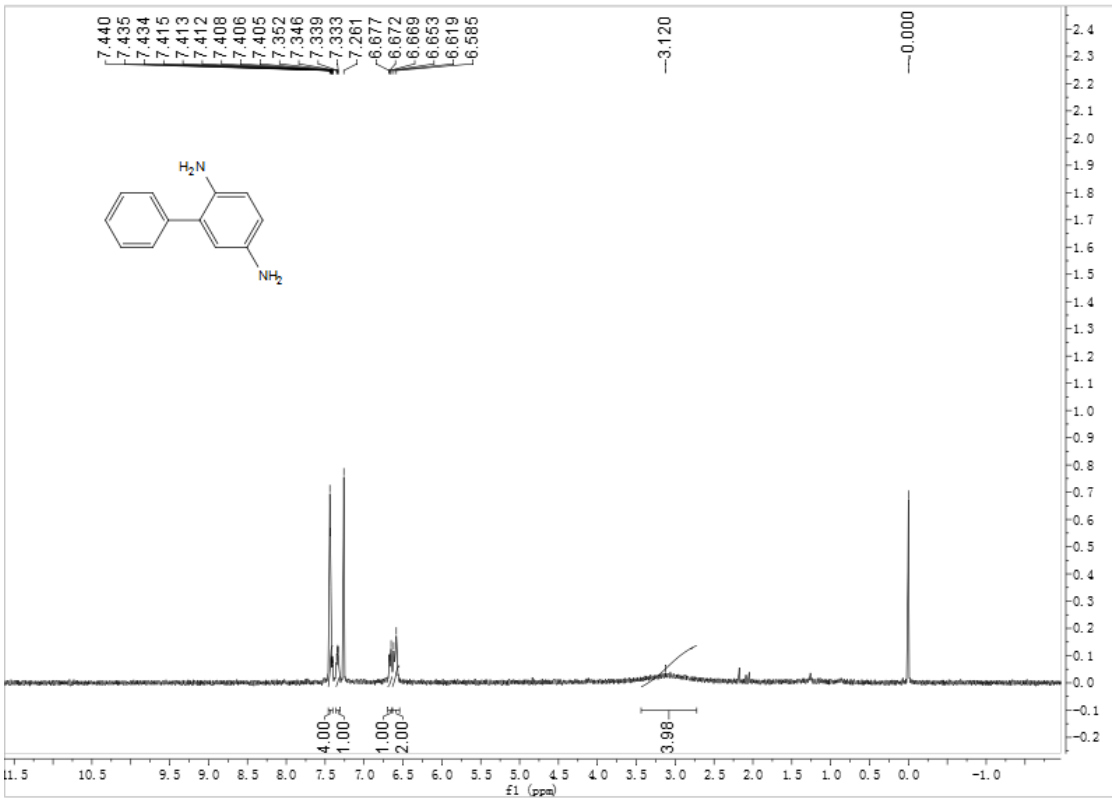

153.519
139.084
135.224
129.883
129.078
128.819
127.427
117.897
115.761
114.371
77.337
77.019
76.702
55.805
NH2
O
CH3
f1 (ppm)

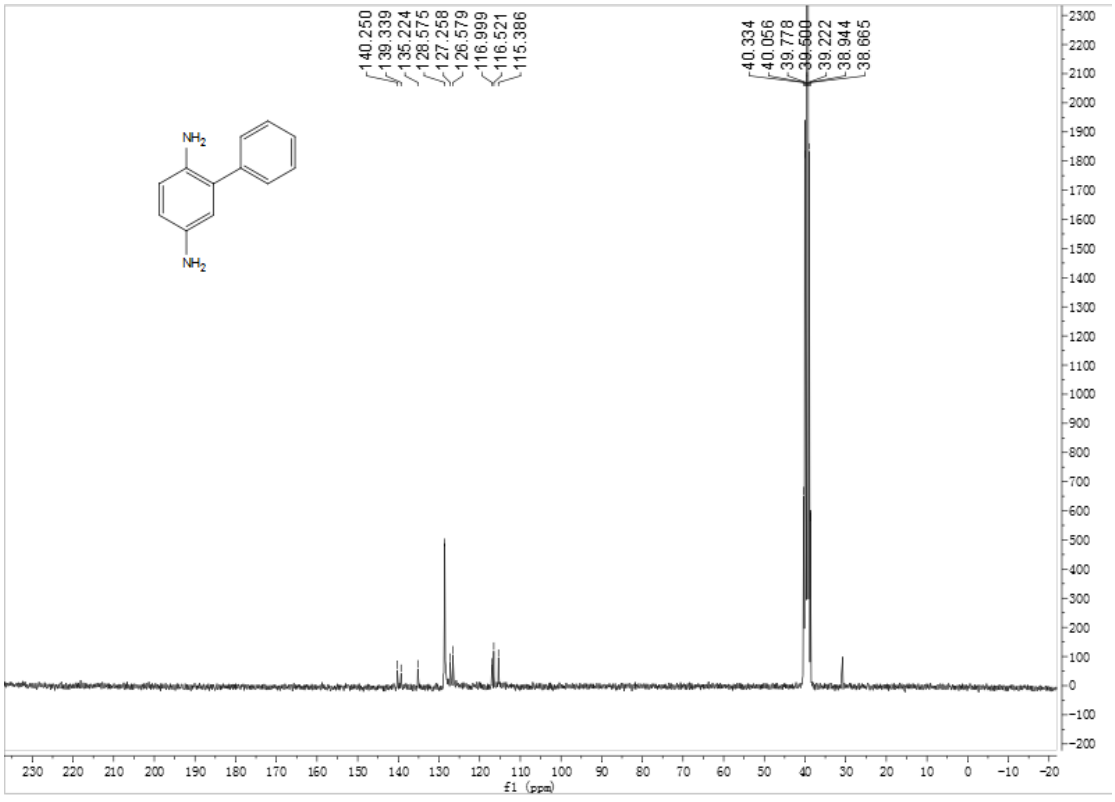
3j


7.474
7.349
7.262
7.242
7.147
6.802
6.781
6.599
6.579
5.022
4.733
3.349
2.503
0.000
NH2
NH2
4.00
1.00
3.00
1.00
1.00
2.00
2.01
2.00
f1 (ppm)

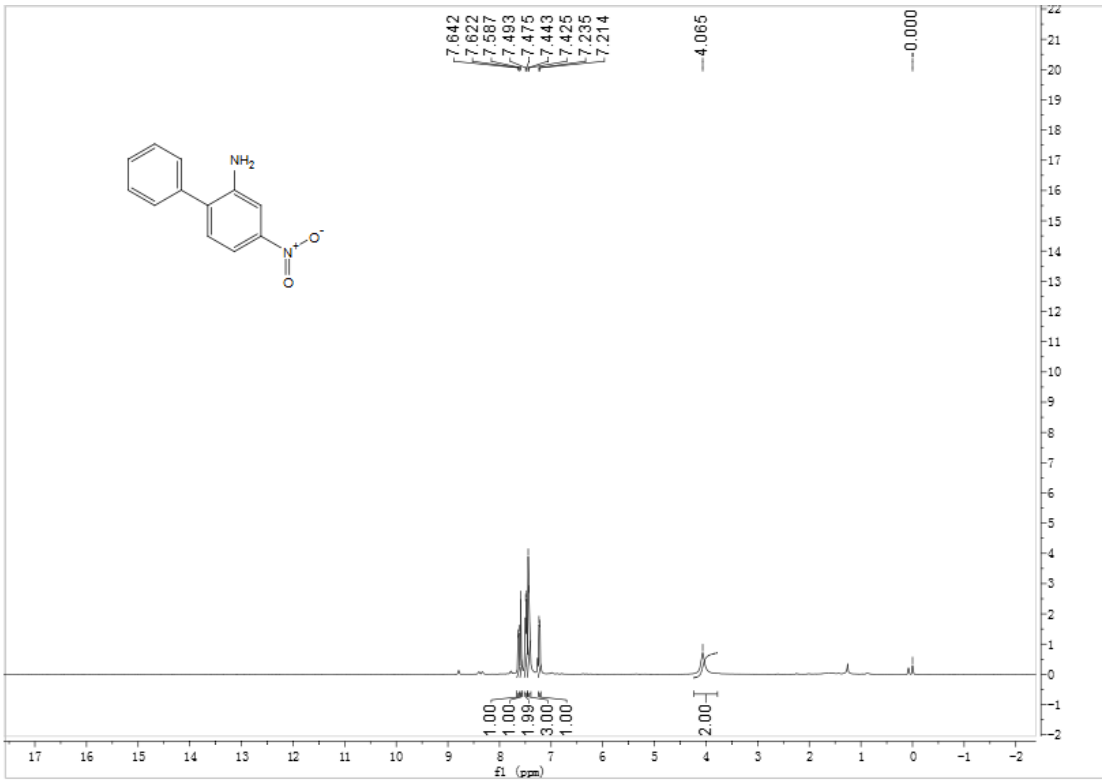

147.554
143.617
140.299
129.192
129.174
127.565
114.760
40.614
40.405
40.197
39.779
39.571
39.362
NH2
NH2
f1 (ppm)

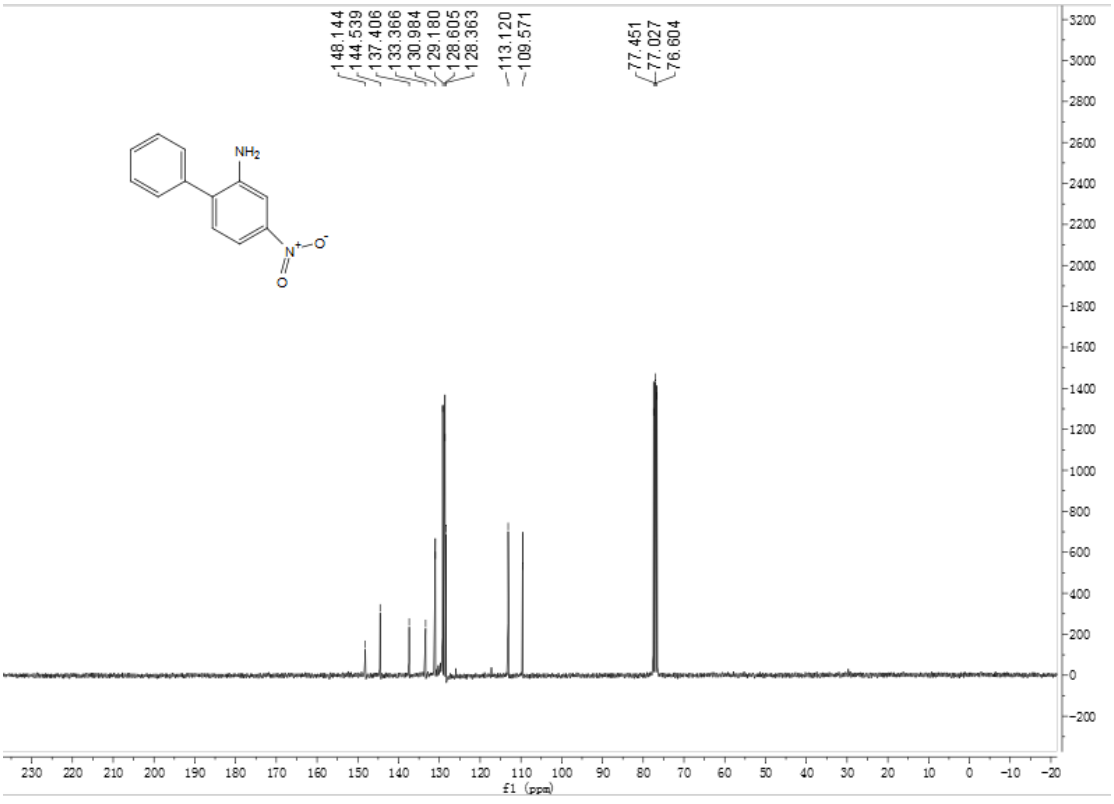
3k


7.440
7.435
7.434
7.415
7.413
7.412
7.408
7.406
7.405
7.352
7.346
7.339
7.333
7.261
6.677
6.672
6.669
6.653
6.619
6.585
3.120
0.000
H2N
NH2
4.00
1.00
1.00
2.00
3.98
f1 (ppm)

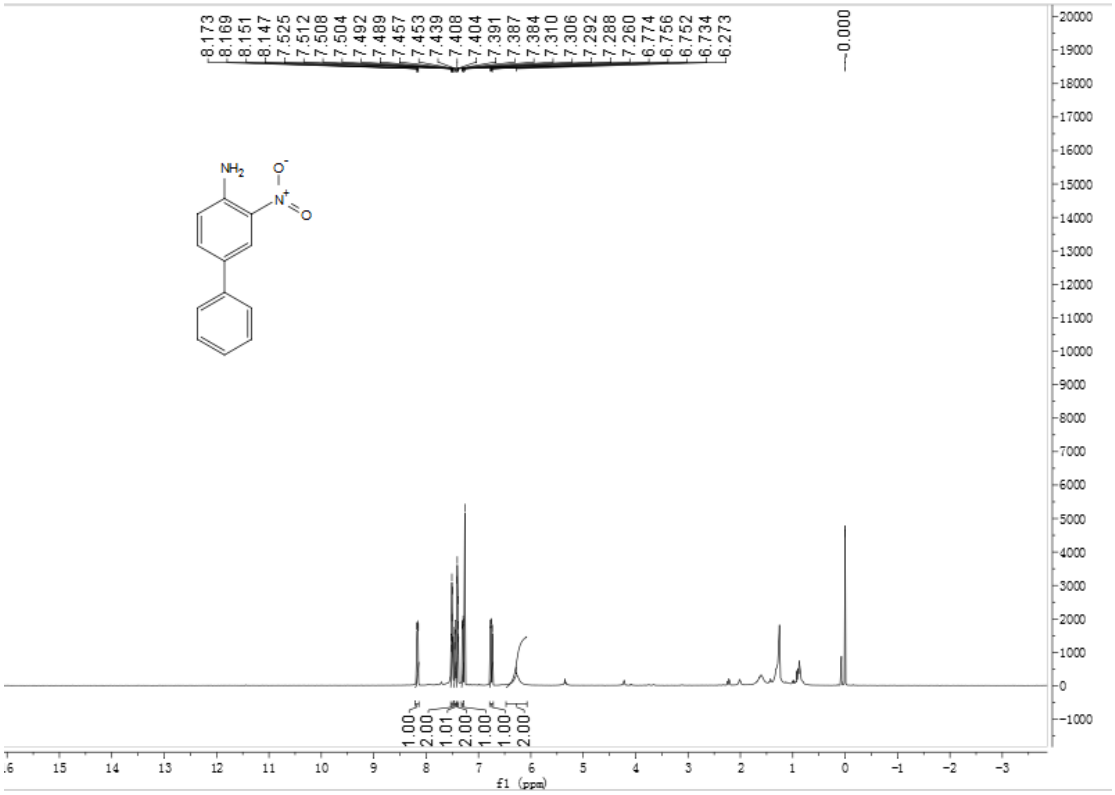

140.250
139.339
135.224
128.575
127.258
126.579
116.999
116.521
115.386
40.334
40.056
39.778
39.600
39.222
38.944
38.665
NH2
NH2
f1 (ppm)

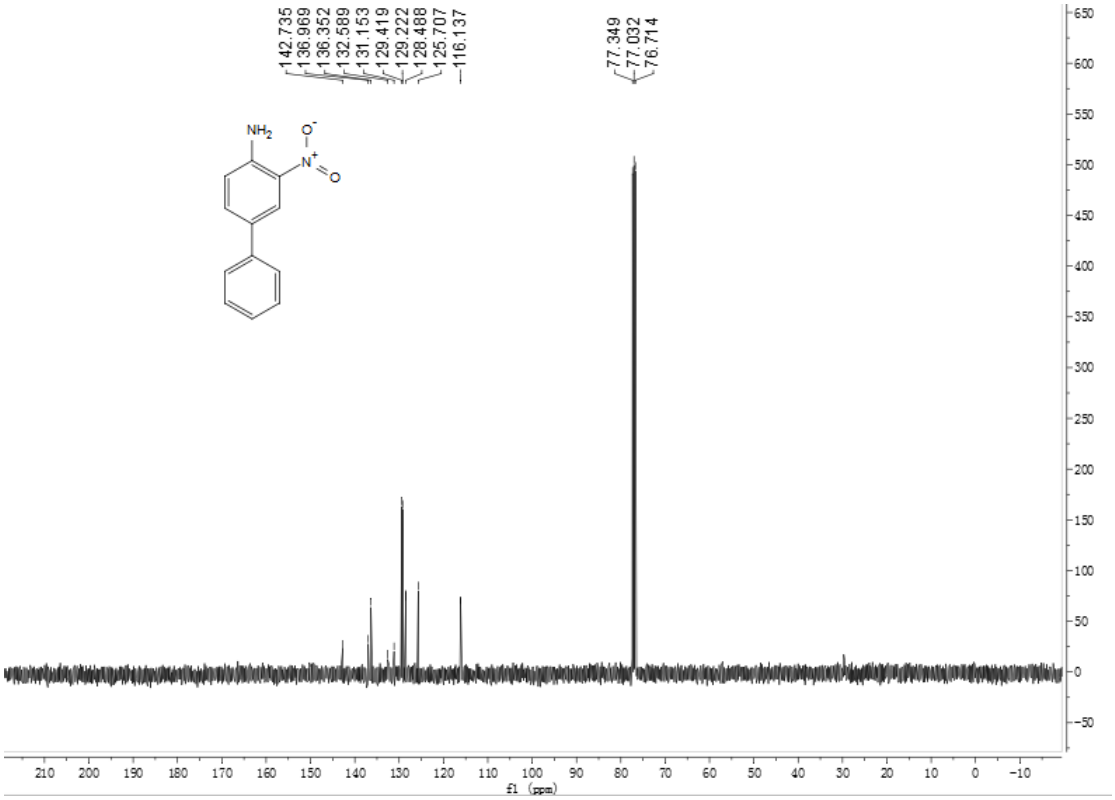
3l


7.642
7.622
7.587
7.493
7.475
7.443
7.425
7.235
7.214
4.065
0.000
NH2
1.00
1.00
1.99
3.00
1.00
2.00
f1 (ppm)

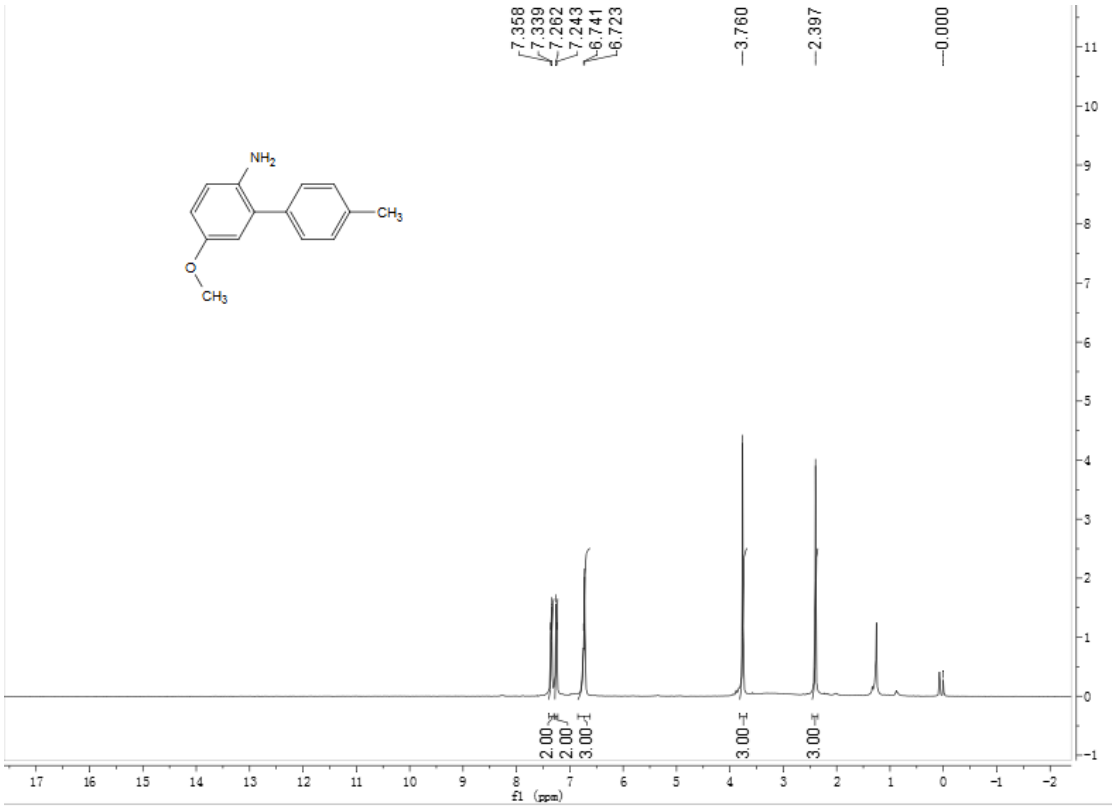

148.144
144.539
137.406
133.366
130.984
129.180
128.605
128.363
113.120
109.571
77.451
77.027
76.604
NH2
f1 (ppm)

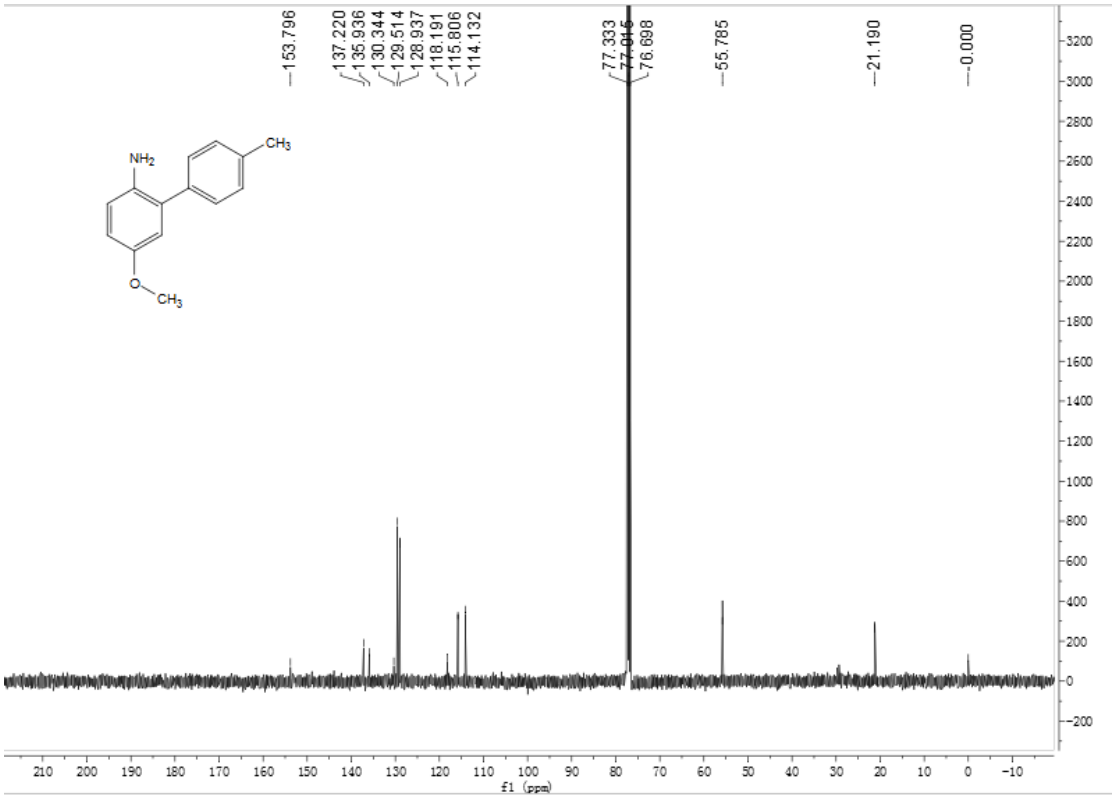
3n


8.173
8.169
8.151
8.147
7.525
7.512
7.508
7.504
7.492
7.489
7.457
7.453
7.439
7.408
7.404
7.391
7.387
7.384
7.310
7.306
7.292
7.288
7.260
6.774
6.756
6.752
6.734
6.273
0.000
NH2
O
N
O
1.00
2.00
1.01
2.00
1.00
1.00
2.00
f1 (ppm)

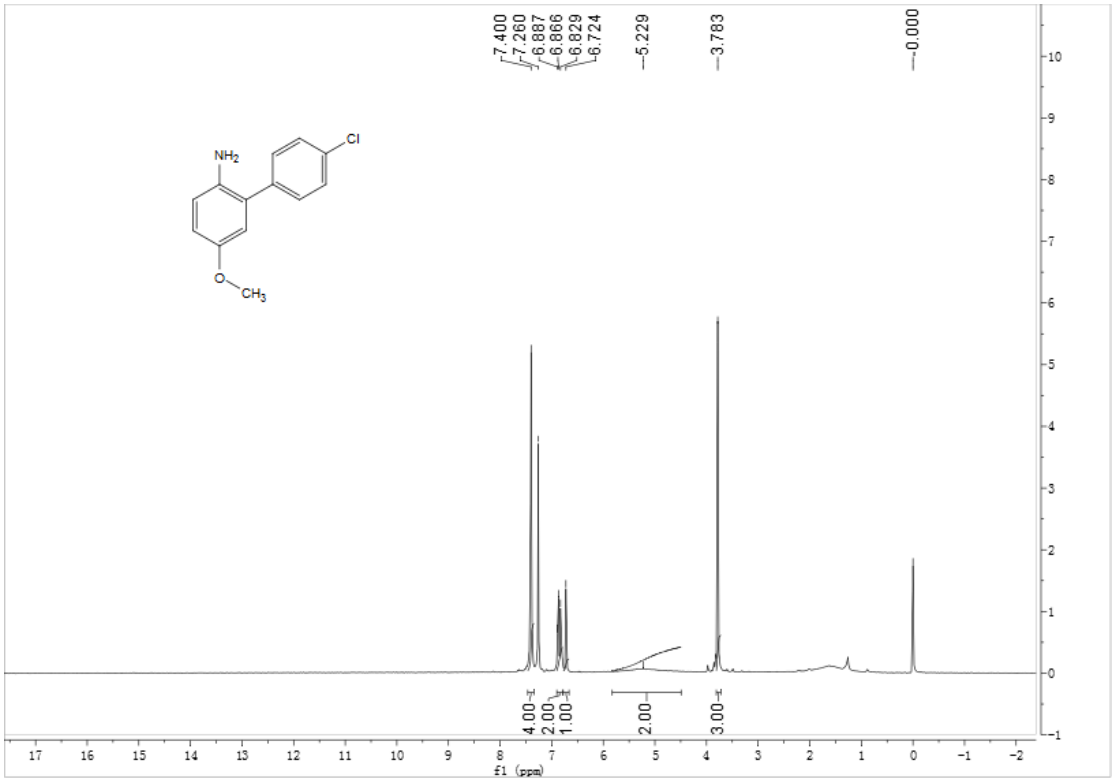

142.735
136.969
136.352
132.589
131.153
129.419
129.222
128.488
125.707
116.137
77.349
77.032
76.714
NH2
O
N
O
f1 (ppm)

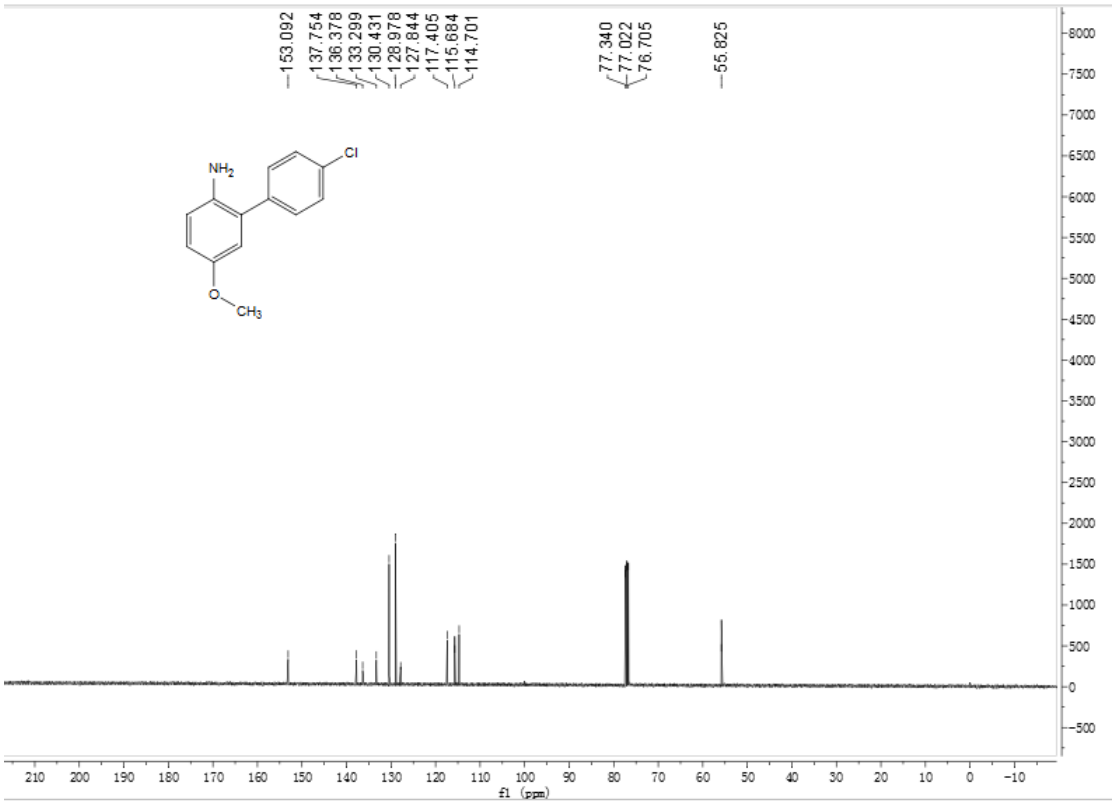
3o


7.358
7.339
7.262
7.243
6.741
6.723
3.760
2.397
0.000
NH2
CH3
O
CH3
2.00
2.00
3.00
3.00
3.00
f1 (ppm)


153.796
137.220
135.936
130.344
129.514
128.937
118.191
115.806
114.132
77.333
77.015
76.698
55.785
21.190
0.000
NH2
CH3
O
CH3
f1 (ppm)

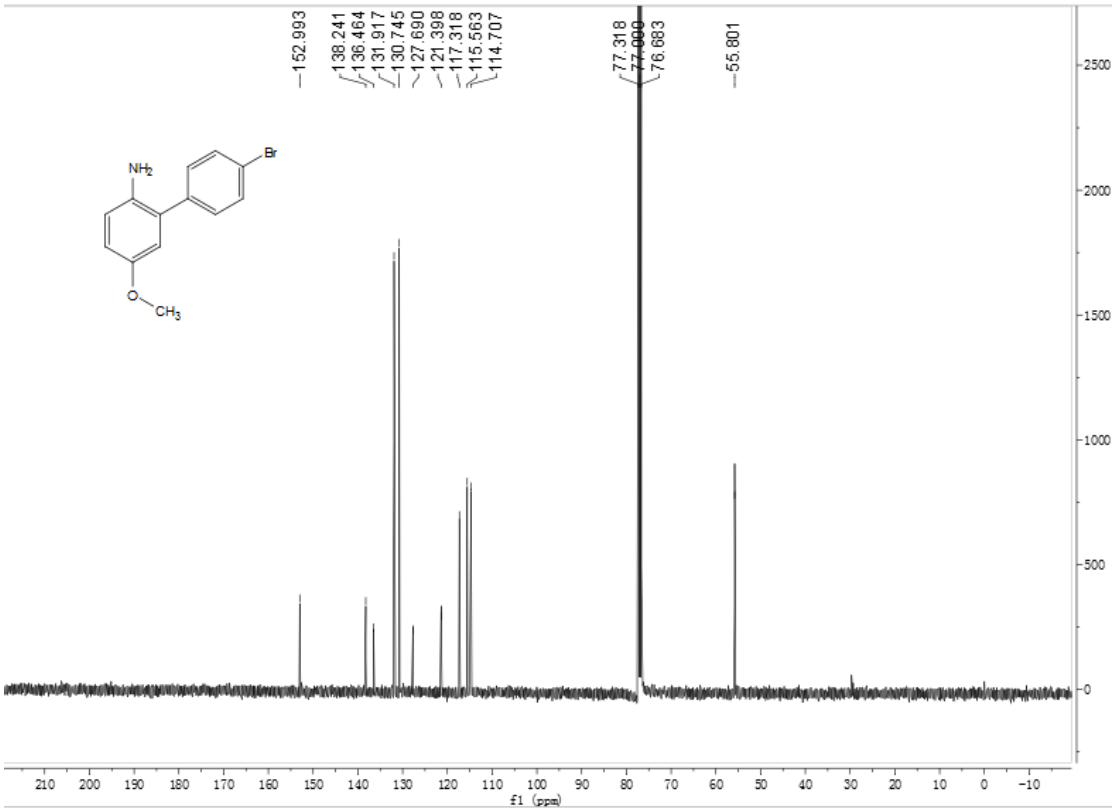
3q


7.400
7.260
6.887
6.866
6.829
6.724
5.229
3.783
0.000
NH2
Cl
O
CH3
4.00
2.00
1.00
2.00
3.00
f1 (ppm)


153.092
137.754
136.378
133.299
130.431
128.978
127.844
117.405
115.684
114.701
77.340
77.022
76.705
55.825
NH2
Cl
O
CH3
f1 (ppm)

3r


7.575
7.554
7.351
7.330
7.257
6.775
6.768
6.744
6.693
6.686
3.764
3.151
0.000
NH2
Br
O
CH3
2.00
2.00
2.00
1.00
3.00
2.00
f1 (ppm)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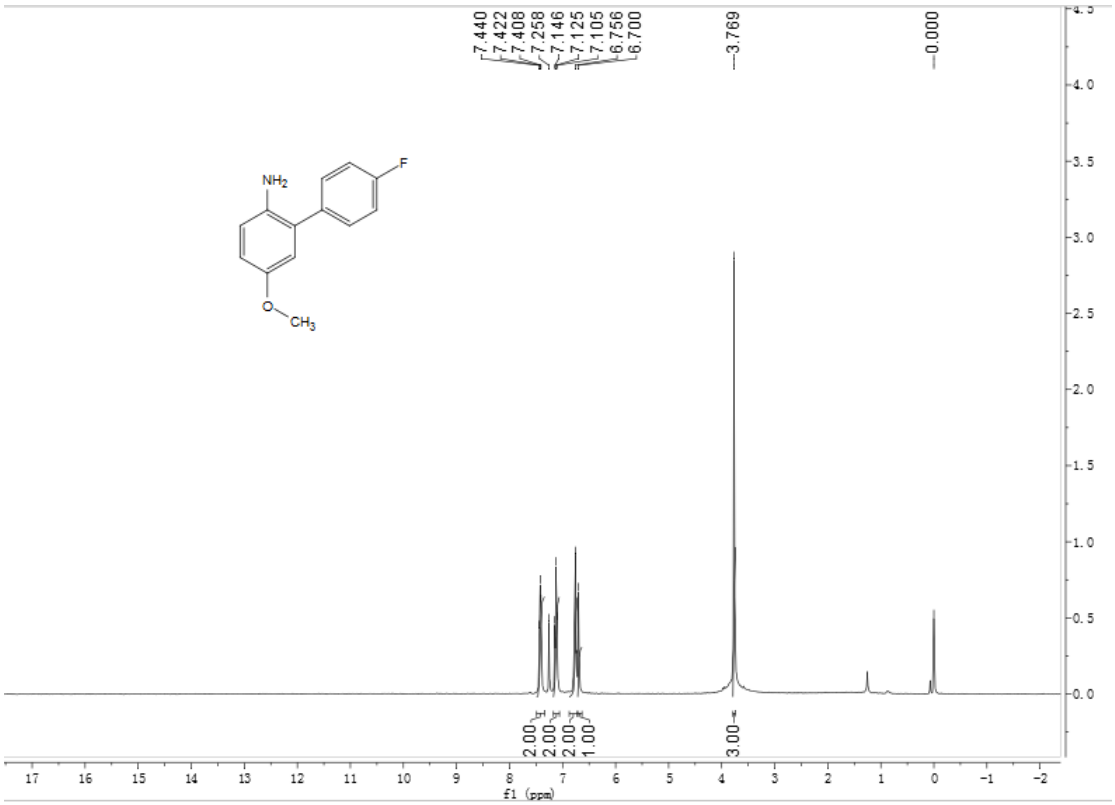
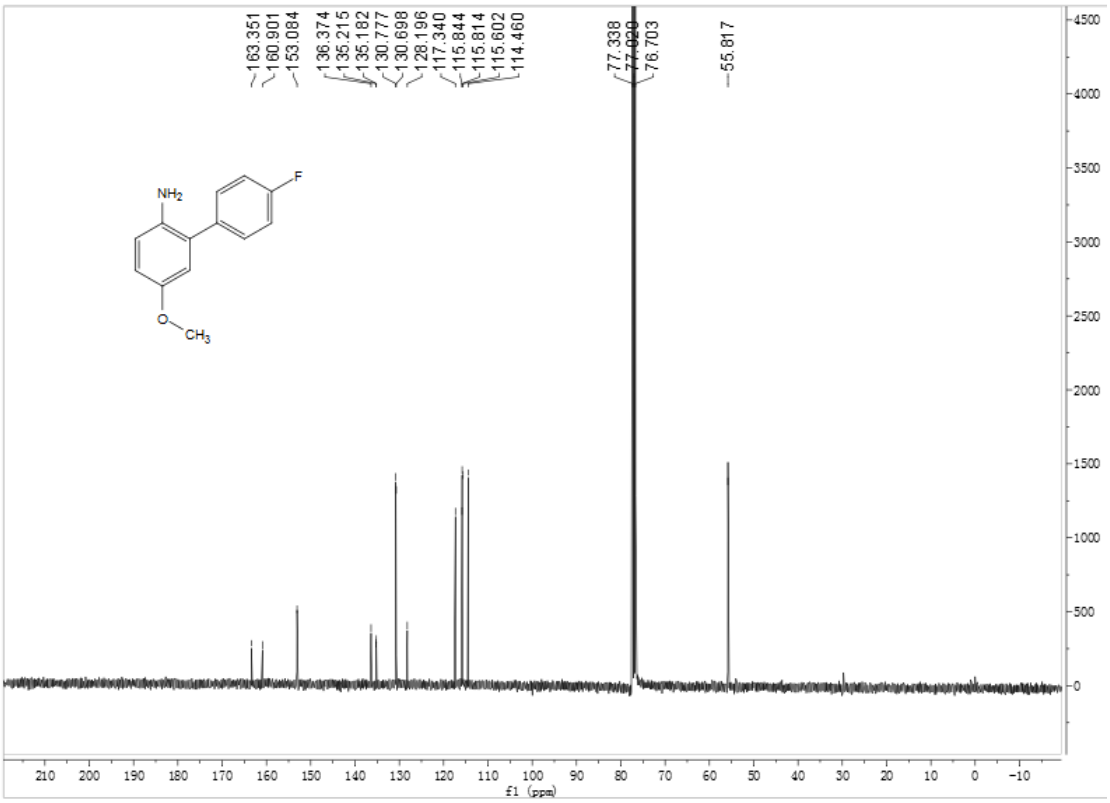
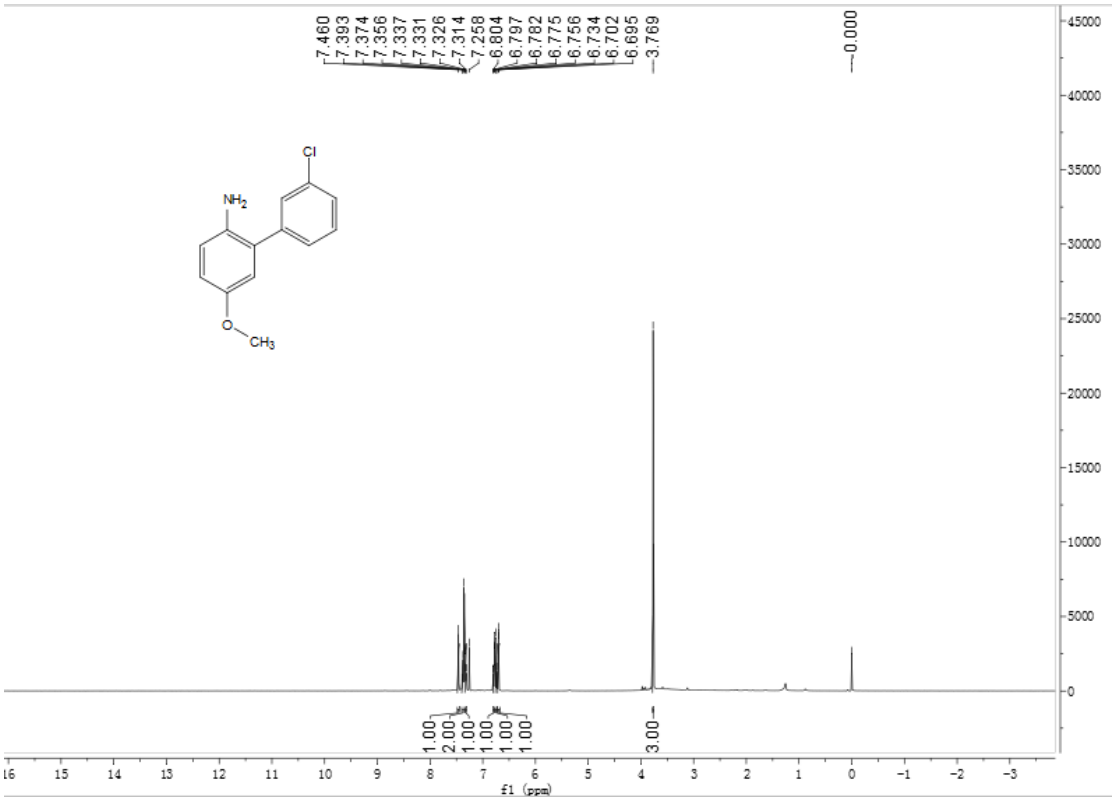
138.241
136.464
131.917
130.745
127.690
121.398
117.318
115.563
114.707
77.318
77.000
76.683
55.801
NH2
Br
O
CH3
f1 (ppm)

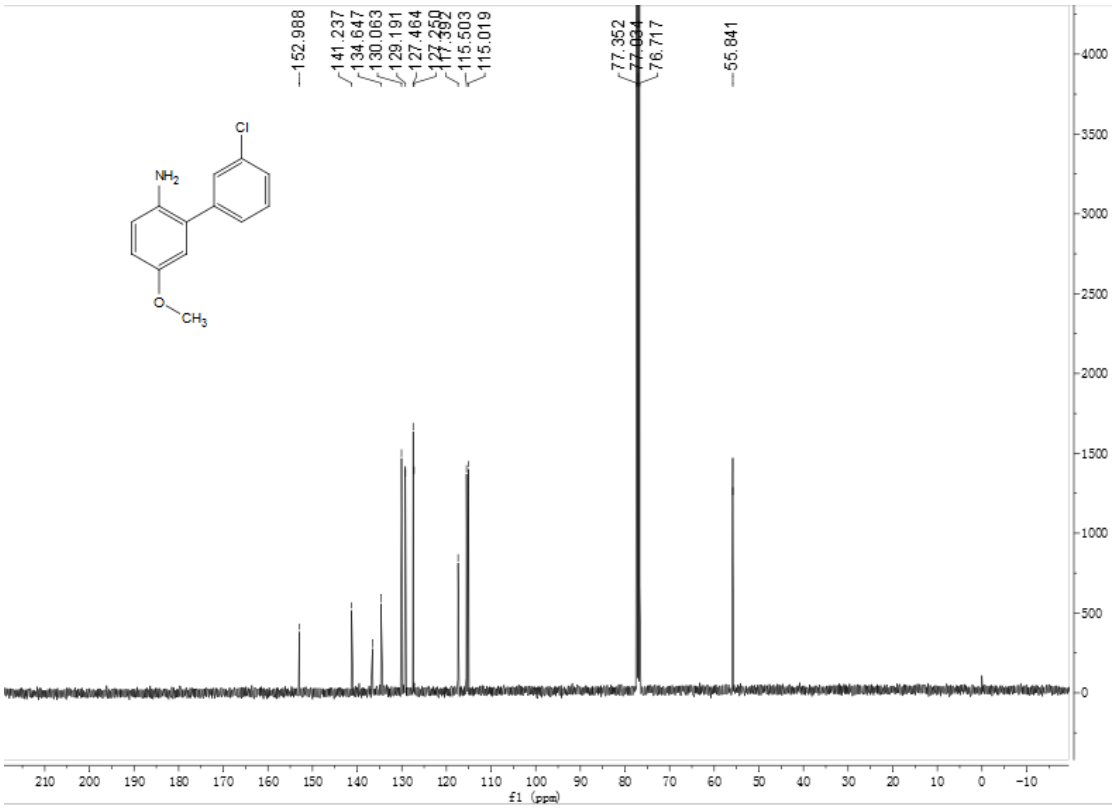
3s


7.440
7.422
7.408
7.258
7.146
7.125
7.105
6.756
6.700
3.769
0.000
NH2
F
O
CH3
2.00
2.00
2.00
1.00
3.00
f1 (ppm)

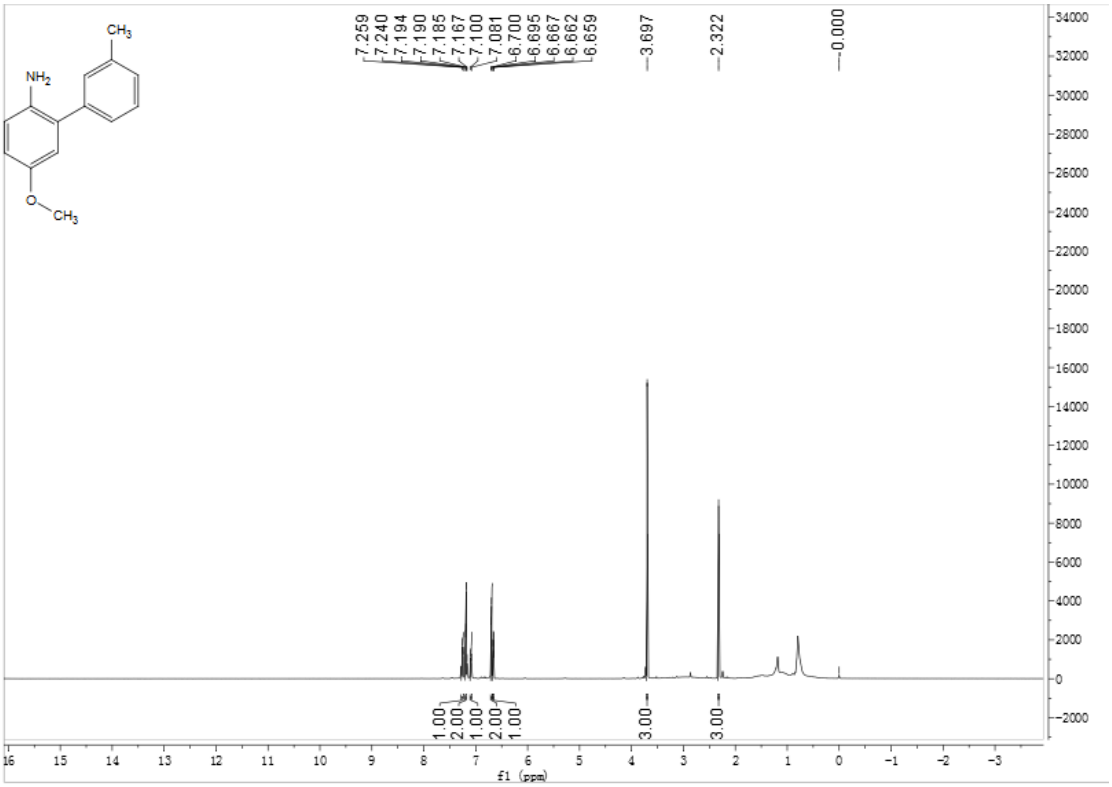

163.351
160.901
153.084
136.374
135.215
135.182
130.777
130.698
128.196
117.340
115.844
115.814
115.602
114.460
77.338
77.020
76.703
55.817
NH2
F
O
CH3
f1 (ppm)

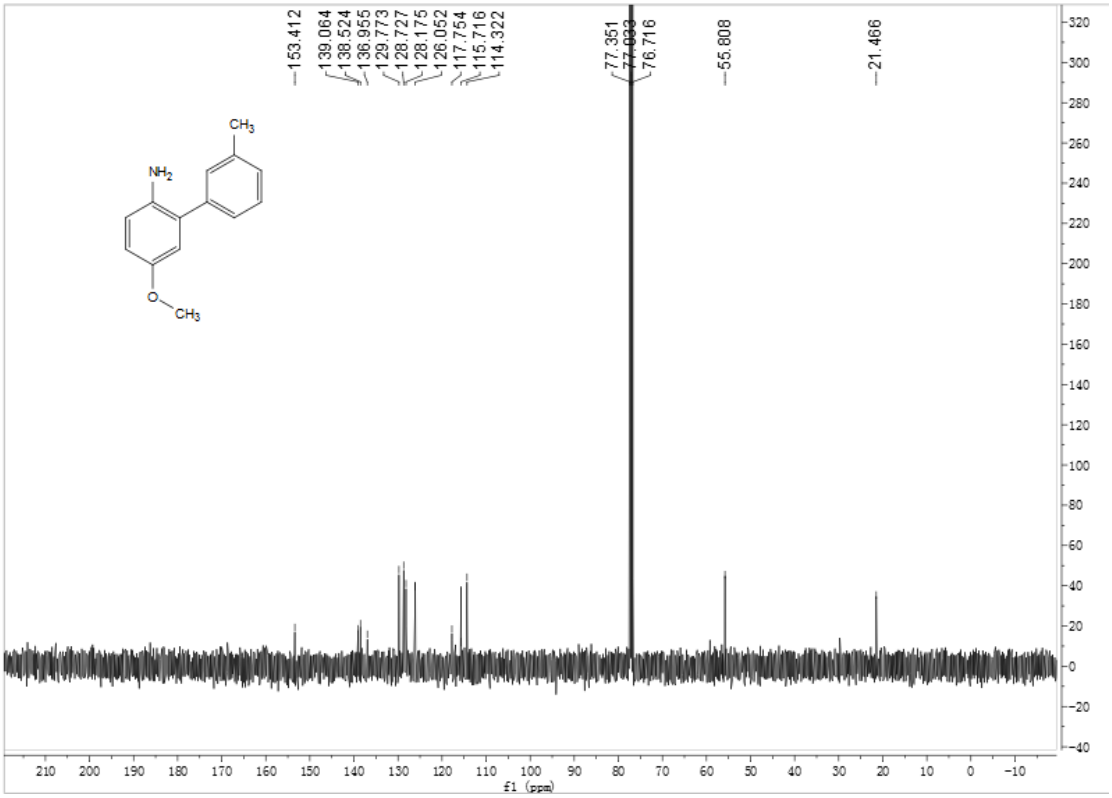
3v


7.460
7.393
7.374
7.356
7.337
7.331
7.326
7.314
7.258
6.804
6.797
6.782
6.775
6.756
6.734
6.702
6.695
3.769
0.000
Cl
NH2
O
CH3
1.00
2.00
1.00
1.00
1.00
3.00
f1 (ppm)


152.988
141.237
134.647
130.063
129.191
127.464
115.503
115.019
77.352
76.717
55.841
Cl
NH2
O
CH3
f1 (ppm)

3w


7.259
7.240
7.194
7.190
7.185
7.167
7.100
7.081
6.700
6.695
6.667
6.662
6.659
3.697
2.322
0.000
1.00
2.00
1.00
2.00
1.00
3.00
3.00
f1 (ppm)


153.412
139.064
138.524
136.955
129.773
128.727
128.175
126.052
117.754
115.716
114.322
77.351
77.033
76.716
55.808
21.466
f1 (ppm)