Supporting Information

Direct arylation of unactivated benzene with aryl acyl peroxides toward biaryls

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1. General experimental details

General Information: All chemicals were used as received without further purification unless stated otherwise. NMR spectra were recorded at ambient temperature on a 400 MHz NMR spectrometer. Chemical shifts (δ) are given in ppm relative to TMS, the coupling constants *J* are given in Hz.

Experimental procedure for the procedure for direct arylation of unactivated benzene with aryl acyl peroxides toward biaryls. Under air, the mixture of aryl acyl peroxides **1** (0.2 mmol) and PhH (1 mL) were added into the sealed tube. The reaction mixture was vigorously stirred at 100 ^{o}C for 12 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on silica gel to give the products.

Take 3aa for example for yield calculation. 0.2 mmol of 4-chlorobenzoic peroxyanhydride was divided into two parts: 0.1 mmol of 4-chlorobenzoic peroxyanhydride was served as aryl radical source to participate the arylation, another 0.1 mmol of 4-chlorobenzoic peroxyanhydride served as oxidant. As 4-chlorobenzoic peroxyanhydride contains two aryl equivalents, thus, the yield calculated on 0.2 mmol scale.

$$\text{Yied of 3aa} = \frac{32.3\ \text{mg}}{188 \times 0.2} \times 100\% = 86\%$$

2. Mechanism Studies

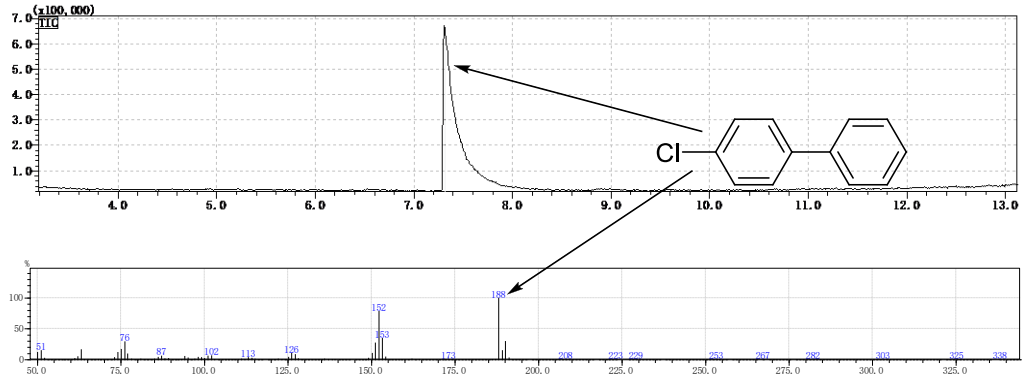
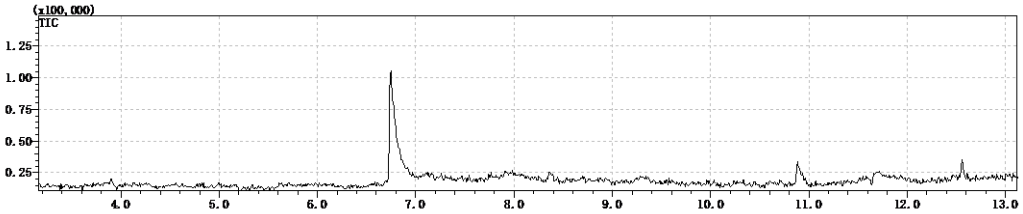


Figure S1 GC-MS spectra of the **3aa**

Standard Procedure + BHT (1.0 equiv)



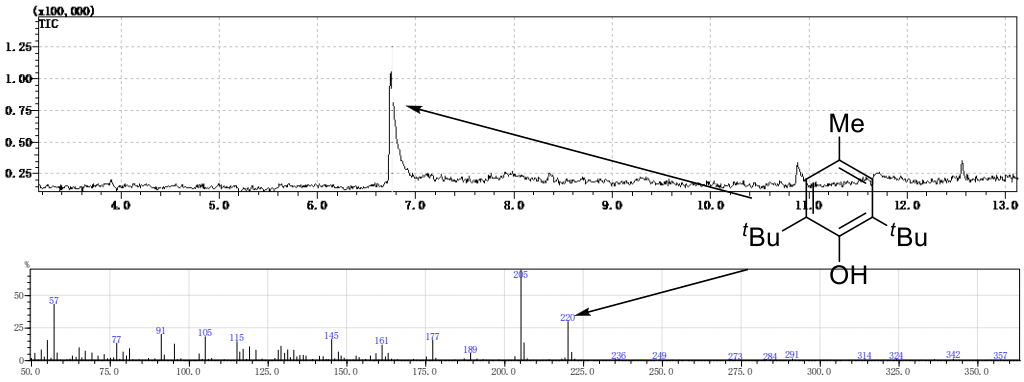
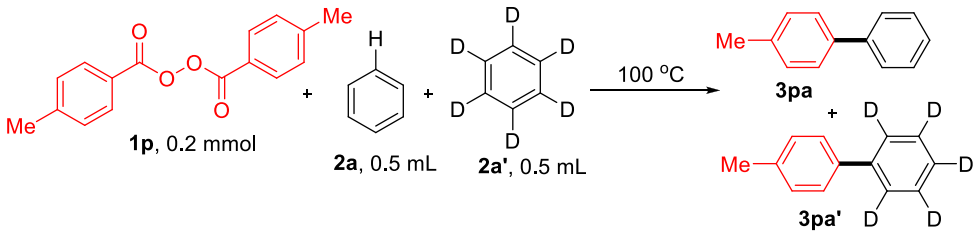
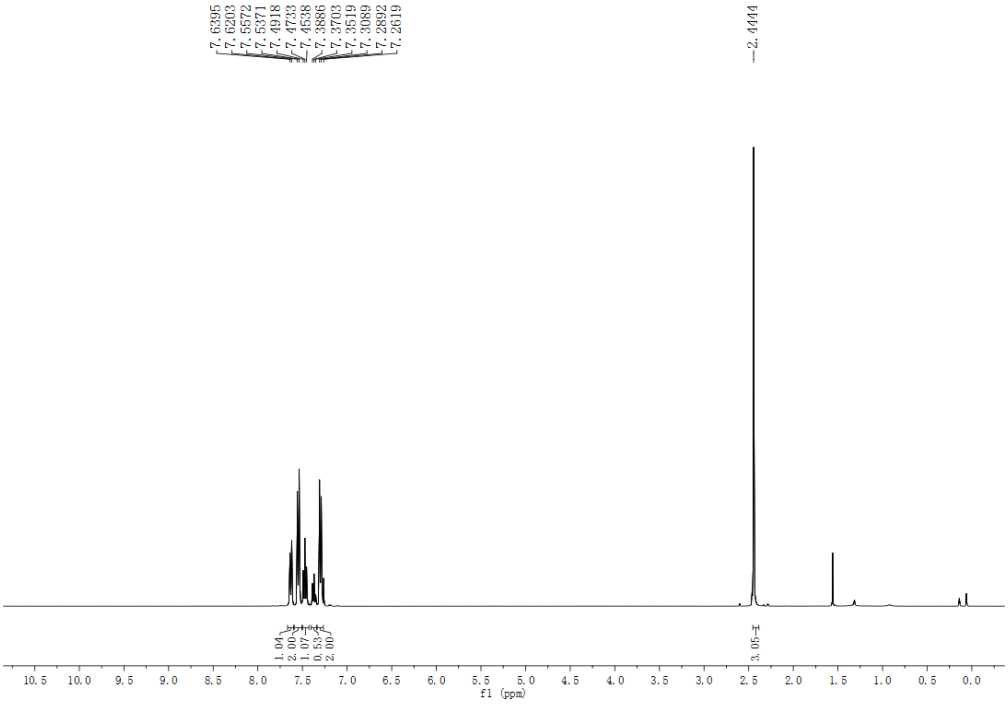


Figure S2 GC-MS spectra of adding BHT

Kinetic isotope effect experiments

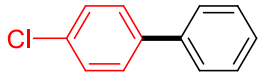


To a sealed tube, the mixture of **1p** (0.2 mmol), benzene-H_6 (0.5 mL) and benzene-D_6 (0.5mL) were added into the flask. The reaction mixture was vigorously stirred at 100 ^{o}C for 12 h. After the completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on silica gel to afford the products **3pa** and **3pa'**. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63 (d, *J* = 7.7 Hz, 1.04H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1.07H), 7.37 (t, *J* = 7.3 Hz, 0.53H), 7.29 (d, *J* = 7.9 Hz, 2H), 2.44 (s, 3H).



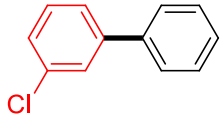
3. Characterization data of the products

4-chloro-1,1'-biphenyl (3aa)[1]



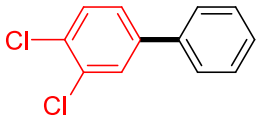
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58-7.51 (m, 4H), 7.48-7.35 (m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.0, 139.7, 133.4, 128.95, 128.93, 128.4, 127.6, 127.0.

3-chloro-1,1'-biphenyl (3ba)[1]



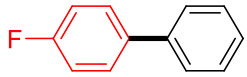
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61-7.58 (m, 3H), 7.50-7.46 (m, 3H), 7.42-7.33 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.1, 139.9, 134.7, 130.0, 128.9, 127.9, 127.4, 127.3, 127.2, 125.4.

3,4-dichloro-1,1'-biphenyl (3ca)[2]



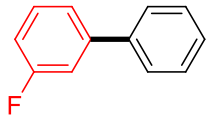
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (d, J = 2.1 Hz, 1H), 7.56-7.53 (m, 2H), 7.52-7.38 (m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.3, 138.8, 132.9, 131.5, 130.7, 129.1, 129.0, 128.2, 127.0, 126.4.

4-fluoro-1,1'-biphenyl (3da)[3]



^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59-7.556 (m, 4H), 7.47 (t, J = 7.3 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 7.16 (t, J = 8.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.5 (d, $J_{C\text{-}F}$ = 244.7 Hz), 140.3, 137.4 (d, $J_{C\text{-}F}$= 3.2 Hz), 128.9, 128.7 (d, $J_{C\text{-}F}$ = 7.9 Hz), 127.3, 127.1, 115.6 (d, $J_{C\text{-}F}$ = 21.3 Hz).

3-fluoro-1,1'-biphenyl (3ea)[4]



^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62-7.59 (m, 2H), 7.50-7.46 (m, 2H), 7.43-7.38 (m, 3H), 7.34-7.31 (m, 1H), 7.09-7.04 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.2 (d, $J_{C\text{-}F}$ = 243.9 Hz),

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[1] A. Kumar and B. Ali Shah, *Org. Lett.*, 2015, **17**, 5232.

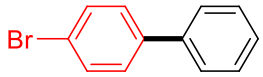
[2] F. Valle ́e, J. J. Mousseau and A. B. Charette, *J. Am. Chem. Soc.*, 2010, **132**, 1514.

[3] O. Y. Yuen, C. M. So, H. W. Man and F. Y. Kwong, *Chem. Eur. J.*, 2016, **22**, 6471.

[4] S. B. Blakey and D. W. C. MacMillan, *J. Am. Chem. Soc.*, 2003, **125**, 6046.

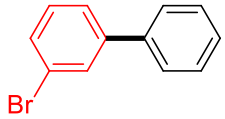
143.5 (d, $J_{C\text{-}F}$= 7.6 Hz), 140.0 (d, $J_{C\text{-}F}$ = 2.1 Hz), 130.3 (d, $J_{C\text{-}F}$ = 8.3 Hz), 128.9, 127.9, 127.1, 122.8 (d, $J_{C\text{-}F}$ = 2.7 Hz), 114.1 (d, $J_{C\text{-}F}$ = 1.6 Hz), 143.5 (d, $J_{C\text{-}F}$ = 2.4 Hz).

4-bromo-1,1'-biphenyl (3fa)[1]



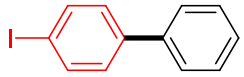
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62-7.59 (m, 4H), 7.51-7.47 (m, 4H), 7.44-7.39 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.2, 140.0, 131.9, 128.9, 128.8, 127.7, 127.0, 121.6.

3-bromo-1,1'-biphenyl (3ga)[1]



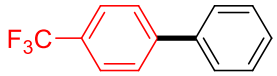
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.78 (t, *J* = 1.8 Hz, 1H), 7.60-7.57 (m, 2H), 7.55-7.46 (m, 4H), 7.43-7.39 (m, 1H), 7.33 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.3, 139.6, 130.2, 130.2, 130.1, 128.9, 127.8, 127.1, 125.7, 122.9.

4-iodo-1,1'-biphenyl (3ha)[5]



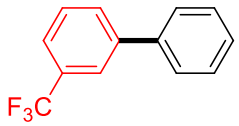
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79-7.76 (m, 2H), 7.58-7.55 (m, 2H), 7.48-7.44 (m, 2H), 7.42-7.33 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.7, 140.1, 137.9, 129.0, 128.9, 127.7, 126.9, 93.1.

4-(trifluoromethyl)-1,1'-biphenyl (3ia)[3]



^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74-7.69 (m, 4H), 7.62 (d, *J* = 7.5 Hz, 2H), 7.52-7.48 (m, 2H), 7.45-7.41 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.8, 139.8, 129.3 (q, $J_{C\text{-}F}$ = 32.2 Hz), 129.0, 128.2, 127.4, 127.3, 125.7 (q, $J_{C\text{-}F}$ = 3.8 Hz), 124.3 (q, $J_{C\text{-}F}$ = 268.9 Hz).

3-(trifluoromethyl)-1,1'-biphenyl (3ja)[6]

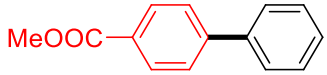


[5] A. Klapars and S. L. Buchwald, *J. Am. Chem. Soc.*, 2002, **124**, 14844.

[6] C.-L. Sun, H. Li, D.-G. Yu, M. Yu, X. Zhou, X.-Y. Lu, K. Huang, S.-F. Zheng, B.-J. Li and Z.-J. Shi, *Nature Chem.*, 2010, **2**, 1044.

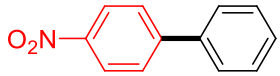
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.65-7.55 (m, 4H), 7.50 (d, *J* = 7.2 Hz, 2H), 7.43 (d, *J* = 7.2 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.1, 139.8, 131.2 (q, $J_{C\text{-}F}$ = 32.9 Hz), 130.5, 130.4, 129.3, 129.0, 128.1, 127.2, 124.3 (q, $J_{C\text{-}F}$ = 270.6 Hz), 123.9 (q, $J_{C\text{-}F}$ = 3.8 Hz).

methyl [1,1'-biphenyl]-4-carboxylate (3ka)[3]



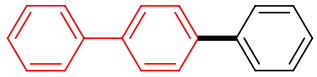
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, *J* = 8.5 Hz, 2H), 7.68-7.62 (m, 4H), 7.47 (t, *J* = 7.1 Hz, 2H), 7.40 (t, *J* = 7.2 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.0, 145.7, 140.0, 130.1, 128.97, 128.91, 128.2, 127.3, 127.1, 52.2.

4-nitro-1,1'-biphenyl (3la)[7]



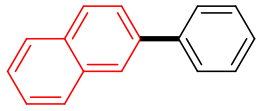
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.29 (d, *J* = 8.8 Hz, 2H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.64-7.62 (m, 2H), 7.53-7.42 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.6, 147.0, 138.8, 129.2, 128.9, 127.8, 127.4, 124.1.

***p*-terphenyl (3ma)**[6]



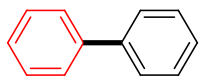
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70-7.65 (m, 8H), 7.50-7.46 (m, 4H), 7.38 (t, *J* = 7.3 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.7, 140.2, 128.8, 127.5, 127.4, 127.1.

2-phenylnaphthalene (3na)[3]



^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.08 (s, 1H), 7.95-7.88 (m, 3H), 7.79-7.74 (m, 3H), 7.55-7.48 (m, 4H), 7.40 (d, *J* = 7.4 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.2, 138.6, 133.7, 132.6, 128.9, 128.5, 128.2, 127.7, 127.5, 127.4, 126.3, 125.9, 125.8, 125.6.

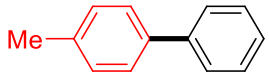
1,1'-biphenyl (3oa)[1]



[7] J.-H. Li, W.-J. Liu and Y.-X. Xie, *J. Org. Chem.*, 2005, **70**, 5409.

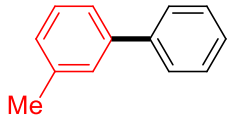
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.64 (d, *J* = 7.7 Hz, 4H), 7.48 (t, *J* = 7.4 Hz, 4H), 7.39 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.3, 128.8, 127.3, 127.2.

4-methyl-1,1'-biphenyl (3pa) [3]



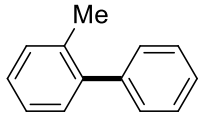
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65 (d, *J* = 7.7 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.2, 138.4, 137.0, 129.5, 128.7, 127.0, 126.9, 21.1.

3-methyl-1,1'-biphenyl (3qa)[3]



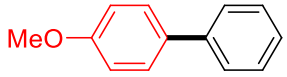
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62 (d, *J* = 7.4 Hz, 2H), 7.48-7.42 (m, 4H), 7.37 (t, *J* = 7.3 Hz, 2H), 7.20 (d, *J* = 7.4 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.4, 141.3, 138.4, 128.8, 128.7, 128.1, 128.0, 127.24, 127.22, 124.3, 21.6.

2-methyl-1,1'-biphenyl (3ra)[3]



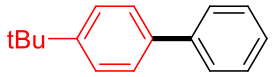
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49-7.44 (m, 2H), 7.40-7.36 (m, 3H), 7.33-7.28 (m, 4H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.0, 141.9, 135.4, 130.3, 129.8, 129.2, 128.1, 127.3, 126.8, 125.8, 20.5.

4-methoxy-1,1'-biphenyl (3sa)[3]



^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59-7.54 (m, 4H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.2, 140.8, 133.8, 128.8, 128.2, 126.8, 126.7, 114.2, 55.4.

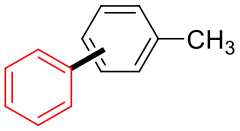
4-(*tert*-butyl)-1,1'-biphenyl (3ta)[8]



[8] W. Liu, H. Cao and A. Lei, *Angew. Chem. Int. Ed.*, 2010, **49**, 2004.

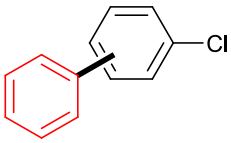
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.64 (d, *J* = 7.2 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 1.41 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.3, 141.1, 138.4, 128.7, 127.1, 127.0, 126.8, 125.9, 34.6, 31.4.

Mixture of 2-methylbiphenyl, 3-methylbiphenyl and 4-methylbiphenyl (3ob)[1]



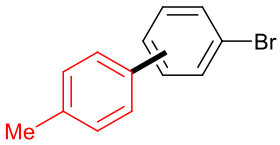
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62-7.59 (m, 1.02H), 7.52 (d, *J* = 8.1 Hz, 0.39H), 7.48-7.42 (m, 2.53H), 7.38-7.34 (m, 2.03H), 7.30-7.25 (m, 2.62H), 7.19 (d, *J* = 7.4 Hz, 0.43H), 2.45 (s, 0.96H), 2.42 (s, 0.6H), 2.30 (s, 1.44H).

Mixture of 2-chloro-1,1'-biphenyl, 3-chloro-1,1'-biphenyl and 4-chloro-1,1'-biphenyl (3oc)[1]



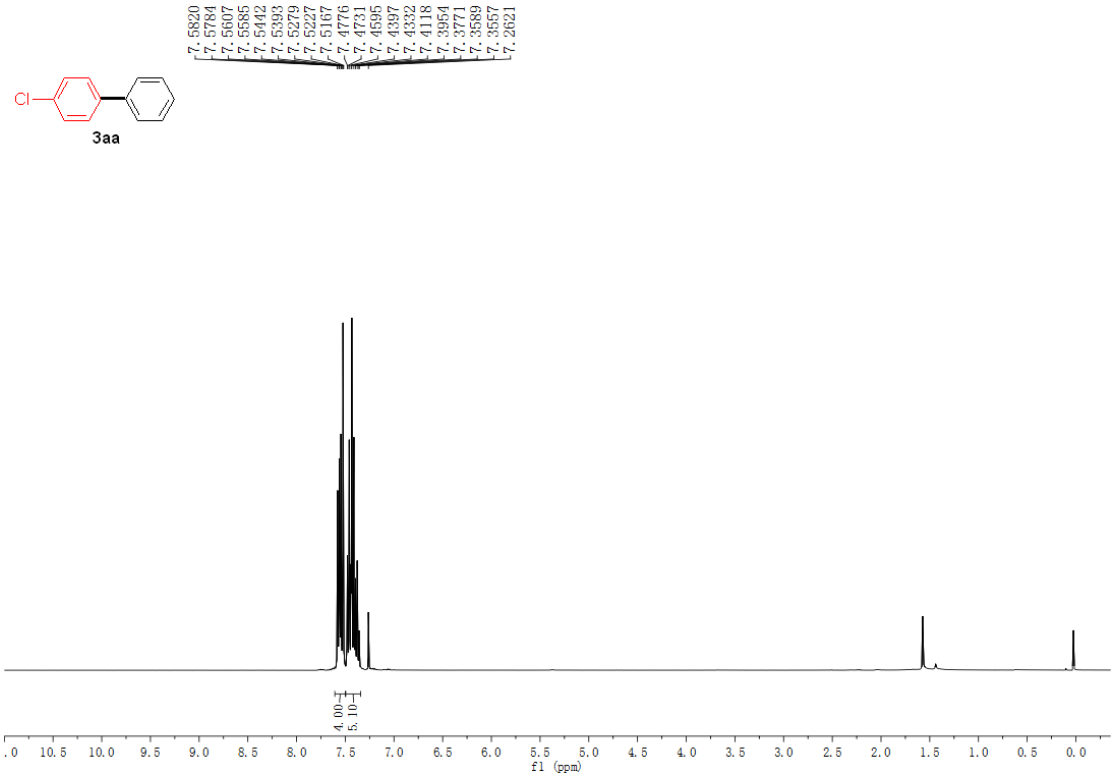
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61-7.28 (m, 9H).

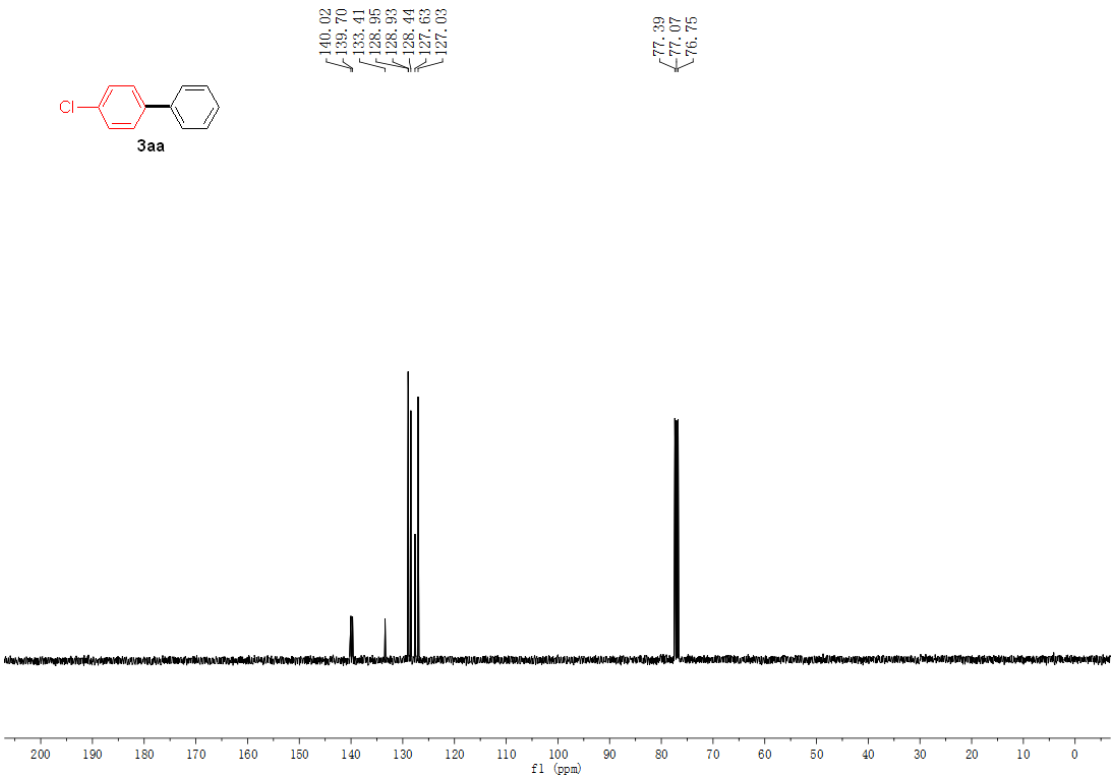
Mixture of 2-bromo-4'-methyl-1,1'-biphenyl, 3-bromo-4'-methyl-1,1'-biphenyl and 4-bromo-4'-methyl-1,1'-biphenyl (3pd)

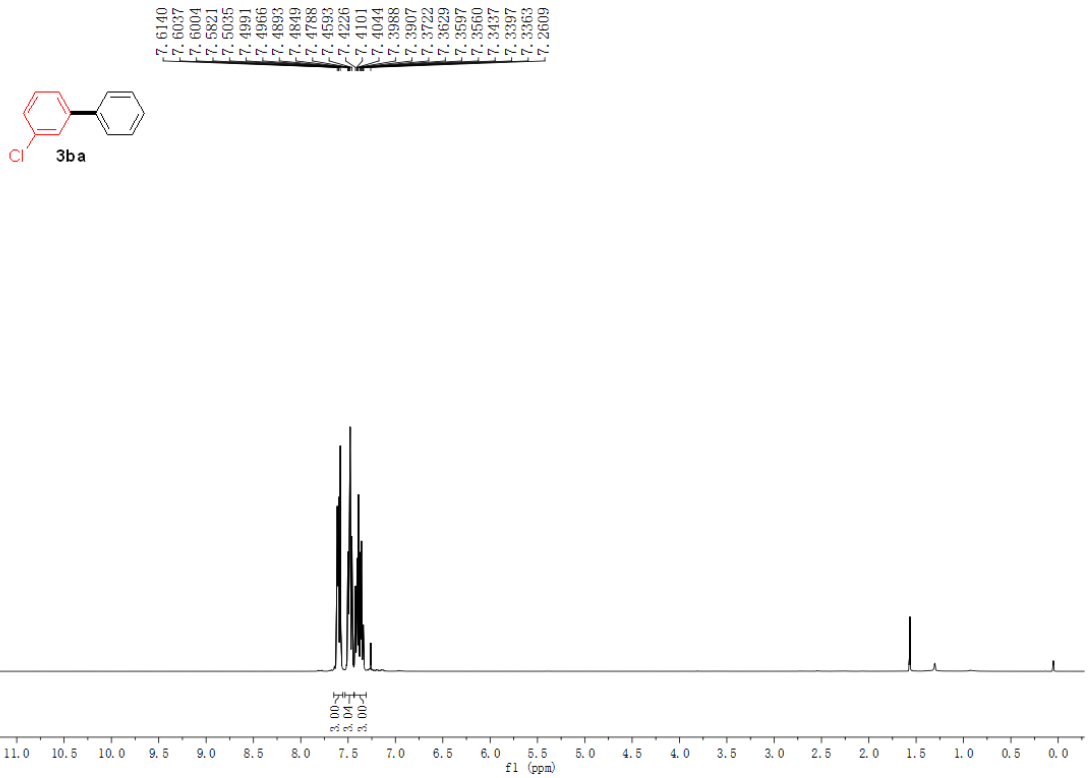


^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70-7.69 (m, 0.69H), 7.65-7.62 (m, 0.53H), 7.53-7.51 (m, 0.37H), 7.48-7.40 (m, 1.73H), 7.34-7.28 (m, 2.33H), 7.23-7.21 (m, 2.08H), 7.18-7.14 (m, 0.56H), 2.39-2.37 (t, 3H).

4. Copies of ^{1}H NMR and ^{13}C NMR spectra of the products



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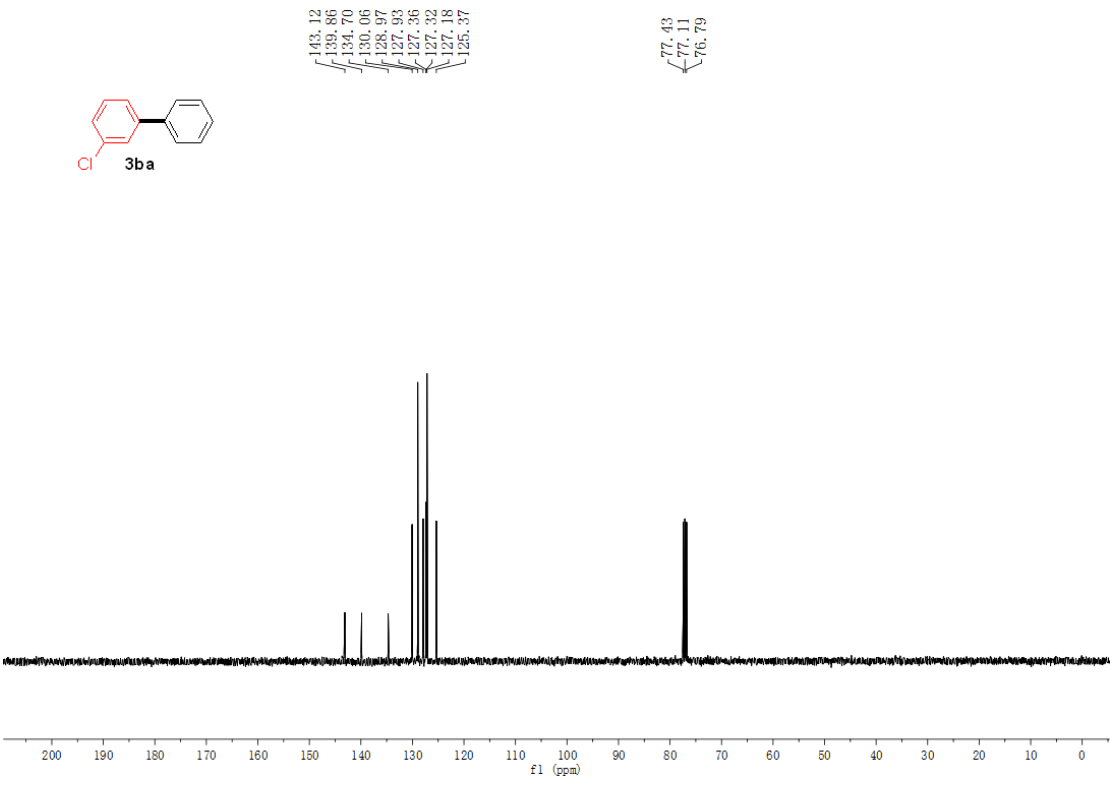
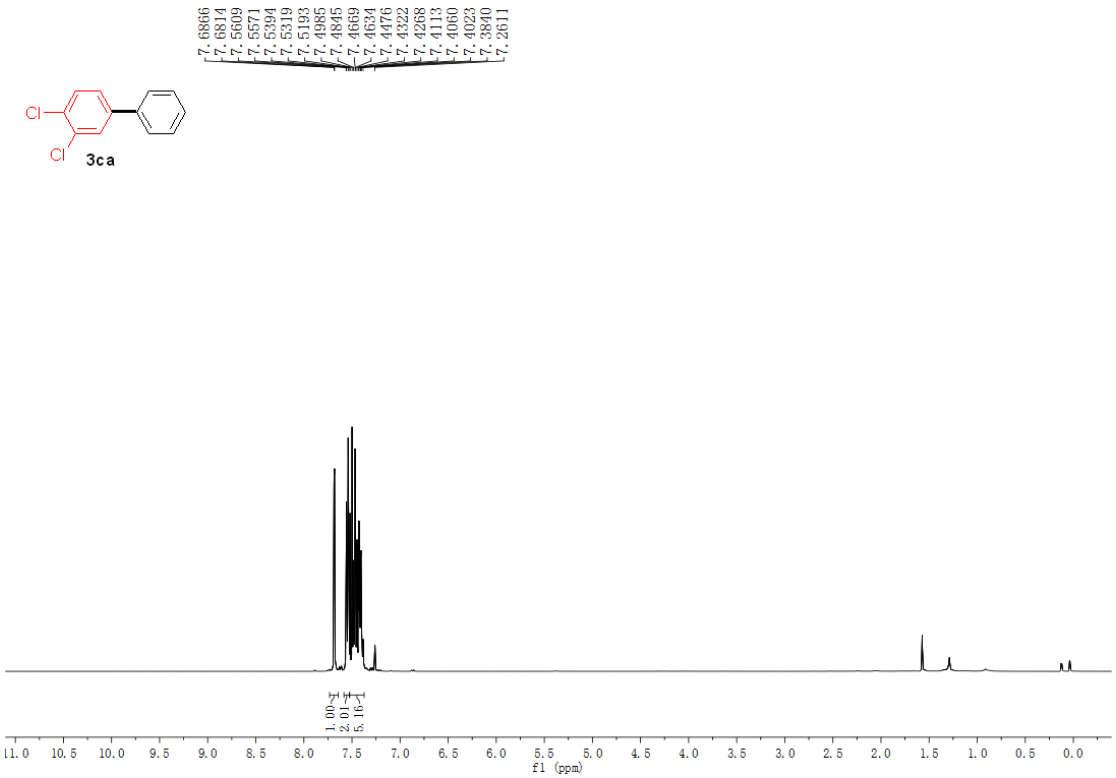
7.6037
7.6004
7.5821
7.5035
7.4991
7.4966
7.4893
7.4849
7.4788
7.4593
7.4226
7.4101
7.4044
7.3988
7.3907
7.3722
7.3629
7.3597
7.3560
7.3437
7.3397
7.3363
7.2609
Cl
3ba
3.00
3.04
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.12
139.86
134.70
130.06
128.97
127.93
127.36
127.32
127.18
125.37
77.43
77.11
76.79
Cl
3ba
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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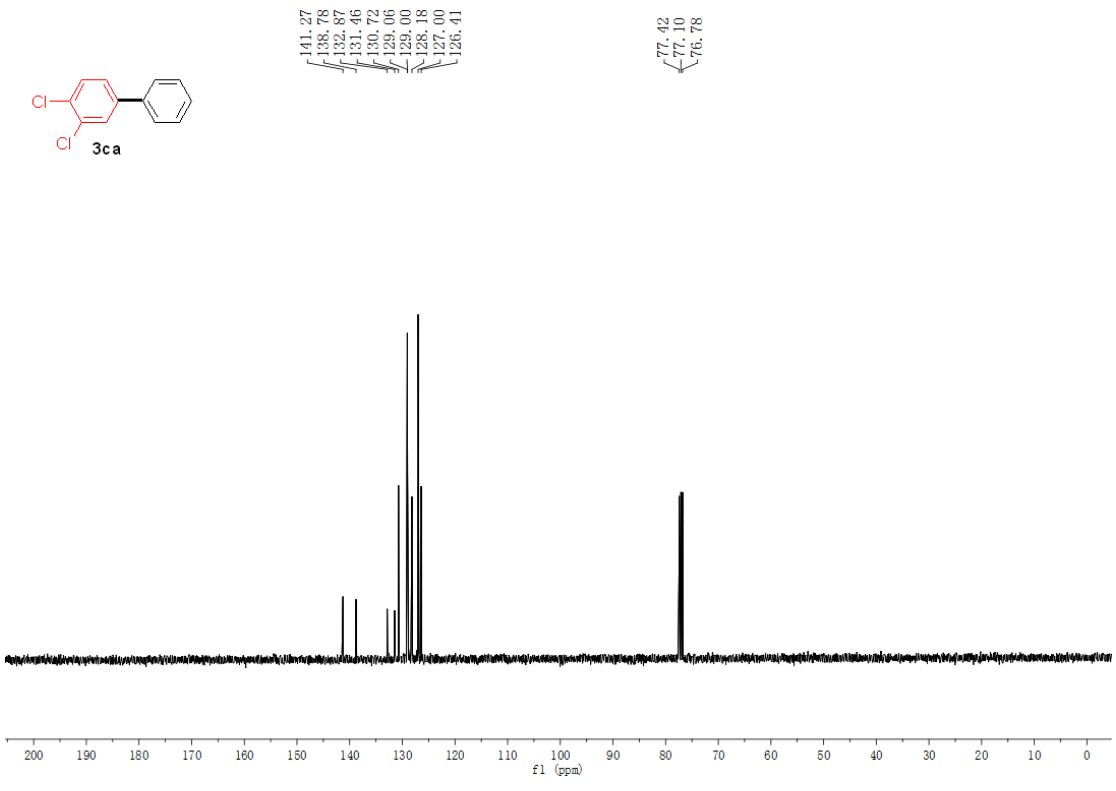
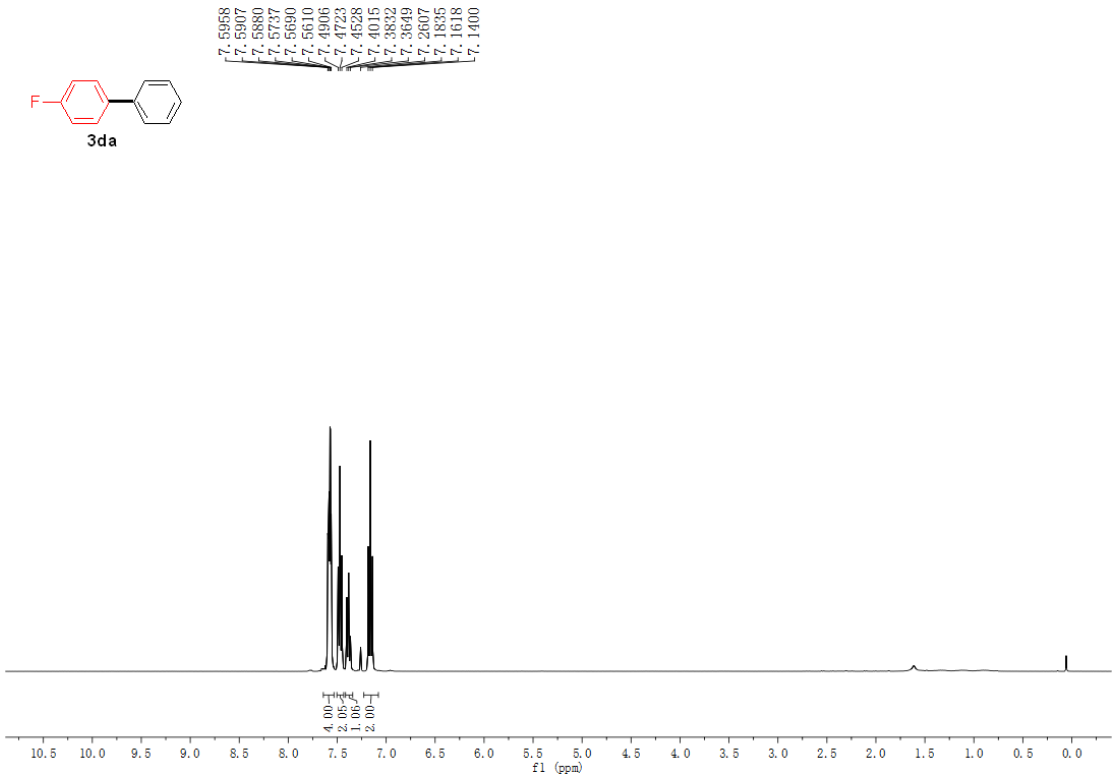
7.6814
7.5609
7.5571
7.5394
7.5319
7.5193
7.4985
7.4845
7.4669
7.4634
7.4476
7.4322
7.4268
7.4113
7.4060
7.4023
7.3840
7.2611
Cl
Cl
3ca
1.00
2.01
5.16
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


141.27
138.78
132.87
131.46
130.72
129.06
129.00
128.18
127.00
126.41
77.42
77.10
76.78
Cl
Cl
3ca
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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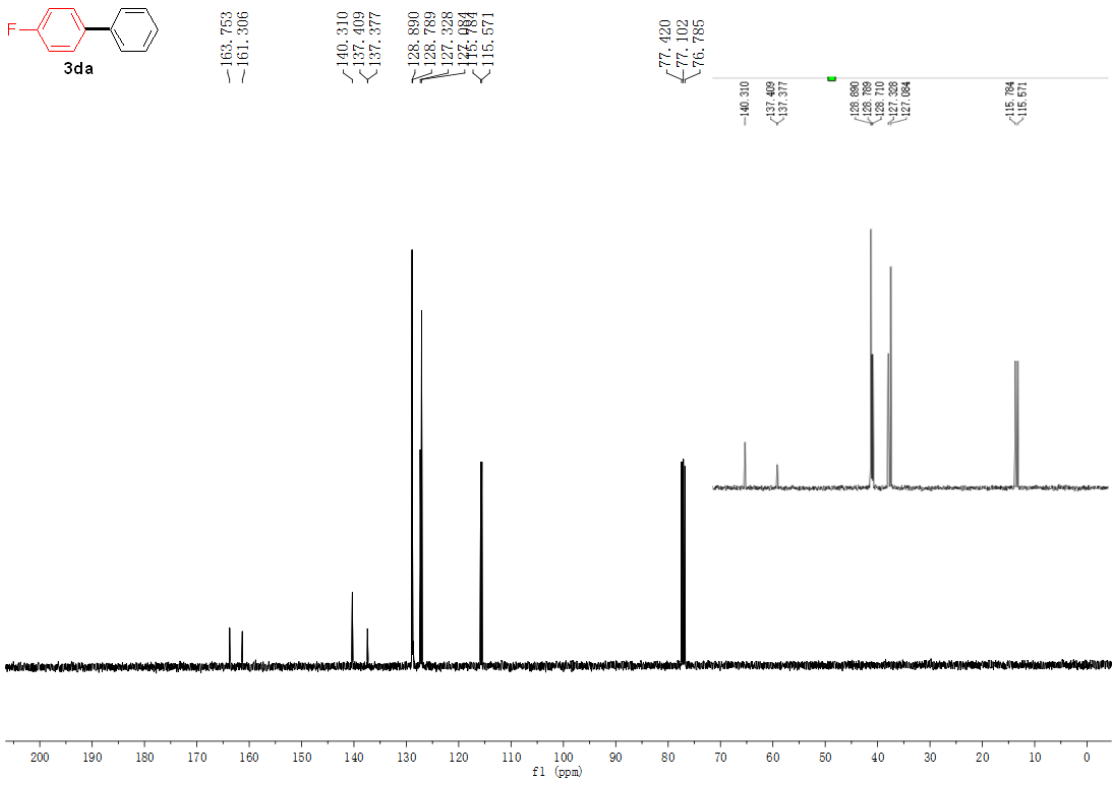
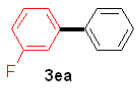
7.5907
7.5880
7.5737
7.5690
7.5610
7.4906
7.4723
7.4528
7.4015
7.3832
7.3649
7.2607
7.1835
7.1618
7.1400
F
3da
4.00
2.05
1.06
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


F
3da
163.753
161.306
140.310
137.409
137.377
128.890
128.789
127.328
127.084
115.784
115.571
77.420
77.102
76.785
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



3ea

7.6191
7.6155
7.6108
7.5976
7.4988
7.4809
7.4775
7.4615
7.4337
7.4140
7.4092
7.4045
7.3858
7.3449
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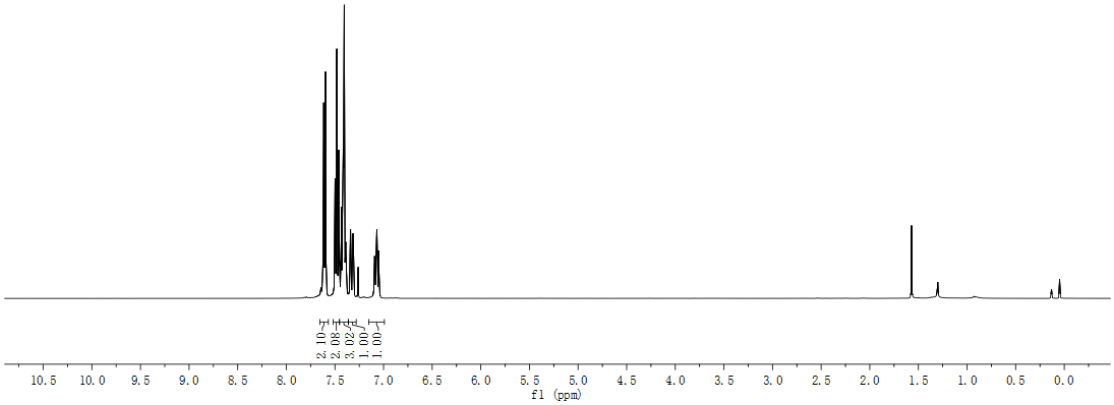
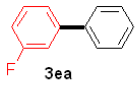
7.3189
7.3111
7.2608
7.0972
7.0922
7.0688
7.0528
7.0464





3ea

164.472
162.033
143.596
143.520
140.002
139.981
128.945
127.905
127.163
122.834
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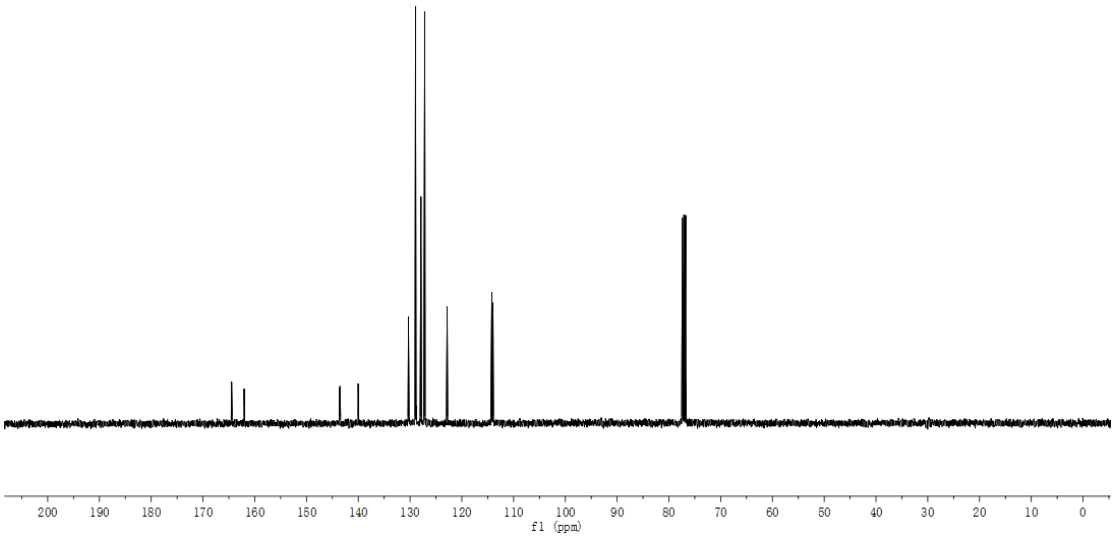
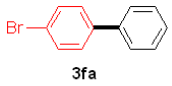
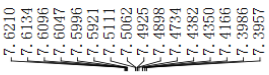
113.989
113.965
77.410
77.092
76.775




Br

3fa


7.6210
7.6134
7.6096
7.6047
7.5996
7.5921
7.5111
7.5062
7.4925
7.4898
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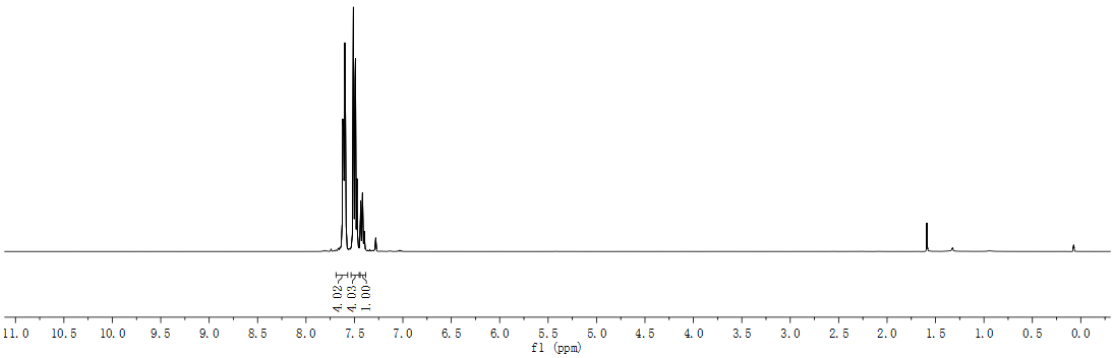
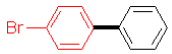
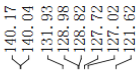
7.4382
7.4350
7.4166
7.3986
7.3957

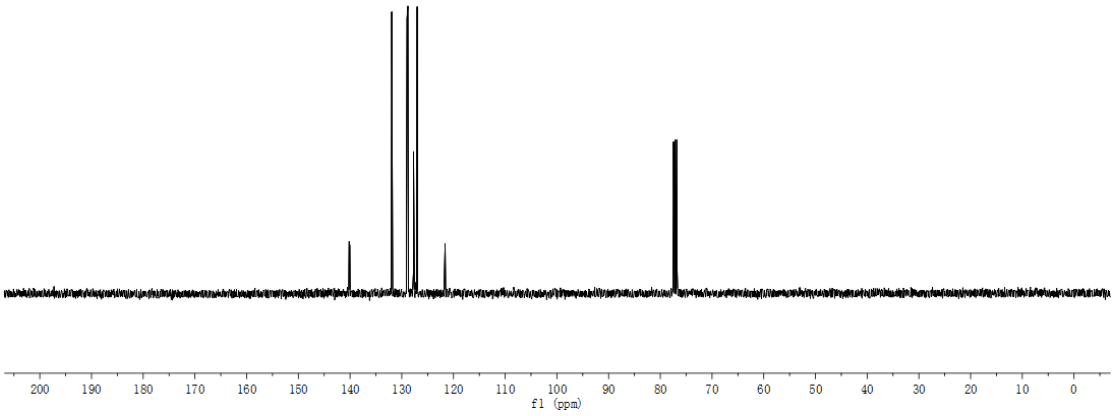

4.02
4.03
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Br

3fa


140.17
140.04
131.93
128.98
128.82
127.72
127.02
121.62


77.44
77.12
76.81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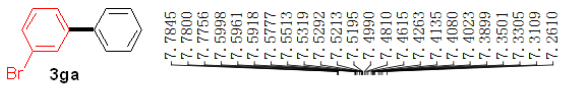
f1 (ppm)


Br
3ga
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7.7800
7.7756
7.5998
7.5961
7.5918
7.5777
7.5513
7.5319
7.5292
7.5213
7.5195
7.4990
7.4810
7.4615
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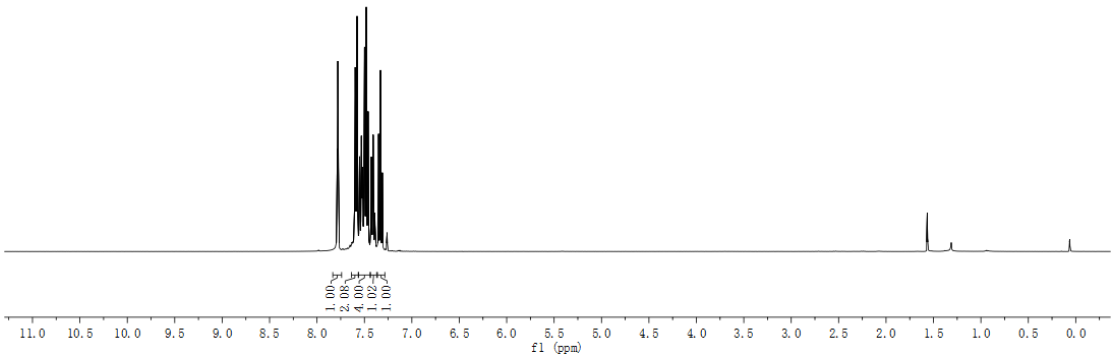
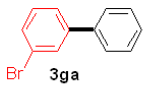
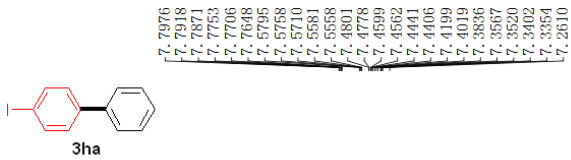
7.4135
7.4080
7.4023
7.3899
7.3501
7.3305
7.3109
7.2610


1.00
2.08
4.00
1.02
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Br
3ga

143.29
139.65
130.24
130.17
130.14
128.86
127.84
127.08
125.72
122.86
77.34
77.02
76.70
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5795
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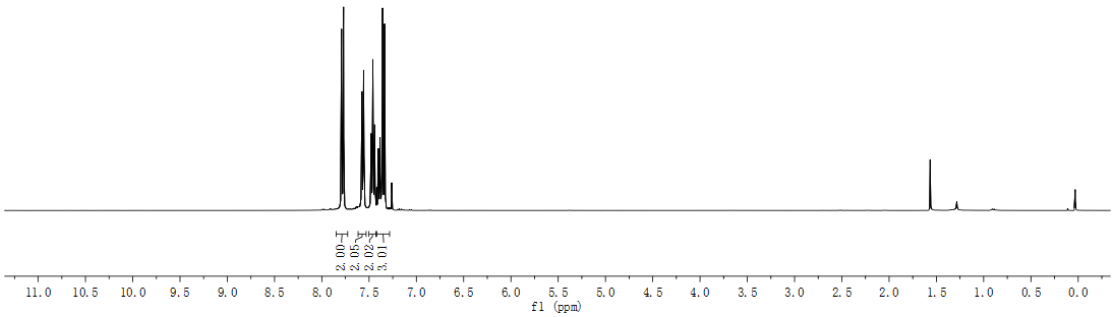
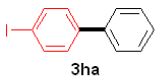
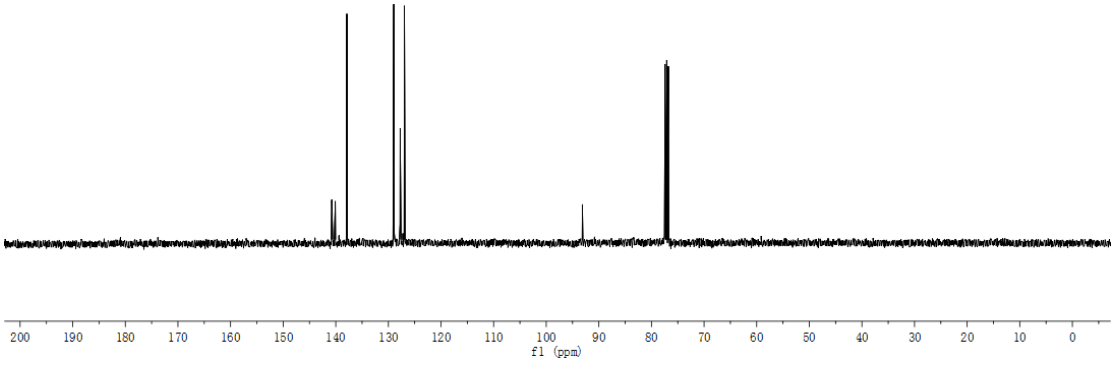
7.5710
7.5581
7.5558
7.4801
7.4778
7.4599
7.4562
7.4441
7.4406
7.4199
7.4019
7.3836
7.3567
7.3520
7.3402
7.3354
7.2610
3ha


2.00
2.05
2.02
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


3ha


140.75
140.09
137.89
129.07
128.97
127.76
126.95
93.13
77.42
77.10
76.78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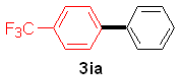
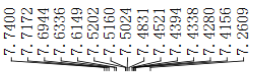
f1 (ppm)


F3C

3ia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7.6336
7.6149
7.5202
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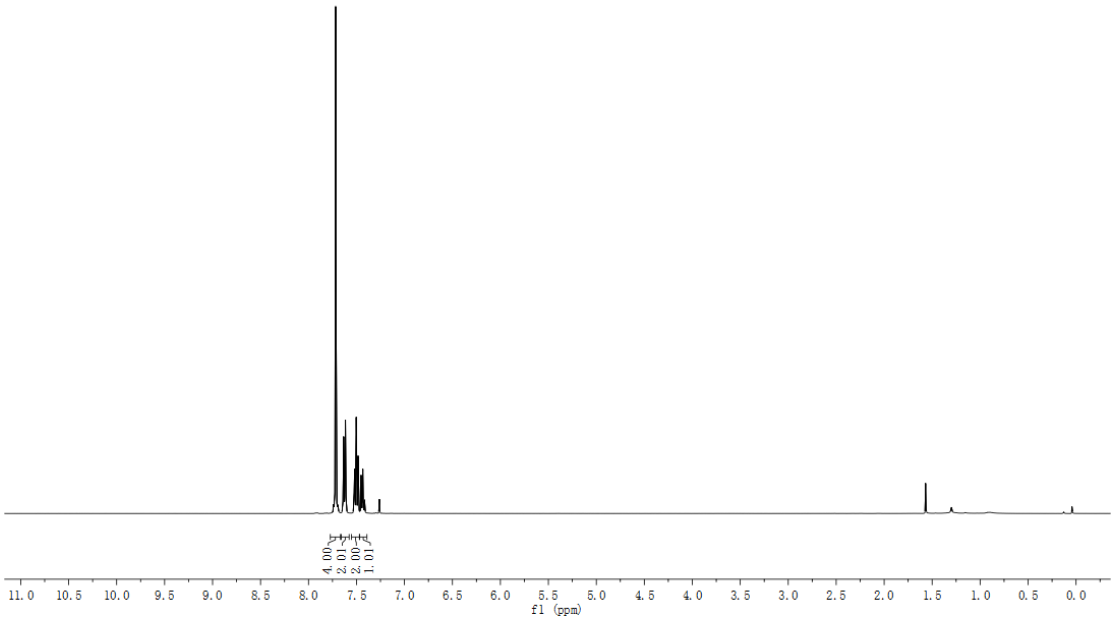
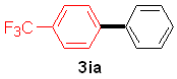
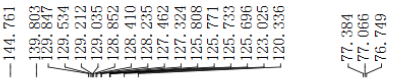
7.4521
7.4394
7.4338
7.4280
7.4156
7.2609


4.00
2.01
2.00
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


F3C

3ia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129.035
128.852
128.410
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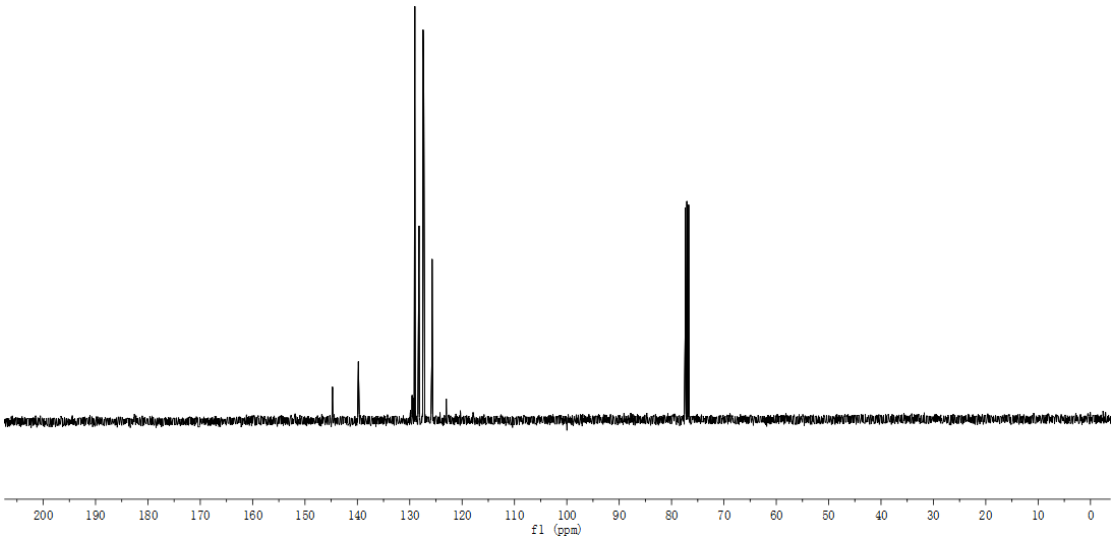
127.462
127.324
125.808
125.771
125.733
125.696
123.025
120.336
77.384
77.066
76.749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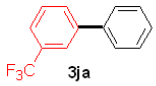
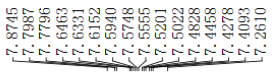
f1 (ppm)


3ja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7.7796
7.6463
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7.6152
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7.5555
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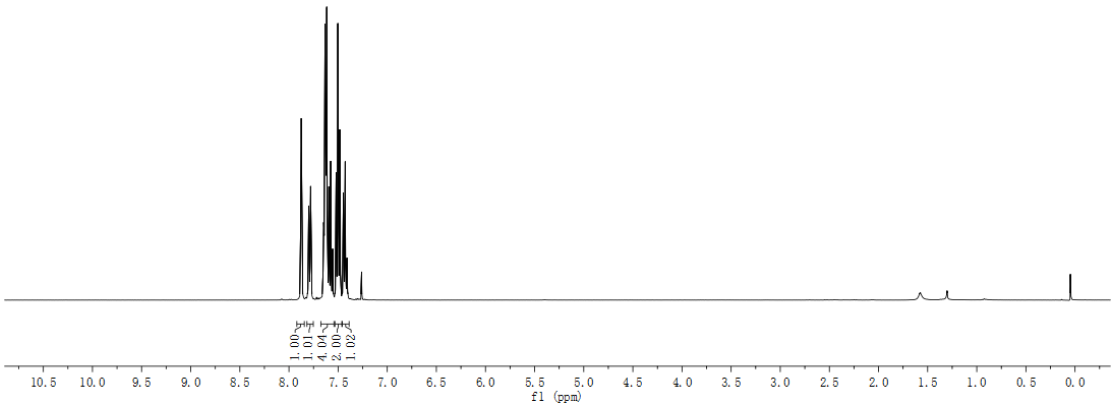
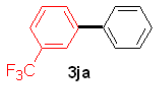
7.5022
7.4828
7.4458
7.4278
7.4093
7.2610


1.00
1.01
4.04
2.00
1.02
f1 (ppm)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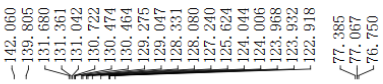
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125.624
124.044
124.006
123.968
123.932
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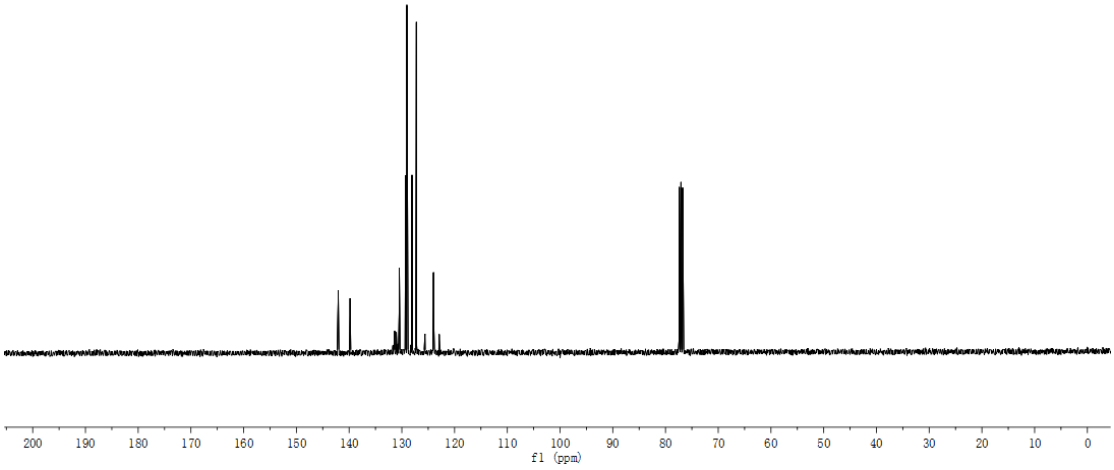
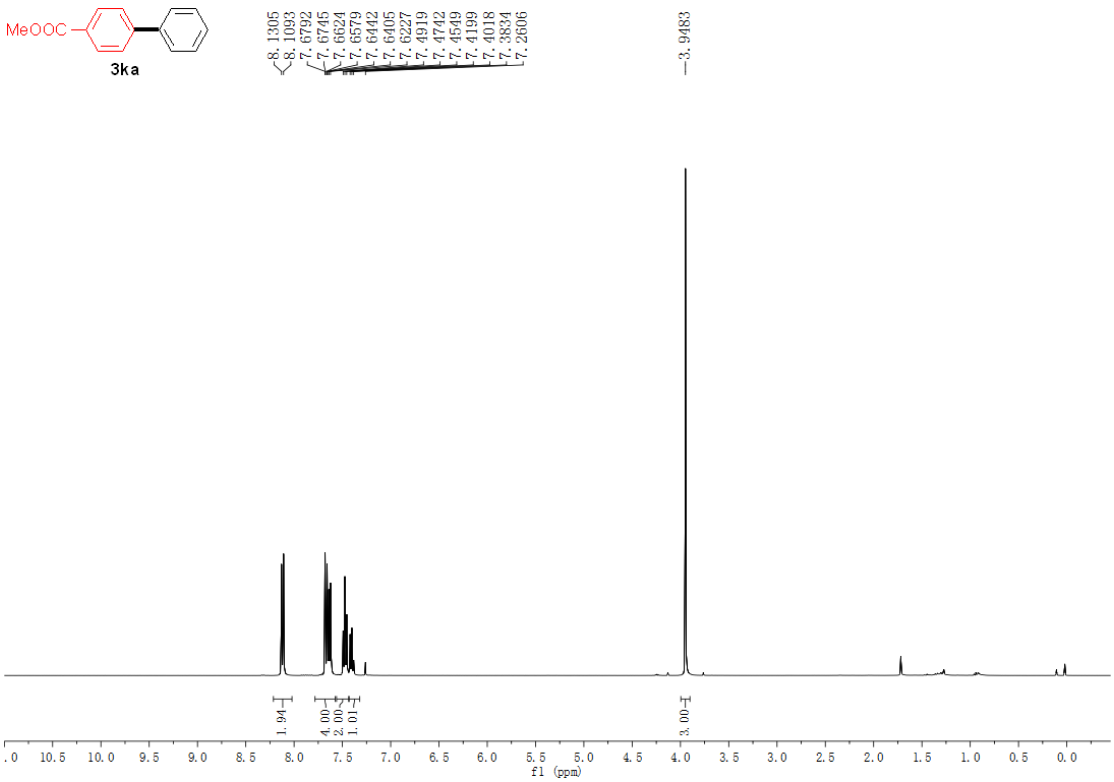
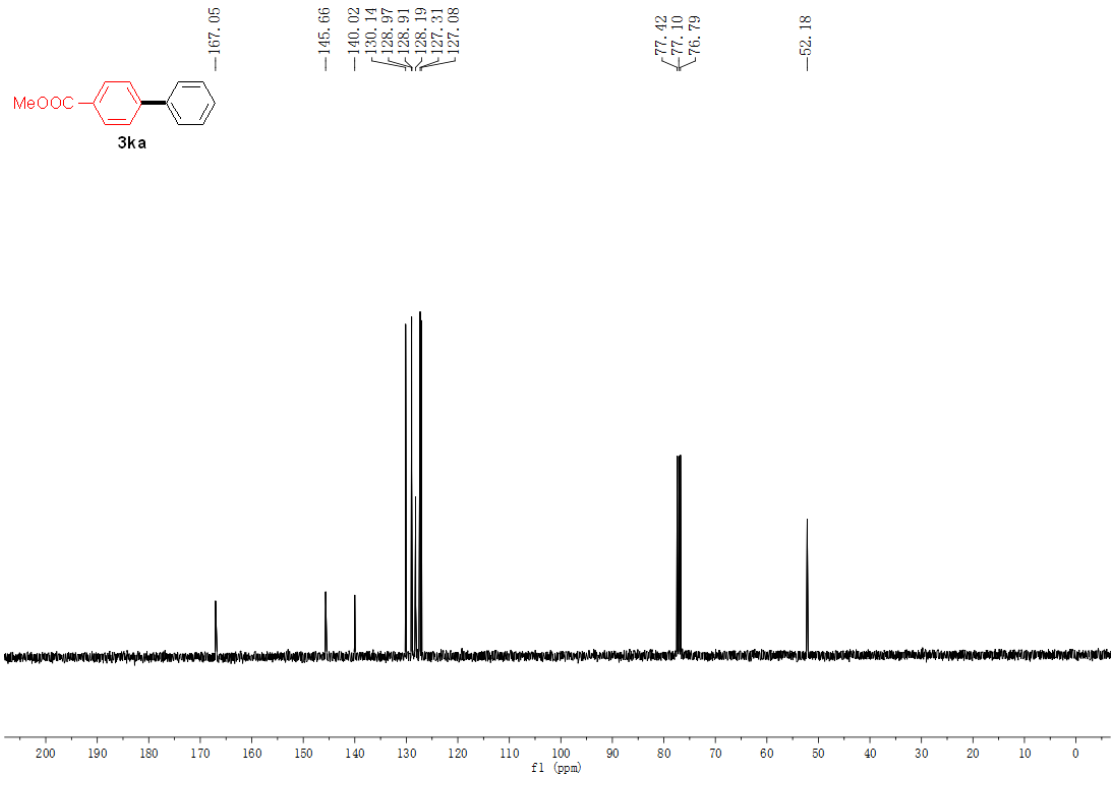
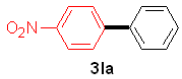
77.385
77.067
76.750

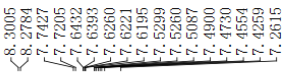

f1 (ppm)

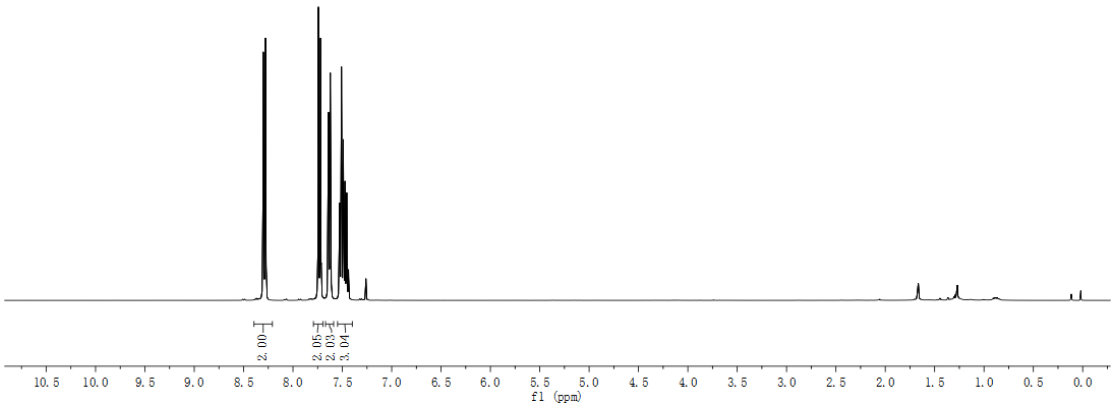

MeOOC
3ka
8.1305
8.1093
7.6792
7.6745
7.6624
7.6579
7.6442
7.6405
7.6227
7.4919
7.4742
7.4549
7.4199
7.4018
7.3834
7.2606
3.9483
1.94
4.00
2.00
1.01
3.00
f1 (ppm)

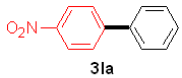

MeOOC
3ka
167.05
145.66
140.02
130.14
128.97
128.91
128.19
127.31
127.08
77.42
77.10
76.79
52.18
f1 (ppm)


O2N

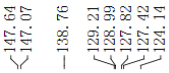
3la


8.3005
8.2784
7.7427
7.7205
7.6432
7.6393
7.6260
7.6221
7.6195
7.5299
7.5260
7.5087
7.4900
7.4730
7.4554
7.4259
7.2615

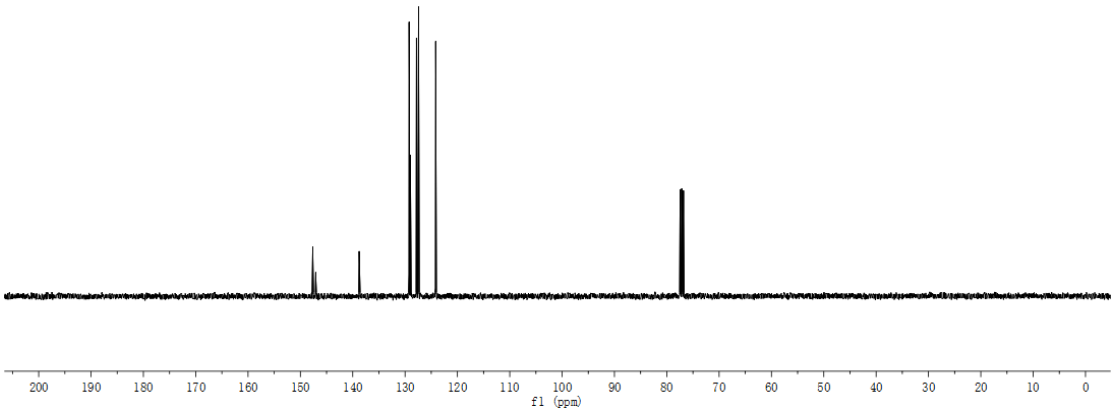

2.00
2.05
2.03
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

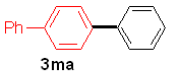

O2N

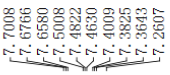
3la

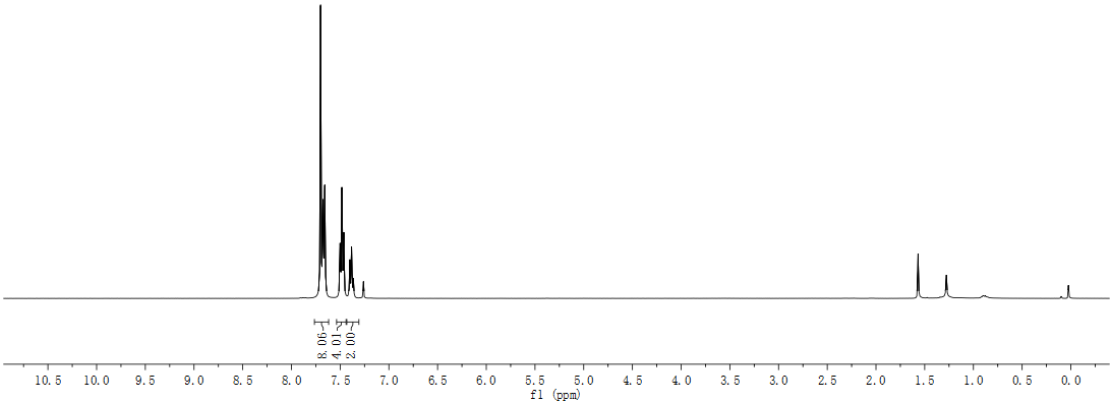

147.64
147.07
138.76
129.21
128.99
127.82
127.42
124.14

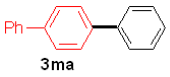

77.46
77.14
76.82

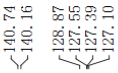

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Ph
3ma

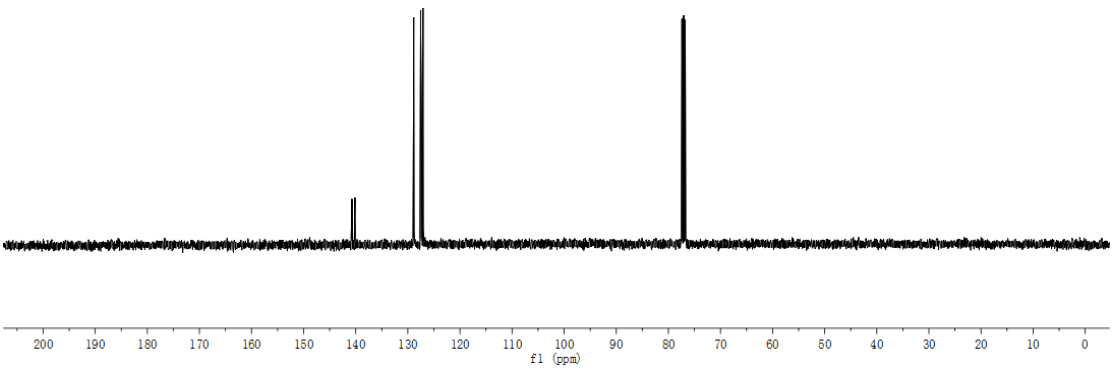

7.7008
7.6766
7.6580
7.5008
7.4822
7.4630
7.4009
7.3825
7.3643
7.2607

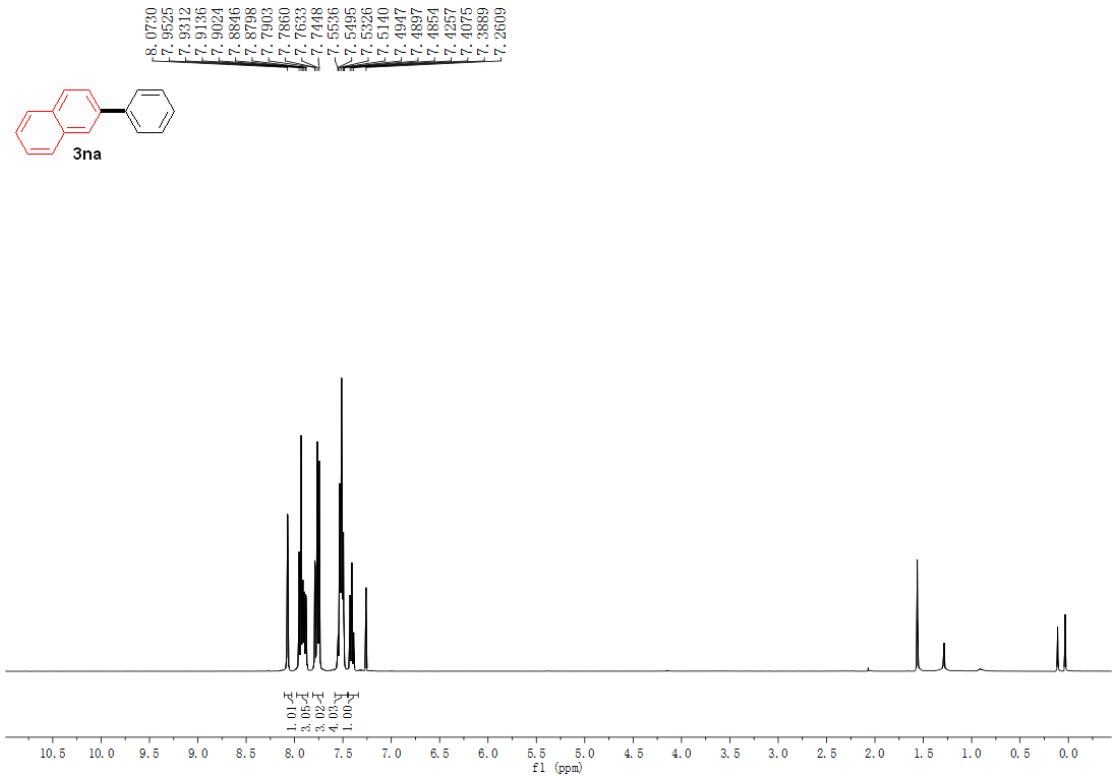

8.06
4.01
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

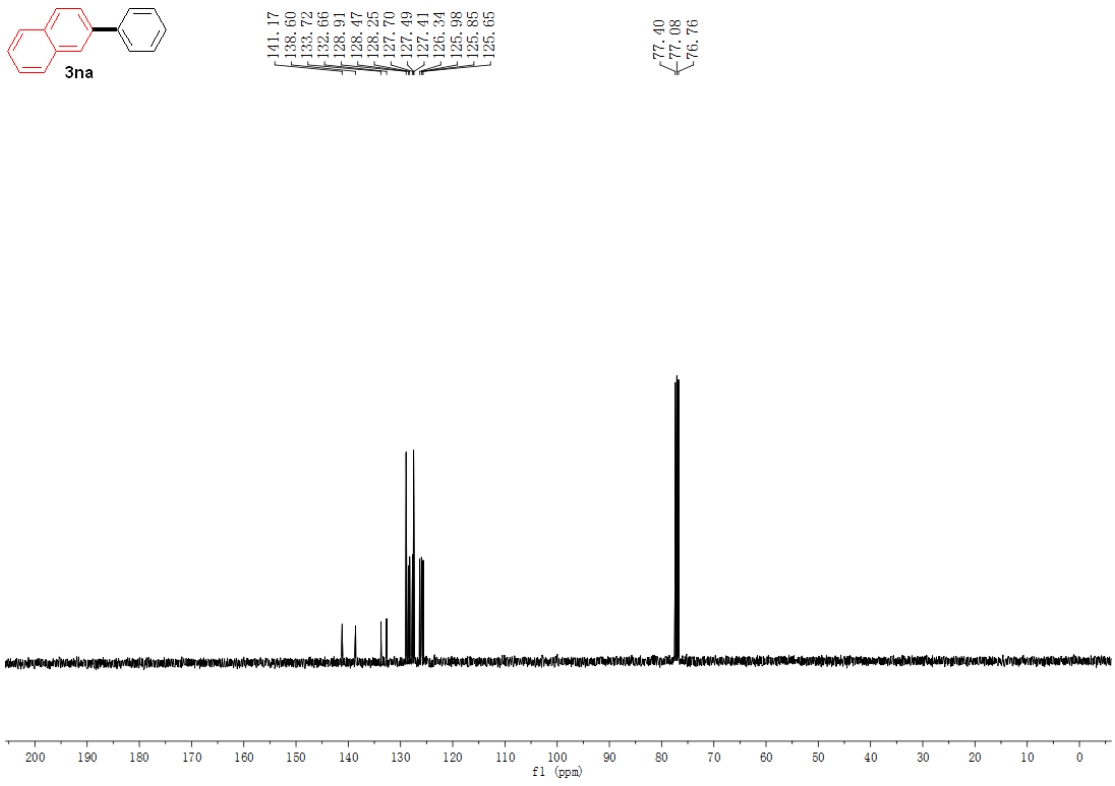

Ph
3ma

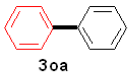

140.74
140.16
128.87
127.55
127.39
127.10

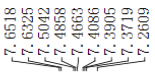

77.39
77.07
76.75

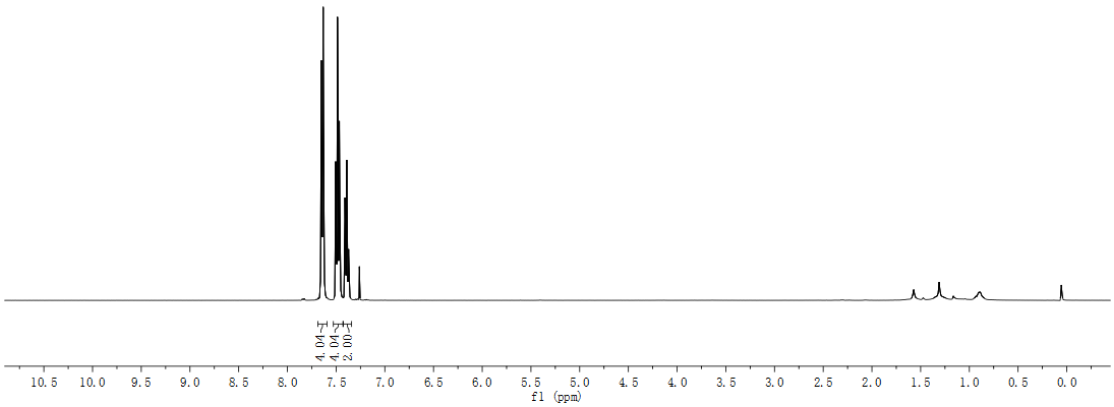

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

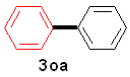

8.0730
7.9525
7.9312
7.9136
7.9024
7.8846
7.8798
7.7903
7.7860
7.7633
7.7448
7.5536
7.5495
7.5326
7.5140
7.4947
7.4897
7.4854
7.4257
7.4075
7.3889
7.2609
3na
1.01
3.05
3.02
4.03
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

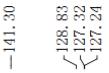

3na
141.17
138.60
133.72
132.66
128.91
128.47
128.25
127.70
127.49
127.41
126.34
125.98
125.85
125.65
77.40
77.08
76.76
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


3oa

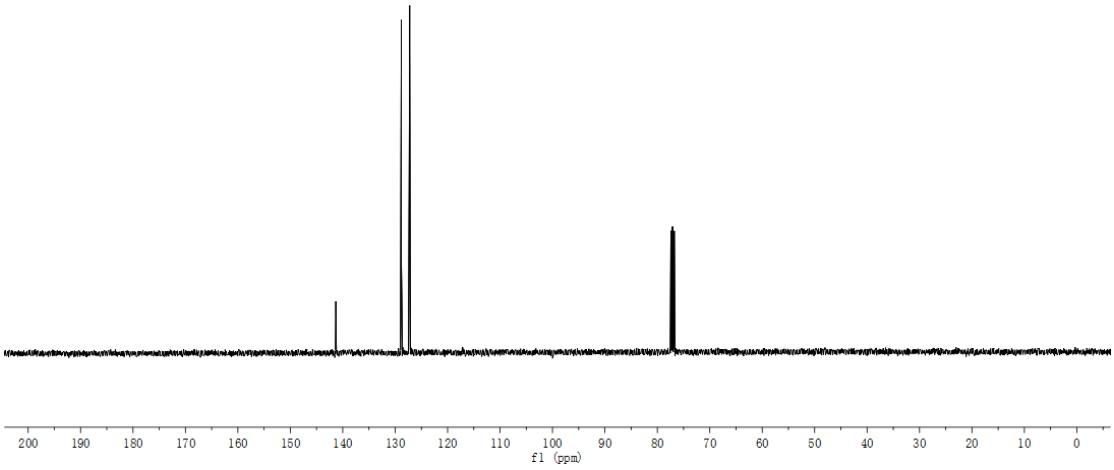

7.6518
7.6325
7.5042
7.4858
7.4663
7.4086
7.3905
7.3719
7.2609

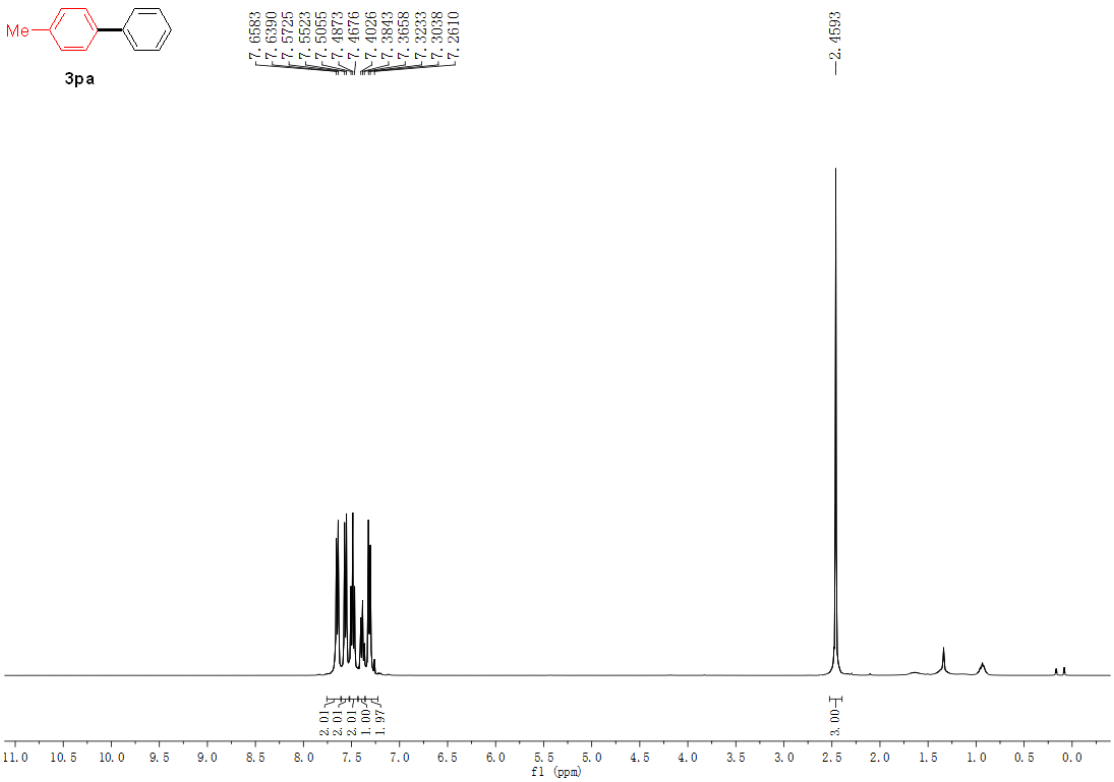

4.04
4.04
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

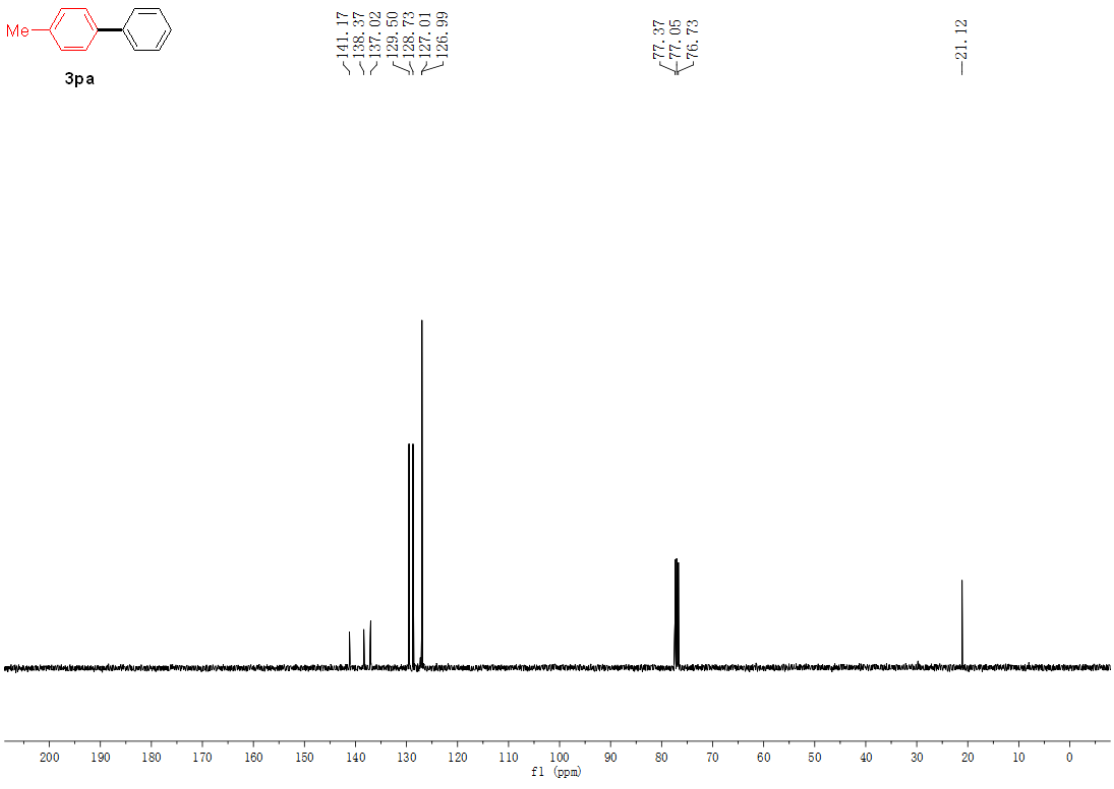

3oa

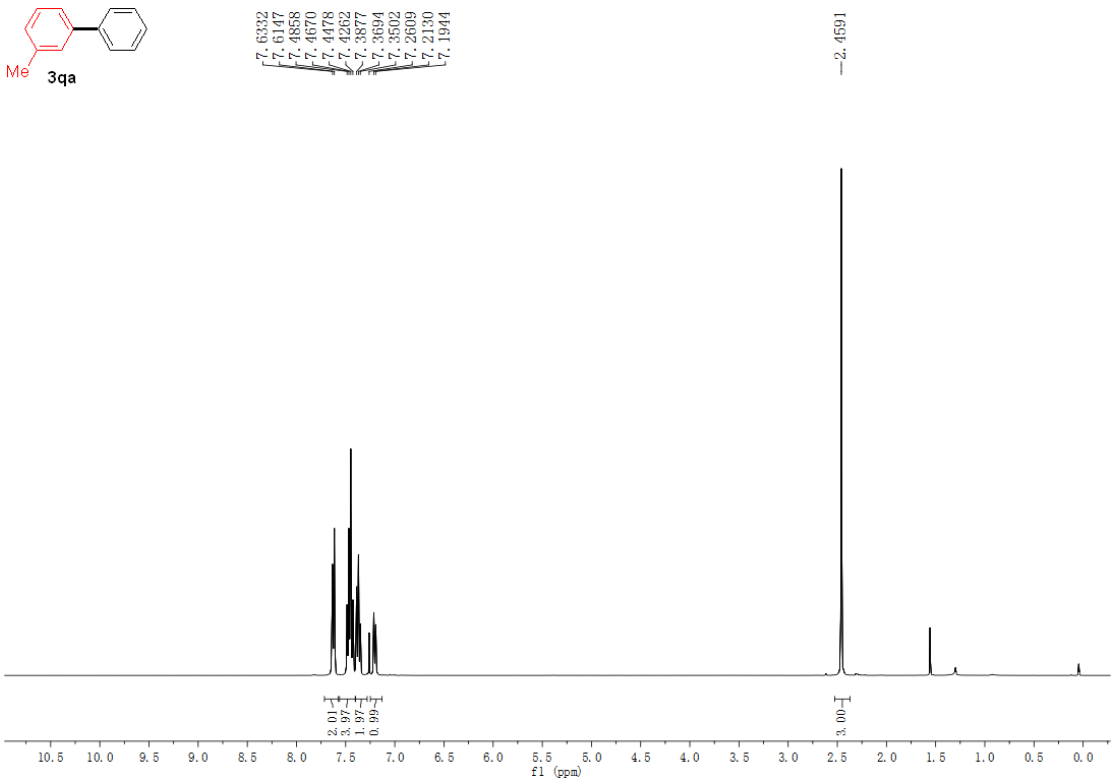

141.30
128.83
127.32
127.24

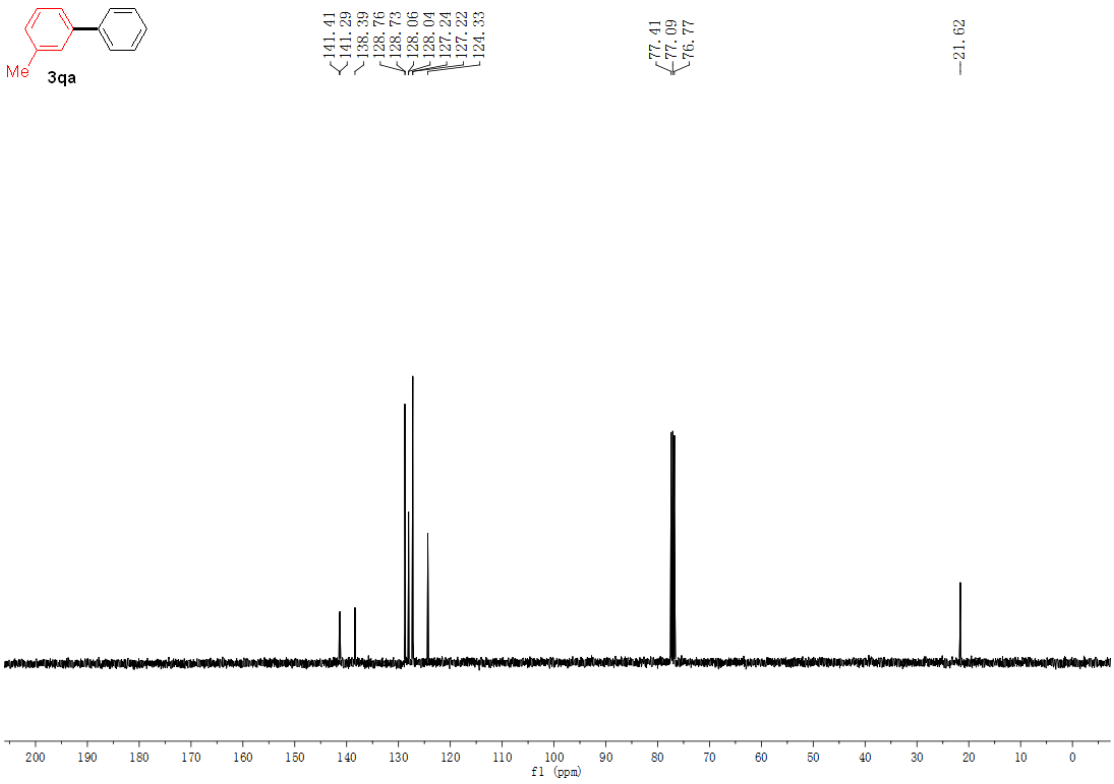

77.42
77.10
76.78

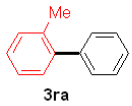

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Me
3pa
7.6583
7.6390
7.5725
7.5523
7.5055
7.4873
7.4676
7.4026
7.3843
7.3658
7.3233
7.3038
7.2610
2.4593
2.01
2.01
2.00
1.97
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

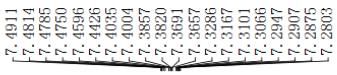

Me
3pa
141.17
138.37
137.02
129.50
128.73
127.01
126.99
77.37
77.05
76.73
21.12
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Me
3qa
7.6332
7.6147
7.4858
7.4670
7.4478
7.4262
7.3877
7.3694
7.3502
7.2609
7.2130
7.1944
2.4591
2.01
3.97
1.97
0.99
3.00
f1 (ppm)

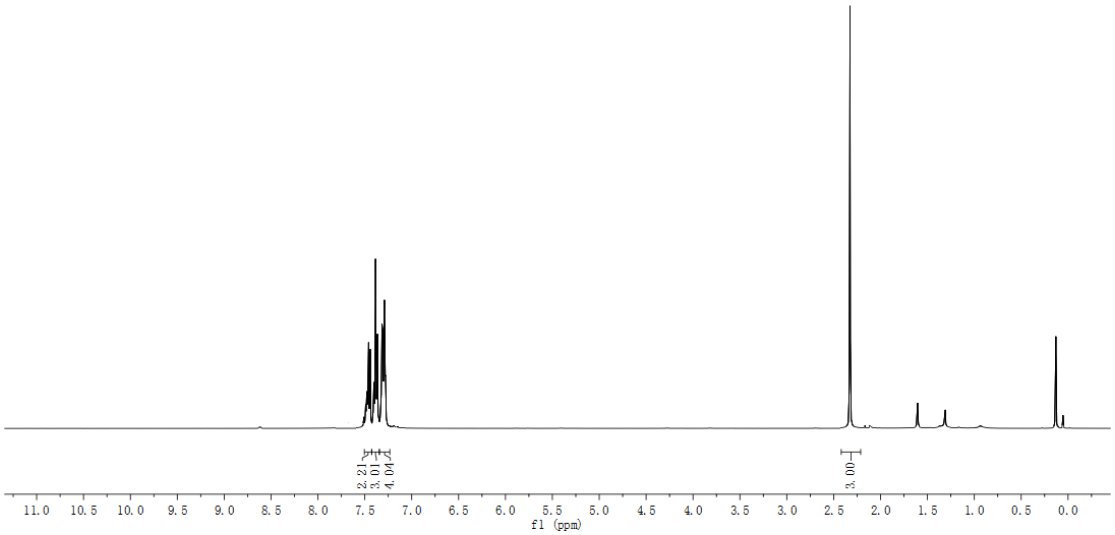

Me
3qa
141.41
141.29
138.39
128.76
128.73
128.06
128.04
127.24
127.22
124.33
77.41
77.09
76.77
21.62
f1 (ppm)

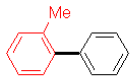

Me

3ra

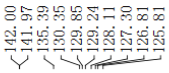

7.4911
7.4814
7.4785
7.4750
7.4596
7.4426
7.4035
7.4004
7.3857
7.3820
7.3691
7.3657
7.3286
7.3167
7.3101
7.3066
7.2947
7.2907
7.2875
7.2803


2.3255


2.21
3.01
4.04
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

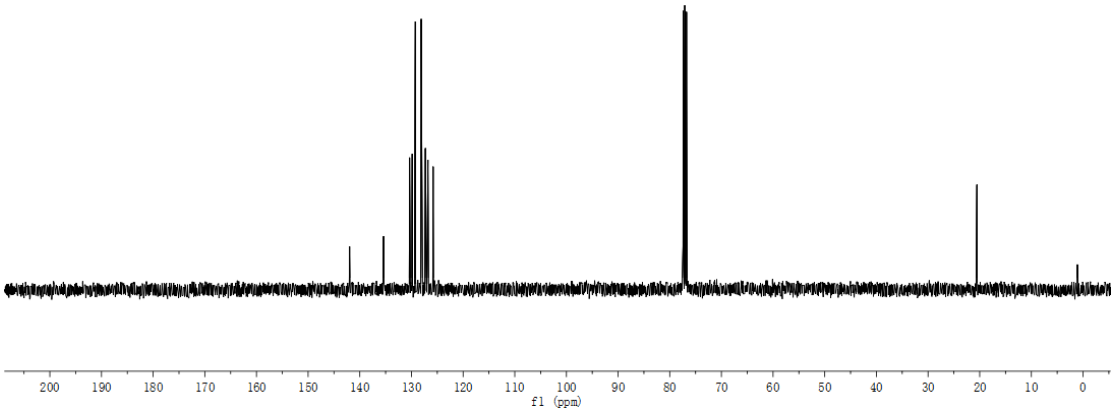

Me

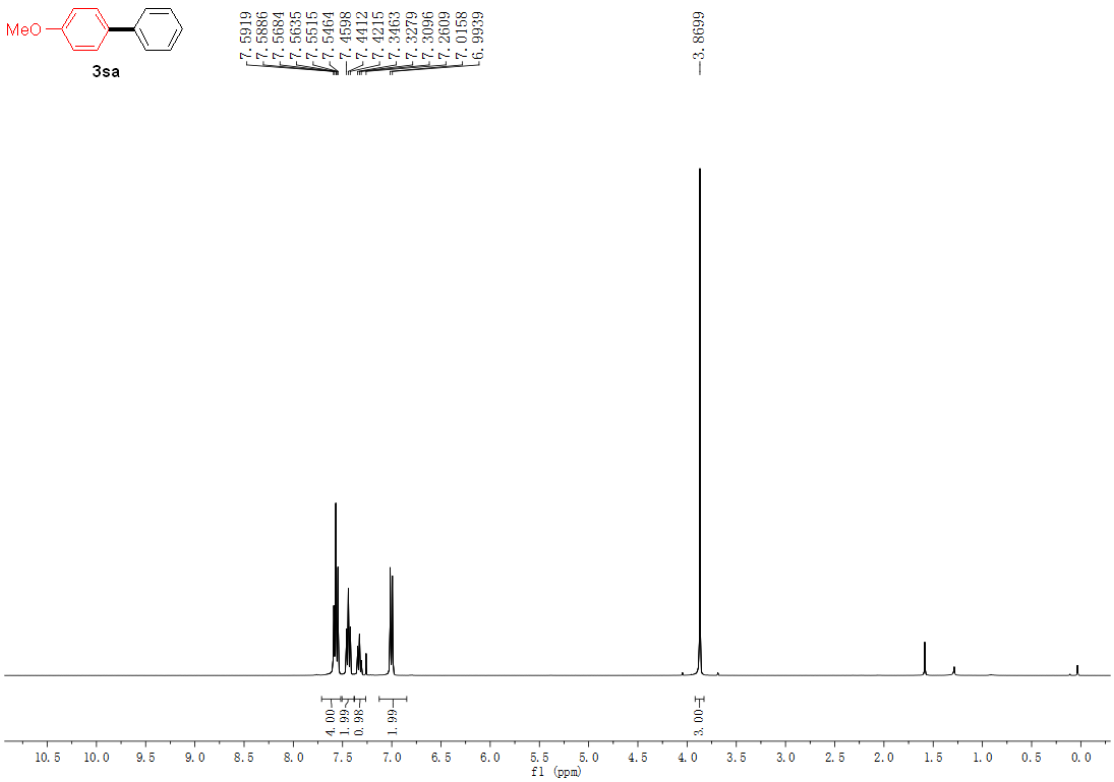
3ra


142.00
141.97
135.39
130.35
129.85
129.24
128.11
127.30
126.81
125.81


77.40
77.08
76.76


20.53


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
3sa
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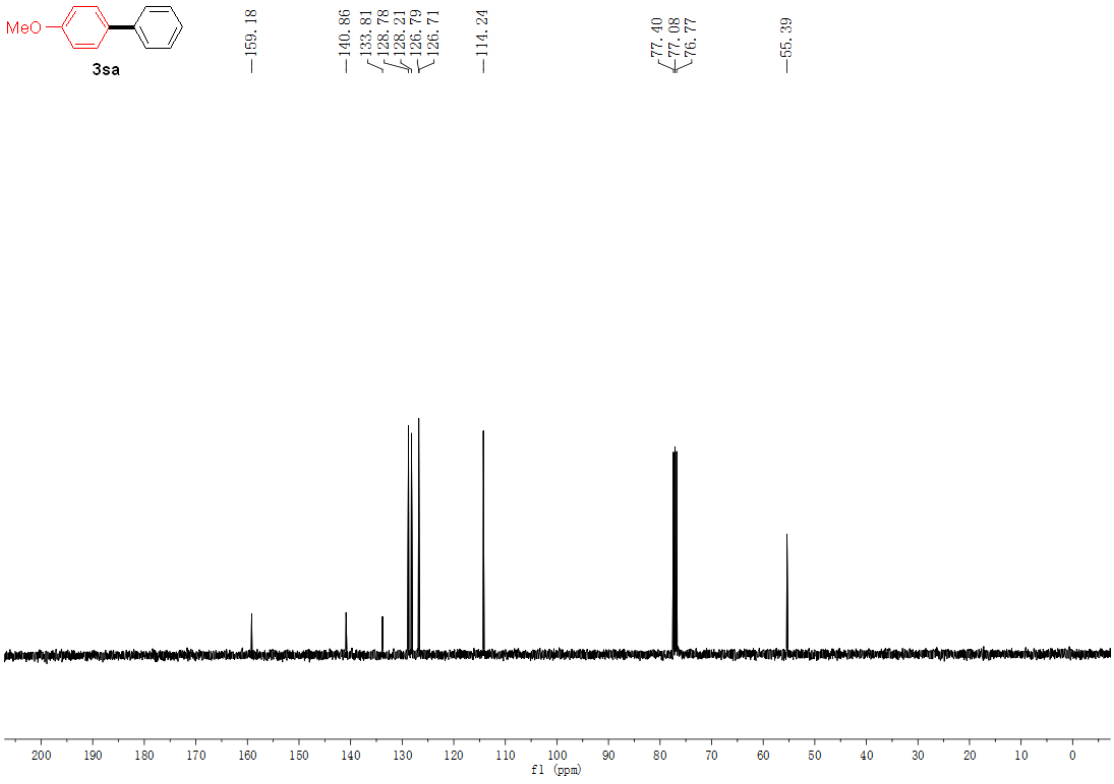
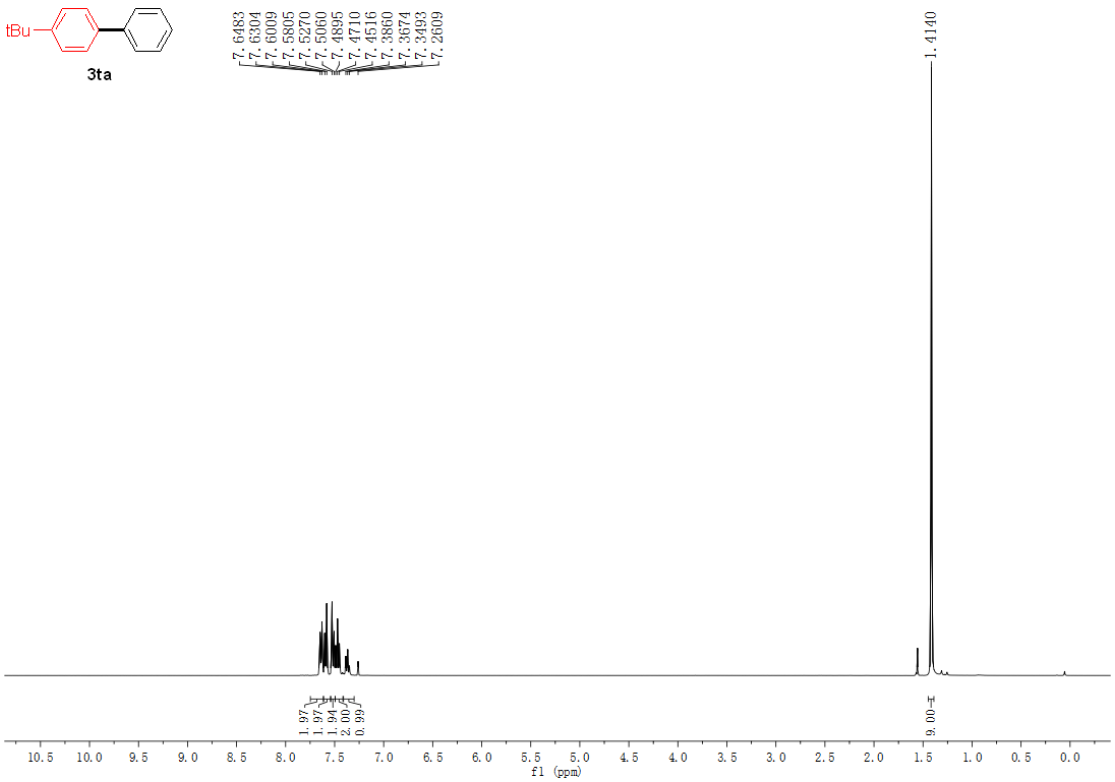
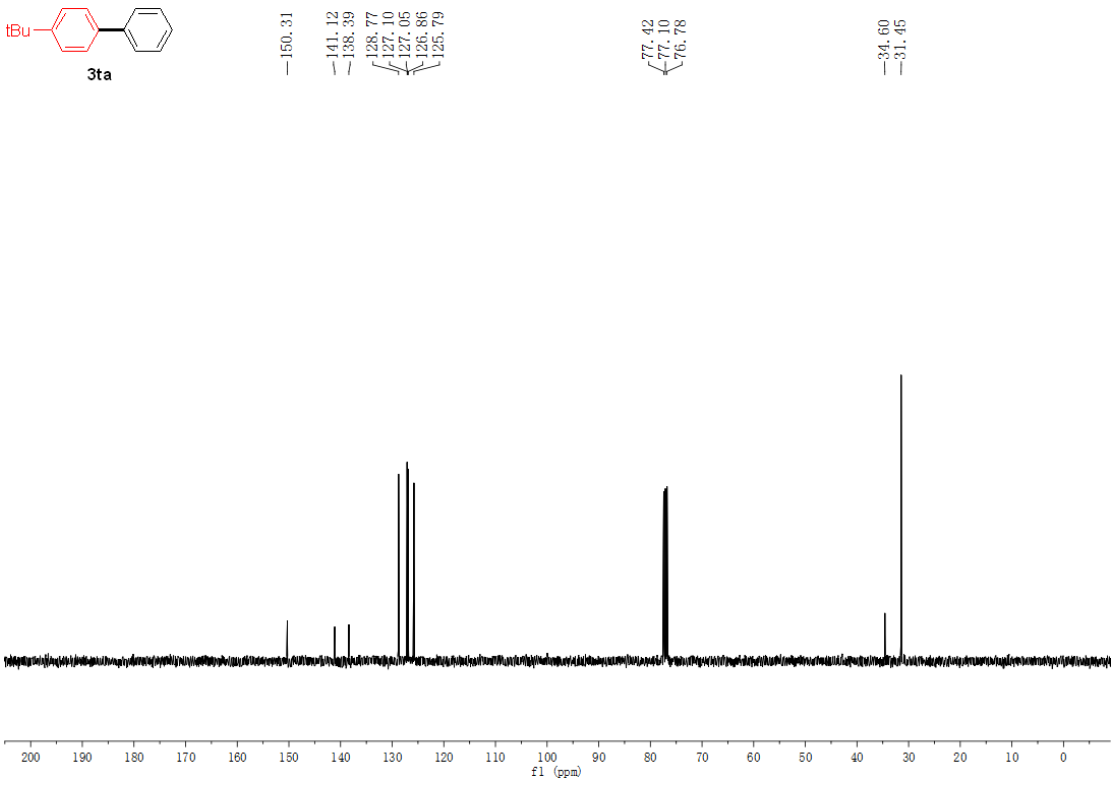
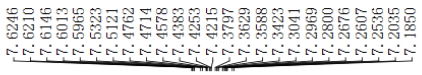
7.5886
7.5684
7.5635
7.5515
7.5464
7.4598
7.4412
7.4215
7.3463
7.3279
7.3096
7.2609
7.0158
6.9939
3.8699
4.00
1.99
0.98
1.99
3.00
f1 (ppm)


MeO
3sa
159.18
140.86
133.81
128.78
128.21
126.79
126.71
114.24
77.40
77.08
76.77
55.39
f1 (ppm)


tBu
3ta
7.6483
7.6304
7.6009
7.5805
7.5270
7.5060
7.4895
7.4710
7.4516
7.3860
7.3674
7.3493
7.2609
1.4140
1.97
1.97
1.94
2.00
0.99
9.00
f1 (ppm)


tBu
3ta
150.31
141.12
138.39
128.77
127.10
127.05
126.86
125.79
77.42
77.10
76.78
34.60
31.45
f1 (ppm)


7.6246
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7.6146
7.6013
7.5965
7.5323
7.5121
7.4762
7.4714
7.4578
7.4383
7.4253
7.4215
7.3797
7.3629
7.3588
7.3423
7.3041
7.2969
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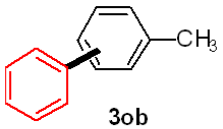
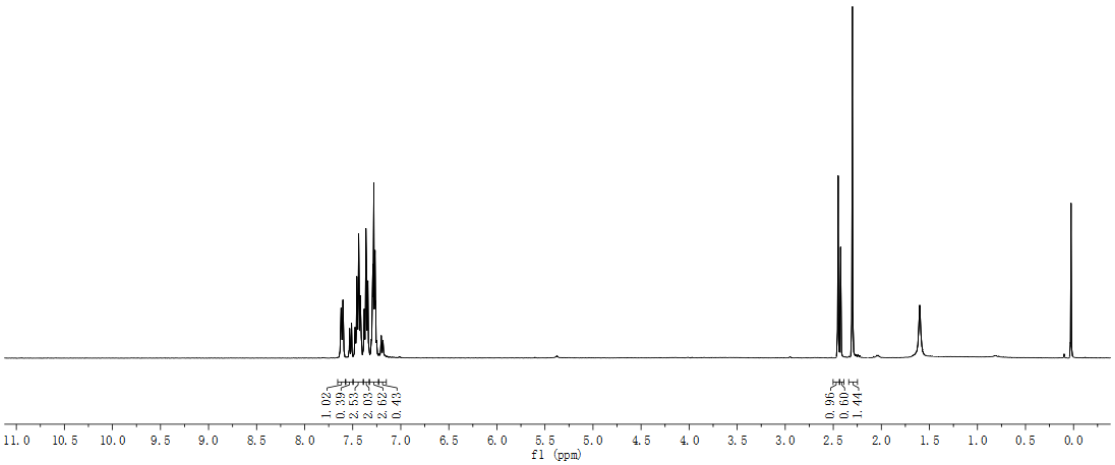
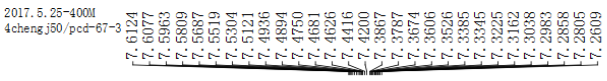
7.2676
7.2607
7.2536
7.2035
7.1850

2.4499
2.4236
2.3017


CH3

3ob


1.02
0.39
2.53
2.03
2.62
0.43
0.96
0.60
1.44
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


2017.5.25-400M
4chengj50/pcd-67-3
7.6124
7.6077
7.5963
7.5809
7.5687
7.5519
7.5304
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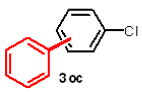
Cl

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11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
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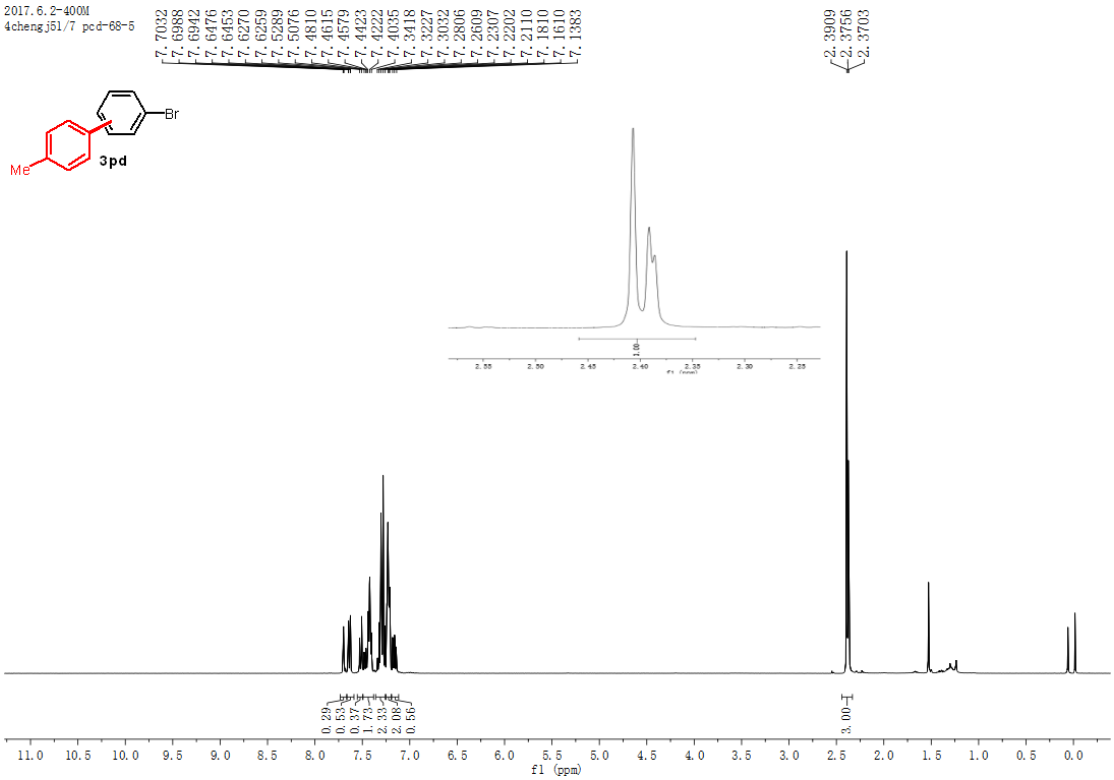
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2.3703
Br
Me
3pd
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0.37
1.73
2.33
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3.00
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10.5
10.0
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8.0
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6.0
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1.5
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f1 (ppm)