Supporting Information

I_2/TBPB mediated oxidative reaction of aryl acetaldehydes with amidines: synthesis of 1,2,5-triaryl-1H-imidazoles

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1.General Remarks.

^{1}H NMR and ^{13}C NMR spectra were determined on 300 MHz and 75 MHz in $CDCl_3$. unknown products were further characterized by HRMS (TOF-ESI), the melting points of solid products were determined on a microscopic apparatus.

2. General experimental procedure.

Typical procedure for the synthesis of **3aa**.

All reactions were performed on a scale relative to 1,2,5-triaryl-1H-imidazoles. The N-phenylbenzimidamide **1a** (0.20 mmol) , phenylacetaldehyde **2a** (0.24 mmol), I_2 (20 mol%), TBPB (1eq) and dioxane (2 mL) were successfully mixed in the flask using a magnetic stir bar and reacted at 100 ^{o}C for 5 h in the presence of air. Then the mixture was removed from the oil bath and cooled to room temperature. The mixture was filtered and washed with ethyl acetate (3×50 mL) and the crude product was obtained by concentrating under reduced pressure. Finally, product **3aa** was isolated as a white solid by silica gel chromatography (petroleum ether/ethyl acetate = 2/1 as the eluent). The remaining substituted imidazoles were prepared in a similar manner. The structures of the products (**3aa**[1]**,3ac**[1]**,3ah**[2]**,3ha**[3]) were identified according to the literature.

3. References

1. A. R. Katritzky, L. Zhu, H. Lang, O. Denisko and Z. Wang, *Tetrahedron*, 1995, **51**, 13271-13276.
2. S. Auricchio, A. M. Truscello, M. Lauria and S. V. Meille, *Tetrahedron*, 2012, **68**, 7441-7449.
3. M. Zibinsky and V. V. Fokin, *Angew. Chem. Int. Ed. Engl.*, 2013, **52**, 1507-1510.

3.Characterization data of 1,2,5-trisubstitued imidazoles

1,2,5-triphenyl-1H-imidazole(**3aa**):0.2 mmol, 55mg, 93%;white solid; mp249-252°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 6H), 7.27 – 7.19 (m, 6H), 7.11 (d, *J* = 6.9 Hz, 4H). ^{13}C NMR (75 MHz, DMSO) δ 148.2, 137.4, 135.2, 130.8, 130.0, 129.6, 129.0, 128.6, 128.44, 128.41, 128.3, 128.2, 127.5. HRMS (ESI)calcd for $C_{21}H_{17}N_3$ $(M + H)^+$ 297.1387, found 297.1389.

2-(4-methoxyphenyl)-1,5-diphenyl-1H-imidazole(**3ba**)：0.2 mmol, 53mg, 81%;white solid; mp 206-210°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 – 7.16 (m, 9H), 7.08 (dd, *J* = 10.8, 6.9 Hz, 4H), 6.75 (d, *J* = 8.5 Hz, 2H), 3.77 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 147.9, 137.2, 134.6, 130.1, 129.8, 129.3, 128.4, 128.35, 128.3, 128.2, 127.7, 127.2, 123.0, 113.5, 55.1. HRMS (ESI)calcd for $C_{22}H_{19}N_2O$ $(M + H)^+$ 327.1492, found 327.1491.

1,5-diphenyl-2-(p-tolyl)-1H-imidazole(**3ca**)0.2 mmol, 53mg, 85%;white solid; mp198-202 °C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (t, *J* = 3.6 Hz, 3H), 7.27 – 7.18 (m, 6H), 7.14 – 7.01 (m, 6H), 2.30 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.0, 137.9, 137.2, 134.7, 130.7, 129.8, 129.2, 128.6, 128.5,128.3,128.2，128.1, 127.9,127.6, 127.1, 21.1. HRMS (ESI)calcd for $C_{22}H_{19}N_2$ $(M + H)^+$ 311.1543, found 311.1545.

1,5-diphenyl-2-(4-(trifluoromethyl)phenyl)-1H-imidazole (**3da**)：0.2 mmol, 57mg, 78%;white solid; mp158-162 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 – 7.32 (m, 8H), 7.22 (s, 3H), 7.12 (d, *J* = 8.5 Hz, 4H).^{13}C NMR (75 MHz, $CDCl_3$) δ 146.3, 136.8, 135.8, 134.0, 130.0, 129.6, 129.55, 129.4, 128.9,128.7,128.6，128.5, 128.3,128.1, 127.6, 125.0 ($J_{C\text{-}F}$ = 3 Hz).HRMS (ESI)calcd for $C_{22}H_{16}F_3N_2$ $(M + H)^+$ 365.1260, found 365.1264.

2-(2-chlorophenyl)-1,5-diphenyl-1H-imidazole(**3ea**)：0.2 mmol, 52mg, 79%;white solid; mp126-128 °C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (s, 1H), 7.37 – 7.15 (m, 10H), 7.12 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.02 (dd, *J* = 7.7, 1.8 Hz, 2H).^{13}C NMR (75 MHz, $CDCl_3$) δ 146.4, 136.7, 135.0, 134.3, 133.0, 130.9, 130.6, 130.0，129.7, 129.1, 128.6, 128.4, 128.3, 128.2, 127.9, 127.6, 126.5. HRMS (ESI)calcd for $C_{21}H_{16}ClN_2$ $(M + H)^+$ 331.1997, found 331.1995.

3-(1,5-diphenyl-1H-imidazol-2-yl)pyridine(**3fa**)：0.2 mmol, 26mg, 44%;white solid; mp209-211 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.59 – 8.45 (m, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.32 (m, 4H), 7.28 – 7.05 (m, 8H).^{13}C NMR (75 MHz, $CDCl_3$) δ 149.4, 149.0, 145.2, 136.7, 135.8, 129.7, 129.4, 129.1, 128.8,128.7，
128.5,128.3,128.2,127.6,126.8, 122.9. HRMS (ESI) calcd for $C_{20}H_{16}N_3$ $(M + H)^+$298.1339, found 298.1341.

1-(4-methoxyphenyl)-2,5-diphenyl-1H-imidazole(**3ga**):0.2 mmol, 62mg, 95%;white solid; mp202-205°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 3H), 7.29 – 7.20 (m, 6H), 7.10 (dd, *J* = 6.9, 2.8 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 3.82 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 148.0, 135.4, 132.8, 130.1, 129.7, 129.4, 129.1, 128.7, 128.6,128.5, 128.3,127.6, 127.2,114.7, 55.6. HRMS (ESI)calcd for $C_{22}H_{19}N_2O$ $(M + H)^+$ 327.1492, found 327.1490.

2,5-diphenyl-1-(p-tolyl)-1H-imidazole (**3ha**):0.2 mmol, 57mg, 92%;white solid; mp218-222°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (d, *J* = 5.3 Hz, 3H), 7.27 – 7.20 (m, 6H), 7.11 (dd, *J* = 11.4, 6.0 Hz, 4H), 6.98 (d, *J*

= 8.2 Hz, 2H), 2.38 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 147.9, 138. 8, 135.2, 134.4, 130.2, 130.1, 129.8, 129.1,128.7, 128.6, 128.4,128.3,128.1, 127.6,127.3, 21.4. HRMS (ESI)calcd for $C_{22}H_{19}N_2$ $(M + H)^+$ 311.1543, found 311.1540.

2,5-diphenyl-1-(o-tolyl)-1H-imidazole(**3ia**):0.2 mmol, 56mg, 90%;white solid; mp148-150^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.39 – 7.28 (m, 3H), 7.26 – 7.14 (m, 9H), 7.07 (dd, *J* = 6.6, 3.0 Hz, 2H), 1.84 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.1 , 136.7, 136.3, 135.2, 131.6, 131.0, 130.2, 129.5,129.4,128.6,128.5,128.4, 128.38, 128.2,127.8 , 127.5, 127.3, 17.8. HRMS (ESI)calcd for $C_{22}H_{19}N_2$ $(M + H)^+$ 311.1543, found 311.1542.

1-(3,4-dimethylphenyl)-2,5-diphenyl-1H-imidazole(**3ja**):0.2 mmol, 60mg, 91%;white solid; mp 216-220 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.32 (m, 3H), 7.26 – 7.16 (m, 6H), 7.08 (dd, *J* = 12.0, 5.5 Hz, 3H), 6.84 (d, *J* = 10.4 Hz, 2H), 2.26 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.2, 138.0, 137.3, 135.3, 135.0, 131.0, 130.6, 130.2, 129.2, 128.8, 128.5, 128.3,128.2,127.3, 125.7, 19.9,19.7. HRMS (ESI)calcd for $C_{23}H_{21}N_2$ $(M + H)^+$ 325.1700, found 325.1702.

1-(2-ethylphenyl)-2,5-diphenyl-1H-imidazole (**3ka**):0.2 mmol, 56mg, 86%;white solid; mp123-125^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 – 7.33 (m, 4H), 7.31 – 7.15 (m, 9H), 7.11 – 7.04 (m, 2H), 2.16 (q, *J* = 7.6 Hz, 2H), 0.84 (td, *J* = 7.6, 1.1 Hz, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 148.2, 141.6, 136.1, 135.4, 131.0, 130.2 , 129.7,129.6,129.5,128.5,128.4,128.37,128.3,128.2, 128.0, 127.5, 127.1, 23.5, 13.3. HRMS (ESI)calcd for $C_{23}H_{21}N_2$ $(M + H)^+$ 325.1700, found 325.1697.

1-(4-fluorophenyl)-2,5-diphenyl-1H-imidazole (**3la**) :0.2 mmol, 54mg, 86%;white solid; mp221-226^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.21 (m, 9H), 7.06 (dd, *J* = 11.9, 6.7 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ161.9 ($J_{C\text{-}F}$=247.5),147.9, 134.92 (s), 133.1, 130.2, 129.8,129.7,129.4,128.6, 128.4, 128.2, 128.1, 128.0, 127.3, 116.3($J_{C\text{-}F}$=22.5). HRMS (ESI)calcd for $C_{21}H_{16}FN_2$ $(M + H)^+$ 315,1292, found 315.1290.

1-(4-chlorophenyl)-2,5-diphenyl-1H-imidazole (**3ma**):0.2 mmol, 59mg, 89%;white solid; mp214-218^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (ddd, *J* = 20.6, 10.3, 6.3 Hz, 11H), 7.12 – 6.96 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.2, 135.9, 135.2, 134.7, 130.4, 129.9, 129.7, 129.1, 128.8, 128.7, 128.6, 128.5, 127.8 .HRMS (ESI)calcd for $C_{21}H_{16}ClN_2$ $(M + H)^+$ 331.0997, found 331.0998.

2-(4-methoxyphenyl)-5-phenyl-1-(p-tolyl)-1H-imidazole (**3na**):0.2 mmol, 63mg, 92%;white solid; mp182-186^{o}C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 – 7.18 (m, 6H), 7.16 – 7.05 (m, 4H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.77 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 148.0, 138.4, 134.7, 130.9, 130.1, 130.0, 128.8, 128.4, 128.2, 128.0, 127.8, 127.1, 123.3, 113.4, 55.1, 21.2. HRMS (ESI)calcd for $C_{23}H_{21}N_2O$ $(M + H)^+$ 341.1649, found 341.1650.

5-phenyl-1,2-di-p-tolyl-1H-imidazole (**3oa**):0.2 mmol, 59mg, 91%;white solid; mp192-196^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (s, 1H), 7.27 – 7.18 (m, 5H), 7.15 – 6.95 (m, 8H), 2.37 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.4, 138.6, 138.2, 135.1, 134.9, 130.3, 130.2, 129.0, 128.9, 128.6, 128.4, 128.3,128.2,128.1, 127.4, 21.5. HRMS (ESI)calcd for $C_{23}H_{21}N_2$ $(M + H)^+$ 325.1700, found 325.1701.

2-(3-bromo-4-methylphenyl)-5-phenyl-1-(p-tolyl)-1H-imidazole (**3pa**):0.2 mmol, 63mg, 78%;white solid; mp210-212°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.33 (s, 1H), 7.27 – 7.14 (m, 5H), 7.12 – 6.96 (m, 6H), 2.39 (s, 3H), 2.34 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ146.8，139.0，138.0，135.6，134.6，132.7，130.4，130.3，130.2，130.0，128.6，128.5，128.4，128.2，127.6，127.4，124.8，22.9，21.5 HRMS (ESI)calcd for $C_{23}H_{20}BrN_2$ $(M + H)^+$ 403.0805, found403.0803.

2-(4-chlorophenyl)-5-phenyl-1-(p-tolyl)-1H-imidazole (**3qa**):0.2 mmol, 52mg, 76%;white solid; mp 193-196°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (dd, *J* = 6.7, 3.0 Hz, 3H), 7.27 – 7.18 (m, 8H), 7.09 (dd, *J* = 6.7, 3.0 Hz, 2H), 6.92 (d, *J* = 2.5 Hz, 2H), 2.27 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 148.0, 139.5, 137.1, 135.1, 130.7, 129.9, 129.3,129.1, 128.7,128.4,128.2, 128.1,128.0, 127.3, 125.4, 21.3. HRMS (ESI)calcd for $C_{22}H_{18}ClN_2$ $(M + H)^+$ 345.1153, found 345.1155.

2-(4-bromophenyl)-5-phenyl-1-(p-tolyl)-1H-imidazole (**3ra**):0.2 mmol, 56mg, 72%;white solid; mp 174-178°C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 3H), 7.27 – 7.06 (m, 9H), 6.97 (d, *J* = 8.3 Hz, 2H), 2.38 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 147.1, 139.0, 135.7, 134.5, 131.5, 130.4, 130.3, 129.9, 129.8, 128.7,128.5,128.4, 128.1, 127.6, 122.7, 21.5. HRMS (ESI)calcd for $C_{22}H_{18}BrN_2$ $(M + H)^+$ 389.0648, found 389.0651.

5-(4-methoxyphenyl)-1,2-diphenyl-1H-imidazole (**3ab**):0.2 mmol, 55mg, 85%;white solid; mp 168-172 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 22.8, 12.2 Hz, 9H), 7.09 (dd, *J* = 7.7, 1.8 Hz, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 8.8 Hz, 2H), 3.76 (s, 3H).^{13}C NMR (75 MHz, DMSO) δ 159.3, 147.9, 137.6, 135.3, 131.0, 130.2, 129.7, 129.1, 128.8, 128.7, 128.4, 127.9, 122.6, 114.1, 55.6. HRMS (ESI)calcd for $C_{22}H_{19}N_2O$ $(M + H)^+$ 327.1492, found 327.1491.

1,2-diphenyl-5-(p-tolyl)-1H-imidazole(**3ac**):0.2 mmol, 51mg, 83%;white solid; mp217-220°C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 – 7.31 (m, 6H), 7.27 – 7.22 (m, 3H), 7.11 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.00 (dd, *J* = 20.4, 8.2 Hz, 4H), 2.30 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 147.8, 137.3, 137.2, 135.2, 130.9, 129.4, 129.0, 128.8,128.5,128.4,128.3, 128.1, 128.0, 127.9,126.9, 21.2. HRMS (ESI)calcd for $C_{22}H_{19}N_2$ $(M + H)^+$ 311.1543, found 311.1542.

1,2-diphenyl-5-(m-tolyl)-1H-imidazole(**3ad**):0.2 mmol, 50mg, 81%;white solid; mp180-184°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.1 Hz, 6H), 7.24 (t, *J* = 5.9 Hz, 3H), 7.15 – 6.94 (m, 5H), 6.80 (d, *J* = 7.3 Hz, 1H), 2.24 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 147.9, 137.8, 137.2, 135.1,130.6, 129.6,129.3,129.2, 128.7,128.4,128.2,128.1,128.03, 128.0,125.4, 21.3. HRMS (ESI)calcd for $C_{22}H_{19}N_2$ $(M + H)^+$ 311.1543, found 311.1541.

1,2-diphenyl-5-(o-tolyl)-1H-imidazole (**3ae**): 0.2 mmol, 48mg, 78%;white solid; mp119-123°C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 2H), 7.29 – 7.04 (m, 11H), 6.97 (d, *J* = 8.2 Hz, 2H), 2.12 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 147.2, 138.3, 137.2, 134.1, 131.9, 131.0, 130.8,130.1,129.6, 129.1, 128.8, 128.6, 128.2, 128.1, 127.8, 125.4, 20. 6. HRMS (ESI) calcd for $C_{22}H_{19}N_2$ $(M + H)^+$ 311.1543, found 311.1545.

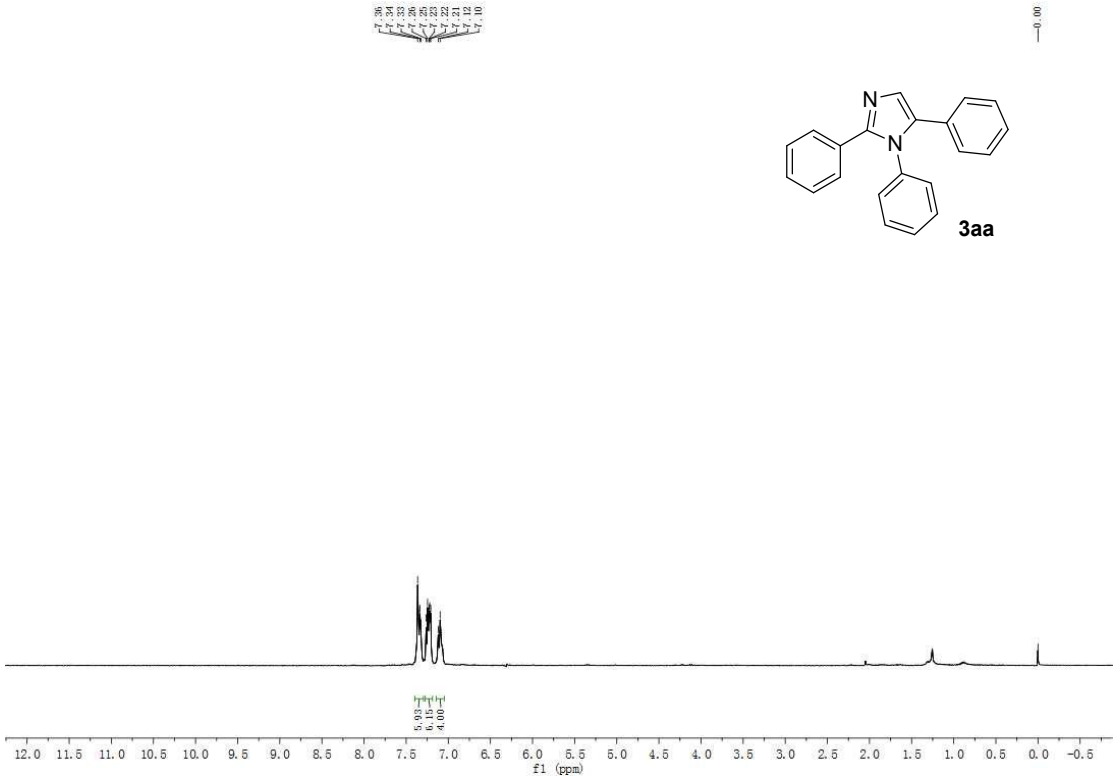
5-(3,4-dimethylphenyl)-1,2-diphenyl-1H-imidazole (**3af**) :0.2 mmol, 52mg,80%;white solid; mp 188 - 192°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.30 (m, 6H), 7.26 – 7.21 (m, 3H), 7.14 – 7.08 (m, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 9.4 Hz, 1H), 2.20 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.6, 137.3, 136.4, 135.8, 135.2, 130.6, 129.6, 129.4, 129.2, 128.7, 128.3, 128.2,128.0, 127.9, 127.7,125.7, 19.6 ,19.4. HRMS (ESI)calcd for $C_{23}H_{21}N_2$ $(M + H)^+$ 325.1700, found 325.1702.

5-(4-ethylphenyl)-1,2-diphenyl-1H-imidazole(**3ag**):0.2 mmol, 52mg, 81%;white solid; mp269-272°C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (d, *J* = 5.0 Hz, 6H), 7.22 (d, *J* = 6.1 Hz, 3H), 7.14 – 6.96 (m, 6H), 2.59 (q, *J* = 7.6 Hz, 2H), 1.19 (t, *J* = 7.6 Hz, 3H).^{13}C NMR (75 MHz, DMSO) δ 147.7, 143.3, 137.2, 135.1, 130.6, 129.3, 128.7, 128.4,128.3,128.2,128.0, 127.9,127.7,127.0, 28.4, 15.2. HRMS (ESI)calcd for $C_{23}H_{21}N_2$ $(M + H)^+$ 325.1700, found 325.1698.

5-(4-fluorophenyl)-1,2-diphenyl-1H-imidazole(**3ah**):0.2 mmol,49mg, 78%;white solid; mp228-232°C;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (td, *J* = 11.4, 6.9 Hz, 9H), 7.12 – 7.00 (m, 4H), 6.92 (t, *J* = 8.7 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ162.3 ($J_{C\text{-}F}$=245.3Hz) ,148.2, 137.2, 134.4, 130.7, 130.5($J_{C\text{-}F}$=8.3Hz),130.1, 129.7, 129.0, 128.9, 128.7,128.5, 128.3, 126.1, 115.6($J_{C\text{-}F}$=21.0Hz). HRMS (ESI)calcd for $C_{21}H_{16}FN_2$ $(M + H)^+$ 315.1292, found 315.1294.

5-(2-fluorophenyl)-1,2-diphenyl-1H-imidazole(**3ai**): 0.2 mmol, 45mg, 72%;white solid; mp198-201°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (ddd, *J* = 16.1, 11.4, 8.4 Hz, 10H), 7.12 – 6.93 (m, 5H). ^{13}C NMR (75 MHz, $CDCl_3$) δ160.1($J_{C\text{-}F}$=246,8Hz), 148.2, 137.2, 131.9, 131.85,131.0,130.6, 130.1,130.0, 129.3, 128.9,128.5,128.4, 128.2, 127. 9, 123.9 (d, *J* = 3.8 Hz),115.8($J_{C\text{-}F}$=21.8Hz). HRMS (ESI)calcd for $C_{21}H_{16}FN_2$ $(M + H)^+$ 315.1292, found 315.1291

4.^{1}H and ^{13}C NMR spectra of the products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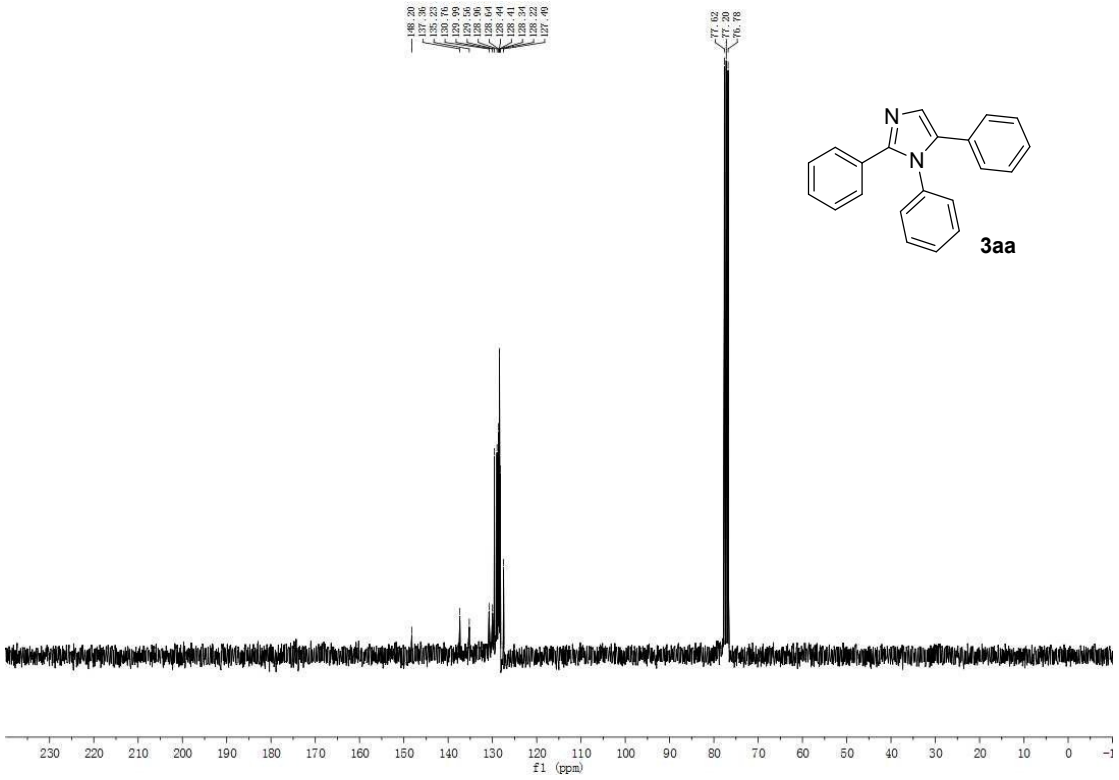
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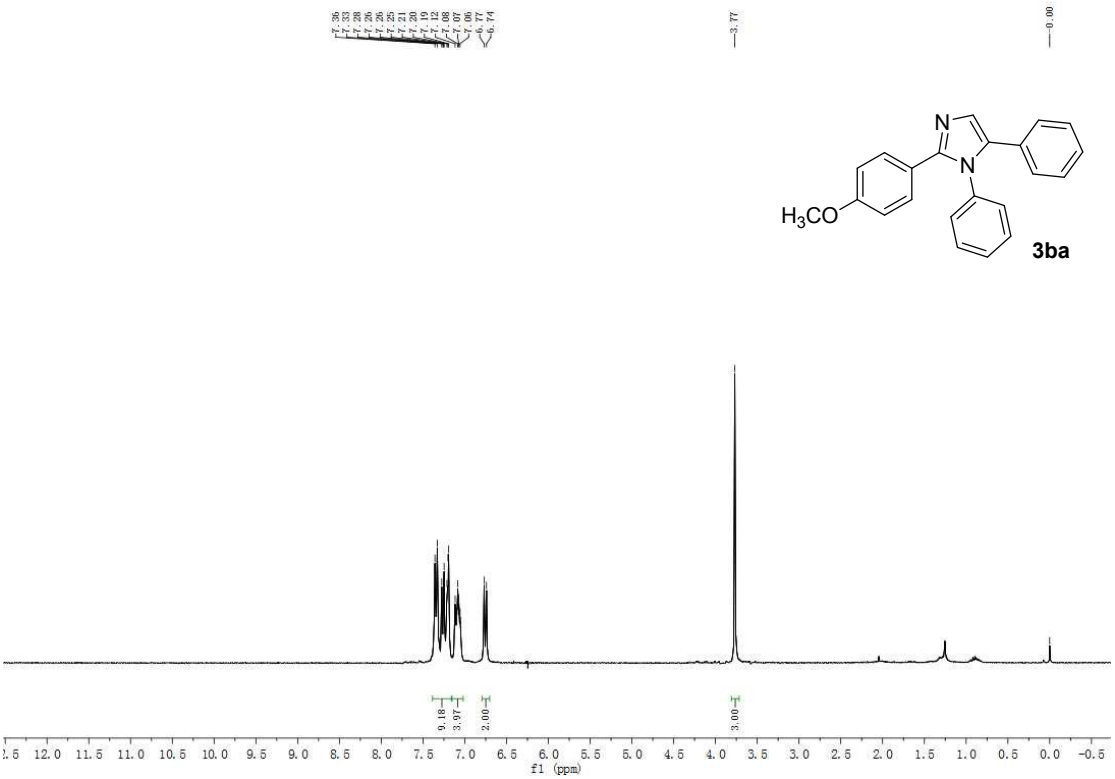
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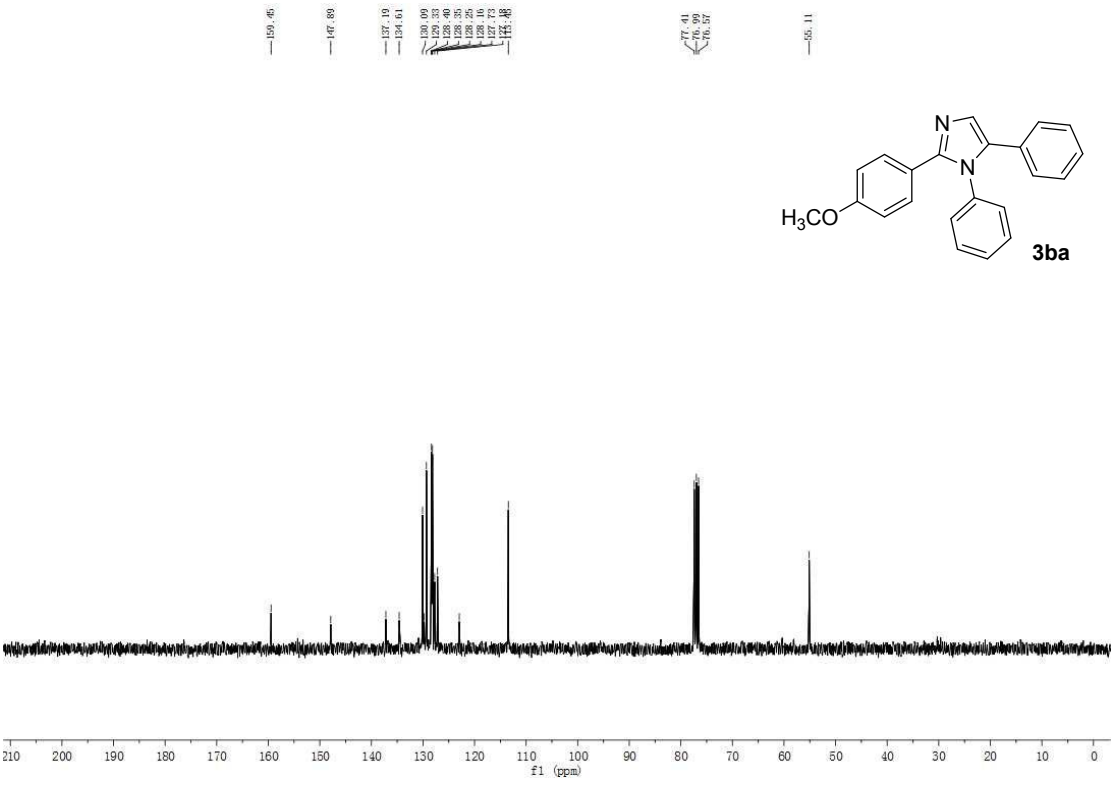
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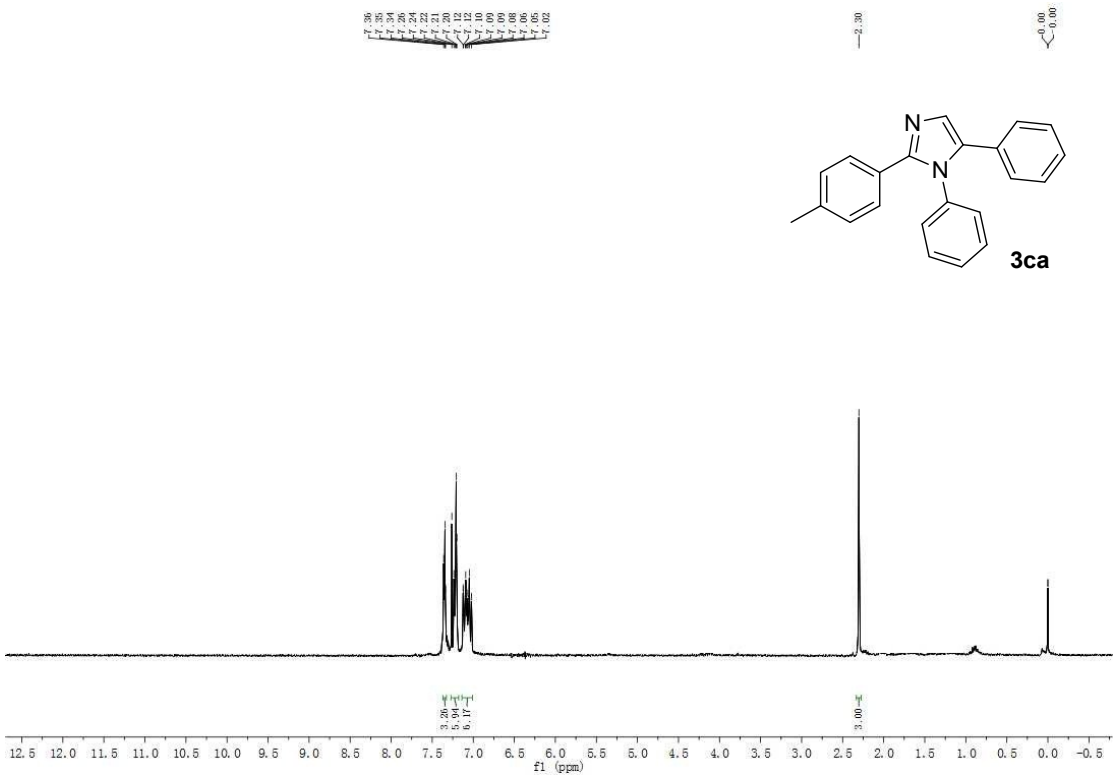
f1 (ppm)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7.20
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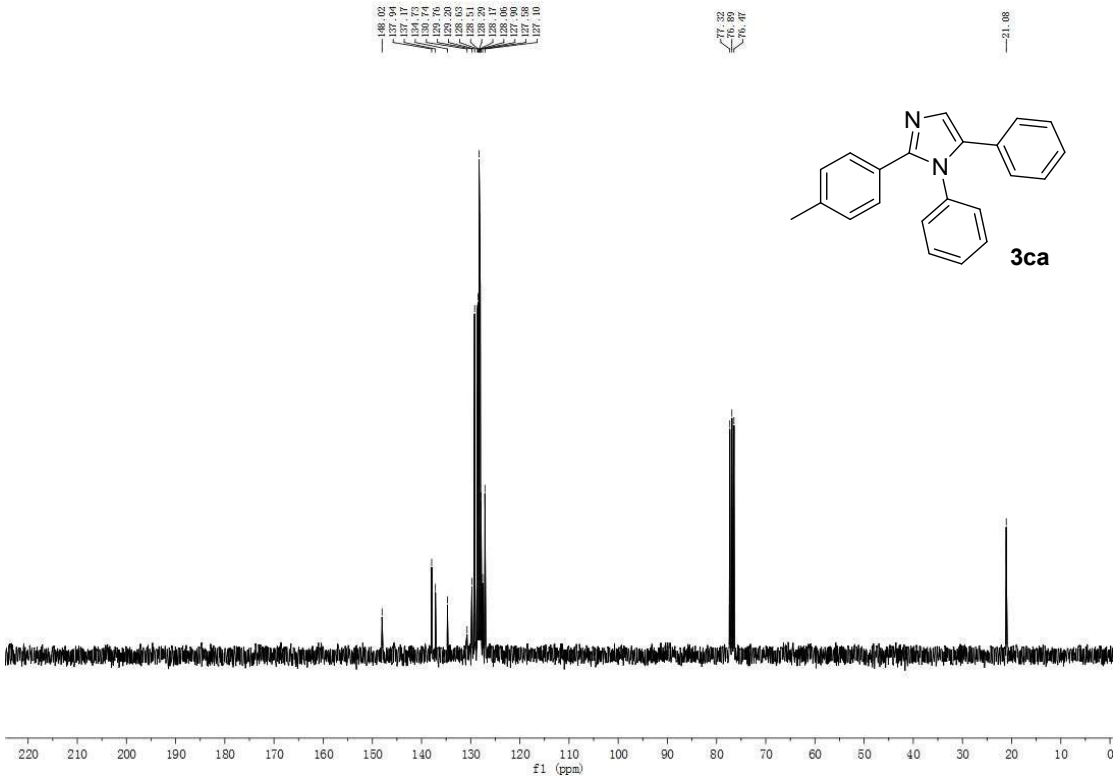
7.12
7.10
7.09
7.09
7.08
7.06
7.05
7.02
2.30
0.00
0.00
N
N
3ca
3.26
5.94
6.17
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.65
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128.29
128.17
127.96
127.59
127.58
127.10
77.32
76.89
76.47
21.08
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N
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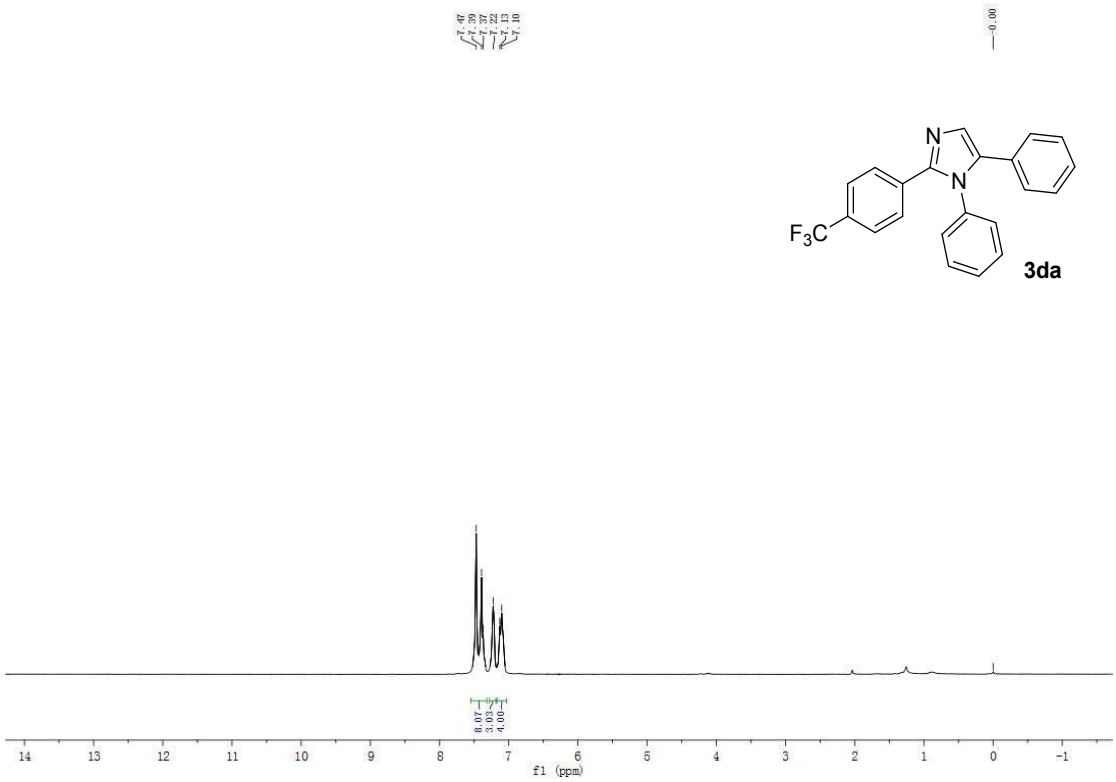
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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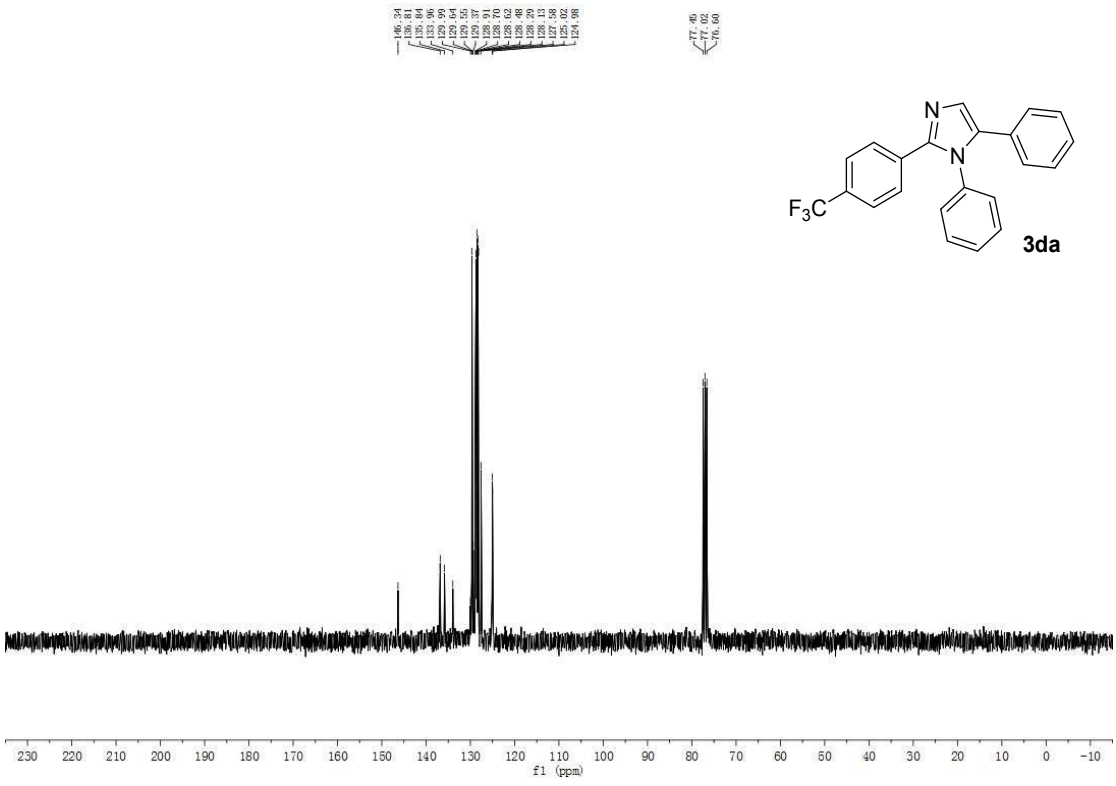
7.39
7.37
7.22
7.13
7.10
0.00
N
N
F3C
3da
8.07
3.03
4.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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129.37
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128.70
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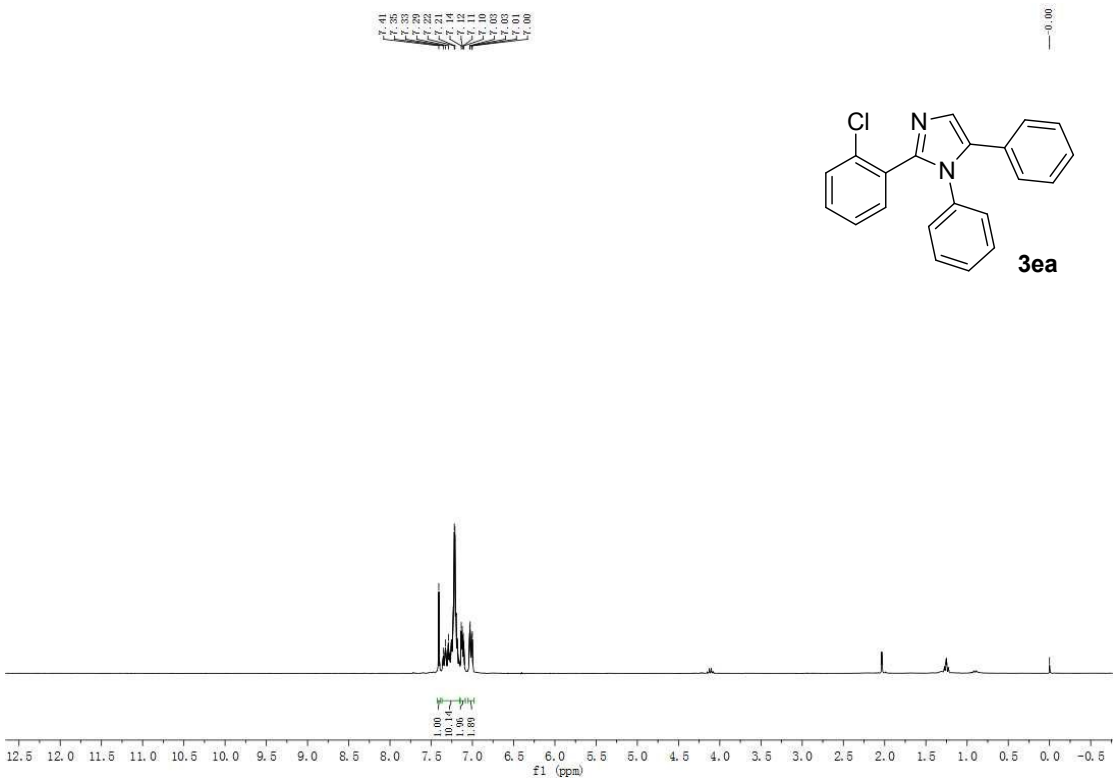
128.48
128.20
128.13
127.58
125.62
124.98
77.45
77.02
76.60
N
N
F3C
3da
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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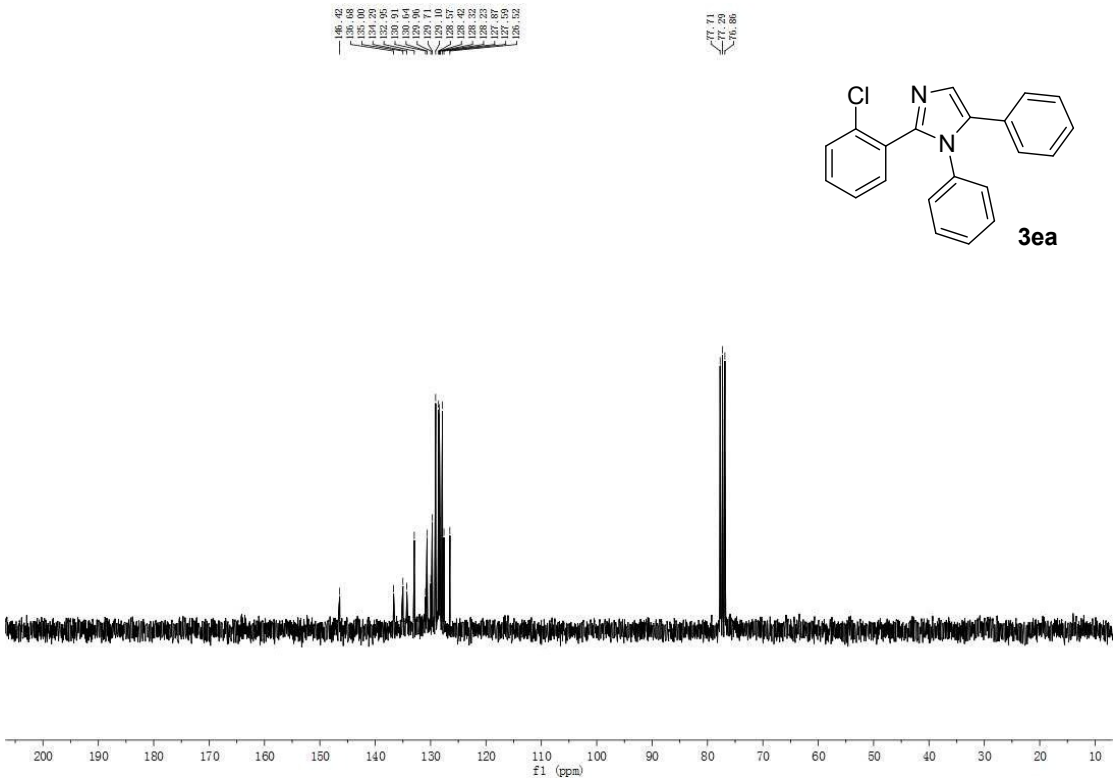
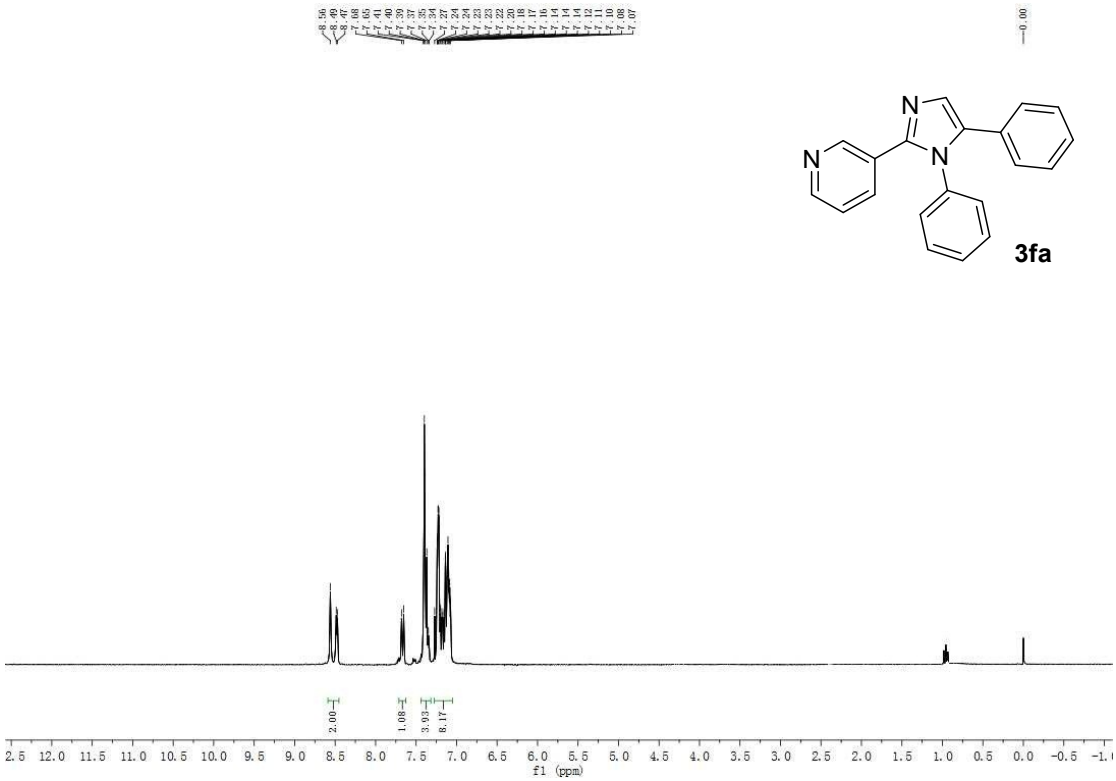
1.89
f1 (ppm)


Cl
N
N
3ea
f1 (ppm)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1.08
3.93
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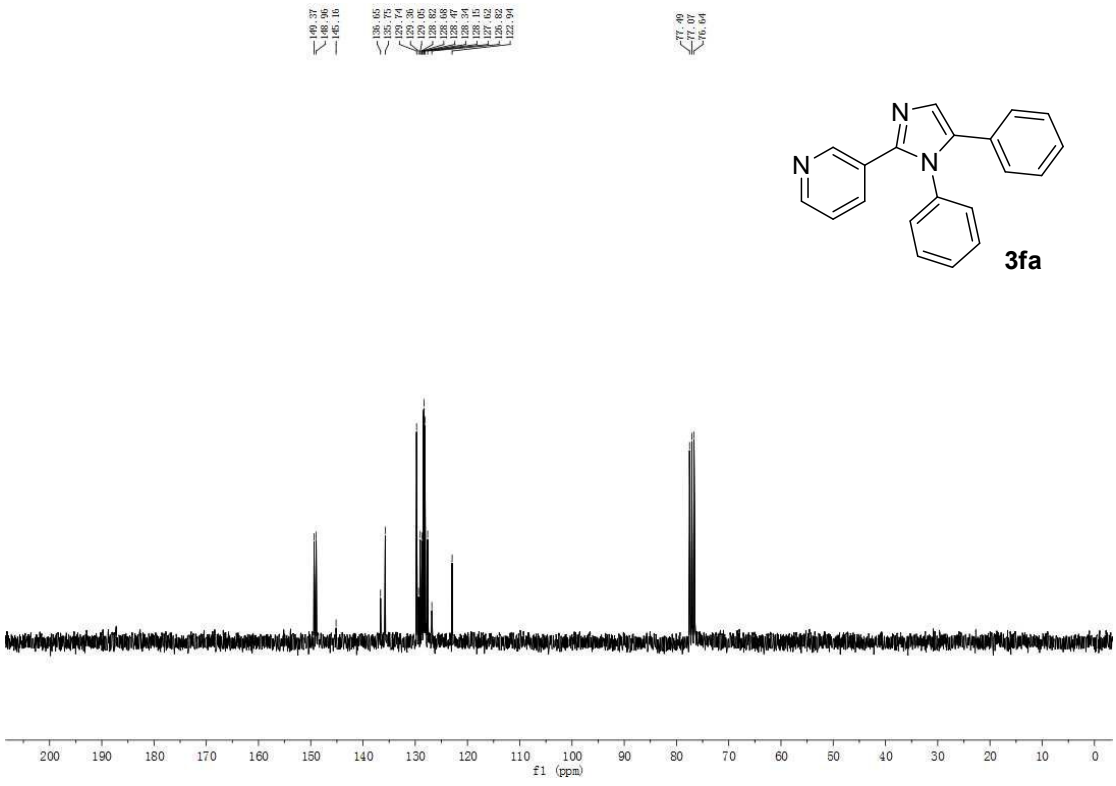
f1 (ppm)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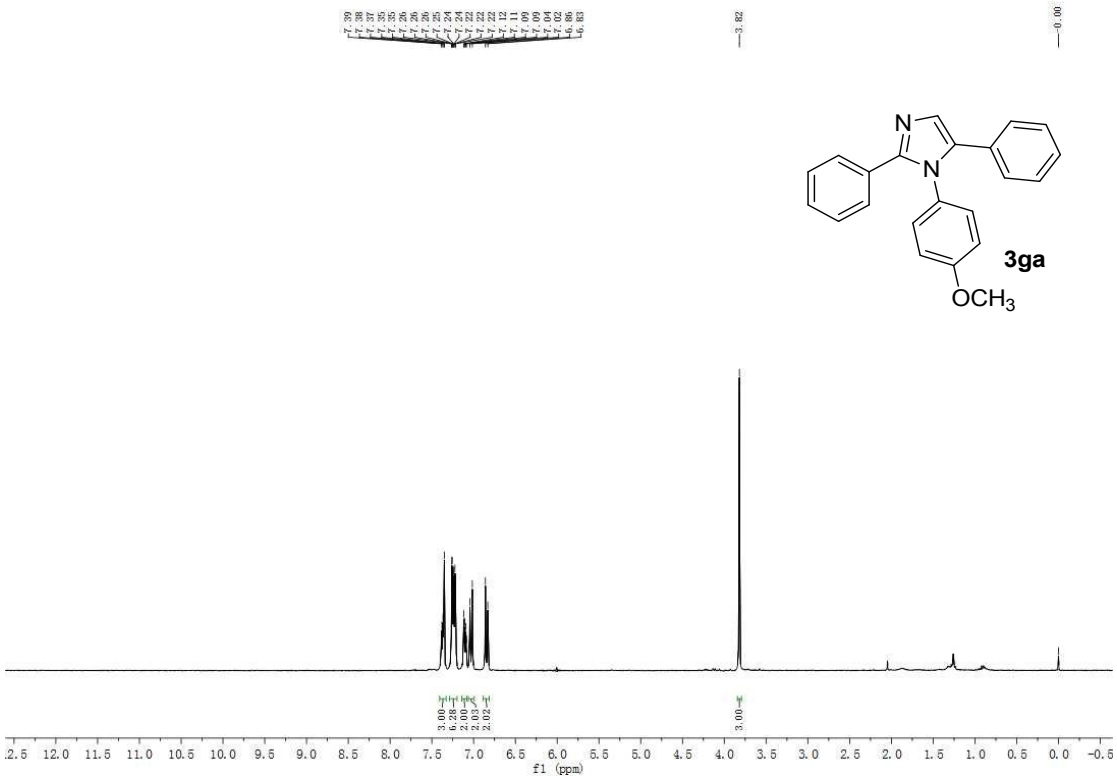
f1 (ppm)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7.22
7.22
7.22
7.12
7.11
7.09
7.09
7.04
7.02
6.86
6.83
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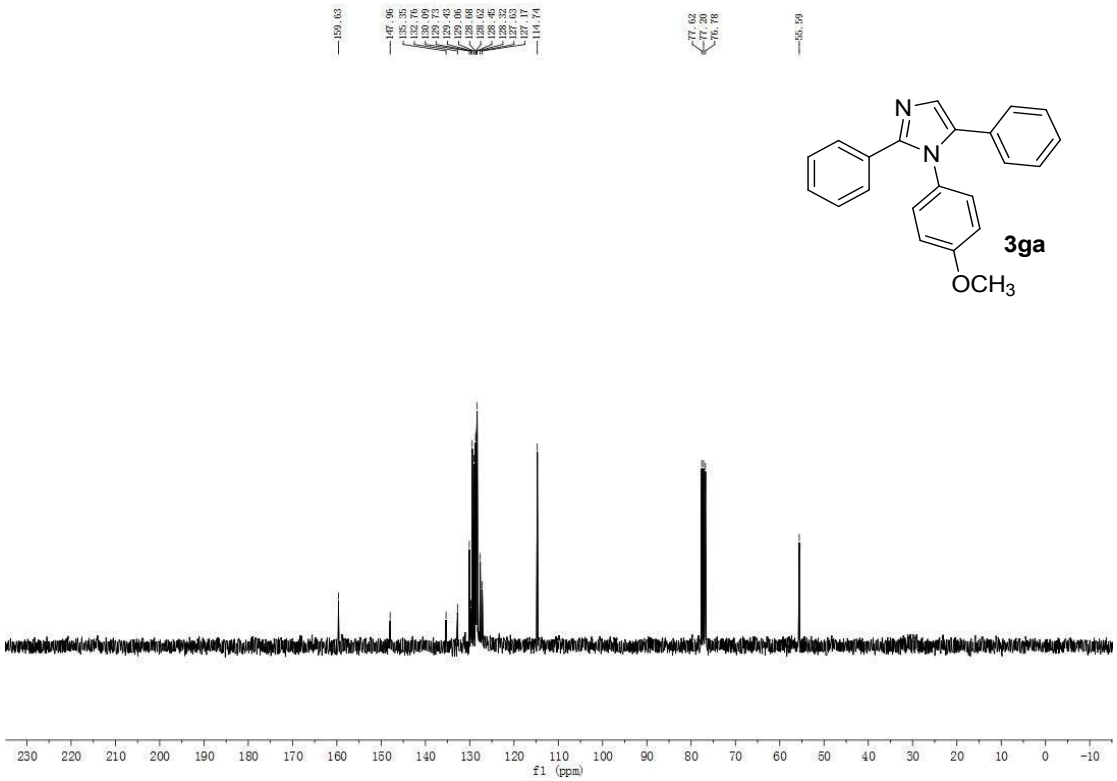
3ga
OCH3
3.00
6.28
2.00
3.03
2.02
3.00
f1 (ppm)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129.06
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128.62
128.45
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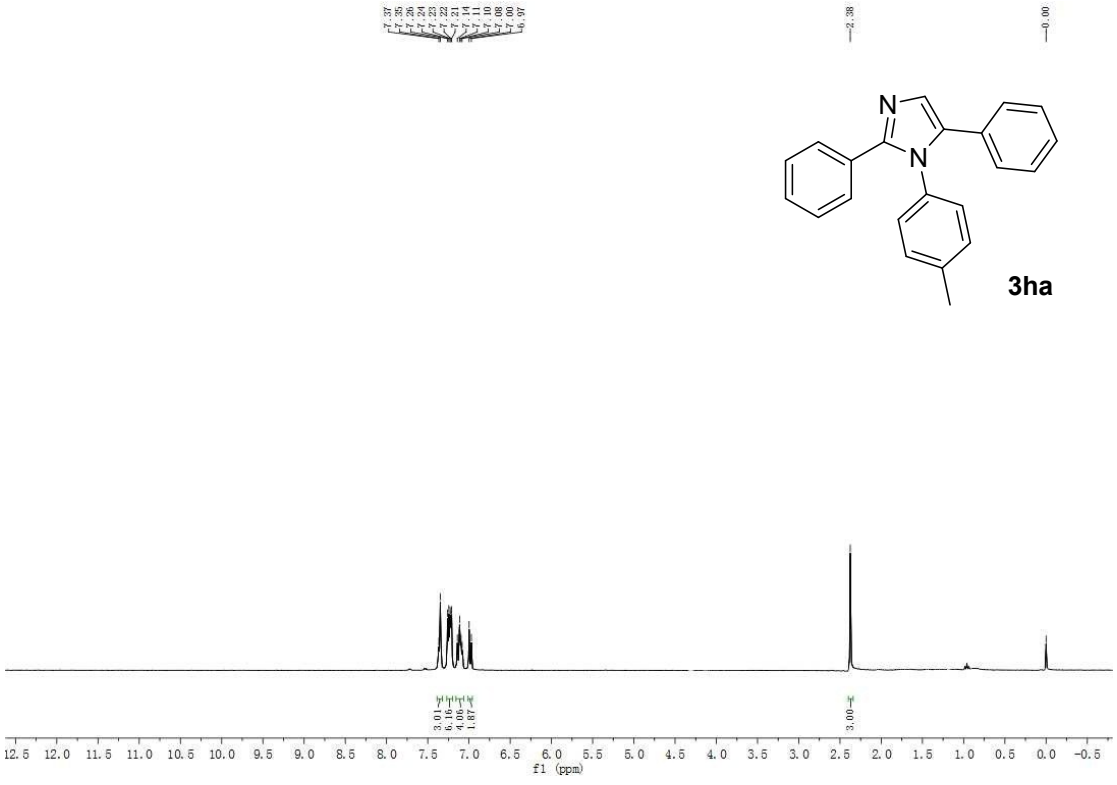
127.63
127.17
114.74
77.62
77.20
76.78
55.59
N
N
3ga
OCH3
f1 (ppm)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7.14
7.11
7.10
7.08
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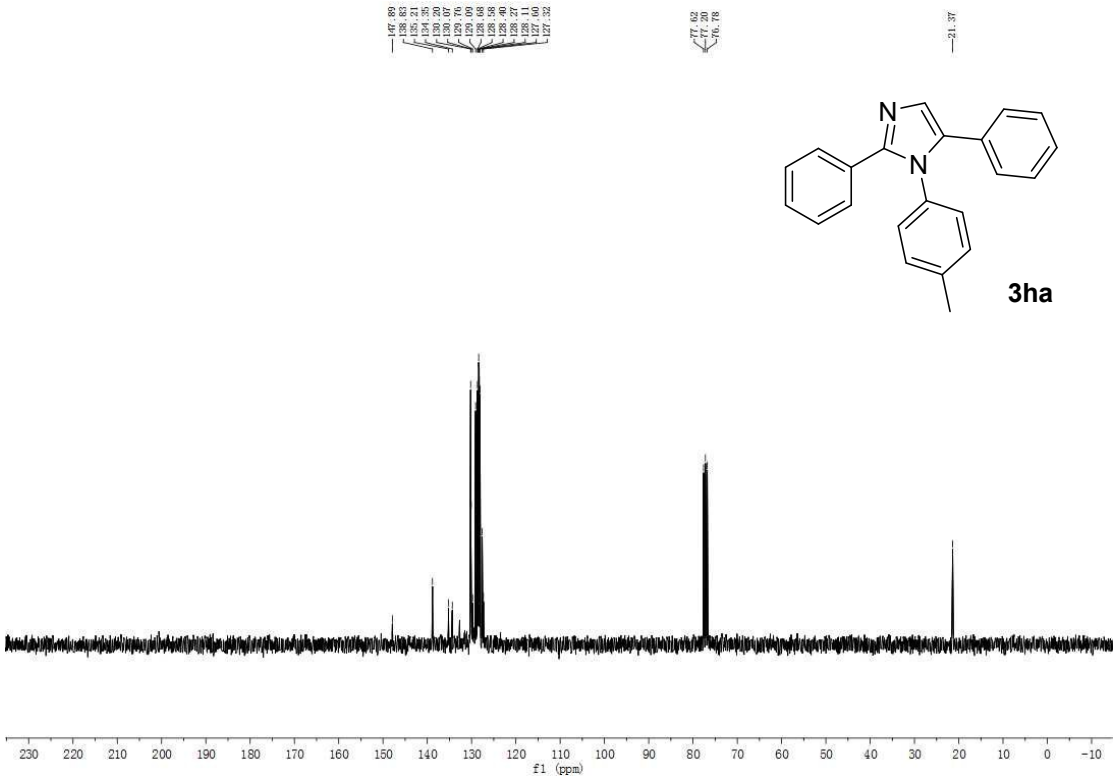
2.38
0.00
3.01
6.16
4.05
1.87
3.00
f1 (ppm)
3ha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129.76
129.09
128.68
128.38
128.40
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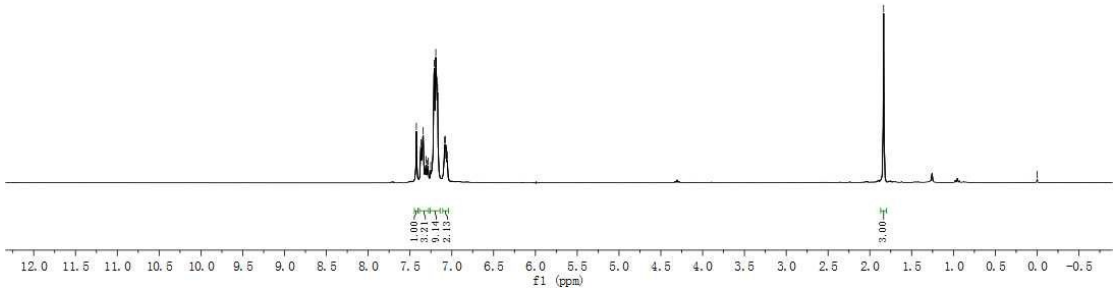
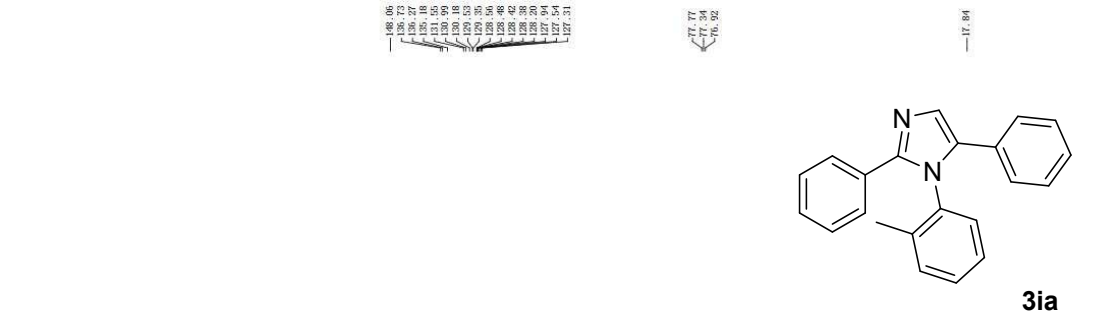
128.11
127.60
127.32
77.62
77.20
76.78
21.37
f1 (ppm)
3ha

3ia





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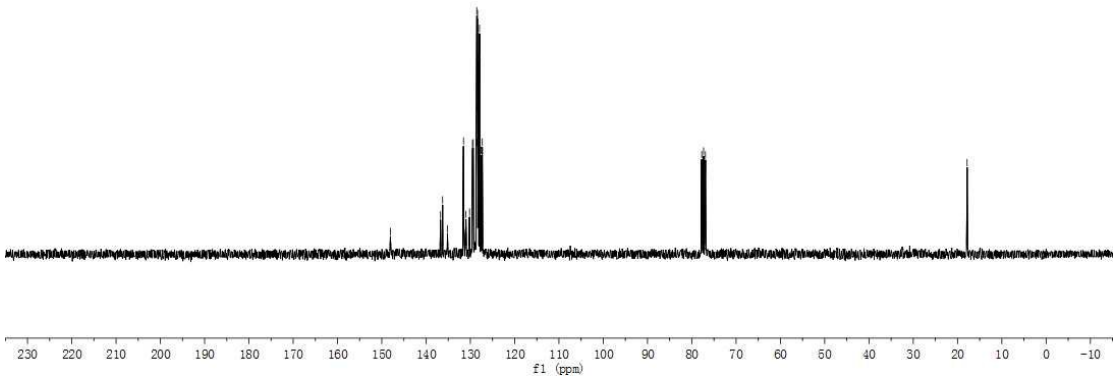

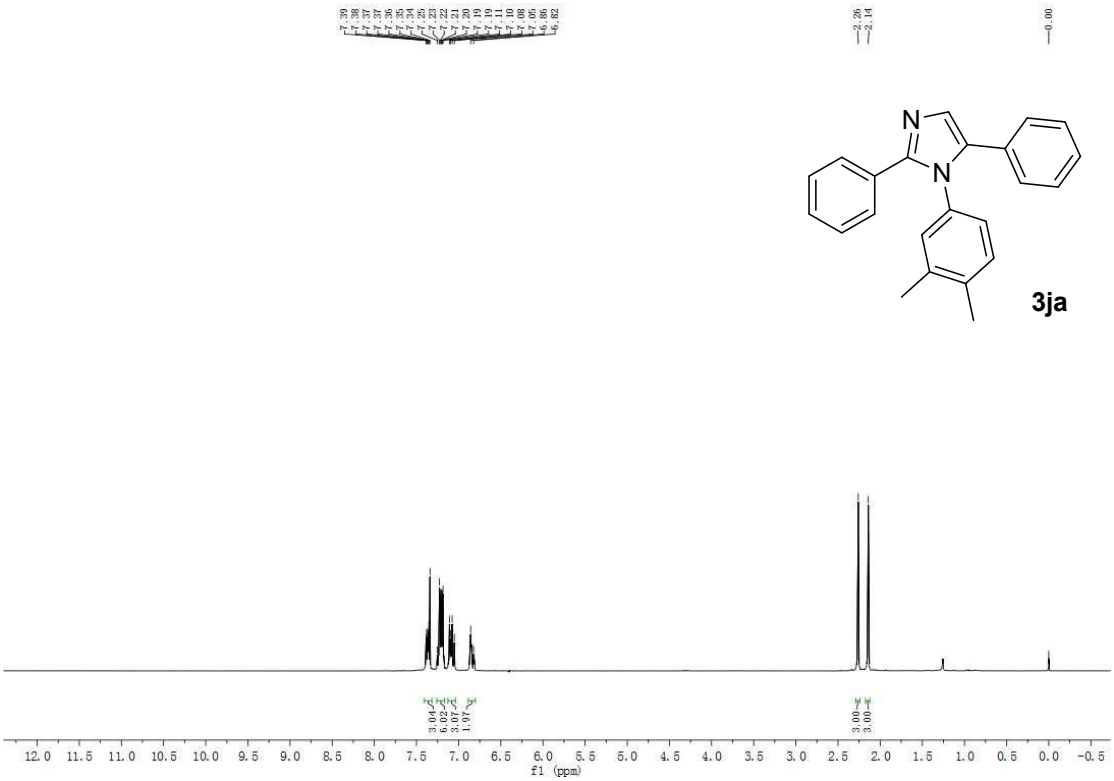
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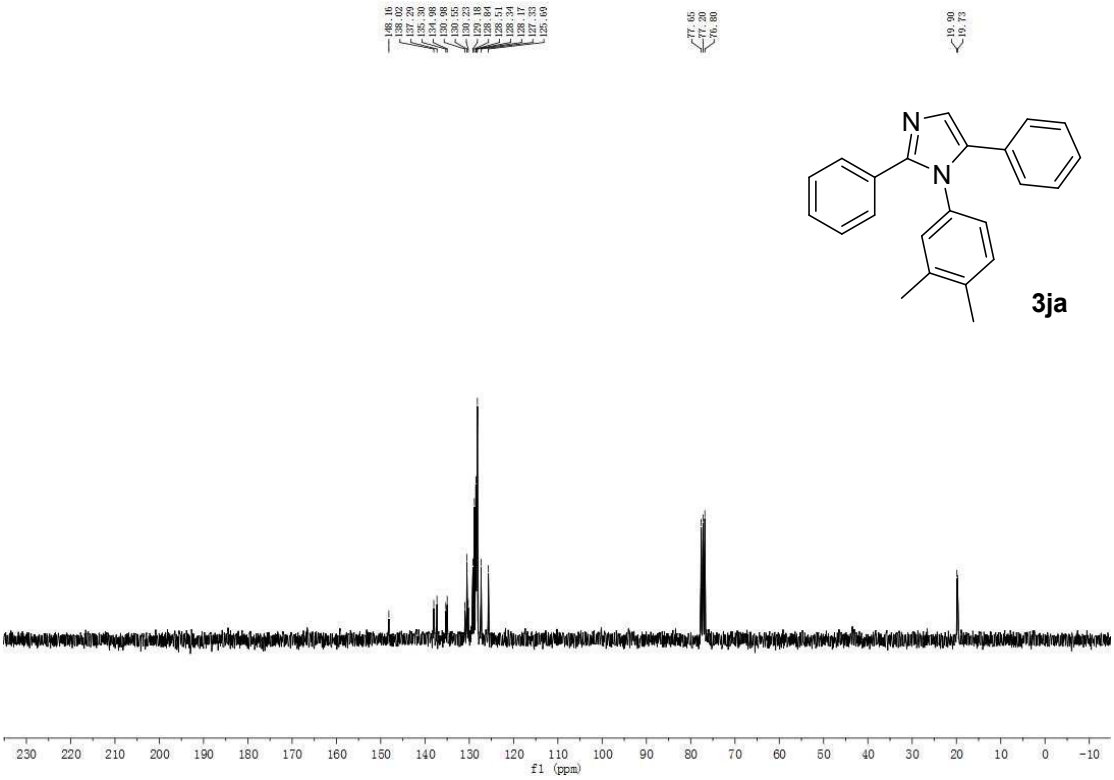
7.21
7.20
7.19
7.19
7.11
7.10
7.08
7.05
6.85
6.82
2.26
2.14
0.00
3.04
3.02
3.07
1.97
3.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
3ja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138.02
137.29
135.30
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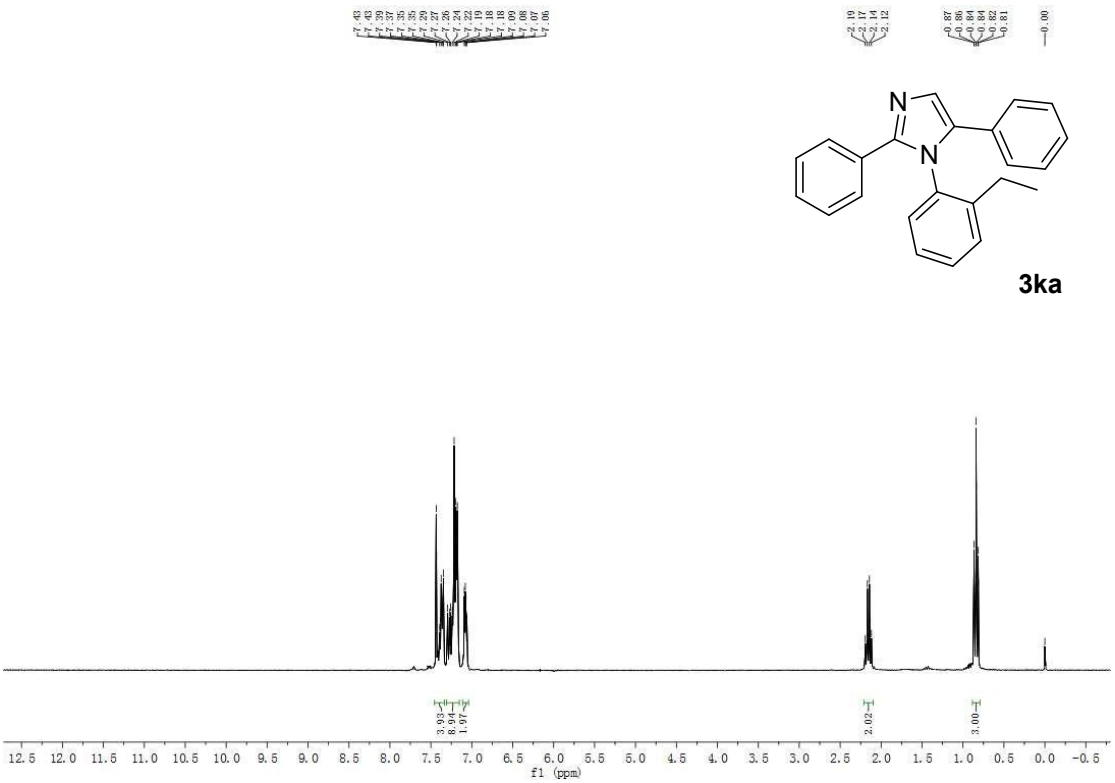
130.55
130.23
129.18
128.64
128.51
128.34
128.17
127.33
125.69
77.65
77.20
76.80
19.90
19.73
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
3ja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7.26
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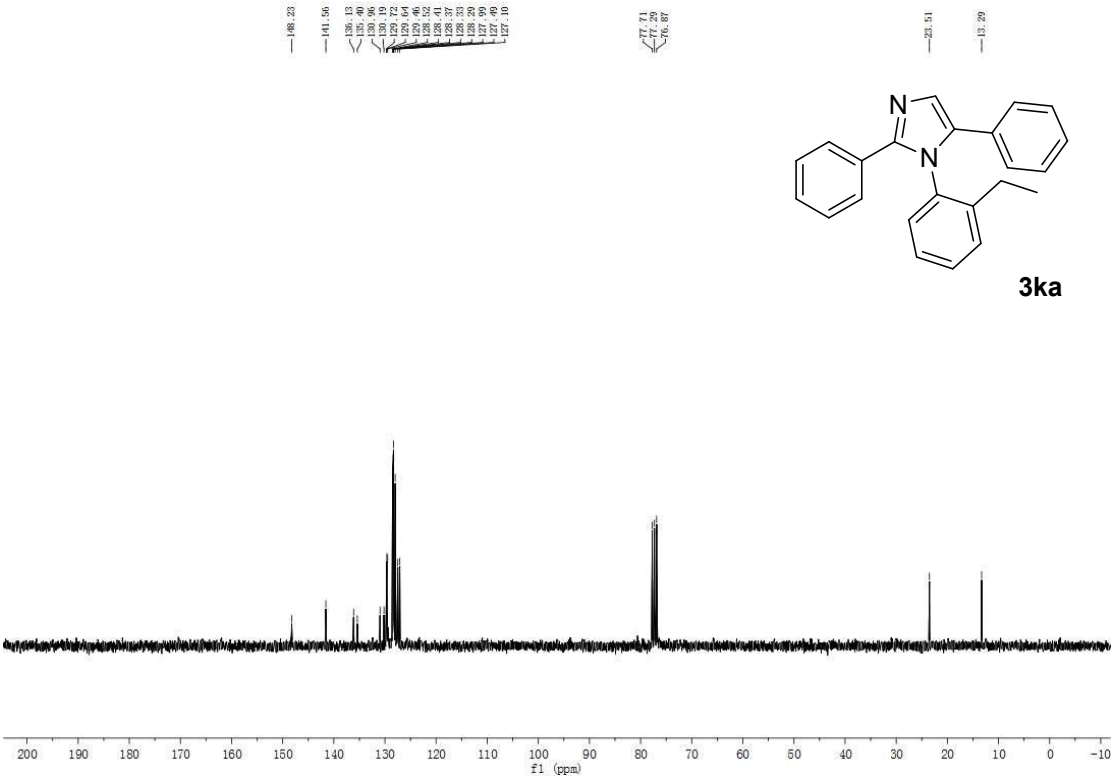
7.22
7.19
7.18
7.10
7.09
7.08
7.07
7.06
2.19
2.17
2.14
2.12
0.87
0.86
0.84
0.84
0.82
0.81
0.00
N
N
3ka
3.93
8.94
1.97
2.02
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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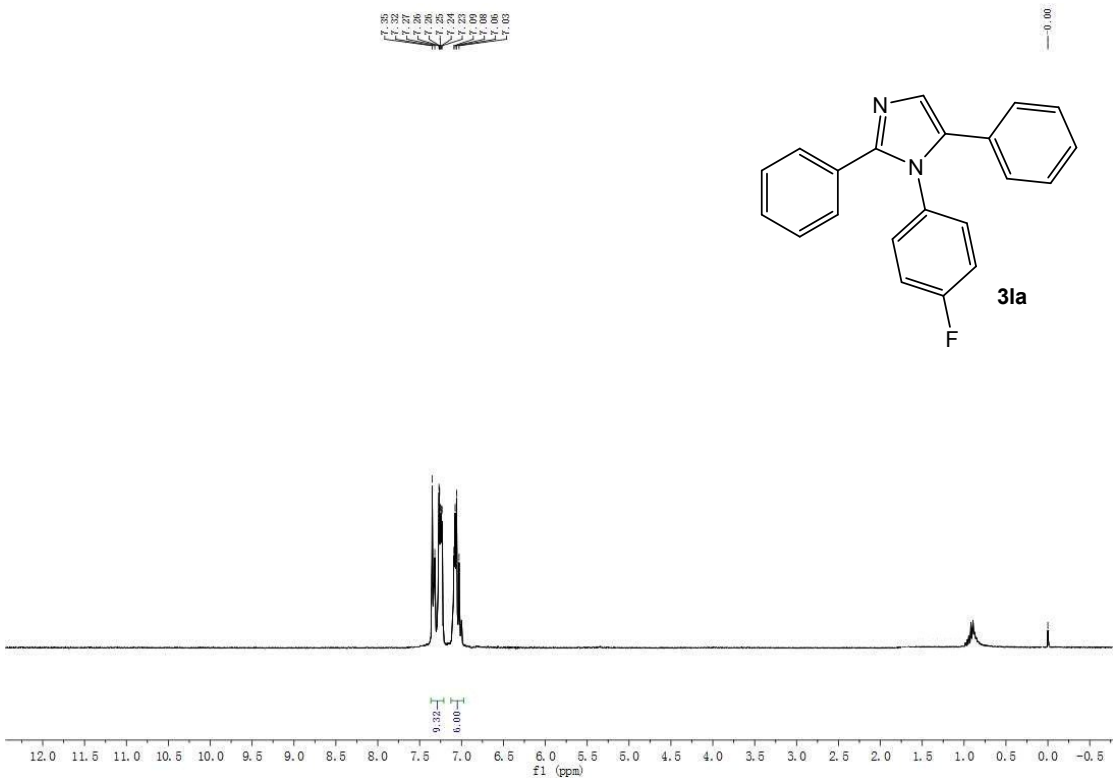
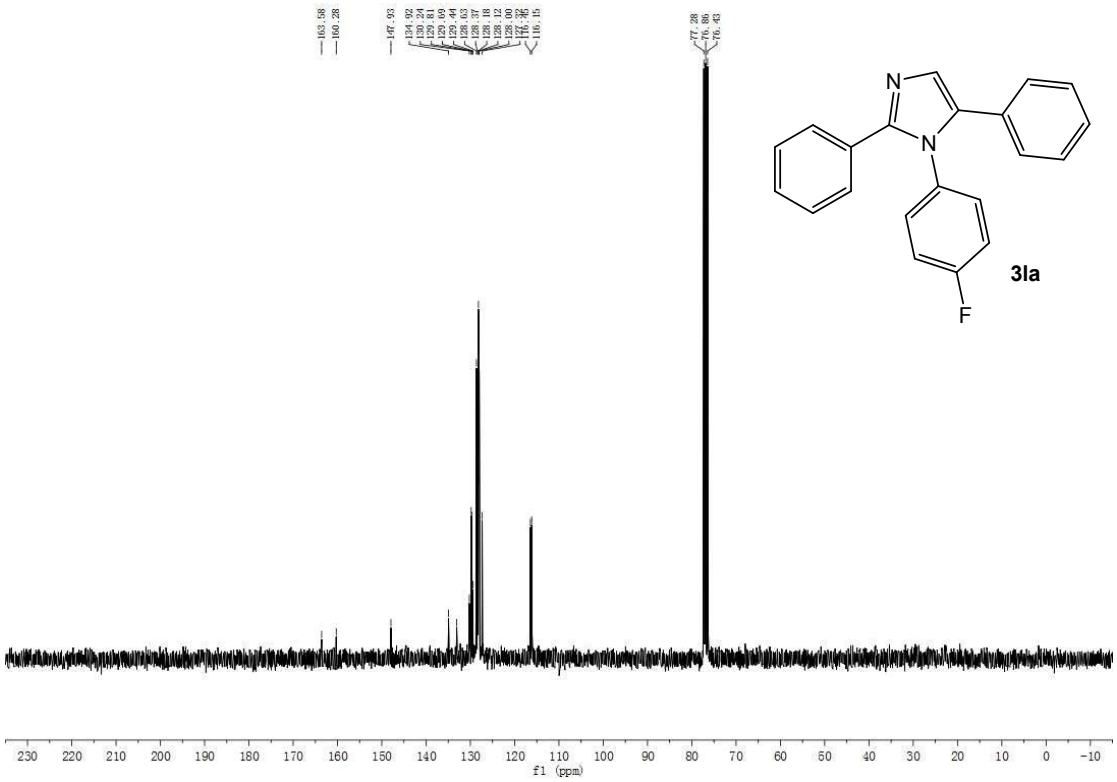
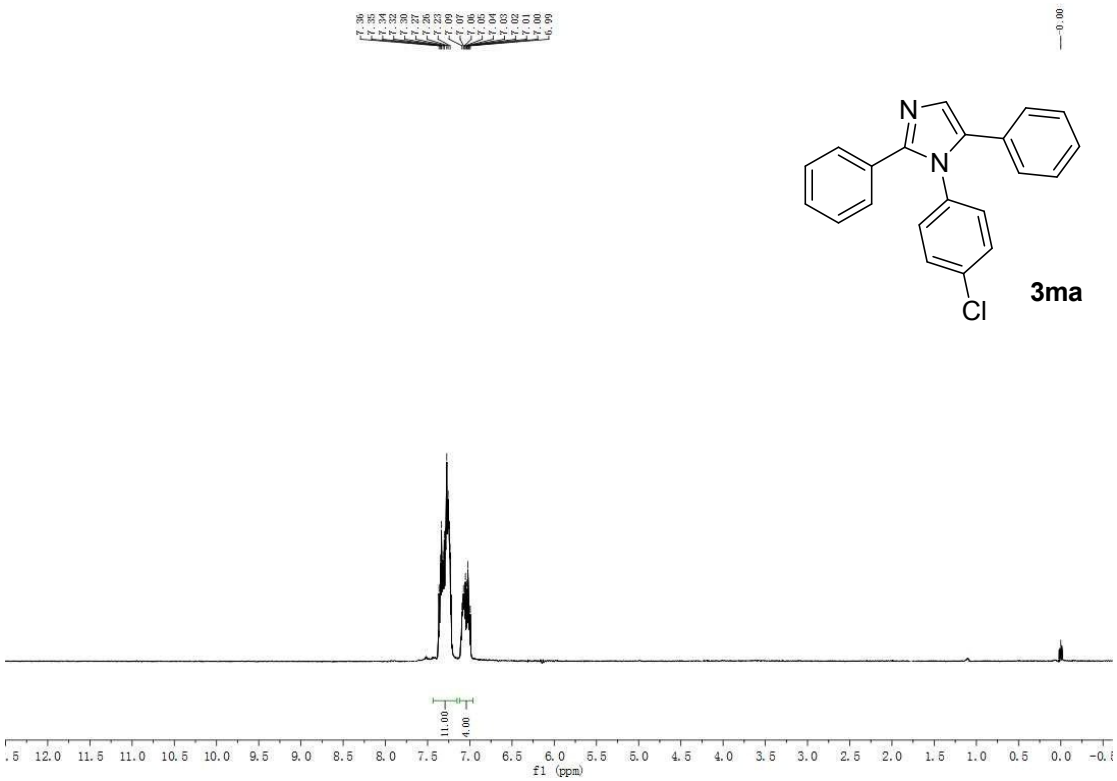
128.33
128.29
127.99
127.49
127.10
77.71
77.29
76.87
23.51
13.29
N
N
3ka
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


N
N
F
3la
9.32
6.00
f1 (ppm)


N
N
F
3la
f1 (ppm)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N
Cl
3ma
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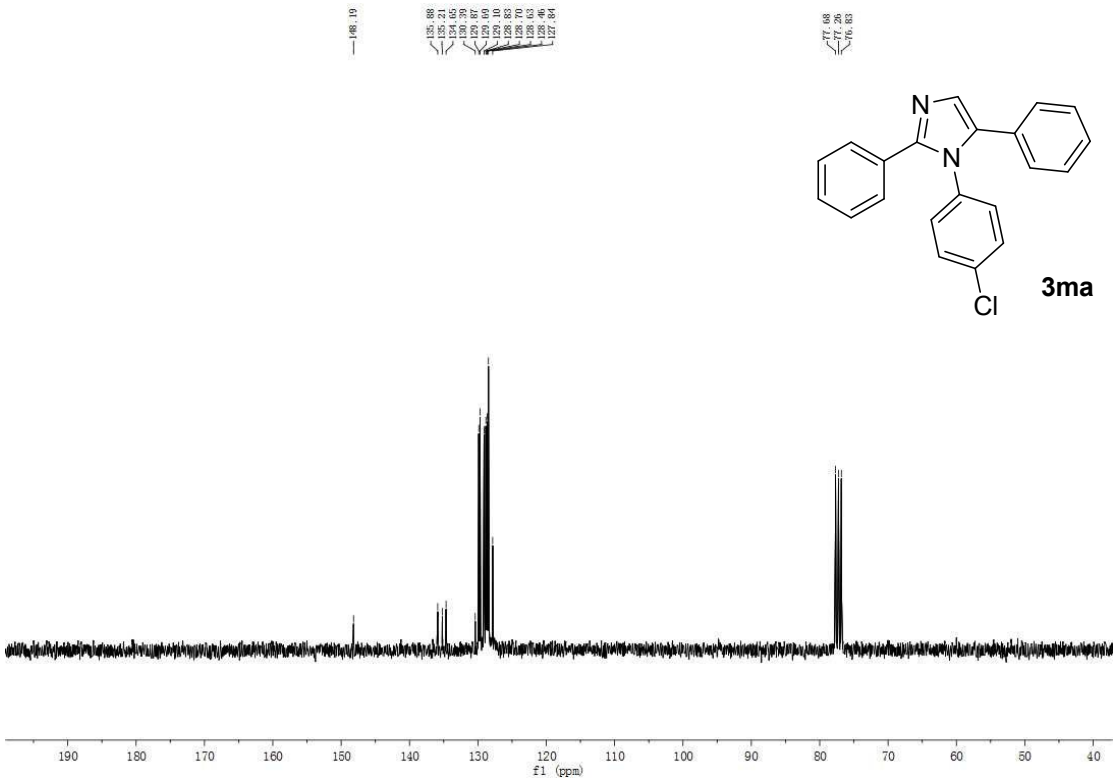
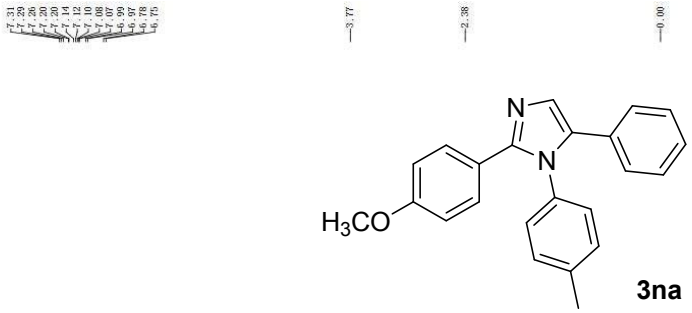
4.00
f1 (ppm)


N
N
Cl
3ma
f1 (ppm)



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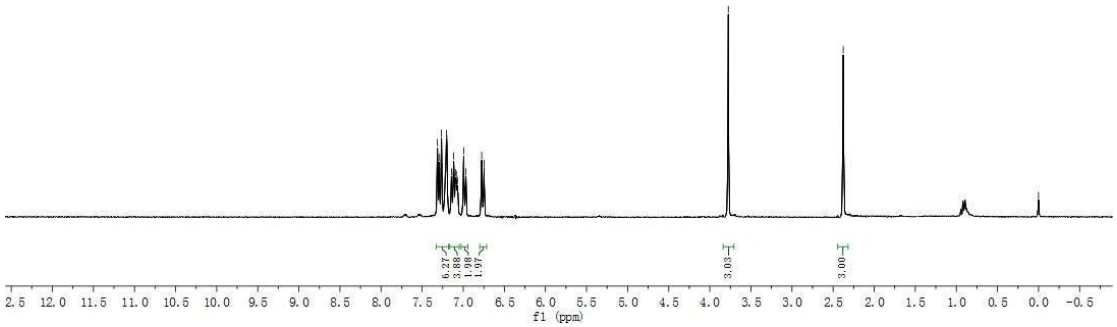

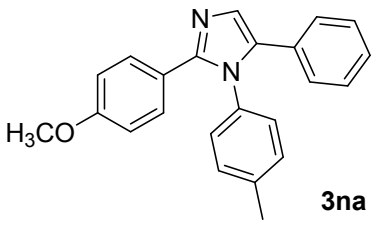

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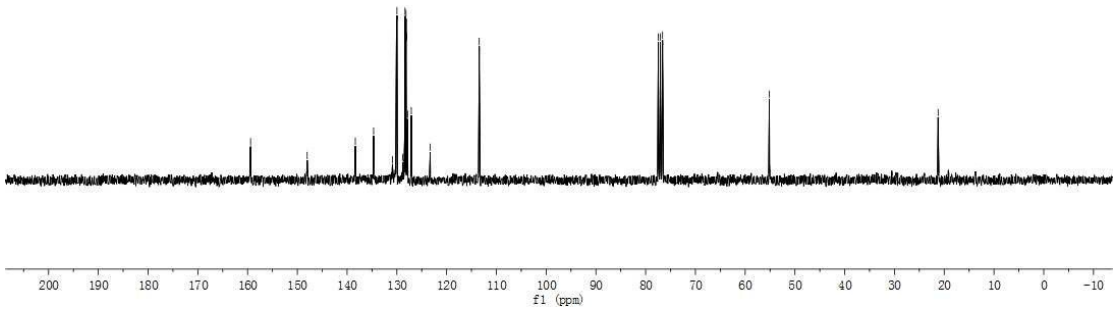

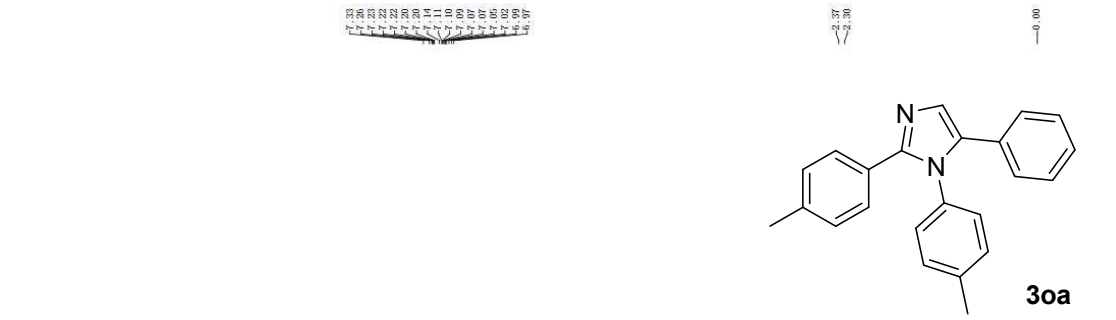
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7.20
7.14
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7.07
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7.05
7.02
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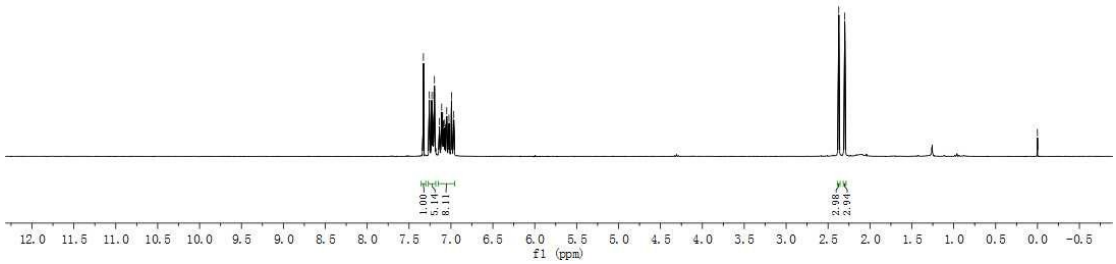
6.97
2.37
2.30
0.00
N
N
3oa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5.14
8.11
2.98
2.94
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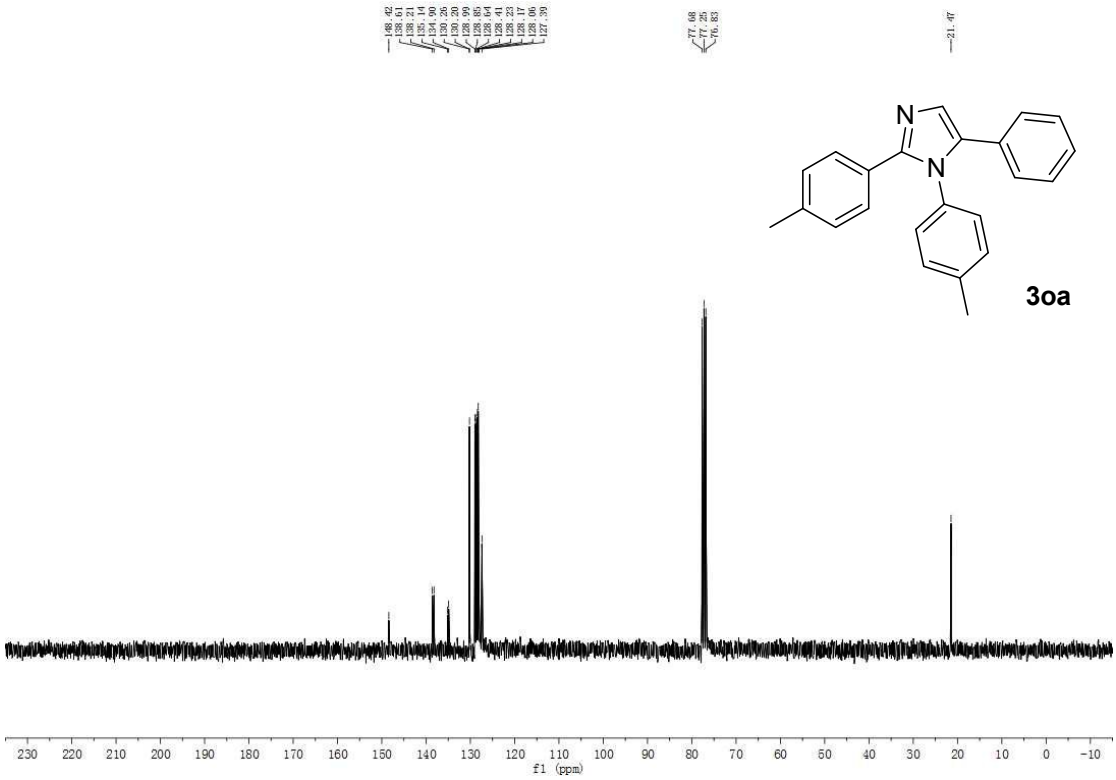
f1 (ppm)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127.99
77.68
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N
N
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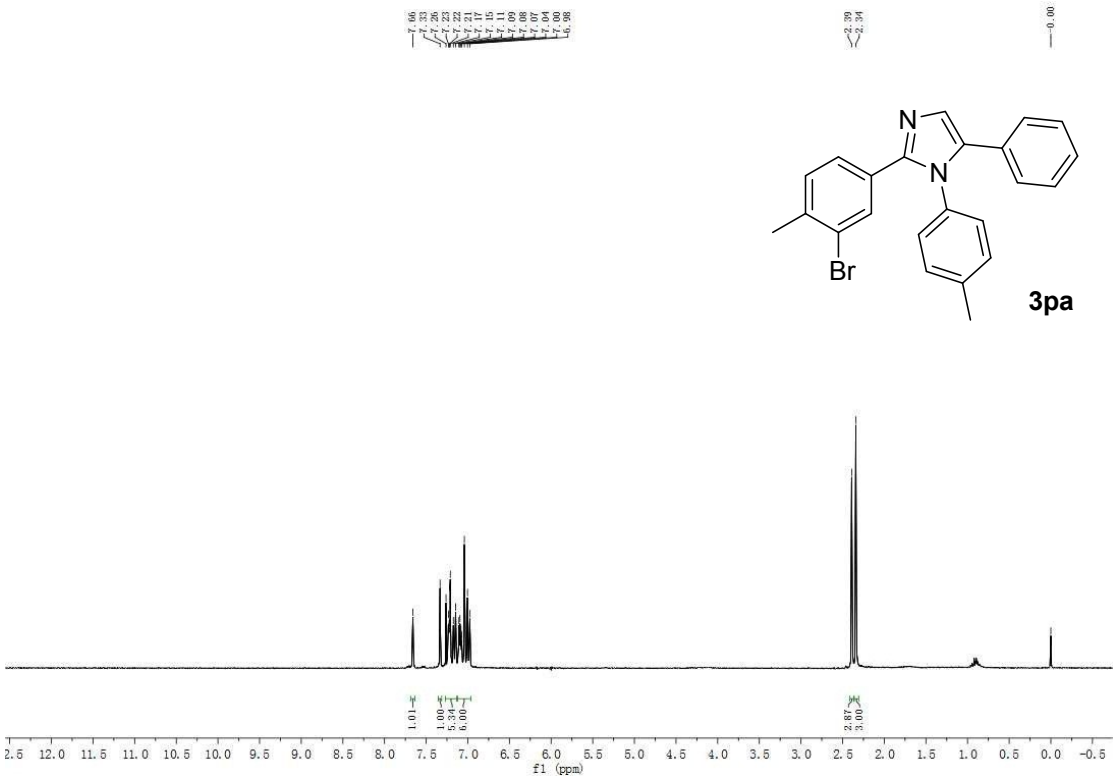
f1 (ppm)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7.07
7.04
7.00
6.98
2.39
2.34
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N
Br
3pa
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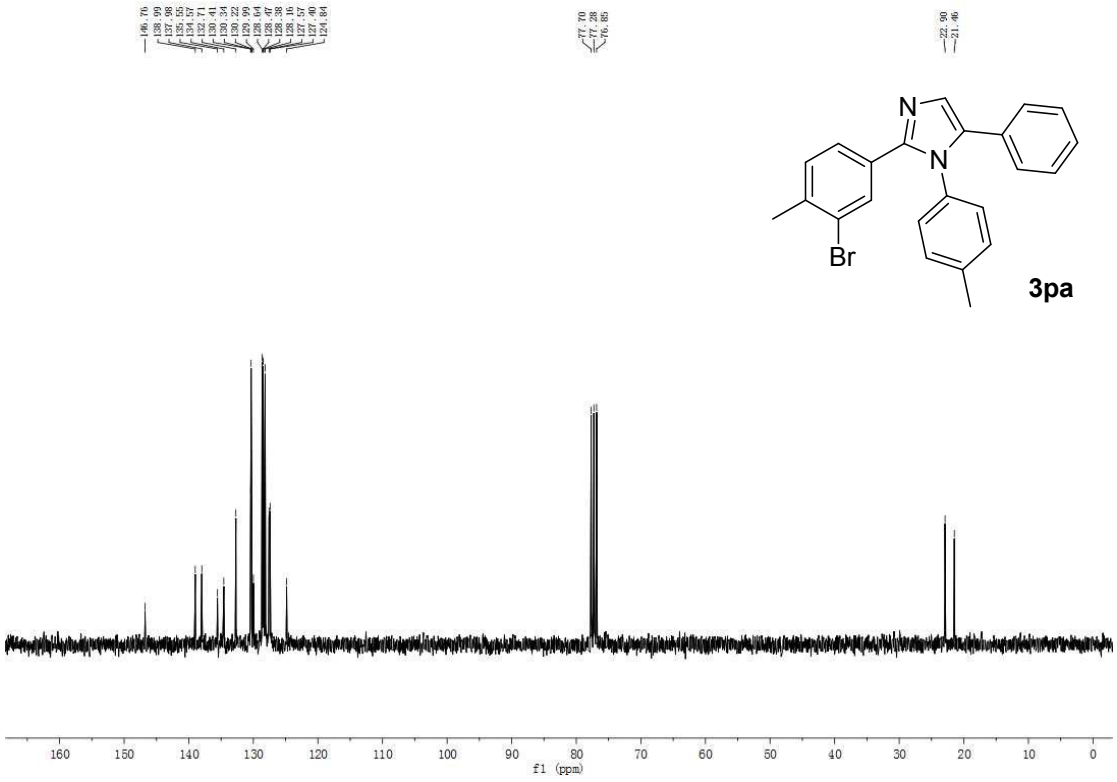
1.00
5.34
6.00
2.87
3.00
f1 (ppm)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76.85
22.90
21.46
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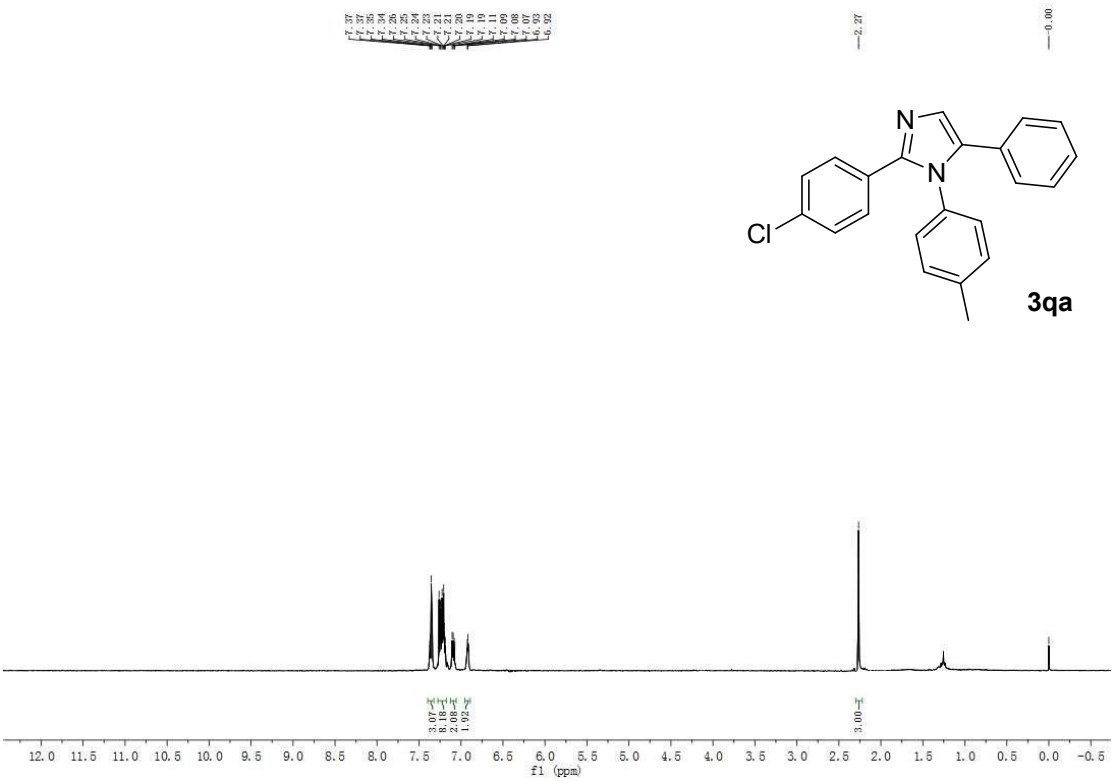
N
Br
3pa
f1 (ppm)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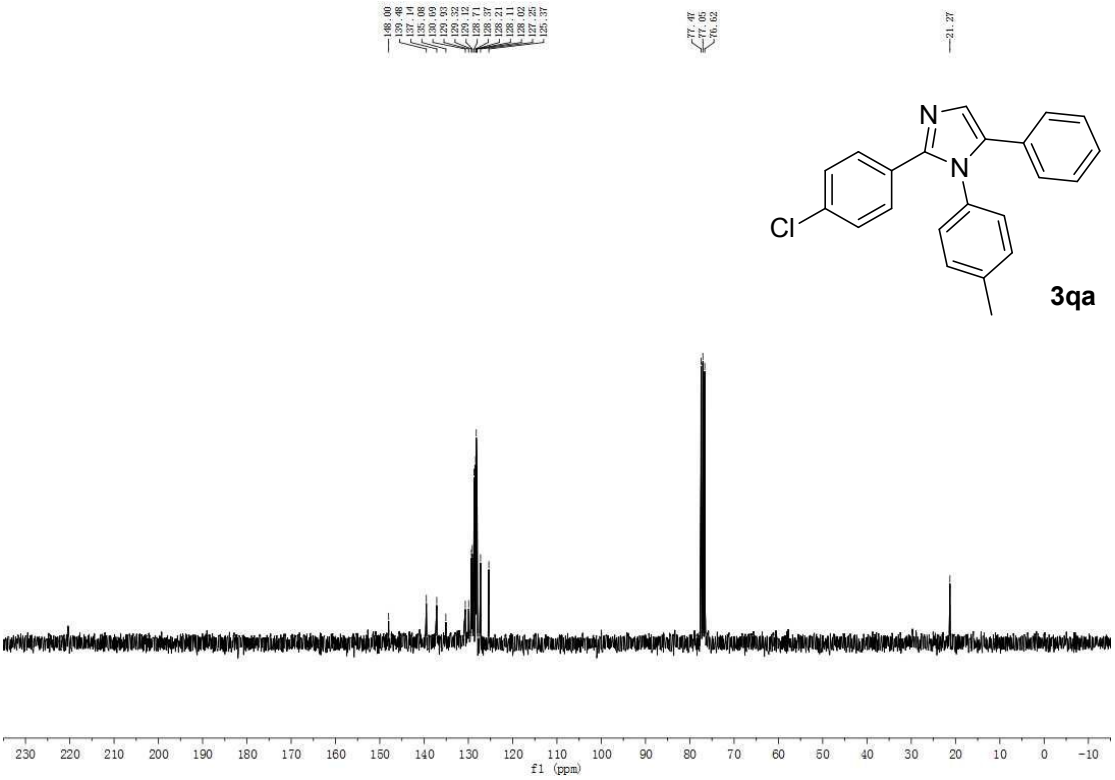
7.09
7.08
7.07
6.93
6.92
2.27
0.00
N
N
Cl
3qa
3.07
8.18
2.08
1.92
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.12
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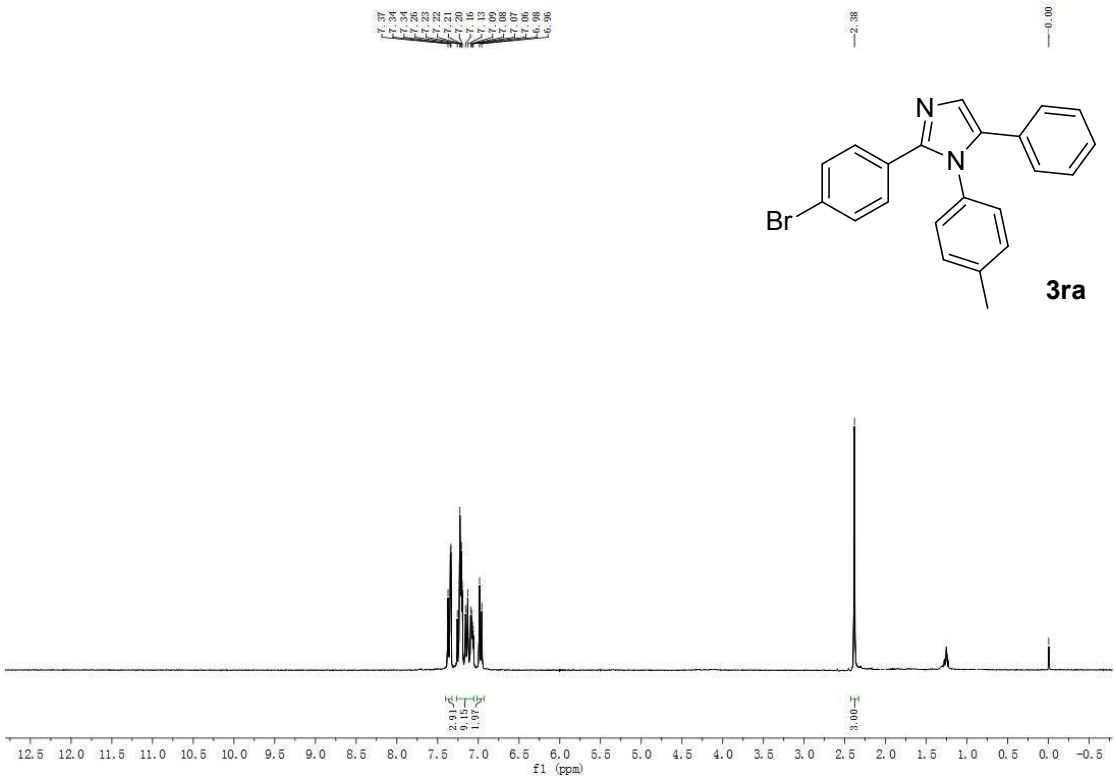
128.21
128.11
128.02
127.25
125.37
77.47
77.05
76.62
21.27
N
N
Cl
3qa
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.37
7.34
7.34
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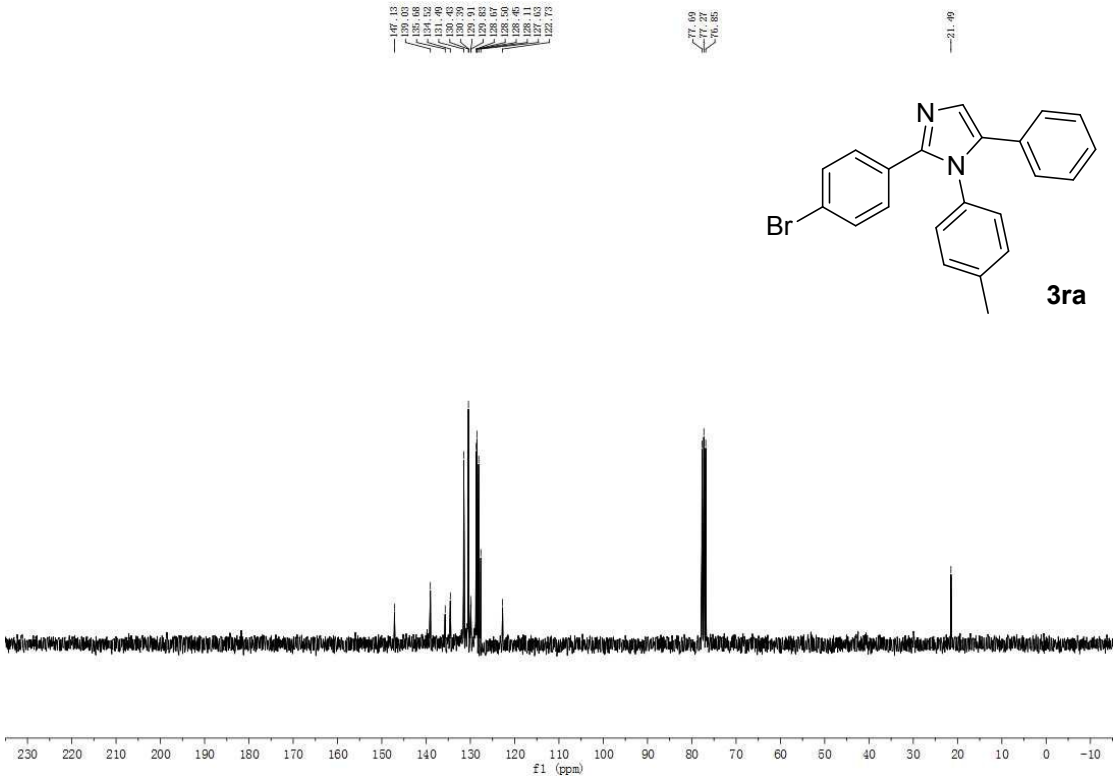
7.16
7.13
7.09
7.08
7.07
7.06
6.98
6.96
2.38
0.00
N
N
Br
3ra
2.91
9.15
1.91
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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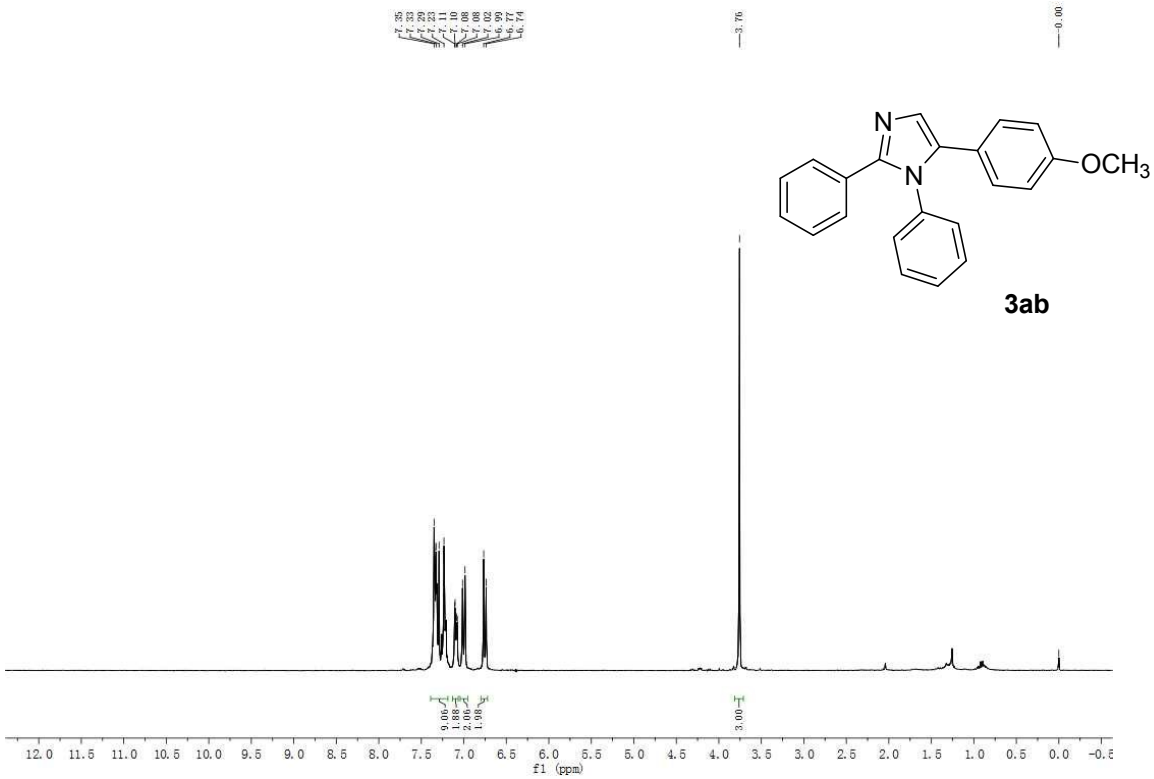
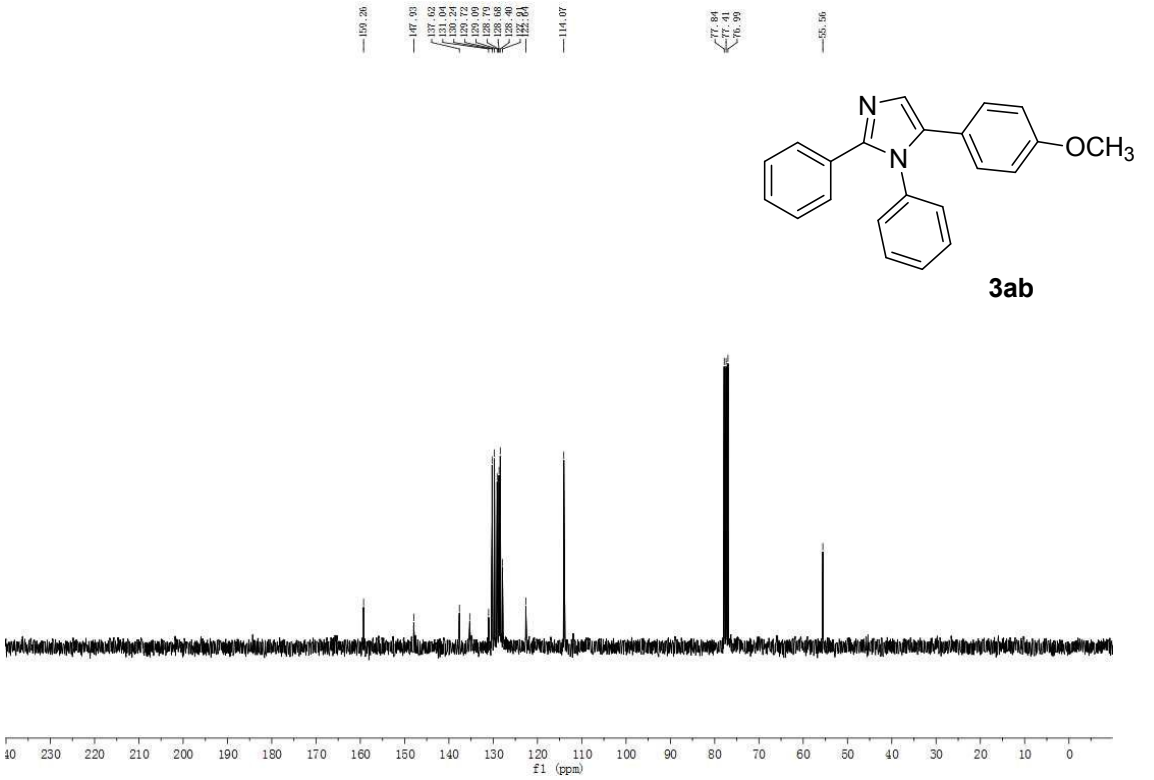
128.67
128.50
128.46
128.11
127.63
122.73
77.69
77.27
76.85
21.49
N
N
Br
3ra
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.35
7.33
7.29
7.23
7.11
7.10
7.08
7.08
7.05
6.99
6.77
6.74
3.76
0.00
N
N
OCH3
9.06
1.88
2.06
1.98
3.00
12.0 11.5 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)

3ab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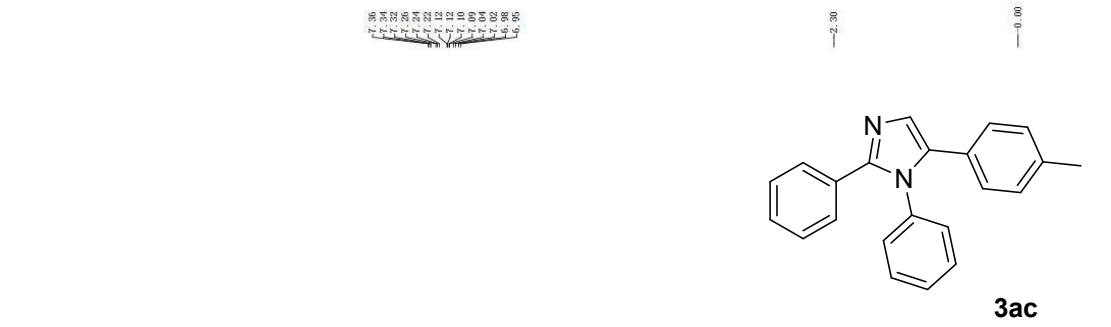
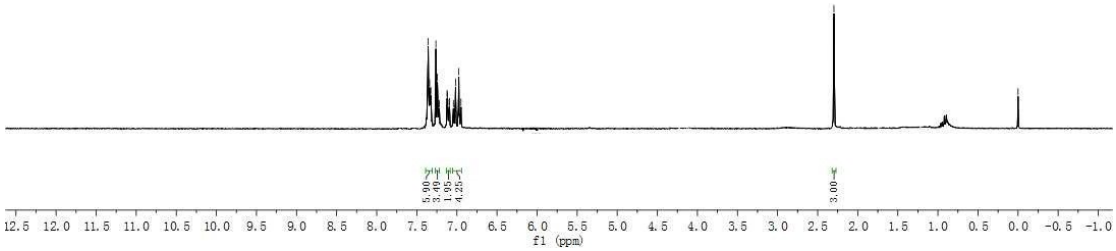
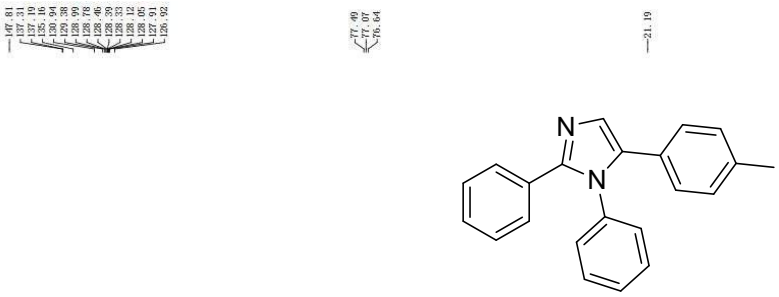
147.93
137.62
131.04
130.24
129.72
129.09
128.79
128.68
128.40
122.21
114.07
77.84
77.41
76.99
55.56
N
N
OCH3
40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ab


7.36
7.34
7.32
7.25
7.24
7.22
7.12
7.10
7.09
7.04
7.02
6.98
6.95
2.39
0.00
N
N

3ac


5.90
3.49
1.95
4.25
3.00
12.5 12.0 11.5 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 -0.5 -1.0
f1 (ppm)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137.31
137.19
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129.38
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128.78
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128.05
127.91
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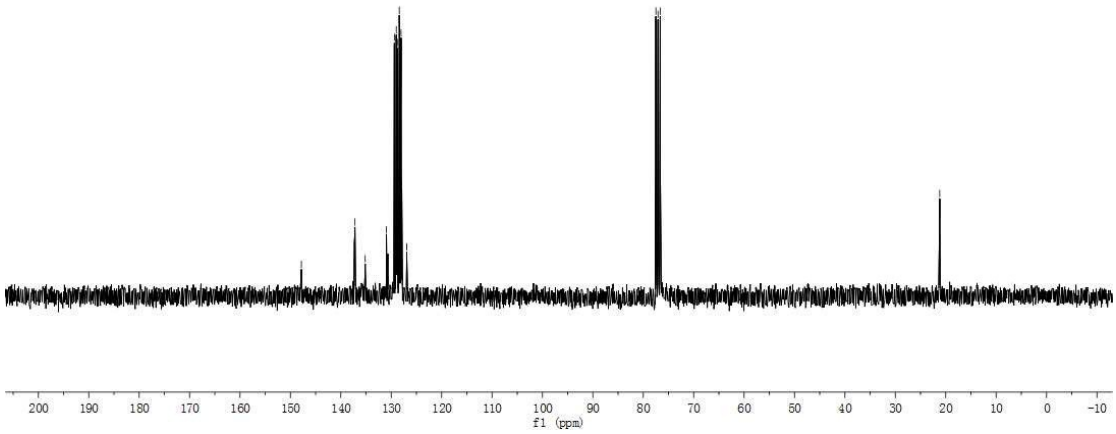
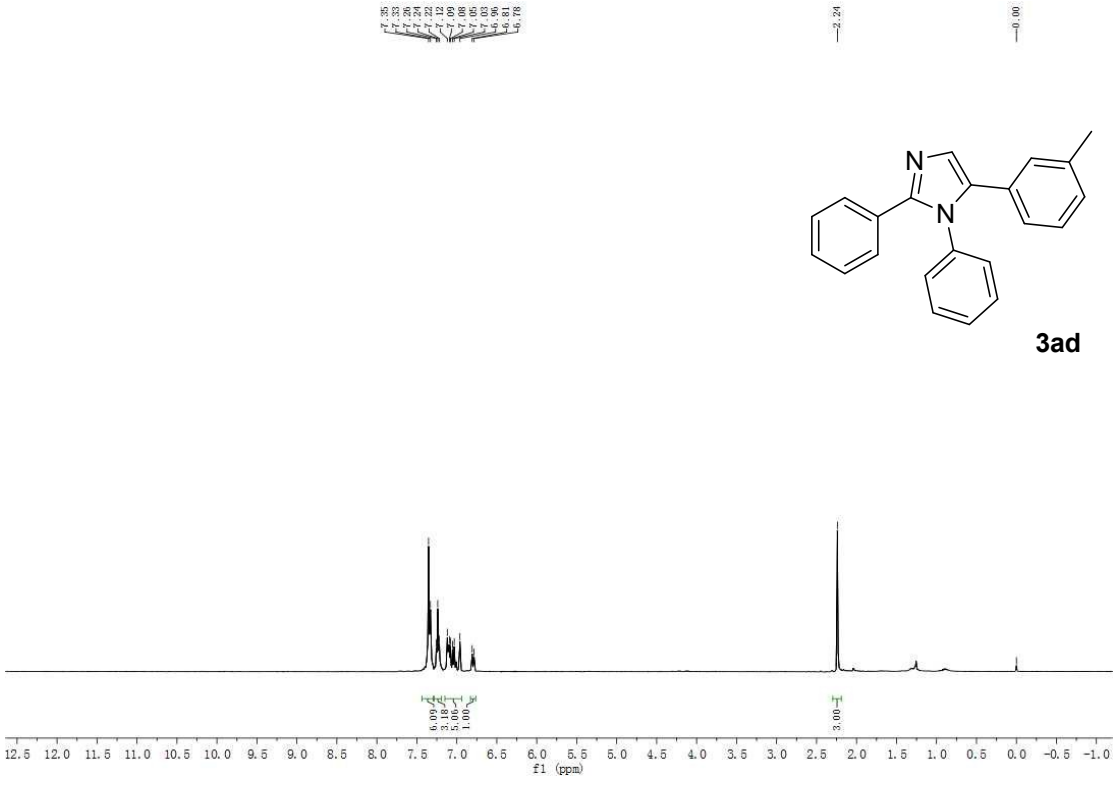
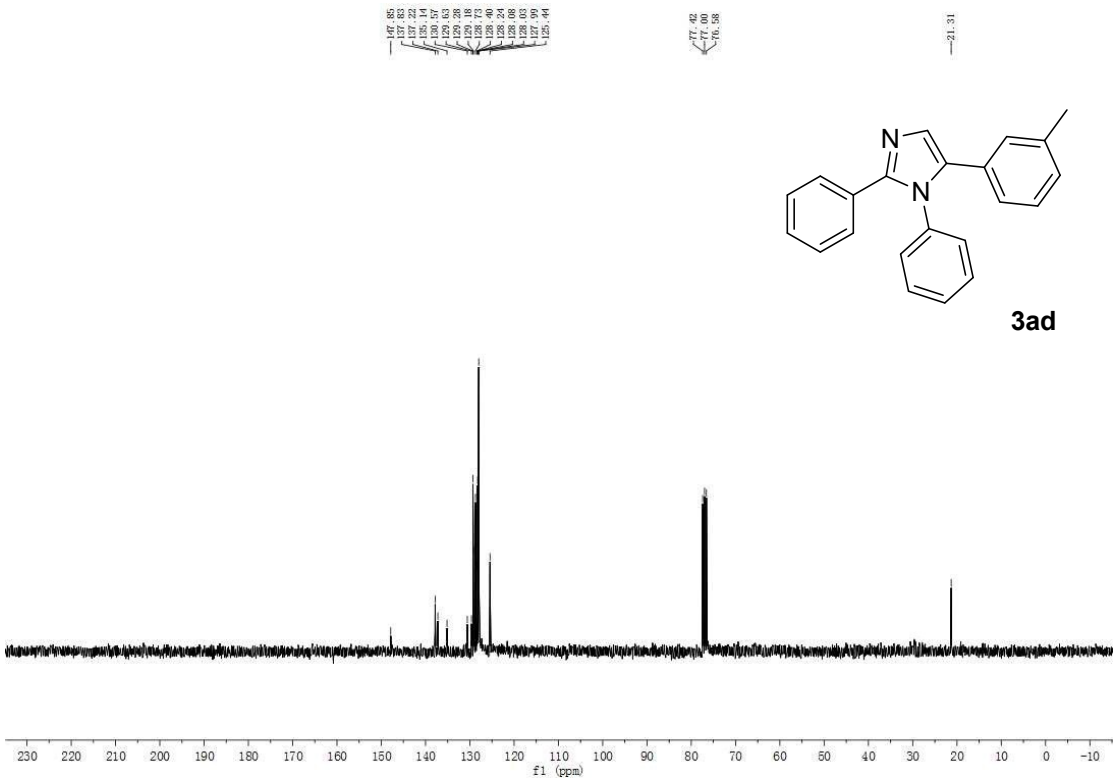
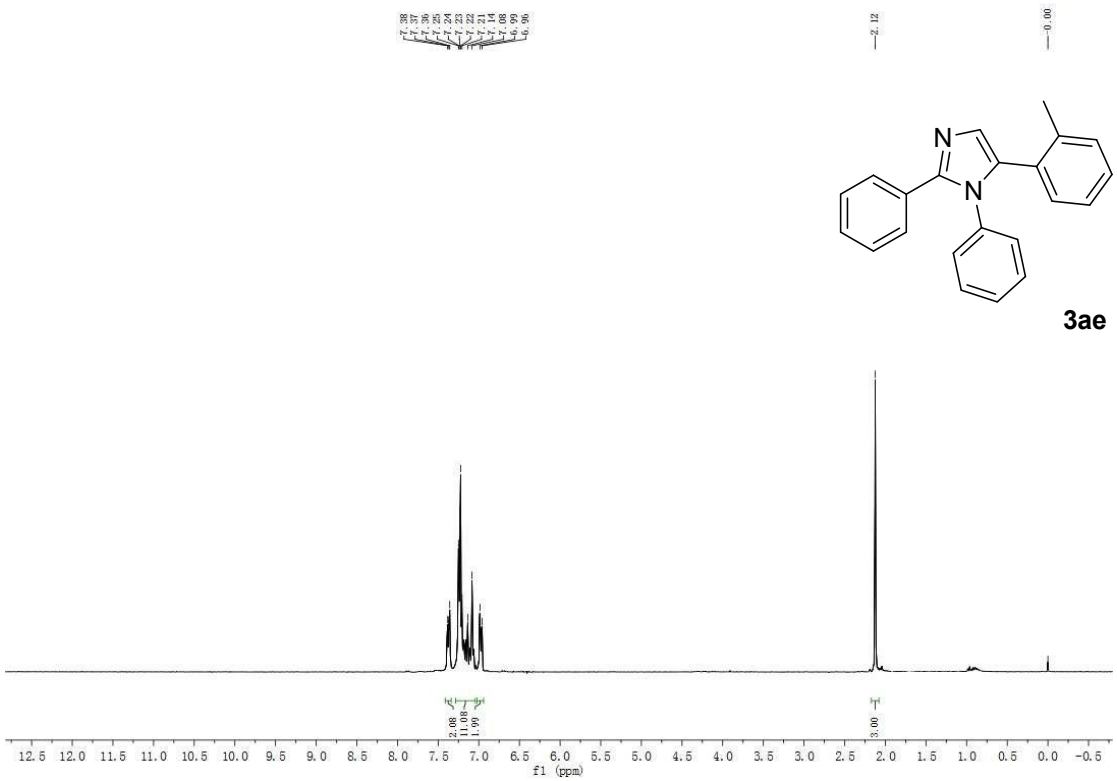
77.07
76.64
21.19
N
N

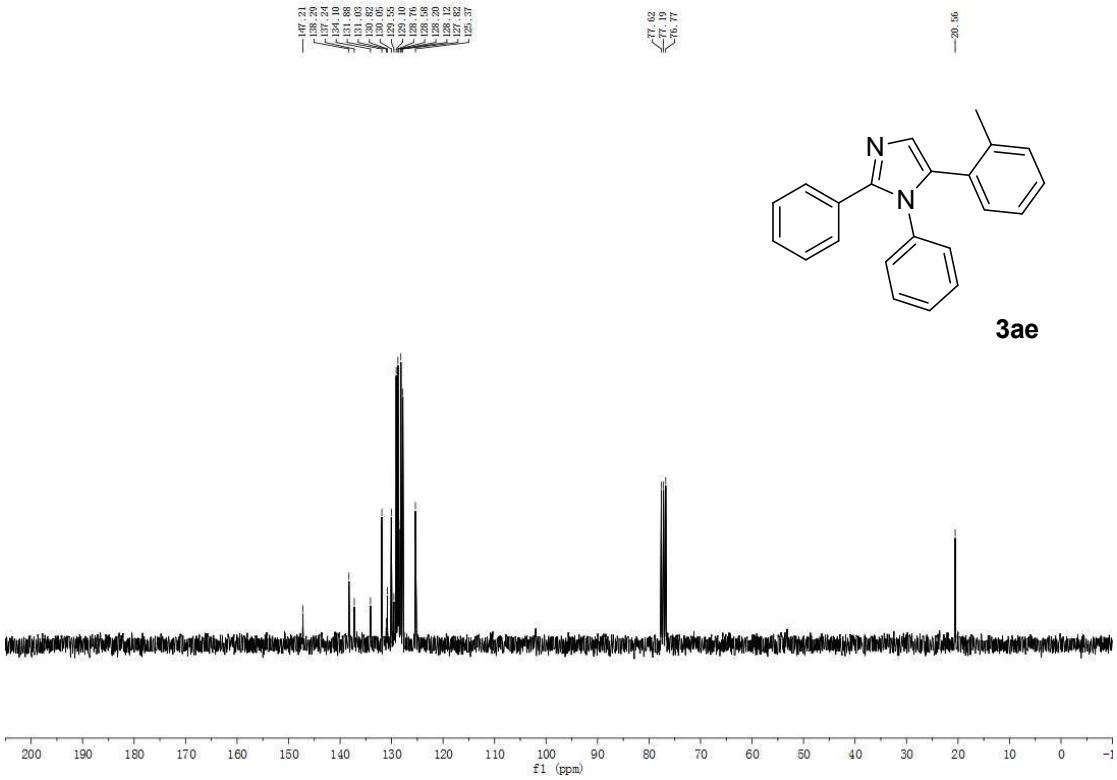
3ac

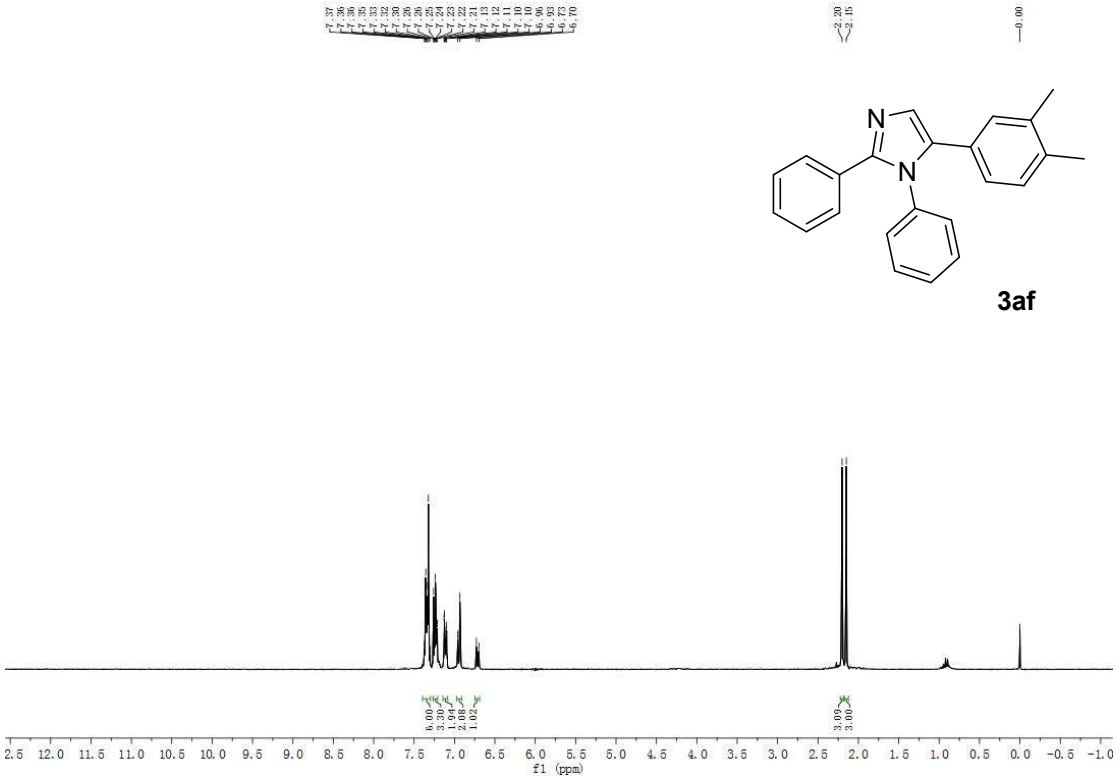

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

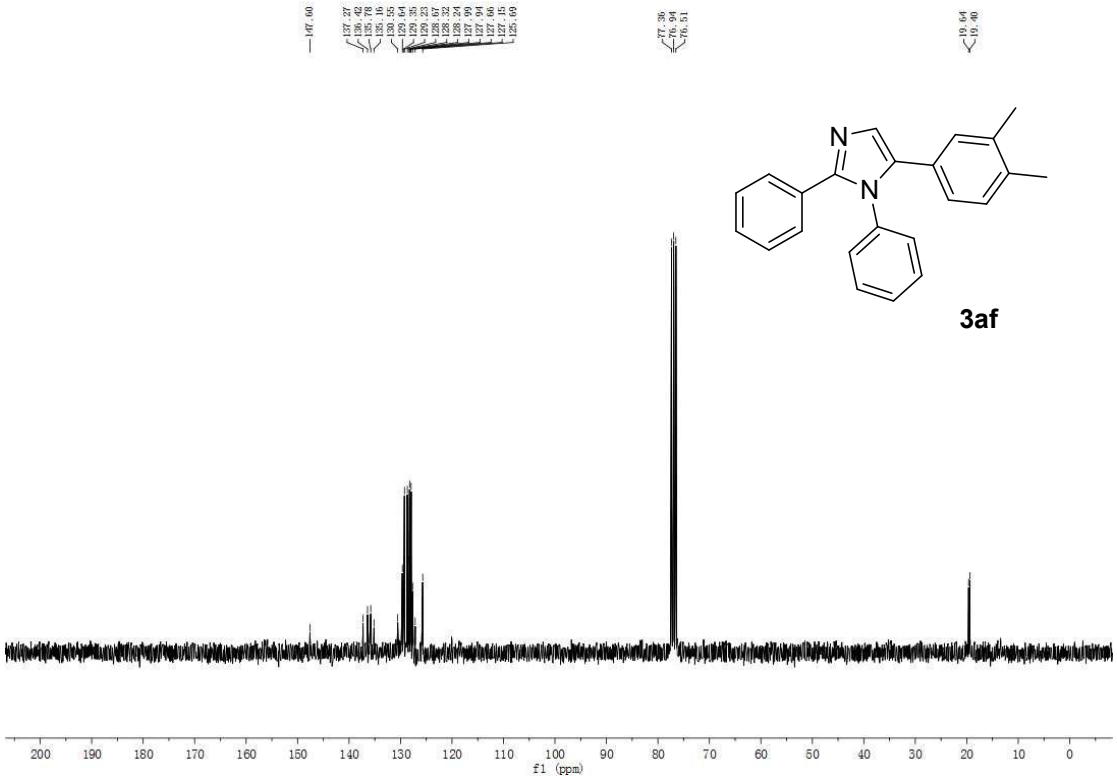

7.35
7.33
7.26
7.24
7.22
7.12
7.09
7.08
7.05
7.03
6.96
6.81
6.78
2.24
0.00
N
N
3ad
6.09
3.18
5.06
1.00
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

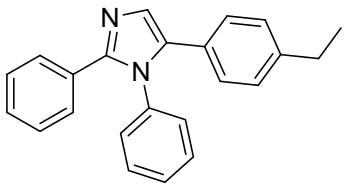

147.85
137.83
137.22
135.14
130.57
129.55
129.28
129.18
128.73
128.49
128.29
128.08
128.03
127.99
125.44
77.42
77.00
76.58
21.31
N
N
3ad
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.38
7.37
7.36
7.25
7.24
7.23
7.22
7.21
7.14
7.08
6.99
6.96
2.12
0.00
N
N
3ae
2.08
11.06
1.99
3.00
12.5 12.0 11.5 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 -0.5
f1 (ppm)

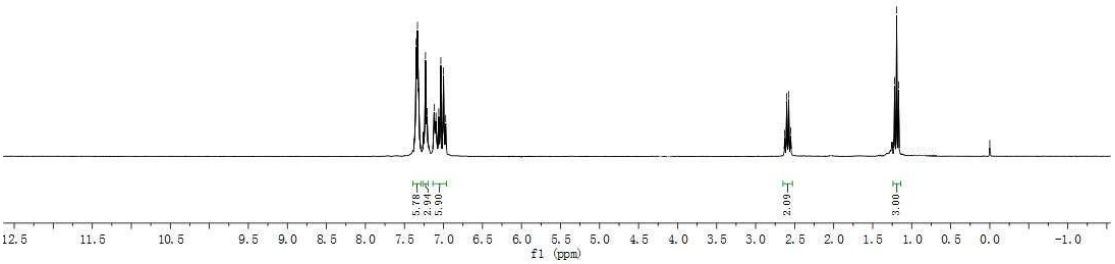

147.21
138.29
137.24
134.19
131.88
131.03
130.82
130.05
129.55
129.10
128.76
128.58
128.29
128.12
127.82
125.37
77.62
77.19
76.77
20.56
N
N
3ae
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

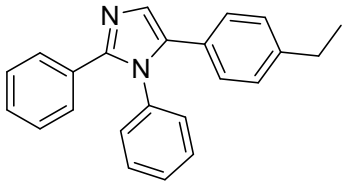

N
N
3af
f1 (ppm)


N
N
3af
f1 (ppm)



3ag





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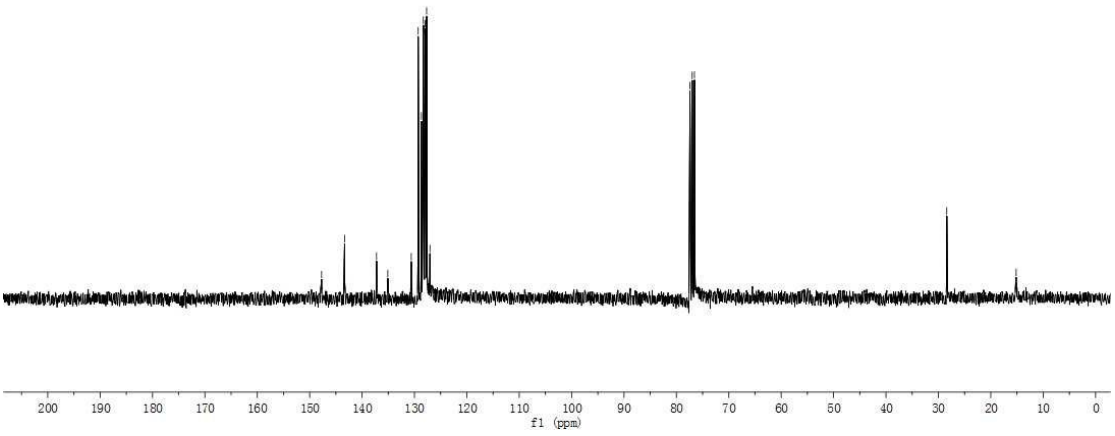
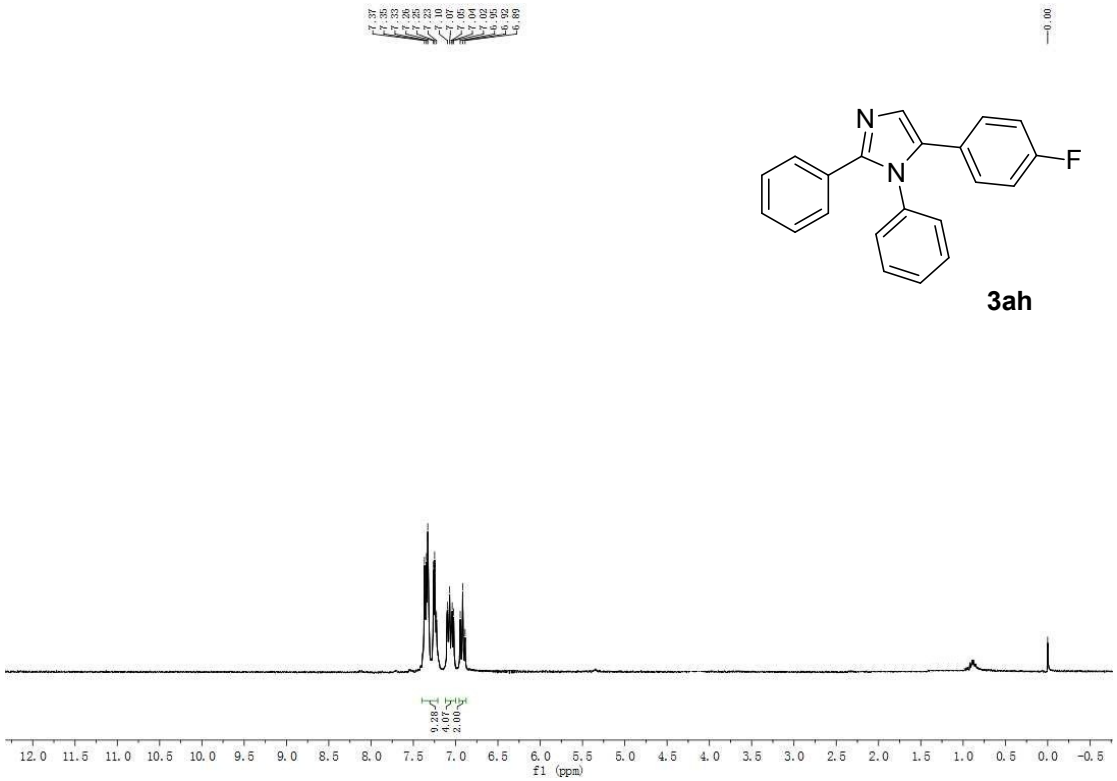
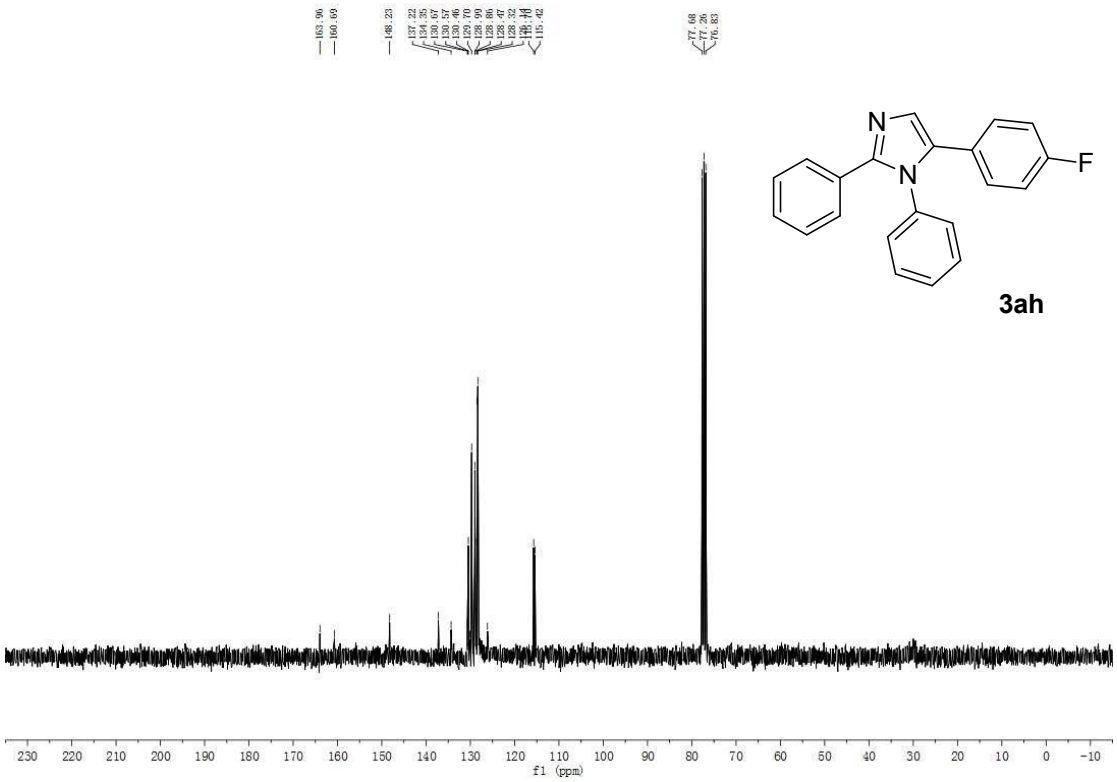
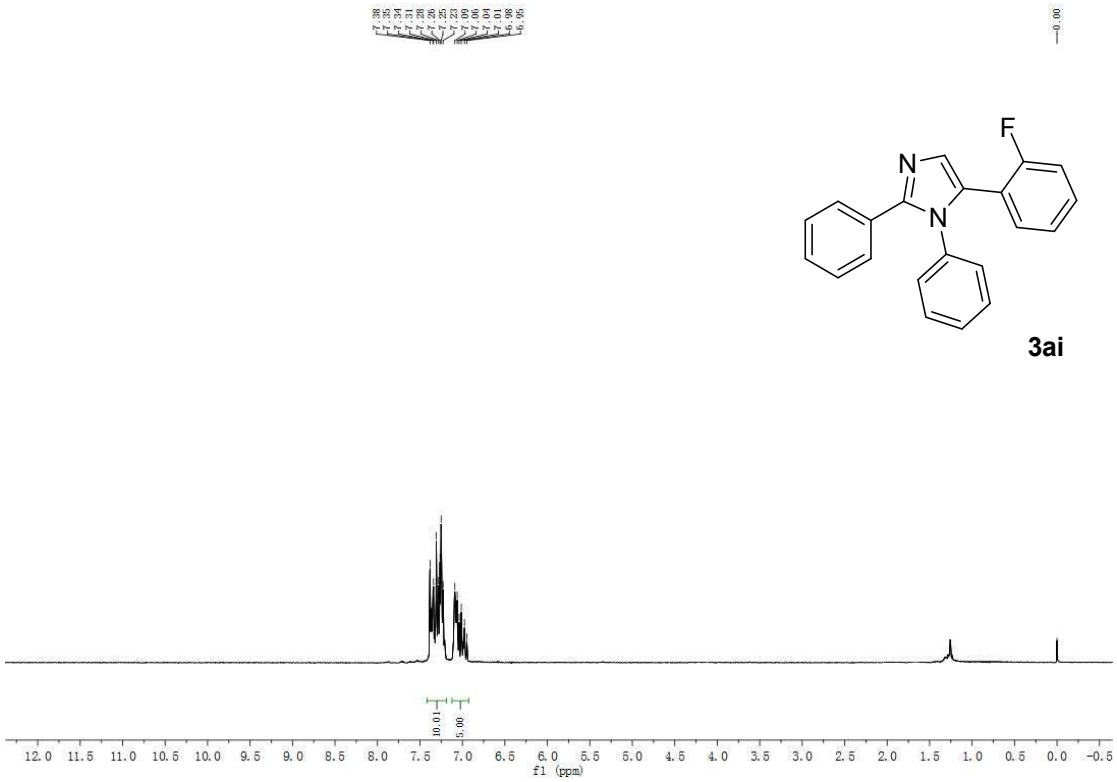
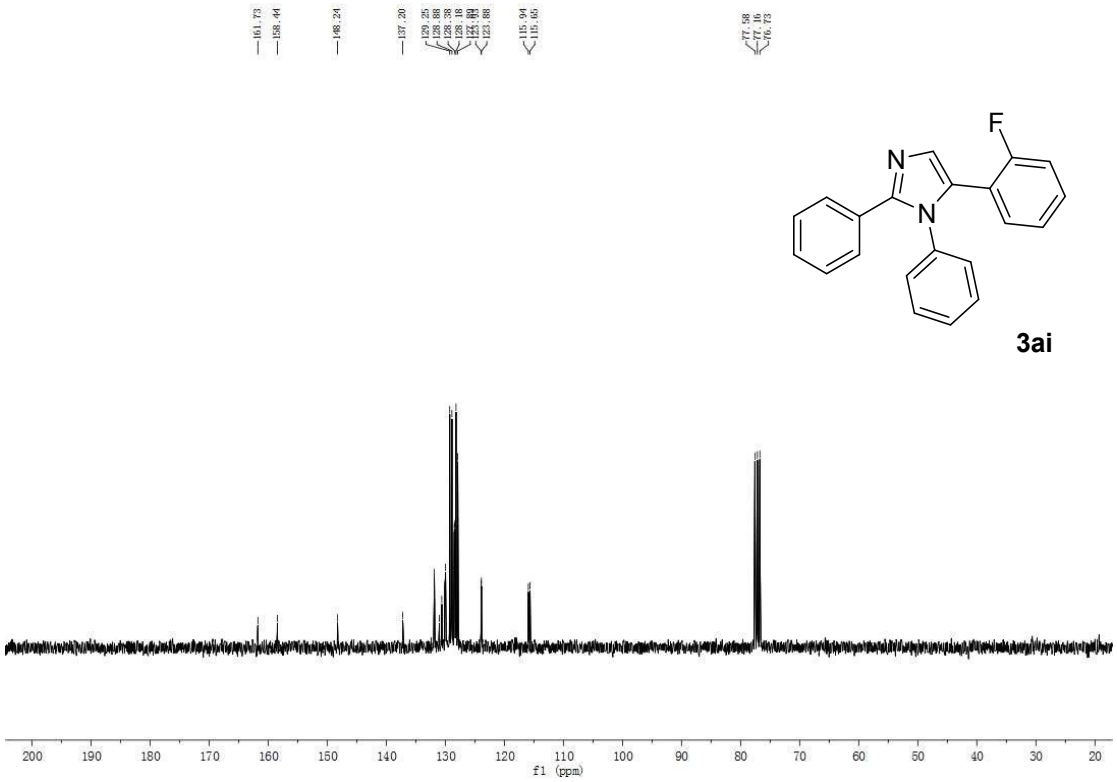



N
N
F
3ah
f1 (ppm)


N
N
F
3ah
f1 (ppm)


F
N
N
3ai
10.01
5.00
f1 (ppm)


F
N
N
3ai
f1 (ppm)