Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Facile and Efficient Method for the Synthesis of 1,2,4-Trisubstituted Imidazoles with Enamides and Benzylamines

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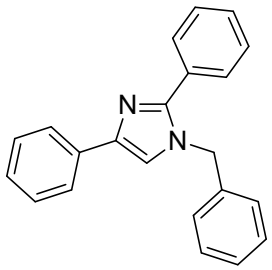
1. General remark

^{1}H-NMR spectra were recorded on Bruker avance III-400 spectrometers. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ as an internal standard. ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.00 ppm). Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. Unless otherwise noted, commercially available reagents and solvents were used without further purification. The enamides were in all cases prepared from the corresponding ketoximes according to reported literature. [19]

2. General experimental procedure

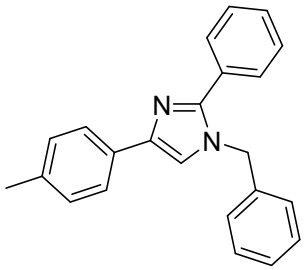
A test tube equipped with a magnetic stir bar was charged with enamides **1a** (0.2 mmol), benzylamine **2a** (0.6 mmol), CuBr (0.02 mmol) and I_2 (0.01 mmol) were mixed in 1, 4-dioxane (2 mL). Then the reaction mixture was stirred at 60 ^{o}C for 8 h. The reaction mixture was cooled down to rt and then extracted with ethyl acetate. The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/EtOAc (10:2-4:1) to afford the desired imidazoles **3aa**.

3. Characterization data of 1,2,4-trisubstituted



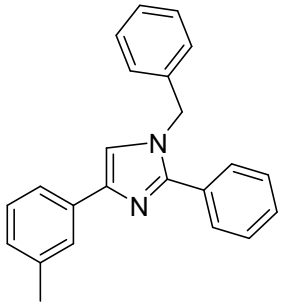
1-benzyl-2, 4-diphenyl-1H-imidazole (3aa).

Yellow Solid, mp: 121-123℃. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84-7.81 (m, 2 H), 7.61-7.58 (m, 2 H), 7.42-7.27 (m, 8 H), 7.24-7.19 (m, 2 H), 7.13-7.11 (m, 2 H), 5.19 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.56, 141.47, 136.80, 134.01, 130.41, 128.96, 128.94, 128.56, 128.47, 127.91, 126.74, 126.61, 124.87, 116.78, 50.42; MS (EI) m/z: 310.



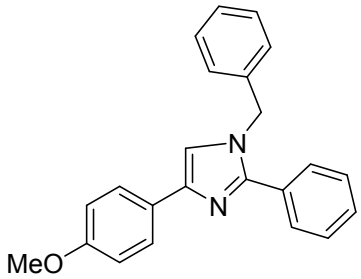
1-benzyl-2-phenyl-4-(p-tolyl)-1H-imidazole (3ba).

Yellow Solid, mp: 138 - 148^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.72-7.70 (m, 2 H), 7.60-7.58 (m, 2 H), 7.42-7.27 (m, 6 H), 7.22-7.15 (m, 3 H), 7.12-7.10 (m, 2 H), 5.17 (s, 2 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.40, 141.59, 136.88, 136.35, 131.25, 130.51, 129.16, 128.97, 128.92, 128.85, 128.53, 127.87, 126.62, 124.81, 116.34, 50.40, 21.15; MS (EI) m/z: 324.



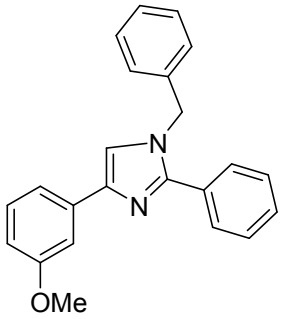
1-benzyl-2-phenyl-4-(m-tolyl)-1H-imidazole (3ca).

Yellow Solid, mp: 130 - 132°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.72-7.70 (m, 2 H), 7.60-7.58 (m, 2 H), 7.42-7.27 (m, 6 H), 7.22-7.15 (m, 3 H), 7.12-7.10 (m, 2 H), 5.17 (s, 2 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.40, 141.59, 136.88, 136.35, 131.25, 130.51, 129.16, 128.97, 128.92, 128.85, 128.53, 127.87, 126.62, 124.81, 116.34, 50.40, 21.15; MS (EI) m/z: 324.



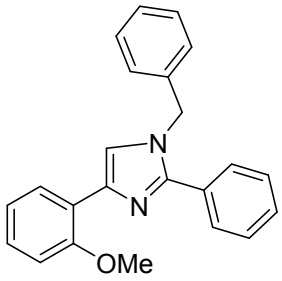
1-benzyl-4-(4-methoxyphenyl)-2-phenyl-1H-imidazole (3ea).

Yellow Solid, mp: 146 - 148°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.76-7.74 (m, 2 H), 7.60-7.58 (m, 2 H), 7.41-7.35 (m, 3 H), 7.33-7.29 (m, 3 H), 7.13-7.11 (m, 3 H), 6.91-6.89 (m, 2 H), 5.18 (s, 2 H), 3.80 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.66, 148.34, 141.35, 136.89, 130.47, 128.95, 128.92, 128.86, 128.54, 127.87, 126.92, 126.61, 126.13, 115.76, 113.91, 55.22, 50.38; MS (EI) m/z: 340.



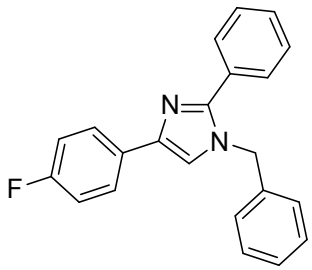
1-benzyl-4-(3-methoxyphenyl)-2-phenyl-1H-imidazole (3fa).

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.62-7.59 (m, 2 H), 7.44-7.39 (m, 4 H), 7.37-7.28 (m, 4 H), 7.26-7.24 (m, 2 H), 7.13-7.12 (m, 2 H), 6.80-6.78 (m, 1 H), 5.21 (s, 2 H), 3.84 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.94, 148.52, 141.37, 136.78, 135.48, 130.39, 129.48, 129.01, 128.98, 128.60, 127.95, 126.64, 117.41, 117.07, 113.01, 109.86, 55.30, 50.47; MS (EI) m/z: 340.



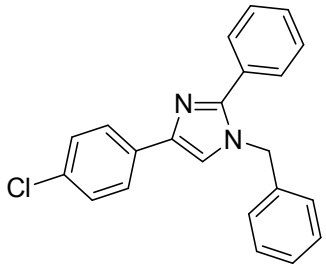
1-benzyl-4-(2-methoxyphenyl)-2-phenyl-1H-imidazole (3ga).

Yellow Solid, mp: 156 - 158^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.36-8.34 (m, 1 H), 7.60-7.58 (m, 3 H), 7.40-7.28 (m, 6 H), 7.24-7.19 (m, 1 H), 7.13-7.11 (m, 2 H), 7.06-7.02 (m, 1 H), 6.94-6.92 (m, 1 H), 5.24 (s, 2 H), 3.89 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.97, 147.36, 137.82, 136.88, 130.66, 128.96, 128.89, 128.77, 128.51, 127.70, 127.56, 127.27, 126.38, 122.73, 121.45, 120.85, 110.53, 55.21, 50.28; MS (EI) m/z: 340.



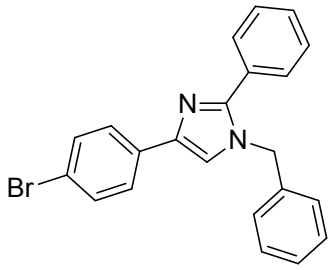
1-benzyl-4-(4-fluorophenyl)-2-phenyl-1H-imidazole (3ha).

Yellow Solid, mp: 107-109 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.80-7.76 (m, 2 H), 7.61-7.58 (m, 2 H), 7.43-7.40 (m, 3 H), 7.38-7.29 (m, 3 H), 7.18 (s, 1 H), 7.14-7.12 (m 2 H), 7.06-7.02 (m, 2 H), 5.20 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.23-160.80 (d, *J* = 243 Hz, 1 C), 148.70, 140.75, 136.79, 130.38-130.35 (d, *J* = 3 Hz), 130.32-129.08 (d, *J* = 124Hz), 129.05-129.02 (d, *J* = 3 Hz), 128.68, 128.05, 126.71, 126.58-126.50 (d, *J* = 8 Hz), 116.44, 115.49-115.28 (d, *J* = 21 Hz), 50.53.; MS (EI) m/z: 328.



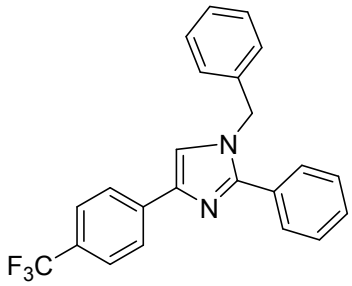
1-benzyl-4-(4-chlorophenyl)-2-phenyl-1H-imidazole (3ia).

Yellow Solid, mp: 125-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.76-7.74 (d, *J* = 8 Hz, 2 H), 7.61-7.58 (m, 2 H), 7.42-7.09 (m, 3 H), 7.35-7.30 (m, 5 H), 7.21 (s, 1 H), 7.13-7.11 (m, 2 H), 5.20 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.82, 140.50, 136.70, 132.66, 132.32, 130.30, 129.15, 129.08, 129.02, 128.70, 128.68, 128.09, 126.74, 126.20, 116.96, 50.58; MS (EI) m/z: 344.



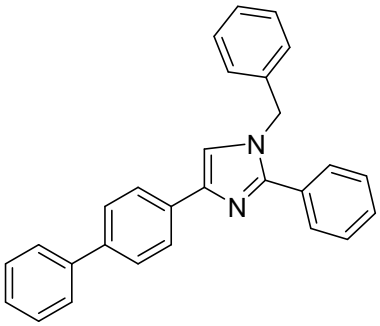
1-benzyl-4-(4-bromophenyl)-2-phenyl-1H-imidazole (3ja).

Yellow Solid, mp: 164-166 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.71-7.68 (m, 2 H), 7.62-7.57 (m, 2 H), 7.49-7.45 (m, 2 H), 7.44-7.40 (m, 3 H), 7.38-7.30 (m, 3 H), 7.24 (s, 1 H), 7.14-7.12 (m, 2 H), 5.21 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.80, 140.44, 136.62, 133.02, 131.55, 130.20, 129.12, 129.03, 128.97, 128.67, 128.05, 126.68, 126.46, 120.38, 116.95, 50.52; MS (EI) m/z: 388.



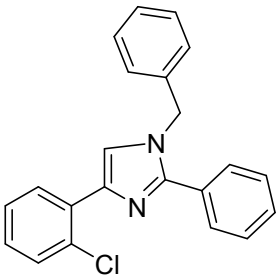
1-benzyl-4-(4-(trifluoromethyl) phenyl) -2-phenyl-1H-imidazole (3ka).

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.93-7.91 (m, 2 H), 7.62-7.59 (m, 4 H), 7.44-7.38 (m, 3 H), 7.36-7.32 (m, 3 H), 7.24 (s, 1 H), 7.14-7.12 (m, 2 H), 5.22 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 149.09, 140.13, 137.51, 136.51, 130.12, 129.23, 129.07, 129.00, 128.70, 128.62, 128.30, 128.12, 126.70, 125.75, 125.65, 125.53, 125.49, 125.46, 125.42, 124.88, 123.05, 117.90, 50.60; MS (EI) m/z: 378.



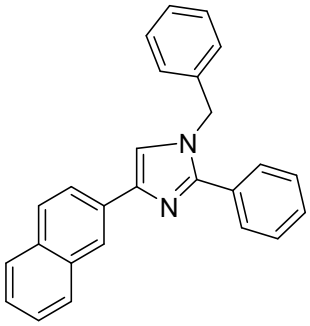
1-benzyl-4-(biphenyl-4-yl) -2-phenyl-1H-imidazole (3la).

Yellow Solid, mp: 128-130 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.91-7.89 (m, 2 H), 7.63-7.59 (m, 6 H), 7.43-7.37 (m, 5 H), 7.36-7.30 (m, 4 H), 7.29 (s, 1 H), 7.26-7.23 (m, 2 H), 5.20 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.68, 141.16, 140.39, 139.39, 136.80, 133.11, 130.41, 129.00, 128.98, 128.68, 128.60, 127.95, 127.17, 127.03, 126.84, 126.64, 125.26, 116.94, 50.48; MS (EI) m/z: 386.



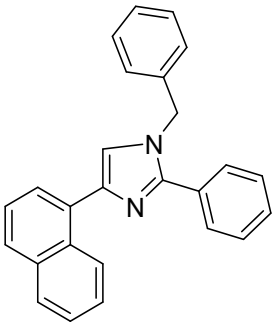
1-benzyl-4-(2-chlorophenyl)-2-phenyl-1H-imidazole (3ma).

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.32-8.30 (m, 1 H), 7.74 (s, 1 H), 7.61-7.58 (m, 2 H), 7.41-7.38 (m, 4 H), 7.37-7.30 (m, 4 H), 7.18-7.12 (m, 3 H), 5.25 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.68, 137.48, 136.82, 132.39, 130.75, 130.29, 130.09, 129.67, 129.01, 128.98, 128.95, 127.91, 127.42, 126.83, 126.48, 121.59, 50.51; MS (EI) m/z: 344.



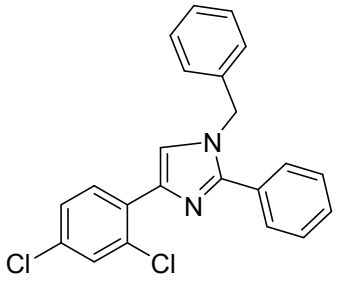
1-benzyl-4-(naphthalen-2-yl)- 2-phenyl-1H-imidazole (3ns):

Yellow solid, mp: 136-138 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.38 (s, 1 H), 7.89-7.86 (m, 2 H), 7.84-7.77 (m, 2 H), 7.65-7.62 (m, 2 H), 7.45-7.39 (m, 5 H), 7.38-7.30 (m, 4 H), 7.15-7.13 (m, 2 H), 5.21 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.87, 141.49, 136.78, 133.85, 132.65, 131.42, 130.45, 129.06, 129.04, 129.01, 128.64, 128.08, 128.04, 127.99, 127.61, 126.71, 126.01, 125.28, 123.69, 123.00, 117.27, 50.54; MS (EI) m/z: 360.



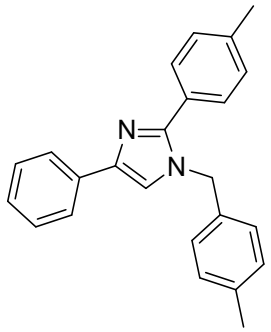
1-benzyl-4-(naphthalen-1-yl)- 2-phenyl-1H-imidazole (3os):

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.64-8.62 (m, 1 H), 7.87-7.85 (m, 1 H), 7.82-7.78 (m, 2 H), 7.70-7.67 (m, 2 H), 7.51-7.40 (m, 5 H), 7.38-7.32 (m, 3 H), 7.27-7.25 (m, 2 H), 7.21-7.19 (m, 2H), 5.32 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.22, 140.89, 136.94, 134.05, 131.93, 131.34, 130.52, 129.05, 128.94, 128.60, 128.43, 128.30, 128.00, 127.62, 126.69, 126.61, 126.06, 125.53, 125.44, 119.97, 50.58; MS (EI) m/z: 360.



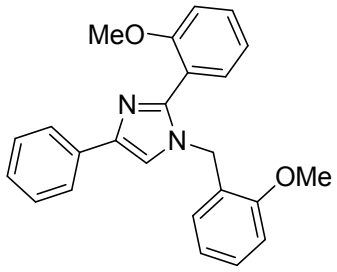
1-benzyl -4-(2, 4-dichlorophenyl)- 2-phenyl -1H-imidazole (3pq):

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.94-7.93 (d, *J* = 2 Hz, 1 H), 7.64-7.58 (m, 3 H), 7.44-7.38 (m, 4 H), 7.36-7.32 (m, 3 H), 7.25-7.23 (m, 1 H), 7.13-7.11 (m, 2 H), 5.20 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.98, 139.32, 136.45, 134.24, 132.62, 130.39, 130.16, 130.05, 129.23, 129.07, 128.96, 128.70, 128.13, 126.71, 126.62, 124.06, 117.40, 50.60; MS (EI) m/z: 378.



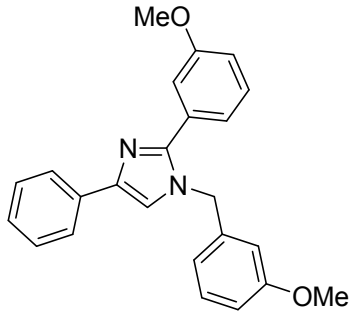
1-(4-methylbenzyl)-4-phenyl-2-(p-tolyl)-1H-imidazole (3ab).

Yellow solid, mp: 94-95 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.50-7.48 (m, 2 H), 7.36-7.32 (m, 2 H), 7.22-7.19 (m, 4 H), 7.14-7.12 (m, 2 H), 7.02-7.00 (m, 2 H), 5.13 (s, 2 H), 2.37 (s, 3 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =148.62, 141.24, 138.81, 137.63, 134.14, 133.85, 129.56, 129.21, 128.86, 128.42, 127.57, 126.63, 126.61, 124.84, 116.56, 50.18, 21.28, 21.03; MS (EI) m/z: 338.



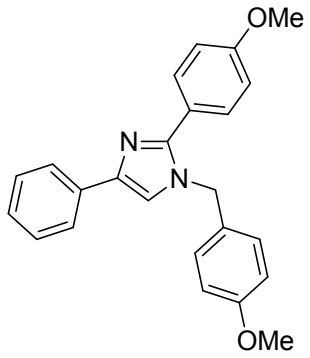
1-(2-methoxybenzyl)-2-(2-methoxyphenyl)-4-phenyl-1H-imidazole (3ae).

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.51-7.48 (m, 1 H), 7.43-7.38 (m, 1 H), 7.34-7.30 (m, 2 H), 7.25 (s, 1 H), 7.23-7.16 (m, 2 H), 7.05-7.01 (m, 1 H), 6.95-6.81 (m, 4 H), 4.97 (s, 2 H), 3.74 (s, 3 H), 3.70 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =157.59, 156.80, 146.14, 141.05, 134.47, 132.59, 130.77, 128.97, 128.88, 128.34, 126.31, 125.32, 124.75, 120.80, 120.48, 120.22, 116.09, 110.79, 110.16, 55.29, 55.19, 45.50; MS (EI) m/z: 370.



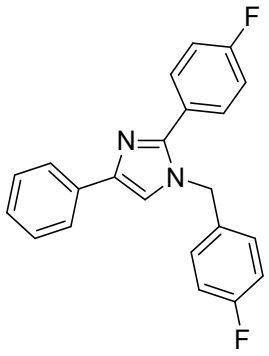
1-(3-methoxybenzyl)-2-(3-methoxyphenyl)-4-phenyl-1H-imidazole (3ad).

Yellow solid, mp: 121-123 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.38-7.21 (m, 6 H), 7.17-7.15 (m, 2 H), 6.97-6.94 (m, 1 H), 6.85-6.82 (m, 1 H), 6.74-6.72 (d, *J* = 7.6 Hz,1 H), 6.67 (s, 1 H), 5.20 (s, 2 H), 3.76 (s, 3 H), 3.75 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.09, 159.66, 148.40, 141.44, 138.47, 133.98, 131.57, 130.10, 129.63, 128.51, 126.79, 124.91, 121.20, 118.82, 116.94, 115.38, 114.05, 113.14, 112.40, 55.25, 55.23, 50.41; MS (EI) m/z: 370.



1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-4-phenyl-1H-imidazole (3ac).

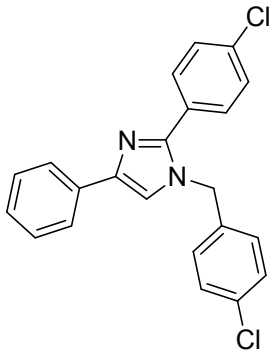
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.54-7.52 (m, 2 H), 7.36-7.32 (m, 2 H), 7.24-7.19 (m 2 H), 7.06-7.04 (m, 2 H), 6.96-6.92 (m, 2 H), 6.88-6.84 (m, 2 H), 5.10 (s, 2 H), 3.82 (s, 3 H), 3.78 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.18, 159.33, 148.44, 141.21, 134.24, 130.45, 128.92, 128.51, 128.13, 126.67, 124.89, 123.09, 116.40, 114.37, 114.05, 55.35, 55.33, 50.01; MS (EI) m/z: 370.



1-(4-fluorobenzyl)-2-(4-fluorophenyl)-4-phenyl-1H-imidazole (3af).

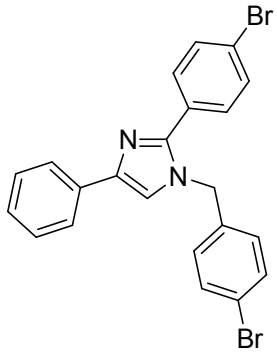
Yellow Solid, mp: 81-83^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.56-7.53 (m, 2 H), 7.38-7.34 (m, 2 H), 7.26-7.22 (m 2 H), 7.13-7.00 (m, 4 H), 5.14 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.40-161.92 (d, *J* = 248 Hz), 163.59-161.13 (d, *J* = 246 Hz), 147.51, 141.60, 133.77, 132.35-132.32 (d, *J* = 3 Hz), 130.92-130.84 (d, *J* = 8 Hz), 128.55, 128.36-128.28 (d, *J* = 8 Hz), 126.94, 126.53-126.50 (d, *J* = 3 Hz), 124.86, 116.67, 116.11-115.89 (d, *J* = 22 Hz), 155.85-155.63 (d,

J = 22 Hz), 49.82; MS (EI) m/z: 346.



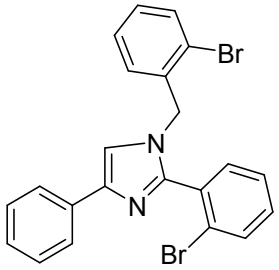
1-(4-chlorobenzyl)-2-(4-chlorophenyl)-4-phenyl-1H-imidazole (3ag).

Yellow Solid, mp: 100-102°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.51-7.49 (m, 2 H), 7.40-7.37 (m, 4 H), 7.35-7.30 (m, 2 H), 7.26-7.23 (m, 2 H), 7.04-7.02 (m, 2 H), 5.15 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.32, 141.88, 135.21, 135.01, 134.01, 133.66, 130.12, 129.26, 128.92, 128.69, 128.58, 127.85, 127.03, 124.89, 116.97, 49.90; MS (EI) m/z: 378.



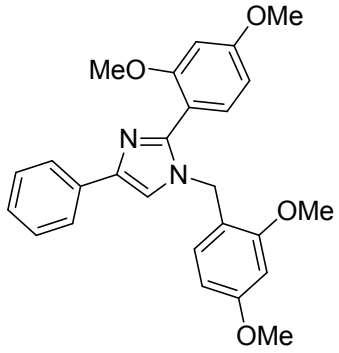
1-(4-bromobenzyl)-2-(4-bromophenyl)-4-phenyl-1H-imidazole (3ah).

Yellow solid, mp: 102-103 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.55-7.52 (m, 2 H), 7.48-7.41 (m, 4 H), 7.38-7.34 (m 2 H), 7.26-7.22 (m, 2 H), 6.97-6.95 (d, J = 8.8 Hz, 2 H), 5.12 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =147.33, 141.91, 135.52, 133.62, 132.21, 131.86, 130.33, 129.10, 128.57, 128.14, 127.05, 124.88, 123.41, 122.07, 117.01, 49.94; MS (EI) m/z: 466.



1-(2-bromobenzyl)-2-(2-bromophenyl)-4-phenyl-1H-imidazole (3ai).

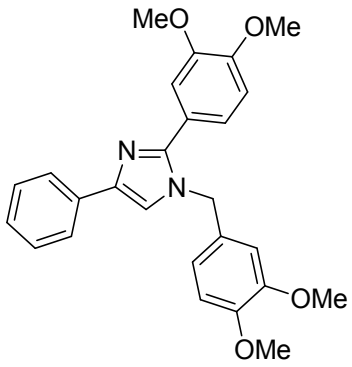
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.83-7.81 (m, 2 H), 7.68-7.66 (m, 1 H), 7.54-7.46 (m, 1 H), 7.44-7.38 (m 1 H), 7.36-7.25 (m, 4 H), 7.24-7.21 (m, 3 H), 7.17-7.13 (m, 1 H), 6.94-6.92 (m, 1 H), 5.09 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =147.18, 141.44, 135.58, 133.86, 133.04, 132.89, 132.87, 132.04, 131.23, 129.71, 129.32, 128.57, 127.91, 127.54, 126.90, 124.92, 124.73, 123.01, 115.64, 50.64; MS (EI) m/z: 466.



1-(2,4-dimethoxybenzyl)-2-(2,4-dimethoxyphenyl)-4-phenyl-1H-imidazole (3aj).

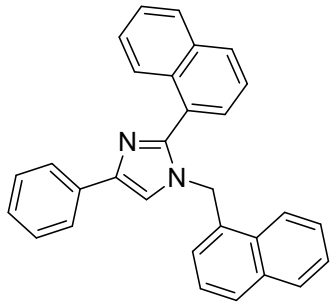
Yellow solid, mp: 106-108 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.80-7.78 (m, 2 H), 7.43-7.41 (d, *J* = 8.4 Hz, 1 H), 7.33-7.30 (m, 2 H), 7.20-7.15 (m, 2 H), 6.84-6.82 (d, *J* = 8 Hz, 1 H), 6.59-6.56 (m, 1 H), 6.52-6.51 (d, *J* = 2.4 Hz, 1 H),6.41-6.36 (m, 2 H), 4.88 (s, 2 H), 3.85 (s, 3 H), 3.78 (s, 3 H), 3.74 (s, 3 H), 3.72 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 161.96, 160.64, 158.76, 157.98, 145.88, 133.25, 129.91, 128.32, 126.24, 124.72, 117.77, 115.77, 104.73, 103.99, 98.47, 98.30, 55.46, 55.38,

55.35, 55.27, 45.09; MS (EI) m/z: 430.



1-(3,4-dimethoxybenzyl)-2-(3,4-dimethoxyphenyl)-4-phenyl-1H-imidazole (3ak).

Yellow solid, mp: 183-185 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.38-7.34 (m, 2 H), 7.25-7.21 (m, 2 H), 7.19-7.18 (d, *J* = 2 Hz, 1 H), 7.13-7.11 (m, 1 H), 6.90-6.88 (m,1 H), 6.84-6.82 (m, 1 H), 6.72-6.69(m, 1H), 6.63-6.62(m, 1H), 5.15 (s, 2 H), 3.90 (s, 3 H), 3.87 (s, 3 H), 3.82 (s, 3 H), 3.80 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 149.65, 149.33, 148.91, 148.66, 148.34, 141.11, 134.02, 129.35, 128.48, 126.71, 124.82, 123.09, 121.36, 118.95, 116.62, 112.27, 111.32, 110.84, 109.64, 55.90, 55.85, 55.81, 50.24; MS (EI) m/z: 430.



2-(naphthalen-1-yl)-1-(naphthalen-1-ylmethyl)-4-phenyl-1H-imidazole (3al).

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.98-7.90 (m, 3 H), 7.85-7.79 (m, 4 H), 7.66-7.60 (m, 2 H), 7.55-7.53 (m, 2 H), 7.51-7.40 (m, 3 H), 7.38-7.32 (m, 3 H), 7.27-7.19 (m, 3 H), 5.40 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.04,

141.44, 134.09, 133.81, 133.62, 132.86, 131.91, 130.60, 129.98, 128.91, 128.85, 128.67, 128.50, 128.34, 127.97, 127.02, 126.74, 126.67, 126.32, 126.07, 125.90, 125.79, 125.39, 125.05, 124.86, 122.47, 115.82, 48.56; MS (EI) m/z: 410.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PROCNO                     1
Date_               20150719
Time                   22.07
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PULPROG                zg30
TD                    65536
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NS                       16
DS                        2
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FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                       101
DW                  62.400 usec
DE                   6.50 usec
TE                   294.7 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
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NUC1                     1H
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WDW                      EM
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LB                     0.30 Hz
GB                        0
PC                     1.00
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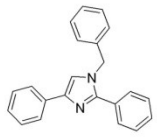
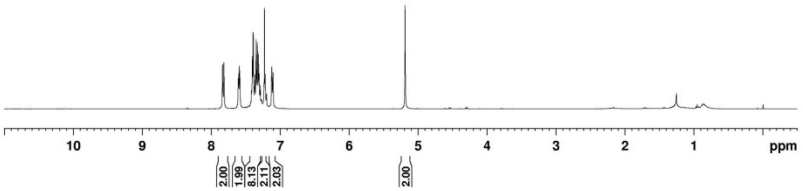


3aa

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EXPNO                     11
PROCNO                     1
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FIDRES             0.366798 Hz
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RG                      1030
DW                  20.800 usec
DE                   6.50 usec
TE                   295.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
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LB                     1.00 Hz
GB                        0
PC                     1.40
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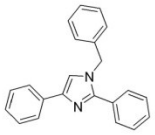
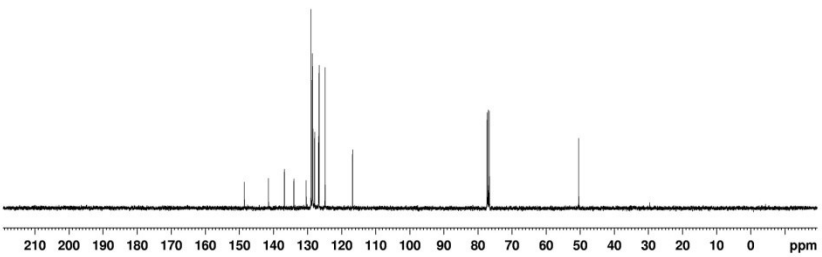


3aa

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7.585
7.581
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7.419
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7.395
7.386
7.382
7.351
7.346
7.329
7.310
7.301
7.290
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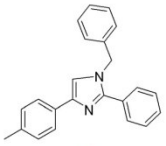

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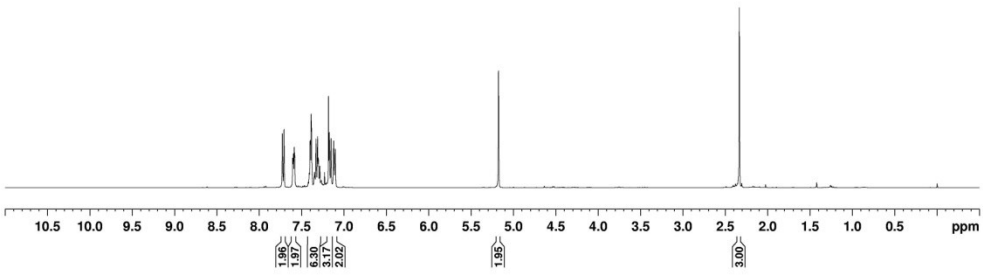
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1.96
1.97
6.30
3.17
2.02
1.95
3.00


148.40
141.59
136.88
136.35
131.25
130.51
129.16
128.97
128.92
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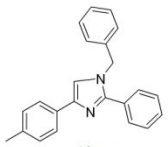
77.00
76.68
50.40
21.15



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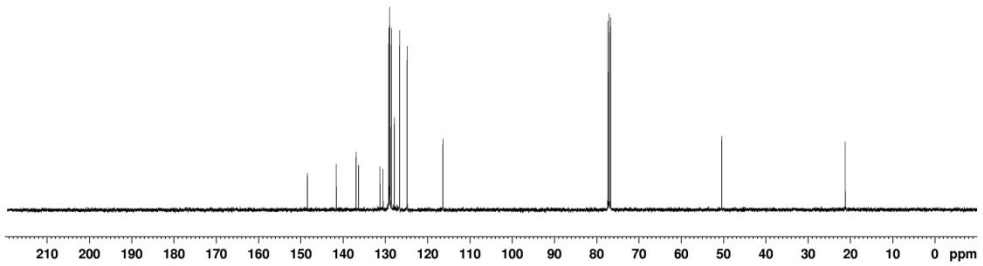
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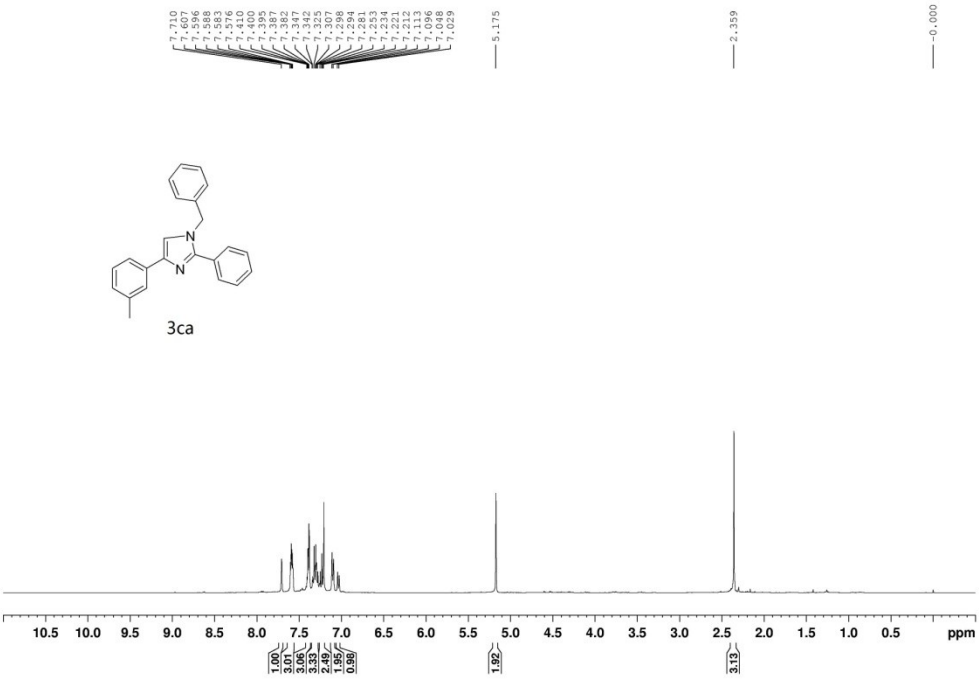
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7.400
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7.387
7.382
7.347
7.332
7.325
7.307
7.298
7.294
7.281
7.253
7.234
7.221
7.212
7.113
7.096
7.048
7.029
5.175
2.359
-0.000
3ca
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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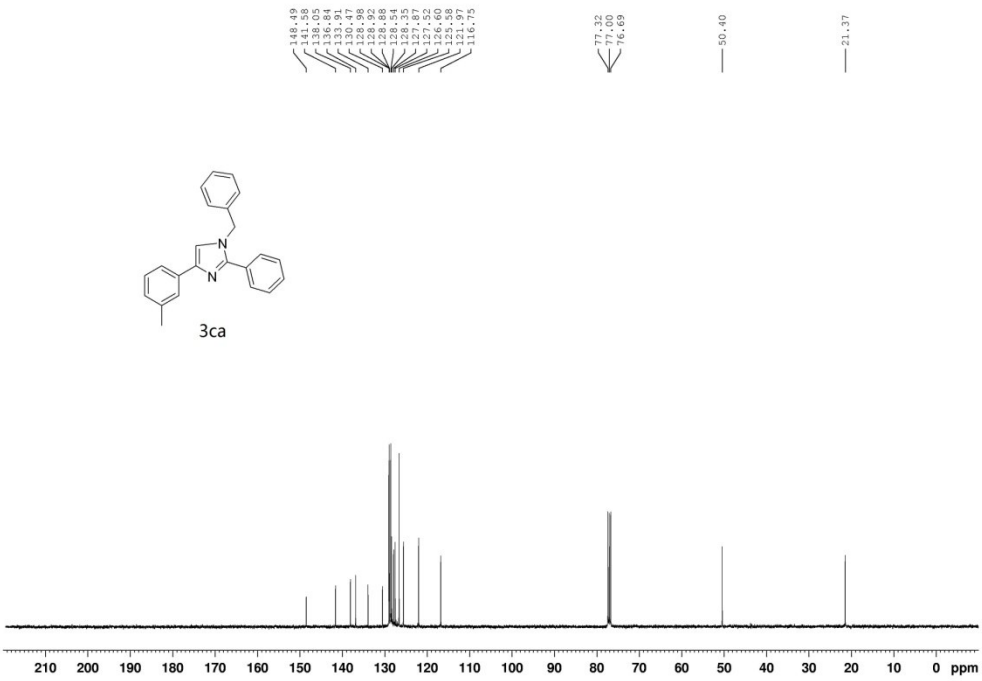
3.06
3.33
2.49
1.95
0.98
1.92
3.13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127.87
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126.60
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121.97
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3ca
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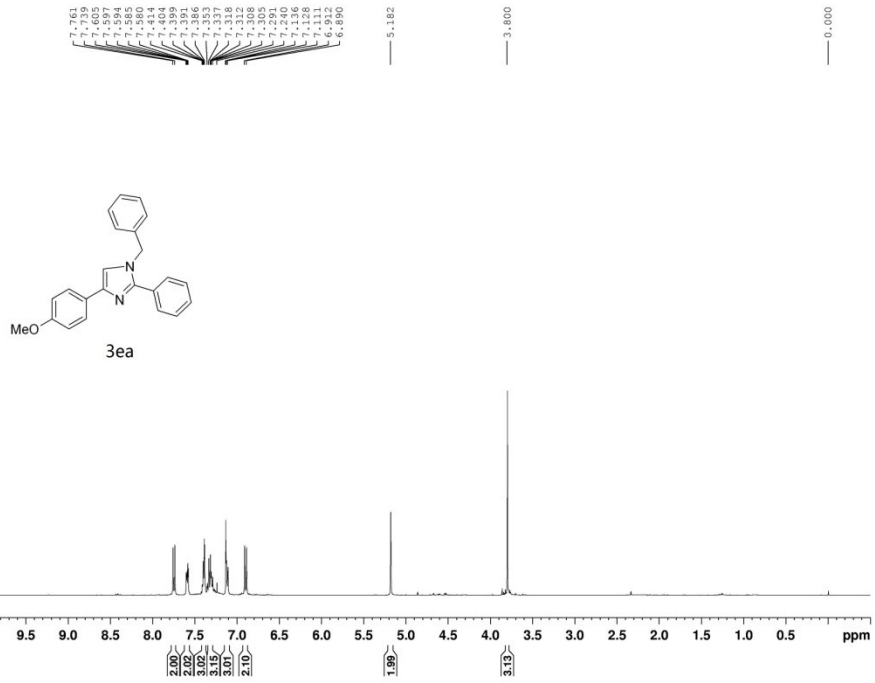
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7.353
7.337
7.318
7.312
7.308
7.305
7.291
7.240
7.136
7.128
7.111
6.912
6.890
5.182
3.800
0.000
MeO
3ea
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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3.15
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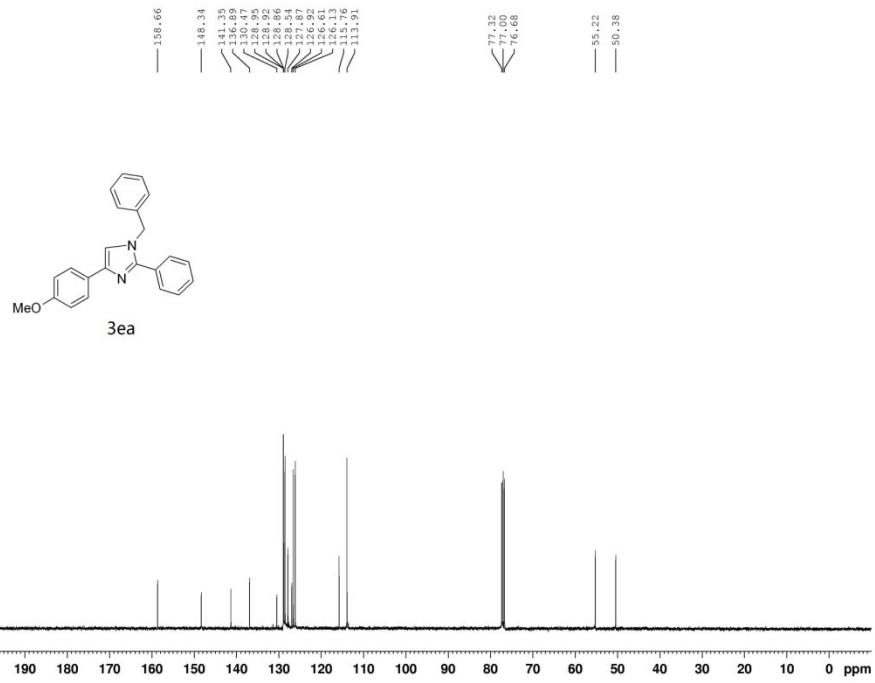
2.10
1.99
3.13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126.61
126.13
115.76
113.91
77.32
77.00
76.68
55.22
50.38
MeO
3ea
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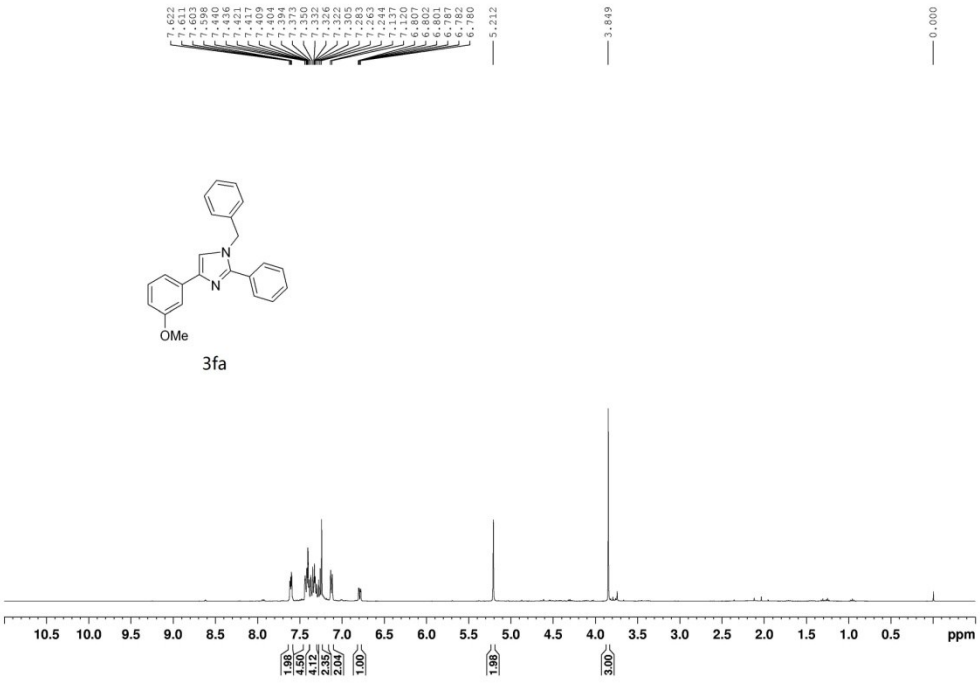
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7.263
7.244
7.137
7.120
6.807
6.802
6.801
6.787
6.782
6.780
5.212
3.849
0.000
N
N
OMe
3fa
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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4.50
4.12
2.35
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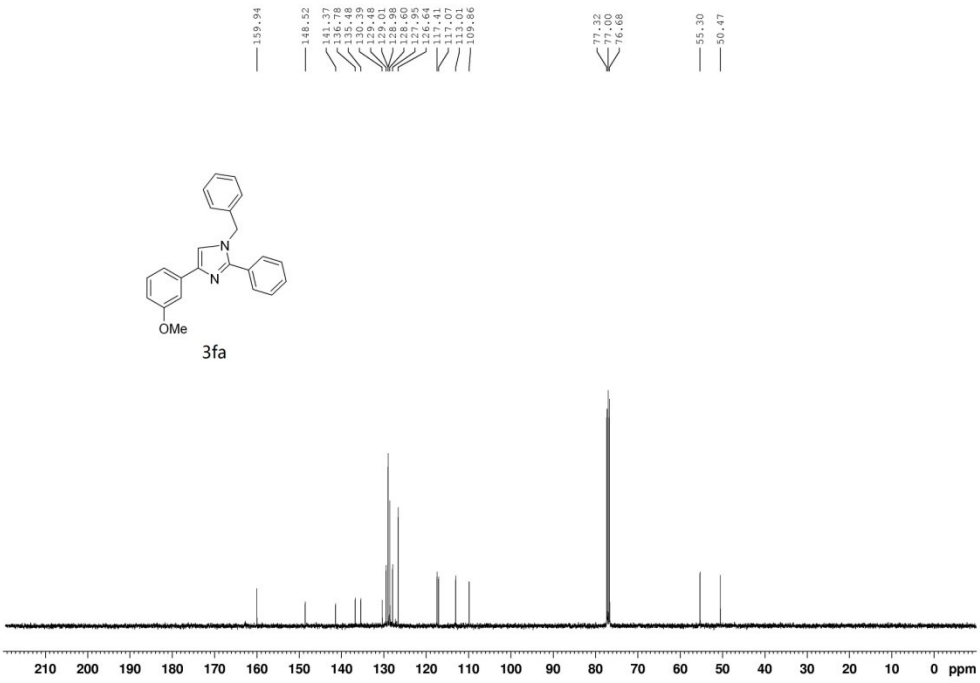
1.00
1.98
3.00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128.60
127.95
126.64
117.41
113.07
111.01
109.86
77.32
77.00
76.68
55.30
50.47
N
N
OMe
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.368
8.364
8.349
8.345
7.608
7.596
7.594
7.586
7.580
7.404
7.394
7.390
7.383
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7.368
7.360
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7.335
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7.237
7.232
7.218
7.216
7.214
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7.194
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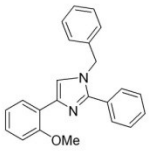
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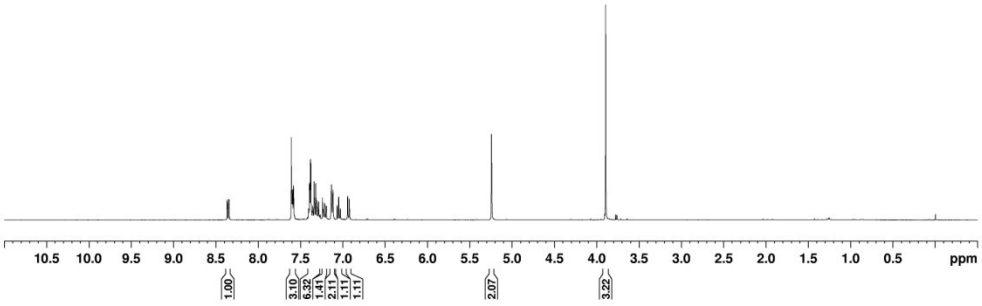
N
OMe

3ga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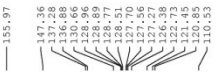
1.41
2.11
1.11
1.11
2.07
3.22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128.77
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127.70
127.56
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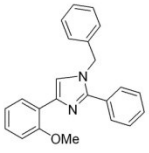
110.53
77.32
77.00
76.68
55.21
50.28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N
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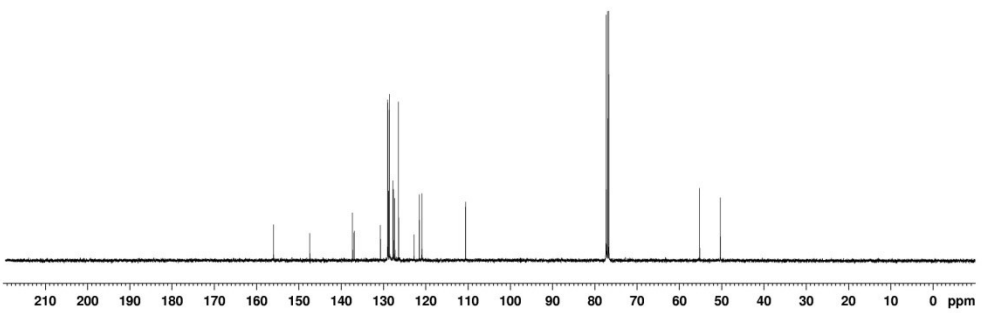
3ga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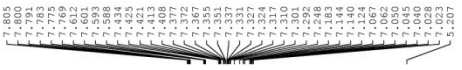
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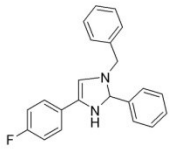
7.791
7.783
7.775
7.769
7.612
7.601
7.593
7.588
7.434
7.425
7.421
7.413
7.409
7.377
7.372
7.367
7.355
7.351
7.337
7.331
7.327
7.324
7.317
7.310
7.301
7.292
7.248
7.183
7.144
7.140
7.124
7.067
7.062
7.050
7.045
7.040
7.028
7.023
5.207
0.000



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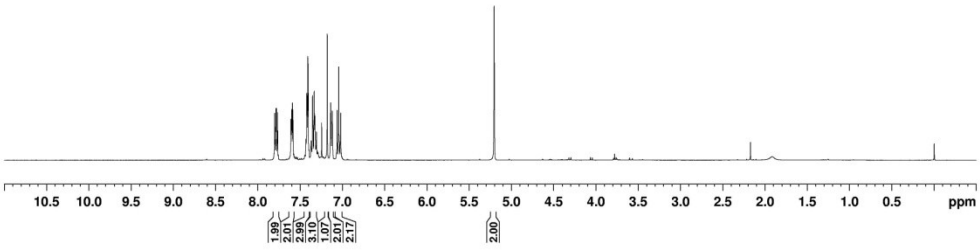
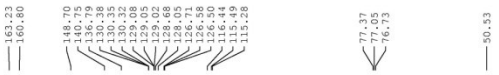
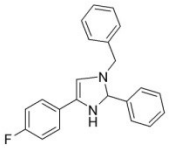
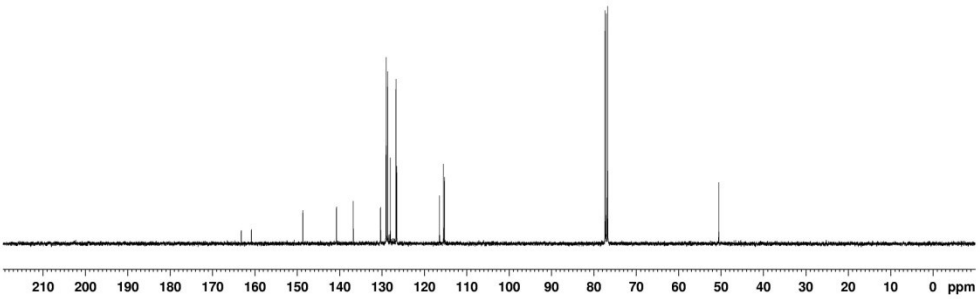
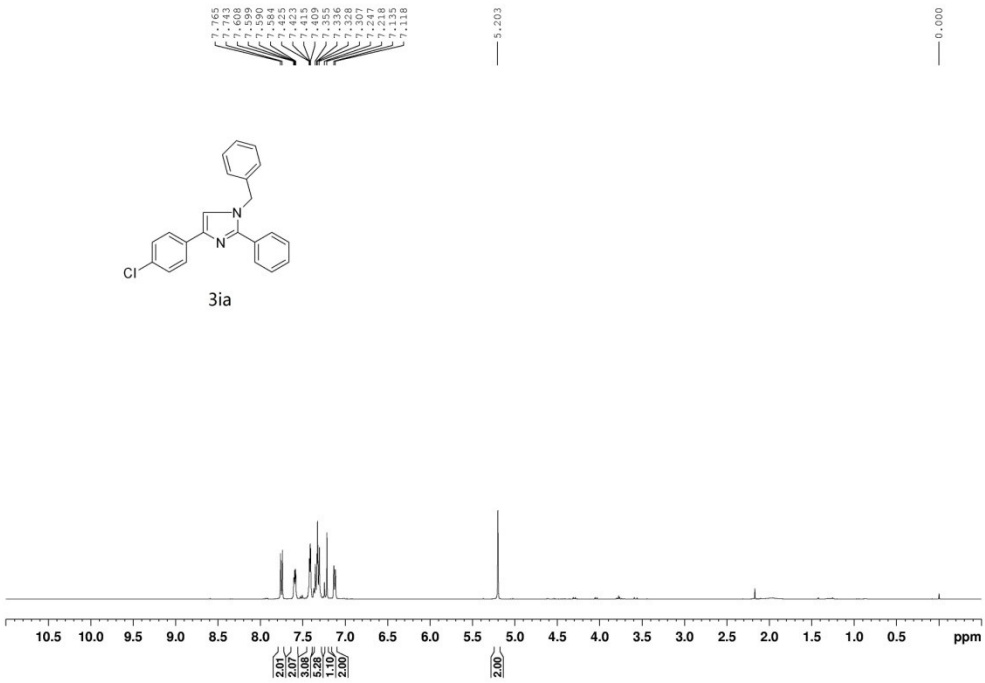

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.99
2.01
2.99
3.10
1.07
2.07
2.17
2.00

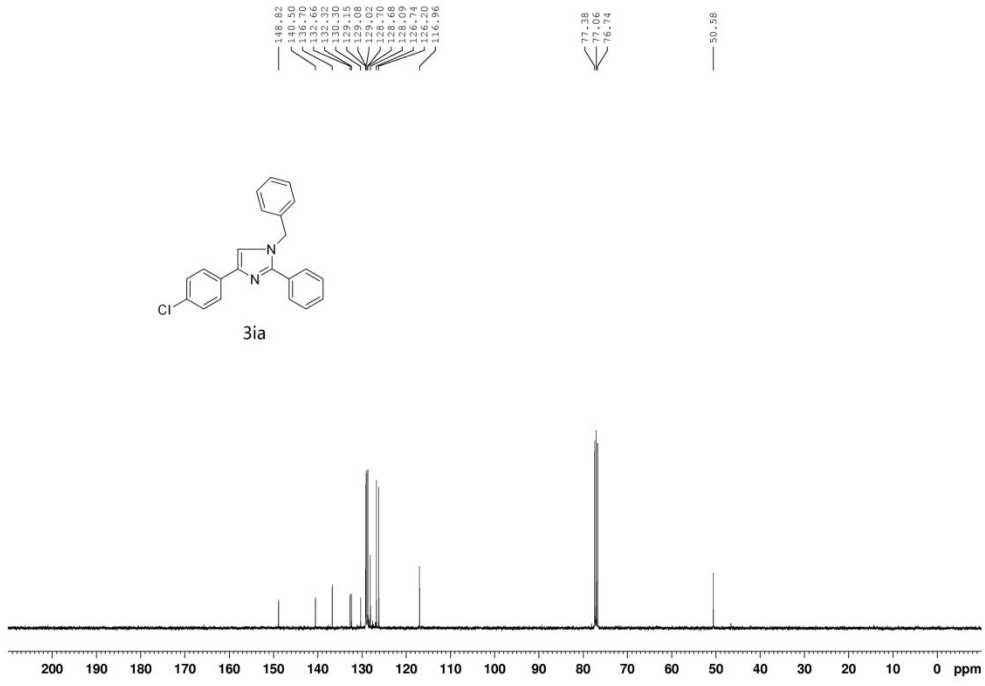

163.23
160.80
148.70
140.75
136.79
130.38
130.35
130.32
129.08
129.05
129.02
128.68
128.05
126.71
126.58
126.50
116.44
115.49
115.28
77.37
77.05
76.73
50.53

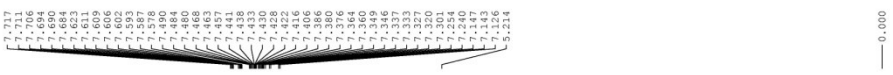


3ha


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.765
7.763
7.608
7.599
7.590
7.584
7.425
7.423
7.415
7.409
7.355
7.336
7.328
7.307
7.247
7.218
7.135
7.118
5.203
0.000
N
N
Cl
3ia
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 ppm
2.01
2.07
3.08
5.28
1.10
2.00
2.00


148.82
140.50
136.70
132.66
132.22
130.30
129.15
129.08
129.02
128.70
128.68
128.09
126.74
126.60
116.96
77.38
77.06
76.74
50.58
N
N
Cl
3ia
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.717
7.711
7.706
7.694
7.690
7.684
7.663
7.611
7.609
7.606
7.602
7.593
7.587
7.578
7.490
7.484
7.480
7.468
7.463
7.457
7.451
7.438
7.433
7.430
7.428
7.422
7.416
7.406
7.386
7.380
7.376
7.366
7.364
7.360
7.349
7.346
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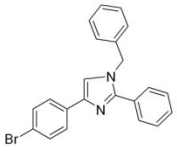
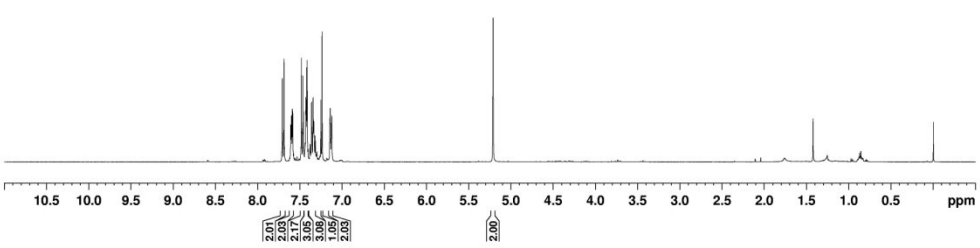
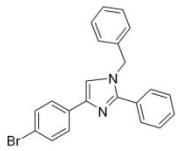
7.240
7.147
7.143
7.126
5.214
0.000


N
N
Br

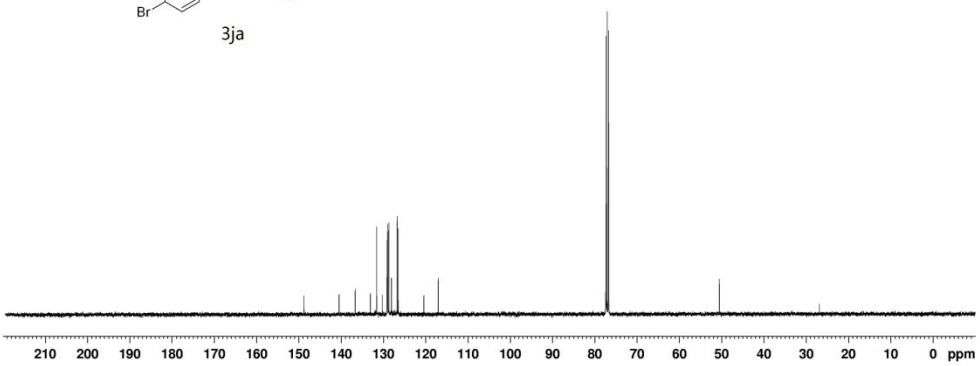
3ja

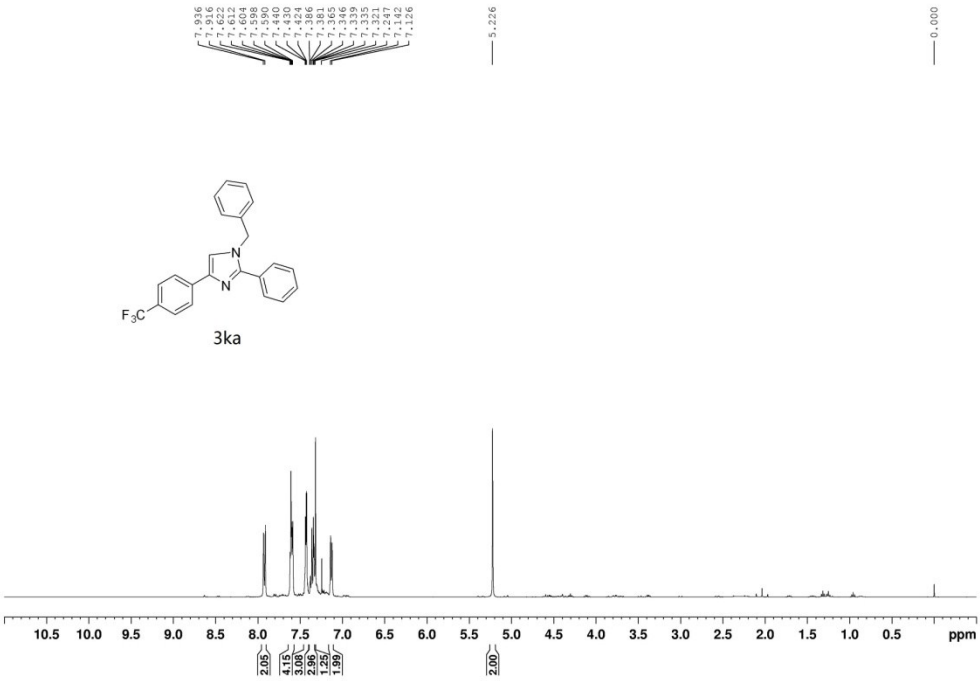

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.01
2.03
2.17
3.16
3.09
1.05
2.03
2.00

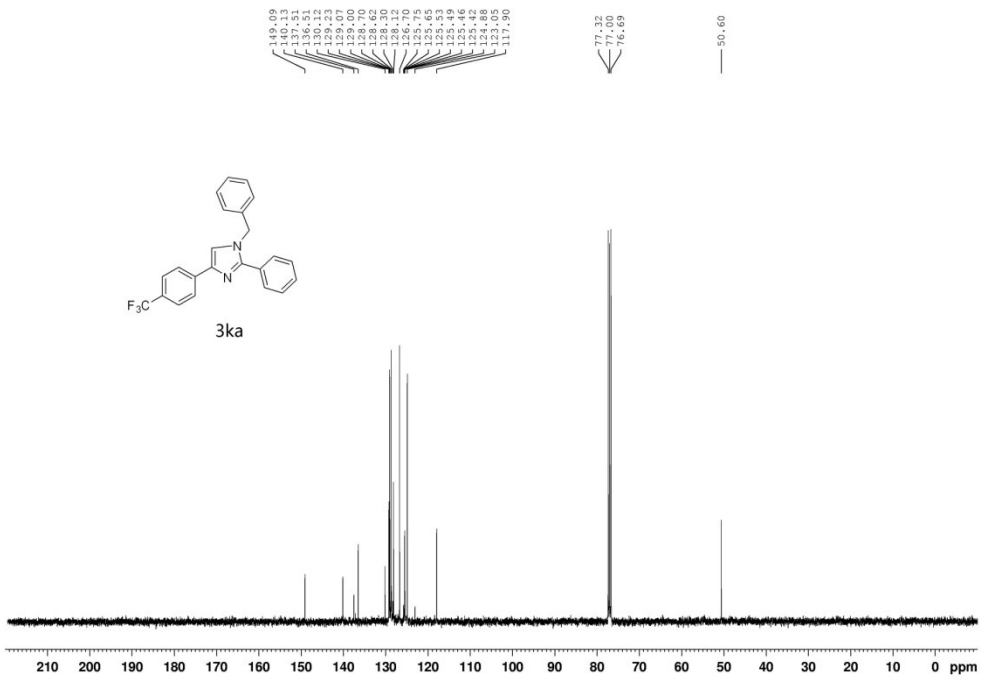

148.80
140.44
136.62
133.02
131.55
130.20
129.12
129.03
128.97
128.67
128.05
126.68
126.46
120.38
116.95
77.32
77.00
76.68
50.52


N
N
Br

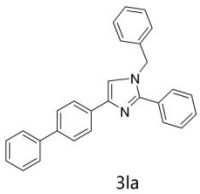
3ja


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

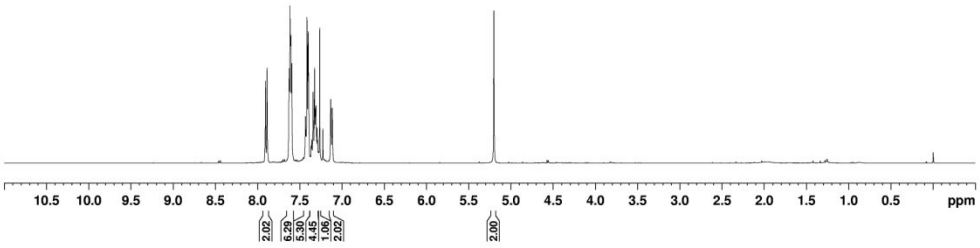

7.936
7.916
7.622
7.612
7.604
7.598
7.590
7.440
7.430
7.424
7.386
7.381
7.365
7.346
7.339
7.335
7.321
7.247
7.142
7.126
5.226
0.000
3ka
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.05
4.15
3.08
2.96
1.25
1.99
2.00


149.09
140.13
137.51
136.51
130.12
129.23
129.07
128.70
128.62
128.30
128.12
126.70
125.75
125.65
125.53
125.49
125.46
125.42
124.88
123.05
117.90
77.32
77.00
76.69
50.60
3ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

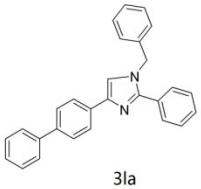

7.911
7.891
7.633
7.629
7.625
7.619
7.612
7.609
7.603
7.598
7.437
7.430
7.418
7.415
7.407
7.402
7.368
7.363
7.346
7.342
7.328
7.322
7.317
7.312
7.301
7.293
7.268
7.230
5.205
0.000



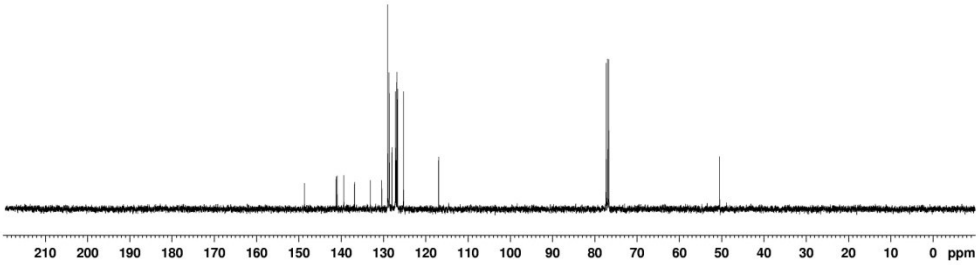
3la

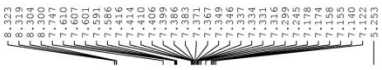

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.02
6.29
5.30
4.45
1.06
2.02
2.00

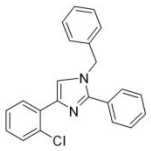

148.68
141.16
140.93
139.39
136.80
133.11
130.41
130.00
128.98
128.68
128.60
127.95
127.17
127.03
126.84
126.64
125.26
116.94
77.32
77.00
76.68
50.48



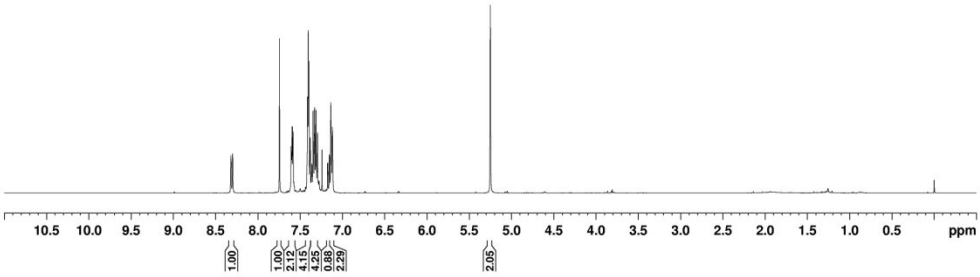
3la

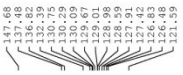

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

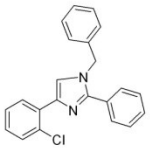

8.323
8.319
8.304
8.300
7.647
7.610
7.607
7.601
7.591
7.466
7.416
7.414
7.410
7.406
7.398
7.386
7.383
7.371
7.367
7.349
7.346
7.337
7.334
7.331
7.316
7.299
7.245
7.178
7.174
7.158
7.155
7.140
7.122
5.253
0.000


N
N
Cl

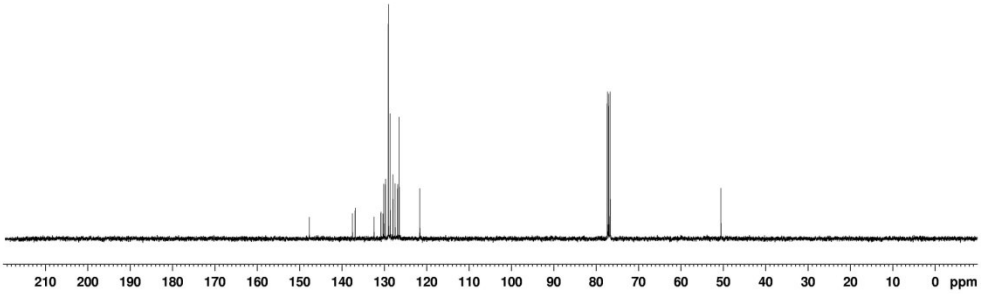
3ma


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 ppm
1.00
1.00
2.12
4.15
4.25
0.88
2.29
2.05

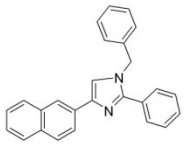

147.68
137.48
136.22
132.39
130.75
130.29
130.09
129.67
129.01
128.98
128.59
128.31
127.91
127.42
126.83
126.48
121.59
77.31
77.00
76.68
50.51


N
N
Cl

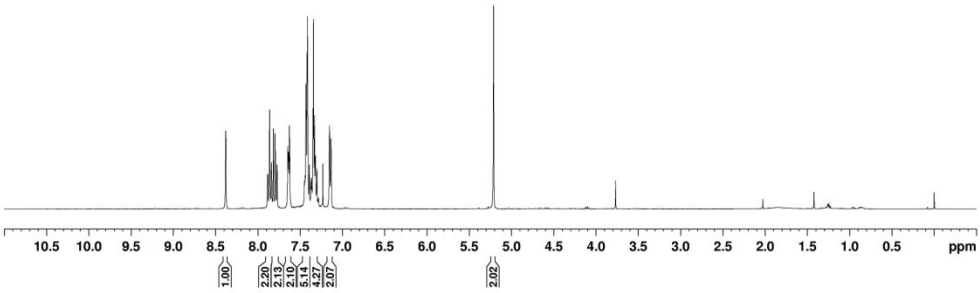
3ma

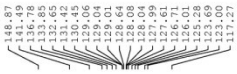

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

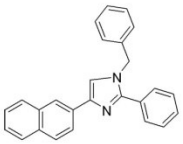

8.383
7.890
7.885
7.868
7.866
7.864
7.843
7.820
7.798
7.777
7.650
7.643
7.639
7.630
7.626
7.455
7.450
7.446
7.442
7.438
7.430
7.421
7.417
7.396
7.385
7.379
7.373
7.368
7.364
7.351
7.337
7.333
7.326
7.322
7.318
7.304
7.235
7.155
7.138
5.215
0.000



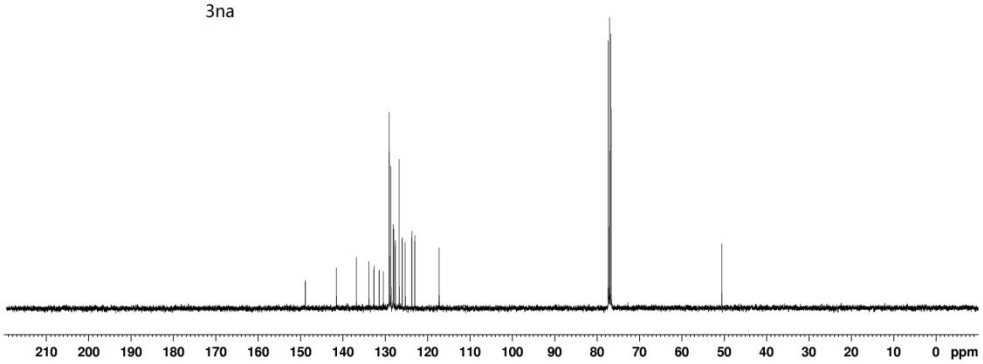
3na

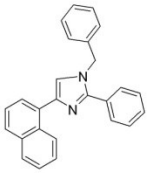

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.20
2.13
2.10
5.14
4.27
2.07
2.02


148.87
141.49
136.78
135.85
132.65
131.42
130.45
129.06
129.04
129.01
128.64
128.08
128.04
127.99
127.61
126.71
126.01
125.58
123.69
123.00
117.27
77.32
77.00
76.68
50.54

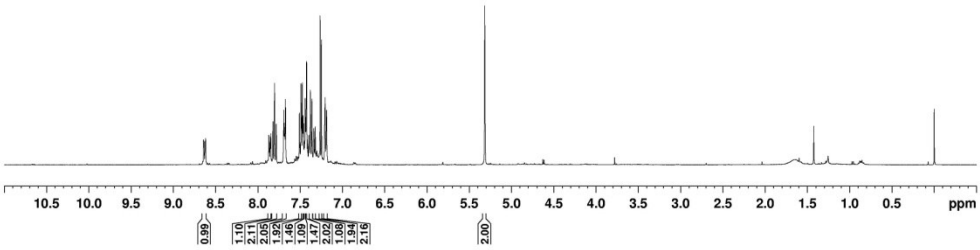


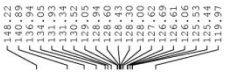
3na

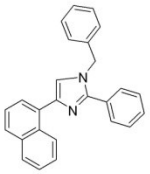

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



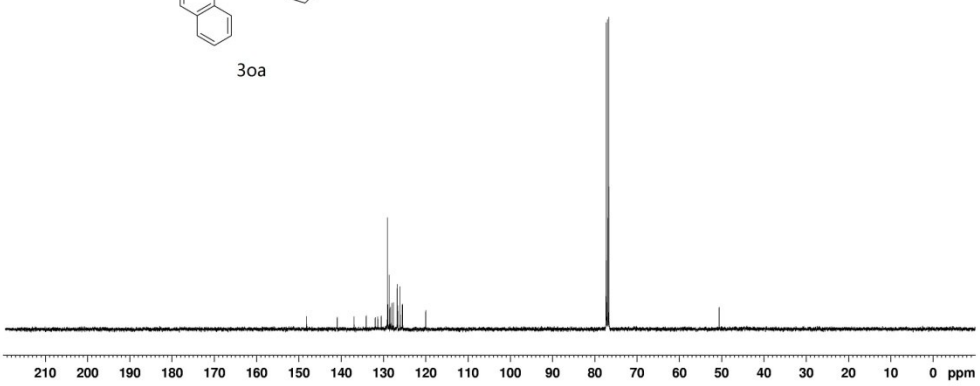
3oa

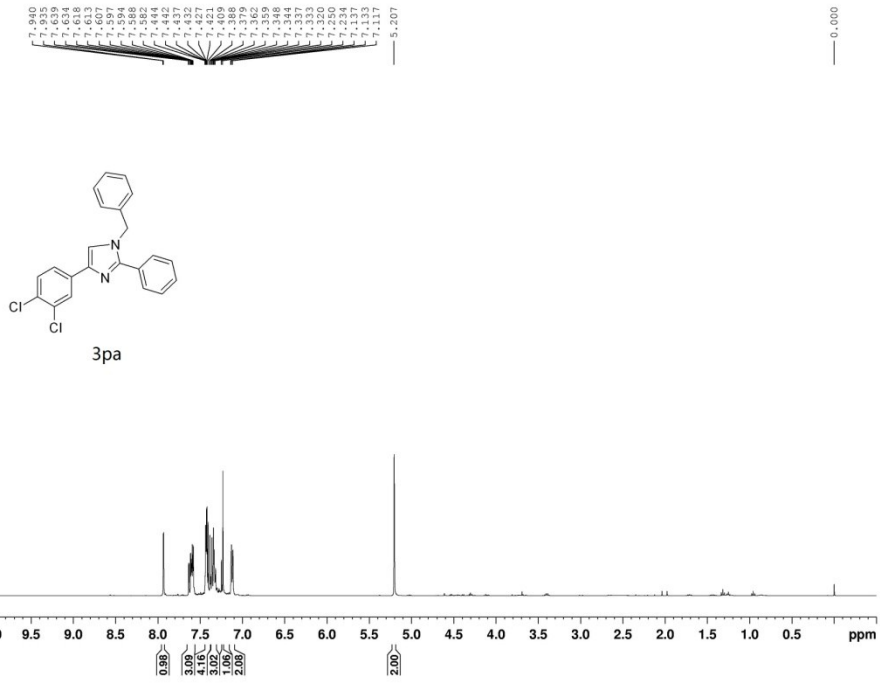




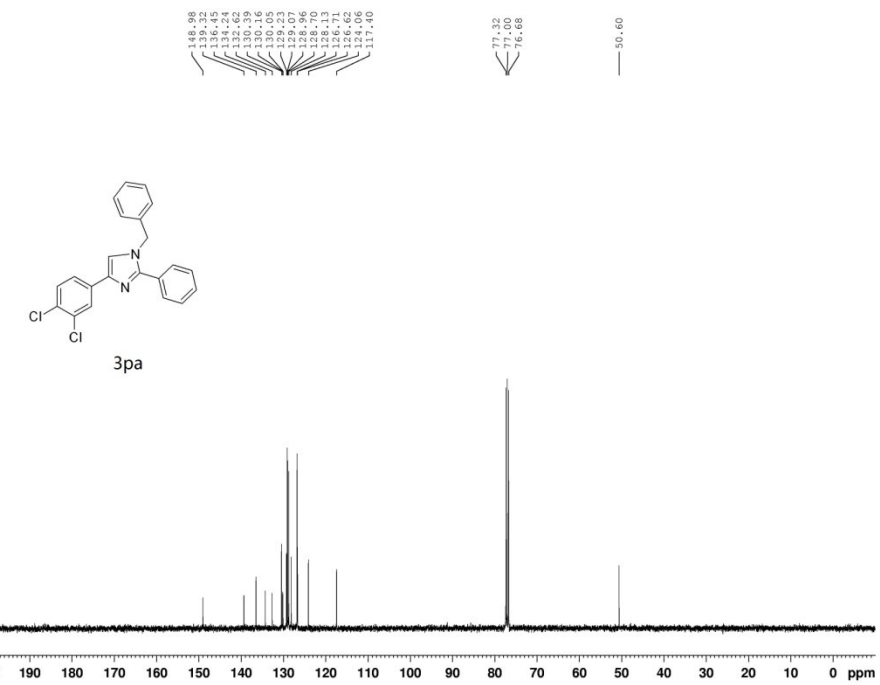


3oa

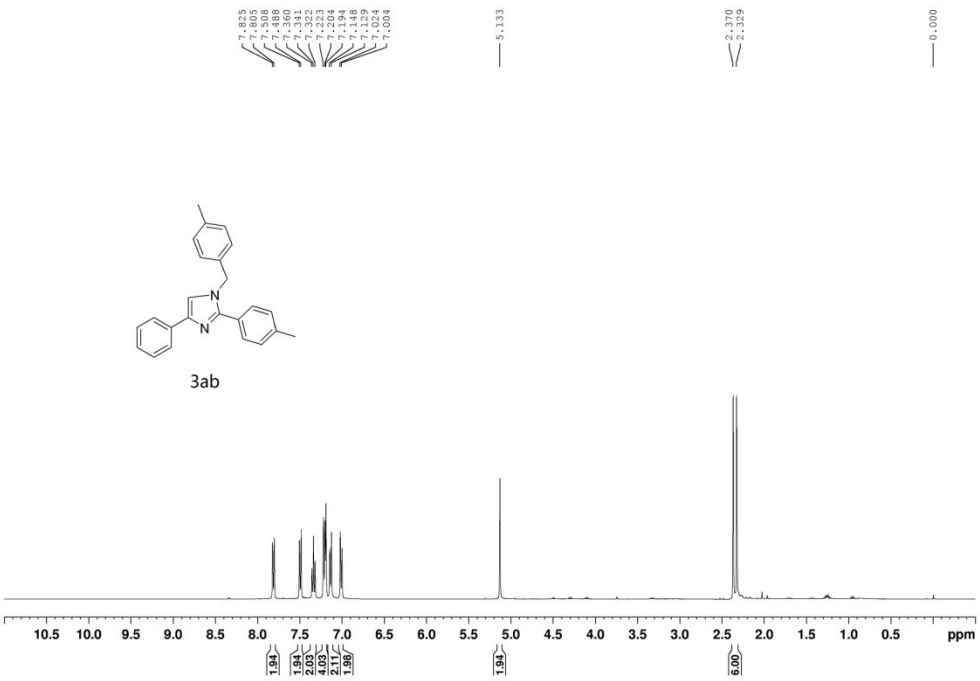


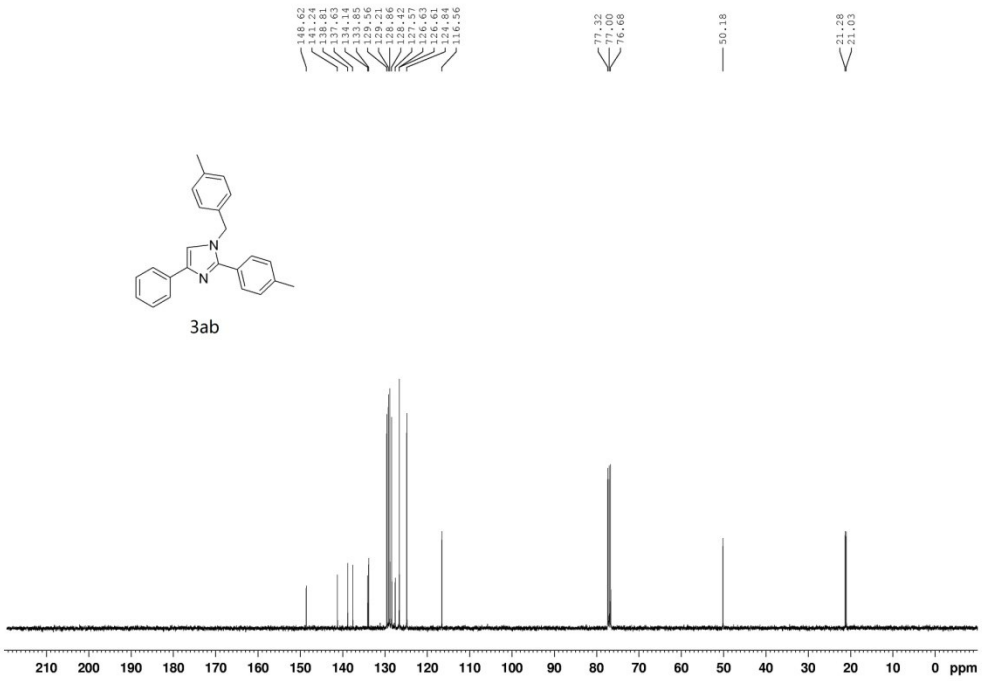

7.940
7.935
7.639
7.634
7.618
7.613
7.607
7.597
7.594
7.588
7.582
7.444
7.442
7.437
7.432
7.427
7.421
7.409
7.388
7.379
7.362
7.359
7.348
7.344
7.337
7.333
7.320
7.250
7.234
7.137
7.133
7.117
5.207
0.000
Cl
Cl
N
N
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.98
3.09
4.16
3.02
1.06
2.08
2.00

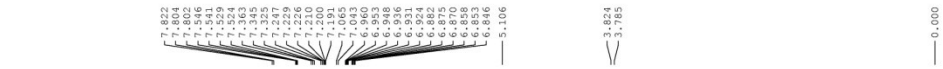
3pa

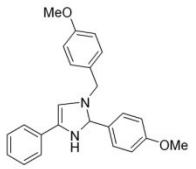

148.98
139.32
136.45
134.24
132.62
130.39
130.16
130.05
129.23
129.07
128.96
128.70
128.13
126.71
126.62
126.06
117.40
77.32
77.00
76.68
50.60
Cl
Cl
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

3pa

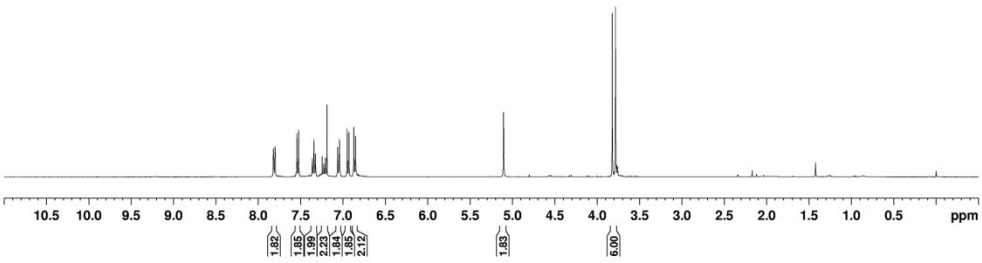

7.825
7.805
7.500
7.488
7.360
7.341
7.222
7.223
7.204
7.194
7.148
7.129
7.024
7.004
5.133
2.370
2.329
0.000
3ab
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.94
1.94
2.03
4.03
2.17
1.98
1.94
6.00

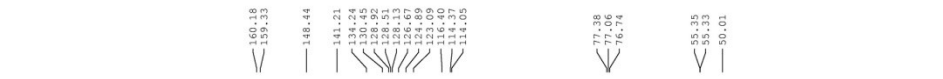

148.62
141.24
138.61
137.63
134.14
133.85
129.56
129.21
128.66
128.42
127.57
126.63
126.61
126.04
116.56
77.32
77.00
76.68
50.18
21.28
21.03
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

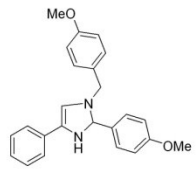

7.822
7.804
7.802
7.546
7.541
7.529
7.524
7.363
7.345
7.325
7.247
7.229
7.226
7.210
7.200
7.191
7.065
7.043
6.960
6.953
6.948
6.936
6.931
6.924
6.882
6.875
6.870
6.858
6.853
6.846
5.106
3.824
3.785
0.000


MeO
N
H
OMe

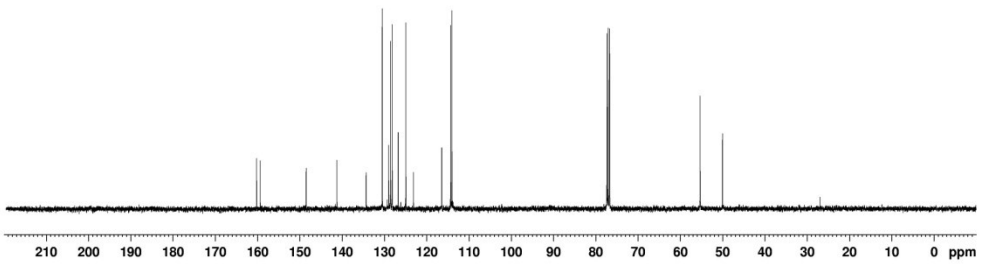
3ac


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 ppm
1.82
1.85
1.99
2.03
1.84
1.85
2.12
1.83
6.00


160.18
159.38
148.44
141.21
134.24
130.45
128.92
128.51
128.13
126.67
124.89
123.09
116.40
114.37
114.05
77.38
77.06
76.74
55.35
55.33
50.01


MeO
N
H
OMe

3ac


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.850
7.847
7.829
7.387
7.368
7.349
7.342
7.301
7.293
7.273
7.266
7.257
7.237
7.218
7.175
7.168
7.164
7.159
7.157
6.970
6.967
6.964
6.961
6.949
6.947
6.942
6.856
6.850
6.835
6.829
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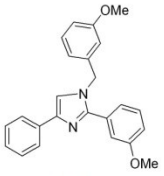
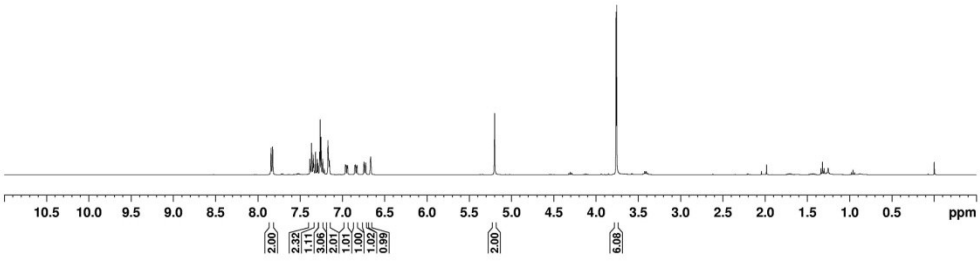
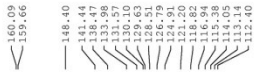
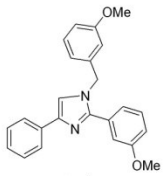
6.728
6.669
5.202
3.765
3.758
0.000


OMe
N
N
OMe

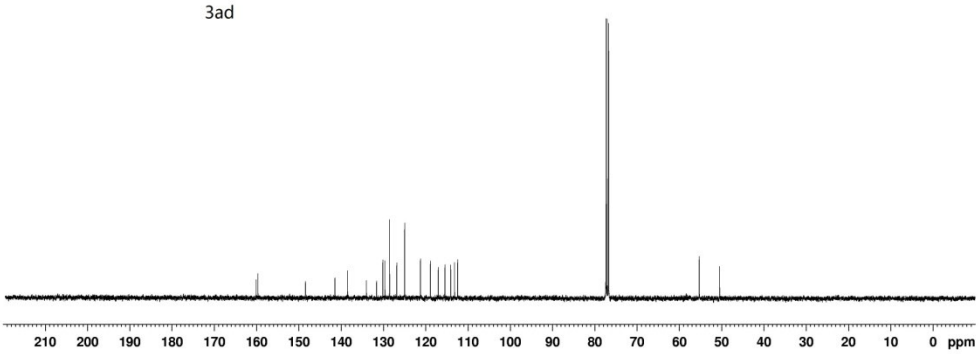
3ad

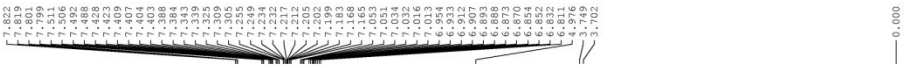

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.32
1.11
1.00
2.01
1.01
1.00
1.02
0.99
2.00
6.00

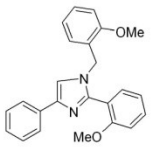

160.09
159.66
148.40
140.44
138.47
133.98
131.57
130.10
129.63
128.91
126.79
124.91
121.20
118.82
116.94
115.38
114.05
113.14
112.40
77.32
77.00
76.68
55.25
55.23
50.41


OMe
N
N
OMe

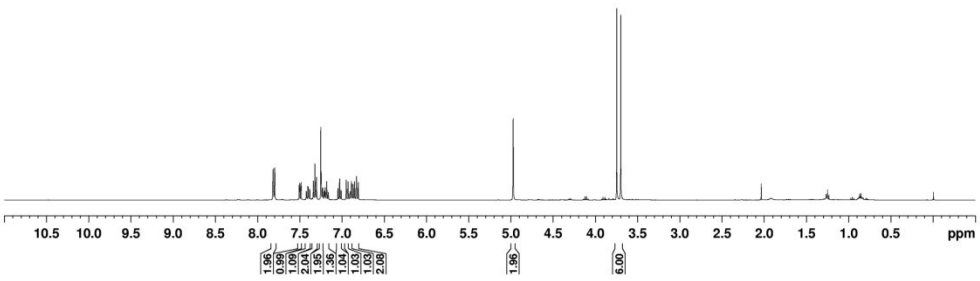
3ad


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

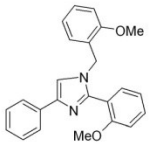

7.822
7.819
7.801
7.799
7.511
7.506
7.492
7.488
7.428
7.423
7.409
7.407
7.404
7.403
7.388
7.384
7.343
7.339
7.325
7.309
7.305
7.255
7.234
7.232
7.217
7.211
7.205
7.202
7.199
7.183
7.168
7.165
7.053
7.051
7.034
7.032
7.016
7.013
6.954
6.933
6.912
6.907
6.893
6.888
6.873
6.870
6.854
6.852
6.832
6.811
4.976
3.749
3.702
0.000


OMe
N
N
MeO

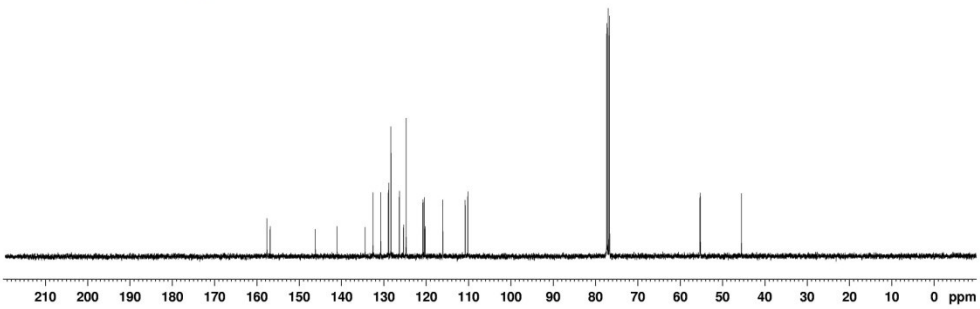
3ae


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 ppm
1.96
0.99
1.00
2.04
1.95
1.36
1.04
1.03
1.03
2.08
1.96
6.00

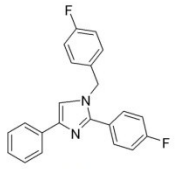

157.59
156.80
146.14
141.05
141.47
132.59
130.77
128.97
128.84
128.34
126.31
125.32
124.75
123.80
120.48
120.22
116.09
110.79
110.16
77.32
77.00
76.68
55.29
55.19
45.50


OMe
N
N
MeO

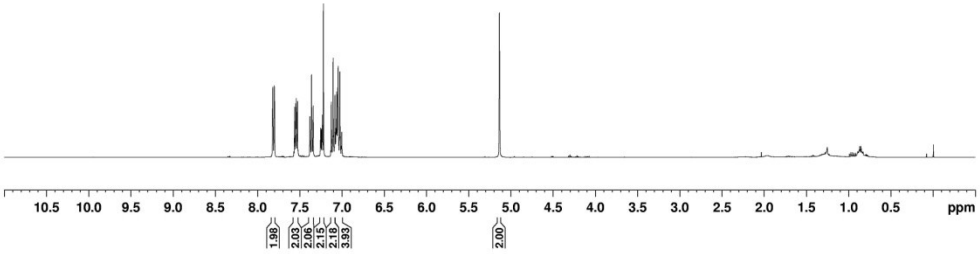
3ae

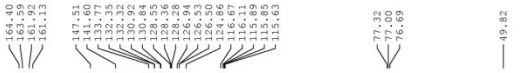

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

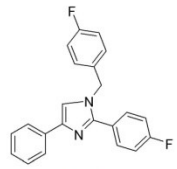

7.826
7.823
7.805
7.803
7.566
7.561
7.553
7.549
7.547
7.544
7.536
7.531
7.383
7.379
7.365
7.345
7.260
7.257
7.254
7.249
7.239
7.234
7.224
7.137
7.130
7.125
7.113
7.108
7.104
7.087
7.074
7.067
7.061
7.053
7.049
7.043
7.033
7.028
7.022
7.012
7.006
5.139
0.000


F
N
N
F

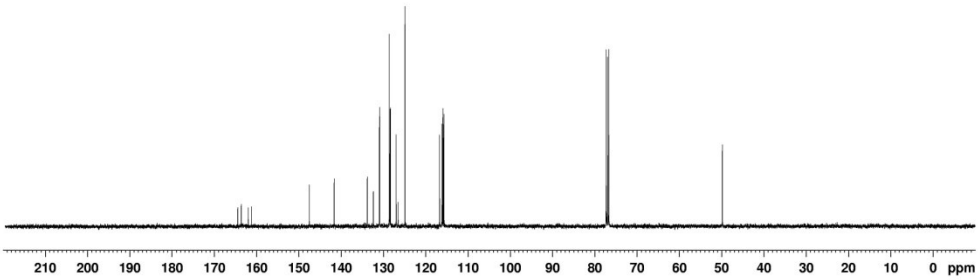
3af

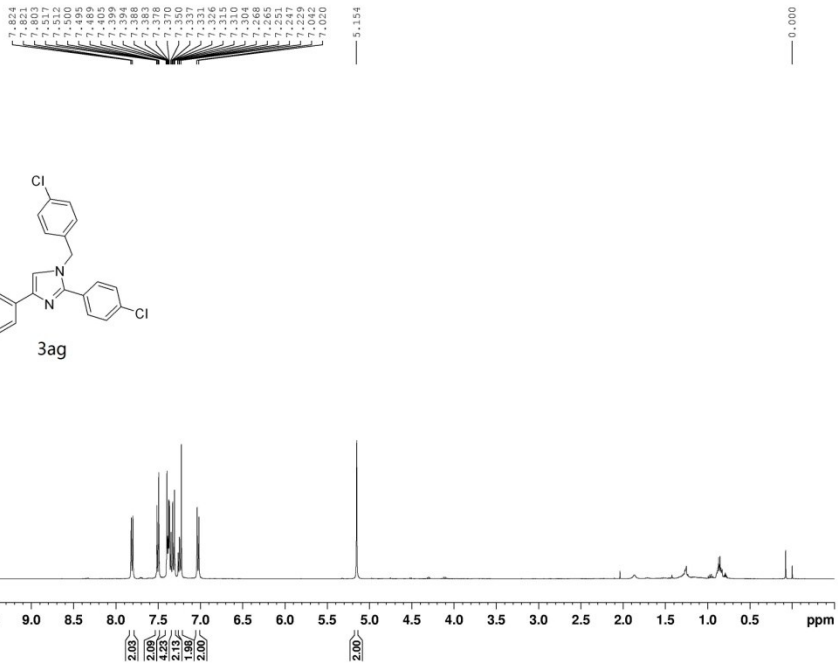

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.98
2.03
2.06
2.15
2.18
3.93
2.00

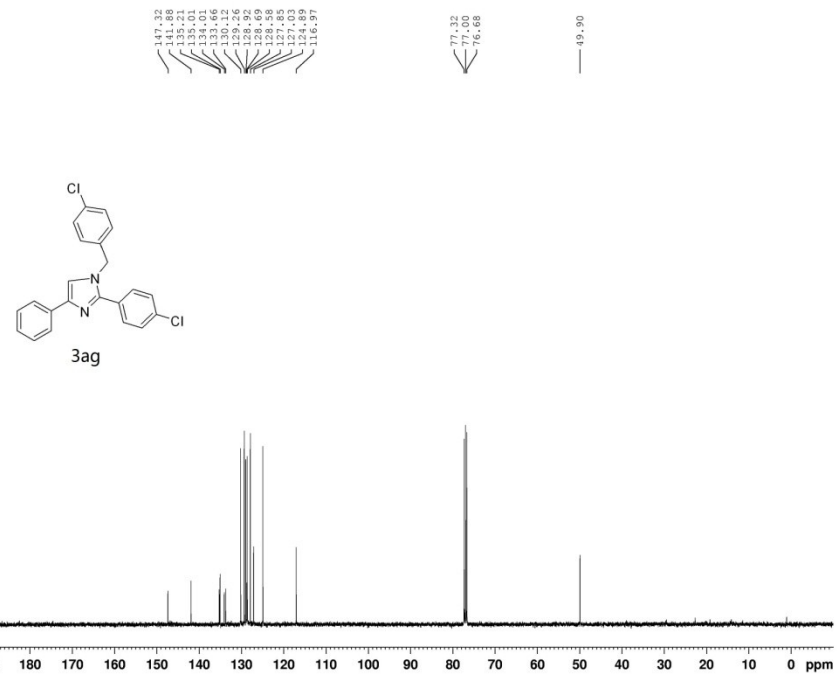

164.40
163.59
161.92
161.13
147.51
141.60
133.77
132.35
132.32
130.92
130.84
128.55
128.36
128.28
126.94
126.53
126.50
124.86
116.67
116.51
115.89
115.85
115.63
77.32
77.00
76.69
49.82

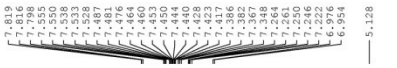

F
N
N
F

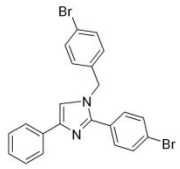
3af


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

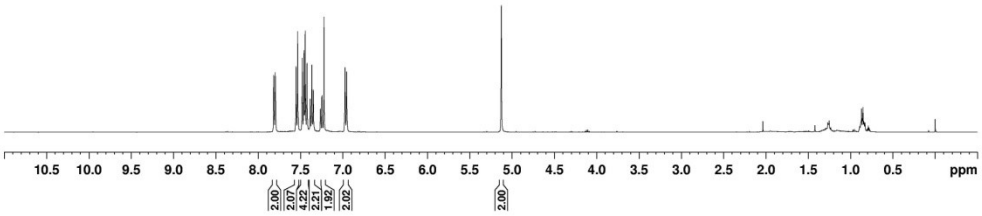

7.824
7.821
7.803
7.517
7.512
7.490
7.489
7.405
7.399
7.394
7.388
7.383
7.378
7.370
7.350
7.337
7.331
7.326
7.315
7.310
7.304
7.268
7.265
7.251
7.247
7.229
7.042
7.020
5.154
0.000
Cl
N
N
Cl
3ag
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.03
2.00
4.23
2.13
1.98
2.00
2.00


147.32
141.88
135.21
133.01
134.01
133.66
130.12
129.56
129.32
128.69
128.58
127.85
127.03
124.89
116.97
77.32
77.00
76.68
49.90
Cl
N
N
Cl
3ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

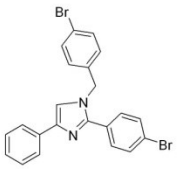

7.819
7.816
7.798
7.555
7.550
7.538
7.533
7.528
7.487
7.481
7.476
7.466
7.460
7.453
7.450
7.444
7.440
7.428
7.423
7.417
7.386
7.382
7.367
7.348
7.264
7.261
7.250
7.246
7.222
6.976
6.954
5.128
0.000


Br
N
N
Br

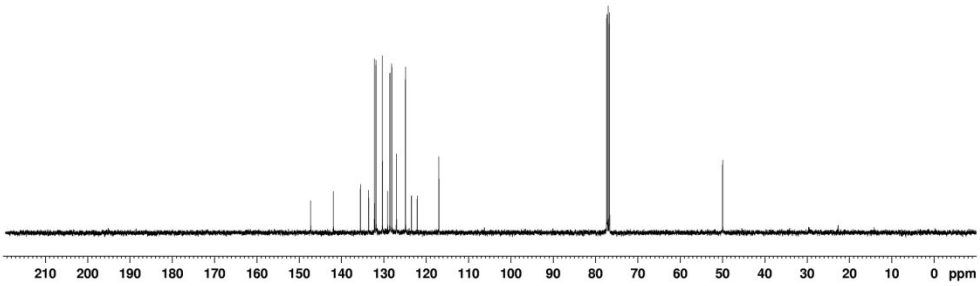
3ah

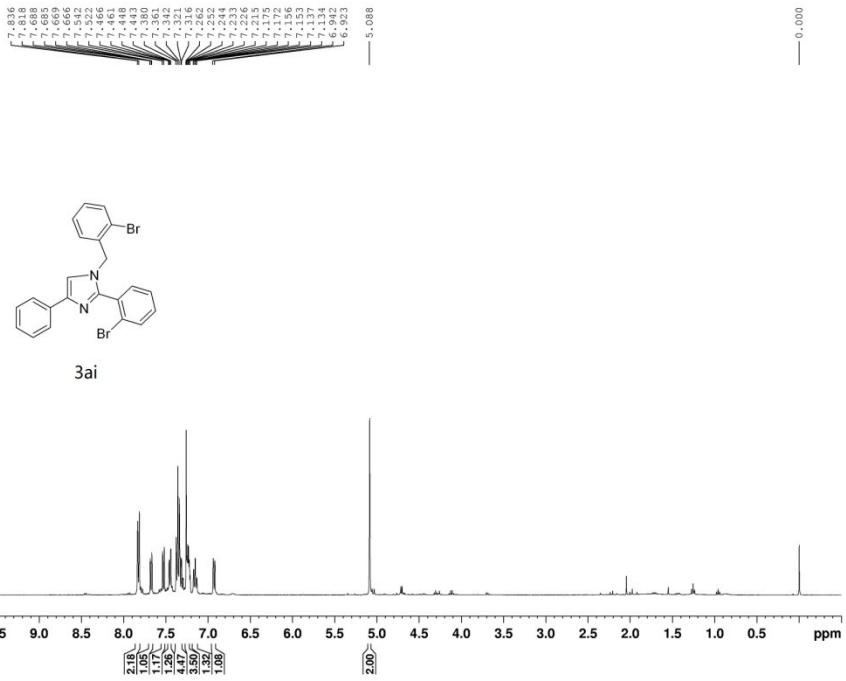

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.07
4.22
2.21
1.92
2.02
2.00

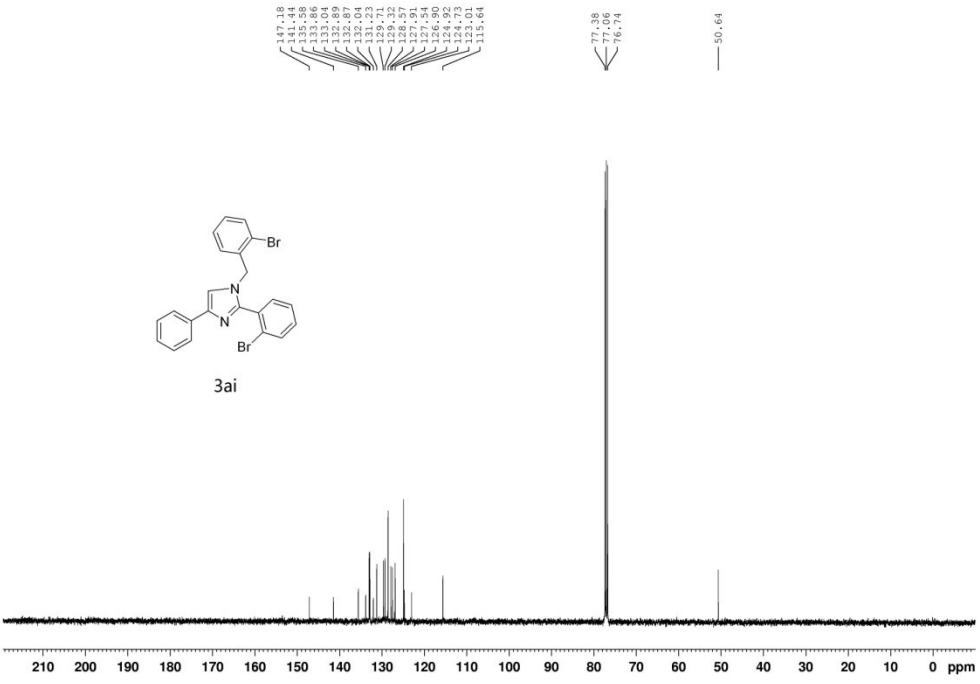

147.33
141.91
135.52
133.62
132.71
131.66
130.33
129.10
128.57
128.14
127.05
124.88
123.47
122.07
117.01
77.32
77.00
76.68
49.94


Br
N
N
Br

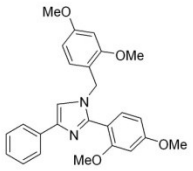
3ah


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

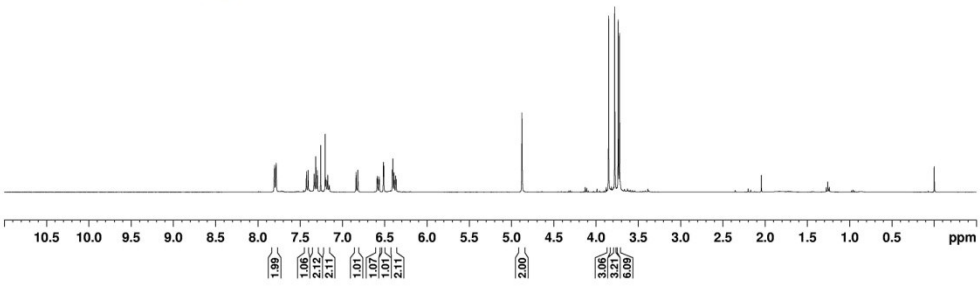

7.836
7.618
7.614
7.688
7.680
7.669
7.666
7.542
7.522
7.466
7.461
7.448
7.443
7.380
7.361
7.342
7.321
7.316
7.262
7.252
7.244
7.233
7.226
7.215
7.175
7.172
7.156
7.153
7.137
7.134
6.942
6.923
5.088
0.000
Br
N
N
Br
3ai
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.18
1.05
1.17
1.26
4.47
3.50
1.32
1.08
2.00


147.18
141.44
135.58
133.86
133.04
132.89
132.67
132.04
131.23
129.71
129.22
128.57
127.91
127.54
126.90
124.22
124.73
123.01
115.64
77.38
77.06
76.74
50.64
Br
N
N
Br
3ai
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.806
7.788
7.430
7.409
7.337
7.319
7.298
7.260
7.207
7.195
7.178
7.158
6.841
6.821
6.593
6.588
6.572
6.567
6.519
6.513
6.412
6.407
6.393
6.387
6.373
6.367
4.879
3.853
3.781
3.741
3.725
0.000


MeO
OMe
N
N
OMe
MeO

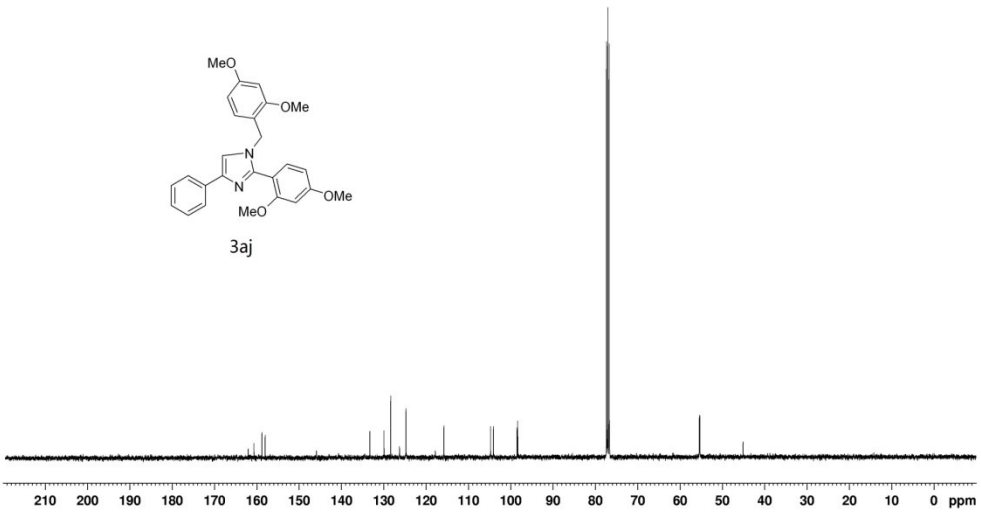
3aj

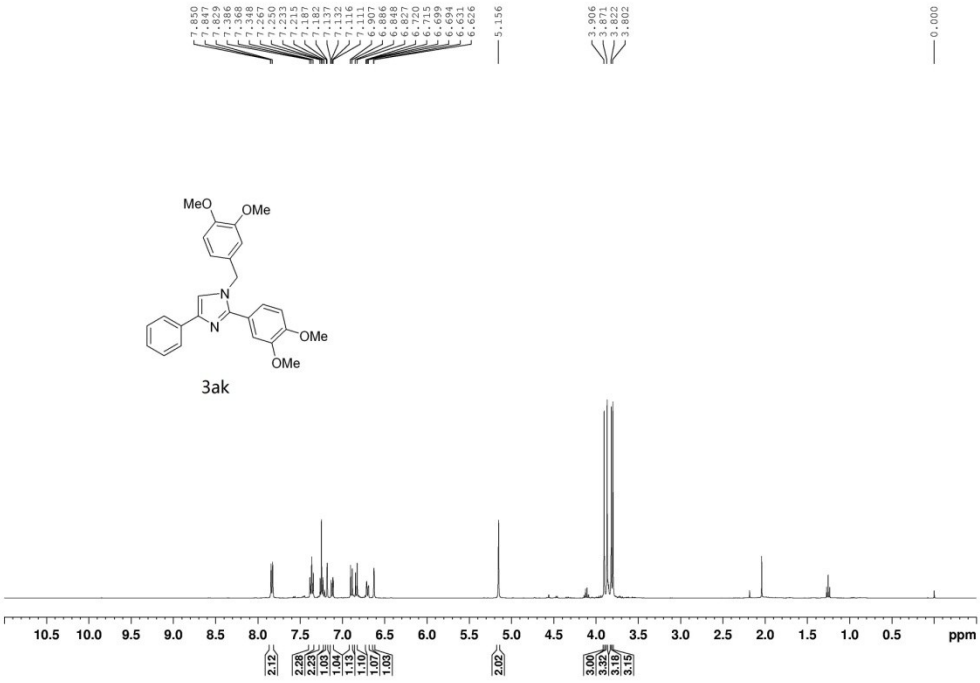

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.99
1.06
2.12
2.11
1.01
1.07
1.01
2.11
2.00
3.06
3.21
6.09

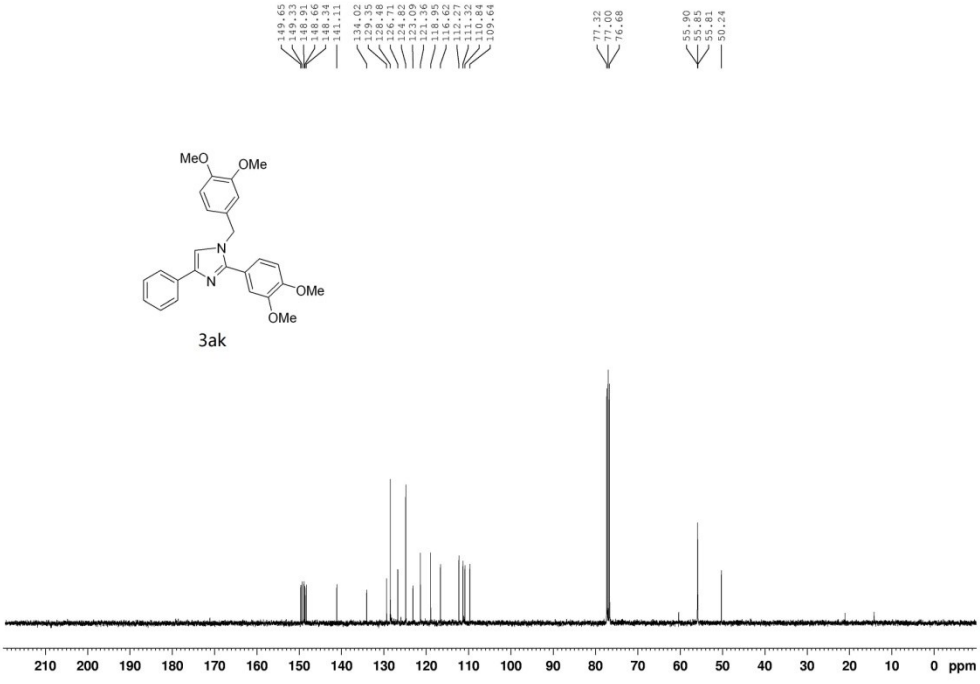

161.96
160.64
158.76
157.98
145.88
133.25
129.31
128.32
126.24
124.72
117.77
115.77
104.73
103.99
98.47
98.30
77.32
77.00
76.68
55.46
55.38
55.35
55.27
45.09

MeO
OMe
N
N
OMe
MeO

3aj


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.850
7.847
7.829
7.386
7.368
7.348
7.267
7.250
7.233
7.215
7.187
7.182
7.137
7.132
7.116
7.111
6.907
6.886
6.848
6.827
6.720
6.715
6.699
6.694
6.671
6.626
5.156
3.906
3.871
3.822
3.802
0.000
MeO
OMe
N
N
OMe
OMe
3ak
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 ppm
2.12
2.28
2.23
1.03
1.04
1.13
1.10
1.07
1.03
2.02
3.00
3.32
3.19
3.19


149.65
149.33
148.91
148.66
148.34
141.11
134.02
129.35
128.48
126.71
124.82
123.09
121.36
118.95
116.62
112.27
111.32
110.84
109.64
77.32
77.00
76.68
55.90
55.85
55.81
50.24
MeO
OMe
N
N
OMe
OMe
3ak
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.983
7.974
7.966
7.959
7.939
7.928
7.920
7.913
7.904
7.855
7.850
7.847
7.829
7.813
7.793
7.661
7.645
7.643
7.623
7.602
7.554
7.546
7.539
7.530
7.515
7.495
7.477
7.458
7.440
7.428
7.409
7.389
7.381
7.378
7.365
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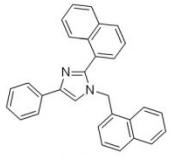
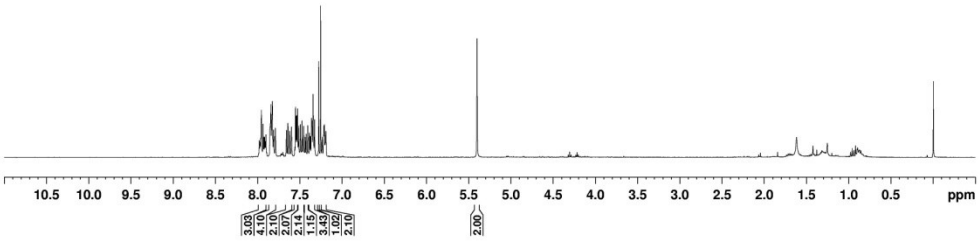
7.347
7.327
7.279
7.257
7.239
7.220
7.212
7.194
5.404
0.000



3al


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 ppm
3.03
4.10
2.10
2.07
2.14
1.15
3.43
1.09
2.19
2.00


147.04
141.44
134.09
133.81
133.62
132.86
131.91
131.60
129.98
128.91
128.85
128.67
128.60
128.34
127.97
127.02
126.74
126.67
126.32
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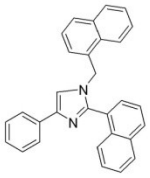
125.38
125.05
124.86
122.47
115.82
77.32
77.00
76.68
48.56



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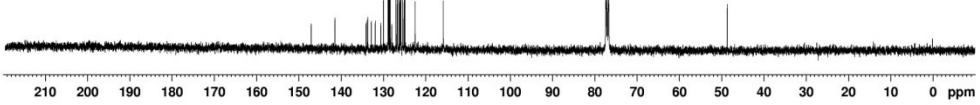
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm