Supporting Information

Metal-Free, Acid-Promoted Synthesis of Imidazole Derivatives via Multicomponent Reaction

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1. Experimental procedures

General Experimental Procedures

The annulation reactions were performed in mild condition. All other reactions, unless otherwise indicated, were carried out under ambient atmosphere in single-neck, round bottom flasks fitted with a rubber septum, equipped with a magnetic stir bar. Air- or water- sensitive solvents were transferred via syringe. When required, solvents were degassed by bubbling of nitrogen through a needle. Organic solutions were concentrated by rotary evaporation at 25-40 °C under reduced pressure (15-30 torr, house vacuum). Analytical Thin Layer Chromatography (TLC) was performed using pre-coated UV 254 plates (0.2 mm) from EM Separations. Visualization was accomplished with a 254 nm UV light source, generally followed by immersion in potassium permanganate ($KMnO_4$) or anisaldehyde solutions, with subsequent heating with a heat gun.

Instrumentation

^1H NMR and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively, using $CDCl_3$ as a solvent. ^1H NMR chemical shifts are referenced to TMS or $CDCl_3$ (0 ; 7.26 ppm). ^{13}C NMR was referenced to $CDCl_3$ (77.0 ppm). Mass spectra and high-resolution mass spectra (HRMS) were measured using the electron-impact (EI, 70 eV, ion trap) technique. Flash chromatography was carried out on silica gel 60 (230-400 mesh). Spectral data are represented in the following order: chemical shift; multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, m = multiplet); coupling constant (*J,* Hz); number of protons.

Materials

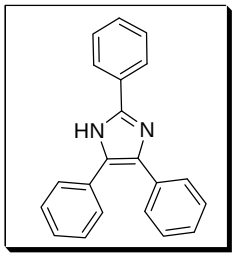
Unless otherwise noted, all reagents, and catalysts were purchased from commercial sources and used as received.

General procedure for the synthesis of 2,4,5-trisubstituted imidazoles.

The starting material 1, 2-diphenylalkyne **1a** 200 mg (1.12 mmol) was dissolved in mixture solvent (dimethylsulfoxide; DMSO, 2 mL) and water (H_2O, 2 mL), followed by benzaldehyde **2a** (114.1 μL, 1.12 mmol), then the ammonium acetate (NH_4OAc, 346 mg, 4.48 mmol), and pivalic acid (PivOH, 126.6 μL, 1.12 mmol) was charged to the reaction mixture and stirred the reaction mixture at 140 ^oC for 24-40 hours.

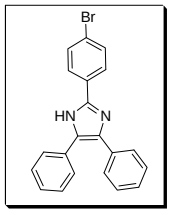
Reaction was monitored by TLC and the reaction mixture was poured out on ice cooled saturated $NaHCO_3$ solution (10 mL) and the aqueous phase was extracted with ethyl acetate (3 X 200 mL), and the combined organic layers were washed with water (3 X 200 mL), brine (1 X 200 mL) and dried over Na_2SO_4, filtered and the volatiles were removed under reduced pressure. The pure compound was obtained by the column chromatography of the crude product on 40-63 mesh silica (Gradient eluent Ethylacetate/Hexane). Purified 2,4,5-trisubstituted imidazole derivatives **4a~4p** (yield 68-90 %).

2,4,5-triphenyl-1*H*-imidazole (4a)[1b,d]



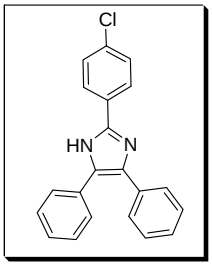
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 276.3 mg (83%). m.p. = 270-272 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 8.11 (d, *J* = 8.4 Hz, 2H)，7.59 (d, *J* = 8.0 Hz, 4H)，7.44 (t, *J* = 8.2 Hz, 2H)，7.35 (t, *J* = 5.2 Hz, 6H) 7.28 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 128.2，128.0，128.0，127.9，126.8，125.4. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{21}H_{17}N_2$, 297.1386; found 297.1390.

2-(4-bromophenyl)-4,5-diphenyl-1*H*-imidazole (4b)[1b]



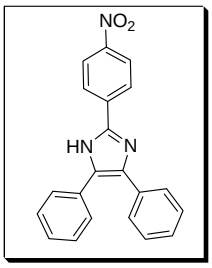
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 337.3mg (80%). m.p. = 257-258 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.77 (d, *J* = 8.4 Hz ,2H)，7.52 (m, 6H)，7.33 (m, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 144.9，131.9，128.6，127.8，127.6，126.9，126.8. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{21}H_{16}N_2Br$, 375.0507; found 375.0491.

2-(4-chlorophenyl)-4,5-diphenyl-1*H*-imidazole(4c)[1b,d]



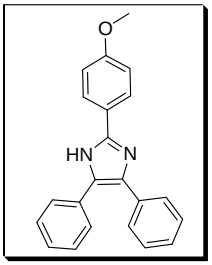
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 308.5 mg (83%). m.p. = 262-264 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.82 (d, *J* = 8.4 Hz, 2H)，7.49 (d, *J* = 7.6 Hz, 4H)， 7.35 (m, 2H)，7.33 (m, 2H)，7.29 (m, 4H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 144.8，134.9，129.1，129.0，128.8，128.5，127.8，127.7，126.7，31.9，31.4，30.1，29.6. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{21}H_{16}N_2Cl$, 331.0997; found 331.1002.

2-(4-nitrophenyl)-4,5-diphenyl-1*H*-imidazole (4d)[1b,d]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 276.1 mg (72%). m.p. = 193-194 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 8.17 (d, *J* = 7.2 Hz, 2H)，7.74 (d, *J* = 7.6 Hz, 2H)，7.72 (d, *J* = 7.6 Hz, 2H)，7.48 (m, 2H)，7.42 (m, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 160.1，136.7，132.5，130.3，128.9，128.7，128.6(2C)，128.5，128.2，128.1，127.3，126.5，126.4. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{21}H_{16}O_2N_3$, 342.3047; found 342.1159.

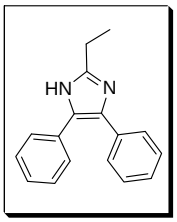
2-(4-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (4e)[1b,d]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 330.0 mg (90%). m.p. = 221-223 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.92 (d, *J* = 8.4 Hz, 2H)，7.485 (d, *J* = 6.8 Hz, 4H)，7.296 (m, 6H)，6.89 (d, *J* = 8.8 Hz, 2H)，3.80(s, 3H). ^{13}C NMR ($CDCl_3$, 100

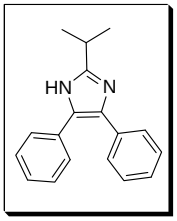
MHz): δ_C 160.0，146.2，132.7，128.4，127.8，127.2，126.8，122.5，114.1，55.3. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{22}H_{19}ON_2$, 327.1506; found 327.1492.

2-ethyl-4,5-diphenyl-1*H*-imidazole (4f)[1g]



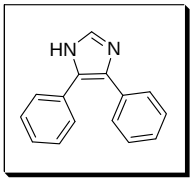
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 189.7 mg (68%). m.p. = 226-228 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.46(d, *J* = 7.6 Hz, 4H)，7.28 (t, *J* = 7.6 Hz, 6H)，2.79 (q, *J* = 7.6 Hz, 2H)，1.28 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 149.4，131.4，130.2，129.0(2C)，128.5，128.3，127.8，127.6，21.0，12.7. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{17}H_{17}N_2$, 249.1392; found 249.1391.

2-isopropyl-4,5-diphenyl-1*H*-imidazole(4g)[1h]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 218.1 mg (74%). m.p. = 162-164 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.50(d, *J* = 7.6 Hz, 4H)，7.31(m, 4H)，7.23(m, 2H)，3.18(m, 1H)，1.38(s, 3H)，1.36(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 168.3，158.5，153.8，128.5，128.1，126.9，29.8，28.6，21.9. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{18}H_{19}N_2$, 263.1543; found 263.1551.

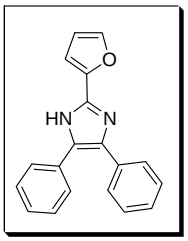
4,5-diphenyl-1*H*-imidazole (4h)[1i]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 183.1 mg (72%). m.p. = 213-215 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.97(s, 1H)，7.48(d, *J* = 7.6 Hz, 4H)，7.31(t, *J* = 9.0 Hz, 6H). ^{13}C NMR

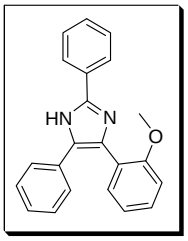
($CDCl_3$, 100 MHz): δ_C 134.1，130.8，130.0，129.2，128.8，128.7，128.3，128.1，127.9. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{15}H_{13}N_2$, 221.1080; found 221.1073.

2-(furan-2-yl)-4,5-diphenyl-1*H*-imidazole(4i)[1d]



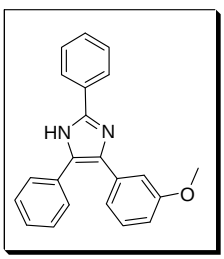
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 267.0 mg (83%). m.p. = 235-237 ^oC. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.52(d, *J* = 7.2 Hz, 5H)，7.35(m, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 135.0，132.9，131.6，128.5，127.9，127.2. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{19}H_{15}N_2O$, 287.1183; found 287.1179.

4-(2-methoxyphenyl)-2,5-diphenyl-1*H*-imidazole(4j)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 300.7 mg (82%). m.p. = 119-121 ^oC. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.94(d, *J* = 7.2 Hz, 2H)，7.51(d, *J* = 7.6 Hz, 2H)，7.41(m, 3H)，7.29(m, 3H)，7.20(t, *J* = 7.2 Hz, 2H)，7.06(d, *J* = 7.2 Hz, 2H)，6.80(d, *J* = 7.2 Hz, 1H)，3.68(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 145.6，129.5，129.1，128.8，128.4，128.0，127.7，125.6，120.2，113.7，112.9，55.1. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{22}H_{19}ON_2$, 327.1502; found 327.1492.

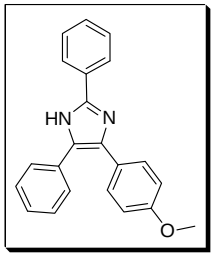
4-(3-methoxyphenyl)-2,5-diphenyl-1*H*-imidazole(4k)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a

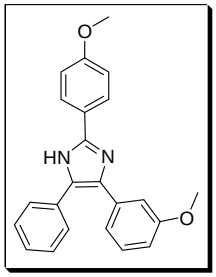
white solid 315.3 mg (86%). m.p. = 143-145 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.84(d, *J* = 7.2 Hz, 2H)，7.48(d, *J* = 7.6 Hz, 2H)，7.29(m, 4H)，7.17(t, 1H)，7.04(m, 2H)，6.89(d, *J* = 7.6 Hz, 2H)，6.78(d, *J* = 8.0 Hz, 1H)，3.80(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 160.2，159.5，145.9，133.5，132.1，129.4，128.4，128.0，127.4，127.1，121.9，120.2，114.1，113.5，112.5，55.3. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{22}H_{19}N_2O$, 327.1497; found 327.1494.

4-(4-methoxyphenyl)-2,5-diphenyl-1*H*-imidazole(4l)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 322.7 mg (88%). m.p. = 155-157 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.92(d, *J* = 7.6 Hz, 2H)，7.51(d, *J* = 8.0 Hz, 2H)，7.42(t, *J* = 8.0 Hz, 4H)，7.37(t, *J* = 8.0 Hz, 2H)，7.29(m, 2H)，6.84(d, *J* = 8.8 Hz, 2H)，3.79(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 159.3，145.8，132.8，129.5，129.1，129.0，128.7，127.9，127.5，125.7，114.6，114.2，55.4. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{22}H_{19}N_2O$, 327.1497; found 327.1495.

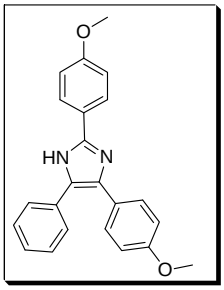
4-(3-methoxyphenyl)-2-(4-methoxyphenyl)-5-phenyl-1*H*-imidazole (4m)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 320.3 mg (80%). m.p. = 224-226 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.84(d, *J* = 7.2 Hz,2H)，7.48(d, *J* = 7.6 Hz, 2H)，7.29(m, 3H)，7.17(t, 1H)，7.04(m, 2H)，6.89(d, *J* = 7.6 Hz, 2H)，6.78(d, *J* = 8.0 Hz, 1H)，3.80(s, 3H) ，3.66(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 160.2，159.5，145.9，133.5，132.1，129.4，128.4，128.0，127.4，127.1，121.9，120.2，114.1，113.5，112.5，55.3，55.1 HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{23}H_{21}N_2O_2$,

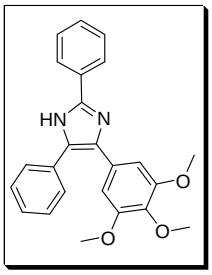
357.1603; found 357.1601.

2,4-bis(4-methoxyphenyl)-5-phenyl-1*H*-imidazole (4n)



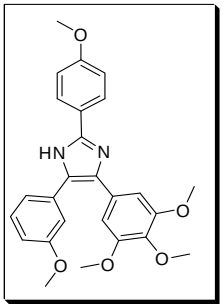
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 332.3 mg (83%). m.p. = 179-181 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.76(d, J = 8.4 Hz, 2H)，7.32(d, J = 7.6 Hz, 2H)，7.22(d, J = 8.0 Hz, 2H)，7.11(m, 3H)，6.69(m, 4H)，3.64(s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 177.4，160.3，159.1，146.3，132.3，132.0，131.7，129.7，128.4，128.2，127.8，127.3，124.5，121.9，114.2，113.9，55.4，55.3. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{23}H_{21}N_2O_2$, 357.1605; found 357.1601.

2-(4-methoxyphenyl)-5-phenyl-4-(3,4,5-trimethoxyphenyl)-1*H*-imidazole (4o)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 373.4 mg (87%). m.p. = 179-181 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.94(d, J = 8.0 Hz, 2H)，7.51(d, J = 7.6 Hz, 2H)，7.39(m, 6H)，6.73(s, 2H)，3.82(s, 3H)，3.64(s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 153.0，145.8，137.1，129.5，128.8，128.7，128.4，128.1，127.6，125.5，104.9，60.8，55.8. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{24}H_{23}O_3N_2$, 387.1703; found 387.1703

5-(3-methoxyphenyl)-2-(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)-1*H*-imida zole(4p)



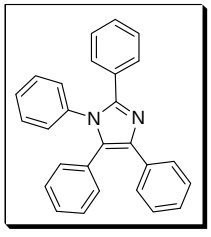
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a yellow solid 431.4 mg (84%). m.p. = 199-201 ^{o}C. ^{1}H NMR

($CDCl_3$, 400 MHz): δ_H 7.85(d, *J* = 8.4 Hz, 2H)，7.19(t, *J* = 8.0 Hz, 1H)，7.05(d, *J* = 7.2 Hz, 2H)，6.85(d, *J* = 8.8 Hz, 2H)，6.79(m, 1H)，6.71(s, 2H)，3.81(s, 3H)，3.78(s, 3H)，3.68(s, 3H)，3.63(s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 160.1，159.4，152.9，146.0，137.0，133.3，129.3，128.1，127.1，122.0，120.5，114.1，113.3，113.1，107.1，105.3，105.0，60.8，55.8，55.4，55.2，55.1. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{26}H_{27}O_5N_2$, 447.1920; found 447.1917.

General procedure for the synthesis of 1,2,4,5-trisubstituted imidazoles.

The starting material 1, 2-diphenylalkyne **1a** (200 mg, 1.12 mmol) was dissolved in mixture solvent (dimethylsulfoxide DMSO, 2 mL) and water (H_2O, 2 mL), followed by benzaldehyde **2a** (114.1 μL, 1.12 mmol), aniline **3a** (102.2 μL, 1.12 mmol) then the ammonium acetate (NH_4OAc, 346 mg, 4.48 mmol),and pivalic acid (PivOH, 126.6 μL, 1.12 mmol) was charged to the reaction mixture and stirred the reaction mixture at 140 ^oC for 24-48 hours. Reaction was monitored by TLC and the reaction mixture was poured out on ice cooled saturated $NaHCO_3$ solution (10 mL) and the aqueous phase was extracted with ethyl acetate (3 X 200 mL), and the combined organic layers were washed with water (3 X 200 mL), brine (1 X 200 mL) and dried over Na_2SO_4, filtered and the volatiles were removed under reduced pressure. The pure compound was obtained by the column chromatography of the crude product on 40-63 mesh silica (Gradient eluent Ethylacetate/Hexane). Purified 1,2,4,5-tetrasubstituted imidazole derivatives **5a~5r** (yield 65-88 %).

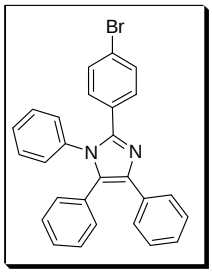
1,2,4,5-tetraphenyl-1*H*-imidazole (5a)[1a,b,d]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a

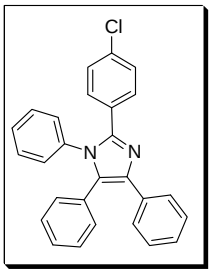
white solid 368.2 mg (88%). m.p. = 218-219 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 8.02(m, 5H)，7.50(m, 4H)，7.37(m, 5H)，7.18(m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 172.7，146.8，138.2，137.7，136.2，134.8，133.5，133.2，132.9，131.0，130.7，130.4，130.0，129.9，129.8，129.7，129.5，129.3，129.2，129.1，129.0，128.9，128.6，128.5，128.3，128.2，128.1，127.9，127.7，127.1，127.0，93.9. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{27}H_{21}N_2$, 373.1703; found 373.1706.

2-(4-bromophenyl)-1,4,5-triphenyl-1*H*-imidazole (5b)[1b]



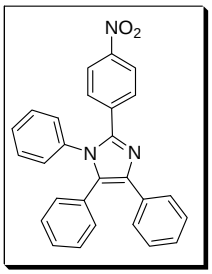
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 380.3 mg (75%). m.p. = 152-154 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.72(m, 1H)，7.66(m, 2H)，7.47(m, 7H)，7.38(d, *J* = 8.0 Hz, 2H)，7.32(m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 144.9，131.9，131.7，129.3，128.6，128.5，128.4，128.2，127.8，127.6，126.9，126.8，123.0，121.6. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{27}H_{20}BrN_2$, 451.1062; found 451.1070.

2-(4-chlorophenyl)-1,4,5-triphenyl-1*H*-imidazole(5c)[1b-d]



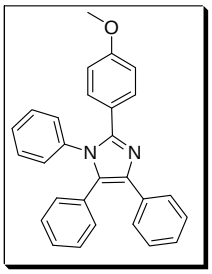
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 324.6 mg (71%). m.p. = 157-158 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.59(d, *J* = 7.6 Hz, 2H)，7.38(d, *J* = 8.4 Hz, 2H)，7.29(m,11H)，7.12(d, *J* = 8.0 Hz, 2H)，7.04(d, *J* = 6.8 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 145.6，136.6，134.5，131.1，130.1，129.2，129.0，128.5，128.3(2C)，128.2，128.1，127.4，127.1，126.8. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$, 407.1315; found 407.1313.

2-(4-nitrophenyl)-1,4,5-triphenyl-1*H*-imidazole (5d)[1b,d]



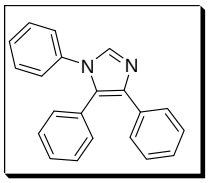
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 304.8 mg (65%). m.p. = 191-193 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 8.41(d, J = 8.8 Hz,2H)，8.28(d, J = 8.8 Hz,2H)，8.07(d, J = 8.8 Hz,2H)，7.59(m, 4 H)，7.45(t, J = 7.6 Hz,2H)，7.37(m,7H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 168.5，147.1，143.5，134.9，132.5，131.5，130.6，129.6，128.7，128.4，128.2，128.1，127.7，127.2，126.3，123.9. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{27}H_{20}O_2N_3$, 418.1708; found 418.1472.

2-(4-methoxyphenyl)-1,4,5-triphenyl-1*H*-imidazole(5e)[1b,d]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 393.4 mg (87%). m.p. = 184-185 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.61(d, J = 9.2 Hz, 2H)，7.38(d, J = 8.8 Hz, 2H)，7.28(m, 9H)，7.12(d, J = 8.0 Hz, 2H)，7.05(d ,J = 7.6 Hz, 2H)，6.78(d, J = 8.0 Hz, 2H)，3.78(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 151.6，133.6，133.3，131.3，130.9，130.2，129.6，126.6，125.8，125.6，125.2，124.0，123.4，122.8，117.7，115.8，113.6，64.3. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{28}H_{23}ON_2$, 403.1805; found 403.1812.

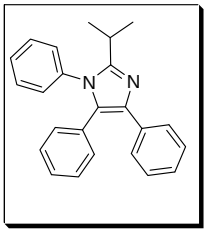
1,4,5-triphenyl-1*H*-imidazole (5f)[1e]



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 243.0 mg (73%). m.p. = 169-171 ^{o}C. ^{1}H NMR ($CDCl_3$, 400

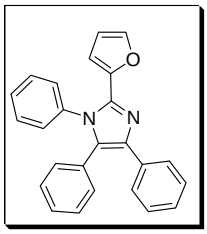
MHz): δ_H 7.81(s, 1H)，7.55(d, *J* = 7.6 Hz, 2H)，7.32(m, 13H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 137.5，134.4，131.0，129.4，128.8，128.4(2C)，128.2，127.4，126.9，126.0. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{21}H_{17}N_2$, 297.1400; found 297.1386.

2-isopropyl-1,4,5-triphenyl-1*H*-imidazole (5g)



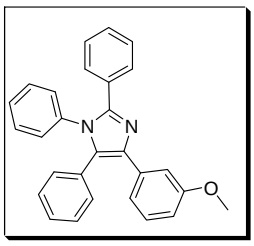
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 296.2 mg (78%). m.p. = 169-171 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.54(d, *J* = 8.4 Hz, 2H)，7.35(m, 3H)，7.24(m, 10H)，2.91(sep, *J* = 6.8 Hz, 1H)，1.33(s, 3H)，1.31(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 153.6，136.8，136.6，134.8，130.8，130.7(2C)，128.9，128.7， 128.3，128.1，128.0，127.4，127.3，127.0，126.1，26.4，21.9(2C). HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{24}H_{23}N_2$, 339.1839; found 339.1856.

2-(furan-2-yl)-1,4,5-triphenyl-1*H*-imidazole(5h)[1d]



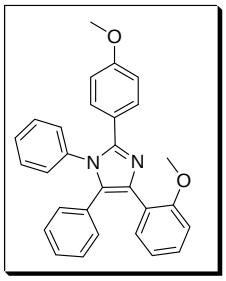
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 325.7 mg (80%). m.p. = 139-141 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.80(m, 1H)，7.546(d, *J* =7.6 Hz, 2H)，7.30(m, 4H)，7.27(m, 6H)，7.19(d, *J* = 6.8 Hz, 1H)，7.15(m, 2H)，7.11(m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 138.6，138.2，137.2，136.2，134.0，130.6(2C)，129.8，129.1，128.6，128.5，128.4，128.2(2C)，128.1，128.0，127.9，127.7，127.2(2C)，126.7，126.6，125.6. $[M+H]^+$ calcd for $C_{25}H_{19}ON_2$, 363.1461; found 363.1467.

4-(3-methoxyphenyl)-1,2,5-triphenyl-1*H*-imidazole (5i)



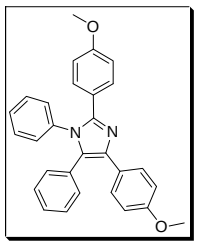
The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 379.8 mg (84%). m.p. = 155-157 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.99(d, *J* = 6.8 Hz, 2H)，7.48(d, *J* = 7.2 Hz, 3H)，7.38(m, 4H)，7.26(m, 5H)，7.15(t, 2H)，7.04(m, 2H)，6.78(d, *J* = 8.1 Hz, 1H)，3.67(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 159.5，145.6，129.4，129.3，128.7，128.4，128.1，127.7，125.6，125.9 ，120.3，113.5，113.8，113.0，55.1. $[M+H]^+$ calcd for $C_{28}H_{23}ON_2$, 403.1703; found 403.1718.

4-(2-methoxyphenyl)-2-(4-methoxyphenyl)-1,5-diphenyl-1*H*-imidazole (5j)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 413.0 mg (85%). m.p. = 129-131 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.86(d, *J* = 8.4 Hz, 2H)，7.59(d, *J* = 8.0 Hz, 2H)，7.34(d, *J* = 7.6 Hz, 2H)，7.28(m, 7H)，6.97(m, 4H)，6.87(t, *J* = 7.6 Hz, 1H)，3.83(s, 3H)，3.81(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 160.1，155.9，145.3，131.5，130.6，130.4，129.0，128.6，128.4，128.2，127.9，127.6，126.9(2C)，120.9，114.2，111.4，55.6，55.3.HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{29}H_{25}O_2N_2$, 433.1911; found 433.1908.

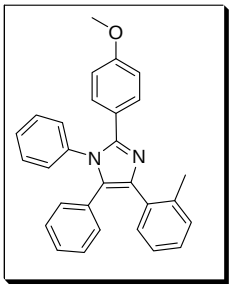
2,4-bis(4-methoxyphenyl)-1,5-diphenyl-1*H*-imidazole (5k)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 427.6 mg (88%). m.p. = 121-123 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H

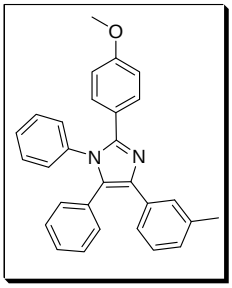
7.80(d, *J* = 8.4 Hz, 2H)，7.48(m, 3H)，7.34(d, *J* = 8.0 Hz, 3H)，7.25(m, 5H)，6.80(m, 5H)，3.74(s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 159.7，158.6，146.1，132.8，130.5，129.2，128.9，128.6，128.1，127.6，127.0，126.7，125.0，122.5，120.0，113.9，113.8，113.6，113.5，113.4，55.1，55.0. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{29}H_{25}O_2N_2$, 433.1894; found 433.1911.

2-(4-methoxyphenyl)-1,5-diphenyl-4-o-tolyl-1*H*-imidazole (5l)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 383.7 mg (82%). m.p. = 145-147 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.98(d, *J* = 7.6 Hz, 1H)，7.90(d, *J* = 8.8 Hz, 2H)，7.52(m, 1H)，7.41(d, *J* = 8.0 Hz, 2H)，7.37(m, 1H)，7.27(t, *J* = 8.0 Hz, 3H)，7.20(m, 6H)，6.88(d, *J* = 8.8 Hz, 2H)，3.76(s, 3H)，2.02(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 160.3，145.6，137.5，132.5，131.2，130.6，130.4，129.7，128.6，128.3，128.0，127.2，126.8，126.2，125.9，121.6，114.2，114.1，55.2. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{29}H_{25}N_2O$, 417.1967; found 417.1964.

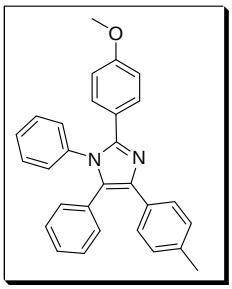
2-(4-methoxyphenyl)-1,5-diphenyl-4-m-tolyl-1*H*-imidazole (5m)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 388.4 mg (83%). m.p. = 172-174 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 7.61(d, *J* = 8.0 Hz, 1H)，7.52(d, *J* = 7.2 Hz, 1H)，7.39(m, 1H)，7.26(d, *J* = 8.8 Hz, 1H)，7.14(m, 6H)，7.03(m, 2H)，6.93(m, 3H)，6.83(d, *J* = 7.6 Hz, 1H)，6.70(m, 2H)，3.64(s, 3H)， 2.18(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 159.4，137.9，137.7，137.6，137.0(2C)，134.5，134.1，131.5，

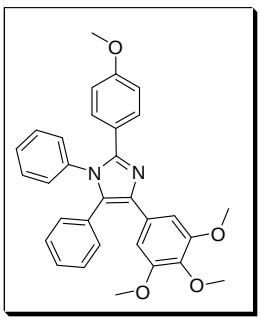
131.0，130.5(2C)，130.4，130.2(2C)，130.0，129.7，129.1，129.0，128.9(2C)，128.8，128.5，128.3，128.2，128.1，128.0，127.9，127.8，127.7，127.6，127.2，127.1，127.0，113.5，113.4，55.0. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{29}H_{25}ON_2$, 417.1961; found 417.1964.

2-(4-methoxyphenyl)-1,5-diphenyl-4-p-tolyl-1*H*-imidazole (5n)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 374.3 mg (80%). m.p. = 162-164 ^oC. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.60(d, J = 7.2 Hz, 1H)，7.48(d, J = 8.0 Hz, 1H)，7.32(d, J = 8.8 Hz, 2H)，7.22(m, 5H)，7.10(m, 2H)，7.01(m, 5H)，6.72(m, 2H)3.68(s, 3H)，2.25(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 159.3，146.6，137.8，137.6，137.4，137.0(2C)，135.9，134.4，131.3，130.9，130.7，130.6，130.4(2C)，130.1(2C)，130.0(2C)，129.9，129.1，129.0，128.9，128.8，128.7，128.3(2C)，128.1(2C)，128.0，127.9(2C)，127.8，127.7，127.6，127.2，127.1，127.0，.6，113.5，113.4，55.0. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{29}H_{25}ON_2$, 417.1961; found 417.1964.

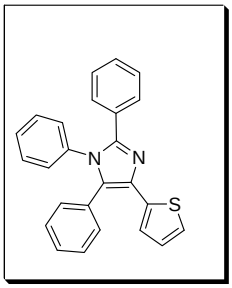
2-(4-methoxyphenyl)-1,5-diphenyl-4-(3,4,5-trimethoxyphenyl)-1H-imidazole (5o)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 487.0 mg (88%). m.p. = 169-171 ^oC. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.67(d, J = 8.0 Hz,2H)，7.37(d, J = 8.0 Hz, 2H)，7.29(m, 4H)，7.24(t, 2H)，7.07(m, 2H)，6.76(d, J = 7.6 Hz, 2H)，6.27(s, 2H)，3.81(s, 3H)，3.71(s, 3H)，3.49(s, 6H). ^{13}C NMR

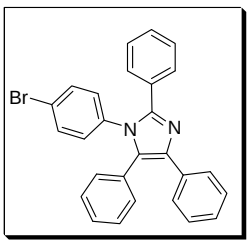
($CDCl_3$, 100 MHz): δ_C 159.4，152.5，146.5，137.4，137.2，137.0，133.9，130.1，129.9，129.8，128.9，128.8，128.7，128.3，128.3，128.1，128.0(2C)，127.9，129.8，128.6，127.5，127.4，127.6，126.4，125.2，122.3，113.2，108.0，107.9，60.5，55.5(2C)，54.8. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{31}H_{29}O_4N_2$, 493.2127; found 493.2125.

1,2,5-triphenyl-4-(thiophen-2-yl)-1*H*-imidazole (5p)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 348.7 mg (82%). m.p. = 141-143 °C. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.70(d, *J* = 7.2 Hz, 2H)，7.46(d, *J* = 7.2 Hz, 2H)，7.31(t, *J* = 7.6 Hz, 6H)，7.24(d, *J* = 7.2 Hz, 4H)，7.14(d, *J* = 7.2 Hz, 2H)，6.92(m, 1H)，6.86(m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 147.6，140.2，136.8，133.9，131.2，131.0，130.9，130.2，130.1，129.2，129.0(2C)，128.9，128.8，128.7，128.6，128.4，128.3，128.2，128.1，128.0(2C)，127.9，127.4，127.3，127.1，127.0，126.9，126.5，123.6. $[M+H]^+$ calcd for $C_{25}H_{19}SN_2$, 379.1812; found 379.1825.

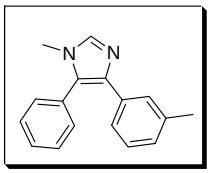
1-(4-bromophenyl)-2,4,5-triphenyl-1*H*-imidazole (5q)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 400.6 mg (79%). m.p. = 239-241 °C. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.72(m, 1H)，7.66(m, 2H)，7.47(m, 7H)，7.38(d, *J* = 8.0 Hz, 2H)，7.32(m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 144.9，131.9，131.7，129.3，128.6，128.5，128.4，128.2，127.8，127.6，

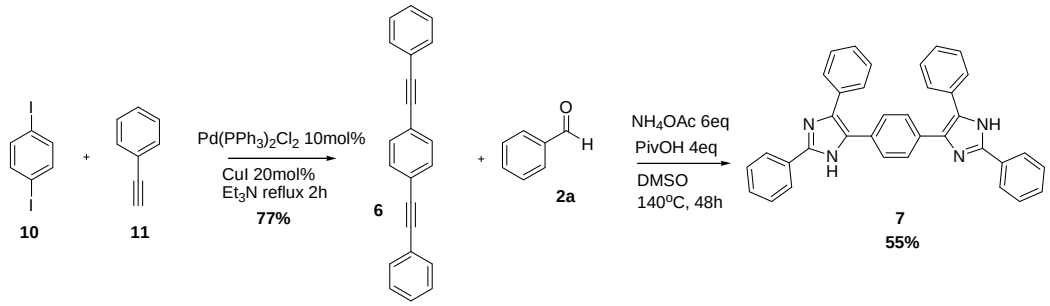
126.9，126.8，123.0，121.6. HRMS (ESI-ion trap, m/z): $[M+H]^+$ calcd for $C_{27}H_{20}BrN_2$, 451.0810; found 451.0808.

1-methyl-5-phenyl-4-m-tolyl-1*H*-imidazole (5r)



The title compound was prepared according to the general procedure and purified by column chromatography to obtain a white solid 228.7 mg (82%). m.p. = 122-124 ^oC. ^1H NMR ($CDCl_3$, 400 MHz): δ_H 7.56 (s, 1H)，7.47(d, J = 8.0 Hz, 2H)，7.42 (m, 2H)，7.31 (m, 2H)，7.20(t, J = 8.0 Hz, 2H)，7.13(m, 1H)，3.43(s, 3H)，2.92(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 137.8，137.2，134.3，131.6，130.4，130.2，128.7，128.4，128.2，127.9，127.2，126.4，126.1，42.3，32.0. $[M+H]^+$ calcd for $C_{17}H_{17}N_2$, 249.1307; found 249.1312.

Synthesis of 4-(4-(2,4-diphenyl-1H-imidazol-5-yl)phenyl)-2,5-diphenyl-1H-imidazole(7)



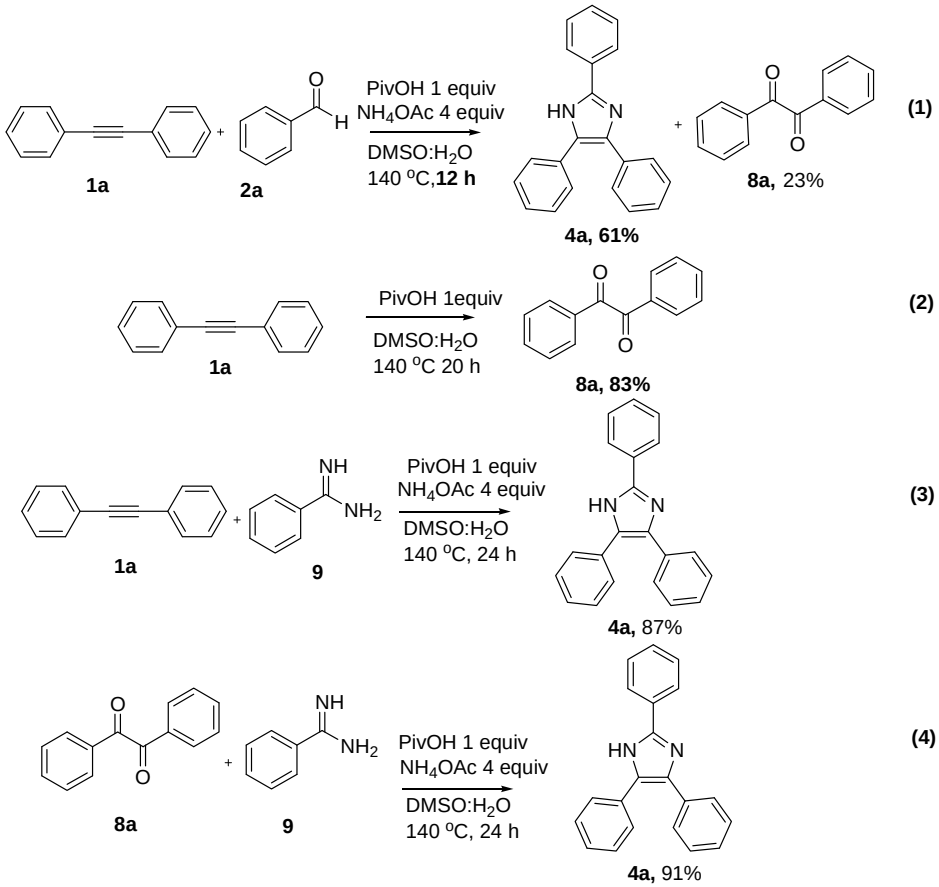
The starting material 1,4-bis(2-phenylethynyl)benzene (**6**) was prepared by reported sonogashira condition, and then treated with benzaldehyde using our methodology to construct bis-imidazole derivatives. The starting material 1,4-bis(2-phenylethynyl) benzene (**6**) 200 mg (0.71 mmol) was dissolved in mixture solvent (dimethylsulfoxide DMSO, 2.0 mL) and water (H_2O, 2.0 mL), followed by benzaldehyde **2a** (146.6 μL, 1.42 mmol), then the ammonium acetate (NH_4OAc, 332 mg, 4.2 mmol), and pivalic

acid (PivOH, 162.1 μL, 1.42 mmol) was charged to the reaction mixture and stirred the reaction mixture at 140 ^{o}C for 48 hours. Reaction was monitored by TLC and the reaction mixture was poured out on ice cooled saturated $NaHCO_3$ solution (10 mL) and the aqueous phase was extracted with ethyl acetate (3 X 200 mL), and the combined organic layers were washed with water (3 X 200 mL), brine (1 X 200 mL) and dried over Na_2SO_4, filtered and the volatiles were removed under reduced pressure. The pure compound was obtained by the column chromatography of the crude product on 40-63 mesh silica (Gradient eluent Ethylacetate: Hexane = 1:1). Purified 4-(4-(2,4-diphenyl-1H-imidazol-5-yl)phenyl) -2,5-diphenyl-1H-imidazole **7** (white solid 203 mg, yield 55 %). m.p. = 127-128 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ_H 8.15(d, *J* = 7.6 Hz, 1H)，8.06 (d, *J* = 8.0 Hz, 2H)，7.57(m, 3H)，7.46(m, 3H)，7.36(m, 3H)，6.19(s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ_C 168.5，132.4，131.8，129.5，128.8，128.7，128.4，128.3，128.1，128.0，127.9，127.2，125.9. $[M+H]^+$ calcd for $C_{36}H_{27}N_4$, 515.2207; found 515.2209.

Reference:

1. (a) Lantos, I.; Zhang, W.-Y.; Shui, X.; Eggleston, D. S. *J. Org. Chem.* **1993** , *58*, 7092. (b) Teimouri, A.; Chermahini, A. N. *J. Mol. Catal. A: Chem.* **2011**, *346*, 39. (c) Kumar, D.; Kommi, D. N.; Bollineni, N.; Patel, A. R.; Chakraborti, A. K. *Green Chem.* **2012**, *14*, 2038. (d) Sivakumar, K.; Kathirvel, A.; Lalitha, A. *Tetrahedron Lett.* **2010**, *51*, 3018. (e) Collibee, W. L.; Anselme, J. P. *Bulletin des Societes Chimiques Belges* **1986**, *95*, 655. (f) Bakibaev, A. A.; Yagovkin, A. Y. *Russian Journal of Organic Chemistry* **1994**, *30*, 143. (g) Wang, L.; Zhong, X.; Zhou, M.; Zhou, W.-Y.; Chen, Q.; He, M.-Y. *Journal of Chemical Research.* **2013**, *37*, 236. (h) Magee, D. I.; Bahramnejad, M.; Dabiri, M. *Tetrahedron Lett.* **2013**, *54*, 2591.(i) Xu, F.; Wang, N.; Tian, Y.; Li, G. *Journal of Heterocyclic Chemistry* **2013**, *50*, 668.

2. Control Experiments



Scheme S1. Control Experiments.

To gain insight into the reaction mechanism, we carried out a few control experiments. First, we started a reaction between **1a** and **2a** in the presence of PivOH and ammonium acetate and observed **4a** as the major product and the benzil product **8a** as the minor one (Scheme S3, eq 1). Then we conducted the experiment without addition of benzaldehyde and ammonium acetate. Based on these reactions, we confirmed that the benzil product **8a** was the intermediate for this transformation (eq 2). With commercially available benzamidine **9** and diphenylacetylene **1a** or benzil **8a**, the desired product **4a** was obtained in 87% and 91% yield, respectively (Scheme S1, eqs 3 and 4).

2. The photo-physical properties of imidazole derivatives

UV Absorption and Fluorescence emission data of imidazole derivatives

The photo-physical properties for some of the representative imidazole derivatives showed a very good fluorescence emission; especially compound **5p** demonstrated maximum absorption at 245 nm, excitation at 291 nm, and emission at 423 nm (Table S1). Indeed, we studied their photoluminescence property in solution of the synthesized compounds. The imidazole product **5p** in different solvents is shown in Figure S1.The emission peaks are slightly changed in different solvents. For example, it emits at 425 nm in DMSO solution, but at 415 nm in EtOH (Fig S1). Our ongoing work will be focused on the synthesis of imidazole attached with heterocycles using this methodology with an emission in the visible or near IR region and will be used for the application of Photo dynamic therapy of skin cancer, and organic electroluminescent devices.

Table S1: The fluorescence and UV absorption of imidazole derivatives.

Entry	cpd	λ **max** Absorption	λ **max** Excitation	λ **max** Emission
1	**4a**	261nm	291nm	385nm
2	**4b**	245nm	289nm	386nm
3	**4g**	236, 285nm	281nm	374nm
4	**4g**	241, 293nm	291nm	378nm
5	**4p**	236, 306nm	304nm	396nm
6	**5a**	245nm	290nm	382nm
7	**5c**	236, 290nm	291nm	382nm
8	**5g**	244nm	235nm	378nm
9	**5h**	243nm	250nm	377nm
10	**5p**	245nm	291nm	423nm
11	**5r**	239, 284nm	281nm	384nm

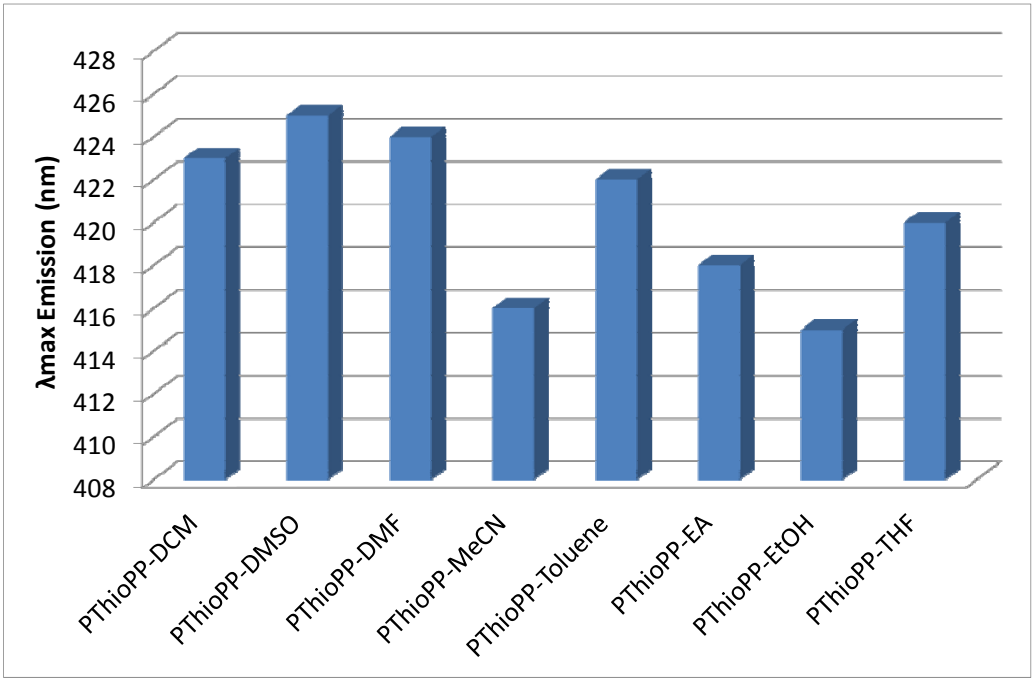
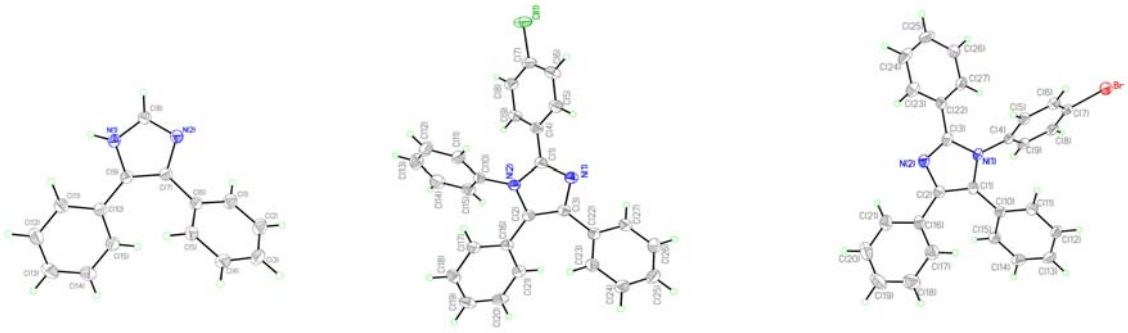


Figure S1: The fluorescein of imidazole derivatives with different solvents.

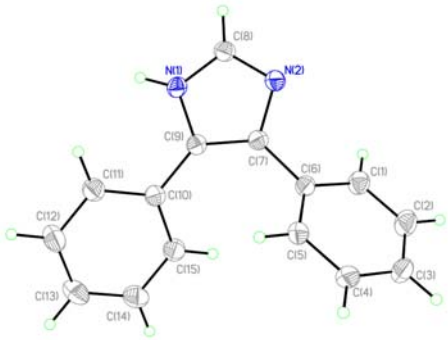
2. ORTEP Diagram of compound **4h**、**5c**、**5q**

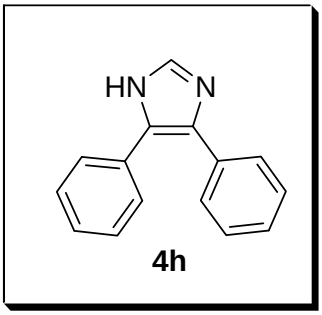
Figure S2. ORTEP diagram of **4h, 5c** and **5q**.



4h **5c** **5q**

The structure of the **4h**、**5c**、**5q** was unambiguously confirmed with X-ray crystallographic technique.





CCDC No of **4h** : 928193

Table 1. Crystal data and structure refinement for **4h**.

Identification code	**4h**
Empirical formula	C15 H12 N2
Formula weight	220.27
Temperature	300(2) K

Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.1711(6) Å	α= 90°.
	b = 9.2671(4) Å	β= 93.572(2)°.
	c = 11.8123(6) Å	γ = 90°.
Volume	1220.48(10) $Å^3$	
Z	4	
Density (calculated)	1.199 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	464	
Crystal size	0.53 x 0.49 x 0.33 mm^3	
Theta range for data collection	2.80 to 26.44°.	
Index ranges	-13<=h<=13, -11<=k<=11, -14<=l<=14	
Reflections collected	20446	
Independent reflections	2506 [R(int) = 0.0428]	
Completeness to theta = 26.44°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9767 and 0.9629	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2506 / 0 / 158	
Goodness-of-fit on F^2	1.080	
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1414	
R indices (all data)	R1 = 0.0655, wR2 = 0.1555	
Largest diff. peak and hole	0.158 and -0.223 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 4h. U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4524(1)	-1363(2)	7659(1)	52(1)
N(2)	5207(1)	768(1)	8212(1)	54(1)
C(1)	4078(2)	2692(2)	9848(2)	63(1)
C(2)	3564(2)	3912(2)	10282(2)	78(1)
C(3)	2424(2)	4321(2)	9914(2)	81(1)
C(4)	1789(2)	3507(2)	9118(2)	73(1)

C(5)	2296(2)	2284(2)	8676(2)	60(1)
C(6)	3450(1)	1862(2)	9035(1)	49(1)
C(7)	4033(1)	624(2)	8514(1)	48(1)
C(8)	5453(2)	-451(2)	7701(2)	55(1)
C(9)	3599(1)	-709(2)	8182(1)	48(1)
C(10)	2452(1)	-1445(2)	8311(1)	51(1)
C(11)	2021(2)	-2460(2)	7518(2)	63(1)
C(12)	944(2)	-3157(3)	7645(2)	78(1)
C(13)	274(2)	-2852(3)	8552(2)	81(1)
C(14)	690(2)	-1852(3)	9342(2)	78(1)
C(15)	1771(2)	-1164(2)	9234(2)	66(1)

Table 3. Bond lengths [Å] and angles [°] for **4h**.

N(1)-C(8)	1.337(2)
N(1)-C(9)	1.377(2)
N(1)-H(1A)	0.87(2)
N(2)-C(8)	1.319(2)
N(2)-C(7)	1.387(2)
C(1)-C(2)	1.380(3)
C(1)-C(6)	1.387(2)
C(1)-H(1)	0.9300
C(2)-C(3)	1.373(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.369(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.384(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.388(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.472(2)
C(7)-C(9)	1.376(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.468(2)
C(10)-C(15)	1.393(2)
C(10)-C(11)	1.392(2)
C(11)-C(12)	1.383(3)
C(11)-H(11)	0.9300

C(12)-C(13)	1.374(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.375(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.378(3)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(8)-N(1)-C(9)	107.97(14)
C(8)-N(1)-H(1A)	127.7(14)
C(9)-N(1)-H(1A)	124.3(14)
C(8)-N(2)-C(7)	105.25(13)
C(2)-C(1)-C(6)	120.48(18)
C(2)-C(1)-H(1)	119.8
C(6)-C(1)-H(1)	119.8
C(3)-C(2)-C(1)	120.51(19)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(4)-C(3)-C(2)	119.74(18)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	120.2(2)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	120.68(18)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	118.37(16)
C(1)-C(6)-C(7)	120.25(15)
C(5)-C(6)-C(7)	121.24(15)
C(9)-C(7)-N(2)	109.58(14)
C(9)-C(7)-C(6)	131.42(14)
N(2)-C(7)-C(6)	118.86(13)
N(2)-C(8)-N(1)	112.00(15)
N(2)-C(8)-H(8)	124.0
N(1)-C(8)-H(8)	124.0
C(7)-C(9)-N(1)	105.19(13)
C(7)-C(9)-C(10)	133.01(14)
N(1)-C(9)-C(10)	121.79(14)

C(15)-C(10)-C(11)	118.09(16)
C(15)-C(10)-C(9)	121.14(15)
C(11)-C(10)-C(9)	120.77(15)
C(12)-C(11)-C(10)	120.64(18)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(13)-C(12)-C(11)	120.5(2)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(12)-C(13)-C(14)	119.36(19)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(15)-C(14)-C(13)	120.71(19)
C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6
C(14)-C(15)-C(10)	120.64(18)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7

Symmetry transformations used to generate equivalent atoms:

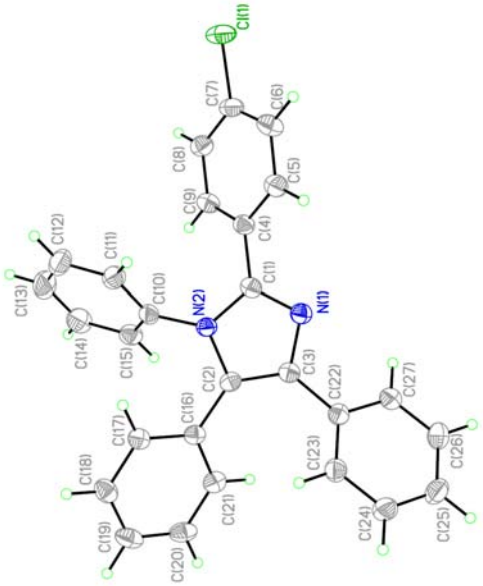
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4h**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

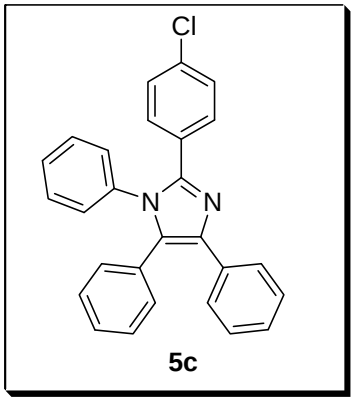
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	60(1)	37(1)	60(1)	1(1)	11(1)	3(1)
N(2)	54(1)	46(1)	63(1)	1(1)	10(1)	-1(1)
C(1)	72(1)	64(1)	52(1)	-6(1)	2(1)	-3(1)
C(2)	99(2)	74(1)	64(1)	-22(1)	13(1)	-10(1)
C(3)	95(2)	56(1)	97(2)	-18(1)	39(1)	-2(1)
C(4)	59(1)	56(1)	106(2)	-3(1)	22(1)	4(1)
C(5)	55(1)	48(1)	77(1)	-6(1)	8(1)	-3(1)
C(6)	57(1)	44(1)	49(1)	1(1)	11(1)	-2(1)
C(7)	50(1)	46(1)	48(1)	4(1)	6(1)	1(1)
C(8)	53(1)	47(1)	67(1)	4(1)	11(1)	4(1)
C(9)	54(1)	42(1)	48(1)	5(1)	6(1)	3(1)

C(10)	55(1)	45(1)	52(1)	6(1)	6(1)	0(1)
C(11)	65(1)	68(1)	57(1)	-4(1)	6(1)	-8(1)
C(12)	75(1)	87(2)	70(1)	-3(1)	-4(1)	-26(1)
C(13)	63(1)	100(2)	79(1)	12(1)	5(1)	-23(1)
C(14)	73(1)	88(2)	75(1)	4(1)	24(1)	-12(1)
C(15)	76(1)	62(1)	62(1)	-1(1)	19(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4h**.

	x	y	z	U(eq)
H(1A)	4485(18)	-2220(20)	7363(17)	68(6)
H(1)	4851	2425	10104	75
H(2)	3994	4460	10827	94
H(3)	2085	5148	10205	97
H(4)	1013	3777	8873	87
H(5)	1860	1740	8133	72
H(8)	6186	-654	7404	66
H(11)	2463	-2671	6897	76
H(12)	670	-3838	7112	93
H(13)	-453	-3317	8632	97
H(14)	237	-1637	9954	93
H(15)	2049	-506	9784	79





CCDC No of **5c** : 928192

Table 1. Crystal data and structure refinement for **5c**.

Identification code	**5c**	
Empirical formula	C27 H19 Cl N2	
Formula weight	406.89	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.1302(5) Å	α= 83.096(2)°.
	b = 10.1424(5) Å	β= 85.781(2)°.
	c = 11.2429(6) Å	γ = 66.007(2)°.
Volume	1047.30(9) $Å^3$	
Z	2	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	0.199 mm^{-1}	
F(000)	424	
Crystal size	0.44 x 0.38 x 0.25 mm^3	
Theta range for data collection	2.20 to 26.39°.	
Index ranges	-12<=h<=12, -12<=k<=12, -14<=l<=14	
Reflections collected	14519	
Independent reflections	4259 [R(int) = 0.0242]	
Completeness to theta = 26.39°	99.2 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9520 and 0.9177
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4259 / 0 / 271
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.1118
R indices (all data)	R1 = 0.0462, wR2 = 0.1191
Largest diff. peak and hole	0.242 and -0.280 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	13119(1)	801(1)	-4349(1)	39(1)
N(1)	9277(1)	2844(1)	838(1)	25(1)
N(2)	7646(1)	2407(1)	-78(1)	22(1)
C(1)	9011(1)	2397(1)	-132(1)	24(1)
C(2)	7012(1)	2895(1)	1018(1)	22(1)
C(3)	8046(1)	3156(1)	1565(1)	23(1)
C(4)	10043(1)	1952(2)	-1153(1)	24(1)
C(5)	10875(2)	2747(2)	-1519(1)	31(1)
C(6)	11847(2)	2384(2)	-2487(1)	34(1)
C(7)	11969(2)	1226(2)	-3091(1)	29(1)
C(8)	11178(2)	403(2)	-2737(1)	28(1)
C(9)	10222(2)	763(2)	-1761(1)	26(1)
C(10)	7048(1)	1877(1)	-935(1)	24(1)
C(11)	6870(2)	2532(2)	-2105(1)	30(1)
C(12)	6393(2)	1935(2)	-2946(2)	39(1)
C(13)	6074(2)	738(2)	-2607(2)	44(1)
C(14)	6221(2)	118(2)	-1431(2)	40(1)
C(15)	6728(2)	679(2)	-586(1)	30(1)
C(16)	5515(1)	3093(1)	1366(1)	22(1)
C(17)	4403(1)	3712(1)	541(1)	24(1)
C(18)	2988(2)	3954(2)	889(1)	29(1)
C(19)	2655(2)	3579(2)	2068(2)	33(1)
C(20)	3752(2)	2945(2)	2887(1)	31(1)
C(21)	5168(2)	2693(2)	2544(1)	26(1)
C(22)	8044(2)	3622(2)	2760(1)	24(1)
C(23)	6816(2)	4604(2)	3310(1)	28(1)
C(24)	6880(2)	4990(2)	4440(1)	33(1)
C(25)	8167(2)	4421(2)	5037(1)	36(1)
C(26)	9401(2)	3457(2)	4497(1)	36(1)
C(27)	9342(2)	3056(2)	3372(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for **5c**.

Cl(1)-C(7)	1.7439(14)
N(1)-C(1)	1.3142(18)
N(1)-C(3)	1.3835(17)
N(2)-C(1)	1.3751(17)
N(2)-C(2)	1.3953(17)
N(2)-C(10)	1.4357(17)
C(1)-C(4)	1.4765(18)
C(2)-C(3)	1.3800(19)
C(2)-C(16)	1.4755(18)
C(3)-C(22)	1.4764(19)
C(4)-C(5)	1.397(2)
C(4)-C(9)	1.399(2)
C(5)-C(6)	1.390(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.384(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.383(2)
C(8)-C(9)	1.389(2)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(15)	1.386(2)
C(10)-C(11)	1.389(2)
C(11)-C(12)	1.392(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.383(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(2)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.3997(19)
C(16)-C(17)	1.4015(19)
C(17)-C(18)	1.3866(19)
C(17)-H(17)	0.9500
C(18)-C(19)	1.390(2)

C(18)-H(18)	0.9500
C(19)-C(20)	1.386(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.384(2)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.396(2)
C(22)-C(27)	1.3987(19)
C(23)-C(24)	1.387(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.381(2)
C(24)-H(24)	0.9500
C(25)-C(26)	1.387(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.387(2)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(1)-N(1)-C(3)	106.16(11)
C(1)-N(2)-C(2)	107.08(11)
C(1)-N(2)-C(10)	126.14(11)
C(2)-N(2)-C(10)	126.51(11)
N(1)-C(1)-N(2)	111.43(12)
N(1)-C(1)-C(4)	124.22(12)
N(2)-C(1)-C(4)	124.35(12)
C(3)-C(2)-N(2)	105.03(11)
C(3)-C(2)-C(16)	132.79(12)
N(2)-C(2)-C(16)	122.13(12)
C(2)-C(3)-N(1)	110.30(12)
C(2)-C(3)-C(22)	130.80(12)
N(1)-C(3)-C(22)	118.82(12)
C(5)-C(4)-C(9)	118.97(13)
C(5)-C(4)-C(1)	118.61(13)
C(9)-C(4)-C(1)	122.42(13)
C(6)-C(5)-C(4)	120.76(14)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(7)-C(6)-C(5)	118.84(14)
C(7)-C(6)-H(6)	120.6

C(5)-C(6)-H(6)	120.6
C(8)-C(7)-C(6)	121.75(13)
C(8)-C(7)-Cl(1)	118.52(12)
C(6)-C(7)-Cl(1)	119.71(12)
C(7)-C(8)-C(9)	119.01(14)
C(7)-C(8)-H(8)	120.5
C(9)-C(8)-H(8)	120.5
C(8)-C(9)-C(4)	120.63(13)
C(8)-C(9)-H(9)	119.7
C(4)-C(9)-H(9)	119.7
C(15)-C(10)-C(11)	121.75(13)
C(15)-C(10)-N(2)	118.91(12)
C(11)-C(10)-N(2)	119.26(12)
C(10)-C(11)-C(12)	118.49(15)
C(10)-C(11)-H(11)	120.8
C(12)-C(11)-H(11)	120.8
C(13)-C(12)-C(11)	120.19(15)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	120.71(15)
C(12)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6
C(13)-C(14)-C(15)	119.81(16)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(10)-C(15)-C(14)	119.01(15)
C(10)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(21)-C(16)-C(17)	118.34(12)
C(21)-C(16)-C(2)	120.45(12)
C(17)-C(16)-C(2)	121.20(12)
C(18)-C(17)-C(16)	120.80(13)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	120.17(14)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(20)-C(19)-C(18)	119.45(13)

C(20)-C(19)-H(19)	120.3
C(18)-C(19)-H(19)	120.3
C(21)-C(20)-C(19)	120.69(14)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(16)	120.52(14)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7
C(23)-C(22)-C(27)	118.18(13)
C(23)-C(22)-C(3)	123.45(12)
C(27)-C(22)-C(3)	118.37(12)
C(24)-C(23)-C(22)	120.74(13)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	120.54(14)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(24)-C(25)-C(26)	119.41(14)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(25)-C(26)-C(27)	120.36(14)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(26)-C(27)-C(22)	120.76(14)
C(26)-C(27)-H(27)	119.6
C(22)-C(27)-H(27)	119.6

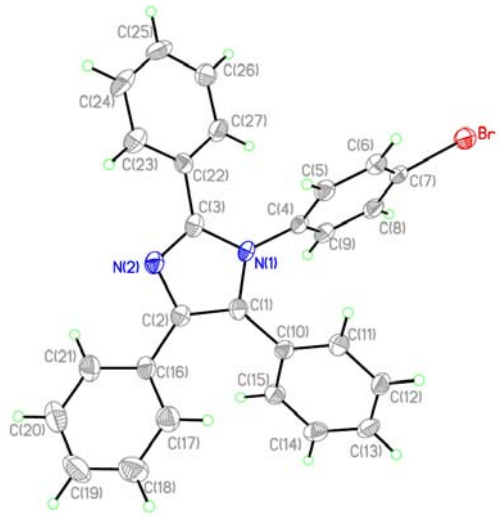
Symmetry transformations used to generate equivalent atoms:

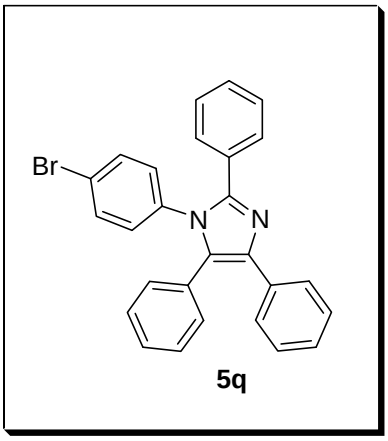
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	35(1)	44(1)	29(1)	0(1)	11(1)	-9(1)
N(1)	24(1)	27(1)	24(1)	-2(1)	0(1)	-11(1)
N(2)	22(1)	24(1)	20(1)	-2(1)	1(1)	-9(1)
C(1)	22(1)	23(1)	25(1)	0(1)	0(1)	-9(1)
C(2)	25(1)	20(1)	20(1)	-1(1)	1(1)	-8(1)
C(3)	23(1)	22(1)	23(1)	0(1)	0(1)	-8(1)
C(4)	21(1)	26(1)	23(1)	0(1)	0(1)	-8(1)
C(5)	30(1)	35(1)	31(1)	-7(1)	3(1)	-16(1)
C(6)	31(1)	38(1)	37(1)	-2(1)	6(1)	-19(1)
C(7)	23(1)	34(1)	23(1)	1(1)	3(1)	-6(1)
C(8)	26(1)	26(1)	26(1)	-2(1)	0(1)	-5(1)
C(9)	23(1)	24(1)	29(1)	0(1)	2(1)	-8(1)
C(10)	19(1)	24(1)	27(1)	-7(1)	0(1)	-6(1)
C(11)	28(1)	30(1)	27(1)	-3(1)	-2(1)	-7(1)
C(12)	38(1)	46(1)	29(1)	-10(1)	-7(1)	-8(1)
C(13)	41(1)	50(1)	46(1)	-24(1)	-4(1)	-16(1)
C(14)	38(1)	37(1)	50(1)	-19(1)	5(1)	-19(1)
C(15)	27(1)	28(1)	33(1)	-7(1)	4(1)	-10(1)
C(16)	24(1)	19(1)	24(1)	-4(1)	2(1)	-9(1)
C(17)	24(1)	22(1)	27(1)	-4(1)	1(1)	-10(1)
C(18)	24(1)	25(1)	39(1)	-6(1)	-1(1)	-10(1)
C(19)	27(1)	30(1)	43(1)	-9(1)	11(1)	-14(1)
C(20)	38(1)	28(1)	30(1)	-6(1)	12(1)	-17(1)
C(21)	32(1)	22(1)	26(1)	-3(1)	2(1)	-12(1)
C(22)	26(1)	24(1)	23(1)	-1(1)	-1(1)	-13(1)
C(23)	26(1)	28(1)	30(1)	-5(1)	-2(1)	-10(1)
C(24)	35(1)	34(1)	33(1)	-11(1)	5(1)	-15(1)
C(25)	44(1)	43(1)	25(1)	-8(1)	-1(1)	-21(1)
C(26)	33(1)	45(1)	32(1)	-3(1)	-9(1)	-15(1)
C(27)	24(1)	35(1)	29(1)	-4(1)	0(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5c**.

	x	y	z	U(eq)
H(5)	10776	3544	-1102	37
H(6)	12417	2921	-2730	41
H(8)	11287	-396	-3156	33
H(9)	9684	196	-1504	32
H(11)	7069	3368	-2325	35
H(12)	6287	2350	-3755	47
H(13)	5751	336	-3187	53
H(14)	5975	-689	-1202	48
H(15)	6855	248	219	36
H(17)	4620	3969	-267	29
H(18)	2244	4377	321	35
H(19)	1685	3755	2311	39
H(20)	3529	2682	3692	38
H(21)	5910	2244	3111	31
H(23)	5926	5012	2905	33
H(24)	6032	5650	4806	40
H(25)	8207	4688	5811	43
H(26)	10292	3070	4900	44
H(27)	10192	2390	3014	36





CCDC No of **5q** : 928194

Table 1. Crystal data and structure refinement for **5q**.

Identification code	**5q**	
Empirical formula	C27 H19 Br N2	
Formula weight	451.35	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 26.4141(14) Å	α= 90°.
	b = 8.1117(5) Å	β= 114.919(6)°.
	c = 21.4876(10) Å	γ = 90°.
Volume	4175.4(4) $Å^3$	
Z	8	
Density (calculated)	1.436 Mg/m^3	
Absorption coefficient	1.985 mm^{-1}	
F(000)	1840	
Crystal size	0.36 x 0.22 x 0.08 mm^3	
Theta range for data collection	2.98 to 29.27°.	
Index ranges	-33<=h<=34, -10<=k<=6, -28<=l<=16	
Reflections collected	10244	
Independent reflections	4827 [R(int) = 0.0419]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	1.00000 and 0.83927
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4827 / 0 / 271
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.0976
R indices (all data)	R1 = 0.1029, wR2 = 0.1186
Largest diff. peak and hole	0.877 and -0.623 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5q**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br	156(1)	139(1)	1694(1)	42(1)
N(1)	2284(1)	-2(3)	4326(1)	23(1)
N(2)	2848(1)	44(3)	5436(1)	25(1)
C(1)	2826(1)	26(4)	4372(2)	22(1)
C(2)	3168(1)	82(4)	5067(2)	23(1)
C(3)	2324(1)	3(4)	4989(2)	25(1)
C(4)	1785(1)	37(4)	3700(2)	22(1)
C(5)	1455(1)	1448(4)	3529(2)	25(1)
C(6)	973(1)	1466(4)	2928(2)	28(1)
C(7)	832(1)	105(4)	2506(2)	27(1)
C(8)	1162(1)	-1289(4)	2664(2)	29(1)
C(9)	1643(1)	-1328(4)	3270(2)	25(1)
C(10)	2943(1)	-72(4)	3759(2)	22(1)
C(11)	2665(1)	895(4)	3172(2)	25(1)
C(12)	2787(1)	752(4)	2610(2)	28(1)
C(13)	3190(1)	-343(4)	2616(2)	30(1)
C(14)	3466(1)	-1315(4)	3190(2)	31(1)
C(15)	3344(1)	-1200(4)	3754(2)	26(1)
C(16)	3780(1)	173(4)	5428(2)	25(1)
C(17)	4108(1)	913(4)	5146(2)	33(1)
C(18)	4683(2)	946(5)	5503(2)	45(1)
C(19)	4942(2)	253(5)	6144(2)	48(1)
C(20)	4621(2)	-468(5)	6438(2)	44(1)
C(21)	4047(2)	-495(4)	6088(2)	34(1)
C(22)	1842(1)	-31(4)	5182(2)	21(1)
C(23)	1926(2)	587(4)	5808(2)	32(1)
C(24)	1498(2)	589(4)	6020(2)	38(1)
C(25)	980(2)	-52(4)	5600(2)	38(1)
C(26)	901(2)	-722(5)	4976(2)	36(1)
C(27)	1327(1)	-722(4)	4761(2)	31(1)

Table 3. Bond lengths [Å] and angles [°] for **5q**.

Br-C(7)	1.900(3)
N(1)-C(3)	1.383(4)
N(1)-C(1)	1.393(4)
N(1)-C(4)	1.432(4)
N(2)-C(3)	1.309(4)
N(2)-C(2)	1.385(4)
C(1)-C(2)	1.382(4)
C(1)-C(10)	1.477(4)
C(2)-C(16)	1.471(4)
C(3)-C(22)	1.498(4)
C(4)-C(5)	1.390(4)
C(4)-C(9)	1.389(4)
C(5)-C(6)	1.380(4)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.376(4)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.379(5)
C(8)-C(9)	1.386(4)
C(8)-H(8A)	0.9500
C(9)-H(9A)	0.9500
C(10)-C(11)	1.402(4)
C(10)-C(15)	1.403(4)
C(11)-C(12)	1.378(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.383(5)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.383(4)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.382(4)
C(14)-H(14A)	0.9500
C(15)-H(15A)	0.9500
C(16)-C(17)	1.386(4)
C(16)-C(21)	1.399(4)
C(17)-C(18)	1.383(5)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.374(5)

C(18)-H(18A)	0.9500
C(19)-C(20)	1.385(6)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.380(5)
C(20)-H(20A)	0.9500
C(21)-H(21A)	0.9500
C(22)-C(23)	1.364(4)
C(22)-C(27)	1.394(5)
C(23)-C(24)	1.386(5)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.383(5)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.380(5)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.384(4)
C(26)-H(26A)	0.9500
C(27)-H(27A)	0.9500
C(3)-N(1)-C(1)	107.1(3)
C(3)-N(1)-C(4)	127.5(3)
C(1)-N(1)-C(4)	125.3(3)
C(3)-N(2)-C(2)	106.9(3)
C(2)-C(1)-N(1)	105.3(3)
C(2)-C(1)-C(10)	132.6(3)
N(1)-C(1)-C(10)	122.1(3)
C(1)-C(2)-N(2)	109.8(3)
C(1)-C(2)-C(16)	130.2(3)
N(2)-C(2)-C(16)	120.0(3)
N(2)-C(3)-N(1)	110.9(3)
N(2)-C(3)-C(22)	123.7(3)
N(1)-C(3)-C(22)	125.4(3)
C(5)-C(4)-C(9)	121.1(3)
C(5)-C(4)-N(1)	119.5(3)
C(9)-C(4)-N(1)	119.3(3)
C(4)-C(5)-C(6)	119.0(3)
C(4)-C(5)-H(5A)	120.5
C(6)-C(5)-H(5A)	120.5
C(7)-C(6)-C(5)	119.6(3)
C(7)-C(6)-H(6A)	120.2

C(5)-C(6)-H(6A)	120.2
C(8)-C(7)-C(6)	121.9(3)
C(8)-C(7)-Br	119.3(3)
C(6)-C(7)-Br	118.8(3)
C(7)-C(8)-C(9)	118.9(3)
C(7)-C(8)-H(8A)	120.5
C(9)-C(8)-H(8A)	120.5
C(4)-C(9)-C(8)	119.4(3)
C(4)-C(9)-H(9A)	120.3
C(8)-C(9)-H(9A)	120.3
C(11)-C(10)-C(15)	117.9(3)
C(11)-C(10)-C(1)	123.1(3)
C(15)-C(10)-C(1)	119.0(3)
C(12)-C(11)-C(10)	120.9(3)
C(12)-C(11)-H(11A)	119.5
C(10)-C(11)-H(11A)	119.5
C(13)-C(12)-C(11)	120.6(3)
C(13)-C(12)-H(12A)	119.7
C(11)-C(12)-H(12A)	119.7
C(12)-C(13)-C(14)	119.2(3)
C(12)-C(13)-H(13A)	120.4
C(14)-C(13)-H(13A)	120.4
C(15)-C(14)-C(13)	120.9(3)
C(15)-C(14)-H(14A)	119.6
C(13)-C(14)-H(14A)	119.6
C(14)-C(15)-C(10)	120.4(3)
C(14)-C(15)-H(15A)	119.8
C(10)-C(15)-H(15A)	119.8
C(17)-C(16)-C(21)	118.1(3)
C(17)-C(16)-C(2)	122.7(3)
C(21)-C(16)-C(2)	119.2(3)
C(16)-C(17)-C(18)	120.5(3)
C(16)-C(17)-H(17A)	119.7
C(18)-C(17)-H(17A)	119.7
C(19)-C(18)-C(17)	121.0(4)
C(19)-C(18)-H(18A)	119.5
C(17)-C(18)-H(18A)	119.5
C(18)-C(19)-C(20)	119.2(4)

C(18)-C(19)-H(19A)	120.4
C(20)-C(19)-H(19A)	120.4
C(21)-C(20)-C(19)	120.1(4)
C(21)-C(20)-H(20A)	119.9
C(19)-C(20)-H(20A)	119.9
C(20)-C(21)-C(16)	121.0(3)
C(20)-C(21)-H(21A)	119.5
C(16)-C(21)-H(21A)	119.5
C(23)-C(22)-C(27)	119.8(3)
C(23)-C(22)-C(3)	117.5(3)
C(27)-C(22)-C(3)	122.6(3)
C(22)-C(23)-C(24)	120.5(4)
C(22)-C(23)-H(23A)	119.7
C(24)-C(23)-H(23A)	119.7
C(25)-C(24)-C(23)	120.3(3)
C(25)-C(24)-H(24A)	119.8
C(23)-C(24)-H(24A)	119.8
C(26)-C(25)-C(24)	119.0(3)
C(26)-C(25)-H(25A)	120.5
C(24)-C(25)-H(25A)	120.5
C(25)-C(26)-C(27)	120.8(4)
C(25)-C(26)-H(26A)	119.6
C(27)-C(26)-H(26A)	119.6
C(26)-C(27)-C(22)	119.5(3)
C(26)-C(27)-H(27A)	120.3
C(22)-C(27)-H(27A)	120.3

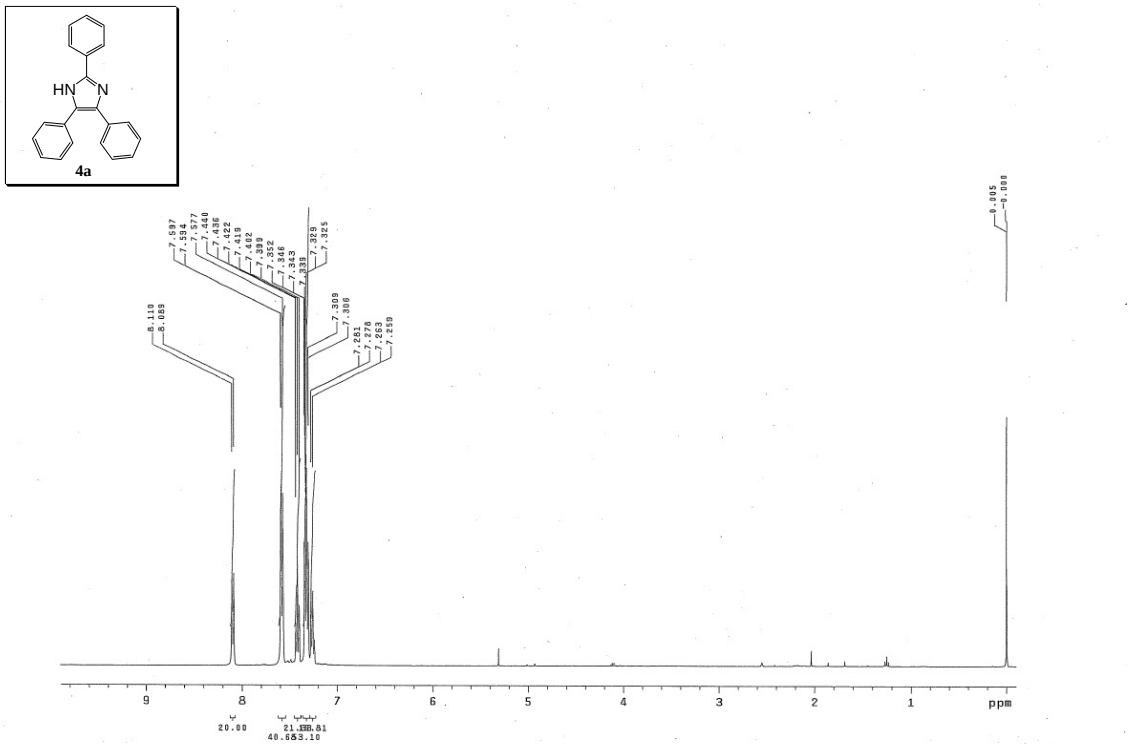
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5q**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br	24(1)	76(1)	23(1)	-4(1)	8(1)	-2(1)
N(1)	25(2)	29(2)	14(1)	-2(1)	10(1)	0(1)
N(2)	26(2)	28(2)	20(1)	-3(1)	9(1)	-2(1)
C(1)	24(2)	21(2)	21(2)	1(1)	8(1)	0(1)
C(2)	26(2)	22(2)	22(2)	0(1)	11(1)	0(1)
C(3)	33(2)	24(2)	20(2)	-2(1)	11(2)	0(2)
C(4)	22(2)	30(2)	18(2)	-1(2)	11(1)	-2(2)
C(5)	26(2)	30(2)	21(2)	-4(2)	12(2)	-1(2)
C(6)	28(2)	33(2)	25(2)	4(2)	15(2)	2(2)
C(7)	23(2)	43(2)	19(2)	3(2)	12(1)	-2(2)
C(8)	31(2)	37(2)	24(2)	-6(2)	16(2)	-6(2)
C(9)	31(2)	24(2)	24(2)	-2(2)	16(2)	0(1)
C(10)	21(2)	27(2)	20(2)	-2(2)	10(1)	-4(1)
C(11)	27(2)	24(2)	24(2)	1(2)	11(2)	0(2)
C(12)	29(2)	34(2)	21(2)	5(2)	11(2)	-6(2)
C(13)	32(2)	37(2)	29(2)	-2(2)	19(2)	-7(2)
C(14)	30(2)	33(2)	35(2)	-5(2)	18(2)	0(2)
C(15)	26(2)	25(2)	27(2)	1(2)	12(2)	3(2)
C(16)	28(2)	24(2)	20(2)	-2(1)	8(1)	2(1)
C(17)	34(2)	33(2)	31(2)	0(2)	12(2)	-2(2)
C(18)	34(2)	50(3)	49(2)	-6(2)	17(2)	-11(2)
C(19)	25(2)	63(3)	45(2)	-9(2)	3(2)	0(2)
C(20)	41(2)	50(3)	30(2)	0(2)	2(2)	6(2)
C(21)	36(2)	37(2)	25(2)	-4(2)	9(2)	-3(2)
C(22)	22(2)	19(2)	22(2)	4(1)	8(1)	4(1)
C(23)	43(2)	29(2)	30(2)	-3(2)	20(2)	-1(2)
C(24)	60(3)	36(2)	31(2)	-2(2)	31(2)	5(2)
C(25)	45(2)	41(2)	42(2)	16(2)	33(2)	17(2)
C(26)	32(2)	47(2)	31(2)	14(2)	15(2)	7(2)
C(27)	37(2)	37(2)	23(2)	5(2)	16(2)	5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5q**.

	x	y	z	U(eq)
H(5A)	1560	2385	3821	30
H(6A)	740	2413	2806	33
H(8A)	1060	-2207	2361	35
H(9A)	1874	-2280	3391	30
H(11A)	2389	1660	3161	30
H(12A)	2592	1412	2216	33
H(13A)	3277	-426	2231	36
H(14A)	3742	-2071	3196	37
H(15A)	3532	-1890	4140	31
H(17A)	3936	1400	4703	40
H(18A)	4902	1456	5301	54
H(19A)	5338	269	6382	58
H(20A)	4796	-946	6882	53
H(21A)	3829	-973	6298	41
H(23A)	2281	1018	6102	39
H(24A)	1560	1033	6455	46
H(25A)	684	-32	5740	45
H(26A)	550	-1189	4689	43
H(27A)	1269	-1189	4331	38


HN
N
4a
8.110
8.089
7.597
7.594
7.577
7.440
7.436
7.422
7.419
7.402
7.399
7.352
7.346
7.343
7.338
7.329
7.325
7.309
7.306
7.281
7.276
7.263
7.259
9.005
9.000
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7
6
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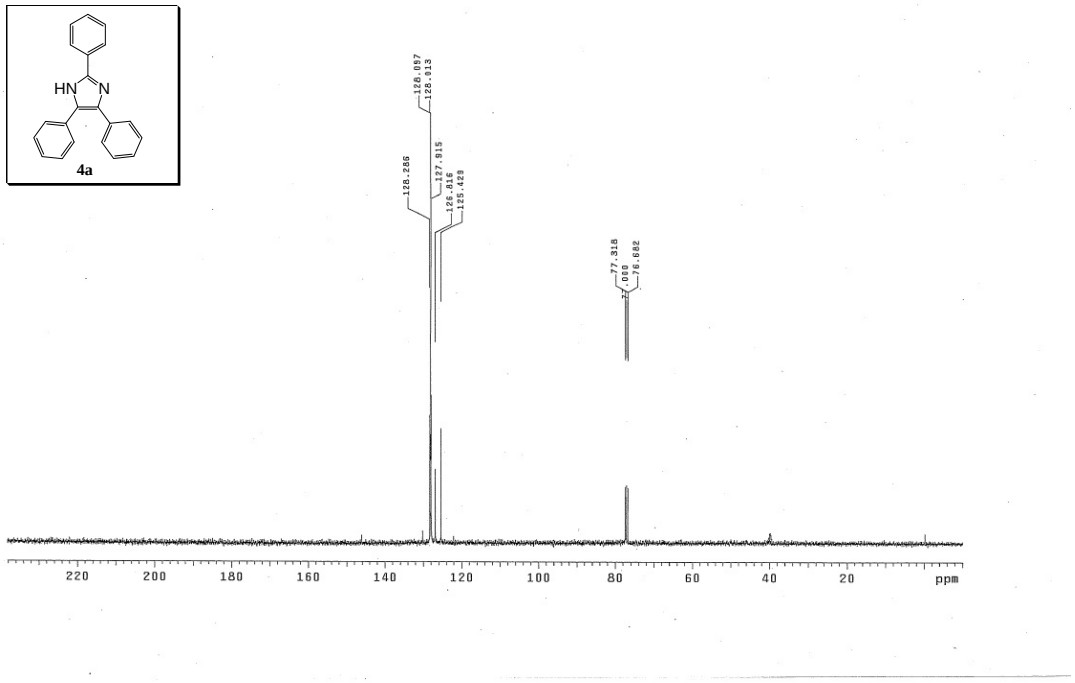
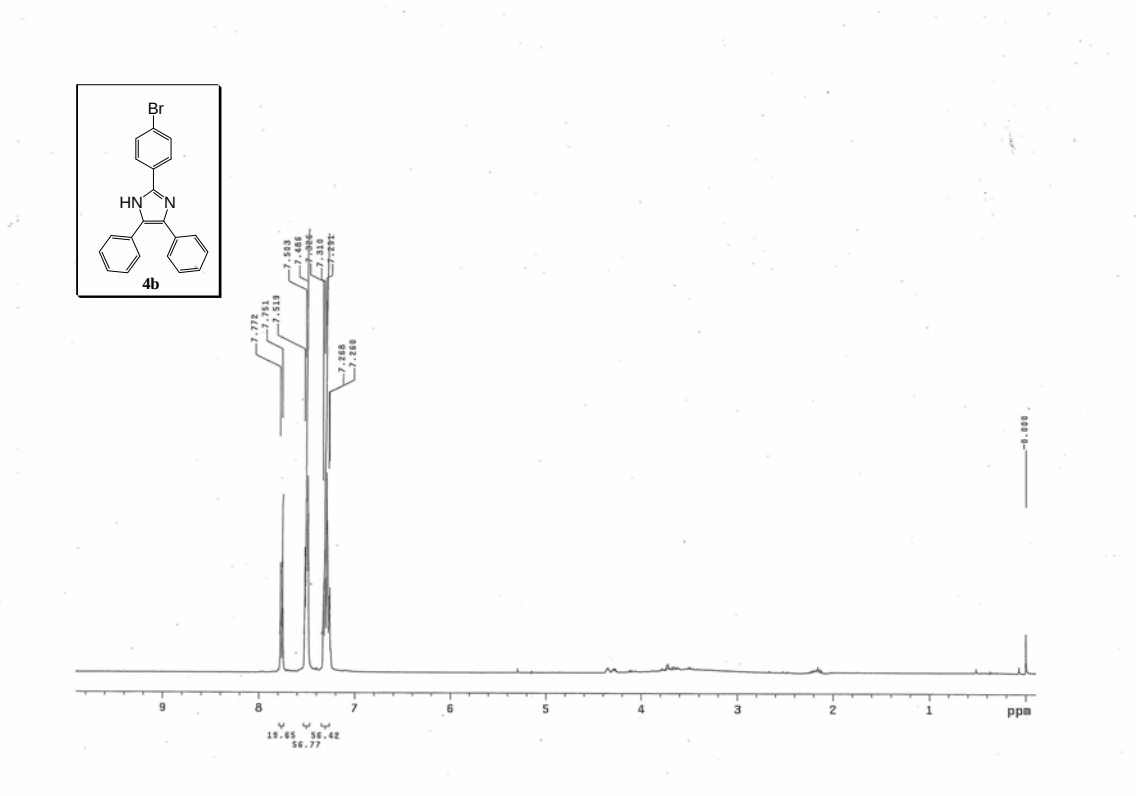
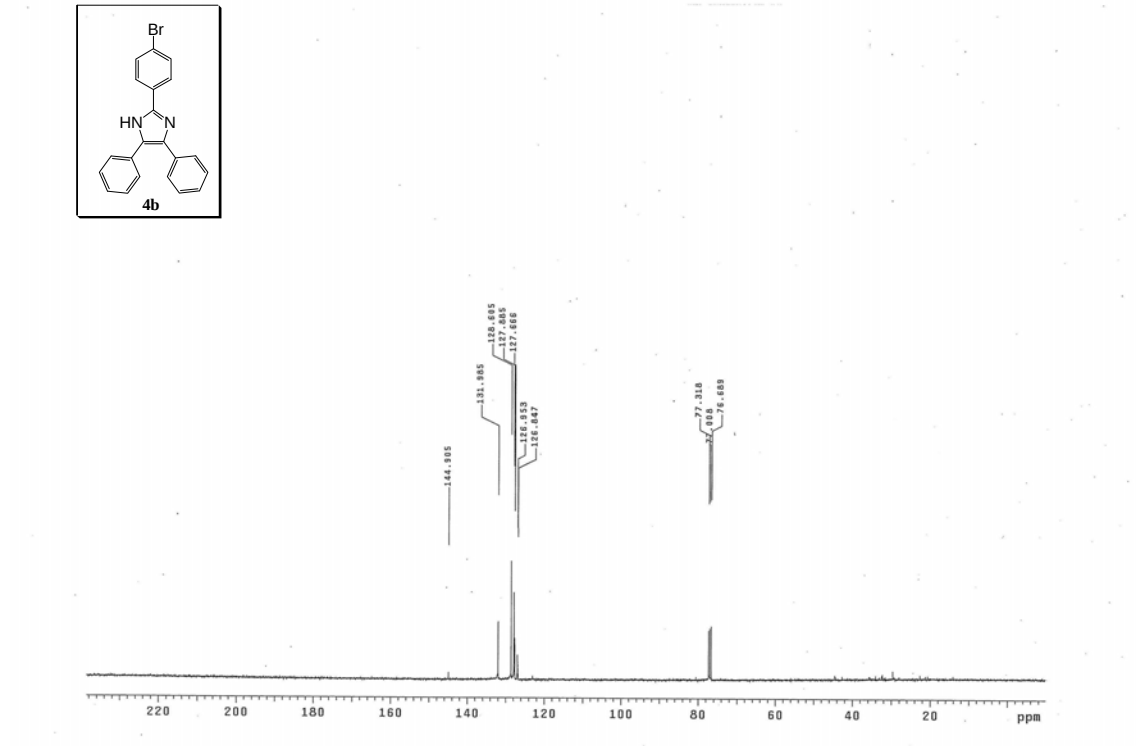
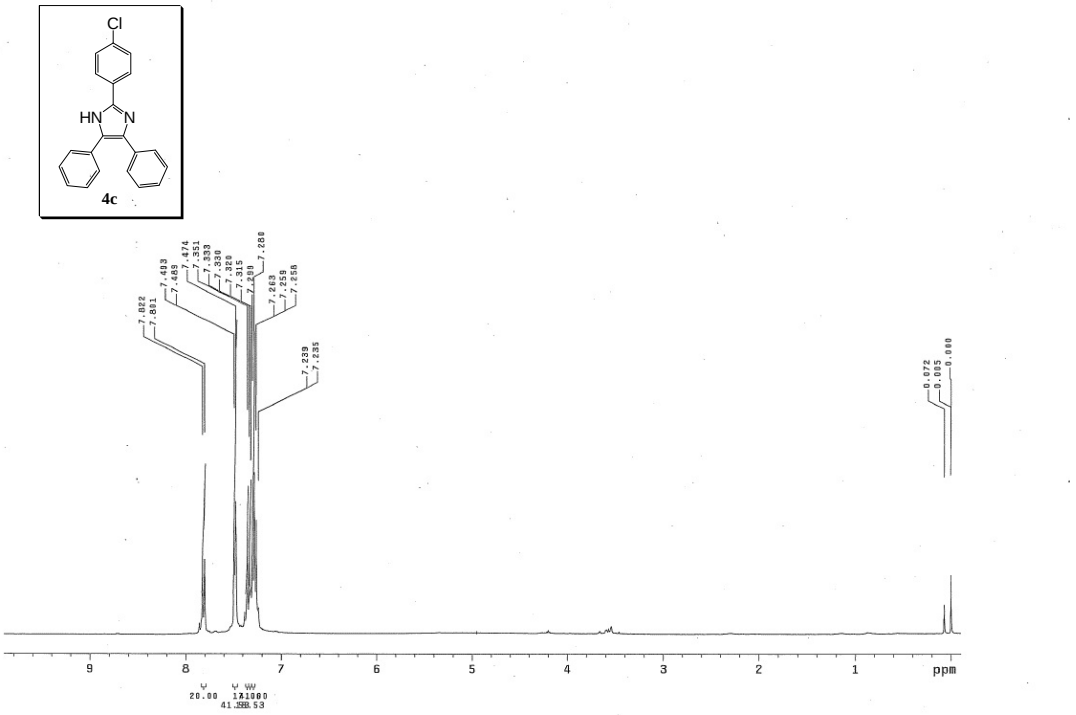
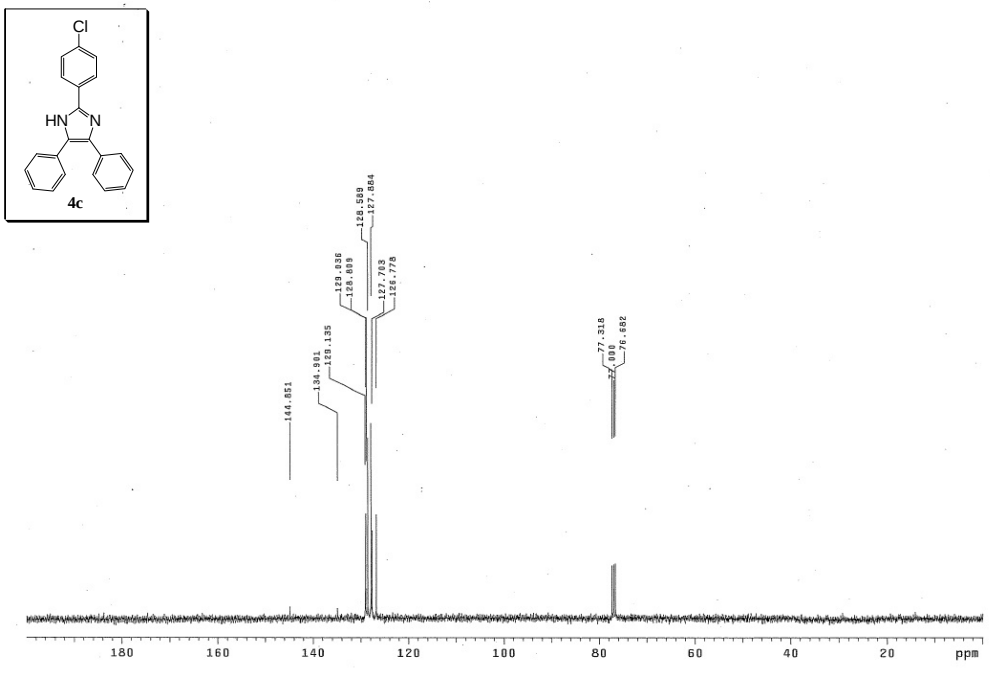
2
1
ppm
20.00
21.88
40.65
3.10

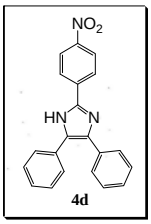

HN
N
4a
126.057
128.013
127.915
126.815
125.428
126.286
77.318
77.000
76.682
220
200
180
160
140
120
100
80
60
40
20
ppm


Br
HN
N
4b
7.772
7.751
7.519
7.503
7.486
7.310
7.288
7.268
0.000
9
8
7
6
5
4
3
2
1
ppm
19.65
56.42
56.77

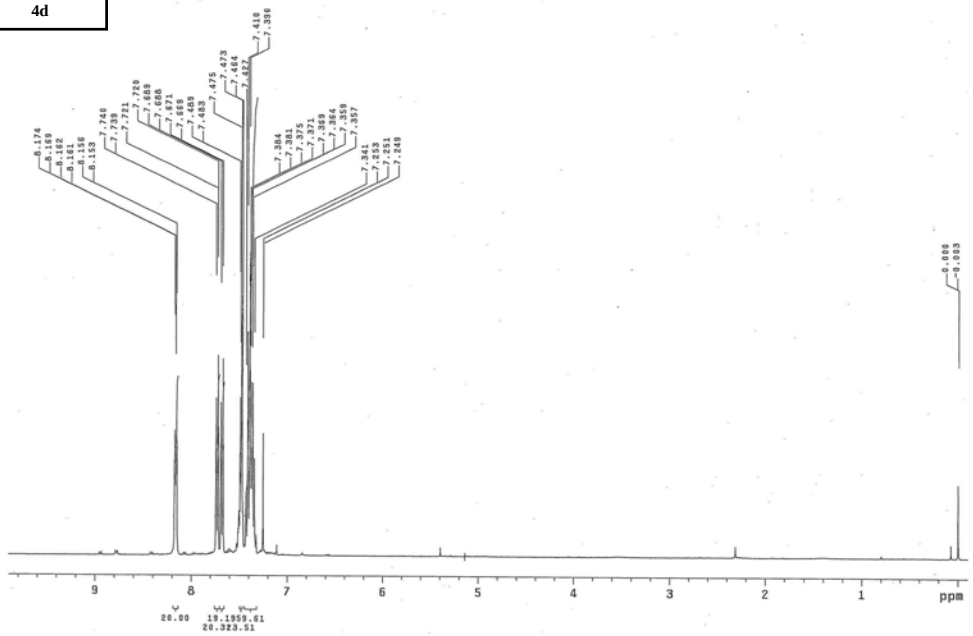

Br
HN
N
4b
144.905
131.985
128.685
127.865
127.665
126.953
126.847
77.318
77.000
76.689
220
200
180
160
140
120
100
80
60
40
20
ppm

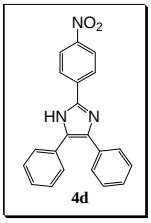

Cl
HN
N
4c
7.872
7.851
7.493
7.489
7.474
7.453
7.338
7.320
7.315
7.280
7.263
7.259
7.188
7.239
7.235
0.072
0.065
0.000
9
8
7
6
5
4
3
2
1
ppm


Cl
HN
N
4c
144.651
134.961
129.135
128.589
127.864
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm

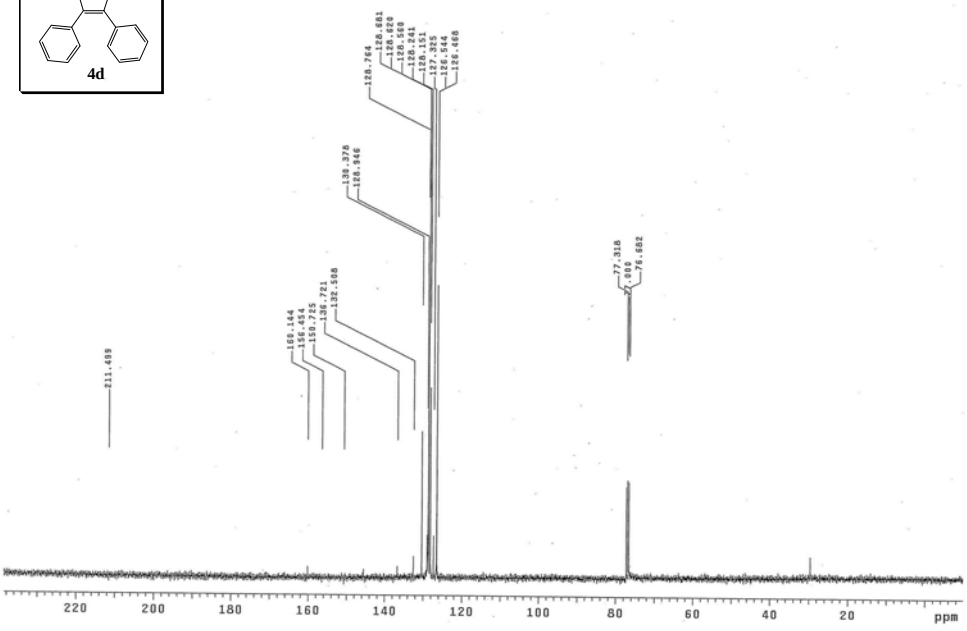

NO2
HN
N

4d


9
8
7
6
5
4
3
2
1
ppm


NO2
HN
N

4d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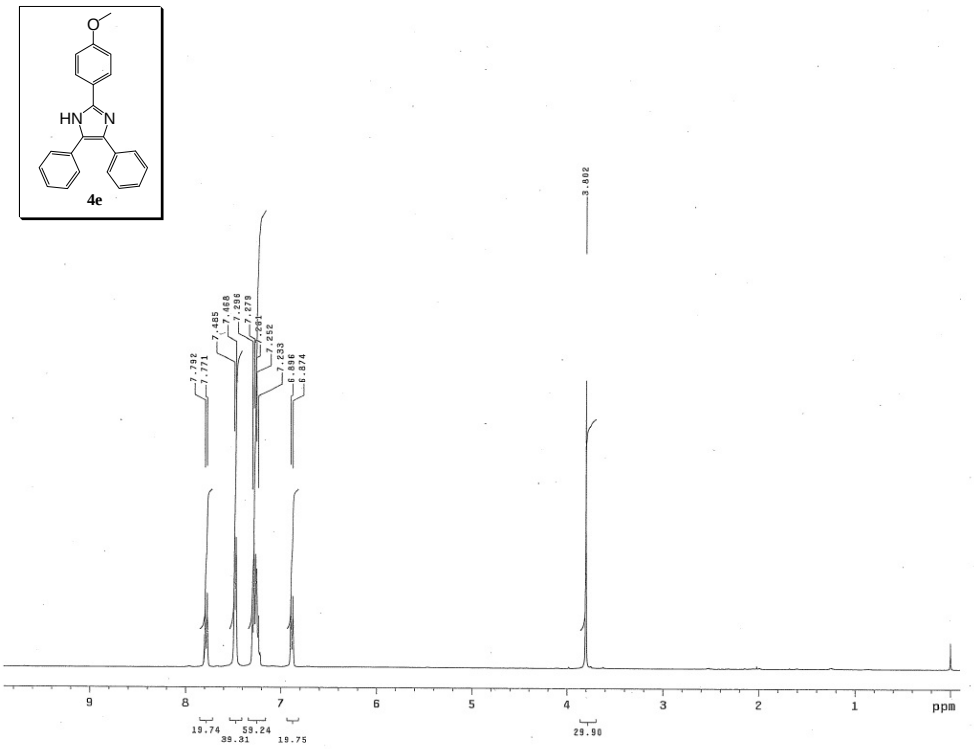
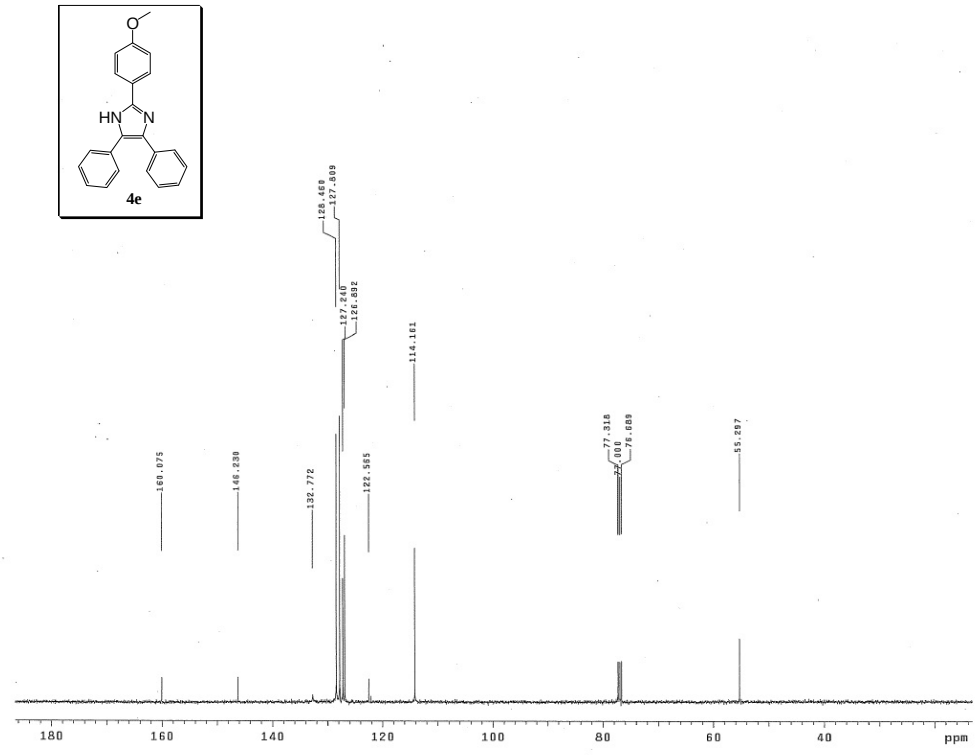
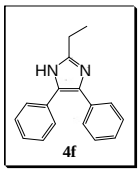
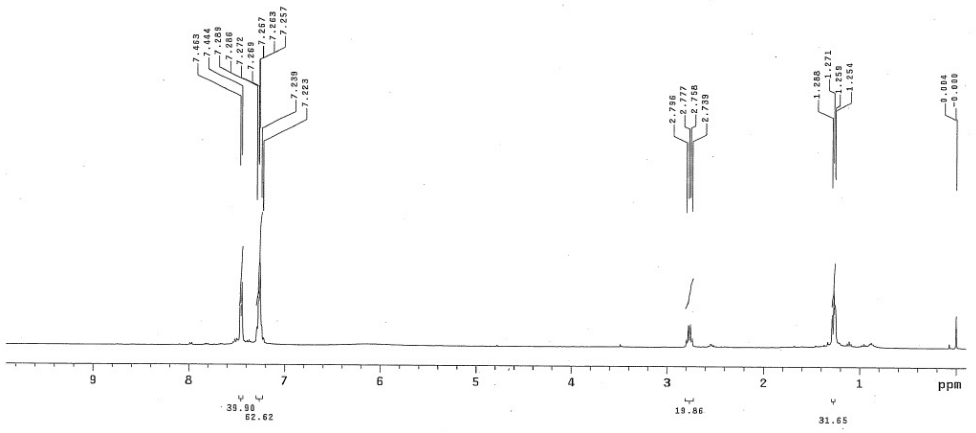
200
180
160
140
120
100
80
60
40
20
ppm

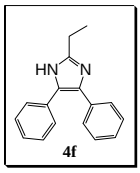

4e
7.732
7.731
7.485
7.466
7.298
7.279
7.261
7.252
7.233
6.896
6.874
3.802
9
8
7
6
5
4
3
2
1
ppm
19.74
39.31
59.24
19.75
29.90


4e
160.075
146.230
132.772
126.468
127.869
127.240
126.892
122.565
114.161
77.318
77.000
76.689
55.267
180
160
140
120
100
80
60
40
ppm

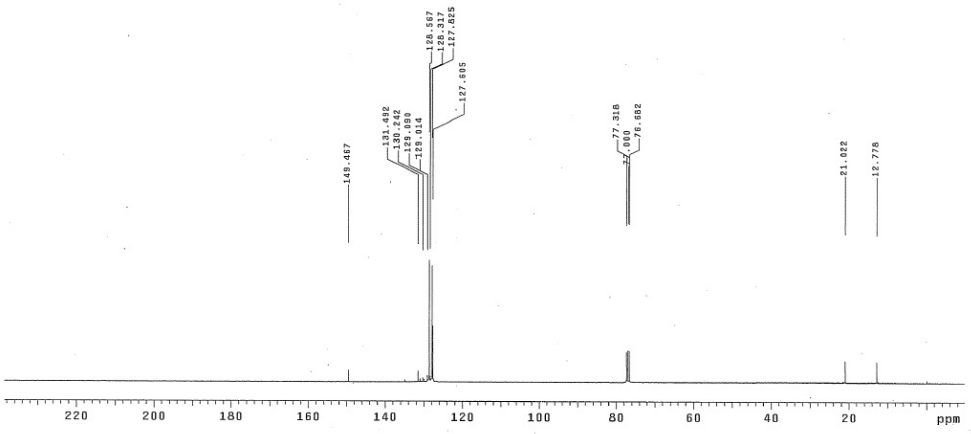

HN
N

4f


7.463
7.444
7.269
7.266
7.222
7.269
7.267
7.263
7.257
7.239
7.223
2.796
2.777
2.758
2.739
1.268
1.271
1.259
1.254
0.004
0.000
9
8
7
6
5
4
3
2
1
ppm
39.90
62.62
19.86
31.65


HN
N

4f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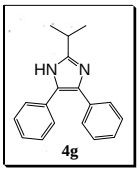
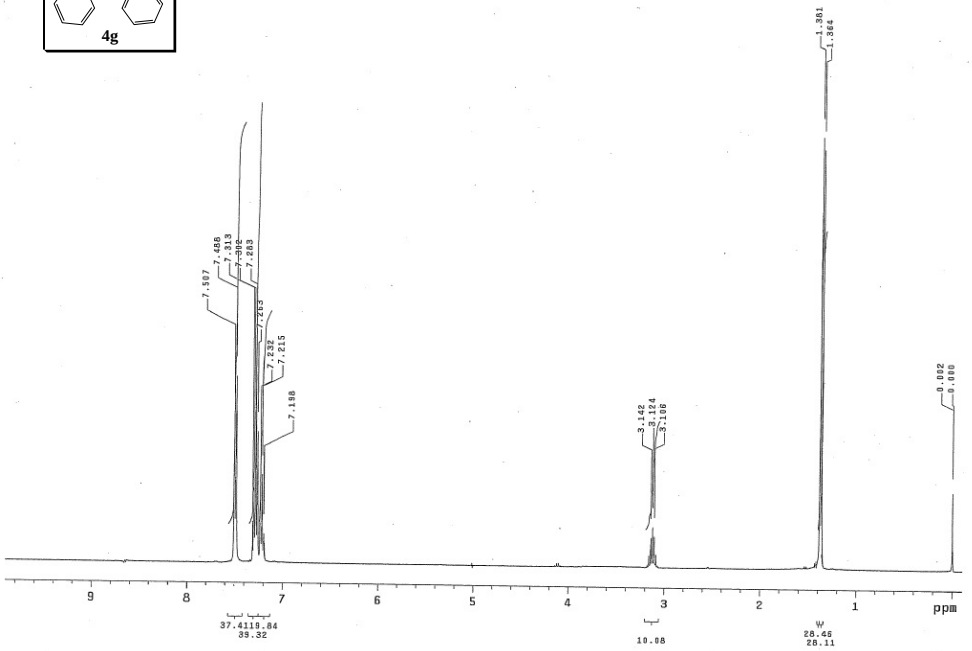
131.492
131.242
129.080
129.014
128.567
128.317
127.825
127.605
77.318
77.000
76.682
21.022
12.778
220
200
180
160
140
120
100
80
60
40
20
ppm


HN
N

4g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7.313
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7.263
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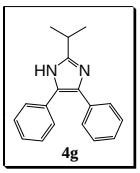
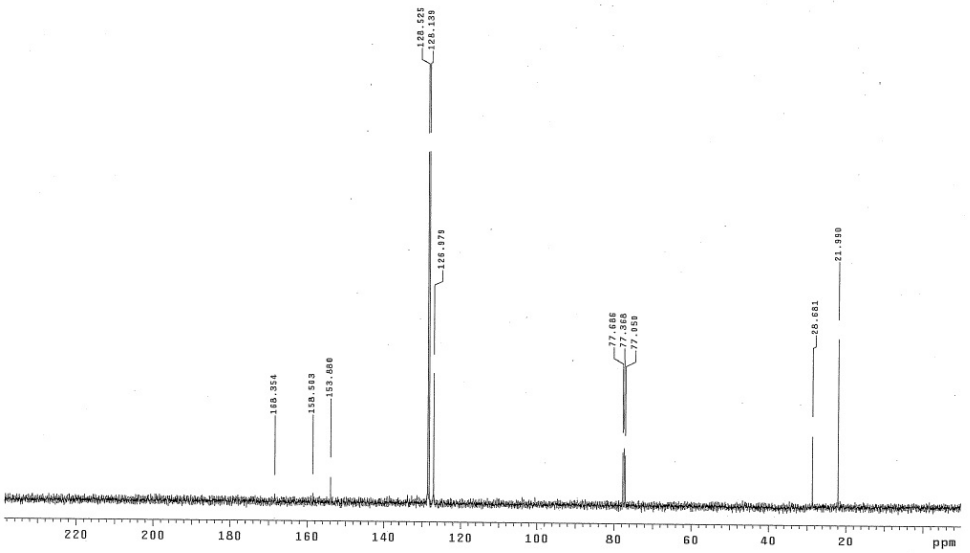
7.215
7.198
3.142
3.124
3.106
1.361
1.364
0.002
0.000
9
8
7
6
5
4
3
2
1
ppm
37.41
19.84
39.32
10.00
28.45
28.11


HN
N

4g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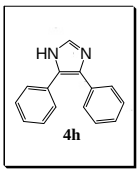
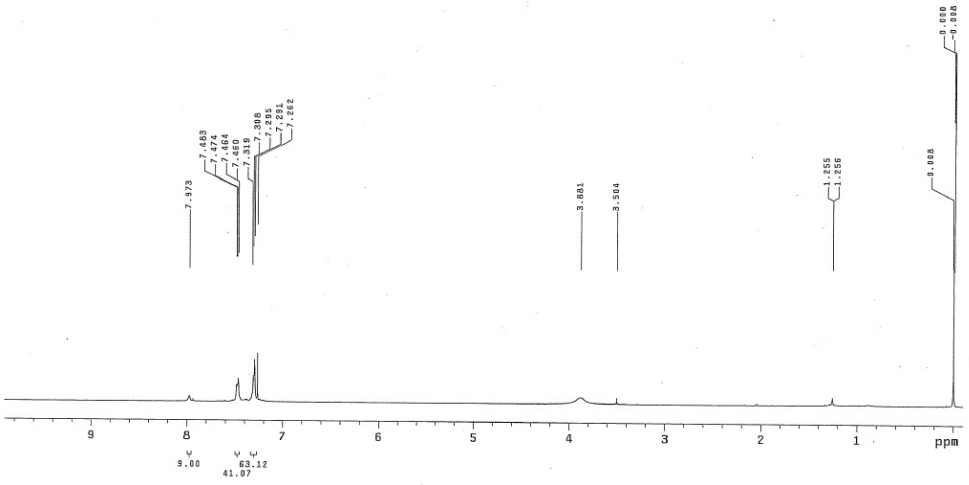
126.079
77.686
77.368
77.059
28.681
21.390
168.354
158.583
153.880
220
200
180
160
140
120
100
80
60
40
20
ppm


HN
N

4h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7.308
7.295
7.291
7.282
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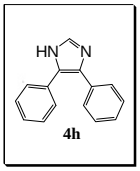
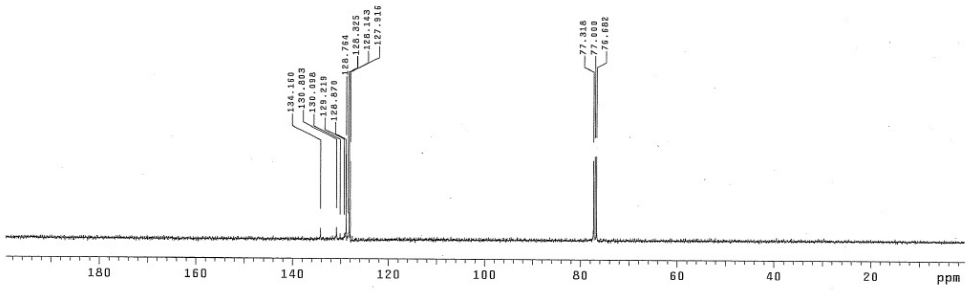
3.504
1.255
1.256
0.088
0.000
0.000
9
8
7
6
5
4
3
2
1
ppm
9.00
63.12
41.07


HN
N

4h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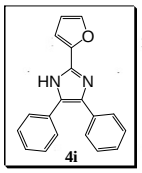
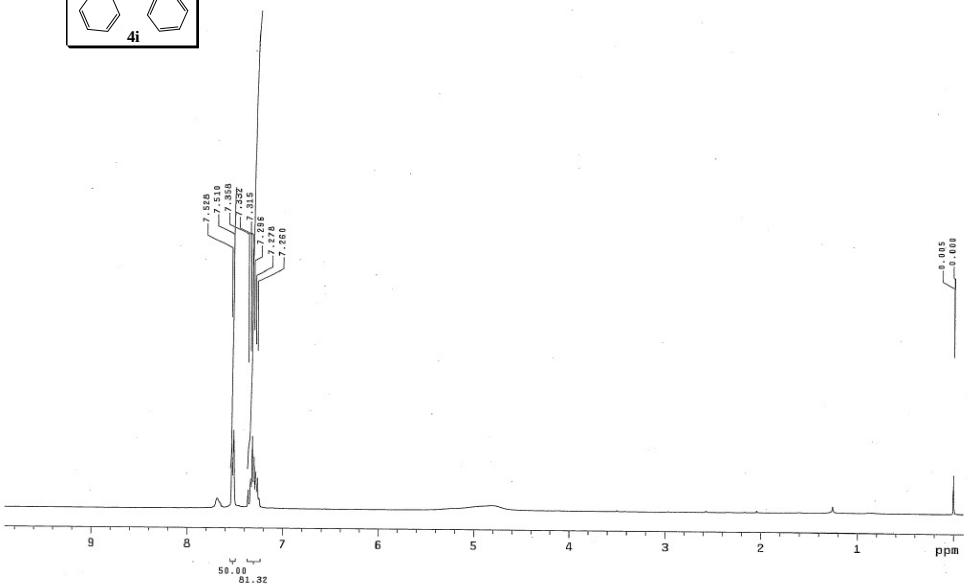
129.218
128.870
128.764
128.325
128.153
127.816
77.316
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm


HN
N
O

4i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7.3032
7.2915
7.2686
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7.2450
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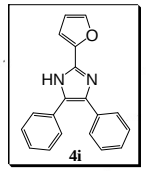
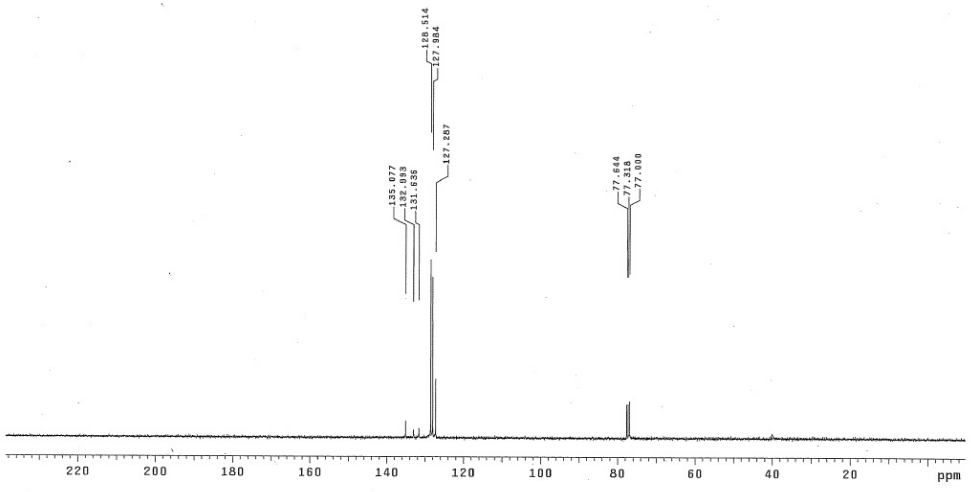
0.000
9
8
7
6
5
4
3
2
1
ppm
50.00
81.32


HN
N
O

4i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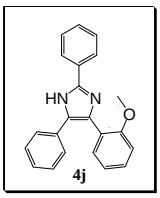
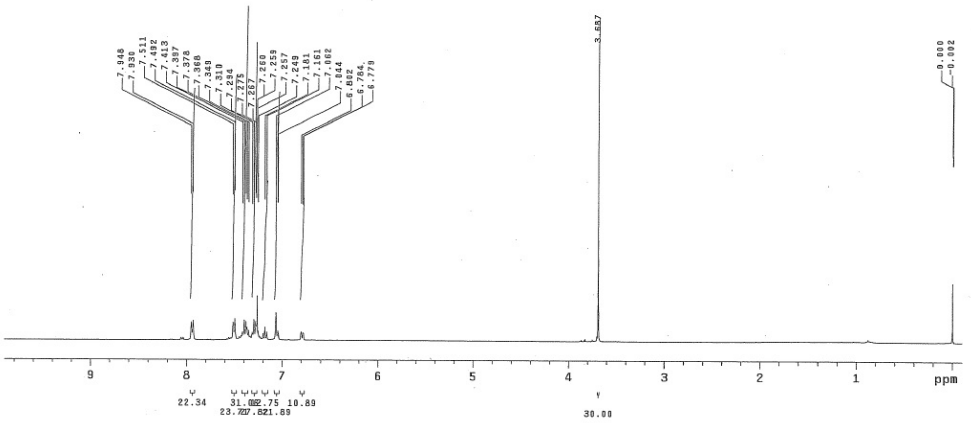
132.093
131.035
77.644
77.318
77.000
220
200
180
160
140
120
100
80
60
40
20
ppm


HN
N
O
4j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7.260
7.259
7.257
7.249
7.161
7.062
7.044
6.815
6.784
6.770
3.687
0.000
-0.002
9
8
7
6
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2
1
ppm
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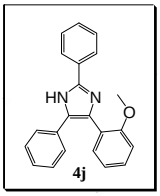
31.08
2.75
10.89
23.72
7.82
1.89
30.00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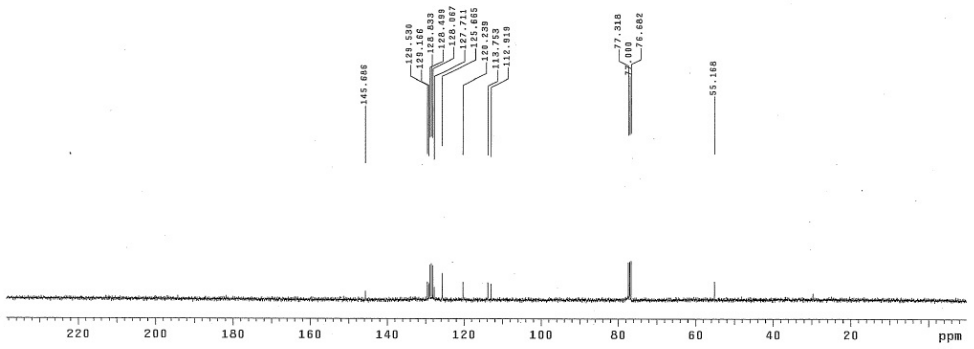
O
4j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128.067
127.711
127.685
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113.753
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77.000
76.682
55.168
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140
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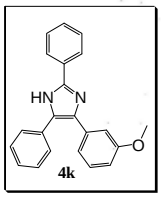
80
60
40
20
ppm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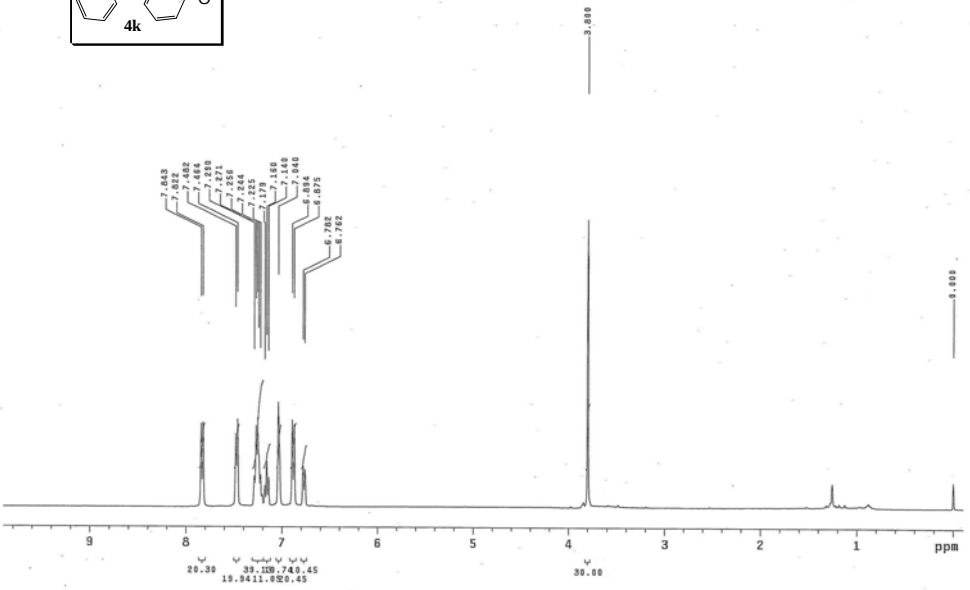
O
4k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7.822
7.482
7.464
7.269
7.261
7.255
7.244
7.225
7.179
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7.148
7.040
6.894
6.875
6.782
6.762
1.000
9
8
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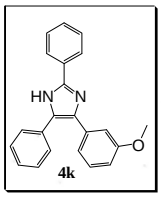
6
5
4
3
2
1
ppm
20.30
39.11
19.94
11.09
20.45
30.00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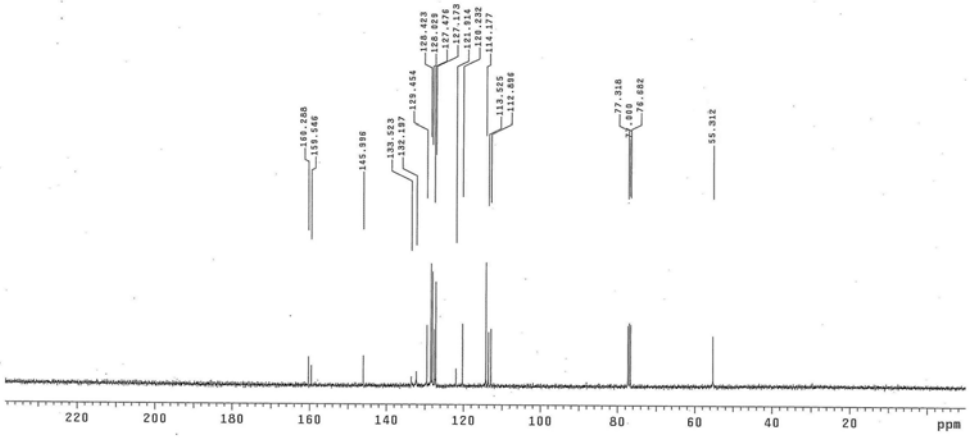
N
O
4k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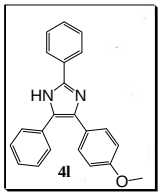
159.646
145.996
133.523
132.197
129.454
128.423
128.029
127.476
127.113
121.914
120.232
114.177
113.926
112.486
77.316
77.000
76.682
55.312
220
200
180
160
140
120
100
80
60
40
20
ppm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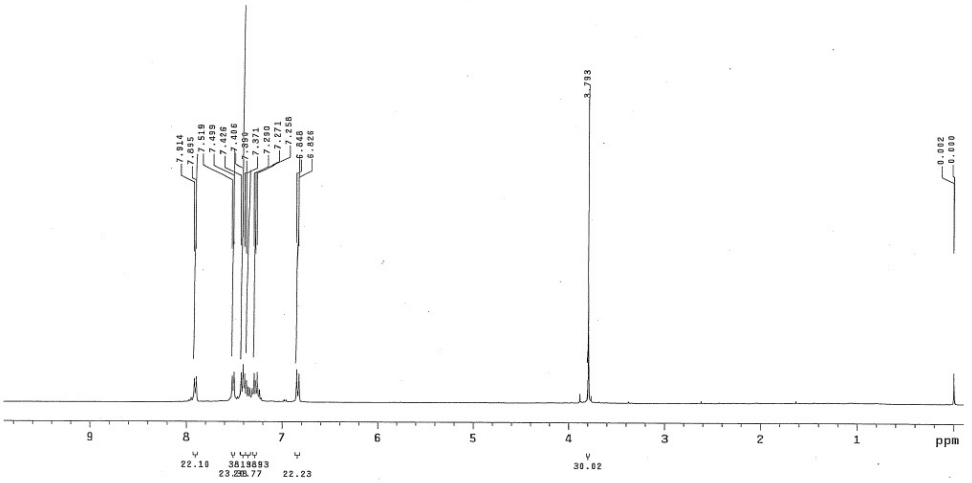
O
4l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7.895
7.519
7.499
7.486
7.406
7.390
7.371
7.293
7.271
7.258
6.846
6.826
3.793
0.022
0.000
9
8
7
6
5
4
3
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1
ppm
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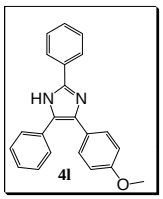
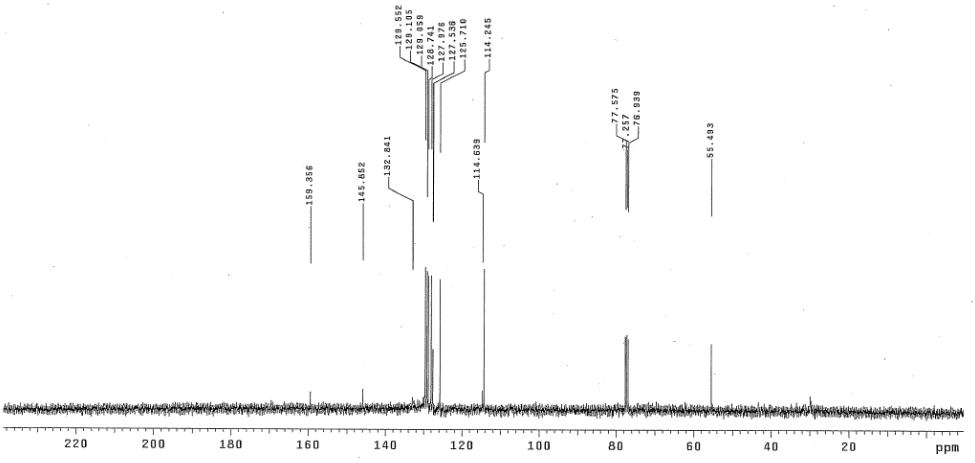
38.77
22.23
30.02


HN
N
O
4l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129.552
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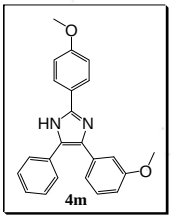
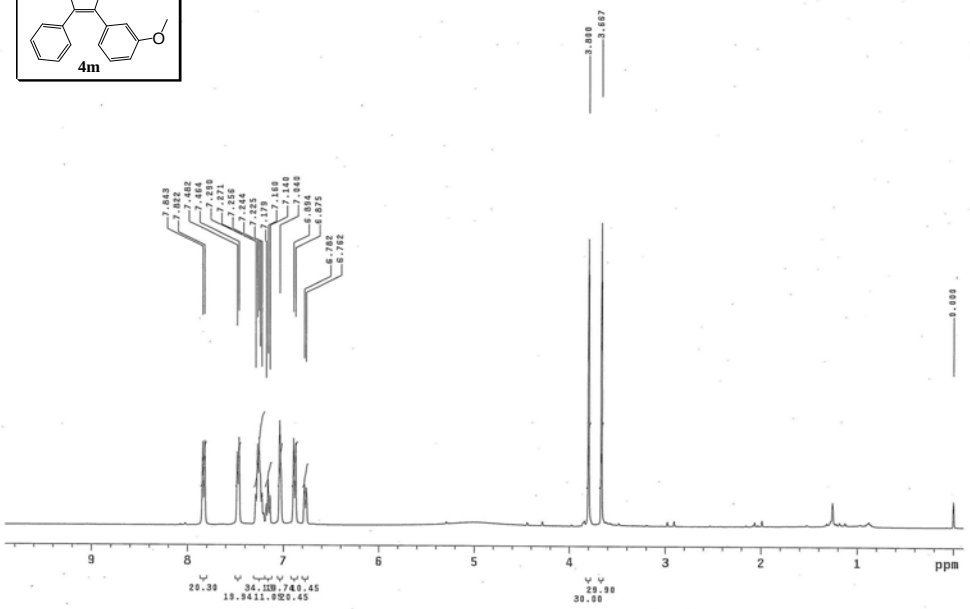
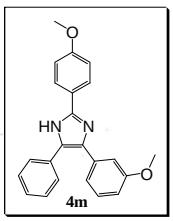
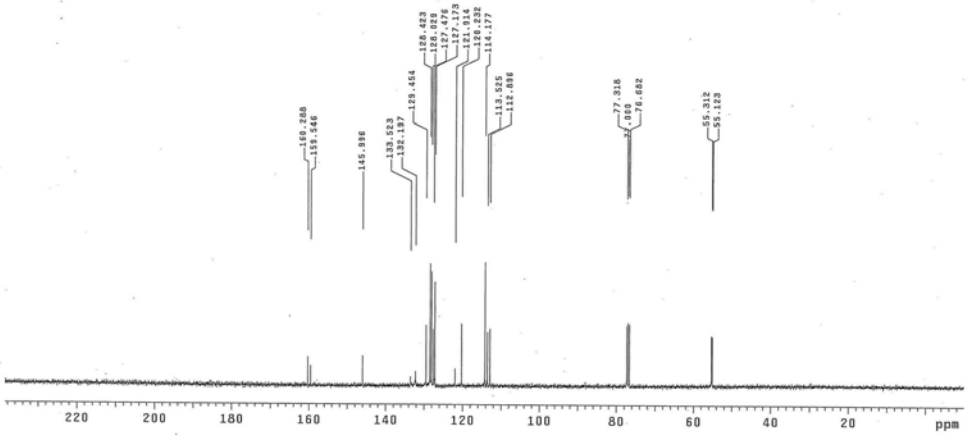
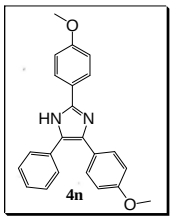
128.888
128.741
127.976
127.538
125.710
114.245
114.639
77.575
77.257
76.938
55.493
220
200
180
160
140
120
100
80
60
40
20
ppm

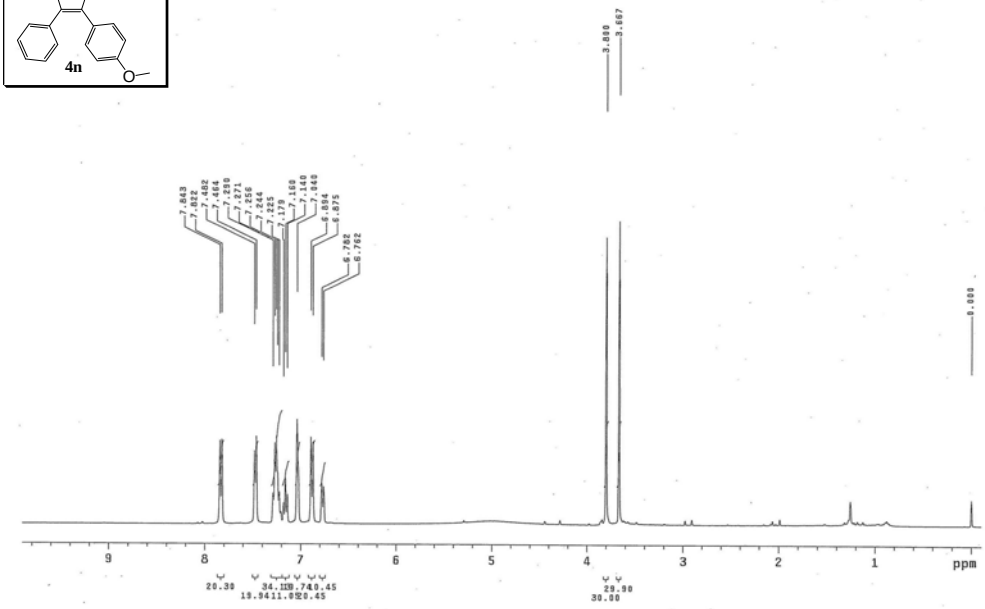

HN
N
O
O
4m


3.000
3.667
9.000
ppm


HN
N
O
O
4m


ppm


HN
N
O
O
4n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3.667
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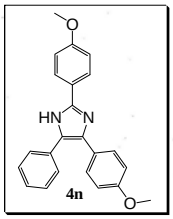
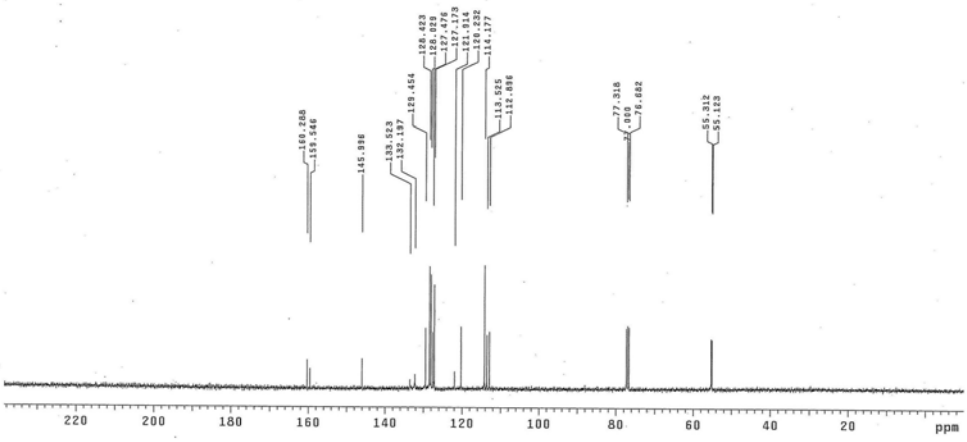
7.482
7.464
7.271
7.256
7.244
7.225
7.179
7.160
7.140
7.046
7.044
6.877
6.875
6.782
6.762
0.000
9
8
7
6
5
4
3
2
1
ppm
20.30
34.11
19.94
11.07
19.74
20.45
19.45
29.98
30.00


HN
N
O
O
4n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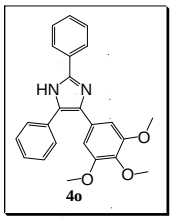
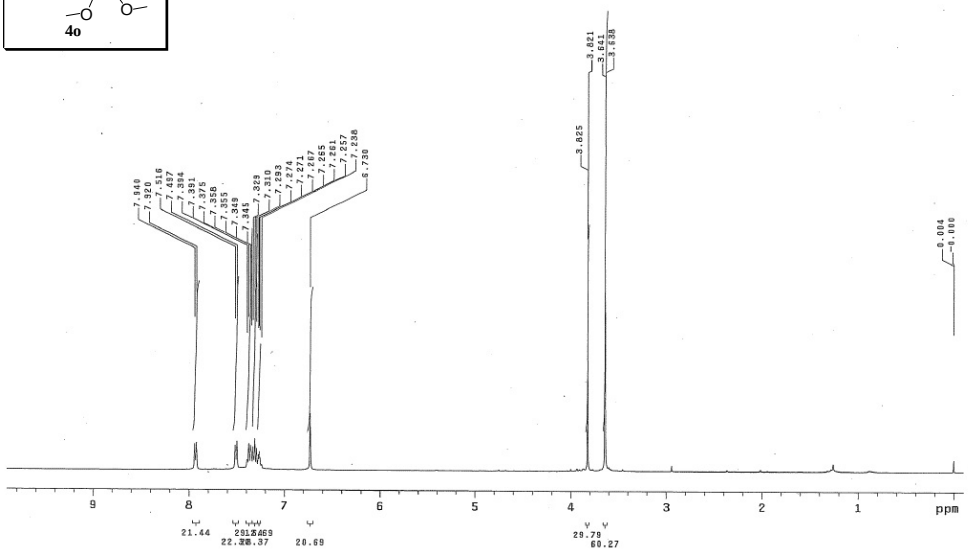
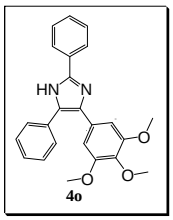
159.546
145.936
133.523
132.197
129.464
128.623
128.438
127.476
127.173
121.014
120.232
114.177
113.525
112.696
77.318
77.000
76.682
55.312
55.123
220
200
180
160
140
120
100
80
60
40
20
ppm

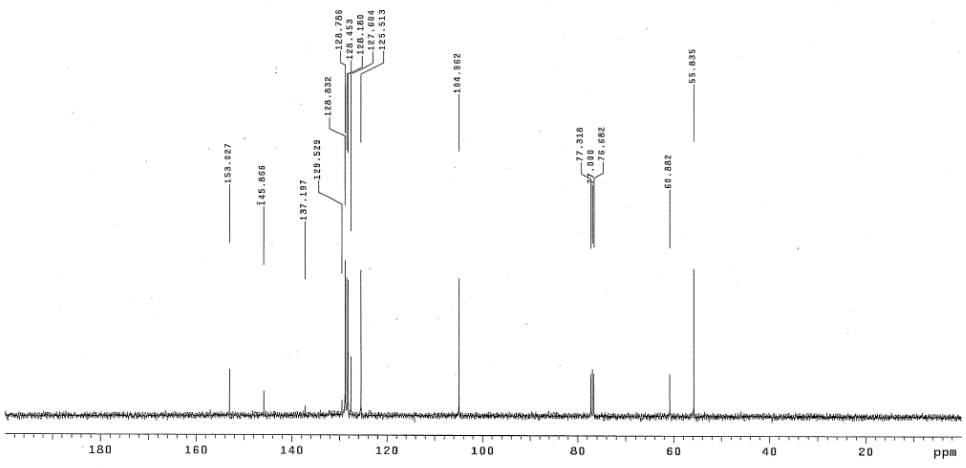

HN
N
O
O
O

4o


7.840
7.820
7.516
7.497
7.394
7.381
7.375
7.356
7.355
7.348
7.343
7.328
7.310
7.293
7.274
7.271
7.267
7.265
7.261
7.257
7.238
6.730
3.825
3.821
3.643
3.638
0.004
0.000
9
8
7
6
5
4
3
2
1
ppm
21.44
28.79
60.27
20.69


HN
N
O
O
O

4o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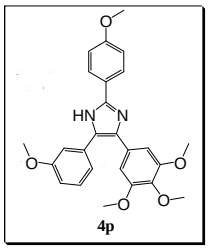
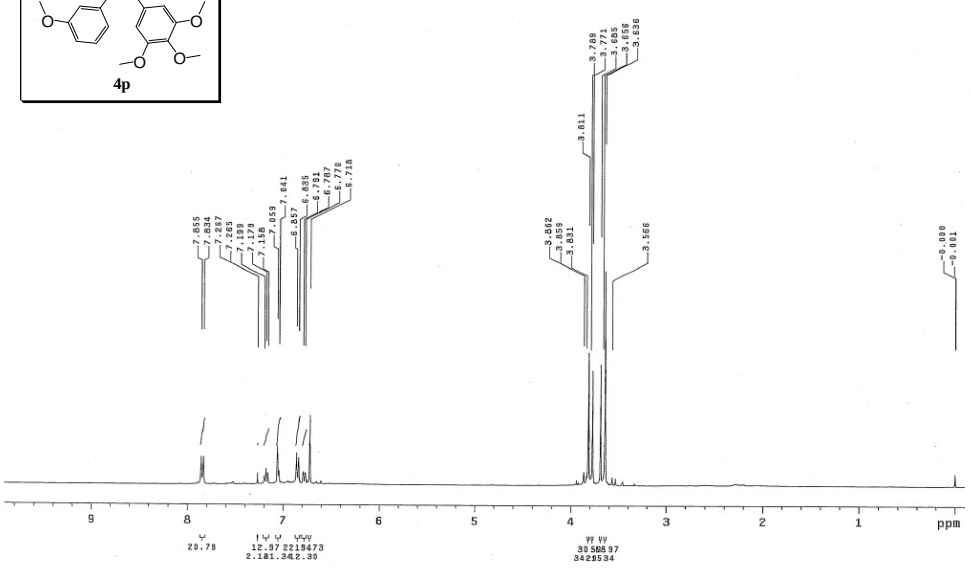
145.865
137.197
129.528
128.832
128.706
128.453
128.180
127.904
125.513
104.962
77.318
77.000
76.682
60.882
55.835
180
160
140
120
100
80
60
40
20
ppm


HN
N
O
O
O
O
O

4p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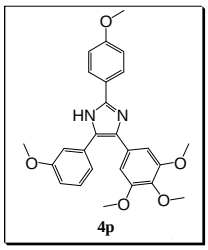
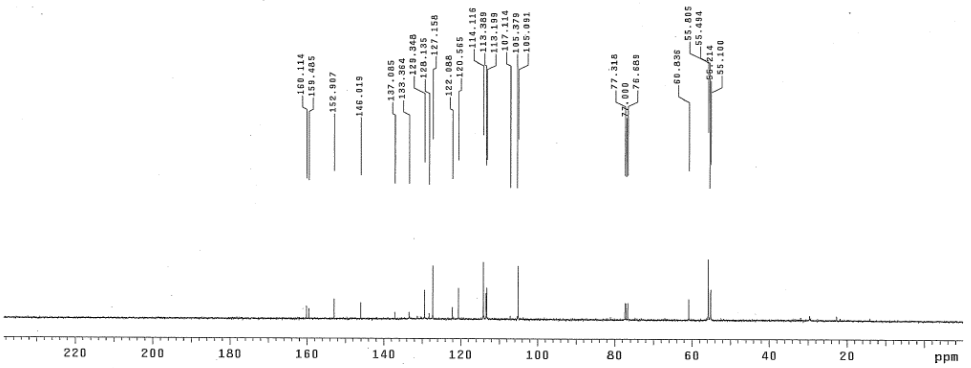
7.834
7.287
7.265
7.199
7.178
7.158
7.059
7.041
6.857
6.835
6.791
6.707
6.779
6.718
3.882
3.858
3.831
3.811
3.789
3.771
3.685
3.658
3.638
3.566
0.000
-0.001
9
8
7
6
5
4
3
2
1
ppm
20.79
12.97
2.18
1.34
2.30
3.29
2.34


HN
N
O
O
O
O
O

4p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159.465
152.907
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137.085
133.364
129.348
128.135
127.158
122.058
120.165
114.116
113.389
113.199
107.114
105.378
105.091
77.318
77.000
76.689
60.838
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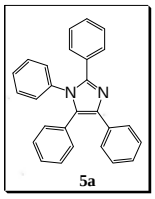
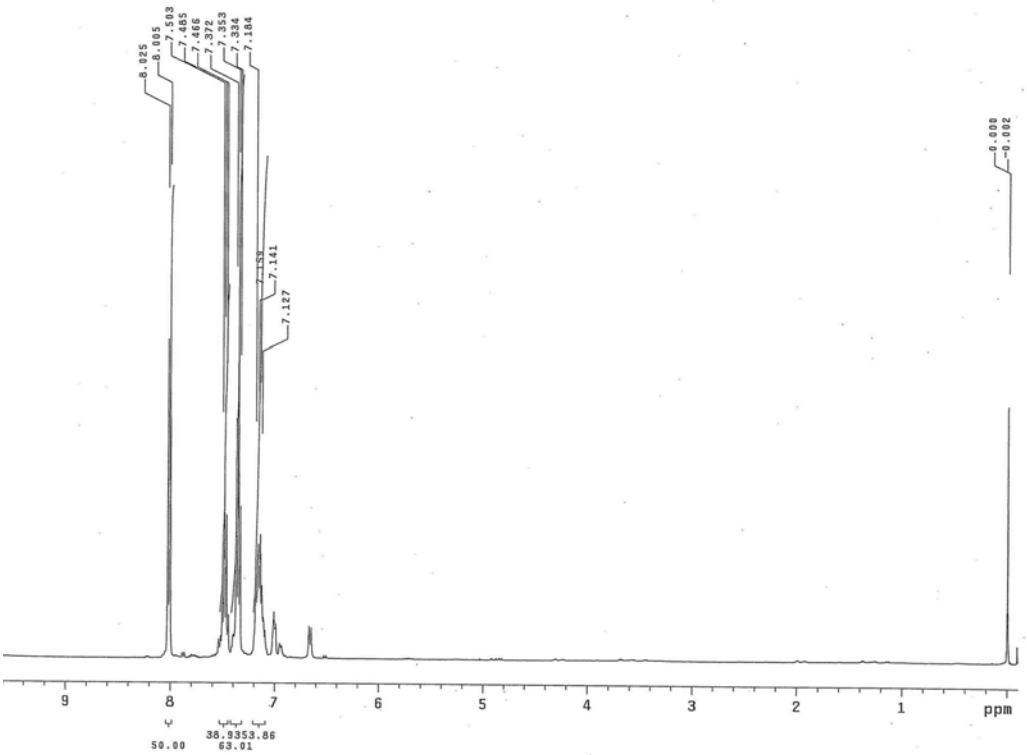
55.214
55.100
220
200
180
160
140
120
100
80
60
40
20
ppm


5a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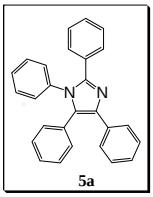
8.005
7.503
7.485
7.466
7.372
7.353
7.334
7.184
7.152
7.141
7.127
0.000
-0.002
9
8
7
6
5
4
3
2
1
ppm
50.00
38.9353.86
63.01


5a

171.791
146.845
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139.258
138.365
131.068
131.036
130.757
130.447
130.080
129.992
129.833
129.572
129.376
129.295
129.120
128.914
128.931
128.689
128.598
128.458
128.355
128.557
128.196
128.166
127.966
127.741
127.196
127.059
139.275
137.765
136.213
134.842
83.974
77.316
77.000
76.682
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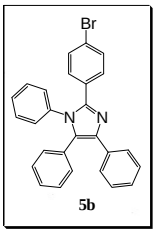
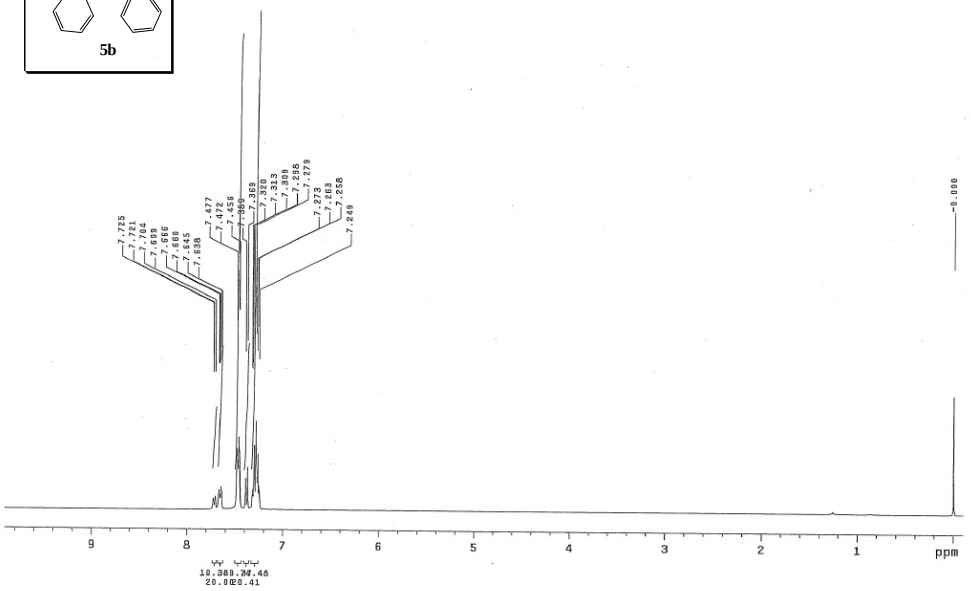
200
180
160
140
120
100
80
60
40
20
ppm


Br
N
N

5b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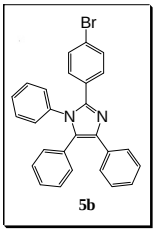
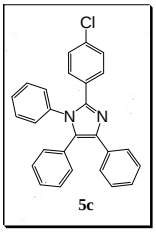
7.660
7.645
7.638
7.477
7.472
7.458
7.389
7.320
7.313
7.309
7.295
7.279
7.273
7.263
7.256
7.249
0.000
9
8
7
6
5
4
3
2
1
ppm

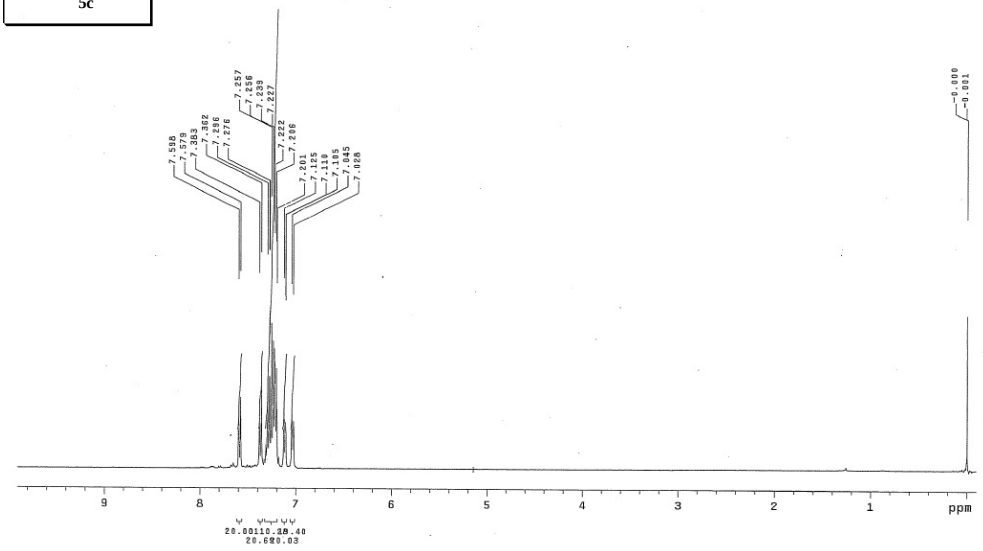

Br
N
N

5b

128.598
128.486
128.372
127.840
131.947
131.720
129.371
128.666
127.666
126.961
126.079
144.881
123.028
121.611
77.318
77.000
76.689
0.014
220
200
180
160
140
120
100
80
60
40
20
ppm


Cl
N
N

5c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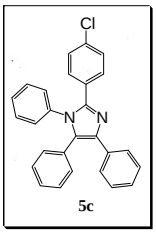
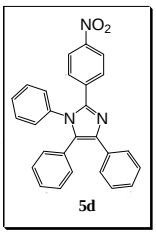
7.256
7.239
7.227
7.382
7.276
7.232
7.206
7.201
7.125
7.115
7.105
7.045
7.028
0.000
0.001
9
8
7
6
5
4
3
2
1
ppm

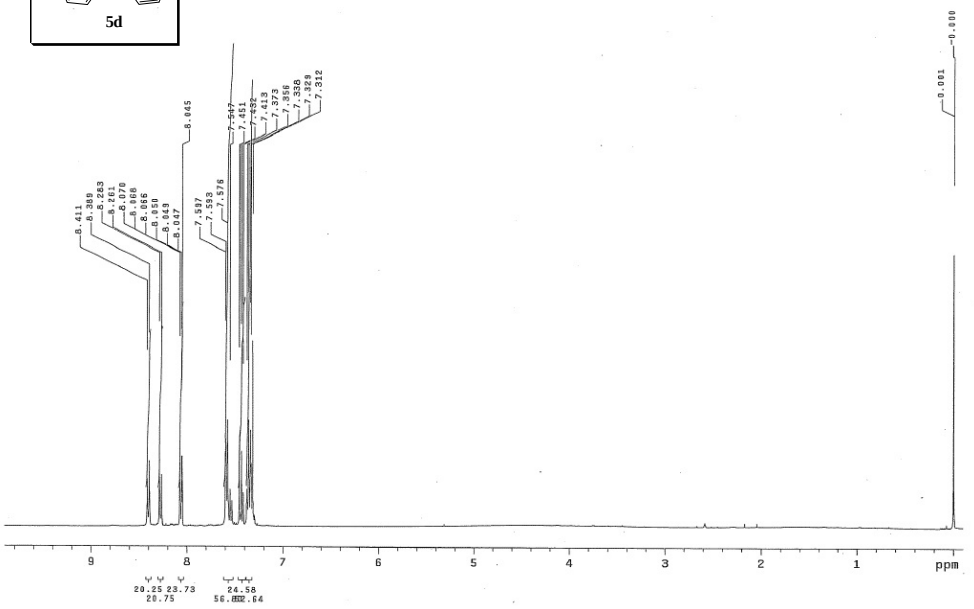

Cl
N
N

5c

126.393
126.302
131.638
130.168
130.264
129.067
128.582
128.211
128.151
127.408
127.173
126.858
145.617
135.645
134.516
131.106
77.318
77.000
76.682
0.014
220
200
180
160
140
120
100
80
60
40
20
ppm


NO2
N
N

5d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8.389
8.283
8.261
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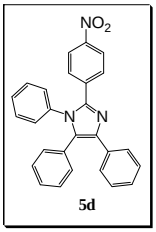
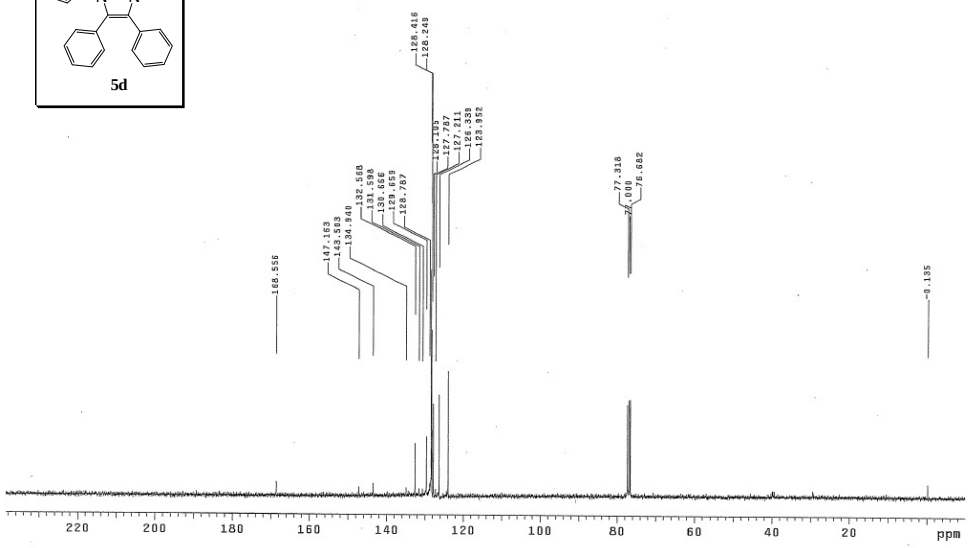
8.066
8.050
8.045
8.040
7.597
7.593
7.576
7.547
7.451
7.433
7.356
7.338
7.329
7.312
0.000
0.001
9
8
7
6
5
4
3
2
1
ppm
20.25 23.73
20.75
24.58
56.82 62.64


NO2
N
N

5d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129.165
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128.416
128.248
127.787
127.211
126.338
123.952
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76.000
76.682
9.135
220
200
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140
120
100
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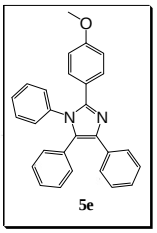
60
40
20
ppm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N
N

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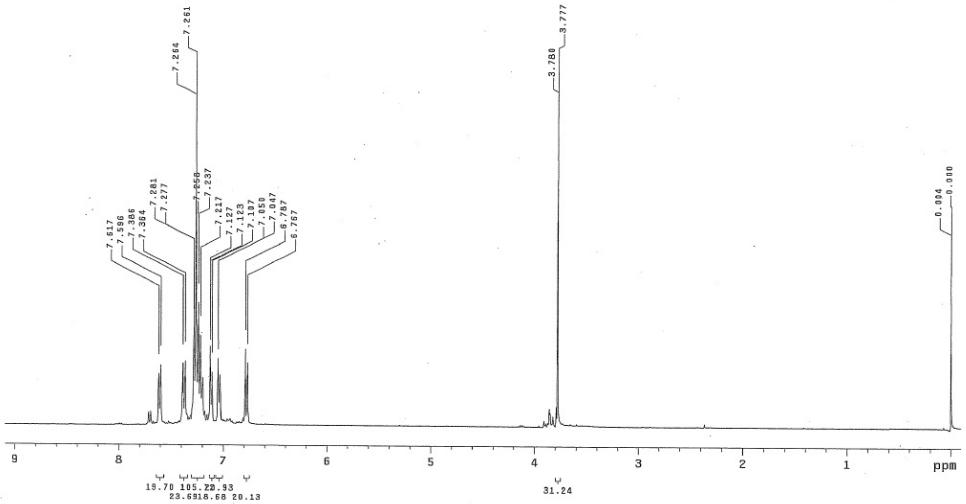
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7.381
7.281
7.277
7.237
7.217
7.127
7.113
7.137
7.059
7.047
6.787
6.767
0.004
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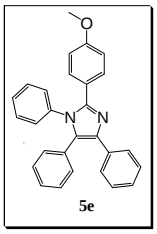
ppm
13.70 105.22 93
23.68 16.68 20.13
31.24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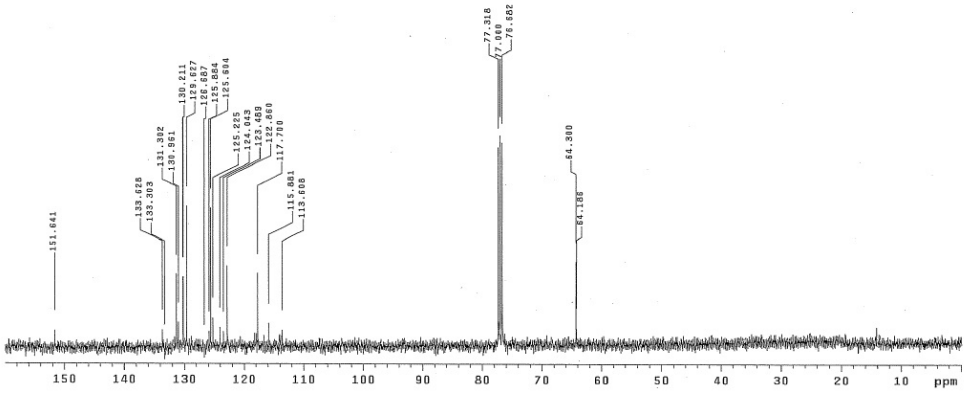
N

5e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125.225
124.043
123.468
120.680
117.780
115.881
115.608
64.380
64.188
151.641
133.628
133.303
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110
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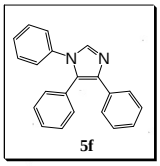
10
ppm



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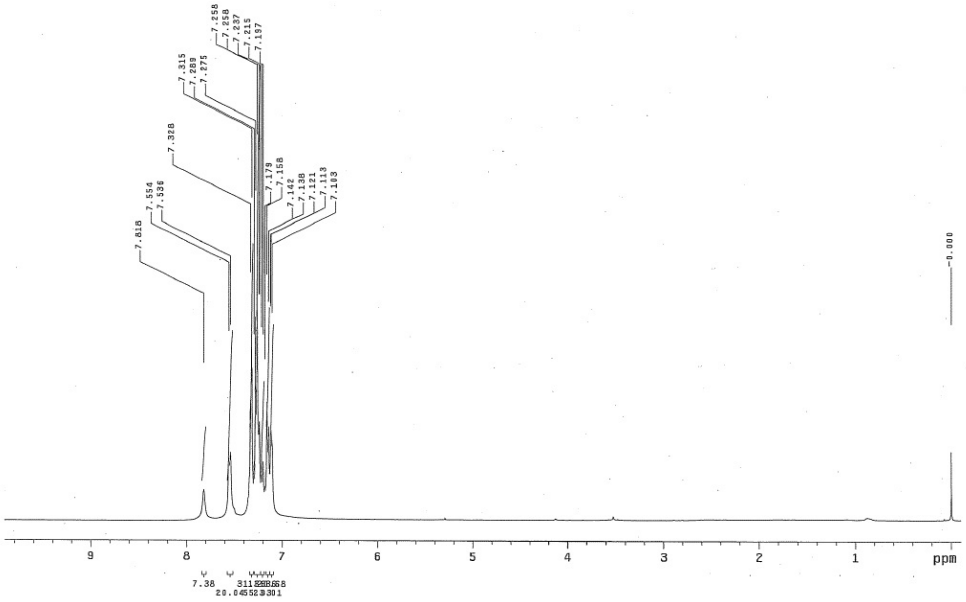
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7.289
7.275
7.258
7.238
7.237
7.215
7.197
7.179
7.158
7.142
7.138
7.121
7.113
7.103
0.000
9
8
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5
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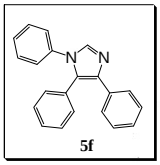
3
2
1
ppm
7.38



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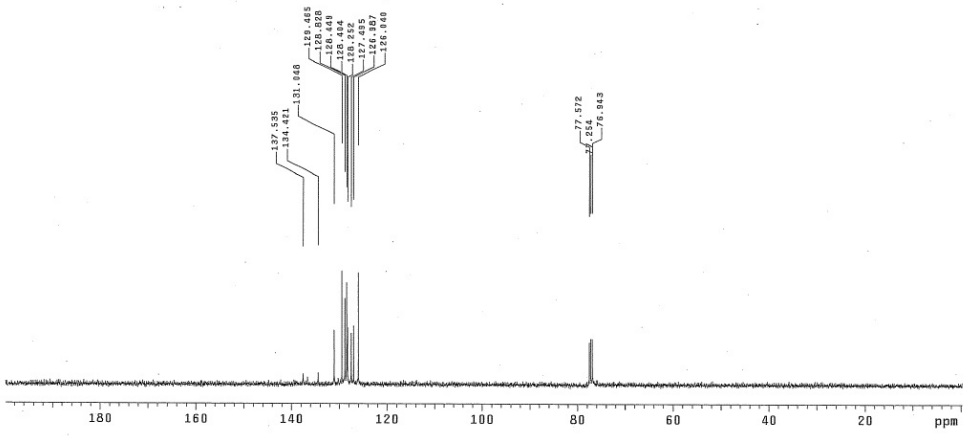
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134.421
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128.449
128.444
128.392
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77.572
77.254
76.943
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60
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20
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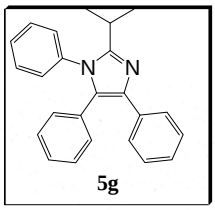

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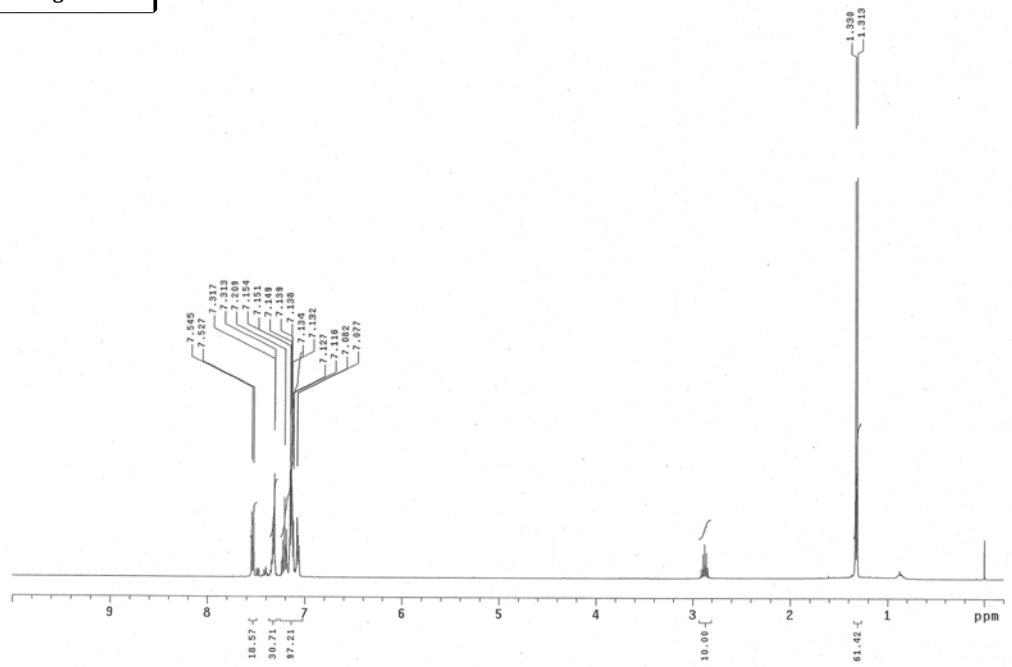
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7.313
7.308
7.154
7.151
7.149
7.139
7.138
7.134
7.132
7.127
7.110
7.102
7.077
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7
6
5
4
3
2
1
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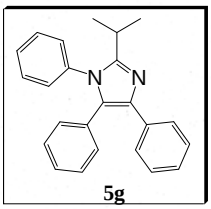
97.21
10.00
61.42



5g

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136.600
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130.752
130.725
128.583
128.381
128.341
128.137
128.008
127.717
127.379
127.068
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77.000
76.682
26.477
21.982
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140
120
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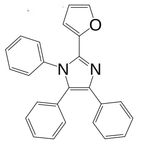
60
40
20
ppm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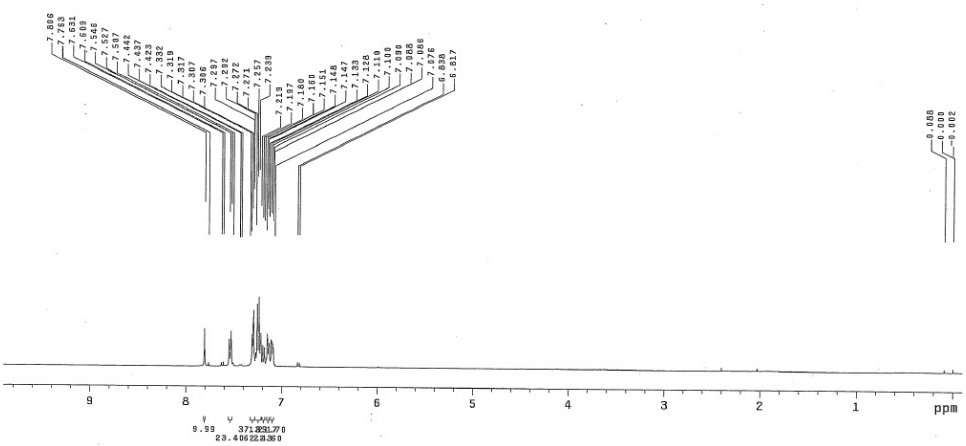
N

5h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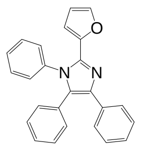
7
6
5
4
3
2
1
ppm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N

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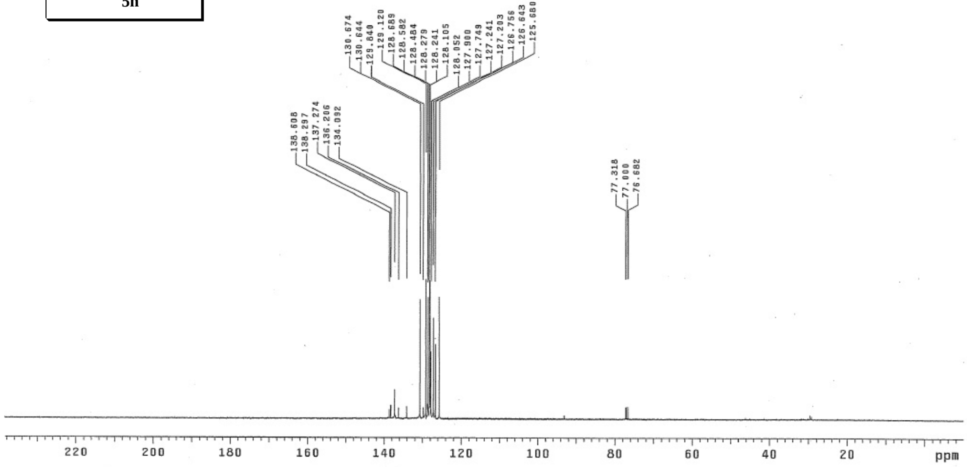
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140
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60
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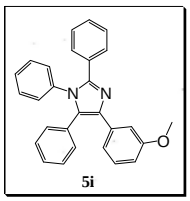
20
ppm



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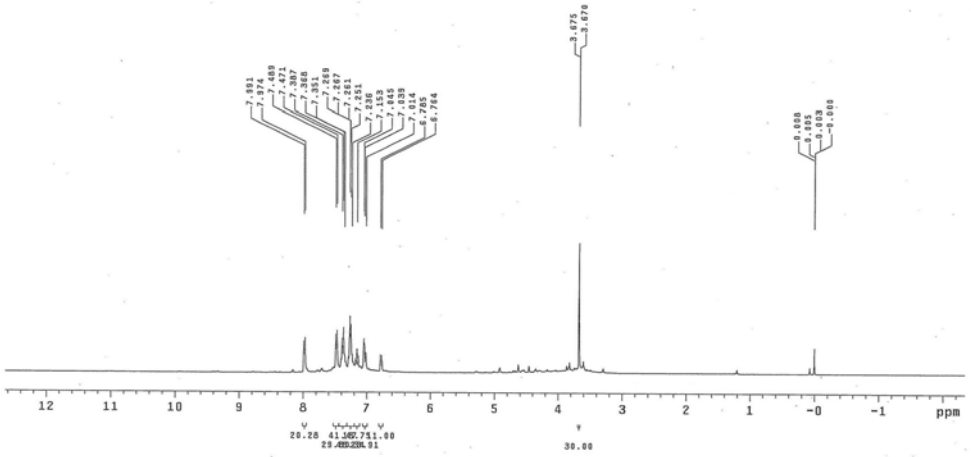

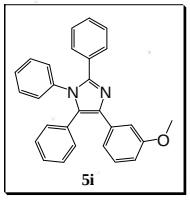

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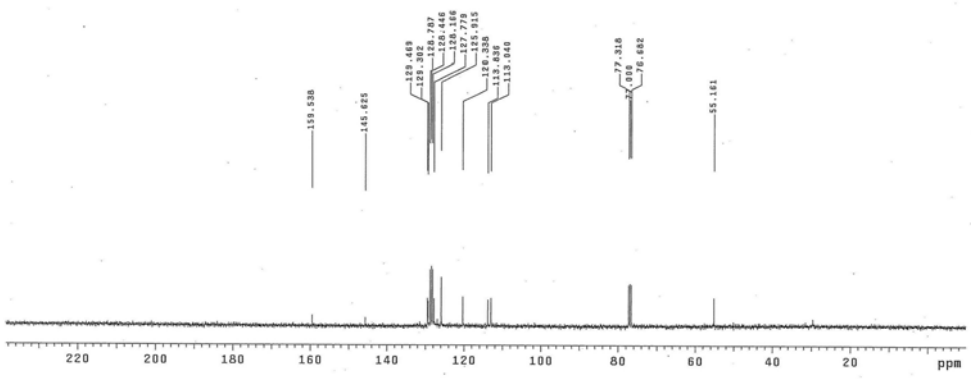

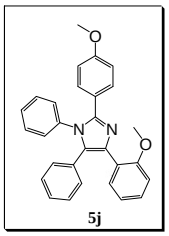
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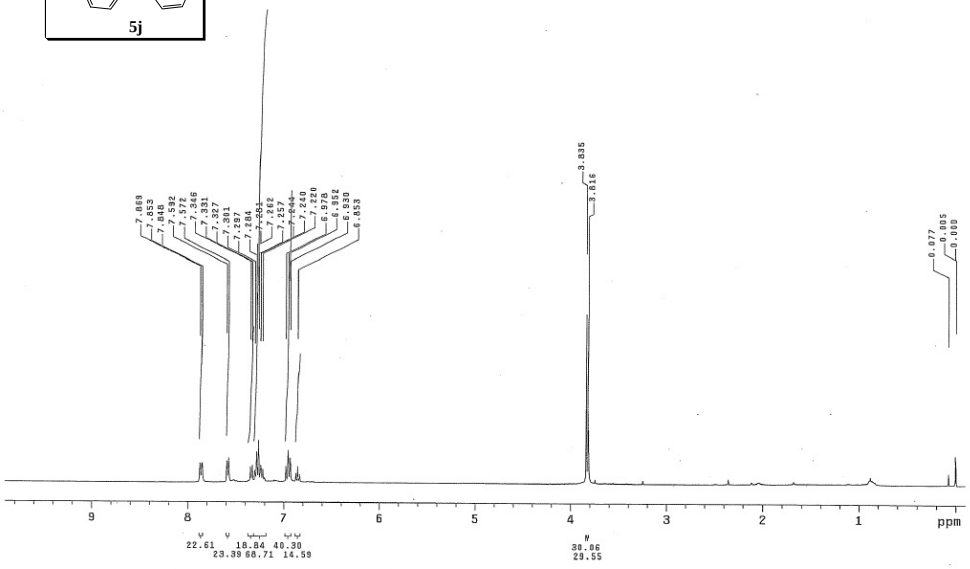
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7.257
7.244
7.220
6.978
6.892
6.830
6.658
3.835
3.616
0.077
0.005
0.000
9
8
7
6
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4
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2
1
ppm
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23.39
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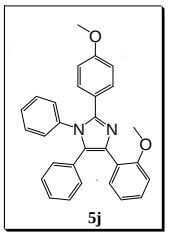
30.06
29.55


5j

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126.425
125.226
127.016
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126.998
126.861
120.987
114.280
111.403
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77.000
76.682
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55.327
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200
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140
120
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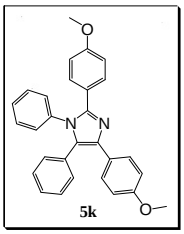
60
40
20
ppm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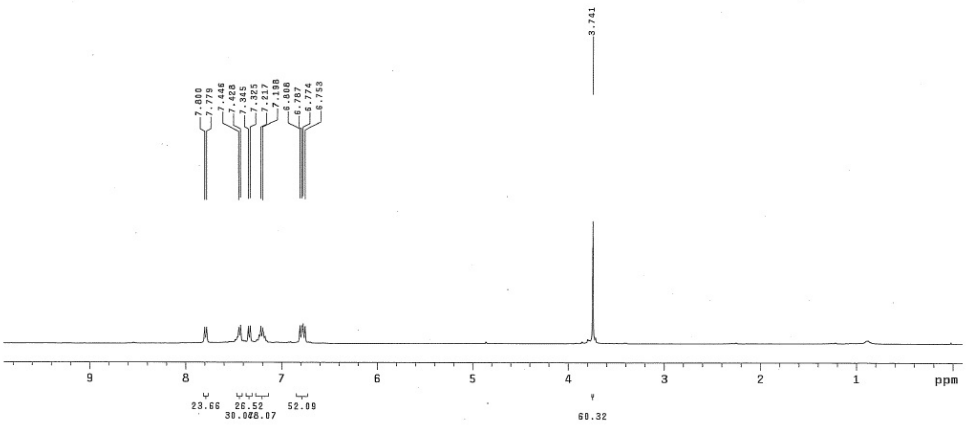
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6.774
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8
7
6
5
4
3
2
1
ppm
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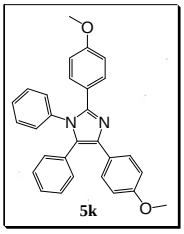
52.09
60.32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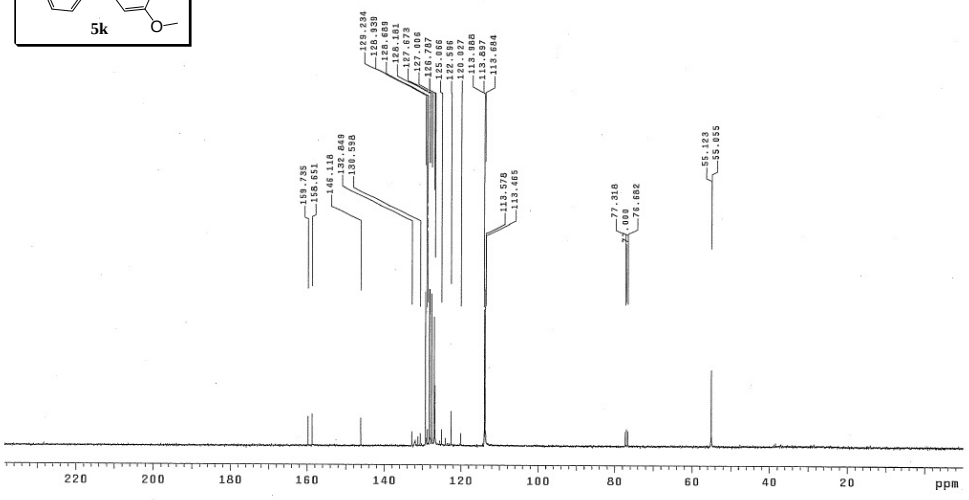
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125.066
122.596
120.077
113.808
113.697
113.694
113.578
113.465
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77.000
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55.055
220
200
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140
120
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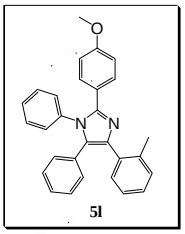
80
60
40
20
ppm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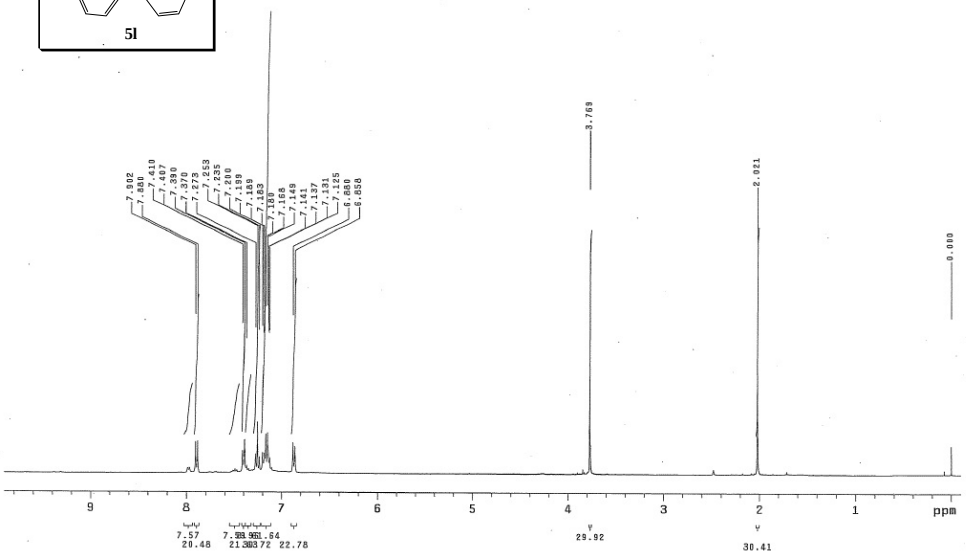
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7.235
7.200
7.189
7.183
7.164
7.154
7.148
7.141
7.137
7.131
7.125
6.886
6.850
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0.000
9
8
7
6
5
4
3
2
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ppm
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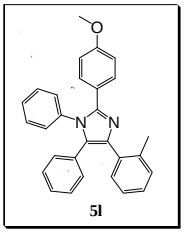
30.41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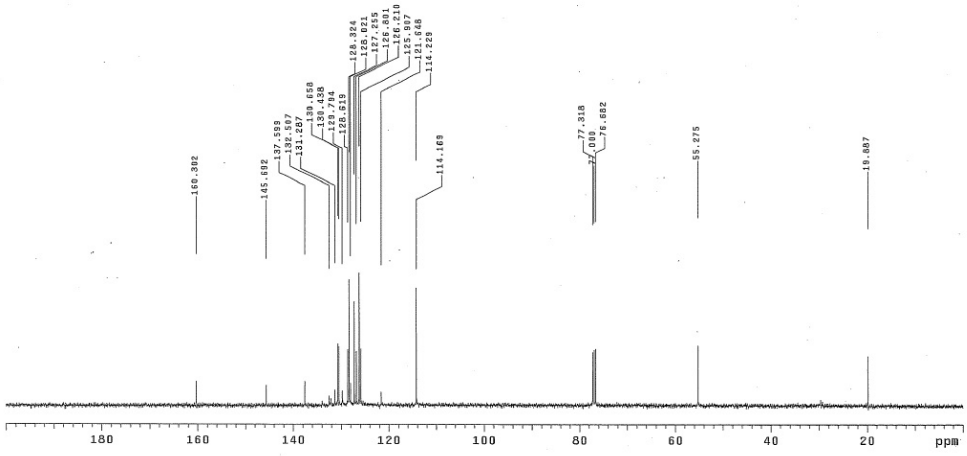
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130.658
130.458
129.794
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128.324
128.021
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126.801
126.210
125.837
121.668
114.229
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77.000
76.682
55.275
19.887
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140
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60
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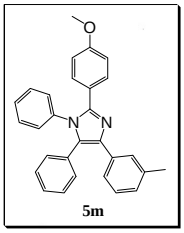
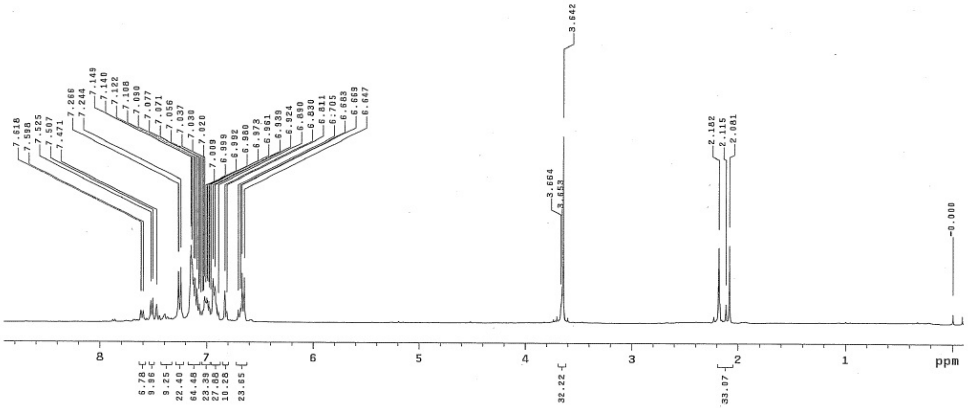
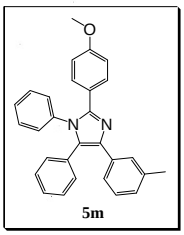
20
ppm



5m





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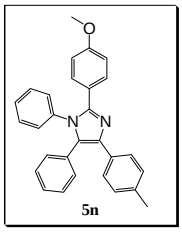
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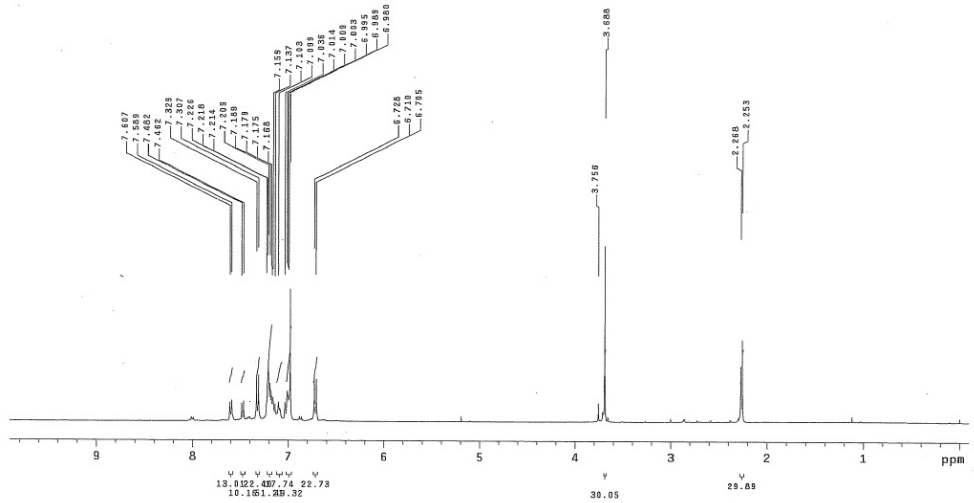
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7.137
7.103
7.038
7.014
7.009
7.003
6.995
6.980
6.728
6.719
6.705
3.688
3.756
2.268
2.253
9
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6
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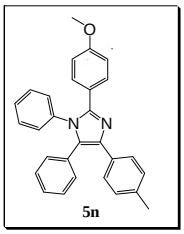
30.05
28.89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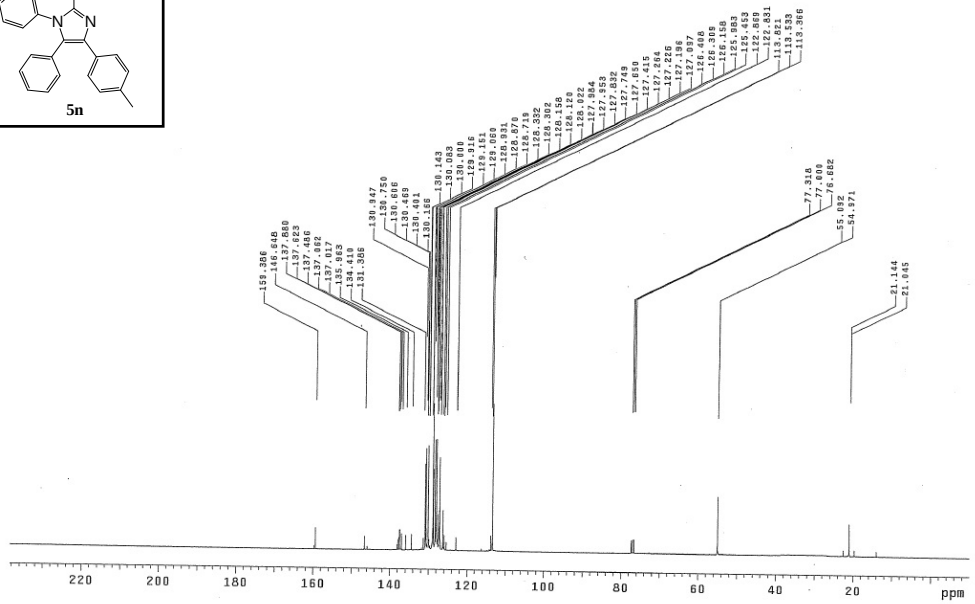
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130.186
130.143
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130.010
129.916
129.151
129.069
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128.870
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126.302
126.158
126.128
126.022
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127.097
127.048
126.305
126.158
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125.463
125.408
122.831
113.821
113.533
113.386
77.316
77.000
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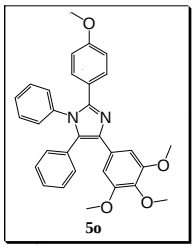
20
ppm



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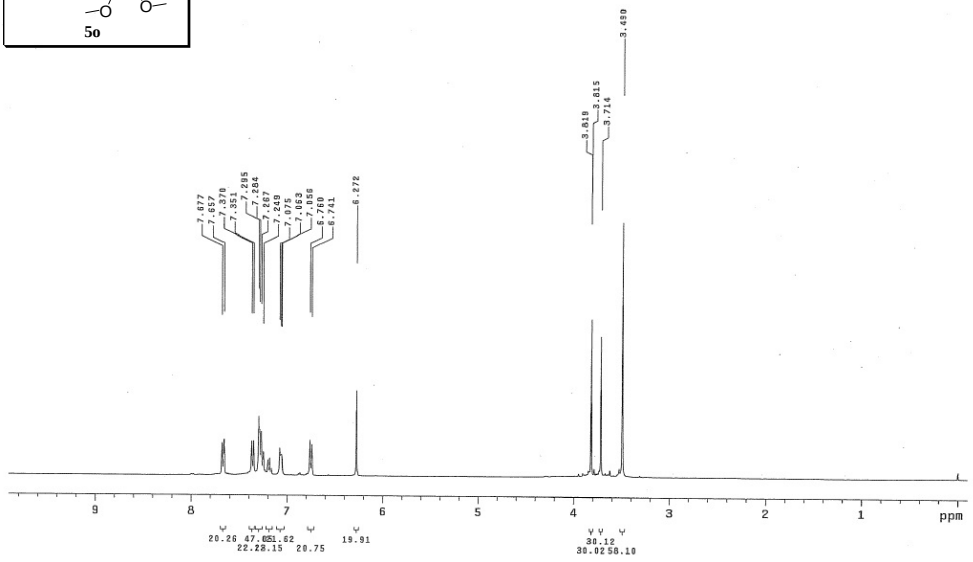
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7.249
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7.056
6.760
6.741
6.272
3.819
3.815
3.714
3.490
9
8
7
6
5
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22.28.15
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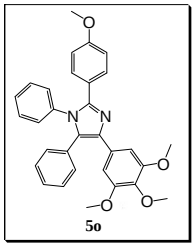
30.02
58.10



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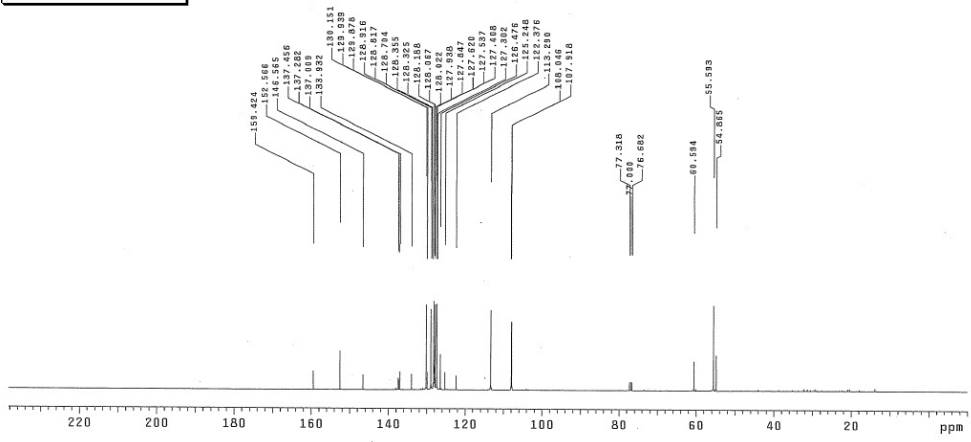
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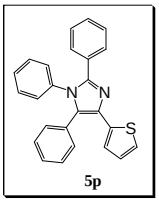
152.666
146.565
137.456
137.282
137.098
136.892
130.151
128.939
128.878
128.816
128.617
128.704
128.355
128.325
128.196
128.067
128.022
127.938
127.847
127.820
127.537
127.468
127.387
127.276
125.248
122.376
113.280
109.466
107.910
77.315
76.682
60.594
55.593
54.865
220
200
180
160
140
120
100
80
60
40
20
ppm



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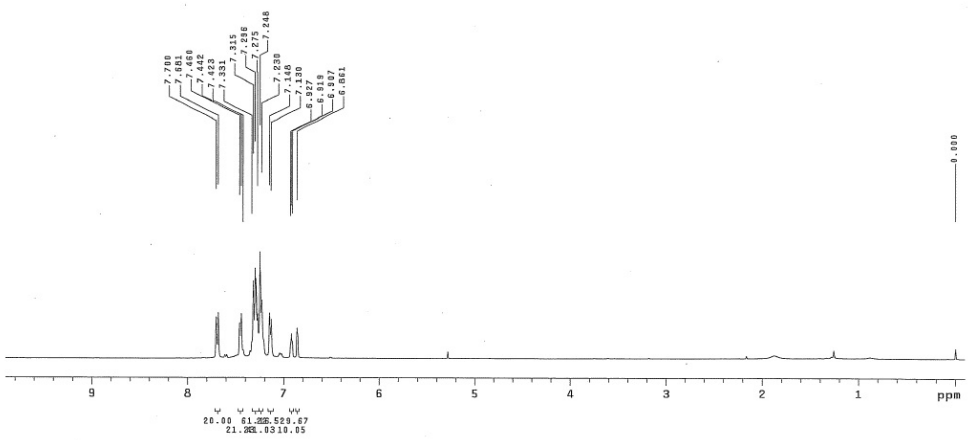
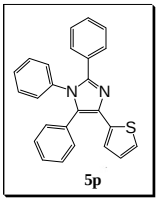

7.700
7.681
7.460
7.442
7.423
7.353
7.315
7.286
7.275
7.248
7.230
7.148
7.130
6.987
6.918
6.861
0.000
9
8
7
6
5
4
3
2
1
ppm



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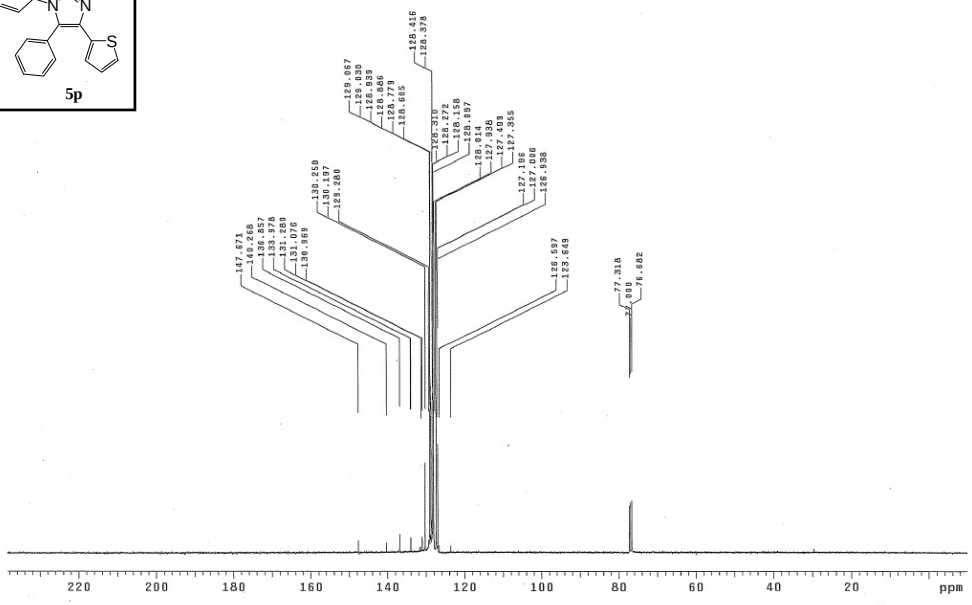
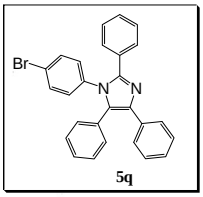
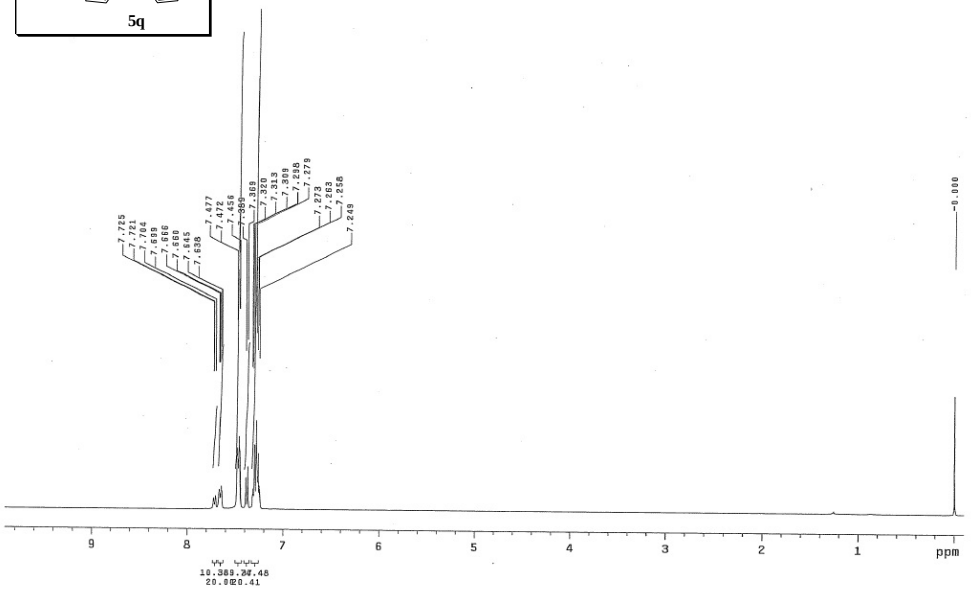

147.671
140.268
136.857
133.976
131.280
131.065
130.969
130.250
130.197
129.260
129.067
129.035
128.938
128.366
128.279
128.065
126.416
126.378
126.272
126.158
125.897
125.014
124.748
127.499
127.355
127.186
127.016
126.938
126.597
123.649
77.318
77.000
76.682
220
200
180
160
140
120
100
80
60
40
20
ppm


Br
N
N

5q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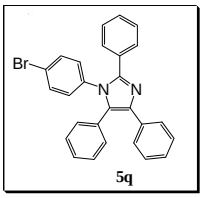
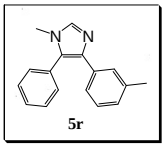
7.721
7.704
7.699
7.698
7.660
7.645
7.638
7.477
7.472
7.456
7.389
7.380
7.313
7.309
7.286
7.279
7.273
7.263
7.256
7.249
8.000
9
8
7
6
5
4
3
2
1
ppm
10.38
9.24
8.45
20.00
20.41

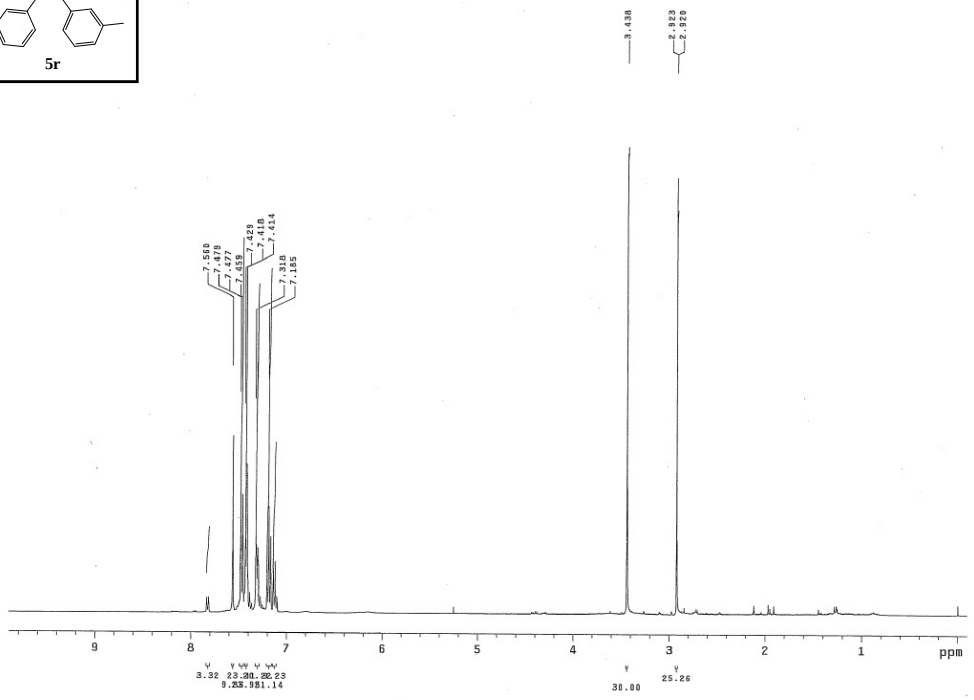

Br
N
N

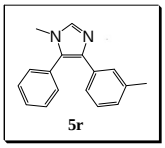
5q

128.598
128.406
128.272
127.840
131.947
131.780
129.371
126.666
127.866
126.961
126.678
144.981
123.028
121.611
77.318
77.000
76.680
8.014
220
200
180
160
140
120
100
80
60
40
20
ppm

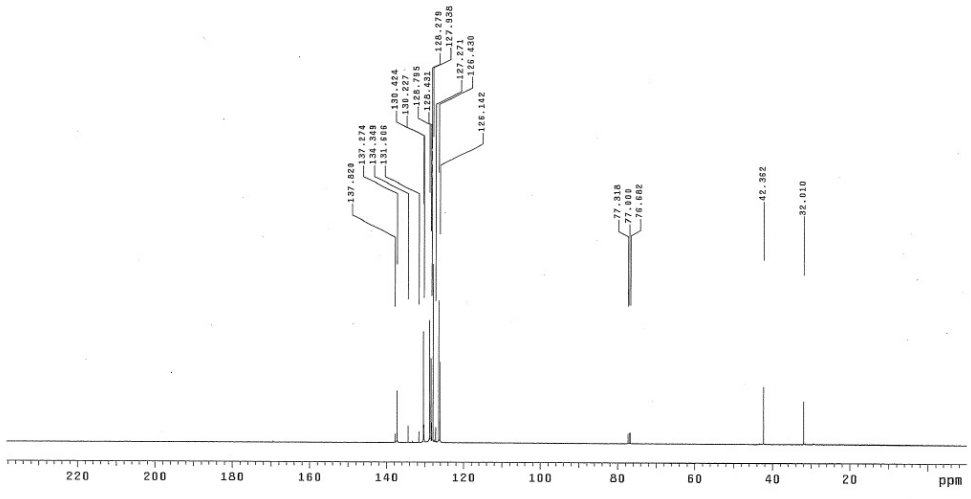


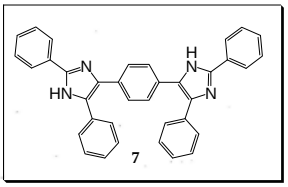
5r

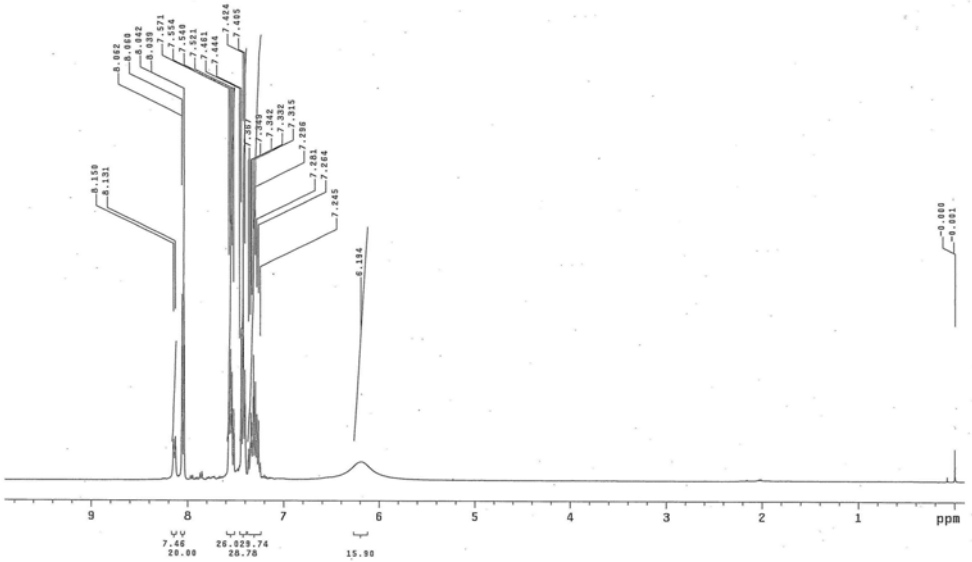

3.438
2.923
2.920
7.560
7.479
7.477
7.459
7.428
7.418
7.414
7.318
7.185
9
8
7
6
5
4
3
2
1
ppm
3.32
23.30
2.23
9.23
1.14
30.00
25.26

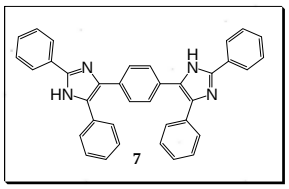


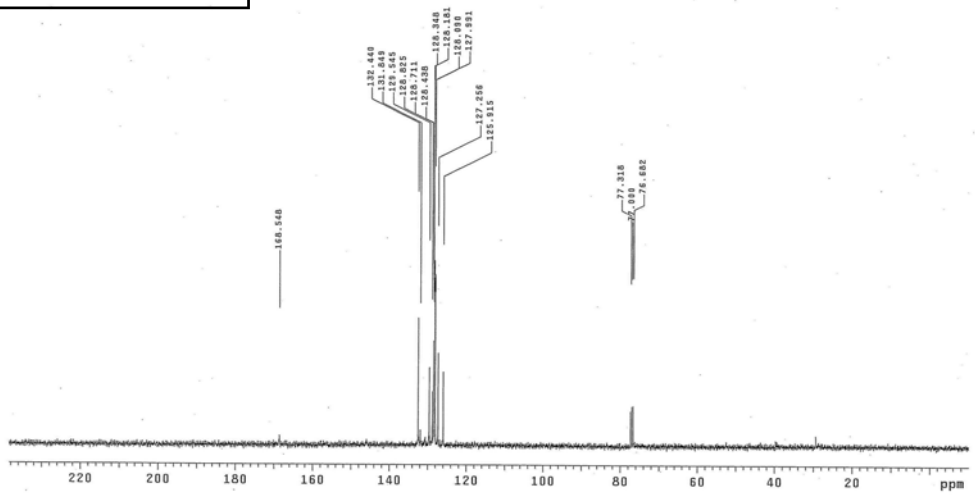
5r


137.823
137.474
134.348
131.606
130.424
130.227
128.795
128.431
128.279
127.938
127.774
126.430
126.142
77.318
77.000
76.682
42.362
32.010
220
200
180
160
140
120
100
80
60
40
20
ppm


HN
N
H
N
7


8.662
8.659
8.642
8.639
7.571
7.554
7.540
7.521
7.461
7.444
7.424
7.405
7.387
7.349
7.342
7.325
7.315
7.296
7.281
7.264
7.245
8.159
8.131
6.194
0.069
0.061
9
8
7
6
5
4
3
2
1
ppm
7.46
20.00
26.029.74
28.78
15.90


HN
N
H
N
7


132.440
131.446
129.545
128.825
128.711
128.438
128.348
128.181
128.050
127.991
127.256
125.915
168.548
77.316
77.000
76.682
220
200
180
160
140
120
100
80
60
40
20
ppm