Supporting Information

Employing TosMIC as a C1N1 'Two-atom Synthon' in Imidazole Synthesis by Neighboring Group Assistance Strategy

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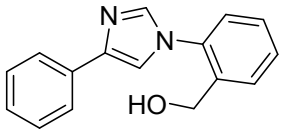
1. General

All substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). ^{1}H spectra were recorded in $CDCl_3$ or DMSO-d_6 on 400/600 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$ or DMSO-d_6 on 100/150 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on an Agilent QTOF 6540 MS/ Bruker 7-tesla FT-ICR MS equipped with an electrospray source.

2. General procedure for the synthesis of 4 (4aa as an example)

A sealed tube was charged with acetophenone (**1a**) (120 mg, 1.0 mmol), iodine (203 mg, 0.8 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 110 °C in metal heating block, after disappearance of the reactant (monitored by TLC), then added 2-aminobenzyl alcohol (**2a**) (123 mg, 1.0 mmol), $FeCl_3$ (162 mg, 1.0 mmol) and TosMIC (195 mg, 1.0 mmol) at 110 ^{o}C for another 1.0 h. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 2/1) to yield the desired product **4aa** as a yellow solid (185.2 mg, 74% yield).

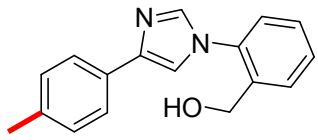
3. Characterization data for compounds 4



4aa

(2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4aa):

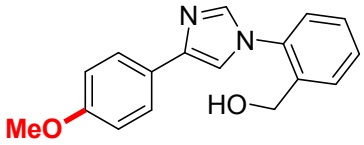
Yield 74%; 185.2 mg; red solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.95 (d, J = 4.8 Hz, 2H), 7.86 (d, J = 7.8 Hz, 2H), 7.68 (d, J = 7.8 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.2 Hz, 1H), 7.42 (d, J= 7.8 Hz, 1H), 7.39 (t, J = 7.8 Hz, 2H), 7.24 (t, J = 7.2 Hz, 1H), 5.44 (t, J = 5.4 Hz, 1H), 4.44 (d, J = 4.2 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 140.9, 138.4, 136.9, 135.1, 134.2, 129.1, 128.6, 128.5, 128.1, 126.6, 125.9, 124.5, 117.4, 58.8; HRMS (ESI) m/z calcd for $C_{16}H_{15}N_2O^+$ $(M+H)^+$ 251.11789, found 251.11797.



4ba

(2-(4-(p-tolyl)-1H-imidazol-1-yl)phenyl)methanol (4ba):

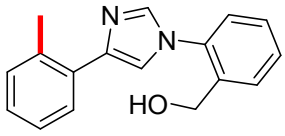
Yield 68%; 177.8 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.94 (s, 1H), 7.89 (s, 1H), 7.77 (d, J = 7.8 Hz, 2H), 7.69 (d, J = 7.2 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.2 Hz, 1H), 7.41 (d, J = 7.8 Hz, 1H), 7.20 (d, J = 7.8 Hz, 2H), 5.48 (s, 1H), 4.46 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 141.1, 138.2, 136.9, 135.7, 135.2, 131.4, 129.2, 128.4, 128.1, 125.8, 124.5, 116.8, 58.9, 20.9; HRMS (ESI) m/z calcd for $C_{17}H_{17}N_2O^+$ $(M+H)^+$ 265.13354, found 265.13364.



4ca

(2-(4-(4-methoxyphenyl)-1H-imidazol-1-yl)phenyl)methanol (4ca):

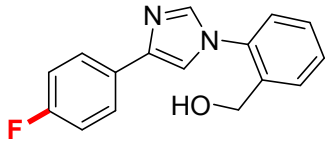
Yield 76%; 213.0 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 2/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 6.6 Hz, 4H), 7.53 (t, J = 7.2 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.40 (s, 1H), 7.33 (d, J = 7.2 Hz, 1H), 6.98 (d, J = 8.4 Hz, 2H), 5.23 (s, 1H), 4.60 (s, 2H), 3.90 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.7, 141.5, 137.8, 136.3, 135.4, 130.0, 128.9, 128.4, 126.04, 125.97, 125.9, 115.7, 113.9, 59.8, 55.1; HRMS (ESI) m/z calcd for $C_{17}H_{17}N_2O_2^+$ $(M+H)^+$ 281.12845, found 281.12823.



4da

(2-(4-(o-tolyl)-1H-imidazol-1-yl)phenyl)methanol (4da):

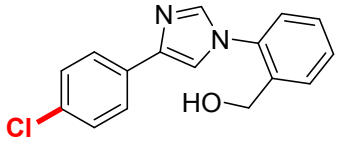
Yield 66%; 174.4 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.18 (s, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.90 (s, 1H), 7.87 (d, J = 7.8 Hz, 1H), 7.71–7.67 (m, 1H), 7.64 (d, J = 4.2 Hz, 1H), 7.47-7.40 (d, J = 3.6 Hz, 2H), 7.36 (t, J = 7.2 Hz, 1H), 5.65 (s, 1H), 4.65 (s, 2H), 2.69 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 140.2, 137.5, 136.9, 135.2, 134.4, 133.3, 130.8, 129.3, 128.5, 128.2, 127.9, 126.5, 125.84, 125.81, 119.6, 58.9, 21.8; HRMS (ESI) m/z calcd for $C_{17}H_{17}N_2O^+$ $(M+H)^+$ 265.13354, found 265.13364.



4ea

(2-(4-(4-fluorophenyl)-1H-imidazol-1-yl)phenyl)methanol (4ea):

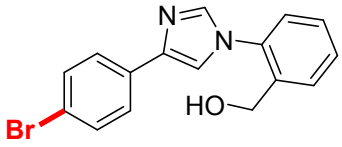
Yield 70%; 187.8 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.01-7.87 (m, 4H), 7.72 (d, J = 6.6 Hz, 1H), 7.54-7.47 (m, 1H), 7.47-7.39 (m, 2H), 7.22 (t, J = 7.2 Hz, 2H), 5.55 (s, 1H), 4.50 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1, 160.5, 140.2, 138.5, 137.0, 135.2, 130.8, 129.3, 128.6, 128.2, 126.41, 126.36, 125.9, 117.2, 115.5, 115.4, 59.0; HRMS (ESI) m/z calcd for $C_{16}H_{14}FN_2O^+$ $(M+H)^+$ 269.1085, found 269.1086.



4fa

(2-(4-(4-chlorophenyl)-1H-imidazol-1-yl)phenyl)methanol (4fa):

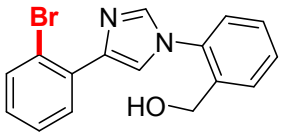
Yield 75%; 213.6 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.00 (s, 1H), 7.96 (s, 1H), 7.87 (d, J = 7.8 Hz, 2H), 7.67 (d, J = 7.8 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.48–7.38 (m, 4H), 5.42 (s, 1H), 4.43 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 139.8, 138.6, 136.9, 135.0, 133.1, 131.2, 130.9, 129.1, 128.6, 128.1, 126.1, 125.9, 117.8, 58.8; HRMS (ESI) m/z calcd for $C_{16}H_{14}ClN_2O^+$ $(M+H)^+$ 285.07892, found 285.07901.



4ga

(2-(4-(4-bromophenyl)-1H-imidazol-1-yl)phenyl)methanol (4ga):

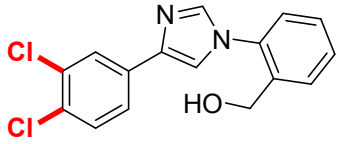
Yield 67%; 220.6 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.00 (d, J = 14.4 Hz, 2H), 7.84 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 7.8 Hz, 1H), 7.58 (d, J = 7.8 Hz, 2H), 7.51 (t, J = 7.2 Hz, 1H), 7.47–7.39 (m, 2H), 5.51 (s, 1H), 4.47 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 139.9, 138.6, 136.9, 135.1, 133.4, 131.5, 129.3, 128.6, 128.1, 126.5, 125.8, 119.5, 117.9, 58.9;HRMS (ESI) m/z calcd for $C_{16}H_{14}BrN_2O^+$ $(M+H)^+$ 329.02840, found 329.02887.



4ha

(2-(4-(2-bromophenyl)-1H-imidazol-1-yl)phenyl)methanole (4ha):

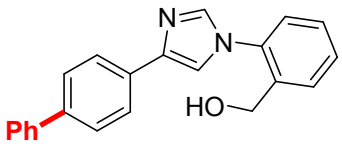
Yield 66%; 217.2 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ8.16–8.11 (m, 2H), 8.06 (s, 1H), 7.73-7.66 (m, 2H), 7.54–7.49 (m, 1H), 7.48–7.42 (m, 3H), 7.19 (t, J = 7.8 Hz, 1H), 5.52 (s, 1H), 4.48 (s, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 138.5, 137.7, 136.8, 135.1, 134.2, 133.6, 130.2, 129.5, 128.6, 128.3, 128.2, 127.7, 125.8, 120.5, 120.0, 59.0; HRMS (ESI) m/z calcd for $C_{16}H_{14}BrN_2O^+$ $(M+H)^+$ 329.02840, found 329.02863.



4ia

(2-(4-(3,4-dichlorophenyl)-1H-imidazol-1-yl)phenyl)methanol (4ia):

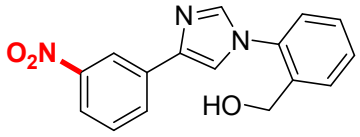
Yield 72%; 225.8 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 2/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.09 (d, J = 9.6 Hz, 2H), 8.00 (s, 1H), 7.83 (d, J= 8.4 Hz, 1H), 7.69 (d, J = 7.2 Hz, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.50 (t, J = 7.2Hz, 1H), 7.46–7.39 (m, 2H), 5.49 (s, 1H), 4.47 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 138.8, 138.7, 136.9, 135.0, 134.9, 131.5, 130.7, 129.2, 128.7, 128.6, 128.1, 126.0, 125.8, 124.4, 118.7, 58.9; HRMS (ESI) m/z calcd for $C_{16}H_{13}Cl_2N_2O^+$ $(M+H)^+$ 319.03994, found 319.04022.



4ja

(2-(4-([1,1'-biphenyl]-4-yl)-1H-imidazol-1-yl)phenyl)methanol (4ja):

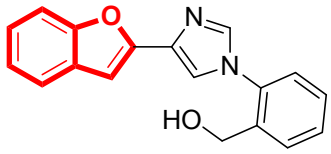
Yield 67%; 218.6 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.19-8.17 (m, 4H), 7.90–7.78 (m, 5H), 7.66-7.61 (m, 1H), 7.57 (d, J = 9.0 Hz, 4H), 7.47 (d, J = 6.6 Hz, 1H), 5.68 (s, 1H), 4.64 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 140.7, 139.9, 138.6, 138.2, 136.9, 135.2, 133.4, 129.3, 129.0, 128.5, 128.1, 127.3, 126.9, 126.4, 125.8, 125.1, 117.6, 59.0; HRMS (ESI) m/z calcd for $C_{22}H_{19}N_2O^+$ $(M+H)^+$ 327.1492, found 327.1496.



4ka

(2-(4-(3-nitrophenyl)-1H-imidazol-1-yl)phenyl)methanol (4ka):

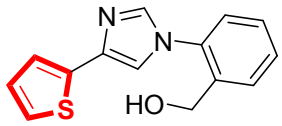
Yield 56%; 165.4 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 2/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.66 (s, 1H), 8.25 (d, J = 7.8 Hz, 1H), 8.20 (s, 1H), 8.05 (d, J = 10.2 Hz, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.64 (t, J = 7.8 Hz, 1H), 7.51 (t, J = 6.6 Hz, 1H), 7.48–7.41 (m, 2H), 5.50 (t, J = 4.8 Hz, 1H), 4.48 (d, J =4.2 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 148.4, 139.0, 138.9, 136.9, 136.0, 135.0, 130.6, 130.1, 129.3, 128.7, 128.2, 125.9, 121.1, 119.1, 118.6, 59.0; HRMS (ESI) m/z calcd for $C_{16}H_{14}N_3O_3^+$ $(M+H)^+$ 296.10297, found 296.10294.



4la

(2-(4-(benzofuran-2-yl)-1H-imidazol-1-yl)phenyl)methanol (4la):

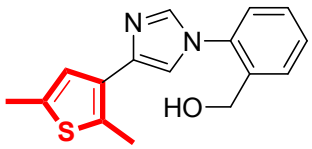
Yield 69%; 200.4 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.52 (d, J =4.8 Hz, 2H), 7.44 (t, J = 7.8 Hz, 1H), 7.39 (d, J = 7.8 Hz, 1H), 7.35 (t, J = 7.8 Hz, 1H), 7.25–7.16 (m, 3H), 6.97 (s, 1H), 4.53 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.3, 150.9, 138.7, 136.2, 135.2, 133.8, 130.3, 129.3, 129.0, 128.7, 126.1, 123.9, 122.8, 120.8, 118.3, 110.8, 101.0, 60.0; HRMS (ESI) m/z calcd for $C_{18}H_{15}N_2O_2^+$ $(M+H)^+$ 291.11280, found 291.11288.



4ma

(2-(4-(thiophen-2-yl)-1H-imidazol-1-yl)phenyl)methanol (4ma):

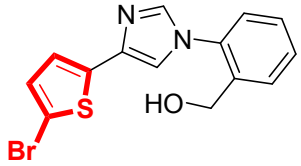
Yield 70%; 179.4 mg; brown solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.92 (s, 1H), 7.83 (s, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.47–7.38 (m, 3H), 7.37-7.33 (m, 1H), 7.11-7.04 (m, 1H), 5.45 (s, 1H), 4.44 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 138.2, 137.9, 136.9, 136.4, 134.9, 129.2, 128.6, 128.1, 127.7, 125.9, 123.7, 121.8, 116.4, 58.9; HRMS (ESI) m/z calcd for $C_{14}H_{13}N_2OS^+$ $(M+H)^+$ 257.07431, found 257.07437.



4na

(2-(4-(2,5-dimethylthiophen-3-yl)-1H-imidazol-1-yl)phenyl)methanol (4na):

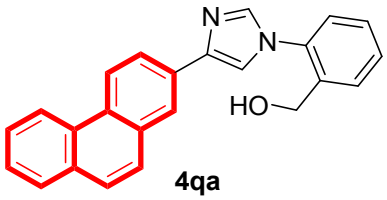
Yield 63%; 179.2 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.92 (s, 1H), 7.67 (d, J = 7.2 Hz, 1H), 7.62 (s, 1H), 7.50 (t, J = 6.6 Hz, 1H), 7.47–7.38 (m, 2H), 7.07 (s, 1H), 5.44 (s, 1H), 4.43 (s, 2H), 2.56 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 138.0, 137.5, 136.9, 135.2, 134.4, 130.8, 129.8, 129.2, 128.4, 128.1, 126.1, 125.8, 117.7, 58.9, 14.9, 14.6; HRMS (ESI) m/z calcd for $C_{16}H_{17}N_2OS^+$ $(M+H)^+$ 285.10561, found 285.10556.



4oa

(2-(4-(5-bromothiophen-2-yl)-1H-imidazol-1-yl)phenyl)methanol (4oa):

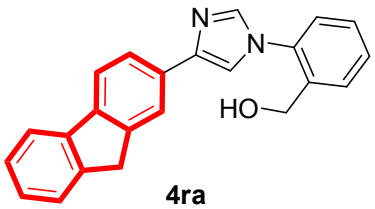
Yield 62%; 207.8 mg; brown oil; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56-7.49 (m, 2H), 7.35 (t, J = 7.8 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 7.17 (s, 1H), 7.13 (d, J = 7.2 Hz, 1H), 6.86 (d, J = 3.6 Hz, 1H), 6.81 (d, J = 3.0 Hz, 1H), 4.56 (s, 1H), 4.38 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.4, 138.0, 136.04, 136.01, 135.2, 130.3, 129.2, 128.7, 126.0, 122.3, 116.2, 110.2, 103.8, 60.0; HRMS (ESI) m/z calcd for $C_{14}H_{12}BrN_2OS^+$ $(M+H)^+$ 334.98482, found 334.98492.



4qa

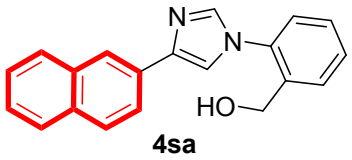
Yield 55%; 175.1 mg; white solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.80 (d, J = 8.4 Hz, 1H), 8.76 (d, J = 7.8 Hz, 1H), 8.58 (s, 1H), 8.24 (d, J = 8.4 Hz, 1H), 8.16 (s, 1H), 8.13 (s, 1H), 7.95 (d, J = 7.8Hz, 1H), 7.92 (d, J =8.4 Hz, 1H), 7.83 (d, J = 9.0 Hz, 1H), 7.78 (d, J = 7.8 Hz, 1H), 7.65 (t, J = 7.2 Hz, 1H), 7.60 (t, J = 7.2 Hz, 1H), 7.54 (t, J = 6.6 Hz, 1H), 7.51–7.44 (m, 2H), 5.63 (s, 1H), 4.59 (s, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 140.9, 138.8, 137.0, 135.2, 132.7, 132.1, 131.5, 129.9, 129.4, 128.59, 128.57, 128.5, 128.2, 127.2, 127.1, 126.9, 126.5,

125.9, 124.0, 123.5, 123.4, 122.8, 118.1, 59.1. HRMS (ESI) m/z calcd for $C_{24}H_{19}N_2O^+$ $(M+H)^+$ 351.1492, found 351.1496.



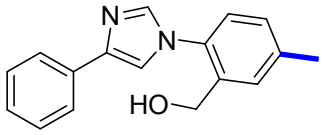
4ra

Yield 61%; 206.3 mg; white solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.11 (s, 1H), 8.00 (s, 2H), 7.96–7.82 (m, 3H), 7.72 (d, J = 6.0 Hz, 1H), 7.57 (t, J = 6.6 Hz, 1H), 7.52 (t, J = 5.4 Hz, 1H), 7.45 (s, 2H), 7.37 (t, J = 7.2 Hz, 1H), 7.30 (t, J = 6.0 Hz, 1H), 5.50 (s, 1H), 4.50 (s, 2H), 3.96 (s, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 143.8, 143.4, 141.6, 141.4, 139.9, 138.6, 137.1, 135.5, 133.2, 129.5, 128.7, 128.4, 127.0, 126.8, 126.1, 125.4, 123.7, 121.4, 120.4, 120.1, 117.6, 59.2, 36.7. HRMS (ESI) m/z calcd for $C_{23}H_{19}N_2O^+$ $(M+H)^+$ 339. 339.1492, found 339.1493.



4sa

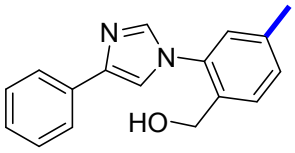
Yield 57%; 171.1 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.81-7.70 (m, 4H), 7.67 (s, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.46-7.35 (m, 3H), 7.31 (t, J = 7.2 Hz, 1H), 7.22 (t, J = 7.8 Hz, 1H), 7.10 (d, J = 7.8 Hz, 1H), 6.17 (s, 1H), 4.46 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.5, 138.2, 136.1, 135.2, 133.5, 132.5, 130.5, 130.0, 129.0, 128.4, 128.2, 128.0, 127.6, 126.1, 125.8, 125.5, 123.5, 123.1, 117.3, 59.7. HRMS (ESI) m/z calcd for $C_{20}H_{17}N_2O^+$ $(M+H)^+$ 301.1335, found 301.1339.



4ab

(5-methyl-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ab):

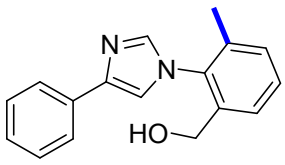
Yield 75%; 198.2mg; yellow oil; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 7.8 Hz, 2H), 7.65 (s, 1H), 7.44 (s, 1H), 7.36-7.30 (m, 3H), 7.22 (t, J = 7.2 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 7.12 (d, J = 7.8 Hz, 1H), 4.45 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.6, 139.2, 138.2, 135.9, 133.3, 133.0, 130.7, 129.1, 128.6, 127.0, 125.9, 124.8, 116.9, 60.0, 21.1. HRMS (ESI) m/z calcd for $C_{17}H_{17}N_2O^+$ $(M+H)^+$ 265.13354, found 265.13385.



4ac

(4-methyl-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ac):

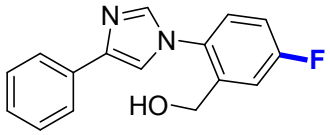
Yield 72%; 190.4 mg; yellow oil; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, J = 7.8 Hz, 2H), 7.64 (s, 1H), 7.48 (d, J =7.8 Hz, 1H), 7.37 (s, 1H), 7.31 (t, J = 7.2 Hz, 2H), 7.24-7.17 (m, 2H), 7.03 (s, 1H), 4.77 (s, 1H), 4.43 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.6, 138.7, 138.0, 135.4, 133.3, 133.1, 130.1, 129.6, 128.5, 126.9, 126.4, 124.8, 116.7, 103.7, 59.7, 20.8; HRMS (ESI) m/z calcd for $C_{17}H_{17}N_2O^+$ $(M+H)^+$ 265.1335, found 265.1338.



4ad

(3-methyl-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ad):

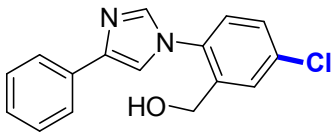
Yield 62%; 163.8 mg; yellow oil; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, J = 7.2 Hz, 2H), 7.48 (d, J = 7.8 Hz, 1H), 7.41 (s, 1H), 7.37 (t, J = 7.8 Hz, 1H), 7.31 (t, J = 7.8 Hz, 2H), 7.26–7.20 (m, 2H), 7.17 (s, 1H), 4.39–4.28 (m, 2H), 2.03 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.5, 138.6, 137.7, 135.1, 133.9, 133.1, 129.5, 129.2, 128.4, 126.7, 126.3, 124.6, 116.2, 59.5, 17.0. HRMS (ESI) m/z calcd for $C_{17}H_{17}N_2O^+$ $(M+H)^+$ 265.1335, found 265.1340.



4ae

(5-fluoro-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ae):

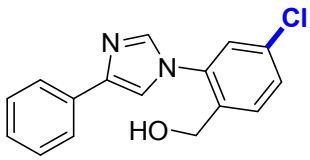
Yield 69%; 185.2 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, J = 7.8 Hz, 2H), 7.52 (s, 1H), 7.37 (d, J =9.0 Hz, 1H), 7.31 (t, J = 7.2 Hz, 2H), 7.25 (s, 1H), 7.24–7.20 (m, 1H), 7.20-7.15 (m, 1H), 7.05–6.99 (m, 1H), 4.42 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.5, 161.8, 142.0, 139.7, 139.6, 138.0, 133.0, 131.0, 128.6, 128.1, 128.0, 127.2, 124.8, 116.8, 116.3, 116.2, 115.2, 115.0, 59.4; HRMS (ESI) m/z calcd for $C_{16}H_{14}FN_2O^+$ $(M+H)^+$ 269.1085, found 269.1088.



4af

(5-chloro-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4af):

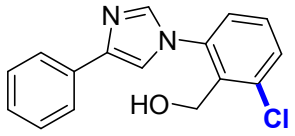
Yield 65%; 185.0 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, J = 7.8 Hz, 2H), 7.51 (s, 1H), 7.48 (s, 1H), 7.21-7.14 (m, 4H), 7.10 (t, J = 7.2 Hz, 1H), 6.99 (d, J = 8.4 Hz, 1H), 5.85 (s, 1H), 4.30 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.7, 138.4, 137.8, 134.8, 133.5, 132.7, 129.7, 128.6, 128.3, 127.2, 124.8, 116.6, 103.7, 59.2; HRMS (ESI) m/z calcd for $C_{16}H_{14}ClN_2O^+$ $(M+H)^+$ 285.07892, found 285.07907.



4ag

(4-chloro-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ag):

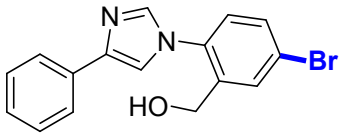
Yield 60%; 170.8 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.01 (d, J = 6.0 Hz, 2H), 7.86 (d, J = 7.2 Hz, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.58 (d, J = 9.6 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.24 (t, J= 7.2 Hz, 1H), 5.56 (s, 1H), 4.44 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 141.1, 138.4, 136.1, 135.9, 133.9, 132.0, 130.7, 128.6, 128.4, 126.7, 125.6, 124.5, 117.2, 58.5; HRMS (ESI) m/z calcd for $C_{16}H_{14}ClN_2O^+$ $(M+H)^+$ 285.07892, found 285.07901.



4ah

(2-chloro-6-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ah):

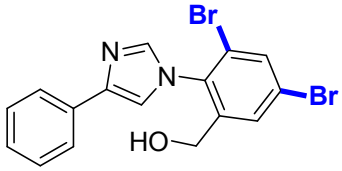
Yield 62%; 176.6 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 3/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.76 (d, J = 6.6 Hz, 2H), 7.48 (d, J =10.2 Hz, 2H), 7.40-7.28 (m, 3H), 7.27–7.18 (m, 2H), 4.58 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 142.1, 138.3, 138.2, 136.6, 133.6, 133.1, 130.1, 129.6, 128.6, 127.1, 124.94, 124.85, 116.9, 57.5; HRMS (ESI) m/z calcd for $C_{16}H_{14}ClN_2O^+$ $(M+H)^+$ 285.0789, found 285.0793.



4ai

(5-bromo-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ai):

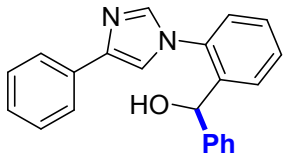
Yield 63%; 207.4 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 2/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.62 (d, J = 7.2 Hz, 2H), 7.52 (s, 1H), 7.42-7.36 (m, 1H), 7.30-7.22 (m, 3H), 7.19 (t, J = 7.2 Hz, 1H), 7.00 (d, J = 8.4 Hz, 1H), 5.35 (s, 1H), 4.38 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.8, 138.5, 137.7, 133.9, 132.7, 132.6, 131.3, 128.5, 127.4, 127.2, 124.7, 122.8, 116.5, 59.1; HRMS (ESI) m/z calcd for $C_{16}H_{14}BrN_2O^+$ $(M+H)^+$ 329.0284, found 329.0286.



4aj

(3,5-dibromo-2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4aj):

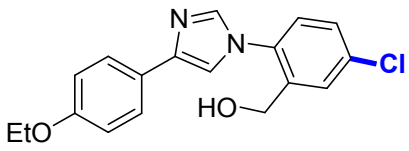
Yield 57%; 232.6 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 2/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.70 (s, 1H), 7.62 (d, J = 7.8 Hz, 2H), 7.33 (s, 1H), 7.28 (t, J = 7.8 Hz, 2H), 7.20 (t, J = 7.2 Hz, 1H), 7.09 (s, 1H), 5.42 (s, 1H), 4.34-4.24 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 142.6, 141.9, 137.7, 134.2, 132.8, 132.5, 131.0, 128.6, 127.3, 124.8, 124.1, 122.8, 116.0, 59.4; HRMS (ESI) m/z calcd for $C_{16}H_{13}Br_2N_2O^+$ $(M+H)^+$ 408.9369, found 408.9366.



4ak

(R)-phenyl(2-(4-phenyl-1H-imidazol-1-yl)phenyl)methanol (4ak):

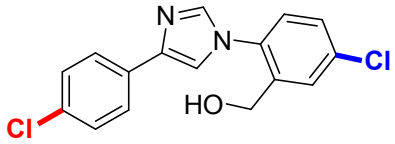
Yield 68%; 222.0 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 2/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.93 (d, J = 7.8 Hz, 2H), 7.87 (s, 1H), 7.82 (s, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.54 (t, J = 7.2 Hz, 1H), 7.47-7.41 (m, 3H), 7.39 (d, J = 7.8 Hz, 1H), 7.31-7.24 (m, 3H), 7.24-7.17 (m, 3H), 6.30 (s, 1H), 5.80 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 144.2, 141.1, 141.0, 138.5, 135.0, 134.2, 129.2, 128.6, 128.5, 128.2, 128.1, 127.0, 126.9, 126.7, 126.3, 124.6, 117.6, 69.2; HRMS (ESI) m/z calcd for $C_{22}H_{19}N_2O^+$ $(M+H)^+$ 327.1492, found 327.1494.



4pf

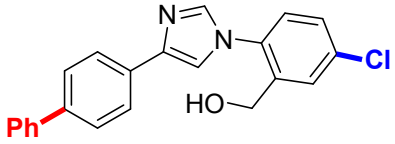
(5-chloro-2-(4-(4-ethoxyphenyl)-1H-imidazol-1-yl)phenyl)methanol (4pf):

Yield 59%; 194.0 mg; yellow oil; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 1/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.91 (s, 1H), 7.81 (s, 1H), 7.75 (d, J = 8.4 Hz, 2H), 7.69 (s, 1H), 7.50 (d, J = 6.6 Hz, 1H), 7.44 (d, J = 8.4 Hz, 1H), 6.94 (d, J = 9.0Hz, 2H), 5.61 (s, 1H), 4.44 (s, 2H), 4.08-3.94 (m, 2H), 1.33 (t, J = 7.2Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 157.6, 141.2, 139.4, 138.1, 133.8, 133.0, 128.3, 127.8, 127.7, 126.6, 125.8, 115.9, 114.5, 63.0, 58.5, 14.8; HRMS (ESI) m/z calcd for $C_{18}H_{18}ClN_2O_2^+$ $(M+H)^+$ 329.1051, found 329.1054.



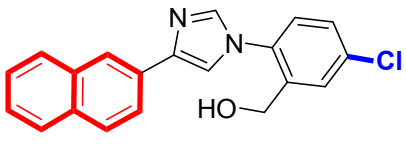
4ff

Yield 52%; 165.4 mg; white solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1);^{1}H NMR (600 MHz, DMSO-d_6) δ 7.98 (d, J = 4.8 Hz, 2H), 7.87 (d, J = 7.8 Hz, 2H), 7.71 (s, 1H), 7.49 (d, J = 7.8 Hz, 1H), 7.44 (t, J = 9.6 Hz, 3H), 5.63 (s, 1H), 4.46 (d, J =4.2 Hz, 2H).^{13}C NMR (150 MHz, DMSO-d_6) δ 140.3, 139.6, 138.8, 133.9, 133.5, 133.1, 131.3, 128.8, 128.7, 128.1, 127.9, 126.4, 117.9, 58.7. HRMS (ESI) m/z calcd for $C_{16}H_{13}Cl_2N_2O^+$ $(M+H)^+$ 319.0399, found 319.0405.



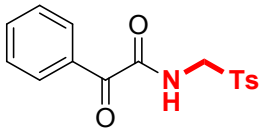
4jf

Yield 60%; 216.1 mg; white solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1);^{1}H NMR (600 MHz, DMSO-d_6) δ 8.03 (d, J = 9.6 Hz, 3H), 7.97 (s, 1H), 7.80 (s, 1H), 7.72 (t, J = 9.6 Hz, 4H), 7.52-7.41 (m, 4H), 7.38-7.32 (m, 1H), 5.81 (s, 1H), 4.57 (s, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 141.3, 140.1, 139.6, 138.8, 138.6, 134.0, 133.5, 133.4, 129.2, 128.9, 128.1, 127.9, 127.5, 127.1, 126.7, 125.4, 117.6, 58.9. HRMS (ESI) m/z calcd for $C_{22}H_{18}ClN_2O^+$ $(M+H)^+$ 361.1102, found 361.1108.



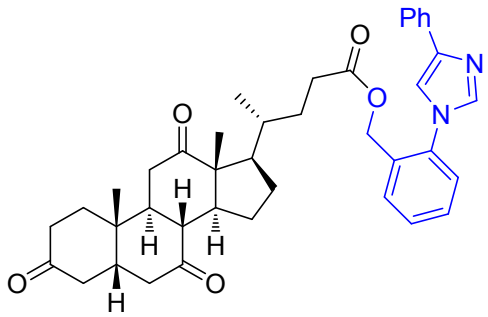
4sf 55%

Yield 55%; 183.7 mg; white solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.48 (s, 1H), 8.08 (d, J = 8.4 Hz, 3H), 7.95 (t, J =9.6 Hz, 2H), 7.88 (d, J = 7.2 Hz, 1H), 7.78 (s, 1H), 7.56-7.40 (m, 4H), 5.76 (s, 1H), 4.57 (s, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 141.3, 139.4, 138.7, 133.8, 133.5, 133.3, 132.2, 131.6, 128.6, 128.2, 127.9, 127.7, 126.4, 125.5, 123.7, 122.4, 121.1, 117.8, 113.0, 58.7. HRMS (ESI) m/z calcd for $C_{20}H_{16}ClN_2O^+$ $(M+H)^+$ 335.0946, found 335.0953.



9a

Yield 45%; 142.8 mg; yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 5/1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.06 (s, 1H), 7.87 (d, J = 7.2 Hz, 2H), 7.79 (d, J = 6.6 Hz, 2H), 7.701 (t, J = 6.6 Hz, 1H), 7.54 (d, J = 6.6 Hz, 2H), 7.47 (d, J = 7.2 Hz, 2H), 4.99 (d, J = 6.0 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.2, 165.1, 145.0, 134.9, 134.6, 132.4, 129.9, 129.8, 128.9, 128.8, 59.8, 21.2; HRMS (ESI) m/z calcd for $C_{16}H_{15}NNaO_4S^+$ $(M+Na)^+$ 340.0614, found 340.0610.

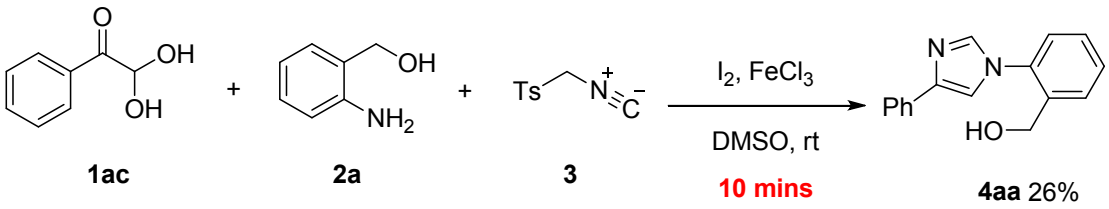


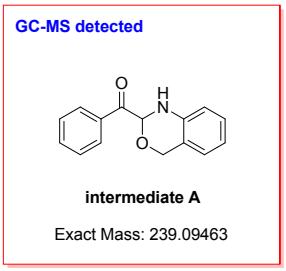
10a

Yield 91%; 288.8 mg (0.5mmol scale); yellow solid; (Flash column chromatography eluent, petroleum ether/ethyl acetate = 1/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, J = 7.8 Hz, 2H), 7.73 (s, 1H), 7.60–7.55 (m, 1H), 7.47 (s, 3H), 7.41–7.32 (m, 3H), 7.25 (t, J = 7.2 Hz, 1H), 5.07–4.96 (m, 2H), 2.92–2.83 (m, 2H), 2.80 (t, J = 12.6 Hz, 1H), 2.43–2.38 (m, 1H), 2.36–2.22 (m, 5H), 2.19–2.06 (m, 4H), 2.00–1.88 (m, 4H), 1.83–1.74 (m, 2H), 1.60–1.53 (m, 1H), 1.35 (s, 4H), 1.28–1.17 (m, 3H), 0.99 (s, 3H), 0.80 (d, J = 6.0 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 211.6, 208.8, 208.4, 172.9, 141.9, 137.7, 136.2, 133.3, 131.2, 130.7, 129.3, 128.8, 128.3, 126.7, 126.4, 124.5, 116.3, 61.4, 56.4, 51.3, 48.5, 46.3, 45.1, 45.0, 44.5, 42.3, 38.2, 36.0, 35.5, 35.0, 34.7, 31.0, 30.0, 27.2, 24.7, 21.4, 18.2, 11.4; HRMS (ESI) m/z calcd for $C_{40}H_{47}N_2O_5^+$ $(M+H)^+$ 635.3480, found 635.3489.

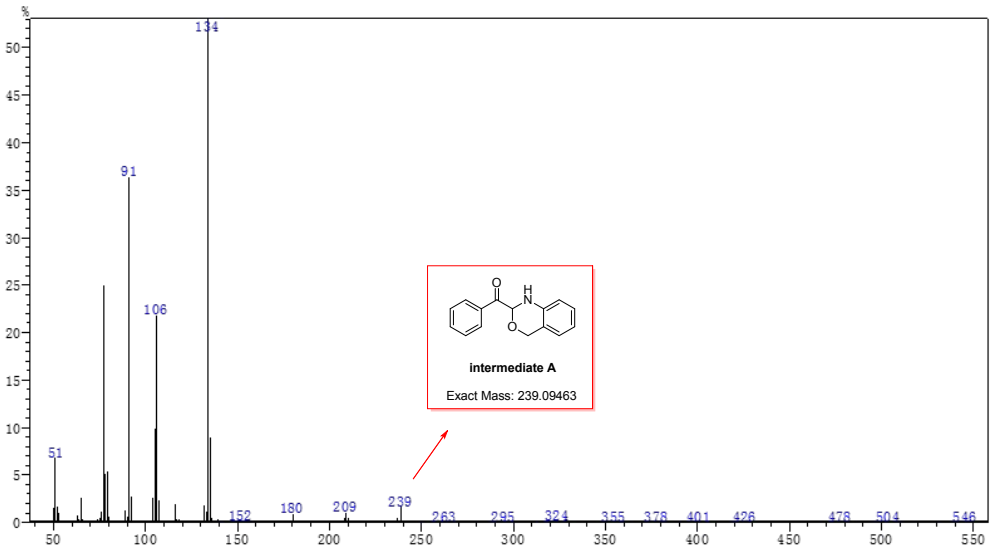
4. Evidence in support of the mechanism.

(1) We used GC-MS to monitor the reaction, and the possible intermediate A was observed (see below).

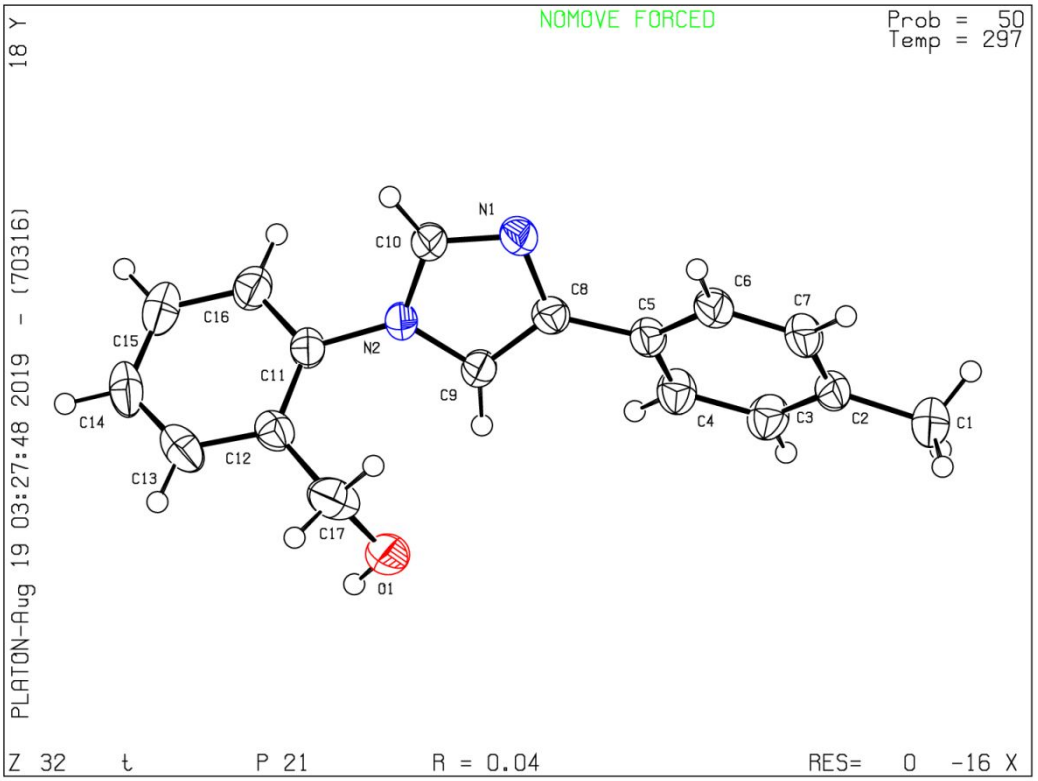


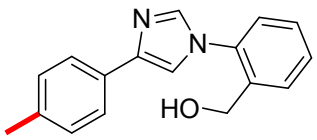


The GC-MS Spectra is listed below:



5. Crystallographic data and molecular structure of compounds 4ba/4ea/9a





4ba

Figure S1. X-ray crystal structure of **4ba.**

Crystal Data for Compound **4ba**: CCDC 1947784 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Bond precision: C-C = 0.0049 A Wavelength=0.71073

Cell: a=8.044(3) b=7.672(3) c=11.656(4)
alpha=90 beta=104.363(5) gamma=90
Temperature: 297 K

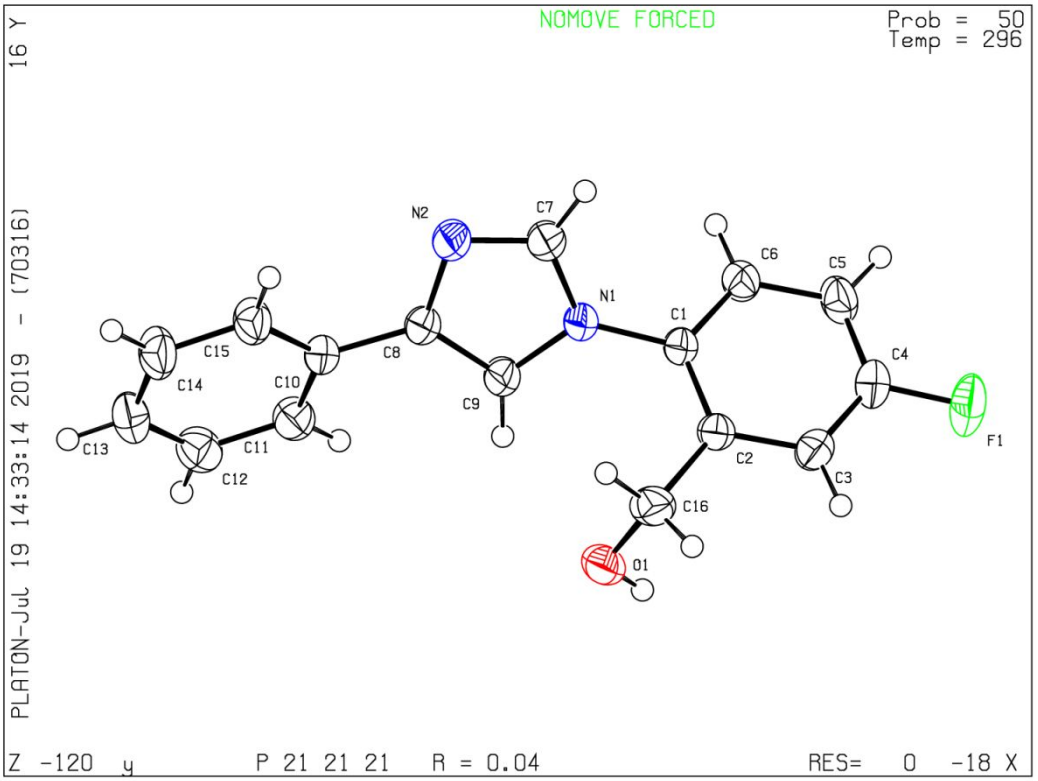
	Calculated	Reported
Volume	696.9(4)	696.8(4)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C17 H16 N2 O	?
Sum formula	C17 H16 N2 O	C17 H16 N2 O
Mr	264.32	264.32
Dx,g cm-3	1.260	1.260
Z	2	2
Mu (mm-1)	0.080	0.080
F000	280.0	280.0
F000'	280.11	
h,k,lmax	9,9,14	9,9,14
Nref	2590[1399]	2381
Tmin,Tmax	0.990,0.992	
Tmin'	0.990	

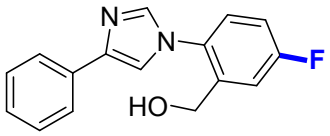
Correction method= Not given

Data completeness= 1.70/0.92 Theta(max)= 25.500

R(reflections)= 0.0385(2272) wR2(reflections)= 0.1447(2381)

S = 1.143 Npar= 184





4ae

Figure S2. X-ray crystal structure of **4ae.**

Crystal Data for Compound **4ae**: CCDC 1941804 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Bond precision: C-C = 0.0025 A Wavelength=0.71073

Cell: a=7.5557(11) b=8.1219(12) c=21.576(3)
alpha=90 beta=90 gamma=90
Temperature: 296 K

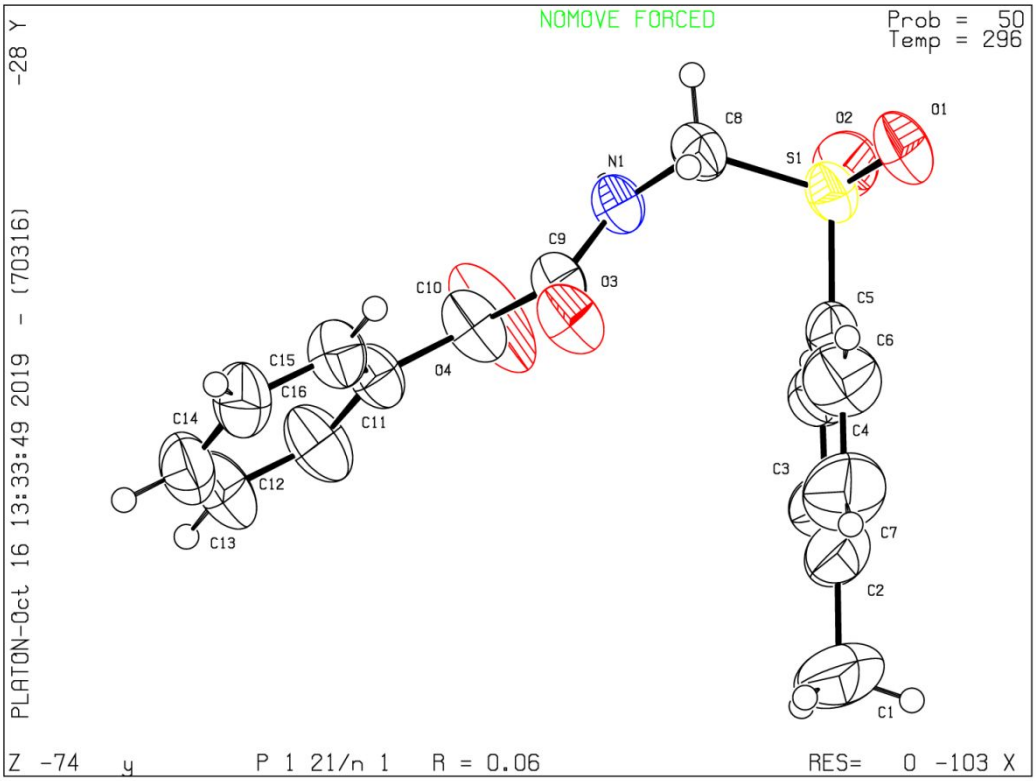
	Calculated	Reported
Volume	1324.1(3)	1324.0(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C16 H13 F N2 O	C16 H13 F N2 O
Sum formula	C16 H13 F N2 O	C16 H13 F N2 O
Mr	268.28	268.28
Dx,g cm-3	1.346	1.346
Z	4	4
Mu (mm-1)	0.095	0.095
F000	560.0	560.0
F000'	560.27	
h,k,lmax	11,12,32	11,11,31
Nref	4550[2609]	4275
Tmin,Tmax	0.989,0.991	0.643,0.746
Tmin'	0.989	

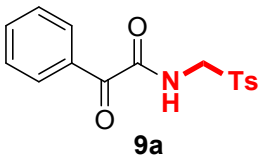
Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.64/0.94 Theta(max)= 31.904

R(reflections)= 0.0448(4028) wR2(reflections)= 0.1181(4275)

S = 1.121 Npar= 183





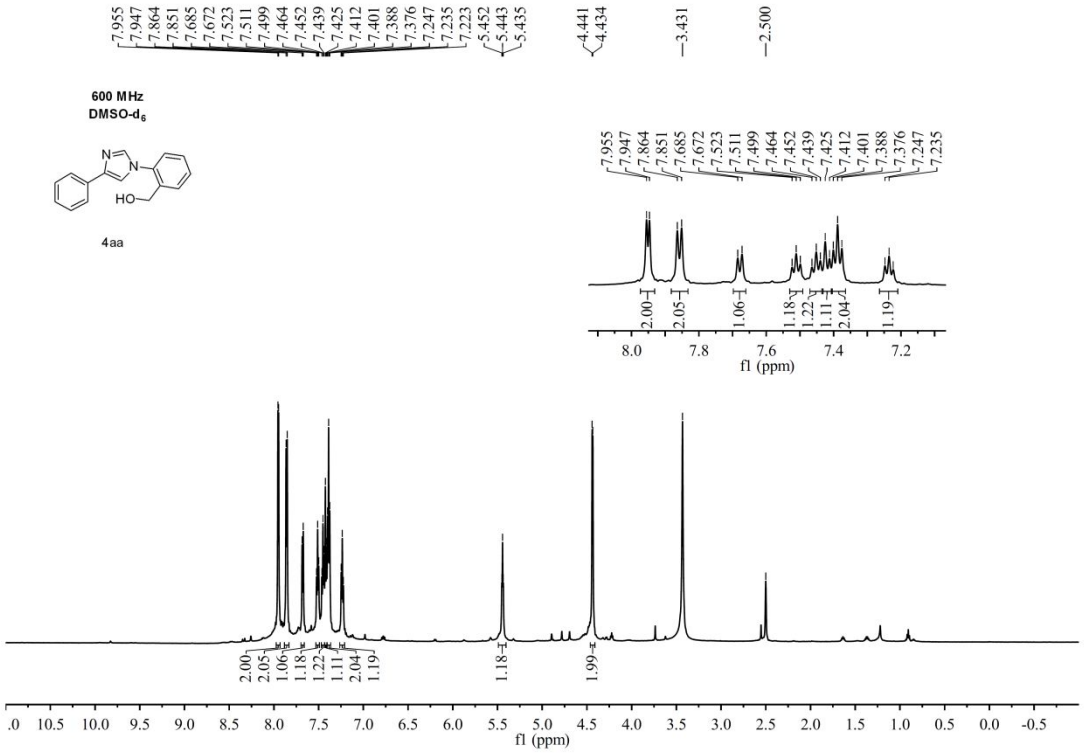
9a

Figure S3. X-ray crystal structure of **9a.**

Crystal Data for Compound **9a**: CCDC 1959657 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

```
Bond precision:  C-C = 0.0055 A          Wavelength=0.71073

Cell:            a=16.377(3)     b=6.4871(12)        c=17.795(3)
                 alpha=90        beta=94.820(3)      gamma=90
Temperature:     296 K

                 Calculated                Reported
Volume           1883.8(6)                 1883.8(6)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C16 H15 N O4 S [+ solvent] C16 H15 N O4 S
Sum formula      C16 H15 N O4 S [+ solvent] C16 H15 N O4 S
Mr               317.35                    317.35
Dx,g cm-3        1.119                     1.119
Z                4                         4
Mu (mm-1)        0.186                     0.186
F000             664.0                     664.0
F000'            664.82
h,k,lmax         19,7,21                   19,7,21
Nref             3319                      3306
Tmin,Tmax        0.978,0.982               0.678,0.746
Tmin'            0.978

Correction method= # Reported T Limits: Tmin=0.678 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 24.999

R(reflections)= 0.0584( 2539)     wR2(reflections)= 0.1882( 3306)

S = 1.065                 Npar= 200
```

6. ^{1}H and ^{13}C NMR spectra of compounds 4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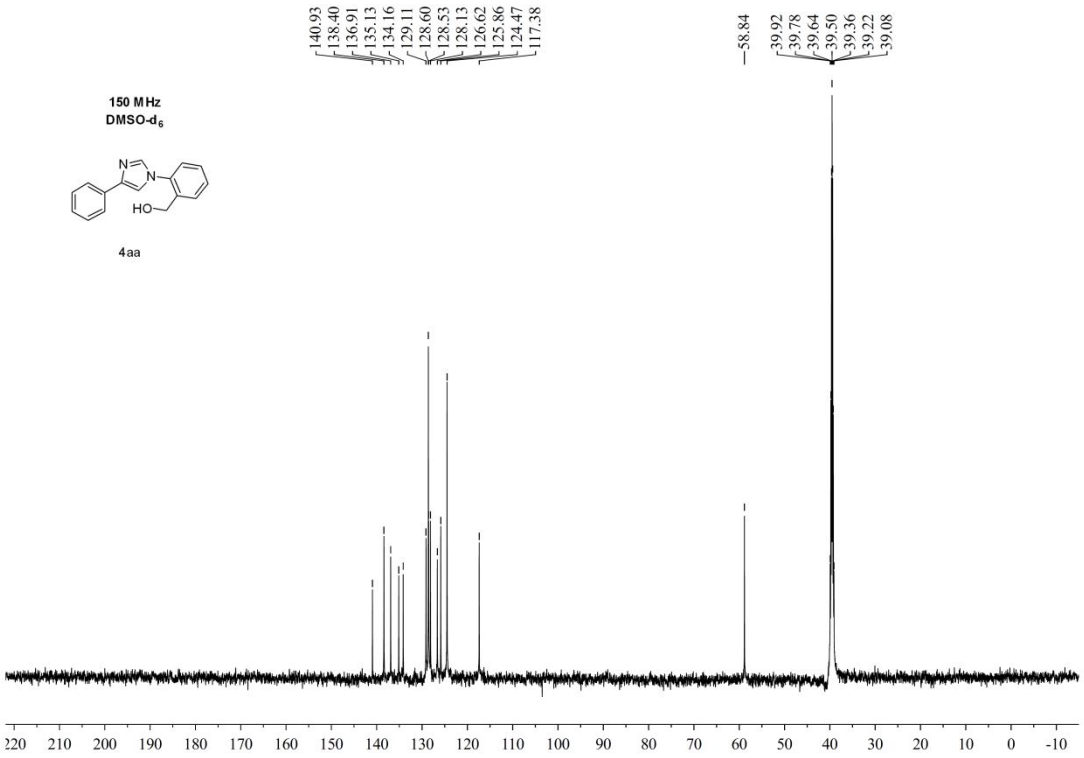
7.864
7.851
7.685
7.672
7.523
7.511
7.499
7.464
7.452
7.439
7.425
7.412
7.401
7.388
7.376
7.247
7.235
7.223
5.452
5.443
5.435
4.441
4.434
3.431
2.500
600 MHz
DMSO-d6
HO
4aa
2.00
2.05
1.06
1.18
1.22
1.11
2.04
1.19
1.18
1.99
fl (ppm)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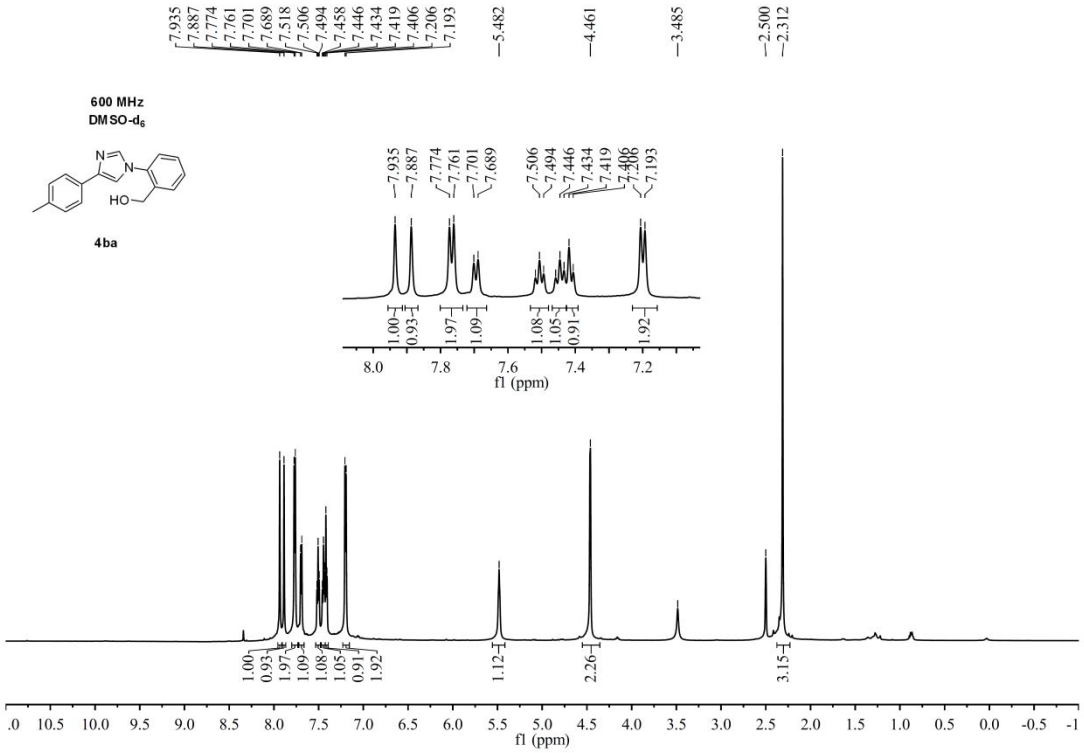
138.40
136.91
135.13
134.16
129.11
128.60
128.53
128.13
126.62
125.86
124.47
117.38
58.84
39.92
39.78
39.64
39.50
39.36
39.22
39.08
150 MHz
DMSO-d6
HO
4aa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7.887
7.774
7.761
7.701
7.689
7.518
7.506
7.494
7.458
7.446
7.434
7.419
7.406
7.206
7.193
5.482
4.461
3.485
2.500
2.312
600 MHz
DMSO-d6
HO
4ba
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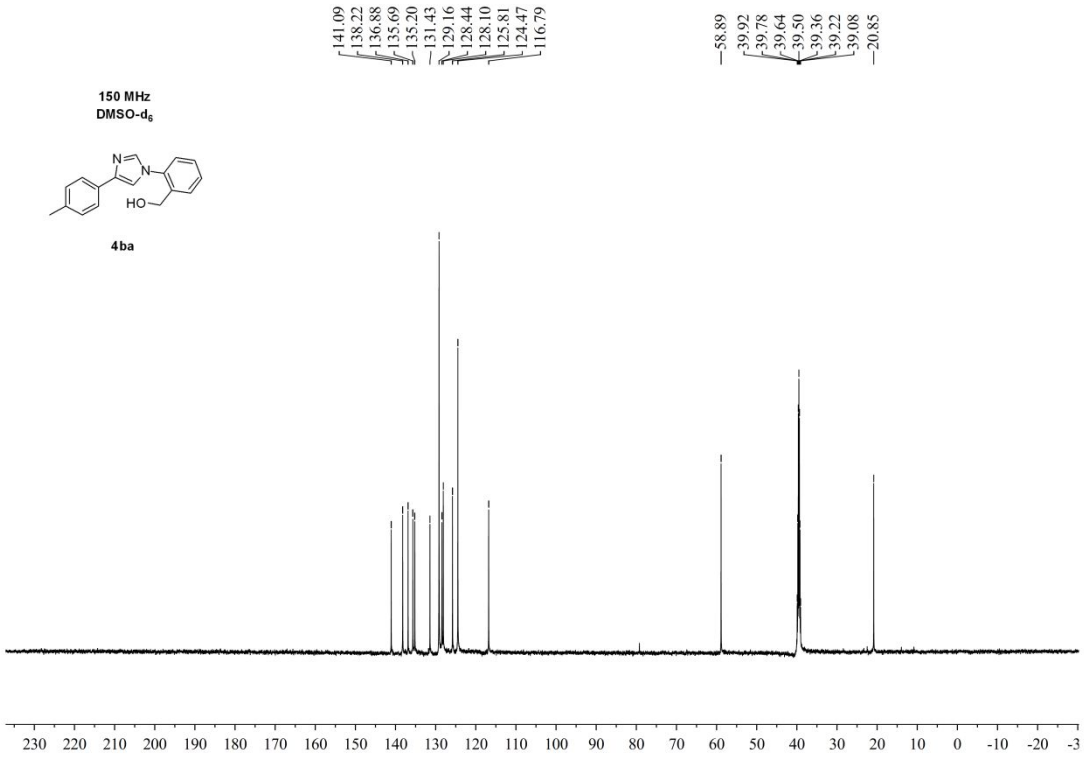
1.09
1.08
1.05
0.91
1.92
1.12
2.26
3.15
f1 (ppm)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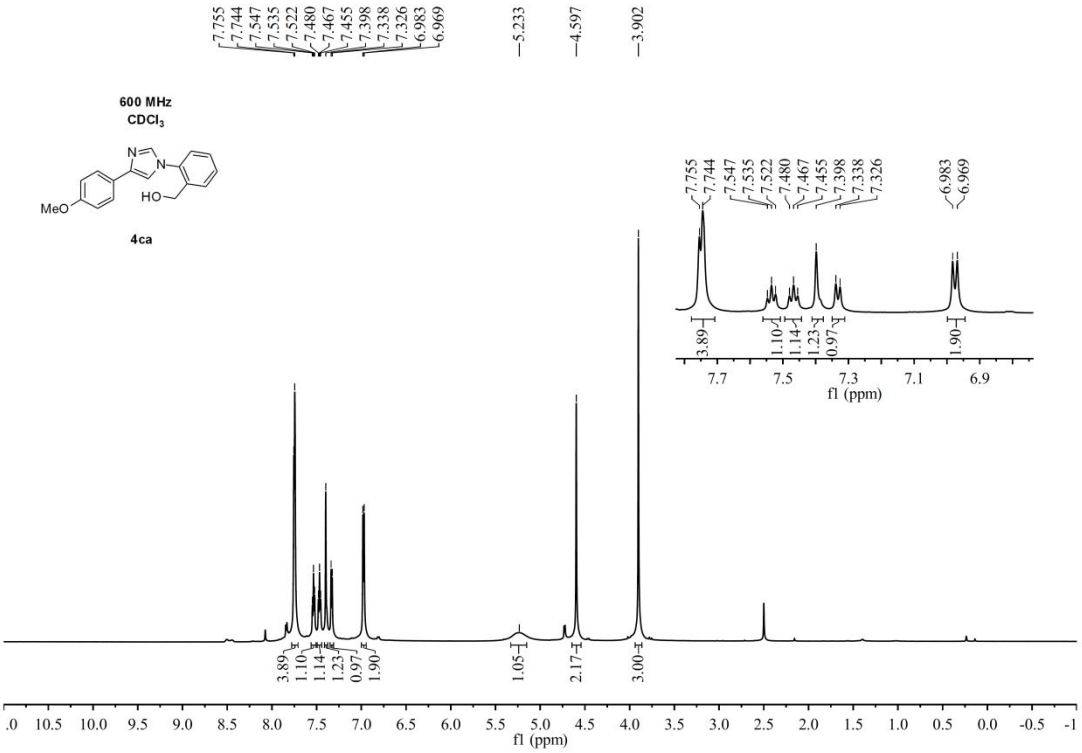
135.20
131.43
129.16
128.44
128.10
125.81
124.47
116.79
58.89
39.92
39.78
39.64
39.50
39.36
39.22
39.08
20.85
150 MHz
DMSO-d6
HO
4ba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HO
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7.535
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7.398
7.338
7.326
6.983
6.969
5.233
4.597
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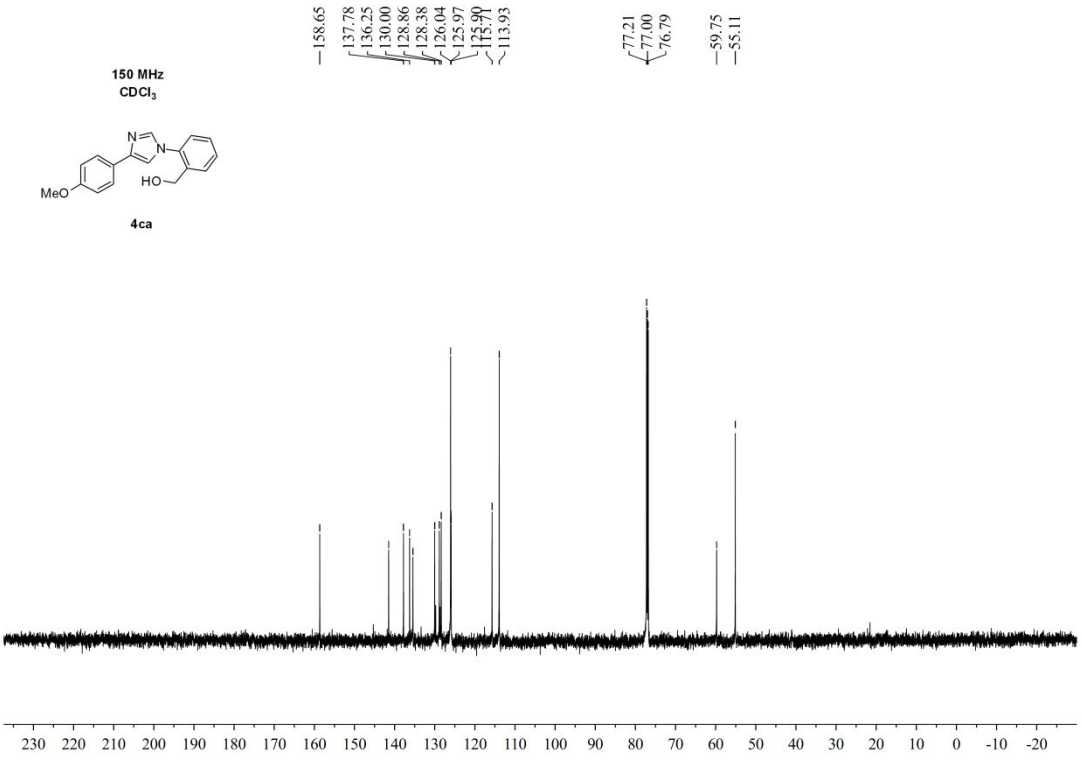
1.10
1.14
1.23
0.97
1.90
1.05
2.17
3.00
f1 (ppm)


150 MHz
CDCl3
MeO
HO
4ca
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137.78
136.25
130.00
128.86
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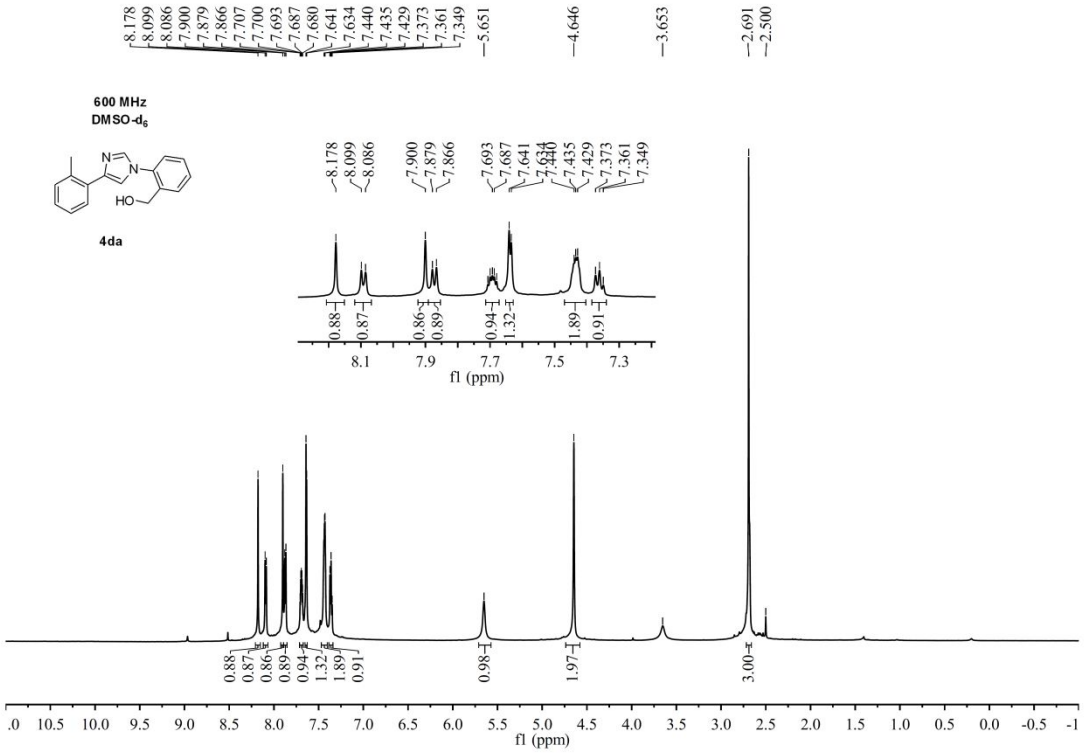
125.97
125.90
125.71
113.93
77.21
77.00
76.79
59.75
55.11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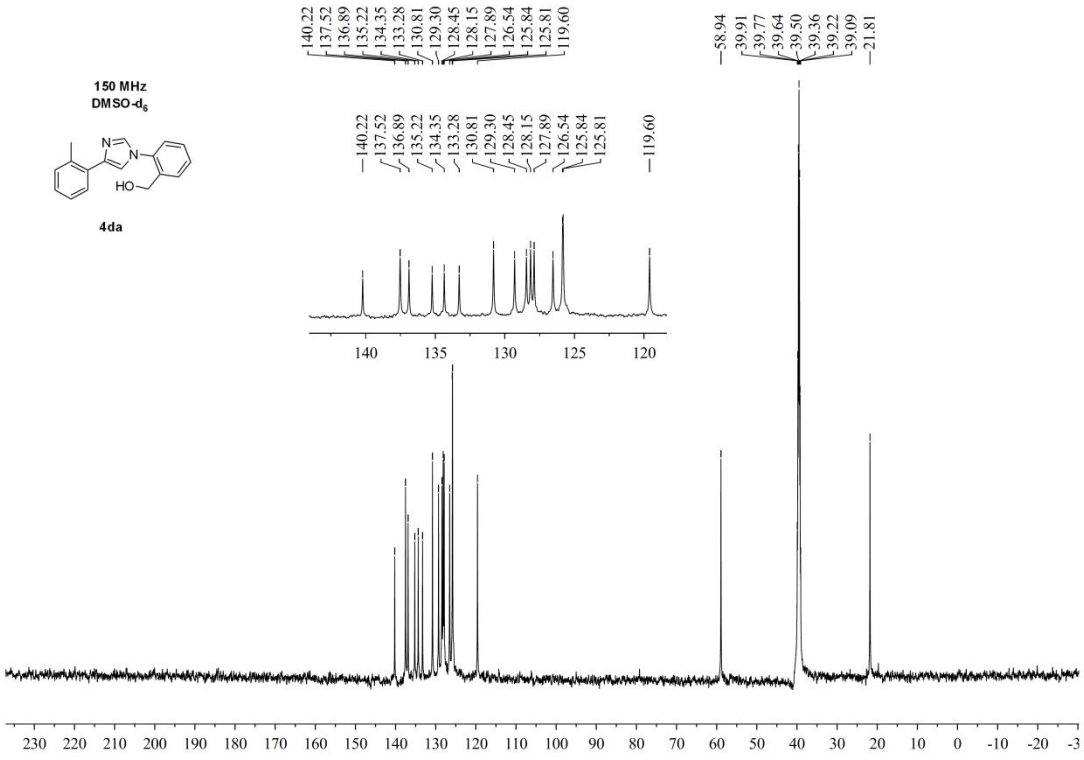
4da
f1 (ppm)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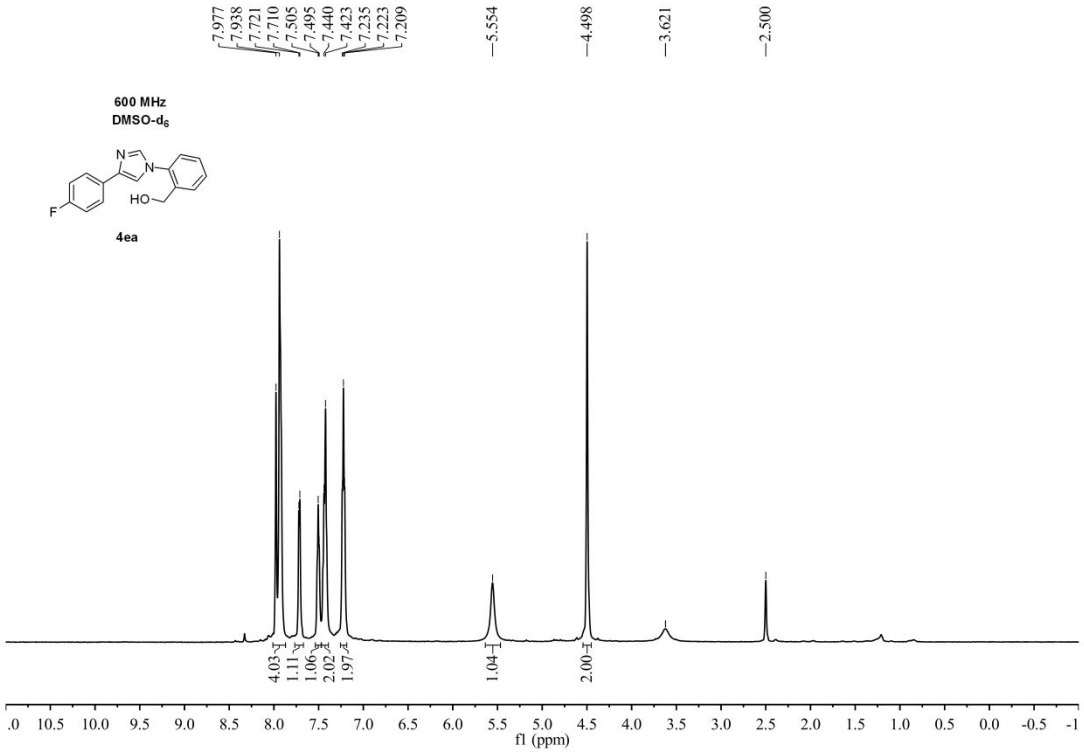
f1 (ppm)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7.495
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7.423
7.235
7.223
7.209
5.554
4.498
3.621
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DMSO-d6
4ea
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2.02
1.97
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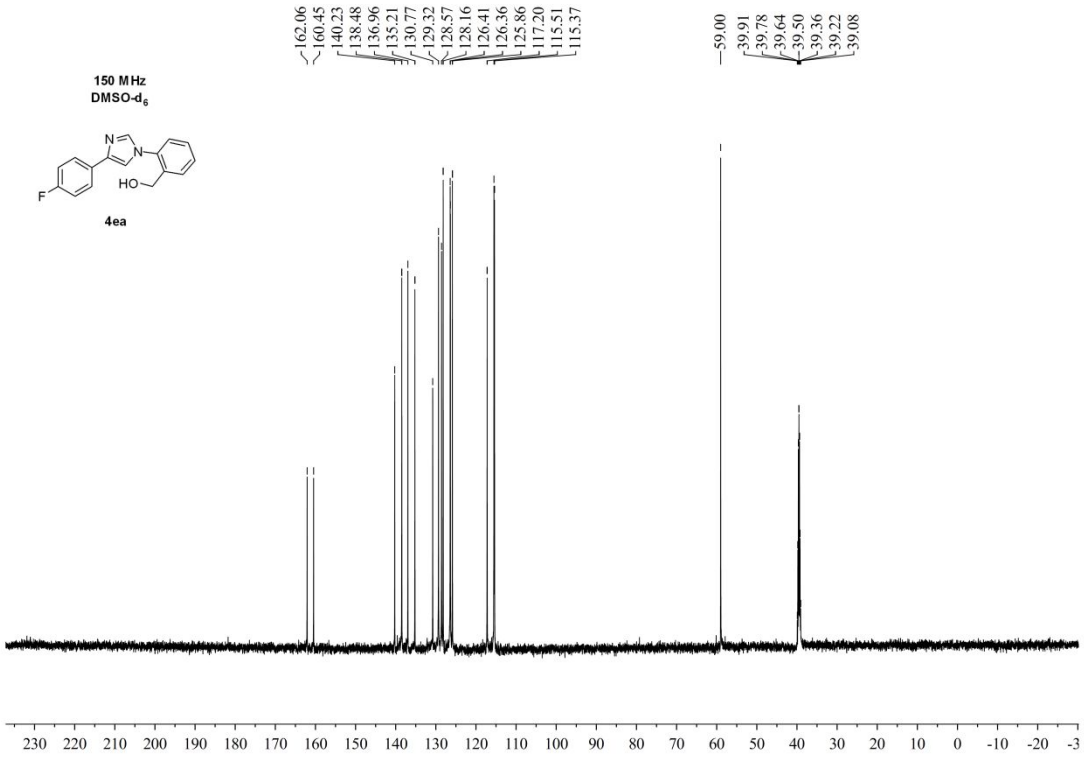
2.00
f1 (ppm)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135.21
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129.32
128.57
128.16
126.41
126.36
125.86
117.20
115.51
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39.78
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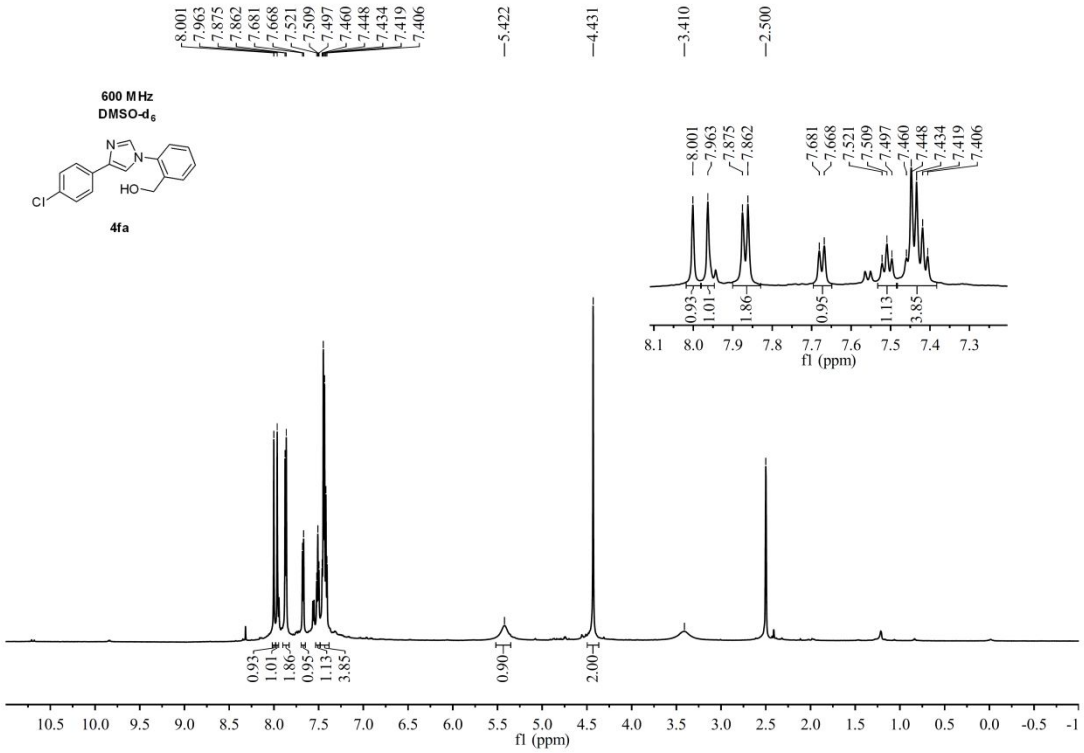
4ea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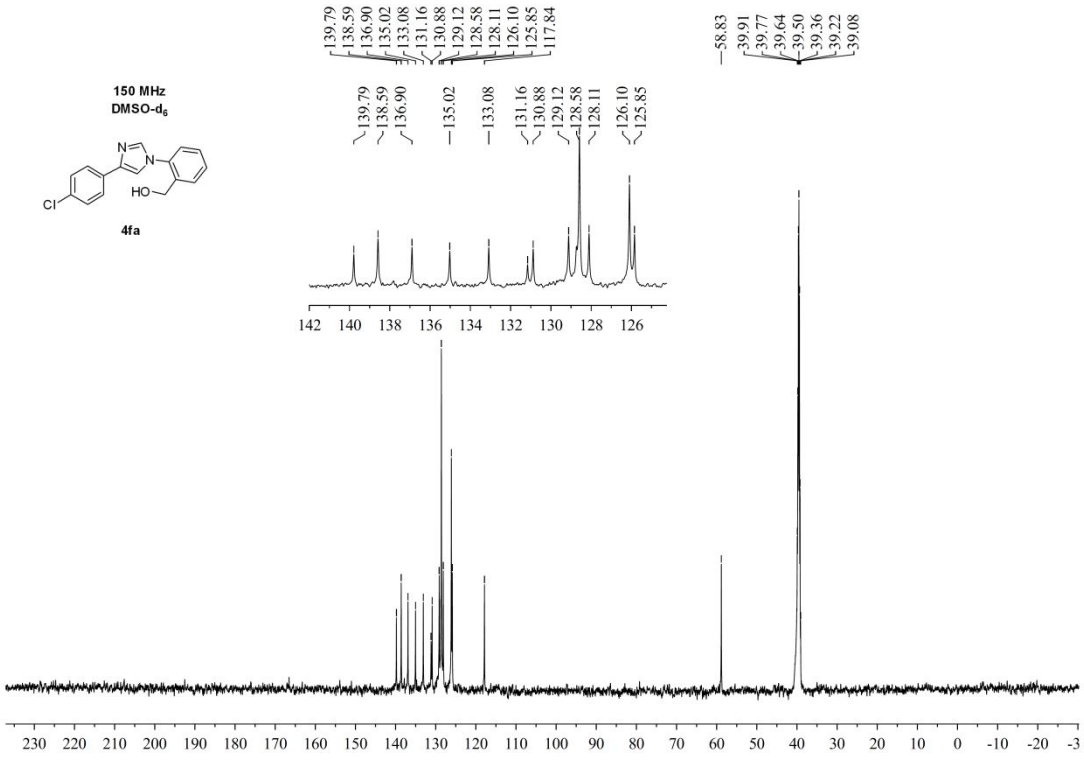
fl (ppm)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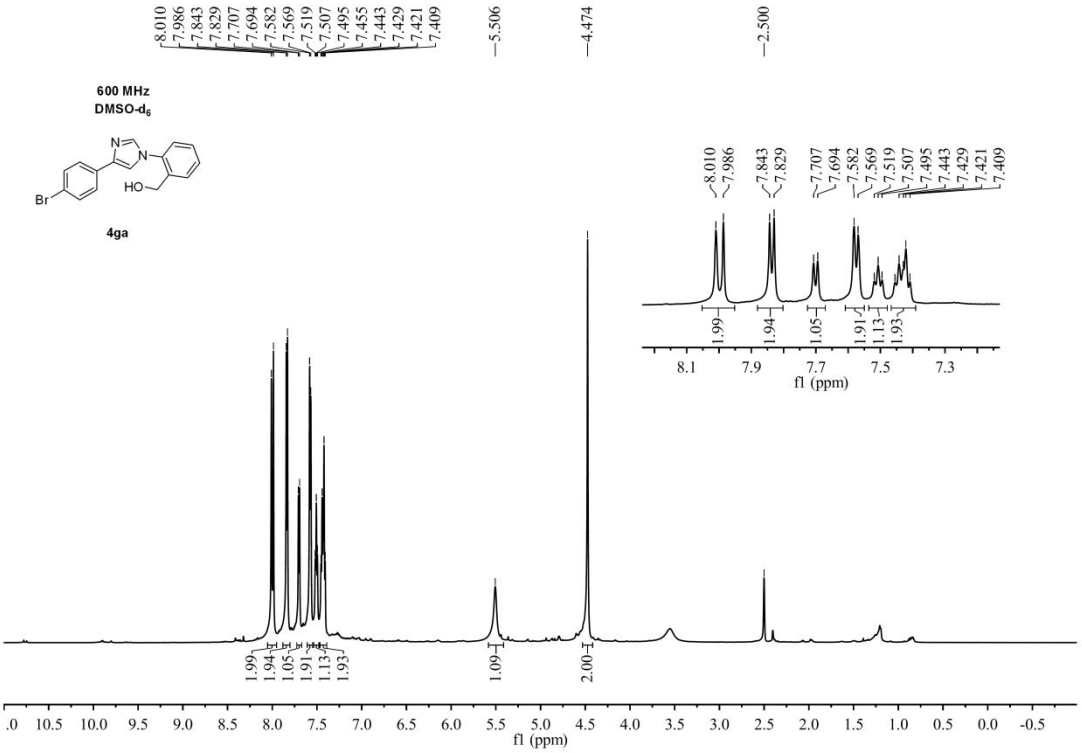
fl (ppm)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7.495
7.455
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7.429
7.421
7.409
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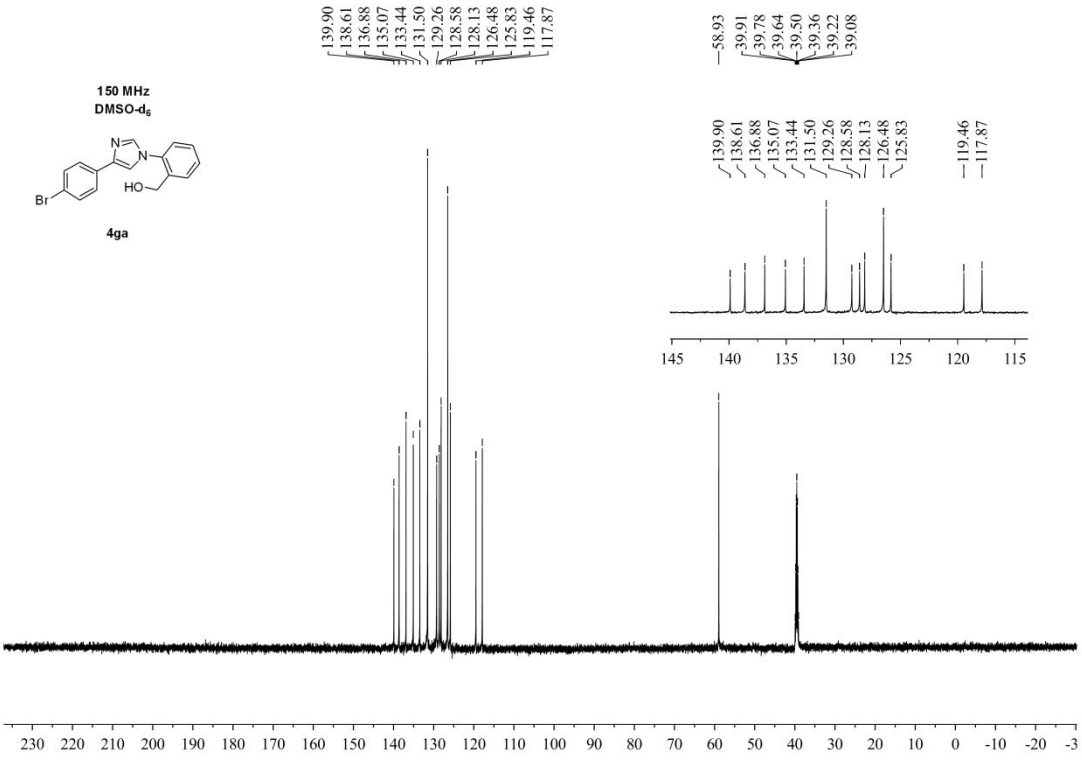
fl (ppm)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39.50
39.36
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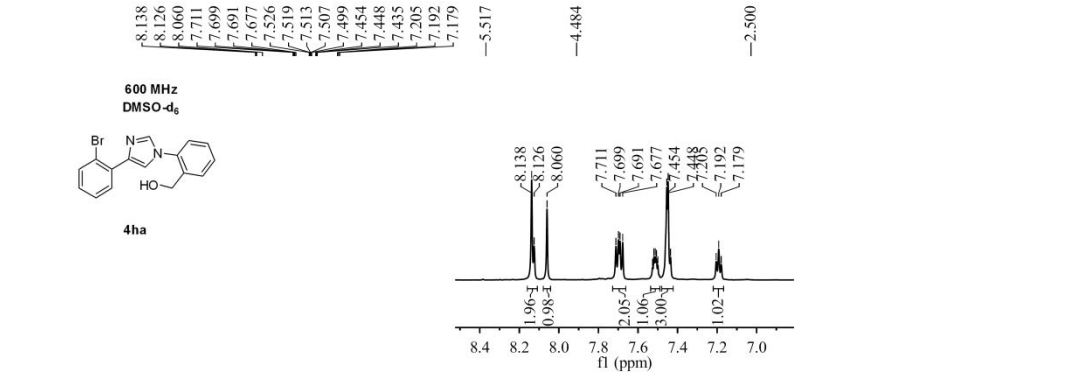
fl (ppm)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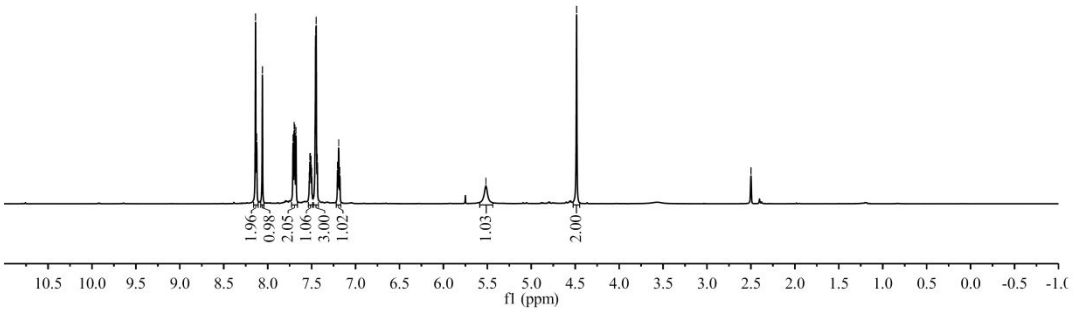
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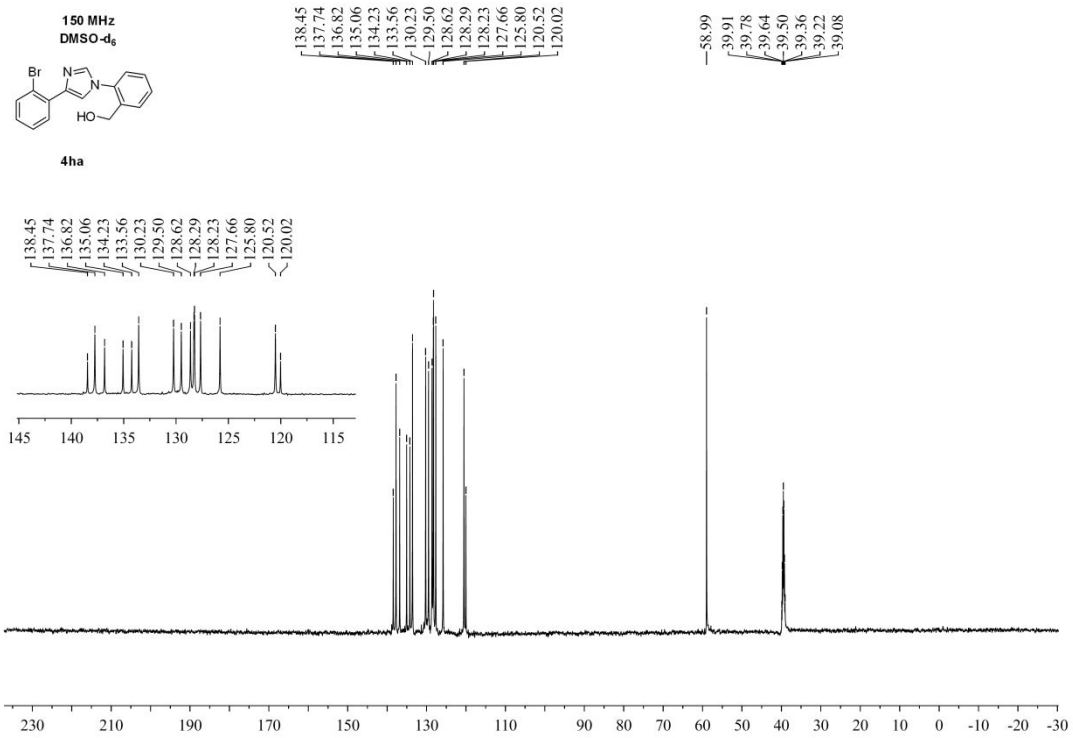
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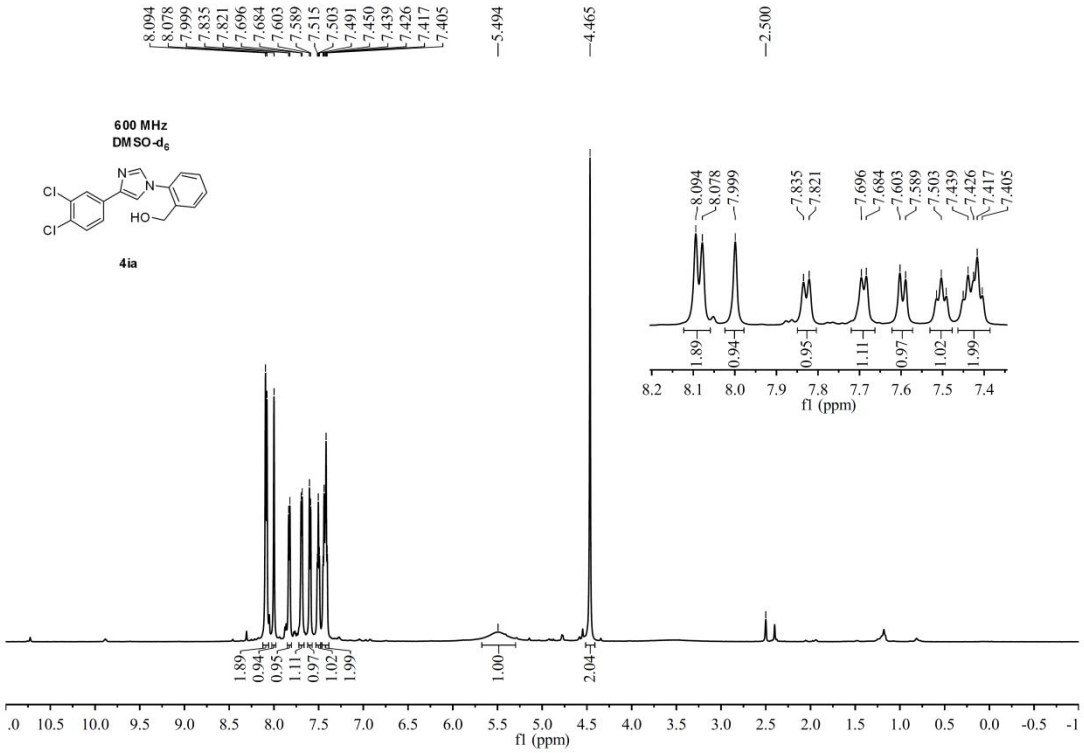
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7.405
5.494
4.465
2.500
600 MHz
DMSO-d6
Cl
Cl
N
N
HO
4ia
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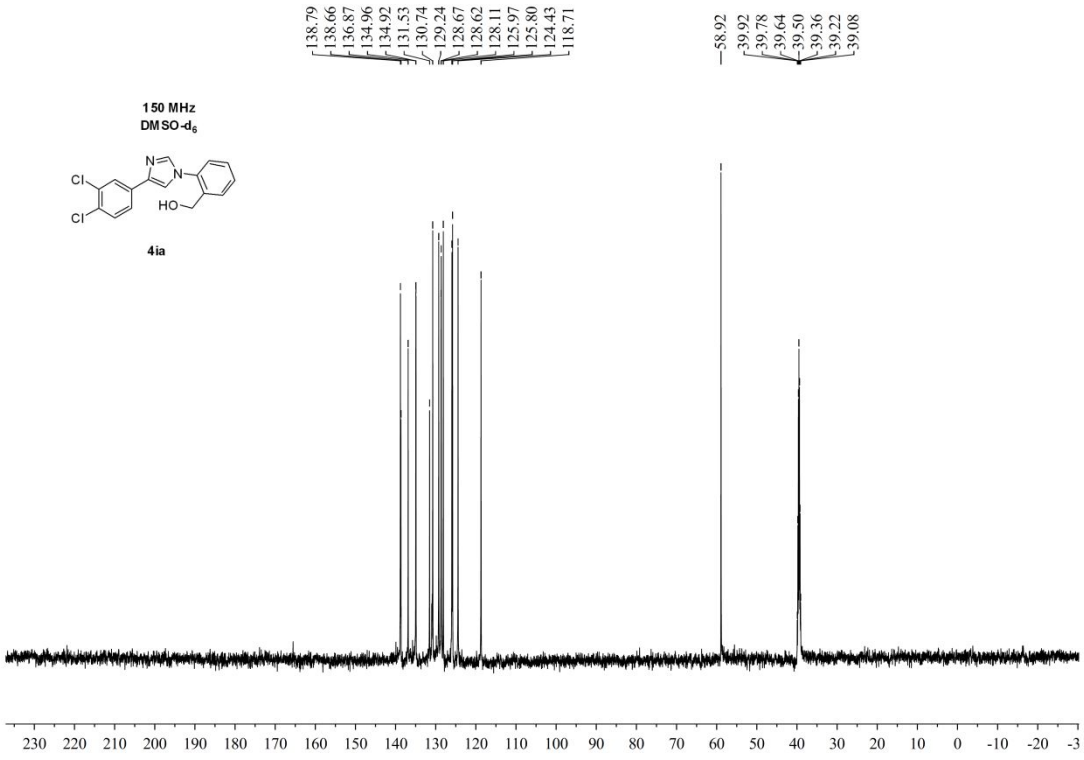
1.02
1.99
1.00
2.04
f1 (ppm)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124.43
118.71
58.92
39.92
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DMSO-d6
Cl
Cl
N
N
HO
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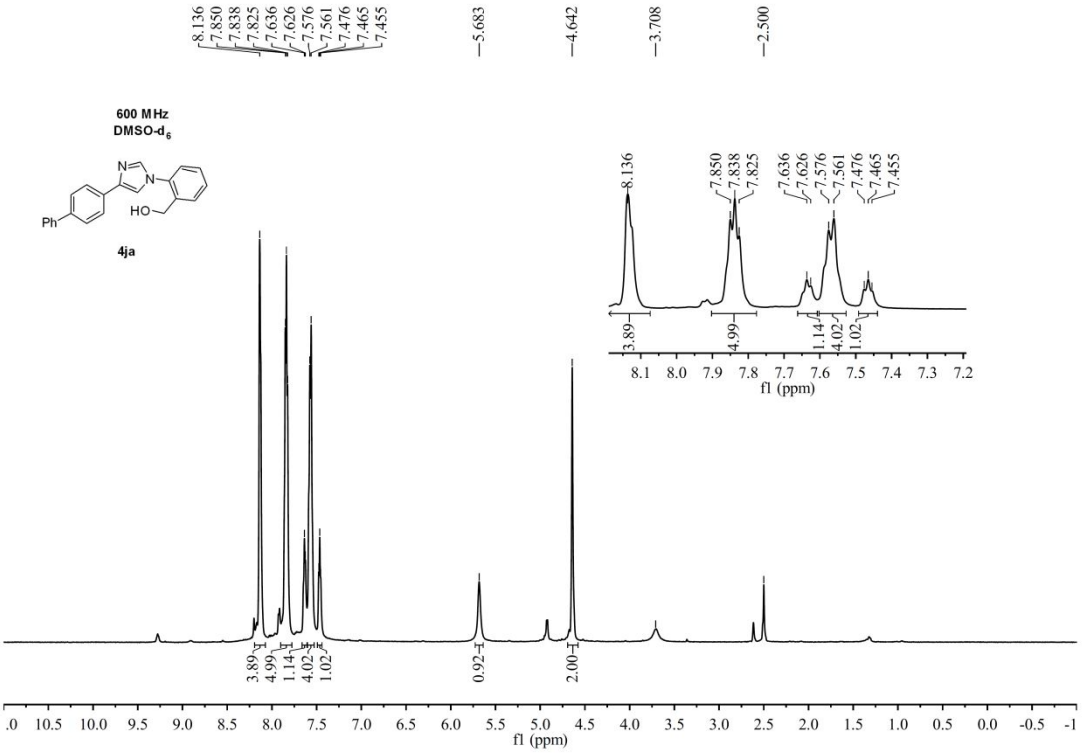
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4.642
3.708
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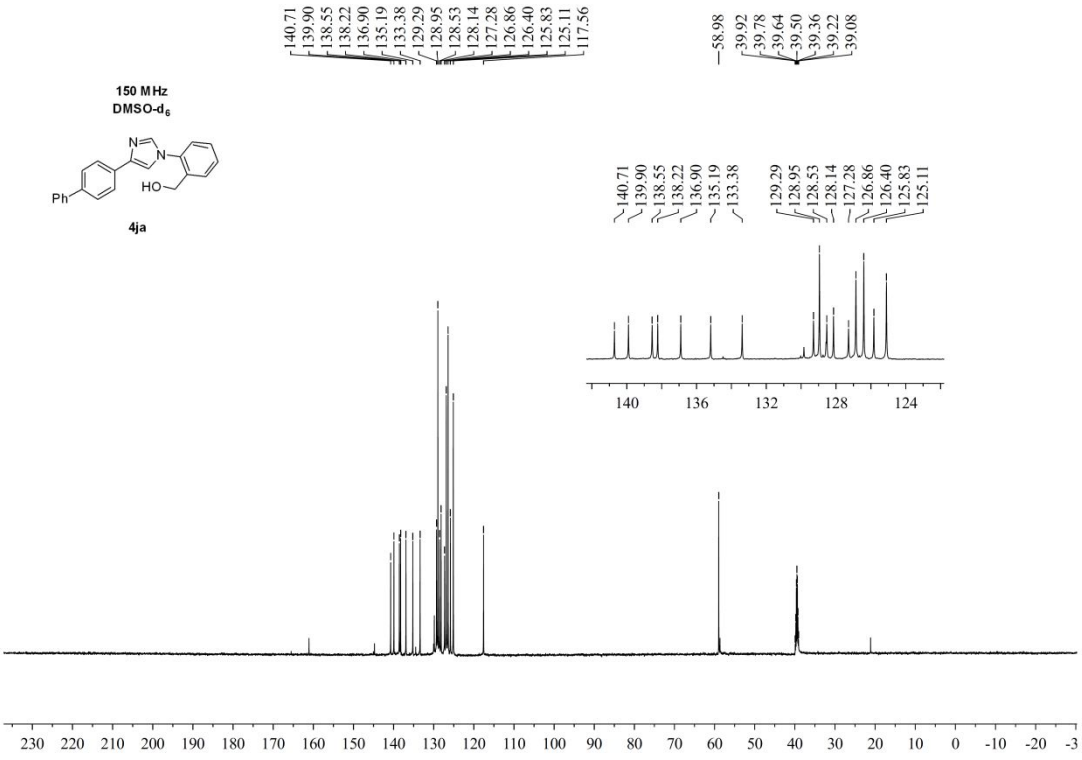
f1 (ppm)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128.14
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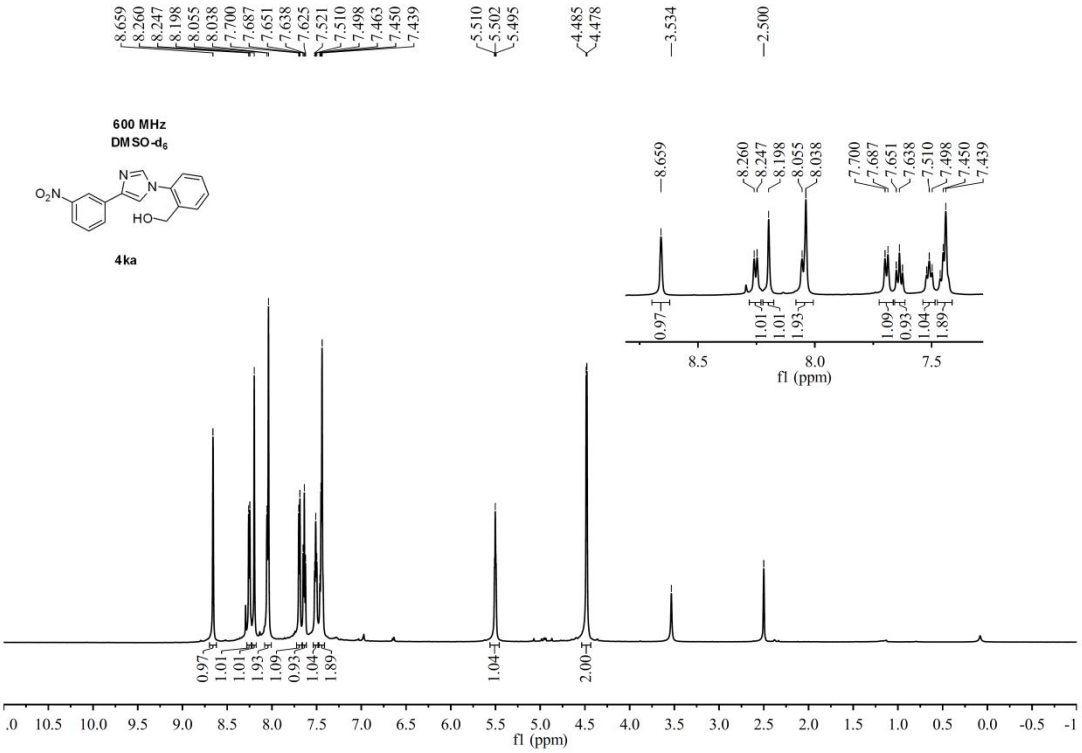
150 MHz
DMSO-d6
Ph
HO
4ja
f1 (ppm)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7.450
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4.485
4.478
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600 MHz
DMSO-d6
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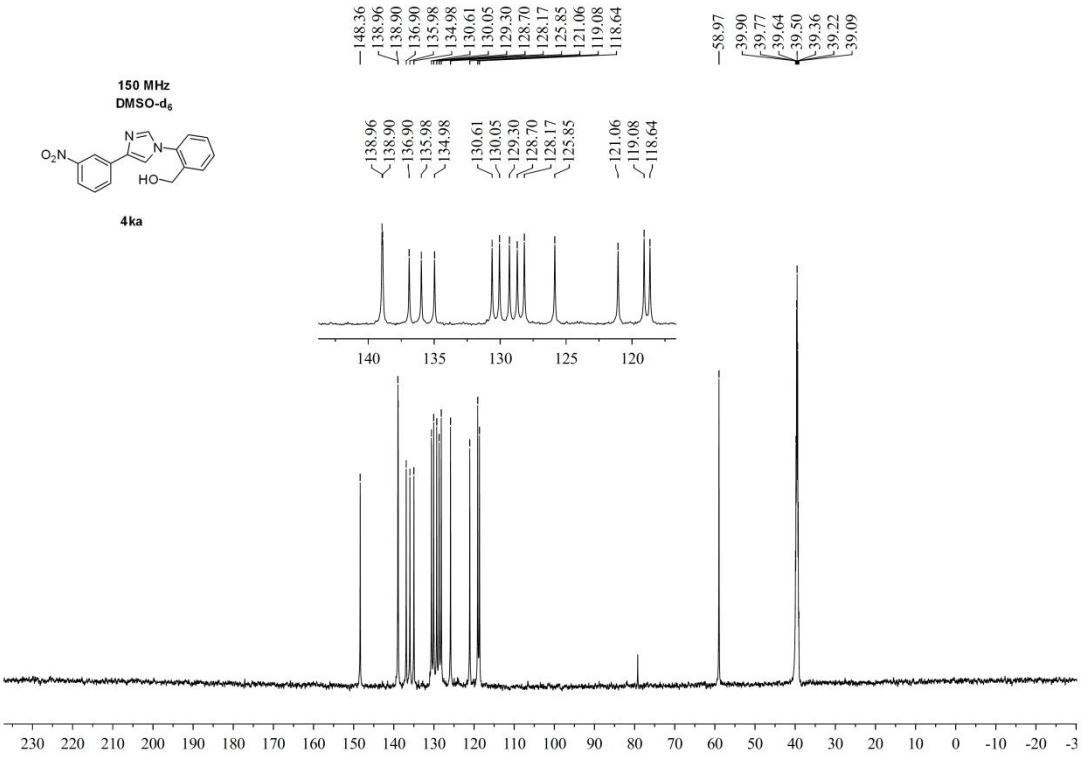
f1 (ppm)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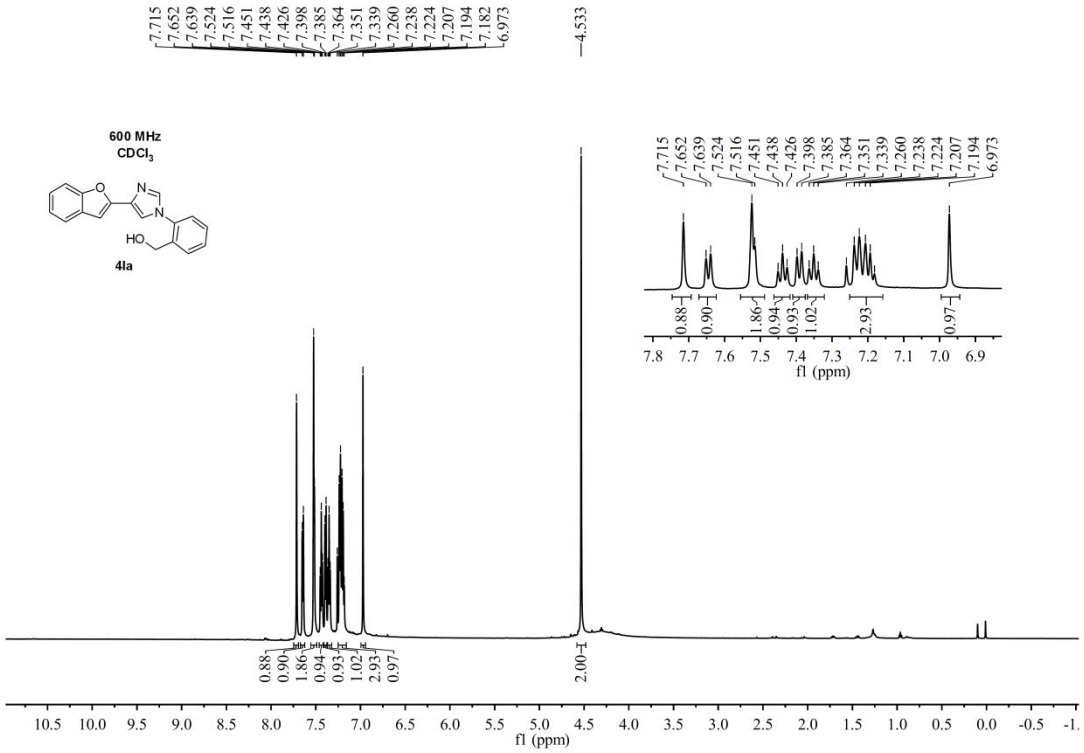
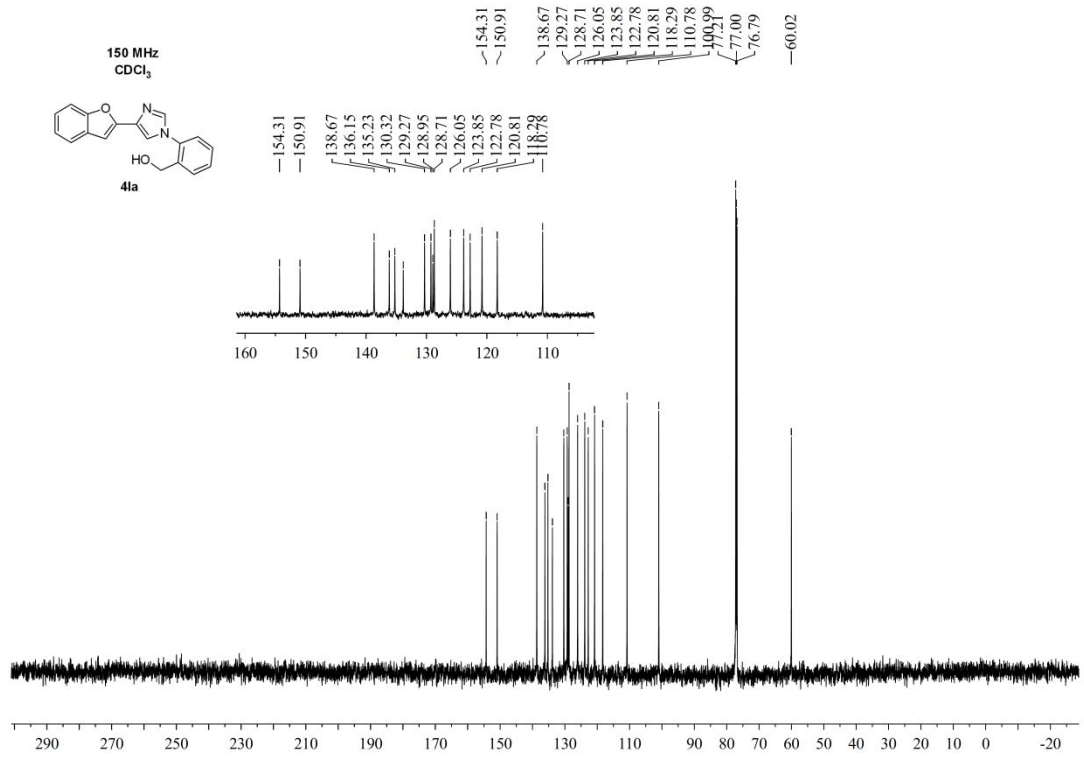
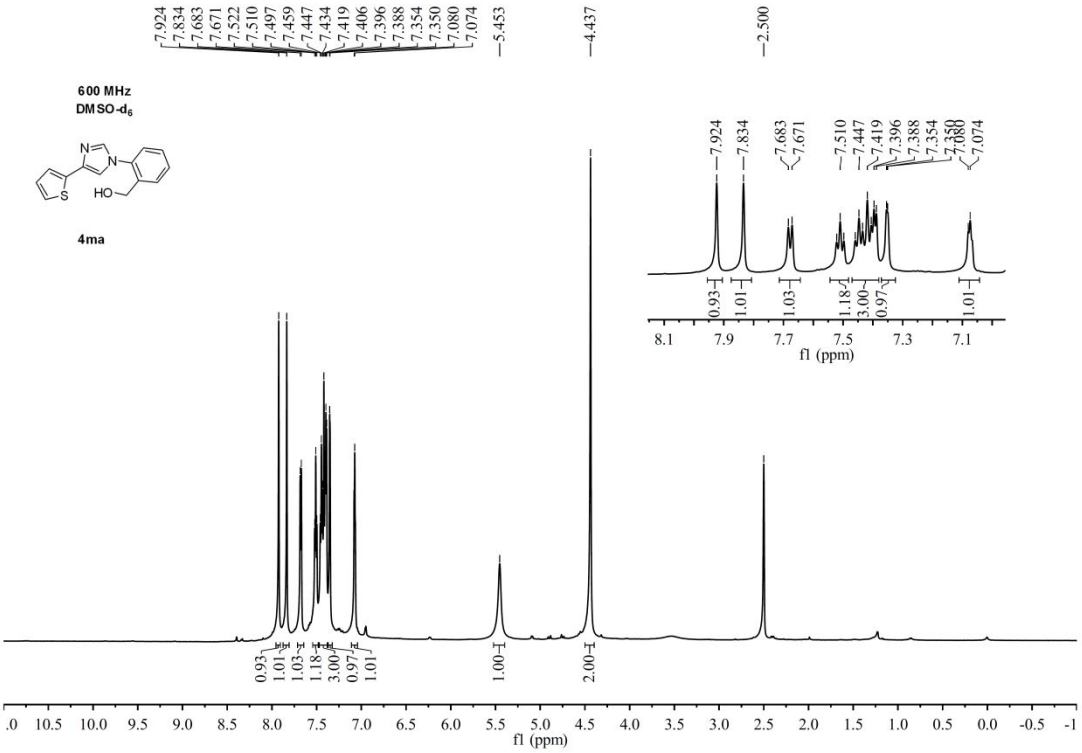
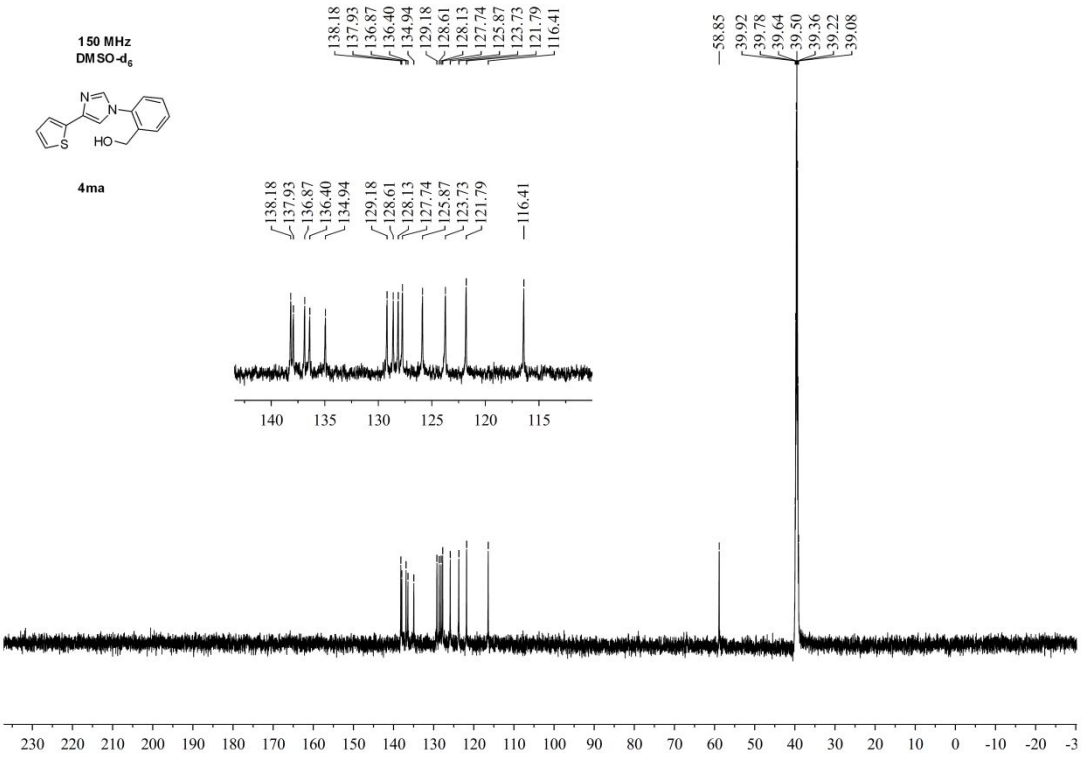
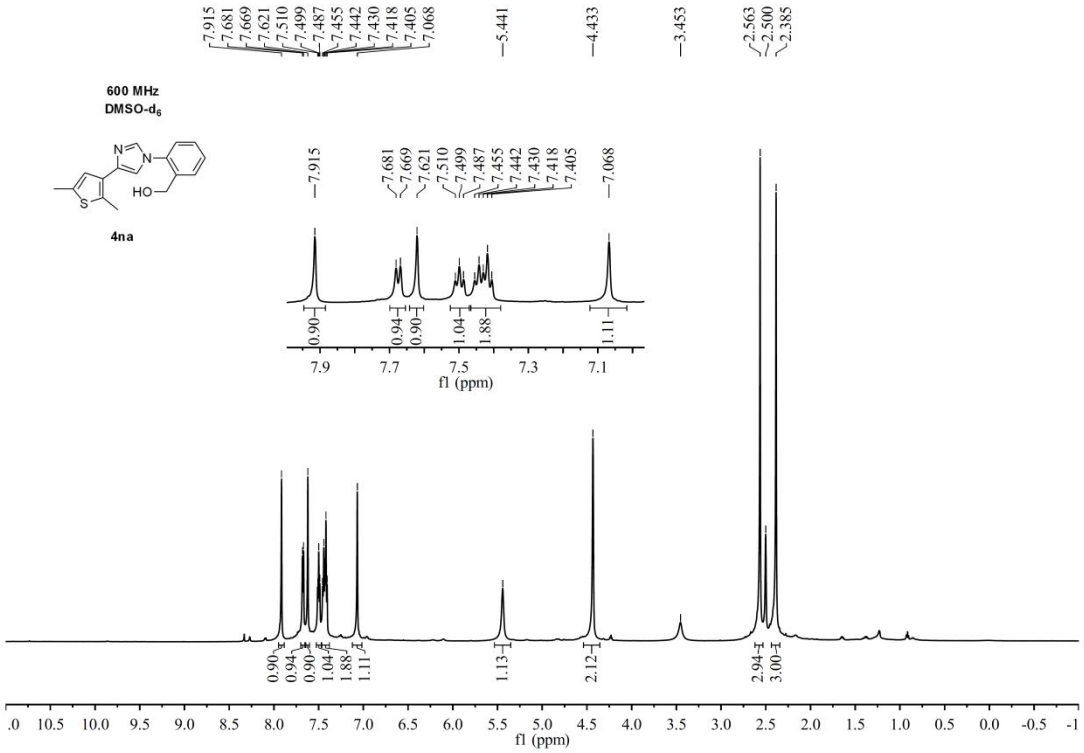
118.64
58.97
39.90
39.77
39.64
39.50
39.36
39.22
39.09
150 MHz
DMSO-d6
4ka
f1 (ppm)

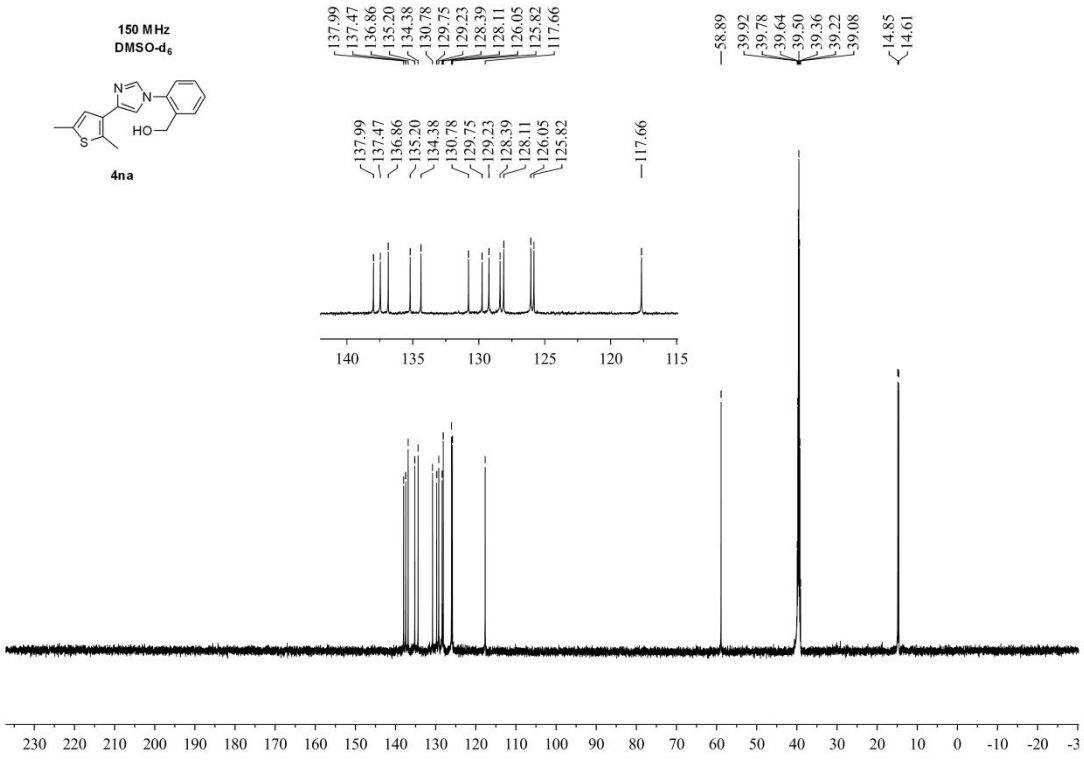

600 MHz
CDCl3
4la
f1 (ppm)


150 MHz
CDCl3
4la
f1 (ppm)


600 MHz
DMSO-d6
4ma
f1 (ppm)


150 MHz
DMSO-d6
4ma
f1 (ppm)


600 MHz
DMSO-d6
4na
f1 (ppm)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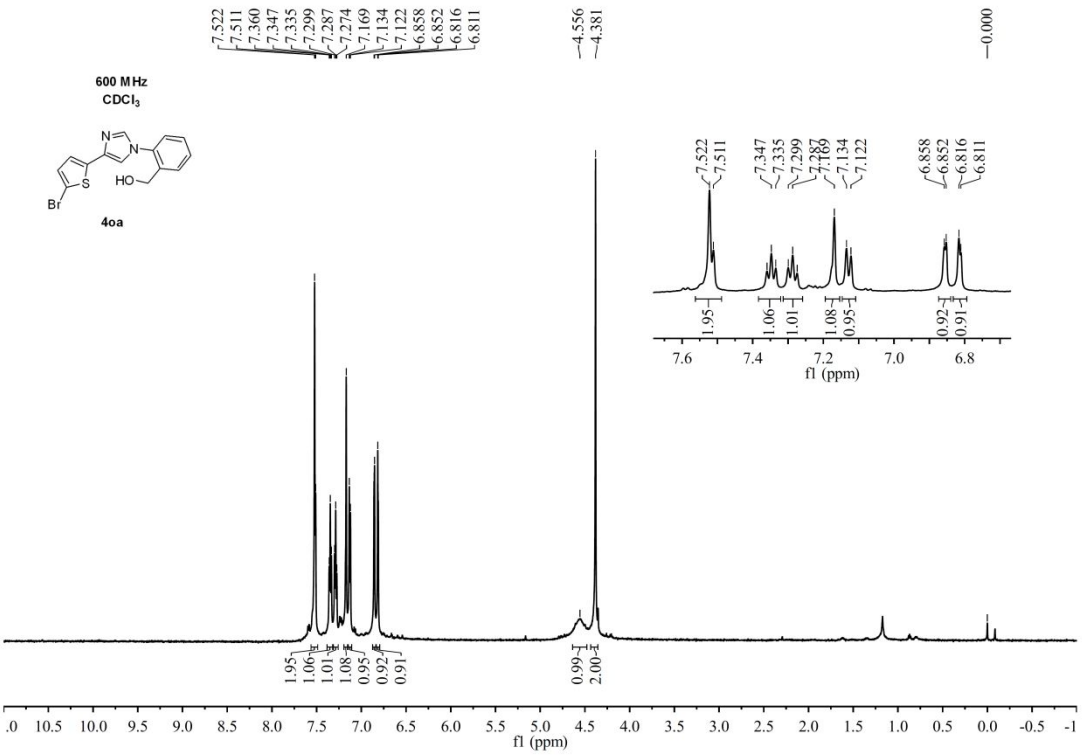
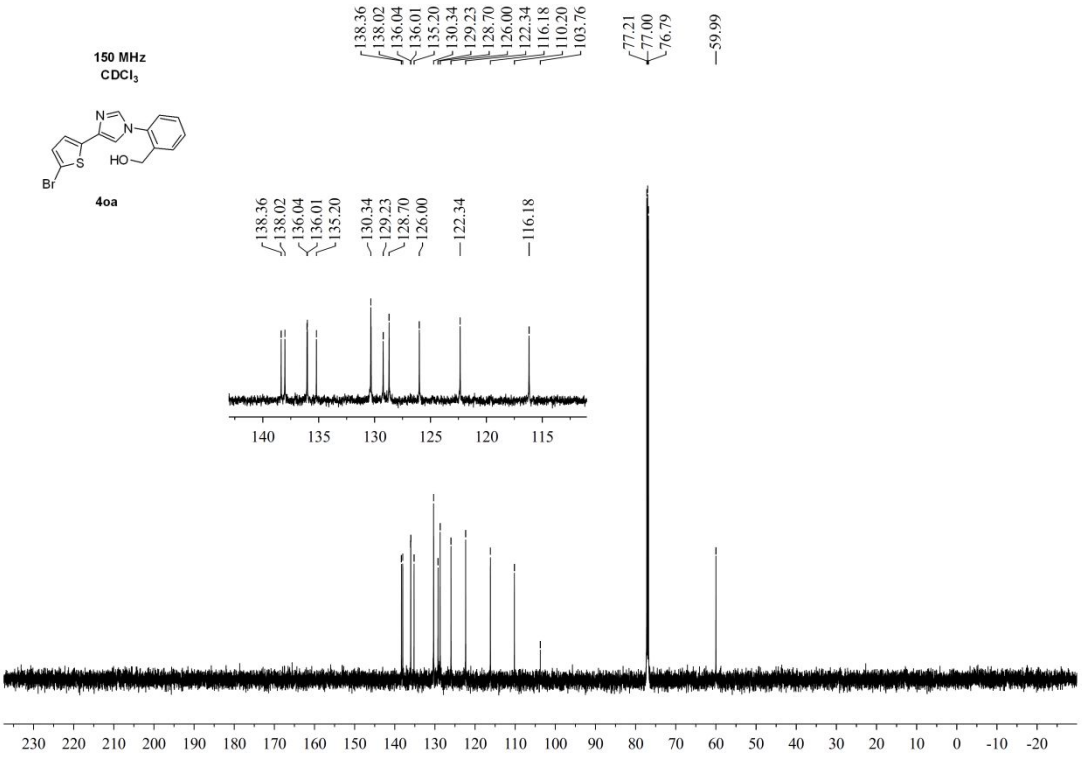
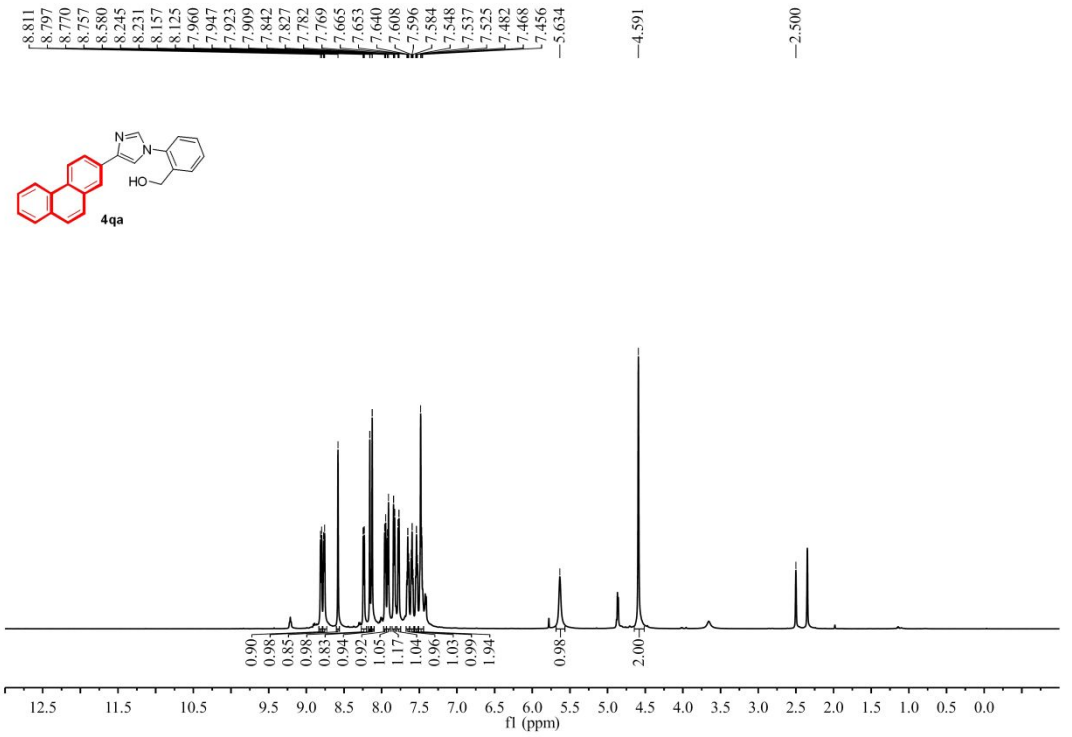
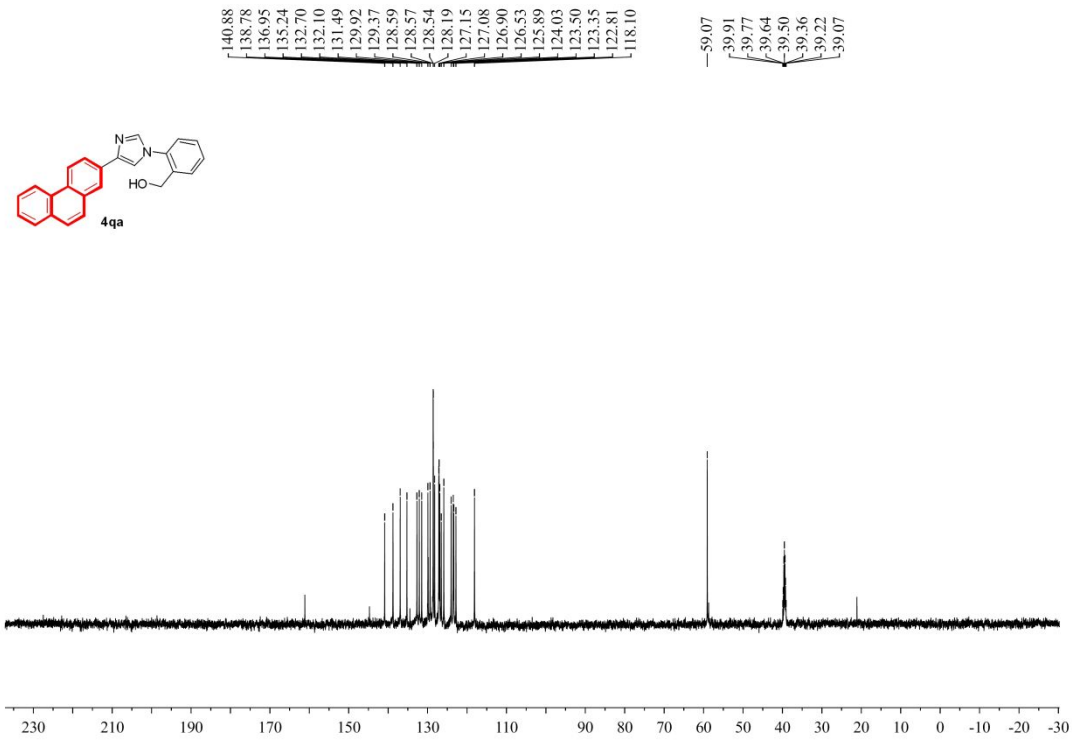
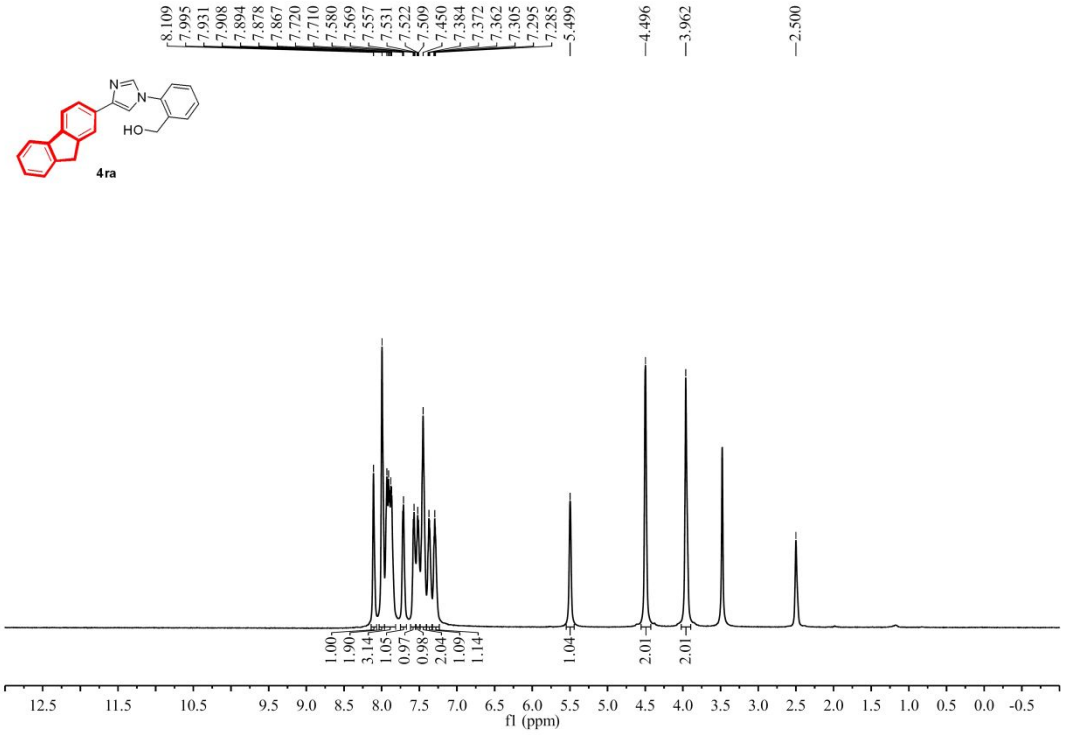
DMSO-d6
4na
f1 (ppm)

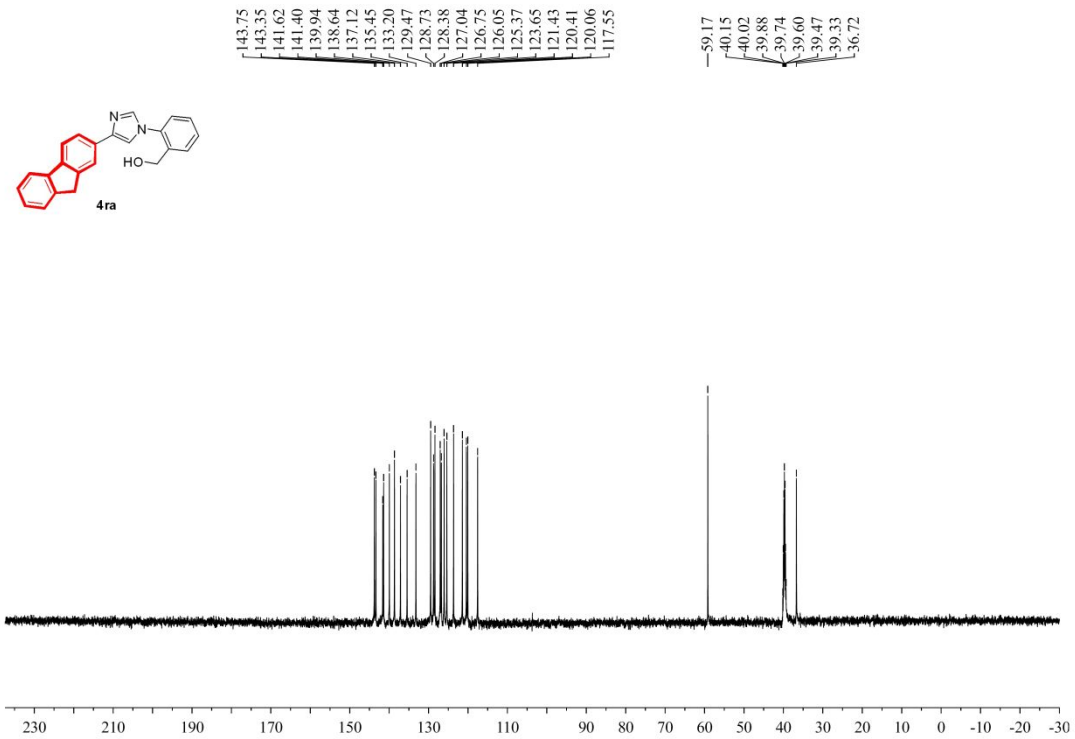

600 MHz
CDCl3
4oa
fl (ppm)

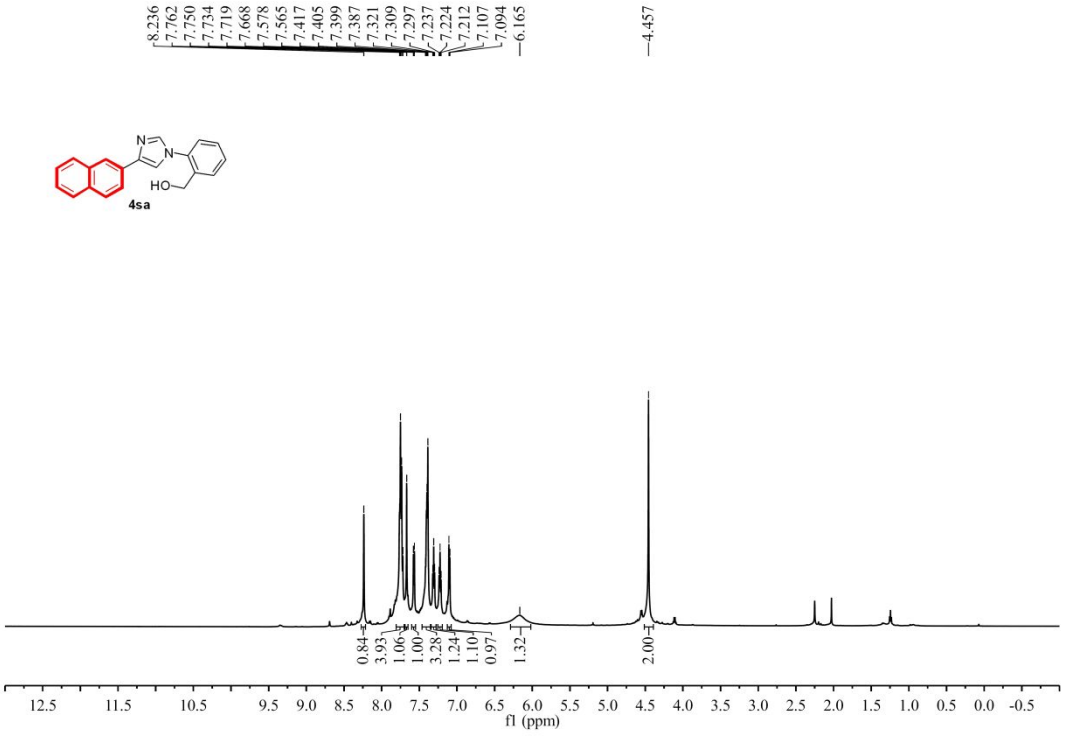

150 MHz
CDCl3
4oa
fl (ppm)

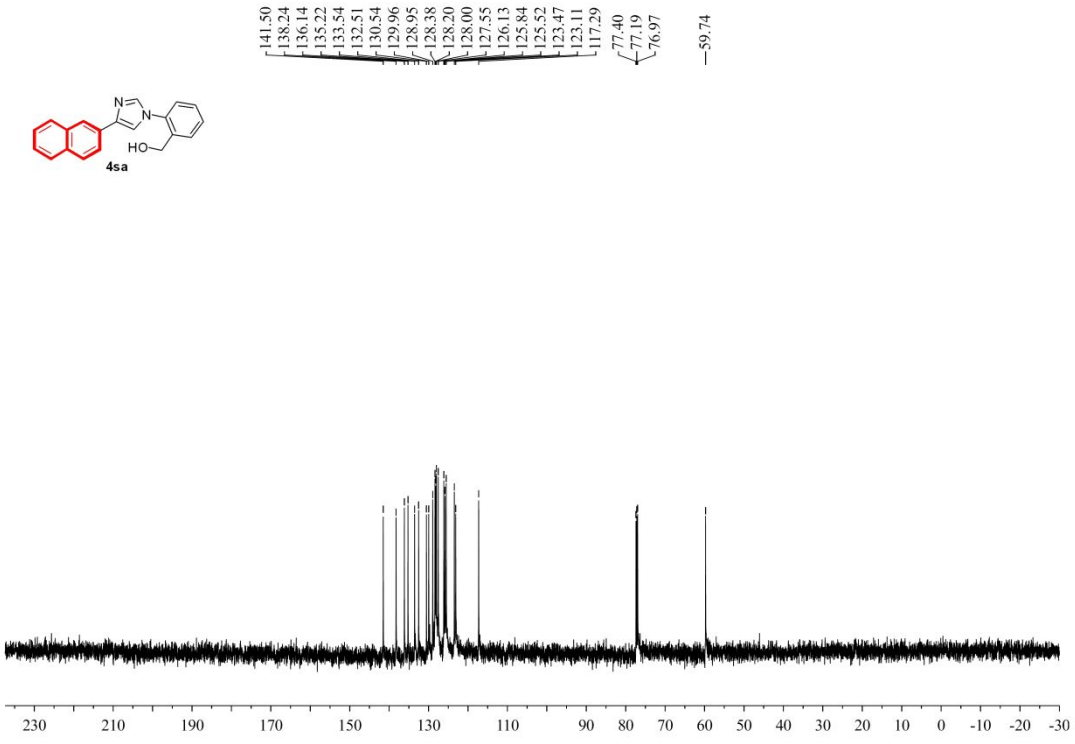

8.811
8.797
8.770
8.757
8.580
8.245
8.231
8.157
8.125
7.960
7.947
7.923
7.909
7.842
7.827
7.782
7.769
7.665
7.653
7.640
7.608
7.596
7.584
7.548
7.537
7.525
7.482
7.468
7.456
5.634
4.591
2.500
HO
4qa
0.90
0.98
0.85
0.98
0.83
0.94
0.92
1.05
1.17
1.04
0.96
1.03
0.99
1.94
0.98
2.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

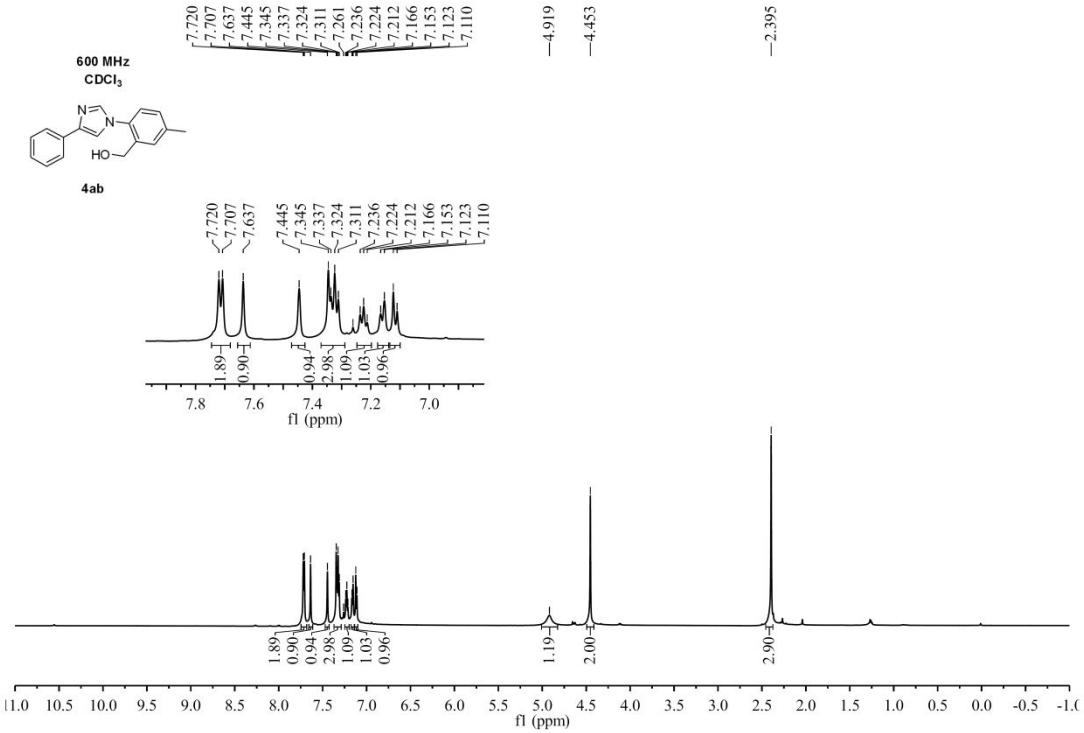

140.88
138.78
136.95
135.24
132.70
132.10
131.49
129.92
129.37
128.59
128.57
128.54
128.19
127.15
127.08
126.90
126.53
125.89
124.03
123.50
123.35
122.81
118.10
59.07
39.91
39.77
39.64
39.50
39.36
39.22
39.07
HO
4qa
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30

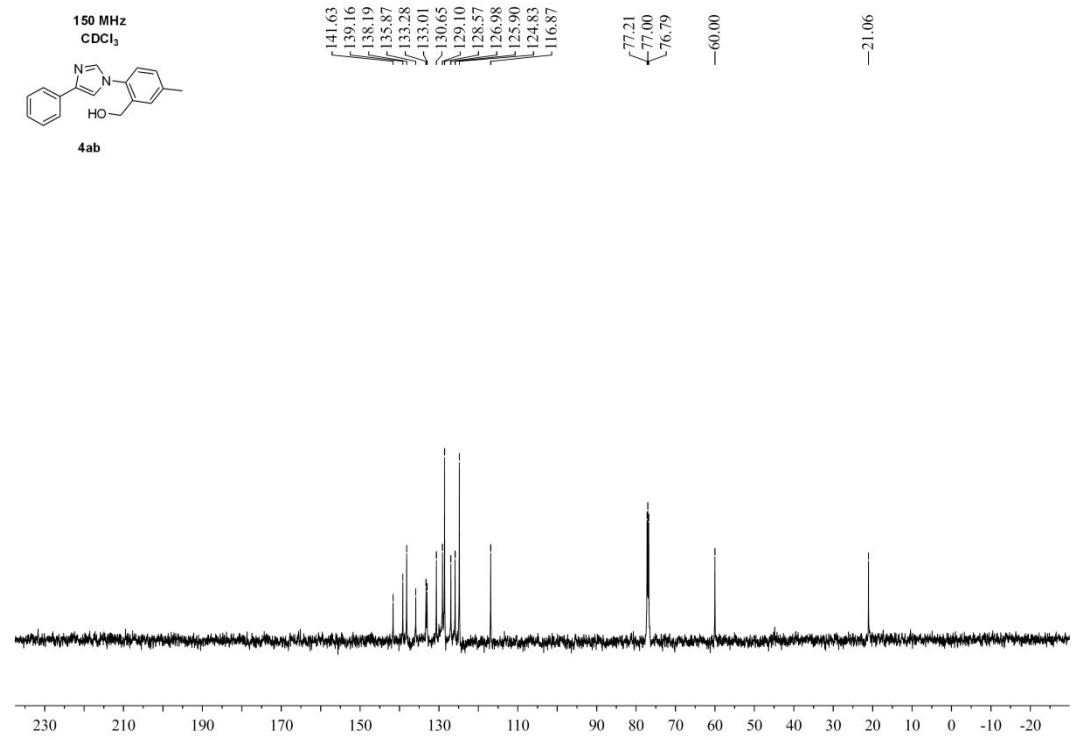

8.109
7.995
7.931
7.908
7.894
7.878
7.867
7.720
7.710
7.580
7.569
7.557
7.531
7.522
7.509
7.450
7.384
7.372
7.362
7.305
7.295
7.285
5.499
4.496
3.962
2.500
HO
4ra
1.00
1.90
3.14
1.05
0.97
0.98
2.04
1.09
1.14
1.04
2.01
2.01
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

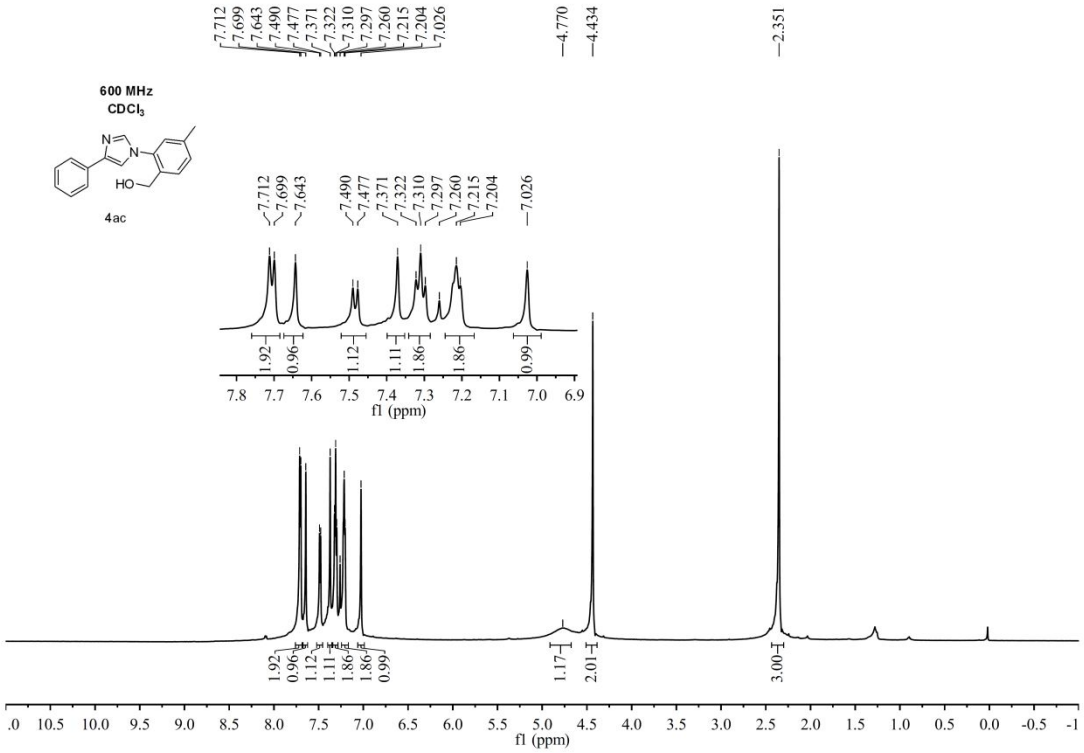

143.75
143.35
141.62
141.40
139.94
138.64
137.12
135.45
133.20
129.47
128.73
128.38
127.04
126.75
126.05
125.37
123.65
121.43
120.41
120.06
117.55
59.17
40.15
40.02
39.88
39.74
39.60
39.47
39.33
36.72
HO
4ra
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20 -30

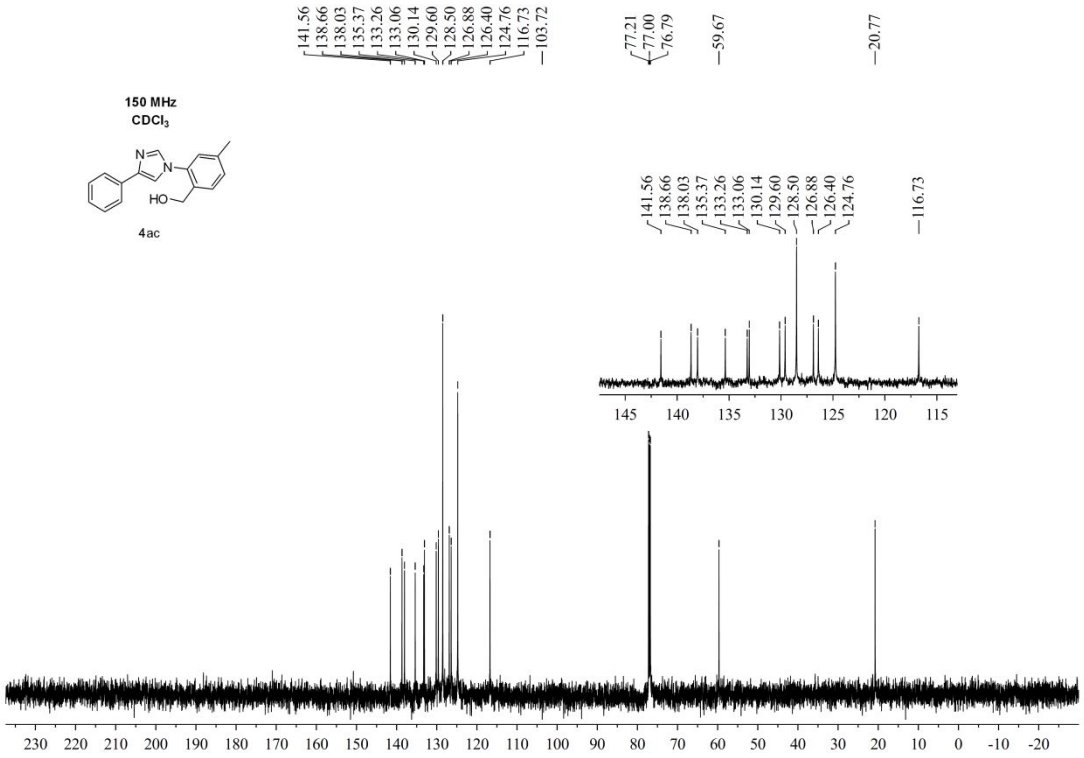

8.236
7.762
7.750
7.734
7.719
7.668
7.578
7.565
7.417
7.405
7.399
7.387
7.321
7.309
7.297
7.237
7.224
7.212
7.107
7.094
6.165
4.457
N
N
HO
4sa
0.84
3.93
1.06
1.00
3.28
1.24
1.10
0.97
1.32
2.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

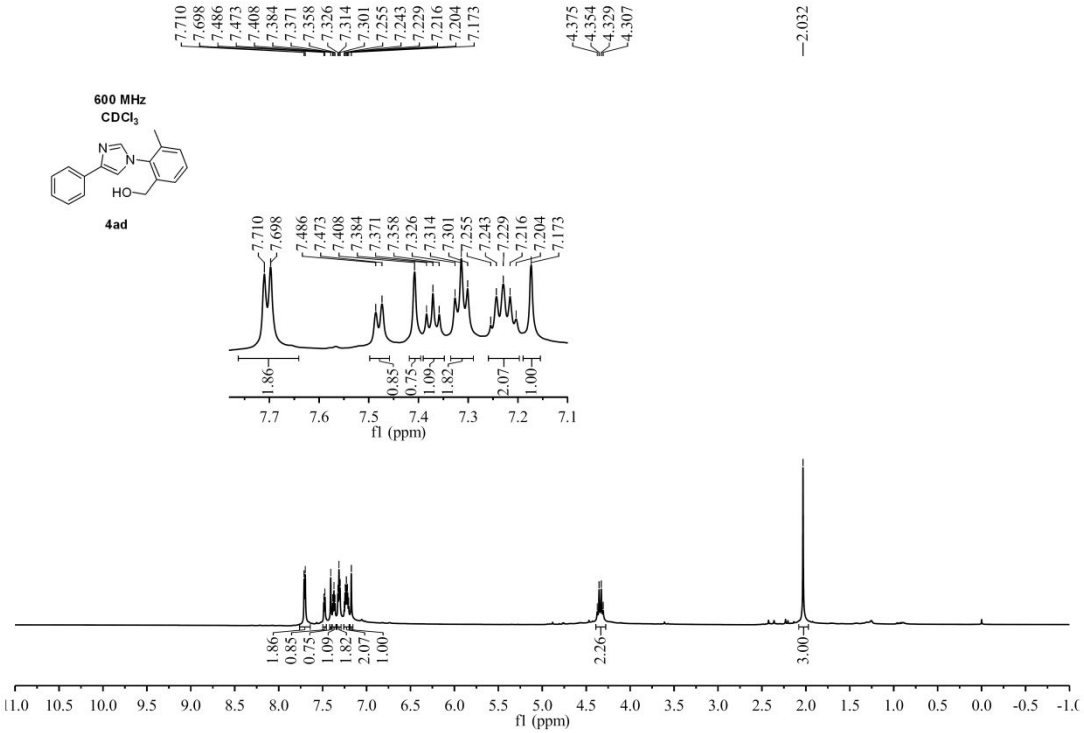

141.50
138.24
136.14
135.22
133.54
132.51
130.54
129.96
128.95
128.38
128.20
128.00
127.55
126.13
125.84
125.52
123.47
123.11
117.29
77.40
77.19
76.97
59.74
N
N
HO
4sa
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20 -30

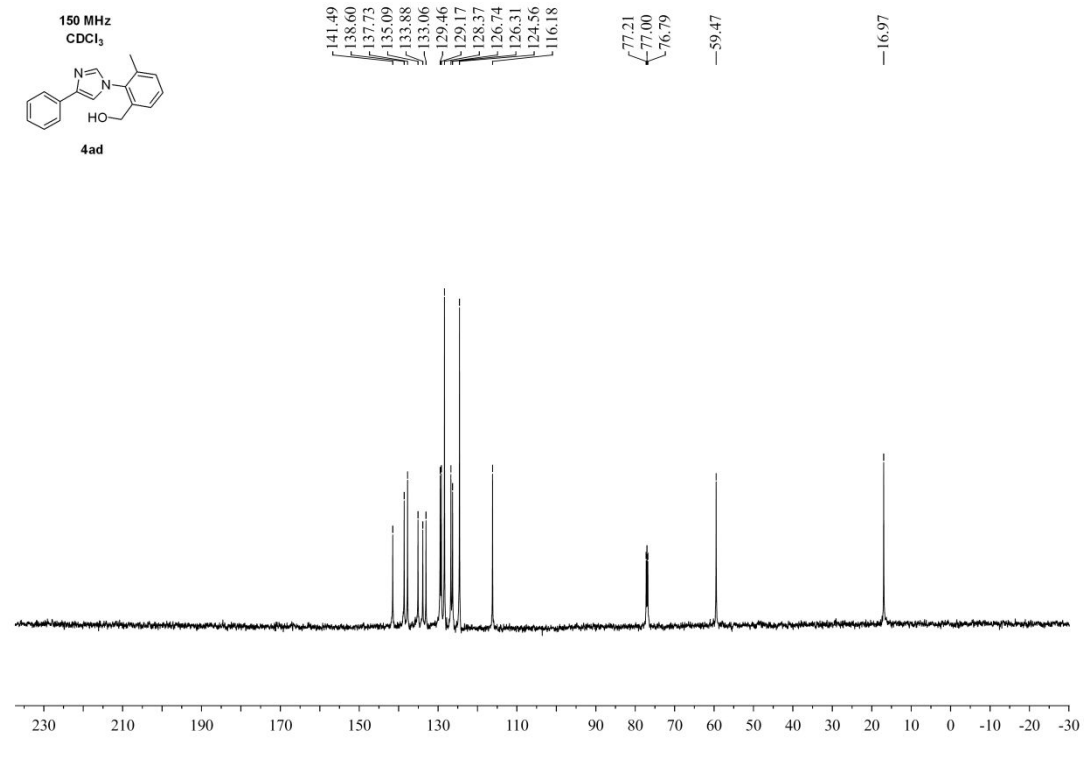

600 MHz
CDCl3
4ab
7.720
7.707
7.637
7.445
7.345
7.337
7.324
7.311
7.261
7.236
7.224
7.212
7.166
7.153
7.123
7.110
4.919
4.453
2.395
1.89
0.90
0.94
2.98
1.09
1.03
0.96
1.19
2.00
2.90
f1 (ppm)


150 MHz
CDCl3
4ab
141.63
139.16
138.19
135.87
133.28
133.01
130.65
129.10
128.57
126.98
125.90
124.83
116.87
77.21
77.00
76.79
60.00
21.06


600 MHz
CDCl3
4ac
7.712
7.699
7.643
7.490
7.477
7.371
7.322
7.310
7.297
7.260
7.215
7.204
7.026
4.770
4.434
2.351
1.92
0.96
1.12
1.11
1.86
1.86
0.99
1.17
2.01
3.00
f1 (ppm)


150 MHz
CDCl3
4ac
141.56
138.66
138.03
135.37
133.26
133.06
130.14
129.60
128.50
126.88
126.40
124.76
116.73
103.72
77.21
77.00
76.79
59.67
20.77
f1 (ppm)


7.710
7.698
7.486
7.473
7.408
7.384
7.371
7.358
7.326
7.314
7.301
7.255
7.243
7.229
7.216
7.204
7.173
4.375
4.354
4.329
4.307
2.032
600 MHz
CDCl3
4ad
1.86
0.85
0.75
1.09
1.82
2.07
1.00
2.26
3.00
f1 (ppm)


150 MHz
CDCl3
4ad
141.49
138.60
137.73
135.09
133.88
133.06
129.46
129.17
128.37
126.74
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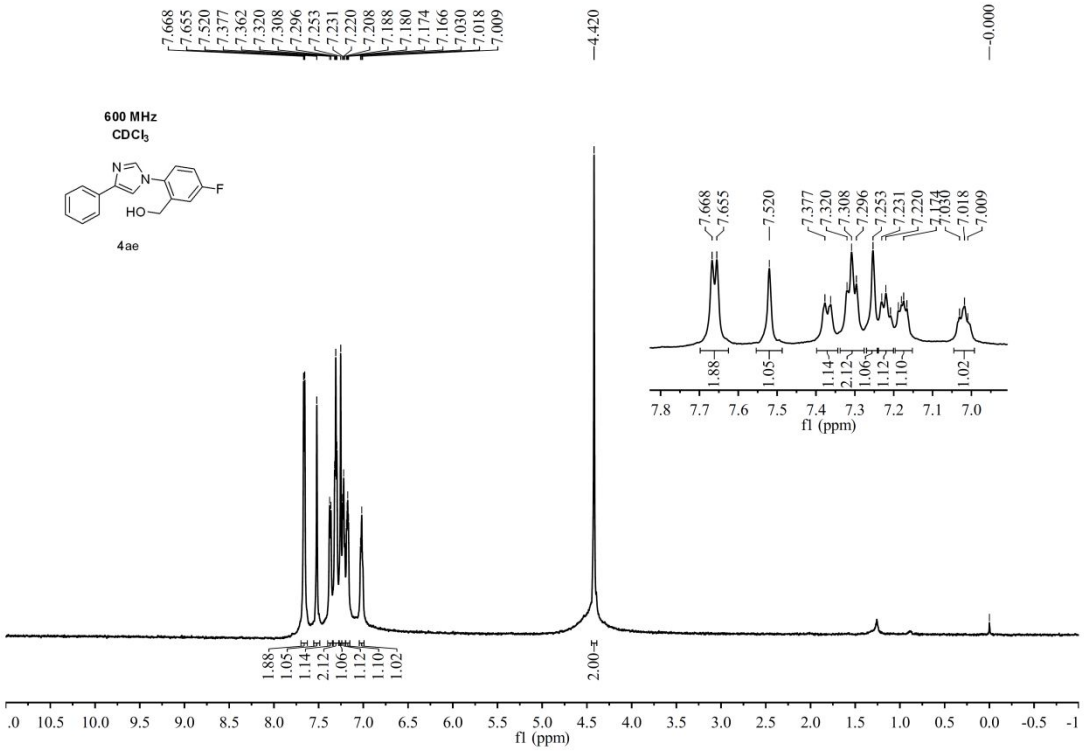
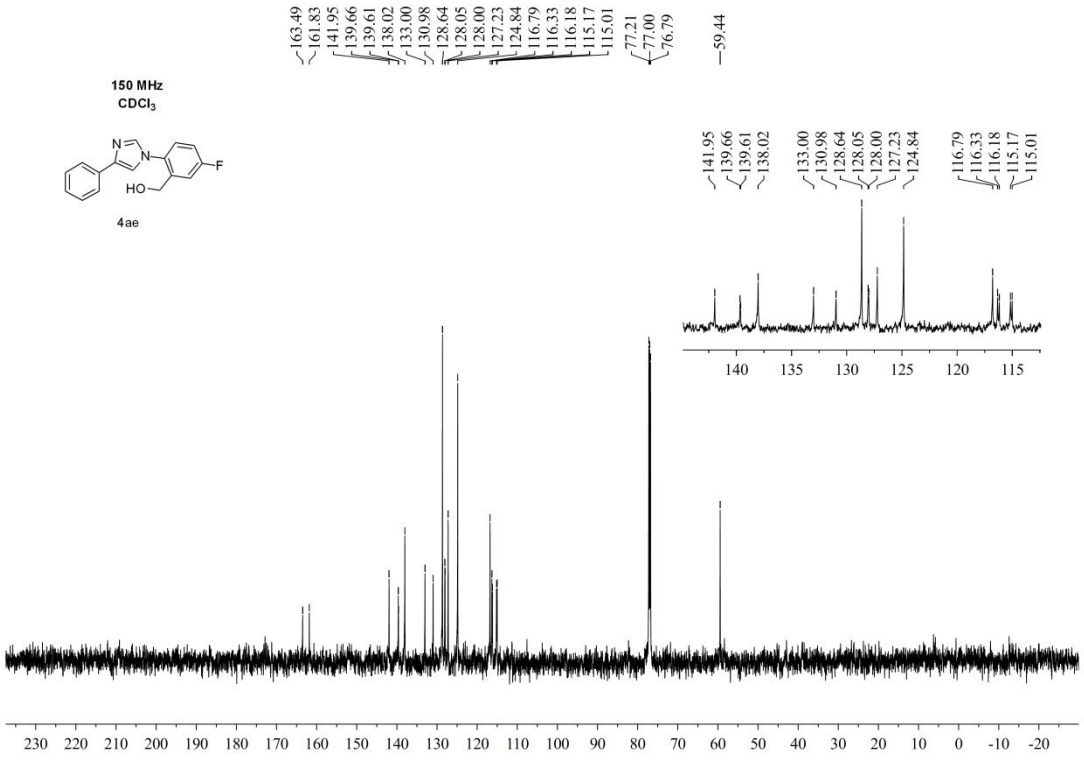
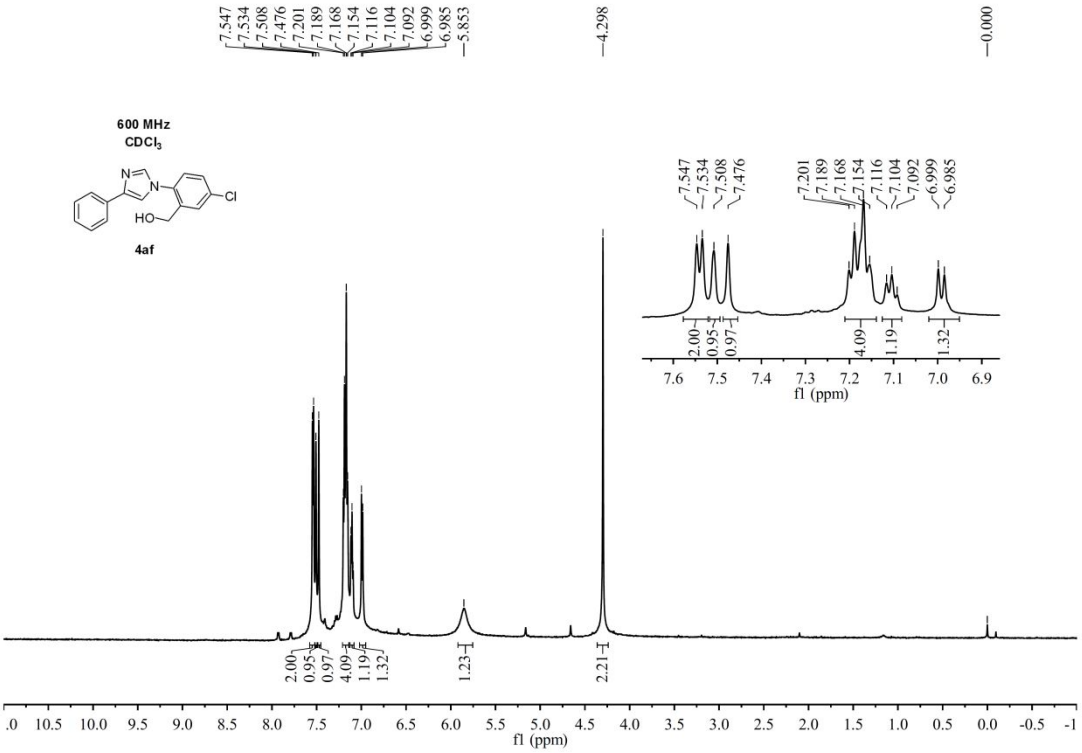
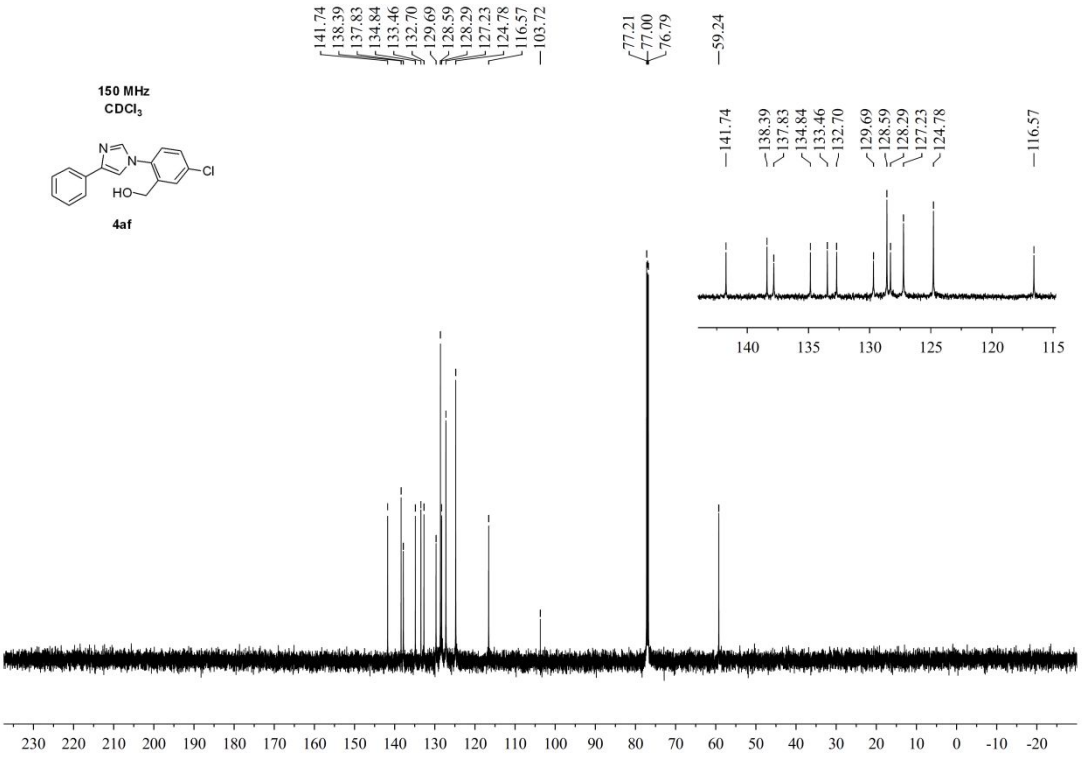
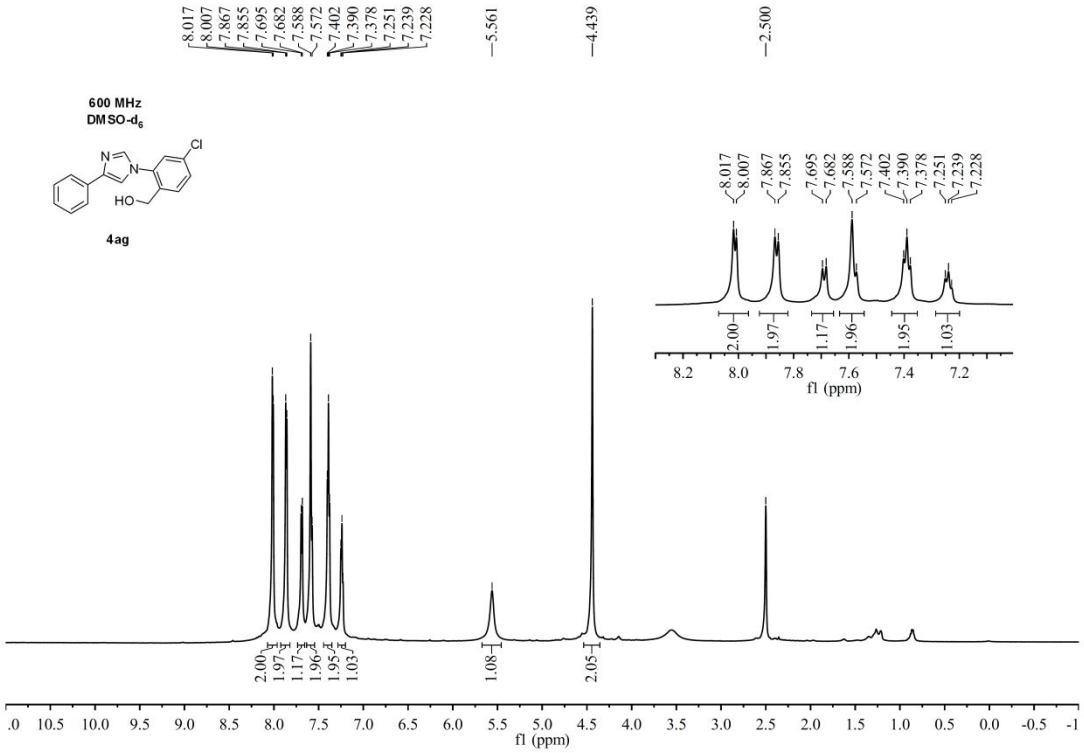
124.56
116.18
77.21
77.00
76.79
59.47
16.97

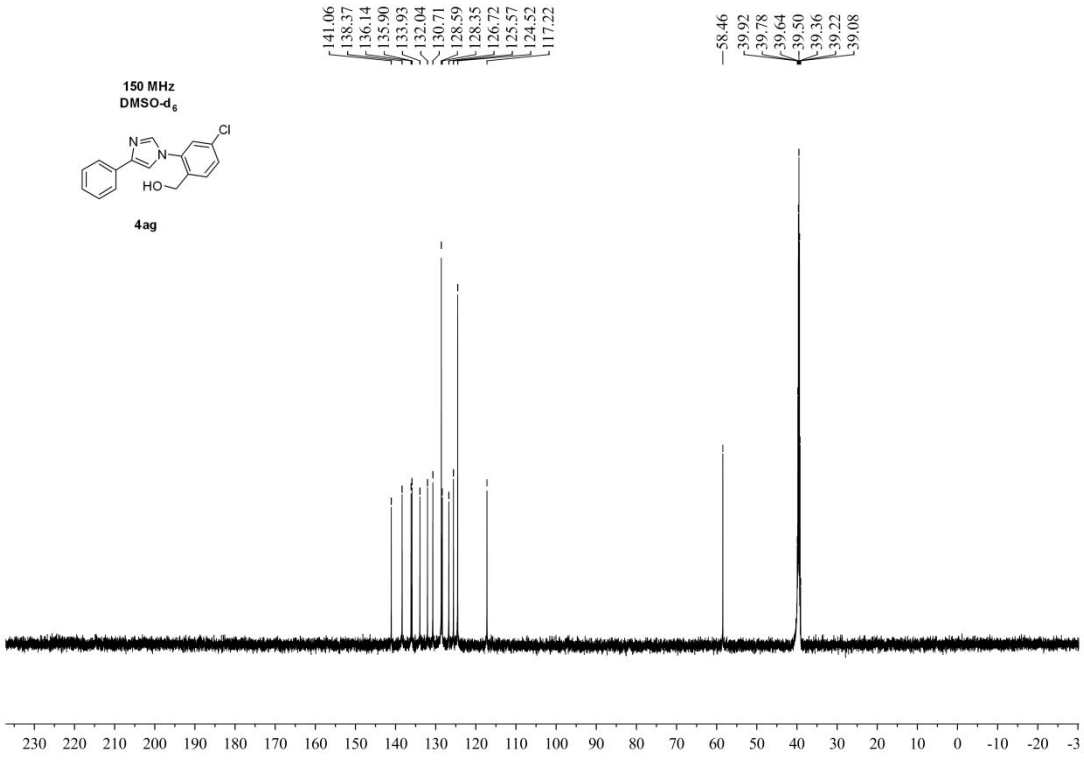

600 MHz
CDCl3
4ae
f1 (ppm)

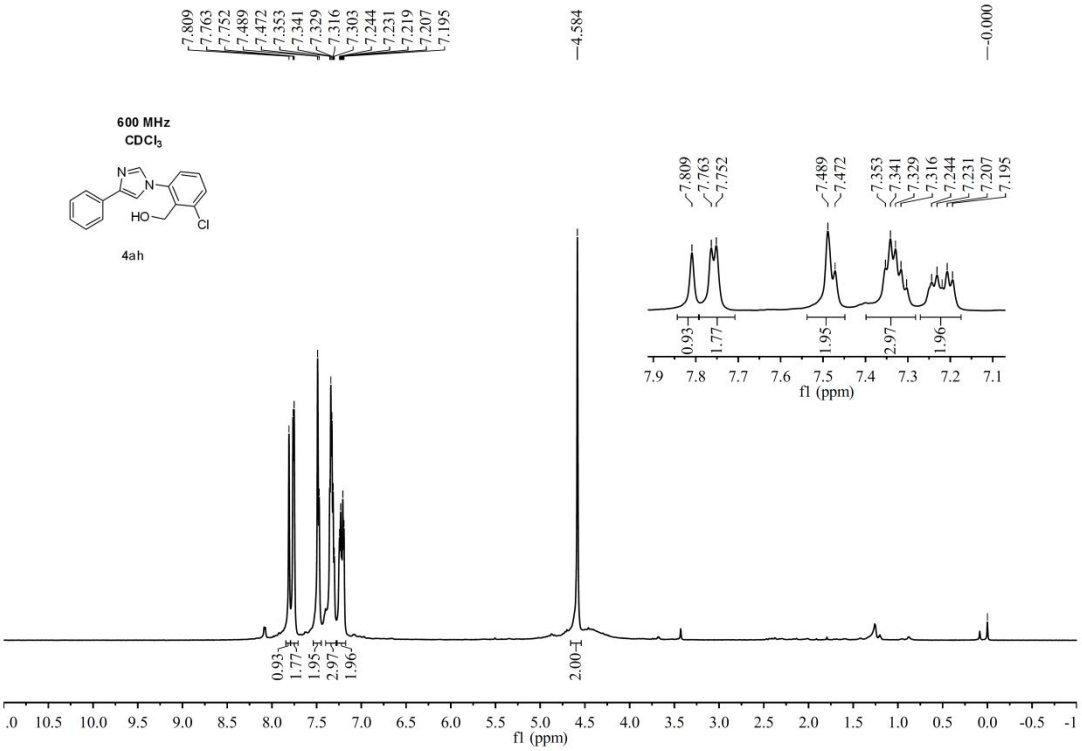

150 MHz
CDCl3
4ae

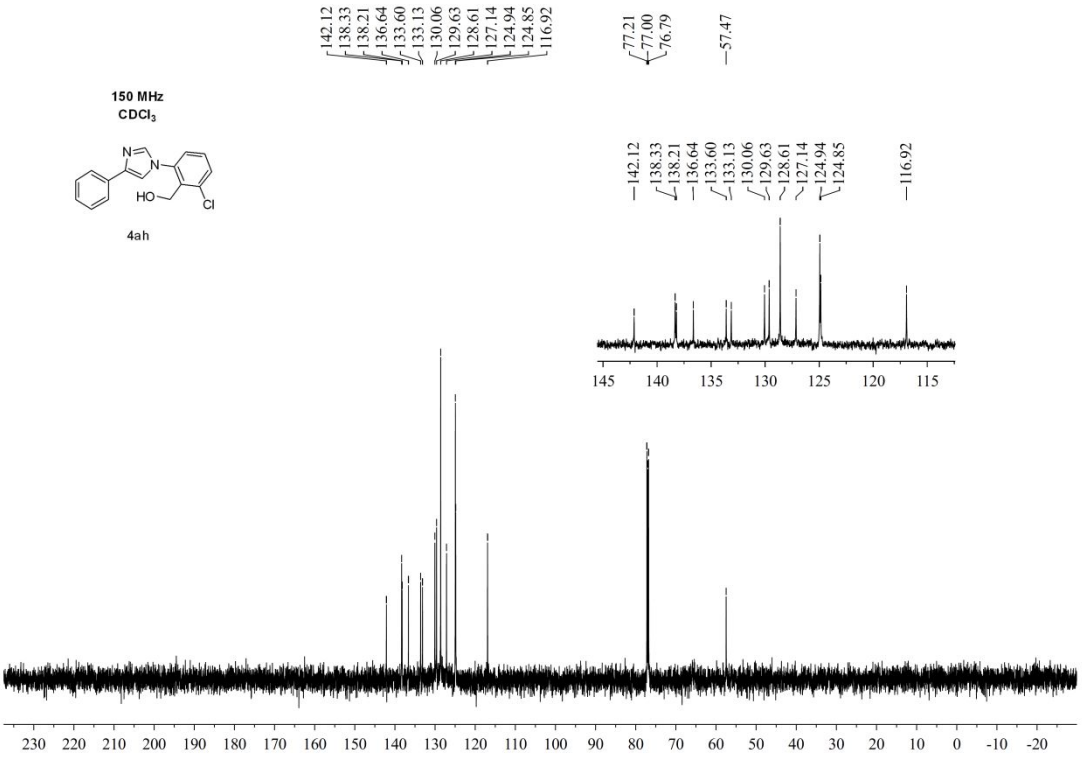

600 MHz
CDCl3
4af
f1 (ppm)

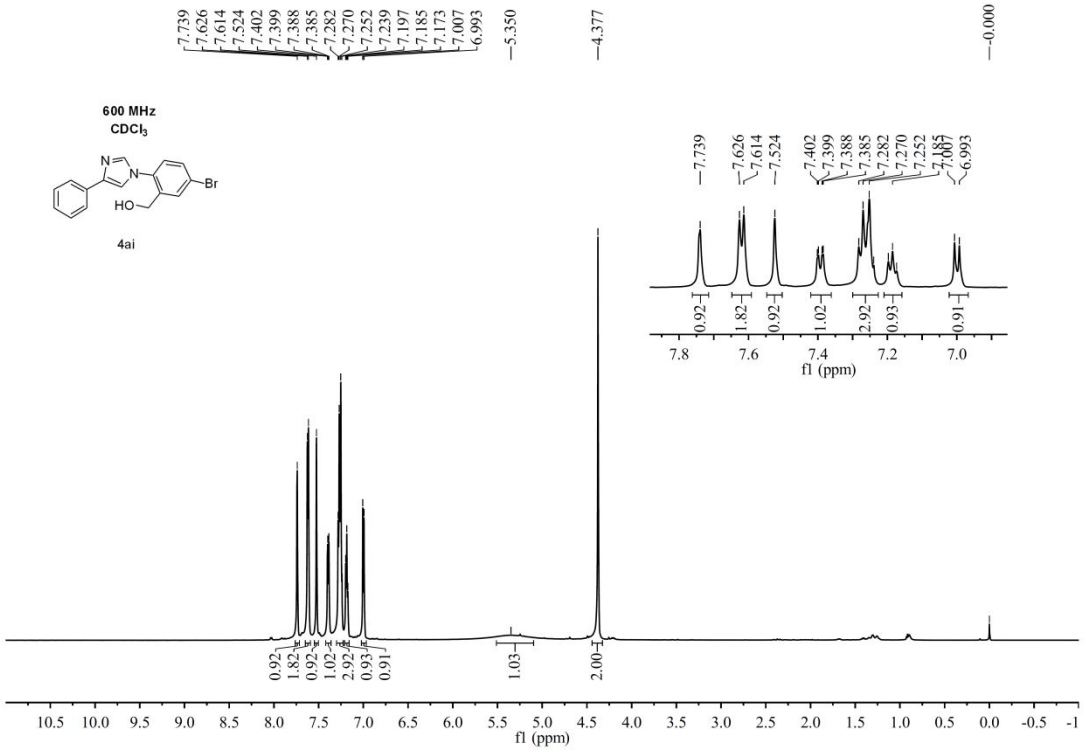

150 MHz
CDCl3
4af
f1 (ppm)

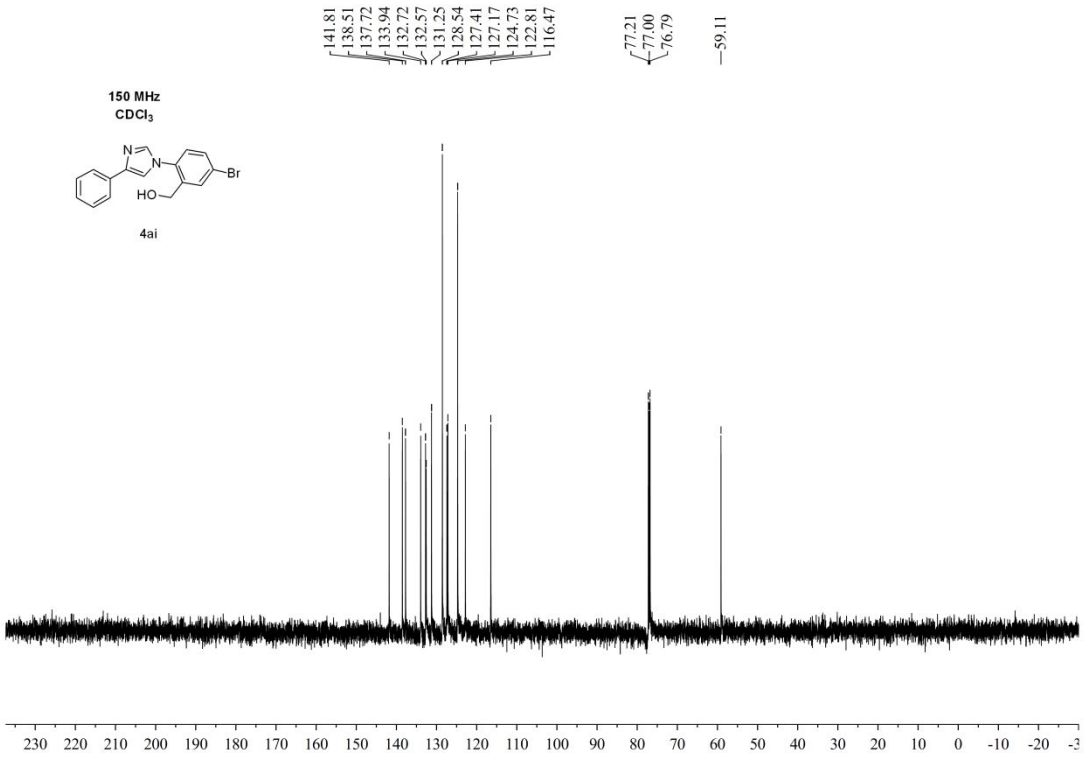

600 MHz
DMSO-d6
4ag
fl (ppm)

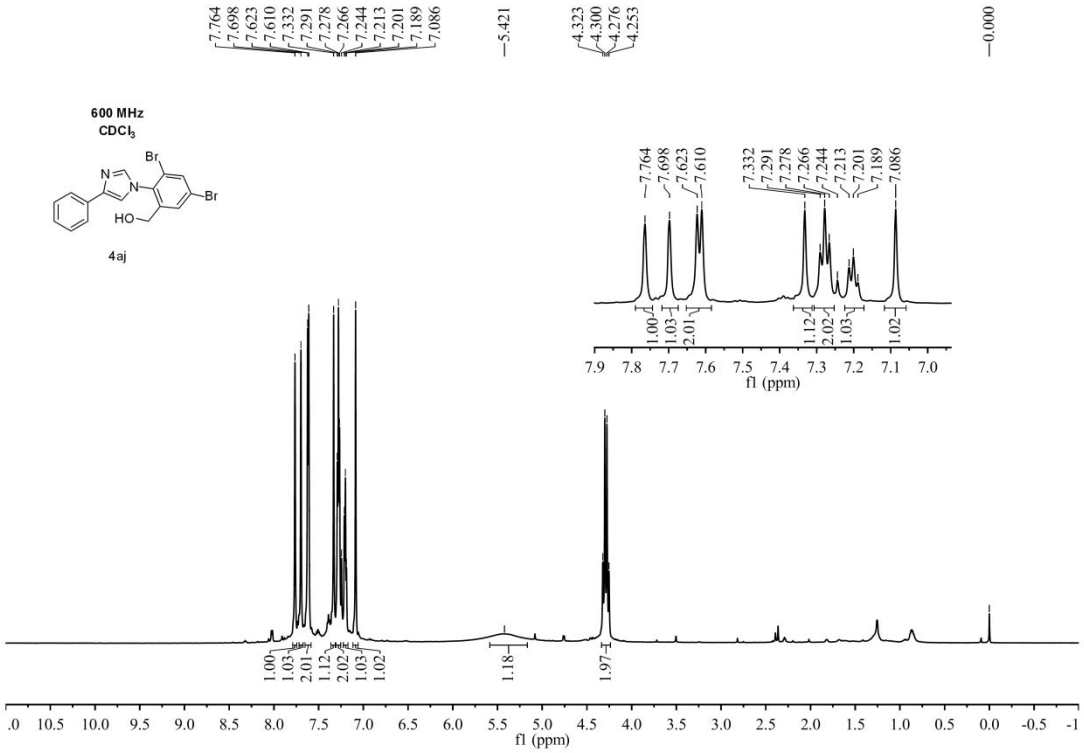

150 MHz
DMSO-d6
4ag

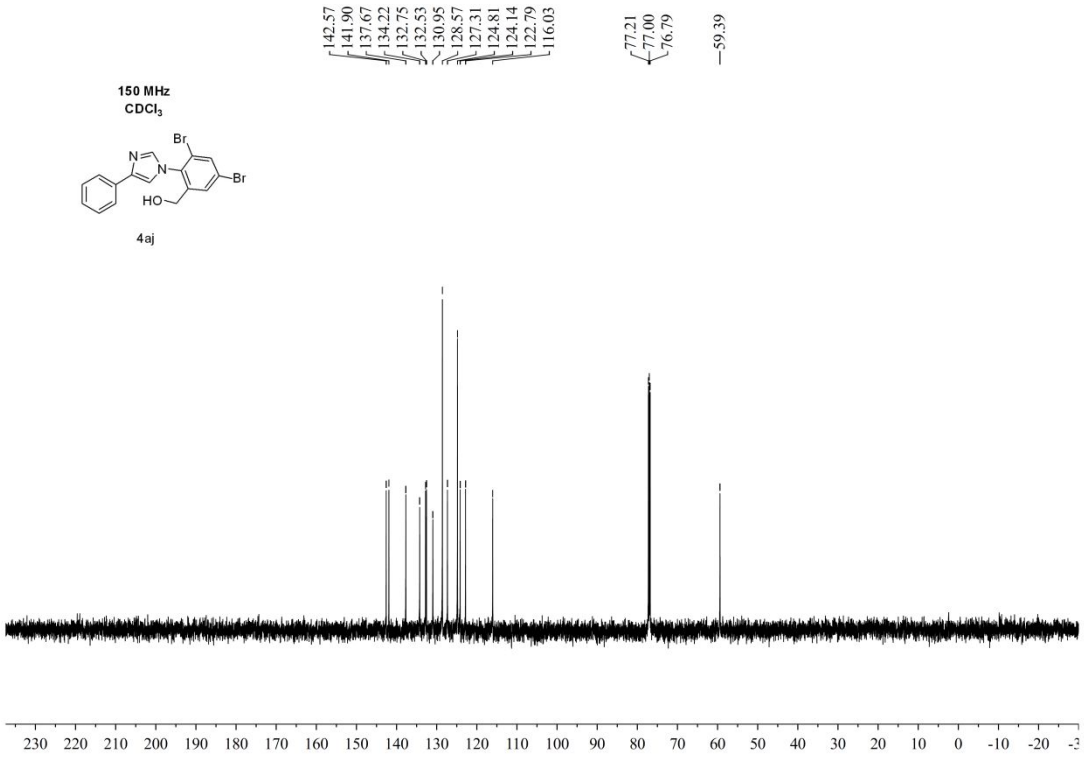

600 MHz
CDCl3
4ah
7.809
7.763
7.752
7.489
7.472
7.353
7.341
7.329
7.316
7.303
7.244
7.231
7.219
7.207
7.195
4.584
0.000
0.93
1.77
1.95
2.97
1.96
2.00
f1 (ppm)

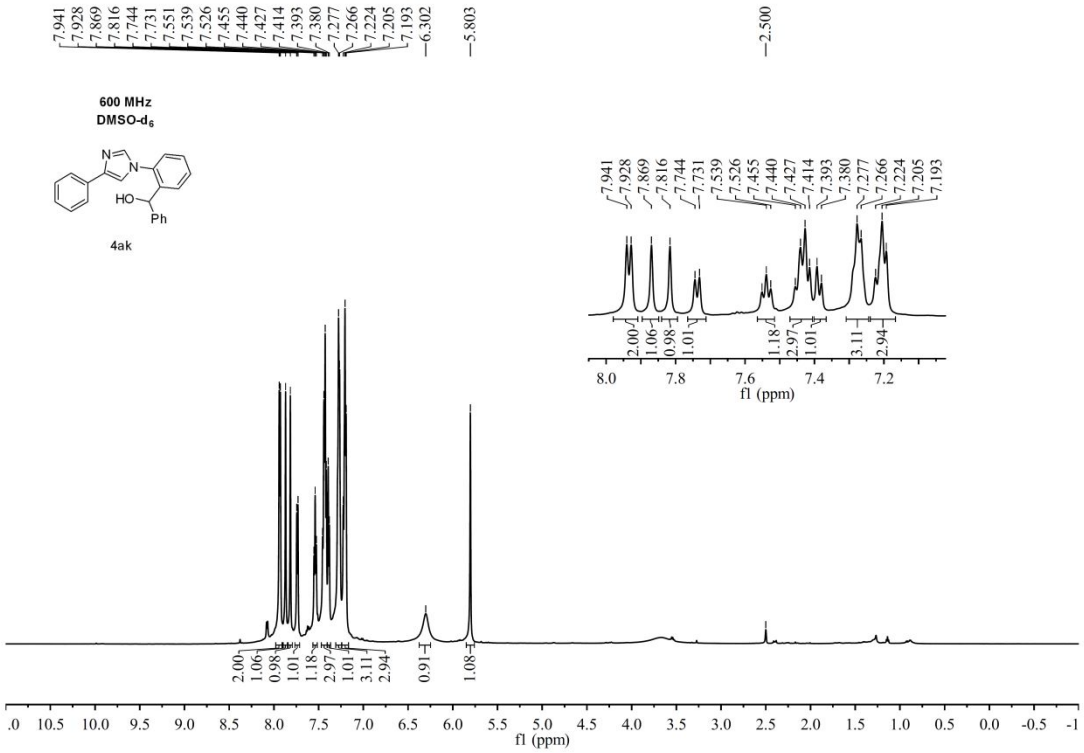

150 MHz
CDCl3
4ah
142.12
138.33
138.21
136.64
133.60
133.13
130.06
129.63
128.61
127.14
124.94
124.85
116.92
77.21
77.00
76.79
57.47

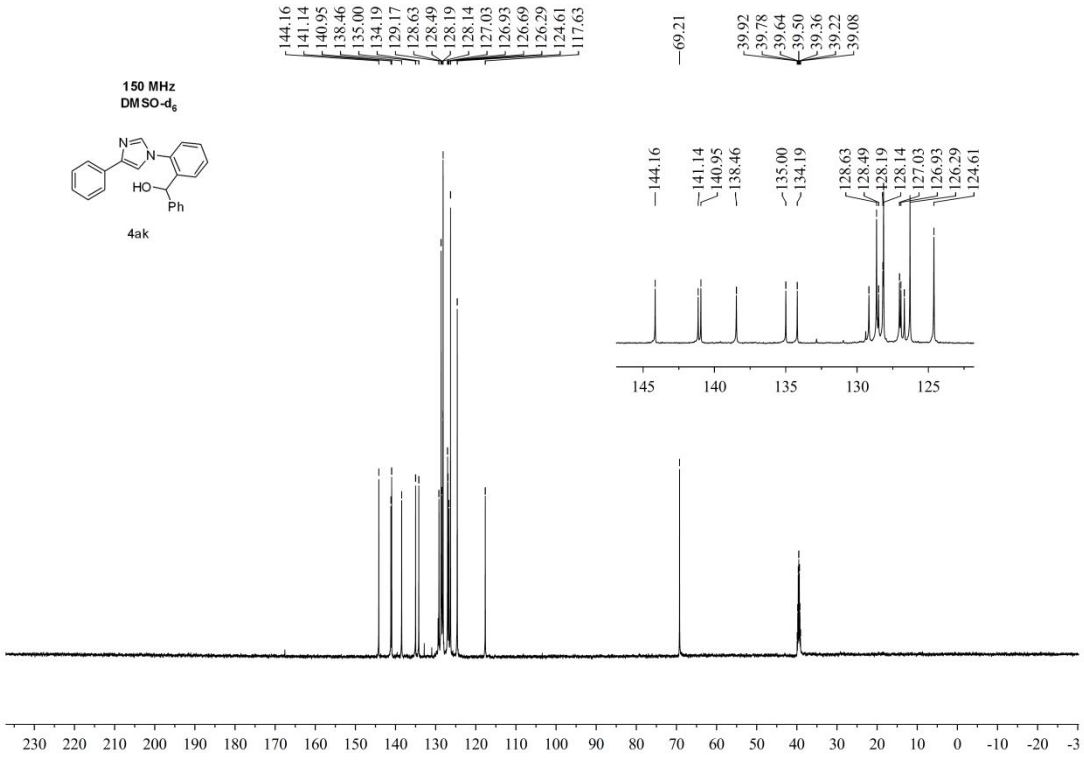

7.739
7.626
7.614
7.524
7.402
7.399
7.388
7.385
7.282
7.270
7.252
7.239
7.197
7.185
7.173
7.007
6.993
5.350
4.377
0.000
600 MHz
CDCl3
N
N
Br
HO
4ai
0.92
1.82
0.92
1.02
2.92
0.93
0.91
1.03
2.00
f1 (ppm)

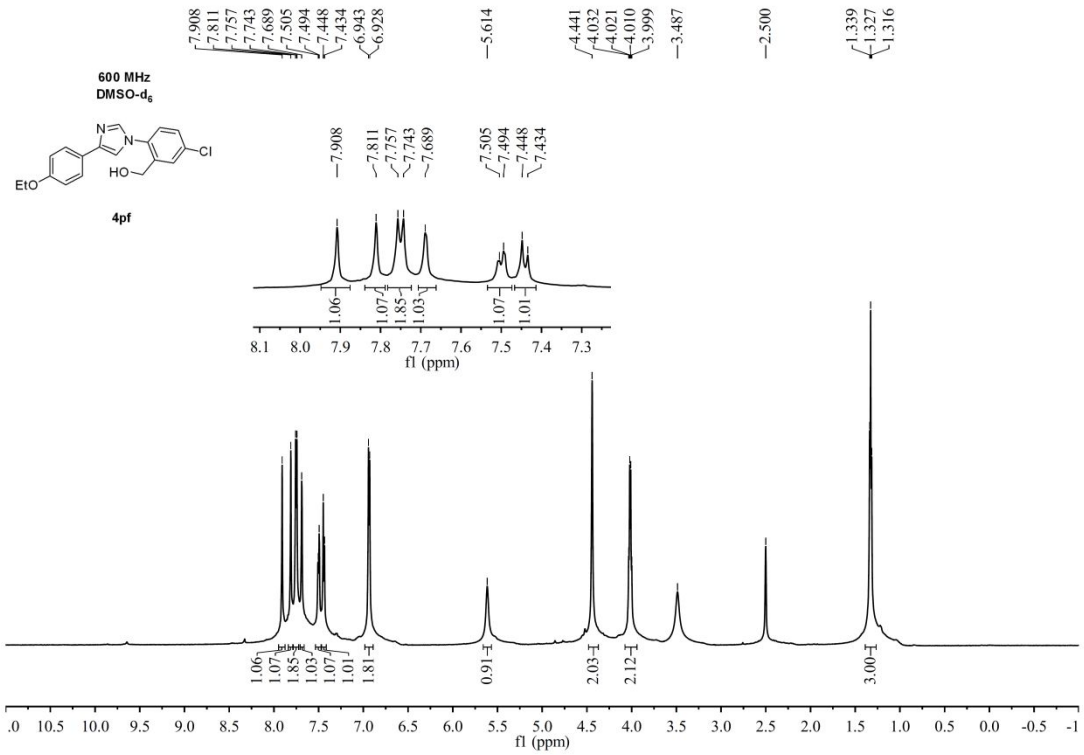

141.81
138.51
137.72
133.94
132.72
132.57
131.25
128.54
127.41
127.17
124.73
122.81
116.47
77.21
77.00
76.79
59.11
150 MHz
CDCl3
N
N
Br
HO
4ai

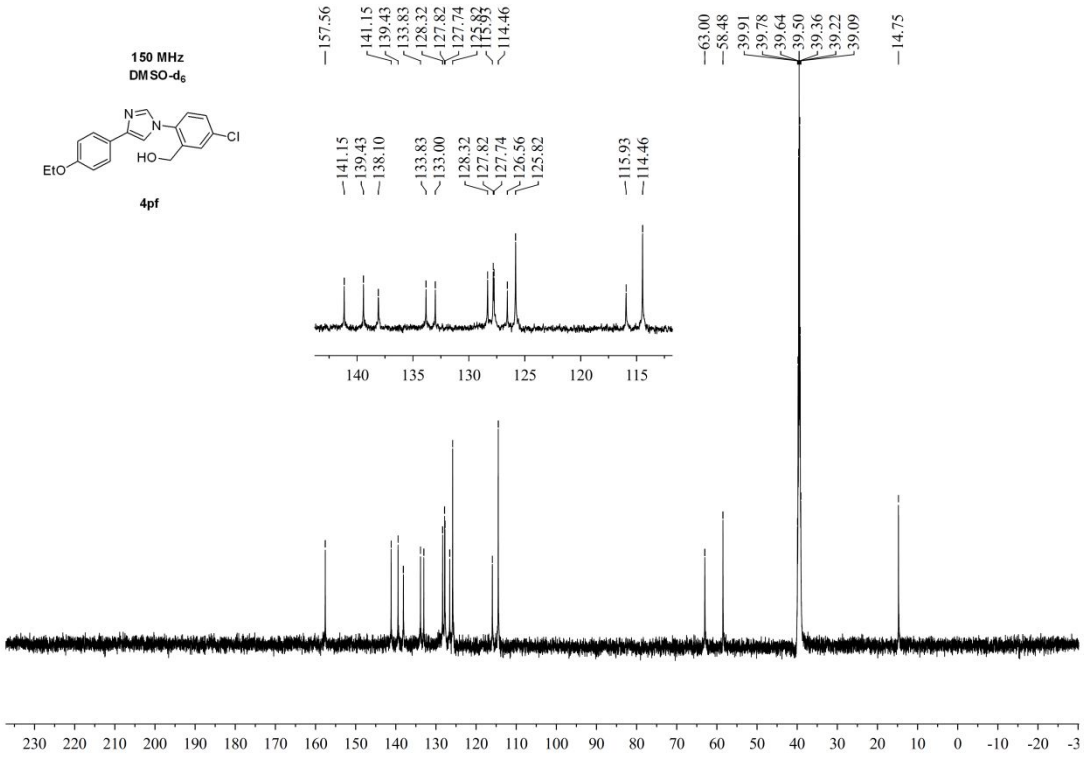

600 MHz
CDCl3
4aj
f1 (ppm)

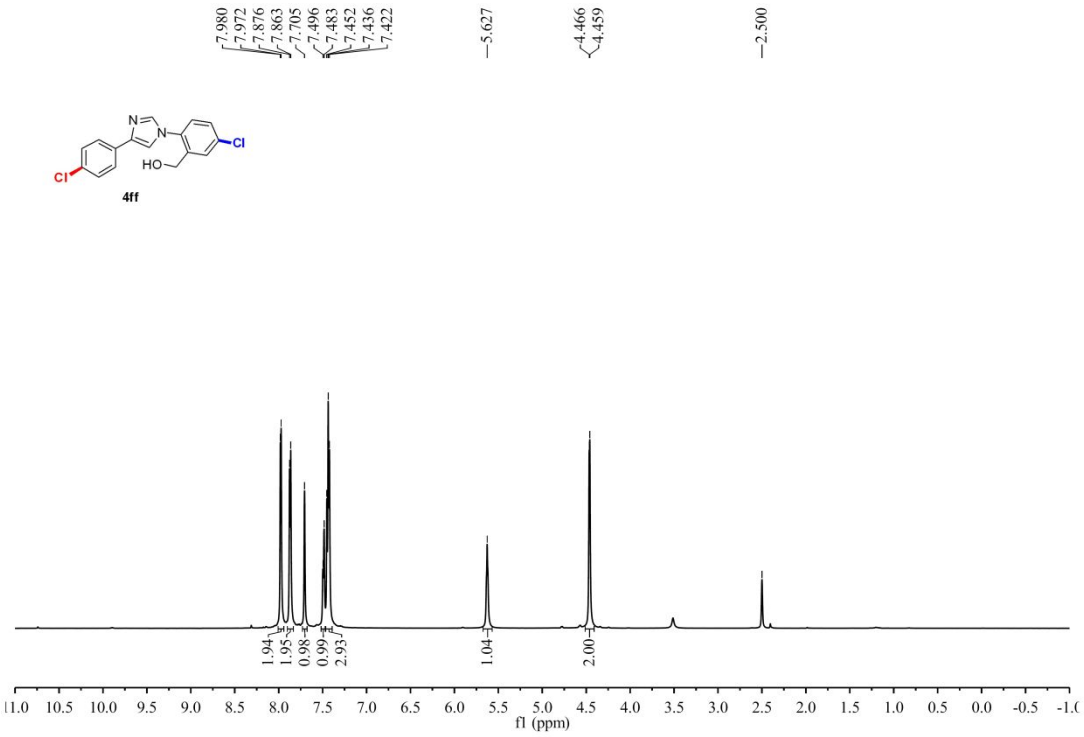

150 MHz
CDCl3
4aj
f1 (ppm)

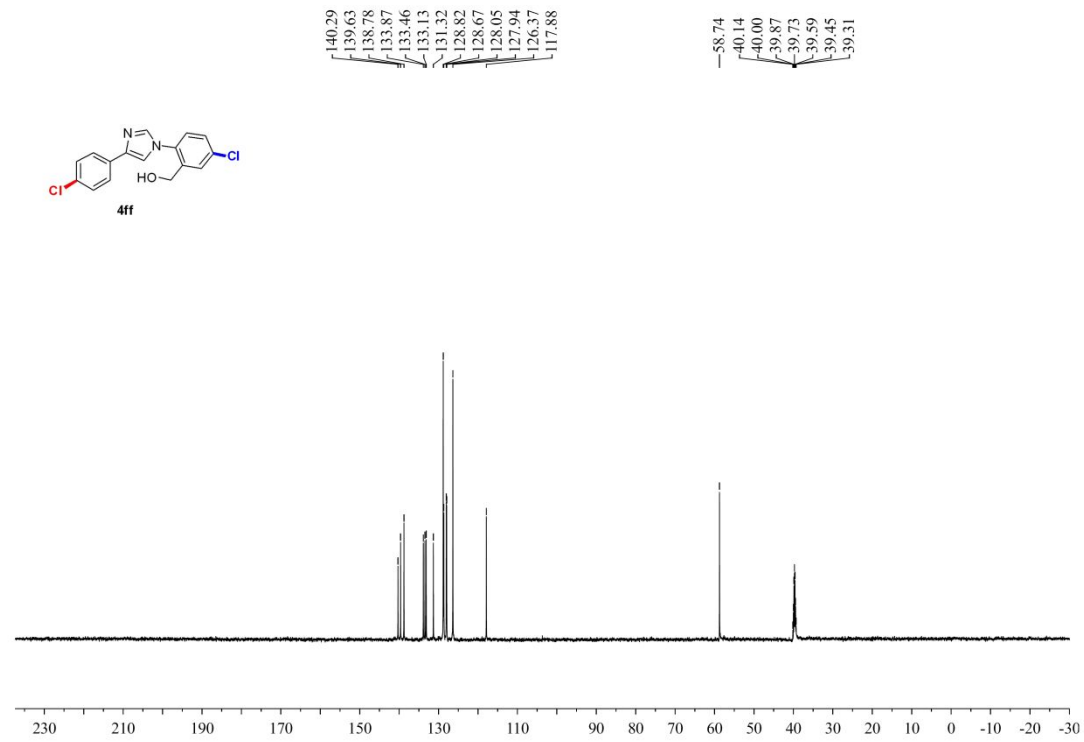

7.941
7.928
7.869
7.816
7.744
7.731
7.551
7.539
7.526
7.455
7.440
7.427
7.414
7.393
7.380
7.277
7.266
7.224
7.205
7.193
6.302
5.803
2.500
600 MHz
DMSO-d6
HO
Ph
4ak
2.00
1.06
0.98
1.01
1.18
2.97
1.01
3.11
2.94
0.91
1.08
fl (ppm)

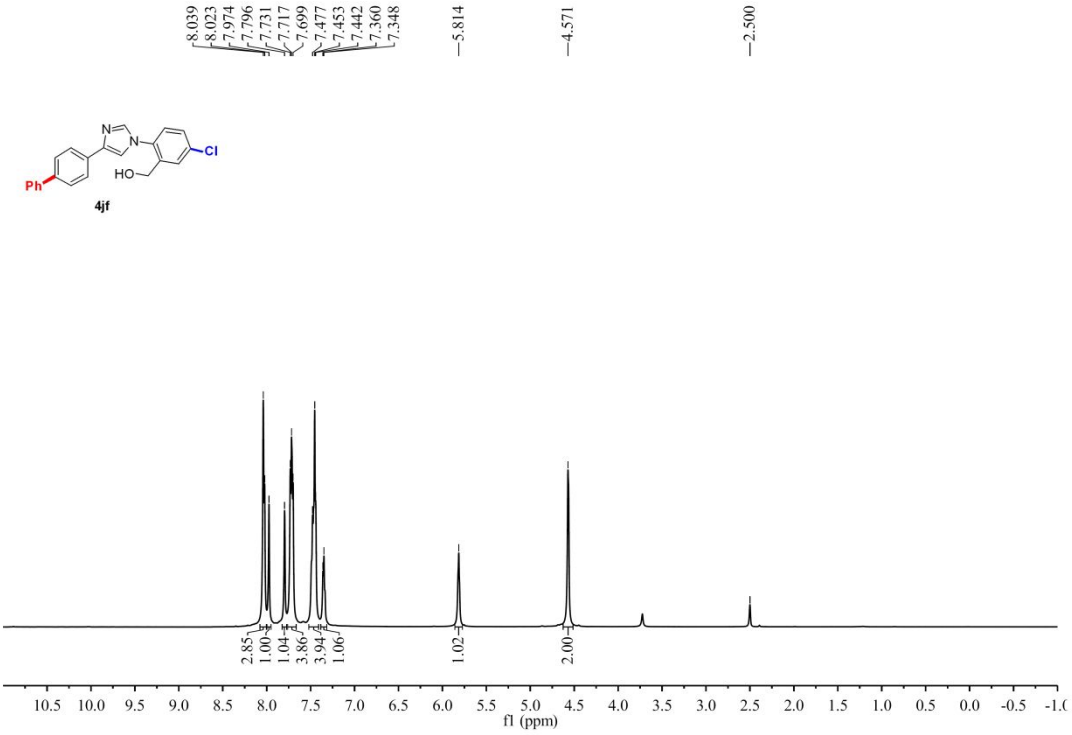

144.16
141.14
140.95
138.46
135.00
134.19
129.17
128.63
128.49
128.19
128.14
127.03
126.93
126.69
126.29
124.61
117.63
69.21
39.92
39.78
39.64
39.50
39.36
39.22
39.08
150 MHz
DMSO-d6
HO
Ph
4ak
fl (ppm)

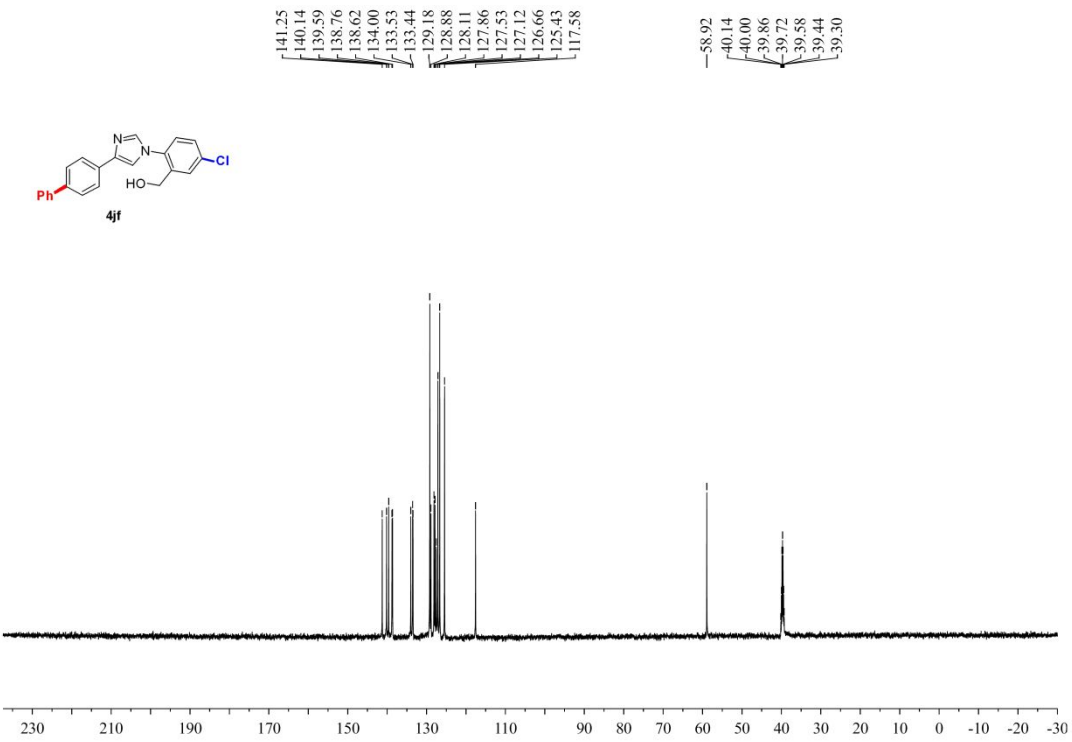

600 MHz
DMSO-d6
4pf
f1 (ppm)

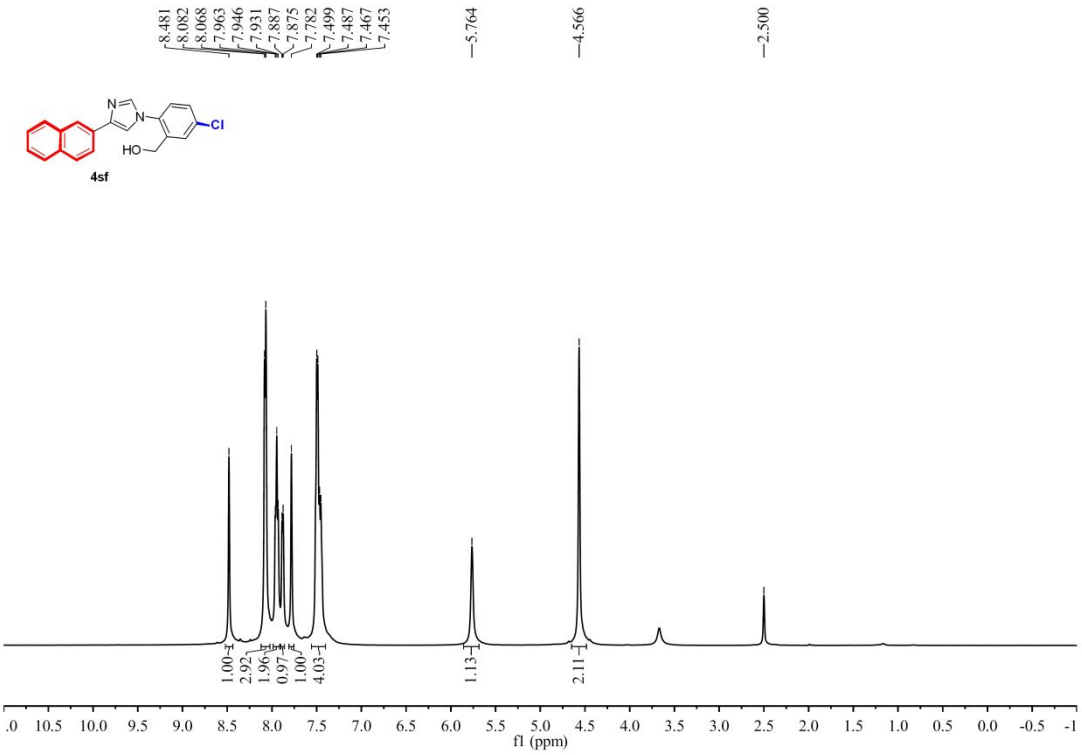

150 MHz
DMSO-d6
4pf
f1 (ppm)

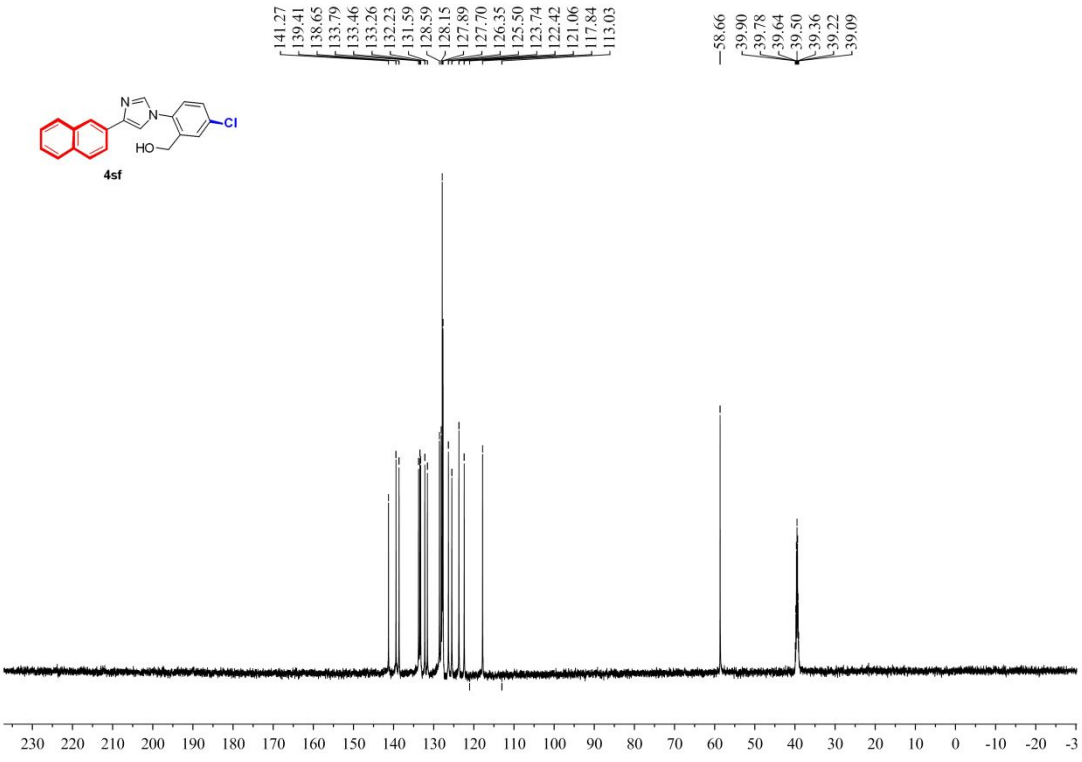

7.980
7.972
7.876
7.863
7.705
7.496
7.483
7.452
7.436
7.422
5.627
4.466
4.459
2.500
N
N
Cl
HO
Cl
4ff
1.94
1.95
0.98
0.99
2.93
1.04
2.00
f1 (ppm)

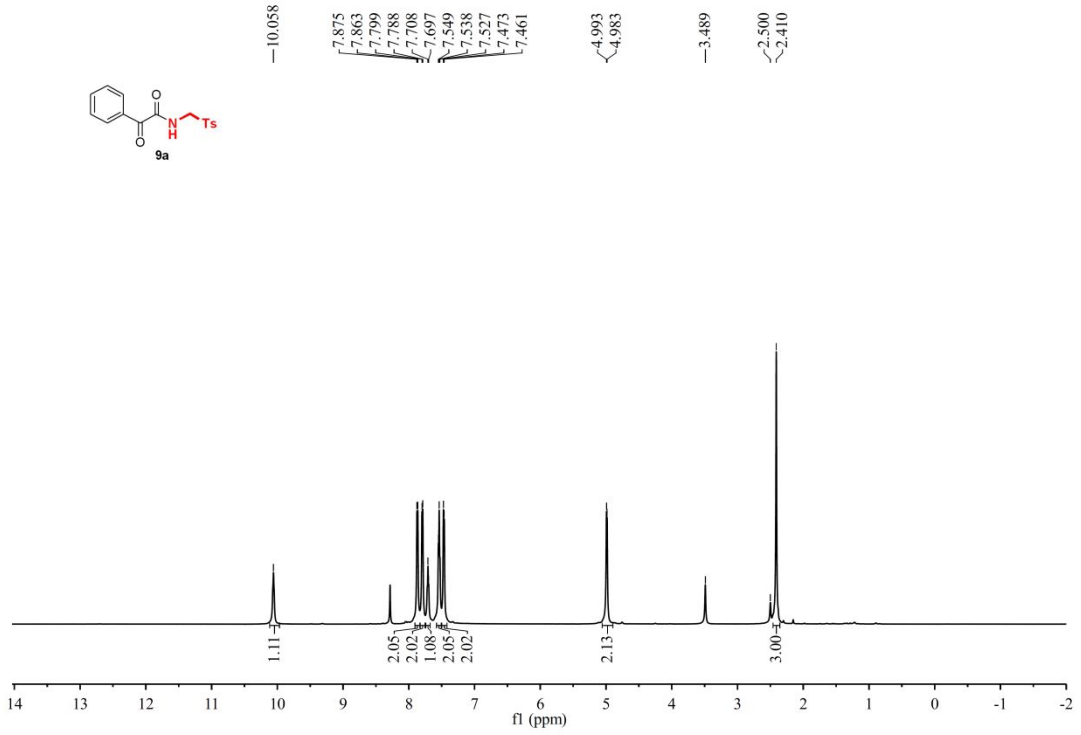

140.29
139.63
138.78
133.87
133.46
133.13
131.32
128.82
128.67
128.05
127.94
126.37
117.88
58.74
40.14
40.00
39.87
39.73
39.59
39.45
39.31
N
N
Cl
HO
Cl
4ff

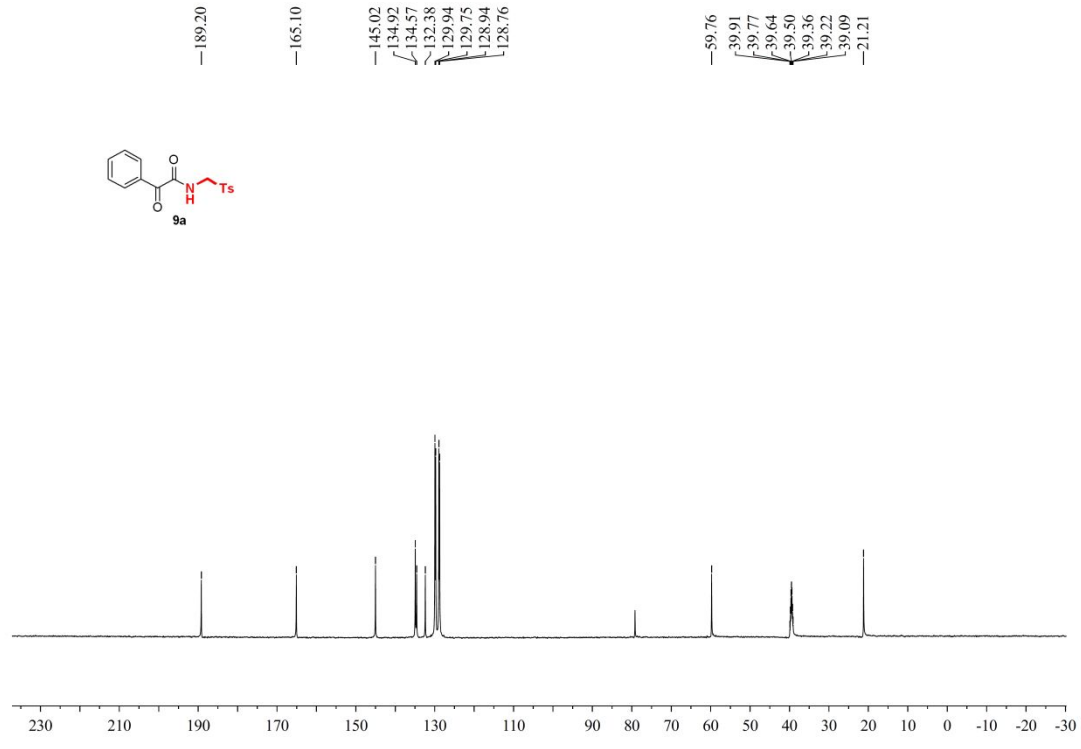

8.039
8.023
7.974
7.796
7.731
7.717
7.699
7.477
7.453
7.442
7.360
7.348
5.814
4.571
2.500
Cl
HO
Ph
4jf
2.85
1.00
1.04
3.86
3.94
1.06
1.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

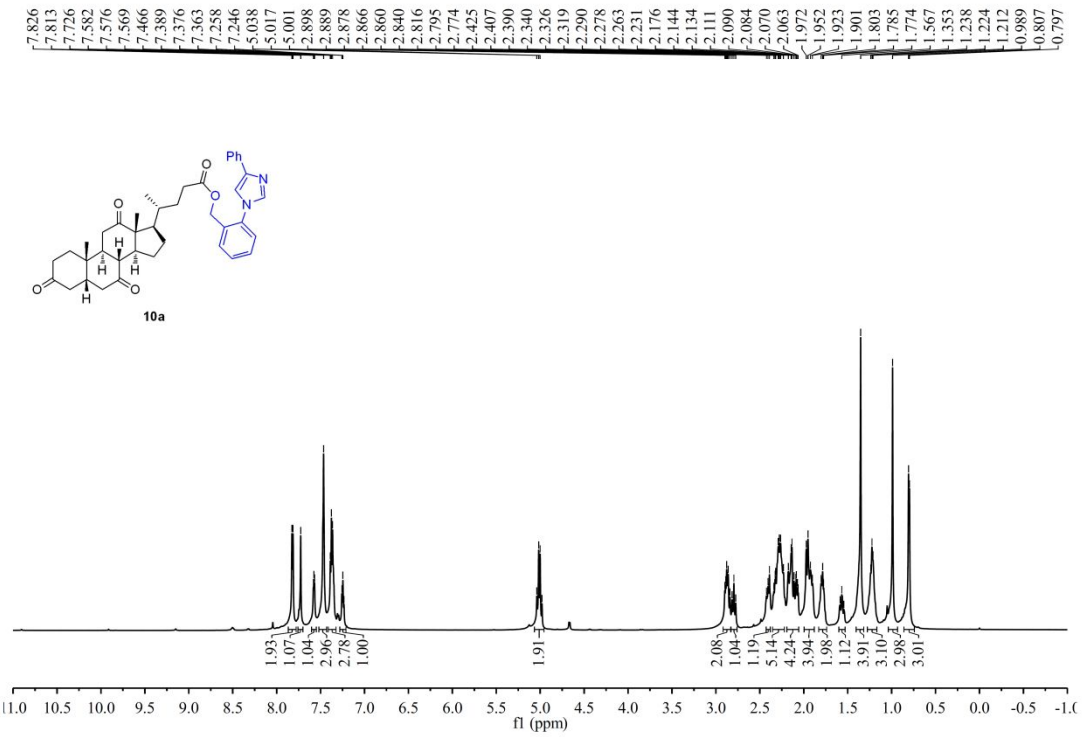

141.25
140.14
139.59
138.76
138.62
134.00
133.53
133.44
129.18
128.88
128.11
127.86
127.53
127.12
126.66
125.43
117.58
58.92
40.14
40.00
39.86
39.72
39.58
39.44
39.30
Cl
HO
Ph
4jf
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20 -30

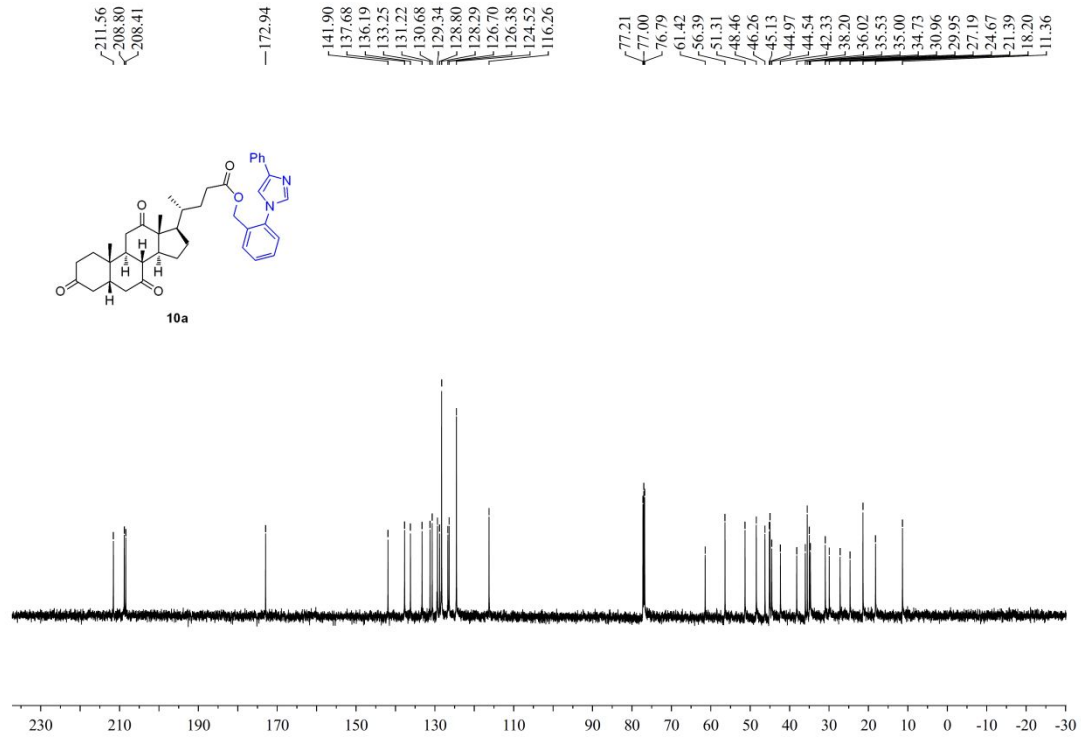

8.481
8.082
8.068
7.963
7.946
7.931
7.887
7.875
7.782
7.499
7.487
7.467
7.453
5.764
4.566
2.500
Cl
HO
4sf
1.00
2.92
1.96
0.97
1.00
4.03
1.13
2.11
f1 (ppm)


141.27
139.41
138.65
133.79
133.46
133.26
132.23
131.59
128.59
128.15
127.89
127.70
126.35
125.50
123.74
122.42
121.06
117.84
113.03
58.66
39.90
39.78
39.64
39.50
39.36
39.22
39.09
Cl
HO
4sf


10.058
7.875
7.863
7.799
7.788
7.708
7.697
7.549
7.538
7.527
7.473
7.461
4.993
4.983
3.489
2.500
2.410
Ts
9a
1.11
2.05
2.02
1.08
2.05
2.02
2.13
3.00
f1 (ppm)


189.20
165.10
145.02
134.92
134.57
132.38
129.94
129.75
128.94
128.76
59.76
39.91
39.77
39.64
39.50
39.36
39.22
39.09
21.21
Ts
9a


7.826
7.813
7.726
7.582
7.576
7.569
7.466
7.389
7.376
7.363
7.258
7.246
5.038
5.017
5.001
2.898
2.889
2.878
2.866
2.860
2.840
2.816
2.795
2.774
2.425
2.407
2.390
2.340
2.326
2.319
2.290
2.278
2.263
2.231
2.176
2.144
2.134
2.111
2.090
2.084
2.070
2.063
1.972
1.952
1.923
1.901
1.803
1.785
1.774
1.567
1.353
1.238
1.224
1.212
0.989
0.807
0.797
Ph
N
O
H
10a
1.93
1.07
1.04
2.96
2.78
1.00
1.91
2.08
1.04
1.19
5.14
4.24
3.94
1.98
1.12
3.91
3.10
2.98
3.01
f1 (ppm)


211.56
208.80
208.41
172.94
141.90
137.68
136.19
133.25
131.22
130.68
129.34
128.80
128.29
126.70
126.38
124.52
116.26
77.21
77.00
76.79
61.42
56.39
51.31
48.46
46.26
45.13
44.97
44.54
42.33
38.20
36.02
35.53
35.00
34.73
30.96
29.95
27.19
24.67
21.39
18.20
11.36
Ph
N
O
H
10a