Supporting Information

Efficient Access to 2,3-diarylimidazo[1,2-a]pyridines via a One-pot, Ligand-free, Palladium-Catalyzed Three-Component Reaction under Microwave Irradiation

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General Information

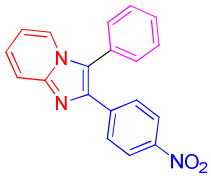
Solvents were purchased from Aldrich or Acros and used without further purification. Other reagents were used as obtained from commercial providers except when otherwise noted. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel plates available from EMD. Visualization was accomplished with UV light. Column chromatography was performed using Biotage chromatographic systems. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian Inova instrument (400 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the residual undeuterated solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, *J*, were reported in Hertz unit (Hz). Low and high resolution mass spectra were obtained using ESI methods.

General procedure for the preparation of compounds 2 and 6

In a 25 mL microwave tube aminopyridine (1, 1 mmol), 2-bromophenylethanone (2, 1 mmol), phenyl bromide (3, 2 mmol), and KoAc (2 mmol) were taken in 6 mL DMF. The above mixture was purged with nitrogen for 1 minute and then $Pd(OAc)_2$ (10 mol %) was added. The tube was sealed with a pressure cap and irradiated in a Bitage microwave for indicated time at 160 ^{o}C. After cooling to room temperature, the mixture was diluted with ethyl acetate (20 mL) and washed with water, brine, and dried over anhydrous Na_2SO_4. The organic solvent was removed under vacuum to get the crude product, which is purified using Biotage chromatographic systems.

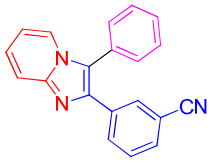
Characterization of 4 and 6

3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine (4aaa)



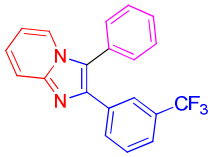
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.27 (m, 2H), 8.08 (dt, *J* = 7.0, 1.2 Hz, 1H), 7.71 (dt, *J* = 9.1, 1.2 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.60 – 7.53 (m, 2H), 7.37 – 7.26 (m, 4H), 6.84 (td, *J* = 6.9, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 145.6, 144.4, 136.6, 133.4, 131.0, 128.5, 128.4, 128.1, 125.6, 124.6, 122.8, 118.7, 117.9, 113.1; $[M+H]^+$ = 316.

3-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzonitrile (4aab)



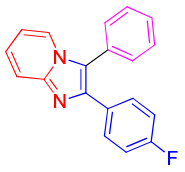
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.92 (m, 1H), 7.77 – 7.70 (m, 2H), 7.69 – 7.65 (m, 2H), 7.61 (dd, *J* = 7.4, 0.8 Hz, 1H), 7.58 – 7.55 (m, 2H), 7.30 – 7.22 (m, 4H), 6.78 (td, *J* = 6.8, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 143.5, 135.1, 133.8, 133.4, 132.1, 131.4, 130.5, 128.4, 128.1, 127.9, 125.3, 122.7, 118.4, 118.0, 117.7, 113.8, 112.9; $[M+H]^+$ = 296.

2-phenyl-3-(3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine (4aac)



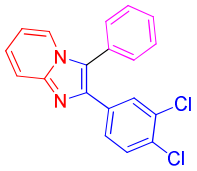
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dt, *J* = 7.1, 1.2 Hz, 1H), 7.75 (s, 1H), 7.75 – 7.69 (m, 2H), 7.66 – 7.54 (m, 4H), 7.32 – 7.19 (m, 4H), 6.76 (td, *J* = 6.9, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 143.1, 134.1 (q, *J* = 1 Hz), 133.5, 131.9 (q, *J* = 33 Hz), 130.7, 130.1, 128.3, 128.1, 127.8, 127.2 (q, *J* = 3 Hz), 125.5 (q, *J* = 4 Hz), 125.2, 123.7 (q, *J* = 271 Hz), 122.8, 119.3, 117.6, 112.8; $[M+H]^+$ = 339.

3-(4-fluorophenyl)-2-phenylimidazo[1,2-a]pyridine (4aad)



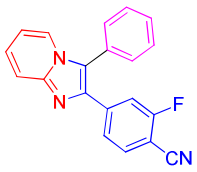
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.0 Hz, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.70 – 7.55 (m, 2H), 7.48 – 7.35 (m, 2H), 7.33 – 7.18 (m, 6H), 6.76 (t, *J* = 6.6 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 248 Hz), 144.5, 142.1, 133.6, 132.7 (d, *J* = 8 Hz), 128.2 (d, *J* = 32 Hz), 128.0, 127.6, 125.6 (d, *J* = 4 Hz), 125.0, 123.1, 119.9, 117.4, 116.9, 116.7; $[M+H]^+$ = 289.

3-(3,4-dichlorophenyl)-2-phenylimidazo[1,2-a]pyridine (4aae)



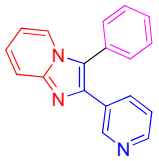
white solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.93 (dt, *J* = 7.0, 1.2 Hz, 1H), 7.67 (dt, *J* = 9.1, 1.2 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.61 – 7.48 (m, 2H), 7.33 – 7.18 (m, 5H), 6.79 – 6.74 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 142.2, 132.6, 132.5, 132.0, 131.0, 130.5, 129.0, 128.8, 127.4, 127.0, 126.8, 124.1, 121.8, 117.3, 116.6, 111.7; $[M+H]^+$ = 339.

2-fluoro-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzonitrile (4aaf)



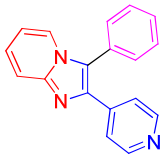
White solid. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.29 (dt, *J* = 6.9, 1.2 Hz, 1H), 8.16 – 8.00 (m, 1H), 7.79 (dd, *J* = 10.3, 1.5 Hz, 1H), 7.71 (dt, *J* = 9.1, 1.2 Hz, 1H), 7.63 – 7.52 (m, 2H), 7.49 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.44 – 7.25 (m, 4H), 6.97 (td, *J* = 6.8, 1.2 Hz, 1H). ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 163.3 (d, *J* = 246 Hz), 145.2, 143.4, 137.5 (d, *J* = 9 Hz), 135.2, 133.9, 128.9, 128.5 (d, *J* = 44 Hz), 128.4, 128.3, 128.0 (d, *J* = 4 Hz), 126.6, 124.5, 118.6 (d, *J* = 30 Hz), 117.5, 114.3, 113.6; $[M+H]^+$ = 314; HRMS calculated for $C_{20}H_{13}FN_3$ $[M+H]^+$, 314.3352; found 314.3356.

2-phenyl-3-(pyridin-3-yl)imidazo[1,2-a]pyridine (4aag)



Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (p, *J* = 4.4, 3.4 Hz, 2H), 7.99 – 7.93 (m, 1H), 7.78 (ddq, *J* = 7.4, 4.0, 1.9 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.62 (dq, *J* = 7.5, 1.8 Hz, 2H), 7.46 (dq, *J* = 7.4, 3.0, 1.6 Hz, 1H), 7.36 – 7.23 (m, 4H), 6.79 (qd, *J* = 5.9, 5.3, 2.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 149.8, 145.3, 143.7, 138.2, 133.5, 128.4, 128.1, 127.8, 125.2, 122.8, 117.7, 117.4, 112.8; $[M+H]^+$ = 272.

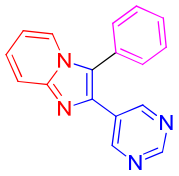
2-phenyl-3-(pyridin-4-yl)imidazo[1,2-a]pyridine (4aah)



Yellow Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 – 8.72 (m, 2H), 8.11 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.71 (dt, *J* = 9.0, 1.2 Hz, 1H), 7.65 – 7.53 (m, 2H), 7.43 – 7.35 (m, 2H), 7.35 – 7.23 (m, 4H), 6.82 (td, *J* = 6.9, 1.2 Hz, 1H). ^{13}C NMR (100 MHz,

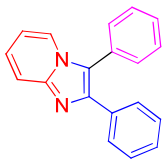
$CDCl_3$) δ 144.7, 142.0, 133.7, 130.7, 129.9, 129.5, 128.8, 128.3, 128.2, 127.5, 125.0, 123.3, 121.0, 117.3, 112.4; $[M+H]^+$ = 272.

2-phenyl-3-(pyrimidin-5-yl)imidazo[1,2-a]pyridine (4aai)



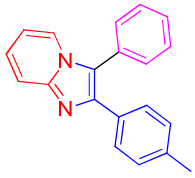
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.31 (d, *J* = 1.1 Hz, 1H), 8.86 (d, *J* = 1.1 Hz, 2H), 8.00 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.74 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.59 – 7.57 (m, 2H), 7.32 (td, *J* = 7.1, 6.6, 1.1 Hz, 4H), 6.88 – 6.85 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 158.1, 145.9, 145.1, 133.0, 128.7, 128.2, 125.7, 125.0, 122.4, 118.1, 113.9, 113.3; $[M+H]^+$ = 273.

2,3-diphenylimidazo[1,2-a]pyridine (4aaj)



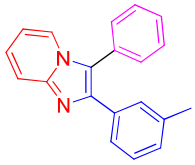
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 1H), 7.77 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.52 – 7.43 (m, 5H), 7.30 – 7.19 (m, 4H), 6.75 – 6.71 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 142.1, 130.7, 129.9, 129.5, 128.9, 128.3, 128.2, 128.1, 127.5, 124.9, 123.2, 117.4, 112.4; $[M+H]^+$ = 271.

2-phenyl-3-p-tolylimidazo[1,2-a]pyridine (4aak)



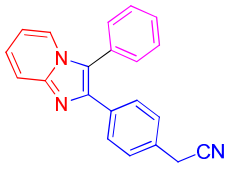
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 6.9, 1.2 Hz, 1H), 7.73 – 7.64 (m, 3H), 7.33 – 7.21 (m, 7H), 7.19 – 7.14 (m, 1H), 6.72 – 6.67 (m, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 142.1, 138.8, 134.1, 130.5, 130.2, 128.2, 127.9, 127.3, 126.6, 124.5, 123.3, 121.1, 117.4, 112.1, 21.4; $[M+H]^+$ = 285.

2-phenyl-3-m-tolylimidazo[1,2-a]pyridine (4aal)



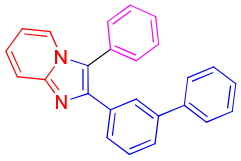
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.75 – 7.58 (m, 3H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.32 – 7.19 (m, 6H), 7.17 (ddd, *J* = 9.1, 6.7, 1.3 Hz, 1H), 6.70 (td, *J* = 6.8, 1.2 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 142.1, 139.2, 134.2, 131.1, 129.7, 129.6, 129.4, 128.2, 128.0, 127.8, 127.4, 124.5, 123.3, 121.2, 117.4, 112.1, 21.4; $[M+H]^+$ = 285.

2-(4-(2-phenylimidazo[1,2-a]pyridin-3-yl)phenyl)acetonitrile (4aam)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.70 (dt, *J* = 9.0, 1.2 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.49 (d, *J* = 1.4 Hz, 4H), 7.32 – 7.20 (m, 4H), 6.76 (td, *J* = 6.8, 1.2 Hz, 1H), 3.86 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 142.7, 133.8, 131.4, 130.6, 129.8, 129.2, 128.3, 128.0, 127.6, 124.9, 123.0, 120.0, 117.6, 117.4, 112.5, 23.5; $[M+H]^+$ = 310.

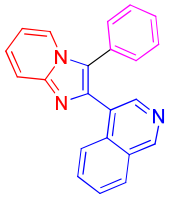
3-(biphenyl-3-yl)-2-phenylimidazo[1,2-a]pyridine (4aan)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.80 – 7.64 (m, 5H), 7.62 – 7.52 (m, 3H), 7.46 – 7.39 (m, 3H), 7.37 – 7.24 (m, 4H), 7.20 (ddd, *J* = 9.1, 6.7, 1.3 Hz, 1H), 6.74 (td, *J* = 6.8, 1.2

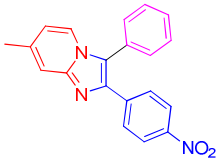
Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 142.5, 142.4, 140.2, 134.0, 130.4, 129.9, 129.5, 129.2, 128.8, 128.3, 128.1, 127.7, 127.6, 127.5, 127.1, 124.6, 123.2, 120.9, 117.6, 112.3; $[M+H]^+$ = 347; HRMS calculated for $C_{25}H_{19}N_2$ $[M+H]^+$, 347.4312; found 347.4310.

4-(2-phenylimidazo[1,2-a]pyridin-3-yl)isoquinoline (4aao)



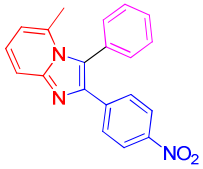
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 – 9.41 (m, 1H), 8.62 (s, 1H), 8.13 (dt, *J* = 8.3, 1.0 Hz, 1H), 7.77 (dt, *J* = 9.1, 1.2 Hz, 1H), 7.67 – 7.56 (m, 4H), 7.49 (dt, *J* = 6.9, 1.2 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.26 – 7.16 (m, 4H), 6.68 – 6.64 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 146.1, 145.5, 144.5, 134.9, 133.6, 131.6, 128.6, 128.4, 128.3, 128.0, 127.7, 127.5, 125.1, 124.0, 123.6, 121.4, 117.6, 115.4, 112.5; $[M+H]^+$ = 322; HRMS calculated for $C_{22}H_{16}N_3$ $[M+H]^+$, 322.3820; found 322.3825.

6-methyl-3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine (4baa)



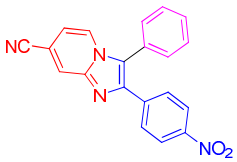
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.31 (m, 2H), 7.86 (dd, *J* = 1.8, 1.0 Hz, 1H), 7.65 – 7.60 (m, 3H), 7.57 – 7.53 (m, 2H), 7.32 – 7.27 (m, 3H), 7.13 (dd, *J* = 9.2, 1.7 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.2, 144.6, 144.0, 136.8, 133.5, 131.0, 128.8, 128.4, 128.3, 128.0, 124.6, 122.9, 120.4, 118.5, 117.2, 18.3; $[M+H]^+$ = 330.

8-methyl-3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine (4caa)



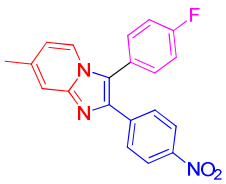
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.22 (m, 2H), 7.68 – 7.59 (m, 3H), 7.47 – 7.37 (m, 2H), 7.23 (dd, *J* = 5.1, 2.0 Hz, 3H), 7.17 (dd, *J* = 9.0, 6.8 Hz, 1H), 6.57 – 6.51 (m, 1H), 2.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 146.6, 144.2, 139.8, 135.9, 133.7, 133.6, 128.3, 128.2, 127.7, 125.3, 122.9, 119.4, 116.0, 114.1, 22.2; $[M+H]^+$ = 330.

3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine-6-carbonitrile (4daa)



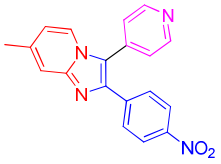
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.35 (m, 2H), 7.80 (dd, *J* = 9.3, 1.0 Hz, 1H), 7.73 – 7.61 (m, 3H), 7.60 – 7.55 (m, 2H), 7.38 (dd, *J* = 9.3, 1.6 Hz, 1H), 7.34 (dd, *J* = 5.1, 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 146.3, 144.6, 134.9, 132.1, 129.0, 128.9, 128.7, 128.4, 125.2, 125.1, 119.7, 118.9, 116.2; $[M+H]^+$ = 341; HRMS calculated for C20H13N4O2 $[M+H]^+$, 341.3423; found 341.3424.

2-(4-fluorophenyl)-6-methyl-3-(4-nitrophenyl)imidazo[1,2-a]pyridine (4bba)



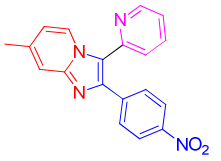
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.28 (m, 2H), 7.85 (q, *J* = 1.3 Hz, 1H), 7.66 – 7.59 (m, 3H), 7.53 (dd, *J* = 8.8, 5.4 Hz, 2H), 7.14 (dd, *J* = 9.2, 1.7 Hz, 1H), 6.99 (t, *J* = 8.7 Hz, 2H), 2.32 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5 (d, *J* = 247 Hz), 147.3, 144.7, 143.2, 136.6, 131.0, 130.1 (d, *J* = 8 Hz), 129.7 (d, *J* = 8 Hz), 128.9, 124.7, 123.0, 120.4, 118.3, 117.1, 115.5 (d, *J* = 21 Hz), 18.3; $[M+H]^+$ = 348.

6-methyl-3-(4-nitrophenyl)-2-(pyridin-4-yl)imidazo[1,2-a]pyridine (4bca)



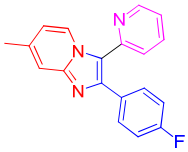
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 – 8.50 (m, 2H), 8.50 – 8.31 (m, 2H), 7.77 (q, *J* = 1.3 Hz, 1H), 7.72 – 7.56 (m, 3H), 7.54 – 7.41 (m, 2H), 7.19 (dd, *J* = 9.2, 1.7 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 147.9, 144.8, 141.3, 140.7, 136.0, 131.3, 129.4, 124.9, 123.6, 122.2, 120.5, 120.0, 117.5, 18.3; $[M+H]^+$ = 331.

6-methyl-3-(4-nitrophenyl)-2-(pyridin-2-yl)imidazo[1,2-a]pyridine (4bda)



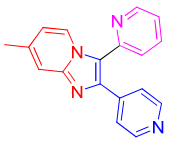
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 8.37 – 8.33 (m, 2H), 8.00 – 7.96 (m, 1H), 7.83 – 7.81 (m, 1H), 7.74 – 7.69 (m, 3H), 7.63 (dd, *J* = 9.2, 0.9 Hz, 1H), 7.18 – 7.13 (m, 2H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 149.1, 147.3, 144.5, 142.7, 137.0, 136.3, 131.6, 129.0, 123.9, 123.1, 122.6, 122.5, 120.6, 117.5, 18.4; $[M+H]^+$ = 331; HRMS calculated for $C_{19}H_{15}N_4O_2$ $[M+H]^+$, 331.3475; found 331.3472.

3-(4-fluorophenyl)-6-methyl-2-(pyridin-2-yl)imidazo[1,2-a]pyridine (4bdd)



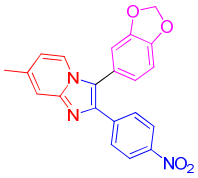
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (ddd, *J* = 4.8, 1.9, 0.9 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.62 – 7.56 (m, 2H), 7.50 – 7.44 (m, 2H), 7.21 (t, *J* = 8.7 Hz, 2H), 7.12 – 7.04 (m, 2H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 250 Hz), 153.3, 149.4. 143.9, 141.6, 135.9, 132.7 (d, *J* = 11 Hz), 128.2, 125.9 (d, *J* = 6 Hz), 122.3, 121.9, 121.6, 120.8, 117.3, 116.1 (d, *J* = 21 Hz), 18.3; $[M+H]^+$ = 304.

6-methyl-2-(pyridin-2-yl)-3-(pyridin-4-yl)imidazo[1,2-a]pyridine (4bdh)



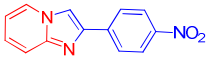
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 – 8.71 (m, 2H), 8.46 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.91 (dt, J = 7.9, 1.1 Hz, 1H), 7.85 (p, J = 1.1 Hz, 1H), 7.68 (td, J = 7.7, 1.8 Hz, 1H), 7.62 (dd, J = 9.2, 0.9 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.19 – 7.09 (m, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 150.3, 149.1, 144.4, 142.6, 138.2, 136.2, 128.9, 125.1, 122.9, 122.4, 121.3, 120.7, 119.9, 117.5, 18.4; $[M+H]^+$ = 287; HRMS calculated for $C_{18}H_{15}N_4$ $[M+H]^+$, 287.3380; found 287.3384.

2-(benzo[d][1,3]dioxol-5-yl)-6-methyl-3-(4-nitrophenyl)imidazo[1,2-a]pyridine (4bea)



Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.30 (m, 2H), 7.84 – 7.80 (m, 1H), 7.67 – 7.58 (m, 3H), 7.12 (dd, *J* = 9.2, 1.7 Hz, 1H), 7.08 – 6.97 (m, 2H), 6.75 (d, *J* = 7.9 Hz, 1H), 5.96 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 147.5, 147.2, 144.6, 144.0, 136.9, 131.0, 128.7, 127.6, 124.7, 122.8, 122.4, 120.3, 117.1, 108.8, 108.4, 101.1, 18.3; $[M+H]^+$ = 374.

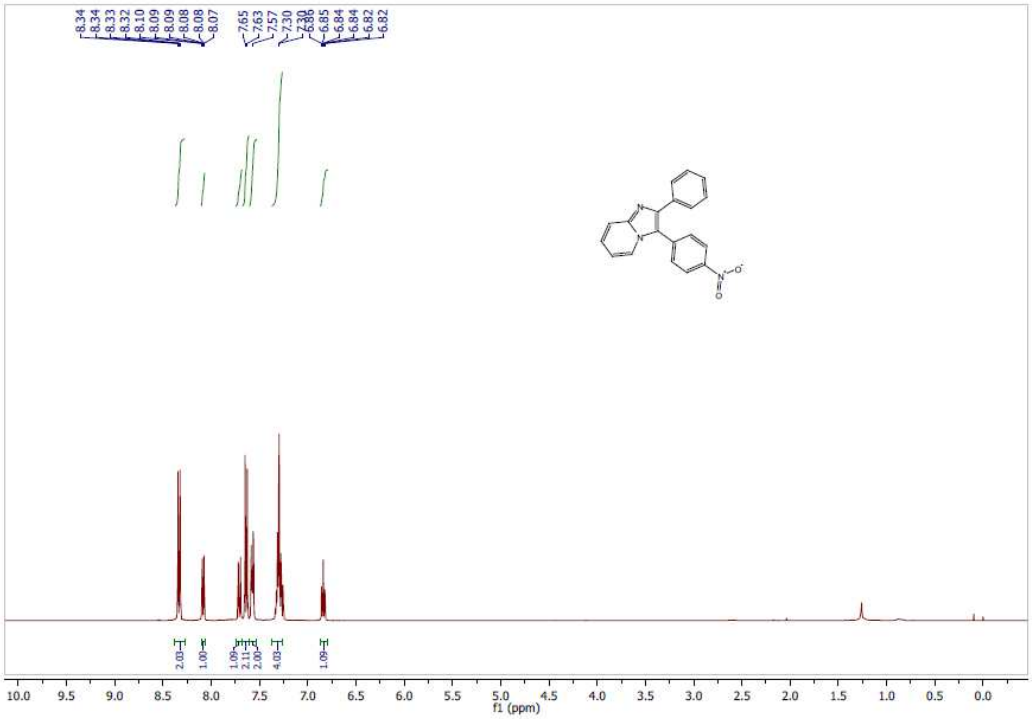
3-(4-nitrophenyl)imidazo[1,2-a]pyridine (6)



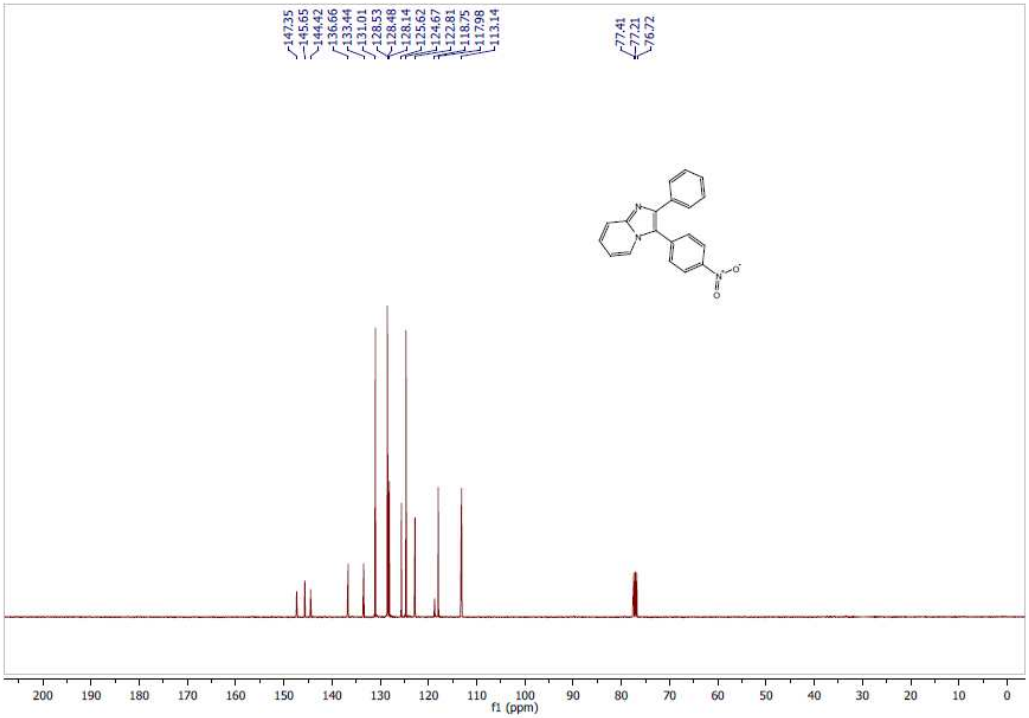
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (dt, *J* = 7.0, 1.2 Hz, 1H), 8.43 – 8.35 (m, 2H), 7.87 (s, 1H), 7.80 – 7.70 (m, 3H), 7.34 – 7.28 (m, 1H), 6.95 (td, *J* = 6.9, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 146.7, 135.8, 134.6, 127.4, 125.4, 124.7, 123.7, 123.2, 118.7, 113.6; $[M+H]^+$ = 240.

Copies of NMR Spectra

^{1}H-NMR of 4aaa



^{13}C-NMR of 4aaa



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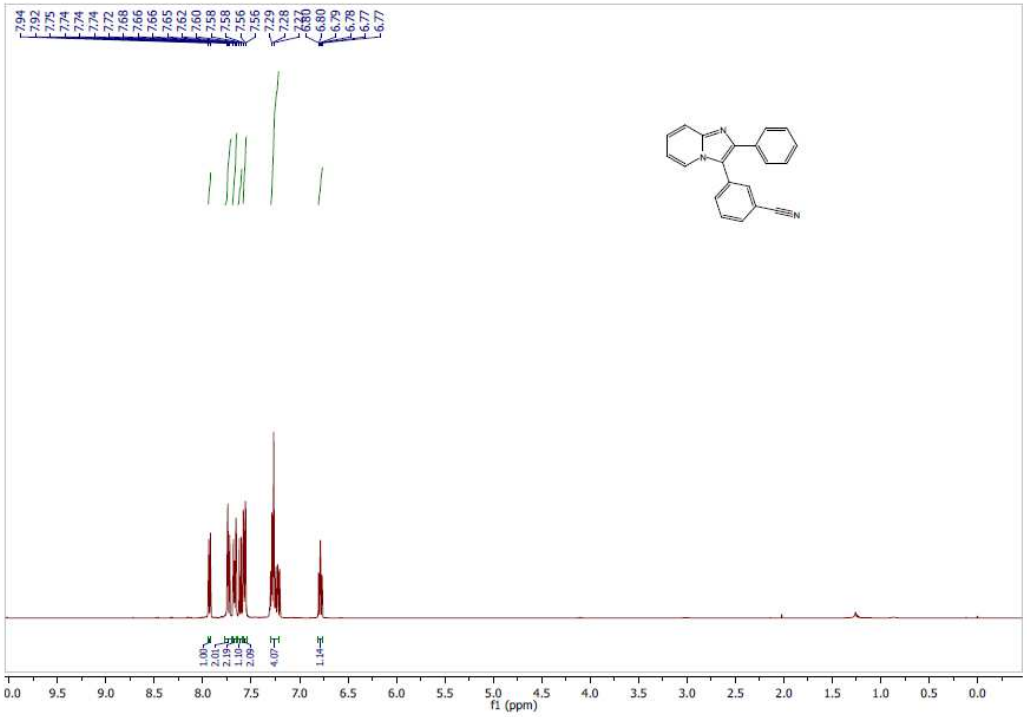

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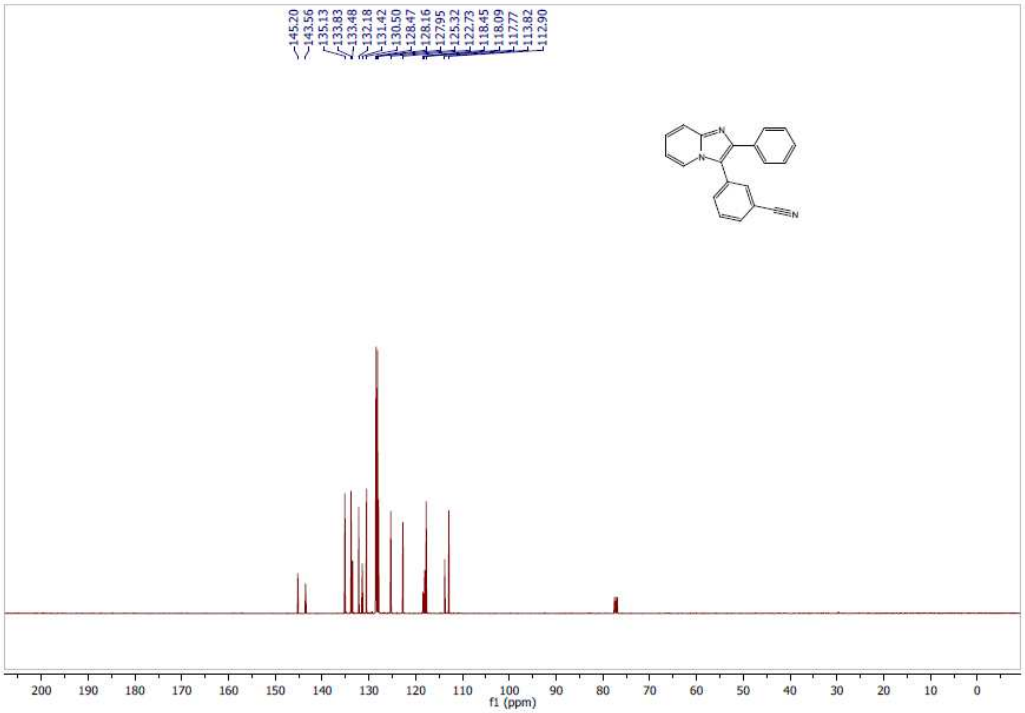

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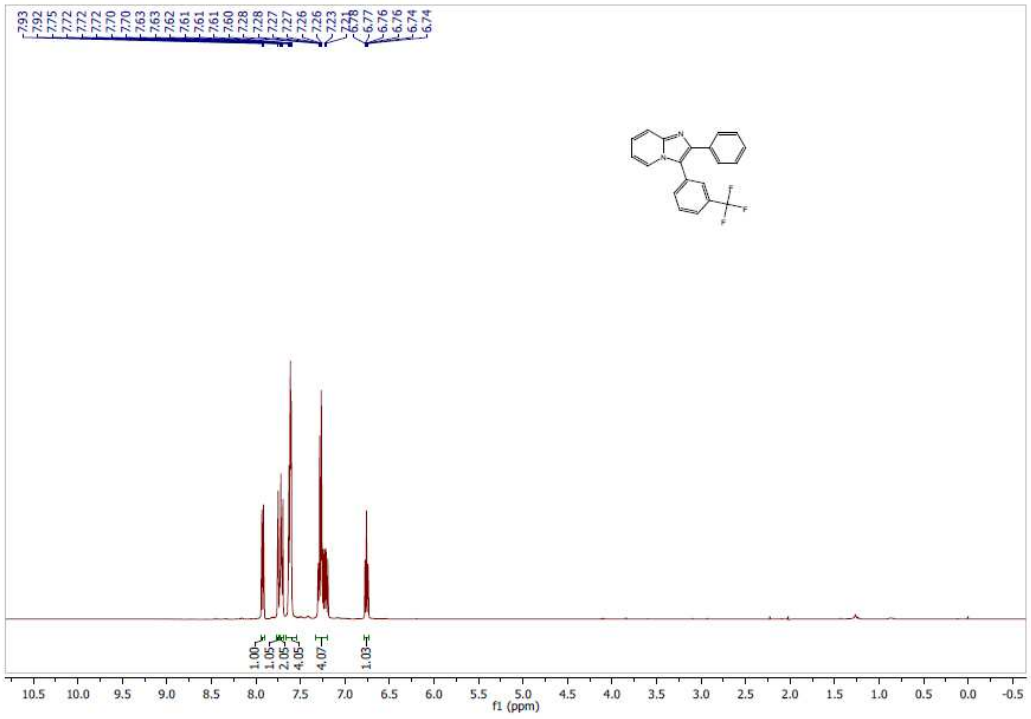

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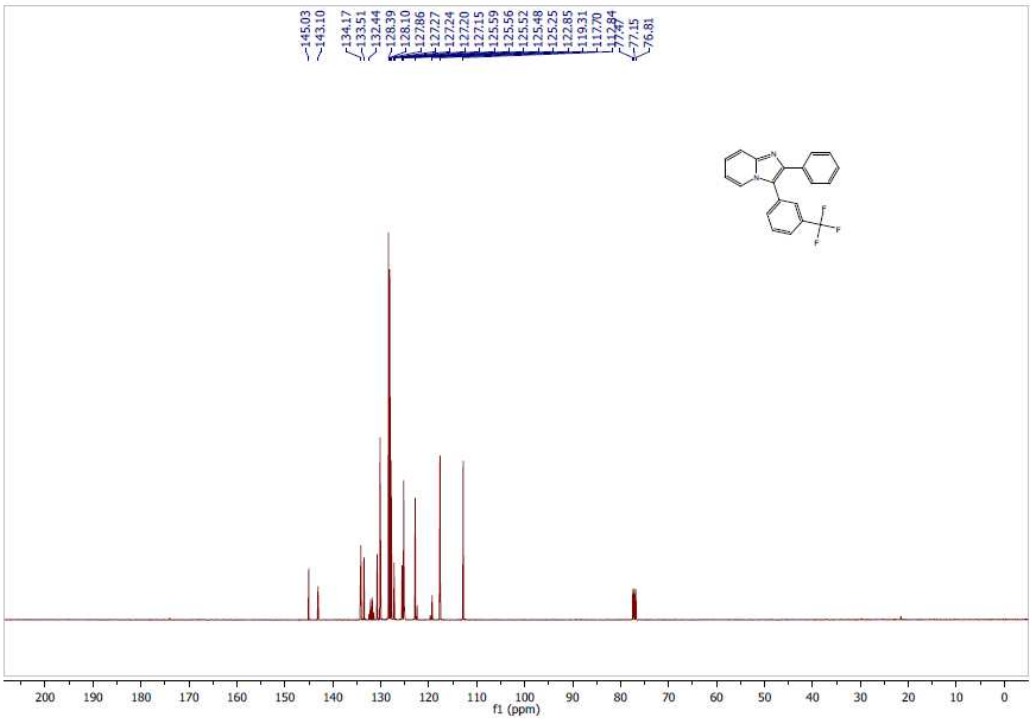

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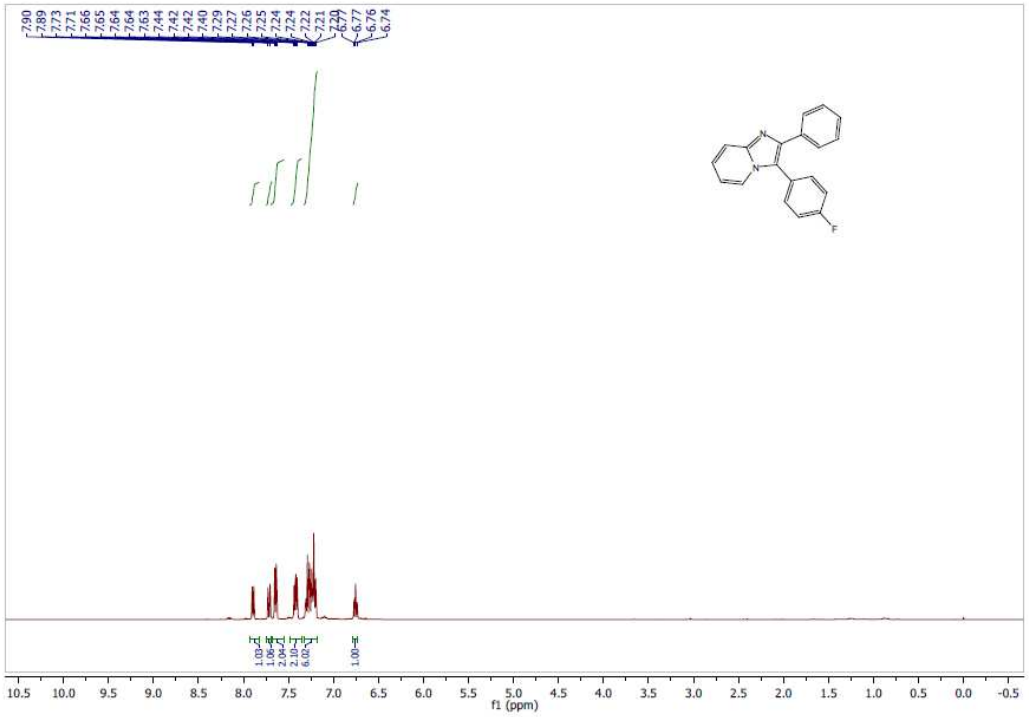

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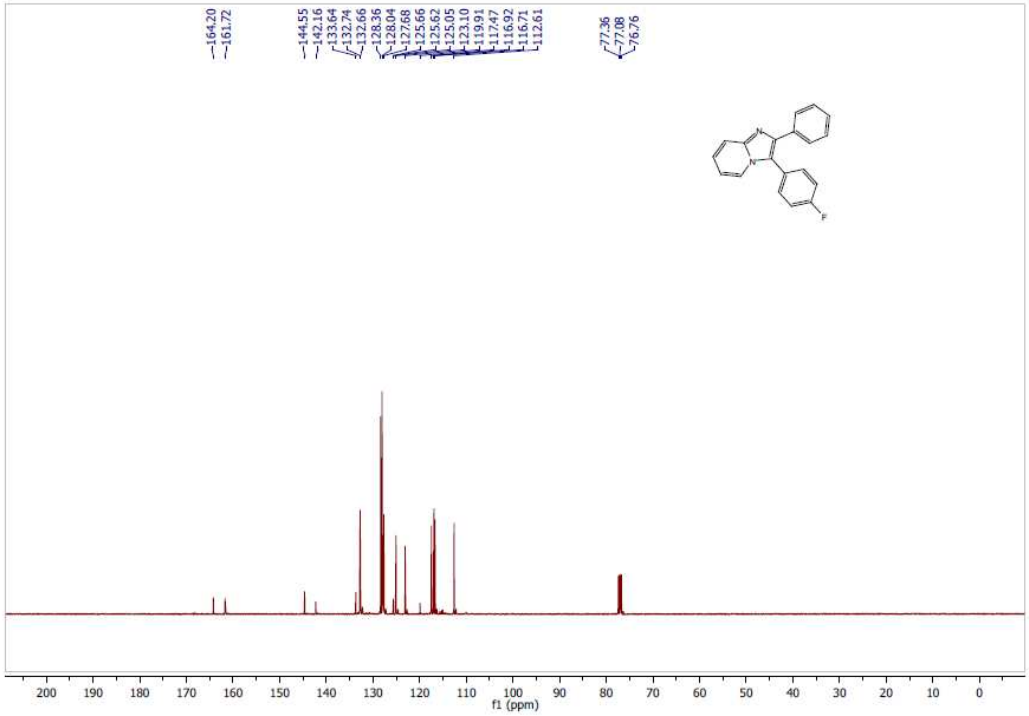

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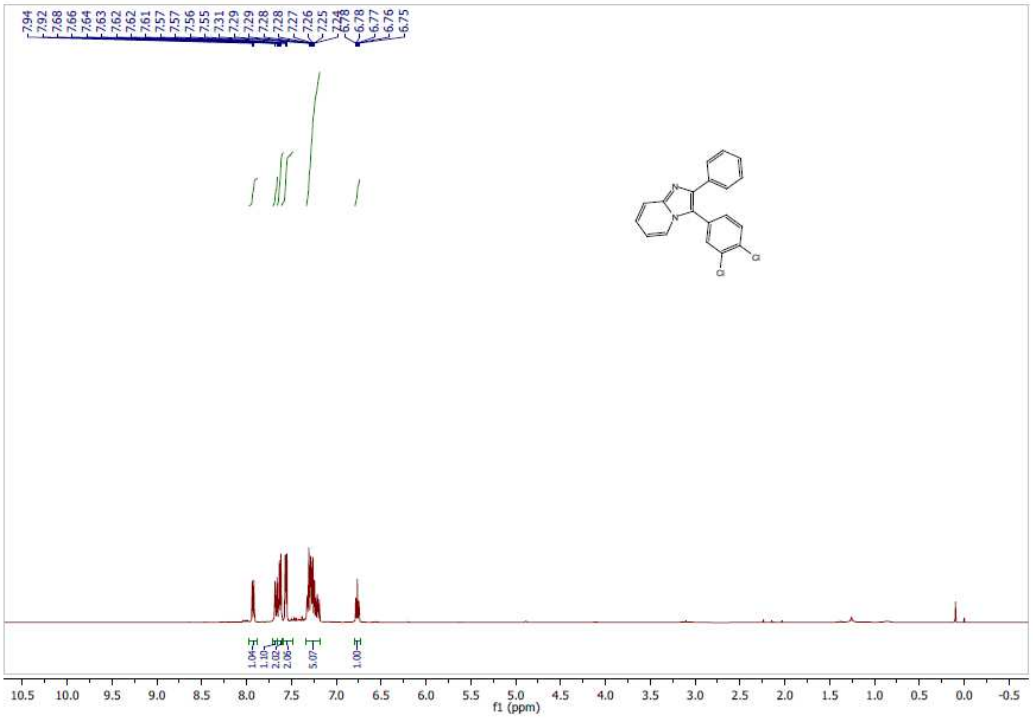

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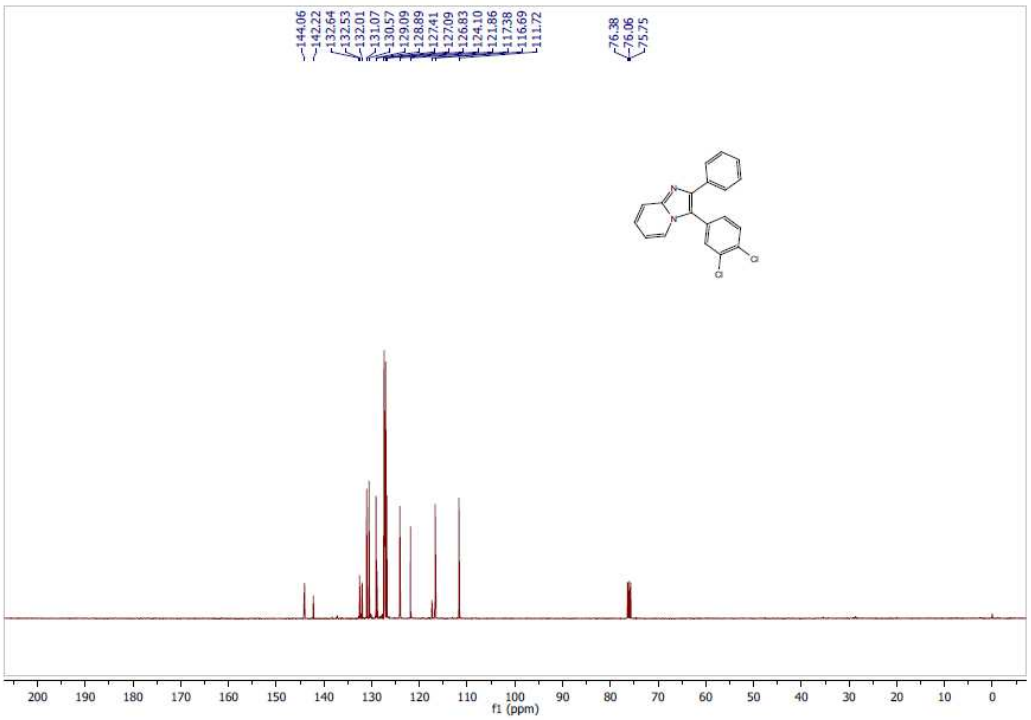

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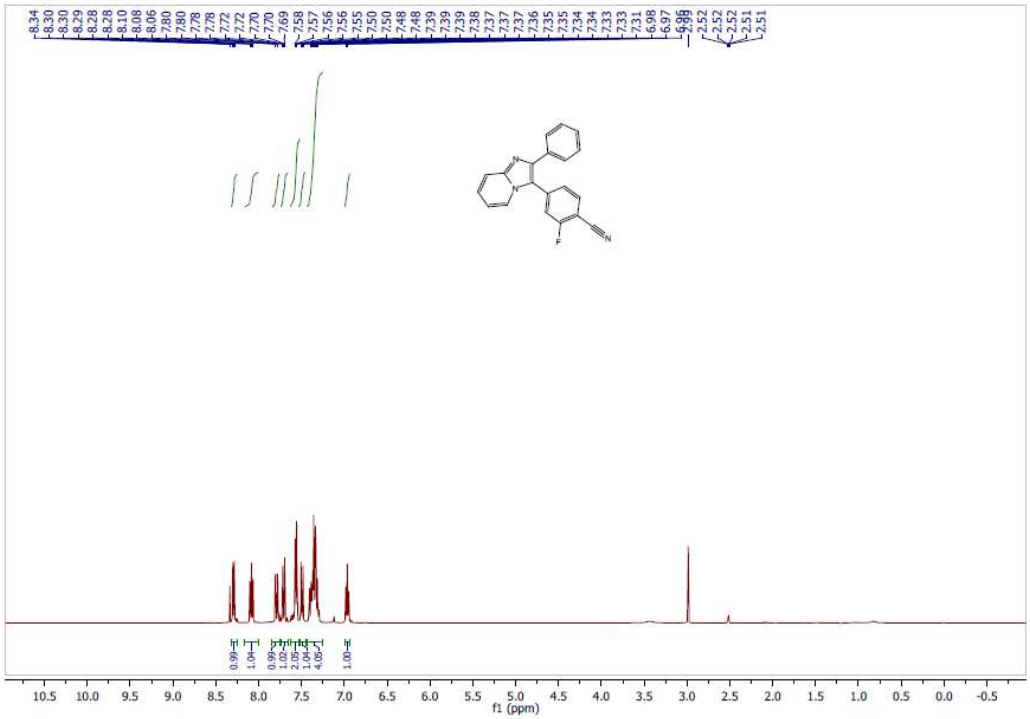

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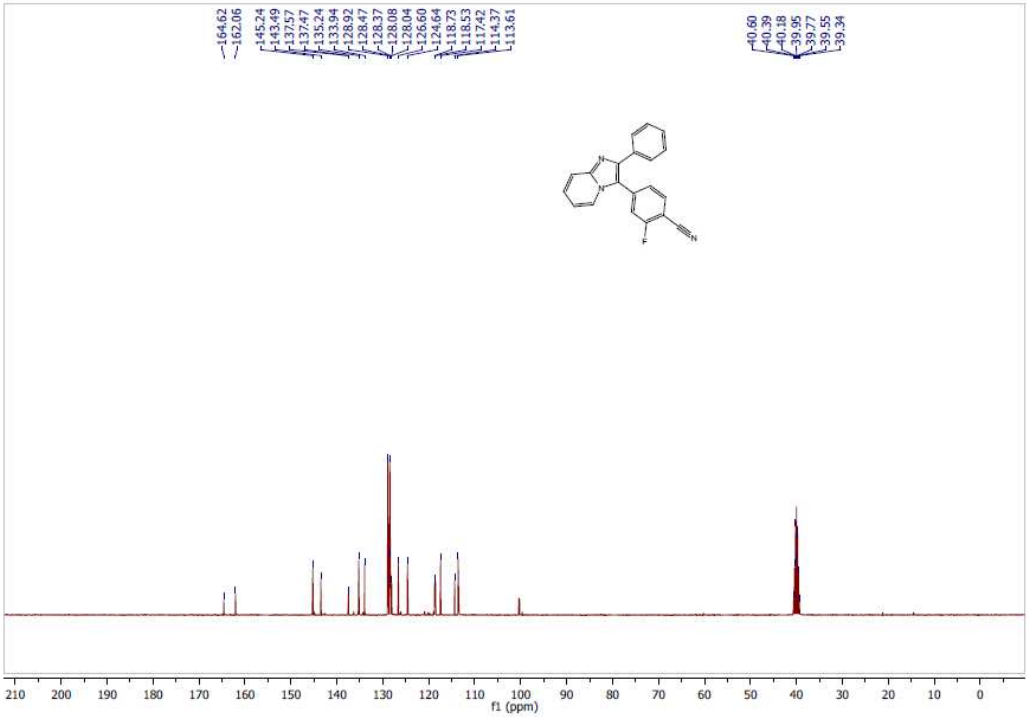

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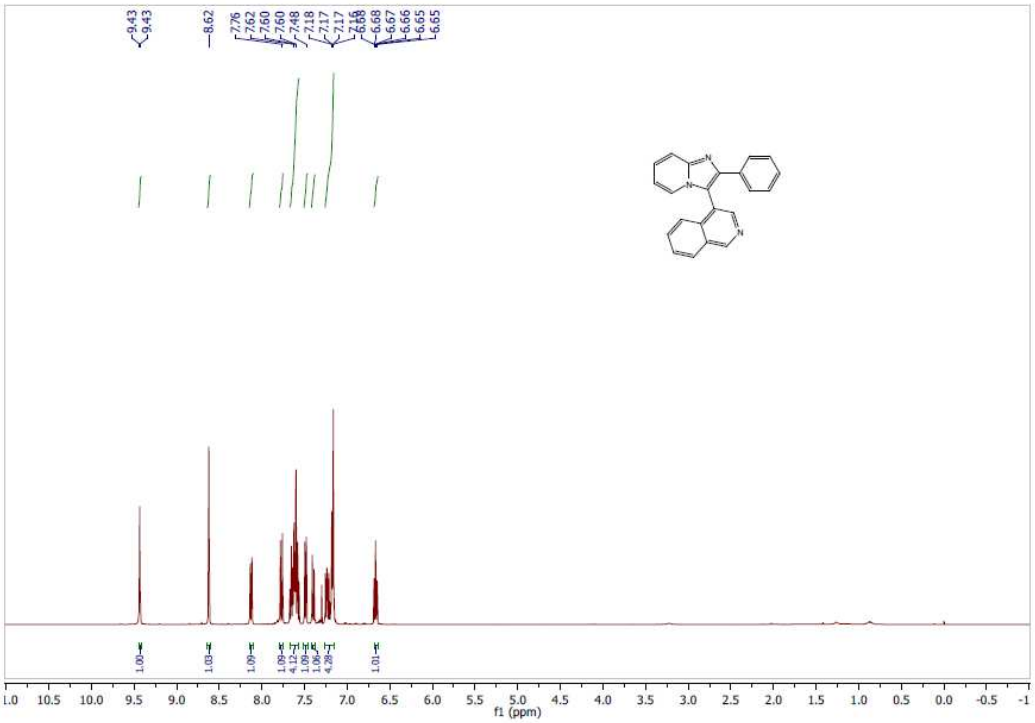

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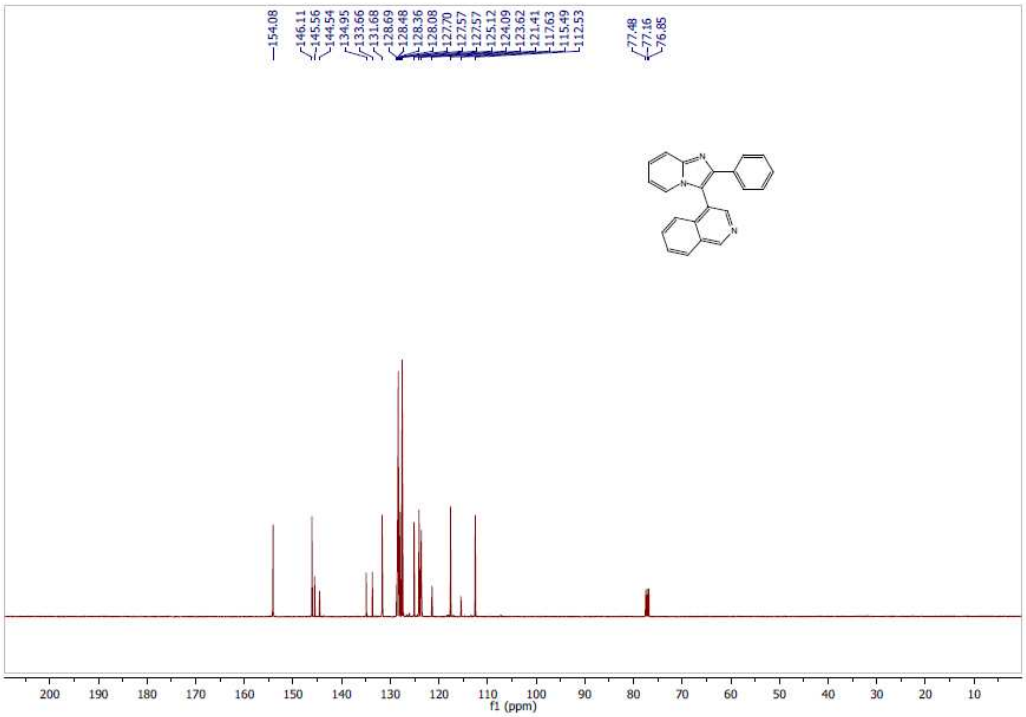

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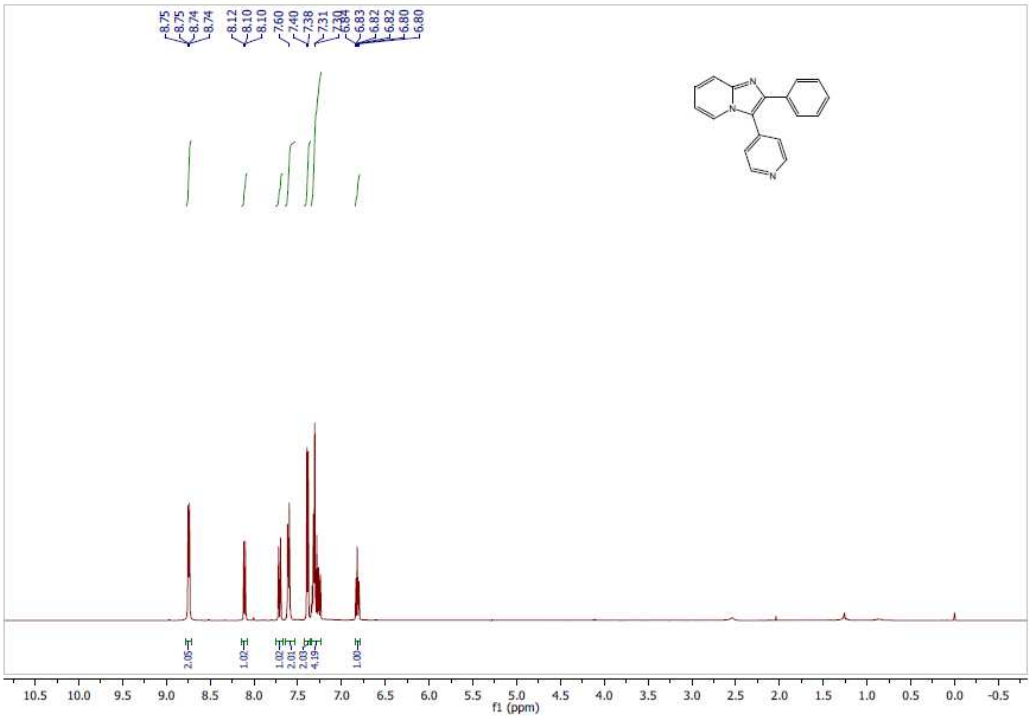

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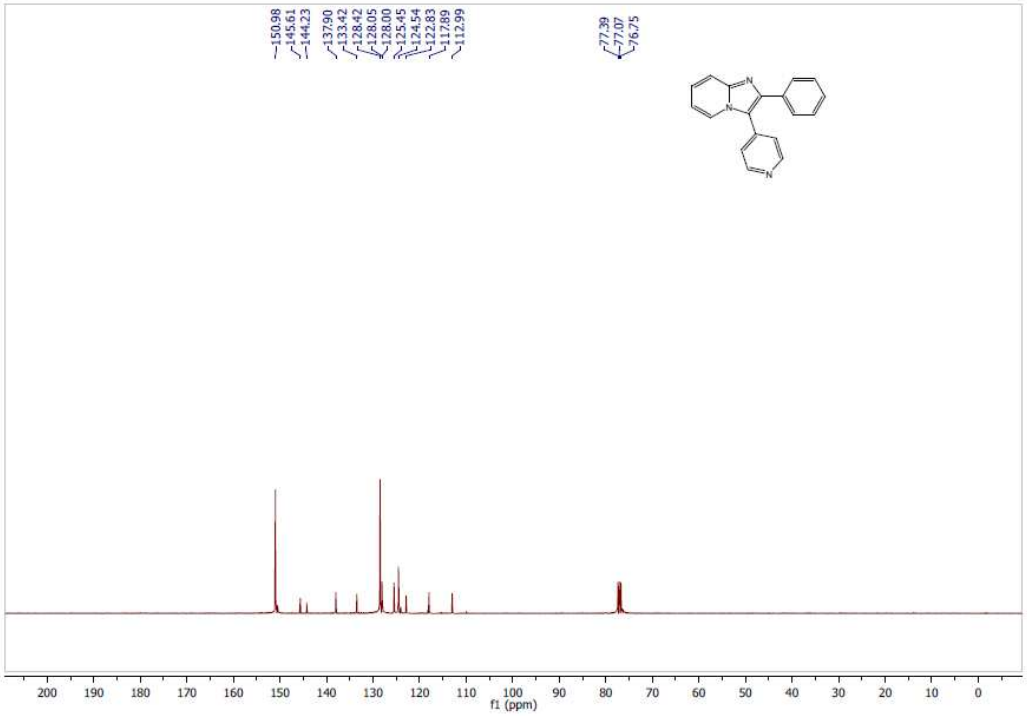

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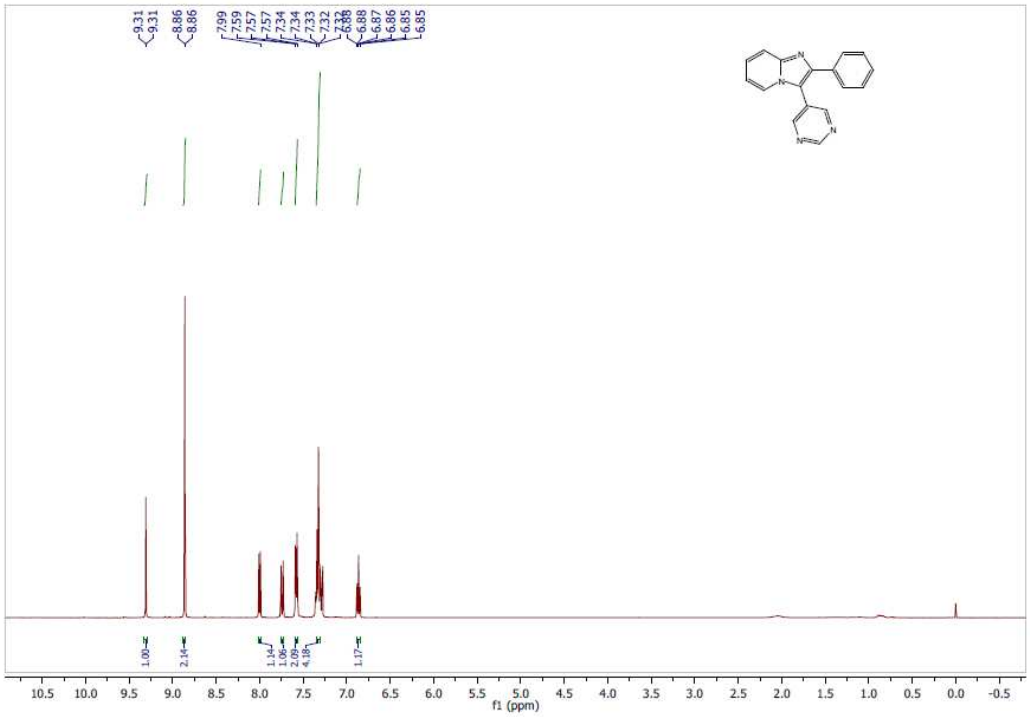

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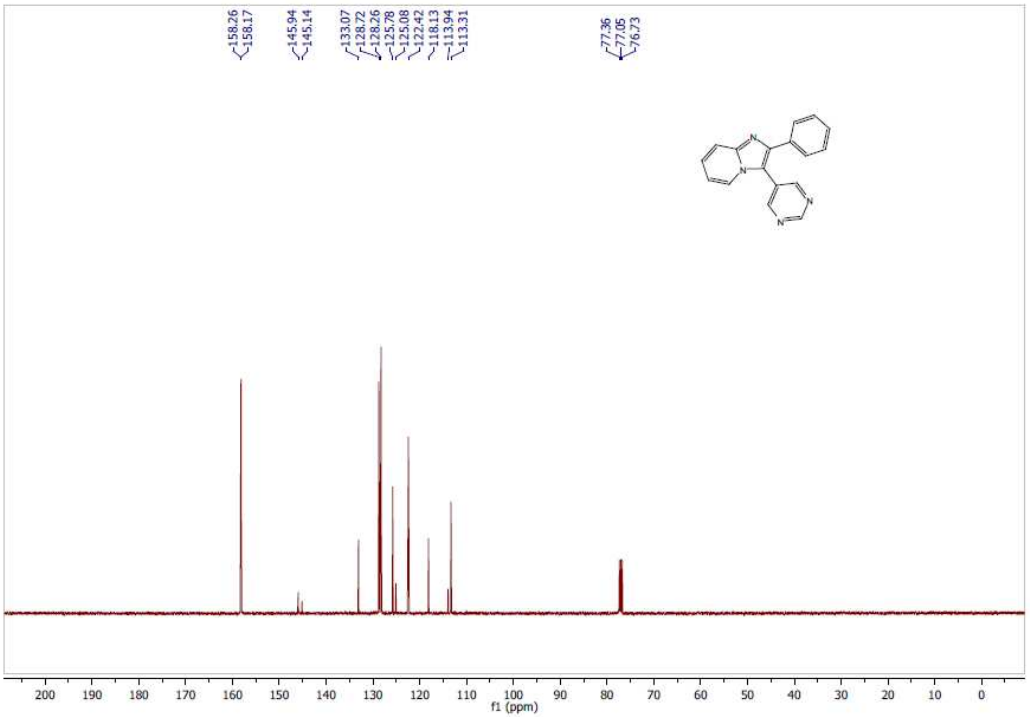

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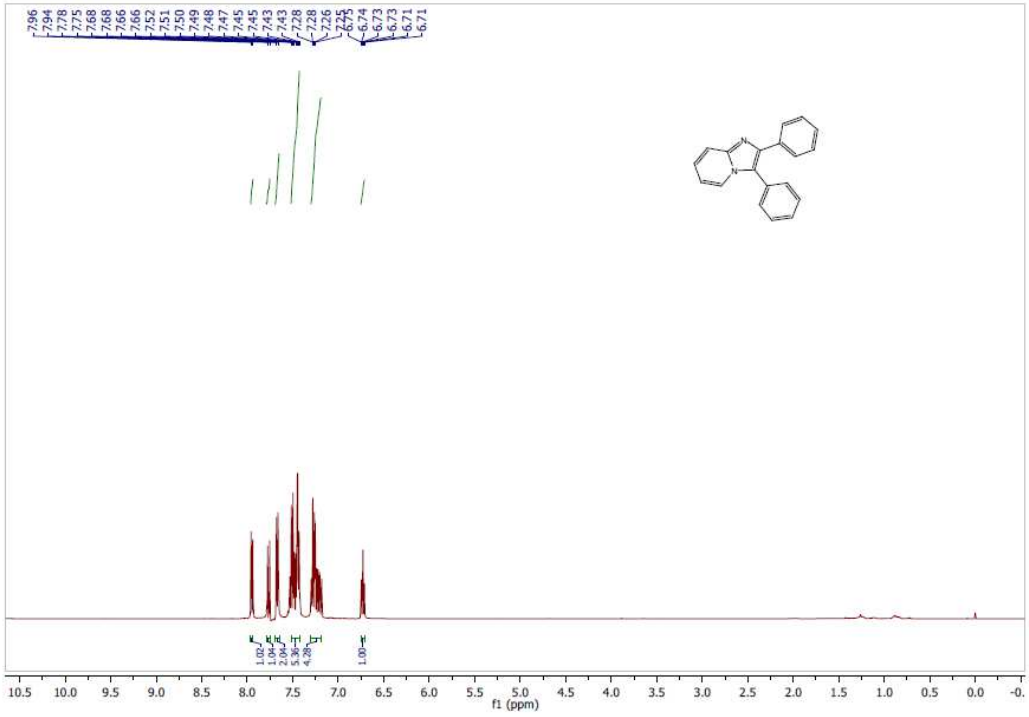

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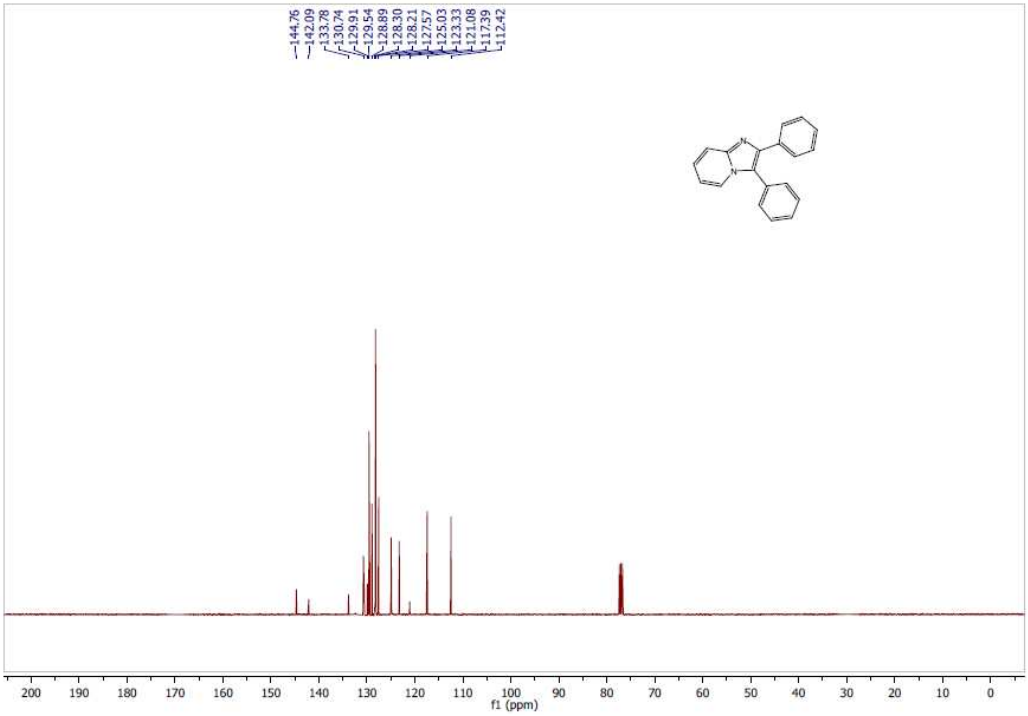

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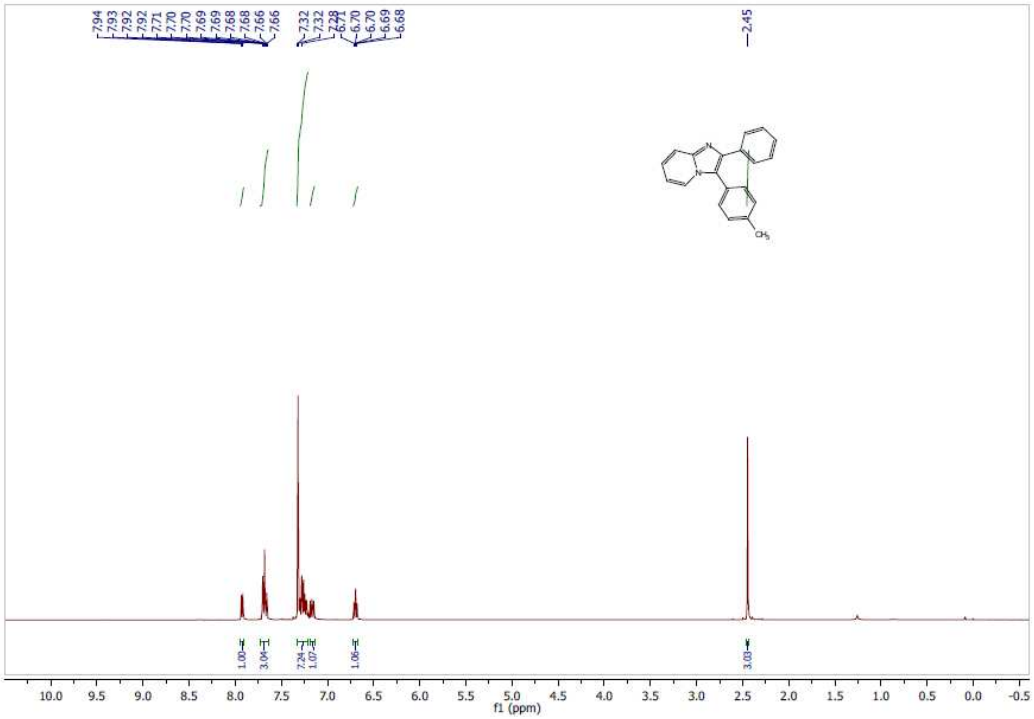

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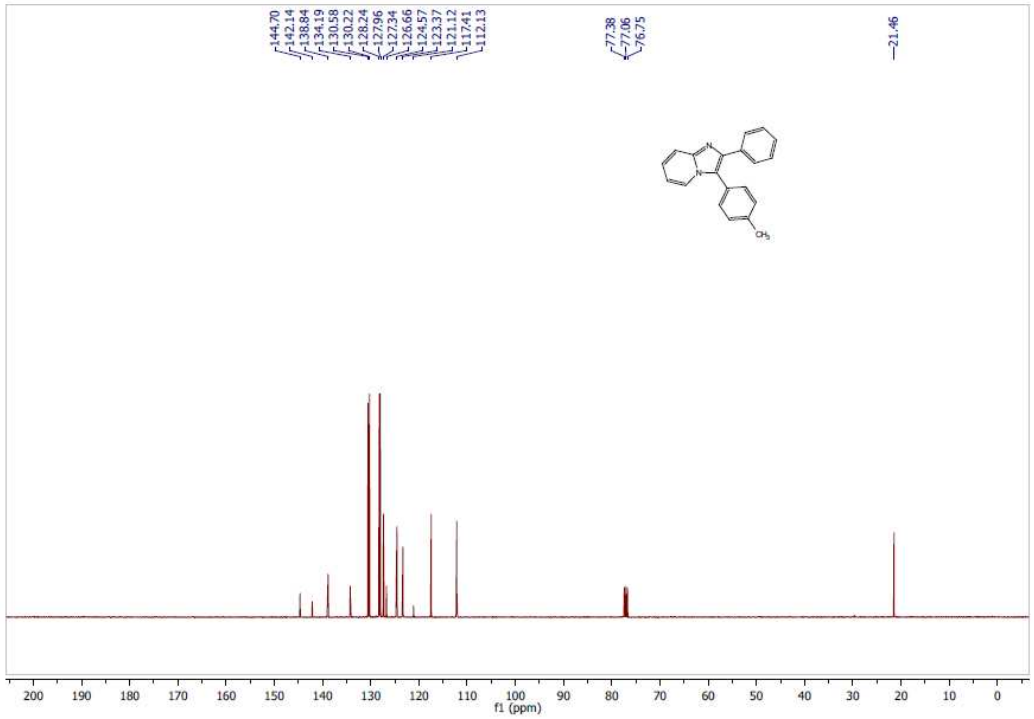

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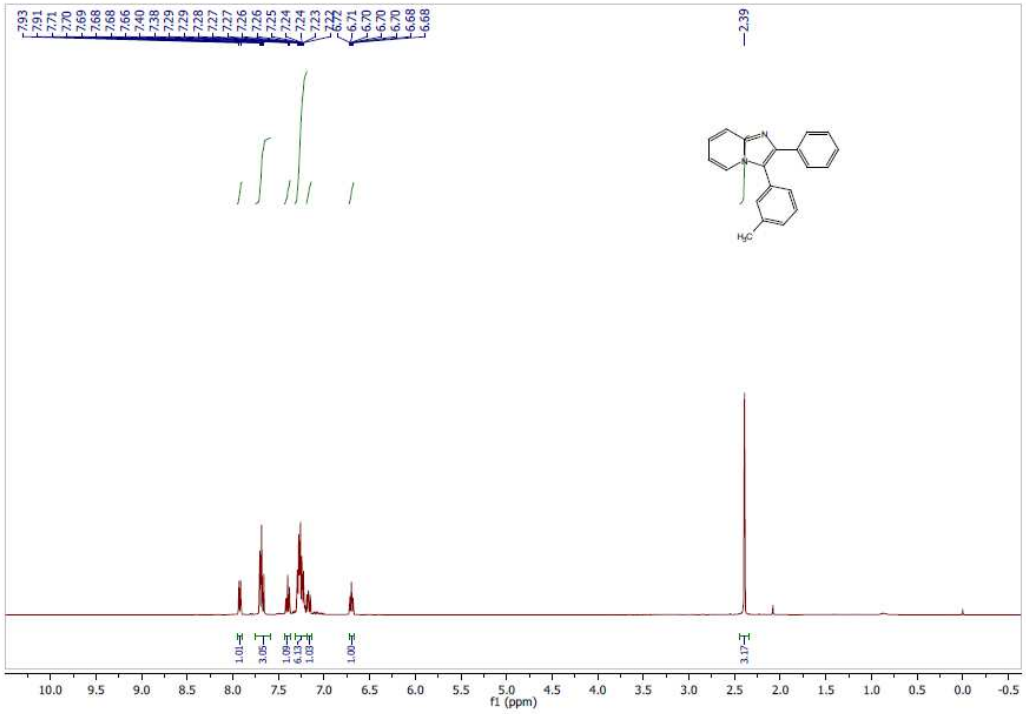

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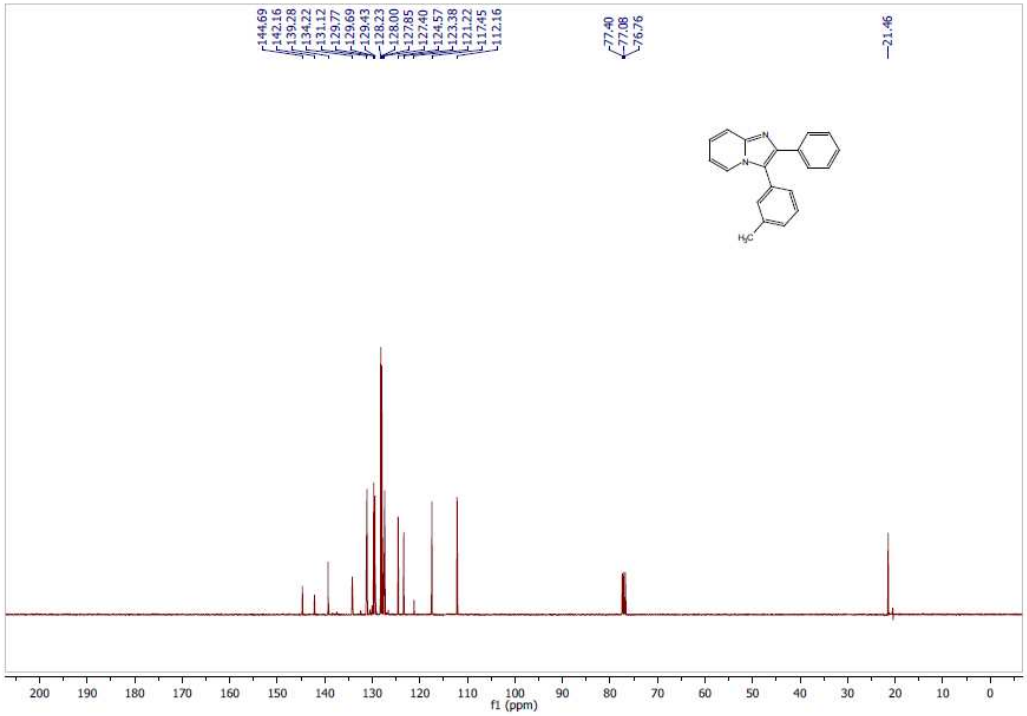

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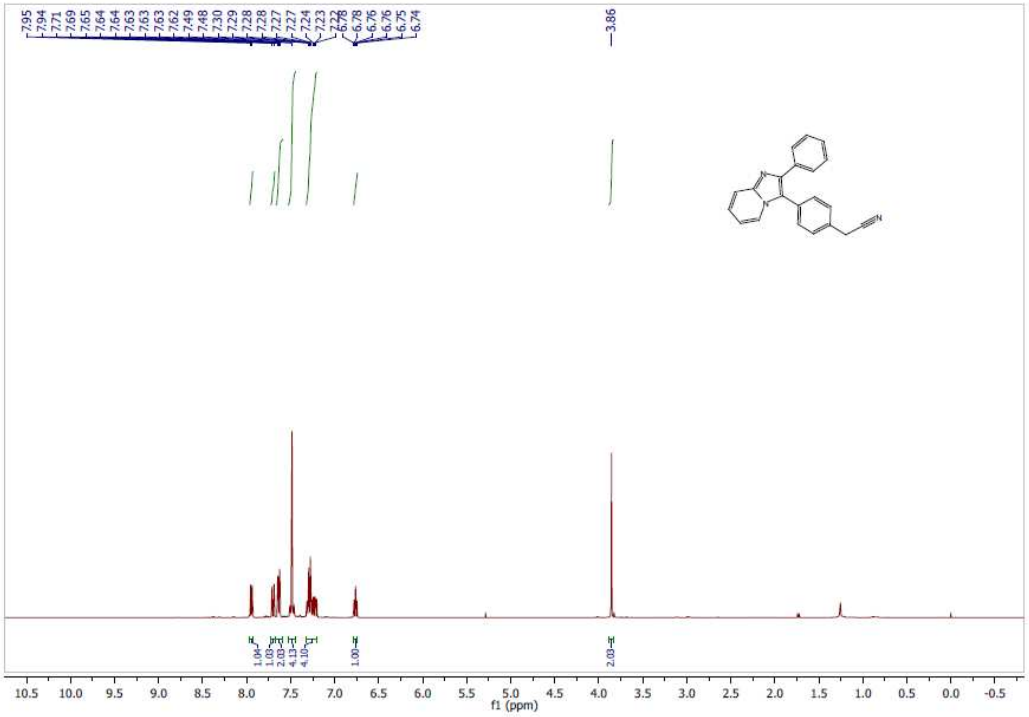

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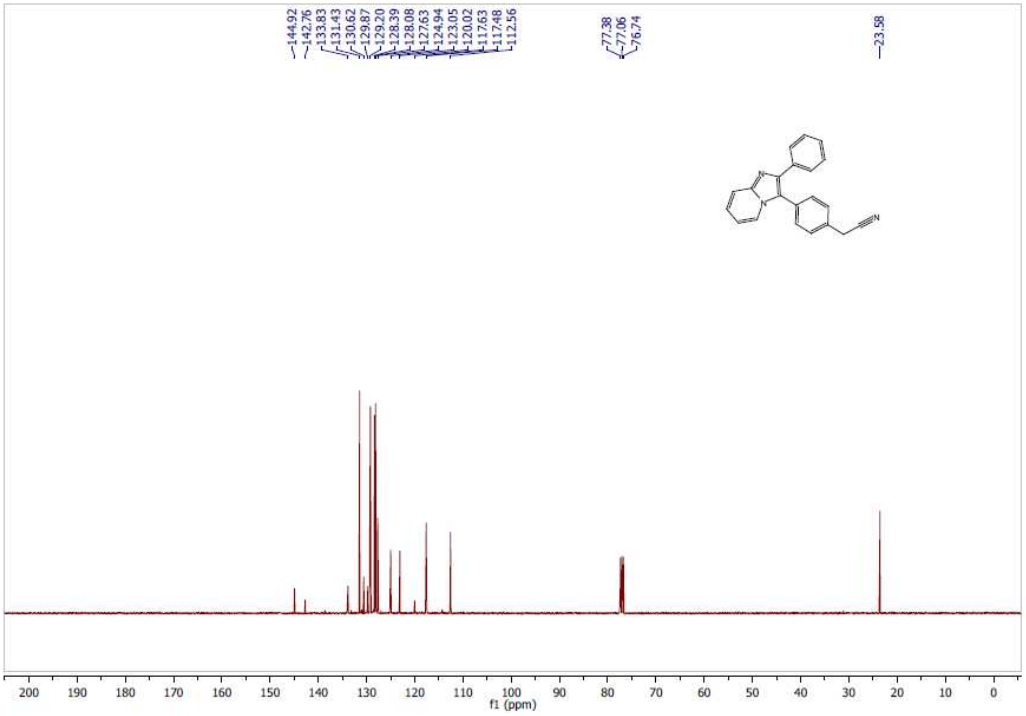

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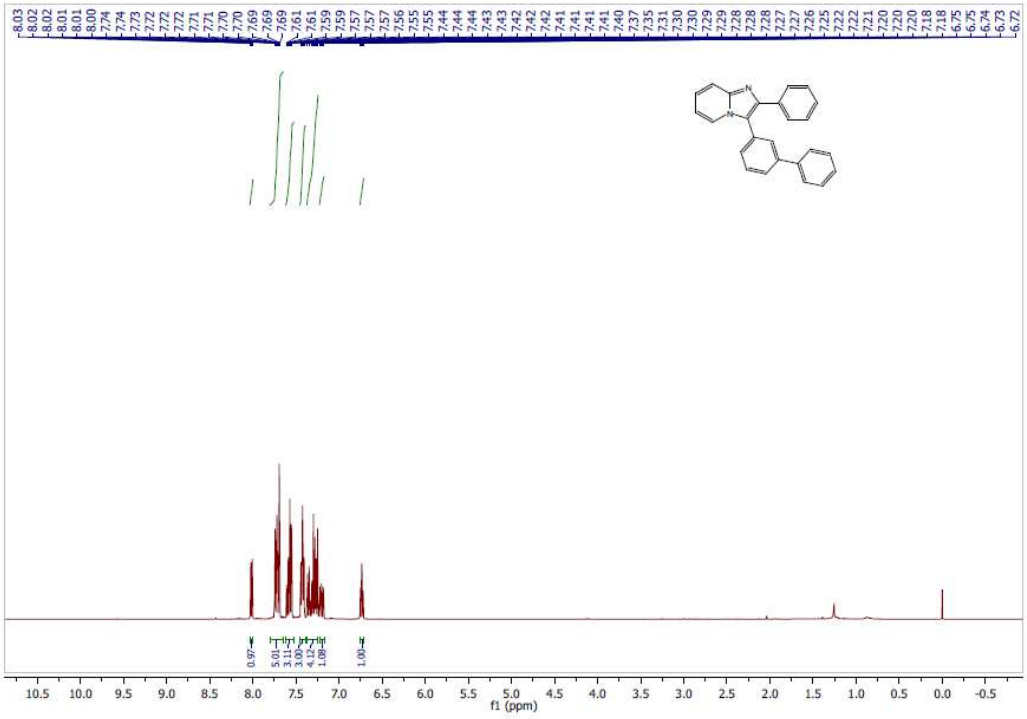

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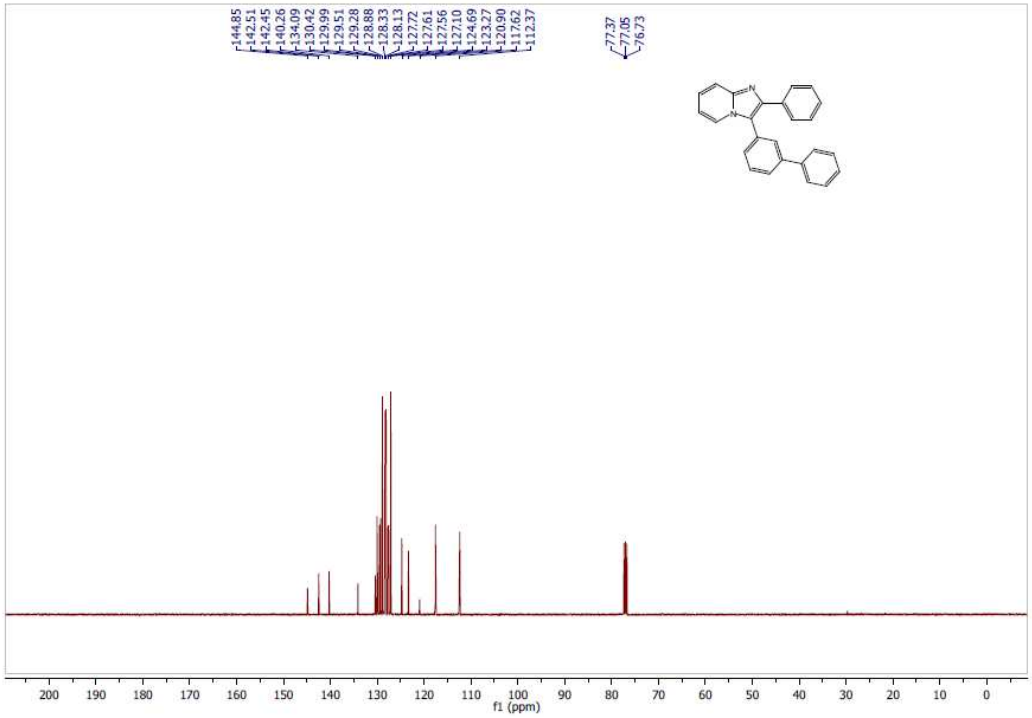

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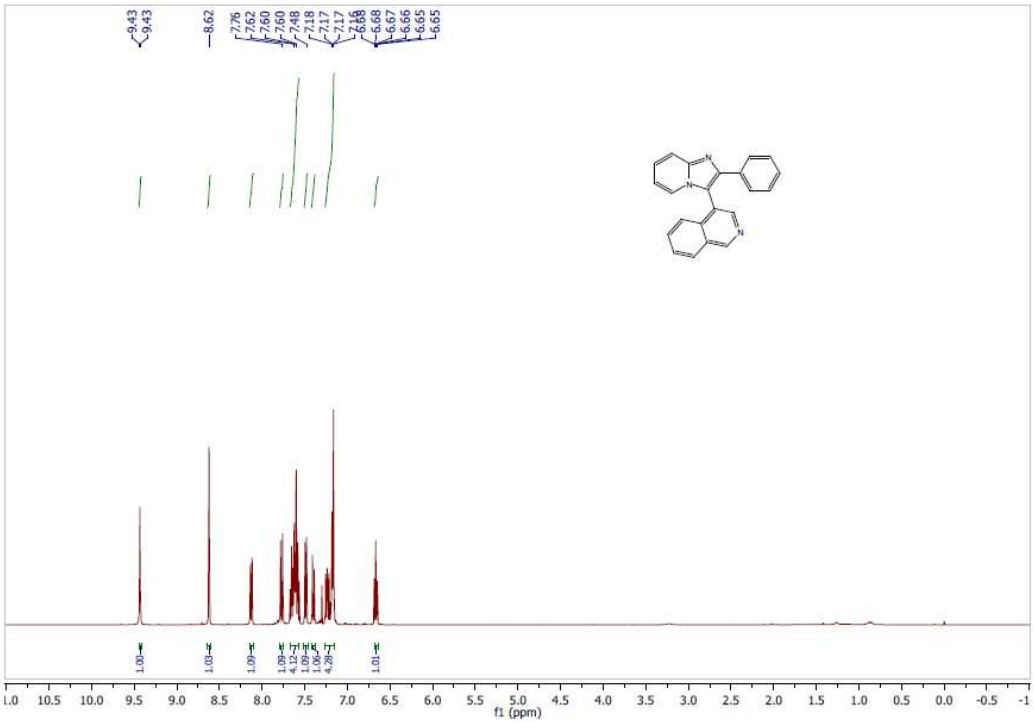

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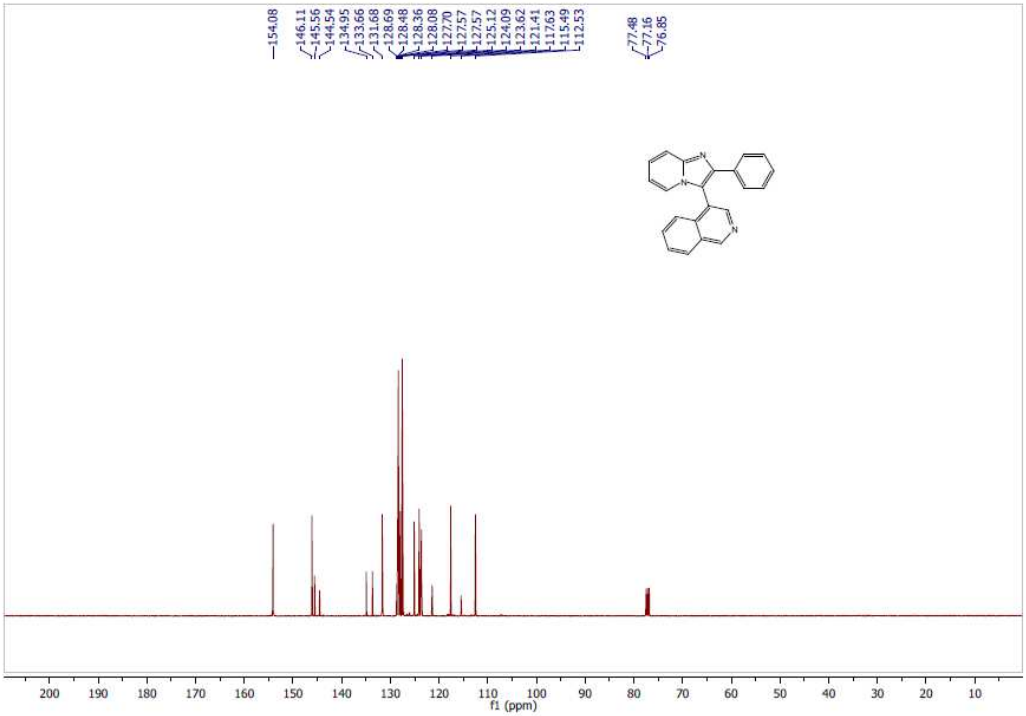

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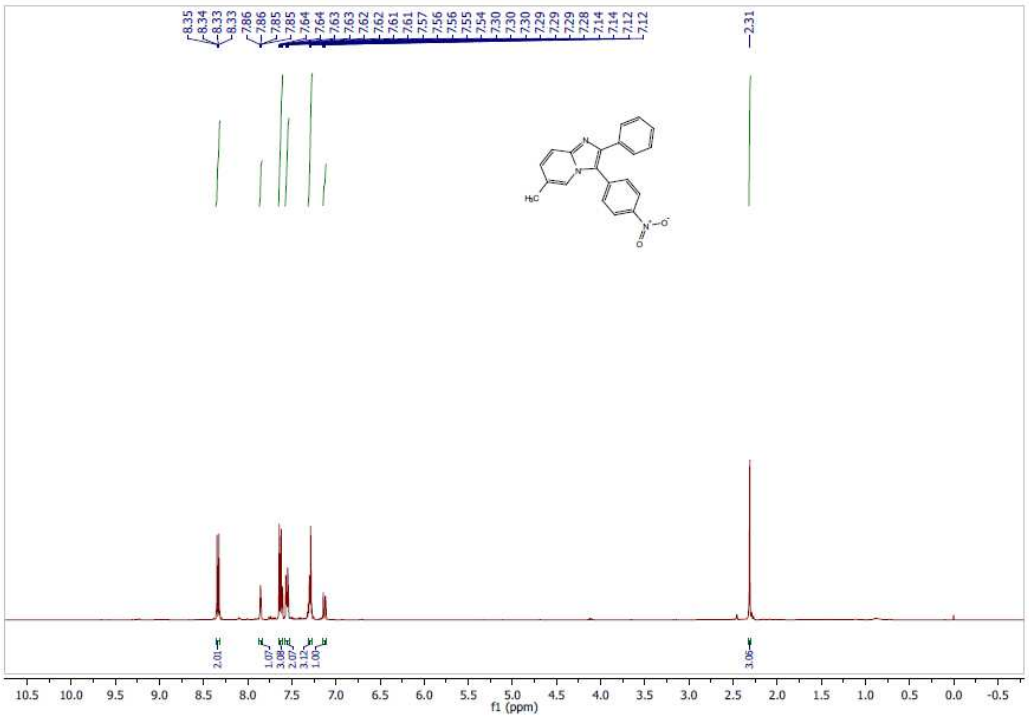

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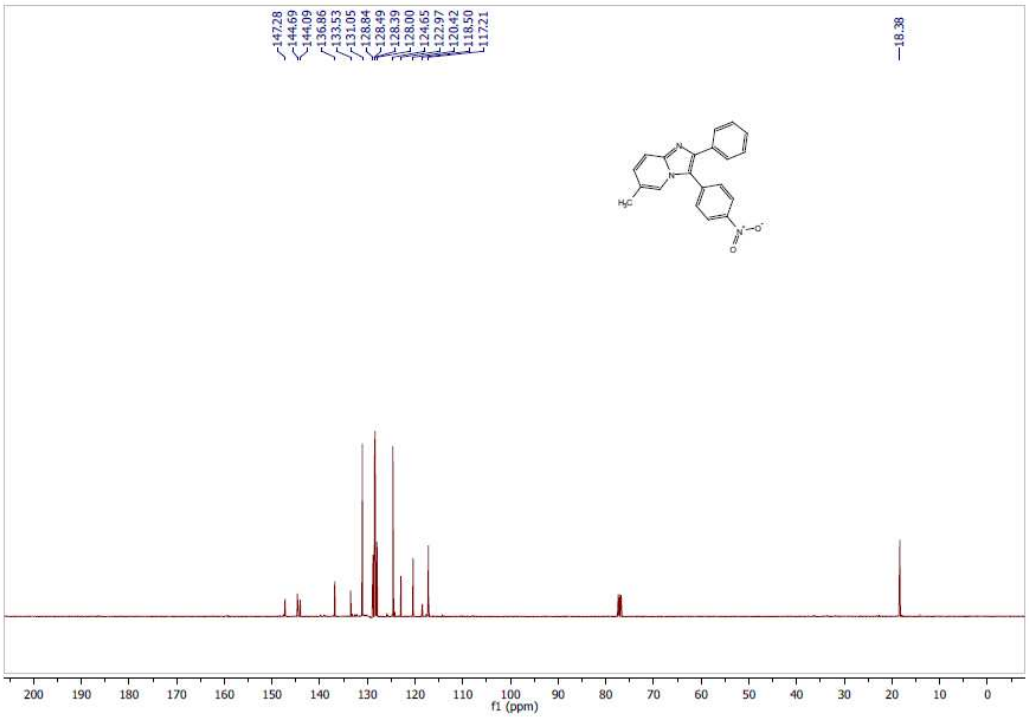
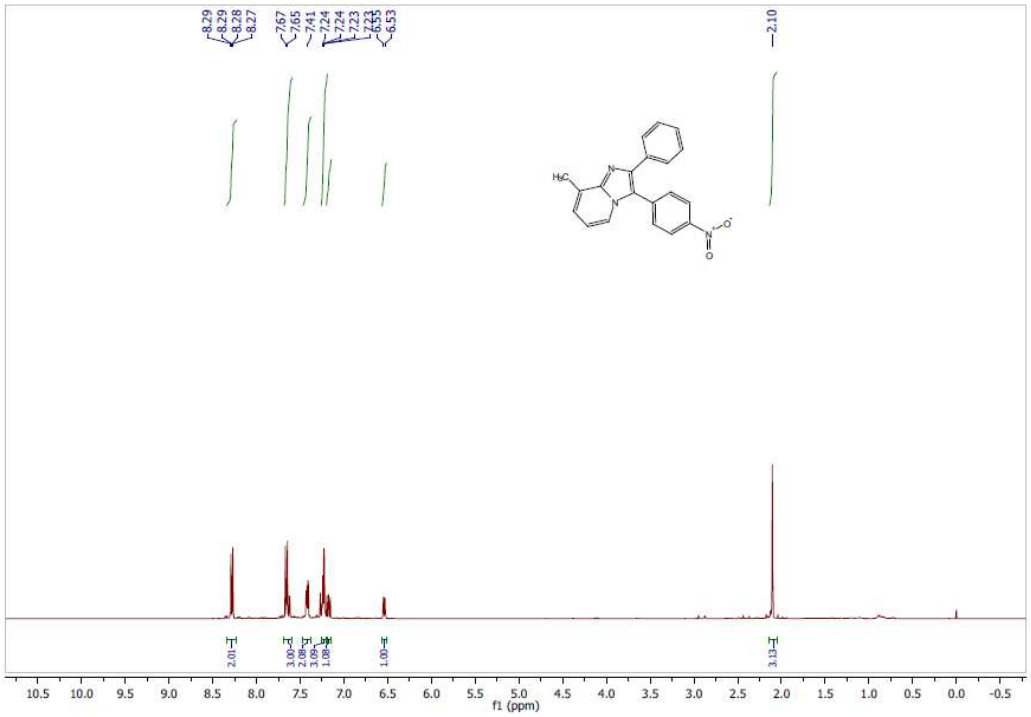
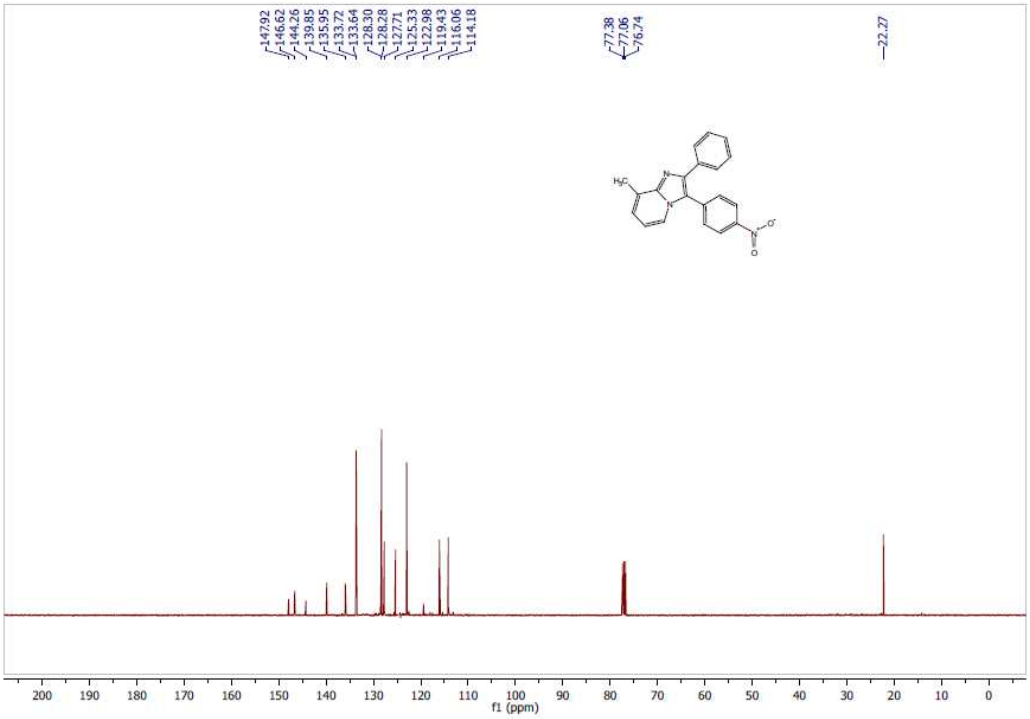


^{1}H-NMR of 4caa



^{13}C-NMR of 4caa



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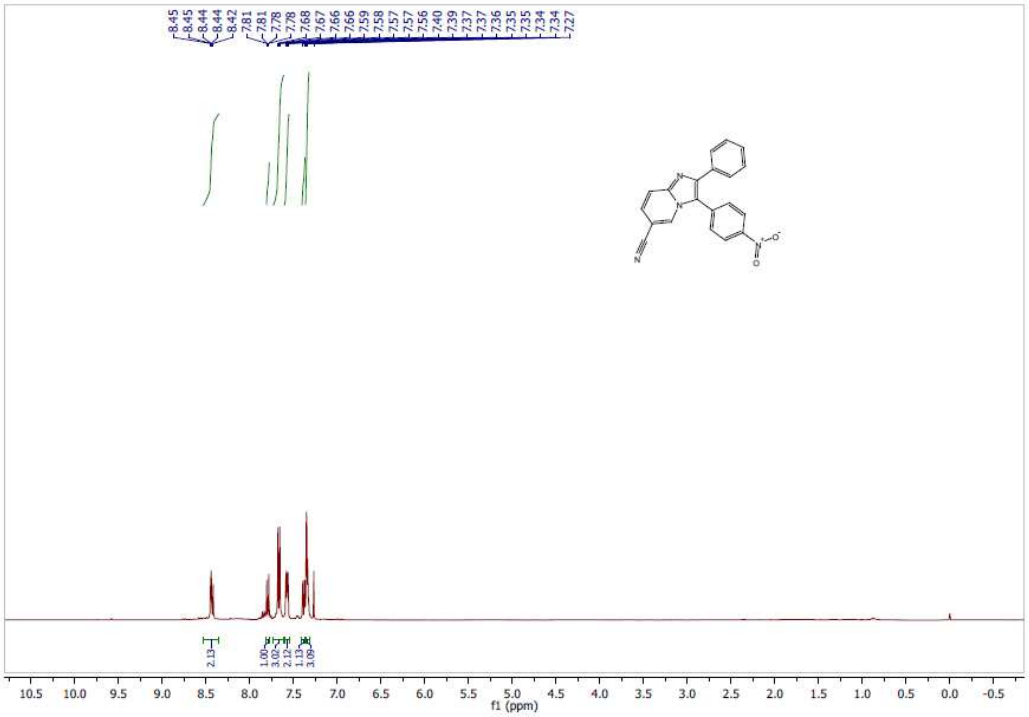

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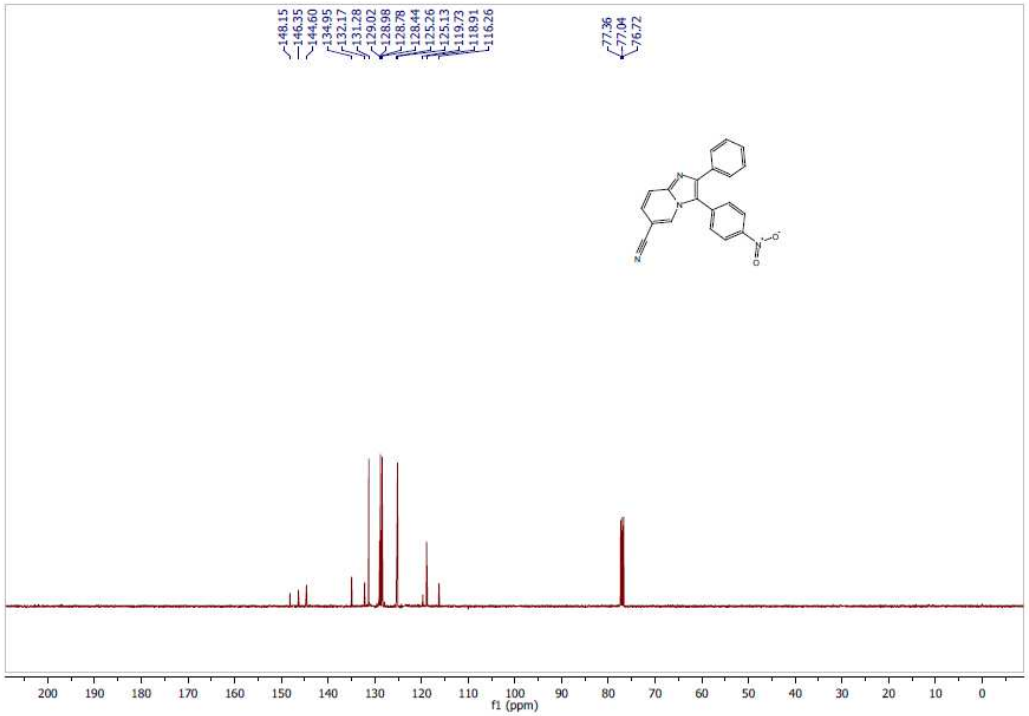

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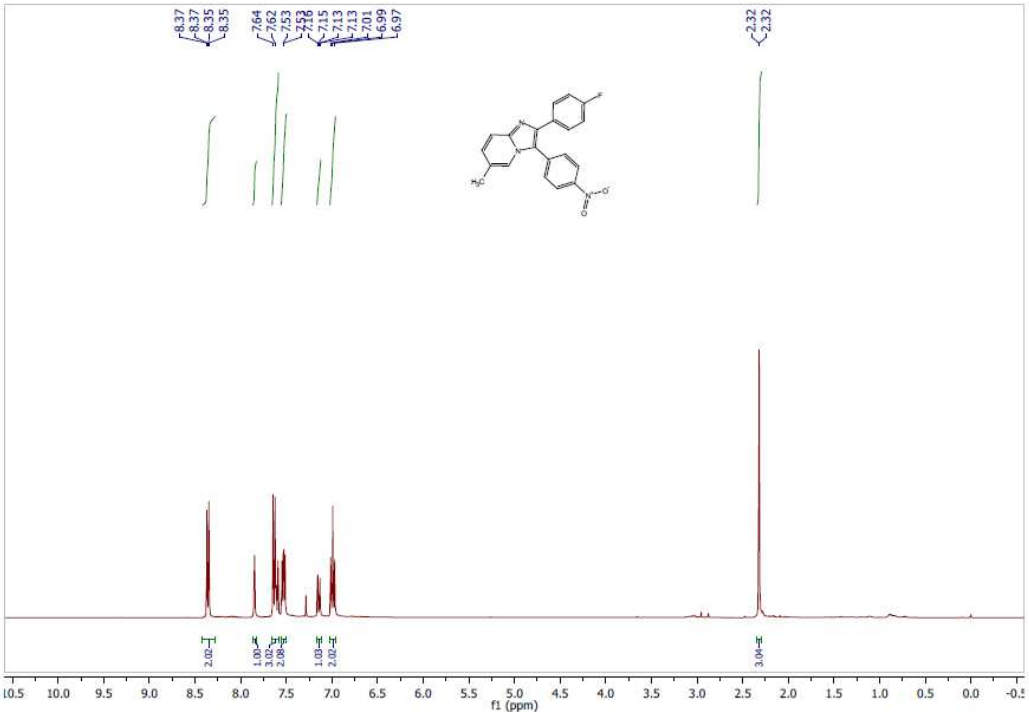
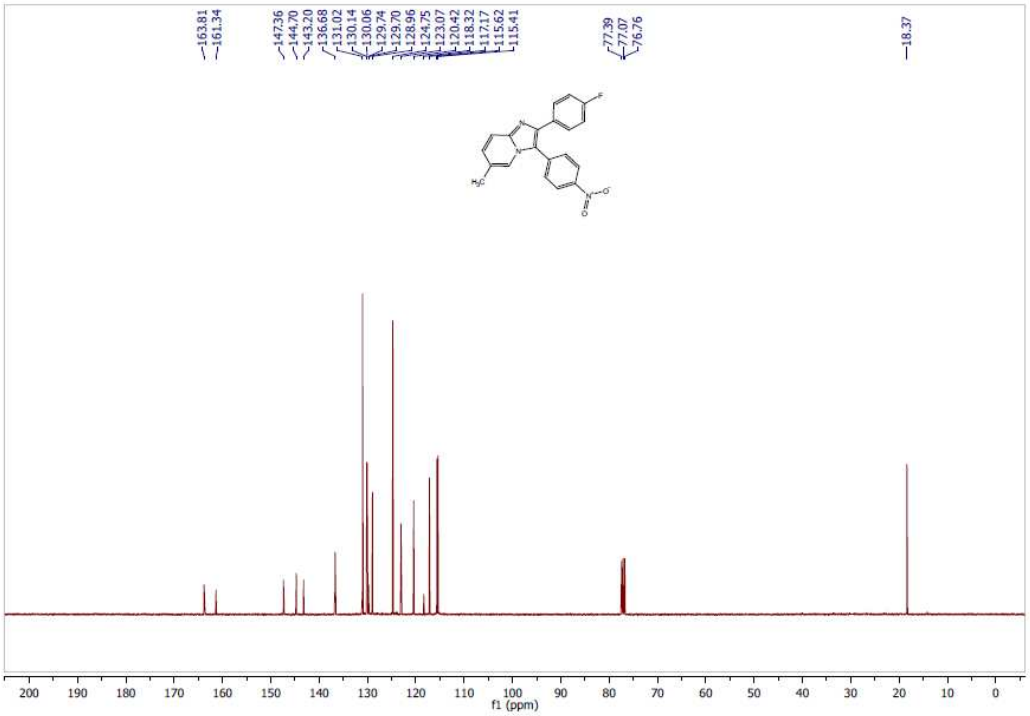
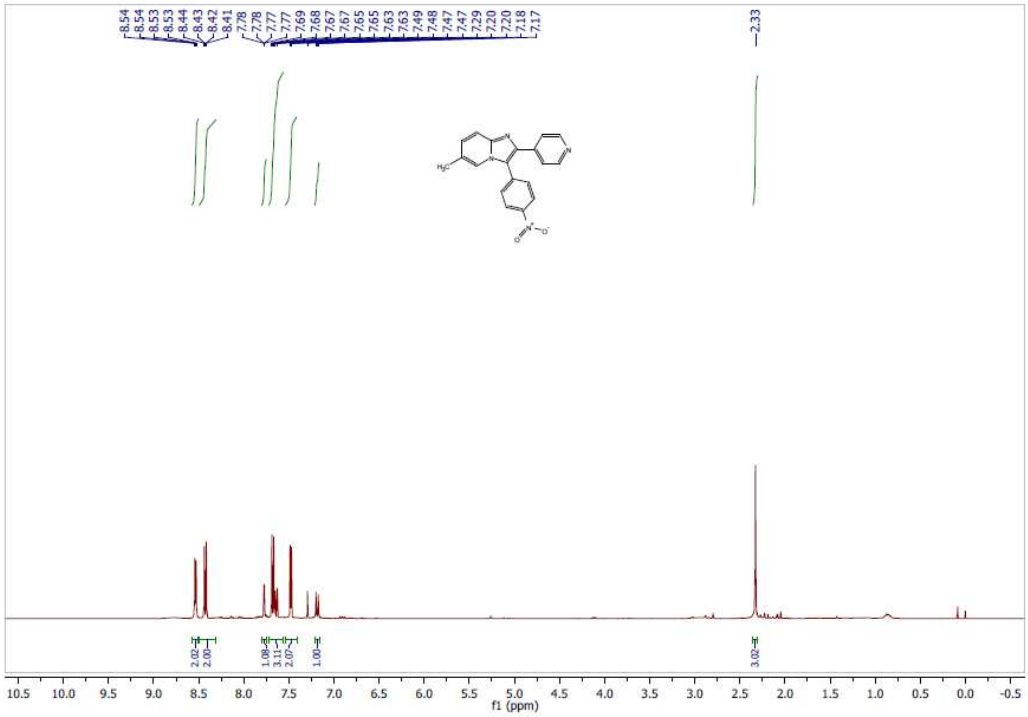


^{13}C-NMR of 4bba



^{1}H-NMR of 4bca



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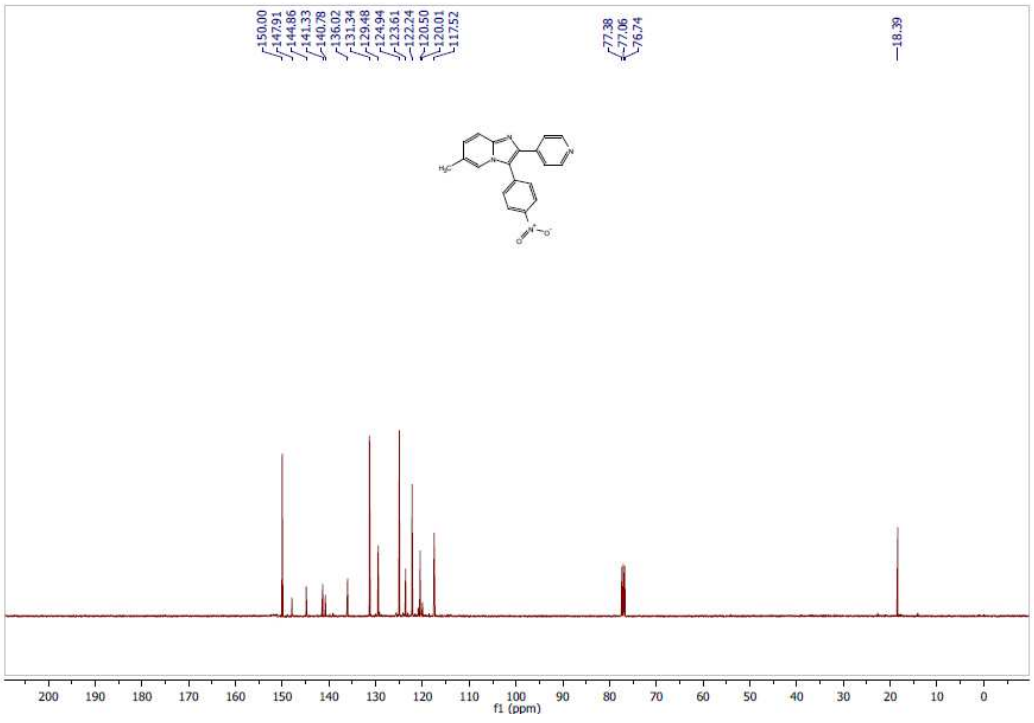

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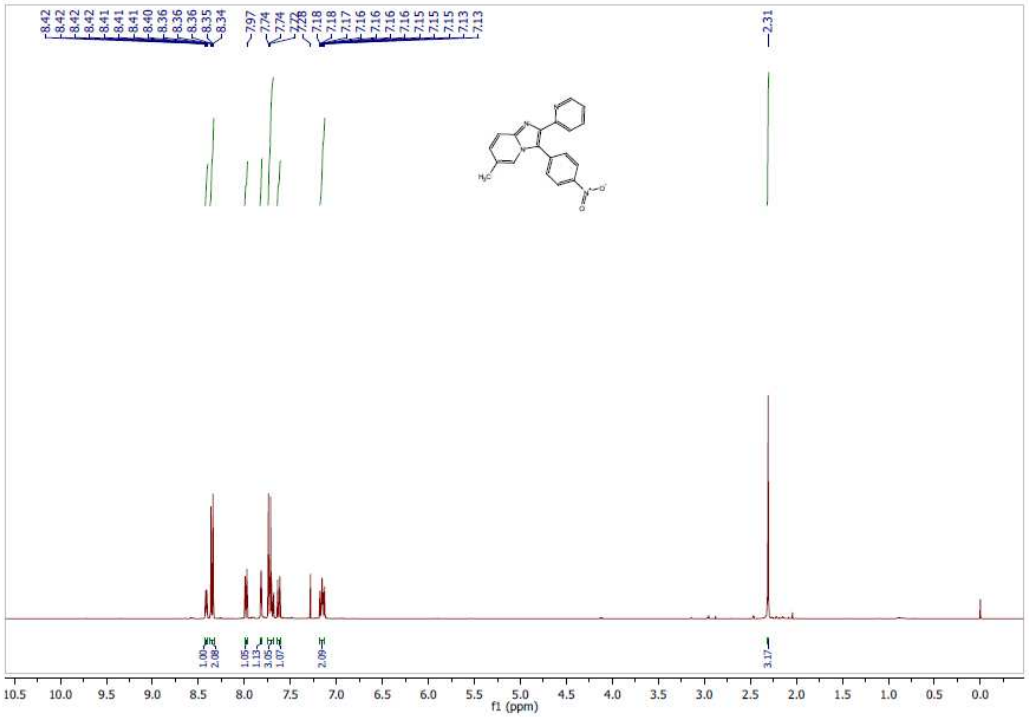

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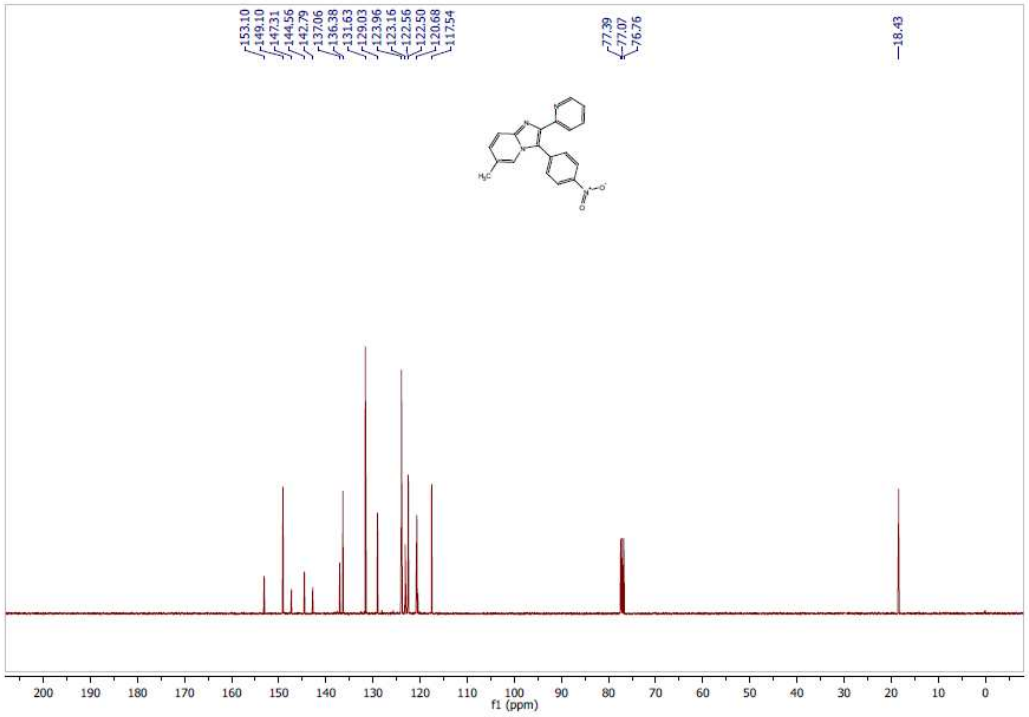

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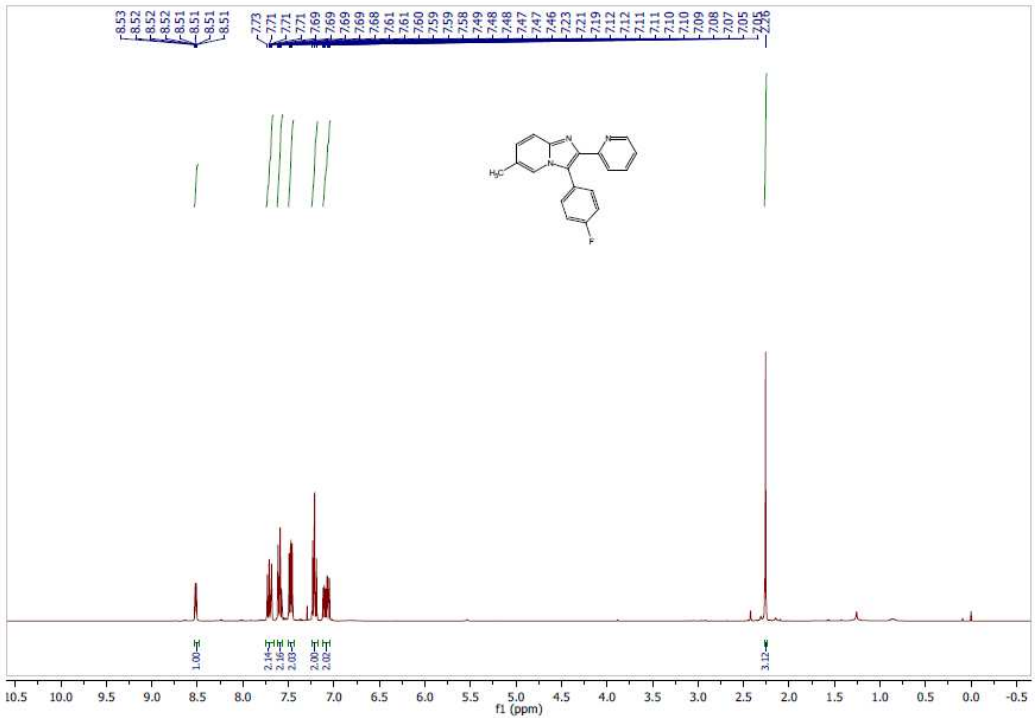

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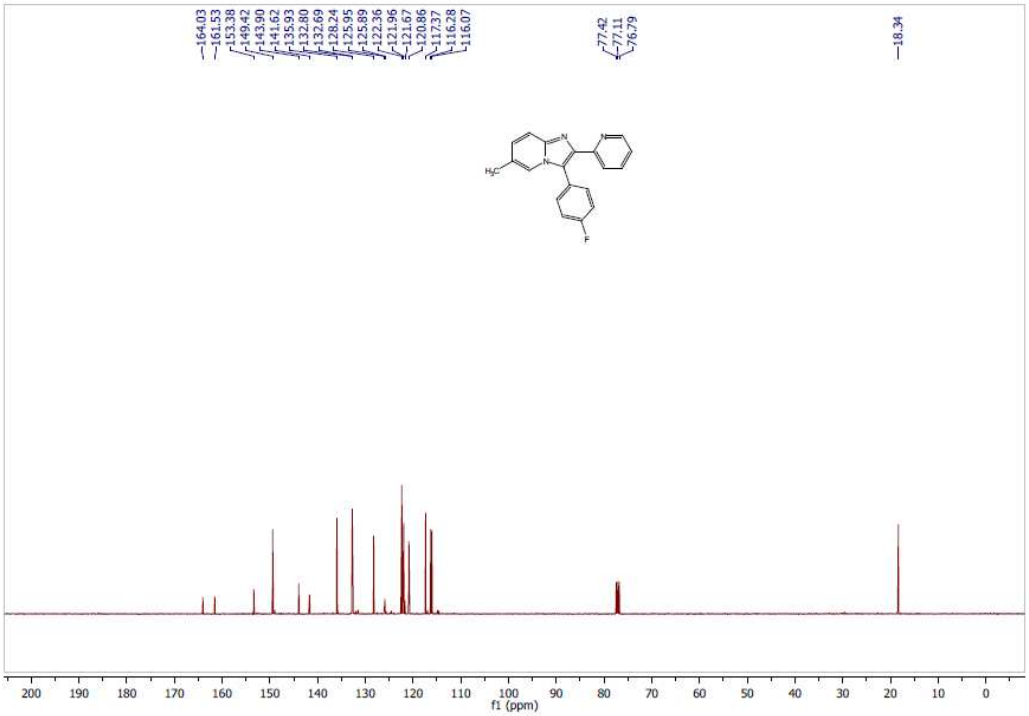

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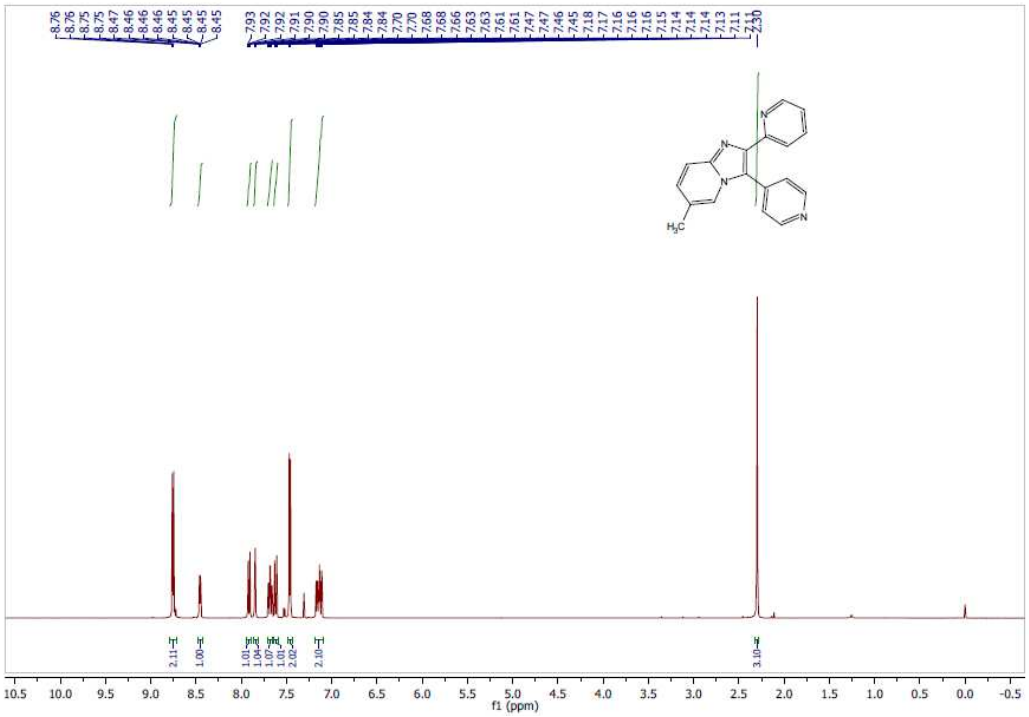

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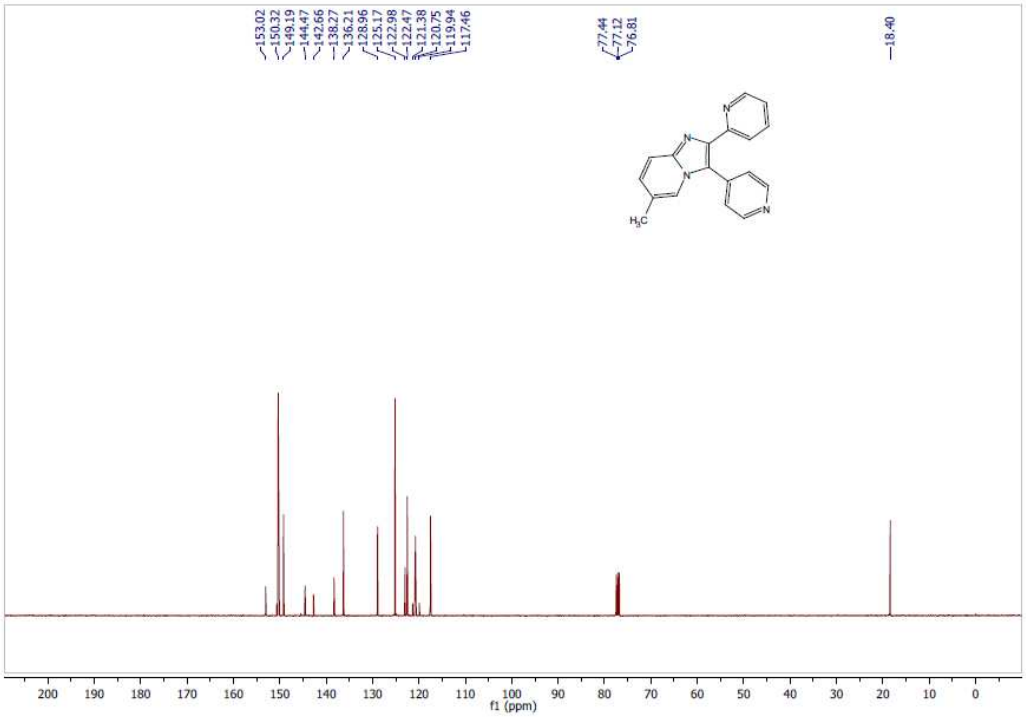

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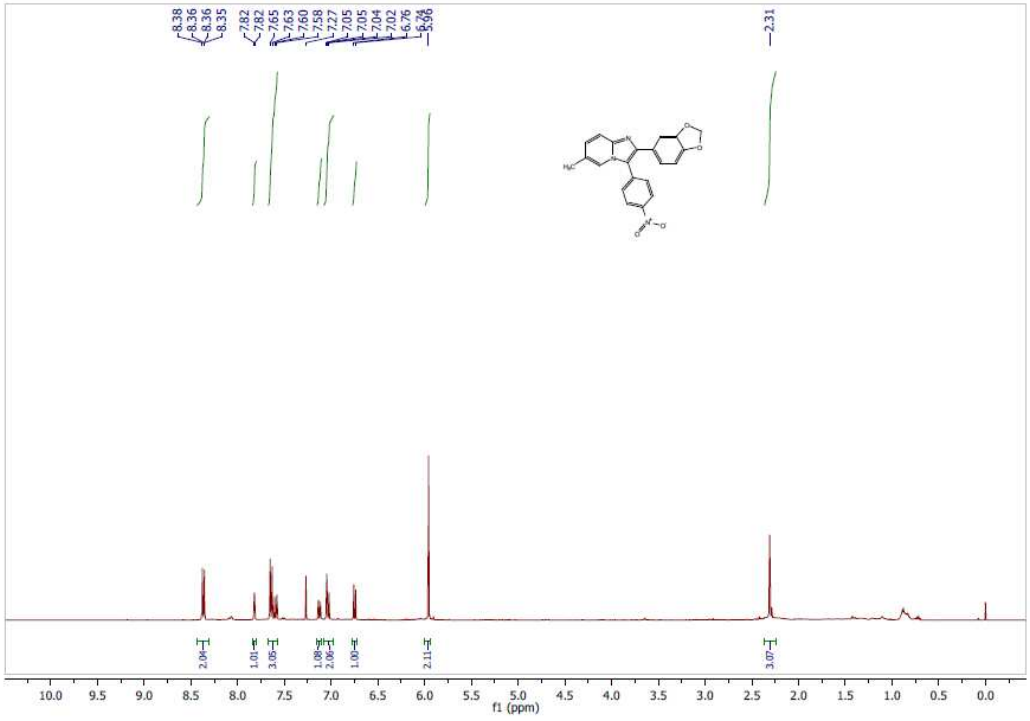

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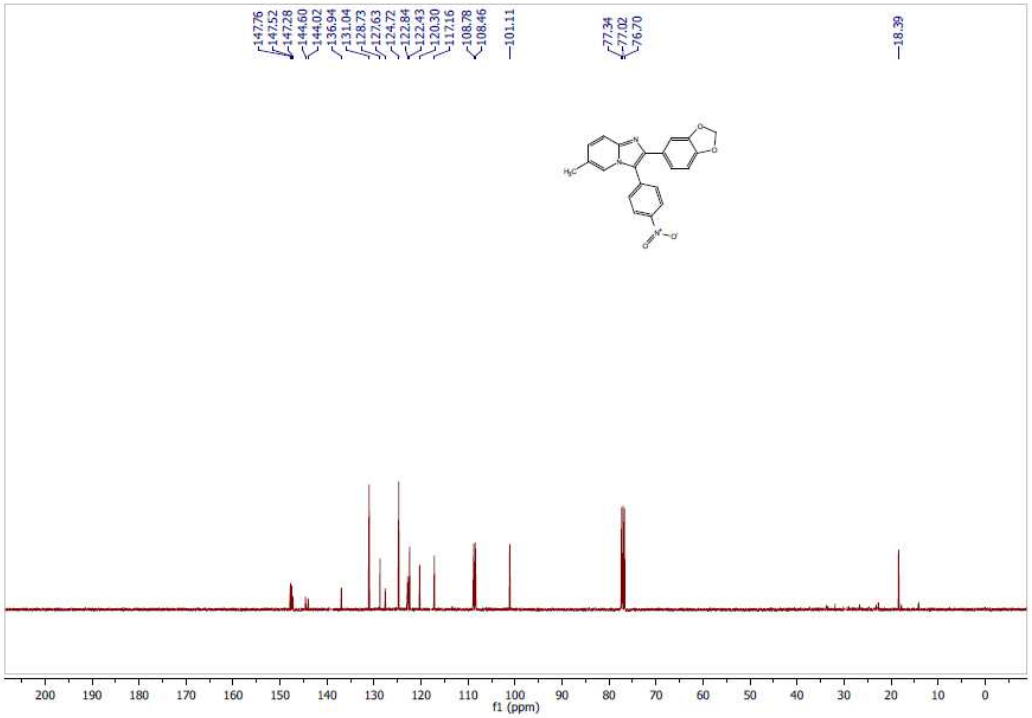
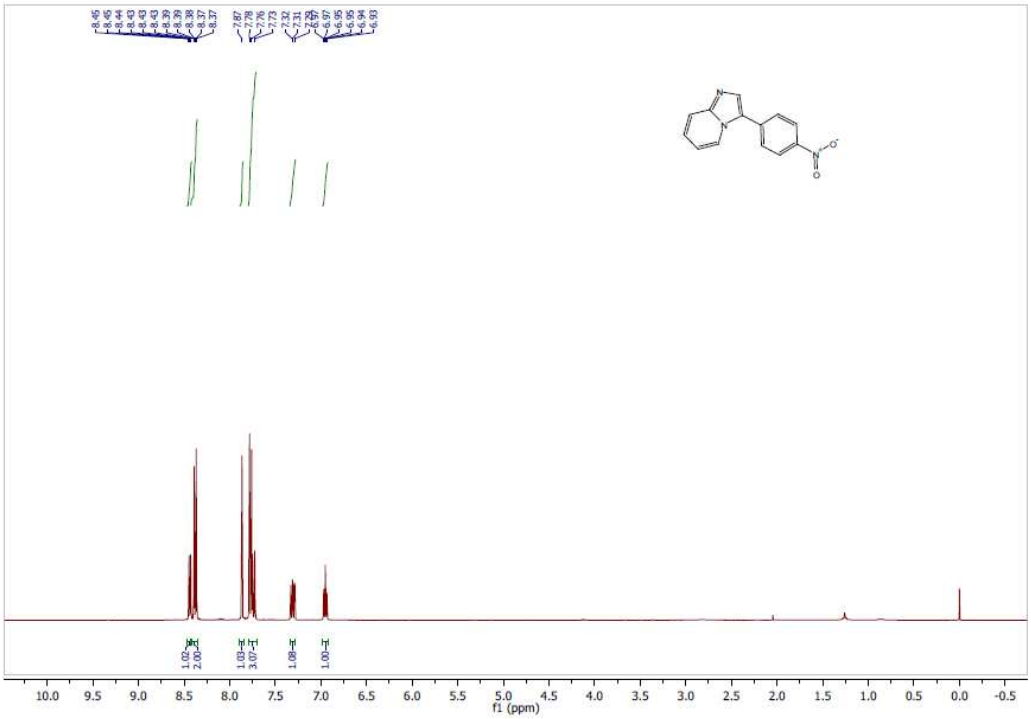
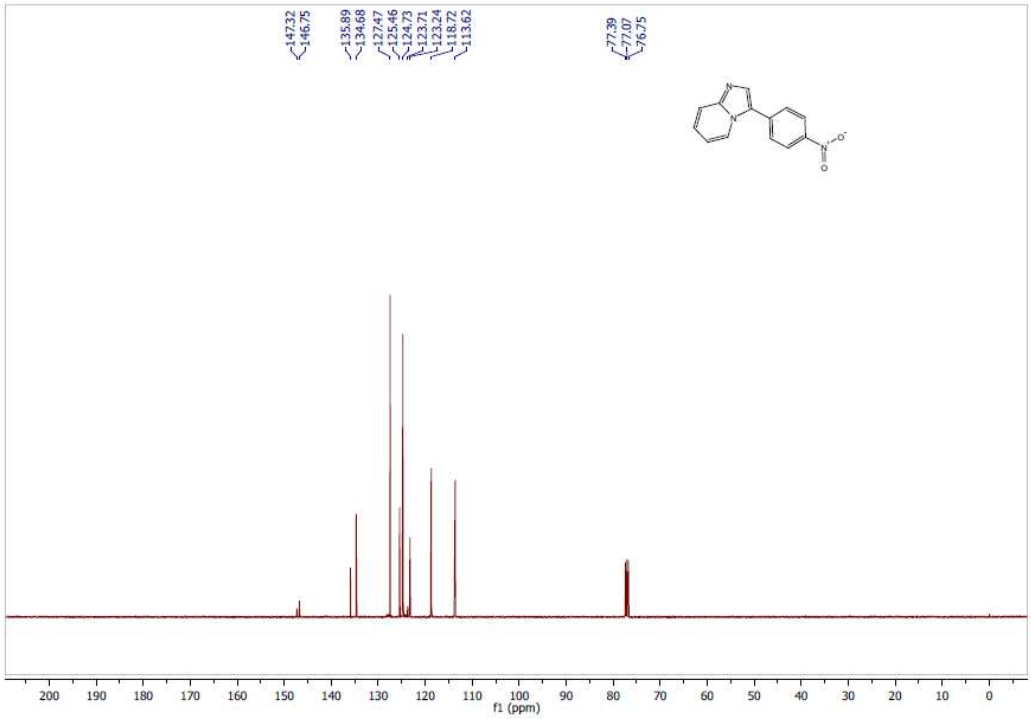


^{1}H-NMR of 6



^{13}C-NMR of 6



TGFβ-R1 Computational Modeling.

Computational modeling studies were completed using AutoDock Vina, AutoDock Tools, and Discovery Studio 3.5. Using AutoDock Tools, the TGFβ-R1 crystal structure (PDB: 3FFA) was prepared as follows: 1) All waters and ligands were removed from the structure, 2) All hydrogens were added as 'Polar Only', and 3) A grid box for the ATP binding site was created (center x = 75.827, center y = 23.317, center z = 93.636 / size x = 18, size y = 22, size z = 22). Compounds to be computationally modeled were assigned appropriate rotatable bonds using AutoDock Tools. To computational model the compounds, AutoDock Vina was employed. After the modeling study, the results were visualized and analyzed with Discovery Studio 3.5.