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Supporting Information

A multi pathway coupled domino strategy: I_2/TBHP-promoted synthesis of imidazopyridines and thiazoles via sp^3, sp^2 and sp C–H functionalization

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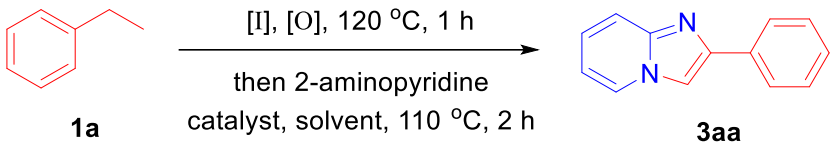
1. General

The Reagents and solvents are commercially purchased and used directly unless otherwise mentioned. All reactions were carried out in a sealed Schlenk tubes and monitored by TLC. Flash column chromatography was performed with silica gel (300–400 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance 400 instrument (400 MHz for ^{1}H and 101 MHz for ^{13}C NMR spectroscopy). Data were reported as chemical shifts in ppm relative to TMS (0.00 ppm) for ^{1}H and $CDCl_3$ (77.16 ppm) or DMSO-d_6 (39.52 ppm) for ^{13}C. HRMS spectra were measured on a Q-TOF instrument in positive-ion mode with an ESI ion source.

2. General procedure for substrates

Ethyl arenes or ethylene arenes or ethyne arenes (1.0 mmol), I_2 (0.40 mmol), tert-butyl hydroperoxide (TBHP, 3.5 mmol, 70% aq. solution) were placed in a sealed tube equipped with a magnetic stirring bar. These mixtures were stirred and reacted at 120°C for 1-1.5 h. After disappearance of the reactant monitored by TLC, 2-aminopyridine (2.0mmol) and $CuCl_2$ (0.5mmol) in DMF (3 ml) was added to the sealed tube at 110 °C and heated for 2 h. After the reaction, 30 ml of saturated $Na_2S_2O_3$ solution was added to the reaction solution to quench the remaining iodine. Then the solution was extracted with ethyl acetate (3 x 30 mL), dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. concentrated under reduced pressure. The residue was purified through silica gel eluting with ethyl acetate/hexanes to give the product.

3. Screening of reaction parameters [a]



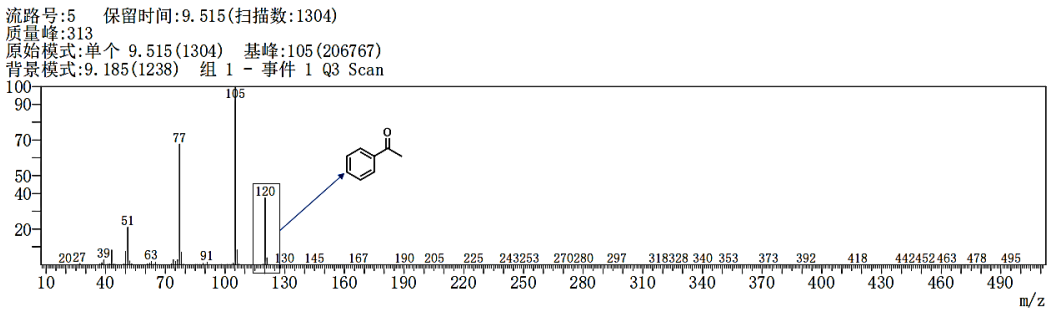
1a **3aa**

Entry	[I]	[O]	catalyst (equiv.)	temperature	solvent	yield, %[b]
Influence of the temperature (the first step)						
1	I_2	TBHP	$CuCl_2$ (0.5)	140 °C	DMF	74
2	**I_2**	**TBHP**	**$CuCl_2$ (0.5)**	**120 °C**	**DMF**	**82**
3	I_2	TBHP	$CuCl_2$ (0.5)	100 °C	DMF	54
4	I_2	TBHP	$CuCl_2$ (0.5)	80 °C	DMF	19
5	I_2	TBHP	$CuCl_2$ (0.5)	60 °C	DMF	None
Influence of the copper salt						
6	I_2	TBHP	-	120 °C	DMF	33
7	I_2	TBHP	CuI (0.5)	120 °C	DMF	41
8	I_2	TBHP	CuCl (0.5)	120 °C	DMF	60
9	I_2	TBHP	$CuSO_4$ (0.5)	120 °C	DMF	47
10	**I_2**	**TBHP**	**$CuCl_2$ (0.5)**	**120 °C**	**DMF**	**82**
11	I_2	TBHP	$Cu(OAc)_2$ (0.5)	120 °C	DMF	57
12	I_2	TBHP	$Cu(NO_3)_2$ (0.5)	120 °C	DMF	Trace
Influence of the equivalent of $CuCl_2$						
13	I_2	TBHP	$CuCl_2$ (0.1)	120 °C	DMF	54
14	I_2	TBHP	$CuCl_2$ (0.1) + **L_1**[c]	120 °C	DMF	75
15	I_2	TBHP	$CuCl_2$ (0.2)	120 °C	DMF	67
16	**I_2**	**TBHP**	**$CuCl_2$ (0.5)**	**120 °C**	**DMF**	**82**
17	I_2	TBHP	$CuCl_2$ (0.8)	120 °C	DMF	77

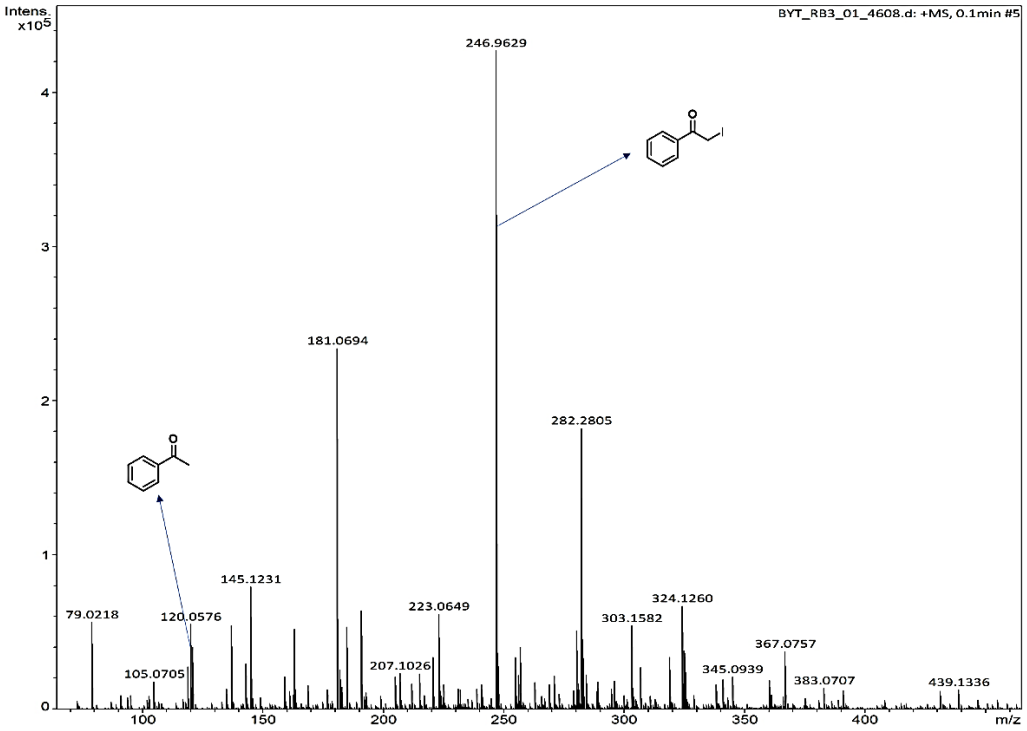
[a] Reaction conditions: **1a** (1 mmol), [I] (0.4 mmol), [O] (3 mmol), 120 °C, 1 h; then 2-aminopyridine (2.0 mmol), $CuCl_2$ (0.5 mmol), solvent (3 mL), 110 °C, 2 h. [b] Isolated yield. [c] L_1 = 1,10-phenanthroline, 0.2 mmol.

4. Monitoring the reaction using GC-MS, HRMS

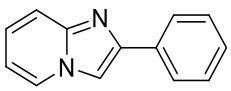
(1) The GC-MC image of ethylbenzene as raw material reacted for 20 minutes:



(2) The HRMS image of α-iodo acetophenone (**1ab**)



5. Characterization Data for the products



3aa

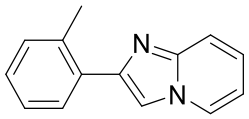
2-Phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 82% isolated yield, mp 135-137 ºC.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.53 (dt, J = 6.8, 1.2 Hz, 1H), 8.40 (s, 1H), 8.02 – 7.94 (m, 2H), 7.59 (dd, J = 9.1, 1.0 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.37 – 7.29 (m, 1H), 7.25 (ddd, J = 9.1, 6.7, 1.3 Hz, 1H), 6.90 (td, J = 6.7, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 145.29, 144.82, 134.39, 129.18, 128.17, 127.35, 126.04, 124.99, 117.11, 112.74, 109.57.

HRMS m/z (ESI): calcd. for $[C_{13}H_{10}N_2+H]^+$: 195.0917 Found: 195.0911



3ba

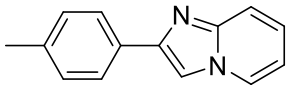
2-(*o*-Tolyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 64% isolated yield, mp = 101-103 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.68 (d, *J* = 6.8 Hz, 1H), 6.47 (d, *J* = 6.7 Hz, 1H), 6.40 – 6.10 (m, 2H), 5.83 (s, 3H), 5.80 – 5.59 (m, 1H), 5.33 (t, *J* = 6.7 Hz, 1H), 1.11 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.24, 144.65, 135.77, 133.22, 130.92, 129.73, 127.81, 126.04, 125.57, 124.66, 117.51, 112.33, 110.78, 22.66.

HRMS m/z (ESI): calcd. for $[C_{14}H_{12}N_2+H]+$: 209.1079 Found:209.1078



3ca

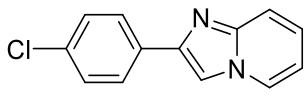
2-(*p*-Tolyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 85% isolated yield, mp 144-145 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 6.7 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.75 (s, 1H), 7.60 (d, *J* = 9.1 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.11 (ddd, *J* = 9.1, 6.8, 1.3 Hz, 1H), 6.69 (td, *J* = 6.7, 1.2 Hz, 1H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.85, 145.59, 137.79, 130.95, 129.45, 125.93, 125.55, 124.52, 117.37, 112.28, 107.80, 21.33.

HRMS m/z (ESI): calcd. for $[C_{14}H_{12}N_2+H]^+$:209.1079 Found:209.1079



3da

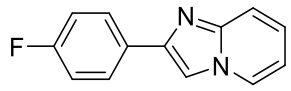
2-(4-Chlorophenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 84% isolated yield, mp 202-205 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 7.91 (m, 2H), 7.80 – 7.70 (m, 2H), 7.53 (d, *J* = 9.1 Hz, 1H), 7.35 (d, *J* = 8.9 Hz, 1H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.13 – 7.05 (m, 1H), 6.69 (t, *J* = 6.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.65, 143.58, 132.68, 131.18, 127.89, 126.23, 124.59, 123.98, 116.52, 111.64, 107.16.

HRMS m/z (ESI): calcd. for $[C_{13}H_9ClN_2+H]^+$:229.0533 Found:229.0524



3ea

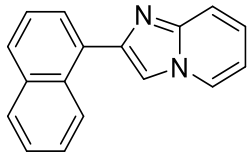
2-(4-Fluorophenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 78% isolated yield, mp 163-165 ºC.

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.25 – 9.21 (m, 1H), 8.77 (s, 1H), 8.02 – 7.94 (m, 4H), 7.61 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.58 – 7.52 (m, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 138.85, 136.65, 132.35, 129.78, 128.88, 128.68, 126.32, 126.28, 125.66, 122.61, 112.98, 110.77.

HRMS m/z (ESI): calcd. for $[C_{13}H_9FN_2+H]^+$:213.0829 Found:213.0813



3fa

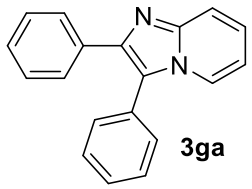
2-(Naphthalen-1-yl)imidazo[1,2-*a*]pyridine

White solid was obtained in 91% isolated yield, mp = 158-160 ºC.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 1.7, 0.8 Hz, 1H), 8.07 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.93 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.90 (d, *J* = 0.7 Hz, 1H), 7.88 – 7.84 (m, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.80 – 7.74 (m, 1H), 7.64 (dq, *J* = 9.1, 1.0 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.14 (ddd, *J* = 9.1, 6.7, 1.3 Hz, 1H), 6.73 (td, *J* = 6.7, 1.2 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.54, 145.27, 133.73, 133.29, 130.51, 128.43, 128.39, 127.72, 126.35, 126.09, 125.70, 125.29, 124.96, 124.10, 117.36, 112.80, 108.60.

HRMS m/z (ESI): calcd. for $[C_{17}H_{12}N_2+H]^+$:245.1079 Found:245.1060



3ga

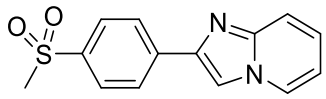
2,3-Diphenylimidazo[1,2-*a*]pyridine

White solid was obtained in 43% isolated yield, mp = 149-151 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 6.9 Hz, 1H), 7.68 (t, *J* = 7.7 Hz, 3H), 7.57 – 7.40 (m, 5H), 7.34 – 7.14 (m, 4H), 6.72 (t, *J* = 6.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.78, 142.33, 134.11, 130.74, 129.84, 129.58, 128.93, 128.30, 128.12, 127.52, 124.78, 123.31, 121.10, 117.53, 112.34.

HRMS m/z (ESI): calcd. for $[C_{19}H_{14}N_2+H]^+$:271.1236 Found:271.1231



3ha

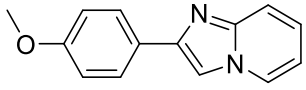
2-(4-(Methylsulfonyl)phenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 73% isolated yield, mp = 242-244 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.13 (m, 3H), 8.05 – 7.96 (m, 3H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.25 (ddd, *J* = 9.1, 6.7, 1.3 Hz, 1H), 6.85 (td, *J* = 6.8, 1.2 Hz, 1H), 3.11 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.98, 143.57, 139.28, 139.26, 127.94, 126.60, 125.86, 125.57, 117.87, 113.11, 109.69, 44.64.

HRMS m/z (ESI): calcd. for $[C_{14}H_{12}N_2O_2S+H]^+$:273.0698 Found:273.0680



3ia

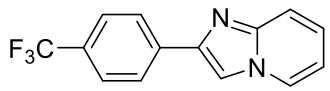
2-(4-Methoxyphenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 89% isolated yield, mp = 133-135 ºC.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (dq, *J* = 6.7, 1.1 Hz, 1H), 7.81 – 7.76 (m, 2H), 7.65 – 7.61 (m, 1H), 7.51 (dt, *J* = 9.1, 1.1 Hz, 1H), 7.03 (ddt, *J* = 9.2, 6.7, 1.3 Hz, 1H), 6.90 – 6.84 (m, 2H), 6.62 (tt, *J* = 6.7, 1.4 Hz, 1H), 3.74 (d, *J* = 1.0 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 159.61, 145.63, 145.57, 127.31, 126.44, 125.49, 124.50, 117.20, 114.15, 112.25, 107.26, 55.31.

HRMS m/z (ESI): calcd. for $[C_{14}H_{12}N_2O+H]^+$:225.1029 Found :225.1029



3ja

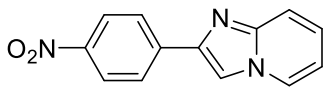
2-(4-(Trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 87% isolated yield, mp = 196-198 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.68 – 6.56 (m, 3H), 6.44 (s, 1H), 6.20 (d, *J* = 8.2 Hz, 3H), 5.76 (dd, *J* = 15.4, 8.7 Hz, 1H), 5.34 (d, *J* = 6.7 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.65, 143.91, 136.91, 129.97, 129.64, 126.16, 125.75 (q, *J*=4.4 Hz), 125.54, 122.90, 117.62, 113.05, 109.05.

HRMS m/z (ESI): calcd. for $[C_{14}H_9F_3N_2+H]^+$:263.0797 Found :263.0794



3ka

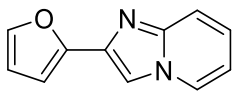
2-(4-Nitrophenyl)imidazo[1,2-*a*]pyridine

Yellow solid was obtained in 85% isolated yield, mp = 258-261ºC.

^{1}H NMR (600 MHz, DMSO-d_6) δ 8.65 (d, *J* = 0.7 Hz, 1H), 8.58 (dt, *J* = 6.8, 1.3 Hz, 1H), 8.34 – 8.29 (m, 2H), 8.26 – 8.21 (m, 2H), 7.63 (dt, *J* = 9.1, 1.0 Hz, 1H), 7.31 (ddd, *J* = 9.1, 6.7, 1.3 Hz, 1H), 6.96 (td, *J* = 6.8, 1.2 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 146.96, 145.73, 142.47, 140.99, 127.74, 126.78, 126.40, 124.67, 117.47, 113.41, 112.17.

HRMS m/z (ESI): calcd. for $[C_{13}H_9N_3O_2+H]^+$:240.0774 Found:240.0766



3la

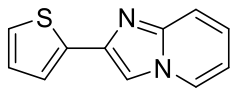
2-(Furan-2-yl)imidazo[1,2-*a*]pyridine

White solid was obtained in 81% isolated yield, mp = 88-90 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (dt, *J* = 6.8, 1.3 Hz, 1H), 7.68 (s, 1H), 7.50 (d, *J* = 9.0 Hz, 1H), 7.38 (d, *J* = 1.1 Hz, 1H), 7.07 (ddd, *J* = 9.2, 6.8, 1.3 Hz, 1H), 6.81 (d, *J* = 2.6 Hz, 1H), 6.66 (td, *J* = 6.8, 1.2 Hz, 1H), 6.42 (dd, *J* = 3.4, 1.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.57, 144.53, 141.02, 136.88, 124.63, 123.95, 116.30, 111.49, 110.56, 106.83, 105.65.

HRMS m/z (ESI): calcd. for $[C_{11}H_8N_2O+H]^+$:185.0716 Found:185.0696



3ma

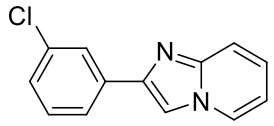
2-(Thiophen-2-yl)imidazo[1,2-*a*]pyridine

White solid was obtained in 76% isolated yield, mp = 136-138 ºC.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (dt, *J* = 6.7, 1.2 Hz, 1H), 7.54 (d, *J* = 0.7 Hz, 1H), 7.44 (dq, *J* = 9.1, 1.0 Hz, 1H), 7.31 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.16 (dd, *J* = 5.0, 1.2 Hz, 1H), 6.99 – 6.91 (m, 2H), 6.55 (td, *J* = 6.7, 1.2 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.35, 140.71, 137.55, 127.78, 125.50, 125.02, 124.86, 123.69, 117.10, 112.51, 107.50.

HRMS m/z (ESI): calcd. for $[C_{11}H_8N_2S+H]^+$:201.0487 Found:201.0468



3na

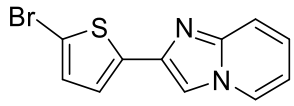
2-(3-Chlorophenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 62% isolated yield, mp = 107-109 ºC.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.89 (t, *J* = 1.9 Hz, 1H), 7.78 (d, *J* = 0.7 Hz, 1H), 7.76 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.58 (dq, *J* = 9.1, 1.0 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.22 (ddd, *J* = 7.9, 2.1, 1.1 Hz, 1H), 7.13 (ddd, *J* = 9.1, 6.7, 1.3 Hz, 1H), 6.74 (td, *J* = 6.7, 1.2 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.55, 144.14, 135.33, 134.79, 130.03, 128.03, 126.13, 125.73, 125.30, 124.14, 117.55, 112.89, 108.55.

HRMS m/z (ESI): calcd. for $[C_{13}H_9ClN_2+H]^+$:229.0533 Found:229.0516



3oa

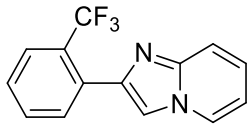
2-(5-Bromothiophen-2-yl)imidazo[1,2-*a*]pyridine

White solid was obtained in 68% isolated yield, mp = 140-142 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60 (d, *J* = 6.8 Hz, 1H), 6.38 – 6.08 (m, 2H), 5.89 – 5.69 (m, 2H), 5.55 (d, *J* = 3.8 Hz, 1H), 5.33 (t, *J* = 6.7 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.14, 139.49, 138.49, 137.85, 130.72, 125.61, 124.23, 117.16, 113.09, 112.16, 107.42.

HRMS m/z (ESI): calcd. for $[C_{11}H_7BrN_2S+H]^+$:278.9592 Found:278.9573



3pa

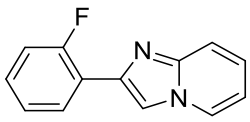
2-(2-(Trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 43% isolated yield, mp: 90-92 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.91 (d, *J* = 7.4 Hz, 1H), 7.73 (s, 1H), 7.68 (d, *J* = 6.6 Hz, 1H), 7.59 – 7.52 (m, 2H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.11 (ddd, *J* = 9.1, 6.8, 1.3 Hz, 1H), 6.72 (td, *J* = 6.8, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.72, 141.27, 132.25, 131.55, 130.72, 126.78, 126.45, 125.05(q, *J* = 5.8 Hz), 124.68, 123.89, 121.96, 116.67, 111.58, 110.41.

HRMS m/z (ESI): calcd. for $[C_{14}H_9F_3N_2+H]^+$:263.0797 Found:263.0796



3qa

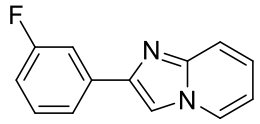
2-(2-Fluorophenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 67% isolated yield， mp: 94-97 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (td, *J* = 7.6, 2.7 Hz, 1H), 8.04 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.97 (d, *J* = 3.9 Hz, 1H), 7.56 (dd, *J* = 9.1, 1.0 Hz, 1H), 7.27 – 7.15 (m, 2H), 7.13 – 7.03 (m, 2H), 6.70 (td, *J* = 6.8, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.51, 158.04, 143.77, 138.07, 127.85 (*J* = 8.6 Hz), 124.71, 123.98, 123.47 (*J* = 3.3 Hz), 120.42 (*J* = 12.2 Hz), 116.39, 114.62 (*J* = 22.1 Hz), 111.46, 111.06 (*J* = 15.2 Hz).

HRMS m/z (ESI): calcd. for $[C_{13}H_9FN_2+H]^+$:213.0829 Found:213.0826



3ra

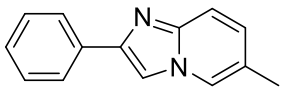
2-(3-Fluorophenyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 65% isolated yield, mp = 101-103 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.83 (s, 1H), 7.77 – 7.57 (m, 3H), 7.38 (td, *J* = 8.0, 5.9 Hz, 1H), 7.17 (ddd, *J* = 9.1, 6.8, 1.3 Hz, 1H), 7.01 (tdd, *J* = 8.4, 2.7, 1.0 Hz, 1H), 6.78 (td, *J* = 6.8, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.49, 162.05, 145.65, 144.56 (*J* = 2.8 Hz), 136.06 (*J* = 8.3 Hz), 130.21 (*J* = 8.3 Hz), 125.66, 125.01, 121.58 (*J* = 2.9 Hz), 117.61, 114.71 (*J* = 21.4 Hz), 112.80 (*J* = 22.1 Hz), 108.54.

HRMS m/z (ESI): calcd. for $[C_{13}H_9FN_2+H]^+$:213.0829 Found:213.0818



3ab

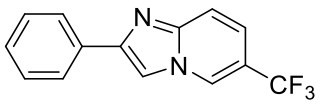
6-Methyl-2-phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 74% isolated yield, mp: 176-177 ºC.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 – 7.84 (m, 2H), 7.81 (dq, *J* = 2.1, 1.1 Hz, 1H), 7.68 (d, *J* = 0.7 Hz, 1H), 7.47 (d, *J* = 9.1 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.27 – 7.21 (m, 1H), 6.94 (dd, *J* = 9.2, 1.7 Hz, 1H), 2.23 (d, *J* = 1.1 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.30, 144.63, 133.71, 128.72, 128.03, 127.89, 125.96, 123.35, 122.19, 116.76, 107.86, 18.12.

HRMS m/z (ESI): calcd. for $[C_{14}H_{12}N_2+H]^+$:209.1079 Found:209.1074



3ac

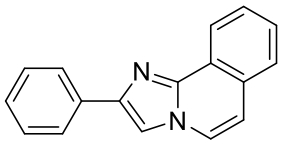
2-Phenyl-6-(trifluoromethyl)imidazo[1,2-*a*]pyridine

White solid was obtained in 67% isolated yield, mp: 165-166 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.88 (dd, *J* = 9.8, 1.6 Hz, 3H), 7.66 (d, *J* = 9.5 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.22 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.69, 144.26, 131.81, 127.86, 127.63, 125.21, 123.55 (q, *J* =5.9 Hz),121.15, 119.61 (q, *J* = 2.7 Hz), 117.10, 115.74, 108.19.

HRMS m/z (ESI): calcd. for $[C_{14}H_9F_3N_2+H]^+$:263.0797 Found:263.0794



3ad

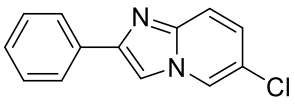
2-Phenylimidazo[2,1-*a*]isoquinoline

White solid was obtained in 62% isolated yield, mp = 144-146 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 7.9 Hz, 1H), 8.01 (d, *J* = 6.8 Hz, 2H), 7.86 (d, *J* = 7.2 Hz, 1H), 7.79 (s, 1H), 7.70 – 7.60 (m, 2H), 7.59 – 7.52 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.00 (d, *J* = 7.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.97, 143.28, 133.95, 129.51, 128.76, 128.20, 128.15, 127.65, 126.97, 125.89, 123.80, 123.55, 122.97, 113.17, 109.88.

HRMS m/z (ESI): calcd. for $[C_{17}H_{12}N_2+H]^+$:245.1079 Found:245.1072



3ae

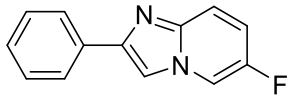
6-Chloro-2-phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 63% isolated yield, mp = 206-209 ºC.

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.25 – 9.21 (m, 1H), 8.77 (s, 1H), 8.02 – 7.98 (m, 3H), 7.96 (dd, *J* = 9.5, 1.9 Hz, 1H), 7.61 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.58 – 7.52 (m, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 138.85, 136.65, 132.35, 129.78, 128.88, 126.32, 126.28, 125.66, 122.61, 112.98, 110.77.

HRMS m/z (ESI): calcd. for $[C_{13}H_9ClN_2+H]^+$:229.0533 Found:229.0525



3af

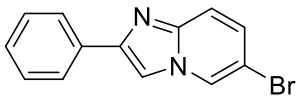
6-Fluoro-2-phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 75% isolated yield, mp = 186-189 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.90 (m, 1H), 7.83 (d, *J* = 6.9 Hz, 2H), 7.74 (s, 1H), 7.56 (dd, *J* = 9.8, 5.1 Hz, 1H), 7.41 – 7.17 (m, 3H), 7.00 (ddd, *J* = 10.2, 8.0, 2.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.27(*J* = 237 Hz), 151.10, 145.83, 142.27, 132.16, 127.77, 127.21, 124.97, 116.25(*J* = 118 Hz), 111.18 (*J* = 41 Hz), 108.49.

HRMS m/z (ESI): calcd. for $[C_{13}H_9FN_2+H]^+$:213.0829 Found:213.0830



3ag

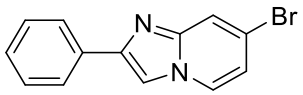
6-Bromo-2-phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 68% isolated yield, mp = 184-186 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.86 (d, *J* = 7.0 Hz, 2H), 7.75 (s, 1H), 7.49 (d, *J* = 9.6 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.17 (dd, *J* = 9.5, 1.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.31, 142.88, 131.86, 127.81, 127.40, 127.34, 125.08, 123.41, 116.98, 107.25, 106.53.

HRMS m/z (ESI): calcd. for $[C_{13}H_9BrN_2+H]^+$:273.0028 Found:273.0031



3ah

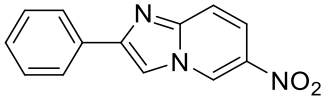
7-Bromo-2-phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 63% isolated yield, mp = 180-182 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.4 Hz, 1H), 7.89 – 7.83 (m, 2H), 7.77 (d, *J* = 3.7 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.32 – 7.17 (m, 1H), 6.83 (dd, *J* = 7.1, 1.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.20, 144.52, 131.81, 127.81, 127.40, 125.08, 124.75, 118.57, 117.63, 115.56, 107.26.

HRMS m/z (ESI): calcd. for $[C_{13}H_9BrN_2+H]^+$:273.0028 Found:273.0030



3ai

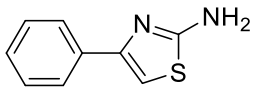
6-Nitro-2-phenylimidazo[1,2-*a*]pyridine

Yellow solid was obtained in 57% isolated yield, mp 171-173 ºC.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.84 (d, *J* = 2.3 Hz, 1H), 8.63 (s, 1H), 8.01 (d, *J* = 6.9 Hz, 2H), 7.96 (dd, *J* = 9.9, 2.3 Hz, 1H), 7.75 (d, *J* = 9.9 Hz, 1H), 7.54 – 7.45 (m, 2H), 7.40 (t, *J* = 7.3 Hz, 1H)

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.91, 145.46, 136.97, 133.16, 129.44, 129.15, 128.55, 126.40, 119.54, 116.52, 112.16.

HRMS m/z (ESI): calcd. for $[C_{13}H_9N_3O_2+H]^+$:240.0774 Found:240.0769



3aj

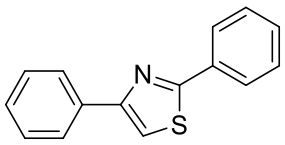
4-Phenylthiazol-2-amine

White solid was obtained in 79% isolated yield, mp 147-149 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.65 (m, 2H), 7.31 (dd, *J* = 8.3, 6.7 Hz, 2H), 7.26 – 7.16 (m, 1H), 6.64 (s, 1H), 5.22 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.42, 150.10, 133.53, 127.58, 126.73, 124.95, 101.70.

HRMS m/z (ESI): calcd. for $[C_9H_8N_2S+H]^+$:177.0487 Found:177.0479



3ak

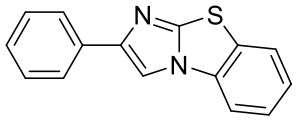
2,4-Diphenylthiazole

White solid was obtained in 86% isolated yield, mp 101-104 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.89 (m, 4H), 7.36 (m, *J* = 7.9, 5.8 Hz, 6H), 7.30 – 7.24 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.90, 156.31, 134.55, 133.79, 130.08, 128.96, 128.78, 128.21, 126.65, 126.49, 112.66.

HRMS m/z (ESI): calcd. for $[C_{15}H_{11}NS+H]^+$:238.0688 Found:238.0680



3al

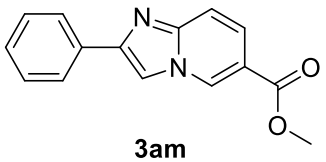
2-Phenylbenzo[*d*]imidazo[2,1-*b*]thiazole

White solid was obtained in 82% isolated yield, mp 142-146 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.79 (d, *J* = 7.0 Hz, 2H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.50 (d, *J* = 9.2 Hz, 1H), 7.39 – 7.29 (m, 3H), 7.28 – 7.15 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.03, 146.57, 132.74, 131.08, 129.21, 127.69, 126.48, 125.14, 124.13, 123.82, 123.33, 111.59, 105.81.

HRMS m/z (ESI): calcd. for $[C_{15}H_{10}N_2S+H]^+$:251.0644 Found:251.0639



3am

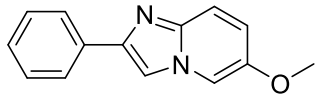
Methyl 2-phenylimidazo[1,2-*a*]pyridine-6-carboxylate

White solid was obtained in 55% isolated yield, mp 174-175 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (dd, *J* = 1.7, 1.0 Hz, 1H), 7.92 – 7.85 (m, 2H), 7.83 (s, 1H), 7.64 (dd, *J* = 9.4, 1.7 Hz, 1H), 7.55 (d, *J* = 9.4 Hz, 1H), 7.37 (dd, *J* = 8.2, 6.7 Hz, 2H), 7.32 – 7.25 (m, 1H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.27, 146.53, 145.04, 131.96, 128.74, 127.80, 127.50, 125.17, 123.38, 115.66, 115.48, 107.91, 51.43.

HRMS m/z (ESI): calcd. for $[C_{15}H_{12}N_2O_2+H]^+$:253.0978 Found:253.0976



3an

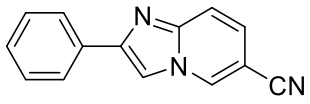
6-Methoxy-2-phenylimidazo[1,2-*a*]pyridine

White solid was obtained in 81% isolated yield, mp 102-105 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.1 Hz, 2H), 7.73 (s, 1H), 7.57 (d, *J* = 2.3 Hz, 1H), 7.47 (d, *J* = 9.8 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.21 (d, *J* = 14.2 Hz, 1H), 6.90 (dd, *J* = 9.7, 2.4 Hz, 1H), 3.75 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.36, 141.59, 132.57, 129.90, 127.71, 126.82, 124.77, 119.04, 116.53, 108.17, 106.40, 55.15.

HRMS m/z (ESI): calcd. for $[C_{14}H_{12}N_2O+H]^+$:225.1029 Found:225.1034



3ao

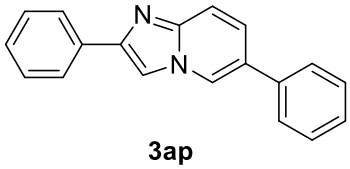
2-Phenylimidazo[1,2-*a*]pyridine-6-carbonitrile

White solid was obtained in 51% isolated yield, mp 240-243 ºC.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.50 (t, *J* = 1.3 Hz, 1H), 7.92 – 7.86 (m, 3H), 7.65 (d, *J* = 9.3 Hz, 1H), 7.40 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.35 – 7.29 (m, 1H), 7.22 (dd, *J* = 9.3, 1.7 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 148.21, 144.69, 132.26, 131.52, 129.06, 128.99, 126.38, 124.72, 118.39, 116.47, 108.97, 98.83.

HRMS m/z (ESI): calcd. for $[C_{14}H_9N_3+H]^+$:220.0875 Found:220.0869



3ap

2,6-Diphenylimidazo[1,2-*a*]pyridine

White solid was obtained in 66% isolated yield, mp 178-180 °C.

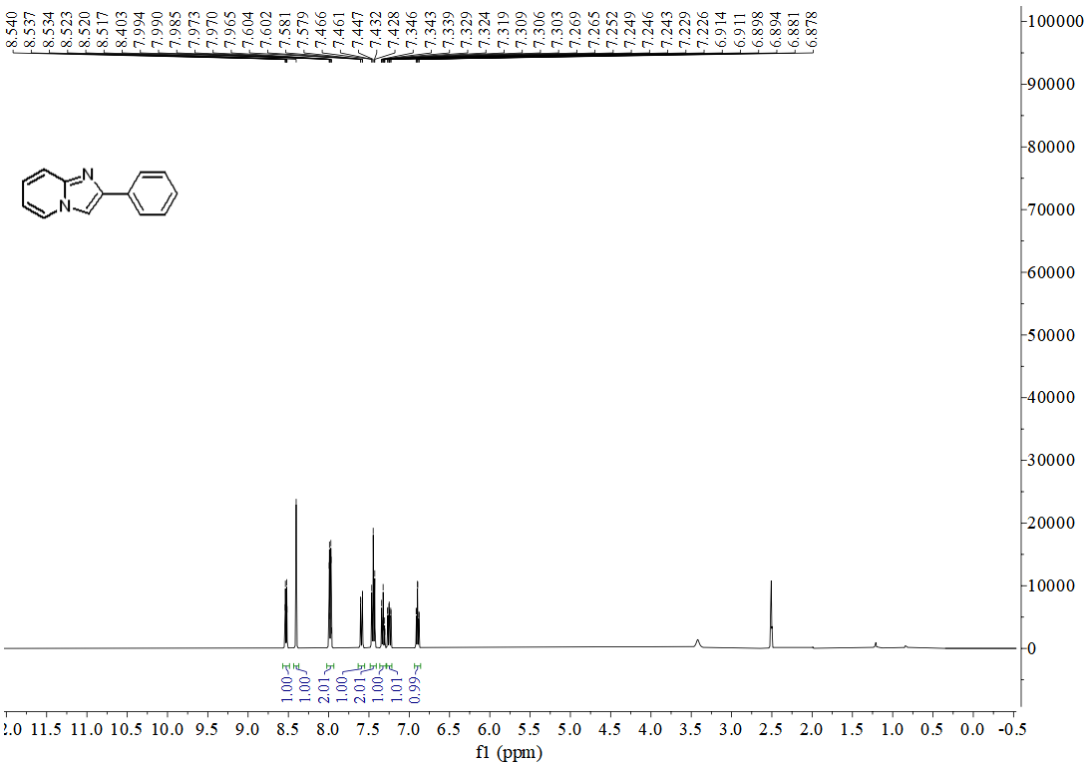
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 9.77 (s, 1H), 9.26 (d, *J* = 10.6 Hz, 1H), 8.50 – 8.16 (m, 5H), 7.75 – 6.94 (m, 5H), 6.86 (d, *J* = 8.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.99, 158.51, 150.01, 149.93, 147.54, 146.39, 137.89, 137.69, 119.19, 118.82, 114.11, 109.50.

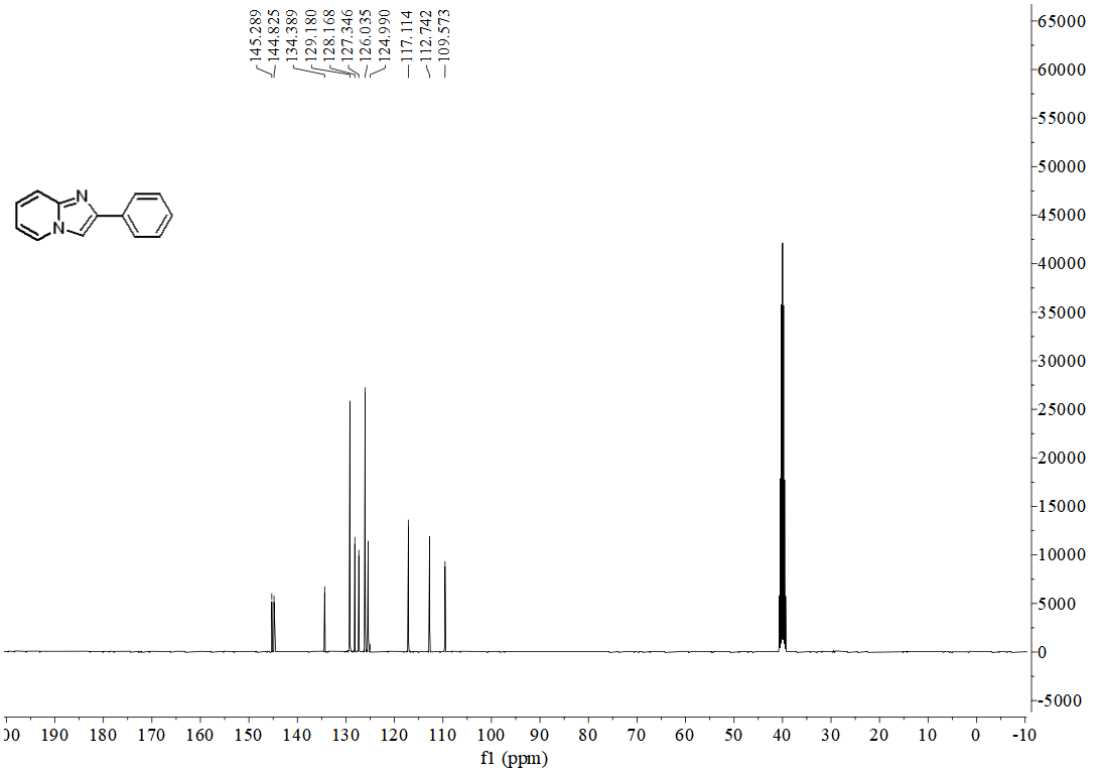
HRMS m/z (ESI): calcd. for $[C_{19}H_{14}N_2+H]^+$:271.1236 Found:271.1243

6. 1H and 13C spectra of products

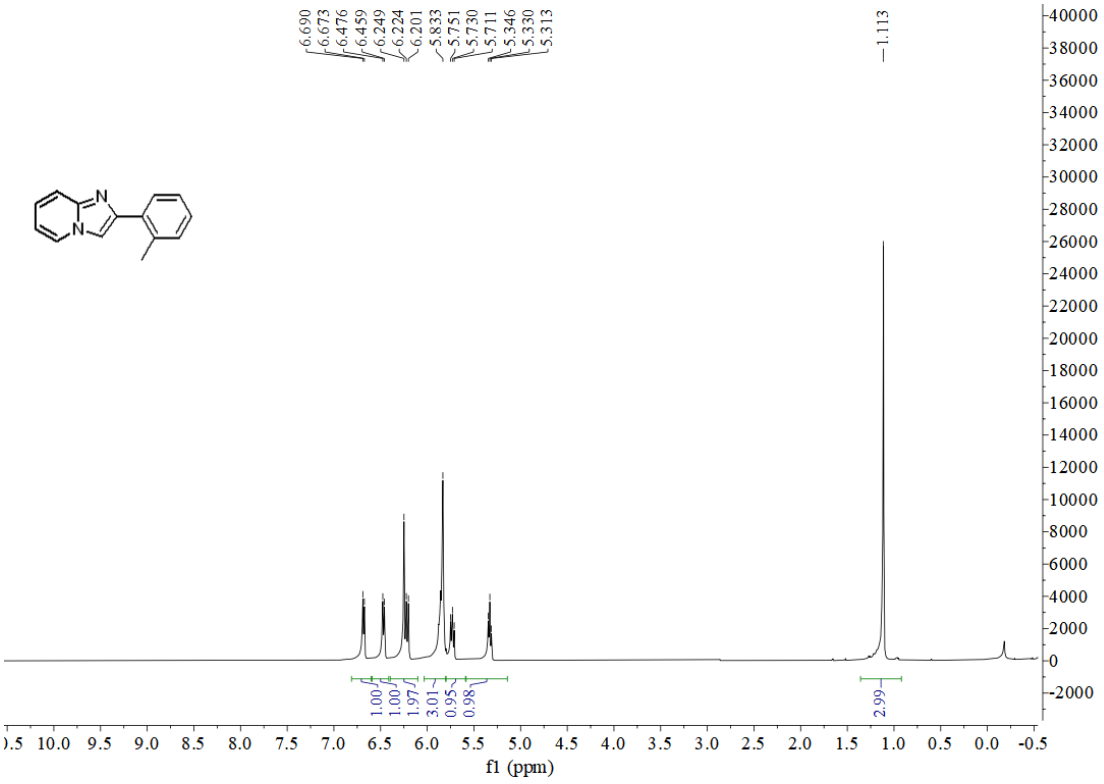
3aa



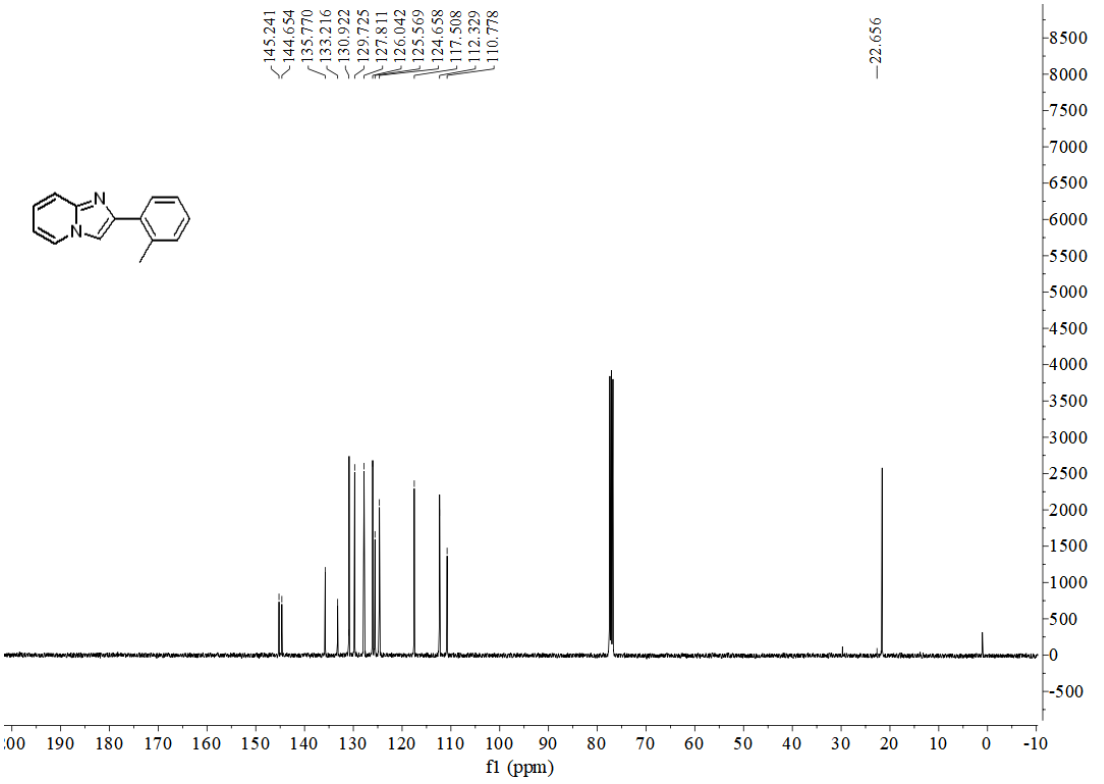
3aa



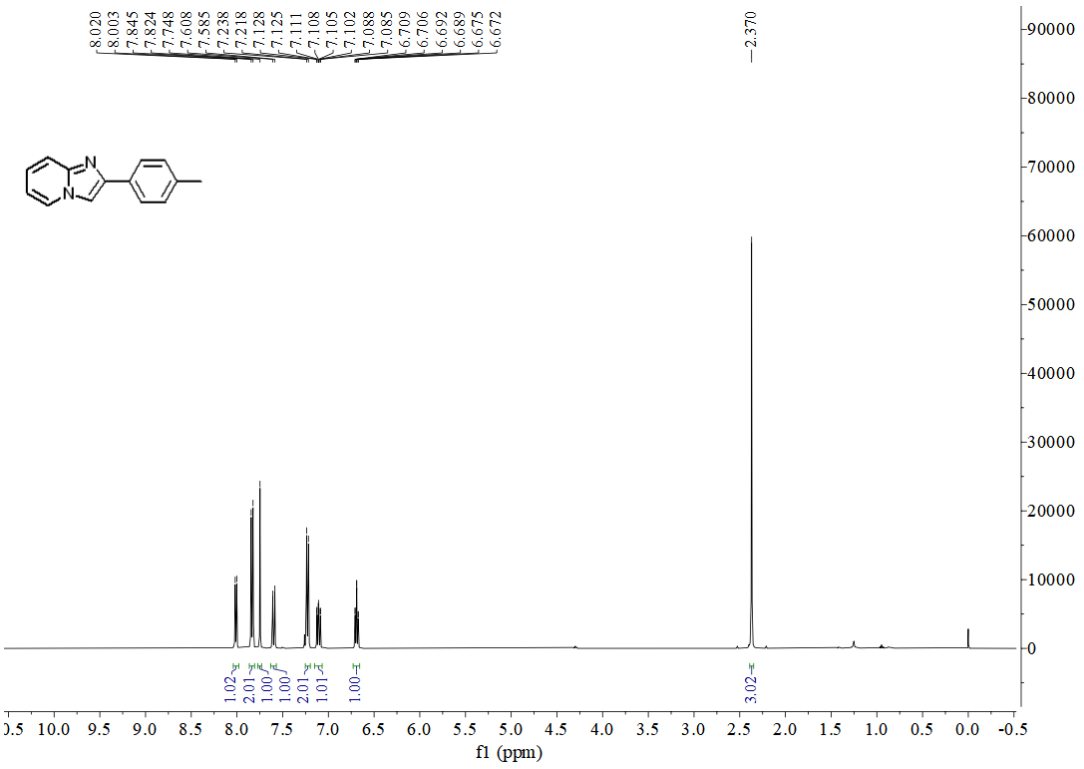
3ba


6.690
6.673
6.476
6.459
6.249
6.224
6.201
5.833
5.751
5.730
5.711
5.346
5.330
5.313
1.113
1.00
1.00
1.97
3.01
0.95
0.98
2.99
f1 (ppm)

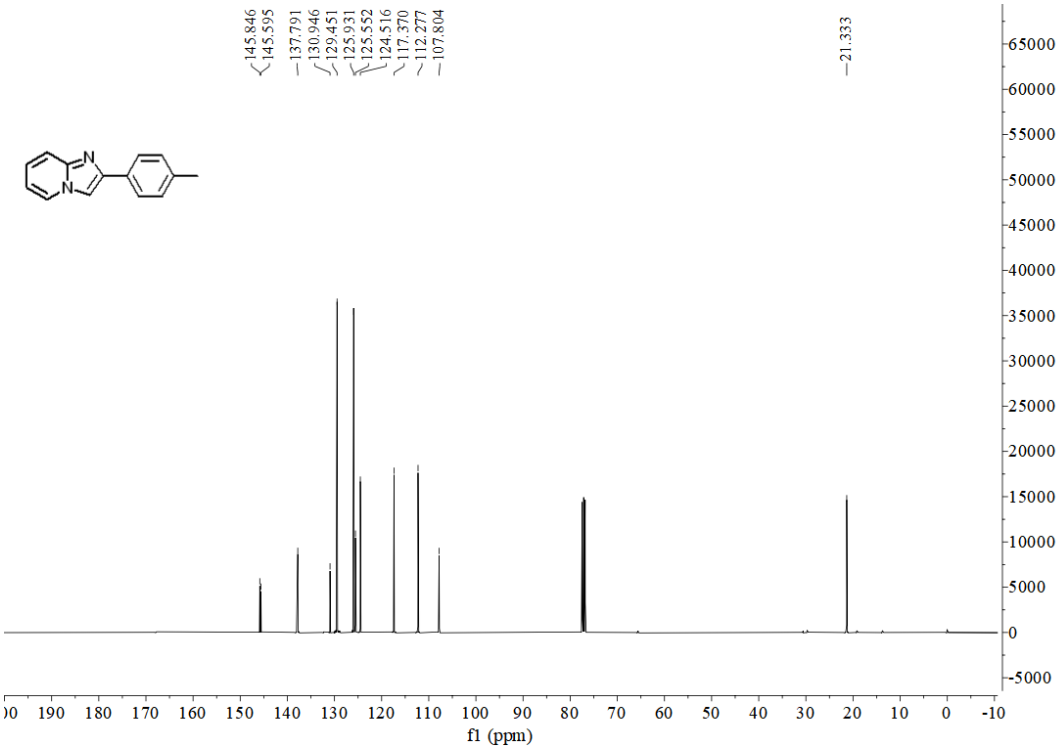
3ba


145.241
144.654
135.770
133.216
130.922
129.725
127.811
126.042
125.569
124.658
117.508
112.329
110.778
22.656
f1 (ppm)

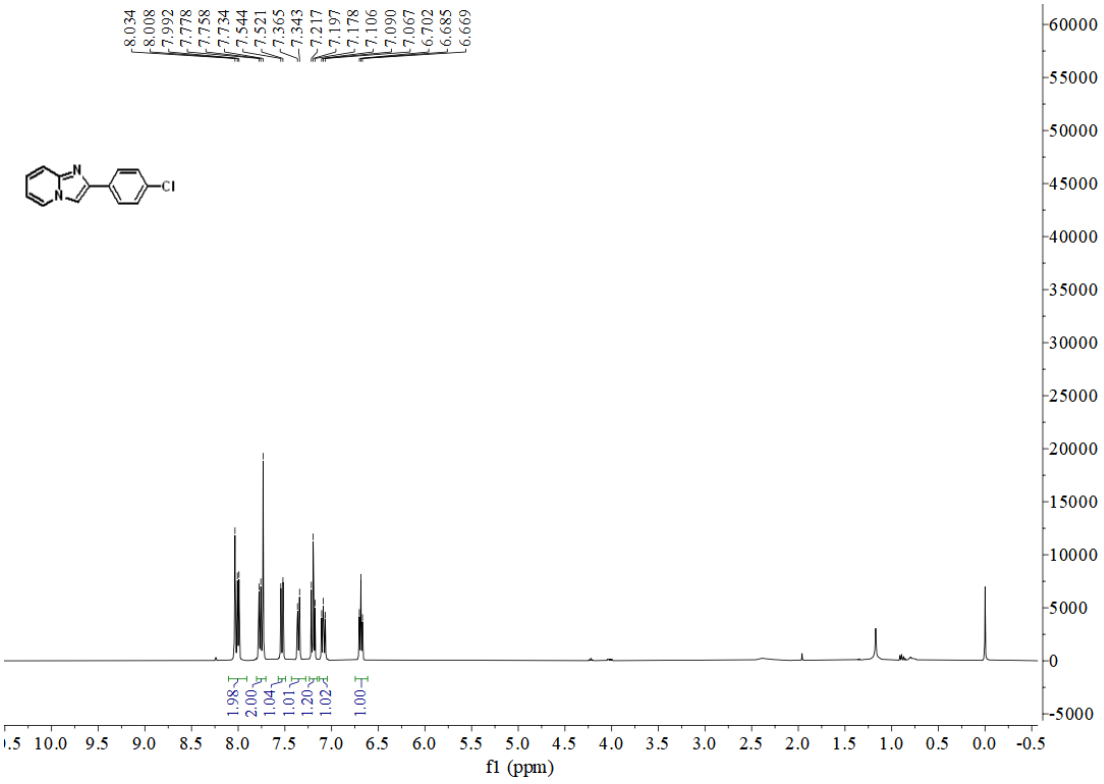
3ca


8.020
8.003
7.845
7.824
7.748
7.608
7.585
7.238
7.218
7.128
7.125
7.111
7.108
7.105
7.102
7.088
7.085
6.709
6.706
6.692
6.689
6.675
6.672
2.370
1.02
2.01
1.00
1.00
2.01
1.01
1.00
3.02
f1 (ppm)

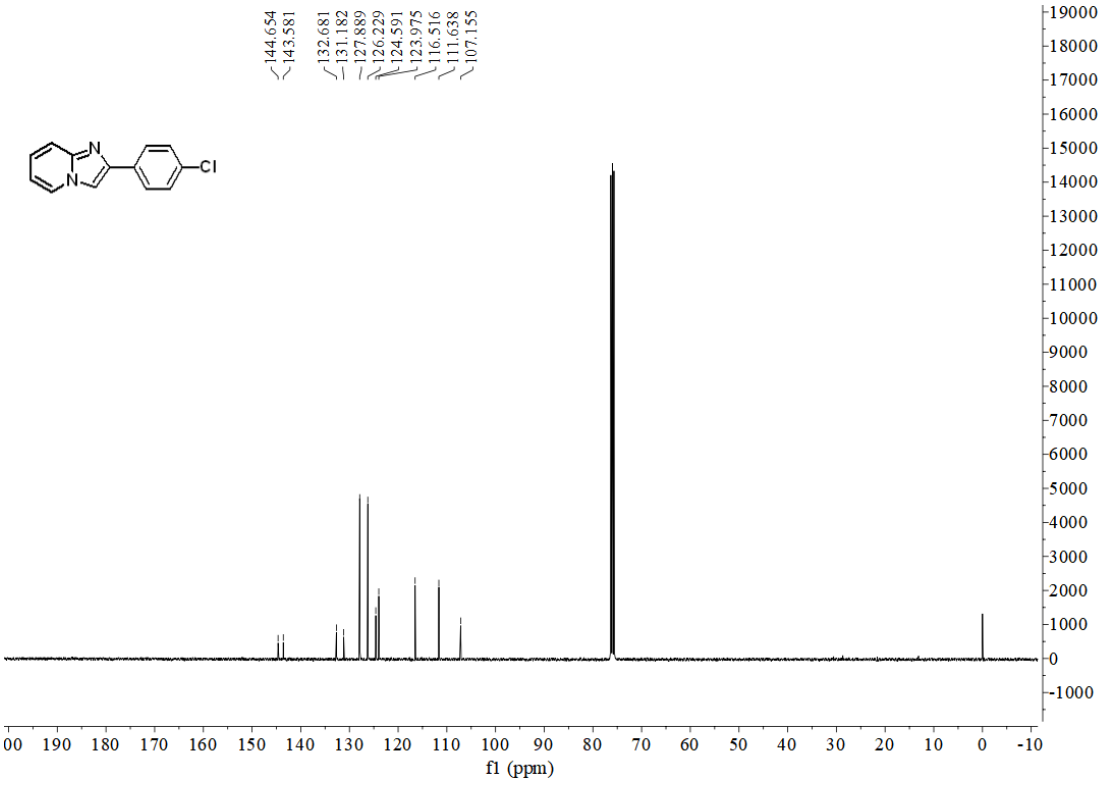
3ca


145.846
145.595
137.791
130.946
129.451
125.931
125.552
124.516
117.370
112.277
107.804
21.333
f1 (ppm)

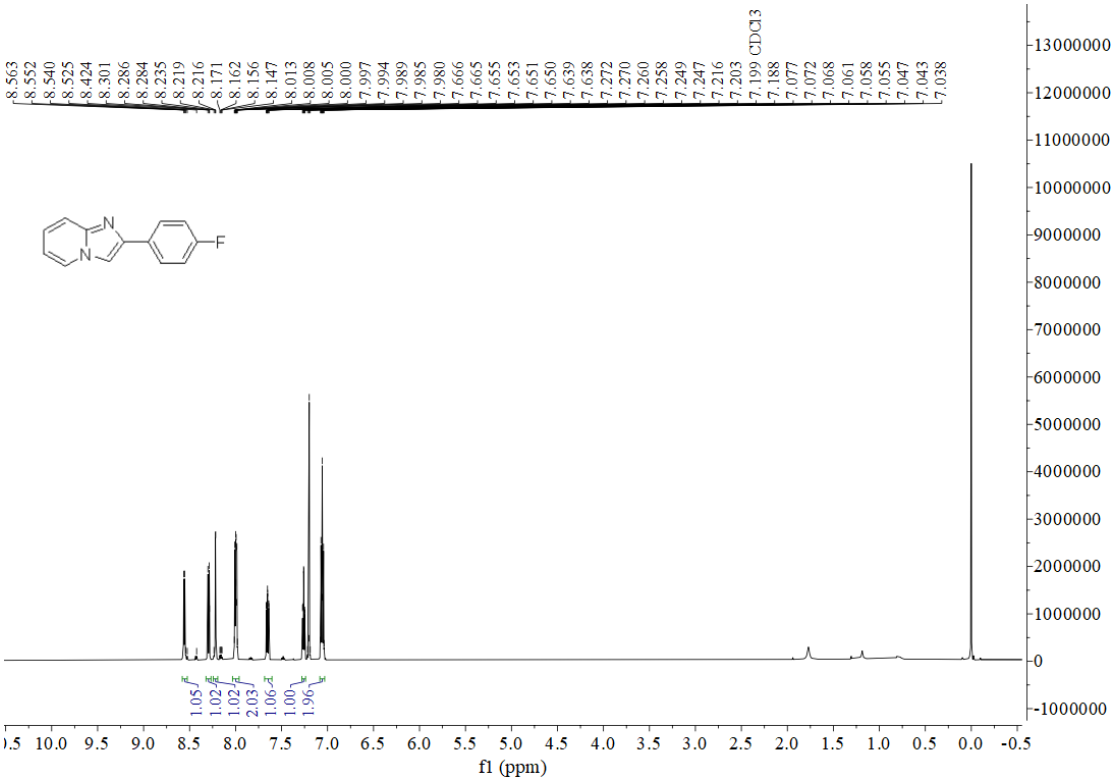
3da


8.034
8.008
7.992
7.778
7.758
7.734
7.544
7.521
7.365
7.343
7.217
7.197
7.178
7.106
7.090
7.067
6.702
6.685
6.669
Cl
1.98
2.00
1.04
1.01
1.20
1.02
1.00
f1 (ppm)

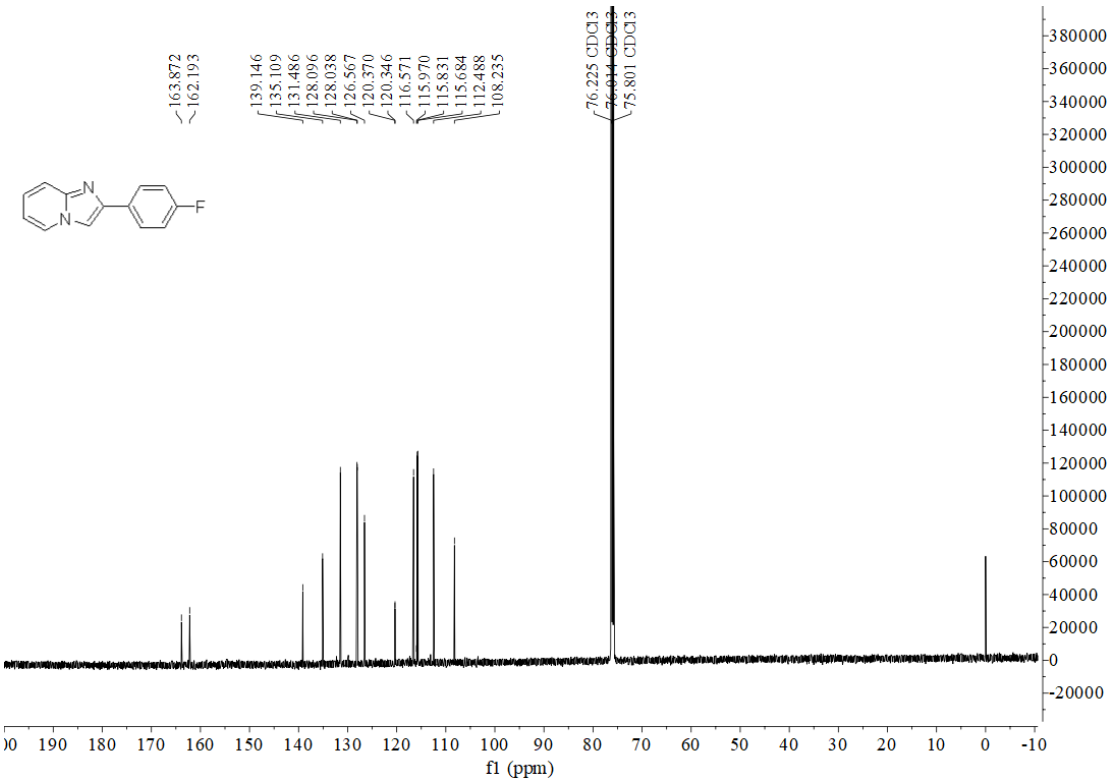
3da


144.654
143.581
132.681
131.182
127.889
126.229
124.591
123.975
116.516
111.638
107.155
Cl
f1 (ppm)

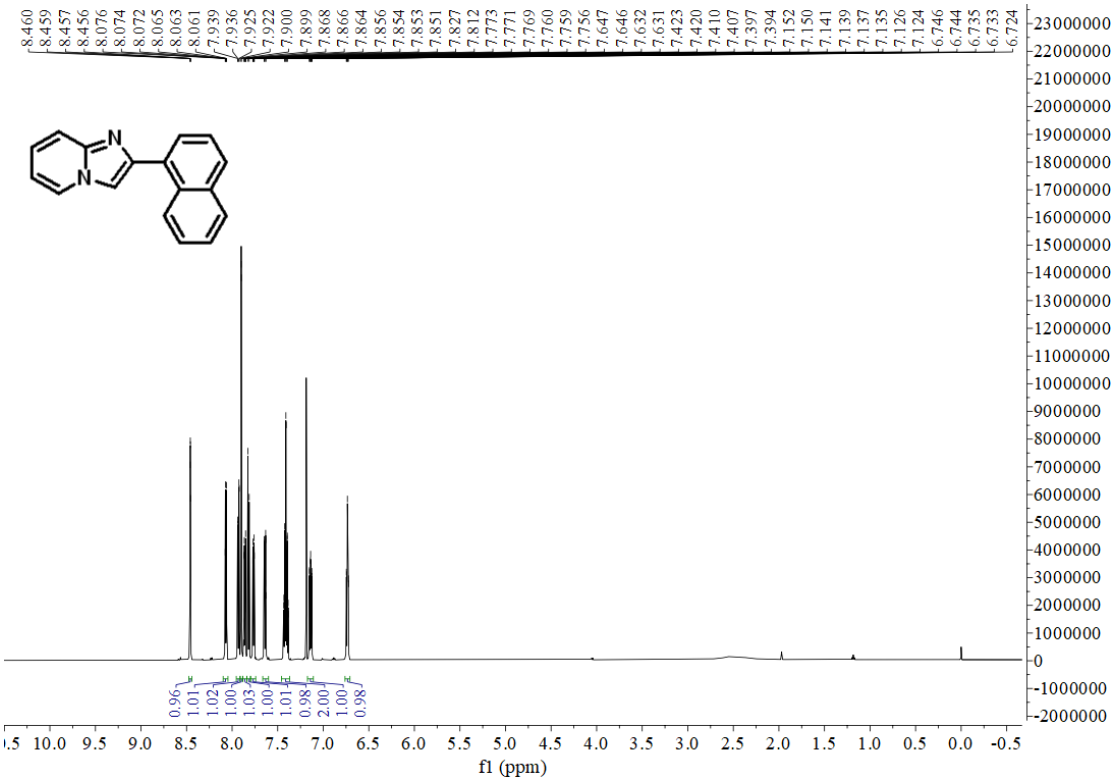
3ea


8.563
8.552
8.540
8.525
8.424
8.301
8.286
8.284
8.235
8.219
8.216
8.171
8.162
8.156
8.147
8.013
8.008
8.005
8.000
7.997
7.994
7.989
7.985
7.980
7.666
7.665
7.655
7.653
7.651
7.650
7.639
7.638
7.272
7.270
7.260
7.258
7.249
7.247
7.216
7.203
7.199 CDCl3
7.188
7.077
7.072
7.068
7.061
7.058
7.055
7.047
7.043
7.038
F
1.05
1.02
1.02
2.03
1.06
1.00
1.96
f1 (ppm)

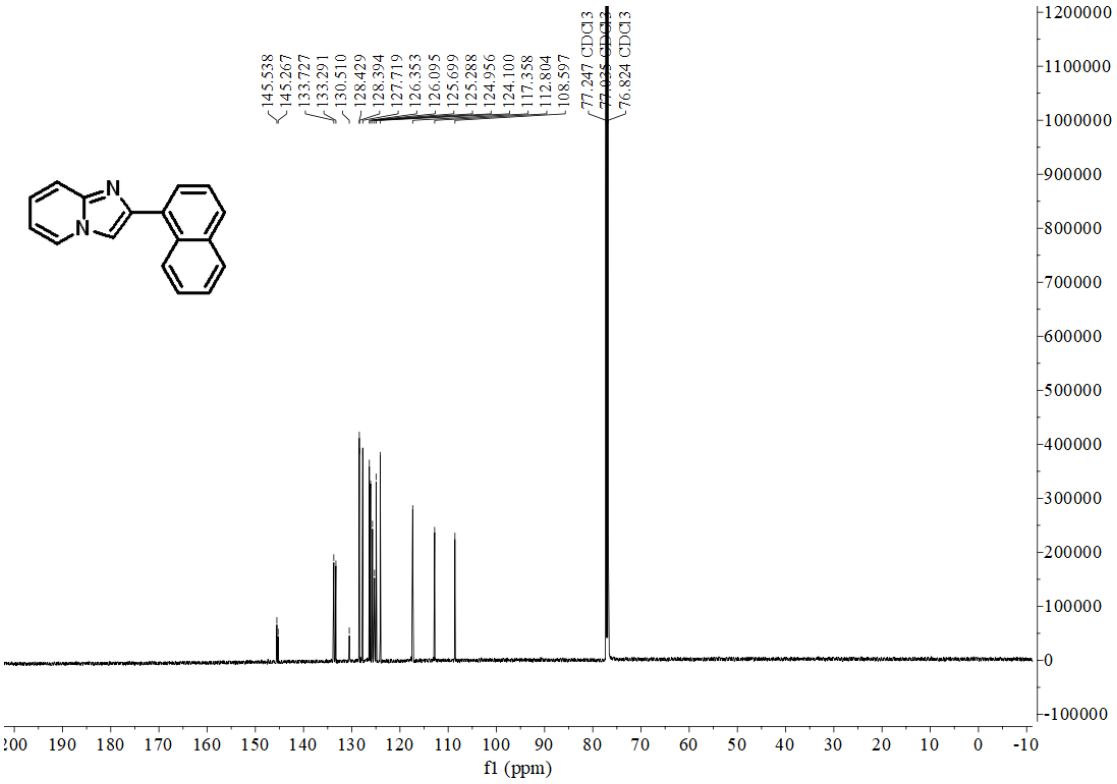
3ea


163.872
162.193
139.146
135.109
131.486
128.096
128.038
126.567
120.370
120.346
116.571
115.970
115.831
115.684
112.488
108.235
76.225 CDCl3
75.801 CDCl3
F
f1 (ppm)

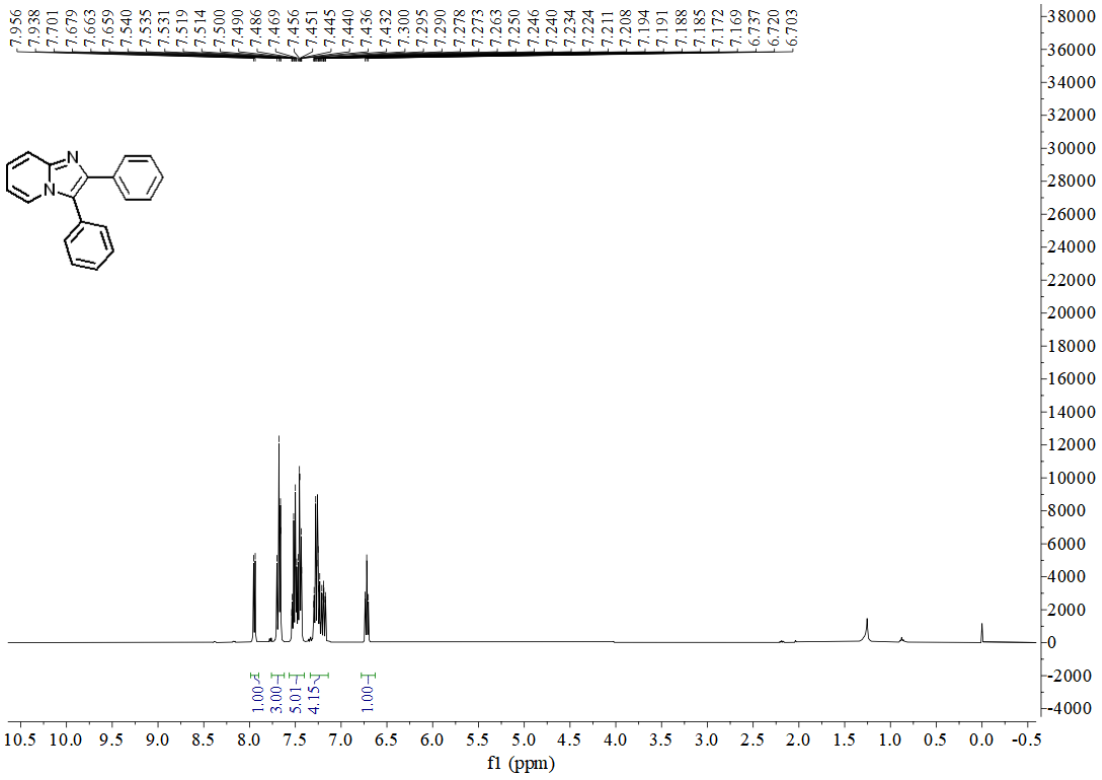
3fa


8.460
8.459
8.457
8.456
8.076
8.074
8.072
8.065
8.063
8.061
7.939
7.936
7.925
7.922
7.900
7.899
7.868
7.866
7.864
7.856
7.854
7.853
7.851
7.827
7.812
7.773
7.771
7.769
7.760
7.759
7.756
7.647
7.646
7.632
7.631
7.423
7.420
7.410
7.407
7.397
7.394
7.152
7.150
7.141
7.139
7.137
7.135
7.126
7.124
6.746
6.744
6.735
6.733
6.724
0.96
1.01
1.02
1.00
1.03
1.00
1.01
0.98
2.00
1.00
0.98
f1 (ppm)

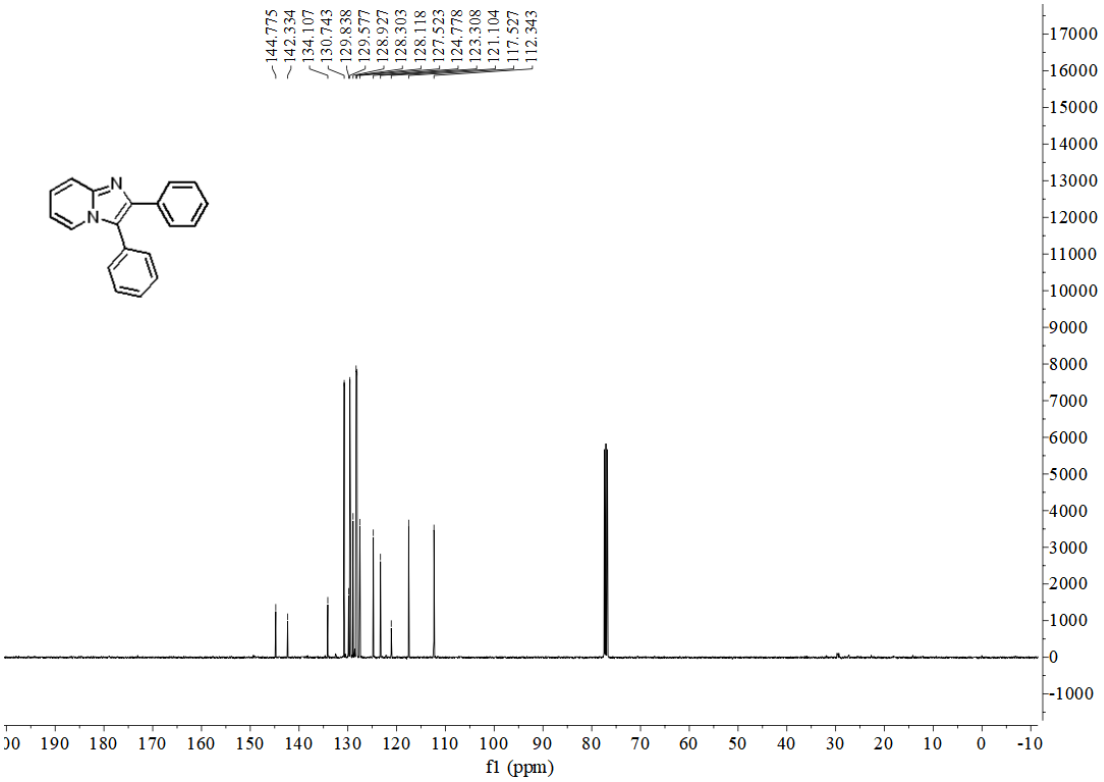
3fa


145.538
145.267
133.727
133.291
130.510
128.429
128.394
127.719
126.353
126.095
125.699
125.288
124.956
124.100
117.358
112.804
108.597
77.247 CDCl3
76.824 CDCl3
f1 (ppm)

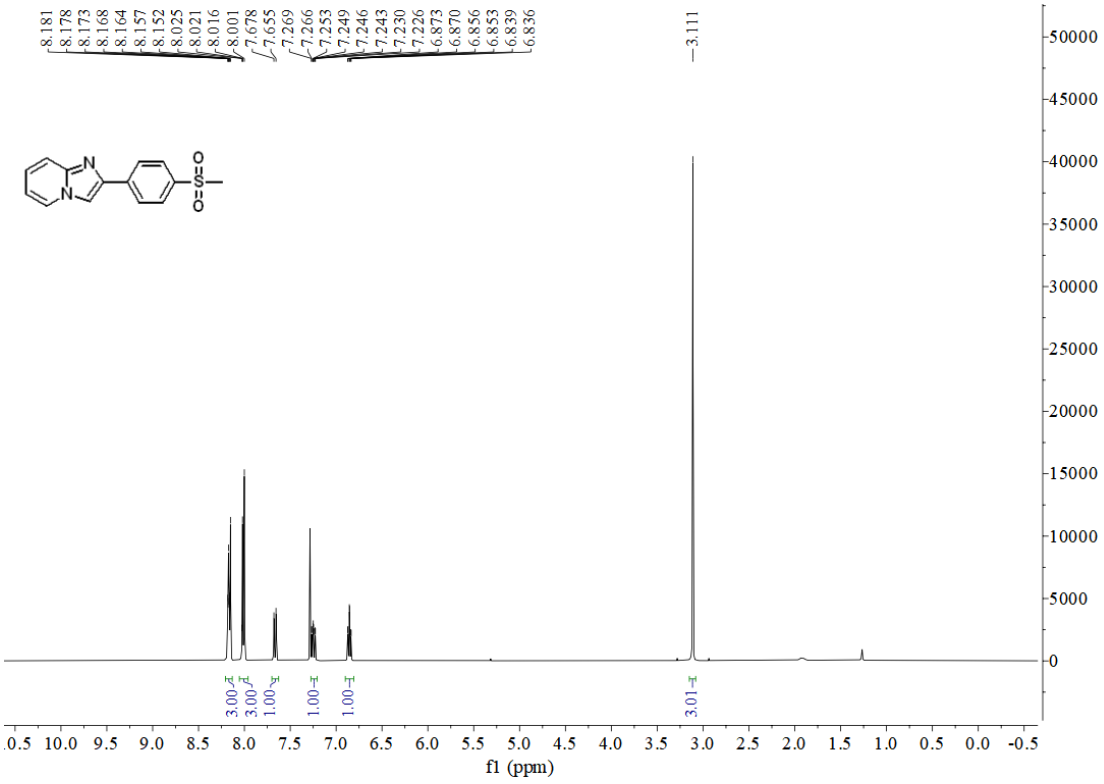
3ga


7.956
7.938
7.701
7.679
7.663
7.659
7.540
7.535
7.531
7.519
7.514
7.500
7.490
7.486
7.469
7.456
7.451
7.445
7.440
7.436
7.432
7.300
7.295
7.290
7.278
7.273
7.263
7.250
7.246
7.240
7.234
7.224
7.211
7.208
7.194
7.191
7.188
7.185
7.172
7.169
6.737
6.720
6.703
1.00
3.00
5.01
4.15
1.00
f1 (ppm)

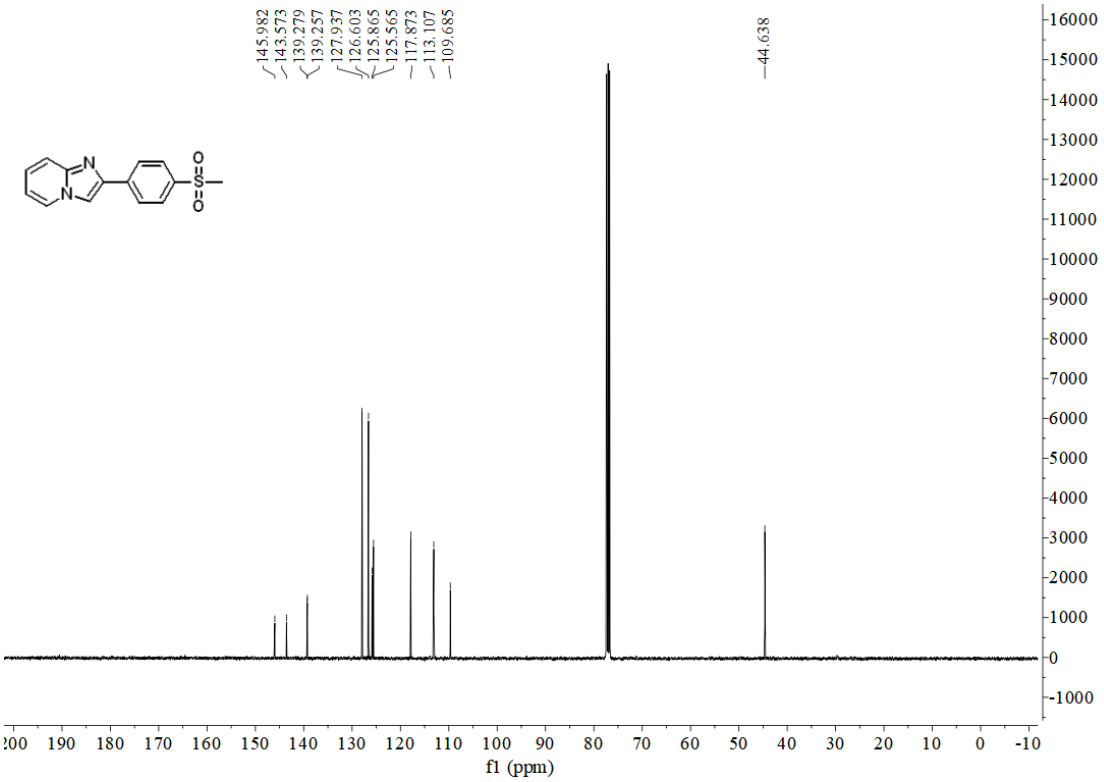
3ga


144.775
142.334
134.107
130.743
129.838
129.577
128.927
128.303
128.118
127.523
124.778
123.308
121.104
117.527
112.343
f1 (ppm)

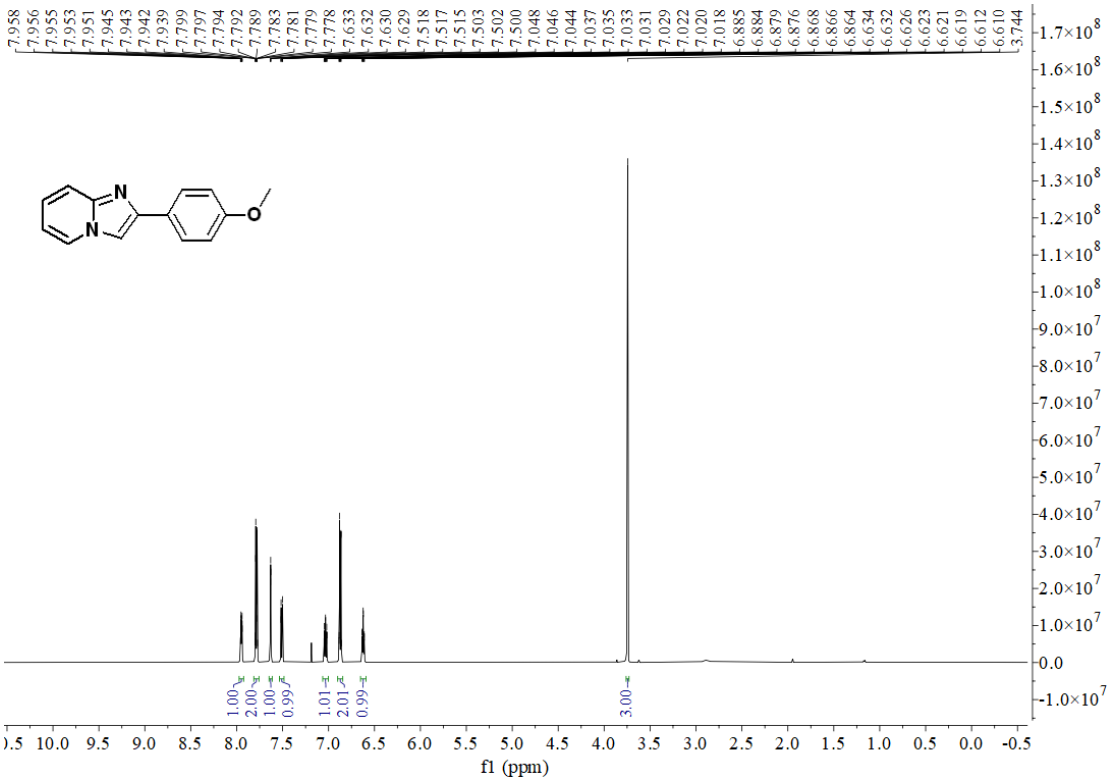
3ha


8.181
8.178
8.173
8.168
8.164
8.157
8.152
8.025
8.021
8.016
8.001
7.678
7.655
7.269
7.266
7.253
7.249
7.246
7.243
7.230
7.226
6.873
6.870
6.856
6.853
6.839
6.836
3.111
3.00
3.00
1.00
1.00
1.00
3.01
f1 (ppm)

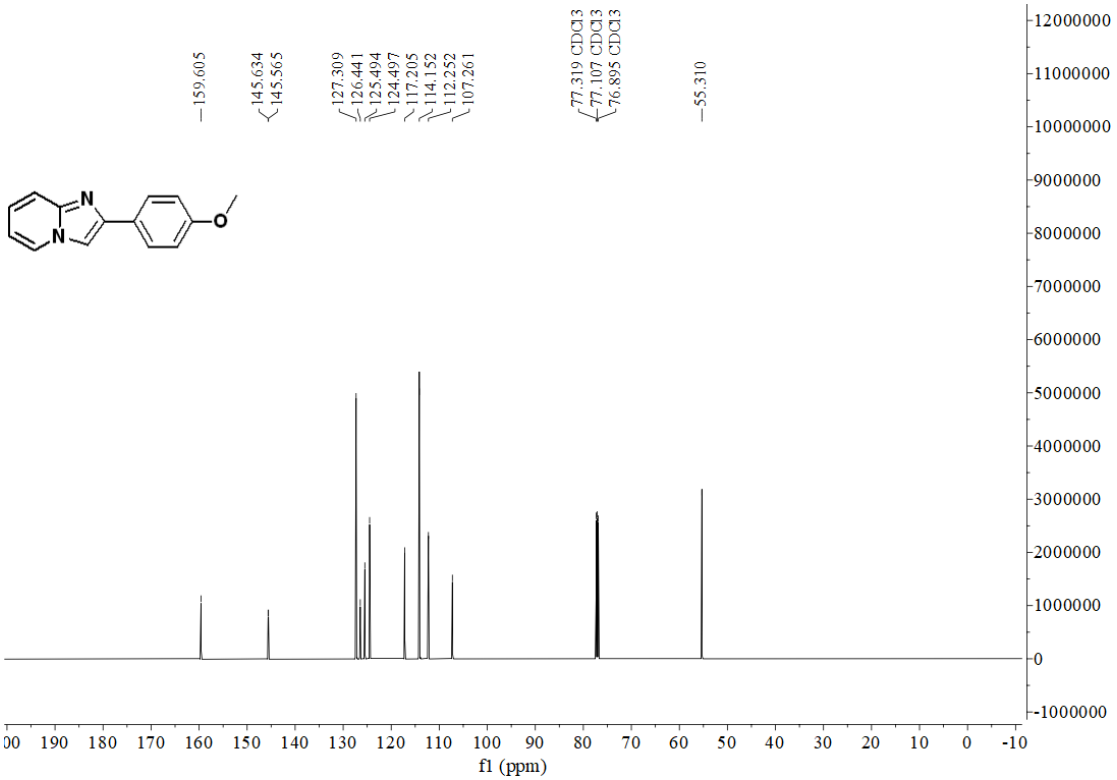
3ha


145.982
143.573
139.279
139.257
127.937
126.603
125.865
125.565
117.873
113.107
109.685
44.638
f1 (ppm)

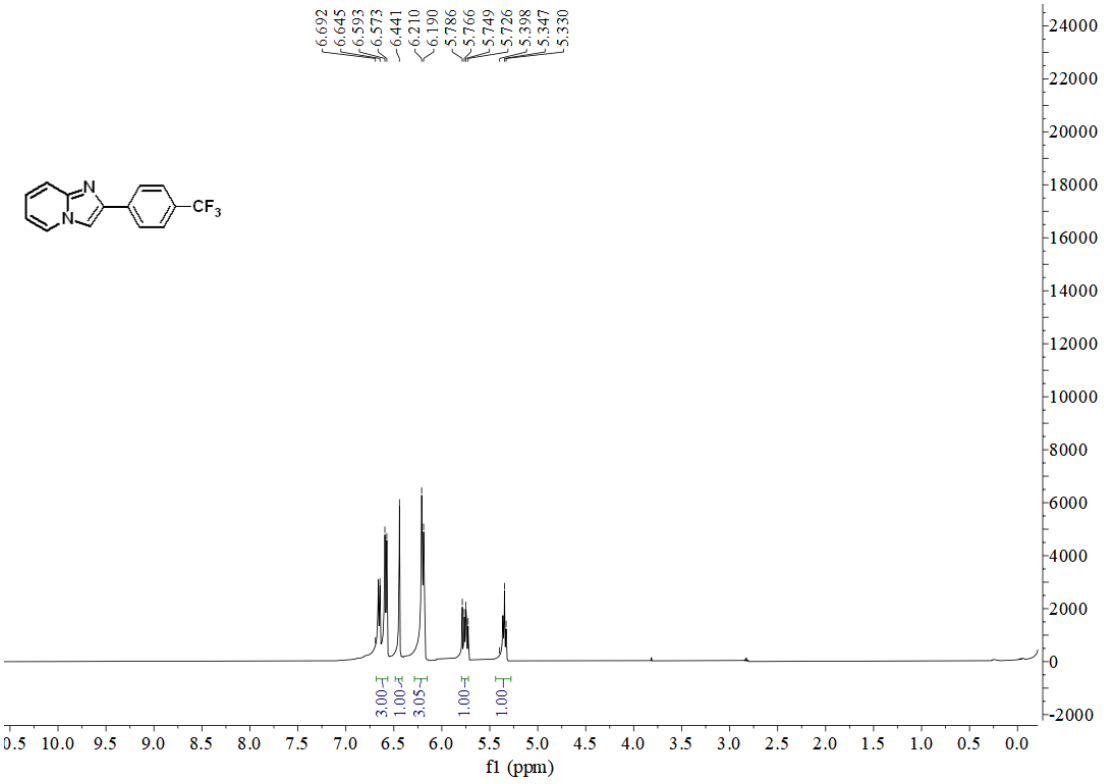
3ia


7.958
7.956
7.955
7.953
7.951
7.945
7.943
7.942
7.939
7.799
7.797
7.794
7.792
7.789
7.783
7.781
7.779
7.778
7.633
7.632
7.630
7.629
7.518
7.517
7.515
7.503
7.502
7.500
7.048
7.046
7.044
7.037
7.035
7.033
7.031
7.029
7.022
7.020
7.018
6.885
6.884
6.879
6.876
6.868
6.866
6.864
6.634
6.632
6.626
6.623
6.621
6.619
6.612
6.610
3.744
1.00
2.00
1.00
0.99
1.01
2.01
0.99
3.00
f1 (ppm)

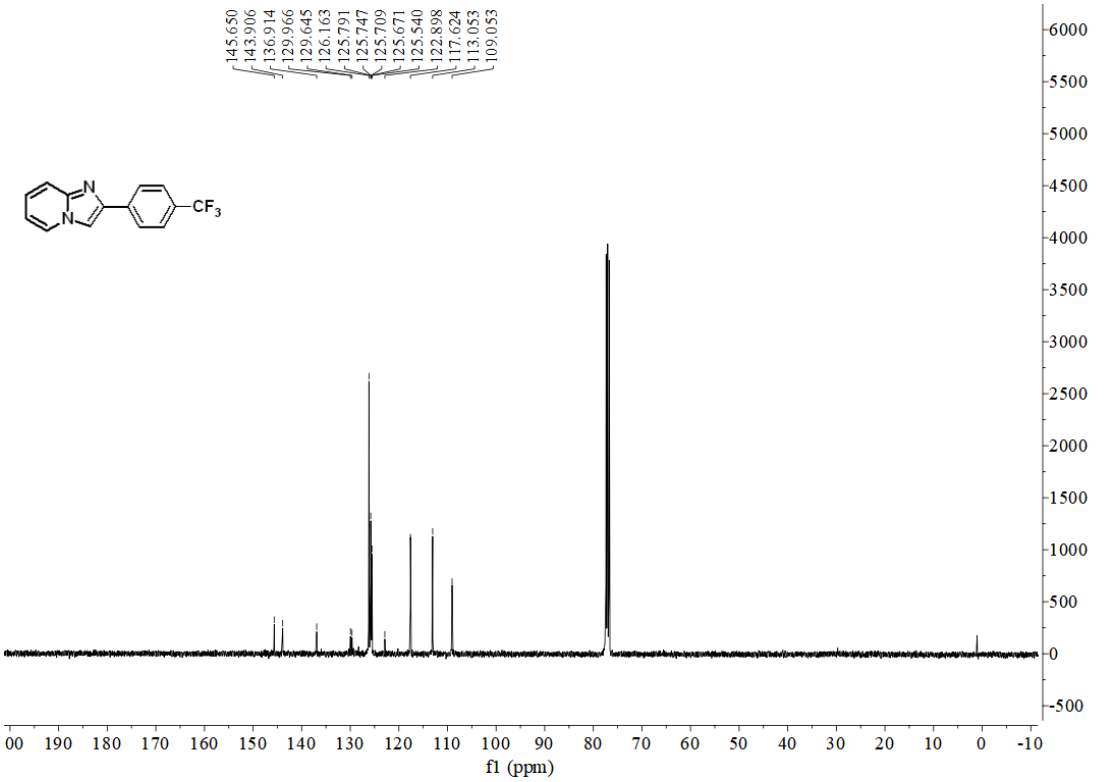
3ia


159.605
145.634
145.565
127.309
126.441
125.494
124.497
117.205
114.152
112.252
107.261
77.319 CDCl3
77.107 CDCl3
76.895 CDCl3
55.310
f1 (ppm)

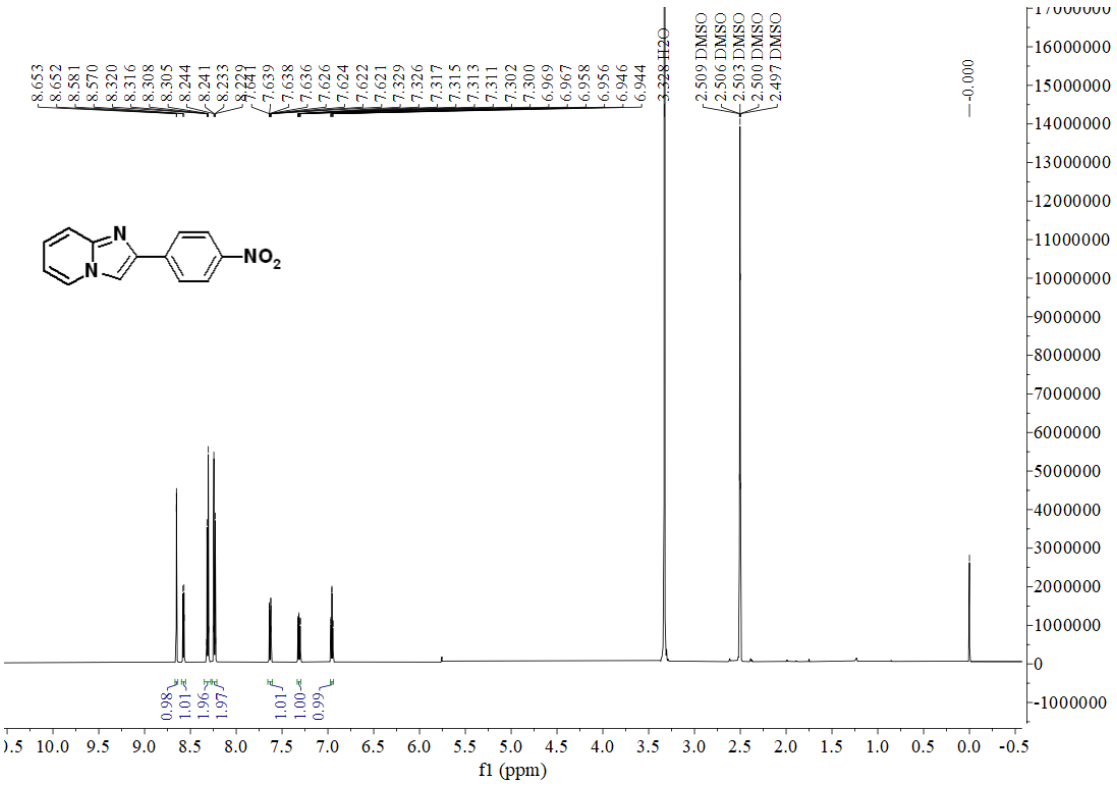
3ja


6.692
6.645
6.593
6.573
6.441
6.210
6.190
5.786
5.766
5.749
5.726
5.398
5.347
5.330
CF3
3.00
1.00
3.05
1.00
1.00
f1 (ppm)

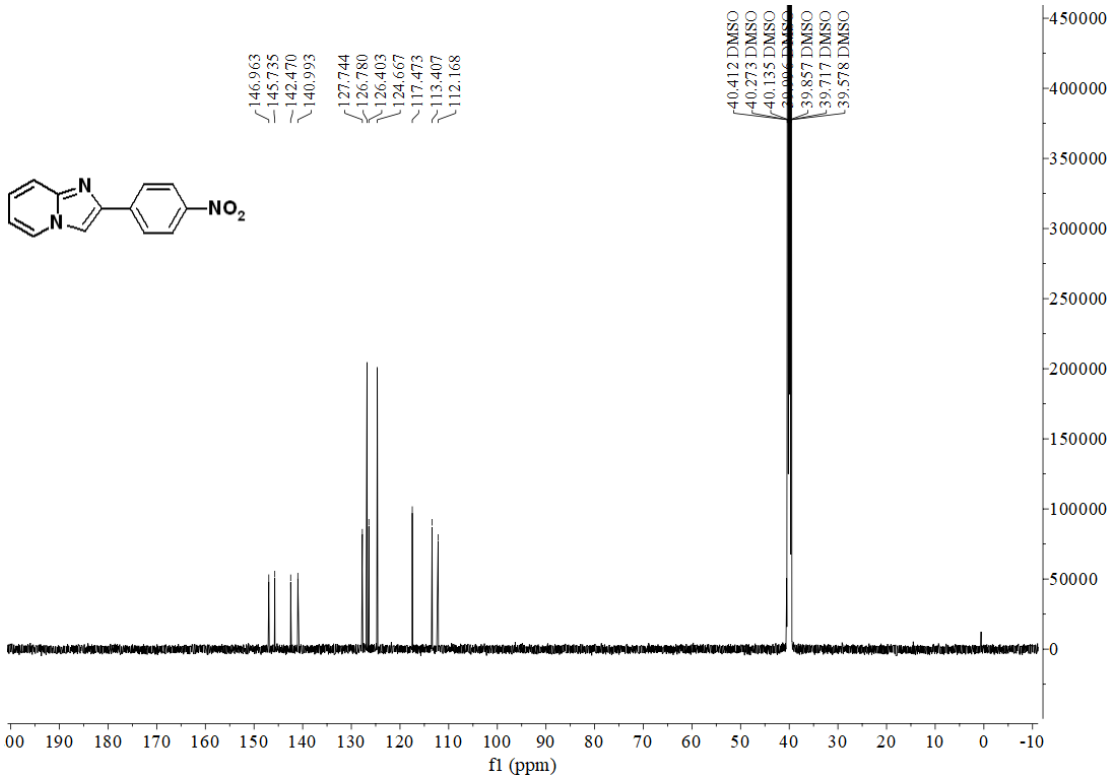
3ja


145.650
143.906
136.914
129.966
129.645
126.163
125.791
125.747
125.709
125.671
125.540
122.898
117.624
113.053
109.053
CF3
f1 (ppm)

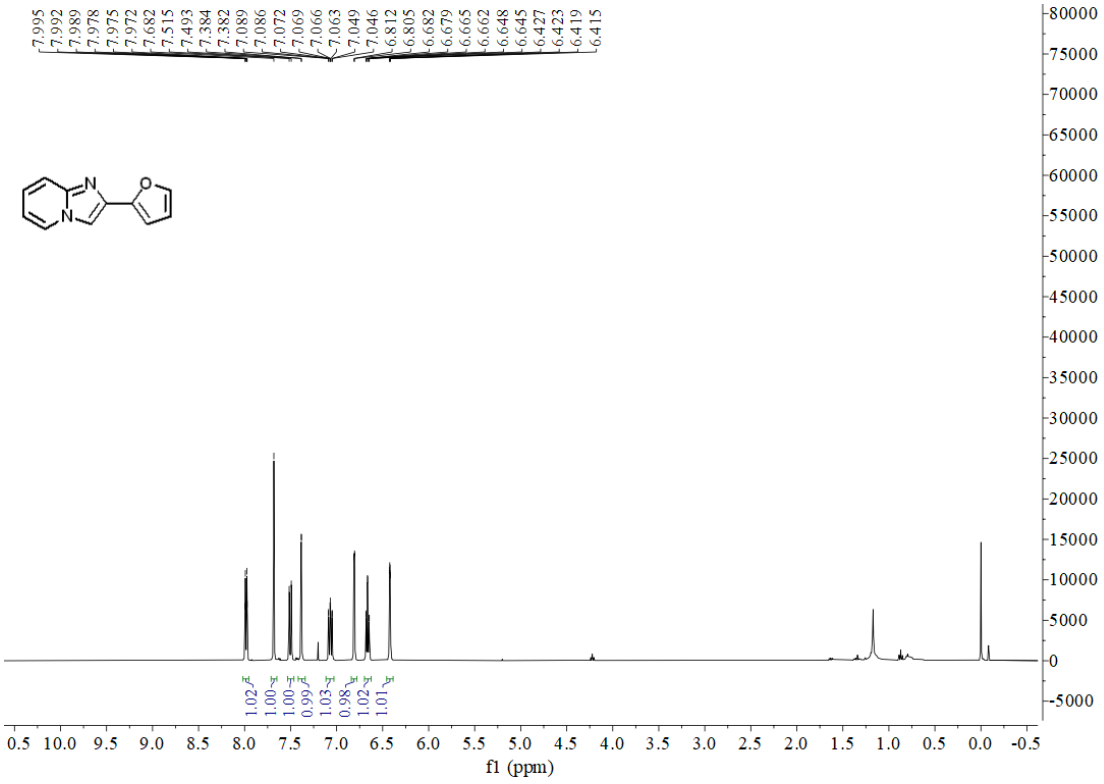
3ka


8.653
8.652
8.581
8.570
8.320
8.316
8.308
8.305
8.244
8.241
8.233
7.639
7.638
7.636
7.626
7.624
7.622
7.621
7.329
7.326
7.317
7.315
7.313
7.311
7.302
7.300
6.969
6.967
6.958
6.956
6.946
6.944
3.328 H2O
2.509 DMSO
2.506 DMSO
2.503 DMSO
2.500 DMSO
2.497 DMSO
-0.000
0.98
1.01
1.96
1.97
1.01
1.00
0.99
NO2
f1 (ppm)

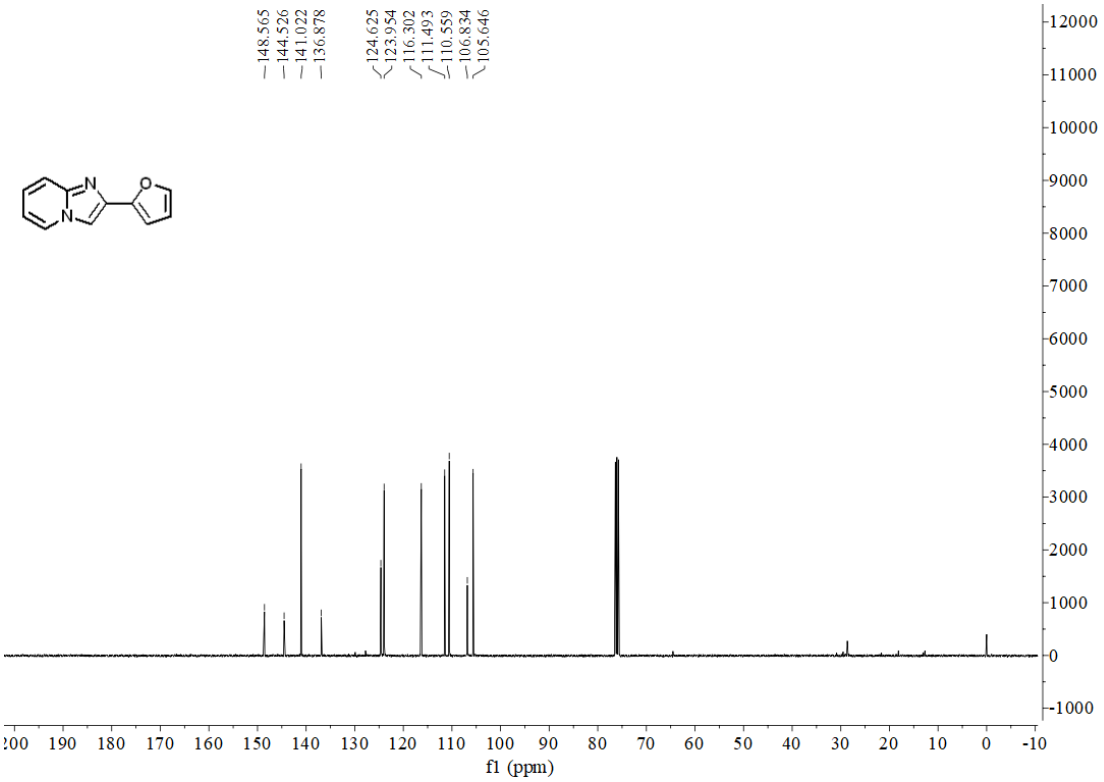
3ka


146.963
145.735
142.470
140.993
127.744
126.780
126.403
124.667
117.473
113.407
112.168
40.412 DMSO
40.273 DMSO
40.135 DMSO
39.857 DMSO
39.717 DMSO
39.578 DMSO
NO2
f1 (ppm)

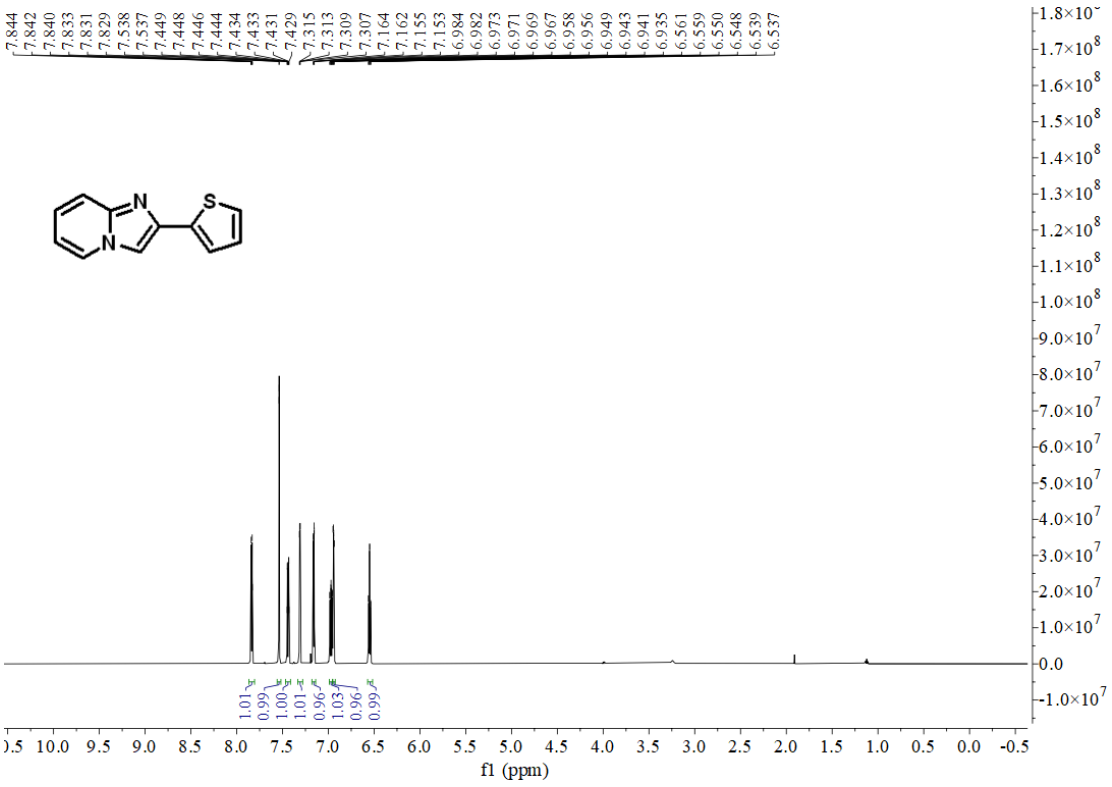
3la


7.995
7.992
7.989
7.978
7.975
7.972
7.682
7.515
7.493
7.384
7.382
7.089
7.086
7.072
7.069
7.066
7.063
7.049
7.046
6.812
6.805
6.682
6.679
6.665
6.662
6.648
6.645
6.427
6.423
6.419
6.415
1.02
1.00
1.00
0.99
1.03
0.98
1.02
1.01
f1 (ppm)

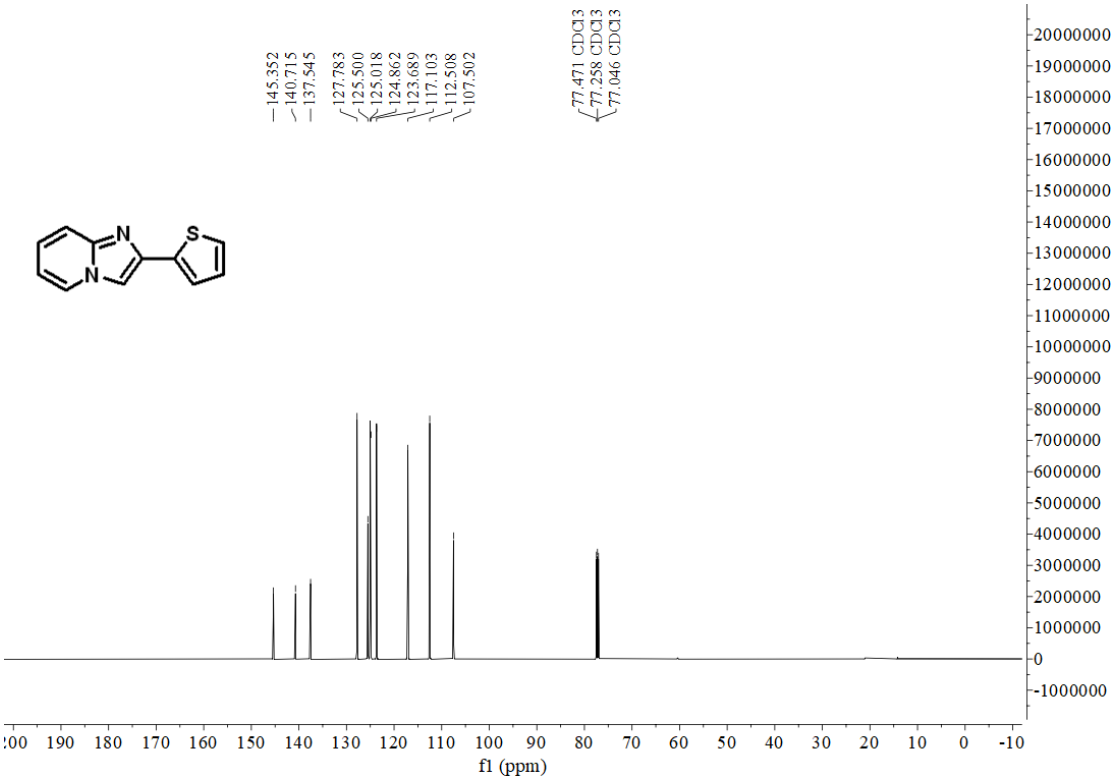
3la


148.565
144.526
141.022
136.878
124.625
123.954
116.302
111.493
110.559
106.834
105.646
f1 (ppm)

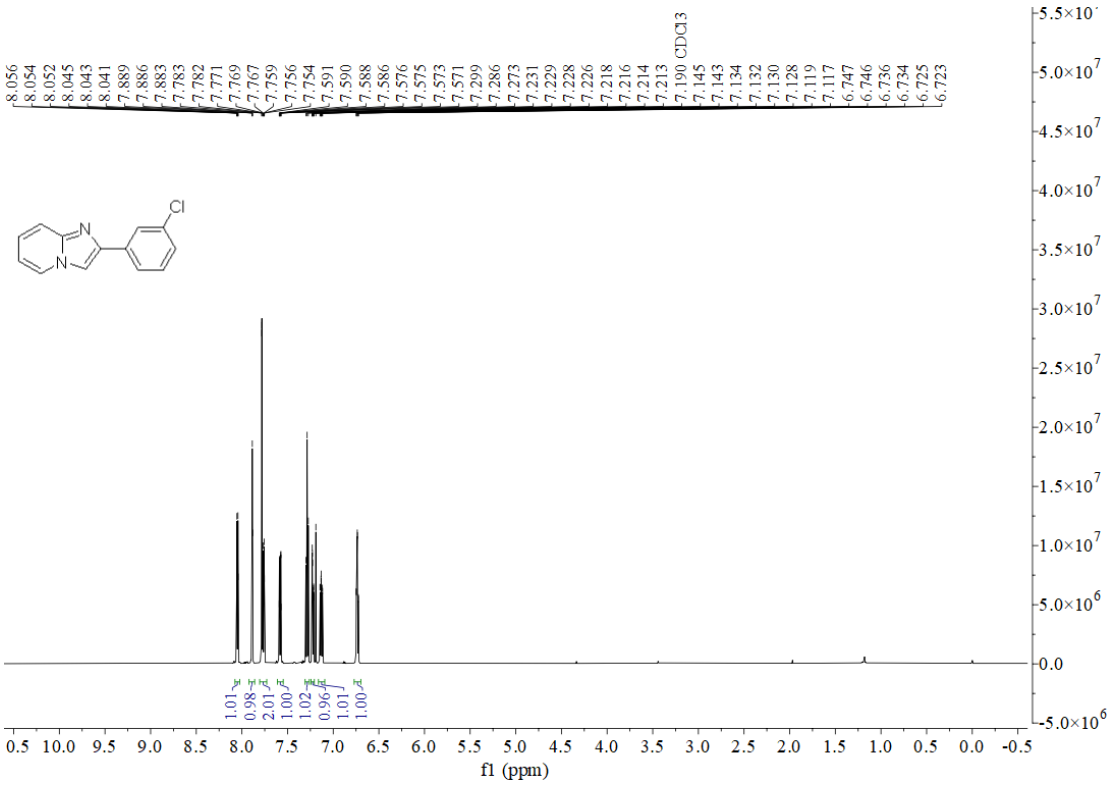
3ma


7.844
7.842
7.840
7.833
7.831
7.829
7.538
7.537
7.449
7.448
7.446
7.444
7.434
7.433
7.431
7.429
7.315
7.313
7.309
7.307
7.164
7.162
7.155
7.153
6.984
6.982
6.973
6.971
6.969
6.967
6.958
6.956
6.949
6.943
6.941
6.935
6.561
6.559
6.550
6.548
6.539
6.537
1.01
0.99
1.00
1.01
0.96
1.03
0.96
0.99
f1 (ppm)

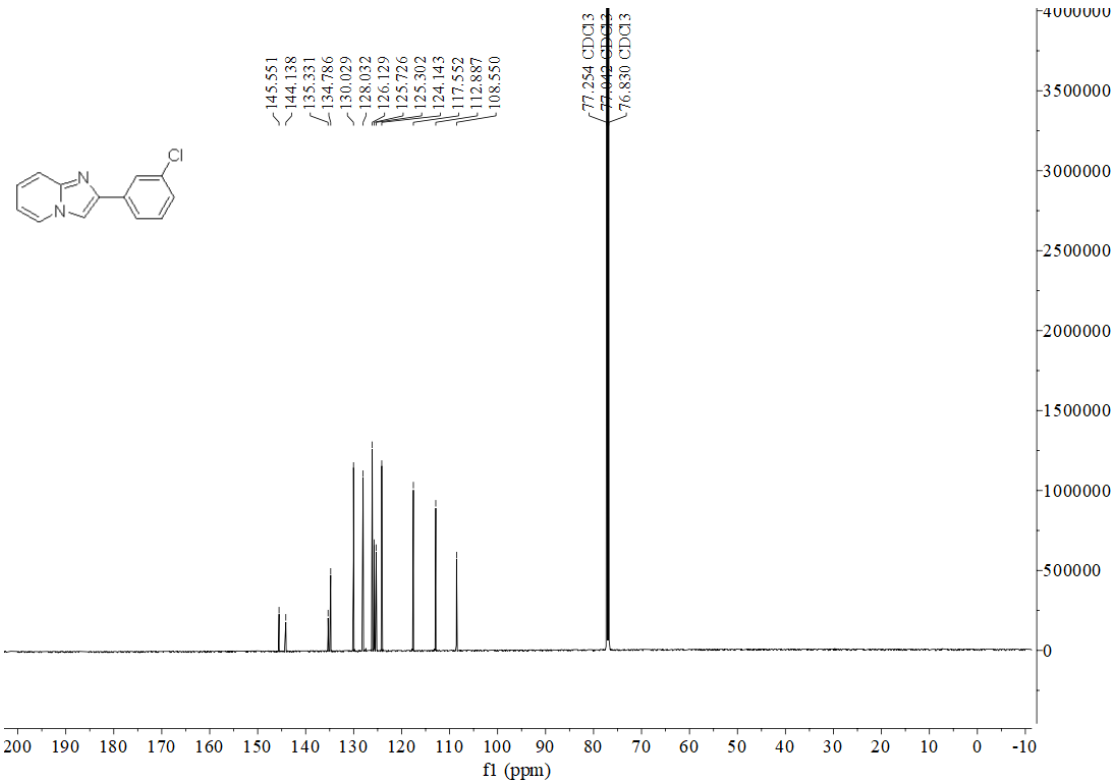
3ma


145.352
140.715
137.545
127.783
125.500
125.018
124.862
123.689
117.103
112.508
107.502
77.471 CDCl3
77.258 CDCl3
77.046 CDCl3
f1 (ppm)

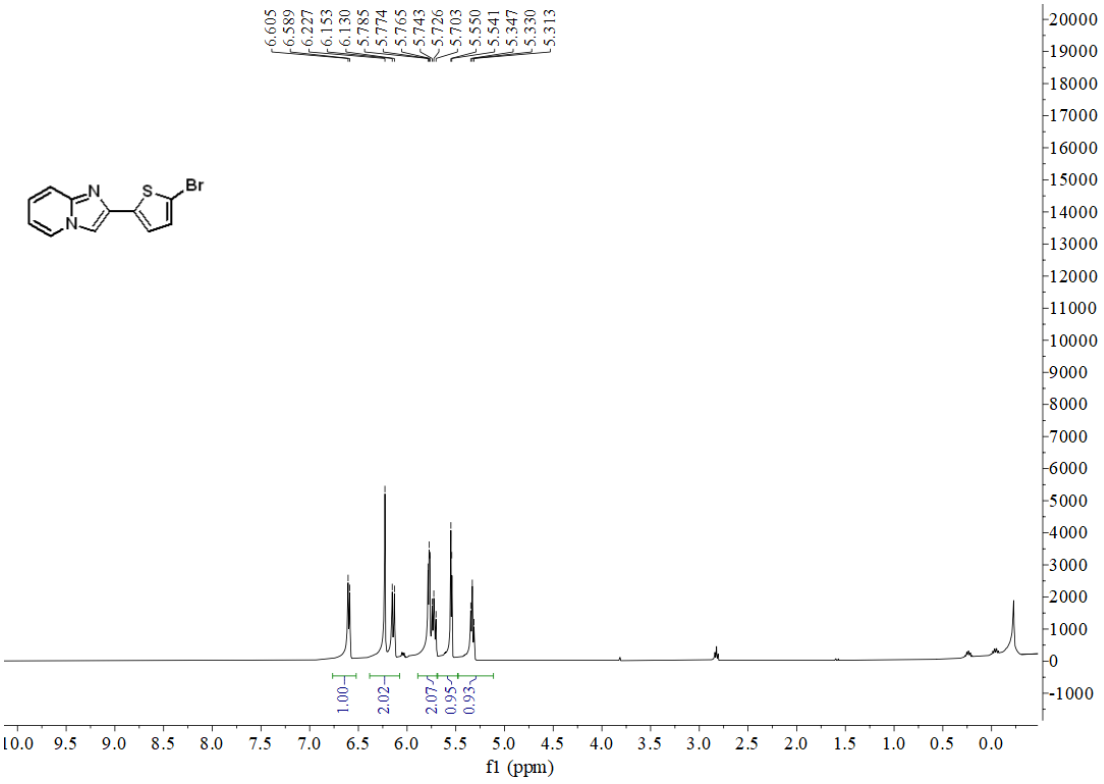
3na


8.056
8.054
8.052
8.045
8.043
8.041
7.889
7.886
7.883
7.783
7.782
7.771
7.769
7.767
7.759
7.756
7.754
7.591
7.590
7.588
7.586
7.576
7.575
7.573
7.571
7.299
7.286
7.273
7.231
7.229
7.228
7.226
7.218
7.216
7.214
7.213
7.190 CDCl3
7.145
7.143
7.134
7.132
7.130
7.128
7.119
7.117
6.747
6.746
6.736
6.734
6.725
6.723
Cl
N
N
1.01
0.98
2.01
1.00
1.02
0.96
1.01
1.00
f1 (ppm)

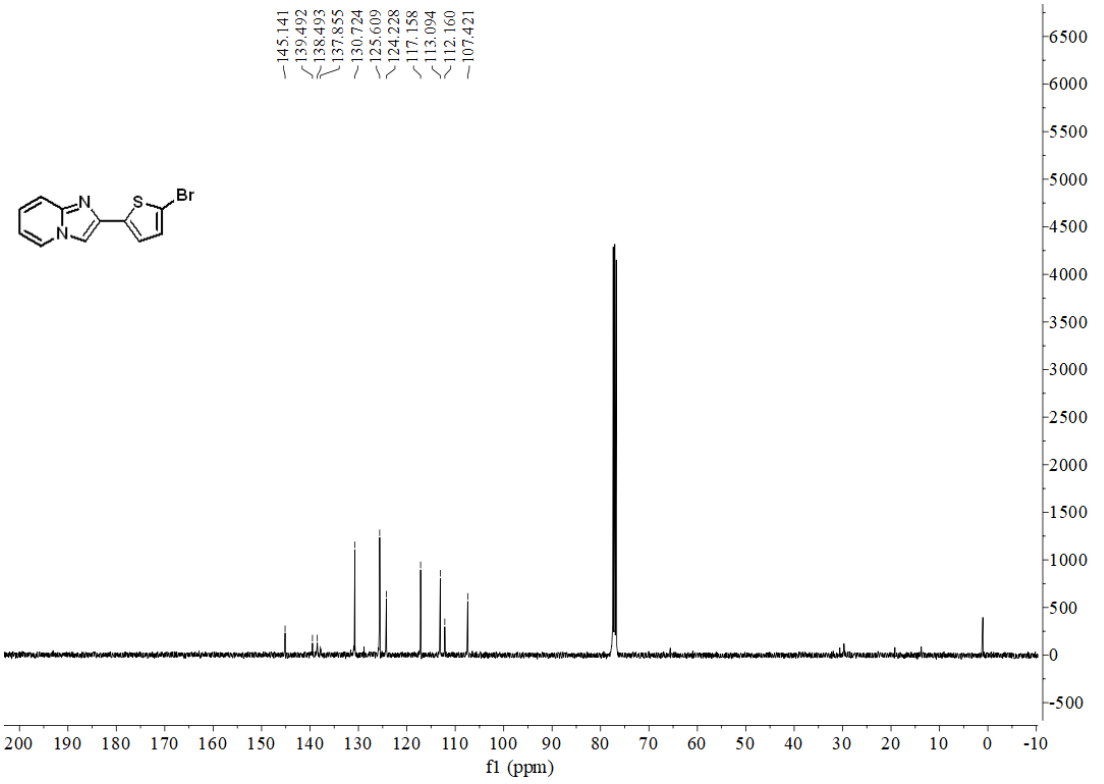
3na


145.551
144.138
135.331
134.786
130.029
128.032
126.129
125.726
125.302
124.143
117.552
112.887
108.550
77.254 CDCl3
77.043 CDCl3
76.830 CDCl3
Cl
N
N
f1 (ppm)

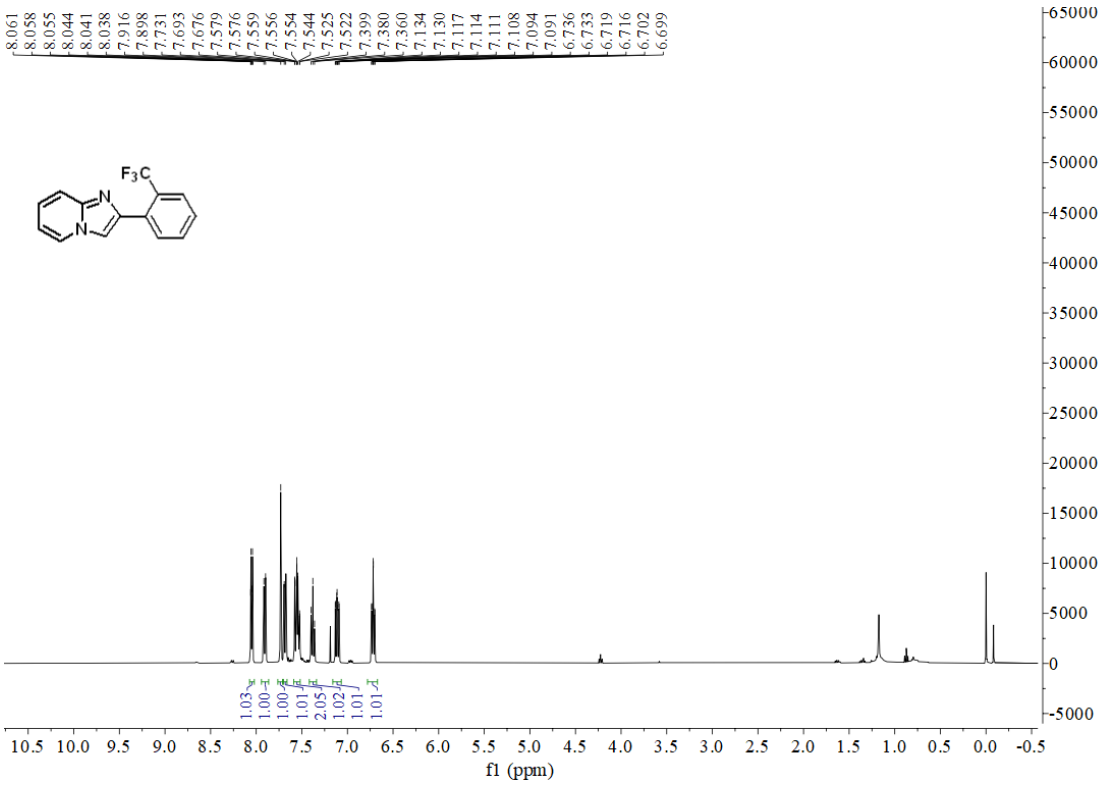
3oa


6.605
6.589
6.227
6.153
6.130
5.785
5.774
5.765
5.743
5.726
5.703
5.550
5.541
5.347
5.330
5.313
N
S
Br
1.00
2.02
2.07
0.95
0.93
f1 (ppm)

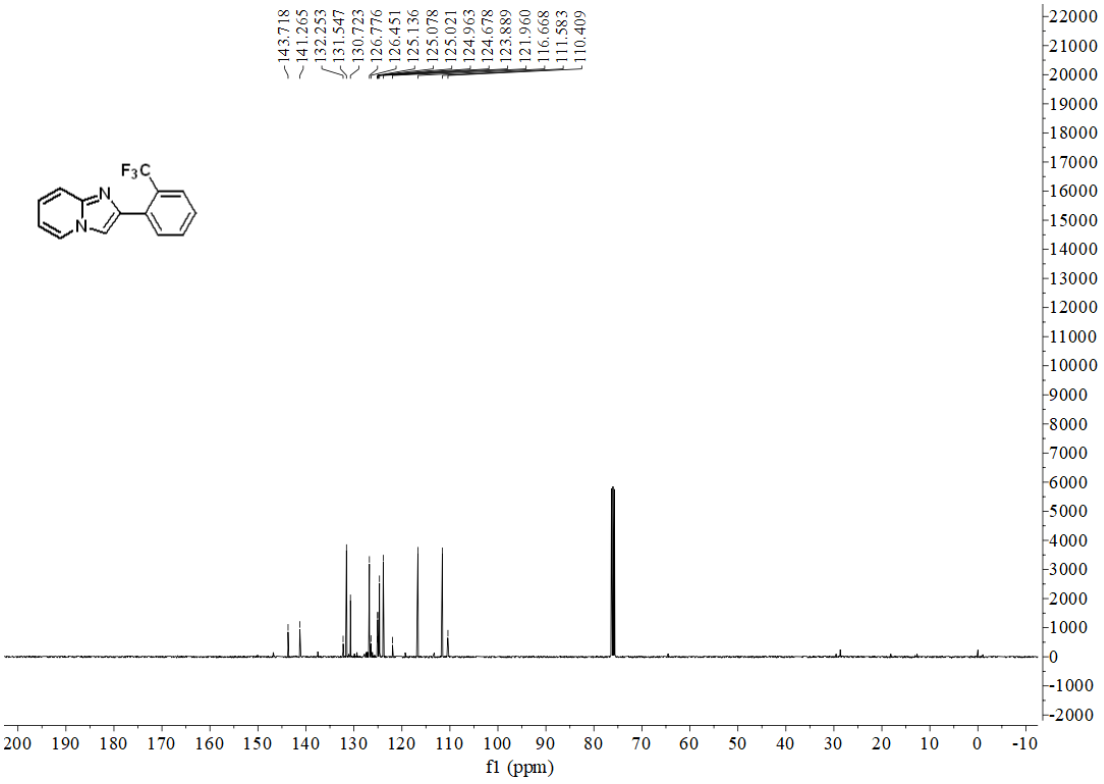
3oa


145.141
139.492
138.493
137.855
130.724
125.609
124.228
117.158
113.094
112.160
107.421
N
S
Br
f1 (ppm)

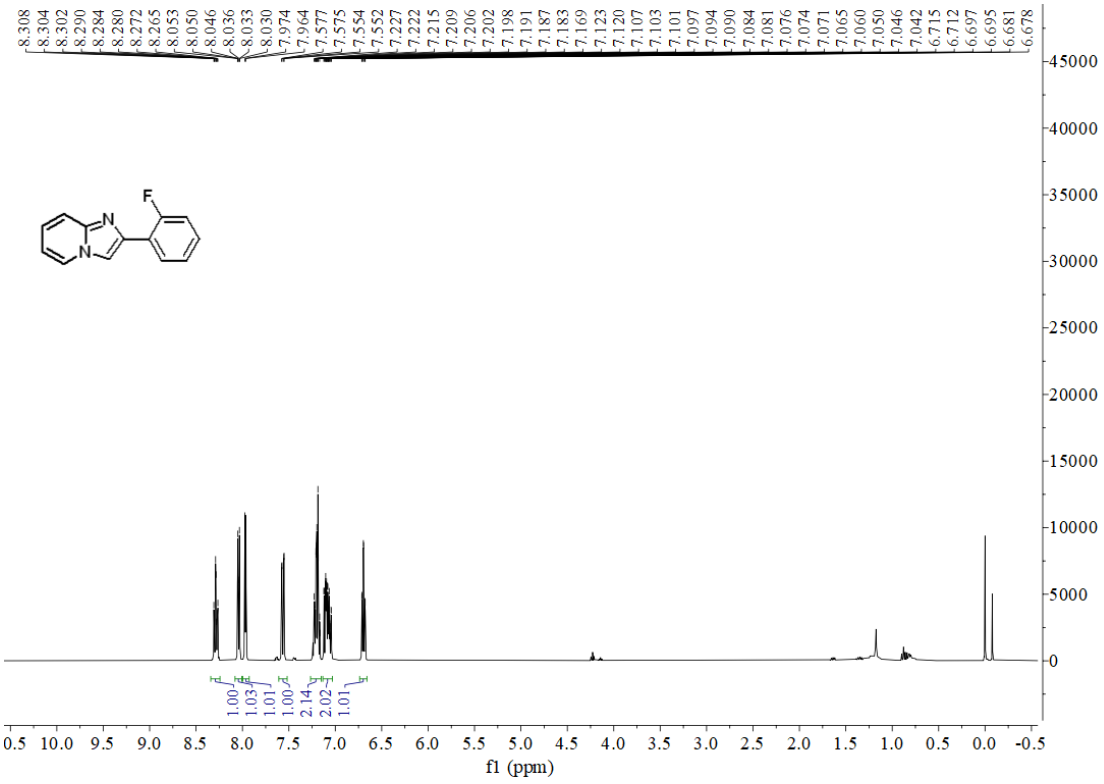
3pa


8.061
8.058
8.055
8.044
8.041
8.038
7.916
7.898
7.731
7.693
7.676
7.579
7.576
7.559
7.556
7.554
7.544
7.525
7.522
7.399
7.380
7.360
7.134
7.130
7.117
7.114
7.111
7.108
7.094
7.091
6.736
6.733
6.719
6.716
6.702
6.699
F3C
N
N
1.03
1.00
1.00
1.01
2.05
1.02
1.01
1.01
f1 (ppm)

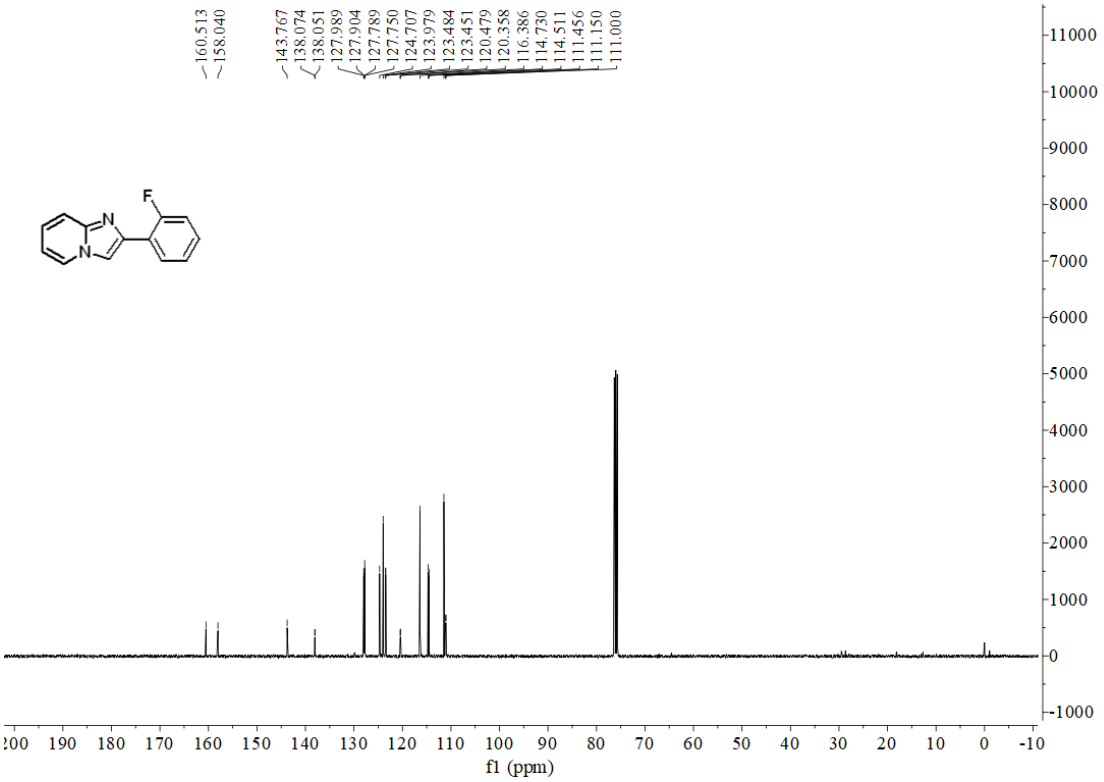
3pa


143.718
141.265
132.253
131.547
130.723
126.776
126.451
125.136
125.078
125.021
124.963
124.678
123.889
121.960
116.668
111.583
110.409
F3C
N
N
f1 (ppm)

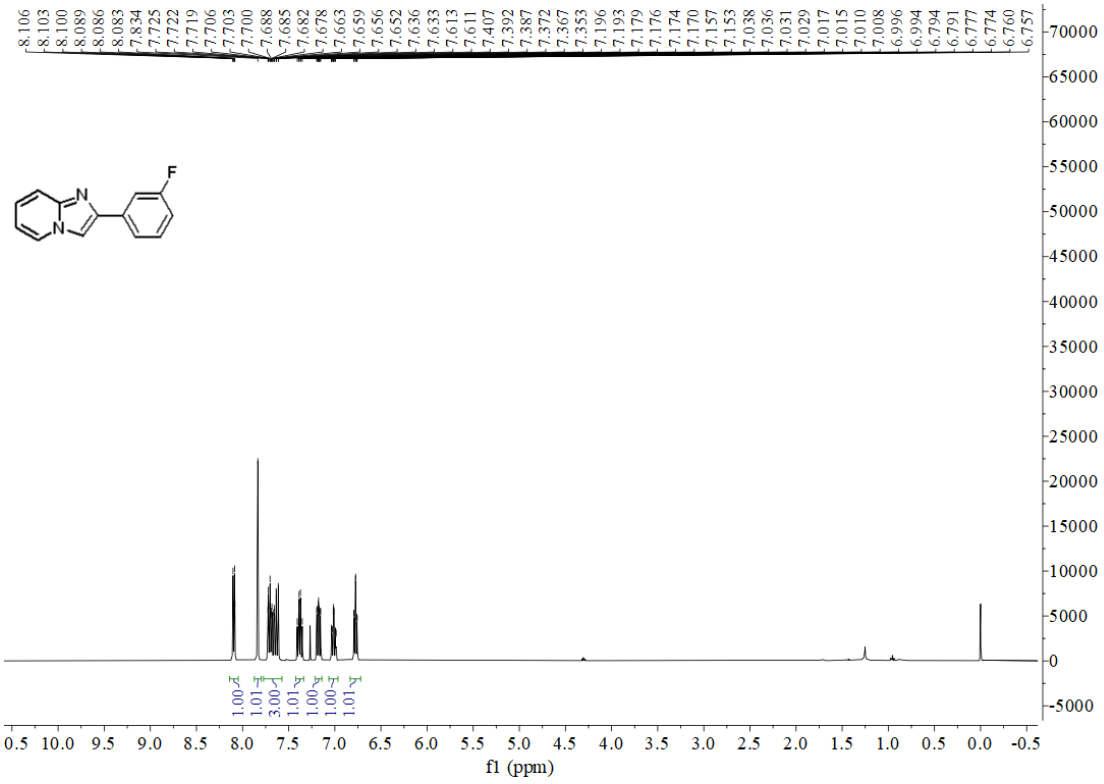
3qa


8.308
8.304
8.302
8.290
8.284
8.280
8.272
8.265
8.053
8.050
8.046
8.036
8.033
8.030
7.974
7.964
7.577
7.575
7.554
7.552
7.227
7.222
7.215
7.209
7.206
7.202
7.198
7.191
7.187
7.183
7.169
7.123
7.120
7.107
7.103
7.101
7.097
7.094
7.090
7.084
7.081
7.076
7.074
7.071
7.065
7.060
7.050
7.046
7.042
6.715
6.712
6.697
6.695
6.681
6.678
F
N
N
1.00
1.03
1.01
1.00
2.14
2.02
1.01
f1 (ppm)

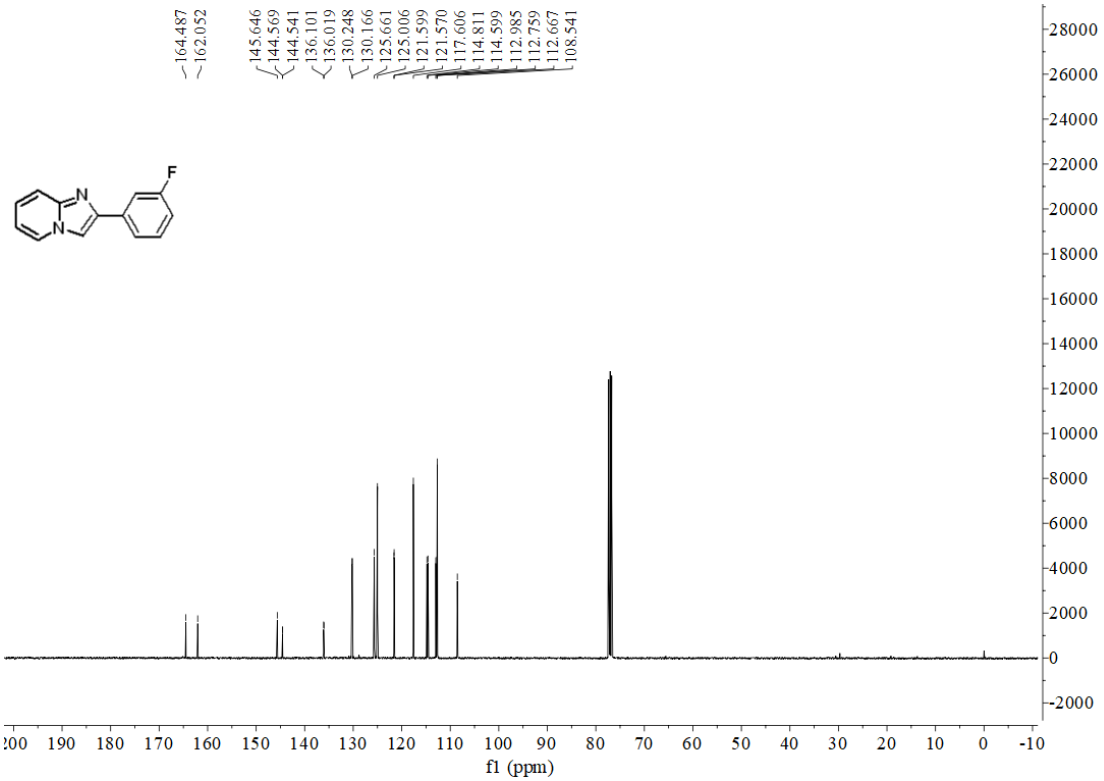
3qa


160.513
158.040
143.767
138.074
138.051
127.989
127.904
127.789
127.750
124.707
123.979
123.484
123.451
120.479
120.358
116.386
114.730
114.511
111.456
111.150
111.000
F
N
N
f1 (ppm)

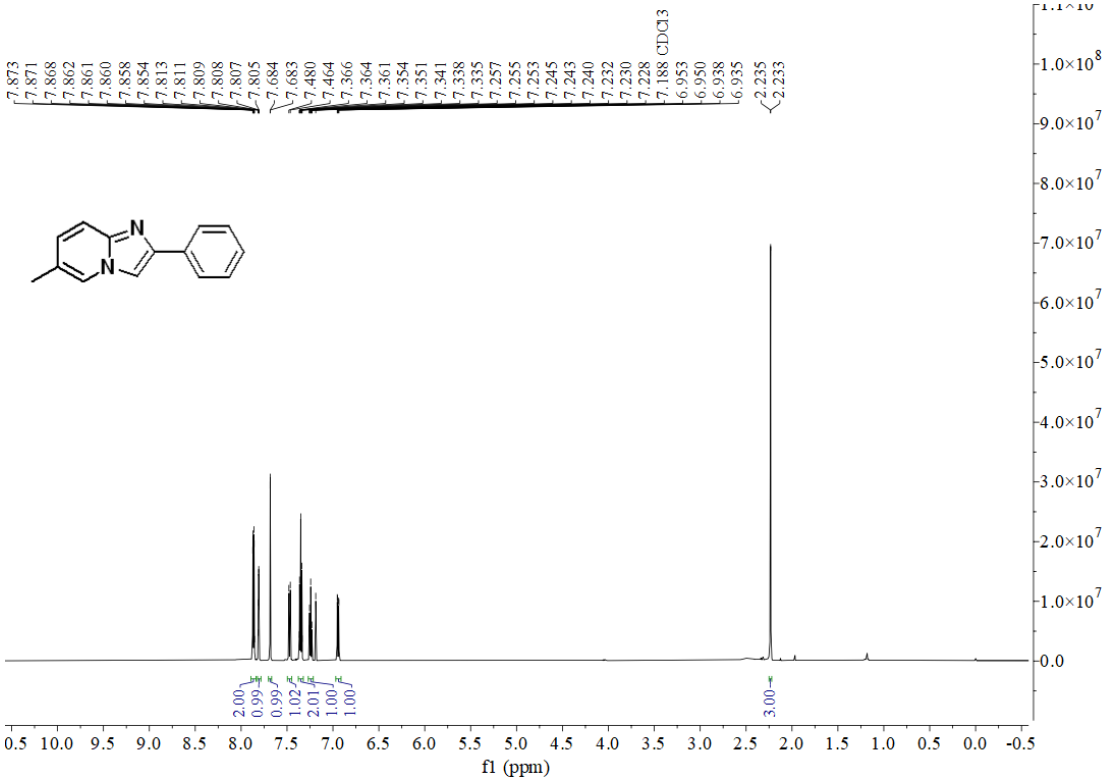
3ra


8.106
8.103
8.100
8.089
8.086
8.083
7.834
7.725
7.722
7.719
7.706
7.703
7.700
7.688
7.685
7.682
7.678
7.663
7.659
7.656
7.652
7.636
7.633
7.613
7.611
7.407
7.392
7.387
7.372
7.367
7.353
7.196
7.193
7.179
7.176
7.174
7.170
7.157
7.153
7.038
7.036
7.031
7.029
7.017
7.015
7.010
7.008
6.996
6.994
6.794
6.791
6.777
6.774
6.760
6.757
F
N
N
1.00
1.01
3.00
1.01
1.00
1.00
1.01
f1 (ppm)

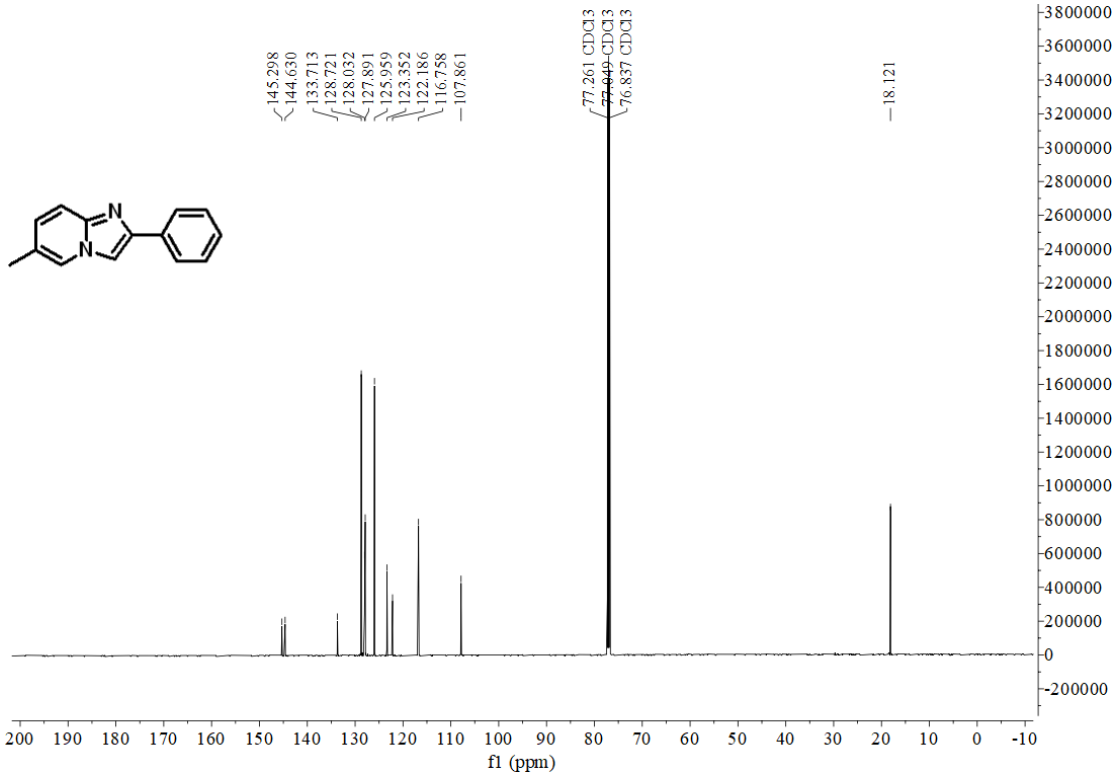
3ra


164.487
162.052
145.646
144.569
144.541
136.101
136.019
130.248
130.166
125.661
125.006
121.599
121.570
117.606
114.811
114.599
112.985
112.759
112.667
108.541
F
N
N
f1 (ppm)

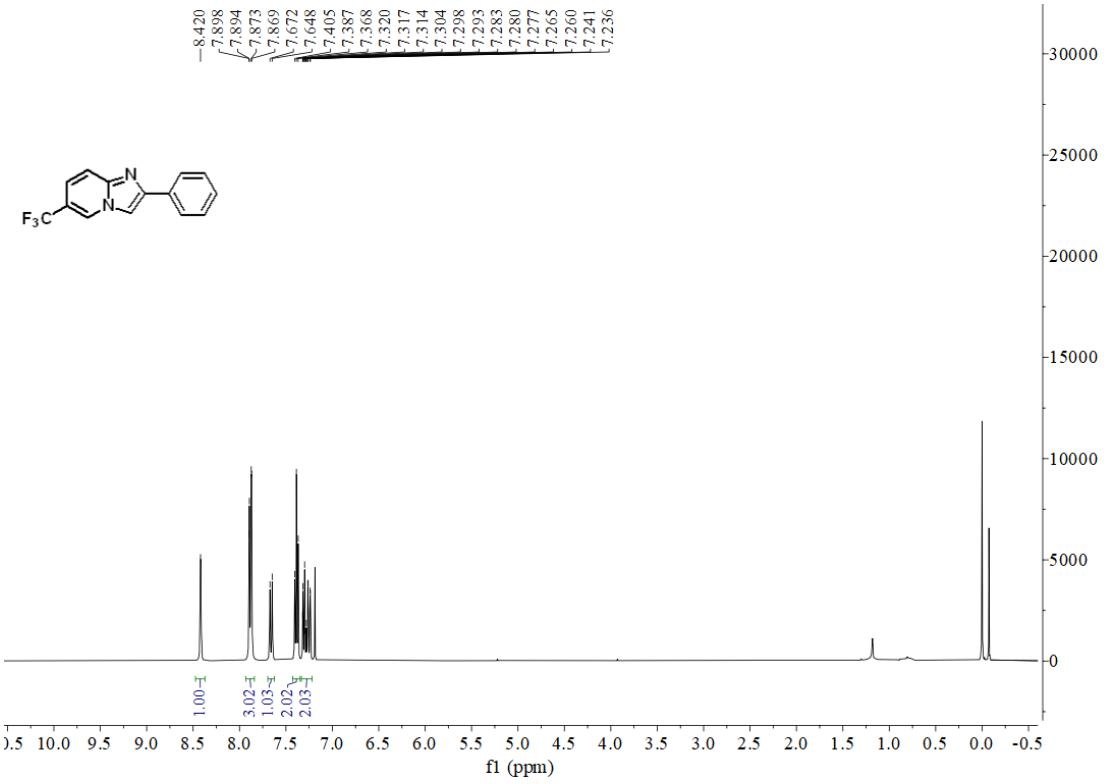
3ab


7.873
7.871
7.868
7.862
7.861
7.860
7.858
7.854
7.813
7.811
7.809
7.808
7.807
7.805
7.684
7.683
7.480
7.464
7.366
7.364
7.361
7.354
7.351
7.341
7.338
7.335
7.257
7.255
7.253
7.245
7.243
7.240
7.232
7.230
7.228
7.188 CDCl3
6.953
6.950
6.938
6.935
2.235
2.233
2.00
0.99
0.99
1.02
2.01
1.00
1.00
3.00
f1 (ppm)

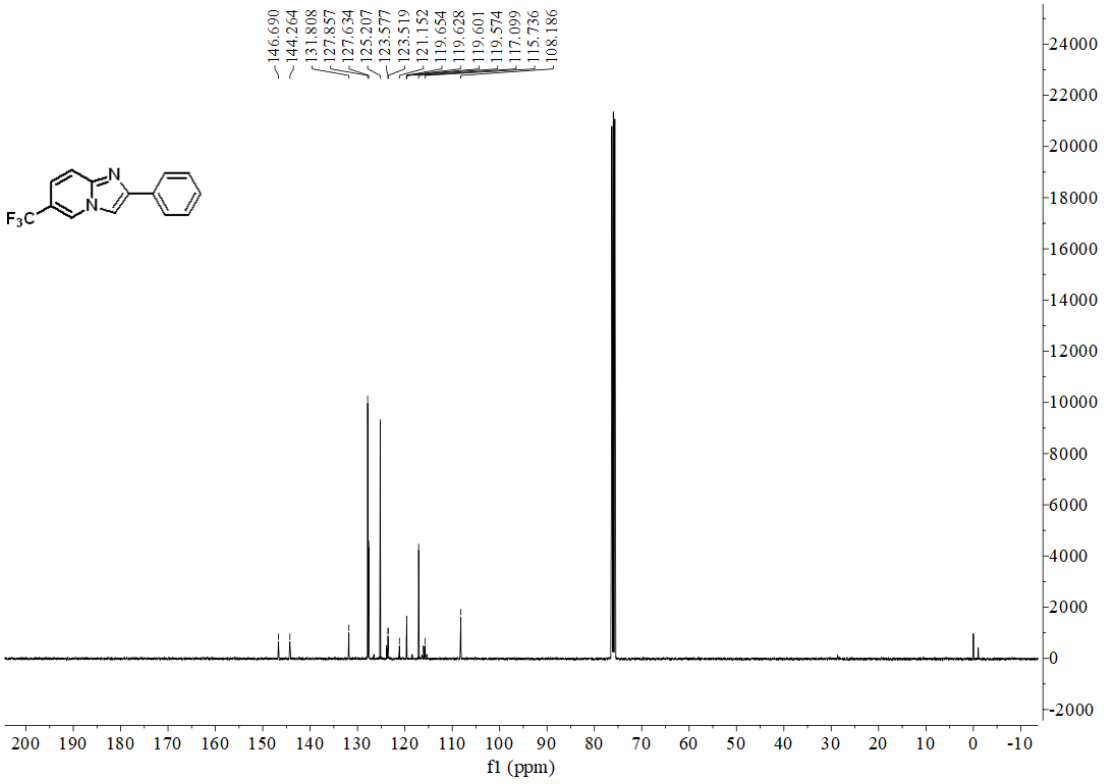
3ab


145.298
144.630
133.713
128.721
128.032
127.891
125.959
123.352
122.186
116.758
107.861
77.261 CDCl3
77.049 CDCl3
76.837 CDCl3
18.121
f1 (ppm)

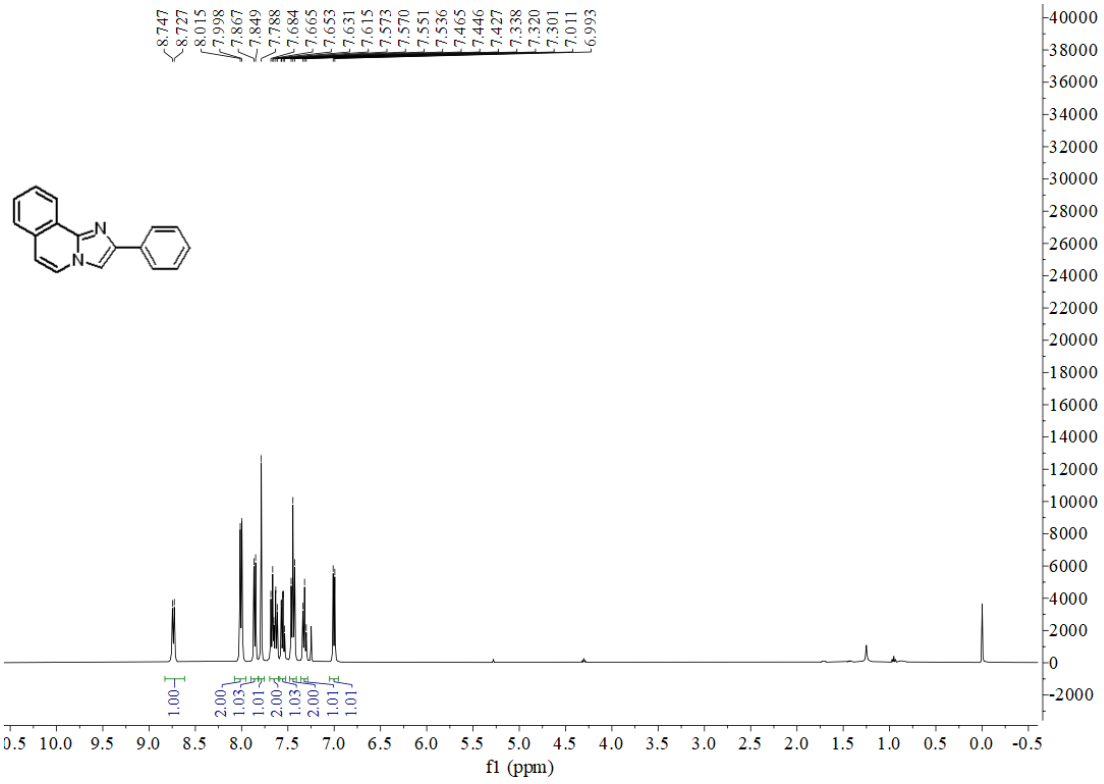
3ac


8.420
7.898
7.894
7.873
7.869
7.672
7.648
7.405
7.387
7.368
7.320
7.317
7.314
7.304
7.298
7.293
7.283
7.280
7.277
7.265
7.260
7.241
7.236
F3C
1.00
3.02
1.03
2.02
2.03
f1 (ppm)

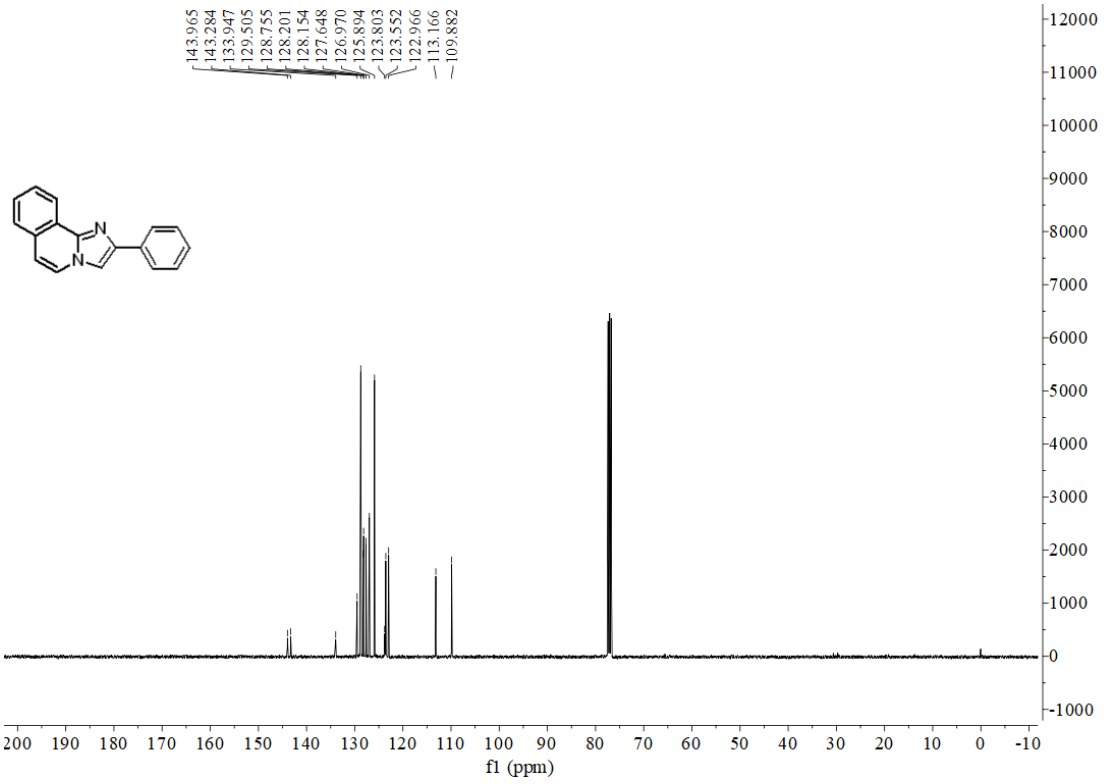
3ac


146.690
144.264
131.808
127.857
127.634
125.207
123.577
123.519
121.152
119.654
119.628
119.601
119.574
117.099
115.736
108.186
F3C
f1 (ppm)

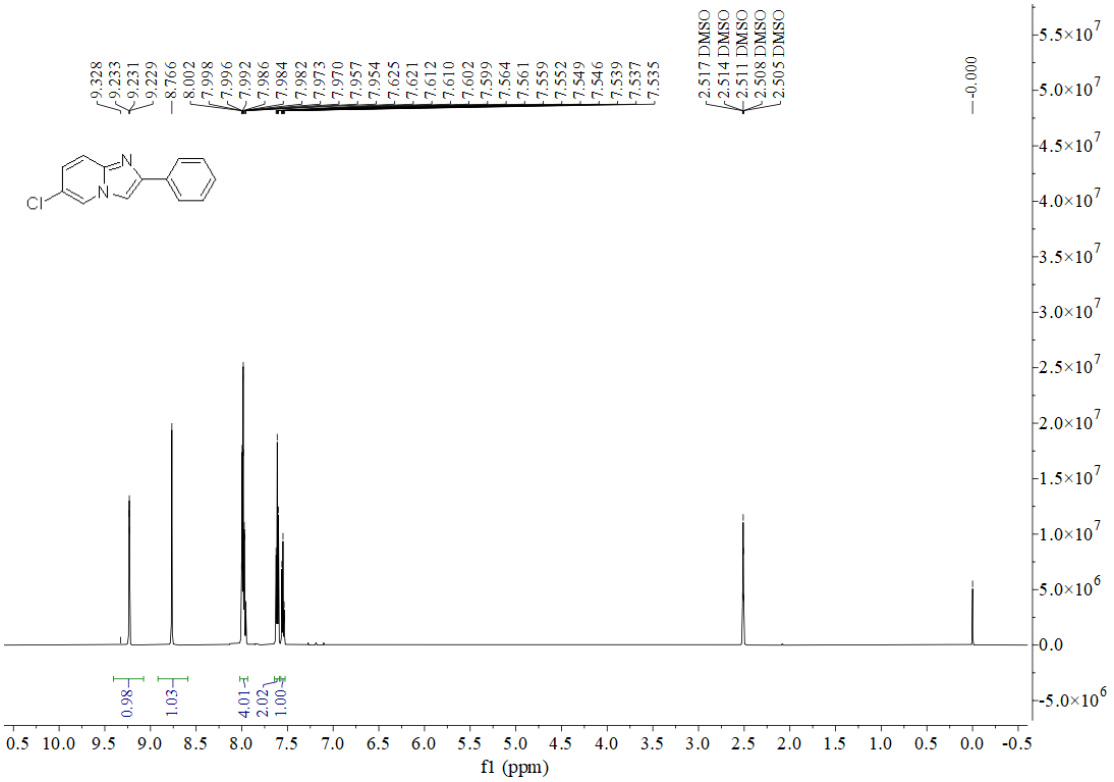
3ad


8.747
8.727
8.015
7.998
7.867
7.849
7.788
7.684
7.665
7.653
7.631
7.615
7.573
7.570
7.551
7.536
7.465
7.446
7.427
7.338
7.320
7.301
7.011
6.993
1.00
2.00
1.03
1.01
2.00
1.03
2.00
1.01
1.01
f1 (ppm)

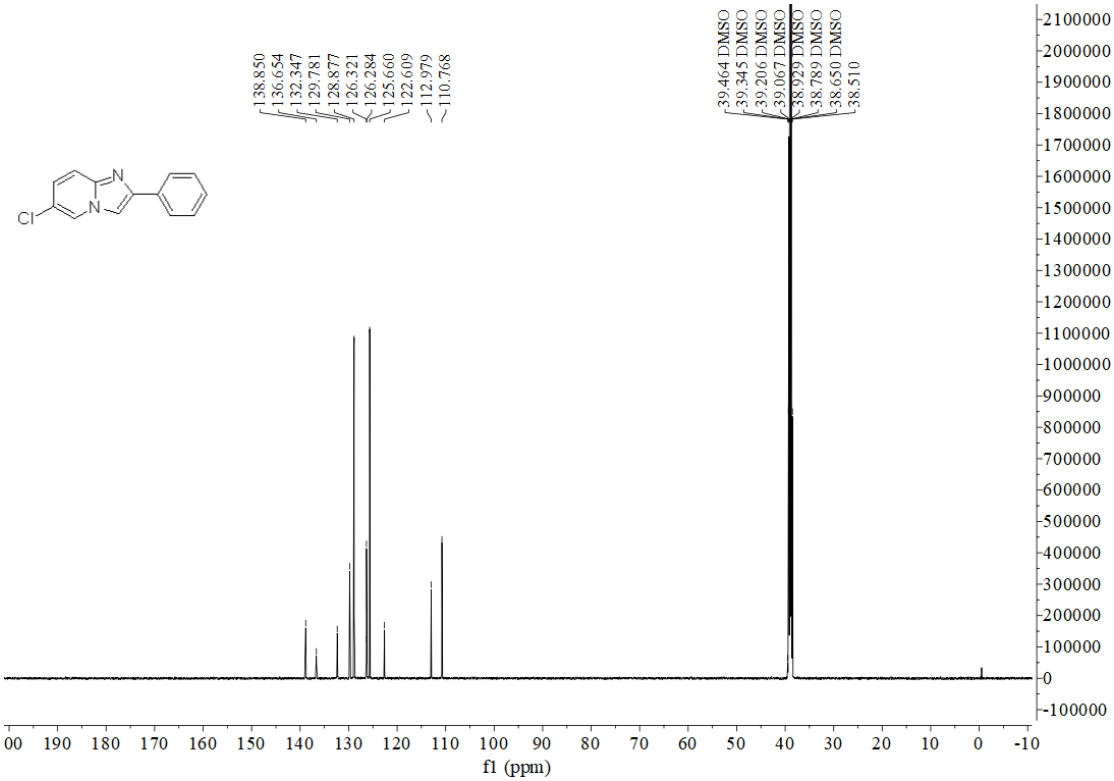
3ad


143.965
143.284
133.947
129.505
128.755
128.201
128.154
127.648
126.970
125.894
123.803
123.552
122.966
113.166
109.882
f1 (ppm)

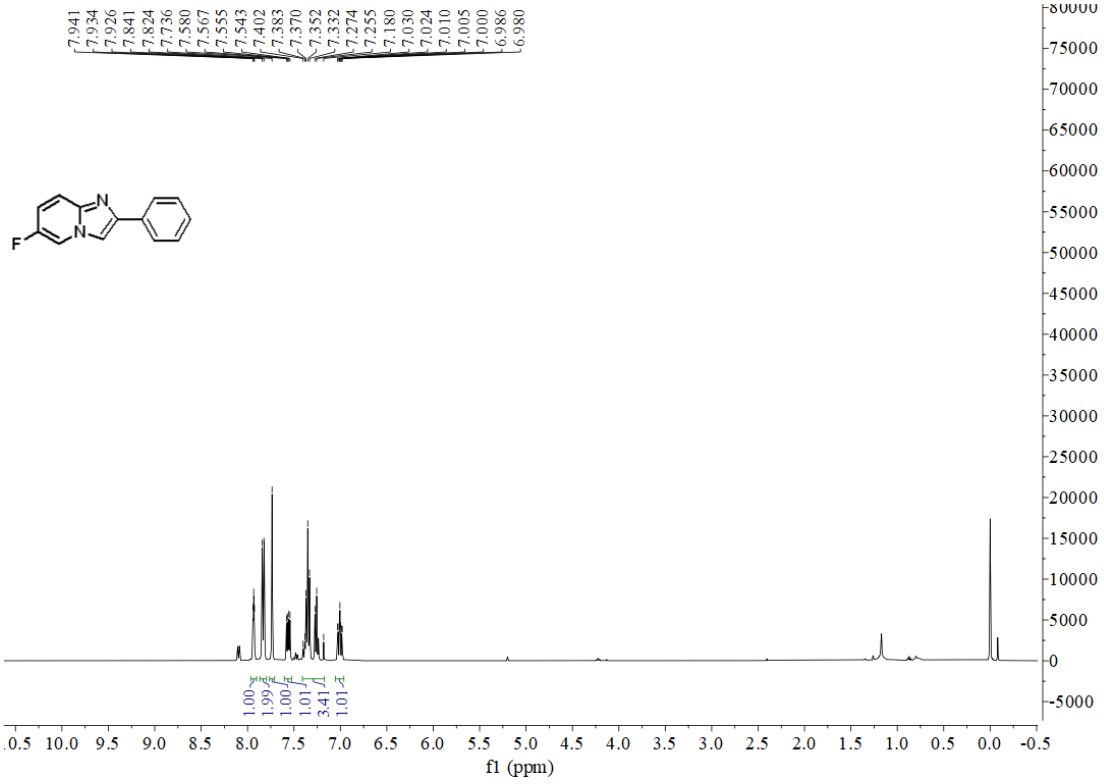
3ae


9.328
9.233
9.231
9.229
8.766
8.002
7.998
7.996
7.992
7.986
7.984
7.982
7.973
7.970
7.957
7.954
7.625
7.621
7.612
7.610
7.602
7.599
7.564
7.561
7.559
7.552
7.549
7.546
7.539
7.537
7.535
2.517 DMSO
2.514 DMSO
2.511 DMSO
2.508 DMSO
2.505 DMSO
-0.000
Cl
N
N
0.98
1.03
4.01
2.02
1.00
f1 (ppm)

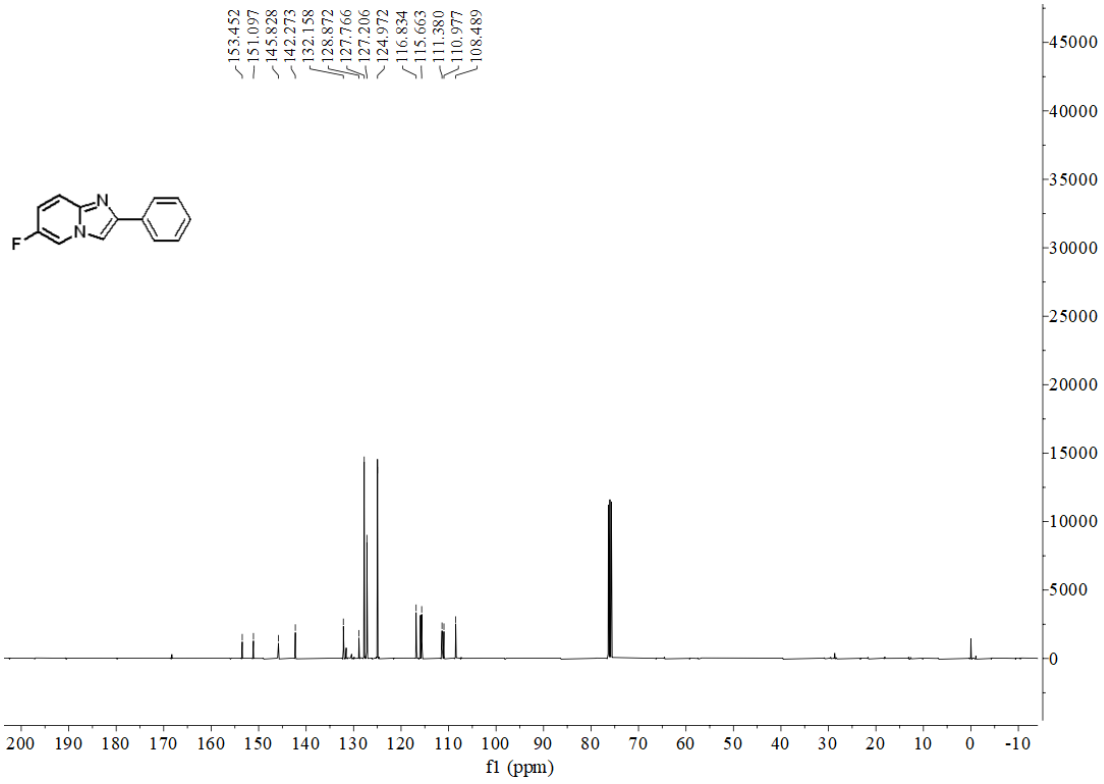
3ae


138.850
136.654
132.347
129.781
128.877
126.321
126.284
125.660
122.609
112.979
110.768
39.464 DMSO
39.345 DMSO
39.206 DMSO
39.067 DMSO
38.929 DMSO
38.789 DMSO
38.650 DMSO
38.510
Cl
N
N
f1 (ppm)

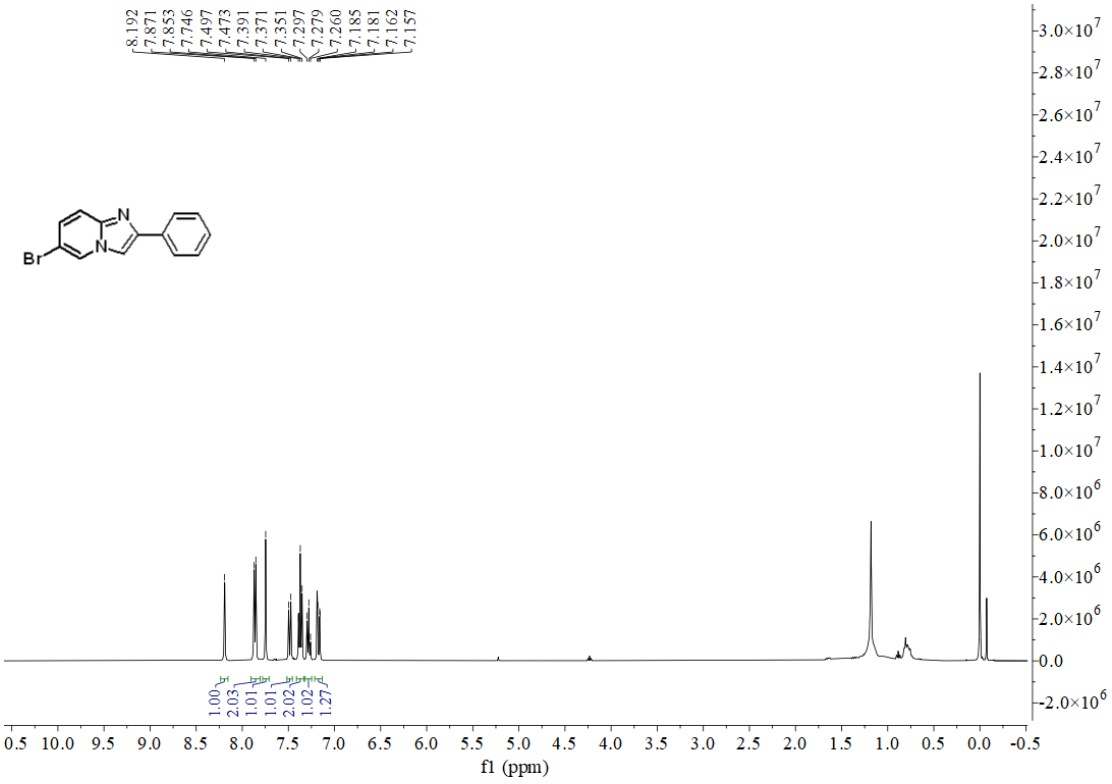
3af


7.941
7.934
7.926
7.841
7.824
7.736
7.580
7.567
7.555
7.543
7.402
7.383
7.370
7.352
7.332
7.274
7.255
7.180
7.030
7.024
7.010
7.005
7.000
6.986
6.980
F
1.00
1.99
1.00
1.01
3.41
1.01
f1 (ppm)

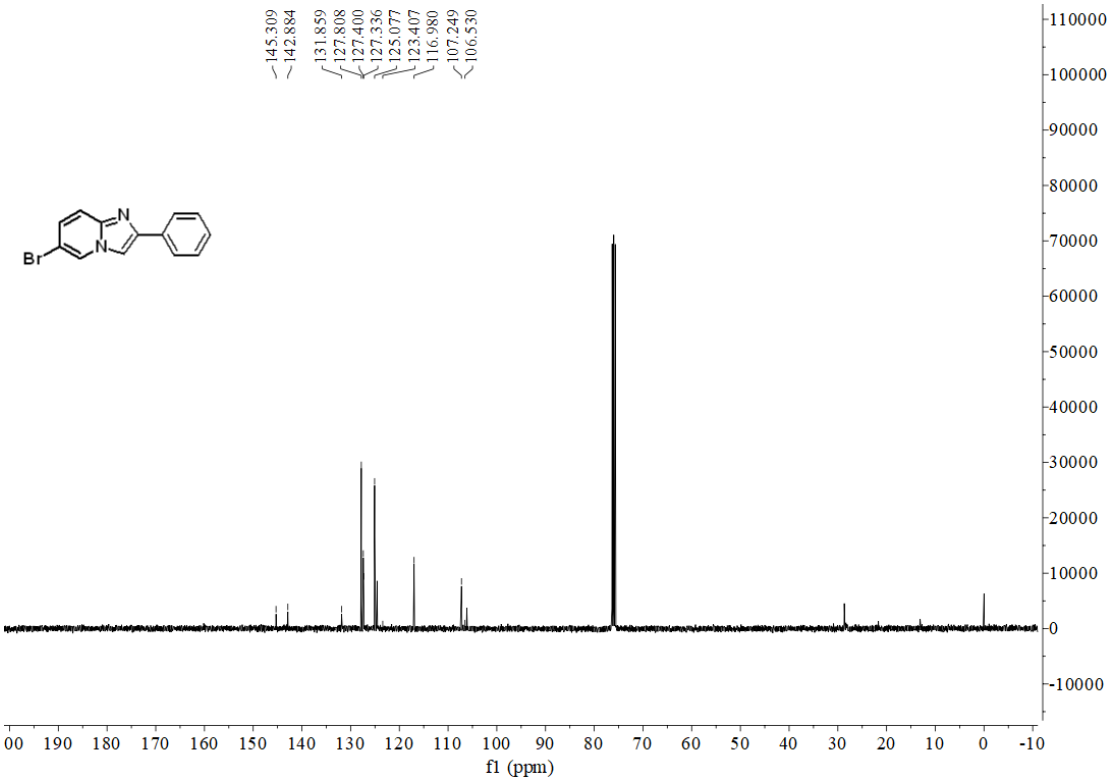
3af


153.452
151.097
145.828
142.273
132.158
128.872
127.766
127.206
124.972
116.834
115.663
111.380
110.977
108.489
F
f1 (ppm)

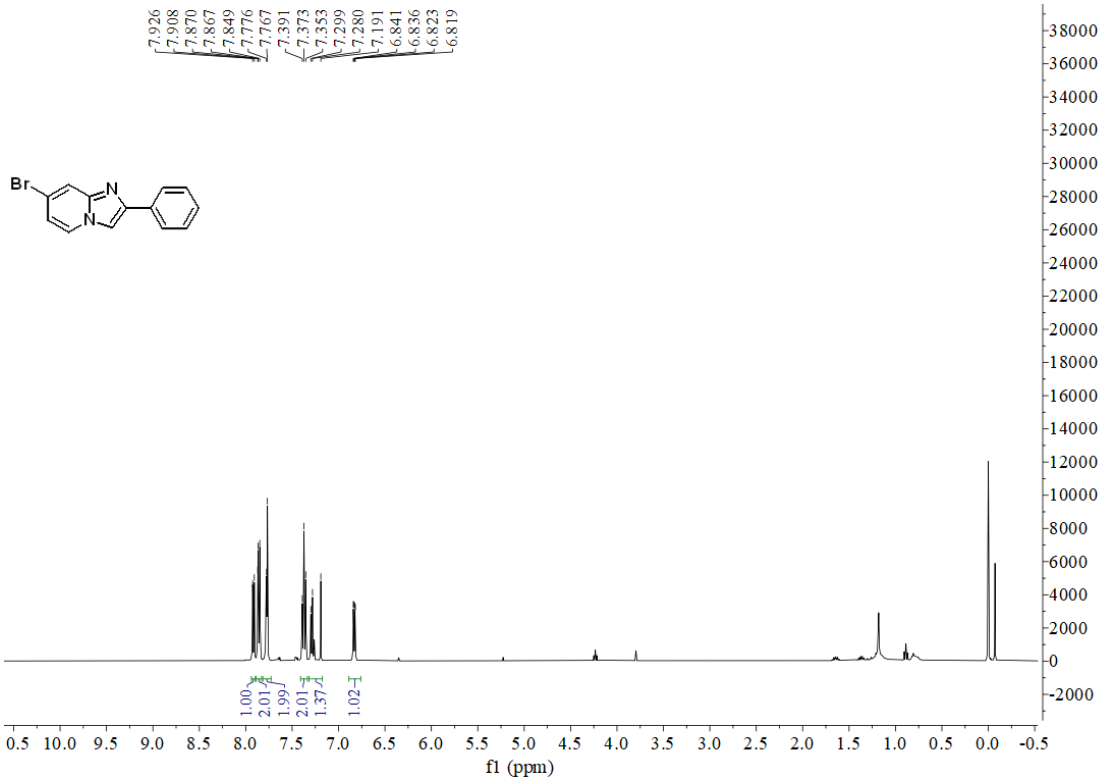
3ag


8.192
7.871
7.853
7.746
7.497
7.473
7.391
7.371
7.351
7.297
7.279
7.260
7.185
7.181
7.162
7.157
Br
N
1.00
2.03
1.01
1.01
2.02
1.02
1.27
f1 (ppm)

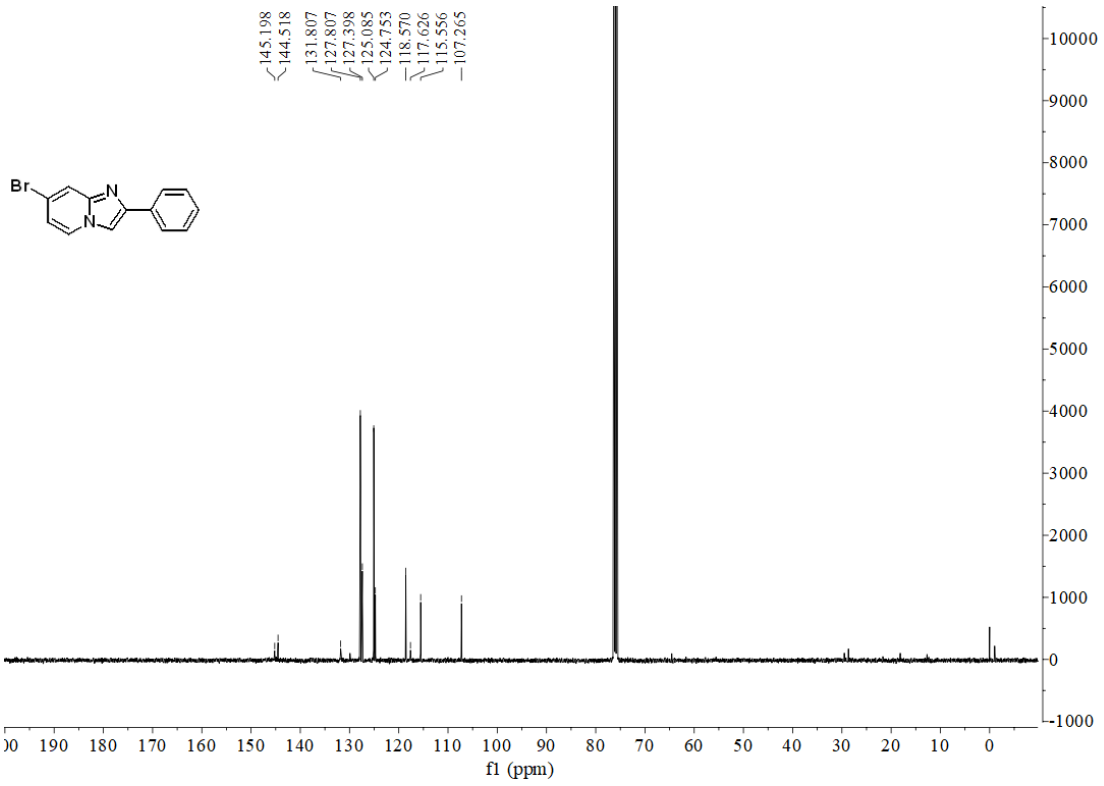
3ag


145.309
142.884
131.859
127.808
127.400
127.336
125.077
123.407
116.980
107.249
106.530
Br
N
f1 (ppm)

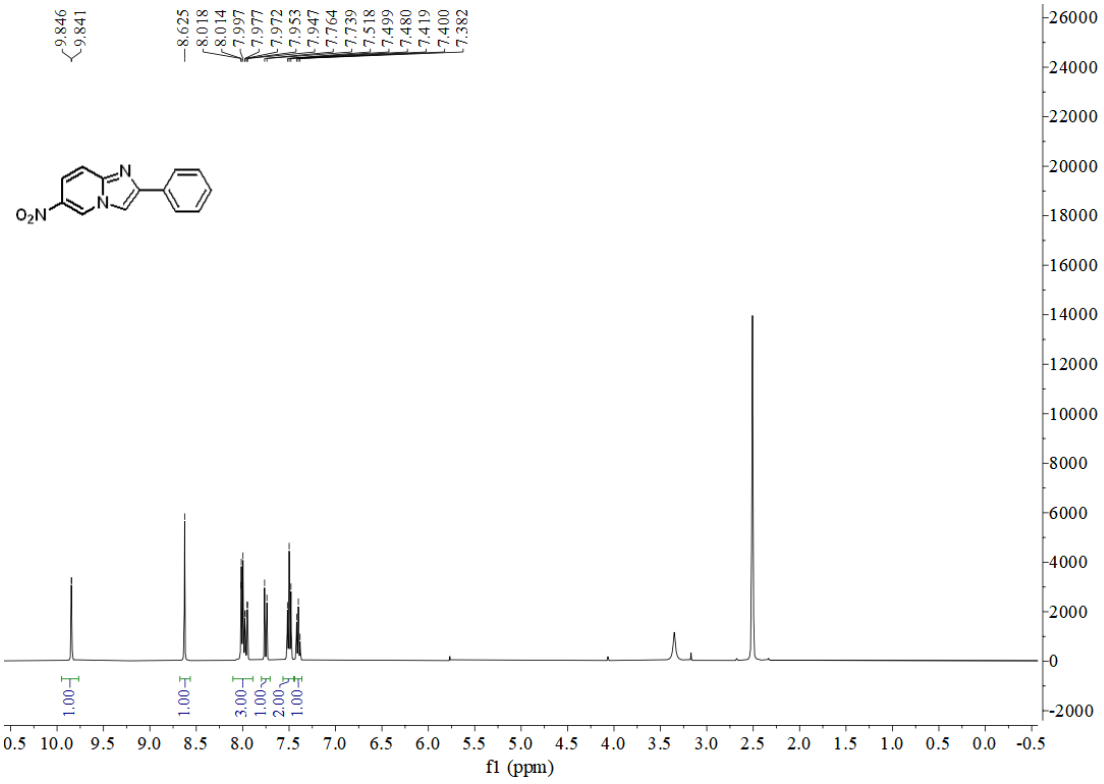
3ah


7.926
7.908
7.870
7.867
7.849
7.776
7.767
7.391
7.373
7.353
7.299
7.280
7.191
6.841
6.836
6.823
6.819
Br
N
N
1.00
2.01
1.99
2.01
1.37
1.02
f1 (ppm)

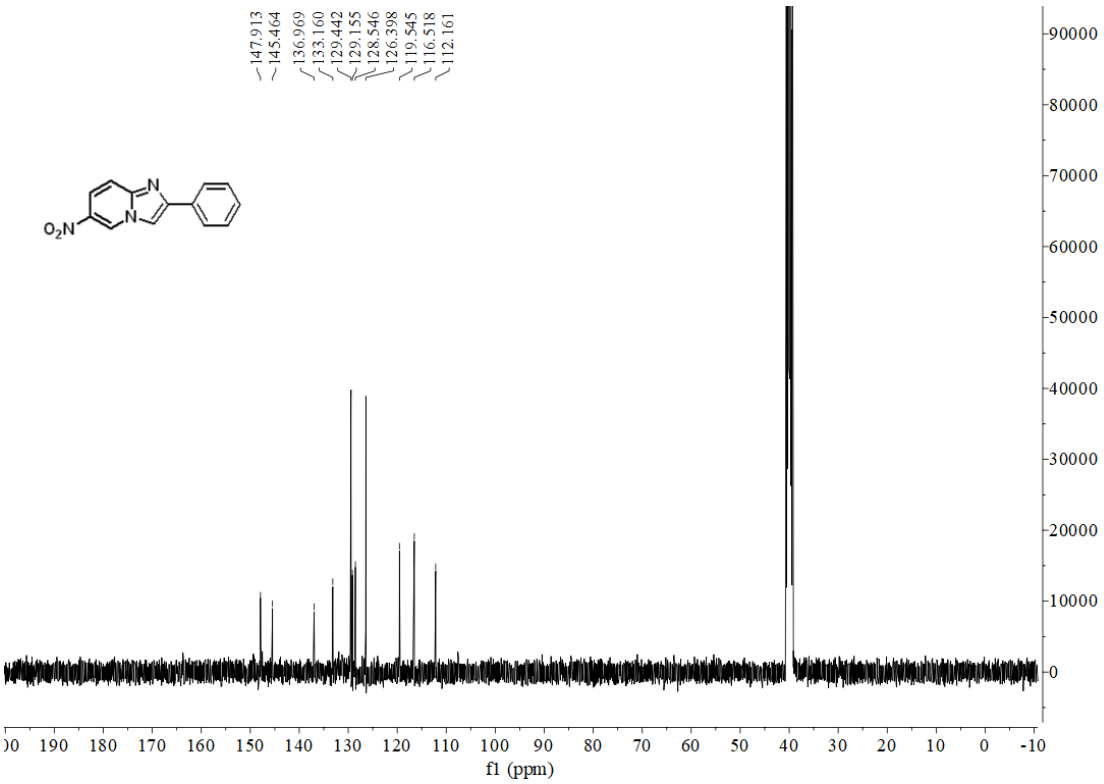
3ah


145.198
144.518
131.807
127.807
127.398
125.085
124.753
118.570
117.626
115.556
107.265
Br
N
N
f1 (ppm)

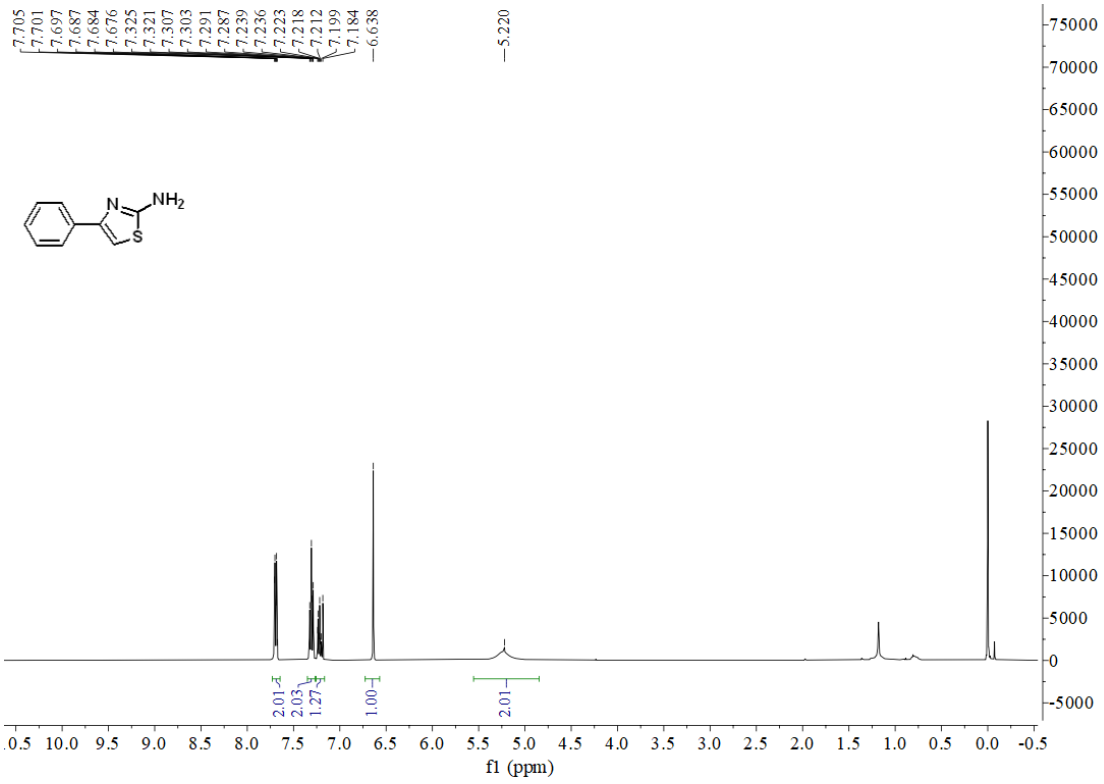
3ai


9.846
9.841
8.625
8.018
8.014
7.997
7.977
7.972
7.953
7.947
7.764
7.739
7.518
7.499
7.480
7.419
7.400
7.382
O2N
1.00
1.00
3.00
1.00
2.00
1.00
f1 (ppm)

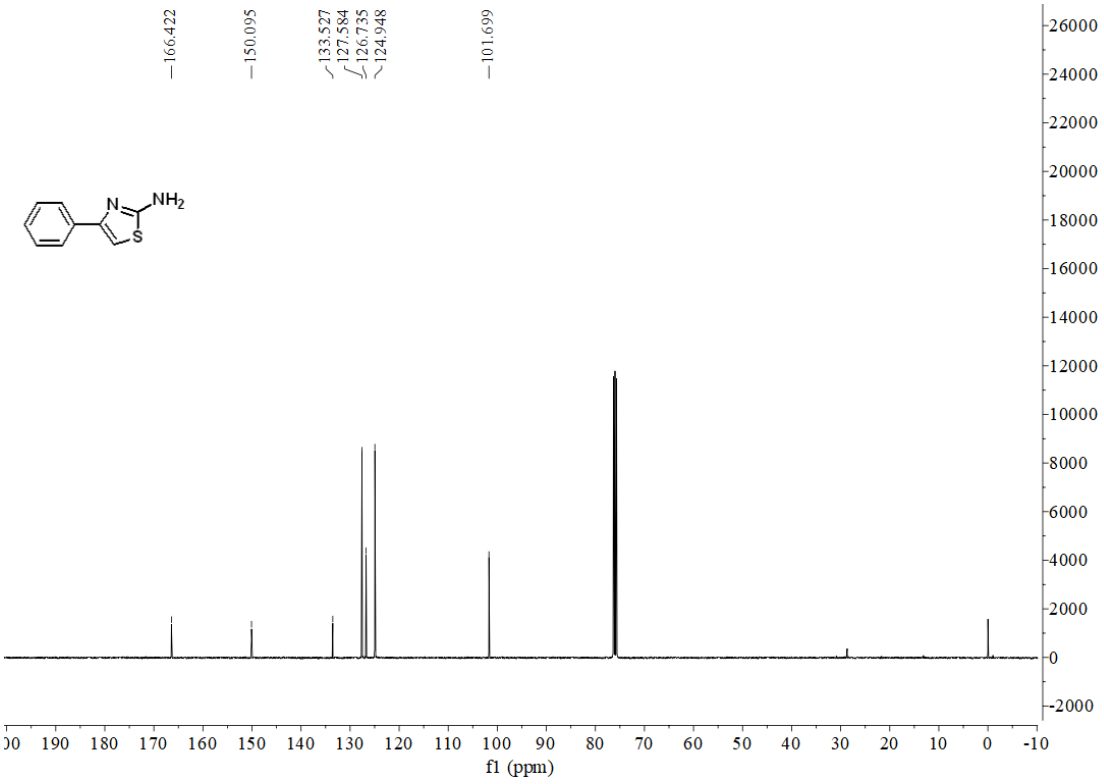
3ai


147.913
145.464
136.969
133.160
129.442
129.155
128.546
126.398
119.545
116.518
112.161
O2N
f1 (ppm)

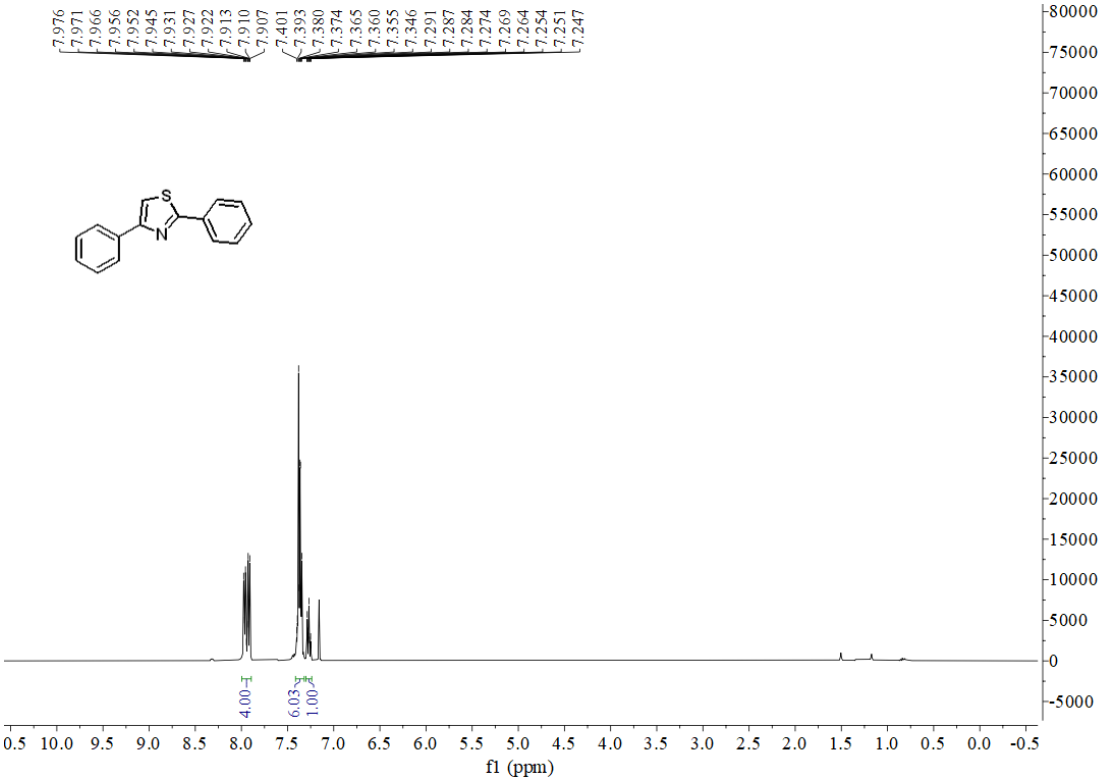
3aj


7.705
7.701
7.697
7.687
7.684
7.676
7.325
7.321
7.307
7.303
7.291
7.287
7.239
7.236
7.223
7.218
7.212
7.199
7.184
6.638
5.220
NH2
N
S
2.01
2.03
1.27
1.00
2.01
f1 (ppm)

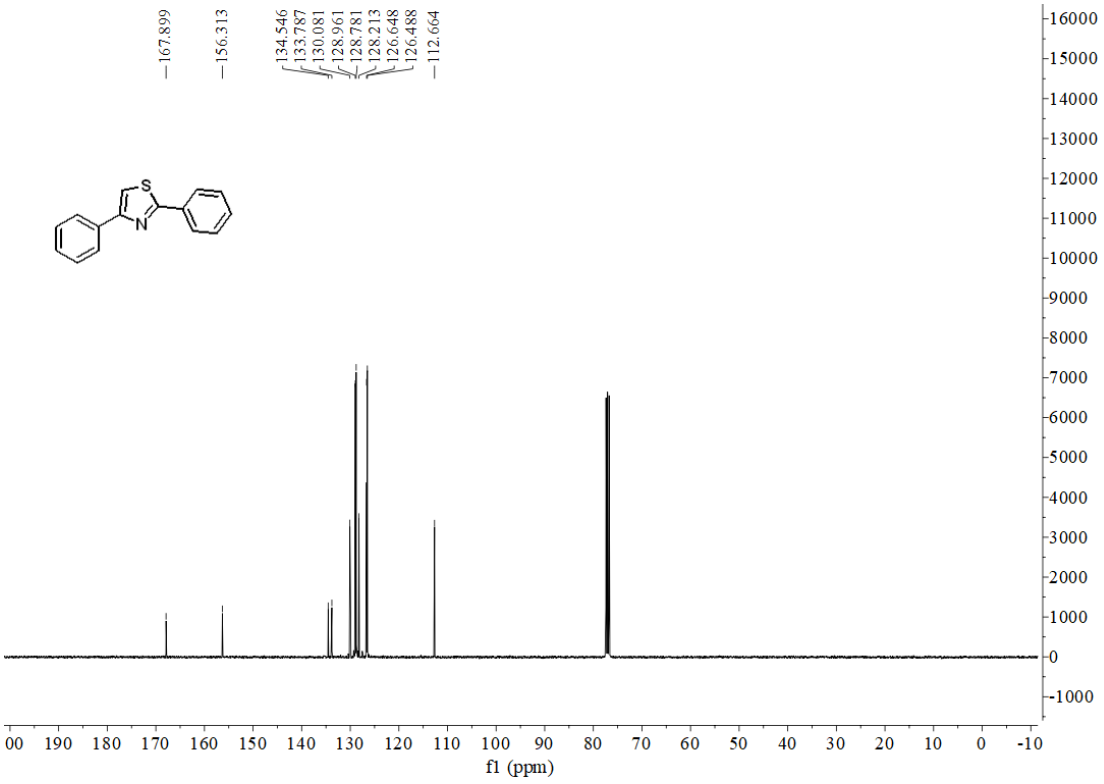
3aj


166.422
150.095
133.527
127.584
126.735
124.948
101.699
NH2
N
S
f1 (ppm)

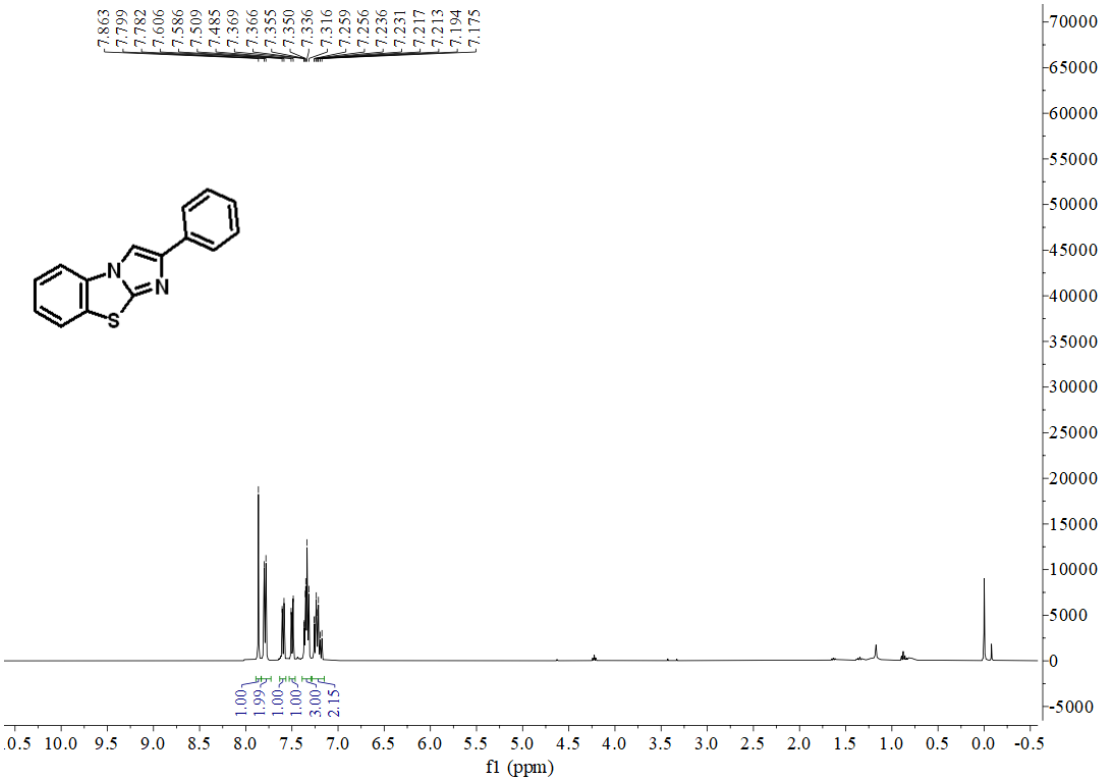
3ak


7.976
7.971
7.966
7.956
7.952
7.945
7.931
7.927
7.922
7.913
7.910
7.907
7.401
7.393
7.380
7.374
7.365
7.360
7.355
7.346
7.291
7.287
7.284
7.274
7.269
7.264
7.254
7.251
7.247
4.00
6.03
1.00
f1 (ppm)

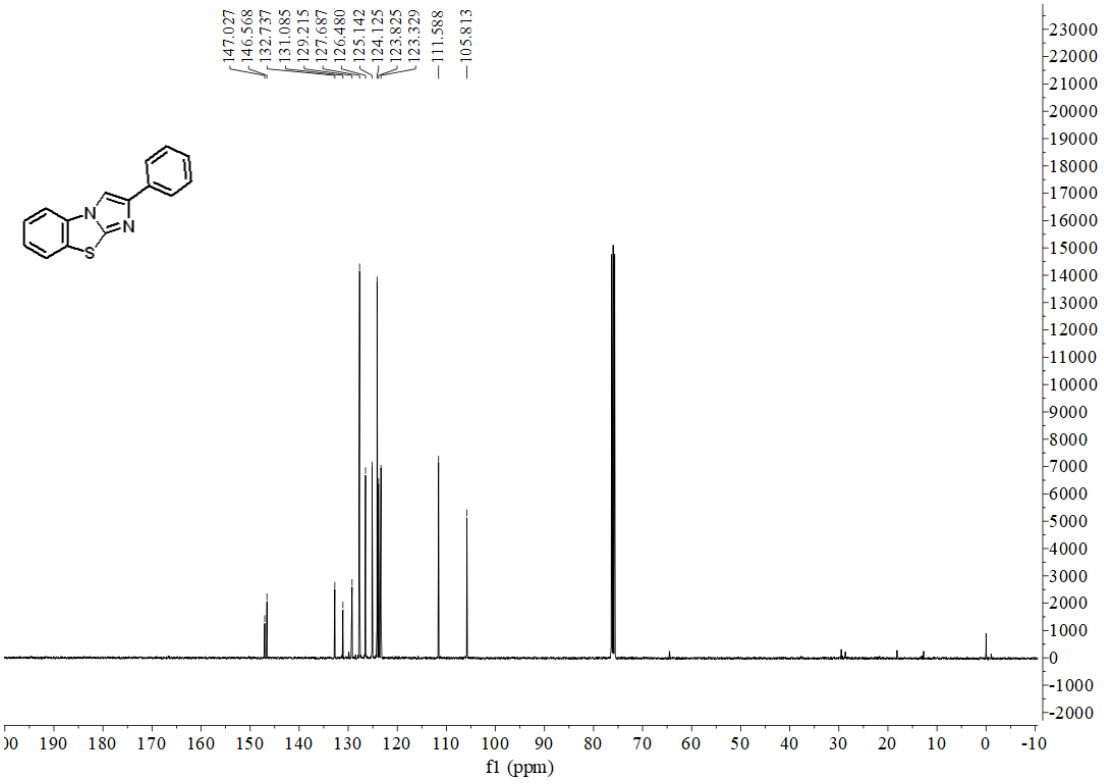
3ak


167.899
156.313
134.546
133.787
130.081
128.961
128.781
128.213
126.648
126.488
112.664
f1 (ppm)

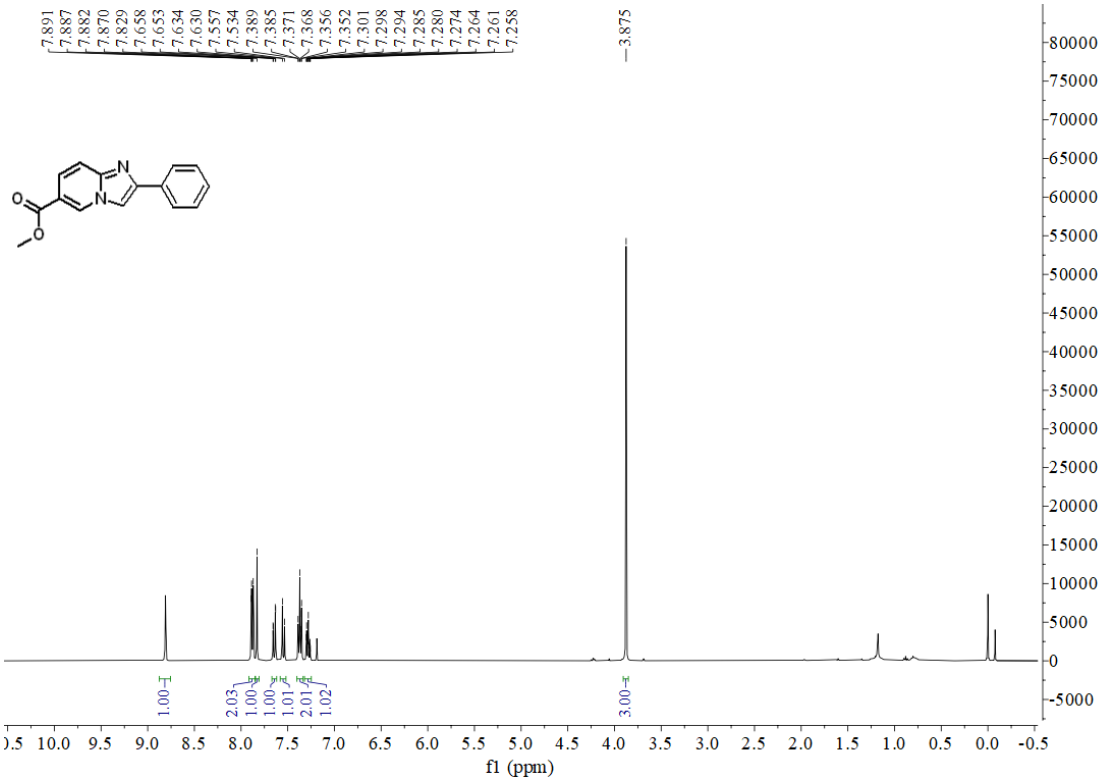
3al


7.863
7.799
7.782
7.606
7.586
7.509
7.485
7.369
7.366
7.355
7.350
7.336
7.316
7.259
7.256
7.236
7.231
7.217
7.213
7.194
7.175
1.00
1.99
1.00
1.00
3.00
2.15
f1 (ppm)

3al


147.027
146.568
132.737
131.085
129.215
127.687
126.480
125.142
124.125
123.825
123.329
111.588
105.813
f1 (ppm)

3am


7.891
7.887
7.882
7.870
7.829
7.658
7.653
7.634
7.630
7.557
7.534
7.389
7.385
7.371
7.368
7.356
7.352
7.301
7.298
7.294
7.285
7.280
7.274
7.264
7.261
7.258
3.875
1.00
2.03
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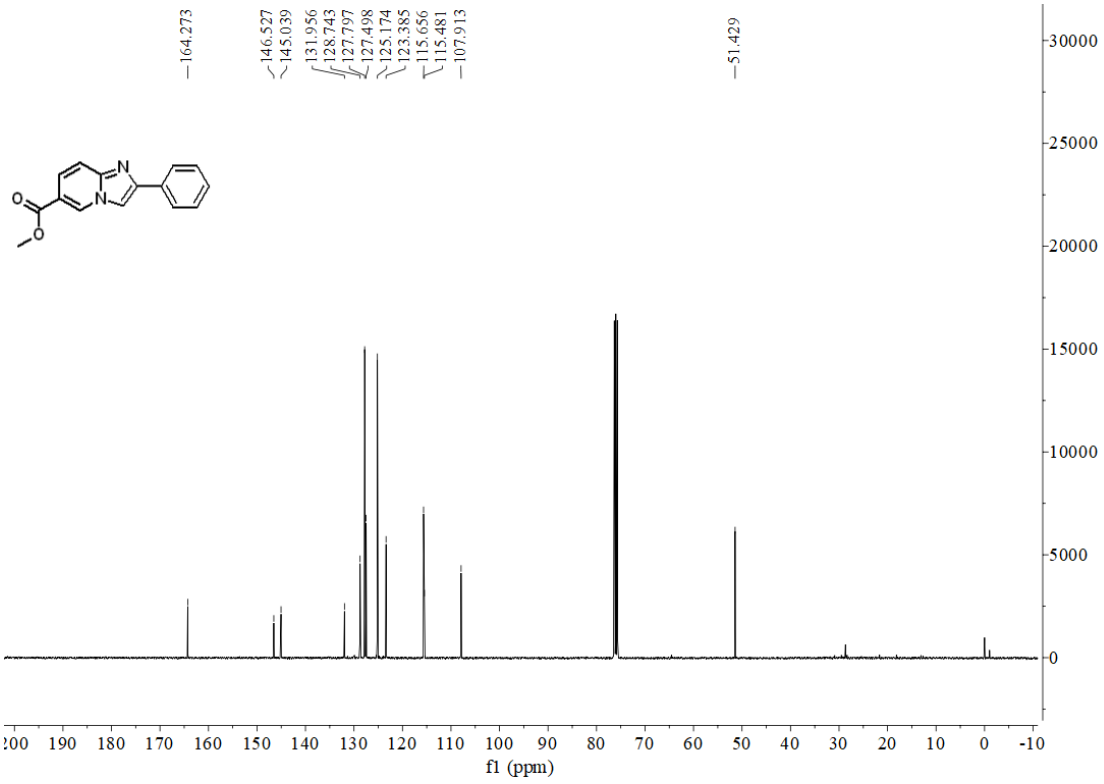
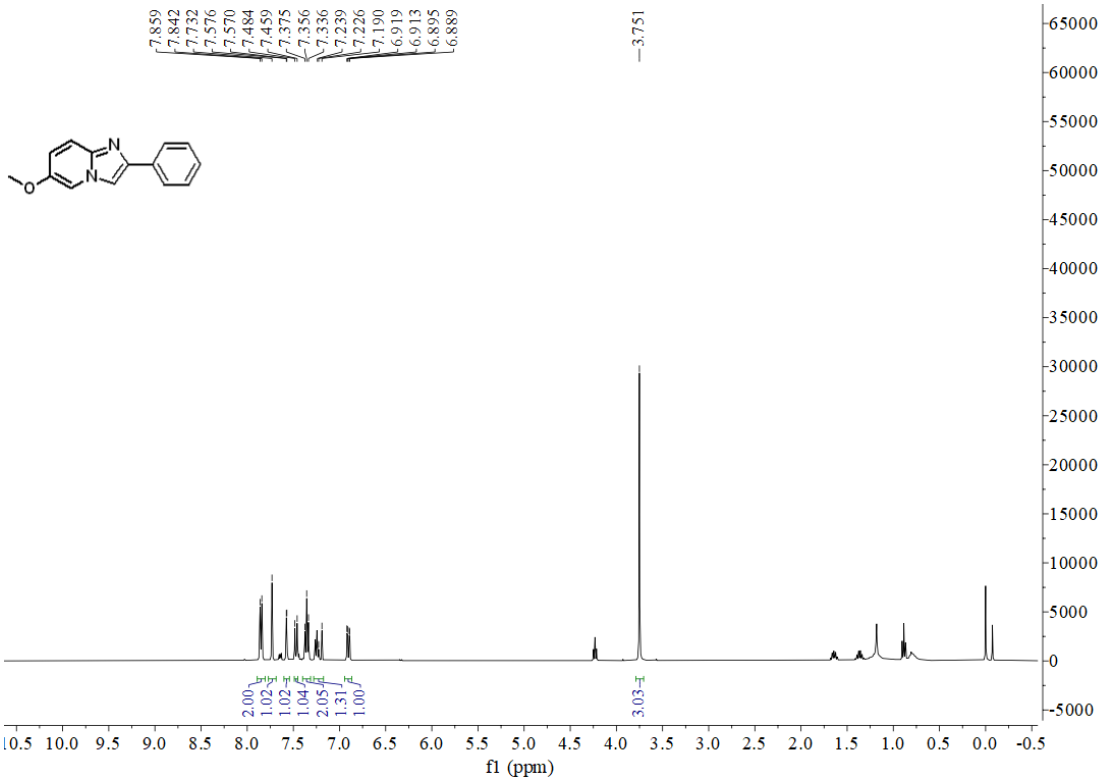
1.00
1.01
2.01
1.02
3.00
f1 (ppm)

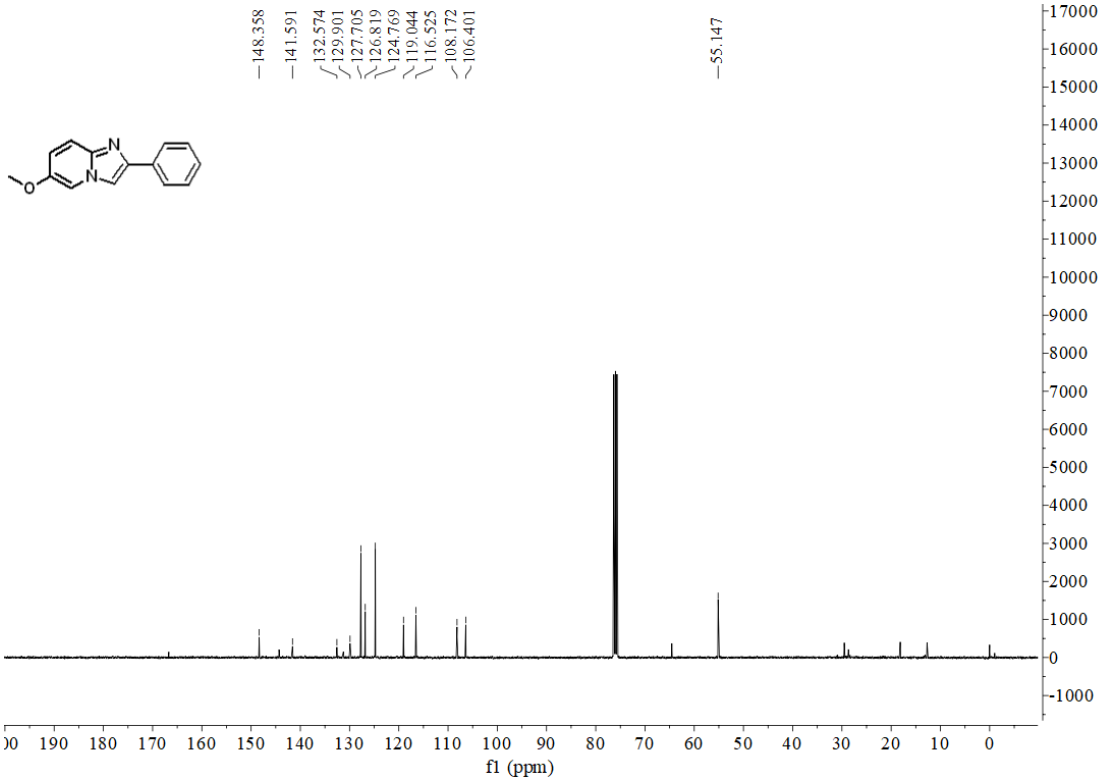
3am


164.273
146.527
145.039
131.956
128.743
127.797
127.498
125.174
123.385
115.656
115.481
107.913
51.429
f1 (ppm)

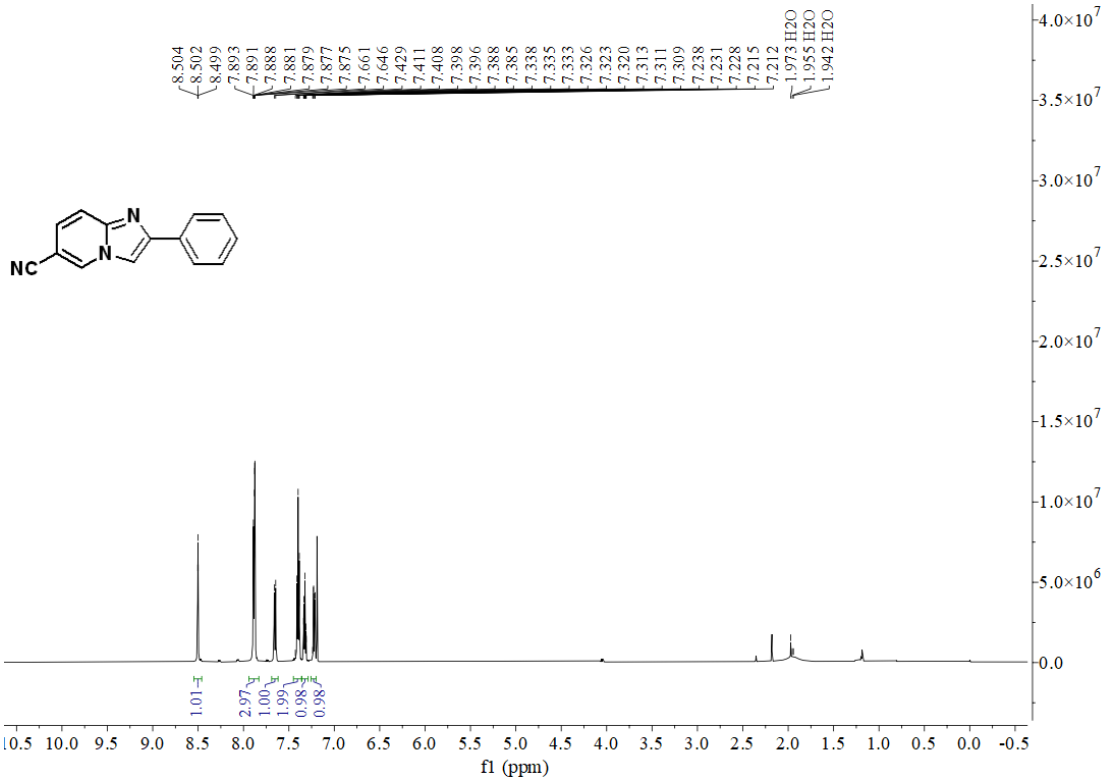
3an


7.859
7.842
7.732
7.576
7.570
7.484
7.459
7.375
7.356
7.336
7.239
7.226
7.190
6.919
6.913
6.895
6.889
3.751
2.00
1.02
1.02
1.04
2.05
1.31
1.00
3.03
f1 (ppm)

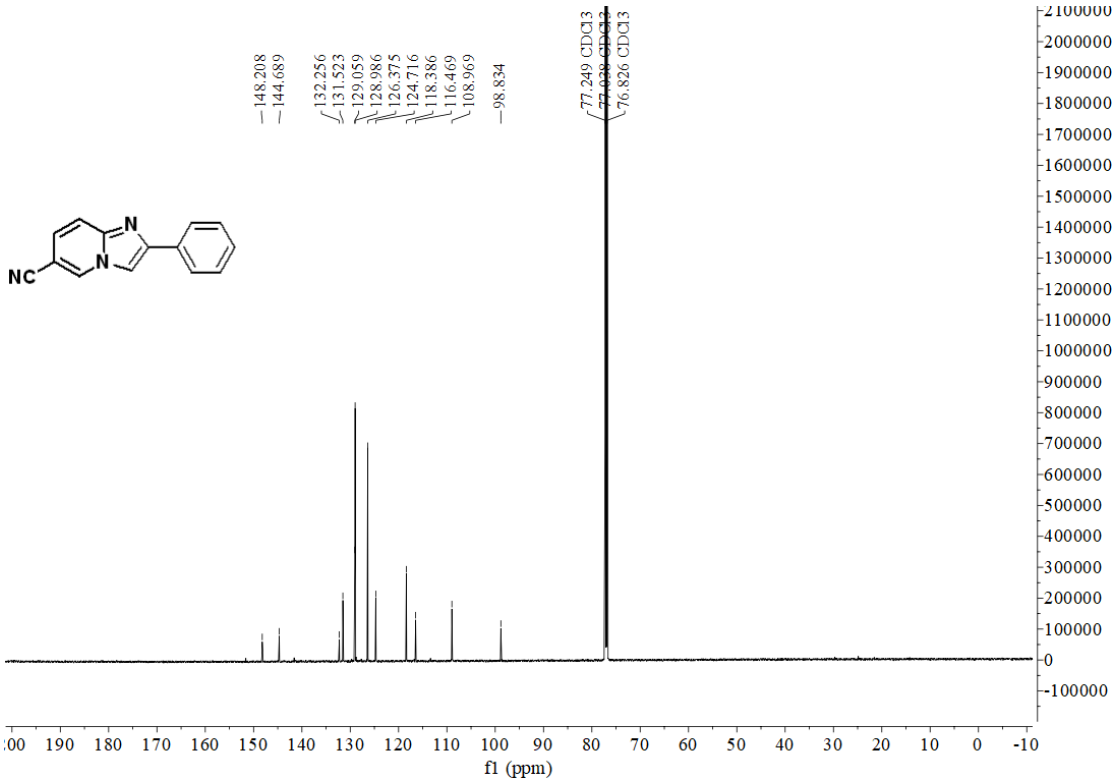
3an


148.358
141.591
132.574
129.901
127.705
126.819
124.769
119.044
116.525
108.172
106.401
55.147
f1 (ppm)

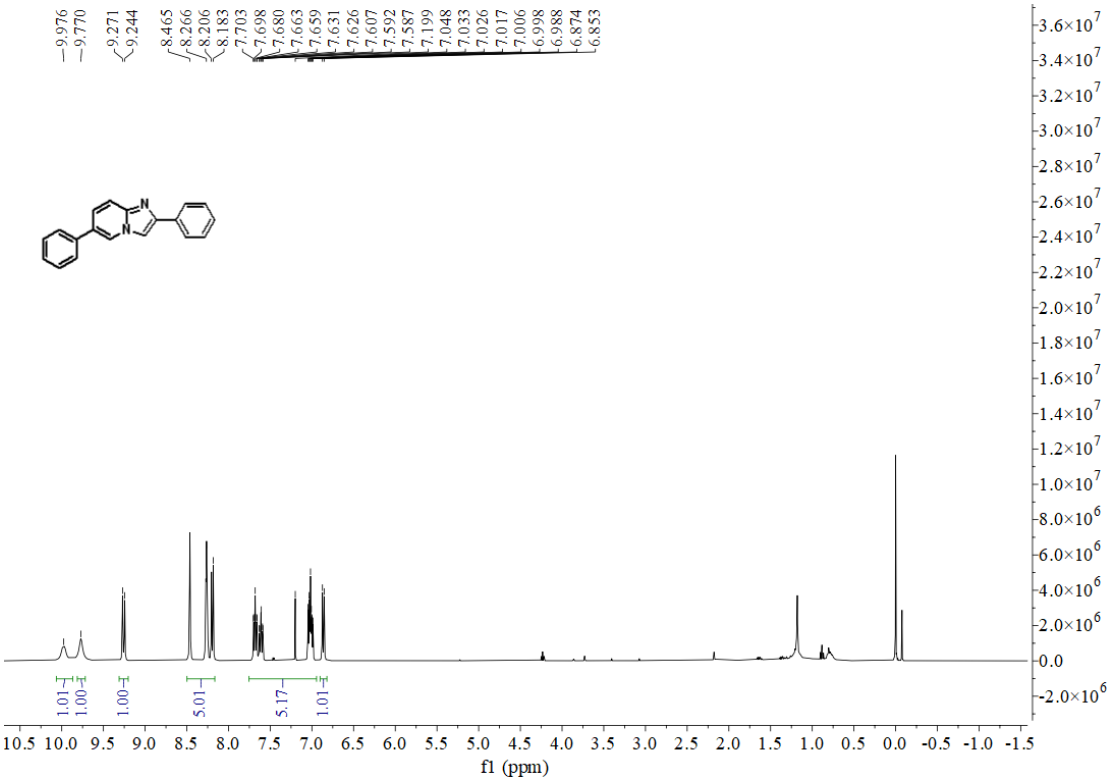
3ao


8.504
8.502
8.499
7.893
7.891
7.888
7.881
7.879
7.877
7.875
7.661
7.646
7.429
7.411
7.408
7.398
7.396
7.388
7.385
7.338
7.335
7.333
7.326
7.323
7.320
7.313
7.311
7.309
7.238
7.231
7.228
7.215
7.212
1.973 H2O
1.955 H2O
1.942 H2O
NC
N
N
1.01
2.97
1.00
1.99
0.98
0.98
f1 (ppm)

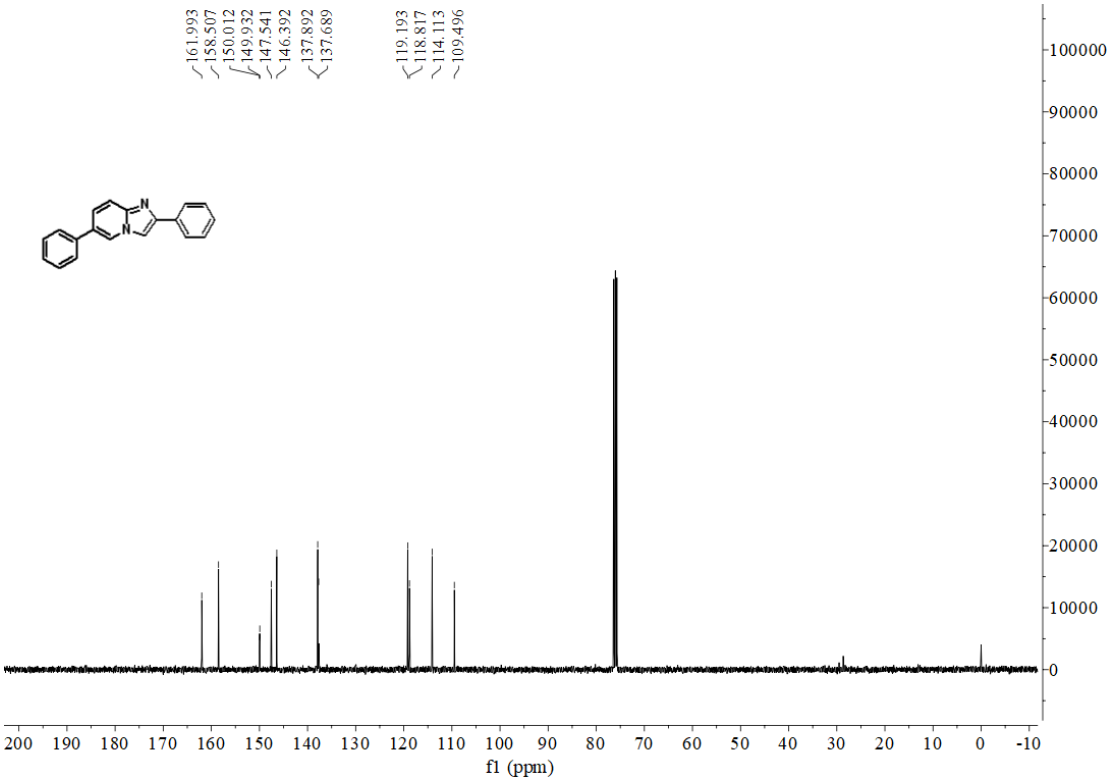
3ao


148.208
144.689
132.256
131.523
129.059
128.986
126.375
124.716
118.386
116.469
108.969
98.834
77.249 CDCl3
77.038 CDCl3
76.826 CDCl3
NC
N
N
f1 (ppm)

3ap


9.976
9.770
9.271
9.244
8.465
8.266
8.206
8.183
7.703
7.698
7.680
7.663
7.659
7.631
7.626
7.607
7.592
7.587
7.199
7.048
7.033
7.026
7.017
7.006
6.998
6.988
6.874
6.853
1.01
1.00
1.00
5.01
5.17
1.01
f1 (ppm)

3ap


161.993
158.507
150.012
149.932
147.541
146.392
137.892
137.689
119.193
118.817
114.113
109.496
f1 (ppm)