Supporting Information

Regiospecific Synthesis of 1,2-Disubstituted (Hetero)aryl Fused Imidazoles with Tunable Fluorescent Emission

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I. General remarks

The ^{1}H NMR (400 MHz or 600 MHz) chemical shifts were measured relative to tetramethylsilane, $CDCl_3$ or DMSO-d_6 as the internal reference. The ^{13}C NMR (100 MHz or 150 MHz) chemical shifts were given using $CDCl_3$ or DMSO-d_6 as the internal standard. Low-resolution mass spectra (MS) were obtained by ESI-MS. High resolution mass spectra (HR-MS) were obtained with a Waters-Q-TOF-Premier (ESI). Absorption spectra were obtained on a HITACHI U-2910 spectrometer. Fluorescence spectra were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer. The photomultiplier voltage was 700 V. To reduce the fluctuation in the excitation intensity, the lamp was kept on for 1 hour prior to the experiment.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. All syntheses and manipulations were carried out under an inert atmosphere in a glove box or using standard Schlenk or vacuum line techniques. Anhydrous caesium carbonate, NaO*t*Bu, KO*t*Bu, LiO*t*Bu was purchased from Acros, and stored in a glove box. Amidines were prepared according to the literature procedure.[1] Solvents were dried by refluxing for at least 24 h over CaH_2 (DMF), or sodium (toluene), and freshly distilled and vigorously purged with N_2 for 1 hour prior to use.

II. General procedure for the synthesis of amidines or diamidines[1]

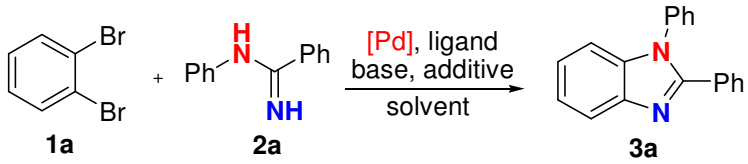
Method A: Under nitrogen gas, to a solution of aniline (20 mmol) in DMSO (10 mL) was added NaH (440 mg, 22 mmol) at room temperature. After the mixture was stirred for 30 min, benzonitrile (20 mmol) was added. The reaction mixture was stirred overnight, and then poured into 200 mL of ice-water. The precipitate was collected by filtration, washed with petroleum ether and dried under vacuum to yield the desired compound as a pale white solid. The residue was either purified by silica gel chromatography or recrystallization using EtOH.

Method B: A baked-out and N_2-purged Schlenk flask was initially charged with 30 mmol or 60 mmol primary amine and 20 mL of absolute THF. The solution was

cooled to -78 ℃, and 12 mL of *n*-BuLi (in hexane, 2.5 M) was added dropwise with stirring. The mixture was allowed to thaw and stirred at room temperature for 30 min, and 30 mmol of nitrile in THF were then slowly added dropwise with vigorous stirring at -78 ℃. Upon completion of addition, stirring was continued at -78 ℃ for 2 h. The mixture was allowed to thaw and hydrolyzed by adding 40 mL of water. The precipitate was collected by filtration, washed with petroleum ether and dried under vacuum to yield the desired compound as a pale white solid. The residue was either purified by silica gel chromatography or recrystallization using EtOH.

III. Optimization of the twofold amination of 1,2-dibromobenzene with *N*-phenylbenzamidine

Table S1: Optimization of the twofold amination of *N*-phenylbenzamidine with 1, 2-dibromobenzene [a]



Entry	Palladium source	Ligand	Base	Solvent	Yield[b]
1	$Pd(OAc)_2$	-	Cs_2CO_3	toluene	n.r
2	$Pd(OAc)_2$	$Cy_3P{\cdot}HBF_4$	Cs_2CO_3	toluene	n.r
3	$Pd(OAc)_2$	X-phos	Cs_2CO_3	toluene	n.r
4	$Pd(OAc)_2$	Daves-phos	Cs_2CO_3	toluene	n.r
5	$Pd(OAc)_2$	Dppf	Cs_2CO_3	toluene	13%
6	$Pd(OAc)_2$	BINAP	Cs_2CO_3	toluene	85%
7	$Pd(OAc)_2$	Xantphos	Cs_2CO_3	toluene	89%
8	$Pd(OAc)_2$	Xantphos	KO*t*Bu	toluene	<5%
9	$Pd(OAc)_2$	Xantphos	LiO*t*Bu	toluene	<5%
10	$Pd(OAc)_2$	Xantphos	NaO*t*Bu	toluene	92%
11[c]	$Pd(OAc)_2$	Xantphos	NaO*t*Bu	toluene	99%
12	$Pd(OAc)_2$	Xantphos	NaO*t*Bu	DMF	trace

13	$Pd(OAc)_2$	Xantphos	NaO*t*Bu	CH_3CN	trace
14	$Pd(OAc)_2$	Xantphos	NaO*t*Bu	DMSO	n.r
15	$Pd_2(dba)_3$	Xantphos	NaO*t*Bu	toluene	trace
16	$PdCl_2$	Xantphos	NaO*t*Bu	toluene	trace
17	$Pd(PPh_3)_4$	Xantphos	NaO*t*Bu	toluene	32%
18[c]	$Pd(dba)_2$	Xantphos	NaO*t*Bu	toluene	98%

[a] Reactions were carried out using [Pd] (2.5 mol%), base (4.0 equiv), ligand (2.5 mol%), *o*-dibromobenzene (0.25 mmol), and *N*-phenylbenzamidine (0.3 mmol) (0.25 M) at 140 ℃ for 24 hours. [b] Yield of isolated product based on *o*-dibromobenzene. [c] 4 Å sieves (100 mg) was added as the additive. $Cy_3P{\cdot}HBF_4$ = tricyclohexylphosphonium tetrafluoroborate, X-phos = 2-dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl, Daves-phos = 2-dicyclohexylphosphino -2'-(N,N-dimethylamino)biphenyl, Dppf = 1,1'-bis(diphenylphosphino)ferrocene; BINAP = (R)-(+)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl, Xantphos = 4,5-bis(diphenylphosphino) -9,9-dimethylxanthene.

IV. General procedure for Tables 1-2

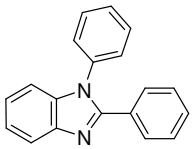
A flame-dried Schlenk test tube with a magnetic stirring bar was charged with $Pddba_2$ or $Pd(OAc)_2$ (2.5-5.0 mol%) , Xantphos (2.5-5.0 mol%), *t*BuONa (96 mg, 1.0 mmol) or Cs_2CO_3 (324 mg, 1.0 mmol), amidine (0.30 mmol), *o*-dihaloarene (0.25 mmol) and toluene (1 mL) in the presence of 4 Å sieves (100 mg) under N_2. A rubber septum was replaced with a glass stopper, and the system was then evacuated three times and back filled with N_2. The reaction mixture was stirred for 10 min at room temperature, and then heated at 140 ℃ for 24 h. The reaction mixture was then cooled to ambient temperature, diluted with 10-15 mL of CH_2Cl_2, filtered through a plug of silica gel, and washed with 10-20 mL of CH_2Cl_2. The combined organic extracts were concentrated and the resulting residue was purified by column chromatography on silica gel to provide the desired product.

V. General procedure for the synthesis of benzobisimidazole

A flame-dried Schlenk test tube with a magnetic stirring bar was charged with $Pd(OAc)_2$ (5.0 mol%), Xantphos (5.0 mol%), *t*BuONa (192 mg, 2.0 mmol), *N*-phenylbenzamidine (118 mg, 0.60 mmol), 1,4-dibromo-2,5-diiodobezene (122 mg,

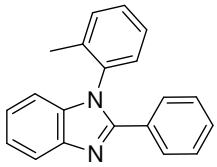
0.25 mmol) or 1,5-dibromo-2,4-diiodobezene (122 mg, 0.25 mmol) and toluene (1 mL) in the presence of 4 Å sieves (100 mg) under N_2. A rubber septum was replaced with a glass stopper, and the system was then evacuated three times and back filled with N_2. The reaction mixture was stirred for 10 min at room temperature, and then heated at 140 ºC for 24 h. The reaction mixture was then cooled to ambient temperature, diluted with 10-15 mL of CH_2Cl_2, filtered through a plug of silica gel, and washed with 10-20 mL of CH_2Cl_2. The combined organic extracts were concentrated and the resulting residue was purified by column chromatography on silica gel to provide the desired product.

VI. Experimental data for the described substances



1,2-Diphenyl-1*H*-benzo[*d*]imidazole (3a)[2]

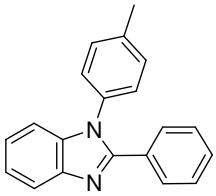
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (1.4 mg, 0.00625 mmol), Xantphos (3.7 mg, 0.00625 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (99% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.26-7.29 (m, 2H), 7.31-7.36 (m, 6H), 7.45-7.52 (m, 3H), 7.56 (d, J = 7.2 Hz, 2H), 7.89 (d, J = 8.0 Hz, 1H) ppm. MS (ESI) m/z: 271.3 $[M+H]^+$.



2-Phenyl-1-*o*-tolyl-1*H*-benzo[*d*]imidazole (3b)

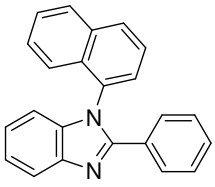
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-*o*-tolylbenzamidine (63.1 mg, 0.30 mmol), $Pd(dba)_2$ (7.2 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc

afforded a white solid (95% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.91 (s, 3H), 7.00 (d, J = 8.0 Hz, 1H), 7.23-7.45 (m, 9H), 7.59-7.61 (m, 2H), 7.90 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 17.6, 110.7, 119.9, 123.0, 123.4, 127.6, 128.5, 128.7, 128.8, 129.5, 129.6, 130.3, 131.8, 136.1, 136.2, 137.2, 143.1, 152.4 ppm. MS (ESI) m/z: 285.1 $[M+H]^+$.



2-Phenyl-1-*p*-tolyl-1*H*-benzo[*d*]imidazole (3c)[3]

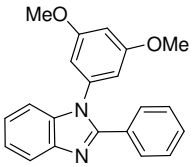
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-*p*-tolylbenzamidine (63.1 mg, 0.30 mmol), $Pd(dba)_2$ (7.2 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.44 (s, 3H), 7.18 (d, J = 8.0 Hz, 2H), 7.22-7.35 (m, 8H), 7.59 (d, J = 7.2 Hz, 2H), 7.88 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.3, 110.6, 119.9, 123.0, 123.3, 127.3, 128.4, 129.46, 129.54, 130.2, 130.6, 134.5, 137.5, 138.7, 143.1, 152.5 ppm. MS (ESI) m/z: 285.1 $[M+H]^+$.



1-(Naphthalen-1-yl)-2-phenyl-1*H*-benzo[*d*]imidazole (3d)

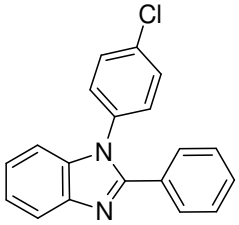
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-phenylnicotinamidine (73.8 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (99% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.85 (d, J = 8.0

Hz, 1H), 7.14-7.18 (m, 3H), 7.22-7.25 (m, 1H), 7.32-7.38 (m, 2H), 7.40 (d, *J* = 3.6 Hz, 2H), 7.50-7.57 (m, 4H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.97 (t, *J* = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 111.1, 119.9, 122.9, 123.1, 123.5, 125.8, 126.7, 127.1, 127.8, 128.4, 128.6, 128.9, 129.6, 129.8, 130.0, 130.3, 133.6, 134.6, 138.3, 143.0, 153.4 ppm. HR-MS (ESI) calcd for $C_{23}H_{17}N_2$ $[M+H]^+$ 321.1392, found: 321.1386.



1-(3,5-Dimethoxyphenyl)-2-phenyl-1*H*-benzo[*d*]imidazole (3e)

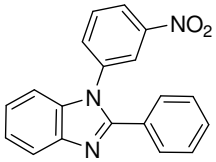
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-(3,5-dimethoxyphenyl)benzamidine (76.89 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (91% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.72 (s, 6H), 6.45 (d, *J* = 2.0 Hz, 2H), 6.54 (d, *J* = 2.0 Hz, 1H), 7.25-7.28 (m, 1H), 7.31-7.38 (m, 5H), 7.63 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.7, 100.7, 105.9, 110.7, 119.9, 123.1, 123.4, 128.4, 129.4, 129.6, 137.2, 138.7, 143.1, 152.4, 161.6 ppm. HR-MS (ESI) calcd for $C_{21}H_{19}N_2O_2$ $[M+H]^+$ 331.1447, found: 331.1442.



1-(4-Chlorophenyl)-2-phenyl-1*H*-benzo[*d*]imidazole (3f)[4]

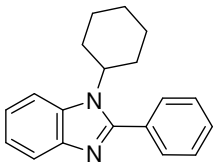
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-(4-chlorophenyl)benzamidine (69.2 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc

afforded a white solid (92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.22-7.28 (m, 4H), 7.30-7.40 (m, 4H), 7.46 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 7.2 Hz, 2H), 7.88 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.3, 120.1, 123.3, 123.7, 128.6, 128.7, 129.6, 129.7, 130.2, 134.5, 135.6, 137.1, 143.1, 152.4 ppm. HR-MS (ESI) calcd for $C_{19}H_{14}ClN_2$ $[M+H]^+$ 305.0846, found: 305.0852.



1-(3-Nitrophenyl)-2-phenyl-1*H*-benzo[*d*]imidazole (3g)

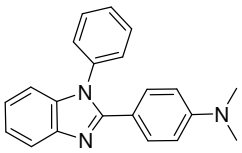
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-(3-nitrophenyl)benzamidine (72.4 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (89% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.25-7.27 (m, 1H), 7.30-7.38 (m, 5H), 7.50 (d, J = 8.0 Hz, 2H), 7.57 (dd, J = 8.0, 1.2 Hz, 1H), 7.65 (t, J = 8.0 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 8.25 (d, J = 2.0 Hz, 1H), 8.30 (d, J = 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 109.9, 120.4, 122.3, 123.3, 123.7, 124.1, 128.7, 129.3, 129.6, 130.0, 130.9, 133.5, 136.5, 138.3, 143.2, 149.1, 152.4 ppm. MS (ESI) m/z: 316.0 $[M+H]^+$. HR-MS (ESI) calcd for $C_{19}H_{14}N_3O_2$ $[M+H]^+$ 316.1086, found: 316.1083.



1-Cyclohexyl-2-phenyl-1*H*-benzo[*d*]imidazole (3h)

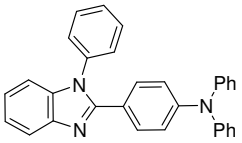
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-cyclohexylbenzamidine (60.69 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc

afforded a white solid (99% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.26-1.38 (m, 3H), 1.75-1.76 (m, 1H), 1.92-1.98 (m, 4H), 2.30-2.38 (m, 2H), 4.32 (m, 1H), 7.24-7.29 (m, 2H), 7.51-7.55 (m, 3H), 7.63-7.65 (m, 3H), 7.81 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 25.4, 26.0, 31.5, 57.1, 112.8, 120.4, 122.1, 122.2, 128.8, 129.6, 129.7, 131.3, 134.1, 143.9, 153.9 ppm. MS (ESI) m/z: 277.1 $[M+H]^+$.



1-Phenyl-2-(4-N,N-dimethylamino-phenyl)-1*H*-benzo[*d*]imidazole (3i)[5]

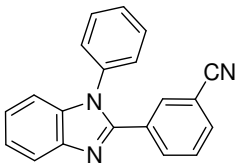
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 4-(dimethylamino)-N-phenylbenzamidine (71.76 mg, 0.30 mmol), $Pd(OAc)_2$ (1.4 mg, 0.00625 mmol), Xantphos (3.7 mg, 0.00625 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (98% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.95 (s, 6H), 6.57 (d, J = 8.8 Hz, 2H), 7.16-7.22 (m, 2H), 7.26-7.29 (m, 1H), 7.33 (d, J = 7.6 Hz, 2H), 7.44-7.53 (m, 5H), 7.83 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.2, 111.1, 111.5, 117.2, 119.2, 122.6, 122.7, 127.7, 128.4, 129.9, 130.6, 137.5, 137.8, 143.3, 151.0, 153.3 ppm. MS (ESI) m/z: 314.1 $[M+H]^+$.



1-Phenyl-2-(4-N,N-diphenylamino-phenyl)-1*H*-benzo[*d*]imidazole (3j)[6]

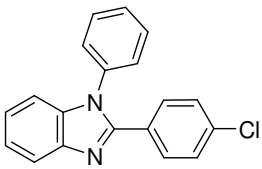
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 4-(diphenylamino)-N-phenylbenzamidine (109.03 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (81%

yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.91 (d, J = 8.8 Hz, 2H), 7.03 (t, J = 7.6 Hz, 2H), 7.08 (d, J = 7.6 Hz, 4H), 7.18 (t, J = 7.0 Hz, 1H), 7.23-7.28 (m, 5H), 7.29-7.34 (m, 1H), 7.35-7.37 (m, 2H), 7.41 (d, J = 8.8 Hz, 2H), 7.46-7.54 (m, 3H), 7.84 (d, J = 8.0 Hz, 1H) ppm. HR-MS (ESI) calcd for $C_{31}H_{24}N_3$ $[M+H]^+$ 438.1970, found: 438.1974.



1-Phenyl-2-(3-cyanophenyl)-1*H*-benzo[*d*]imidazole (3k)[7]

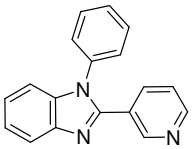
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 3-cyano-N-phenylbenzamidine (66.4 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol), and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (87% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.27 (d, J = 4.0 Hz, 1H), 7.31-7.32 (m, 3H), 7.37-7.45 (m, 2H), 7.52-7.59 (m, 3H), 7.63 (d, J = 7.6 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 7.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.8, 112.9, 118.2, 120.3, 123.6, 124.3, 127.4, 129.36, 129.37, 130.4, 131.6, 132.8, 132.9, 133.4, 136.4, 137.4, 142.9, 149.9 ppm. HR-MS (ESI) calcd for $C_{20}H_{14}N_3[M+H]^+$ 296.1188, found: 296.1190.



1-Phenyl-2-(4-chlorophenyl)-1*H*-benzo[*d*]imidazole (3l)[7]

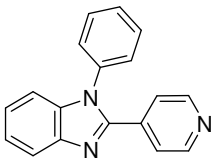
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 4-chloro-N-phenylbenzamidine (69.2 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.28-7.40 (m,

7H), 7.50-7.58 (m, 5H), 7.90 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.6, 120.0, 123.3, 123.7, 127.5, 128.6, 128.8, 128.9, 130.1, 130.8, 135.8, 136.9, 137.4, 143.0, 151.3 ppm. HR-MS (ESI) calcd for $C_{19}H_{14}ClN_2$ $[M+H]^+$ 305.0846, found: 305.0840.



1-Phenyl-2-(pyridin-3-yl)-1*H*-benzo[*d*]imidazole (3m) [2]

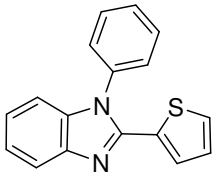
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-phenylnicotinamidine (59.17 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (96% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.27-7.40 (m, 6H), 7.50-7.57 (m, 3H), 7.91-7.95 (m, 2H), 8.58 (dd, J = 4.8, 1.6 Hz, 1H), 8.78 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.7, 120.1, 123.2, 123.4, 124.0, 126.4, 127.5, 129.2, 130.3, 136.5, 136.6, 137.4, 143.1, 149.6, 150.1, 150.3 ppm. MS (ESI) m/z: 272.1 $[M+H]^+$.



1-Phenyl-2-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole (3n)[8]

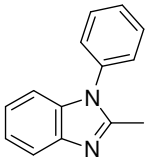
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-phenylisonicotinamidine (59.17 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (94% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.25-7.27 (m, 1H), 7.30-7.40 (m, 4H), 7.45 (d, J = 6.0 Hz, 2H), 7.52-7.59 (m, 3H), 7.91 (d, J = 8.0 Hz, 1H), 8.56 (d, J = 6.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.8, 120.4,

123.2, 123.6, 124.5, 127.4, 129.3, 130.3, 136.4, 137.55, 137.56, 142.9, 149.4, 150.0 ppm. HR-MS (ESI) calcd for $C_{18}H_{14}N_3$ $[M+H]^+$ 272.1188, found: 272.1182.



1-Phenyl-2-(thiophen-2-yl)-1*H*-benzo[*d*]imidazole (3o)[7]

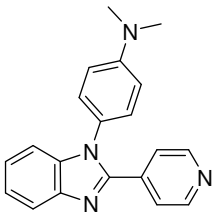
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-phenylthiophene-2-carboxamidine (60.9 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (82% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.85 (dd, J = 3.6, 0.8 Hz, 1H), 6.90 (t, J = 4.8 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 7.21 (t, J = 7.2 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 7.35 (d, J = 5.6 Hz, 1H), 7.42-7.44 (m, 2H), 7.59-7.61 (m, 3H), 7.84 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.3, 119.6, 123.2, 123.5, 127.7, 128.3, 128.48, 128.50, 129.7, 130.3, 132.8, 136.6, 137.8, 143.0, 147.5 ppm. MS (ESI) m/z: 277.0 $[M+H]^+$.



2-Methyl-1-phenyl-1*H*-benzo[*d*]imidazole (3p)[2]

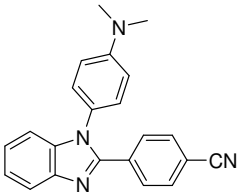
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-phenylacetamidine (40.25 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (99% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.28 (s, 3H), 6.88 (d, J = 8.0 Hz, 1H), 6.94 (t, J = 7.2 Hz, 1H), 7.01 (t, J = 7.2 Hz, 1H), 7.12 (d, J = 7.6 Hz, 2H), 7.28 (d, J = 7.2 Hz, 1H), 7.33 (t, J = 7.2 Hz, 2H), 7.50 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.5, 110.0, 119.1, 122.5, 122.7, 127.2, 128.9,

130.0, 136.2, 136.5, 142.7, 151.6 ppm. MS (ESI) m/z: 209.1 $[M+H]^+$.



1-(4-N,N-Dimethylamino-phenyl)-2-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole (3q)

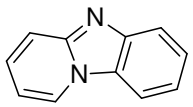
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), N-(4-(dimethylamino)phenyl)isonicotinamidine (72.09 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a white-yellow solid (93% yield). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.06 (s, 6H), 6.78 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 9.0 Hz, 2H), 7.22 (d, J = 8.4 Hz, 1H), 7.28 (t, J = 7.2 Hz, 1H), 7.33 (t, J = 7.8 Hz, 1H), 7.53 (d, J = 6.0 Hz, 2H), 7.88 (d, J = 7.8 Hz, 1H), 8.56 (d, J = 6.0 Hz, 2H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 40.5, 111.1, 112.8, 120.2, 123.2, 123.3, 124.1, 124.5, 128.1, 138.0, 138.4, 142.8, 149.7, 150.0, 150.7 ppm. HR-MS (ESI) calcd for $C_{20}H_{19}N_4[M+H]^+$ 315.1610, found: 315.1616.



1-(4-N,N-Dimethylamino-phenyl)-2-(4-cyanophenyl)-1*H*-benzo[*d*]imidazole (3r)

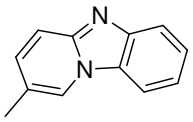
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 4-cyano-N-(4-(dimethylamino)phenyl)benzamidine (79.3 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (91% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.06 (s, 6H), 6.76 (d, J = 8.8 Hz,

2H), 7.12 (d, J = 8.8 Hz, 2H), 7.23-7.36 (m, 3H), 7.59 (d, J = 8.0 Hz, 2H), 7.76 (d, J = 8.0 Hz, 2H), 7.87 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.5, 111.1, 112.7, 112.8, 118.7, 120.1, 123.3, 124.0, 124.6, 128.1, 129.8, 132.1, 134.9, 138.3, 142.9, 150.4, 150.6 ppm. HR-MS (ESI) calcd for $C_{22}H_{19}N_4[M+H]^+$ 339.1610, found: 339.1607.



Pyrido[1,2-*a*]benzimidazole (3s)[9]

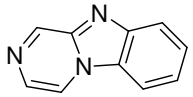
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 2-aminopyridine (28.2 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), K_3PO_4 (106 mg, 0.5 mmol), *t*BuONa (48 mg, 0.5 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/acetone afforded a white solid (86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.82 (t, J = 6.4 Hz, 1H), 7.35-7.42 (m, 2H), 7.51 (t, J = 8.0 Hz, 1H), 7.68 (d, J = 9.2 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 8.43 (d, J = 6.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.4, 110.5, 118.2, 120.1, 121.1, 125.3, 125.8, 128.8, 129.4, 144.6, 148.6 ppm. MS (ESI) m/z: 169.1 $[M+H]^+$.



2-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3t)[9]

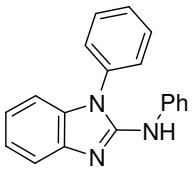
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 5-methyl-2-aminopyridine (32.4 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), K_3PO_4 (106 mg, 0.5 mmol), *t*BuONa (48 mg, 0.5 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.35 (s, 3H), 7.21 (d, J = 9.2 Hz, 1H), 7.28 (t, J = 7.6 Hz, 1H), 7.45 (t, J = 7.2 Hz, 1H), 7.55 (d, J = 9.2 Hz, 1H), 7.78 (d, J = 9.2 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 8.14 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 18.0, 110.2, 117.1, 119.7,

119.8, 120.6, 122.5, 125.2, 128.5, 132.5, 144.5, 147.6 ppm. MS (ESI) m/z: 183.1$[M+H]^+$.



Benzo[4,5]imidazo[1,2-*a*]pyrazine (3u)

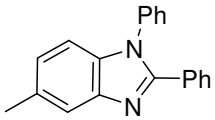
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 2-aminopyrazine (29 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), K_3PO_4 (106 mg, 0.5 mmol), *t*BuONa (48 mg, 0.5 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (87% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.50 (t, J = 7.6 Hz, 1H), 7.63 (t, J = 8.0 Hz, 1H), 7.97 (d, J = 2.8 Hz, 1H), 7.99 (s, 1H), 8.06 (d, J = 8.4 Hz, 1H), 8.36 (d, J = 4.0 Hz, 1H), 9.30 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 111.2, 117.9, 121.6, 123.3, 127.16, 127.20, 127.8, 142.2, 144.3, 145.8 ppm. MS (ESI) m/z: 170.1 $[M+H]^+$.



1-Phenyl-2-phenylamino-1*H*-benzo[*d*]imidazole (3v)[10]

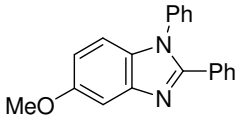
1,2-Dibromobenzene (58.98 mg, 0.25 mmol), 1,3-diphenylguanidine (63.4 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), K_3PO_4 (106 mg, 0.5 mmol), *t*BuONa (48 mg, 0.5 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (84% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.30 (br, 1H), 7.01-7.05 (m, 2H), 7.07 (t, J = 7.6 Hz, 1H), 7.20 (t, J = 7.6 Hz, 1H), 7.33 (t, J = 7.6 Hz, 2H), 7.50 (d, J = 7.2 Hz, 2H), 7.56 (t, J = 7.2 Hz, 1H), 7.64 (d, J = 7.6 Hz, 5H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 108.4, 117.6, 118.3, 121.0, 122.3, 122.6, 127.5, 129.3, 129.4, 130.8, 134.56, 134.61, 139.3, 142.4, 149.1

ppm. MS (ESI) m/z: 286.1 $[M+H]^+$.



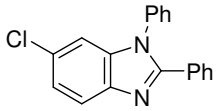
5-Methyl-1,2-diphenyl-1*H*-benzo[*d*]imidazole (4a)[11]

2-Bromo-1-chloro-4-methylbenzene (51.37 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (95% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.52 (s, 3H), 7.08 (d, J = 8.4 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.27-7.36 (m, 5H), 7.43-7.50 (m, 3H), 7.55 (d, J = 7.6 Hz, 2H), 7.67 (s, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 21.7, 110.1, 119.7, 124.9, 127.5, 128.4, 128.5, 129.4, 129.6, 129.9, 130.2, 132.8, 135.5, 137.3, 143.5, 152.5 ppm. HR-MS (ESI) calcd for $C_{20}H_{17}N_2$ $[M+H]^+$ 285.1392, found: 285.1386.



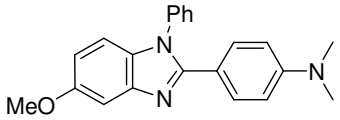
5-Methoxy-1,2-diphenyl-1*H*-benzo[*d*]imidazole (4b)

2-Bromo-1-chloro-4-methoxybenzene (55.37 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(dba)_2$ (7.2 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (97% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.90 (s, 3H), 6.89 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.12 (d, J = 8.8 Hz, 1H), 7.27-7.36 (m, 6H), 7.44-7.50 (m, 3H), 7.54 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 56.0, 102.0, 111.0, 113.5, 126.9, 127.5, 128.4, 128.6, 129.5, 130.0, 130.2, 132.1, 137.2, 143.9, 152.7, 156.9 ppm. HR-MS (ESI) calcd for $C_{20}H_{17}N_2O$ $[M+H]^+$ 301.1341, found: 301.1335.



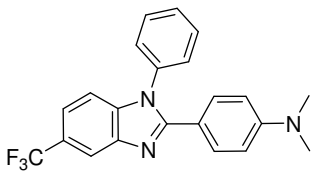
6-Chloro-1,2-diphenyl-1*H*-benzo[*d*]imidazole (4c)

1-Bromo-2,4-dichlorobenzene (56.5 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (81% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.23 (s, 1H), 7.29-7.38 (m, 6H), 7.49-7.58 (m, 5H), 7.77 (d, J = 8.4 Hz, 1H) ppm. HR-MS (ESI) calcd for $C_{19}H_{14}ClN_2[M+H]^+$ 305.0846, found: 305.0855.



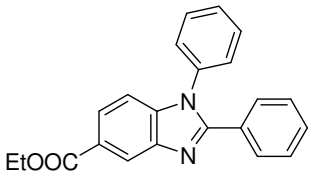
1-Phenyl-2-(4-N,N-dimethylamino-phenyl)-1*H*-5-methoxy-benzo[*d*]imidazole (4d)

2-Bromo-1-chloro-4-methoxybenzene (55.37 mg, 0.25 mmol), 4-(dimethylamino)-N-phenylbenzamidine (71.76 mg, 0.30 mmol), $Pd(dba)_2$ (7.2 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (94% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.04 (s, 6H), 3.88 (s, 3H), 6.75 (d, J = 8.8 Hz, 2H), 6.91 (dd, J = 8.8 Hz, 2.0 Hz, 1H), 7.08-7.13 (m, 3H), 7.33 (d, J = 2.4 Hz, 1H), 7.49 (d, J = 5.6 Hz, 2H), 8.54 (d, J = 5.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ =40.3, 55.7, 101.5, 111.3, 112.6, 114.4, 122.8, 124.4, 127.8, 130.8, 133.0, 137.8, 143.3, 149.4, 149.8, 150.5, 156.8 ppm. MS (ESI) m/z: 344.1 $[M+H]^+$.



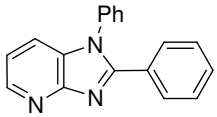
1-Phenyl-2-(4-N,N-dimethylamino-phenyl)-1*H*-5-trifluoromethyl-benzo[*d*]imidazole (4e)

2-Bromo-1-chloro-4-(trifluoromethyl)benzene (64.86 mg, 0.25 mmol), 4-(dimethylamino)-N-phenylbenzamidine (71.76 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (96% yield). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 2.97 (s, 6H), 6.57 (d, J = 9.0 Hz, 2H), 7.21 (d, J = 8.4 Hz, 1H), 7.33 (d, J = 7.2 Hz, 2H), 7.42-7.44 (m, 3H), 7.49-7.56 (m, 3H), 8.10 (s, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 40.1, 110.4, 111.6, 116.2, 116.8, 119.4, 124.1, 125.1, 125.3, 125.9, 127.6, 129.0, 130.2, 130.7, 137.2, 139.4, 142.8, 151.3, 155.3 ppm. HR-MS (ESI) calcd for $C_{22}H_{19}F_3N_3$ $[M+H]^+$ 382.1531, found: 382.1524.



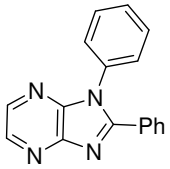
Ethyl 1,2-diphenyl-1*H*-benzo[*d*]imidazole-5-carboxylate (4f)

Ethyl 3-bromo-4-chlorobenzoate (66 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (90% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.37 (t, J = 7.2 Hz, 3H), 4.35 (q, J = 6.8 Hz, 2H), 7.29-7.40 (m, 5H), 7.49-7.59 (m, 5H), 7.87 (d, J = 8.4 Hz, 1H), 7.96 (s, 1H), 8.05 (d, J = 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.5, 61.1, 112.9, 119.5, 124.6, 125.7, 127.6, 128.5, 129.1, 129.5, 129.7, 130.1, 130.2, 136.6, 137.2, 146.5, 155.1, 167.1 ppm. HR-MS (ESI) calcd for $C_{22}H_{19}N_2O_2$ $[M+H]^+$ 343.1447, found: 343.1439.



1,2-Diphenyl-1*H*-imidazo[4,5-*b*]pyridine (4g)[12]

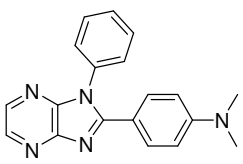
2-Bromo-3-chloropyridine (48.11 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a white solid (92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29 (m, 3H), 7.37 (t, *J* = 7.2 Hz, 3H), 7.45-7.52 (m, 3H), 7.58 (d, *J* = 7.6 Hz, 2H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.39 (d, *J* = 4.0 Hz, 1H) ppm. MS (ESI) m/z: 272.1 $[M+H]^+$.



1,2-Diphenyl-1*H*-imidazo[4,5-*b*]pyrazine (4h)

2,3-Dichloropyrazine (37.25 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.34-7.39 (m, 4H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 6.8 Hz, 3H), 7.68 (d, *J* = 8.0 Hz, 2H), 8.31 (d, *J* = 2.0 Hz, 1H), 8.59 (d, *J* = 2.4 Hz, 1H) ppm. HR-MS (ESI) calcd for $C_{17}H_{13}N_4$ $[M+H]^+$ 273.1140, found: 273.1144.

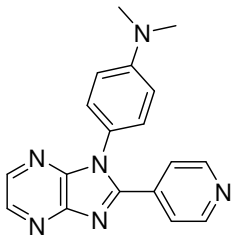
Exact Mass:



1-Phenyl-2-(4-N,N-dimethylamino-phenyl)-1*H*-imidazo[4,5-*b*]pyrazine (4i)

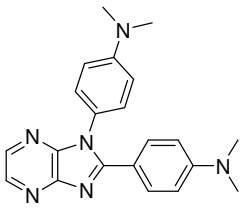
2,3-Dichloropyrazine (37.25 mg, 0.25 mmol),

4-(dimethylamino)-N-phenylbenzamidine (71.76 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (88% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.99 (s, 6H), 6.56 (d, *J* = 9.2 Hz, 2H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.49-7.59 (m, 5H), 8.17 (d, *J* = 2.4 Hz, 1H), 8.46 (d, *J* = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.1, 111.3, 115.3, 127.8, 129.2, 130.0, 131.3, 135.7, 137.4, 140.2, 143.3, 149.7, 151.9, 157.4 ppm. HR-MS (ESI) calcd for $C_{19}H_{18}N_5[M+H]^+$ 316.1562, found: 317.1558.



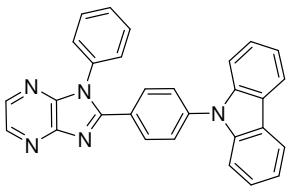
1-(4-N,N-Dimethylamino-phenyl)-2-(pyridin-4-yl)-1*H*-imidazo[4,5-*b*]pyrazine (4j)

2,3-Dichloropyrazine (37.25 mg, 0.25 mmol), N-(4-(dimethylamino)phenyl)isonicotinamidine (72.1 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (90% yield). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.06 (s, 6H), 6.80 (d, *J* = 9.0 Hz, 2H), 7.18 (d, *J* = 9.0 Hz, 2H), 7.65 (d, *J* = 6.0 Hz, 2H), 8.36 (d, *J* = 2.4 Hz, 1H), 8.61 (d, *J* = 2.4 Hz, 1H), 8.64 (d, *J* = 6.0 Hz, 2H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 40.5, 112.9, 122.0, 123.4, 128.2, 136.8, 139.9, 141.4, 143.3, 148.6, 150.3, 151,2, 153.5 ppm. HR-MS (ESI) calcd for $C_{18}H_{17}N_6[M+H]^+$ 317.1515, found: 317.1512.



1,2-Di(4-N,N-dimethylamino-phenyl)-1*H*-imidazo[4,5-*b*]pyrazine (4k)

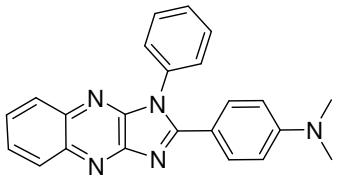
2,3-Dichloropyrazine (37.25 mg, 0.25 mmol), 4-(dimethylamino)-N-(4-(dimethylamino)phenyl)benzamidine (84.714 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (79% yield). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 2.99 (s, 6H), 3.03 (s, 6H), 6.59 (d, J = 9.0 Hz, 2H), 6.80 (d, J = 9.0 Hz, 2H), 7.21 (d, J = 9.0 Hz, 2H), 7.70 (d, J = 7.8 Hz, 2H), 8.15 (d, J = 3.0 Hz, 1H), 8.42 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 40.1, 40.5, 111.3, 113.0, 115.9, 123.8, 128.4, 131.2, 137.3, 139.8, 143.9, 149.7, 150.7, 151.8, 157.5 ppm. HR-MS (ESI) calcd for $C_{21}H_{23}N_6[M+H]^+$ 359.1984, found: 359.1992.



9-(4-(1-Phenyl-1*H*-imidazo[4,5-*b*]pyrazin-2-yl)phenyl)-9*H*-carbazole (4l)

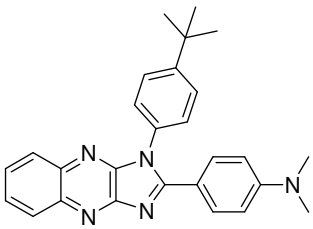
2,3-Dichloropyrazine (37.25 mg, 0.25 mmol), 4-(9H-carbazol-9-yl)-N-phenylbenzamidine (108.4 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (82% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29 (t, J = 7.6 Hz, 2H), 7.40-7.50 (m, 6H), 7.57-7.65 (m, 5H), 7.94 (d, J = 8.4 Hz, 2H), 8.12 (d, J = 8.0 Hz, 2H), 8.35 (d, J = 2.8 Hz, 1H), 8.62 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 109.9, 120.6, 120.7, 123.9, 126.3, 126.7, 127.3, 127.8, 129.7, 130.3, 131.5, 134.8, 139.1,

140.3, 140.4, 141.2, 142.9, 149.1, 155.5 ppm. HR-MS (ESI) calcd for $C_{29}H_{20}N_5$ $[M+H]^+$438.1719, found:438.1722.



1-Phenyl-2-(4-N,N-dimethylamino-phenyl)-1*H*-imidazo[4,5-*b*]quinoxaline (**4m**)

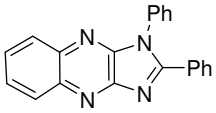
2,3-Dibromoquinoxaline (72 mg, 0.25 mmol), N-phenyl-4-(dimethylamino)benzamidine (73.9 mg, 0.30 mmol), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol), Xantphos (14.6 mg, 0.025 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (85% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.03 (s, 6H), 6.59 (d, J = 9.2 Hz, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.56-7.64 (m, 4H), 7.68 (d, J = 9.2 Hz, 3H), 8.02 (d, J = 8.0 Hz, 1H), 8.22 (d, J = 8.0 Hz, 1H) ppm. HR-MS (ESI) calcd for $C_{23}H_{20}N_5$ $[M+H]^+$ 366.1719, found: 366.1721.



1-(4-*Tert*-butylphenyl)-2-(4-N,N-dimethylamino-phenyl)-1*H*-imidazo[4,5-*b*]quino xaline (4n)

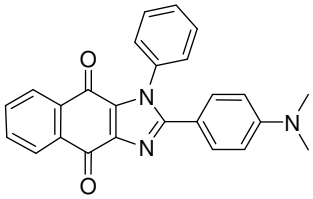
2,3-Dibromoquinoxaline (72 mg, 0.25 mmol), N-(4-tert-butylphenyl)-4-(dimethylamino)benzamidine (88.6 mg, 0.30 mmol), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol), Xantphos (14.6 mg, 0.025 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (88% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.42 (s, 9H), 3.03 (s,

6H), 6.59 (d, J = 8.8 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.62 (t, J = 9.2 Hz, 2H), 7.69 (d, J = 8.8 Hz, 2H), 8.03 (d, J = 8.0 Hz, 1H), 8.22 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.4, 34.9, 40.0, 111.1, 115.2, 126.9, 127.2, 127.3, 127.5, 128.2, 129.3, 131.8, 133.0, 139.8, 141.8, 144.6, 150.5, 152.1, 152.3, 162.6 ppm. HR-MS (ESI) calcd for $C_{27}H_{28}N_5[M+H]^+$ 422.2345, found: 422.2339.



1,2-Diphenyl-1*H*-imidazo[4,5-*b*]quinoxaline (4o)

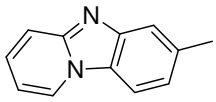
2,3-Dichloroquinoxaline (49.75 mg, 0.25 mmol), N-phenylbenzamidine (59 mg, 0.30 mmol), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol), Xantphos (14.6 mg, 0.025 mmol), 4 Å sieve (100 mg), *t*BuONa (96 mg, 1.0 mmol) and toluene (2 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a yellow solid (81% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37 (t, J = 7.6 Hz, 2H), 7.45-7.50 (m, 3H), 7.52-7.59 (m, 3H), 7.66-7.74 (m, 2H), 7.77 (d, J = 7.6 Hz, 2H), 8.08 (d, J = 8.0 Hz, 1H), 8.29 (d, J = 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 127.9, 128.0, 128.4, 128.5, 128.7, 128.9, 129.3, 129.8, 130.0, 130.4, 131.7, 135.1, 140.4, 142.1, 143.8, 149.9, 161.9 ppm. HR-MS (ESI) calcd for $C_{21}H_{15}N_4$ $[M+H]^+$ 323.1297, found: 323.1300.



2-(4-(Dimethylamino)phenyl)-1-phenyl-1*H*-naphtho[2,3-*d*]imidazole-4,9-dione (4p)[13]

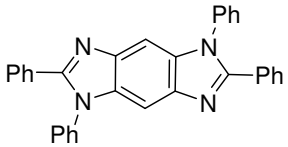
2,3-Dichloronaphthalene-1,4-dione (56.8 mg, 0.25 mmol), 4-(dimethylamino)-N-phenylbenzamidine (71.76 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), Cs_2CO_3 (324

mg, 1.0 mmol) and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (91% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.95 (s, 6H), 6.50 (d, J = 8.8 Hz, 2H), 7.39-7.42 (m, 4H), 7.52-7.59 (m, 3H), 7.65 (m, 2H), 8.00 (dd, J = 7.2, 1.2 Hz, 1H), 8.26 (dd, J = 7.2, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.1, 111.2, 114.5, 126.5, 127.0, 127.8, 129.7, 129.8, 130.7, 132.9, 133.5, 133.6, 133.6, 136.9, 144.1, 151.4, 154.9, 175.1, 179.8 ppm. HR-MS (ESI) calcd for $C_{25}H_{20}N_3O_2[M+H]^+$ 394.1556, found: 394.1559.



7-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (4q)[9]

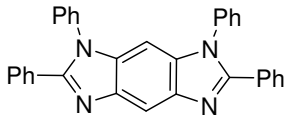
2-Bromo-1-chloro-4-methylbenzene (51.37 mg, 0.25 mmol), 2-aminopyridine (28.2 mg, 0.30 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), sieve (100 mg), K_3PO_4 (106 mg, 0.5 mmol), *t*BuONa (48 mg, 0.5 mmol) and toluene (1 mL). Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (91% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.51 (s, 3H), 6.95 (t, J = 6.8 Hz, 1H), 7.18 (d, J = 8.4 Hz, 1H), 7.50 (t, J = 8.6 Hz, 1H), 7.60 (s, 1H), 7.62 (d, J = 9.2 Hz, 1H), 8.16 (d, J = 8.4 Hz, 1H), 9.02 (d, J = 6.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 22.0, 110.5, 111.9, 117.3, 118.9, 122.6, 127.2, 127.4, 130.2, 135.2, 144.9, 148.3 ppm. MS (ESI) m/z: 183.0$[M+H]^+$.



1,2,5,6-Tetraphenyl-1,5-dihydrobenzo[1,2-*d*:4,5-*d'*]diimidazole (5a)[14]

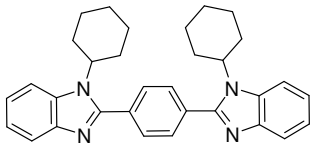
1,4-Dibromo-2,5-diiodobenzene (122 mg, 0.25 mmol), *N*-phenylbenzamidine (118 mg, 0.60 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (192 mg, 2.0 mmol) and toluene (2 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc

afforded a white solid (88% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.28-7.35 (m, 6H), 7.38 (d, J = 6.8 Hz, 4H), 7.47-7.55 (m, 6H), 7.60 (d, J = 6.8 Hz, 4H), 7.67 (s, 2H) ppm. HR-MS (ESI) calcd for $C_{32}H_{23}N_4[M+H]^+$463.1923, found: 463.1922.



1,2,6,7-Tetraphenyl-1,7-dihydrobenzo[1,2-*d*:4,5-*d'*]diimidazole (5b)[15]

1,5-Dibromo-2,4-diiodobenzene (122 mg, 0.25 mmol), *N*-phenylbenzamidine (118 mg, 0.60 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), Xantphos (7.3 mg, 0.0125 mmol), 4 Å sieve (100 mg), *t*BuONa (192 mg, 2.0 mmol), and toluene (1 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/EtOAc afforded a white solid (85% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.95 (s, 1H), 7.28-7.36 (m, 10H), 7.41-7.49 (m, 6H), 7.55 (d, J = 7.6 Hz, 4H), 8.36 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 90.2, 109.4, 127.7, 128.4, 128.6, 129.5, 129.6, 130.1, 130.2, 135.9, 137.5, 140.8, 153.3 ppm. HR-MS (ESI) calcd for $C_{32}H_{23}N_4[M+H]^+$463.1923, found: 463.1920.



1-Cyclohexyl-2-(4-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)-1*H*-benzo[*d*]imidazole (6a)

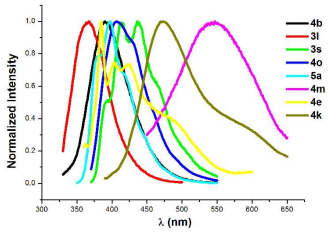
1,2-Dibromobenzene (141.54 mg, 0.6 mmol), N^1,N^4-dicyclohexylterephthalamidine (81.62 mg, 0.25 mmol), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol), Xantphos (14.6 mg, 0.025 mmol), 4 Å sieve (100 mg), *t*BuONa (192 mg, 2.0 mmol) and toluene (2 mL) at 140 ºC for 24 h. Purification via silica gel column chromatography using petroleum ether/CH_2Cl_2/EtOAc afforded a white solid (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.33-1.41 (m, 6H), 1.79-1.81 (m, 2H), 1.93-2.07 (m, 8H), 2.32-2.41 (m, 4H), 4.38 (t, J = 12.0 Hz, 2H), 7.29-7.31 (m, 4H), 7.69-7.71 (m, 2H), 7.80 (s, 4H), 7.83-7.85 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 25.5, 26.0, 31.7, 57.4, 112.9, 120.5, 122.3,

122.6, 130.0, 132.6, 134.1, 143.9, 153.1 ppm. HR-MS (ESI) calcd for $C_{32}H_{35}N_4[M+H]^+$ 475.2862, found: 475.2858.

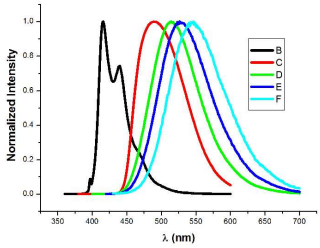
VII. Absorption and Fluorescence emission spectroscopy

***Table S2*:** The UV absorption and fluorescence emission maximum of selected benzimidazoles in CH_3CN.

Compd.	$\lambda_{abs}/\lambda_{em}$ [nm]	Stokes shift [nm]	Compd.	$\lambda_{abs}/\lambda_{em}$ [nm]	Stokes shift [nm]
4b	268/391	123	**4k**	371/472	101
4o	348/409	61	**4j**	309/405	96
3l	295/367	72	**4e**	332/406	74
3j	339/444	105	**3q**	299/556	257
5a	330/397	67	**3i**	325/397	72
4i	371/477	106	**3r**	308/586	278
4m	411/528	117	**4n**	411/529	118
4l	339/490	151	**3s**	344/414	70



Figures S1. The fluorescent emission spectra of selected benzimidazoles in CH_3CN, excited at the absorption maximum (Signal intensities have been normalized).



Figures S2. The fluorescent emissions spectra of **4m** in different solvents, excited at the excitation maximum (Signal intensities have been normalized). From left to right: hexane, CH_2Cl_2, acetone, CH_3CN, and DMSO. Excitation and emission slit widths were 1.0 nm and 1.0 nm, respectively.

VIII. Cell culture experiments and imaging of living-cell

The human hepatocellular carcinoma cells (SMMC-7721) and human lung adenocarcinoma epithelial cells (A549) lines were purchased from American Type Culture Collection. One day before imaging, cells were seeded in 8 tissue culture wells. Then cells were cultured following ATCC protocols and maintained at 37 ºC, 5% CO_2 atmosphere in Dublecco's Minimum Essential Medium (DMEM) medium (containing 1% dimethylsulfoxide) supplemented with 10% FBS, 2 mM L-glutamine, 100 units/mL of penicillin, and 100 mg/mL of streptomycin overnight. For imaging experiments, live cells were coincubated with donor-acceptor 1,2-disubstituted (hetero)aryl fused imidazoles (20 μM) in DMEM without PBS for 40 min at 37 ºC. The cells were then washed twice with culture medium. Fluorescence images were observed with a Fluorescence Inverted Microscope (IX71, OLYMPUS) by excitation of SMMC-7721 and A549 cells with UV-light (300-450 nm) and photographed by using Spot Flex. Worthy of note is that there were not obvious cell necrosis when the live cells were coincubated with 1,2-disubstituted (hetero)aryl fused imidazoles. It implied that these compounds exhibited relatively low toxicity to cultured cells.

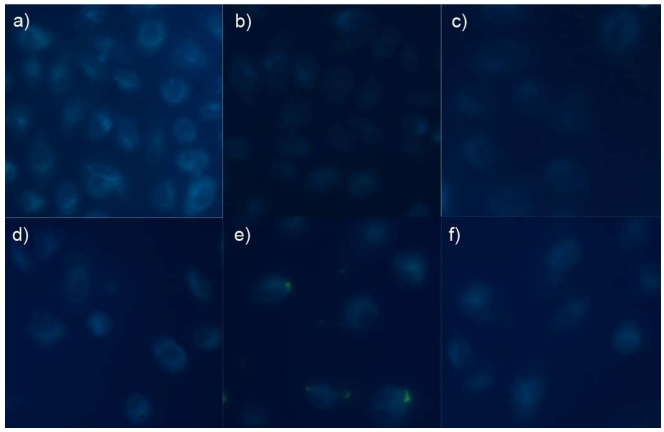


Figure S3. a) Fluorescence image of SMMC-7721 cells incubated with **4m** (20 μM). b) Fluorescence image of SMMC-7721 cells incubated with **4n** (20 μM). c) Fluorescence image of SMMC-7721 cells incubated with **3r** (20 μM). d) Fluorescence image of A549 cells incubated with **4m** (20 μM). e) Fluorescence image of A549 cells incubated with **4n** (20 μM). f) Fluorescence image of A549 cells incubated with **4i** (20 μM).

IX. References

(1) (a) Takahashi, F.; Terasaka, T.; Morita, M.; Konishi, N.; Nakamura, K. US

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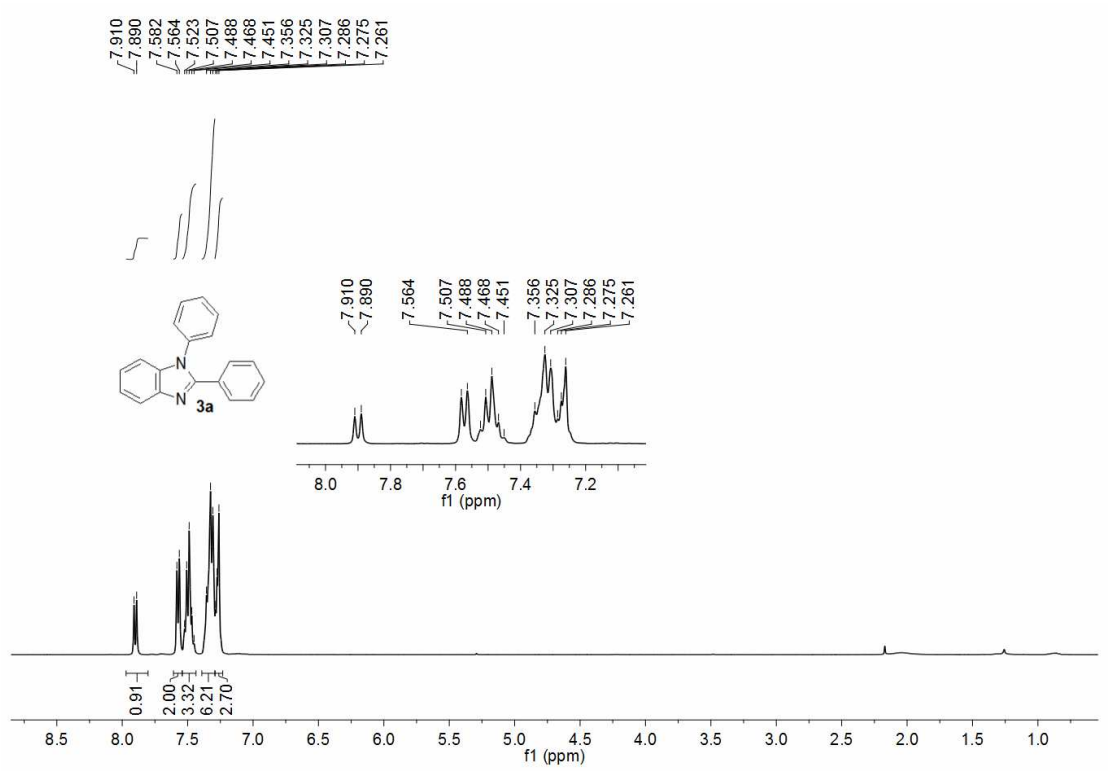
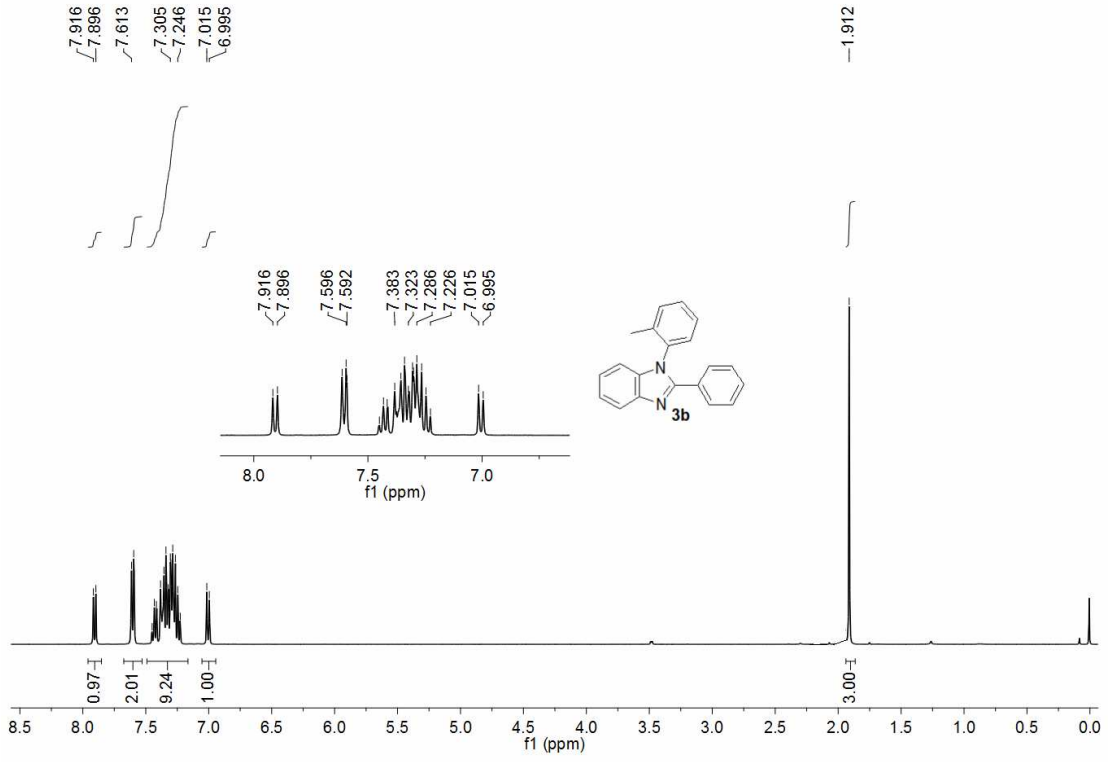
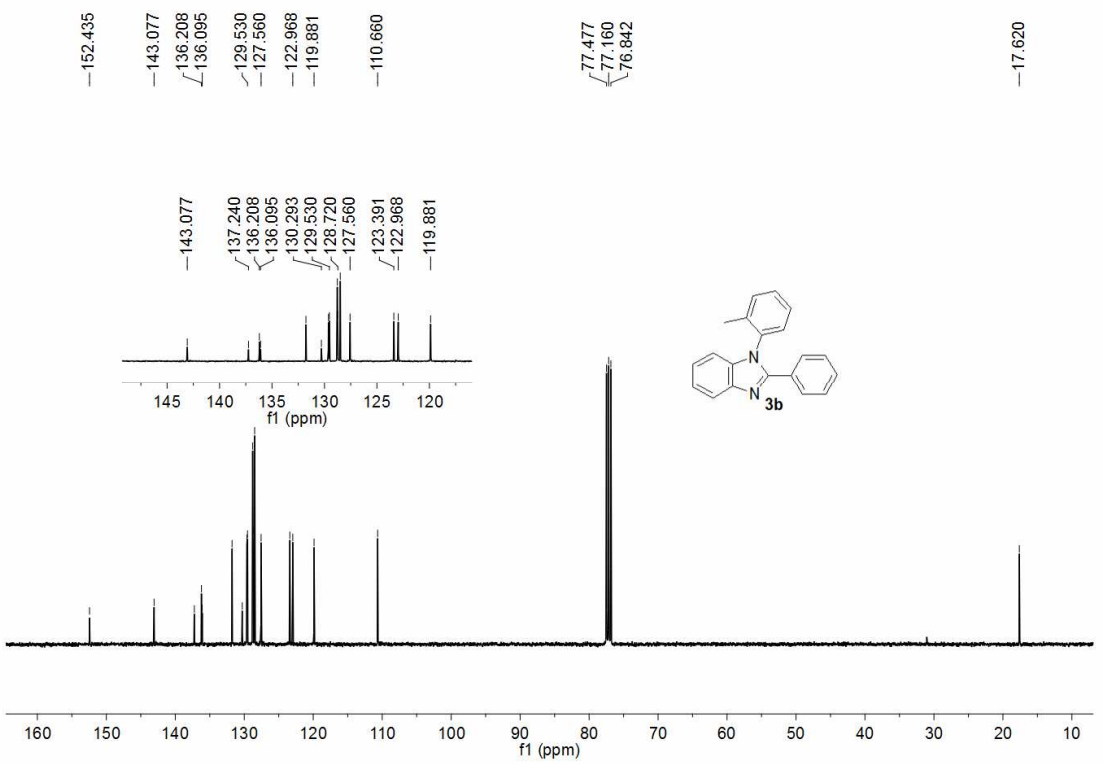
X. Copies of ^{1}H NMR and ^{13}C NMR spectra



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17.620
143.077
137.240
136.208
136.095
130.293
129.530
128.720
127.560
123.391
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119.881
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f1 (ppm)
3b
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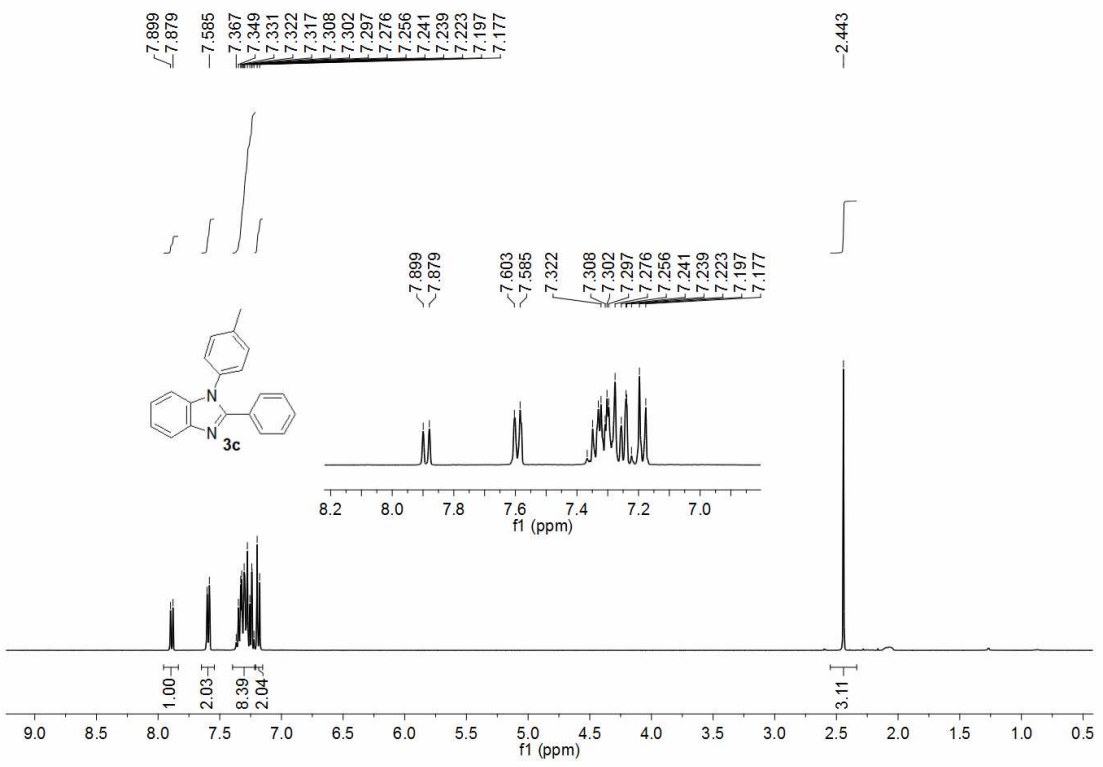
f1 (ppm)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7.308
7.302
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7.197
7.177
3c
8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
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2.03
8.39
2.04
3.11
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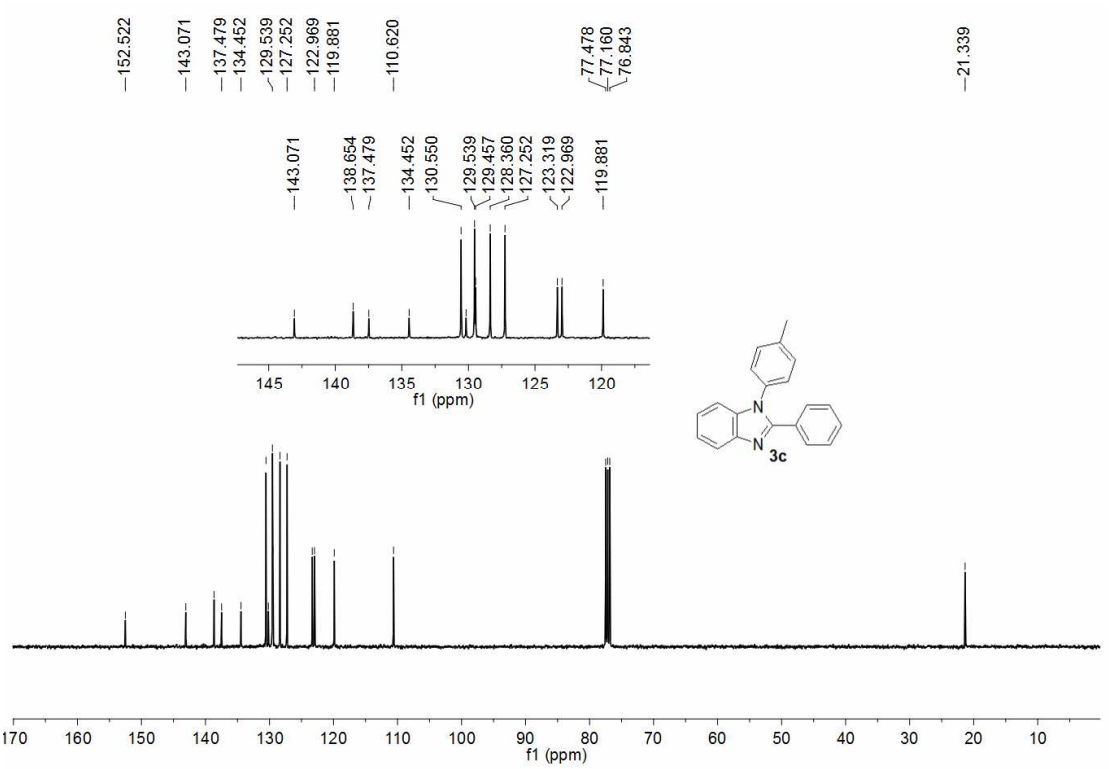
f1 (ppm)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145 140 135 130 125 120
f1 (ppm)
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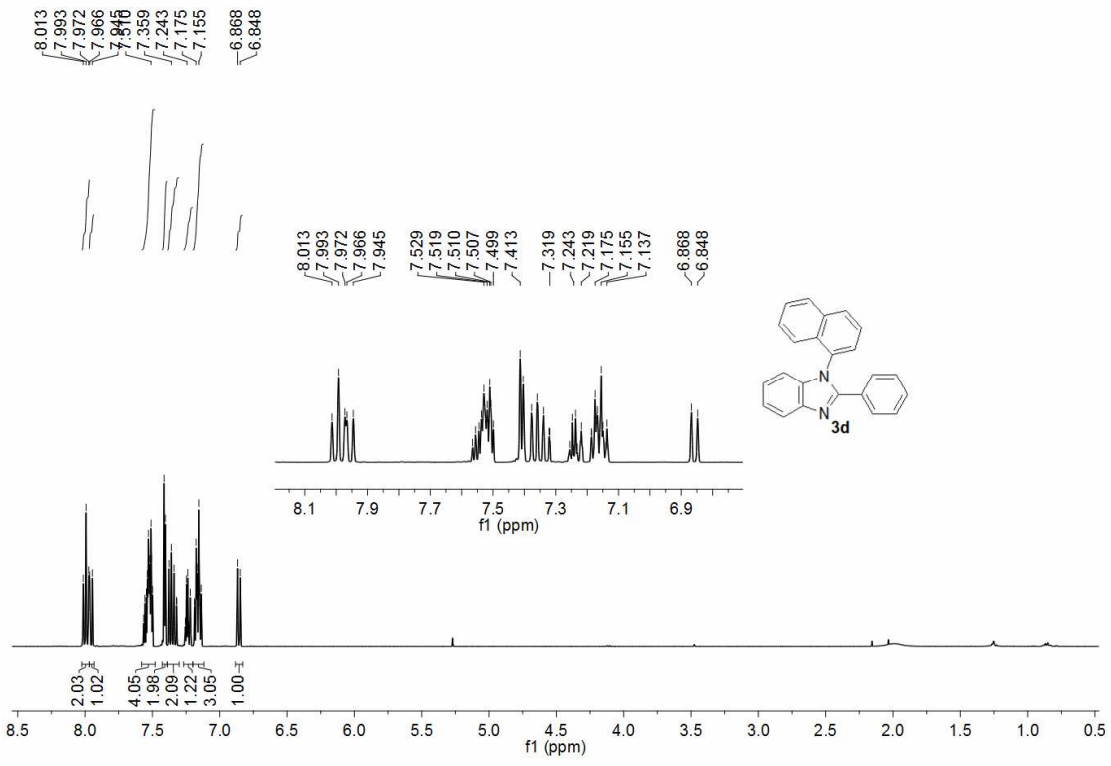
f1 (ppm)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7.507
7.499
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7.319
7.243
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7.137
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6.848
8.1 7.9 7.7 7.5 7.3 7.1 6.9
f1 (ppm)
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1.22
3.05
1.00
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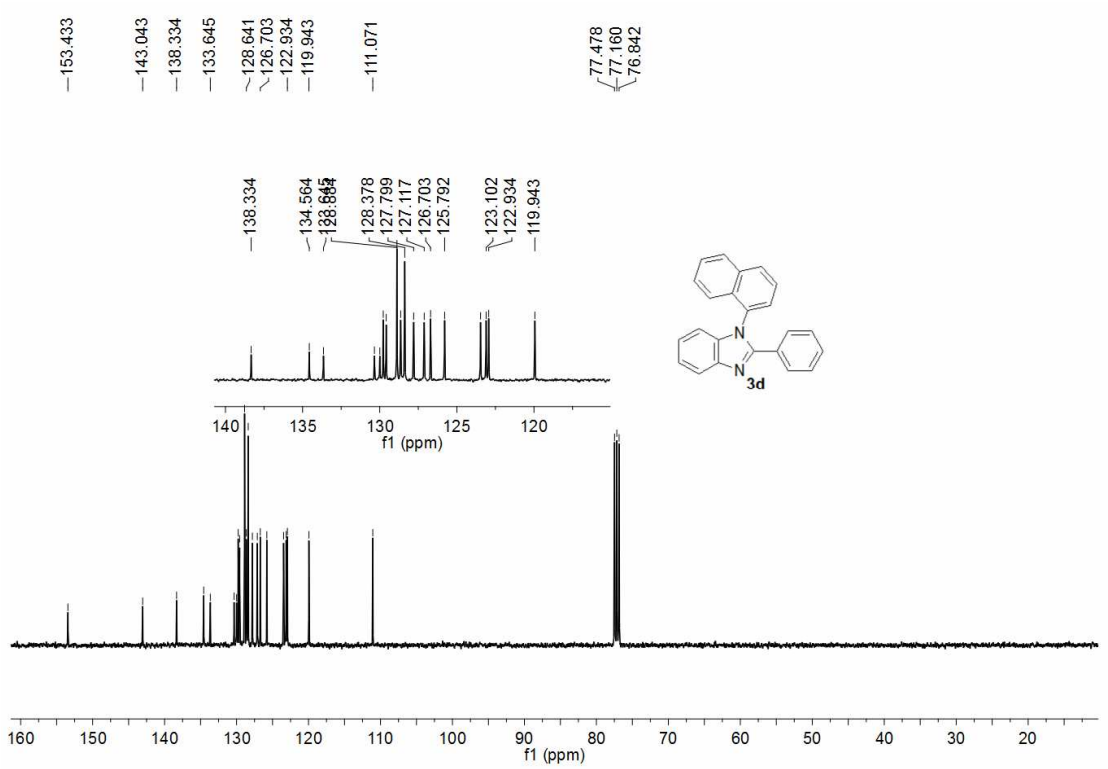
f1 (ppm)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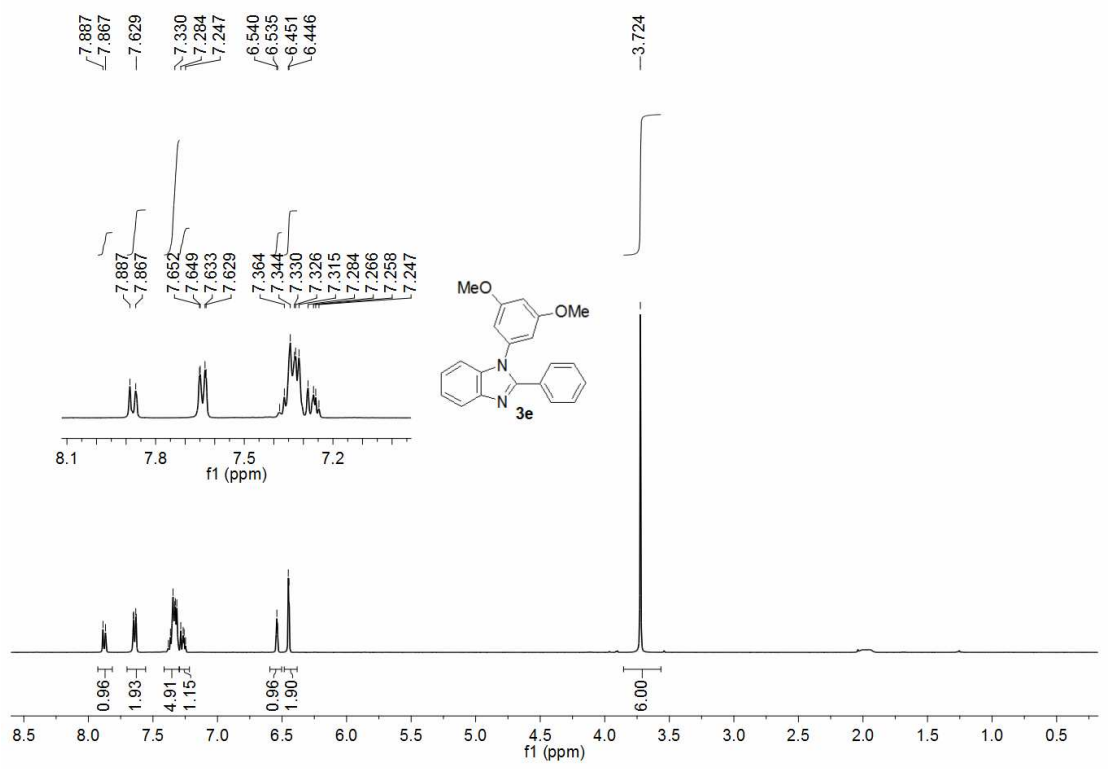
3d
f1 (ppm)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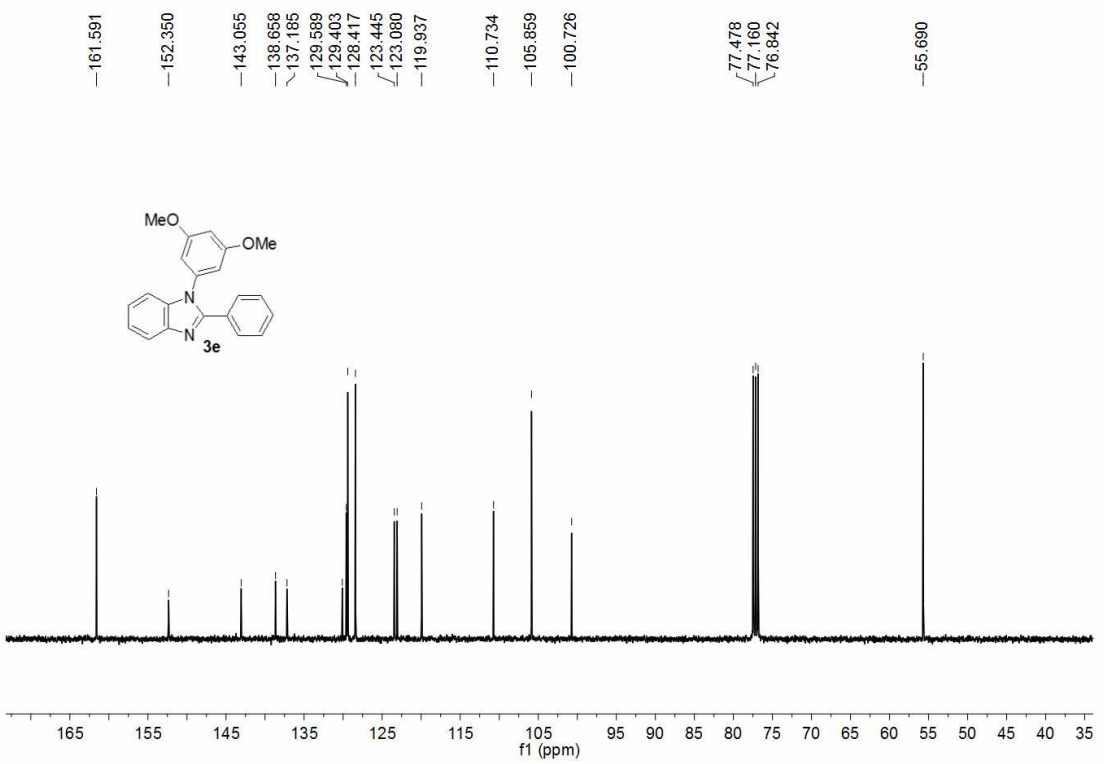
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MeO
OMe
N
N
3e
165
155
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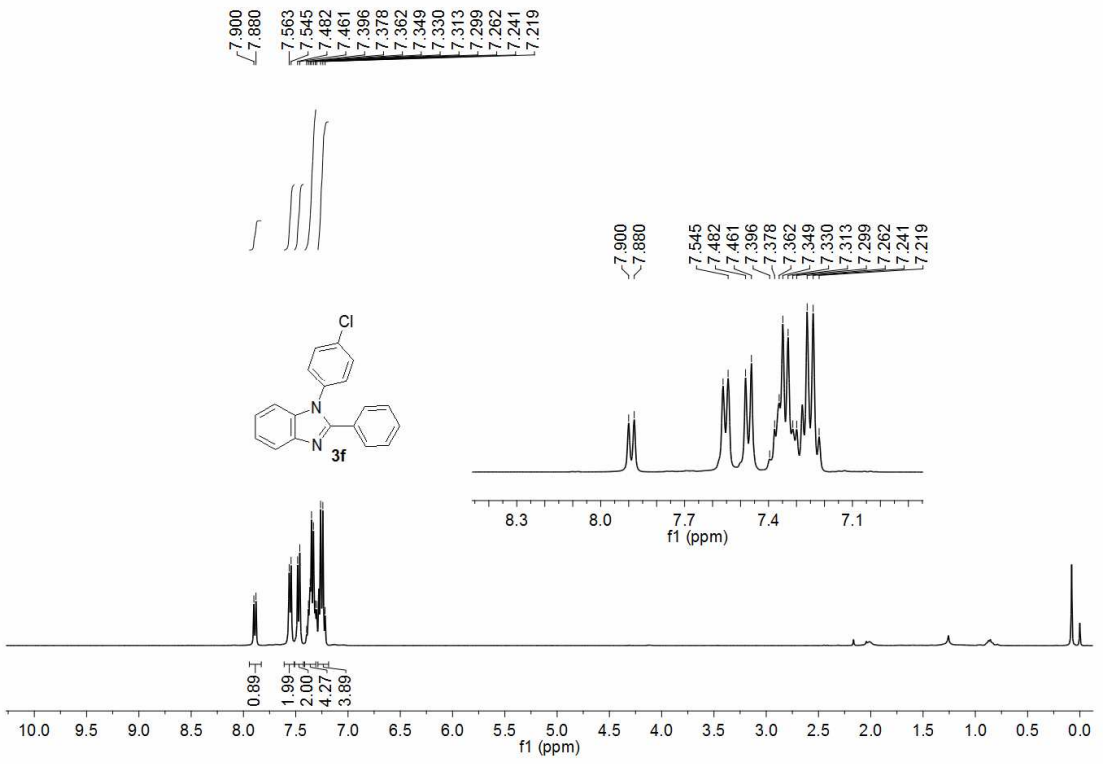
f1 (ppm)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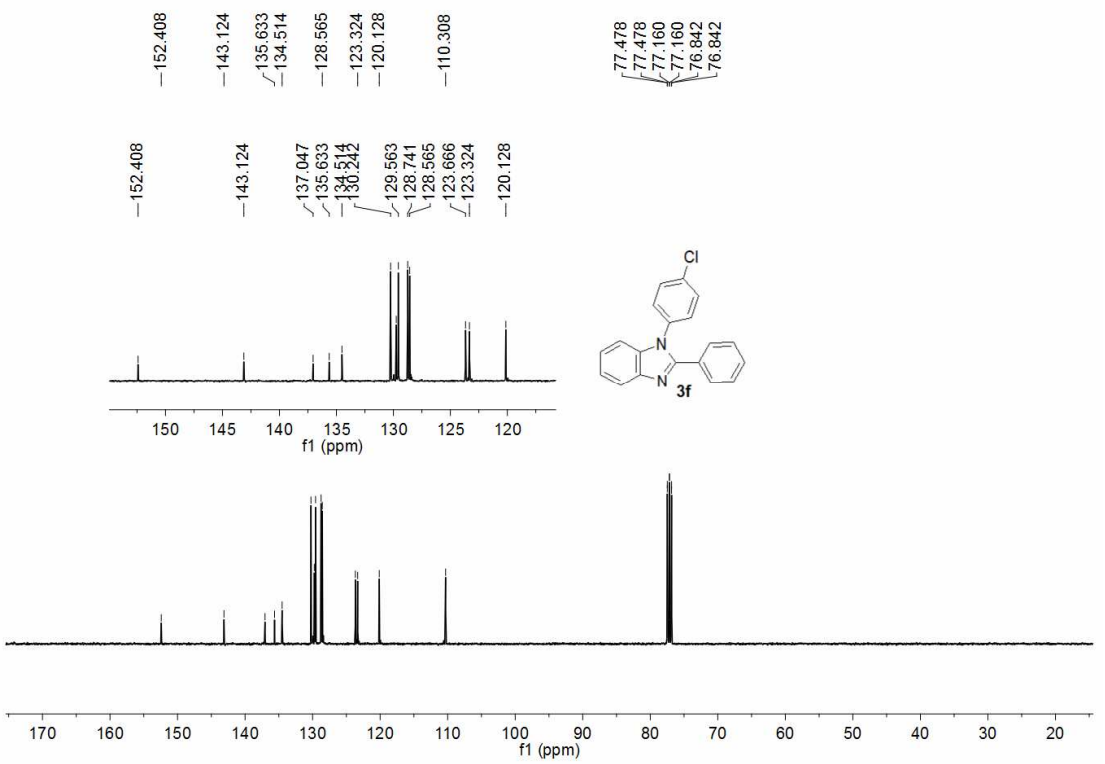
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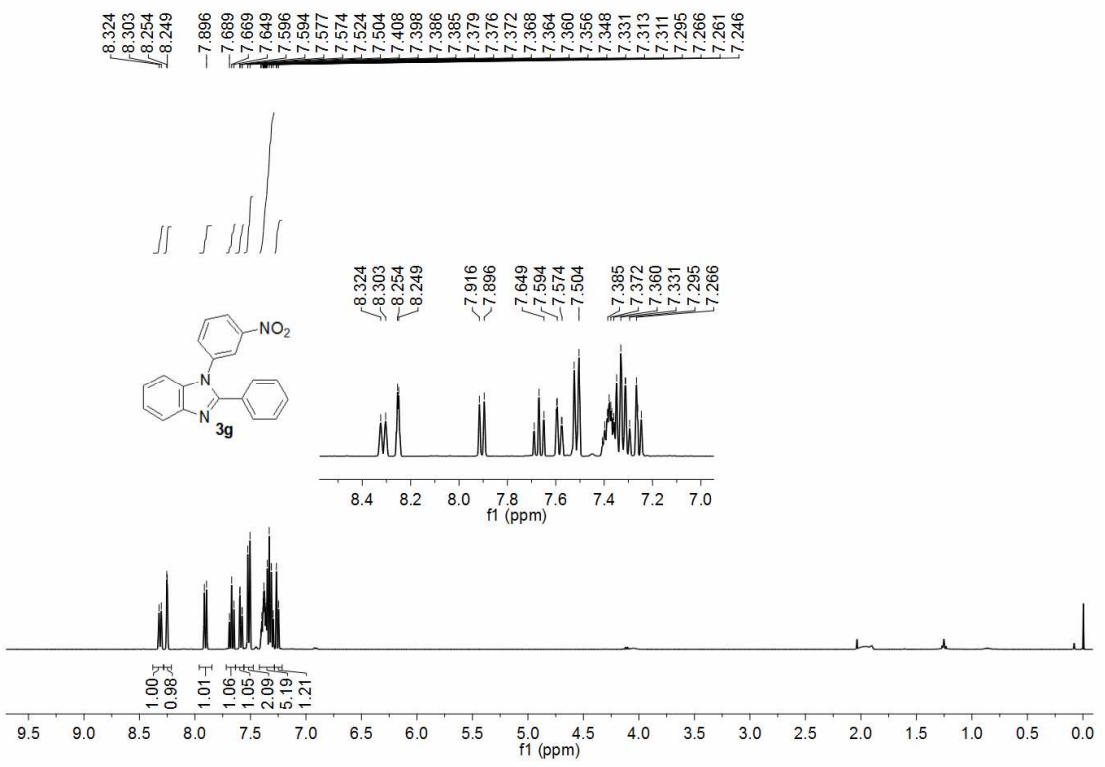
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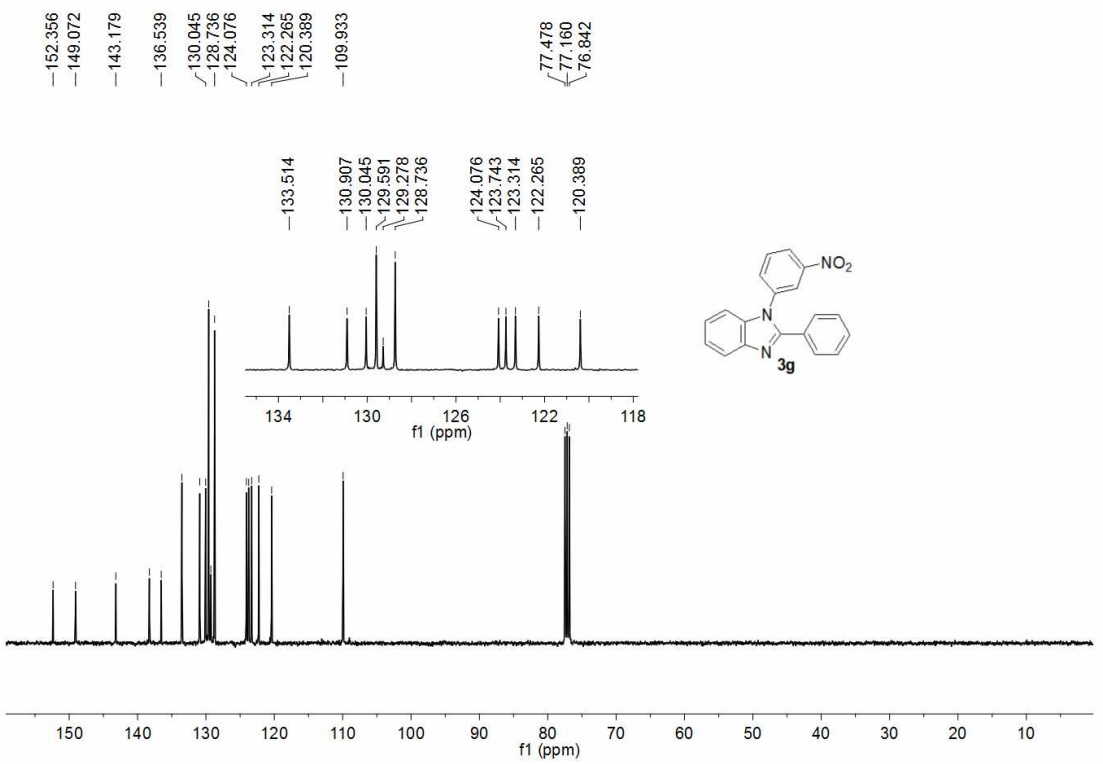
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50
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20
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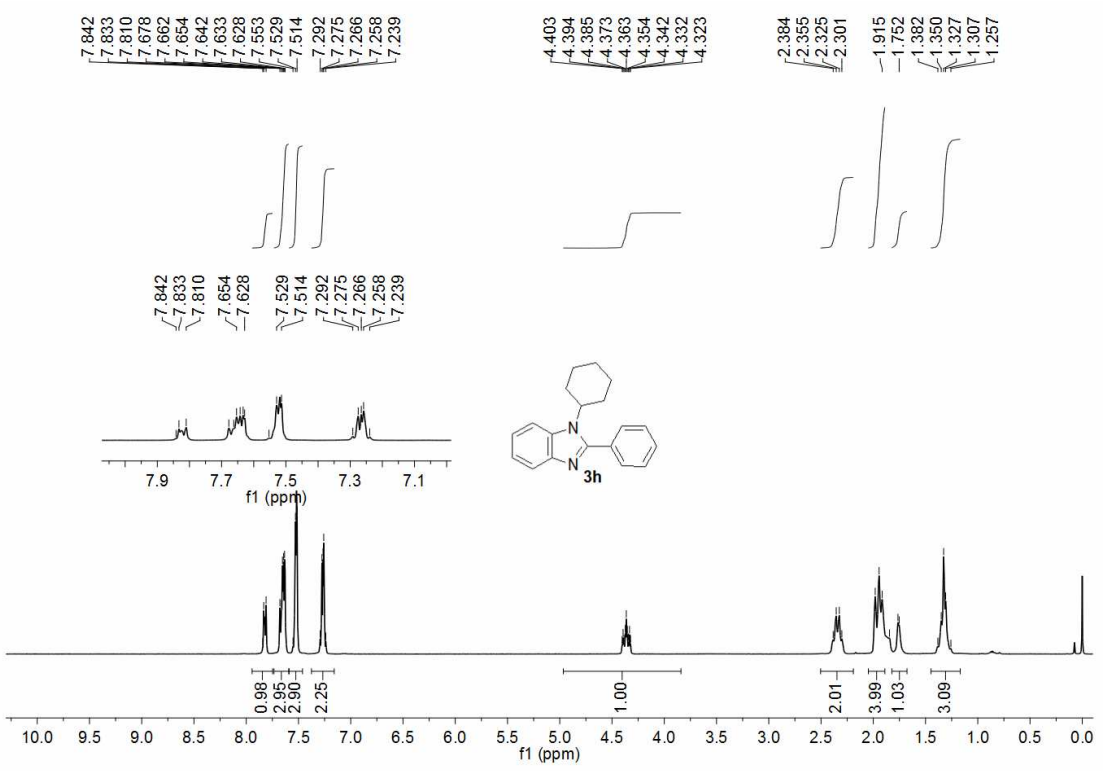
f1 (ppm)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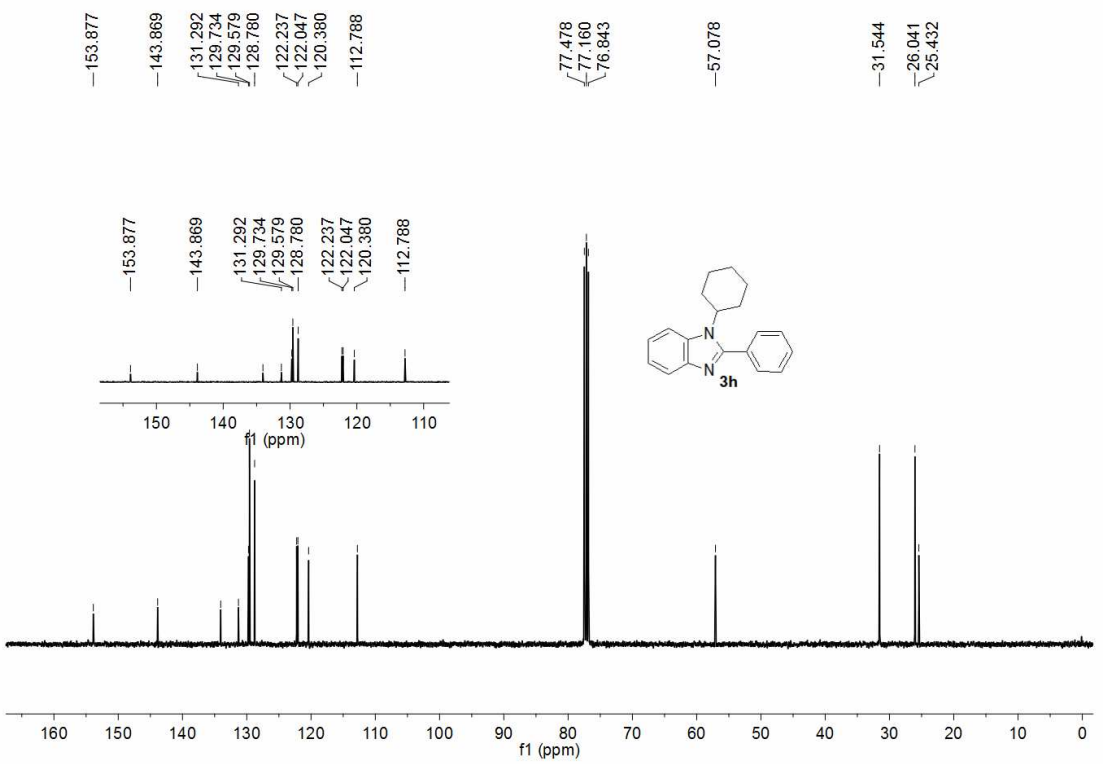
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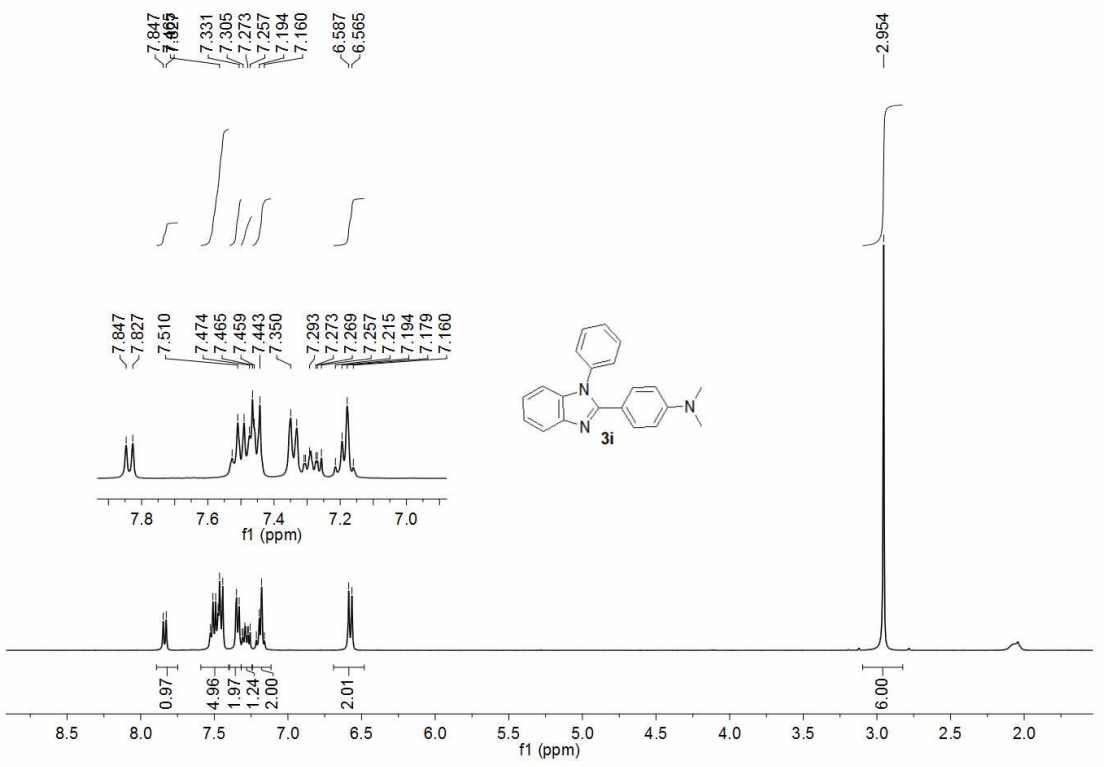
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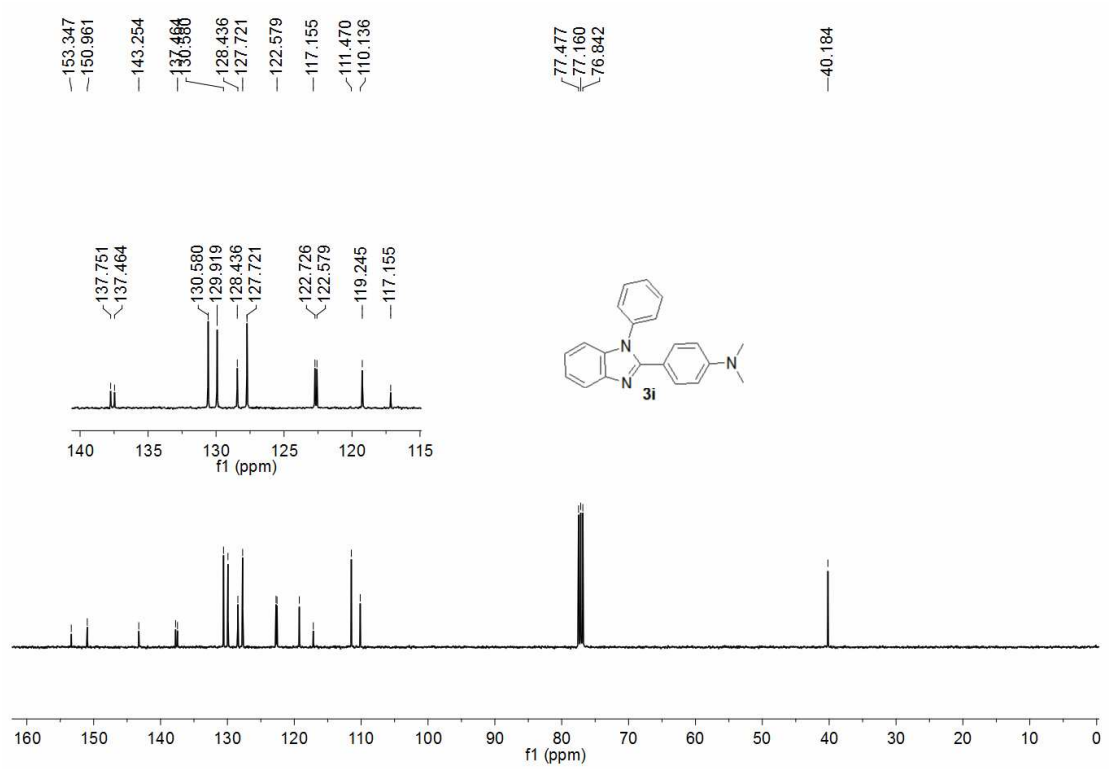
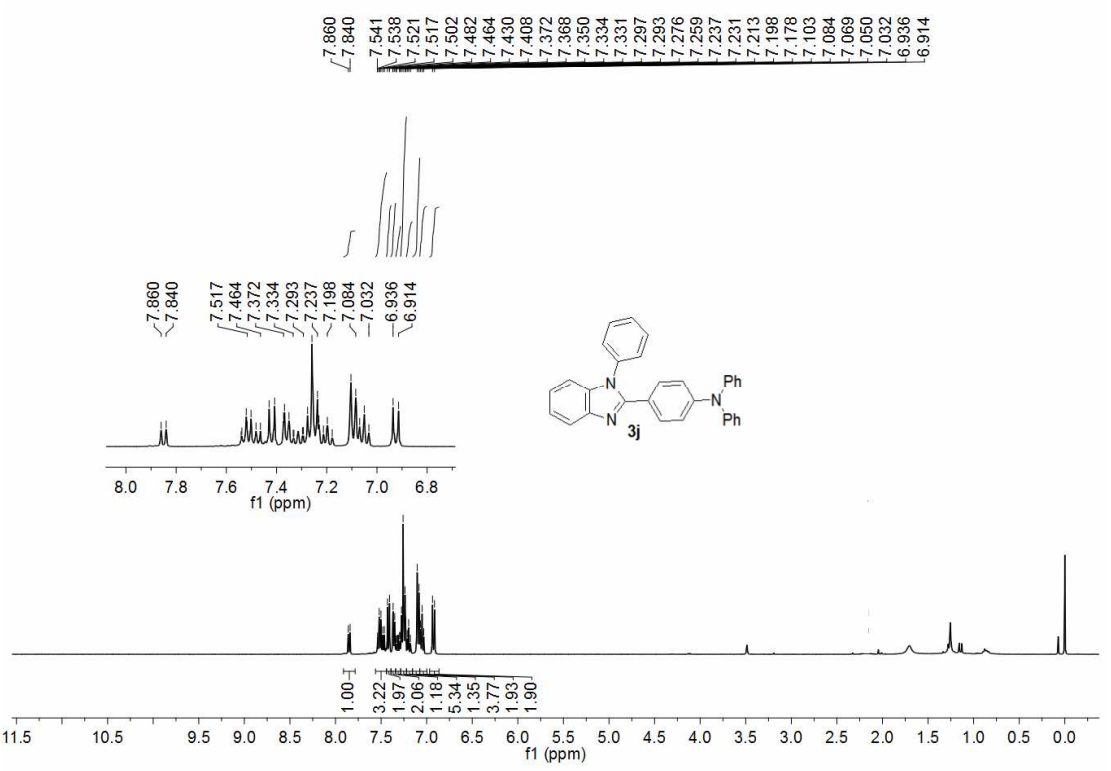
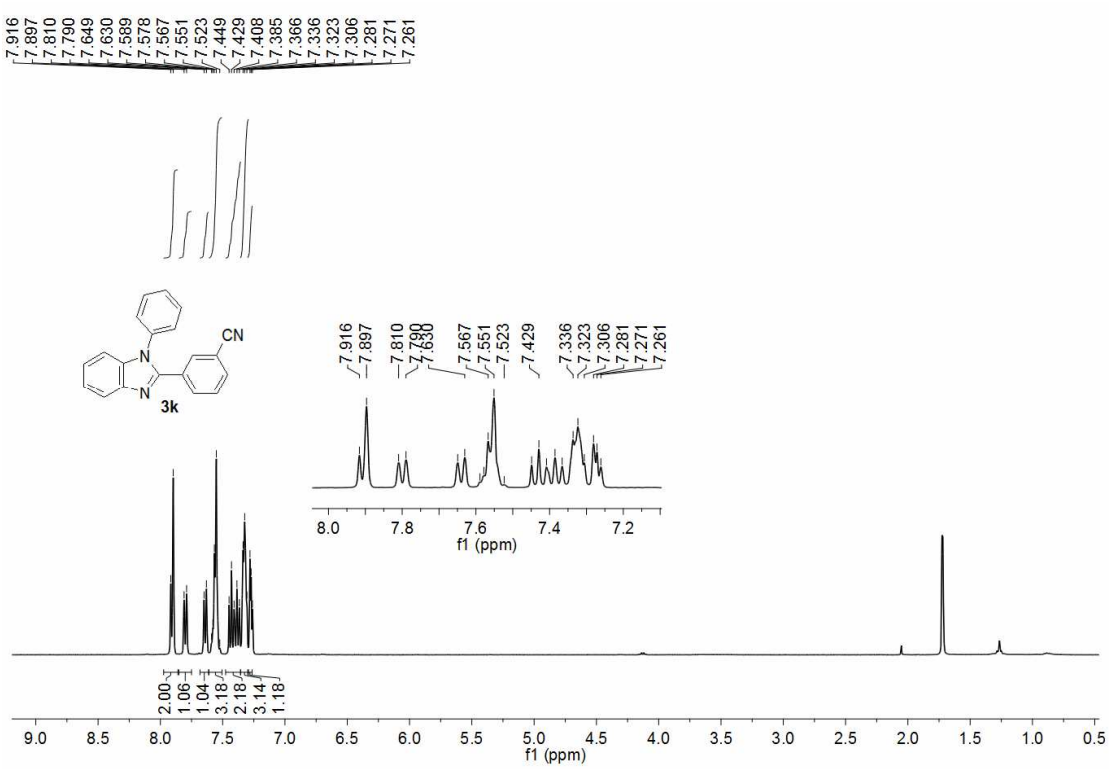
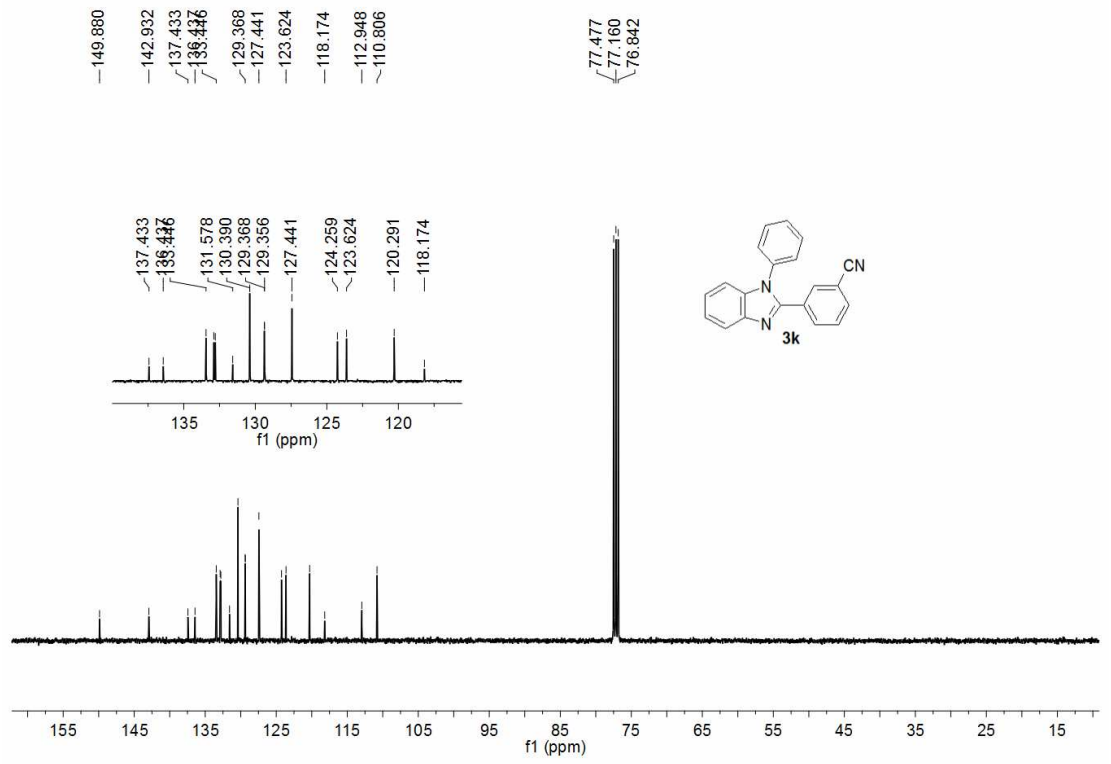
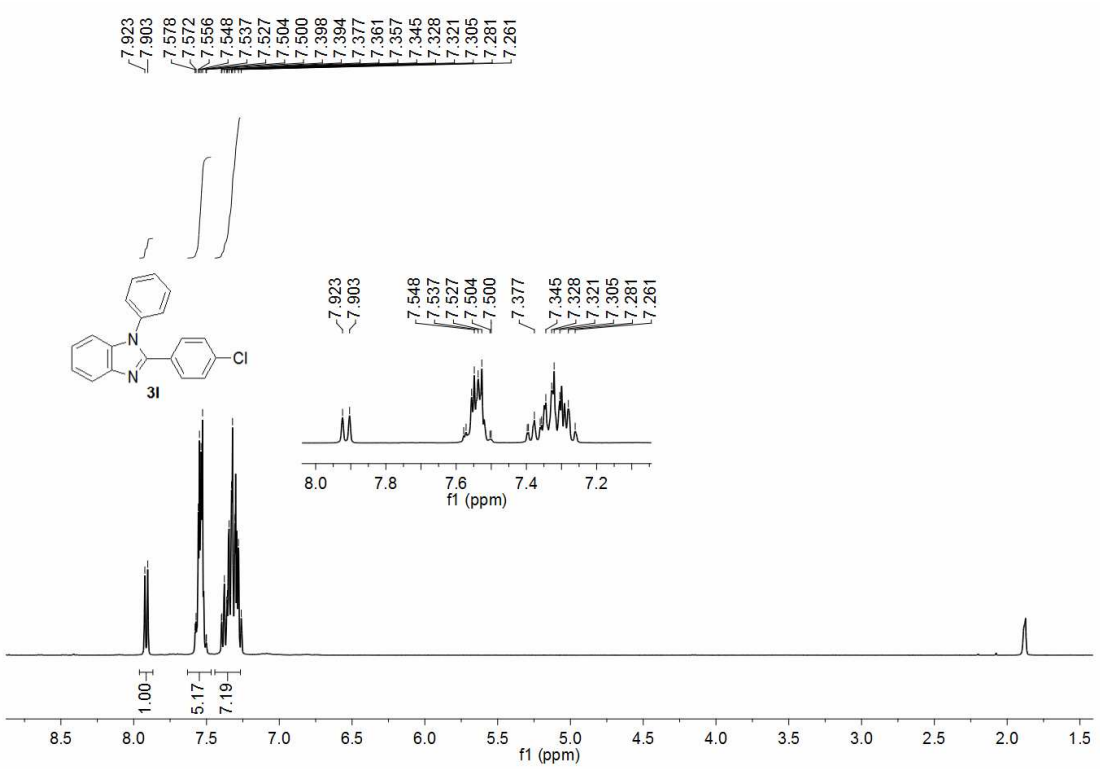
3i
0.97
4.96
1.97
1.24
2.00
2.01
6.00
f1 (ppm)

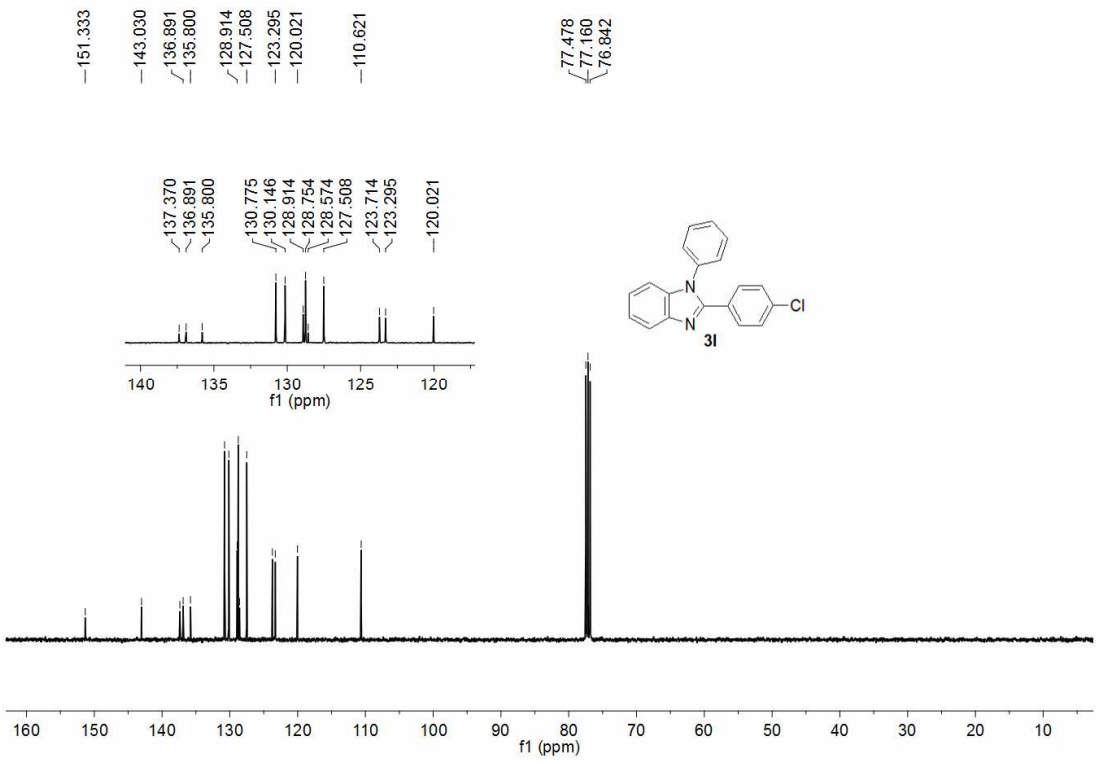

153.347
150.961
143.254
137.464
130.580
128.436
127.721
122.579
117.155
111.470
110.136
77.477
77.160
76.842
40.184
137.751
137.464
130.580
129.919
128.436
127.721
122.726
122.579
119.245
117.155
f1 (ppm)
3i
f1 (ppm)

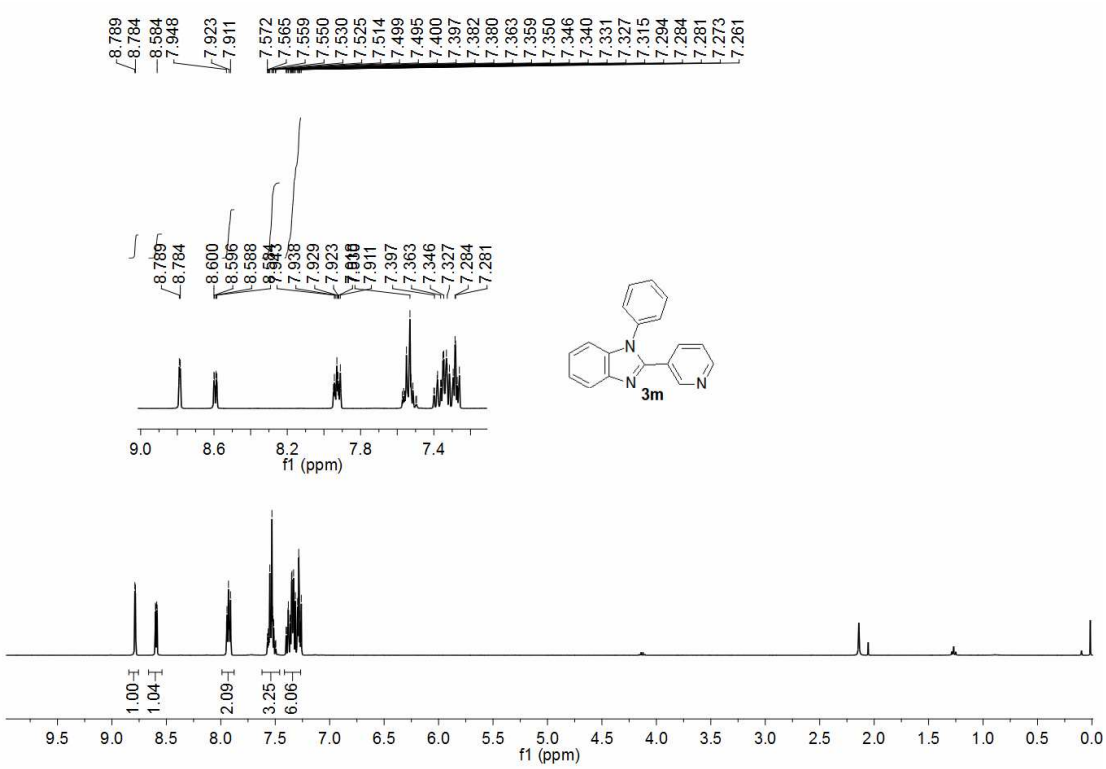

7.860
7.840
7.541
7.538
7.521
7.517
7.502
7.482
7.464
7.430
7.408
7.372
7.368
7.350
7.334
7.331
7.297
7.293
7.276
7.259
7.237
7.231
7.213
7.198
7.178
7.103
7.084
7.069
7.050
7.032
6.936
6.914
7.860
7.840
7.517
7.464
7.372
7.334
7.293
7.237
7.198
7.084
7.032
6.936
6.914
f1 (ppm)
Ph
Ph
3j
1.00
3.22
1.97
2.06
1.18
5.34
1.35
3.77
1.93
1.90
f1 (ppm)

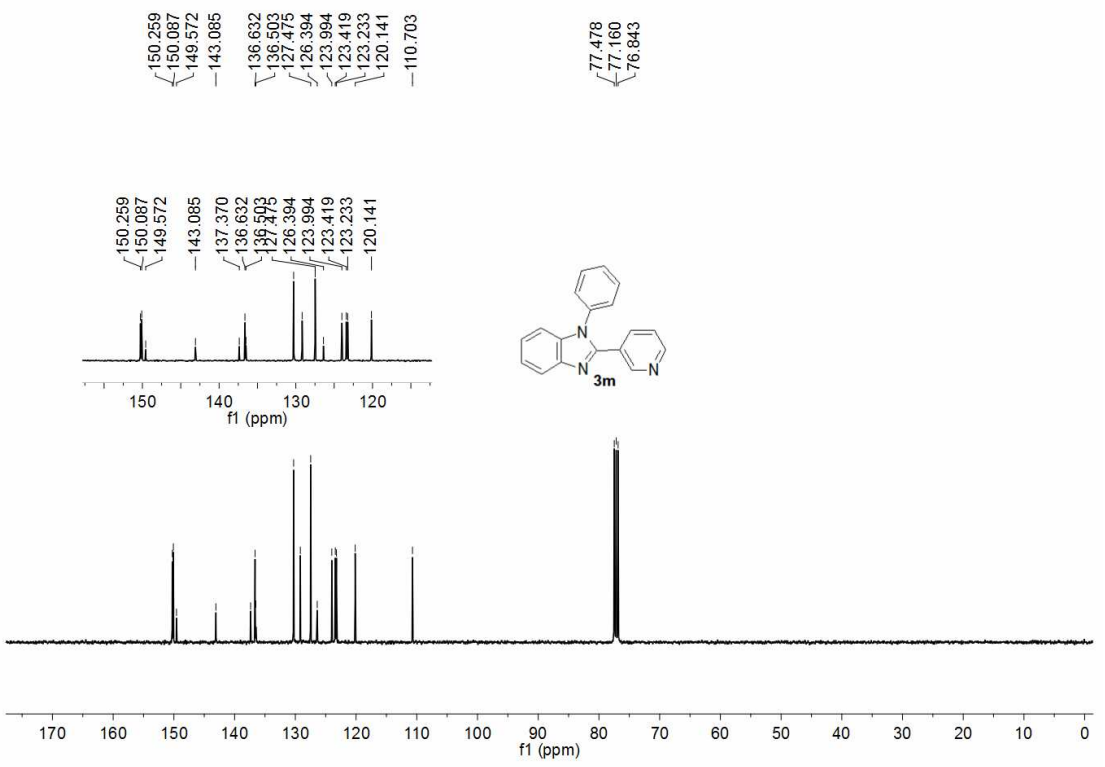

7.916
7.897
7.810
7.790
7.649
7.630
7.589
7.578
7.567
7.551
7.523
7.449
7.429
7.408
7.385
7.366
7.336
7.323
7.306
7.281
7.271
7.261
CN
N
N
3k
2.00
1.06
1.04
3.18
2.18
3.14
1.18
f1 (ppm)

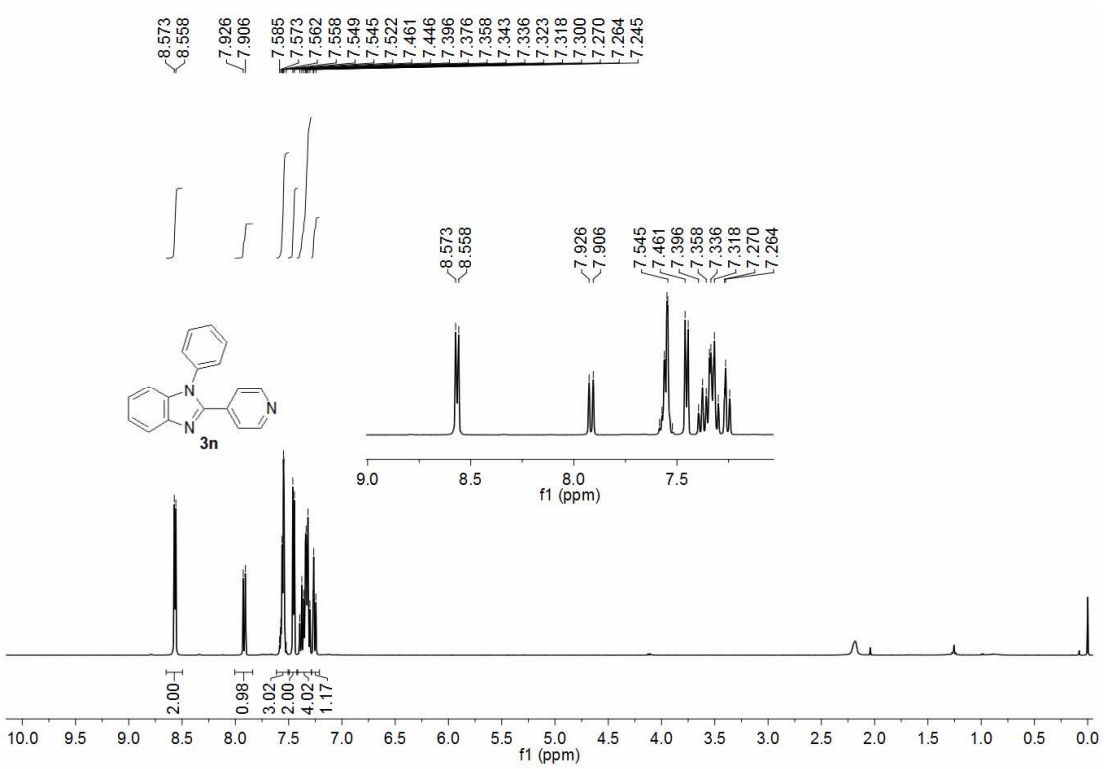

149.880
142.932
137.433
136.437
133.446
129.368
127.441
123.624
118.174
112.948
110.806
77.477
77.160
76.842
131.578
130.390
124.259
120.291
CN
N
N
3k
f1 (ppm)

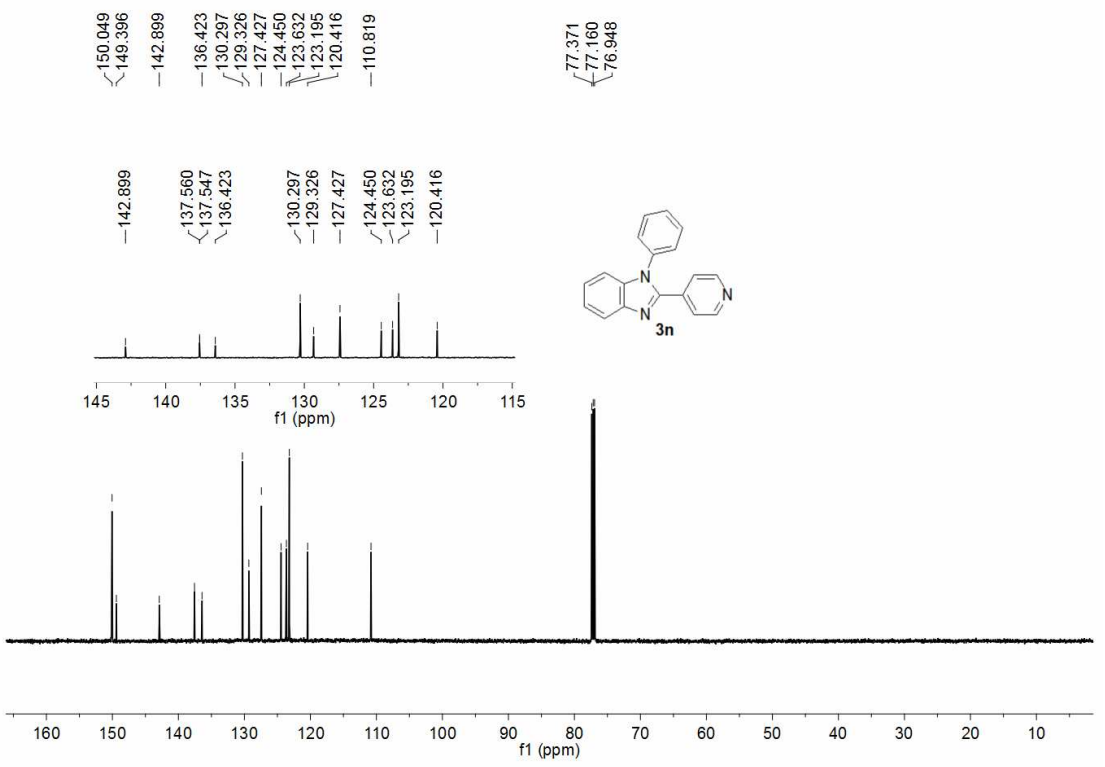

7.923
7.903
7.578
7.572
7.556
7.548
7.537
7.527
7.504
7.500
7.398
7.394
7.377
7.361
7.357
7.345
7.328
7.321
7.305
7.281
7.261
N
N
Cl
3l
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
1.00
5.17
7.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

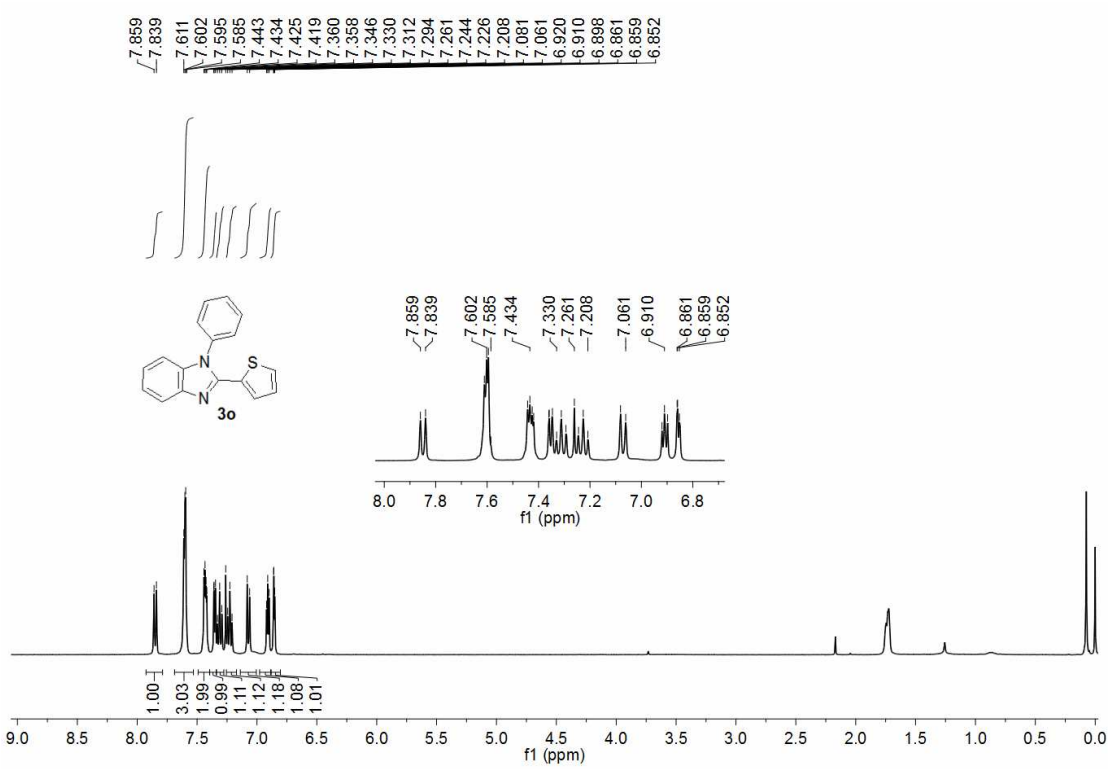

151.333
143.030
136.891
135.800
128.914
127.508
123.295
120.021
110.621
77.478
77.160
76.842
137.370
136.891
135.800
130.775
130.146
128.914
128.754
128.574
127.508
123.714
123.295
120.021
N
N
Cl
3l
140
135
130
125
120
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

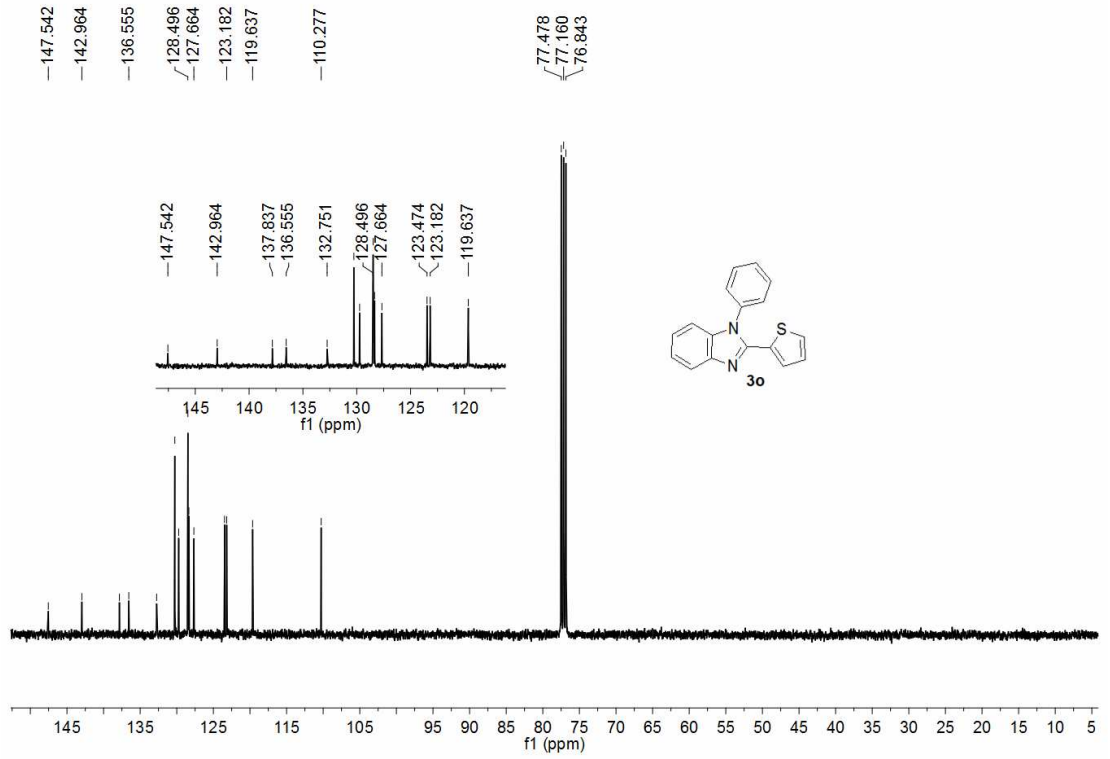

8.789
8.784
8.584
7.948
7.923
7.911
7.572
7.565
7.559
7.550
7.530
7.525
7.514
7.499
7.495
7.400
7.397
7.382
7.380
7.363
7.359
7.350
7.346
7.340
7.331
7.327
7.315
7.294
7.284
7.281
7.273
7.261
8.600
8.596
8.588
7.938
7.929
7.923
7.397
7.363
7.346
7.327
7.284
7.281
3m
f1 (ppm)
1.00
1.04
2.09
3.25
6.06
f1 (ppm)

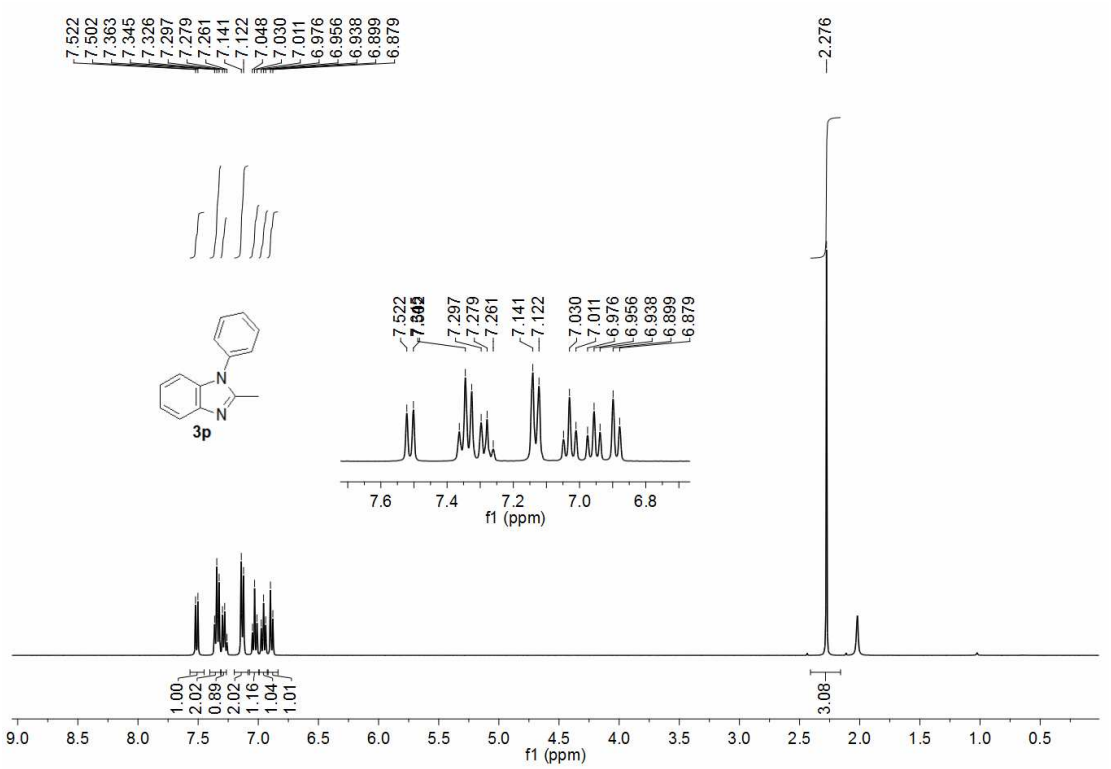

150.259
150.087
149.572
143.085
136.632
136.503
127.475
126.394
123.994
123.419
123.233
120.141
110.703
77.478
77.160
76.843
137.370
3m
f1 (ppm)
f1 (ppm)

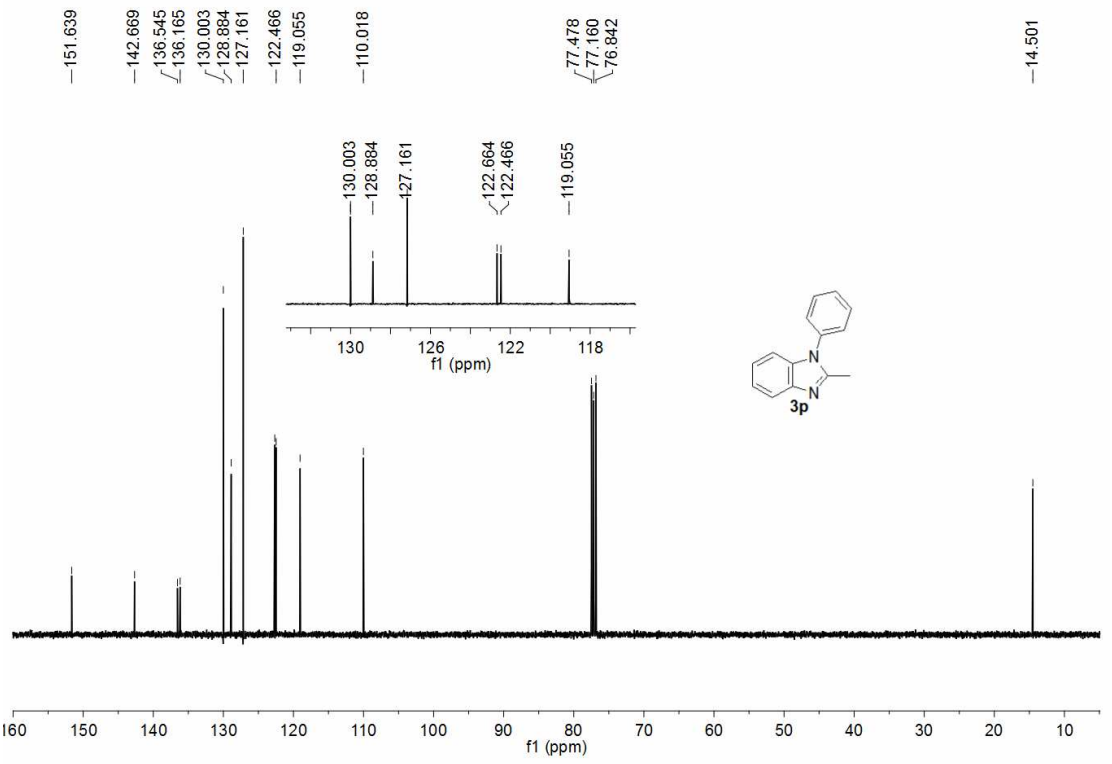

8.573
8.558
7.926
7.906
7.585
7.573
7.562
7.558
7.549
7.545
7.522
7.461
7.446
7.396
7.376
7.358
7.343
7.336
7.323
7.318
7.300
7.270
7.264
7.245
3n
f1 (ppm)
2.00
0.98
3.02
2.00
4.02
1.17
f1 (ppm)

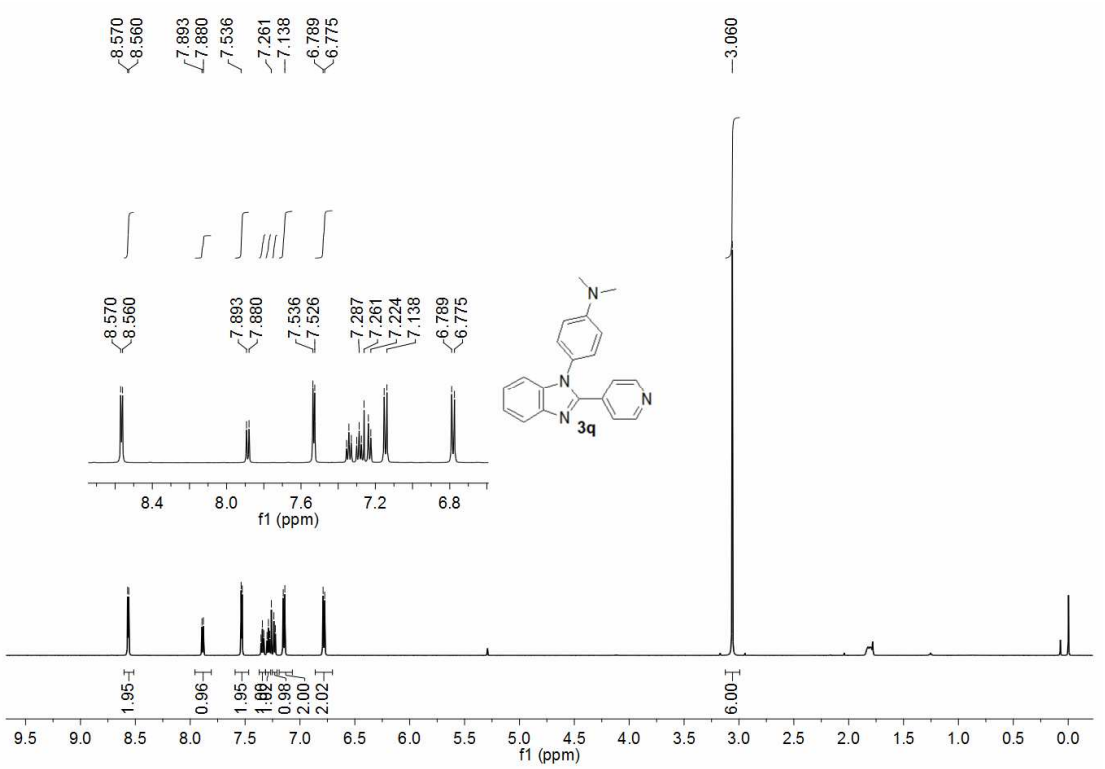

150.049
149.396
142.899
136.423
130.297
129.326
127.427
124.450
123.632
123.195
120.416
110.819
77.371
77.160
76.948
3n
f1 (ppm)
f1 (ppm)

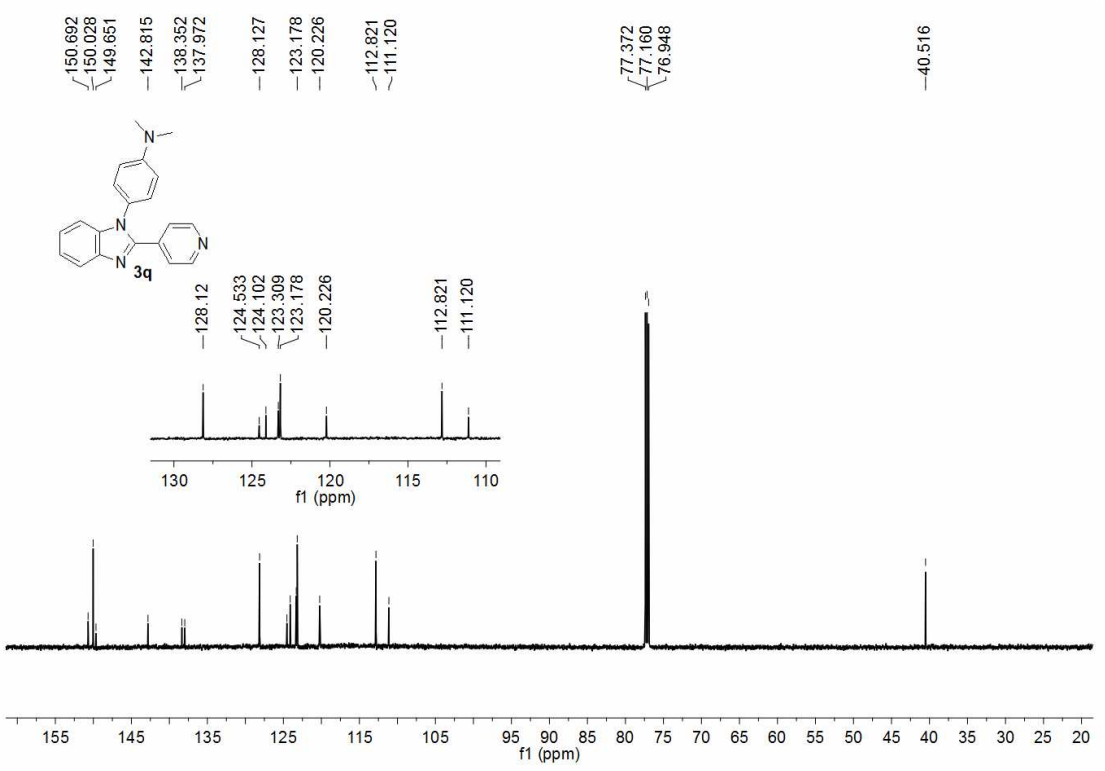

7.859
7.839
7.611
7.602
7.595
7.585
7.443
7.434
7.425
7.419
7.360
7.358
7.346
7.330
7.312
7.294
7.261
7.244
7.226
7.208
7.081
7.061
6.920
6.910
6.898
6.861
6.859
6.852
3o
1.00
3.03
1.99
0.99
1.11
1.12
1.18
1.08
1.01
f1 (ppm)

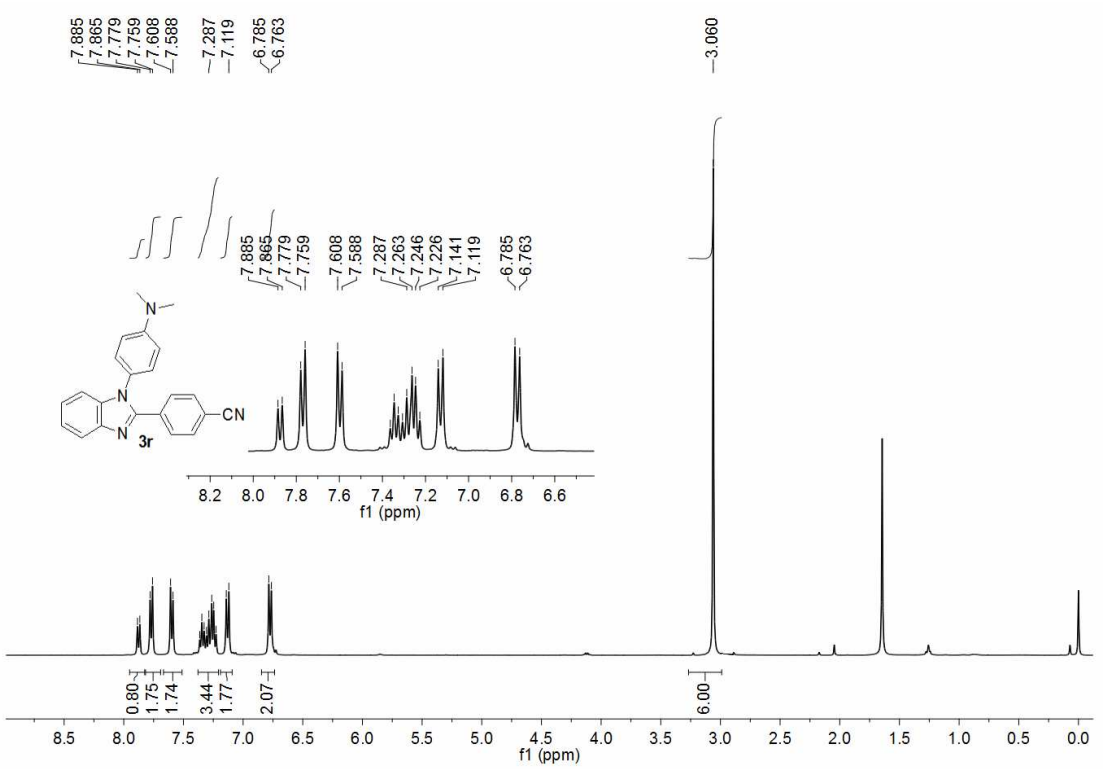

147.542
142.964
136.555
128.496
127.664
123.182
119.637
110.277
77.478
77.160
76.843
137.837
132.751
123.474
3o
f1 (ppm)

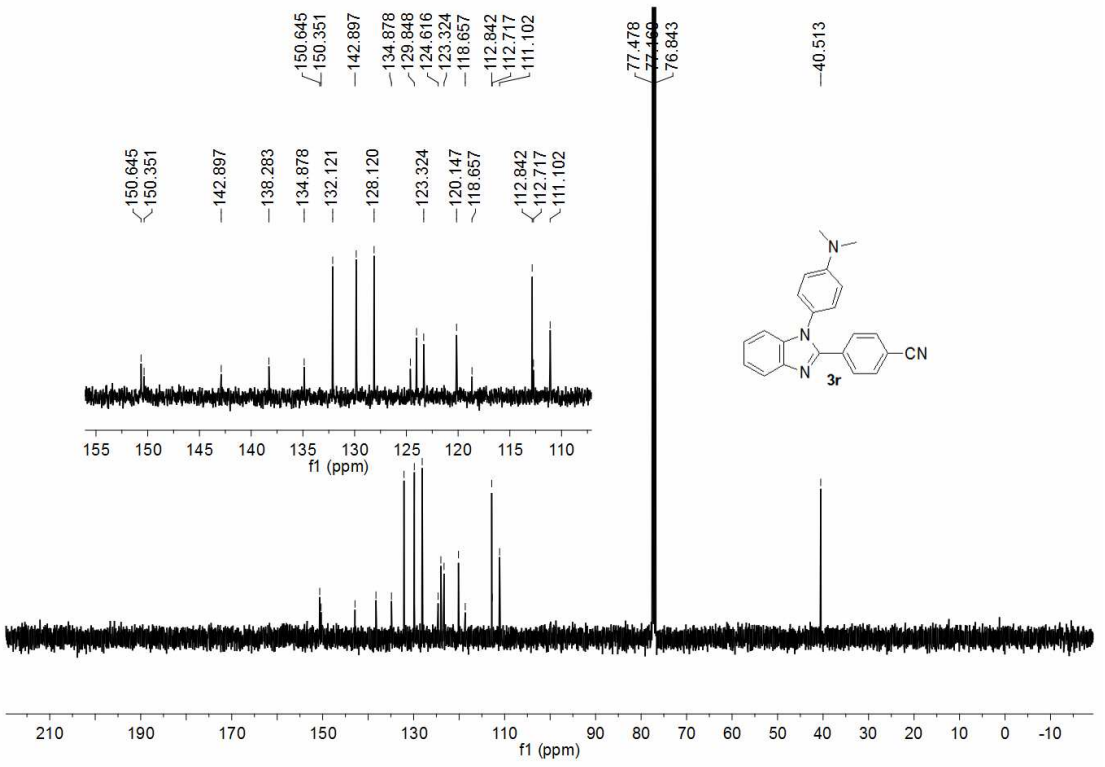

7.522
7.502
7.363
7.345
7.326
7.297
7.279
7.261
7.141
7.122
7.048
7.030
7.011
6.976
6.956
6.938
6.899
6.879
2.276
3p
f1 (ppm)
1.00
2.02
0.89
2.02
1.16
1.04
1.01
3.08

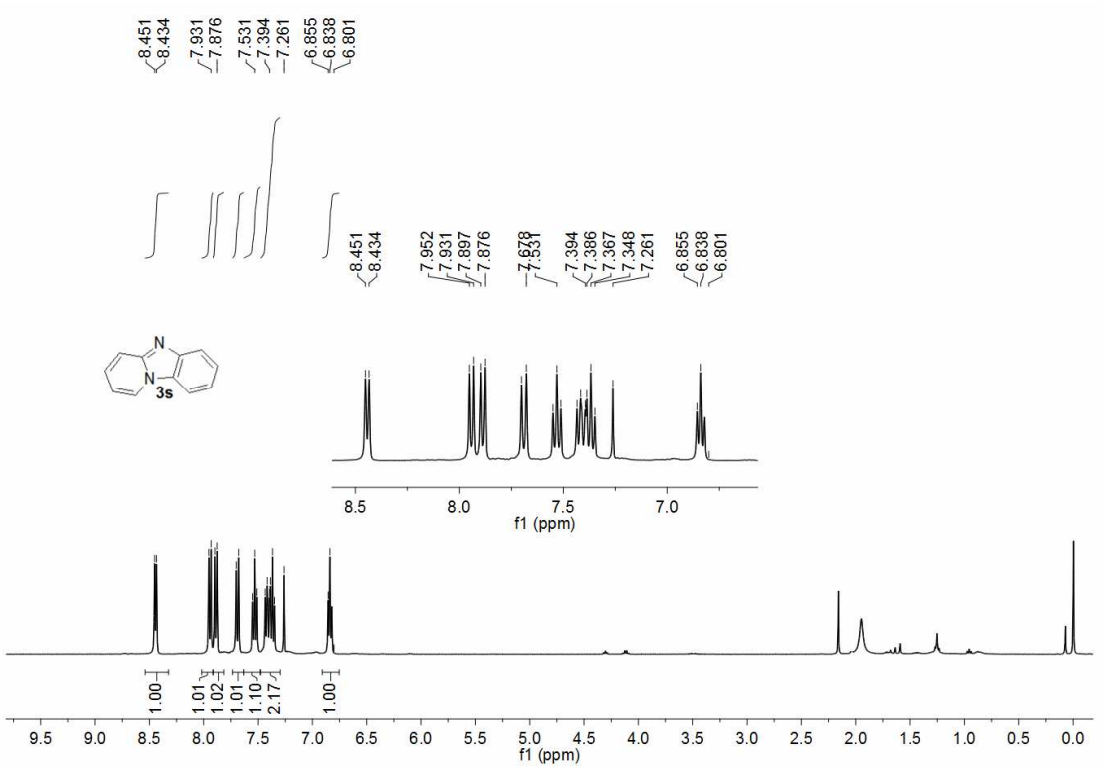

151.639
142.669
136.545
136.165
130.003
128.884
127.161
122.466
119.055
110.018
77.478
77.160
76.842
14.501
3p
f1 (ppm)

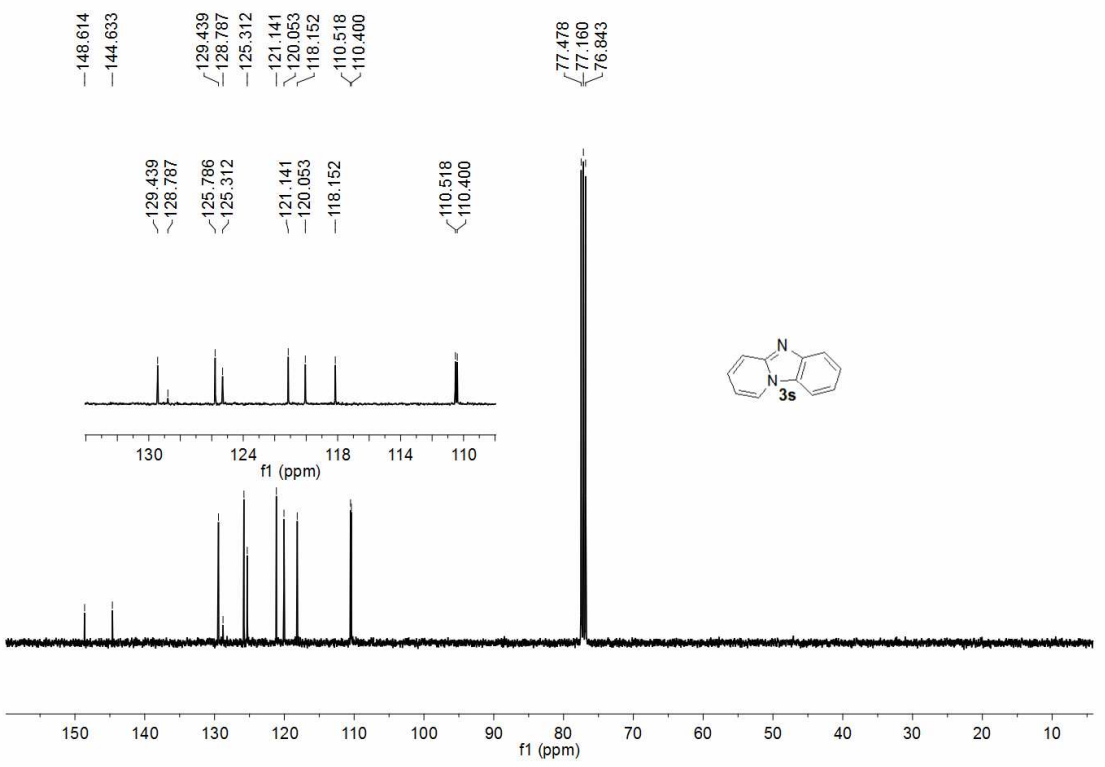

8.570
8.560
7.893
7.880
7.536
7.261
7.138
6.789
6.775
3.060
3q
f1 (ppm)
1.95
0.96
1.95
0.98
2.00
2.02
6.00

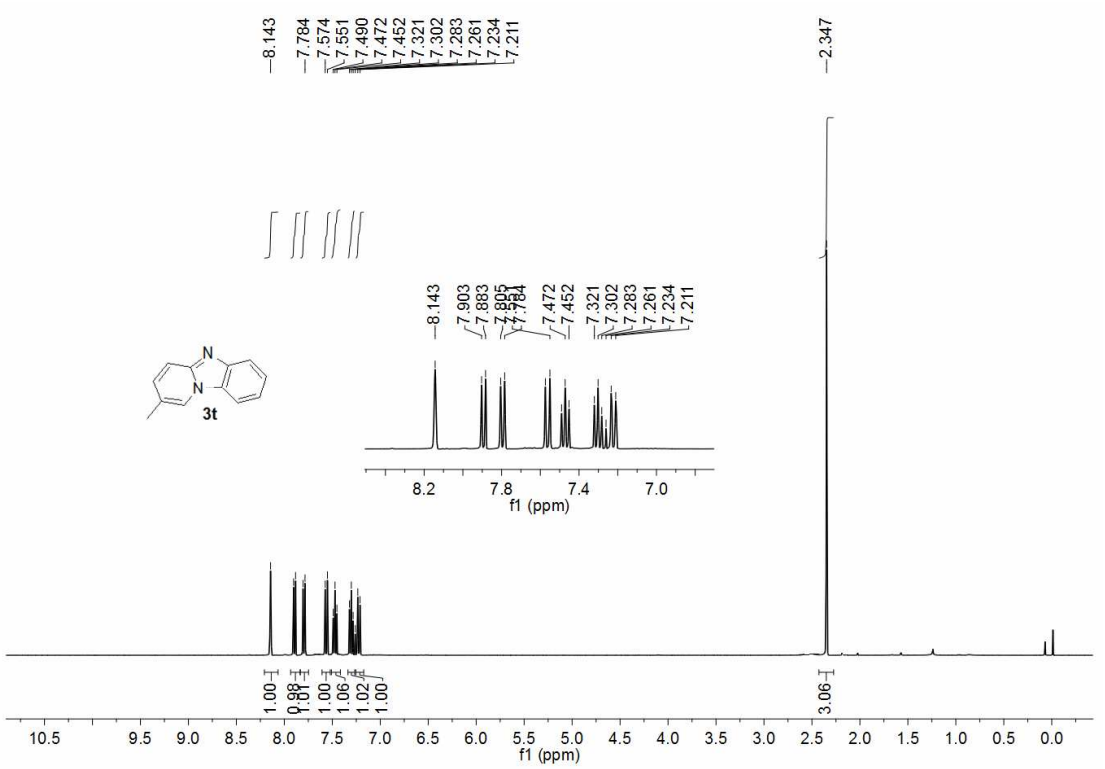

150.692
150.028
149.651
142.815
138.352
137.972
128.127
123.178
120.226
112.821
111.120
77.372
77.160
76.948
40.516
3q
f1 (ppm)


7.885
7.865
7.779
7.759
7.608
7.588
7.287
7.119
6.785
6.763
3.060
N
N
N
CN
3r
0.80
1.75
1.74
3.44
1.77
2.07
6.00
f1 (ppm)


150.645
150.351
142.897
138.283
134.878
132.121
128.120
123.324
120.147
118.657
112.842
112.717
111.102
77.478
77.160
76.843
40.513
N
N
N
CN
3r
f1 (ppm)


8.451
8.434
7.931
7.876
7.531
7.394
7.261
6.855
6.838
6.801
7.952
7.897
7.678
7.348
3s
f1 (ppm)
1.00
1.01
1.02
1.01
1.10
2.17
1.00


148.614
144.633
129.439
128.787
125.312
121.141
120.053
118.152
110.518
110.400
77.478
77.160
76.843
125.786
3s
f1 (ppm)


8.143
7.784
7.574
7.551
7.490
7.472
7.452
7.321
7.302
7.283
7.261
7.234
7.211
2.347
3t
f1 (ppm)
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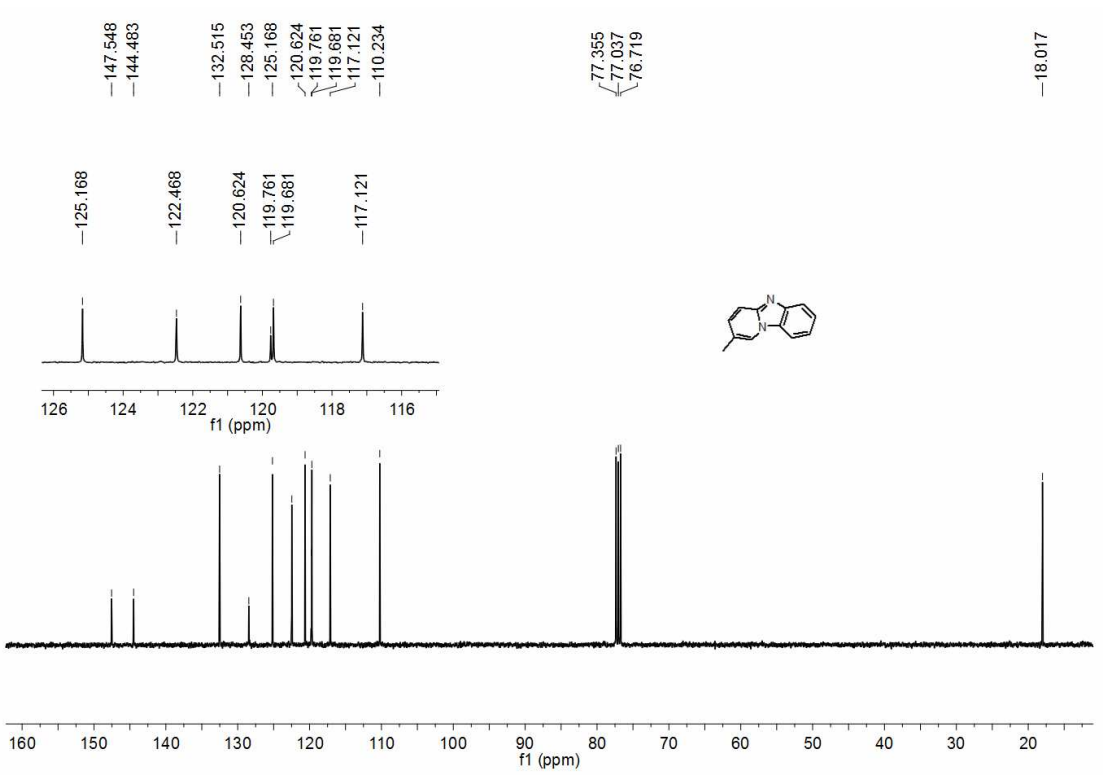
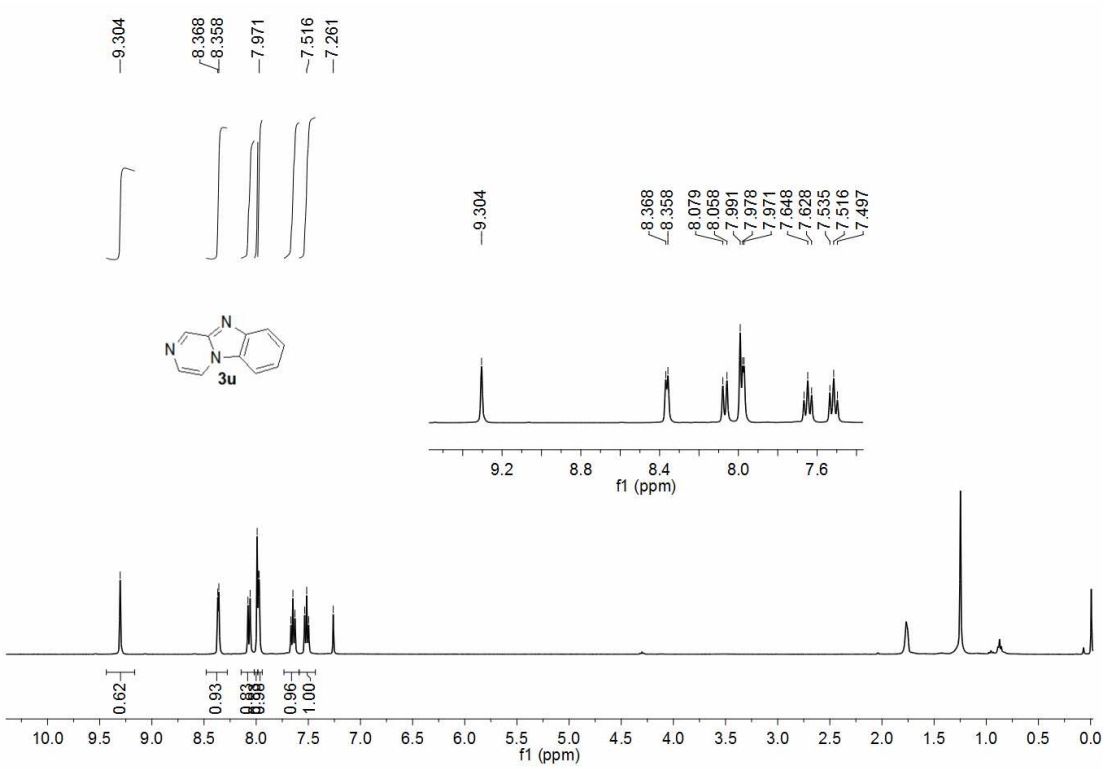
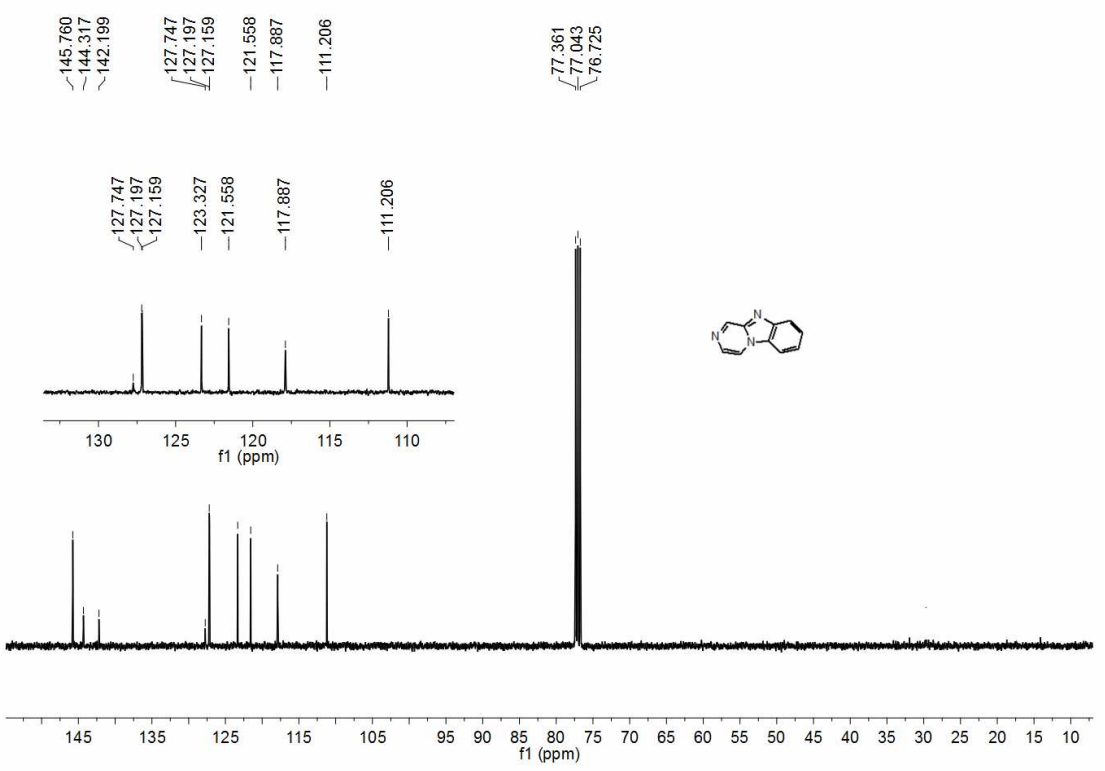
0.88
1.00
1.06
1.02
1.00
3.06


147.548
144.483
132.515
128.453
125.168
120.624
119.761
119.681
117.121
110.234
77.355
77.037
76.719
18.017
f1 (ppm)


9.304
8.368
8.358
7.971
7.516
7.261
3u
f1 (ppm)


145.760
144.317
142.199
127.747
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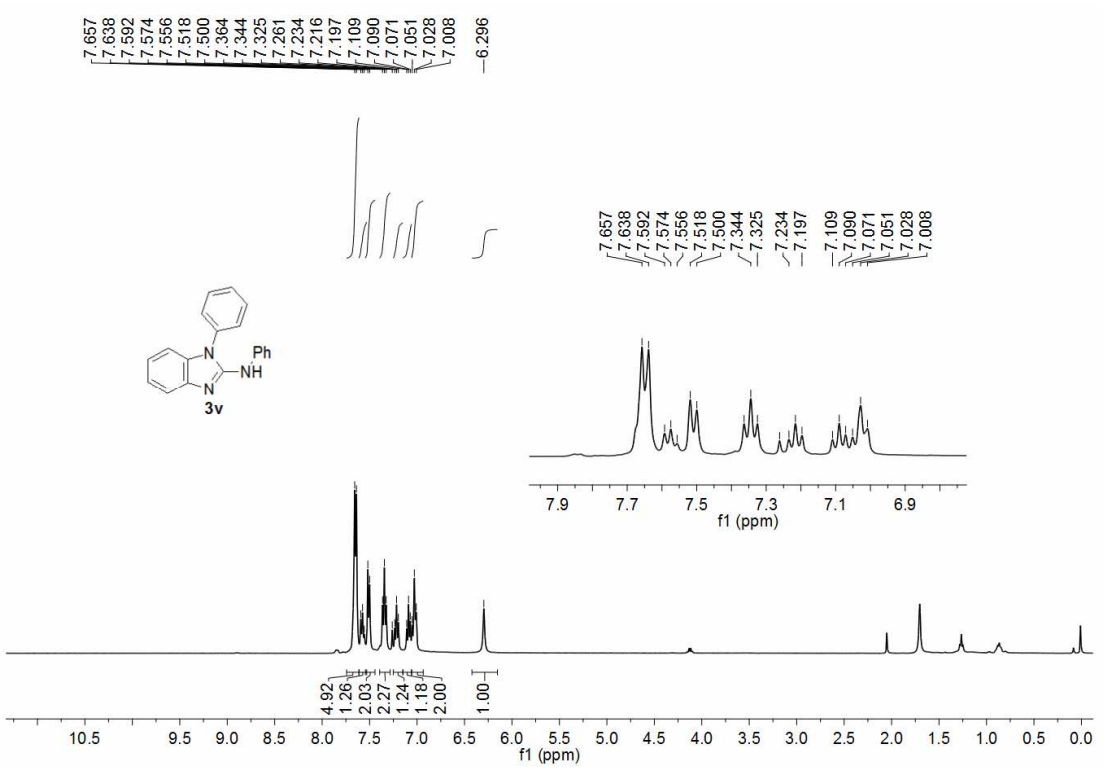
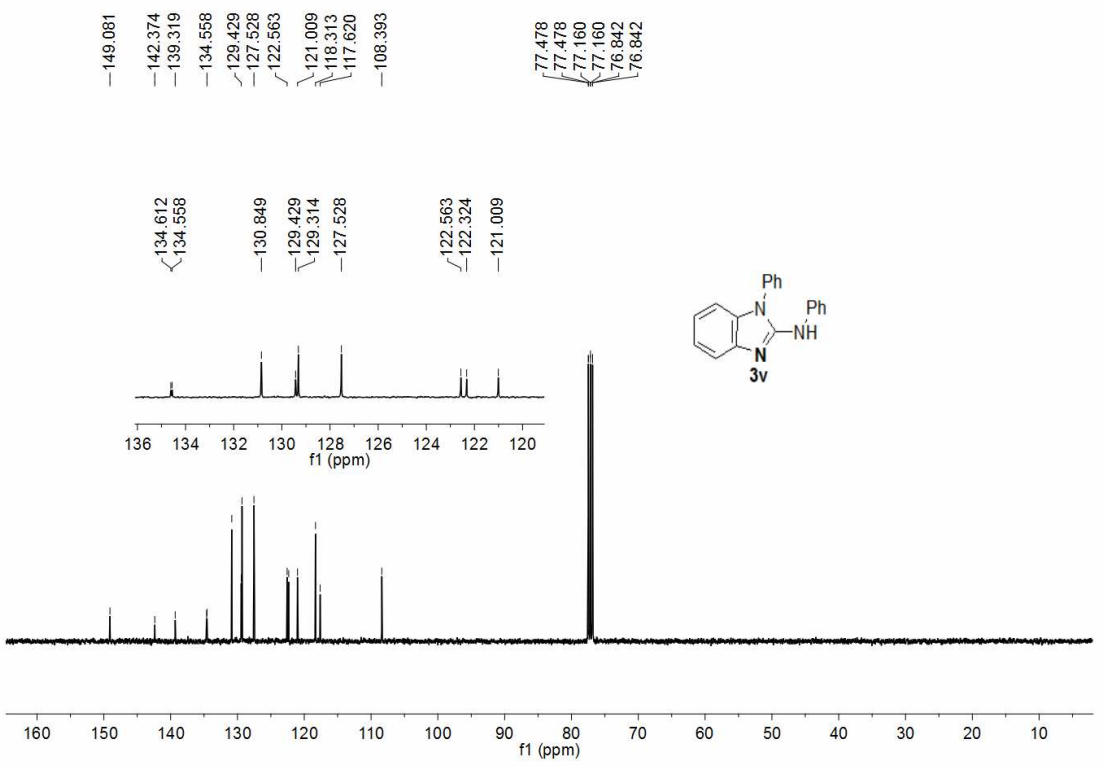
127.159
121.558
117.887
111.206
77.361
77.043
76.725
123.327
f1 (ppm)


7.657
7.638
7.592
7.574
7.556
7.518
7.500
7.364
7.344
7.325
7.261
7.234
7.216
7.197
7.109
7.090
7.071
7.051
7.028
7.008
6.296
Ph
NH
N
3v
4.92
1.26
2.03
2.27
1.24
1.18
2.00
1.00
f1 (ppm)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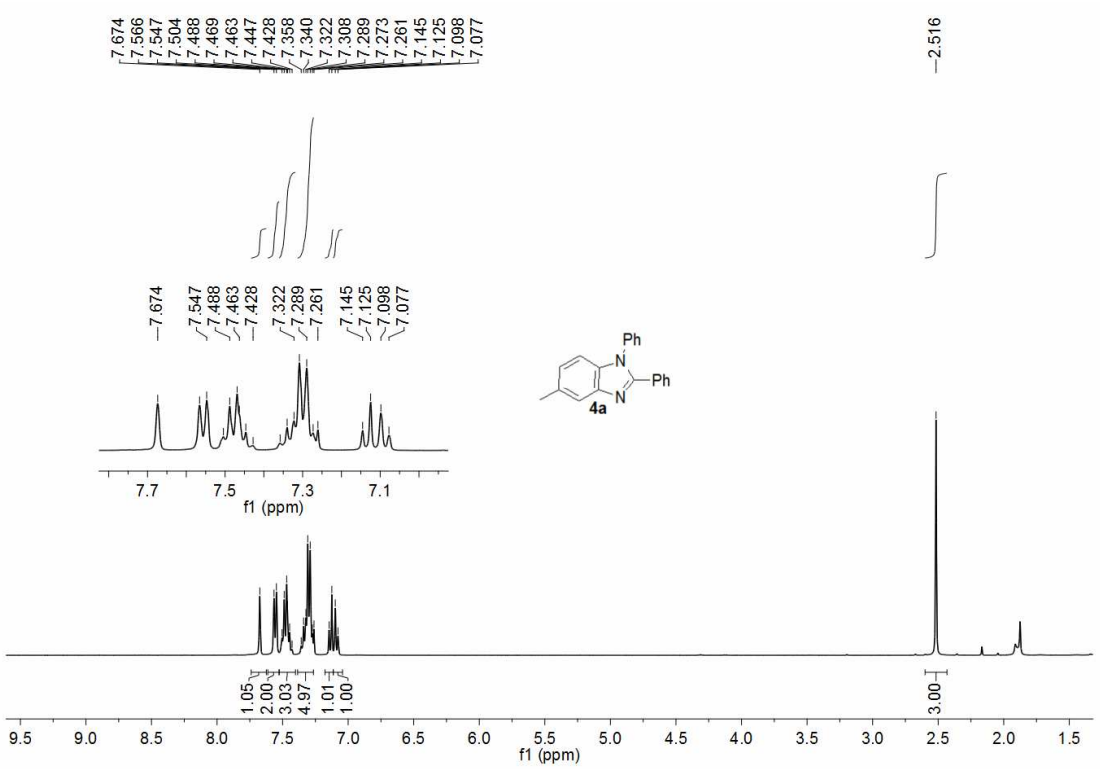
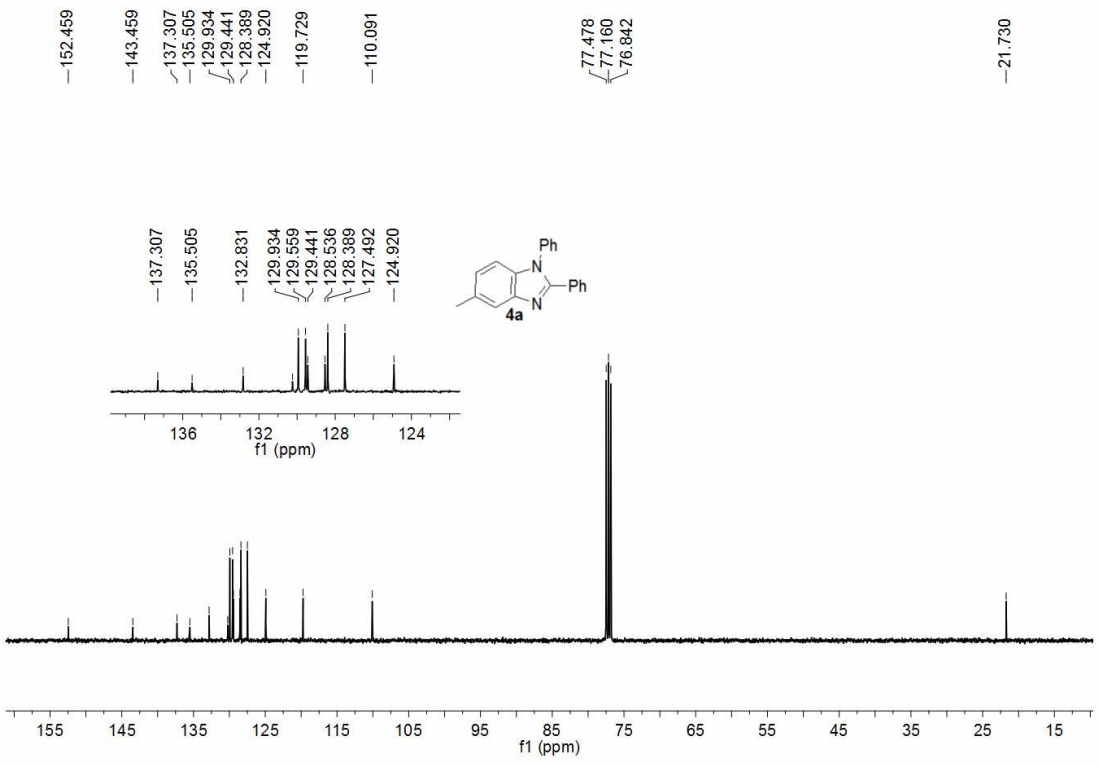
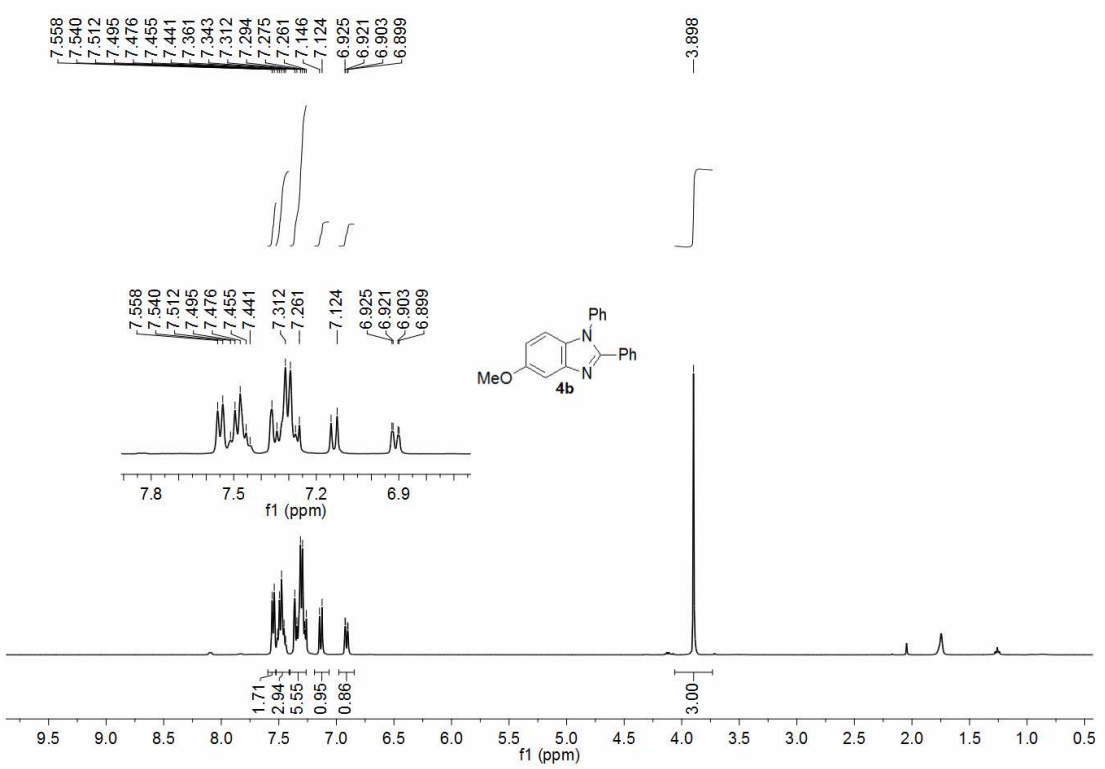
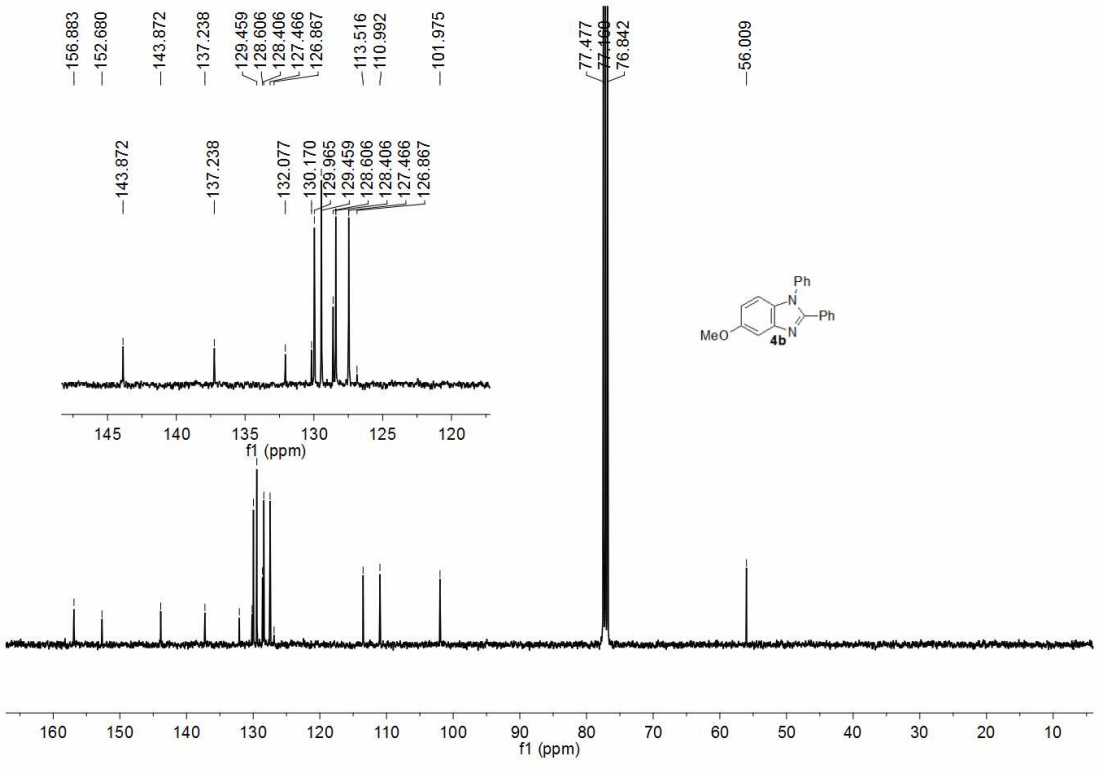
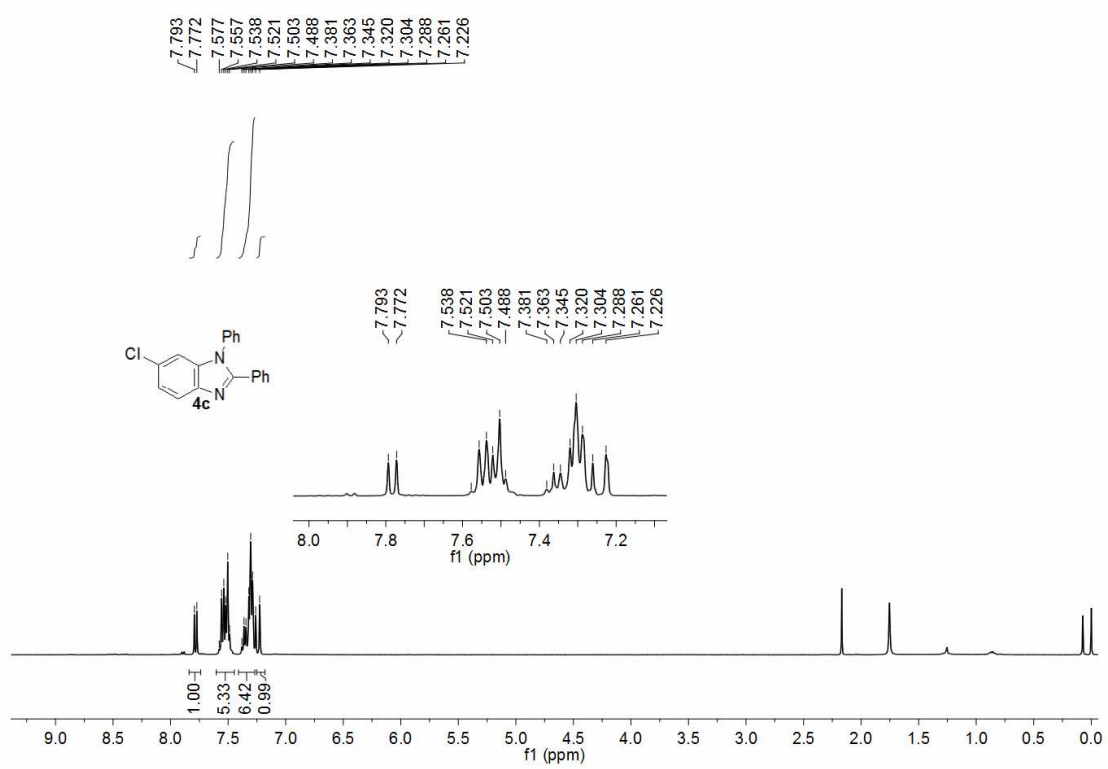
142.374
139.319
134.558
129.429
127.528
122.563
121.009
118.313
117.620
108.393
77.478
77.160
76.842
134.612
130.849
129.429
129.314
127.528
122.563
122.324
121.009
Ph
Ph
NH
N
3v
f1 (ppm)

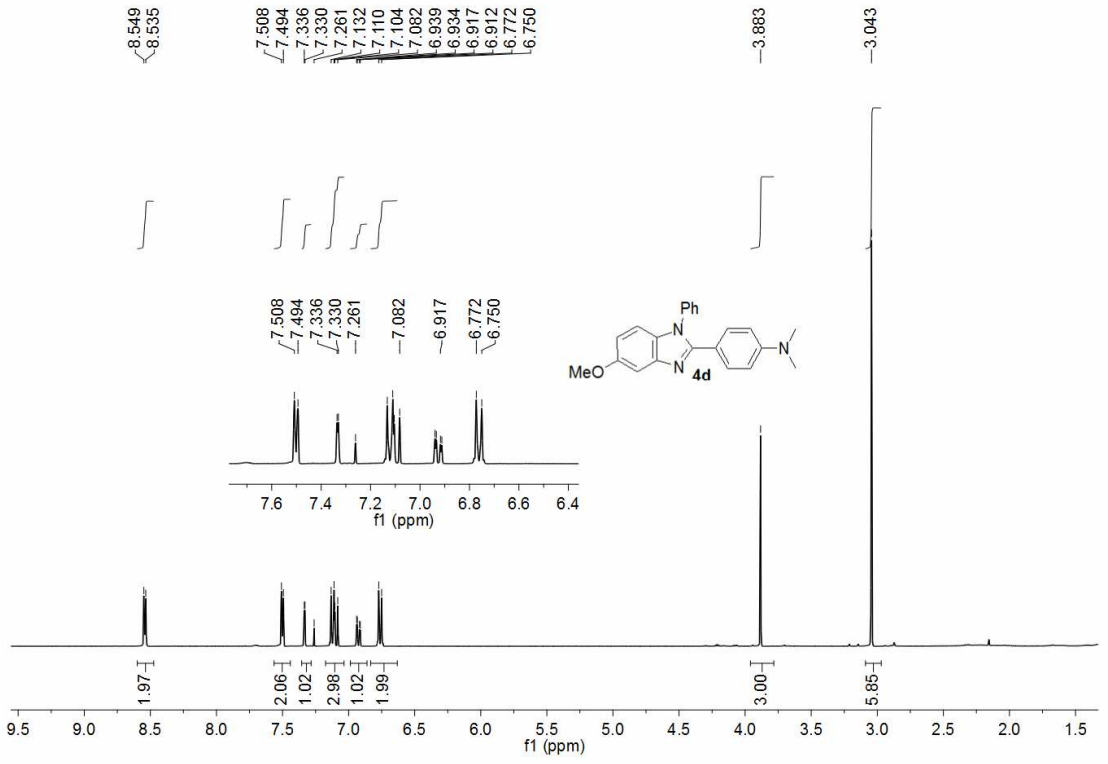

7.674
7.566
7.547
7.504
7.488
7.469
7.463
7.447
7.428
7.358
7.340
7.322
7.308
7.289
7.273
7.261
7.145
7.125
7.098
7.077
2.516
Ph
N
Ph
N
4a
f1 (ppm)
1.05
2.00
3.03
4.97
1.01
1.00
3.00
f1 (ppm)

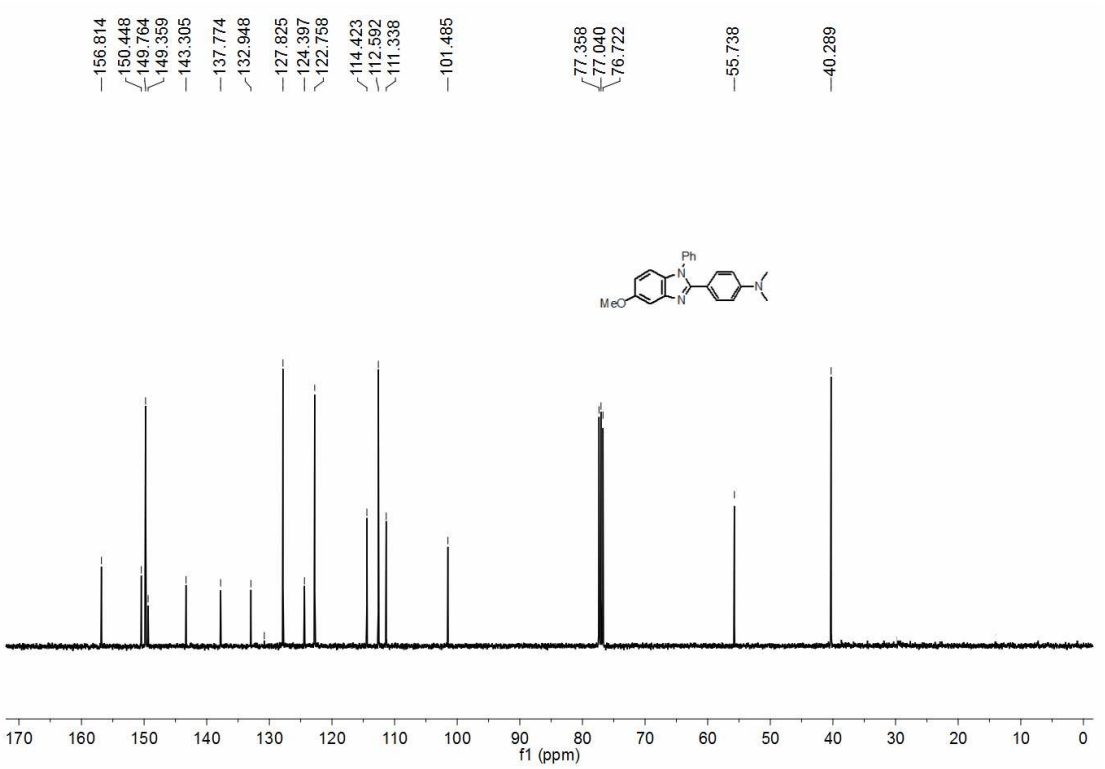

152.459
143.459
137.307
135.505
129.934
129.441
128.389
124.920
119.729
110.091
77.478
77.160
76.842
21.730
Ph
N
Ph
N
4a
f1 (ppm)
f1 (ppm)

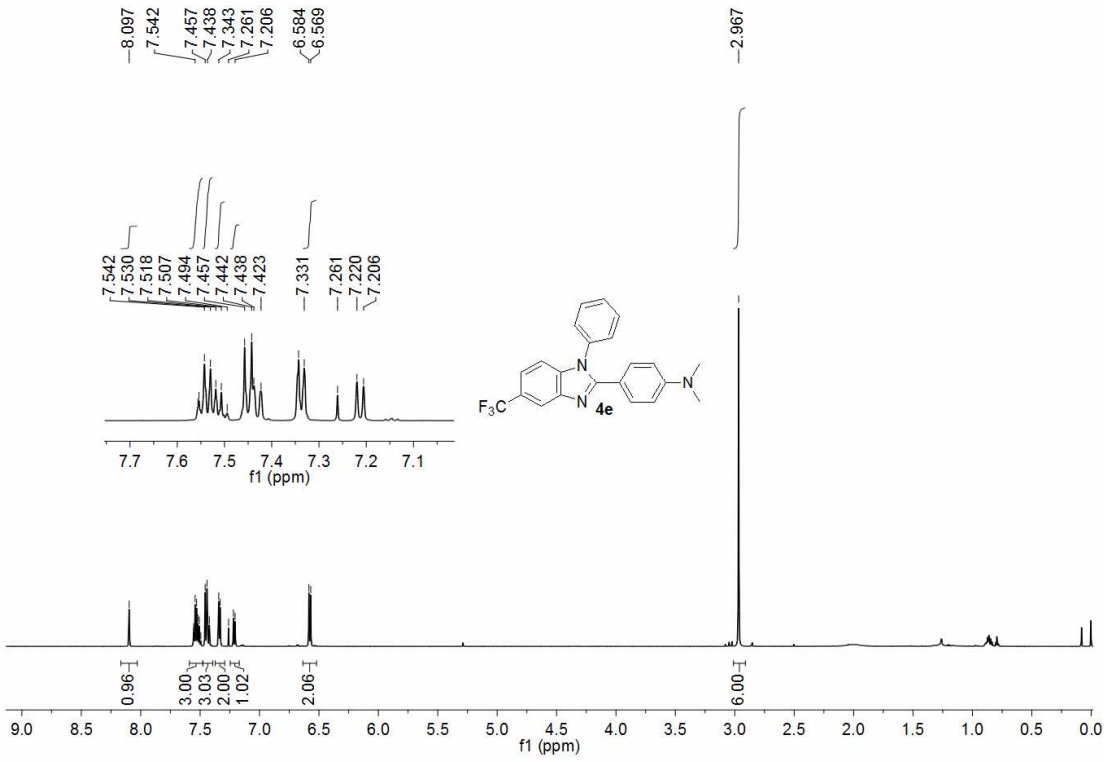

7.558
7.540
7.512
7.495
7.476
7.455
7.441
7.361
7.343
7.312
7.294
7.275
7.261
7.146
7.124
6.925
6.921
6.903
6.899
3.898
Ph
N
Ph
N
MeO
4b
1.71
2.94
5.55
0.95
0.86
3.00
f1 (ppm)

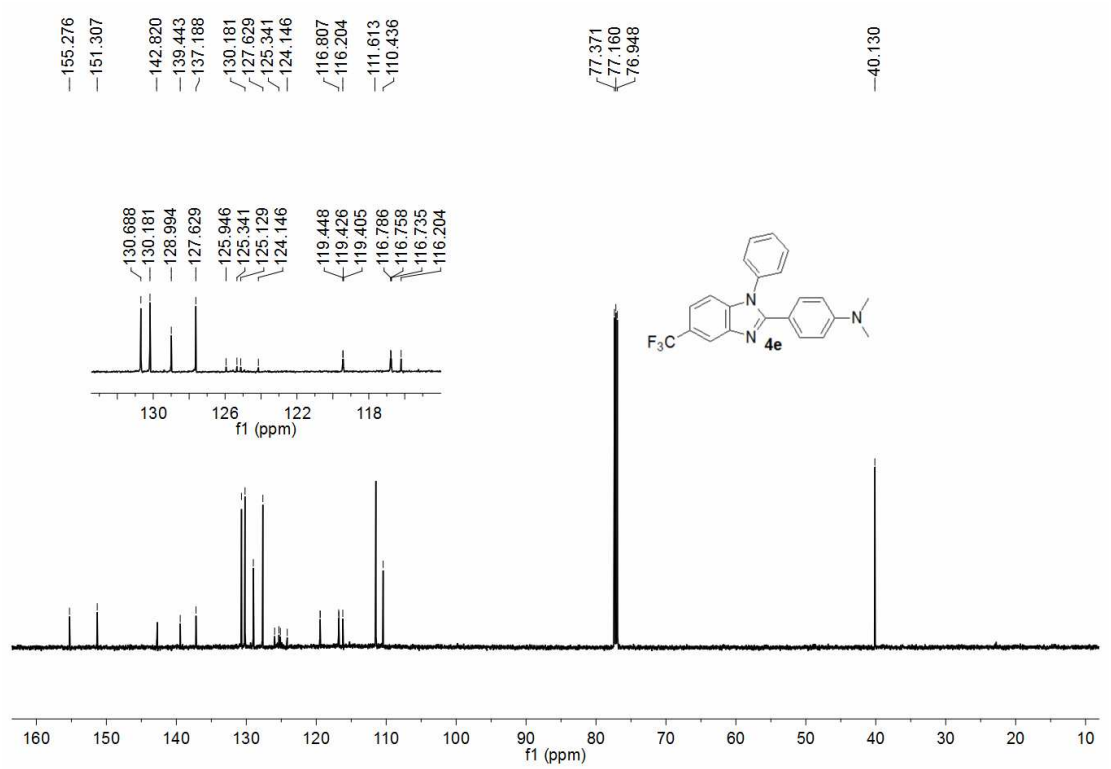

156.883
152.680
143.872
137.238
129.459
128.606
128.406
127.466
126.867
113.516
110.992
101.975
77.477
77.160
76.842
56.009
132.077
130.170
129.965
Ph
N
Ph
N
MeO
4b
f1 (ppm)

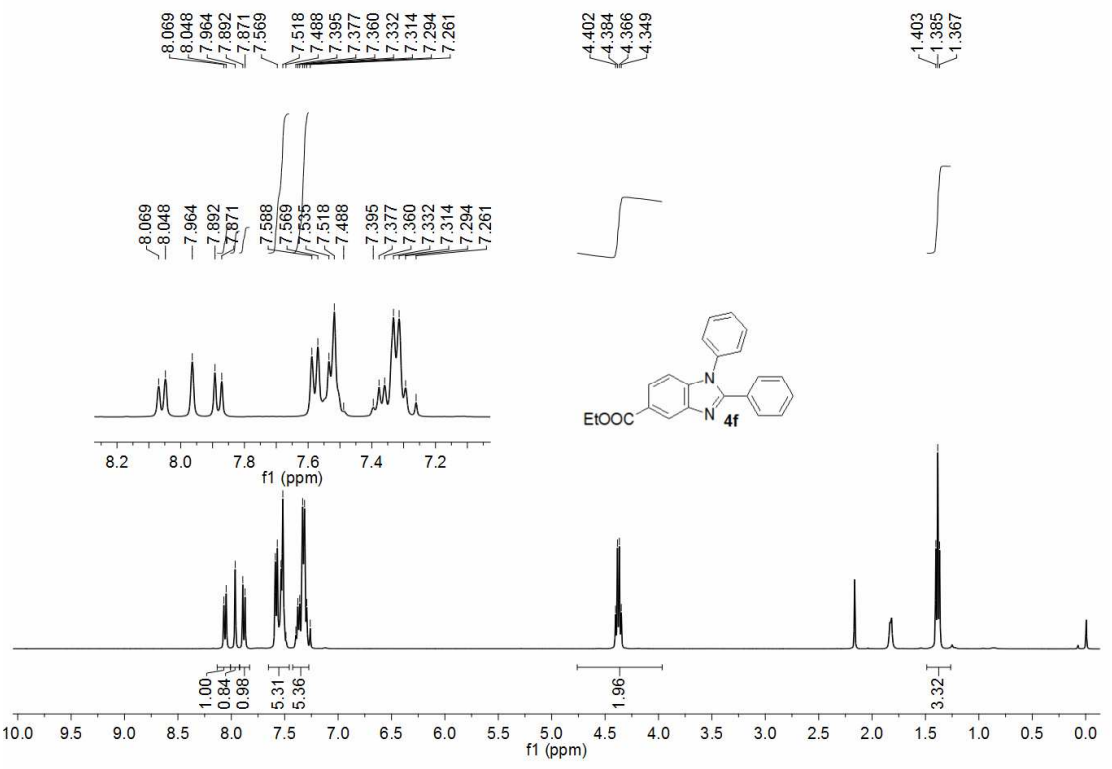

7.793
7.772
7.577
7.557
7.538
7.521
7.503
7.488
7.381
7.363
7.345
7.320
7.304
7.288
7.261
7.226
Ph
Cl
N
Ph
N
4c
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
1.00
5.33
6.42
0.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

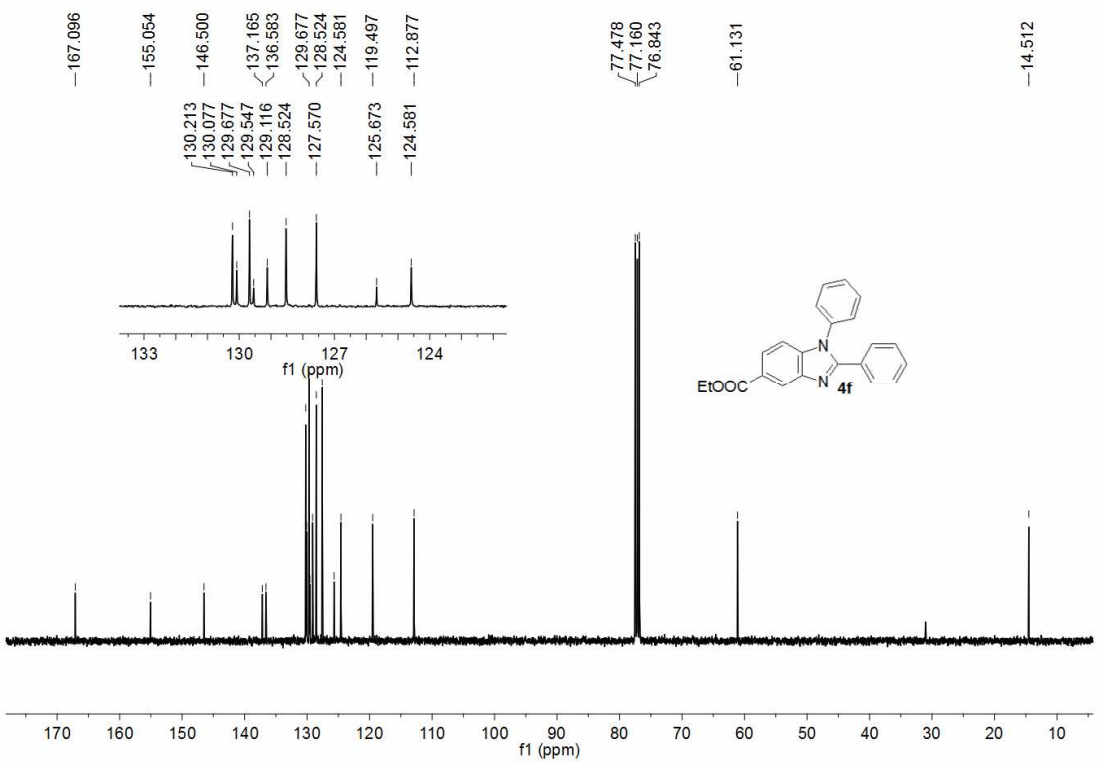

8.549
8.535
7.508
7.494
7.336
7.330
7.261
7.132
7.110
7.104
7.082
6.939
6.934
6.917
6.912
6.772
6.750
3.883
3.043
Ph
N
N
MeO
N
4d
7.6
7.4
7.2
7.0
6.8
6.6
6.4
f1 (ppm)
1.97
2.06
1.02
2.98
1.02
1.99
3.00
5.85
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

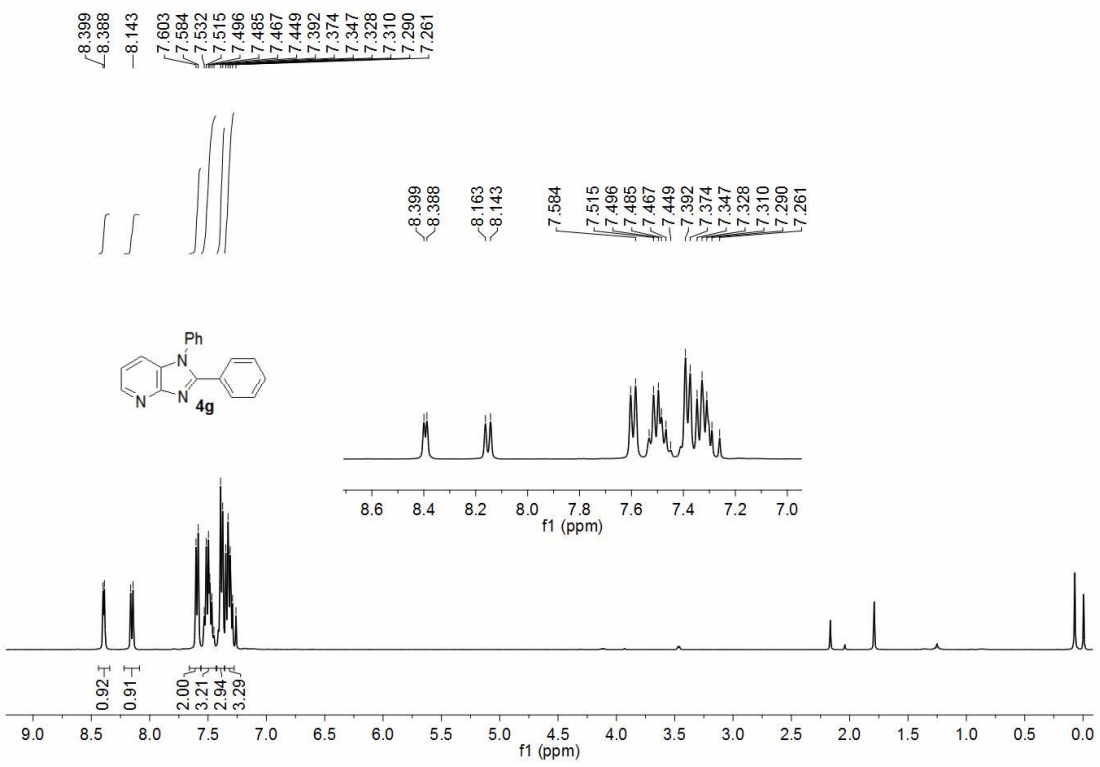

156.814
150.448
149.764
149.359
143.305
137.774
132.948
127.825
124.397
122.758
114.423
112.592
111.338
101.485
77.358
77.040
76.722
55.738
40.289
Ph
MeO
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

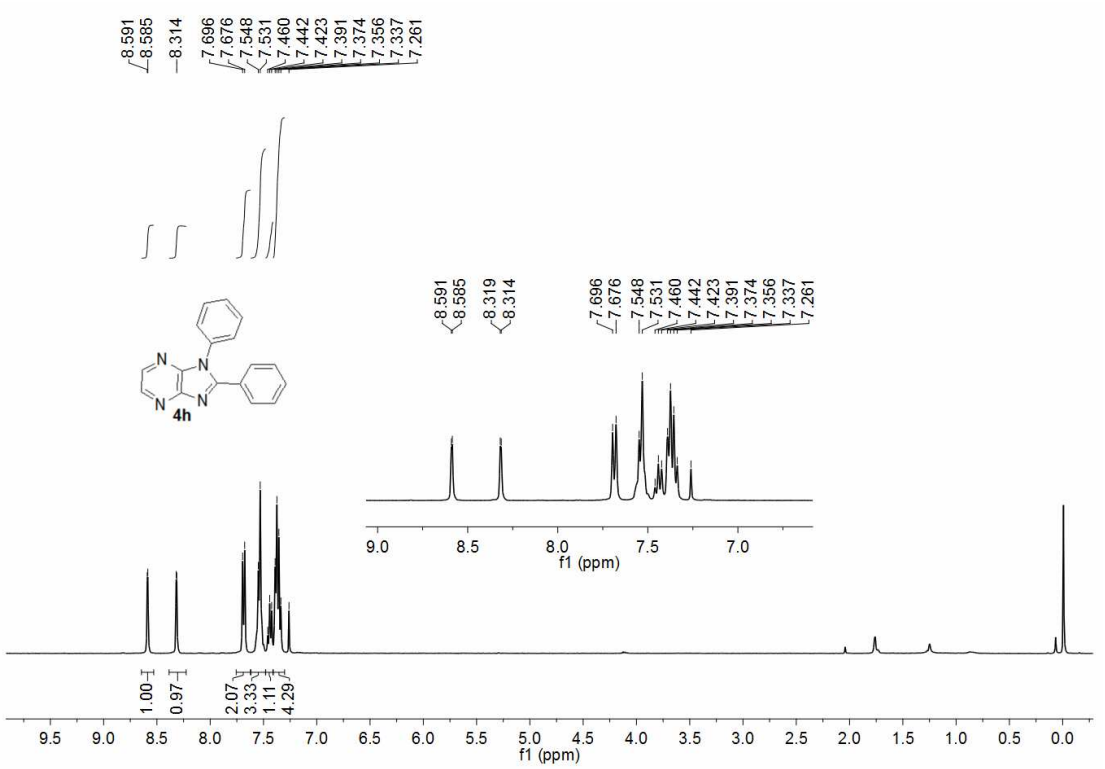

8.097
7.542
7.457
7.438
7.343
7.261
7.206
6.584
6.569
2.967
7.542
7.530
7.518
7.507
7.494
7.457
7.442
7.438
7.423
7.331
7.261
7.220
7.206
7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
F3C
4e
0.96
3.00
3.03
2.00
1.02
2.06
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

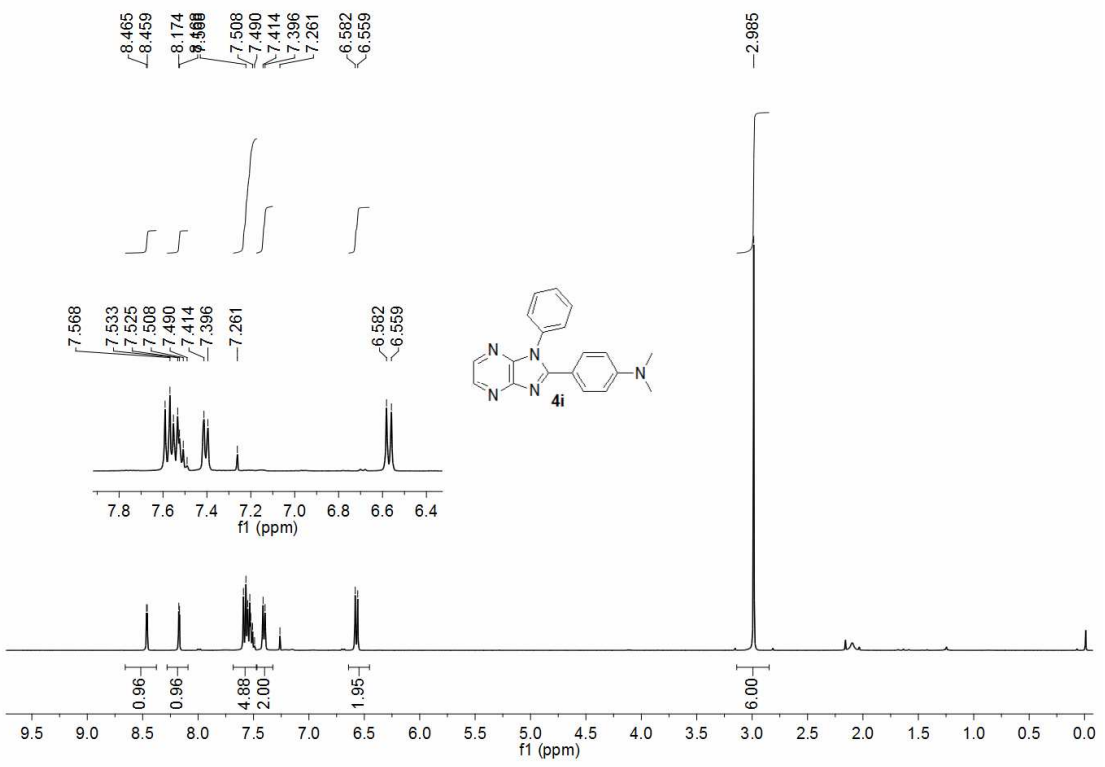

155.276
151.307
142.820
139.443
137.188
130.181
127.629
125.341
124.146
116.807
116.204
111.613
110.436
77.371
77.160
76.948
40.130
130.688
130.181
128.994
127.629
125.946
125.341
125.129
124.146
119.448
119.426
119.405
116.786
116.758
116.735
116.204
F3C
N
N
N
4e
f1 (ppm)
f1 (ppm)

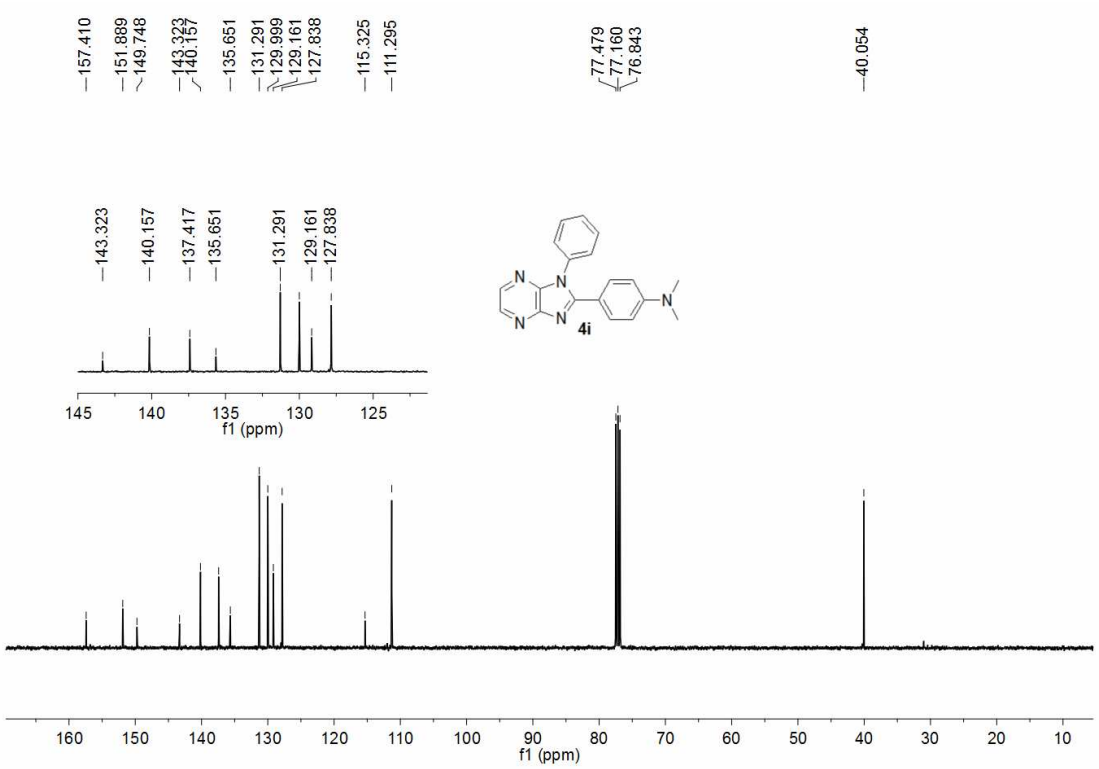

8.069
8.048
7.964
7.892
7.871
7.569
7.518
7.488
7.395
7.377
7.360
7.332
7.314
7.294
7.261
4.402
4.384
4.366
4.349
1.403
1.385
1.367
EtOOC
N
N
4f
1.00
0.84
0.98
5.31
5.36
1.96
3.32
f1 (ppm)
f1 (ppm)

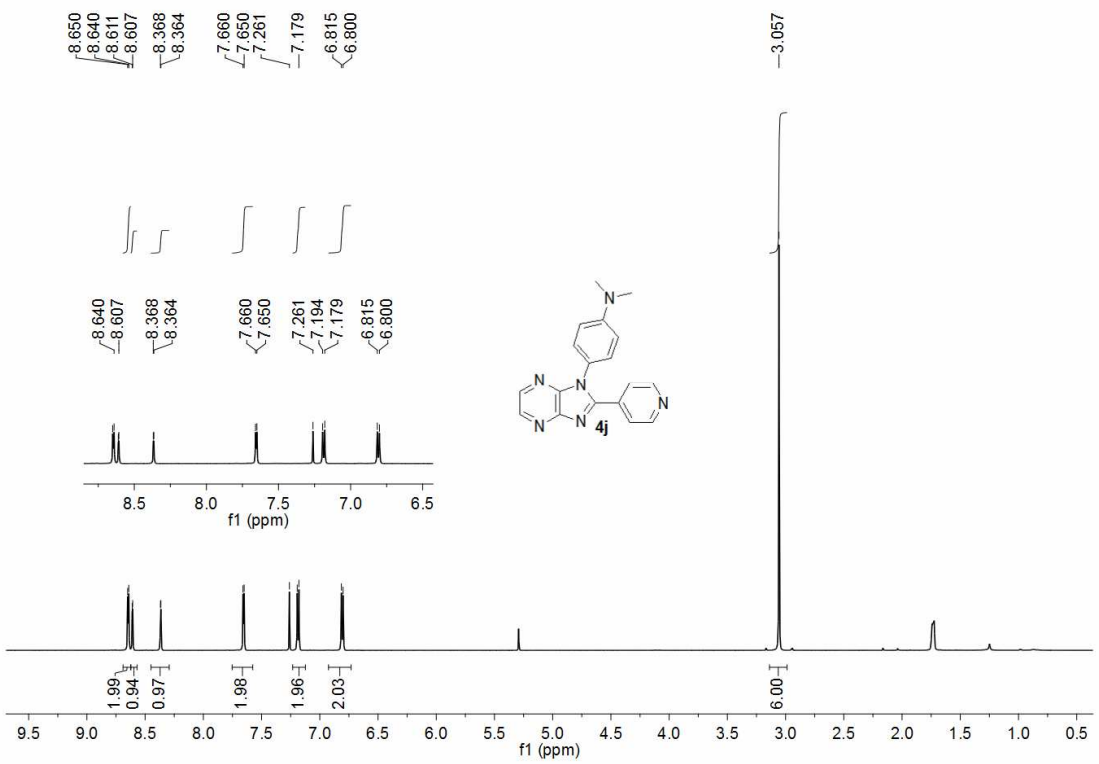

167.096
155.054
146.500
137.165
136.583
129.677
128.524
124.581
119.497
112.877
77.478
77.160
76.843
61.131
14.512
130.213
130.077
129.677
129.547
129.116
128.524
127.570
125.673
124.581
133
130
127
124
f1 (ppm)
EtOOC
N
N
4f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

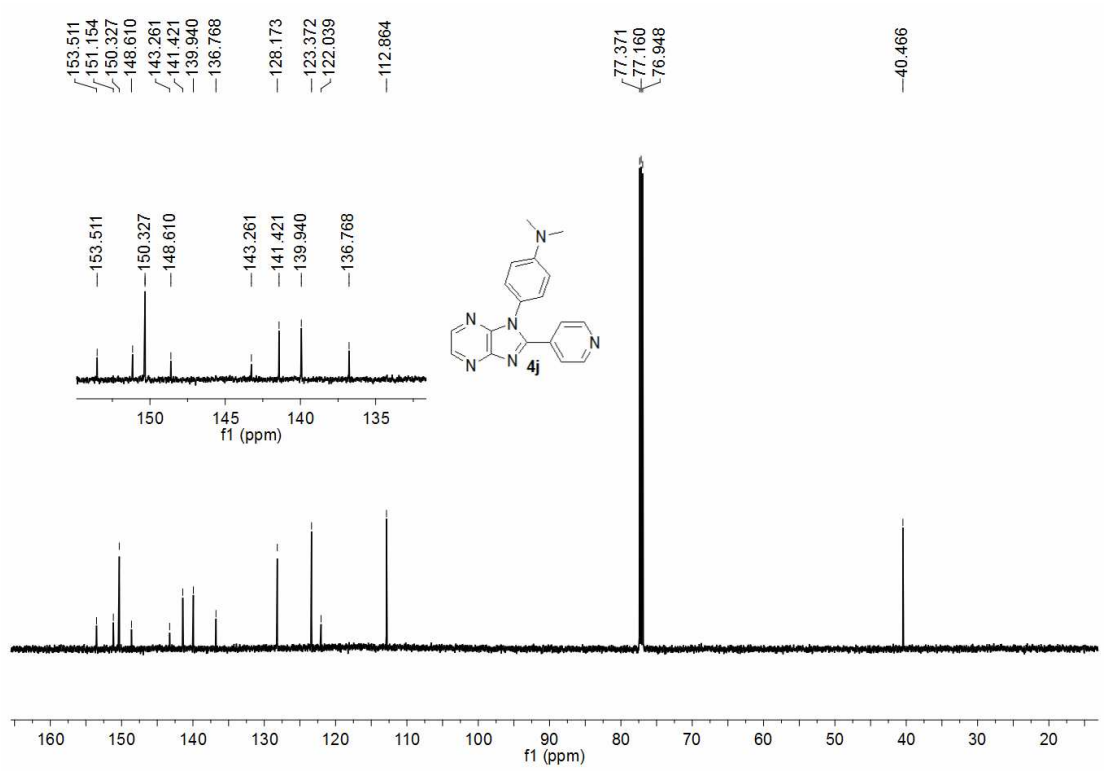

8.399
8.388
8.143
7.603
7.584
7.532
7.515
7.496
7.485
7.467
7.449
7.392
7.374
7.347
7.328
7.310
7.290
7.261
Ph
N
N
N
4g
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
0.92
0.91
2.00
3.21
2.94
3.29
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

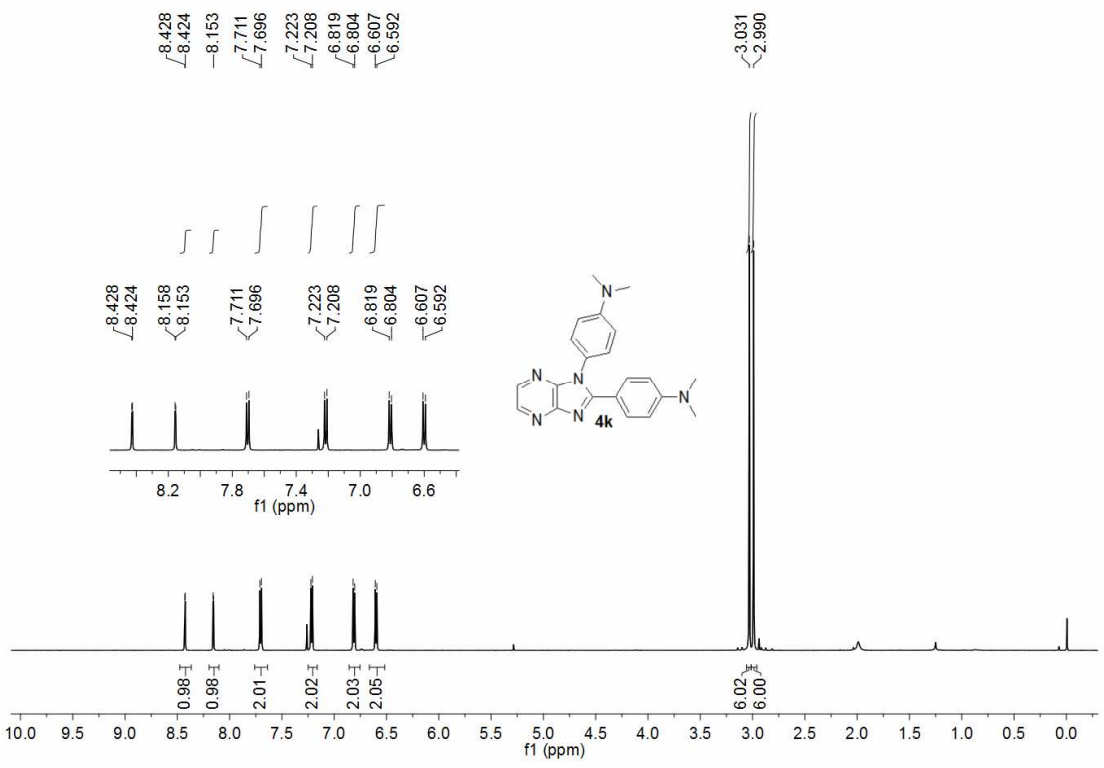

8.591
8.585
8.314
7.696
7.676
7.548
7.531
7.460
7.442
7.423
7.391
7.374
7.356
7.337
7.261
4h
8.319
f1 (ppm)
1.00
0.97
2.07
3.33
1.11
4.29

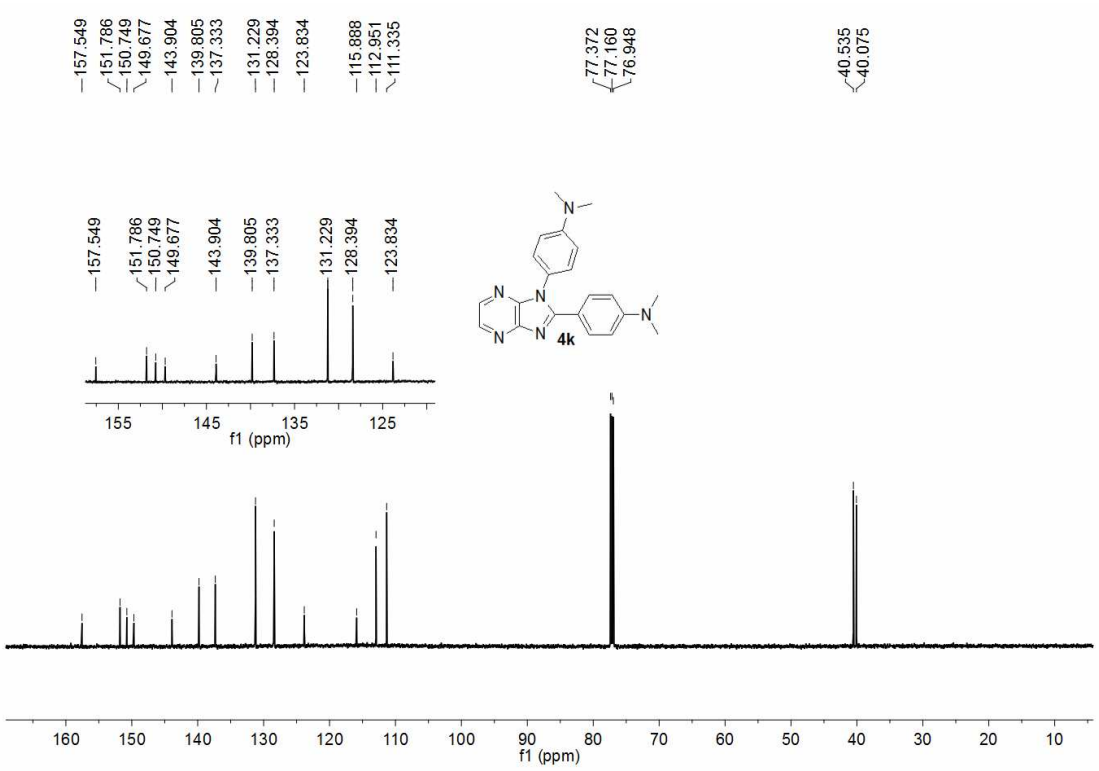

8.465
8.459
8.174
7.508
7.490
7.414
7.396
7.261
6.582
6.559
2.985
7.568
7.533
7.525
4i
f1 (ppm)
0.96
0.96
4.88
2.00
1.95
6.00

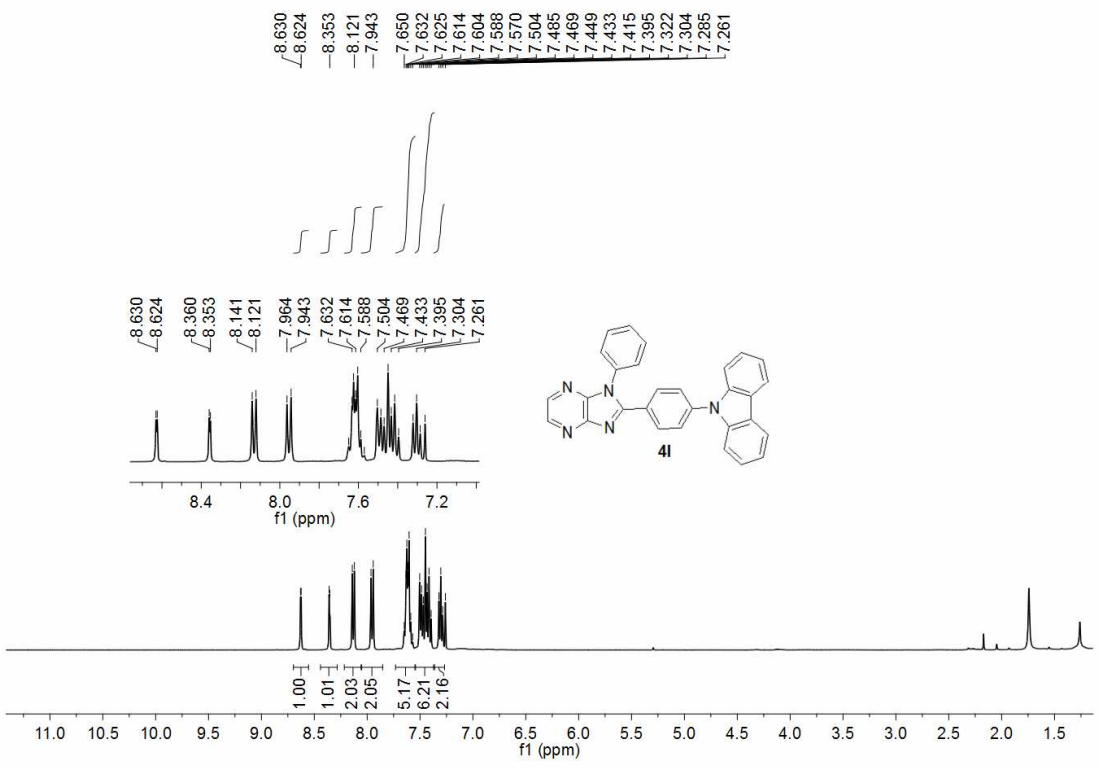

157.410
151.889
149.748
143.323
140.157
135.651
131.291
129.999
129.161
127.838
115.325
111.295
77.479
77.160
76.843
40.054
143.323
140.157
137.417
135.651
131.291
129.161
127.838
4i
f1 (ppm)
f1 (ppm)

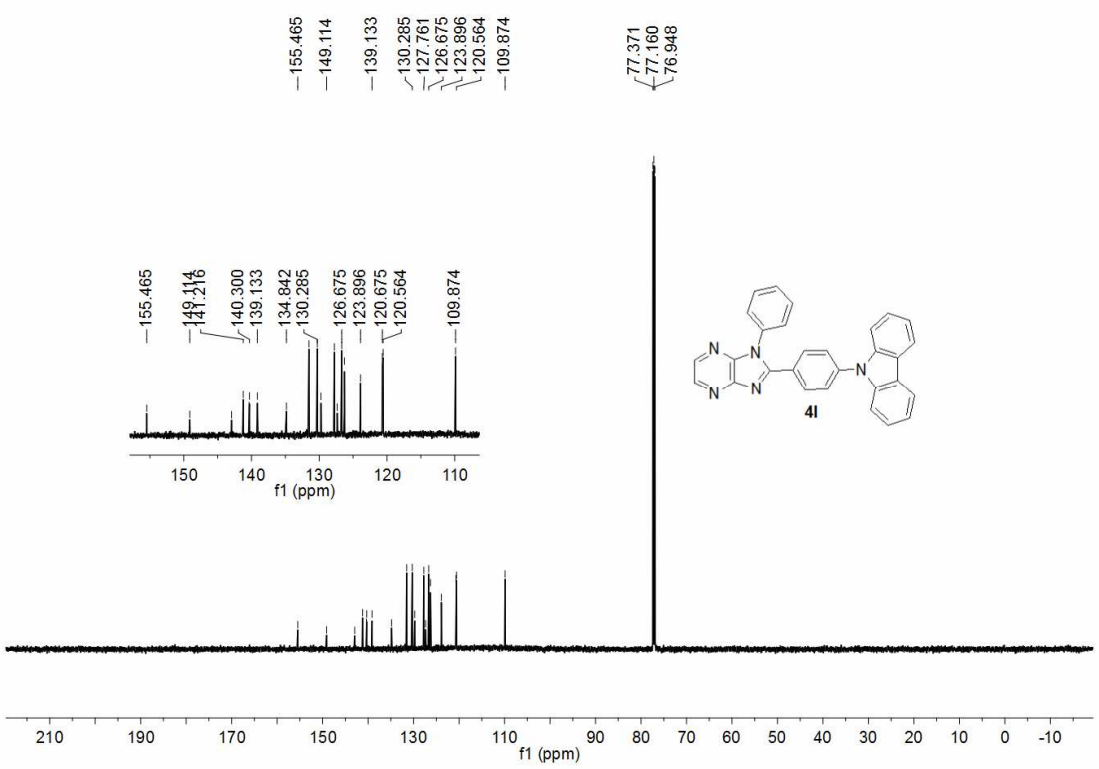

8.650
8.640
8.611
8.607
8.368
8.364
7.660
7.650
7.261
7.179
6.815
6.800
3.057
8.640
8.607
8.368
8.364
7.660
7.650
7.261
7.194
7.179
6.815
6.800
4j
f1 (ppm)
1.99
0.94
0.97
1.98
1.96
2.03
6.00
f1 (ppm)

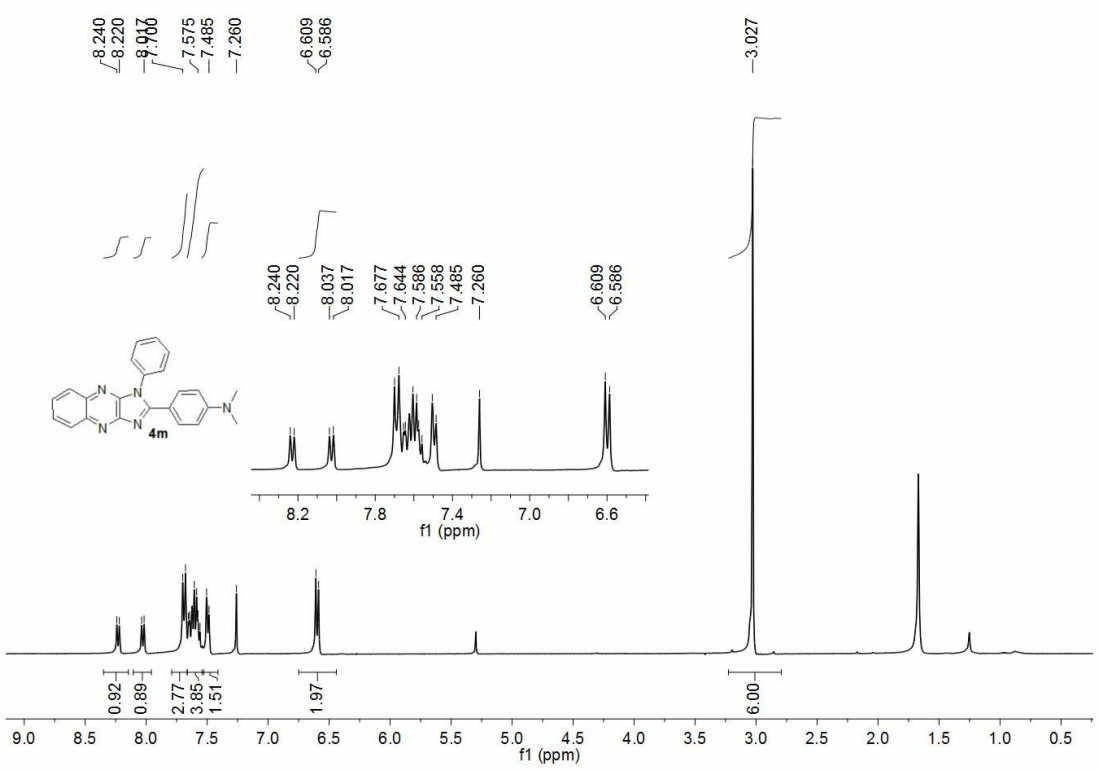

153.511
151.154
150.327
148.610
143.261
141.421
139.940
136.768
128.173
123.372
122.039
112.864
77.371
77.160
76.948
40.466
4j
f1 (ppm)

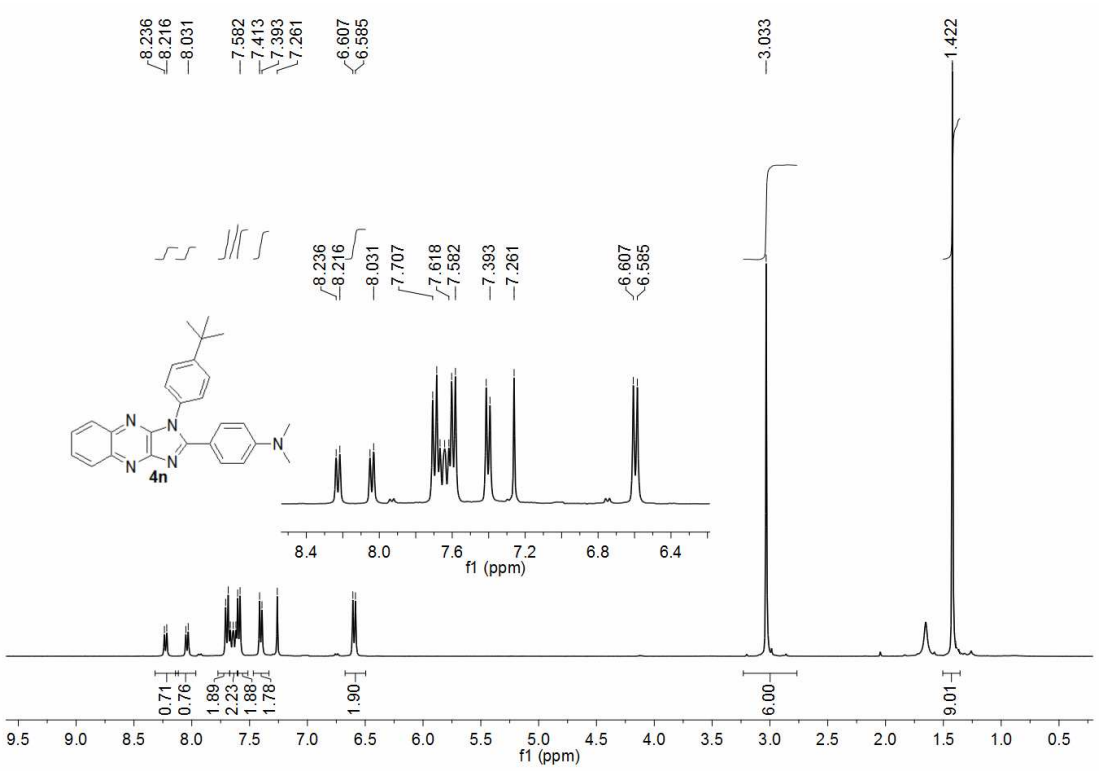

8.428
8.424
8.153
7.711
7.696
7.223
7.208
6.819
6.804
6.607
6.592
3.031
2.990
4k
0.98
0.98
2.01
2.02
2.03
2.05
6.02
6.00
f1 (ppm)

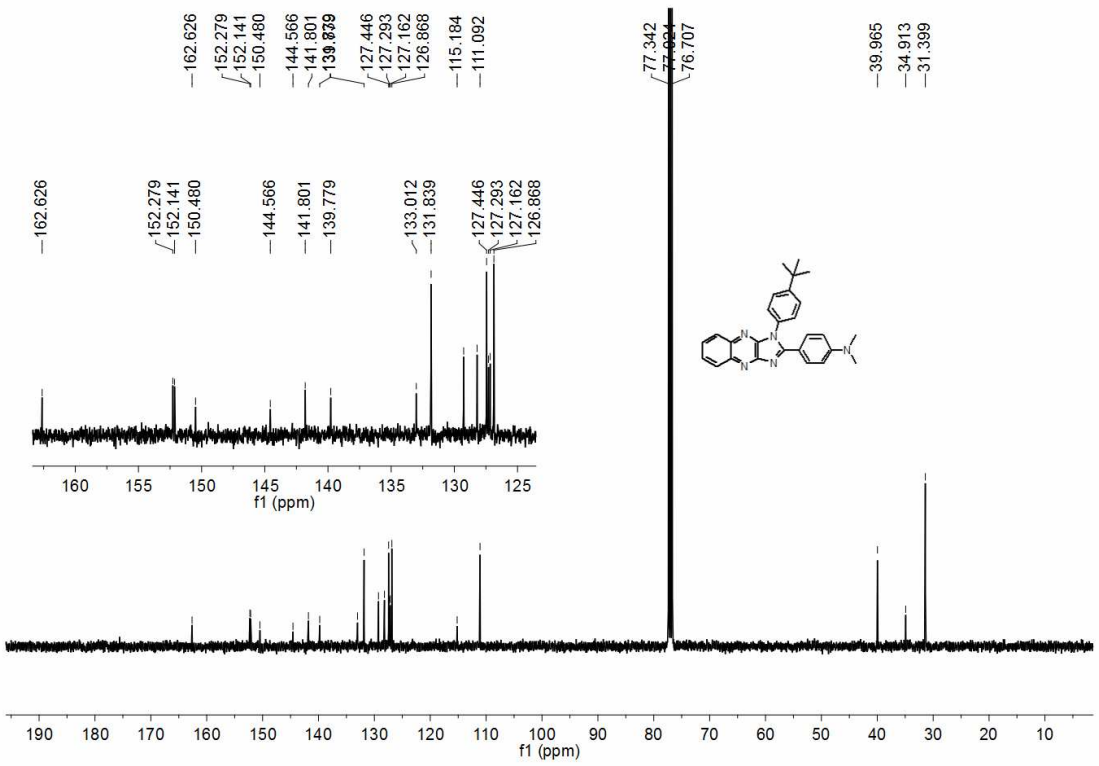

157.549
151.786
150.749
149.677
143.904
139.805
137.333
131.229
128.394
123.834
115.888
112.951
111.335
77.372
77.160
76.948
40.535
40.075
4k
f1 (ppm)

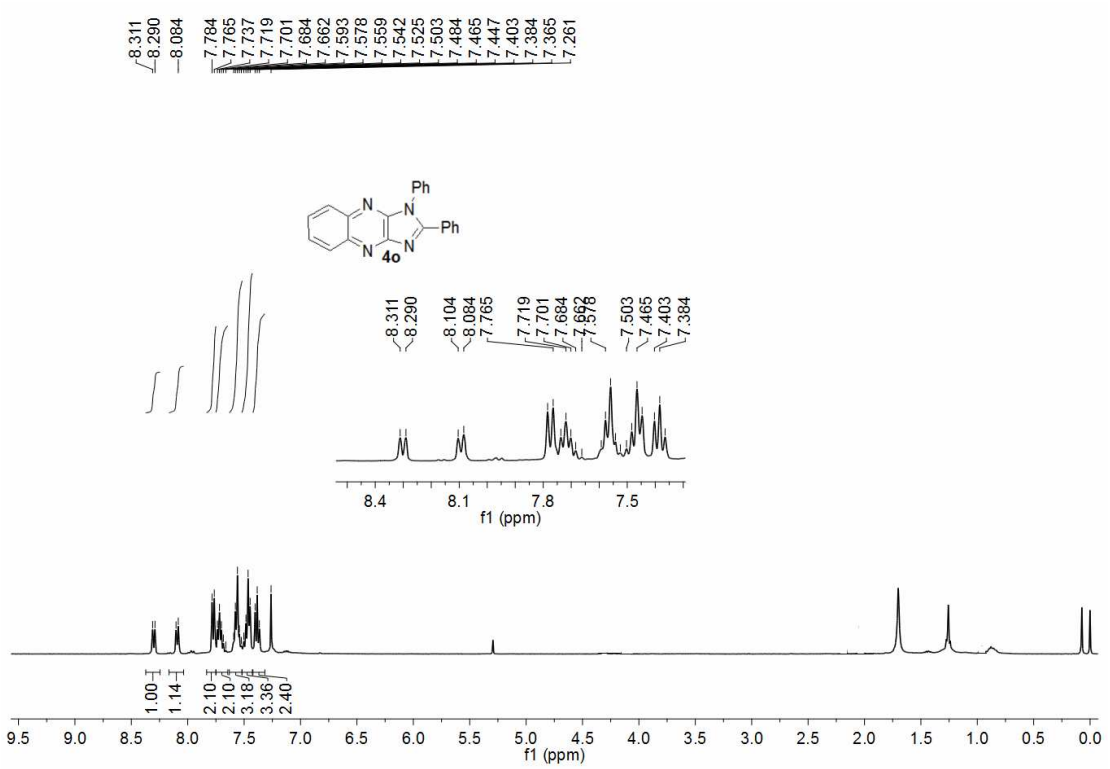

8.630
8.624
8.360
8.353
8.141
8.121
7.964
7.943
7.632
7.614
7.588
7.504
7.469
7.433
7.395
7.304
7.261
4l
1.00
1.01
2.03
2.05
5.17
6.21
2.16
f1 (ppm)

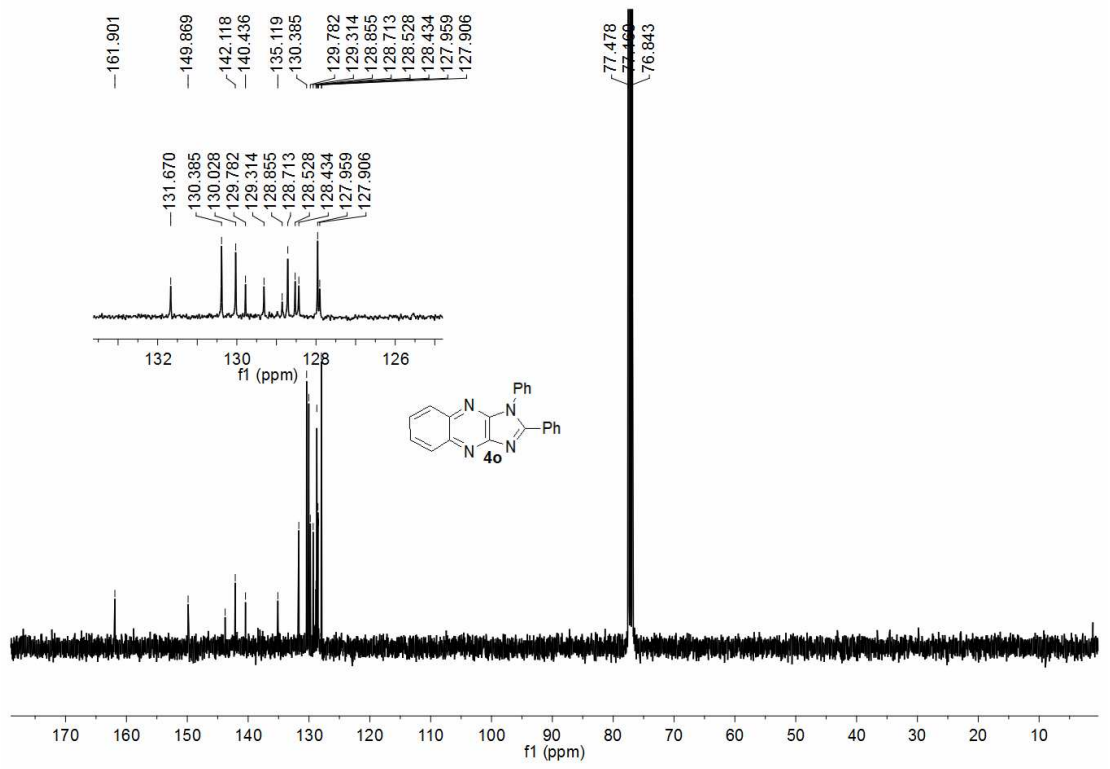

155.465
149.114
139.133
130.285
127.761
126.675
123.896
120.564
109.874
77.371
77.160
76.948
155.465
149.114
141.216
140.300
139.133
134.842
130.285
126.675
123.896
120.675
120.564
109.874
150
140
130
120
110
f1 (ppm)
4l
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

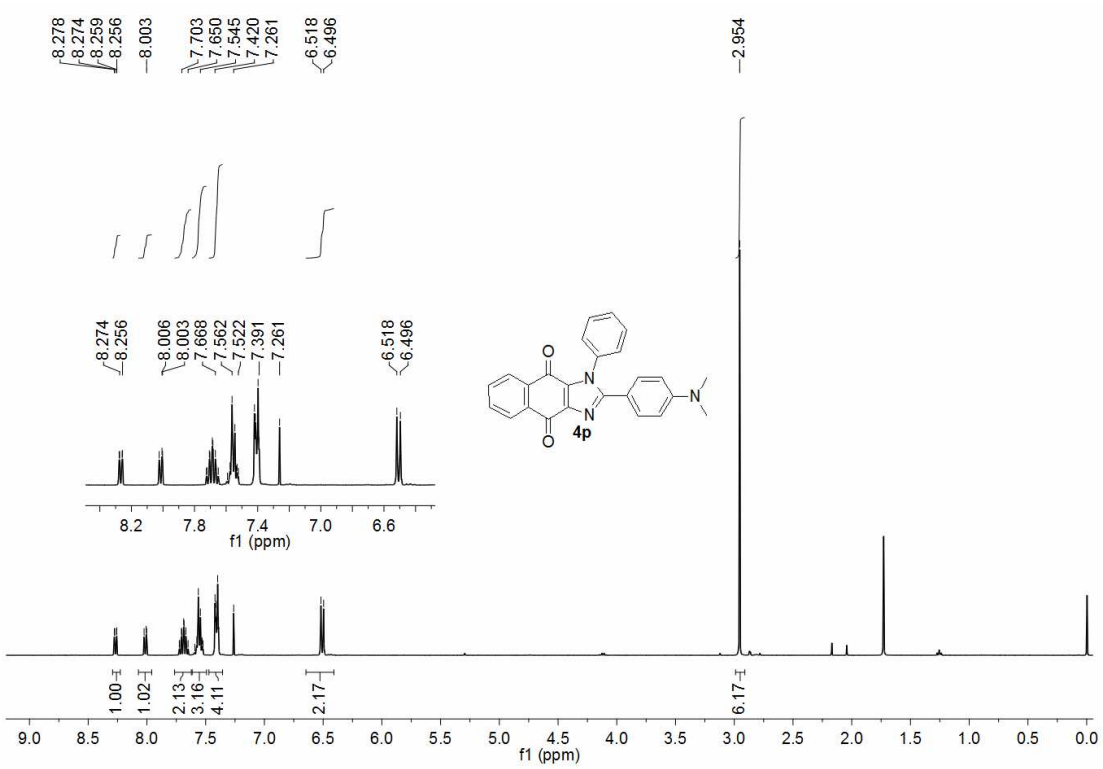

8.240
8.220
8.017
8.000
7.575
7.485
7.260
6.609
6.586
3.027
8.240
8.220
8.037
8.017
7.677
7.644
7.586
7.558
7.485
7.260
6.609
6.586
4m
8.2
7.8
7.4
7.0
6.6
f1 (ppm)
0.92
0.89
2.77
3.85
1.51
1.97
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

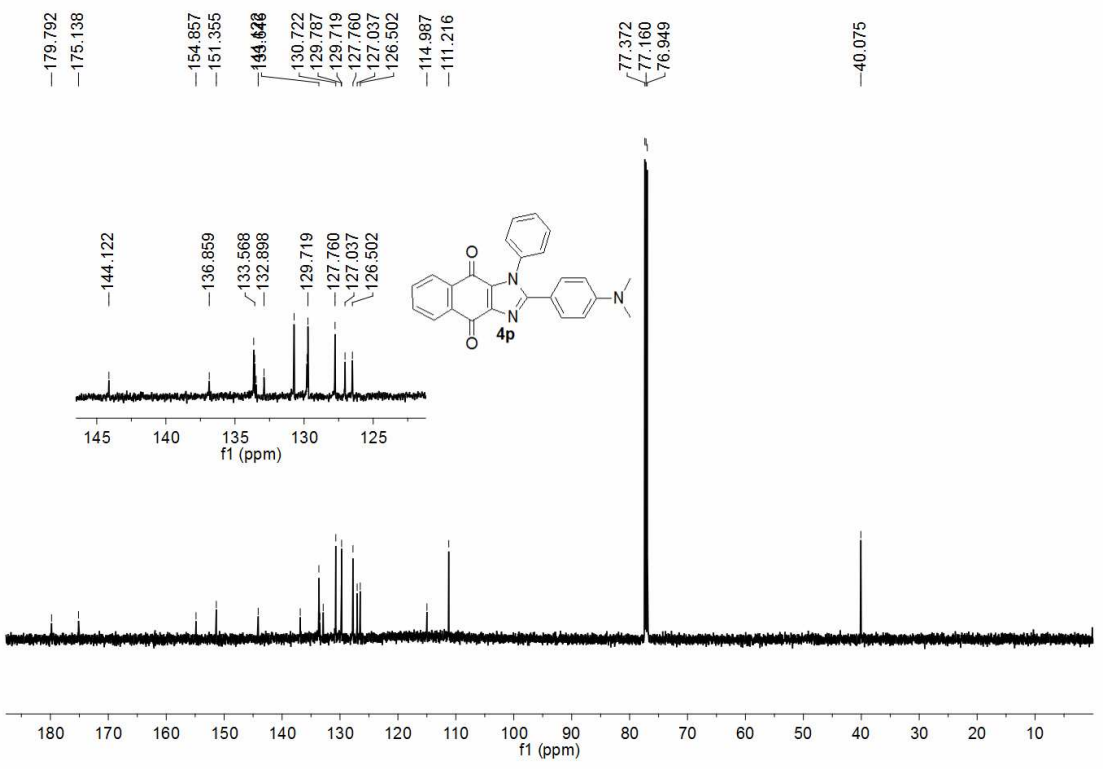

8.236
8.216
8.031
7.582
7.413
7.393
7.261
6.607
6.585
3.033
1.422
4n
f1 (ppm)
0.71
0.76
1.89
2.23
1.88
1.78
1.90
6.00
9.01

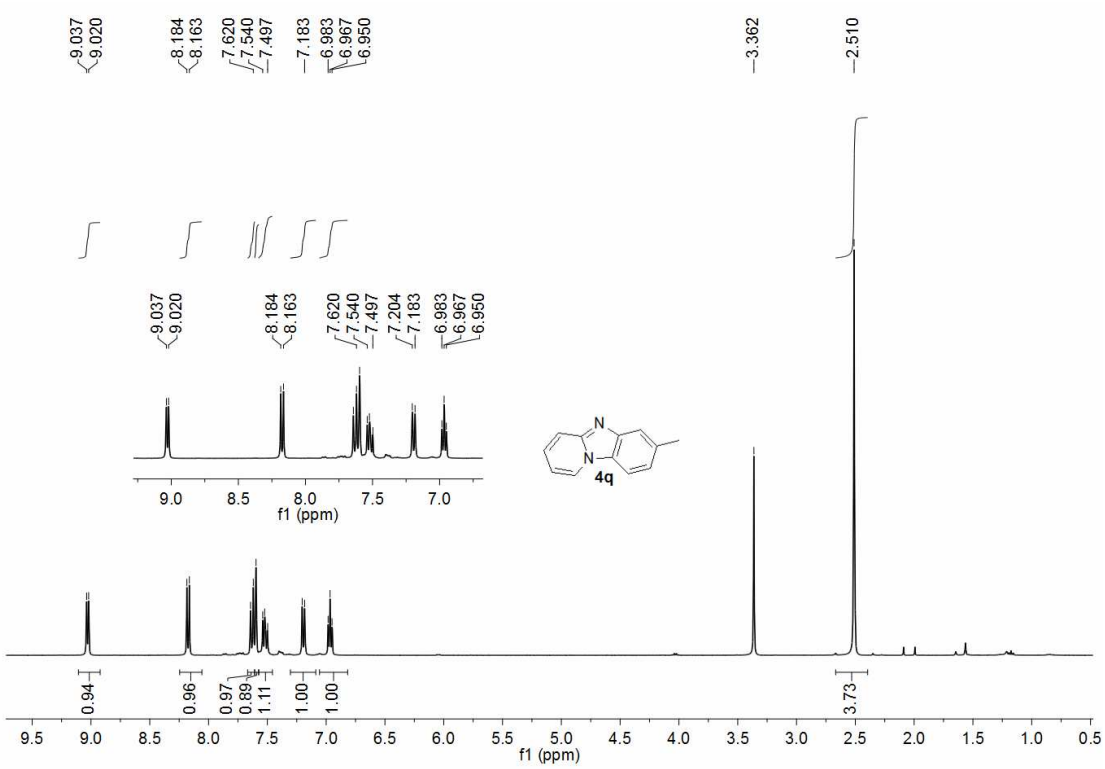

162.626
152.279
152.141
150.480
144.566
141.801
139.779
133.012
131.839
127.446
127.293
127.162
126.868
115.184
111.092
77.342
76.707
39.965
34.913
31.399
f1 (ppm)

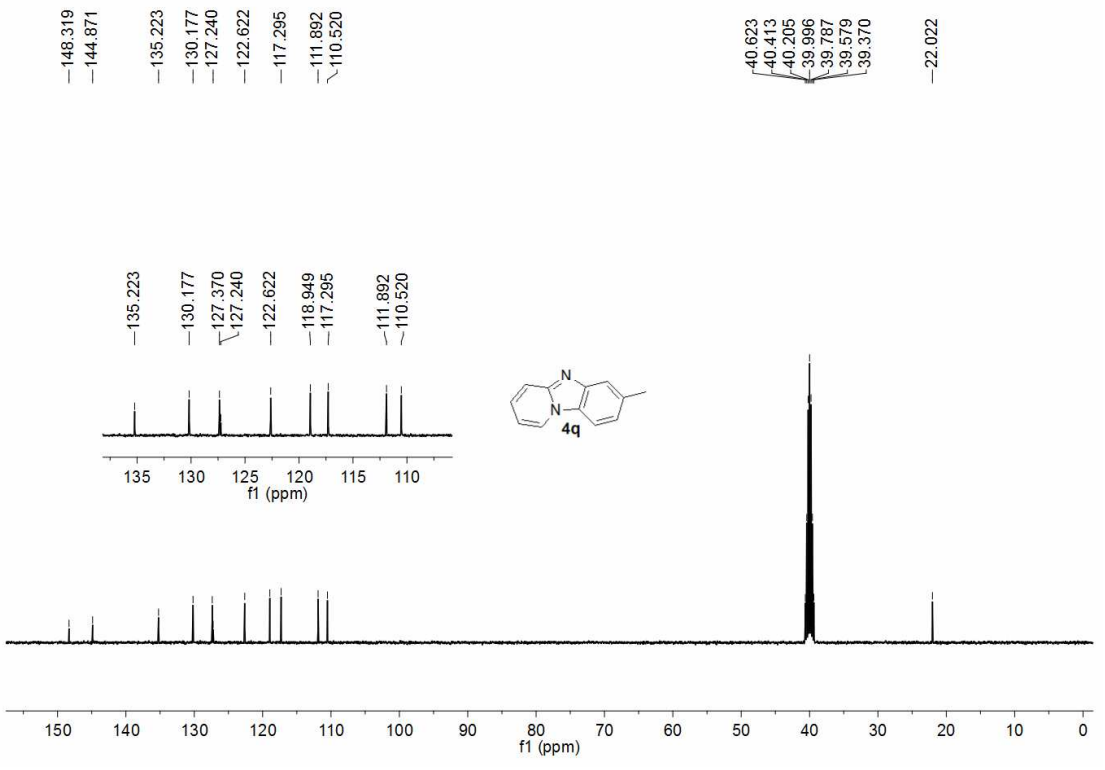

8.311
8.290
8.084
7.784
7.765
7.737
7.719
7.701
7.684
7.662
7.593
7.578
7.559
7.542
7.525
7.503
7.484
7.465
7.447
7.403
7.384
7.365
7.261
Ph
Ph
4o
8.104
8.084
7.765
7.719
7.701
7.684
7.503
7.465
7.403
7.384
8.4
8.1
7.8
7.5
f1 (ppm)
1.00
1.14
2.10
2.10
3.18
3.36
2.40
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

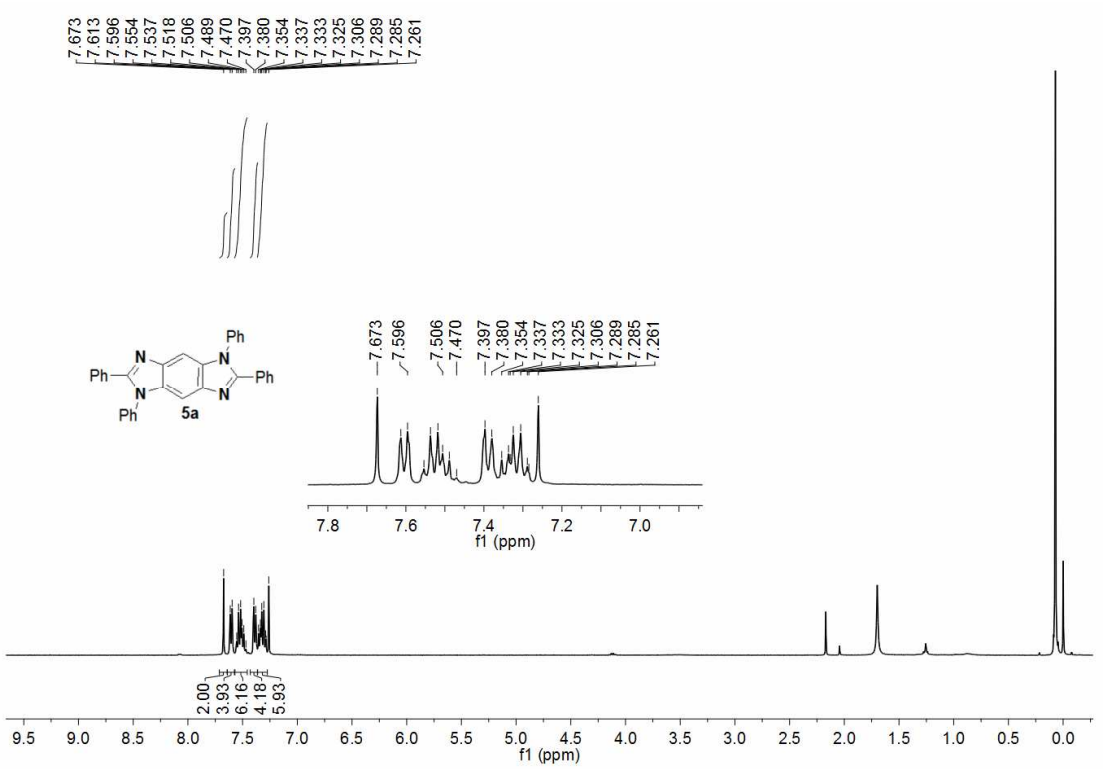

161.901
149.869
142.118
140.436
135.119
130.385
129.782
129.314
128.855
128.713
128.528
128.434
127.959
127.906
77.478
77.160
76.843
131.670
130.385
130.028
129.782
129.314
128.855
128.713
128.528
128.434
127.959
127.906
132
130
128
126
f1 (ppm)
Ph
Ph
4o
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

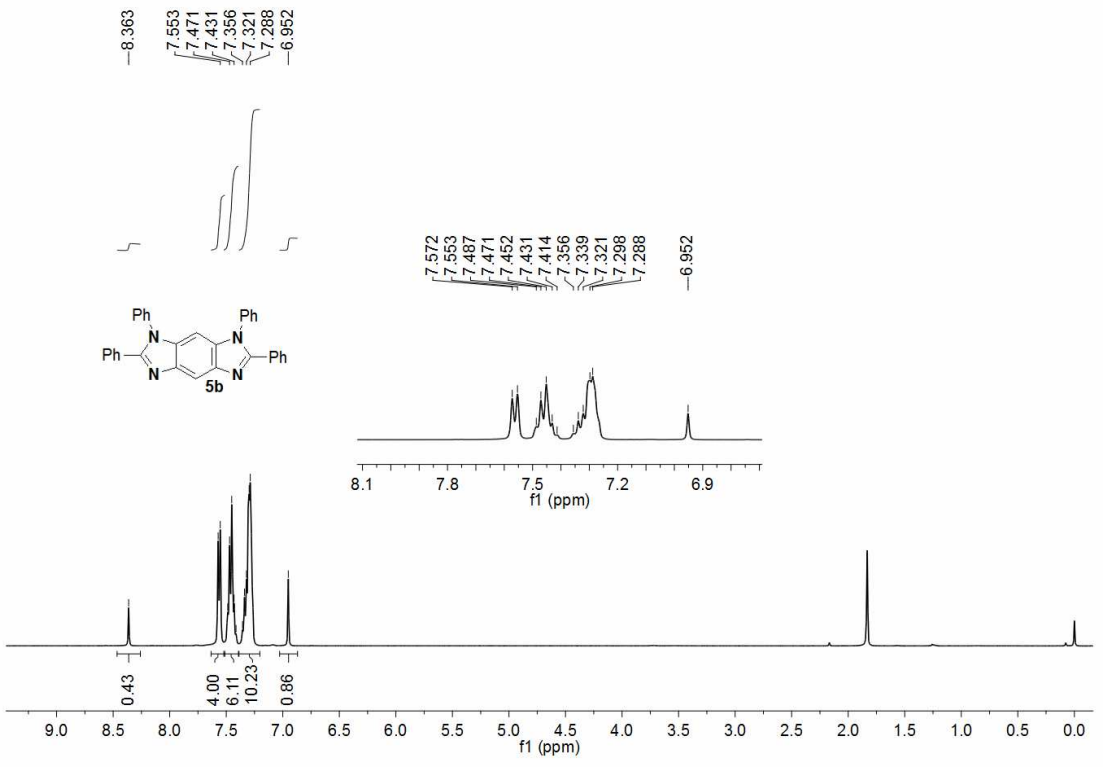

8.278
8.274
8.259
8.256
8.003
7.703
7.650
7.545
7.420
7.261
6.518
6.496
2.954
8.274
8.256
8.006
8.003
7.668
7.562
7.522
7.391
7.261
6.518
6.496
4p
8.2
7.8
7.4
7.0
6.6
f1 (ppm)
1.00
1.02
2.13
3.16
4.11
2.17
6.17
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

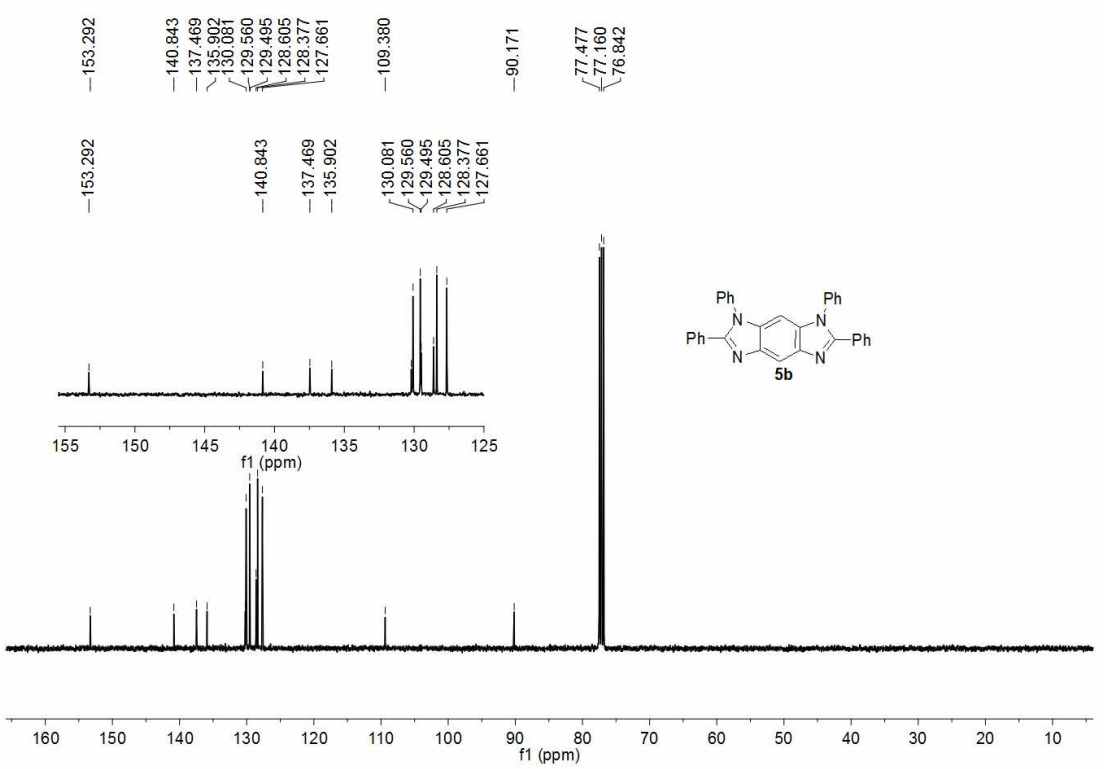

179.792
175.138
154.857
151.355
130.722
129.787
129.719
127.760
127.037
126.502
114.987
111.216
77.372
77.160
76.949
40.075
144.122
136.859
133.568
132.898
129.719
127.760
127.037
126.502
4p
145
140
135
130
125
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

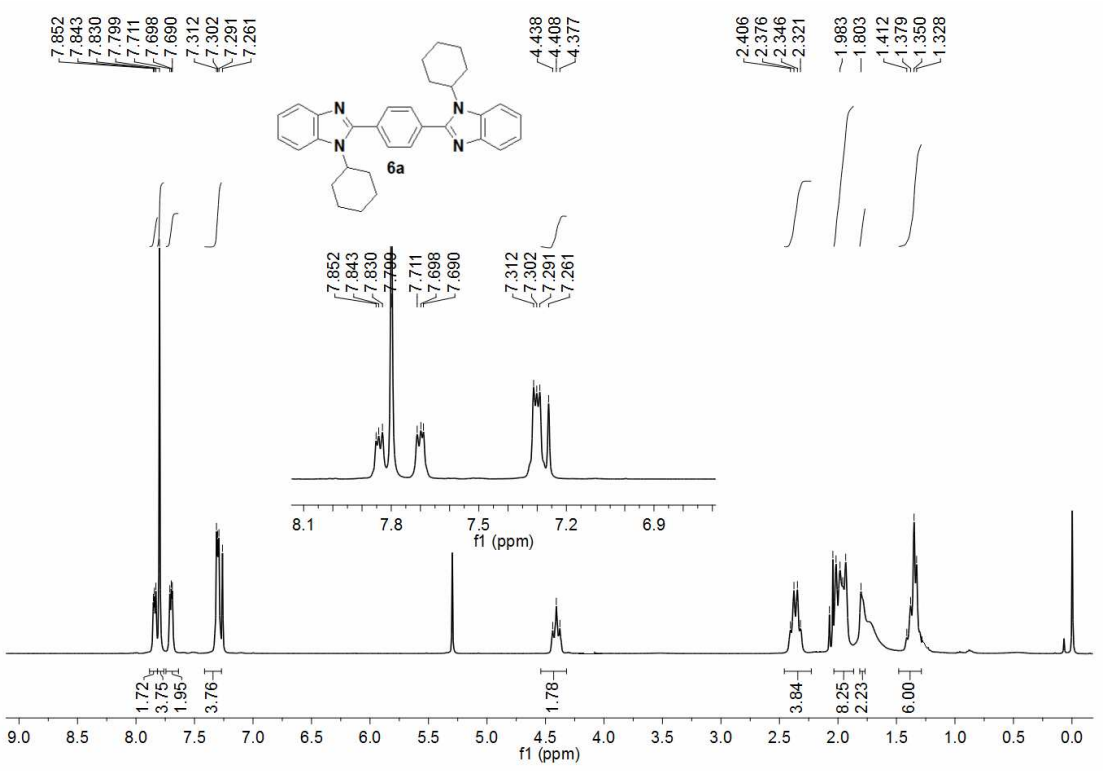

9.037
9.020
8.184
8.163
7.620
7.540
7.497
7.204
7.183
6.983
6.967
6.950
3.362
2.510
4q
f1 (ppm)
0.94
0.96
0.97
0.89
1.11
1.00
1.00
3.73

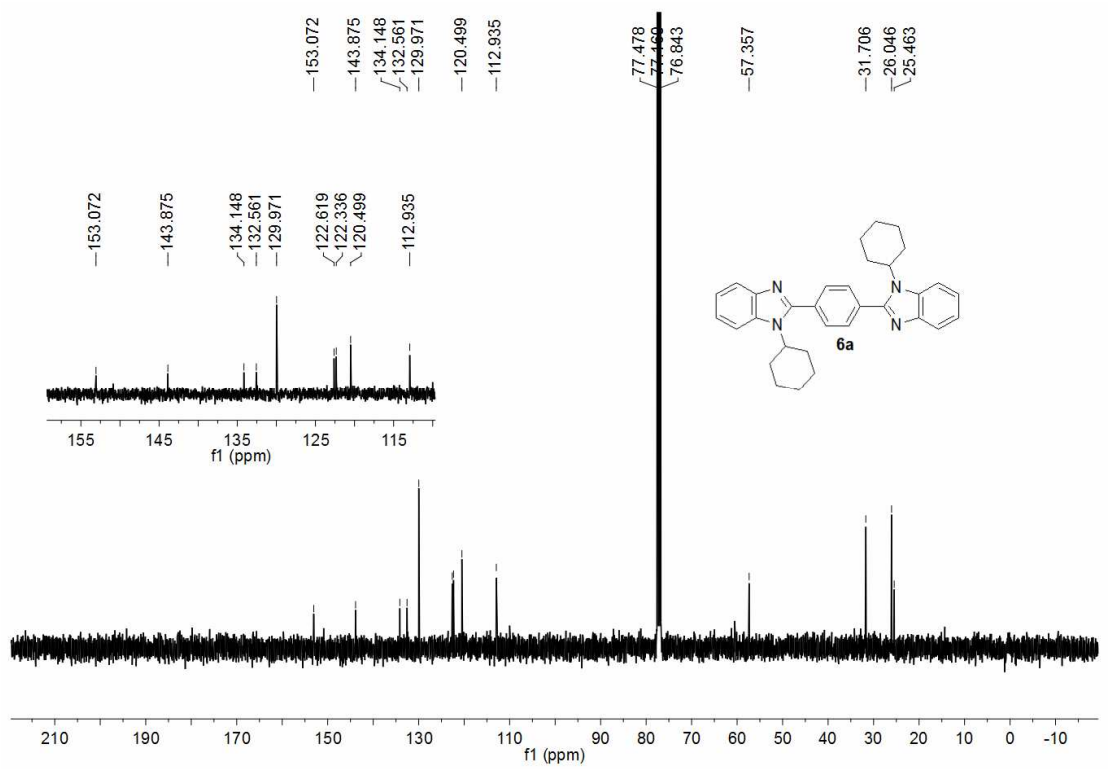

148.319
144.871
135.223
130.177
127.240
122.622
117.295
111.892
110.520
40.623
40.413
40.205
39.996
39.787
39.579
39.370
22.022
127.370
118.949
4q
f1 (ppm)


7.673
7.613
7.596
7.554
7.537
7.518
7.506
7.489
7.470
7.397
7.380
7.354
7.337
7.333
7.325
7.306
7.289
7.285
7.261
Ph
N
Ph
N
Ph
N
Ph
N
5a
7.673
7.596
7.506
7.470
7.397
7.380
7.354
7.337
7.333
7.325
7.306
7.289
7.285
7.261
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
2.00
3.93
6.16
4.18
5.93
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


8.363
7.553
7.471
7.431
7.356
7.321
7.288
6.952
Ph
Ph
N
Ph
N
Ph
N
Ph
N
5b
7.572
7.553
7.487
7.471
7.452
7.431
7.414
7.356
7.339
7.321
7.298
7.288
6.952
8.1
7.8
7.5
7.2
6.9
f1 (ppm)
0.43
4.00
6.11
10.23
0.86
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.292
140.843
137.469
135.902
130.081
129.560
129.495
128.605
128.377
127.661
109.380
90.171
77.477
77.160
76.842
Ph
Ph
Ph
Ph
N
N
N
N
5b
f1 (ppm)


7.852
7.843
7.830
7.799
7.711
7.698
7.690
7.312
7.302
7.291
7.261
4.438
4.408
4.377
2.406
2.376
2.346
2.321
1.983
1.803
1.412
1.379
1.350
1.328
N
N
N
N
6a
f1 (ppm)
1.72
3.75
1.95
3.76
1.78
3.84
8.25
2.23
6.00


153.072
143.875
134.148
132.561
129.971
120.499
112.935
77.478
77.160
76.843
57.357
31.706
26.046
25.463
122.619
122.336
6a
f1 (ppm)
f1 (ppm)