Supporting Information

N-Benzylhydroxylamine as a novel synthetic block in "C1N1" embedding reaction *via* α–C(sp^3)−H activation strategy

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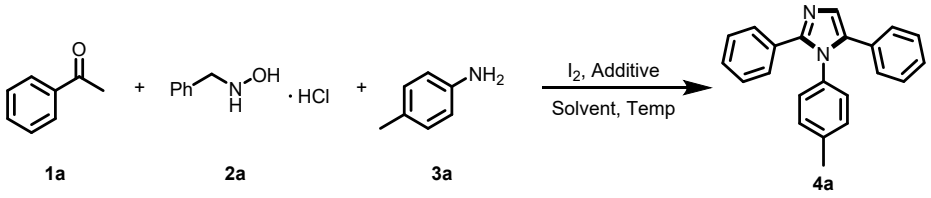
1. General

All of the substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Flash column chromatography was performed on silica gel (200–300 mesh). ^{1}H NMR spectra were determined at 25 °C on a Varian Mercury 400 MHz spectrometer. Chemical shifts were provided in ppm relative to the internal standard of tetramethylsilane (TMS). ^{13}C spectra were recorded in $CDCl_3$ on 100 MHz NMR spectrometers and resonances (δ) in ppm. The data is being reported as s = singlet, d = doublet, t = triplet, m = multiplet or unresolved coupling constant(s) in Hz, integration. HRMS were obtained on Thermo Scientific Q Exactive equipped with an electron spray ionization source. Melting points were determined by using an electrothermal capillary melting point apparatus and not corrected. The X-ray crystal-structures were obtained on a Bruker APEX DUO CCD system.

2. Experimental procedures

2.1 Optimization of the reaction conditions [a,b]

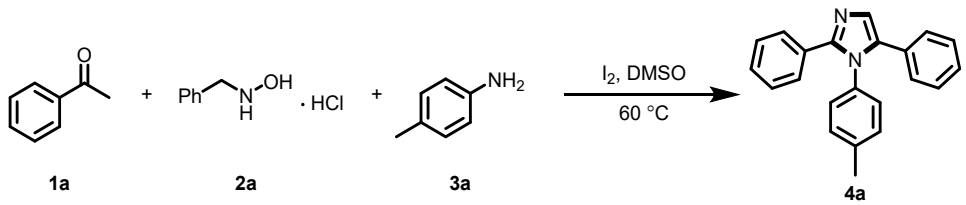


1a 2a 3a 4a

Entry	**1a**:**2a:3a**	I_2 (equiv.)	Additive (equiv.)	solvent	Temp (°C)	Yield[b] (%)
1	1:1:1	1.6		DMSO	100	41
2	1:1:1	1.6		DMSO	120	29
	1:1:1	1.6		DMSO	140	25
3	1:1:1	1.6		DMSO	80	50
4	1:1:1	1.6		DMSO	60	63
5	1:1:1	1.6		DMSO	40	26
6	1:1:1	1.6	TFA (1.0)	DMSO	60	46
7	1:1:1	1.6	TfOH (1.0)	DMSO	60	40
8	1:1:1	1.6	HI (1.0)	DMSO	60	31
9	1:1:1	1.6	TsOH (1.0)	DMSO	60	37
10	1:1:1	1.6	PhCOOH (1.0)	DMSO	60	49
11	1:1:1	1.6	$ZnCl_2$ (1.0)	DMSO	60	28
12	1:1:1	1.6	$FeCl_3$ (1.0)	DMSO	60	43
13	1:1:1	1.6	$CuBr_2$ (1.0)	DMSO	60	trace
14	1:1:1	1.6	Morpholine (1.0)	DMSO	60	50
15	1:1:1	1.6	DABCO (1.0)	DMSO	60	46
16	1:1:1	1.6	Cs_2CO_3 (1.0)	DMSO	60	33
17	1:1:1	1.6	$NaHCO_3$ (1.0)	DMSO	60	47
18	2:1:1	1.6		DMSO	60	56
19	1:2:1	1.6		DMSO	60	31
20	1:1:2	1.6		DMSO	60	43
21	**1:2:2**	**1.6**		**DMSO**	**60**	**70**
22	1:3:2	1.6		DMSO	60	54
23	1:2:2	0		DMSO	60	ND
24	1:2:2	0.8		DMSO	60	59
25	1:2:2	1.2		DMSO	60	64
26	1:2:2	2.0		DMSO	60	57
27	1:2:2	1.6		THF	60	ND
28	1:2:2	1.6		MeCN	60	ND
29	1:2:2	1.6		EtOH	60	ND
30	1:2:2	1.6		H_2O	60	ND
31	1:2:2	1.6		DMF	60	ND
32	1:2:2	1.6		1,4-Dioxane	60	ND
33	1:2:2	1.6		DCM	60	ND
34	1:2:2	1.6		DCE	60	ND

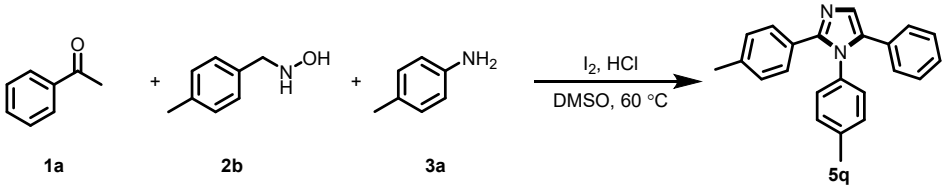
[a]Reaction conditions: **1a** (0.5 mmol, 1.0 equiv.), **2a** (equiv.), **3a** (equiv.), I_2 (equiv.), additive (equiv.) and indicated temperature heated in solvent (3mL) for 8 h. [b]Products were obtained in isolated yields.

2.2 General procedure for the synthesis of 4 or 5a-5p (4a as an example)



A tube equipped with a magnetic stirring bar was charged with acetophenone (**1a**) (60.0 mg, 0.5 mmol), *N*-Benzylhydroxylamine hydrochloride (**2a**) (160.0 mg, 1.0 mmol), *p*-toluidine (**3a**) (107.0 mg, 1.0 mmol), and iodine (203.0 mg, 0.8 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 60 °C for 8 h and monitored by TLC. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) to yield the desired product **4a** (108.6 mg, yield 70%) as light yellow solid.

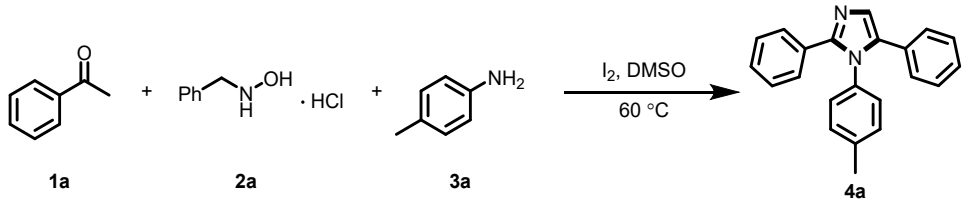
2.3 General procedure for the synthesis of 5q



A tube equipped with a magnetic stirring bar was charged with acetophenone (**1a**) (60.0 mg, 0.5 mmol), *N*-(4-methylbenzyl)hydroxylamine (**2b**) (137.0 mg, 1.0 mmol), *p*-toluidine (**3a**) (107.0 mg, 1.0 mmol), and iodine (203.0 mg, 0.8 mmol) at room temperature, and DMSO (3 mL) was added, followed by the dropwise addition of a 12 N HCl (36 mg, 1.0 mmol, 2.0 equiv) at 60 °C. The resulting mixture was stirred at 60 °C for 8 h and monitored by TLC. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 8:1) to yield the desired product **5q** (76.2 mg, yield 47%) as light

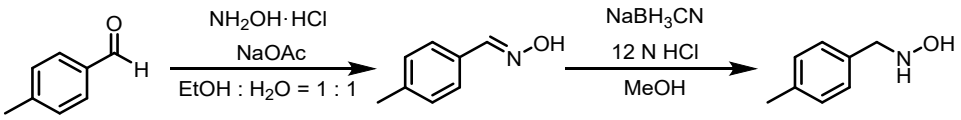
yellow solid.

2.4 General procedure for the synthesis of 4a in a 10.0 mmol scale



A 100 mL round-bottomed flask was charged with acetophenone (**1a**) (1.20 g, 10.0 mmol), *N*-Benzylhydroxylamine hydrochloride (**2a**) (3.20 g, 20.0 mmol), *p*-toluidine (**3a**) (2.14 g, 20.0 mmol), and iodine (4.06 g, 16.0 mmol) at room temperature, and DMSO (50 mL) was added. The resulting mixture was stirred at 60 °C for 8 h in oil bath and monitored by TLC. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (200 mL), extracted with EtOAc (3 × 200 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) to yield the desired product **4a** (1.98 g, yield 64%) as light yellow solid.

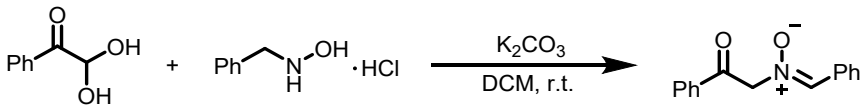
2.5 Preparation of hydroxylamines from aldehydes [1]



To a solution of an aldehyde (1.2g, 10 mmol, 1.0 equiv.) and hydroxylammonium chloride (0.83 g, 12 mmol, 1.2 equiv.) in ethanol-water (10 mL:10 mL) was added sodium acetate (1.64 g, 20 mmol, 2.0 equiv). The solution was stirred until the aldehyde was fully consumed. The solvent was removed under vacuum, and the residue was separated between water and EtOAc. The aqueous layer was washed with EtOAc (2× 50 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated to afford oxime that was used for the next step without further purification. The oxime obtained in the previous step was suspended in MeOH (20 mL), to which sodium cyanoborohydride (0.75g, 12 mmol, 1.2 equiv.) was added, followed by the dropwise addition of a 12 N HCl (8.3 mL, 100 mmol, 10.0 equiv.) at 0 °C. After stirring for 4 h at room temperature, the reaction mixture was poured into water and the whole mixture was neutralized with KOH pellet at 0 °C. Then, extractive work-up was performed with EtOAc, and the organic extracts

were washed with brine, dried over anhydrous Na_2SO_4, and concentrated. The hydroxylamine could be used directly without further purification.

2.6 Procedure for the synthesis of 6 [2]

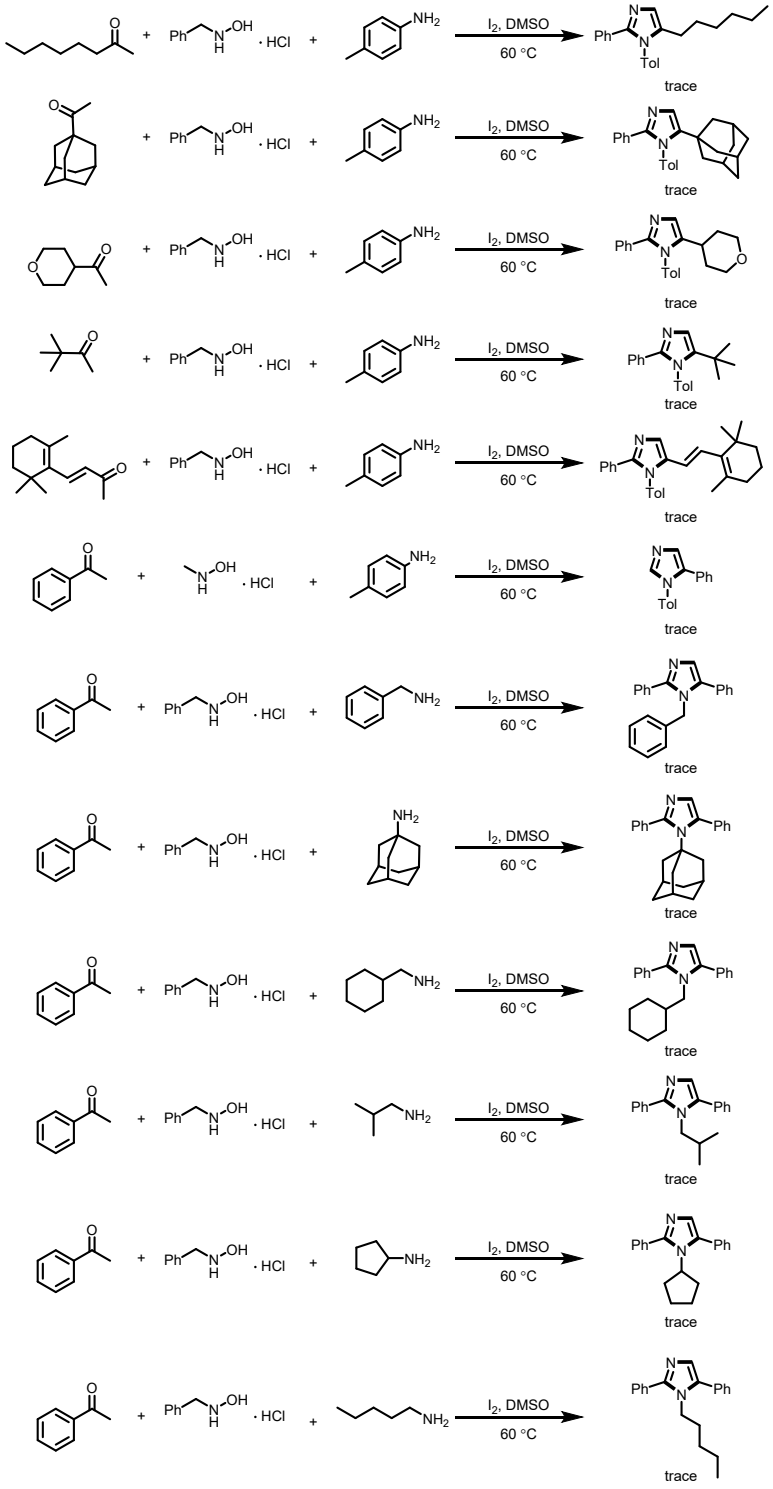


1ac **2a** **6**

To a stirred solution of *N*-Benzylhydroxylamine hydrochloride **2a** (319 mg, 1.0 equiv., 2 mmol) and K_2CO_3 (828 mg, 3.0 equiv., 6 mmol) in DCM was added phenylglyoxal monohydrate **1ac** (334mg, 1.1 equiv., 2.2 mmol) at room temperature. The mixture was stirred overnight, and then filtrated on celite, evaporation under vacuum. The residue was then crystallized from dichloromethane and petroleum ether, to give the product **6** (454.1 mg, yield 95%) as orange solid.

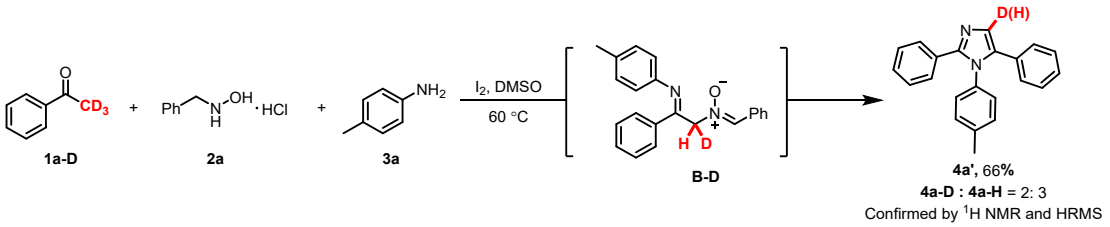
3. Substrate scope of alkyl reactants

We employed some alkyl reactants under the optimized reaction conditions, to our disappointment, the aliphatic ketones, alkyl hydroxylamine, and aliphatic amines were not compatible with this transformation, and the trace desired products only could be detected in the crude reaction extract by HRMS analysis.

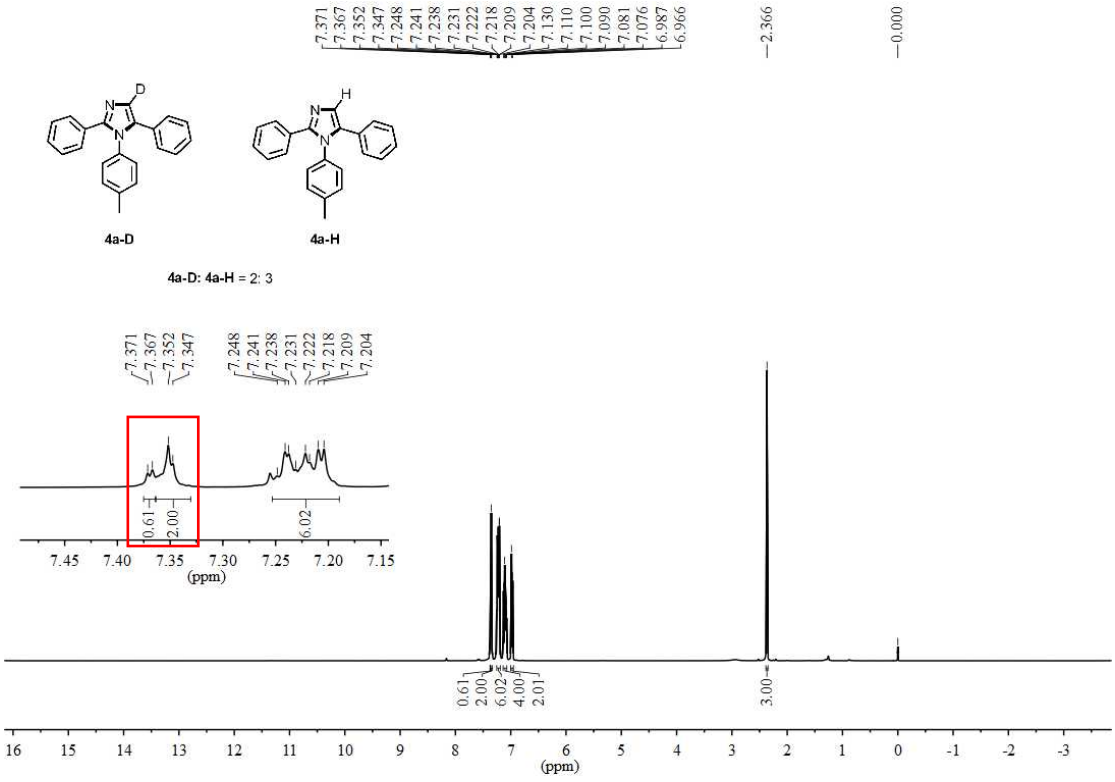


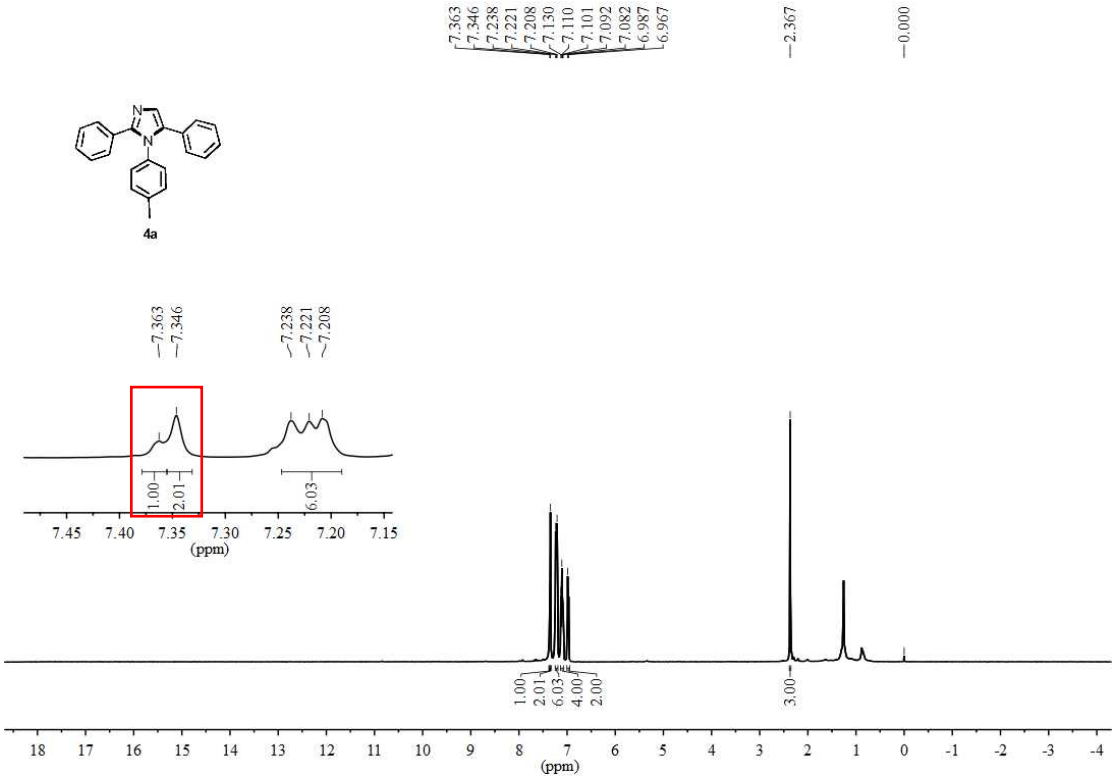
4. Mechanistic study

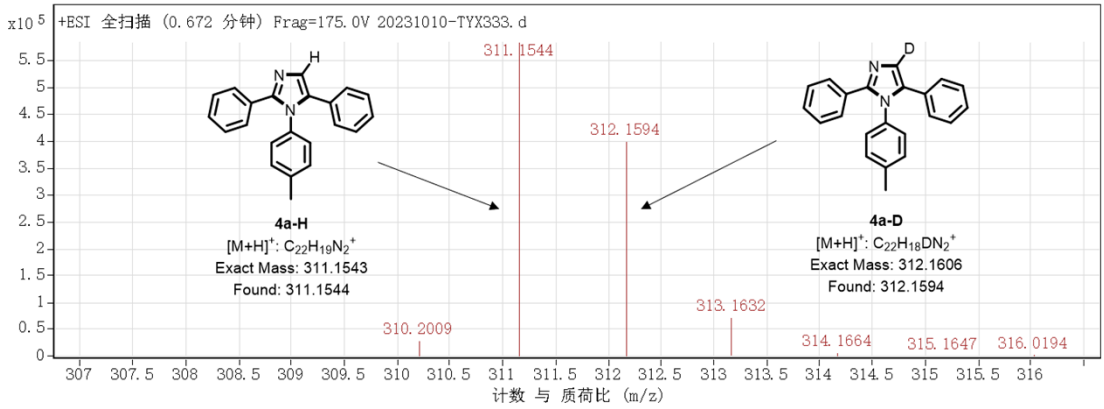
4.1 Isotope labeling experiment



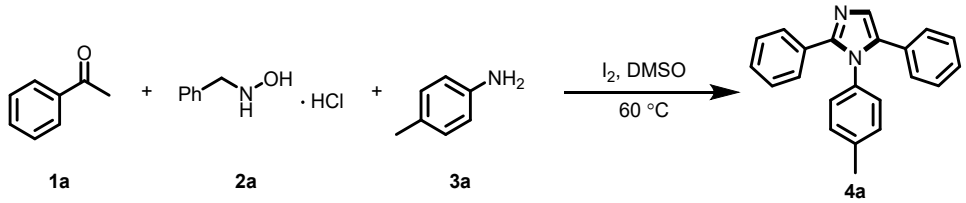
A tube equipped with a magnetic stirring bar was charged with CD_3-labeled acetophenone (**1a-D**) (62.0 mg, 0.5 mmol), *N*-Benzylhydroxylamine hydrochloride (**2a**) (160.0 mg, 1.0 mmol), *p*-toluidine (**3a**) (107.0 mg, 1.0 mmol) and iodine (203.0 mg, 0.8 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 60 °C for 8 h and monitored by TLC. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) to yield the desired product (102.6 mg, yield 66%) as yellow solid.



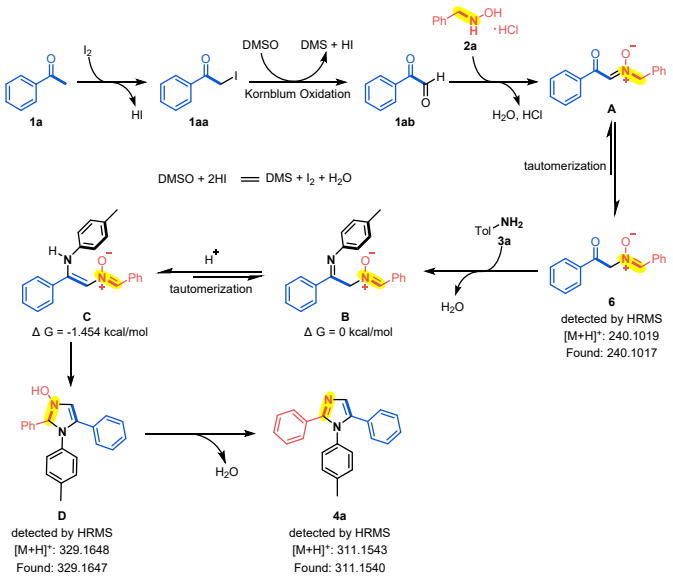


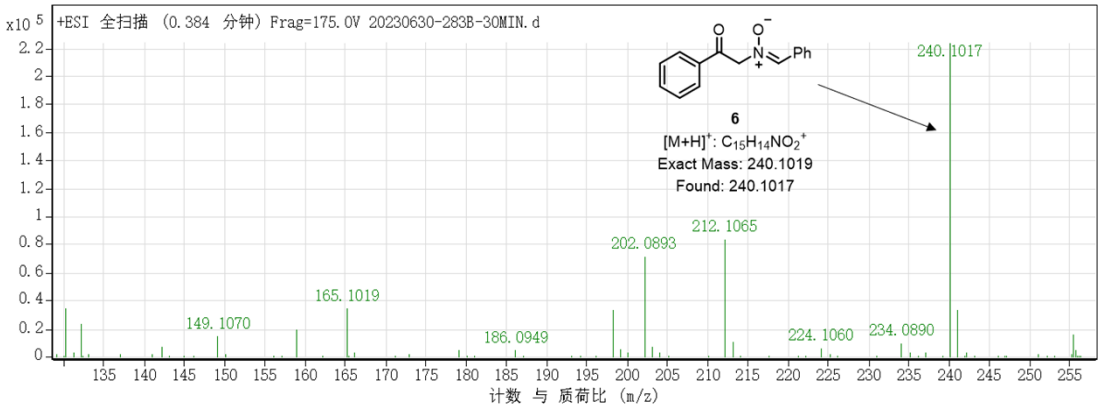


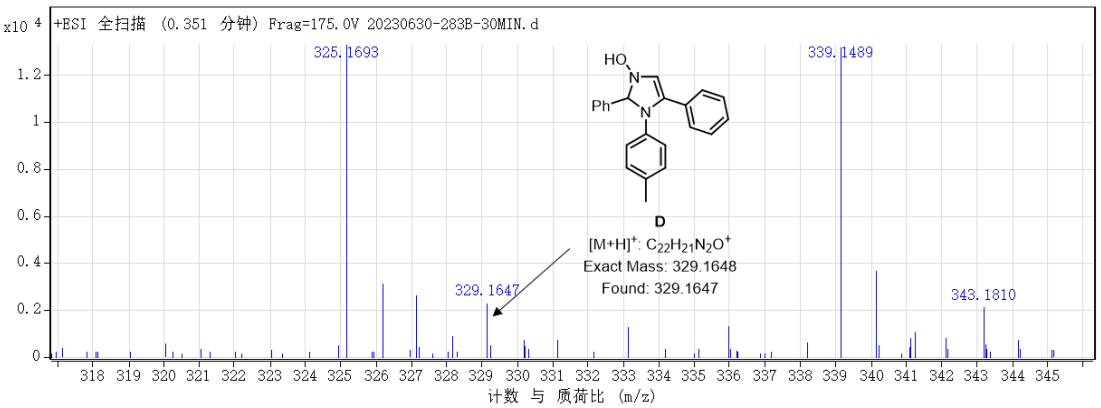
4.2 The mechanism of HRMS

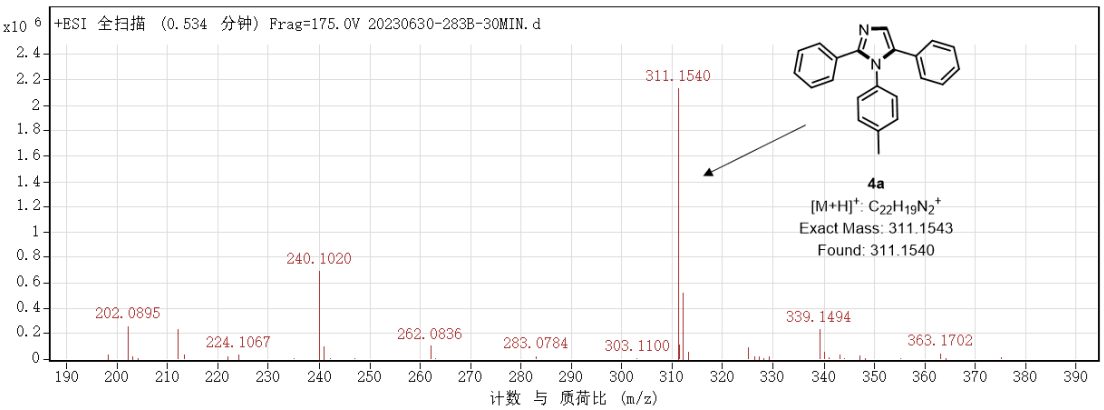


A tube equipped with a magnetic stirring bar was charged with acetophenone (**1a**) (60.0 mg, 0.5 mmol), *N*-Benzylhydroxylamine hydrochloride (**2a**) (160.0 mg, 1.0 mmol), *p*-toluidine (**3a**) (107.0 mg, 1.0 mmol) and iodine (203.0 mg, 0.8 mmol) at room temperature, and DMSO (3 mL) was added. The resulting mixture was stirred at 60 °C for 30 min. Then, the 0.5 mL of the reaction solution was diluted with 1.5 mL of EtOAc. The samples were immediately monitored by HRMS.


1a
I2
HI
1aa
DMSO
DMS + HI
Kornblum Oxidation
1ab
2a
·HCl
H2O, HCl
A
tautomerization
DMSO + 2HI = DMS + I2 + H2O
Tol
NH2
3a
H2O
6
detected by HRMS
[M+H]+: 240.1019
Found: 240.1017
H+
tautomerization
B
Δ G = 0 kcal/mol
C
Δ G = -1.454 kcal/mol
H2O
D
detected by HRMS
[M+H]+: 329.1648
Found: 329.1647
4a
detected by HRMS
[M+H]+: 311.1543
Found: 311.1540

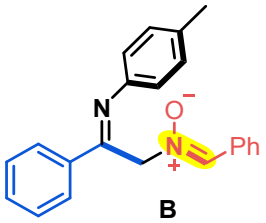

+ESI 全扫描 (0.384 分钟) Frag=175.0V 20230630-283B-30MIN.d
x10 5
6
[M+H]+: C15H14NO2+
Exact Mass: 240.1019
Found: 240.1017
240.1017
212.1065
202.0893
165.1019
149.1070
186.0949
224.1060
234.0890
计数 与 质荷比 (m/z)


+ESI 全扫描 (0.351 分钟) Frag=175.0V 20230630-283B-30MIN.d
x10 4
D
[M+H]+: C22H21N2O+
Exact Mass: 329.1648
Found: 329.1647
325.1693
339.1489
329.1647
343.1810
计数 与 质荷比 (m/z)


+ESI 全扫描 (0.534 分钟) Frag=175.0V 20230630-283B-30MIN.d
x10 6
4a
[M+H]+: C22H19N2+
Exact Mass: 311.1543
Found: 311.1540
311.1540
240.1020
202.0895
224.1067
262.0836
283.0784
303.1100
339.1494
363.1702
计数 与 质荷比 (m/z)

4.3 The free energies of the key intermediates B and C

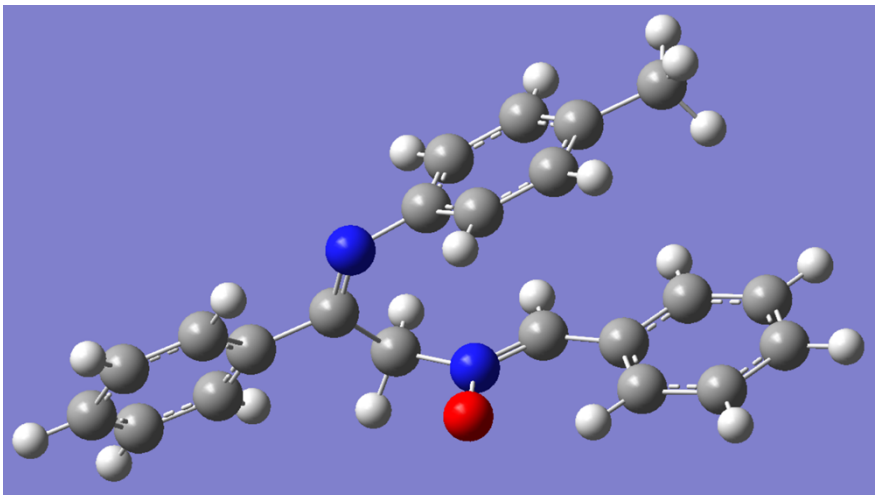
We calculated the free energies of the key intermediates **B** and **C**. It turns out that the energy difference between the two was 1.454 kcal/mol, with **C** having less energy than **B**, thus, the conversion of **B** to **C** is thermodynamically advantageous (Software: Gaussian 09W; Method: b3lyp/lanl2dz).

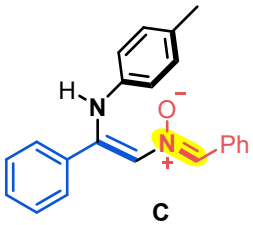


B

Free energy:
-1034.68440659 hartree
= -649274.8119792909 kcal/mol

Relative value: 0 kcal/mol

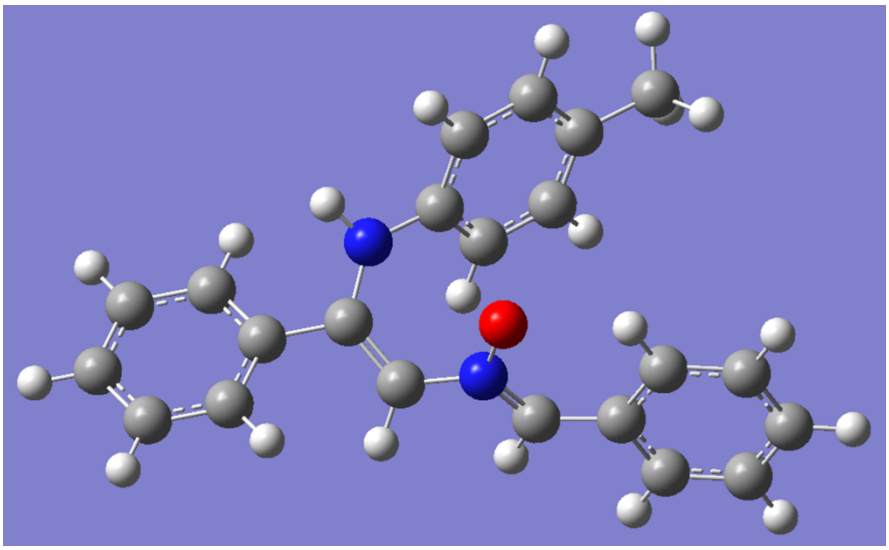




C

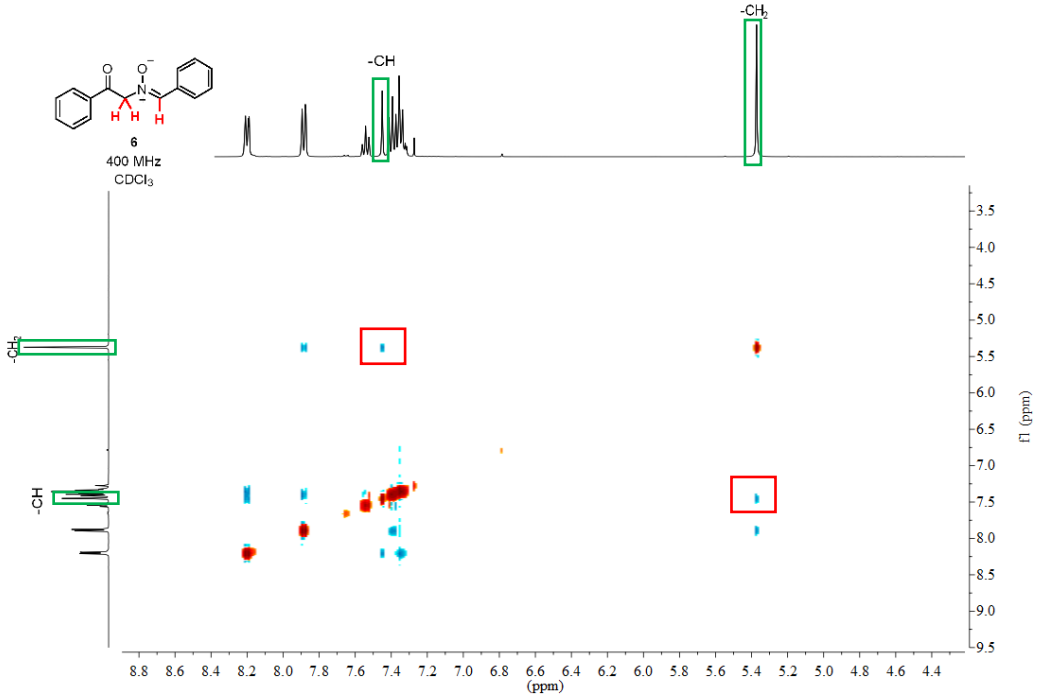
Free energy:
-1034.68672411 hartree
= -649276.2662462661 kcal/mol

Relative value: -1.454 kcal/mol



4.4 The 2D NMR spectra (NOESY) of intermediate 6

We have performed the 2D NMR spectra (NOESY) of intermediate **6**, the spectrum indicated that -CH_2 and -CH were exist a spatial long-range coupling, thus indirectly showing that the two groups -Ph and $PhCOCH_2$- were in trans-configuration.

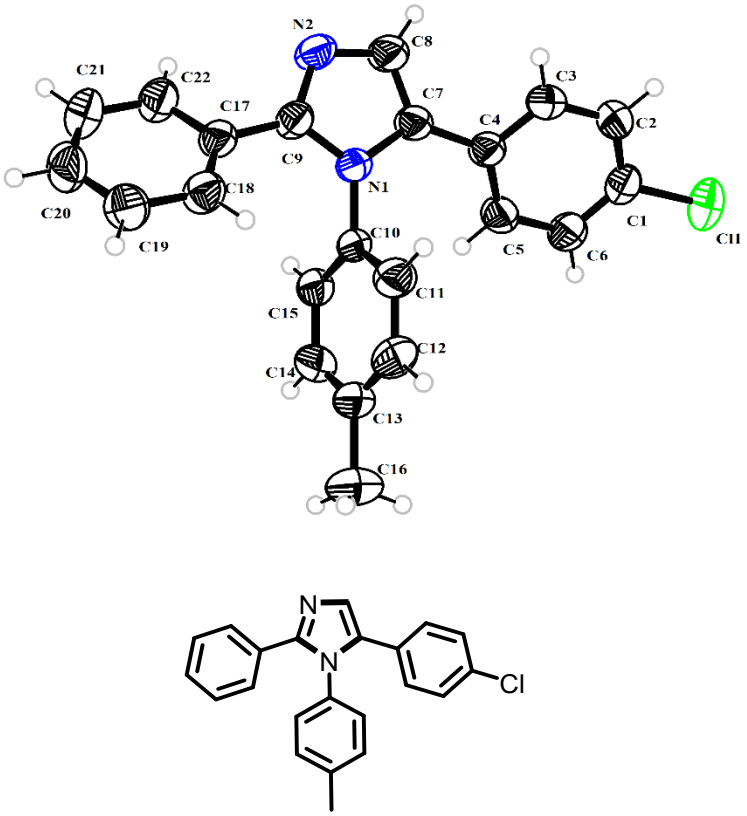


Reference

[1] (a) Sun, H.; Gong, L.; Tian, Y.; Wu, J.; Zhang, X.; Liu, J.; Fu, Z.; Niu, D. Metal- and Base-Free Room-Temperature Amination of Organoboronic Acids with *N*-Alkyl Hydroxylamines. *Angew. Chem. Int. Ed.*, **2018**, *57*, 9456−9460; (b) Zhang, Z.; Sabat, N.; Frison, G.; Marinetti, A.; Guinchard, X. Enantioselective Au(I)-Catalyzed Multicomponent Annulations via Tethered Counterion-Directed Catalysis. *ACS Catal.*, **2022**, *12*, 4046−4053

[2] (a) Zhang, Z.; Sabat, N.; Frison, G.; Marinetti, A.; Guinchard, X. *ACS Catal.,* **2022**, *12*, 4046-4053; (b) Zhang, M.; Kumagai, N.; Shibasaki, M. *Chemistry A European J,* **2017**, *23*, 12450-12455.

5. The crystallographic data



4u

Figure S1. X-ray crystal structure of **4u** ORTEP (50%) drawing

Crystal Data for Compound **4u**: CCDC 2342462 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Sample preparation: In a 10 mL glass bottle, 15 mg of pure **4u** was completely dissolved in the mixed solvent of 3 mL $CHCl_3$, and then 2 mL of n-hexane was added slowly. After a week of solvent evaporation, some yellow transparent crystals were obtained. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature.

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=16.652(3) b=14.997(2) c=21.130(3)
alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	5276.8(14)	5277.0(14)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C22 H18 Cl N2, C2 H F3 O2, C2 F3 O2	C22 H18 Cl N2, C2 H F3 O2, C2 F3 O2
Sum formula	C26 H19 Cl F6 N2 O4	C26 H19 Cl F6 N2 O4
Mr	572.88	572.88
Dx,g cm-3	1.442	1.442
Z	8	8
Mu (mm-1)	0.222	0.222
F000	2336.0	2336.0
F000'	2338.82	
h,k,lmax	19,17,25	19,17,25
Nref	4647	4625
Tmin,Tmax	0.974,0.978	0.605,0.745
Tmin'	0.974	

Correction method= # Reported T Limits: Tmin=0.605 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 24.997

R(reflections)= 0.0611(3441) wR2(reflections)= 0.1894(4625)

S = 1.051 Npar= 405

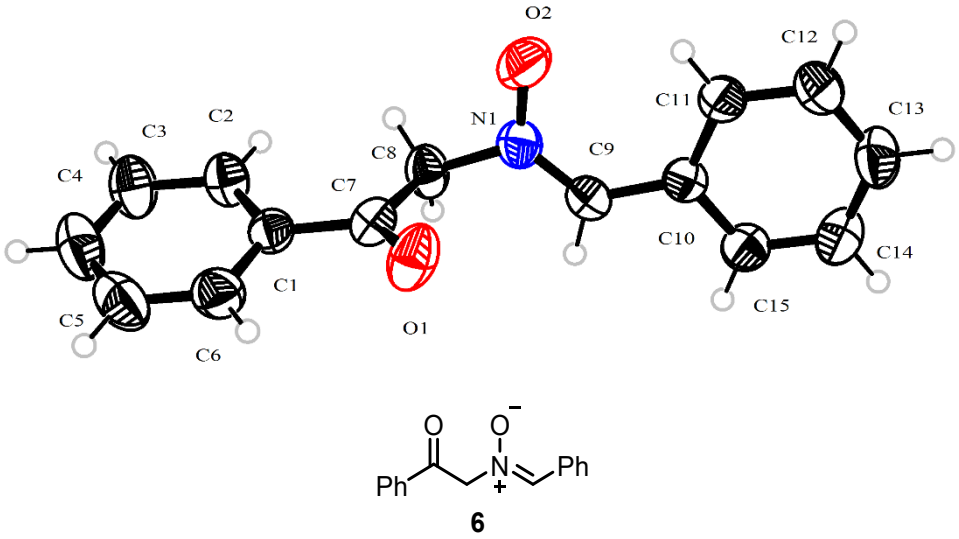


Figure S1. X-ray crystal structure of **6** ORTEP (50%) drawing

Crystal Data for Compound **6**: CCDC 2359610 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Sample preparation: In a 10 mL glass bottle, 15 mg of pure **6** was completely dissolved in the mixed solvent of 3 mL $CHCl_3$, and then 2 mL of n-hexane was added slowly. After a week of solvent evaporation, some yellow transparent crystals were obtained. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature.

Bond precision: C-C = 0.0023 A Wavelength=0.71073

Cell: a=12.719(3) b=13.852(3) c=14.156(4)
alpha=90 beta=97.096(4) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	2475.0(11)	2474.9(11)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C15 H13 N O2	C15 H13 N O2
Sum formula	C15 H13 N O2	C15 H13 N O2
Mr	239.26	239.26
Dx,g cm-3	1.284	1.284
Z	8	8
Mu (mm-1)	0.086	0.086
F000	1008.0	1008.0
F000'	1008.46	
h,k,lmax	17,18,19	17,18,19
Nref	3305	3298
Tmin,Tmax	0.989,0.991	0.692,0.746
Tmin'	0.989	

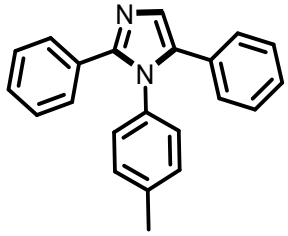
Correction method= # Reported T Limits: Tmin=0.692 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 29.020

R(reflections)= 0.0490(2212) wR2(reflections)= 0.1470(3298)

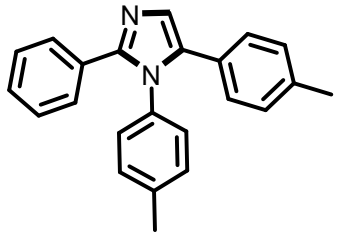
S = 1.024 Npar= 163

6. Spectroscopic data



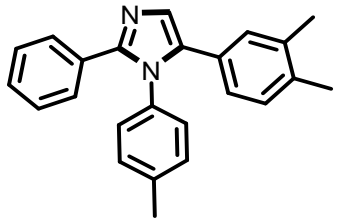
2,5-Diphenyl-1-(*p*-tolyl)-1*H*-imidazole (4a)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (15:1 v/v) as eluent afforded **4a** (108.6 mg , yield 70%) as light yellow solid; m.p. 239-241 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.35 (s, 2H), 7.25–7.19 (m, 6H), 7.14–7.07 (m, 4H), 6.98 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 138.5, 135.1, 134.4, 130.5, 130.0, 129.8, 128.7, 128.4, 128.2, 128.1, 128.0, 127.9, 127.3, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{19}N_2^+$ 311.1543; Found 311.1539.



2-Phenyl-1,5-di-*p*-tolyl-1*H*-imidazole (4b)

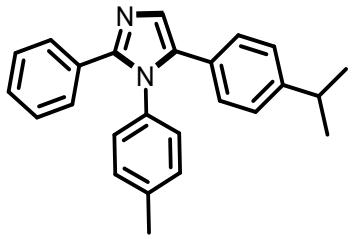
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **4b** (101.5 mg, yield 68%) as white solid; m.p. 146-148 °C; ^{1}H NMR (400 MHz, $CDCl_3$, CF_3COOD) δ 7.68 (s, 1H), 7.43 (d, J = 7.6 Hz, 3H), 7.38–7.32 (m, 2H), 7.22 (d, J = 8.0 Hz, 2H), 7.10 (d, J = 7.6 Hz, 2H), 7.02–6.96 (m, 4H), 2.40 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, CF_3COOD) δ 144.7, 140.8, 139.6, 135.8, 131.3, 131.1, 130.6, 129.4, 129.1, 128.9, 128.8, 127.3, 123.3, 123.1, 118.8, 21.15, 21.12; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2^+$ 325.1699; Found 325.1697.



5-(3,4-Dimethylphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4c)

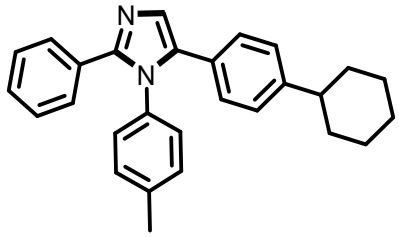
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4c** (101.5mg, yield 60%) as light yellow solid; m.p. 160-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 7.2 Hz, 2H), 7.32 (s, 1H), 7.26–7.22 (m, 3H), 7.13 (d, J = 7.6 Hz, 2H), 7.01f–6.93 (m, 4H), 6.71 (d, J = 7.6 Hz, 1H), 2.38 (s, 3H), 2.21 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 138.4, 136.5, 135.9, 135.3, 134.6, 130.4, 129.9, 129.7, 129.4, 128.7, 128.1,

128.02, 127.98, 127.3, 127.2, 125.8, 21.2, 19.7, 19.4; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_2^+$ 339.1856; Found 339.1853.



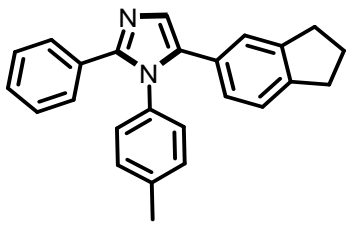
5-(4-Isopropylphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4d)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4d** (114.4 mg, yield 65%) as white solid; m.p. 164-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.33 (m, 2H), 7.32 (s, 1H), 7.23–7.20 (m, 3H), 7.12 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.4 Hz, 2H), 7.02–6.97 (m, 4H), 2.88–2.80 (m, 1H), 2.37 (s, 3H), 1.20 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.81, 147.76, 138.3, 135.1, 134.6, 130.7, 129.9, 128.7, 128.2, 127.94, 127.91, 127.8, 127.2, 126.2, 33.6, 23.8, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{25}N_2^+$ 353.2012; Found 353.2011.



5-(4-Cyclohexylphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4e)

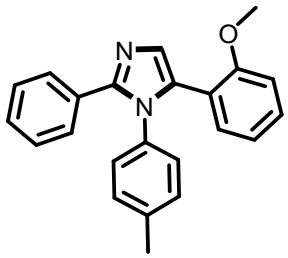
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4e** (123.6 mg, yield 63%) as white solid; m.p. 190-192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.33 (m, 2H), 7.32 (s, 1H), 7.23–7.19 (m, 3H), 7.12 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.4 Hz, 2H), 7.01–6.96 (m, 4H), 2.46–2.39 (m, 1H), 2.37 (s, 3H), 1.85–1.79 (m, 4H), 1.72 (d, J = 12.4 Hz, 1H), 1.39–1.30 (m, 4H), 1.27–1.21 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 147.1, 138.3, 135.1, 134.6, 130.7, 129.9, 128.7, 128.2, 127.94, 127.93, 127.7, 127.2, 126.6, 44.1, 34.2, 26.8, 26.0, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{29}N_2^+$ 393.2325; Found 393.2323.



5-(2,3-Dihydro-1*H*-inden-5-yl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4f)

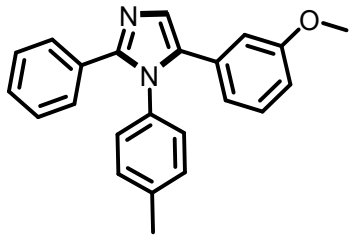
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **4f** (103.3 mg, yield 59%) as white solid; m.p. 177-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.33 (m, 2H), 7.30 (s, 1H), 7.24–7.20 (m, 3H), 7.12 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 7.6 Hz, 2H), 6.98 (d, J = 8.4 Hz, 2H), 6.77 (d, J = 8.0 Hz, 1H), 2.87–2.78 (m, 4H), 2.36 (s, 3H),

2.07–1.99 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 144.2, 143.5, 138.3, 135.6, 134.6, 130.7, 129.9, 128.7, 128.0, 127.7, 127.6, 126.4, 124.5, 124.0, 32.7, 32.5, 25.2, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{23}N_2^+$ 351.1856; Found 351.1854.



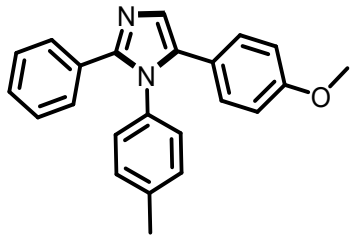
5-(2-Methoxyphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4g)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4g** (95.2 mg, yield 56%) as light yellow solid; m.p. 140-142 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.35 (m, 2H), 7.28–7.25 (m, 2H), 7.24–7.19 (m, 4H), 7.01 (d, J = 8.4 Hz, 2H), 6.92–6.87 (m, 3H), 6.72 (d, J = 8.4 Hz, 1H), 3.42 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 147.2, 137.5, 135.1, 132.1, 132.0, 130.8, 129.8, 129.2, 128.7, 128.5, 127.9, 127.1, 120.2, 119.1, 110.5, 54.7, 21.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O^+$ 341.1648; Found 341.1647.



5-(3-Methoxyphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4h)

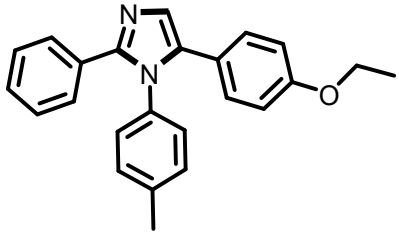
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4h** (103.7 mg, yield 61%) as white solid; m.p. 160-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 3H), 7.25–7.20 (m, 3H), 7.15–7.10 (m, 3H), 6.99 (d, J = 7.6 Hz, 2H), 6.75 (d, J = 8.4 Hz, 1H), 6.70 (d, J = 7.6 Hz, 1H), 6.59 (s, 1H), 3.60 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 148.0, 138.4, 134.z9, 134.5, 131.0, 130.5, 129.9, 129.2, 128.7, 128.0, 127.94, 127.89, 120.8, 113.4, 113.2, 54.9, 21.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O^+$ 341.1648; Found 341.1644.



5-(4-Methoxyphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4i)

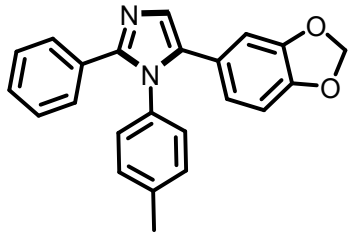
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4i** (98.6 mg, yield 58%) as white solid; m.p. 173-175 °C; ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.35 (s, 2H), 7.29–7.20 (m, 4H), 7.11 (s, 2H), 7.04–6.94 (m, 4H), 6.76 (s, 2H), 3.76 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 147.5, 138.3, 134.9, 134.5, 130.7, 129.9, 129.8, 128.6, 128.0, 127.3, 122.3, 113.6, 55.1, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O^+$ 341.1648; Found 341.1646.



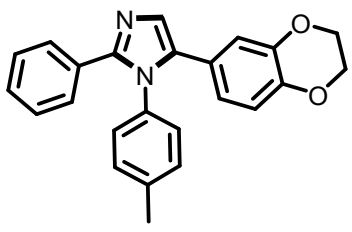
5-(4-Ethoxyphenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4j)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4j** (100.9 mg, yield 57%) as white solid; m.p. 155-157 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.38–7.33 (m, 2H), 7.28 (s, 1H), 7.23 (s, 3H), 7.12 (d, J = 8.0 Hz, 2H), 7.01–6.94 (m, 4H), 6.74 (d, J = 8.4 Hz, 2H), 4.01–3.94 (m, 2H), 2.36 (s, 3H), 1.38 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 147.4, 138.3, 135.0, 134.5, 130.6, 129.9, 129.8, 128.7, 127.99, 127.97, 127.9, 127.1, 122.1, 114.1, 63.3, 21.2, 14.8; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_2O^+$ 355.1805; Found 355.1803.



5-(Benzo[*d*][1,3]dioxol-5-yl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4k)

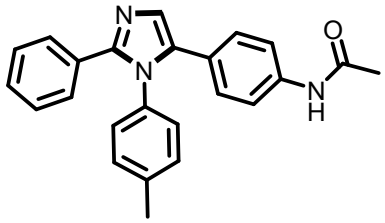
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4k** (109.8 mg, yield 62%) as light yellow solid; m.p. 207-209 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36–7.32 (m, 2H), 7.26 (s, 1H), 7.22 (s, 3H), 7.12 (d, J = 7.6 Hz, 2H), 6.97 (d, J = 7.6 Hz, 2H), 6.67 (d, J = 8.0 Hz, 1H), 6.59 (d, J = 8.0 Hz, 1H), 6.54 (s, 1H), 5.89 (s, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 147.3, 146.9, 138.4, 134.8, 134.4, 130.6, 130.0, 128.6, 128.0, 127.9, 127.8, 127.6, 123.6, 122.5, 109.0, 108.1, 101.0, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{19}N_2O_2^+$ 355.1441; Found 355.1440.



5-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4l)

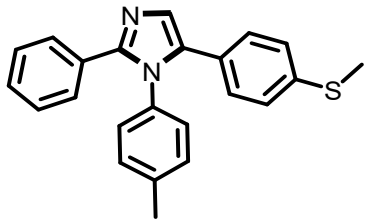
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4l** (112.0 mg, yield 64%) as light yellow solid; m.p. 227-229 °C; ^1H NMR (400

MHz, $CDCl_3$) δ 7.34 (s, 2H), 7.28–7.19 (m, 4H), 7.12 (s, 2H), 6.98 (s, 2H), 6.67 (s, 2H), 6.50 (s, 1H), 4.20 (s, 4H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 143.1, 143.0, 138.4, 134.7, 134.5, 130.7, 129.9, 128.6, 127.9, 127.5, 123.2, 121.8, 117.4, 117.0, 64.3, 64.2, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{21}N_2O_2^+$ 369.1598; Found 369.1599.



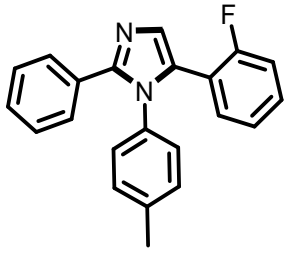
***N*-(4-(2-phenyl-1-(*p*-tolyl)-1*H*-imidazol-5-yl)phenyl)acetamide (4m)**

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (1:1 v/v) as eluent afforded **4m** (112.0 mg, yield 61%) as yellow solid; m.p. 140-142 °C; ^1H NMR (400 MHz, $CDCl_3$, CF_3COOD) δ 8.86 (s, 1H), 7.55–7.47 (m, 4H), 7.40–7.31 (m, 4H), 7.22 (d, J = 6.8 Hz, 2H), 7.07–6.98 (m, 4H), 2.38 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, CF_3COOD) δ 172.1, 145.1, 141.7, 139.0, 138.9, 136.2, 132.4, 131.0, 130.1, 129.8, 129.3, 129.1, 127.2, 121.9, 121.3, 120.6, 120.5, 117.0, 23.43, 23.38, 21.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{22}N_3O^+$ 368.1757; Found 368.1755.



5-(4-(Methylthio)phenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4n)

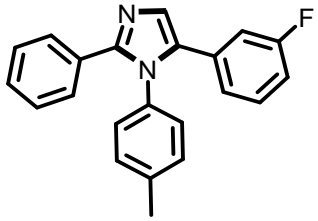
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4n** (105.1 mg, yield 59%) as white solid; m.p. 171-173 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.37–7.33 (m, 2H), 7.28–7.22 (m, 4H)), 7.14 (d, J = 7.6 Hz, 2H), 7.10 (s, 1H), 7.08 (s, 1H), 7.01–6.96 (m, 4H), 2.45 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 138.6, 137.8, 134.7, 134.3, 130.3, 130.1, 128.73, 128.67, 128.2, 128.1, 127.9, 127.6, 126.4, 125.9, 21.2, 15.4; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2S^+$ 357.1420; Found 357.1418.



5-(2-Fluorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4o)

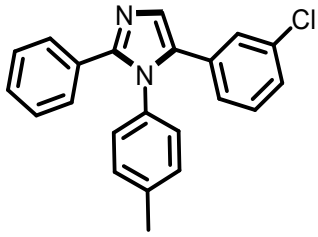
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4o** (106.6 mg, yield 65%) as light yellow solid; m.p. 164-166 °C; ^1H NMR (400

MHz, $CDCl_3$) δ 7.39–7.34 (m, 3H), 7.26–7.19 (m, 4H), 7.06 (d, J = 7.6 Hz, 3H), 7.02–6.92(m, 4H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9 (d, J = 247.0 Hz, $^1J_{CF}$), 148.0, 138.2, 134.4, 131.7 (d, J = 2.0 Hz, $^4J_{CF}$), 130.5, 129.7 (d, J = 11.0 Hz, $^3J_{CF}$), 129.69, 129.6, 128.8, 128.6, 128.1, 128.0, 127.4, 123.7 (d, J = 4.0 Hz, $^3J_{CF}$), 118.0 (d, J = 15.0 Hz, $^2J_{CF}$), 115.6 (d, J = 22.0 Hz, $^2J_{CF}$), 21.1; ^{19}F NMR (376 MHz, CDCl3) δ -111.80; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}FN_2^+$ 329.1449; Found 329.1448.



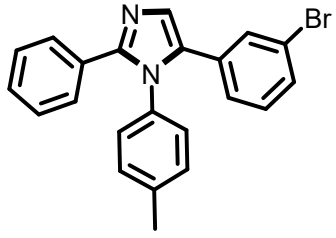
5-(3-Fluorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4p)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4p** (109.9 mg, yield 67%) as light yellow solid; m.p. 179-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.34 (m, 3H), 7.25–7.20 (m, 3H), 7.18–7.11 (m, 3H), 6.99 (d, J = 8.0 Hz, 2H), 6.92–6.85 (m, 2H), 6.76 (d, J = 10.0 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4 (d, J = 244.0 Hz, $^1J_{CF}$), 148.4, 138.8, 134.2, 133.8 (d, J = 2.0 Hz, $^4J_{CF}$), 131.9 (d, J = 8.0 Hz, $^3J_{CF}$), 130.4, 130.1, 129.7 (d, J = 8.0 Hz, $^3J_{CF}$), 128.7, 128.6, 128.2, 128.0, 127.8, 123.9 (d, J = 3.0 Hz, $^4J_{CF}$), 115.0 (d, J = 23.0 Hz, $^2J_{CF}$), 114.0 (d, J = 20.0 Hz, $^2J_{CF}$), 21.2; ^{19}F NMR (376 MHz, CDCl3) δ -112.78; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}FN_2^+$ 329.1449; Found 329.1445.



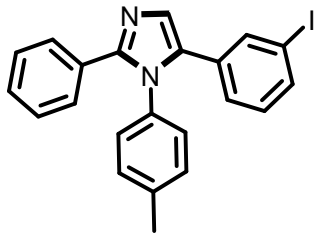
5-(3-Chlorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4q)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4q** (110.1 mg, yield 64%) as white solid; m.p. 158-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.33 (m, 3H), 7.26–7.19 (m, 3H), 7.18–7.09 (m, 5H), 6.98 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 7.6 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 138.8, 134.1, 134.0, 133.6, 131.6, 130.3, 130.1, 129.4, 128.7, 128.5, 128.3, 128.2, 128.0, 127.8, 127.2, 126.3, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}ClN_2^+$ 345.1153; Found 345.1152.



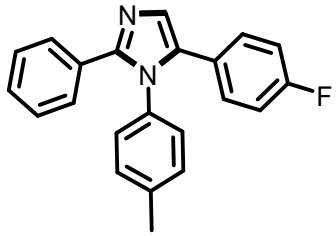
5-(3-Bromophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4r)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4r** (120.3 mg, yield 62%) as light yellow solid; m.p. 166-168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.29 (m, 5H), 7.28–7.21 (m, 3H), 7.15 (d, J = 7.6 Hz, 2H), 7.07–7.02 (m, 1H), 6.98 (d, J = 7.6 Hz, 2H), 6.91 (d, J = 7.2 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 138.8, 134.1, 133.5, 131.8, 131.1, 130.2, 130.1, 129.6, 128.7, 128.4, 128.3, 128.0, 127.8, 126.7, 122.2, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}BrN_2^+$ 389.0648; Found 389.0644.



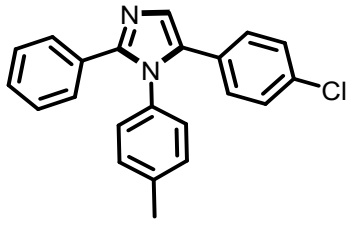
5-(3-Iodophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4s)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **4s** (141.7 mg, yield 65%) as light yellow solid; m.p. 150-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$, CF_3COOD) δ 7.70 (s, 1H), 7.67–7.61 (m, 1H), 7.53 (s, 1H), 7.46–7.39 (m, 3H), 7.36–7.31 (m, 2H), 7.24 (d, J = 8.0 Hz, 2H), 7.05–6.98 (m, 4H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, CF_3COOD) δ 145.4, 140.8, 137.9, 137.4, 133.7, 131.1, 130.7, 130.6, 130.0, 128.9, 128.8, 128.1, 127.8, 127.2, 123.4, 120.1, 93.9, 21.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}IN_2^+$ 437.0509; Found 437.0506.



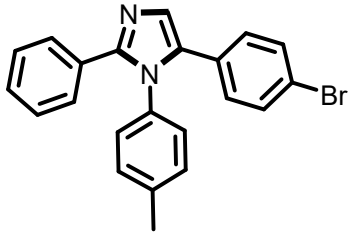
5-(4-Fluorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4t)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (12:1 v/v) as eluent afforded **4t** (100.1mg, yield 61%) as light yellow solid; m.p. 200-202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 6.4 Hz, 2H), 7.31 (s, 1H), 7.27–7.21 (m, 3H), 7.13 (d, J = 7.6 Hz, 2H), 7.09–7.02 (m, 2H), 6.99–6.87 (m, 4H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, J = 246.0 Hz, $^1J_{CF}$), 148.0, 138.6, 134.3, 134.1, 130.6, 130.3, 130.2, 130.1, 128.7, 128.1, 128.03, 127.98, 127.9, 126.1 (d, J = 4.0 Hz, $^3J_{CF}$), 115.3 (d, J = 21.0 Hz, $^2J_{CF}$), 21.2; ^{19}F NMR (376 MHz, CDCl3) δ -114.34; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}FN_2^+$ 329.1449; Found 329.1446.



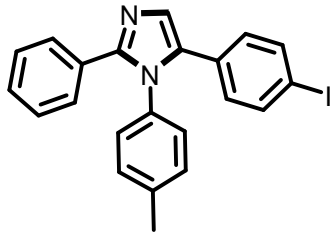
5-(4-Chlorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4u)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4u** (108.4 mg, yield 63%) as light yellow solid; m.p. 120-122 °C; ^{1}H NMR (400 MHz, $CDCl_3$, CF_3COOD) δ 7.70 (s, 1H), 7.52–7.46 (m, 1H), 7.38 (d, J = 4.0 Hz, 4H), 7.31 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 3.2 Hz, 1H), 7.24 (s, 1H), 7.09–7.00 (m, 4H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, CF_3COOD) δ 145.3, 141.6, 136.4, 135.2, 132.3, 131.0, 130.4, 130.2, 129.3, 129.2, 127.3, 123.8, 121.9, 117.8, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}ClN_2^+$ 345.1153; Found 345.1150.



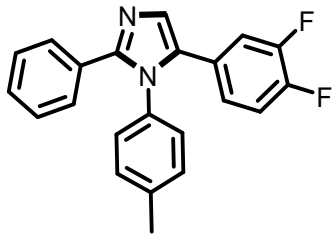
5-(4-Bromophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4v)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (15:1 v/v) as eluent afforded **4v** (116.4 mg, yield 60%) as yellow solid; m.p. 204-206 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.4 Hz, 5H), 7.27–7.23 (m, 3H), 7.15 (d, J = 8.0 Hz, 2H), 7.00–6.92 (m, 4H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.3, 138.8, 134.1, 133.9, 131.4, 130.2, 129.8, 128.7, 128.3, 128.1, 128.0, 127.8, 121.5, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}BrN_2^+$ 389.0648; Found 389.0647.



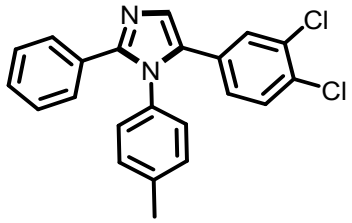
5-(4-Iodophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4w)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **4w** (114.2 mg, yield 62%) as white solid; m.p. 210-212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 2H), 7.34 (s, 3H), 7.23 (s, 3H), 7.13 (s, 2H), 6.97 (s, 2H), 6.80 (d, J = 4.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 138.7, 137.3, 134.2, 133.9, 130.4, 130.1, 129.9, 129.4, 128.7, 128.3, 128.2, 128.0, 127.8, 93.0, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}IN_2^+$ 437.0509; Found 437.0507.



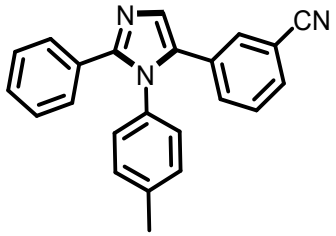
5-(3,4-Difluorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4x)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4x** (114.2 mg, yield 66%) as light yellow solid; m.p. 161-163 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.31 (m, 3H), 7.24 (s, 3H), 7.16 (d, J = 7.2 Hz, 2H), 7.05–6.95 (m, 3H), 6.90–6.79 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8 (dd, $^1J_{CF}$ = 247.0 Hz, $^2J_{CF}$ = 27.0 Hz), 149.6 (dd, $^1J_{CF}$ = 247.0 Hz, $^2J_{CF}$ = 26.0 Hz), 148.4, 138.9, 134.0, 133.0, 130.3, 130.2, 128.6, 128.4, 128.3, 128.0, 127.8, 126.9 (dd, $^3J_{CF}$ = 6.0 Hz, $^4J_{CF}$ = 2.0 Hz), 124.5 (dd, $^3J_{CF}$ = 6.0 Hz, $^4J_{CF}$ = 4.0 Hz), 117.2 (dd, $^2J_{CF}$ = 18.0 Hz, $^3J_{CF}$ = 8.0 Hz), 21.1; ^{19}F NMR (376 MHz, CDCl3) δ -137.25, -137.30, -138.96, -139.02; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{17}F_2N_2^+$ 347.1354; Found 347.1356.



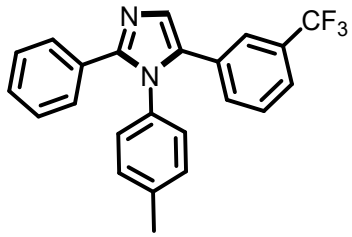
5-(3,4-Dichlorophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4y)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4y** (109.6 mg, yield 58%) as white solid; m.p. 178-180 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.33 (m, 3H), 7.25 (d, J = 8.0 Hz, 5H), 7.17 (d, J = 7.2 Hz, 2H), 6.99 (d, J = 7.2 Hz, 2H), 6.81 (d, J = 8.0 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 139.1, 133.9, 132.7, 132.4, 131.3, 130.3, 130.2, 130.1, 129.9, 128.72, 128.65, 128.4, 128.1, 127.8, 127.3, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{17}Cl_2N_2^+$ 379.0763; Found 379.0761.



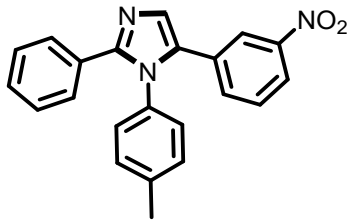
3-(2-Phenyl-1-(*p*-tolyl)-1*H*-imidazol-5-yl)benzonitrile (4z)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4z** (103.9 mg, yield 62%) as white solid; m.p. 161-163 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 6.8 Hz, 1H), 7.41 (s, 1H), 7.38–7.30 (m, 5H), 7.28–7.22 (m, 3H), 7.17 (d, J = 8.0 Hz, 2H), 6.98 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 139.1, 133.8, 132.7, 132.2, 131.3, 130.5, 130.3, 130.1, 129.1, 128.7, 128.4, 128.1, 127.7, 118.3, 112.5, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{18}N_3^+$ 336.1495; Found 336.1491.



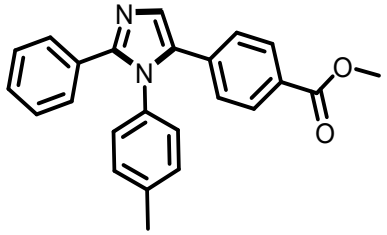
2-Phenyl-1-(*p*-tolyl)-5-(3-(trifluoromethyl)phenyl)-1*H*-imidazole (4aa)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4aa** (109.7 mg, yield 58%) as white solid; m.p. 187-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47–7.42 (m, 2H), 7.40–7.36 (m, 2H), 7.35–7.30 (m, 2H), 7.28–7.22 (m, 4H), 7.16 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 8.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 139.0, 134.1, 133.6, 131.3, 130.7, 130.6 (q, J = 32.0 Hz, $^2J_{CF}$), 130.3, 130.2, 128.73, 128.69, 128.67, 128.3, 128.1, 127.8, 124.9 (q, J = 4.0 Hz, $^3J_{CF}$), 123.75 (q, J = 271.0 Hz, $^1J_{CF}$), 123.73 (q, J = 4.0 Hz, $^3J_{CF}$), 21.1; ^{19}F NMR (376 MHz, $CDCl_4$) δ -62.98; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{18}F_3N_2^+$ 379.1417; Found 379.1415.



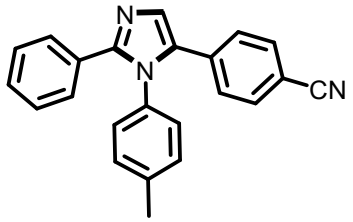
5-(3-Nitrophenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4ab)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4ab** (133.0 mg, yield 61%) as light yellow solid; m.p.156-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08–8.02 (m, 1H), 7.93 (d, J = 1.2 Hz, 1H), 7.48 (s, 1H), 7.41–7.36 (m, 4H), 7.28–7.24 (m, 3H), 7.19 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.4 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 148.0, 139.3, 133.8, 133.7, 132.6, 131.6, 130.4, 130.1, 129.24, 129.19, 128.7, 128.5, 128.1, 127.8, 122.6, 121.8, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}N_3O_2^+$ 356.1394; Found 356.1391.



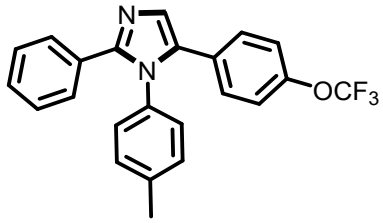
Methyl 4-(2-phenyl-1-(*p*-tolyl)-1*H*-imidazol-5-yl)benzoate (4ac)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4ac** (110.4 mg, yield 60%) as white solid; m.p. 187-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.4 Hz, 2H), 7.45 (s, 1H), 7.38–7.34 (m, 2H), 7.26–7.21 (m, 3H), 7.16–7.11 (m, 4H), 6.98 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 148.8, 138.8, 134.3, 134.2, 133.9, 130.3, 130.1, 129.4, 129.2, 128.7, 128.4, 128.2, 128.0, 127.8, 127.7, 52.0, 21.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{21}N_2O_2^+$ 369.1598; Found 369.1599.



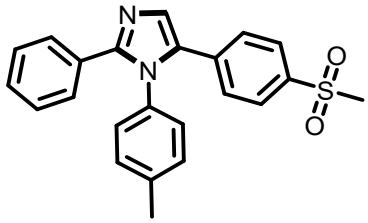
4-(2-Phenyl-1-(*p*-tolyl)-1*H*-imidazol-5-yl)benzonitrile (4ad)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4ad** (95.5 mg, yield 57%) as white solid; m.p. 212-214 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.46 (m, 3H), 7.38–7.33 (m, 2H), 7.28–7.23 (m, 3H), 7.20–7.14 (m, 4H), 7.00 (d, J = 8.4 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 139.2, 134.4, 133.9, 133.1, 132.1, 130.4, 130.0, 129.7, 128.8, 128.6, 128.13, 128.12, 127.8, 118.7, 110.5, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{18}N_3^+$ 336.1495; Found 336.1492.



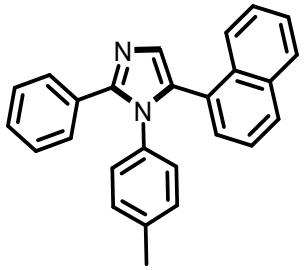
2-Phenyl-1-(*p*-tolyl)-5-(4-(trifluoromethoxy)phenyl)-1*H*-imidazole (4ae)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4ae** (116.3 mg, yield 59%) as white solid; m.p. 164-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.33 (m, 3H), 7.26–7.20 (m, 3H), 7.15 (d, J = 8.0 Hz, 2H), 7.12–7.05 (m, 4H), 6.98 (d, J = 8.4 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 148.3, 138.8, 134.2, 133.7, 130.4, 130.2, 129.6, 128.7, 128.6, 128.4, 128.2, 128.0, 127.9, 120.6, 120.4 (q, J = 256.0 Hz, $^1J_{CF}$), 21.2; ^{19}F NMR (376 MHz, $CDCl_4$) δ -57.78; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{18}F_3N_2O^+$ 395.1366; Found 395.1362.



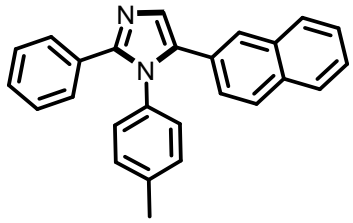
5-(4-(Methylsulfonyl)phenyl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4af)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (2:1 v/v) as eluent afforded **4af** (122.3 mg, yield 63%) as white solid; m.p. 230-232 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.4 Hz, 2H), 7.48 (s, 1H), 7.36 (d, J = 7.2 Hz, 2H), 7.28–7.22 (m, 5H), 7.18 (d, J = 8.0 Hz, 2H), 7.00 (d, J = 8.0 Hz, 2H), 3.02 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 139.0, 138.3, 135.2, 133.8, 132.9, 130.3, 129.9, 129.7, 128.6, 128.3, 128.1, 127.9, 127.6, 127.2, 44.2, 21.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O_2S^+$ 389.1318; Found 389.1315.



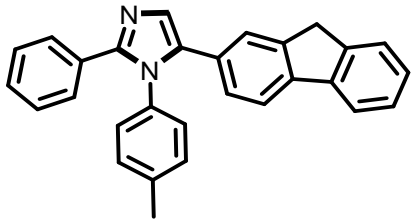
5-(Naphthalen-1-yl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4ag)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4ag** (111.7 mg, yield 62%) as yellow solid; m.p. 163-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.80–7.71 (m, 2H), 7.43 (s, 4H), 7.38 (s, 1H), 7.29 (s, 1H), 7.24 (s, 3H), 7.19 (d, J = 5.6 Hz, 1H), 6.85 (s, 4H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 138.0, 134.2, 133.3, 133.0, 132.6, 130.2, 129.50, 129.46, 129.2, 128.62, 128.57, 128.2, 128.0, 127.2, 127.1, 126.3, 125.8, 125.7, 124.7, 20.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{21}N_2^+$ 361.1699; Found 361.1700.



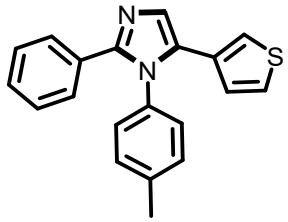
5-(Naphthalen-2-yl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4ah)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4ah** (108.0 mg, yield 60%) as yellow solid; m.p. 180-182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.60 (s, 1H), 7.46 (s, 1H), 7.44–7.36 (m, 4H), 7.25 (s, 3H), 7.16–7.08 (m, 3H), 7.01 (d, J = 7.2 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 138.5, 135.1, 134.6, 133.1, 132.2, 130.7, 130.0, 128.7, 128.5, 128.1, 128.0, 127.9, 127.7, 127.5, 127.3, 127.2, 126.2, 126.1, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{21}N_2^+$ 361.1699; Found 361.1698.



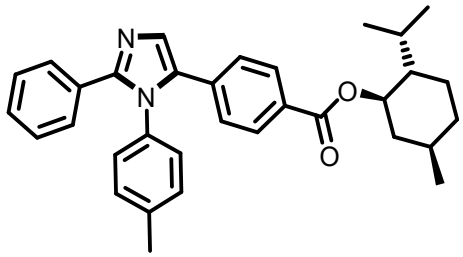
5-(9*H*-fluoren-2-yl)-2-phenyl-1-(*p*-tolyl)-1*H*-imidazole (4ai)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded **4ai** (99.5 mg, yield 50%) as light yellow solid; m.p. 200-202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 6.8 Hz, 1H), 7.60 (d, J = 7.2 Hz, 1H), 7.50 (d, J = 6.8 Hz, 1H), 7.40 (d, J = 12.4 Hz, 3H), 7.34–7.30 (m, 2H), 7.26 (s, 4H), 7.13 (d, J = 6.4 Hz, 2H), 7.02 (s, 3H), 3.80 (s, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 143.3, 143.2, 141.1, 140.9, 138.5, 135.5, 134.4, 130.3, 130.0, 128.8, 128.2, 128.1, 128.0, 127.5, 127.3, 126.9, 126.8, 125.2, 125.0, 119.9, 119.5, 36.8, 21.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{29}H_{23}N_2^+$ 399.1856; Found 399.1860.



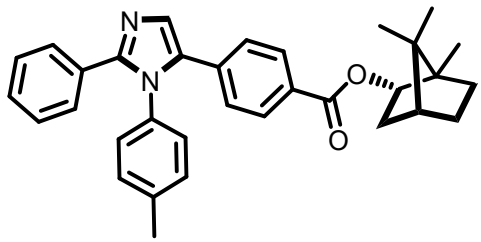
2-Phenyl-5-(thiophen-3-yl)-1-(*p*-tolyl)-1*H*-imidazole (4aj)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **4aj** (78.0 mg, yield 52%) as yellow solid; m.p. 210-212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.38 (d, J = 2.4 Hz, 1H), 7.26–7.19 (m, 7H), 7.09 (d, J = 8.0 Hz, 2H), 6.90 (d, J = 4.8 Hz, 1H), 6.64 (d, J = 2.0 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 139.2, 134.7, 131.1, 130.2, 130.0, 128.5, 128.2, 128.11, 128.08, 127.21, 127.16, 125.3, 121.2, 21.3; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{17}N_2S^+$ 317.1107; Found 317.1106.



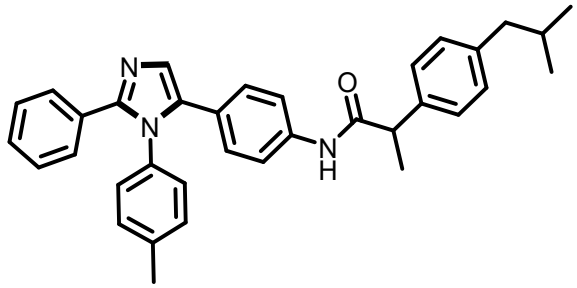
(1R,2R,5R)-2-isopropyl-5-methylcyclohexyl 4-(2-phenyl-1-(*p*-tolyl)-1H-imidazol-5-yl)benzoate (4ak)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **4ak** (150.1 mg, yield 61%) as yellow solid; m.p. 188-190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.4 Hz, 2H), 7.44 (s, 1H), 7.39–7.33 (m, 2H), 7.27–7.23 (m, 3H), 7.18–7.13 (m, 4H), 7.00 (d, J = 8.4 Hz, 2H), 4.95–4.87 (m, 1H), 2.40 (s, 3H), 2.10 (d, J = 11.6 Hz, 1H), 1.99–1.90 (m, 1H), 1.72 (d, J = 11.6 Hz, 2H), 1.58–1.48 (m, 2H), 1.17–1.04 (m, 2H), 0.94–0.88 (m, 7H), 0.78 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 148.8, 138.8, 134.3, 134.11, 134.05, 130.3, 130.2, 129.5, 129.16, 129.15, 128.7, 128.3, 128.0, 127.8, 127.7, 74.8, 47.2, 40.9, 34.2, 31.4, 26.4, 23.5, 22.0, 21.2, 20.7, 16.4; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{33}H_{37}N_2O_2^+$ 493.2850; Found 493.2846.

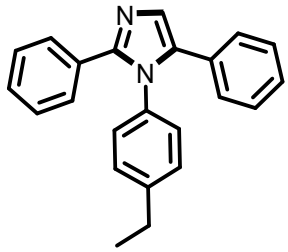


(1*R*,2*R*,4*R*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 4-(2-phenyl-1-(*p*-tolyl)-1*H*-imidazol-5-yl)benzoate (4al)

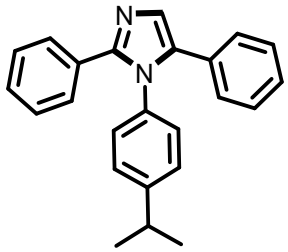
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **4al** (161.8 mg, yield 66%) as light yellow solid; m.p. 178-180 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 8.4 Hz, 2H), 7.44 (s, 1H), 7.38–7.33 (m, 2H), 7.27–7.22 (m, 3H), 7.16 (d, J = 8.4 Hz, 4H), 7.01 (d, J = 8.4 Hz, 2H), 5.09 (d, J = 9.2 Hz, 1H), 2.49–2.43 (m, 1H), 2.40 (s, 3H), 2.15–2.05 (m, 1H), 1.83–1.71 (m, 2H), 1.42–1.26 (m, 2H), 1.12–1.06 (m, 1H), 0.96 (s, 3H), 0.91 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 148.8, 138.8, 134.22, 134.16, 134.0, 130.3, 130.2, 129.4, 129.17, 129.16, 128.7, 128.3, 128.0, 127.8, 127.7, 80.5, 49.0, 47.8, 44.9, 36.8, 28.0, 27.3, 21.2, 19.6, 18.8, 13.5; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{33}H_{35}N_2O_2^+$ 491.2693; Found 491.2689.



2-(4-Isobutylphenyl)-*N*-(4-(2-phenyl-1-(*p*-tolyl)-1*H*-imidazol-5-yl)phenyl)propanamide (4am)
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (3:1 v/v) as eluent afforded **4am**(141.2 mg, yield 55%) as light yellow solid; m.p. 210-212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 1.6 Hz, 1H), 7.32 (s, 2H), 7.30 (s, 1H), 7.28 (s, 1H), 7.26 (s, 1H), 7.24–7.21 (m, 4H), 7.16–7.08 (m, 4H), 7.00–6.92 (m, 4H), 3.71–3.64 (m, 1H), 2.46 (d, J = 7.2 Hz, 2H), 2.36 (s, 3H), 1.91–1.79 (m, 1H), 1.55 (d, J = 7.2 Hz, 3H), 1.26 (s, 1H), 0.91 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 147.7, 141.1, 138.7, 137.9, 137.3, 134.7, 134.2, 130.1, 129.8, 128.9, 128.7, 128.3, 128.1, 127.9, 127.4, 127.1, 125.3, 119.3, 47.7, 45.0, 30.1, 22.4, 21.2, 18.4; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{35}H_{36}N_3O^+$ 514.2853; Found 514.2852.

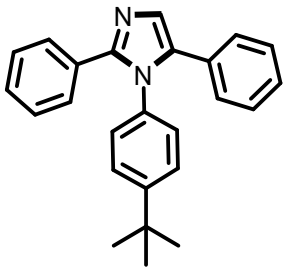


1-(4-Ethylphenyl)-2,5-diphenyl-1*H*-imidazole (5a)
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5a** (108.6 mg , yield 67%) as light yellow solid; m.p. 175-177 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (s, 3H), 7.26–7.19 (m, 6H), 7.15 (d, J = 8.0 Hz, 2H), 7.11–7.06 (m, 2H), 7.00 (d, J = 8.0 Hz, 2H), 2.67 (q, J = 7.6 Hz, 2H), 1.24 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 144.7, 135.1, 134.6, 130.6, 129.9, 128.7, 128.4, 128.2, 128.1, 128.0, 127.2, 28.4, 15.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2^+$ 325.1699; Found 325.1700.



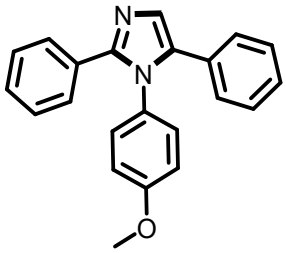
1-(4-Isopropylphenyl)-2,5-diphenyl-1*H*-imidazole (5b)
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5b** (104.8 mg yield 62%) as light yellow solid; m.p. 180-182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.33 (m, 3H), 7.26–7.19 (m, 7H), 7.17 (s, 1H), 7.11–7.06 (m, 2H), 7.02 (d, J

= 8.4 Hz, 2H), 2.97–2.88 (m, 1H), 1.26 (s, 3H), 1.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 147.9, 135.1, 134.6, 130.4, 129.8, 128.8, 128.4, 128.2, 128.0, 127.8, 127.34, 127.26, 33.7, 23.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_2^+$ 339.1856; Found 339.1855.



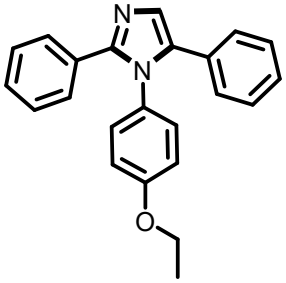
1-(4-(*Tert*-butyl)phenyl)-2,5-diphenyl-1*H*-imidazole (5c)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5c** (110.9 mg, yield 63%) as light yellow solid; m.p. 197-199 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.31 (m, 5H), 7.24–7.18 (m, 6H), 7.10–7.06 (m, 2H), 7.02 (d, J = 8.4 Hz, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 148.0, 135.1, 134.4, 130.6, 129.9, 128.7, 128.3, 128.1, 128.0, 127.9, 127.7, 127.2, 126.2, 34.7, 31.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{25}N_2^+$ 353.2012; Found 353.2010.



1-(4-Methoxyphenyl)-2,5-diphenyl-1*H*-imidazole (5d)

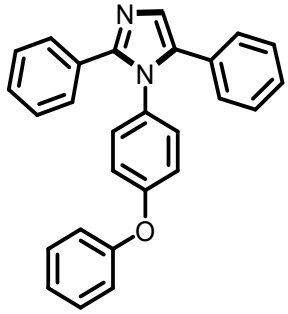
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5d** (104.4 mg, yield 64%) as light yellow solid; m.p. 210-212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.33 (m, 3H), 7.26–7.18 (m, 6H), 7.10 (s, 2H), 7.00 (d, J = 8.4 Hz, 2H), 6.82 (d, J = 8.4 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 148.0, 135.1, 130.6, 129.80, 129.78, 129.2, 128.6, 128.3, 128.1, 128.0, 127.9, 127.2, 114.4, 55.3; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{19}N_2O^+$ 327.1492; Found 327.1491.



1-(4-Ethoxyphenyl)-2,5-diphenyl-1*H*-imidazole (5e)

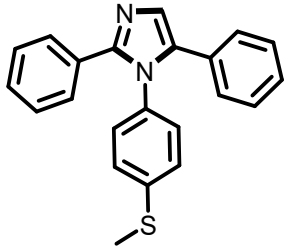
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5e** (103.7 mg, yield 61%) as white solid; m.p. 173-175 °C; ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.40–7.33 (m, 3H), 7.26–7.18 (m, 6H), 7.13–7.07 (m, 2H), 7.00 (d, J = 8.8 Hz, 2H), 6.82 (d, J = 8.8 Hz, 2H), 4.01 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 148.1, 135.2, 130.7, 129.9, 129.7, 129.2, 128.7, 128.3, 128.2, 128.0, 127.2, 114.9, 63.6, 14.7; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O^+$ 341.1648; Found 341.1644.



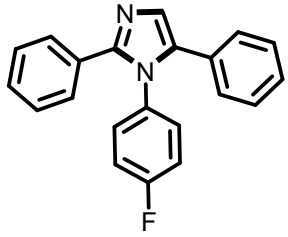
1-(4-Phenoxyphenyl)-2,5-diphenyl-1*H*-imidazole (5f)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5f** (114.5 mg, yield 59%) as light yellow solid; m.p. 220-222 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43–7.33 (m, 5H), 7.30–7.24 (m, 6H), 7.17–7.10 (m, 3H), 7.08–6.99 (m, 4H), 6.97–6.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 156.2, 148.0, 135.2, 131.8, 130.3, 129.9, 129.7, 129.6, 128.8, 128.5, 128.35, 128.29, 128.1, 127.8, 127.5, 124.1, 119.3, 119.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{27}H_{21}N_2O^+$ 389.1648; Found 389.1647.



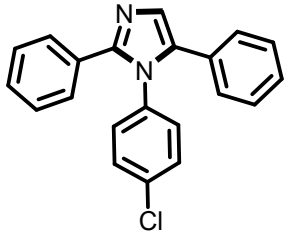
1-(4-(Methylthio)phenyl)-2,5-diphenyl-1*H*-imidazole (5g)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5g** (102.6 mg, yield 60%) as white solid; m.p. 217-219 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (s, 3H), 7.28–7.20 (m, 6H), 7.15 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 4.0 Hz, 2H), 6.99 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 139.5, 135.0, 133.7, 130.4, 129.7, 128.7, 128.41, 128.36, 128.24, 128.15, 128.09, 128.06, 127.3, 126.3, 15.2; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{19}N_2S^+$ 343.1263; Found 343.1262.



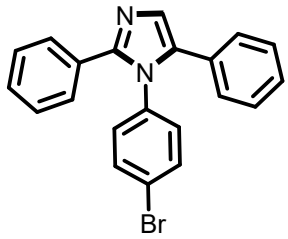
1-(4-Fluorophenyl)-2,5-diphenyl-1*H*-imidazole (5h)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5h** (103.7 mg, yield 66%) as white solid; m.p. 130-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$, CF_3COOD) δ 7.66 (s, 1H), 7.41 (s, 3H), 7.39–7.28(m, 5H), 7.19–7.06 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, CF_3COOD) δ 162.9 (d, J = 251.0 Hz, $^{1}J_{CF}$), 145.2, 135.7, 131.5, 129.7 (d, J = 9.0 Hz, $^{3}J_{CF}$), 129.62, 129.56, 129.2, 129.1, 129.0, 128.7, 125.8, 123.0, 119.3, 117.2 (d, J = 23.0 Hz, $^{2}J_{CF}$); ^{19}F NMR (376 MHz, $CDCl_3$, CF_3COOD) -109.21. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{16}FN_2^+$ 315.1292; Found 315.1289.



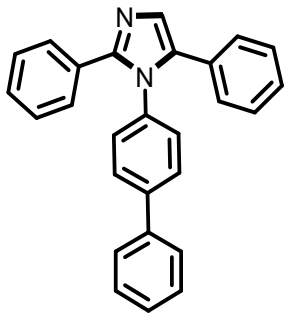
1-(4-Chlorophenyl)-2,5-diphenyl-1*H*-imidazole (5i)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5i** (102.3 mg, yield 62%) as light yellow solid; m.p. 220-222 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.30 (m, 4H), 7.29–7.23 (m, 7H), 7.10–7.05 (m, 2H), 7.02 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 135.6, 134.9, 134.3, 130.2, 129.6, 129.4, 128.8, 128.5, 128.4, 128.3, 128.2, 127.5; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{16}ClN_2^+$ 331.0997; Found 331.0996.



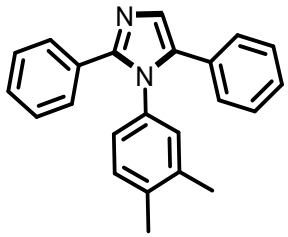
1-(4-Bromophenyl)-2,5-diphenyl-1*H*-imidazole (5j)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5j** (121.6 mg, yield 65%) as light yellow solid; m.p. 208-210 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45–7.40 (m, 2H), 7.35–7.30 (m, 3H), 7.27–7.21 (m, 6H), 7.08–7.04 (m, 2H), 6.93 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 136.1, 134.8, 132.5, 130.2, 129.6, 129.3, 128.7, 128.4, 128.35, 128.28, 128.1, 127.4, 122.3; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{16}BrN_2^+$ 375.0491; Found 375.0490.



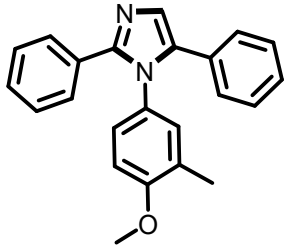
1-([1,1'-Biphenyl]-4-yl)-2,5-diphenyl-1*H*-imidazole (5k)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5k** (107.9 mg, yield 58%) as light yellow solid; m.p. 246-248 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63–7.54 (m, 4H), 7.28–7.20 (m, 6H), 7.47–7.34 (m, 6H), 7.15 (d, J = 8.8 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 141.1, 139.4, 136.1, 135.1, 130.4, 129.7, 128.9, 128.8, 128.5, 128.3, 128.1, 127.9, 127.8, 127.4, 126.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{27}H_{21}N_2^+$ 373.1699; Found 373.1697.



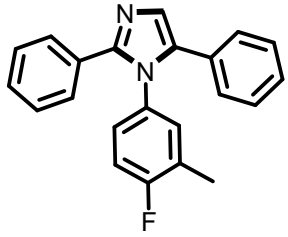
1-(3,4-Dimethylphenyl)-2,5-diphenyl-1*H*-imidazole (5l)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5l** (105.4 mg, yield 65%) as white solid; m.p. 211-213 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.33 (m, 3H), 7.25–7.18 (m, 6H), 7.11–7.04 (m, 3H), 6.88–6.81 (m, 2H), 2.26 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 137.8, 137.1, 135.1, 134.7, 130.7, 130.3, 130.0, 128.9, 128.6, 128.3, 128.1, 127.99, 127.95, 127.9, 127.1, 125.4, 19.7, 19.5; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2^+$ 325.1699; Found 325.1698.



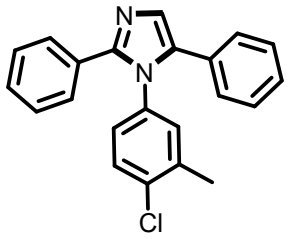
1-(4-Methoxy-3-methylphenyl)-2,5-diphenyl-1*H*-imidazole (5m)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5m** (103.7 mg, yield 61%) as white solid; m.p. 164-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.36 (m, 2H), 7.34 (s, 1H), 7.25–7.17 (m, 6H), 7.13–7.07 (m, 2H), 6.93–6.87 (m, 2H), 6.73 (d, J = 8.4 Hz, 1H), 3.83 (s, 3H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 148.1, 135.2, 130.8, 130.04, 130.02, 129.4, 128.6, 128.3, 128.2, 128.0, 127.9, 127.8, 127.1, 126.5, 110.0, 55.4, 16.1; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O^+$ 341.1648; Found 341.1647.



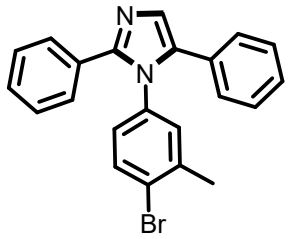
1-(4-Fluoro-3-methylphenyl)-2,5-diphenyl-1*H*-imidazole (5n)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5n** (103.4 mg, yield 63%) as white solid; m.p. 221-223 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.0 Hz, 3H), 7.27–7.20 (m, 6H), 7.12–7.06 (m, 2H), 6.99–6.87 (m, 3H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7 (d, J = 246.0 Hz, $^1J_{CF}$), 159.4, 148.0, 135.1, 132.9 (d, J = 2.0 Hz, $^4J_{CF}$), 131.0 (d, J =5.0 Hz, $^3J_{CF}$), 130.5, 129.7, 128.6, 128.4, 128.2, 128.1 (d, J = 4.0 Hz, $^3J_{CF}$), 128.0, 127.3, 127.1 (d, J = 9.0 Hz, $^3J_{CF}$), 126.3 (d, J = 18.0 Hz, $^2J_{CF}$), 115.8 (d, J = 23.0 Hz, $^2J_{CF}$), 14.45, 14.43; ^{19}F NMR (376 MHz, $CDCl_3$) -116.32; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}FN_2^+$ 329.1449; Found 329.1446.



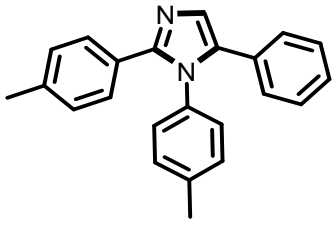
1-(4-Chloro-3-methylphenyl)-2,5-diphenyl-1*H*-imidazole (5o)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5o** (103.2 mg, yield 60%) as light yellow solid; m.p. 214-216 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.33 (m, 3H), 7.28–7.22 (m, 7H), 7.09–7.06 (m, 2H), 6.95 (d, J = 2.4 Hz, 1H), 6.89–6.84 (m, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 137.5, 135.5, 134.9, 134.4, 130.32, 130.28, 129.8, 129.5, 128.7, 128.4, 128.29, 128.27, 128.2, 128.1, 127.4, 126.8, 20.0; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}ClN_2^+$ 345.1153; Found 345.1152.



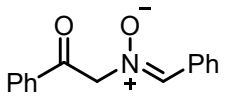
1-(4-Bromo-3-methylphenyl)-2,5-diphenyl-1*H*-imidazole (5p)

Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **5p** (128.1 mg, yield 66%) as light yellow solid; m.p. 212-214 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.4 Hz, 1H), 7.37–7.32 (m, 3H), 7.27–7.21 (m, 6H), 7.10–7.06 (m, 2H), 6.95 (d, J = 2.0 Hz, 1H), 6.81–6.76 (m, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 139.4, 136.2, 134.9, 133.1, 130.3, 130.1, 129.5, 128.7, 128.4, 128.3, 128.2, 128.1, 127.4, 127.0, 124.8, 22.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}BrN_2^+$ 389.0648; Found 389.0642.



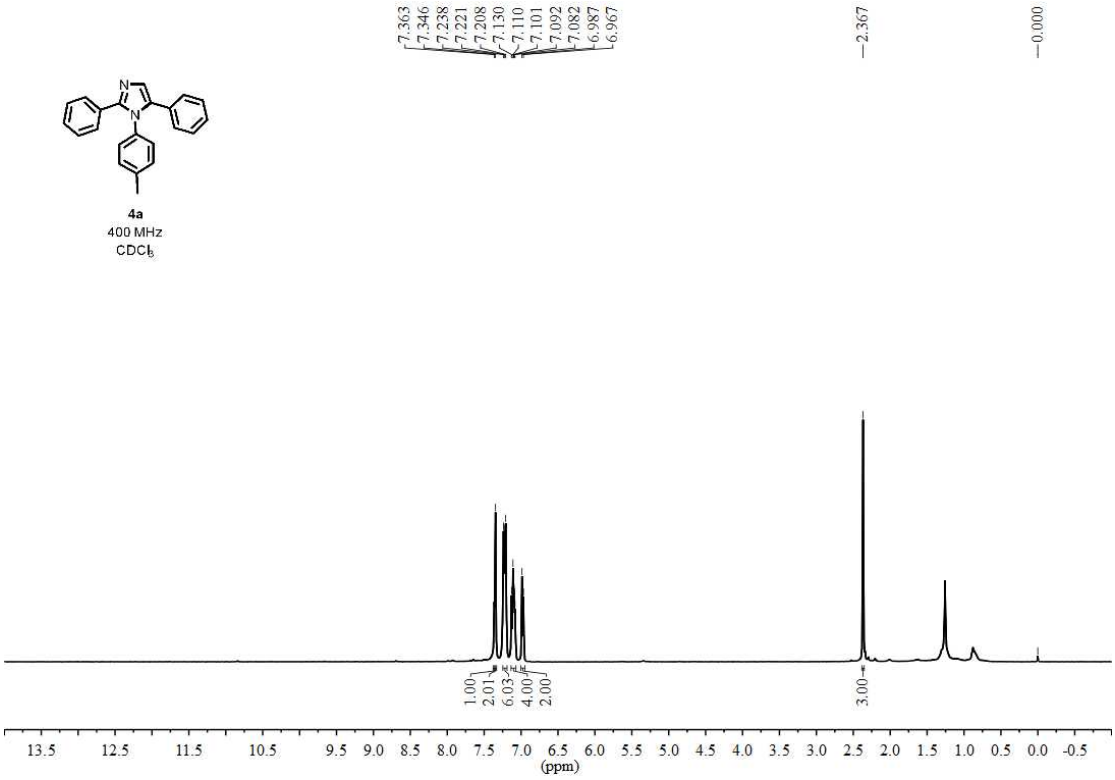
5-Phenyl-1,2-*di*-p-tolyl-1H-imidazole (5q)

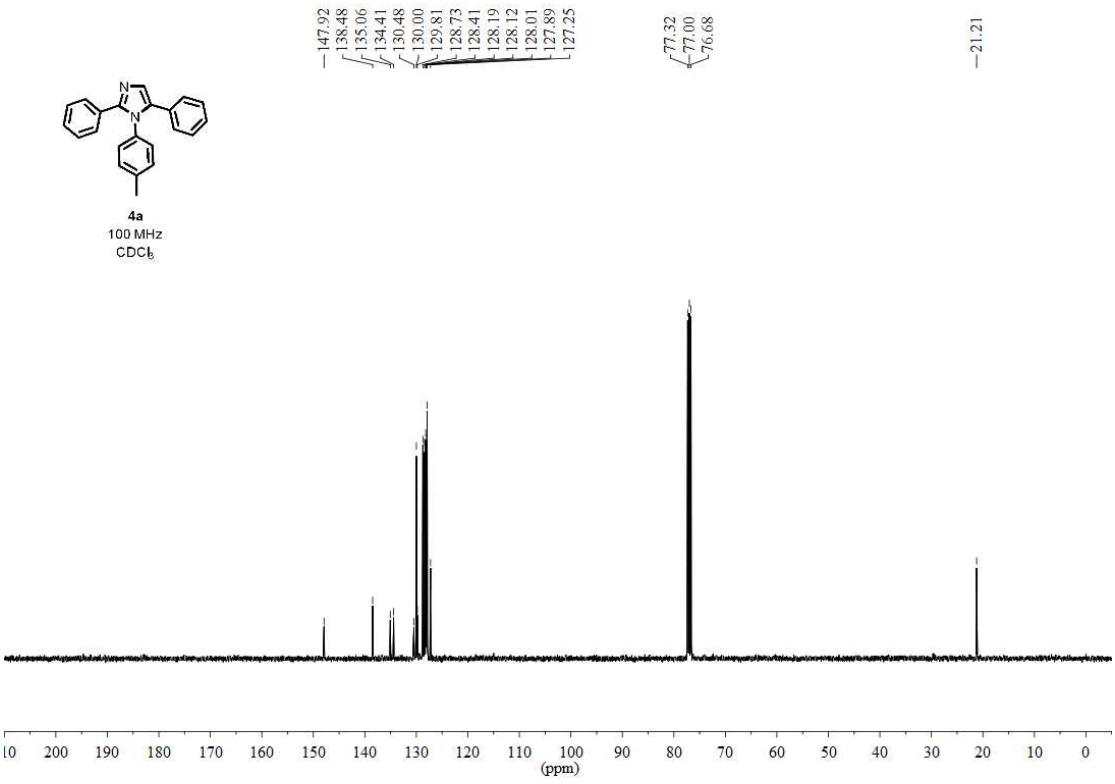
Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (8:1 v/v) as eluent afforded **5q** (76.2 mg, yield 47%) as light yellow solid; m.p. 160-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (s, 1H), 7.26 (s, 1H), 7.23 (s, 1H), 7.22–7.19 (m, 3H), 7.13 (s, 1H), 7.11 (s, 1H), 7.10–7.06 (m, 2H), 7.04 (d, J = 8.0 Hz, 2H), 6.98 (d, J = 8.4 Hz, 2H), 2.37 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 138.4, 138.0, 134.9, 134.6, 130.0, 128.8, 128.6, 128.4, 128.2, 128.0, 127.8, 127.7, 127.2, 21.22, 21.21; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2^+$ 325.1699; Found 325.1703.

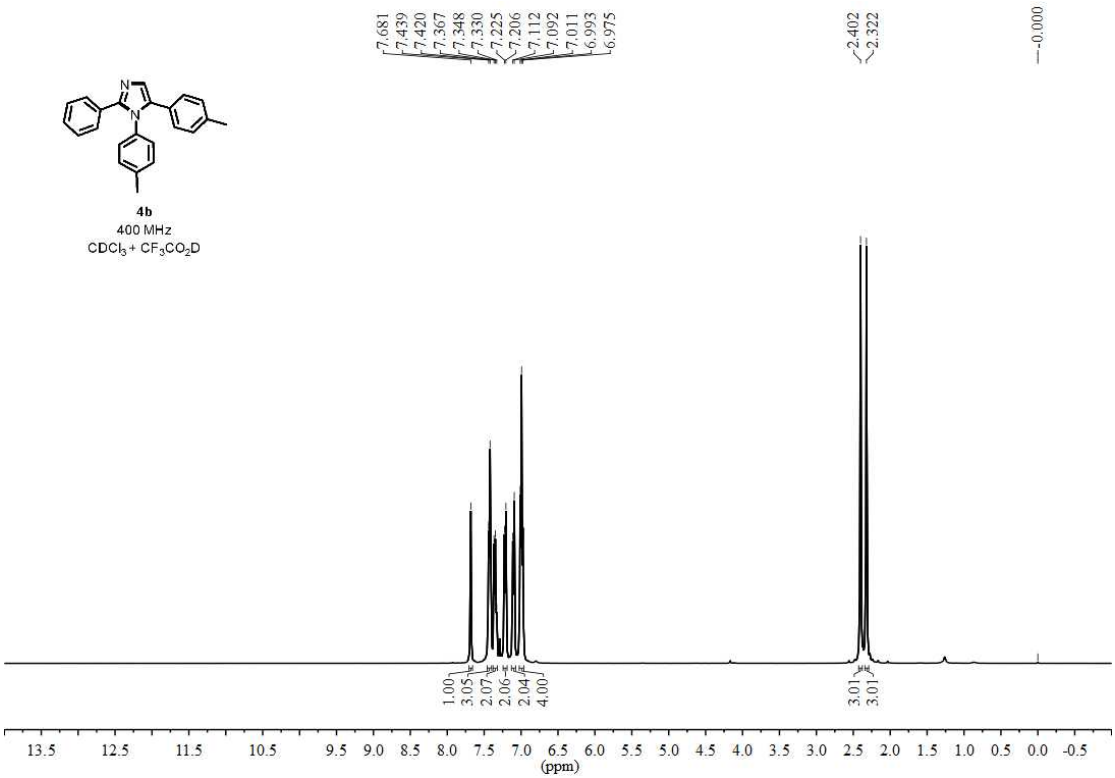


(*Z*)-*N*-(2-oxo-2-phenylethyl)-1-phenylmethanimine oxide (6): (Orange solid, 454.1 mg, yield 95%); m.p. 97-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22–8.17 (m, 2H), 7.91–7.86 (m, 2H), 7.57–7.51 (m, 1H), 7.45 (s, 1H), 7.41–7.32 (m, 5H), 5.37 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.2, 137.3, 134.3, 133.9, 130.4, 129.9, 128.6, 128.4, 128.1, 127.9, 71.9; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}NO_2^+$ 240.1019; Found 240.1018.

7. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra



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7.367
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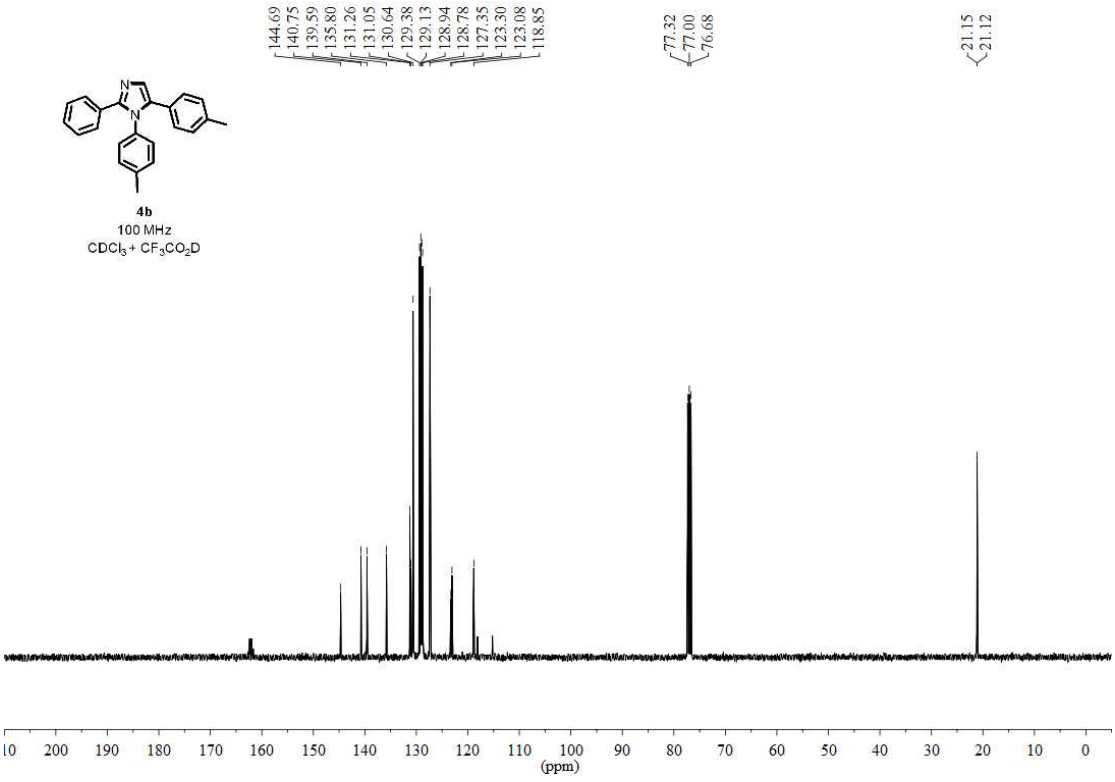
7.330
7.225
7.206
7.112
7.092
7.011
6.993
6.975
2.402
2.322
0.000
4b
400 MHz
CDCl3 + CF3CO2D
1.00
3.05
2.07
2.06
2.04
4.00
3.01
3.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)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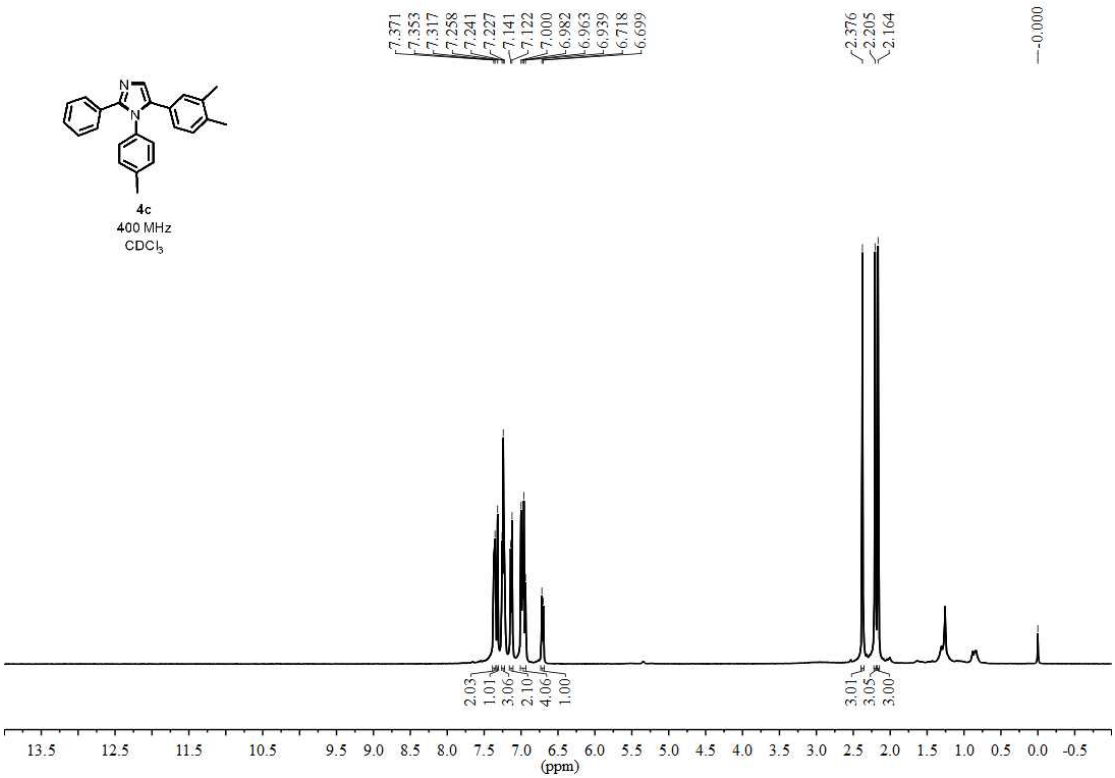
140.75
139.59
135.80
131.26
131.05
130.64
129.38
129.13
128.94
128.78
127.35
123.30
123.08
118.85
77.32
77.00
76.68
21.15
21.12
4b
100 MHz
CDCl3 + CF3CO2D
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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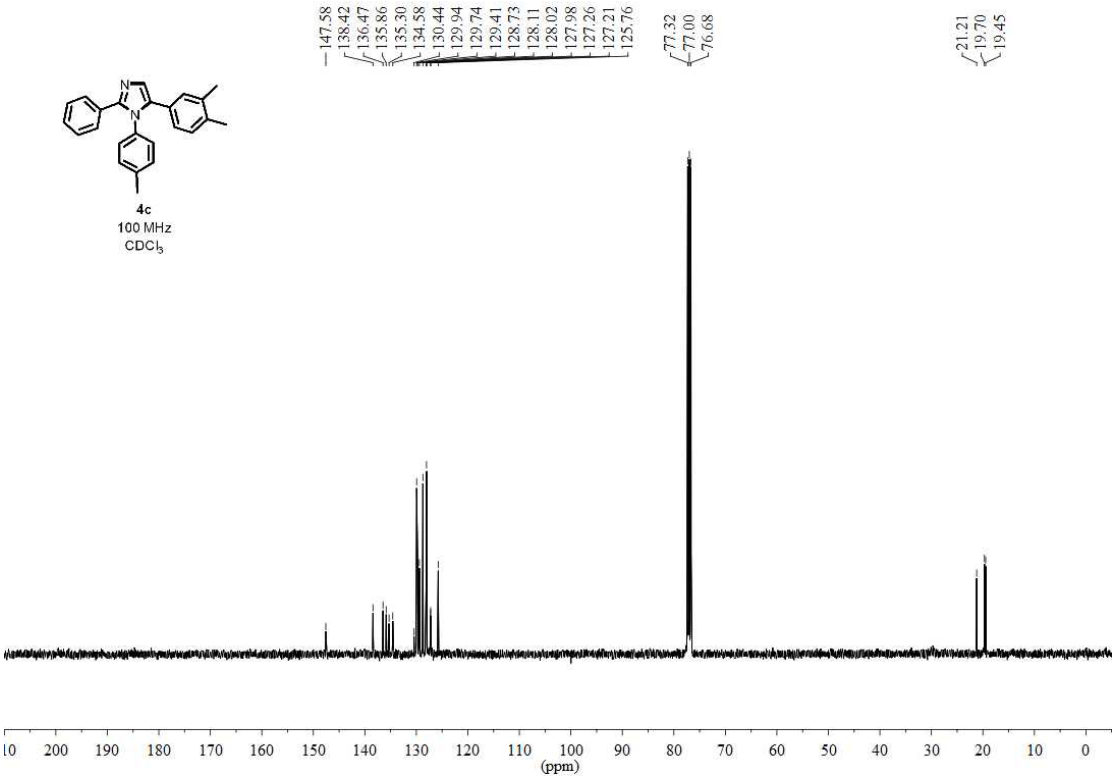
7.227
7.141
7.122
7.000
6.982
6.963
6.939
6.718
6.699
2.376
2.205
2.164
-0.000
4c
400 MHz
CDCl3
2.03
1.01
3.06
2.10
4.06
1.00
3.01
3.05
3.00
(ppm)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138.42
136.47
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134.58
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129.94
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129.41
128.73
128.11
128.02
127.98
127.26
127.21
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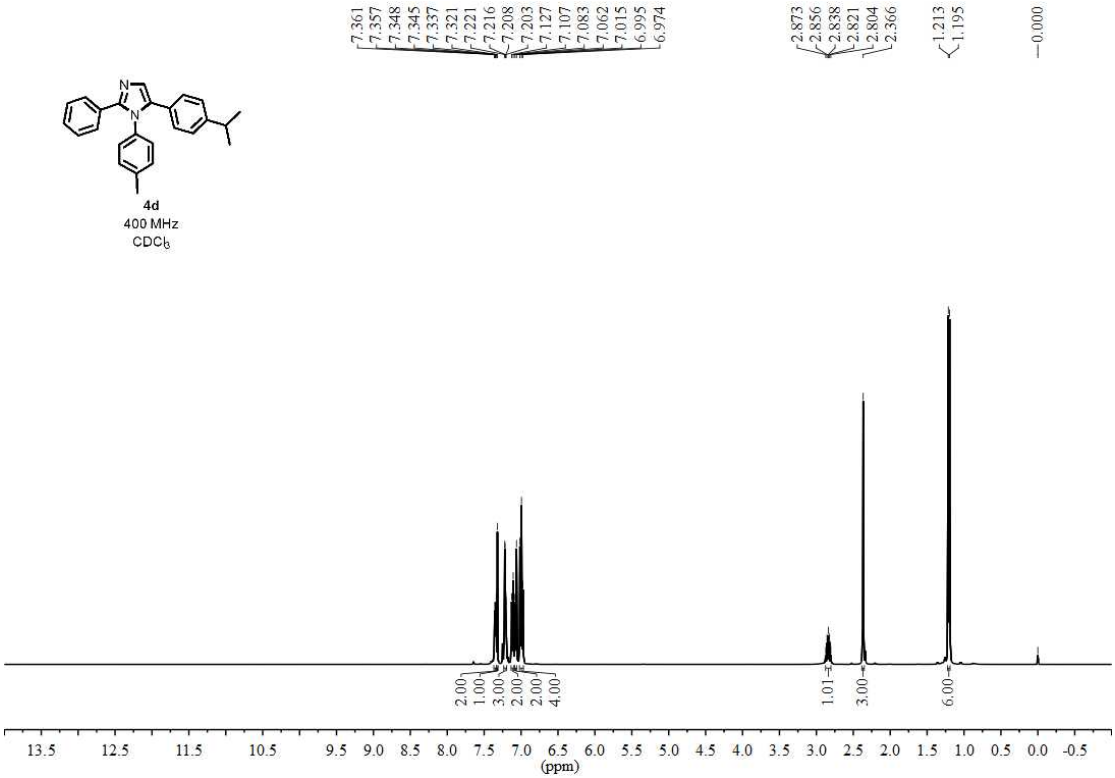
77.32
77.00
76.68
21.21
19.70
19.45
4c
100 MHz
CDCl3
(ppm)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7.321
7.221
7.216
7.208
7.203
7.127
7.107
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7.062
7.015
6.995
6.974
2.873
2.856
2.838
2.821
2.804
2.366
1.213
1.195
0.000
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4.00
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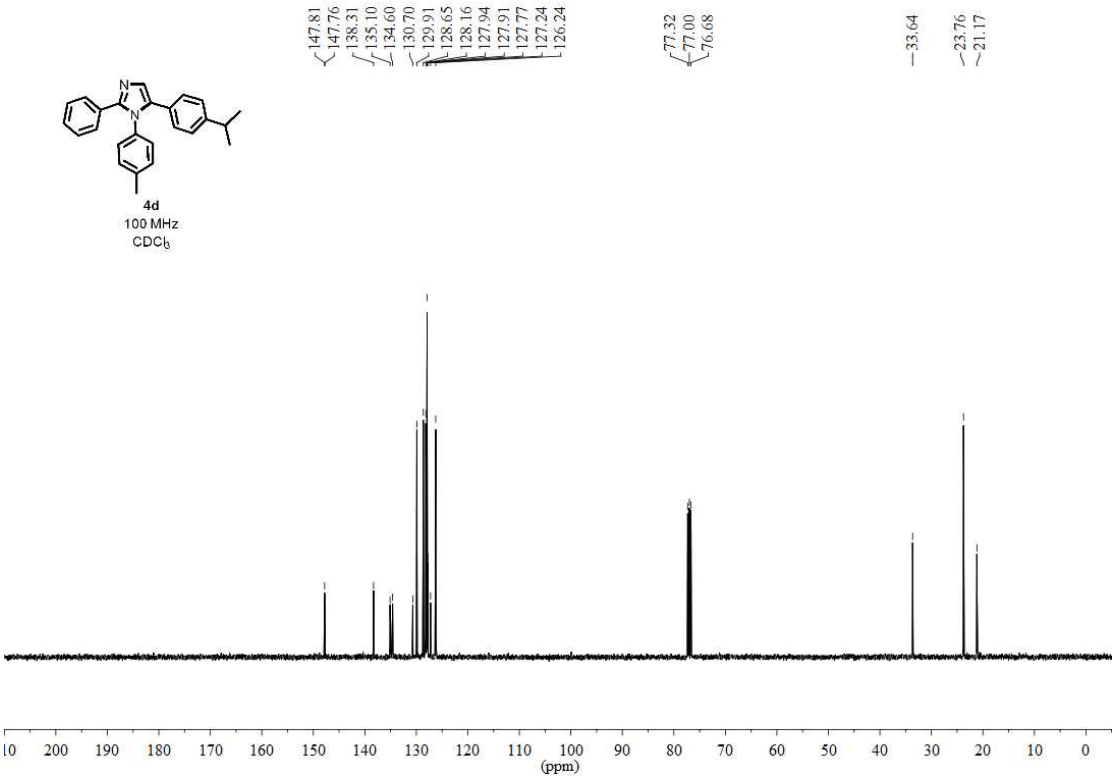
3.00
6.00
(ppm)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127.94
127.91
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77.32
77.00
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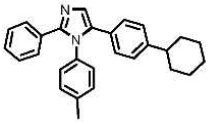
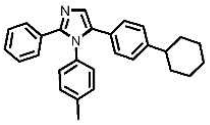
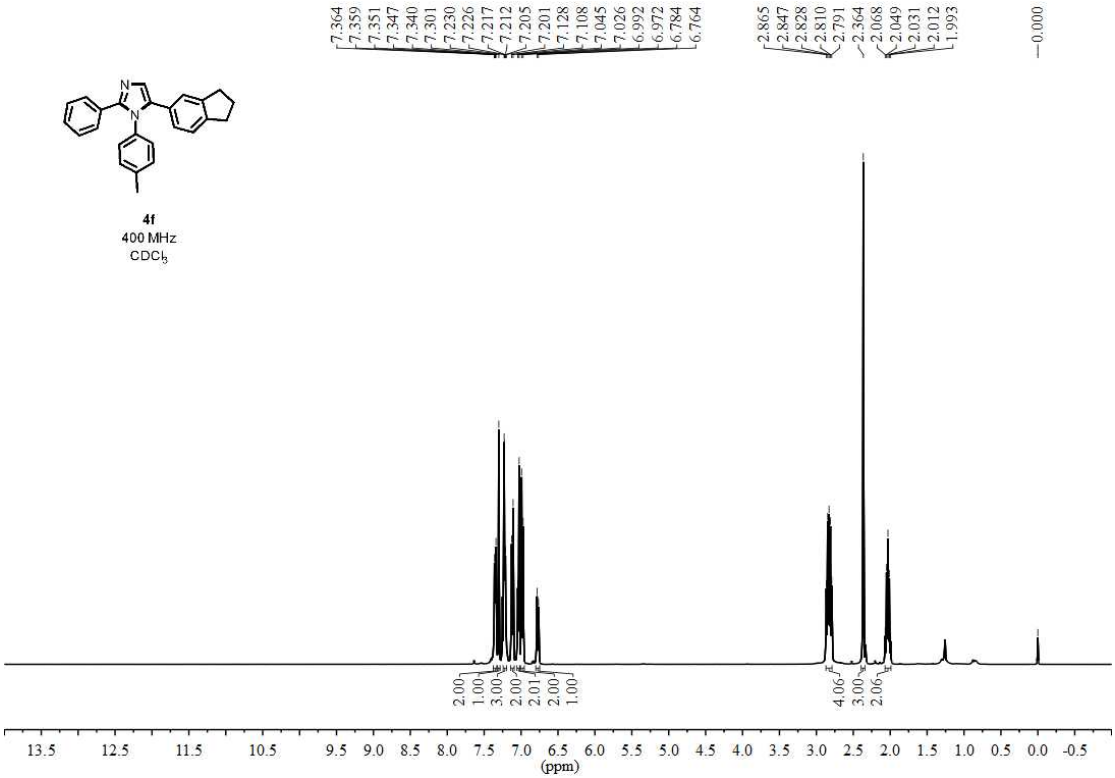
23.76
21.17
4d
100 MHz
CDCl3
(ppm)



4e
400 MHz
$CDCl_3$



4e
100 MHz
$CDCl_3$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7.226
7.217
7.212
7.205
7.201
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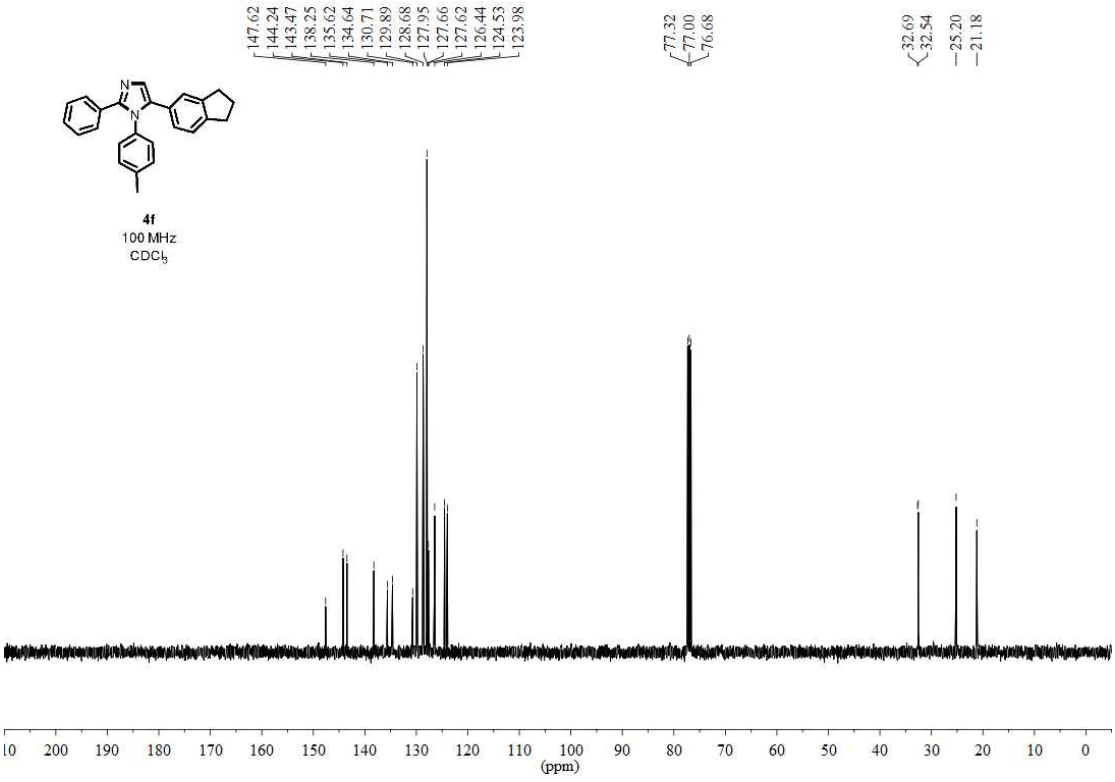
7.108
7.045
7.026
6.992
6.972
6.784
6.764
2.865
2.847
2.828
2.810
2.791
2.364
2.068
2.049
2.031
2.012
1.993
0.000
4f
400 MHz
CDCl3
2.00
1.00
3.00
2.00
2.01
2.00
1.00
4.06
3.00
2.06
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)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144.24
143.47
138.25
135.62
134.64
130.71
129.89
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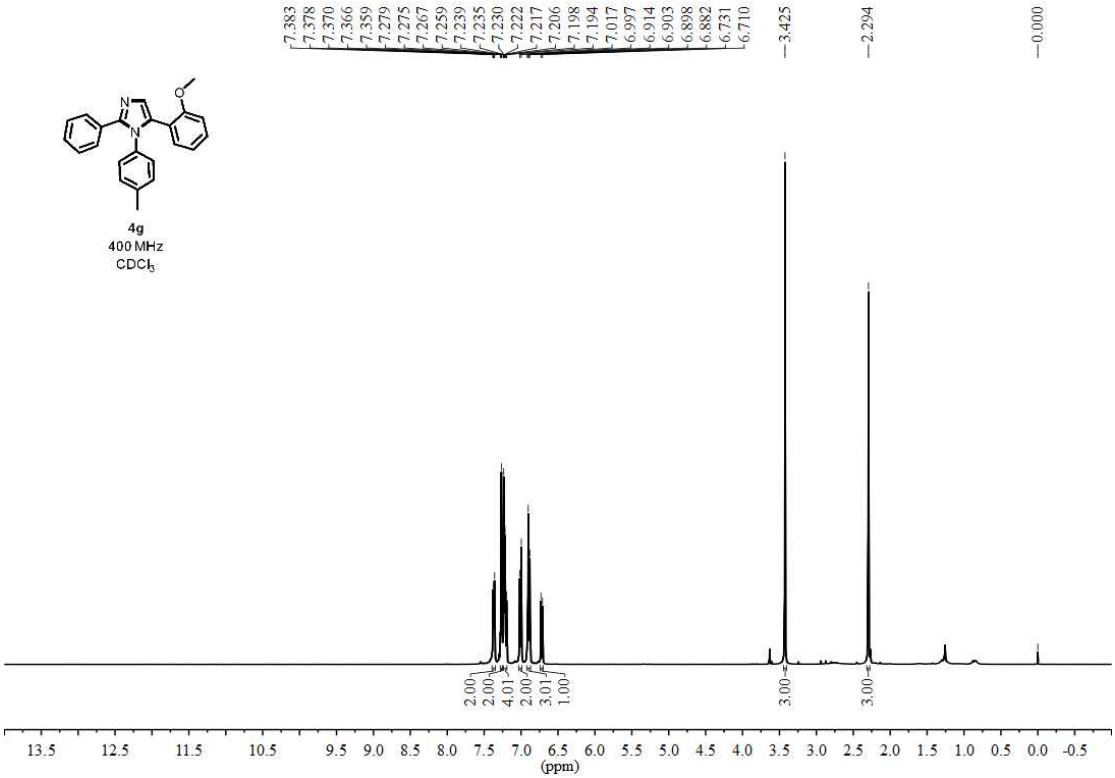
127.62
126.44
124.53
123.98
77.32
77.00
76.68
32.69
32.54
25.20
21.18
4f
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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7.366
7.359
7.279
7.275
7.267
7.259
7.239
7.235
7.230
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7.217
7.206
7.198
7.194
7.017
6.997
6.914
6.903
6.898
6.882
6.731
6.710
3.425
2.294
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400 MHz
CDCl3
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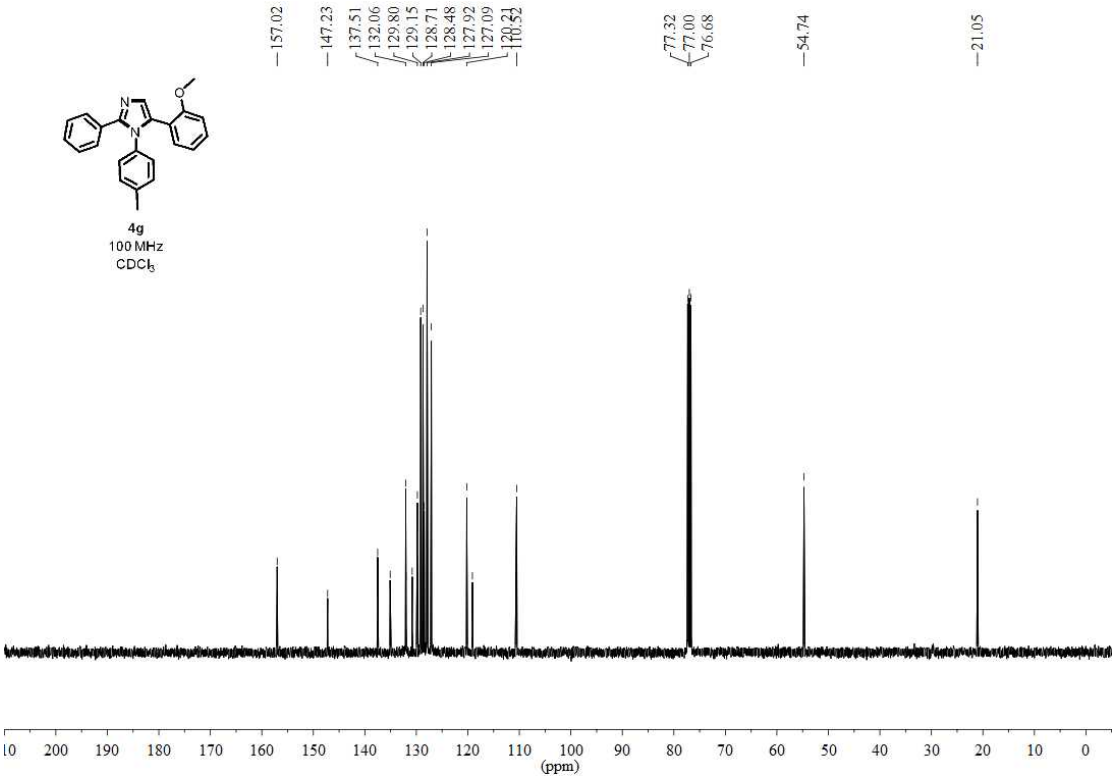
2.00
4.01
2.00
3.01
1.00
3.00
3.00
(ppm)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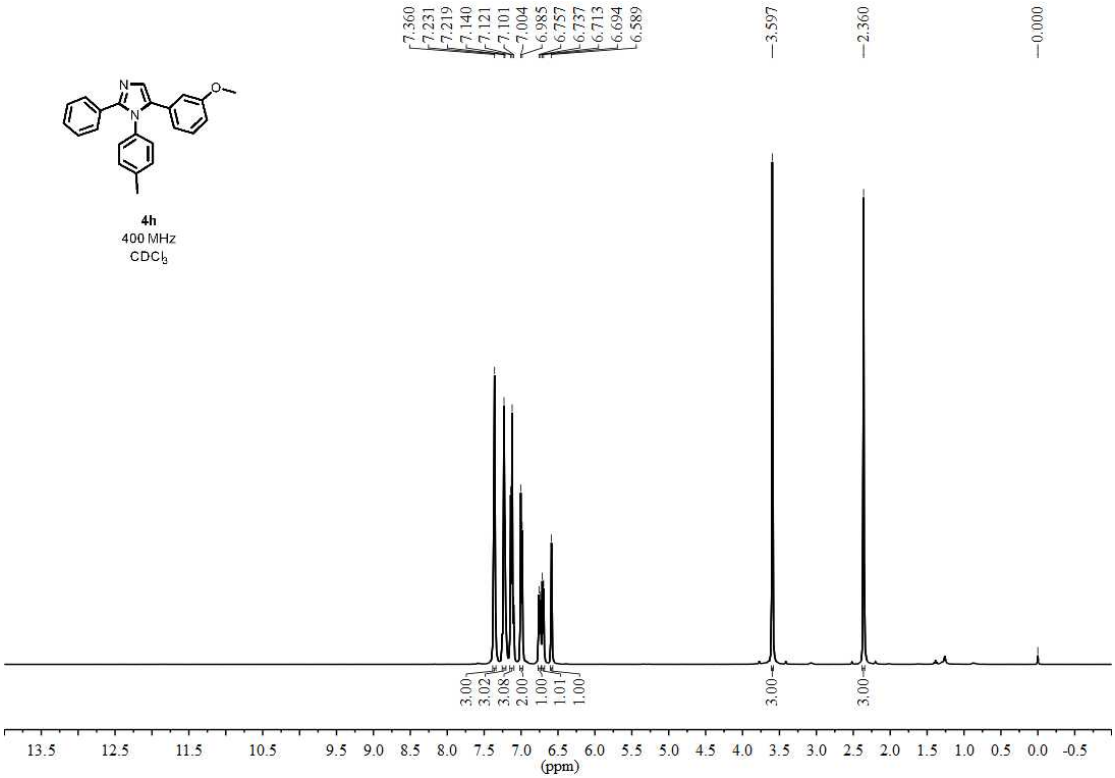
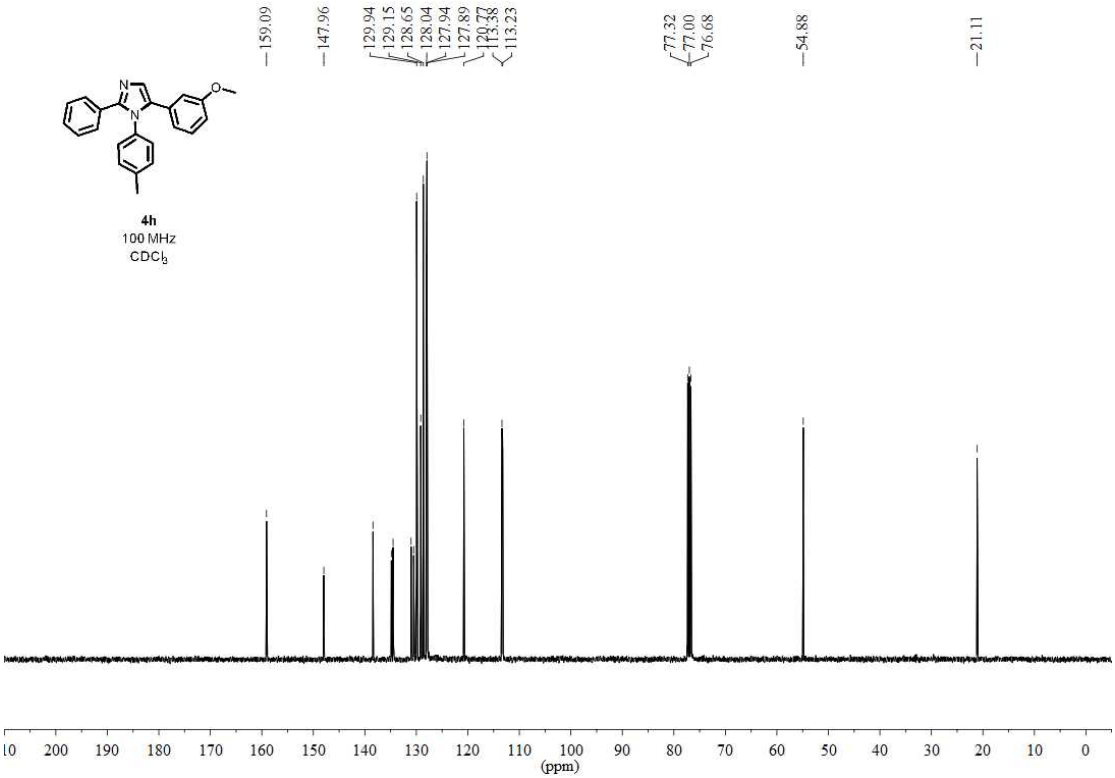
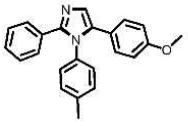
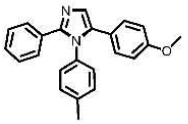
77.00
76.68
54.74
21.05
4g
100 MHz
CDCl3
(ppm)


7.360
7.231
7.219
7.140
7.121
7.101
7.004
6.985
6.757
6.737
6.713
6.694
6.589
3.597
2.360
0.000
4h
400 MHz
CDCl3
3.00
3.02
3.08
2.00
1.00
1.01
1.00
3.00
3.00
(ppm)

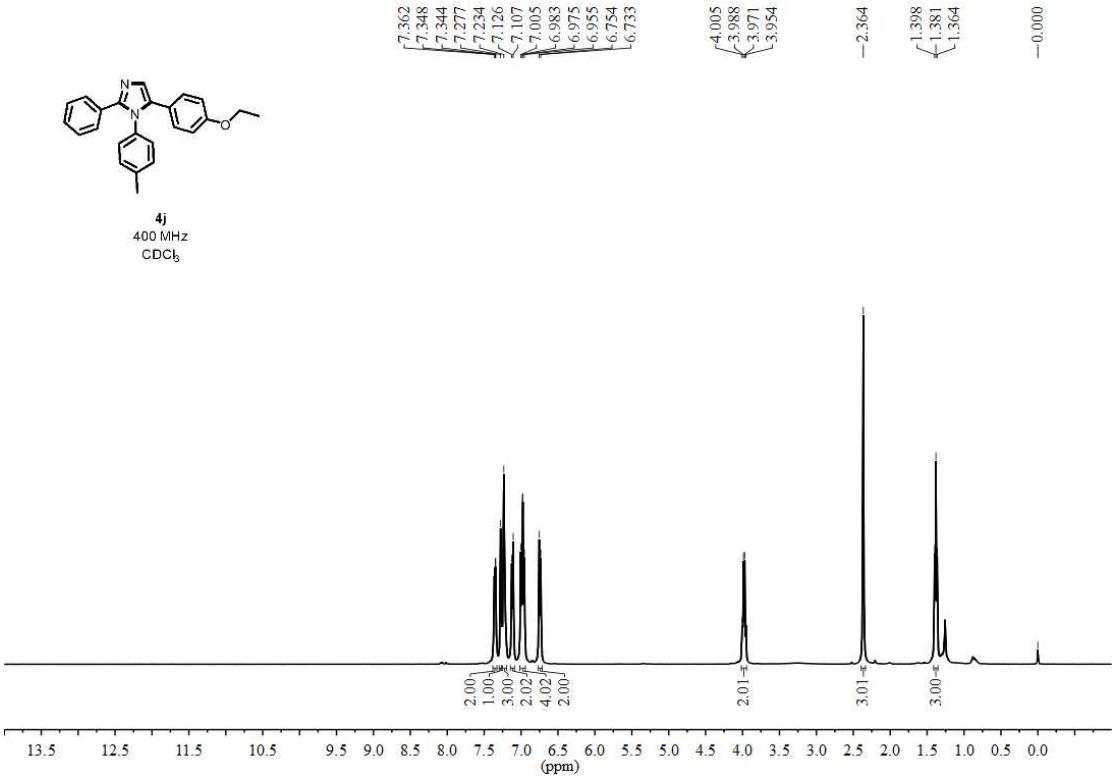

159.09
147.96
129.94
129.15
128.65
128.04
127.94
127.89
120.77
113.38
113.23
77.32
77.00
76.68
54.88
21.11
4h
100 MHz
CDCl3
(ppm)

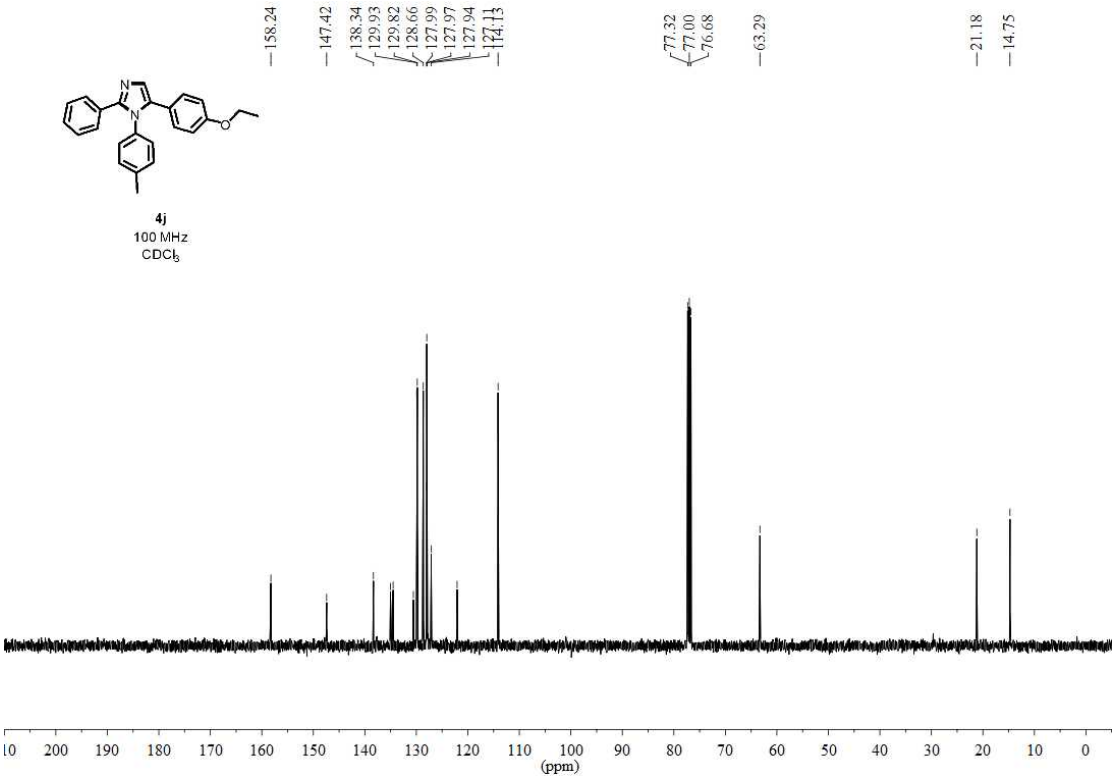


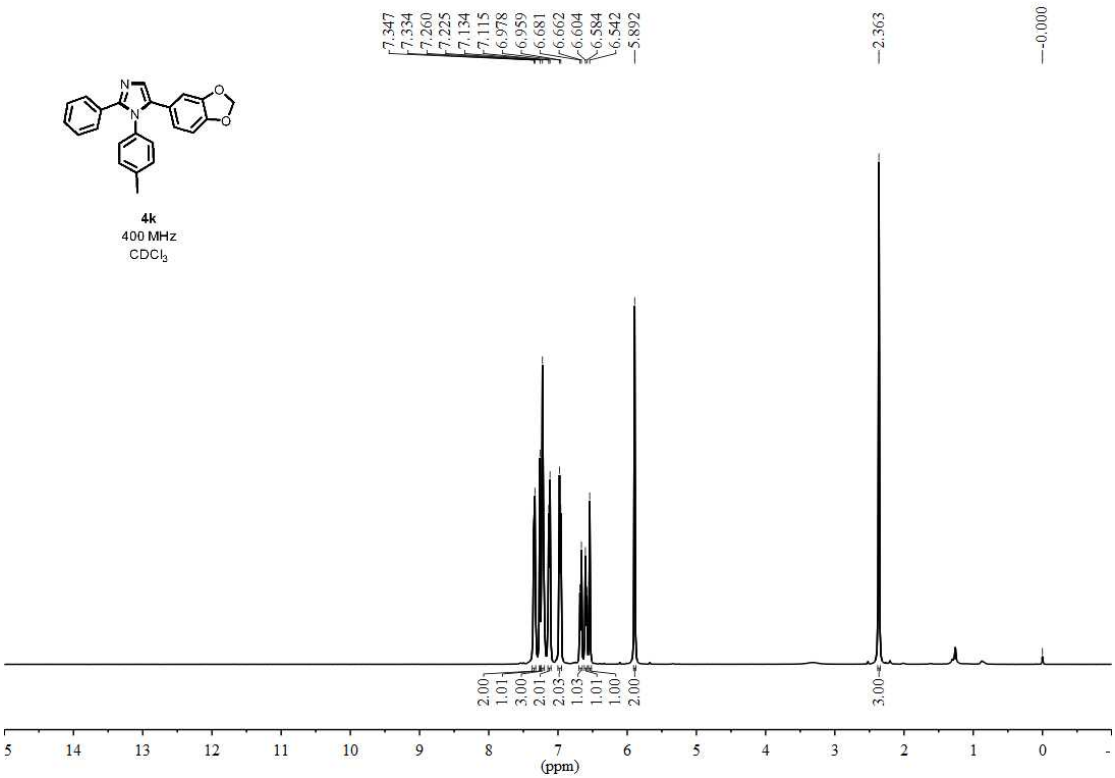
4i
400 MHz
$CDCl_3$

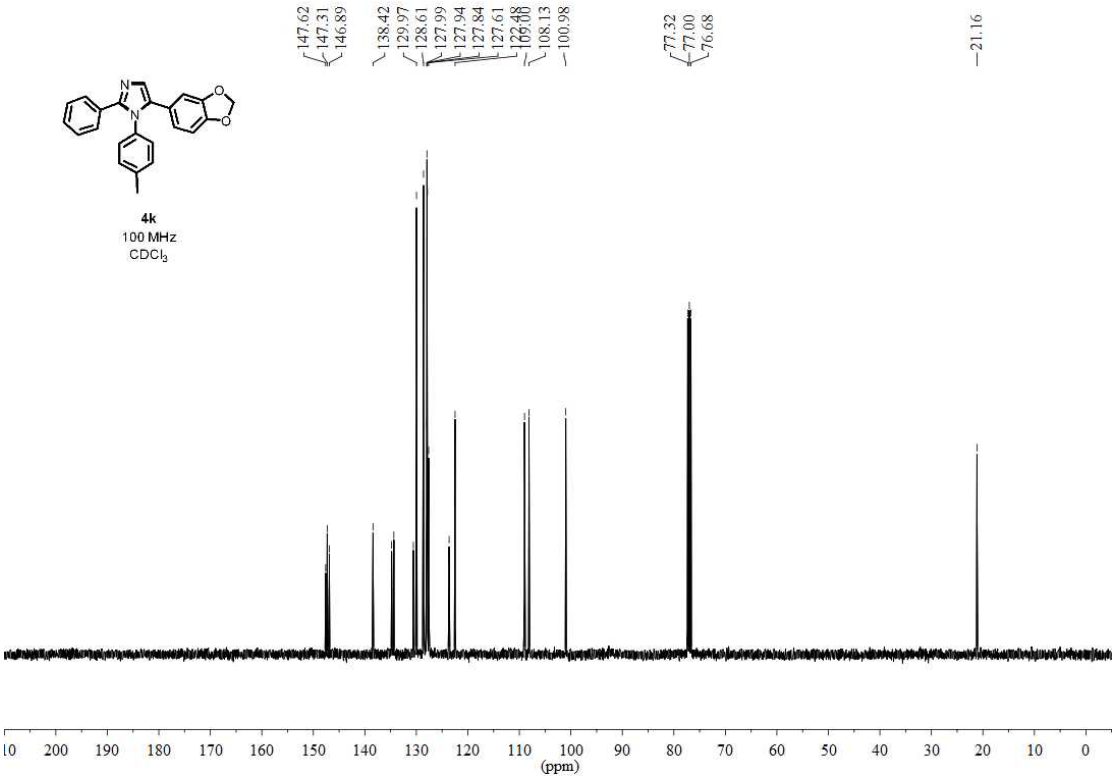


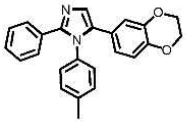
4i
100 MHz
$CDCl_3$


7.362
7.348
7.344
7.277
7.234
7.126
7.107
7.005
6.983
6.975
6.955
6.754
6.733
4.005
3.988
3.971
3.954
2.364
1.398
1.381
1.364
0.000
4j
400 MHz
CDCl3
2.00
1.00
3.00
2.02
4.02
2.00
2.01
3.01
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

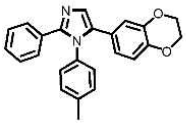

158.24
147.42
138.34
129.93
129.82
128.66
127.99
127.97
127.94
127.11
114.13
77.32
77.00
76.68
63.29
21.18
14.75
4j
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.347
7.334
7.260
7.225
7.134
7.115
6.978
6.959
6.681
6.662
6.604
6.584
6.542
5.892
2.363
0.000
4k
400 MHz
CDCl3
2.00
1.01
3.00
2.01
2.03
1.03
1.01
1.00
2.00
3.00
(ppm)

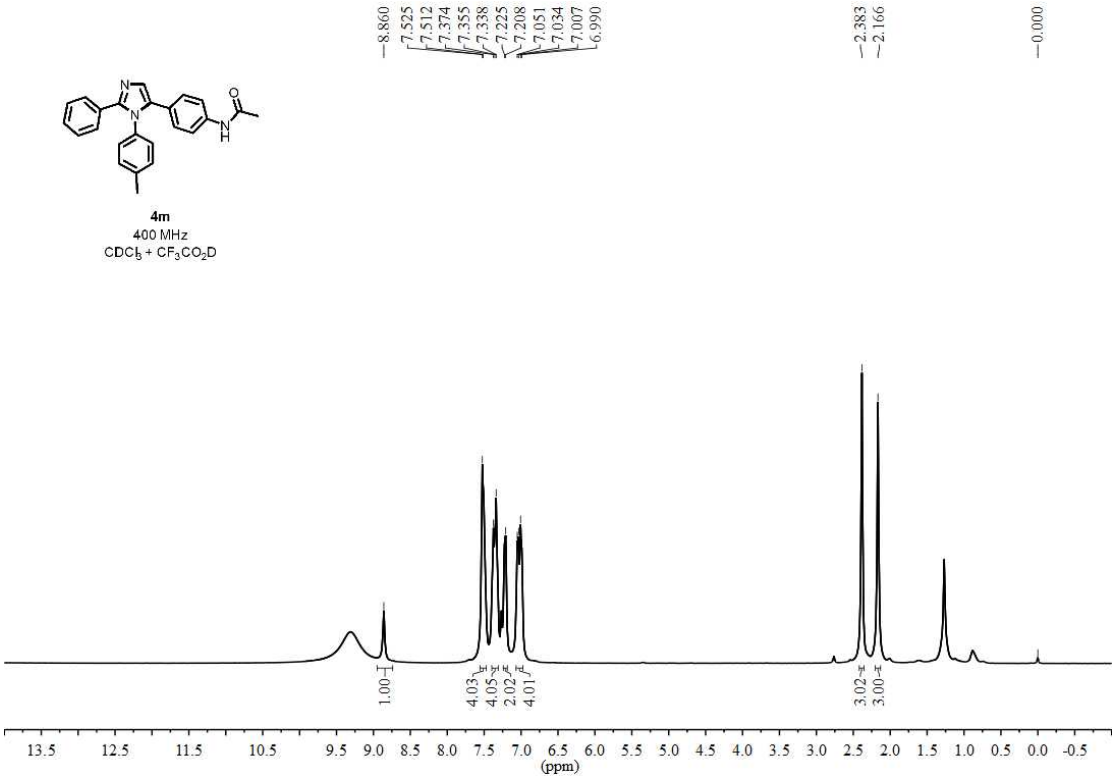

147.62
147.31
146.89
138.42
129.97
128.61
127.99
127.94
127.84
127.61
122.48
109.00
108.13
100.98
77.32
77.00
76.68
21.16
4k
100 MHz
CDCl3
(ppm)



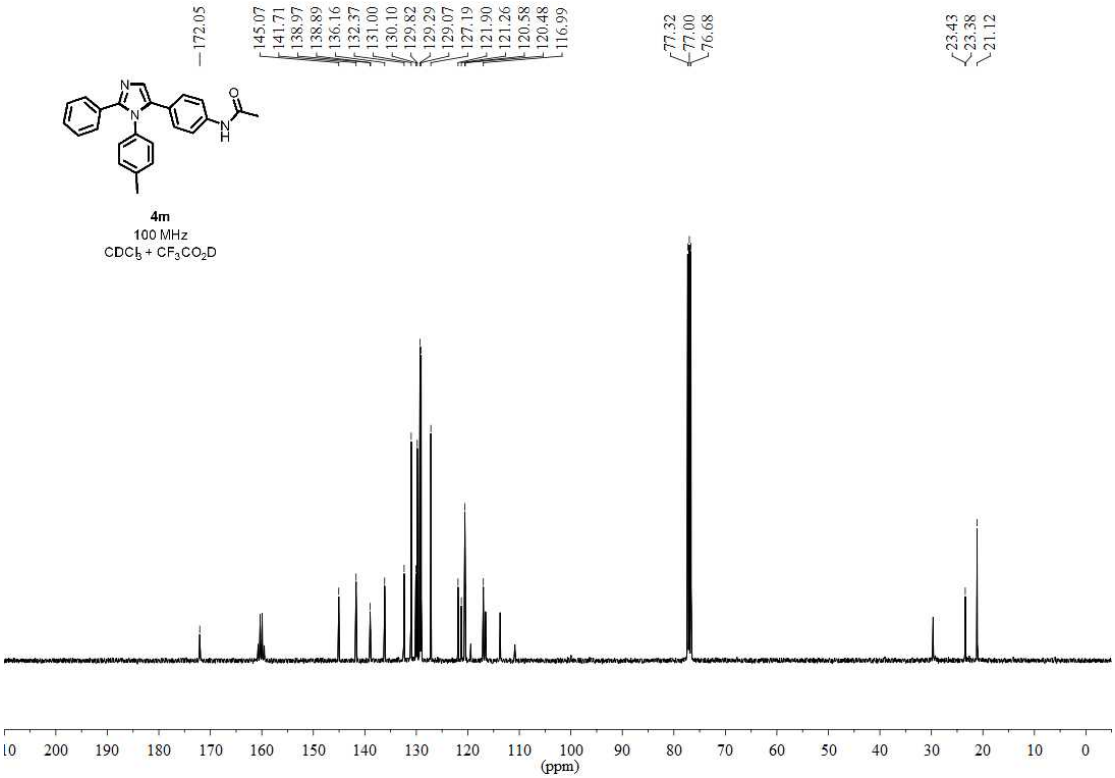
4l
400 MHz
$CDCl_3$



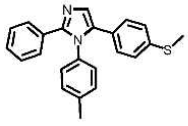
4l
100 MHz
$CDCl_3$



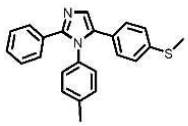
4m
400 MHz
$CDCl_3 + CF_3CO_2D$



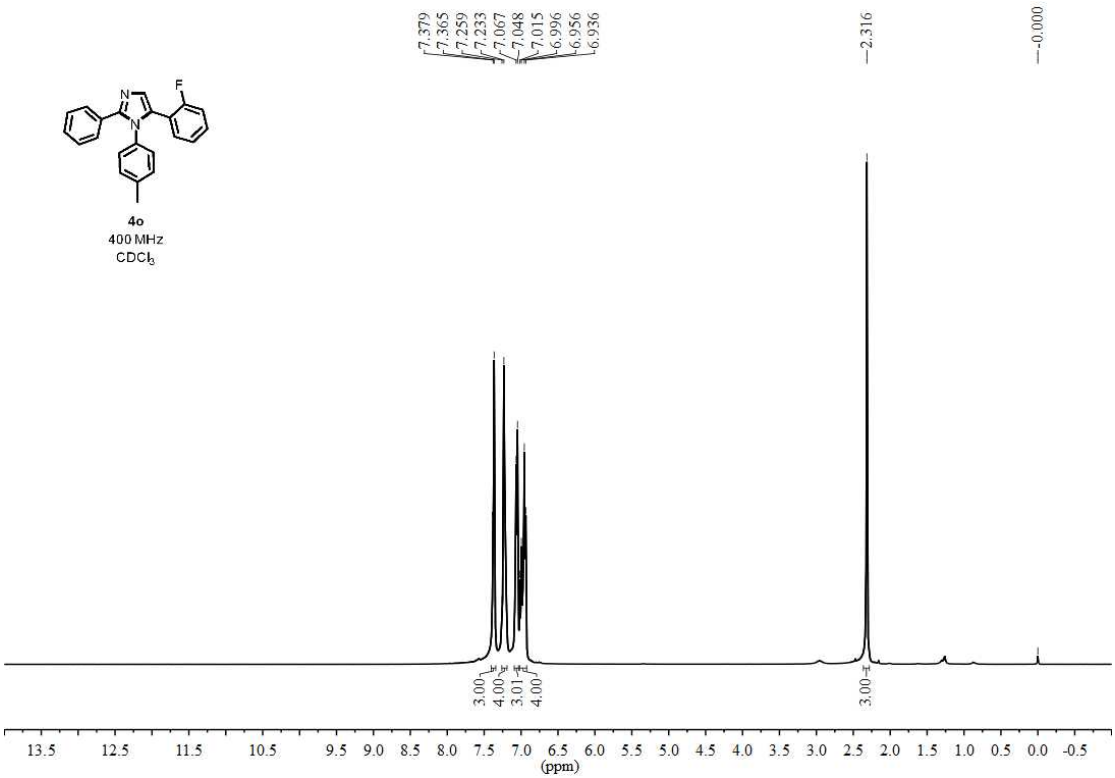
4m
100 MHz
$CDCl_3 + CF_3CO_2D$

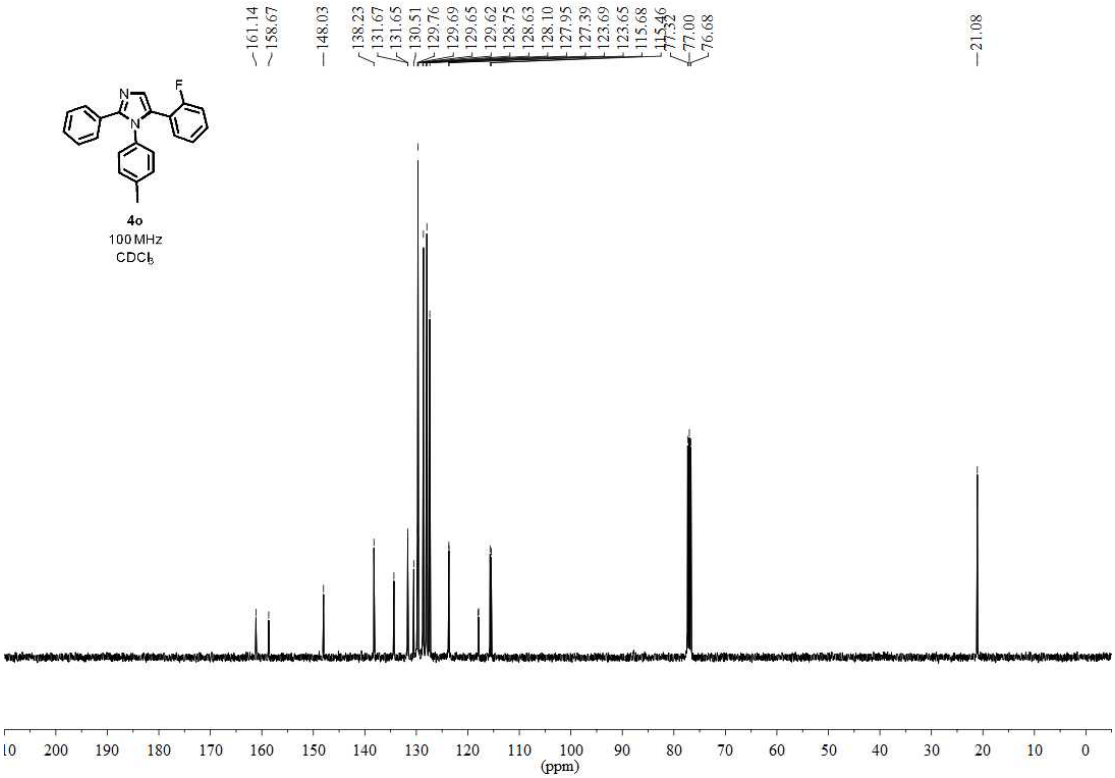


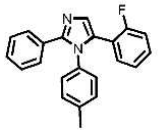
4n
400 MHz
$CDCl_3$



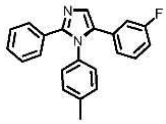
4n
100 MHz
$CDCl_3$


7.379
7.365
7.259
7.233
7.067
7.048
7.015
6.996
6.956
6.936
2.316
0.000
4o
400 MHz
CDCl3
3.00
4.00
3.01
4.00
3.00
(ppm)

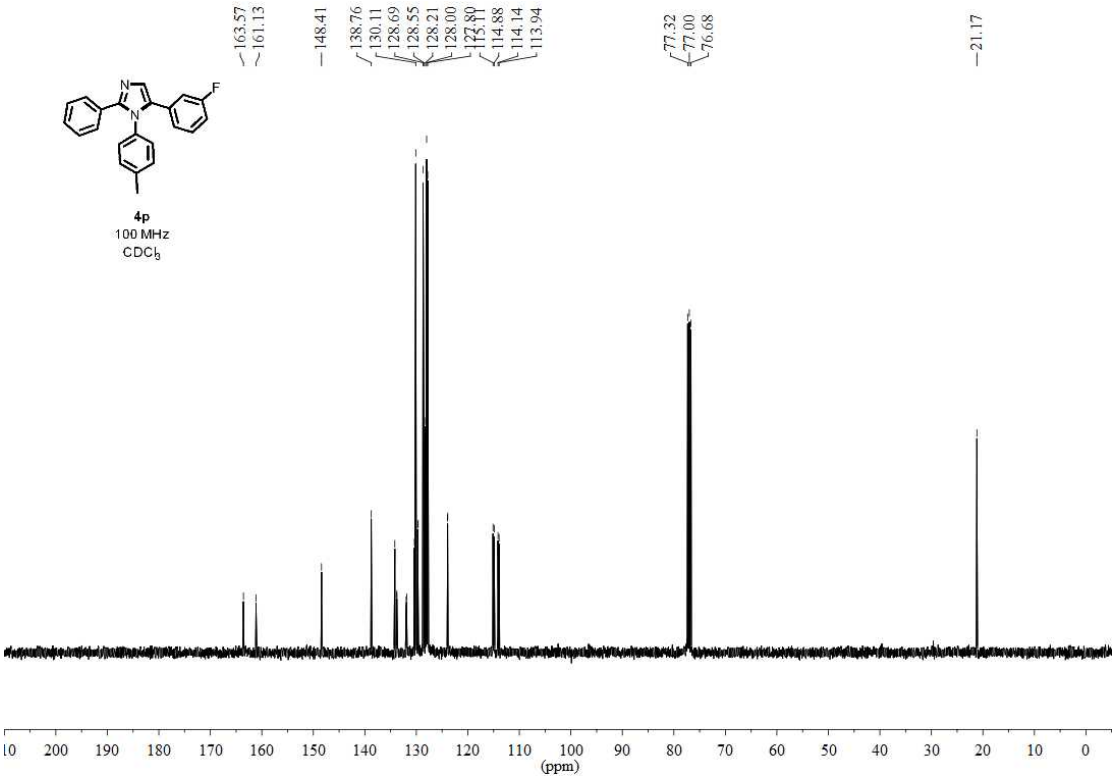

161.14
158.67
148.03
138.23
131.67
131.65
130.51
129.76
129.69
129.65
129.62
128.75
128.63
128.10
127.95
127.39
123.69
123.65
115.68
115.46
77.32
77.00
76.68
21.08
4o
100 MHz
CDCl3
(ppm)

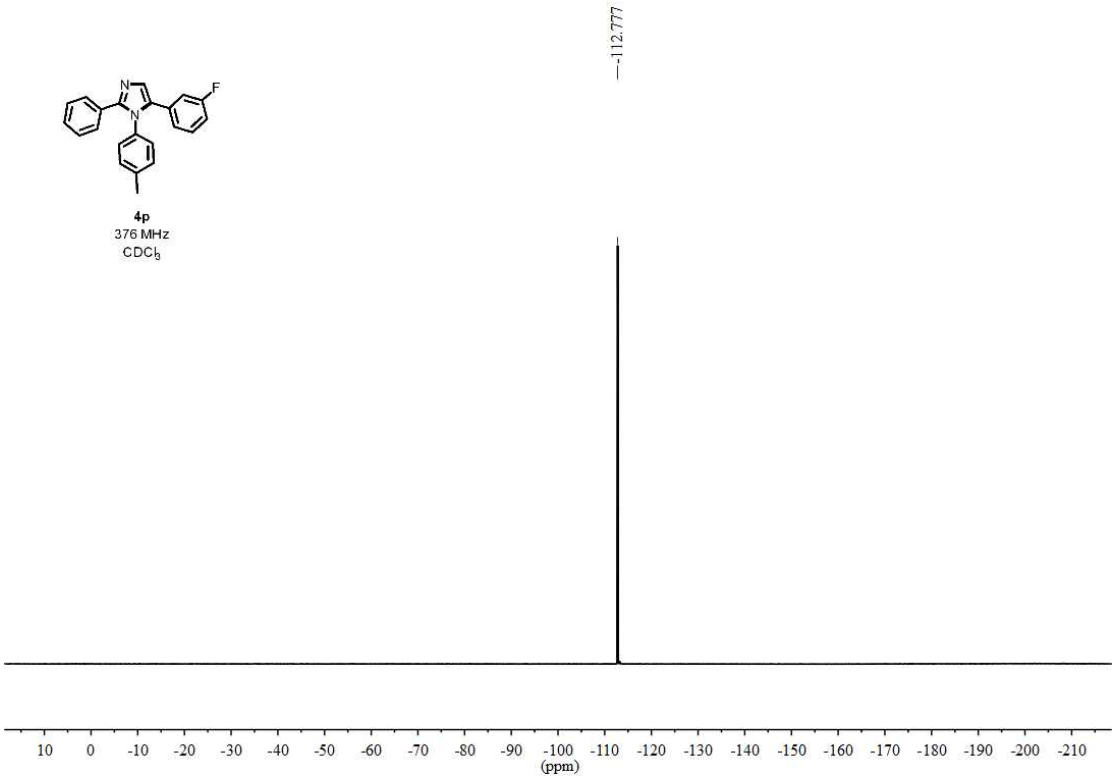


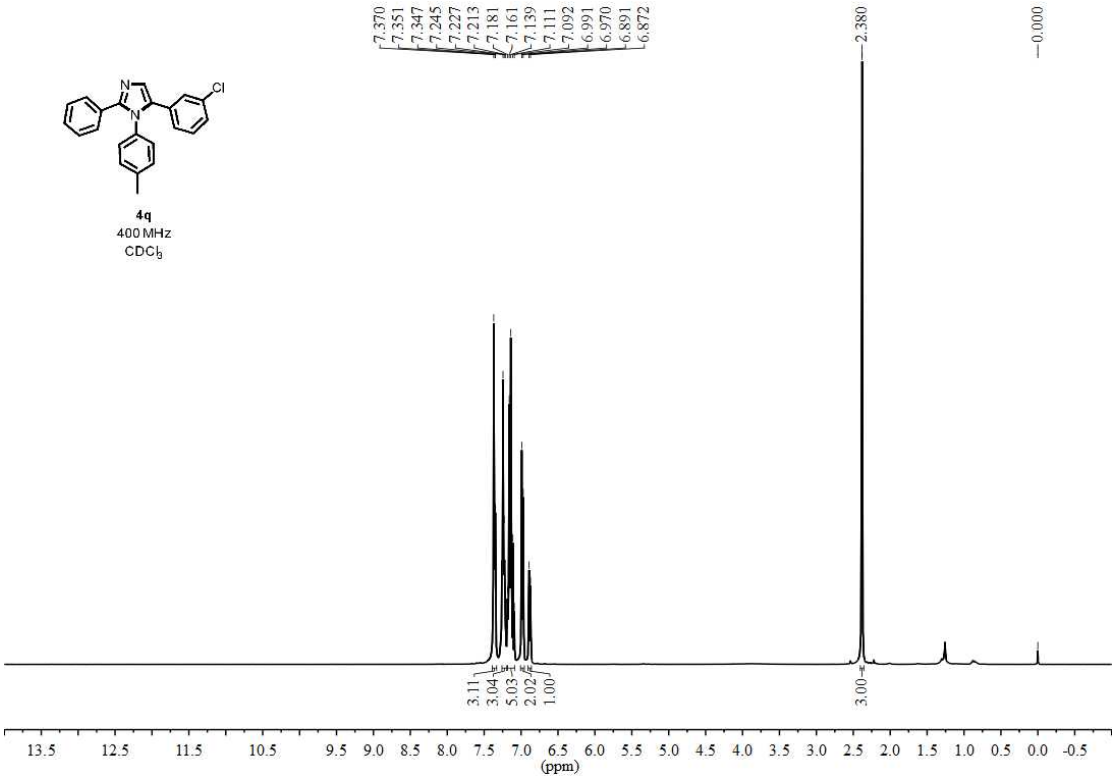
4o
376 MHz
$CDCl_3$

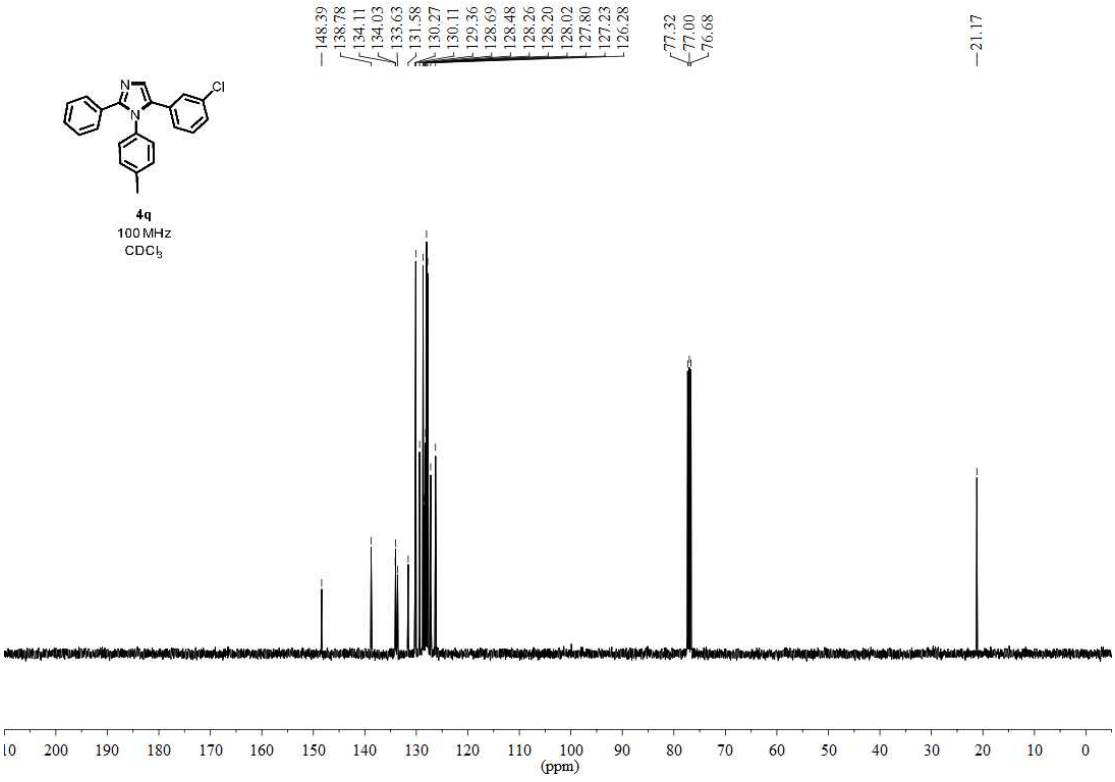


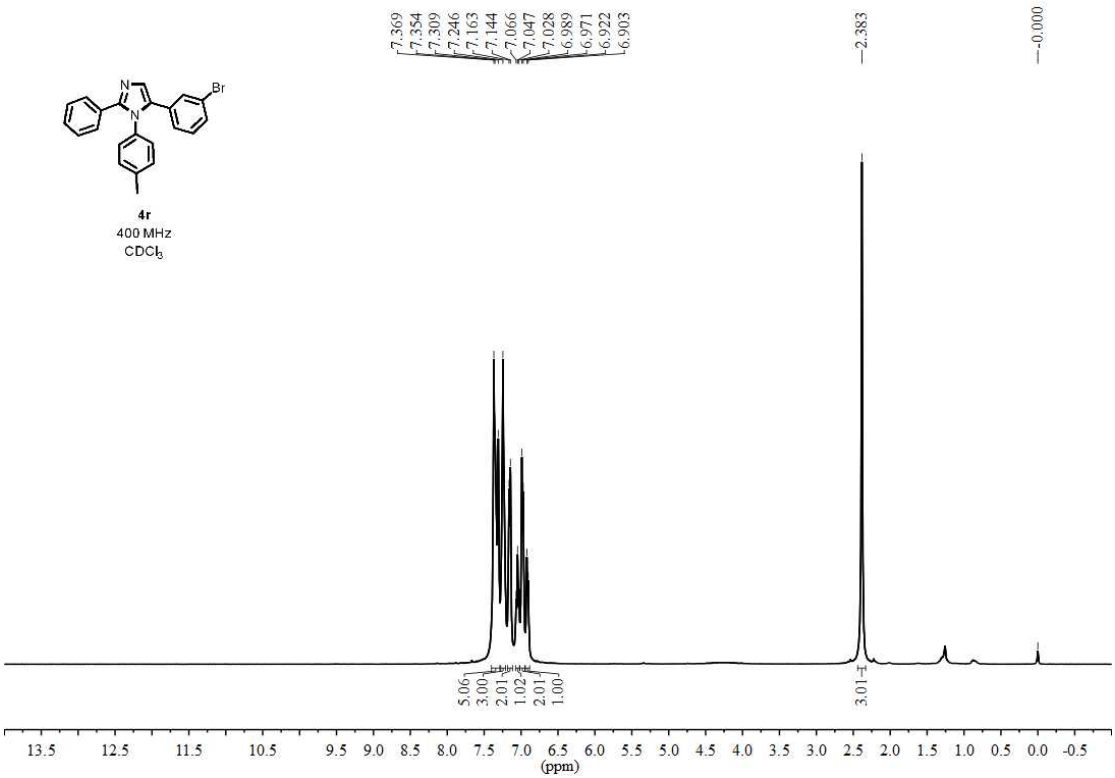
4p
400 MHz
$CDCl_3$

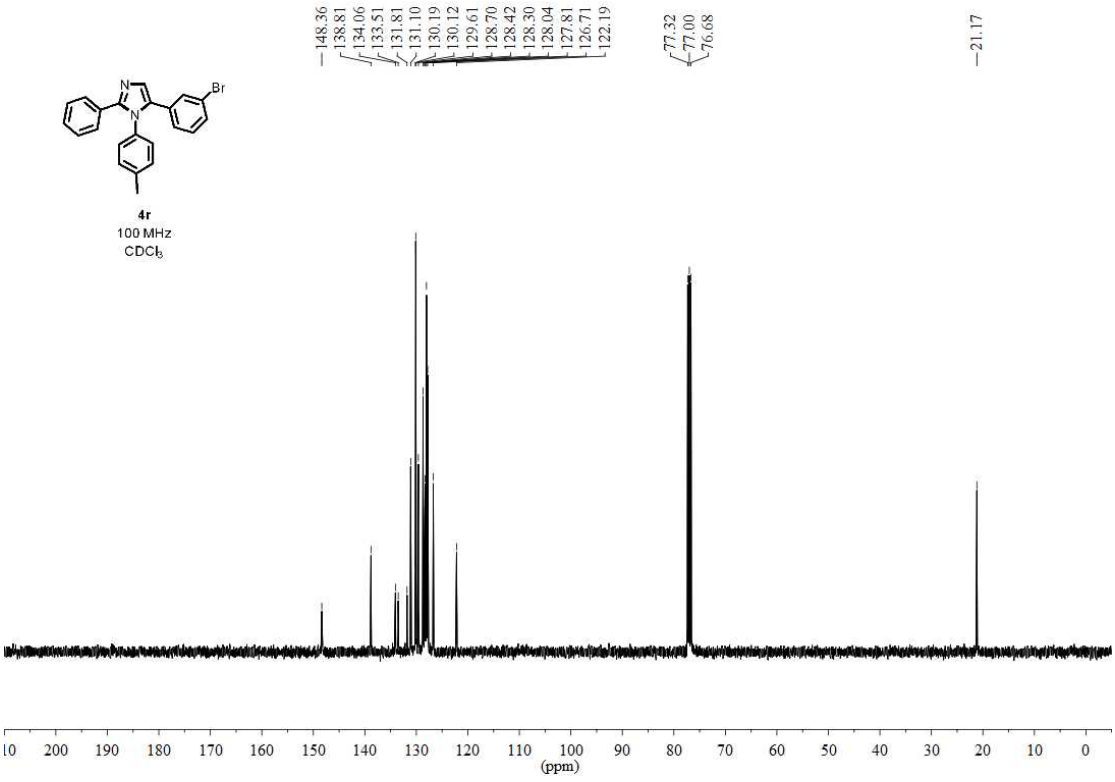

163.57
161.13
148.41
138.76
130.11
128.69
128.55
128.21
128.00
115.11
114.88
114.14
113.94
77.32
77.00
76.68
21.17
4p
100 MHz
CDCl3
(ppm)

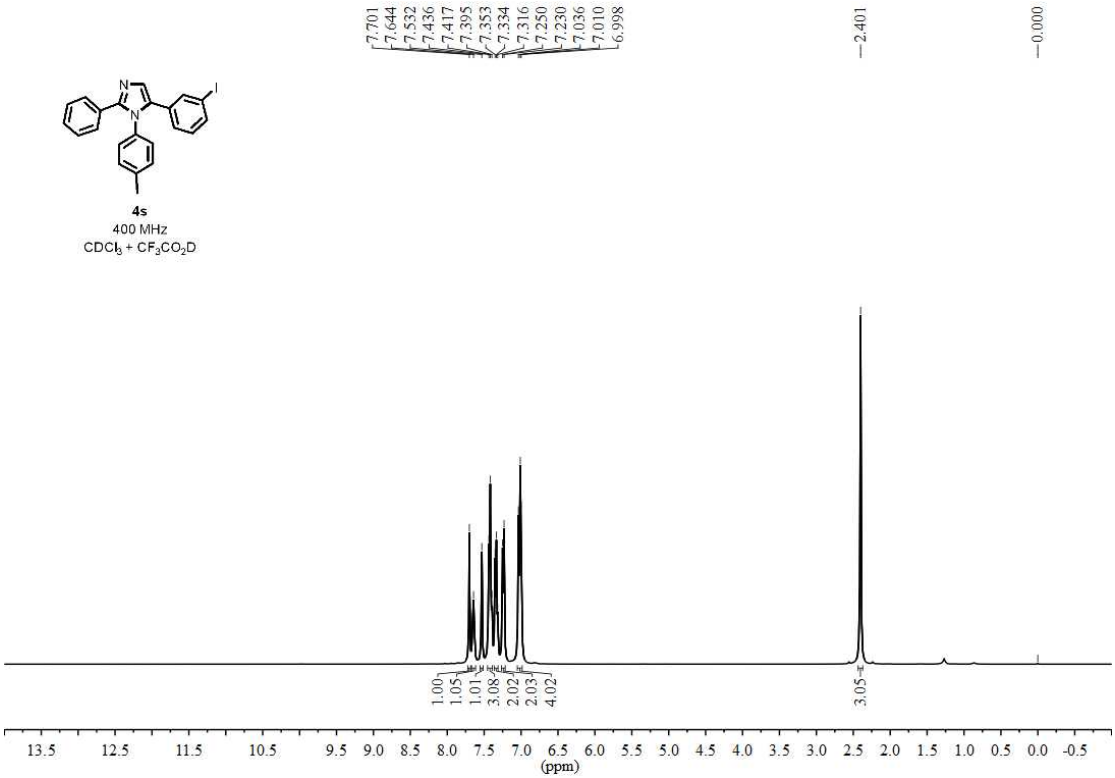

-112.777
4p
376 MHz
CDCl3
(ppm)

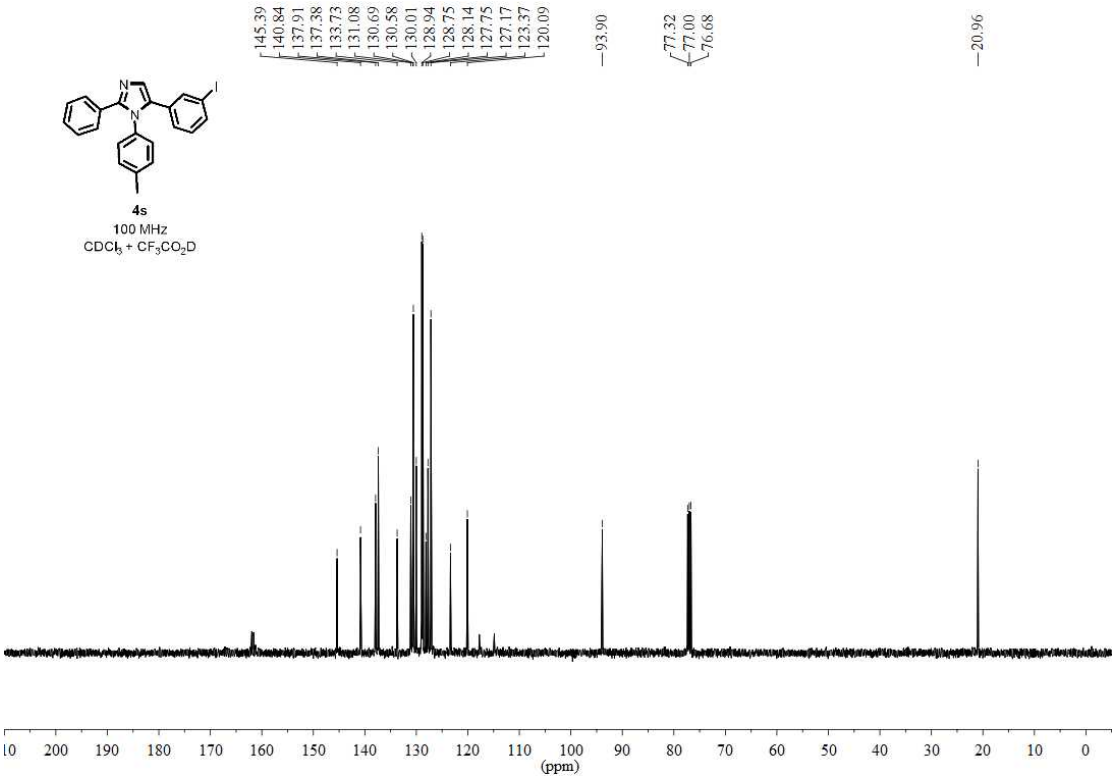

7.370
7.351
7.347
7.245
7.227
7.213
7.181
7.161
7.139
7.111
7.092
6.991
6.970
6.891
6.872
2.380
0.000
4q
400 MHz
CDCl3
3.11
3.04
5.03
2.02
1.00
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

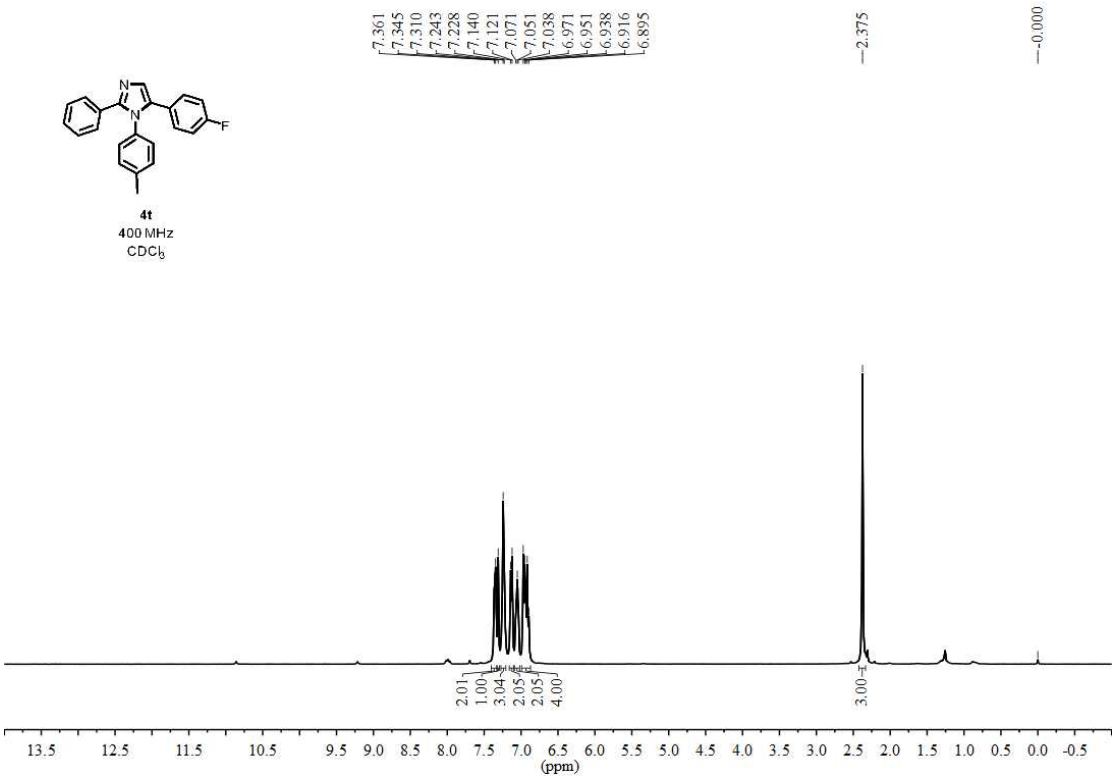

148.39
138.78
134.11
134.03
133.63
131.58
130.27
130.11
129.36
128.69
128.48
128.26
128.20
128.02
127.80
127.23
126.28
77.32
77.00
76.68
21.17
4q
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

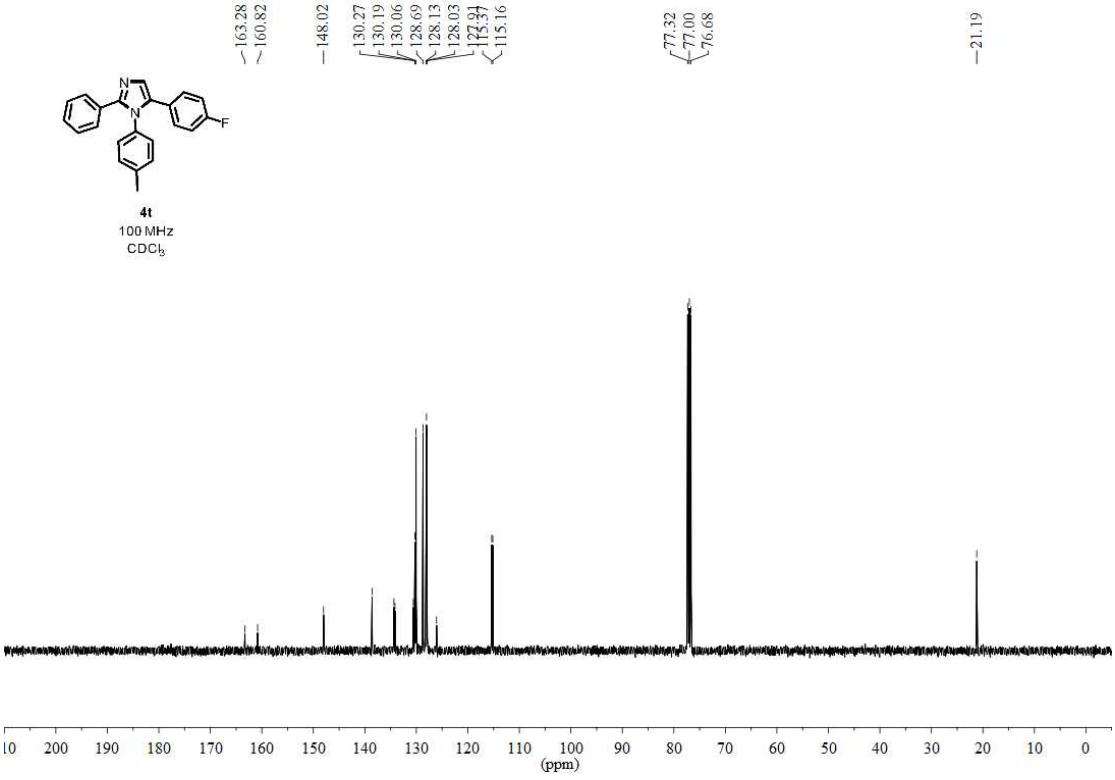

7.369
7.354
7.309
7.246
7.163
7.144
7.066
7.047
7.028
6.989
6.971
6.922
6.903
2.383
0.000
4r
400 MHz
CDCl3
5.06
3.00
2.01
1.02
2.01
1.00
3.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

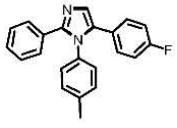

148.36
138.81
134.06
133.51
131.81
131.10
130.19
130.12
129.61
128.70
128.42
128.30
128.04
127.81
126.71
122.19
77.32
77.00
76.68
21.17
4r
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.701
7.644
7.532
7.436
7.417
7.395
7.353
7.334
7.316
7.250
7.230
7.036
7.010
6.998
2.401
0.000
4s
400 MHz
CDCl3 + CF3CO2D
1.00
1.05
1.01
3.08
2.02
2.03
4.02
3.05
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

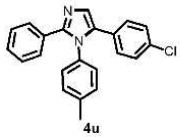

145.39
140.84
137.91
137.38
133.73
131.08
130.69
130.58
130.01
128.94
128.75
128.14
127.75
127.17
123.37
120.09
93.90
77.32
77.00
76.68
20.96
4s
100 MHz
CDCl3 + CF3CO2D
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.361
7.345
7.310
7.243
7.228
7.140
7.121
7.071
7.051
7.038
6.971
6.951
6.938
6.916
6.895
2.375
0.000
4t
400 MHz
CDCl3
2.01
1.00
3.04
2.05
2.05
4.00
3.00
(ppm)

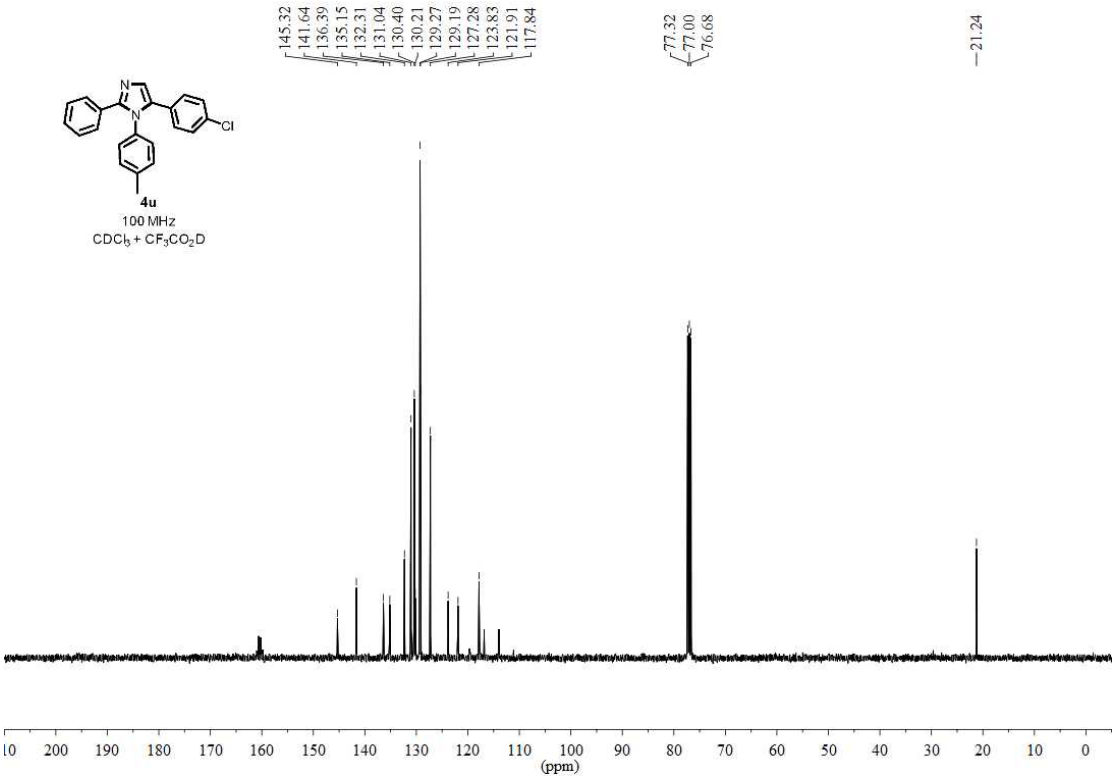

163.28
160.82
148.02
130.27
130.19
130.06
128.69
128.13
128.03
127.91
115.37
115.16
77.32
77.00
76.68
21.19
4t
100 MHz
CDCl3
(ppm)

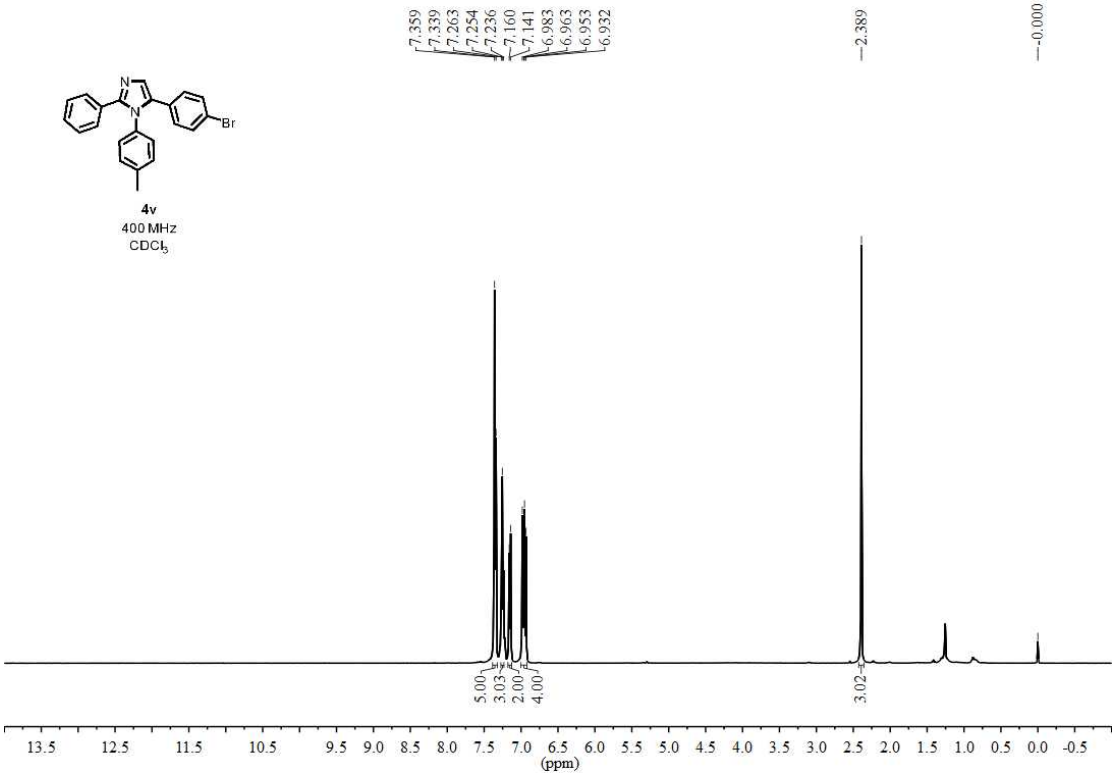


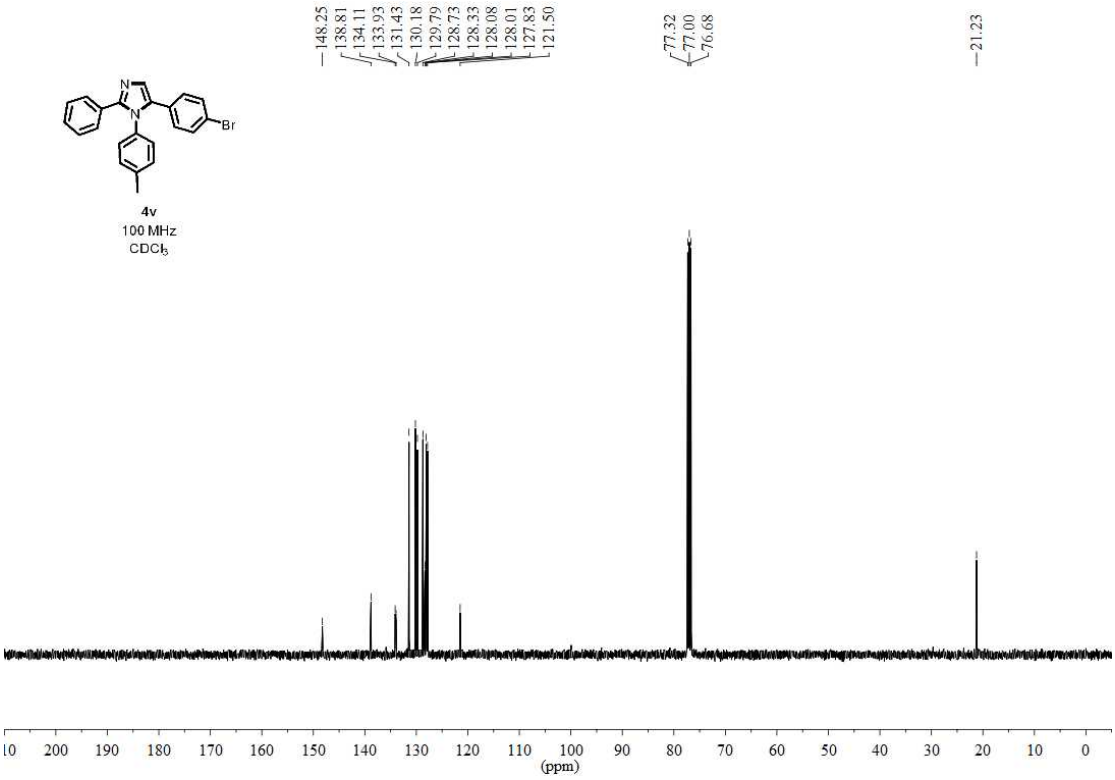
4t
376 MHz
$CDCl_3$

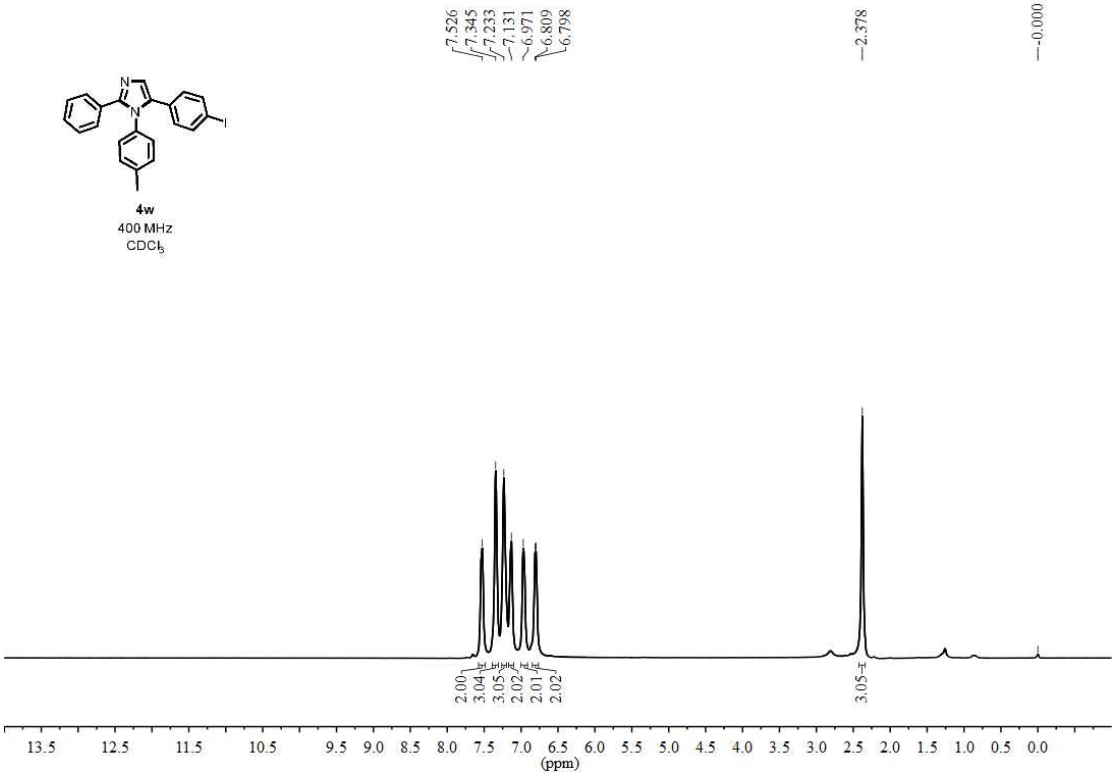


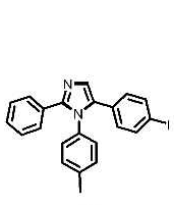
4u
400 MHz
$CDCl_3 + CF_3CO_2D$


145.32
141.64
136.39
135.15
132.31
131.04
130.40
130.21
129.27
129.19
127.28
123.83
121.91
117.84
77.32
77.00
76.68
21.24
Cl
4u
100 MHz
CDCl3 + CF3CO2D
(ppm)

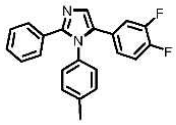

7.359
7.339
7.263
7.254
7.236
7.160
7.141
6.983
6.963
6.953
6.932
2.389
-0.000
Br
4v
400 MHz
CDCl3
5.00
3.03
2.00
4.00
3.02
(ppm)


148.25
138.81
134.11
133.93
131.43
130.18
129.79
128.73
128.33
128.08
128.01
127.83
121.50
77.32
77.00
76.68
21.23
Br
4v
100 MHz
CDCl3
(ppm)

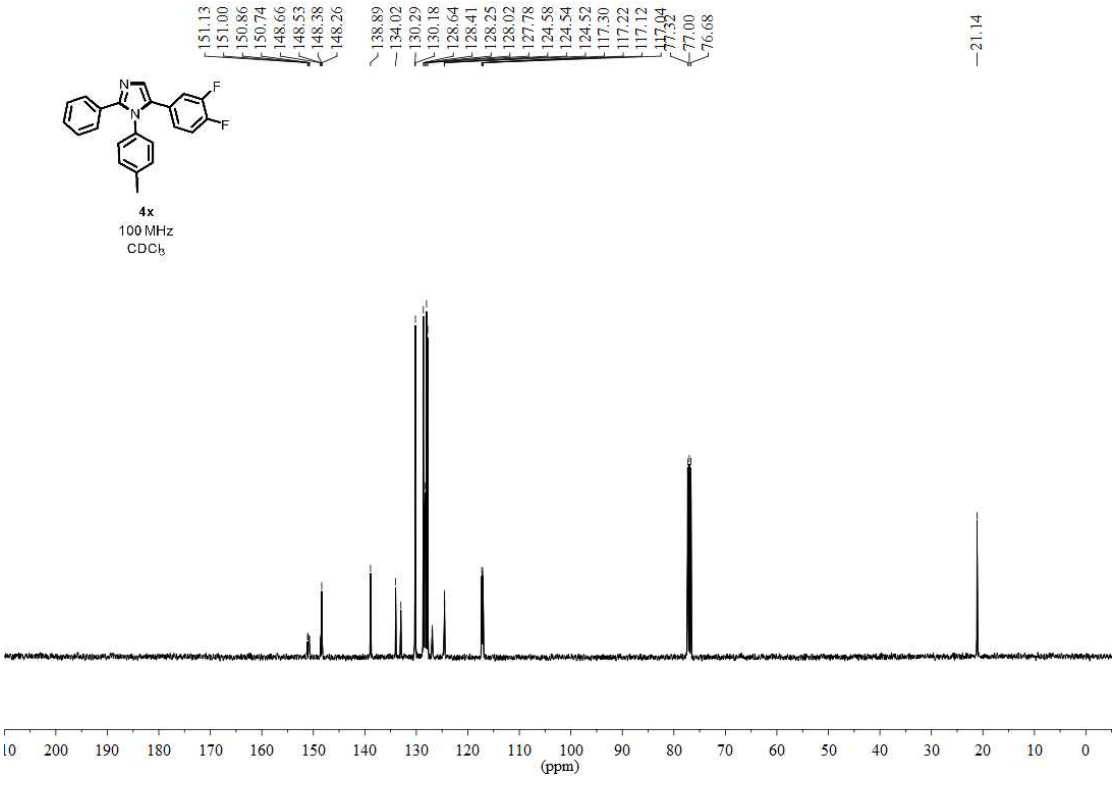

7.526
7.345
7.233
7.131
6.971
6.809
6.798
2.378
0.000
I
4w
400 MHz
CDCl3
2.00
3.04
3.05
2.02
2.01
2.02
3.05
(ppm)

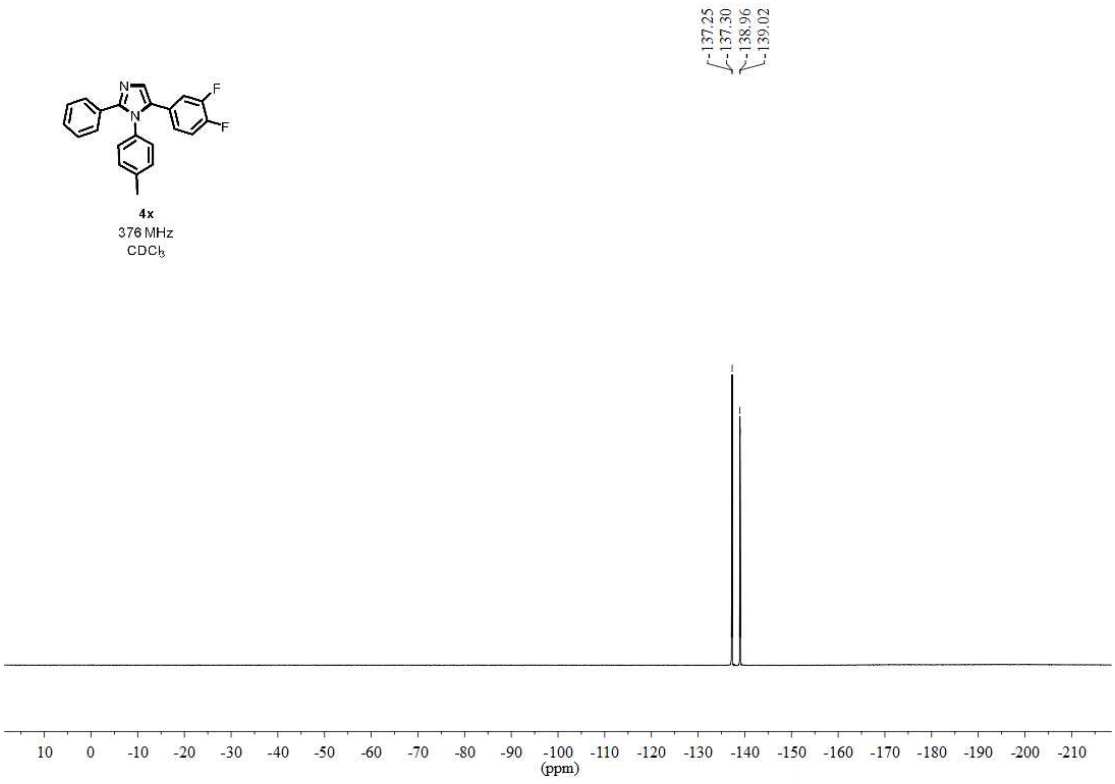


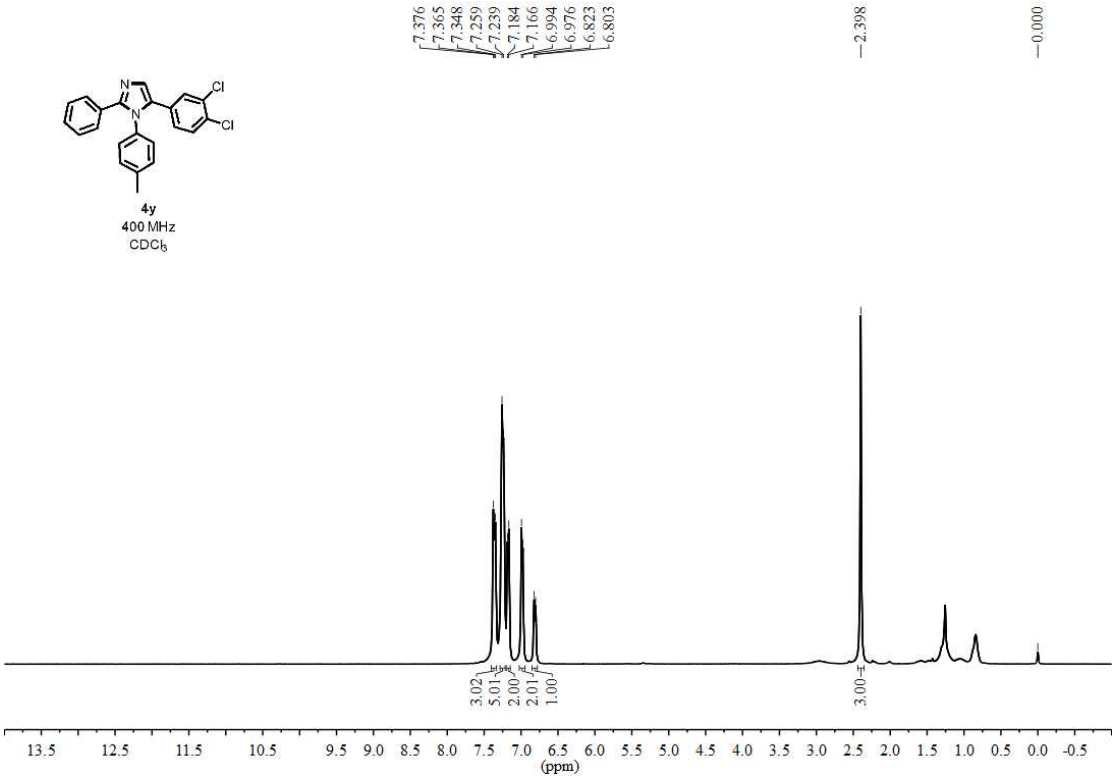
4w
100 MHz
$CDCl_3$

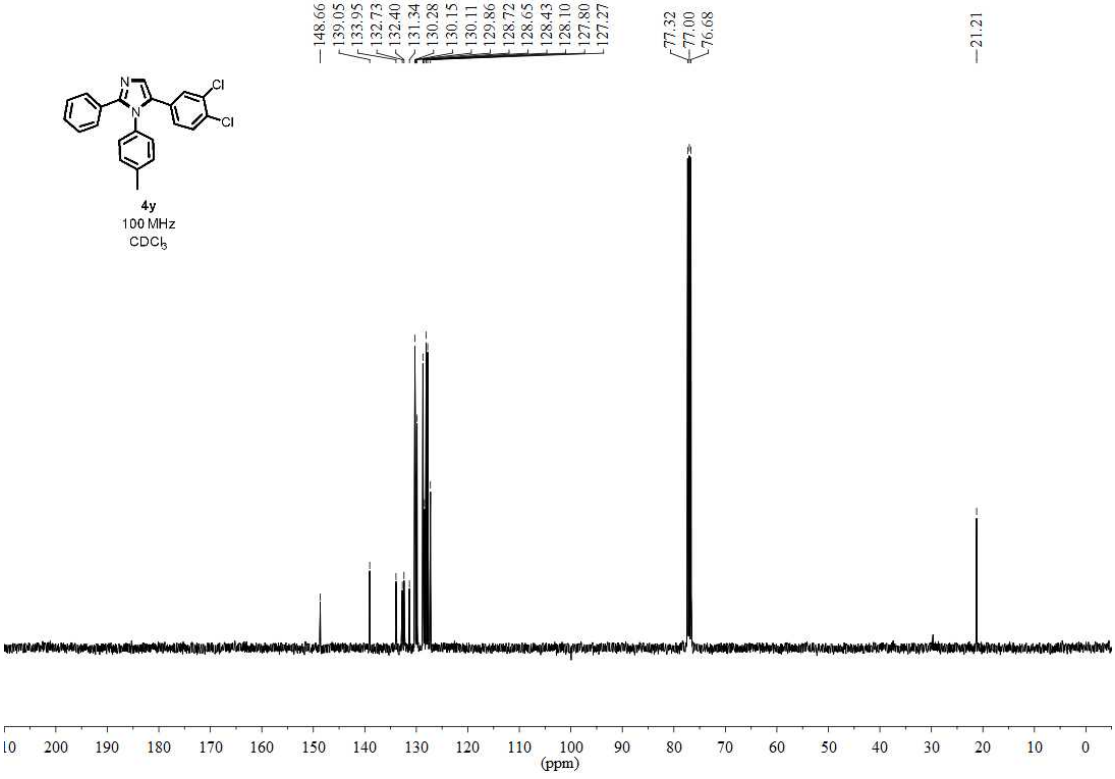


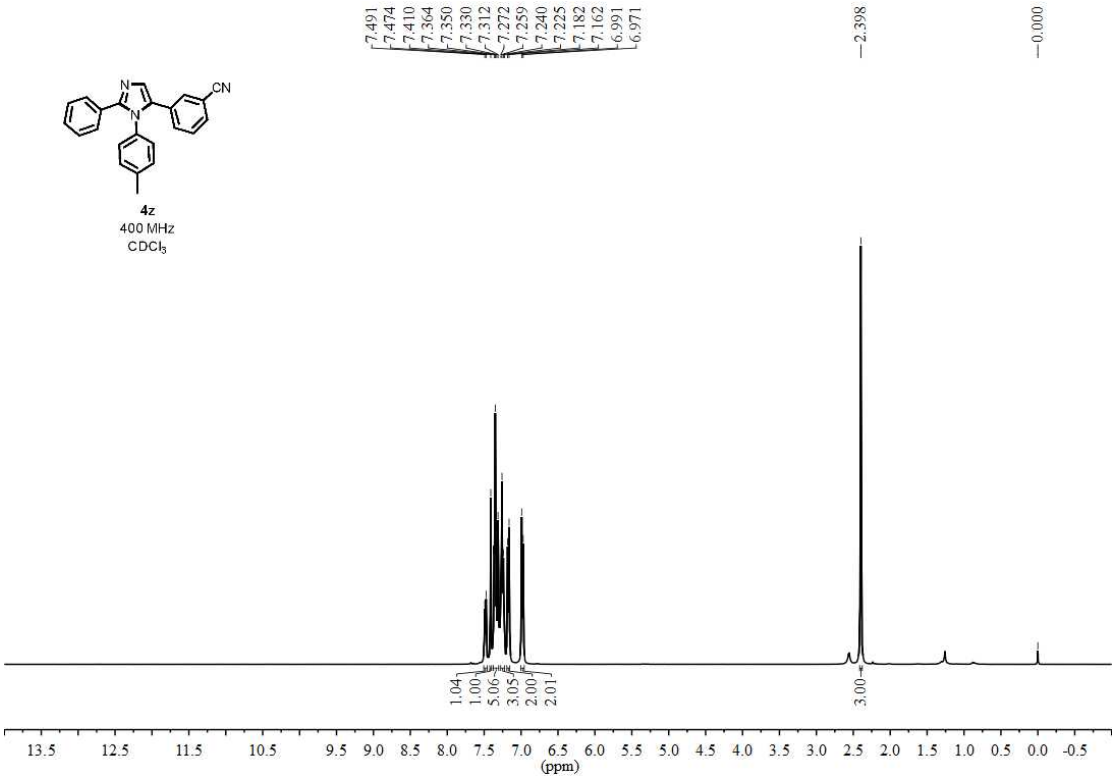
4x
400 MHz
$CDCl_3$

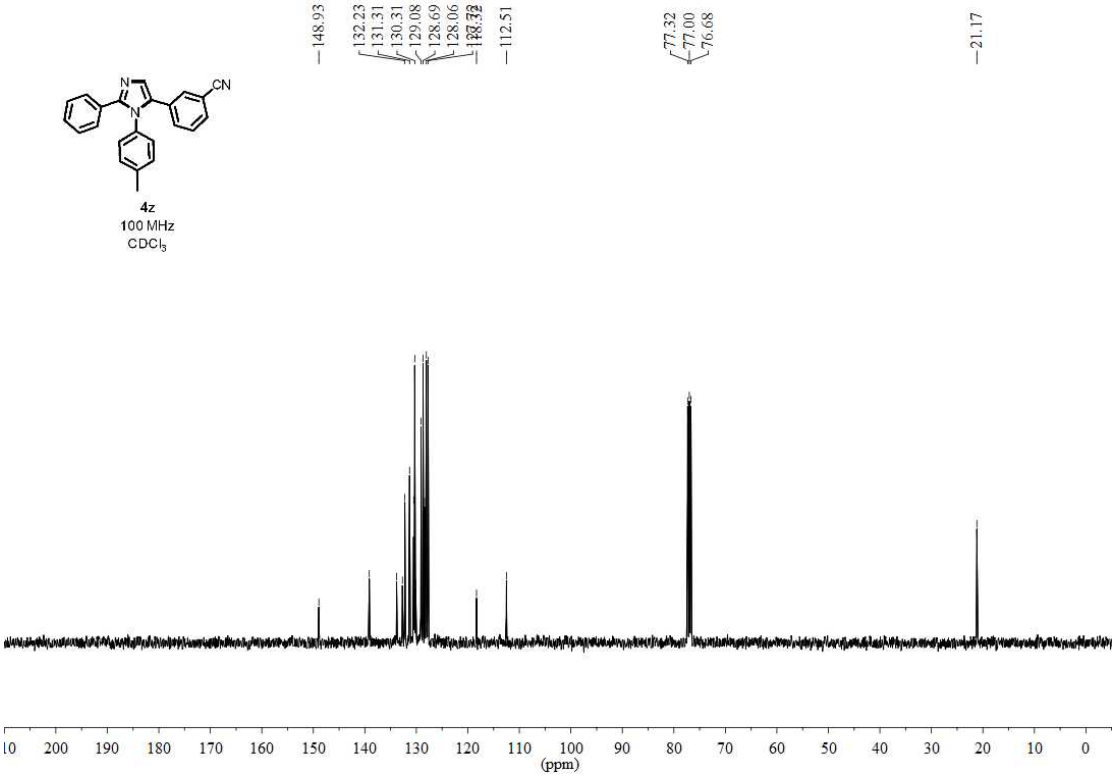

151.13
151.00
150.86
150.74
148.66
148.53
148.38
148.26
138.89
134.02
130.29
130.18
128.64
128.41
128.25
128.02
127.78
124.58
124.54
124.52
117.30
117.22
117.12
117.04
77.32
77.00
76.68
21.14
F
F
N
4x
100 MHz
CDCl3
(ppm)

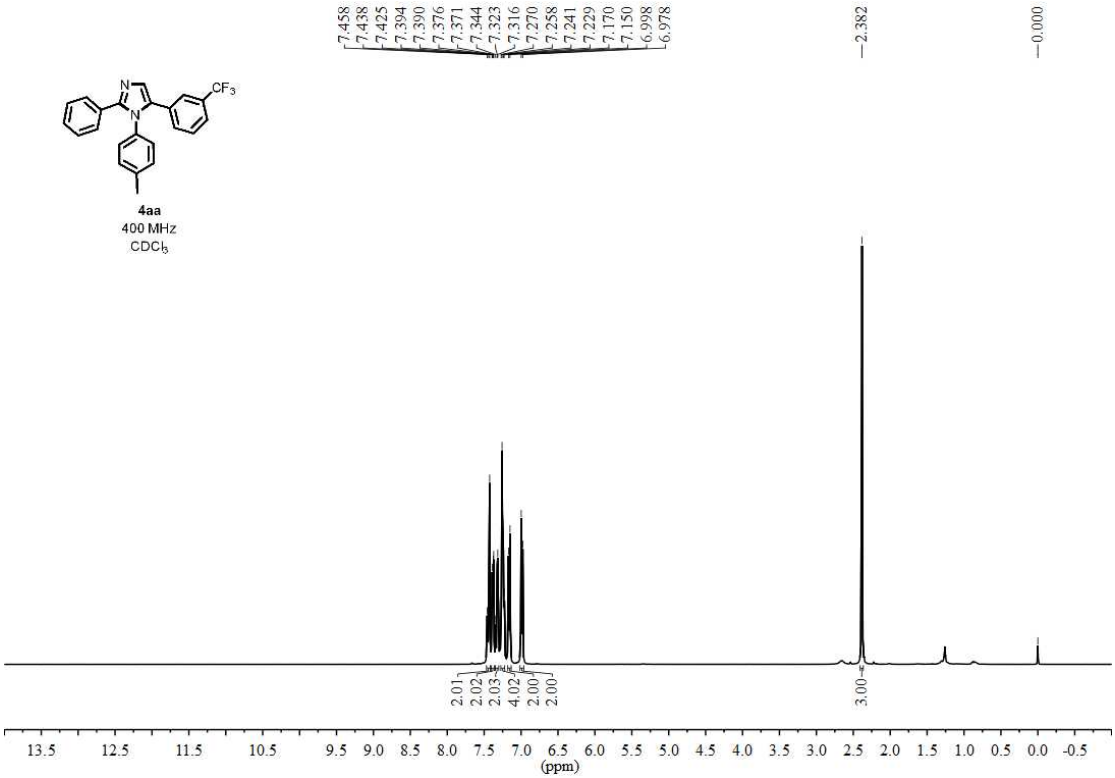

137.25
137.30
138.96
139.02
F
F
N
4x
376 MHz
CDCl3
(ppm)

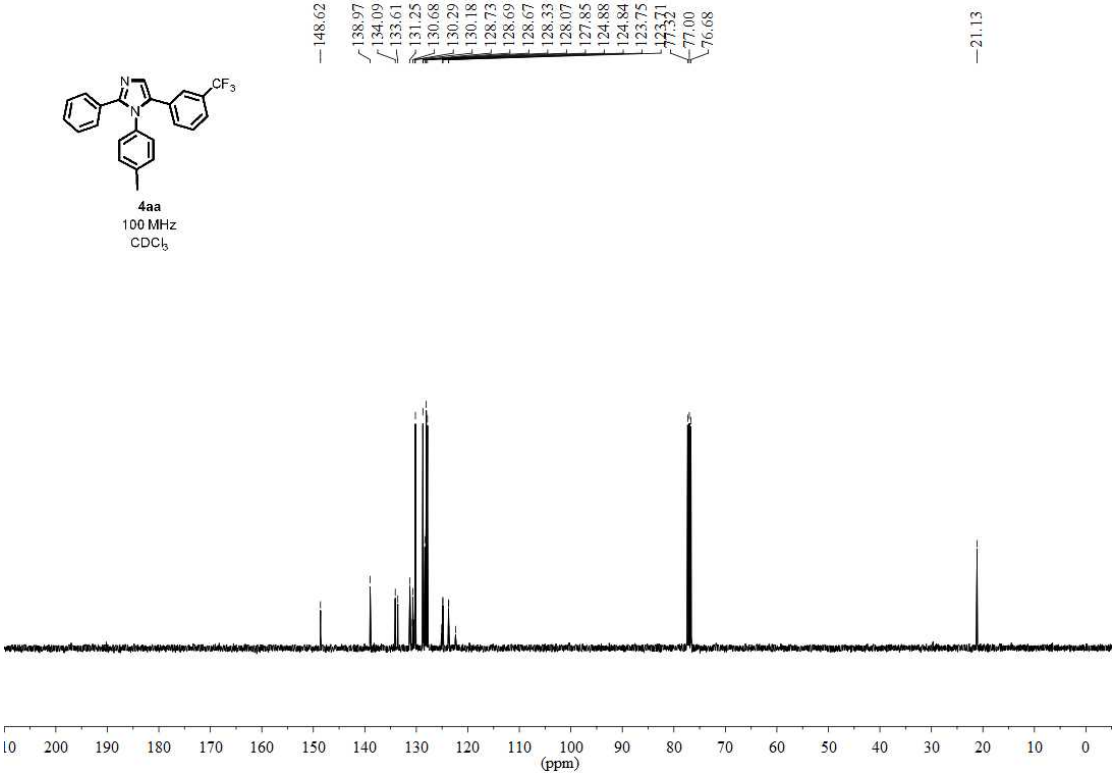

7.376
7.365
7.348
7.259
7.239
7.184
7.166
6.994
6.976
6.823
6.803
2.398
0.000
4y
400 MHz
CDCl3
3.02
5.01
2.00
2.01
1.00
3.00
(ppm)

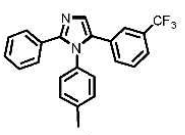

148.66
139.05
133.95
132.73
132.40
131.34
130.28
130.15
130.11
129.86
128.72
128.65
128.43
128.10
127.80
127.27
77.32
77.00
76.68
21.21
4y
100 MHz
CDCl3
(ppm)


7.491
7.474
7.410
7.364
7.350
7.330
7.312
7.272
7.259
7.240
7.225
7.182
7.162
6.991
6.971
2.398
0.000
CN
4z
400 MHz
CDCl3
1.04
1.00
5.06
3.05
2.00
2.01
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

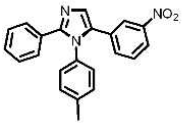

148.93
132.23
131.31
130.31
129.08
128.69
128.06
112.51
77.32
77.00
76.68
21.17
CN
4z
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.458
7.438
7.425
7.394
7.390
7.376
7.371
7.344
7.323
7.316
7.270
7.258
7.241
7.229
7.170
7.150
6.998
6.978
2.382
0.000
4aa
400 MHz
CDCl3
2.01
2.02
2.03
4.02
2.00
2.00
3.00
(ppm)

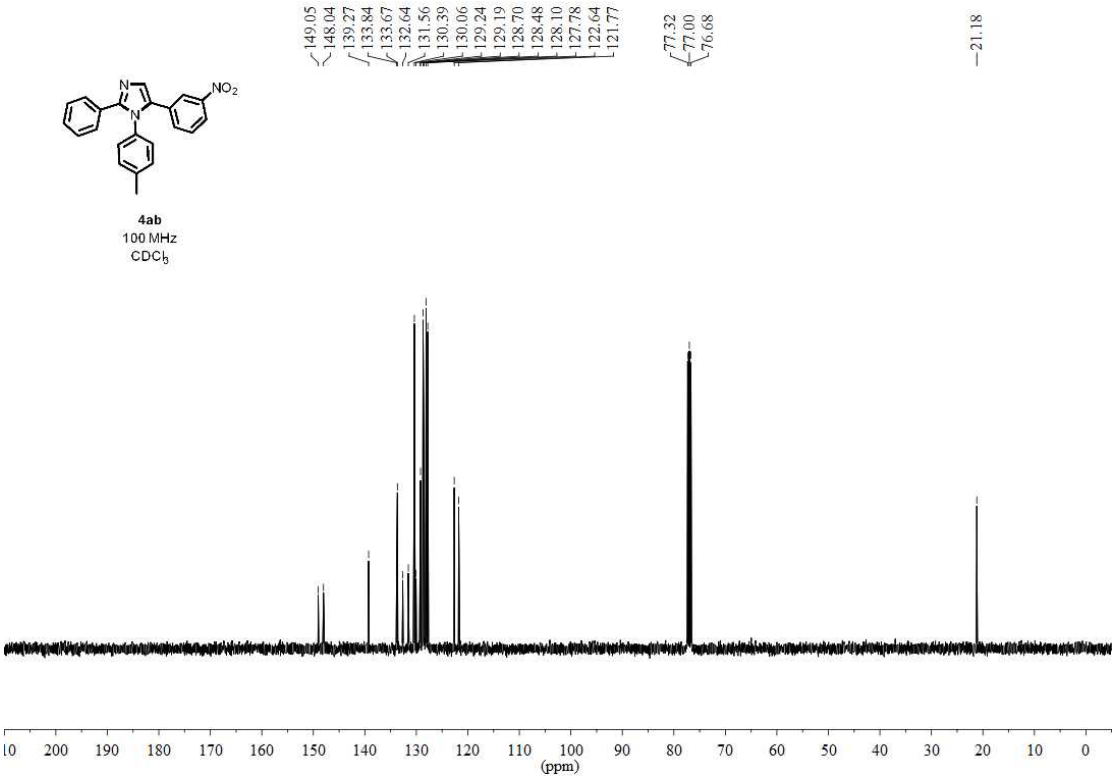

148.62
138.97
134.09
133.61
131.25
130.68
130.29
130.18
128.73
128.69
128.67
128.33
128.07
127.85
124.88
124.84
123.75
123.71
77.32
77.00
76.68
21.13
4aa
100 MHz
CDCl3
(ppm)

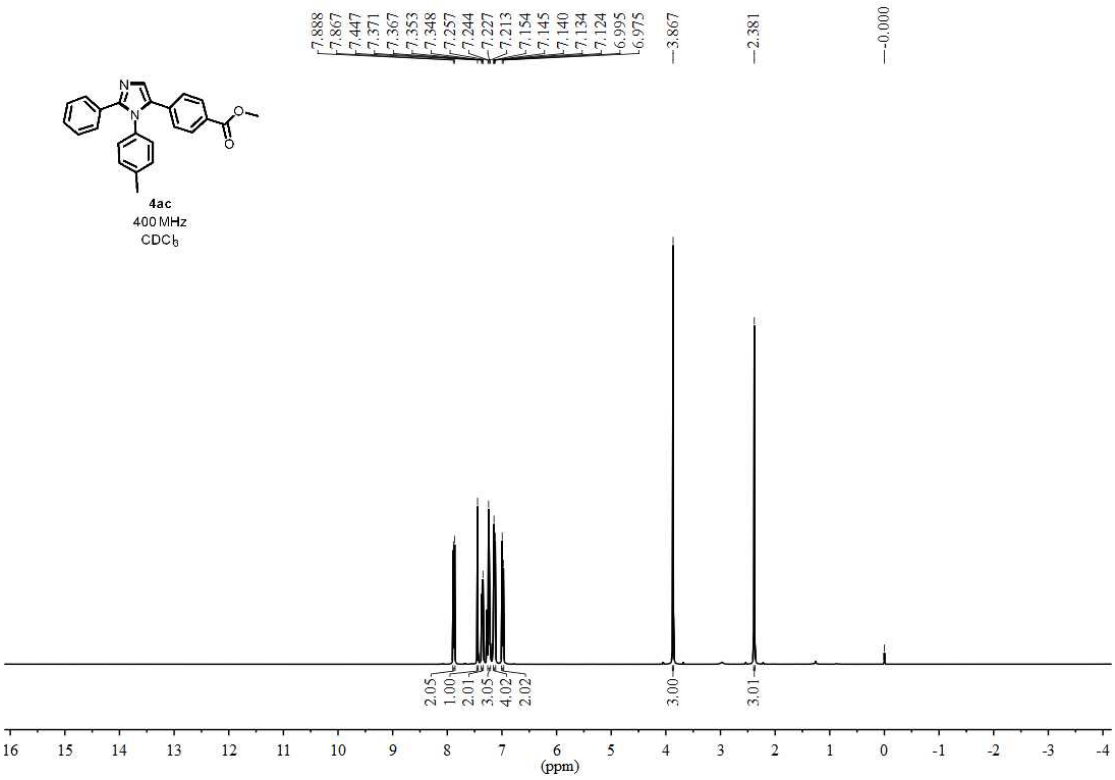


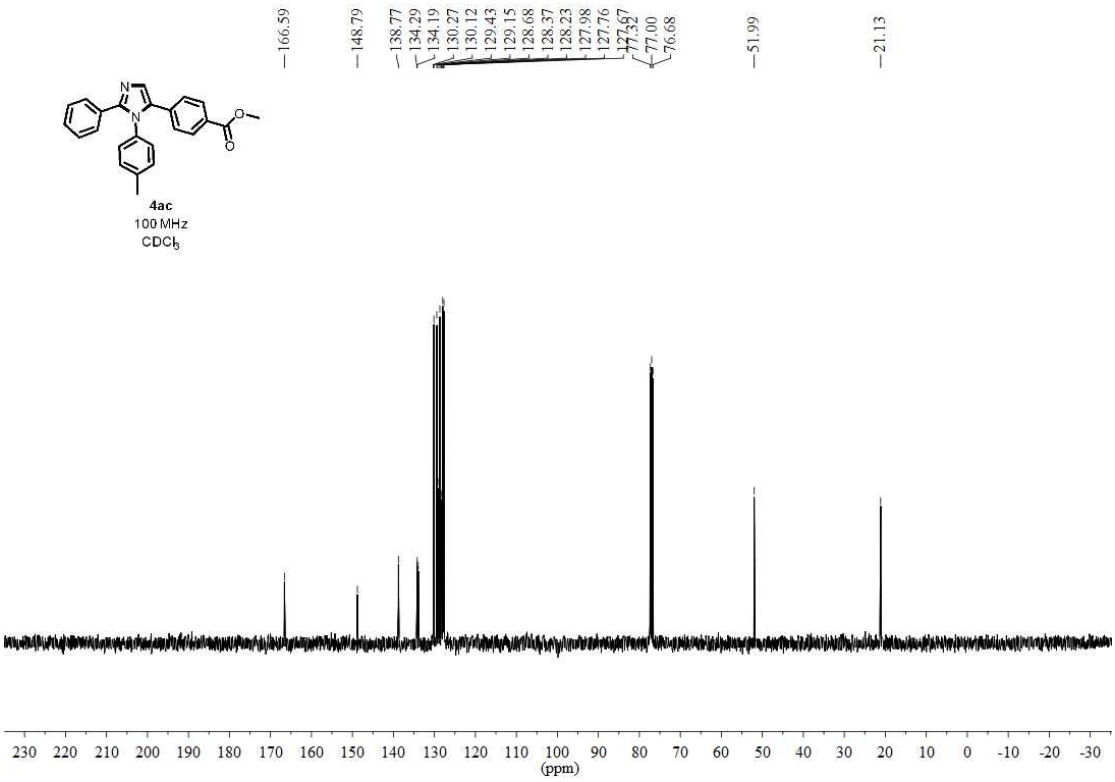
4aa
376 MHz
$CDCl_3$

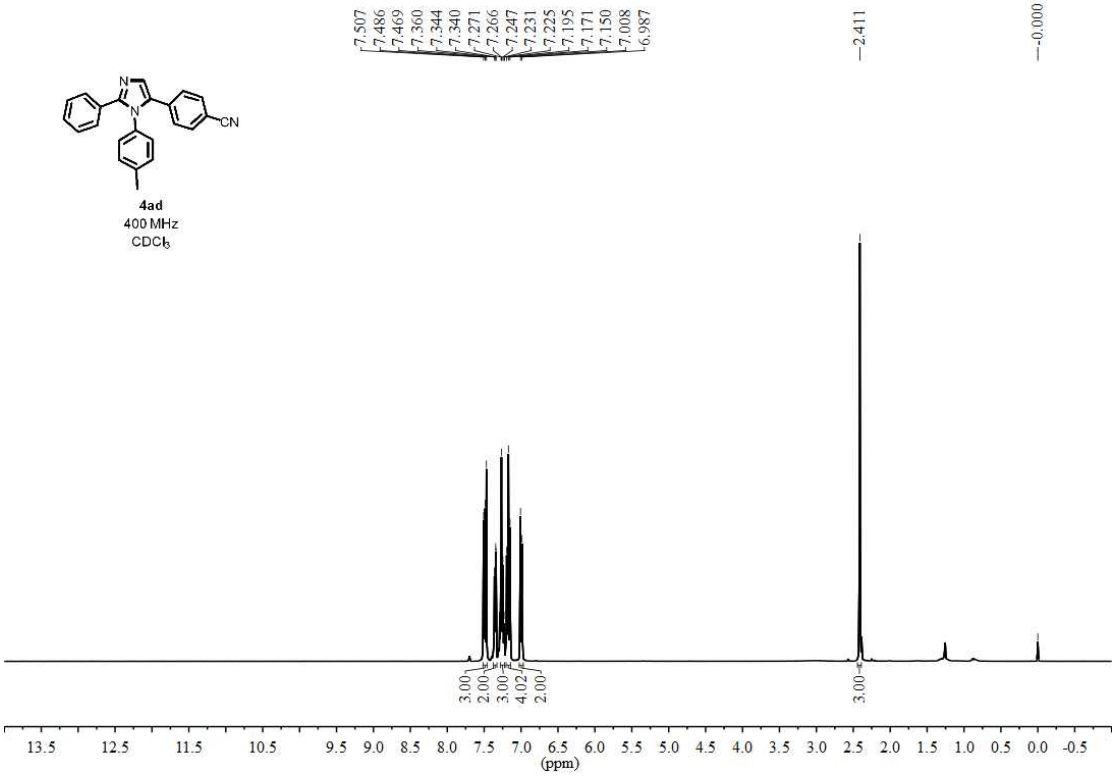


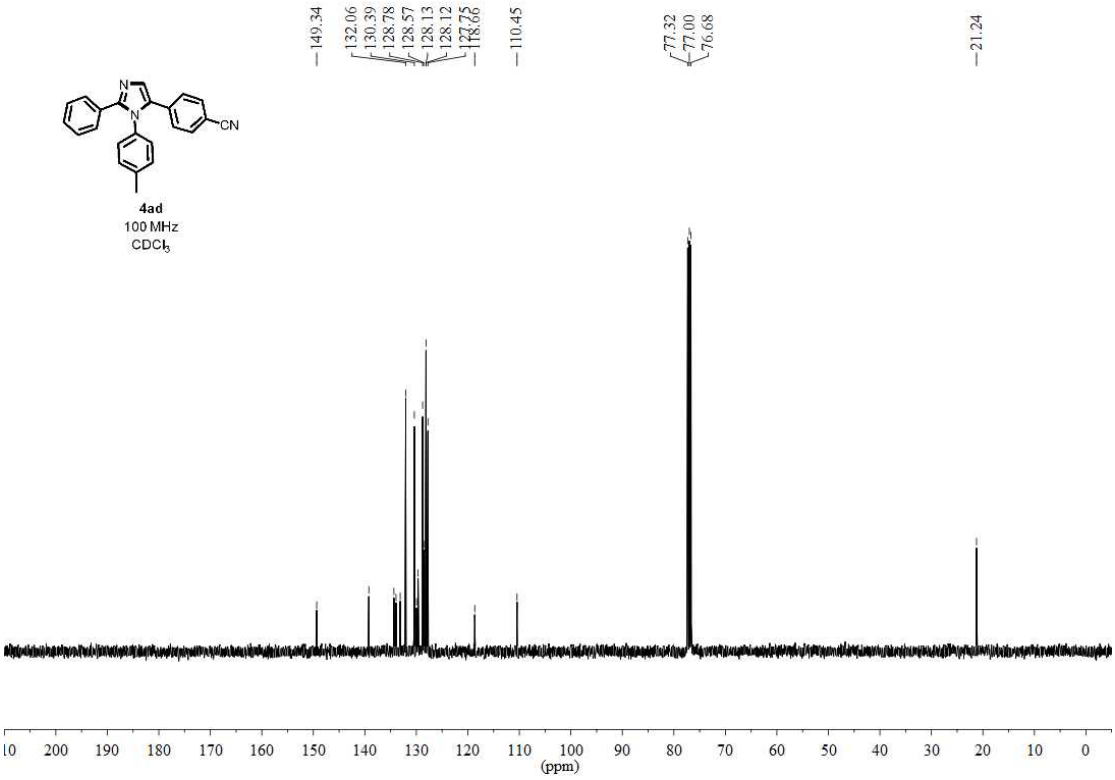
4ab
400 MHz
$CDCl_3$

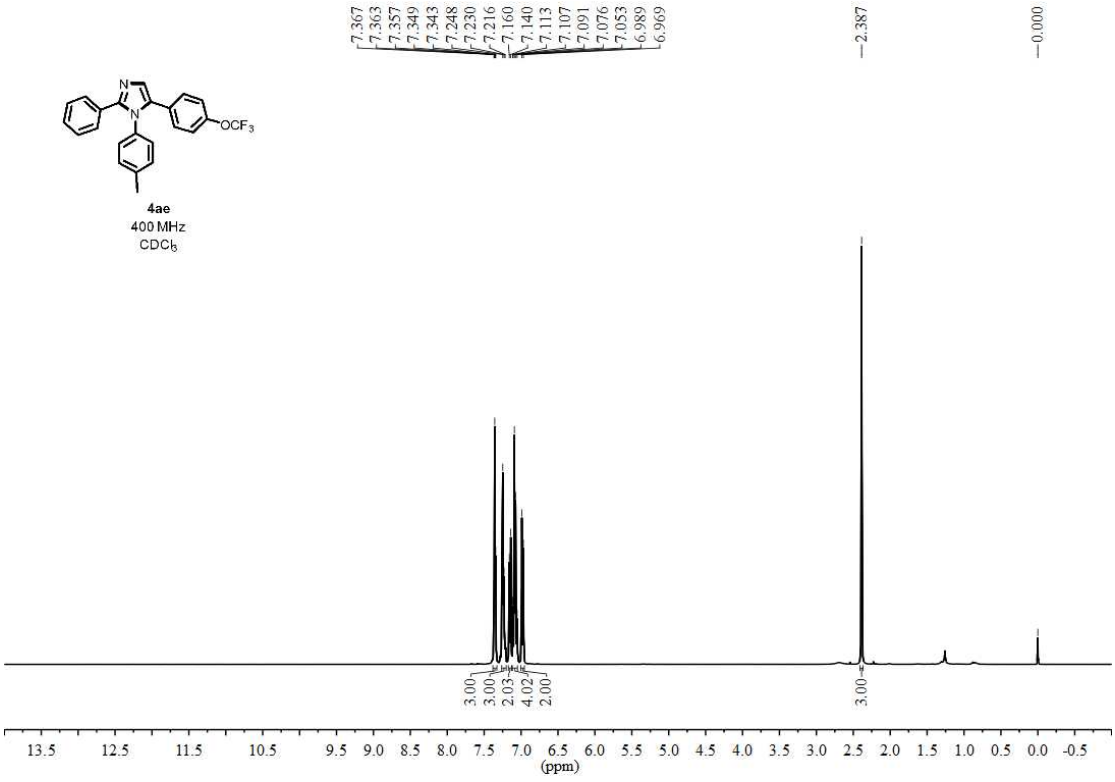

149.05
148.04
139.27
133.84
133.67
132.64
131.56
130.39
130.06
129.24
129.19
128.70
128.48
128.10
127.78
122.64
121.77
77.32
77.00
76.68
21.18
NO2
4ab
100 MHz
CDCl3
(ppm)

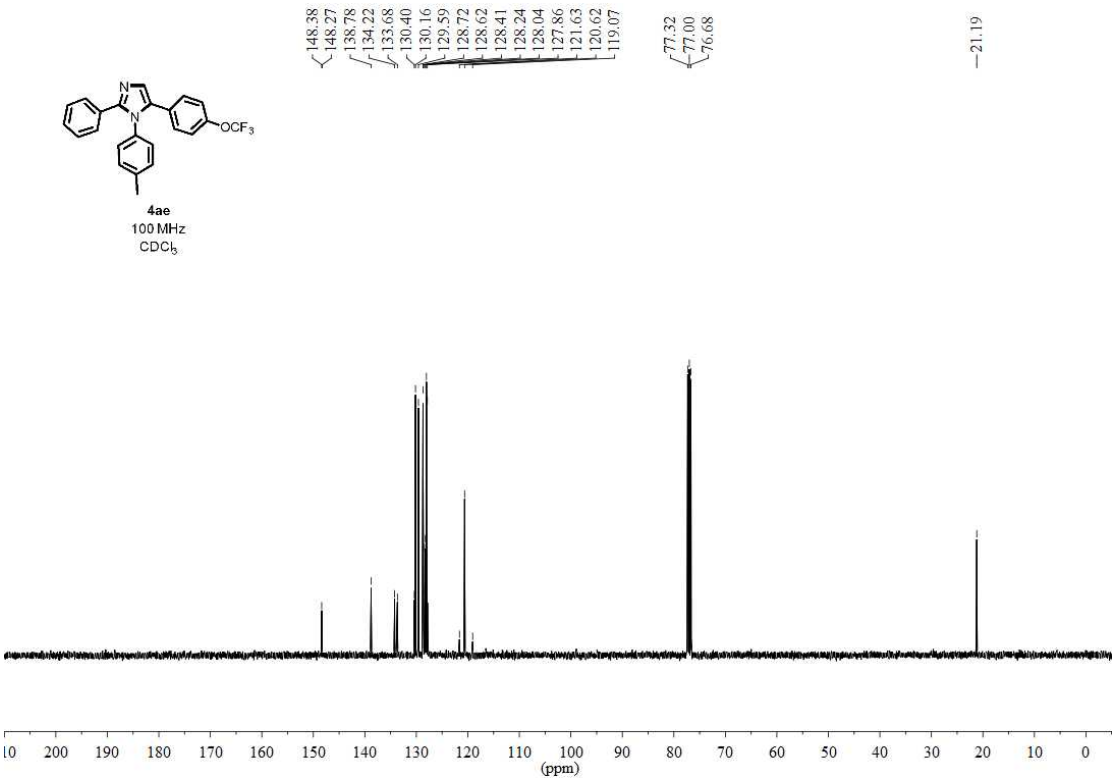

7.888
7.867
7.447
7.371
7.367
7.353
7.348
7.257
7.244
7.227
7.213
7.154
7.145
7.140
7.134
7.124
6.995
6.975
3.867
2.381
0.000
O
4ac
400 MHz
CDCl3
2.05
1.00
2.01
3.05
4.02
2.02
3.00
3.01
(ppm)

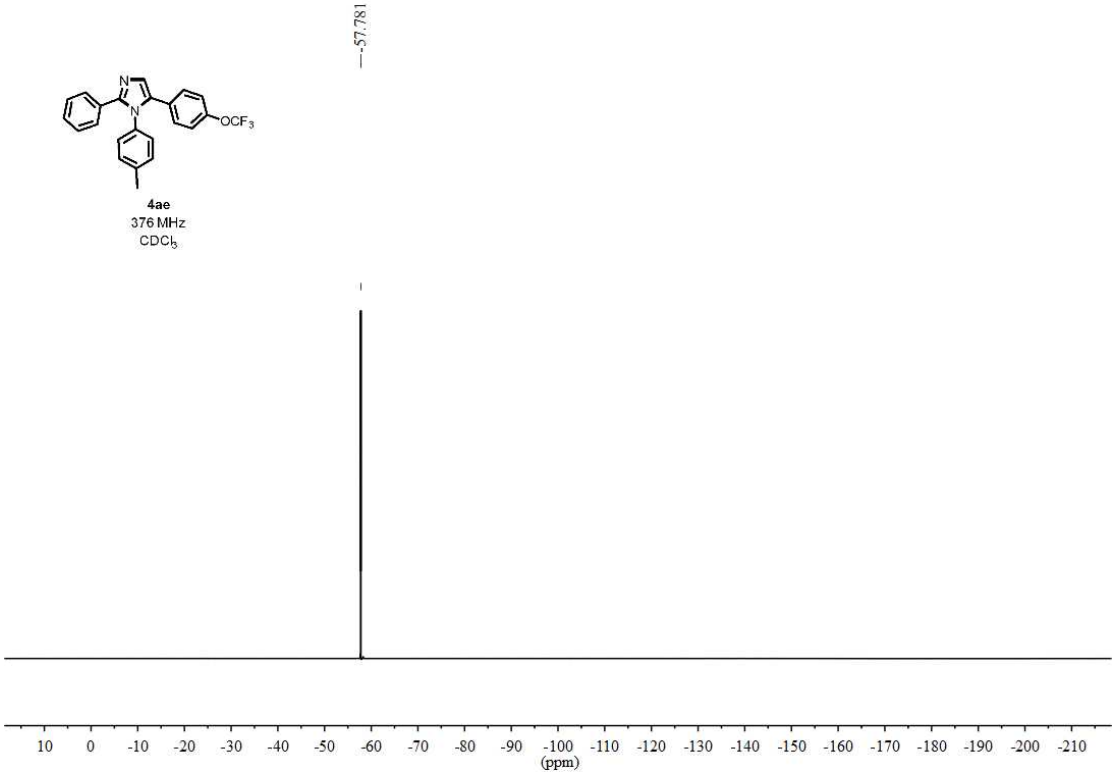

166.59
148.79
138.77
134.29
134.19
130.27
130.12
129.43
129.15
128.68
128.37
128.23
127.98
127.76
77.32
77.00
76.68
51.99
21.13
4ac
100 MHz
CDCl3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
(ppm)

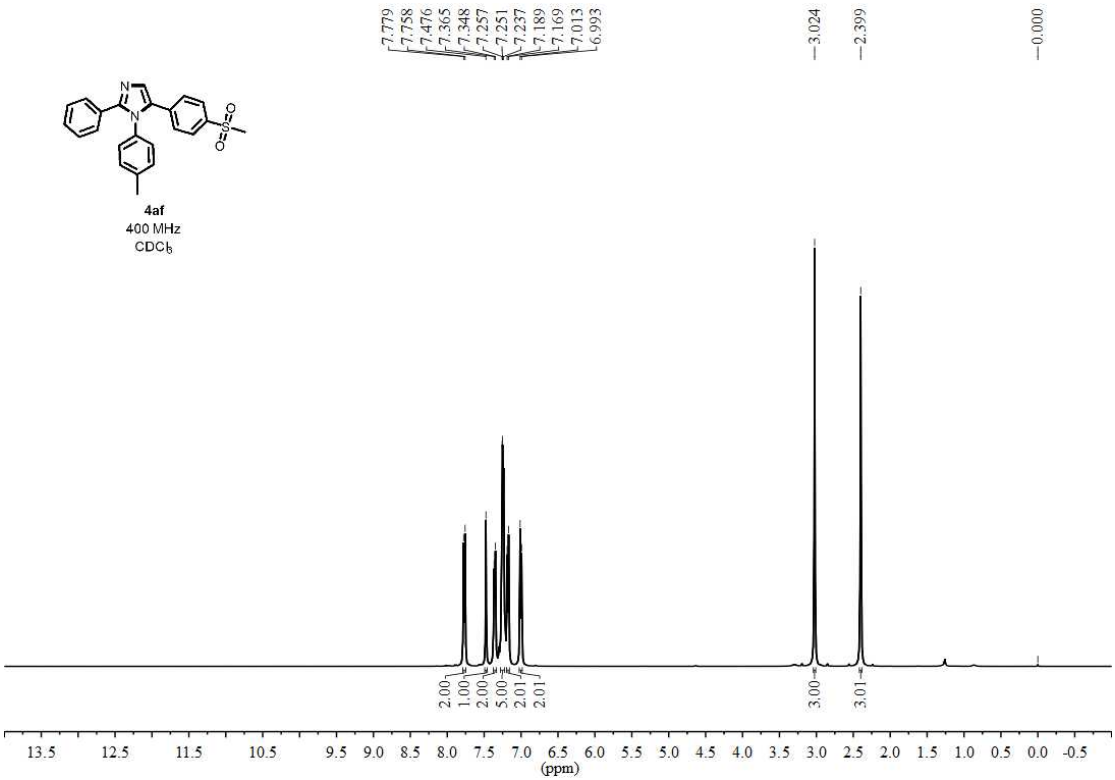

7.507
7.486
7.469
7.360
7.344
7.340
7.271
7.266
7.247
7.231
7.225
7.195
7.171
7.150
7.008
6.987
2.411
-0.000
CN
4ad
400 MHz
CDCl3
3.00
2.00
3.00
4.02
2.00
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

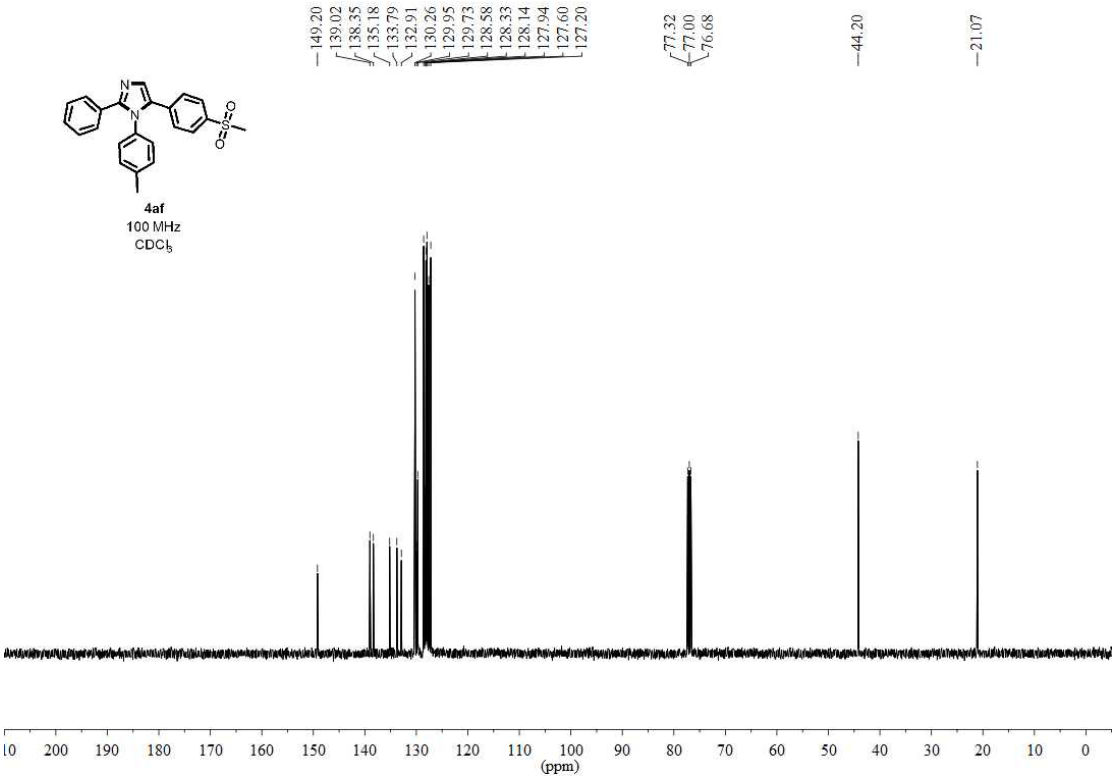

149.34
132.06
130.39
128.78
128.57
128.13
128.12
118.66
110.45
77.32
77.00
76.68
21.24
CN
4ad
100 MHz
CDCl3
(ppm)

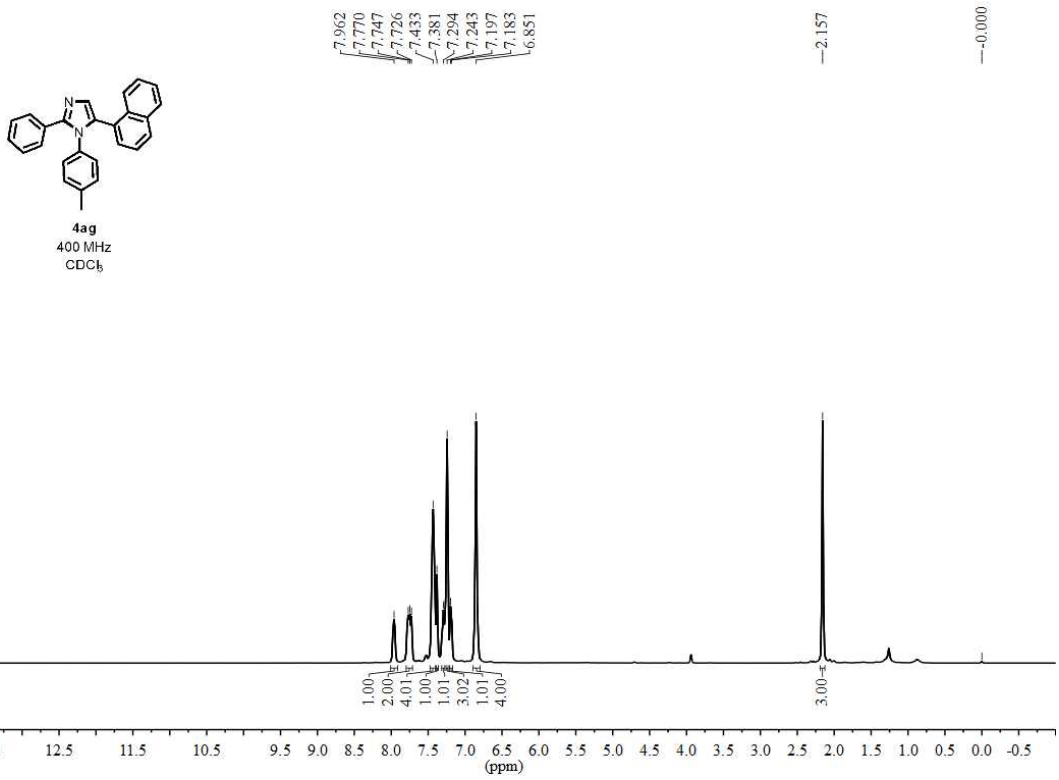

7.367
7.363
7.357
7.349
7.343
7.248
7.230
7.216
7.160
7.140
7.113
7.107
7.091
7.076
7.053
6.989
6.969
2.387
0.000
OCF3
4ae
400 MHz
CDCl3
3.00
3.00
2.03
4.02
2.00
3.00
(ppm)

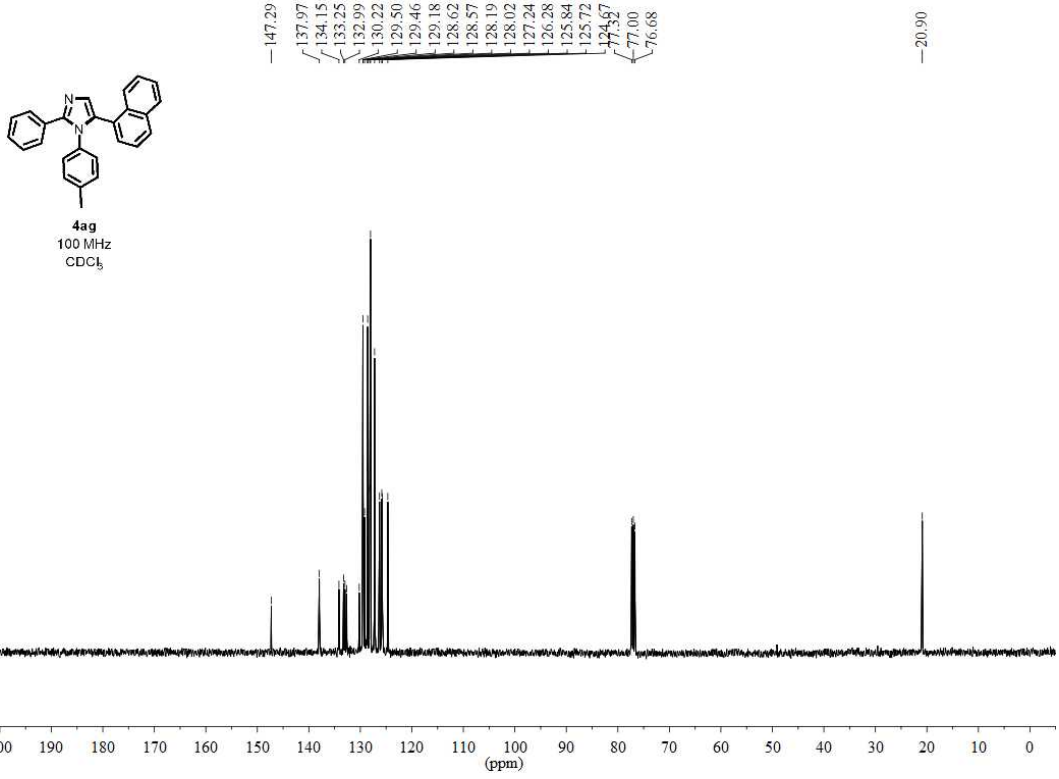

148.38
148.27
138.78
134.22
133.68
130.40
130.16
129.59
128.72
128.62
128.41
128.24
128.04
127.86
121.63
120.62
119.07
77.32
77.00
76.68
21.19
OCF3
4ae
100 MHz
CDCl3
(ppm)

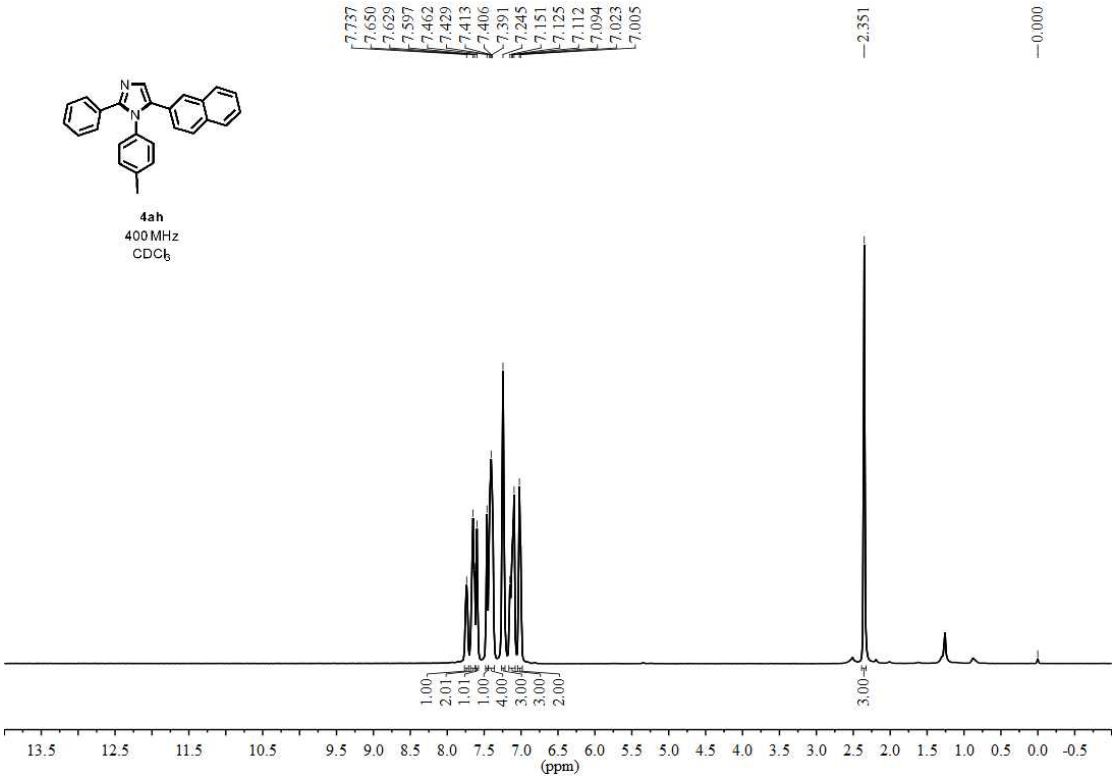

-57.781
OCF3
4ae
376 MHz
CDCl3
(ppm)

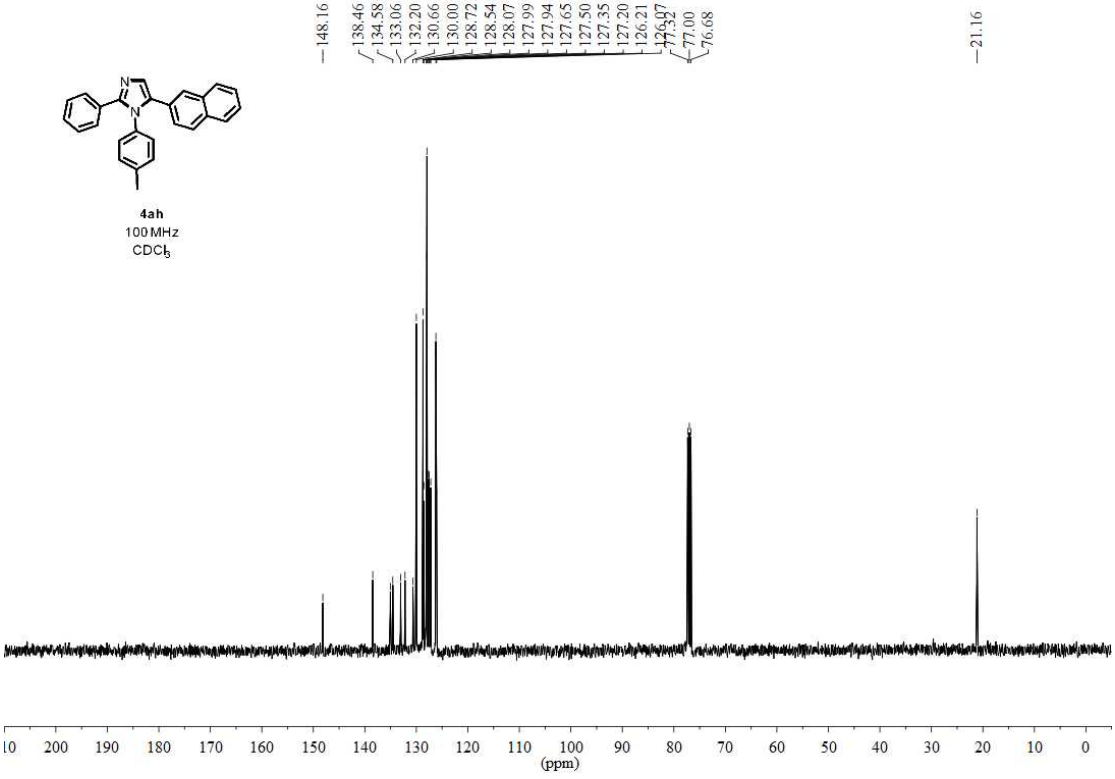

7.779
7.758
7.476
7.365
7.348
7.257
7.251
7.237
7.189
7.169
7.013
6.993
3.024
2.399
0.000
4af
400 MHz
CDCl3
2.00
1.00
2.00
5.00
2.01
2.01
3.00
3.01
(ppm)

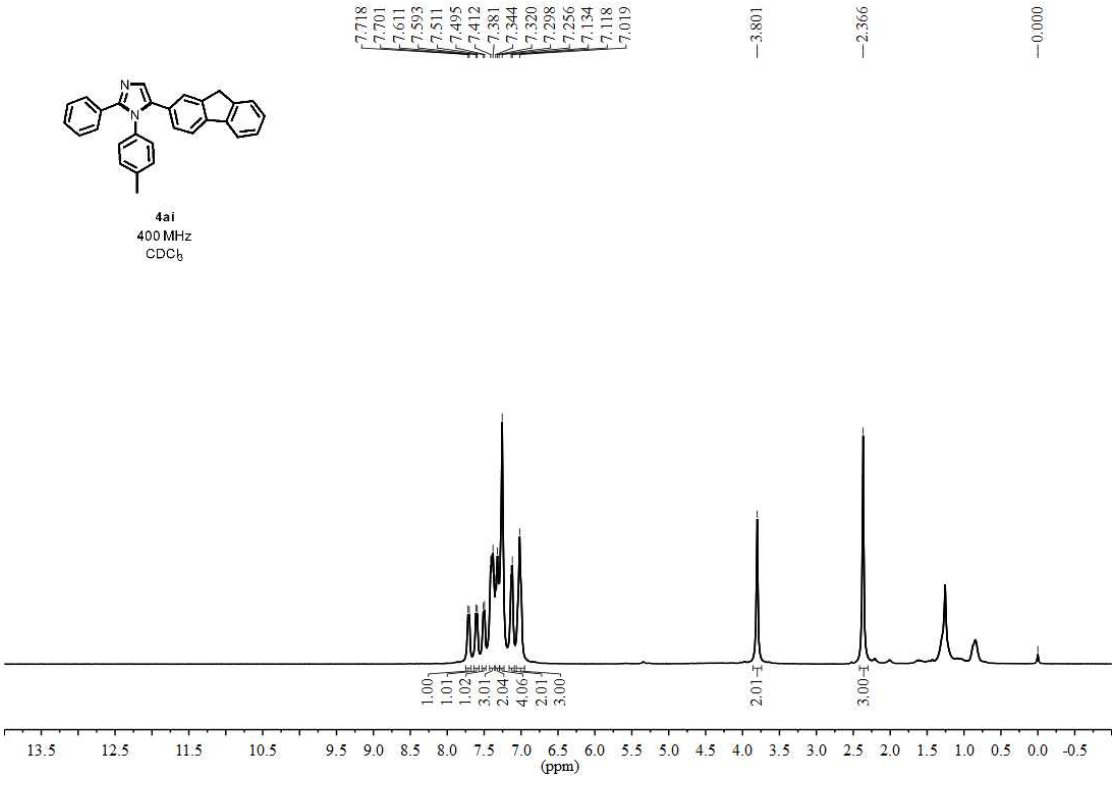

149.20
139.02
138.35
135.18
133.79
132.91
130.26
129.95
129.73
128.58
128.33
128.14
127.94
127.60
127.20
77.32
77.00
76.68
44.20
21.07
4af
100 MHz
CDCl3
(ppm)

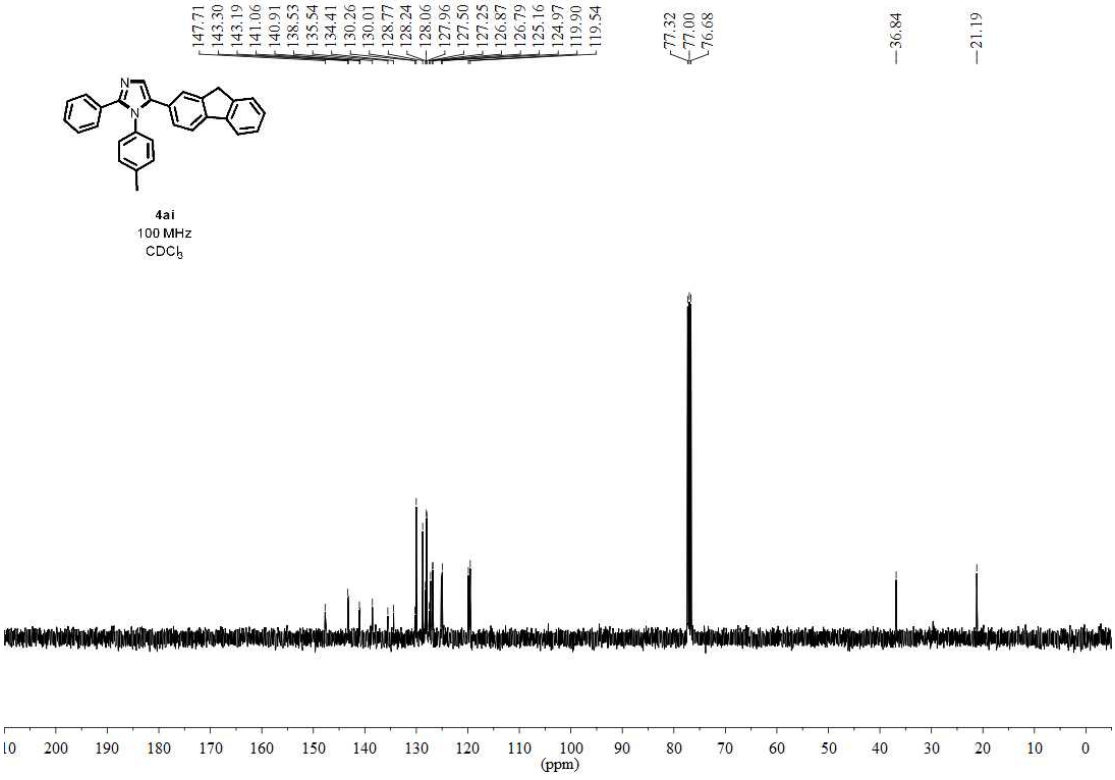

7.962
7.770
7.747
7.726
7.433
7.381
7.294
7.243
7.197
7.183
6.851
2.157
0.000
4ag
400 MHz
CDCl3
1.00
2.00
4.01
1.00
1.01
3.02
1.01
4.00
3.00
(ppm)

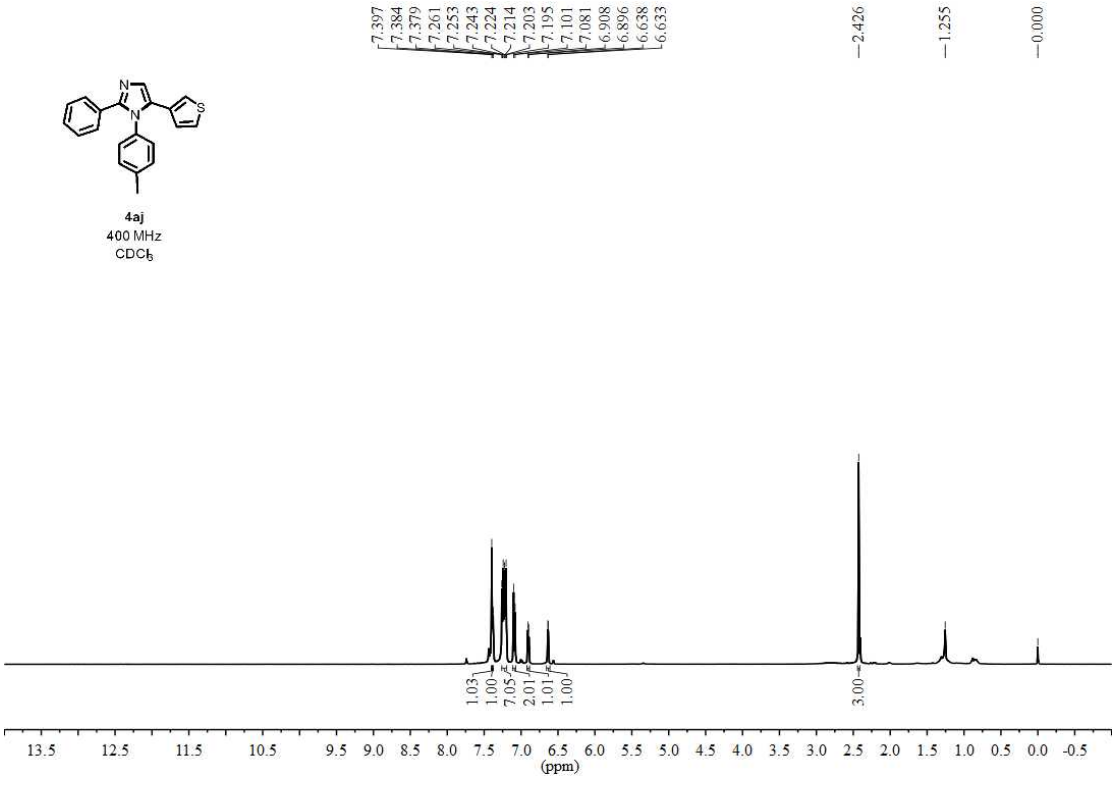

147.29
137.97
134.15
133.25
132.99
130.22
129.50
129.46
129.18
128.62
128.57
128.19
128.02
127.24
126.28
125.84
125.72
124.67
77.32
77.00
76.68
20.90
4ag
100 MHz
CDCl3
(ppm)

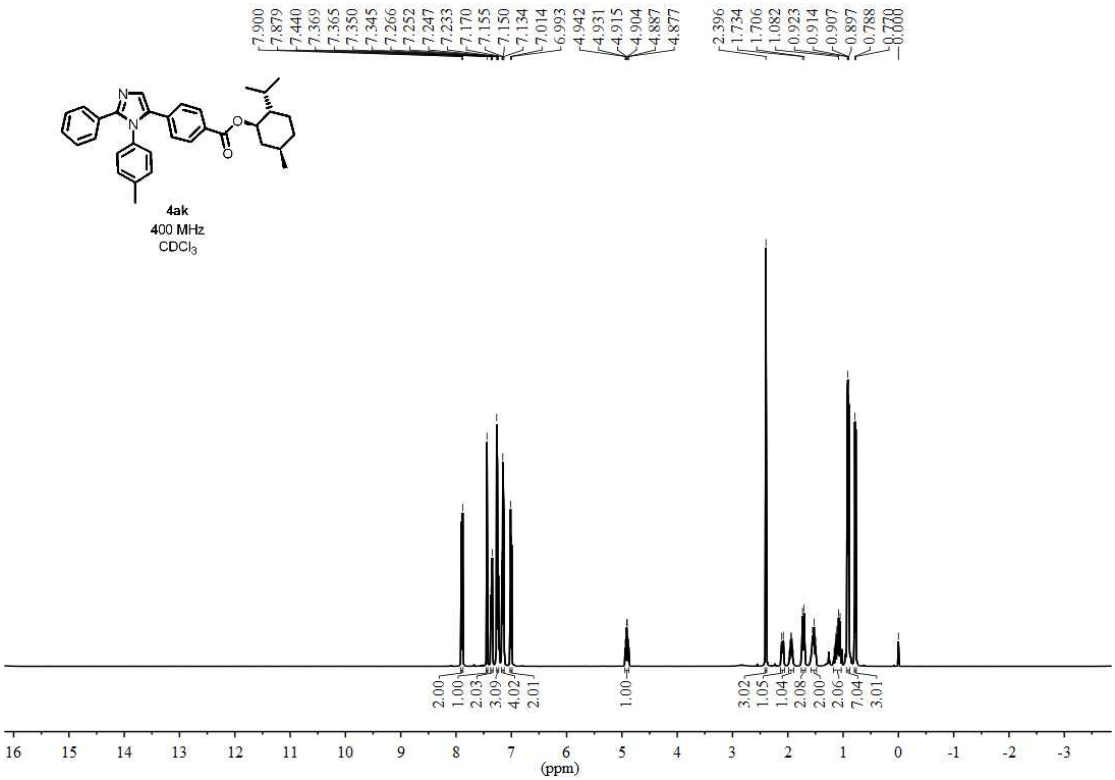

7.737
7.650
7.629
7.597
7.462
7.429
7.413
7.406
7.391
7.245
7.151
7.125
7.112
7.094
7.023
7.005
2.351
0.000
4ah
400 MHz
CDCl3
1.00
2.01
1.01
1.00
4.00
3.00
3.00
2.00
3.00
(ppm)


148.16
138.46
134.58
133.06
132.20
130.66
130.00
128.72
128.54
128.07
127.99
127.94
127.65
127.50
127.35
127.20
126.21
126.07
77.32
77.00
76.68
21.16
4ah
100 MHz
CDCl3
(ppm)


7.718
7.701
7.611
7.593
7.511
7.495
7.412
7.381
7.344
7.320
7.298
7.256
7.134
7.118
7.019
3.801
2.366
0.000
4ai
400 MHz
CDCl3
1.00
1.01
1.02
3.01
2.04
4.06
2.01
3.00
2.01
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)


147.71
143.30
143.19
141.06
140.91
138.53
135.54
134.41
130.26
130.01
128.77
128.24
128.06
127.96
127.50
127.25
126.87
126.79
125.16
124.97
119.90
119.54
77.32
77.00
76.68
36.84
21.19
4ai
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.397
7.384
7.379
7.261
7.253
7.243
7.224
7.214
7.203
7.195
7.101
7.081
6.908
6.896
6.638
6.633
2.426
1.255
0.000
4aj
400 MHz
CDCl3
1.03
1.00
7.05
2.01
1.01
1.00
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)
147.64
139.16
134.66
131.07
130.24
130.00
128.53
128.24
128.11
128.08
127.21
127.16
125.29
121.15
77.32
77.00
76.68
21.30
4aj
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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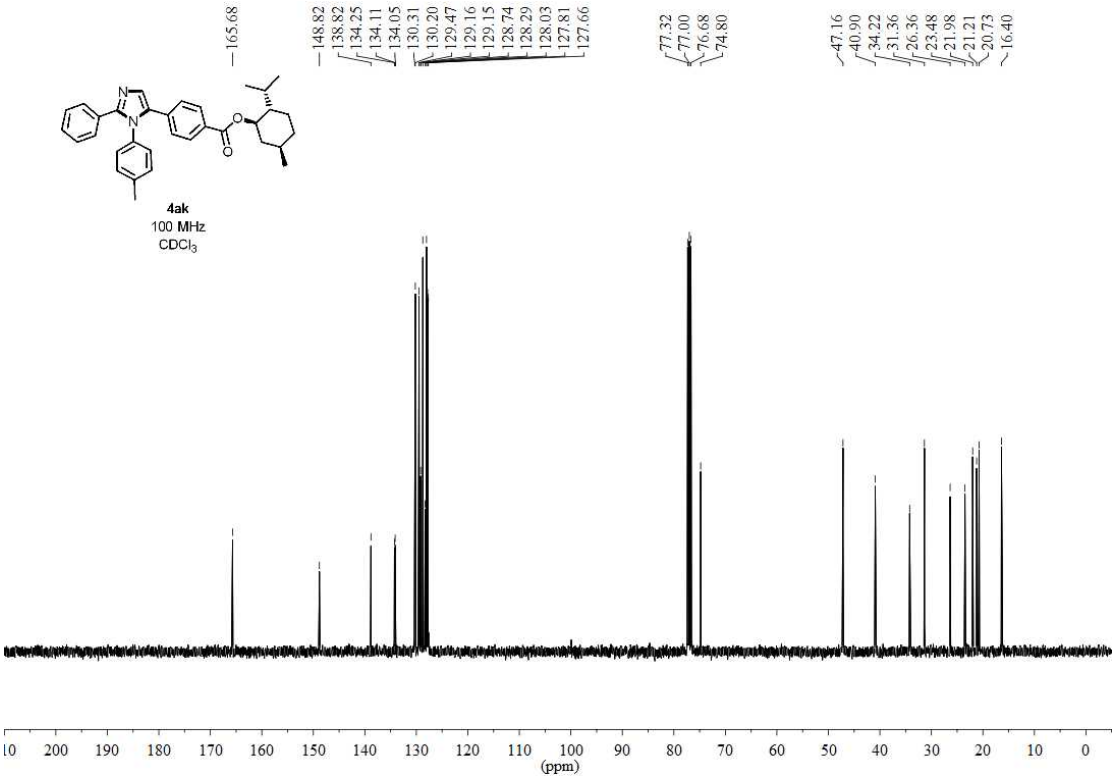
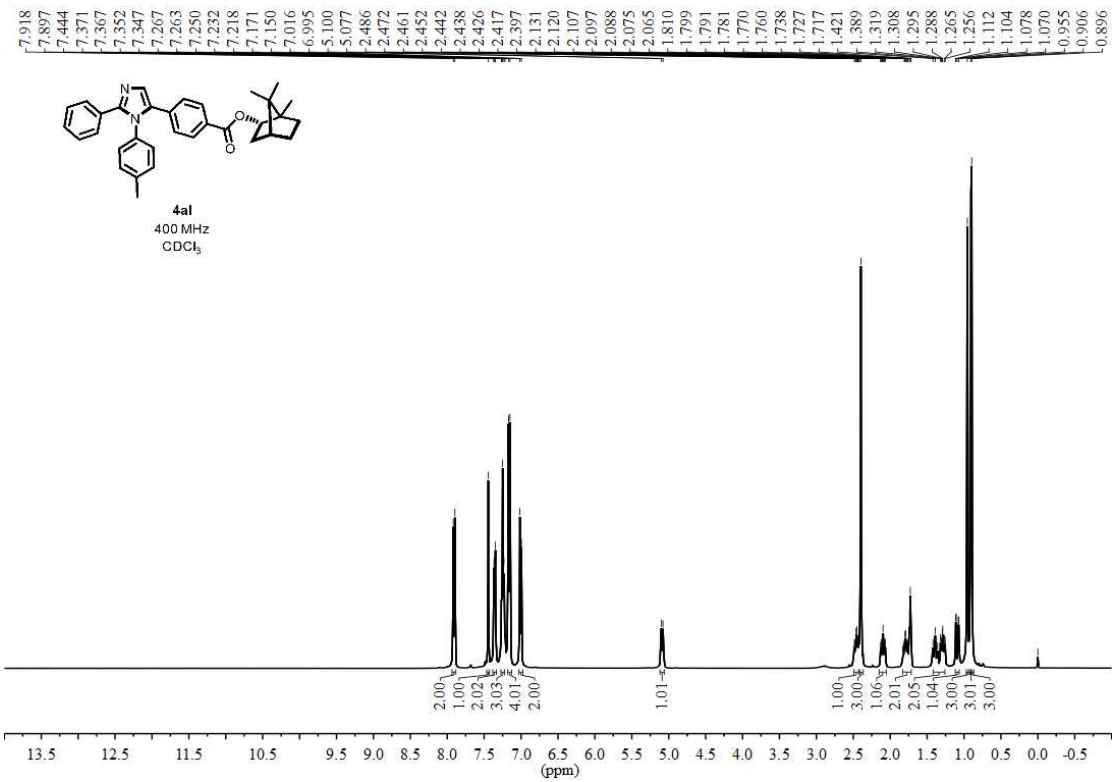
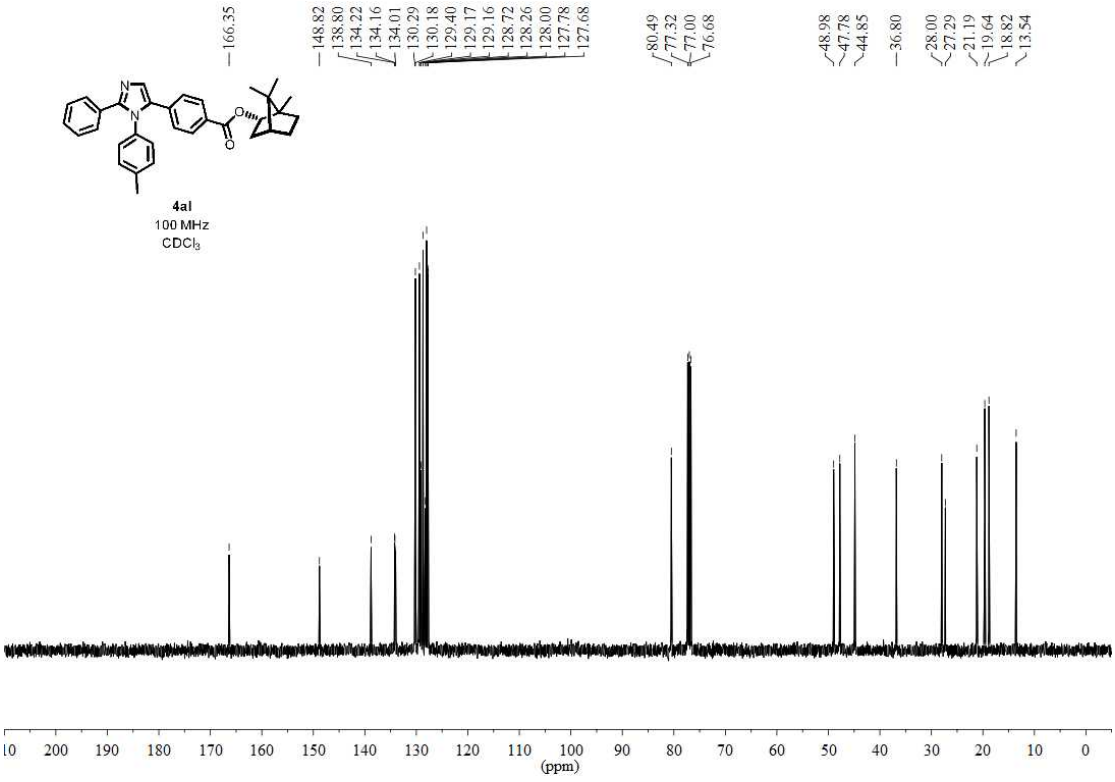
7.369
7.365
7.350
7.345
7.266
7.252
7.247
7.233
7.170
7.155
7.150
7.134
7.014
6.993
4.942
4.931
4.915
4.904
4.887
4.877
2.396
1.734
1.706
1.082
0.923
0.914
0.907
0.897
0.788
0.778
0.000
4ak
400 MHz
CDCl3
2.00
1.00
2.03
3.09
4.02
2.01
1.00
3.02
1.05
1.04
2.08
2.00
2.06
7.04
3.01
(ppm)


165.68
148.82
138.82
134.25
134.11
134.05
130.31
130.20
129.47
129.16
129.15
128.74
128.29
128.03
127.81
127.66
77.32
77.00
76.68
74.80
47.16
40.90
34.22
31.36
26.36
23.48
21.98
21.21
20.73
16.40
4ak
100 MHz
CDCl3
(ppm)


7.918
7.897
7.444
7.371
7.367
7.352
7.347
7.267
7.263
7.250
7.232
7.218
7.171
7.150
7.016
6.995
5.100
5.077
2.486
2.472
2.461
2.452
2.442
2.438
2.426
2.417
2.397
2.131
2.120
2.107
2.097
2.088
2.075
2.065
1.810
1.799
1.791
1.781
1.770
1.760
1.738
1.727
1.717
1.421
1.389
1.319
1.308
1.295
1.288
1.265
1.256
1.112
1.104
1.078
1.070
0.955
0.906
0.896
4al
400 MHz
CDCl3
2.00
1.00
2.02
3.03
4.01
2.00
1.01
1.00
3.00
1.06
2.01
2.05
1.04
3.00
3.01
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)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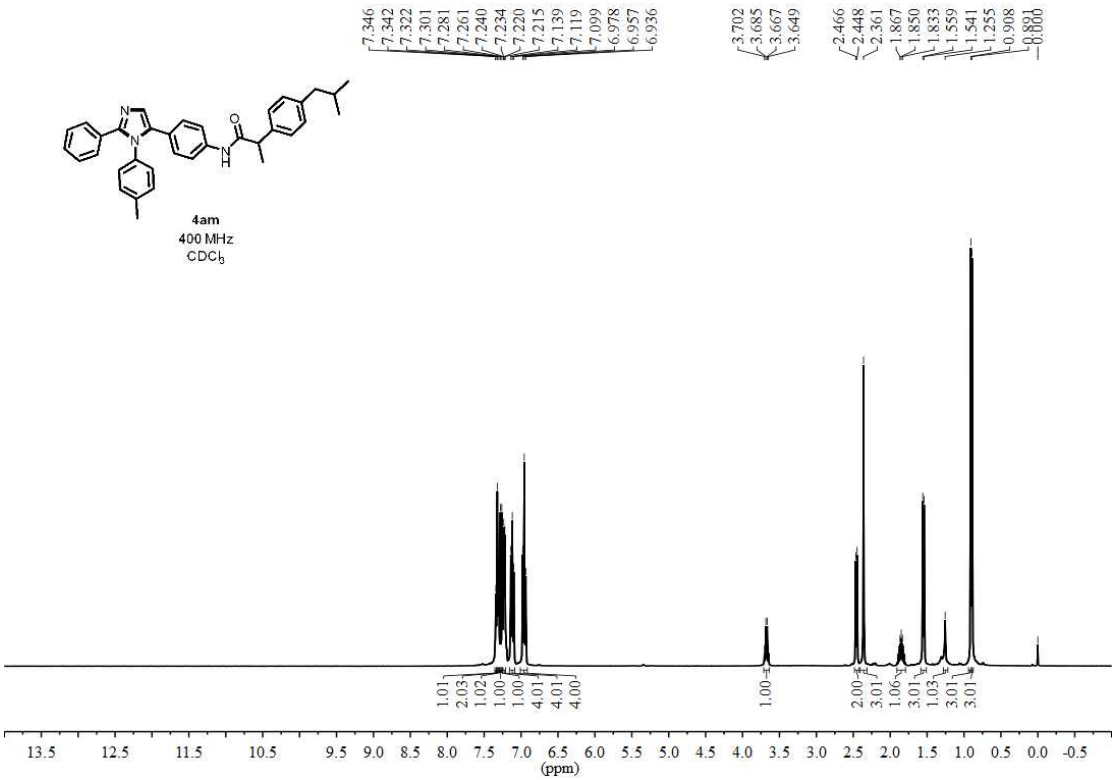
148.82
138.80
134.22
134.16
134.01
130.29
130.18
129.40
129.17
129.16
128.72
128.26
128.00
127.78
127.68
80.49
77.32
77.00
76.68
48.98
47.78
44.85
36.80
28.00
27.29
21.19
19.64
18.82
13.54
4al
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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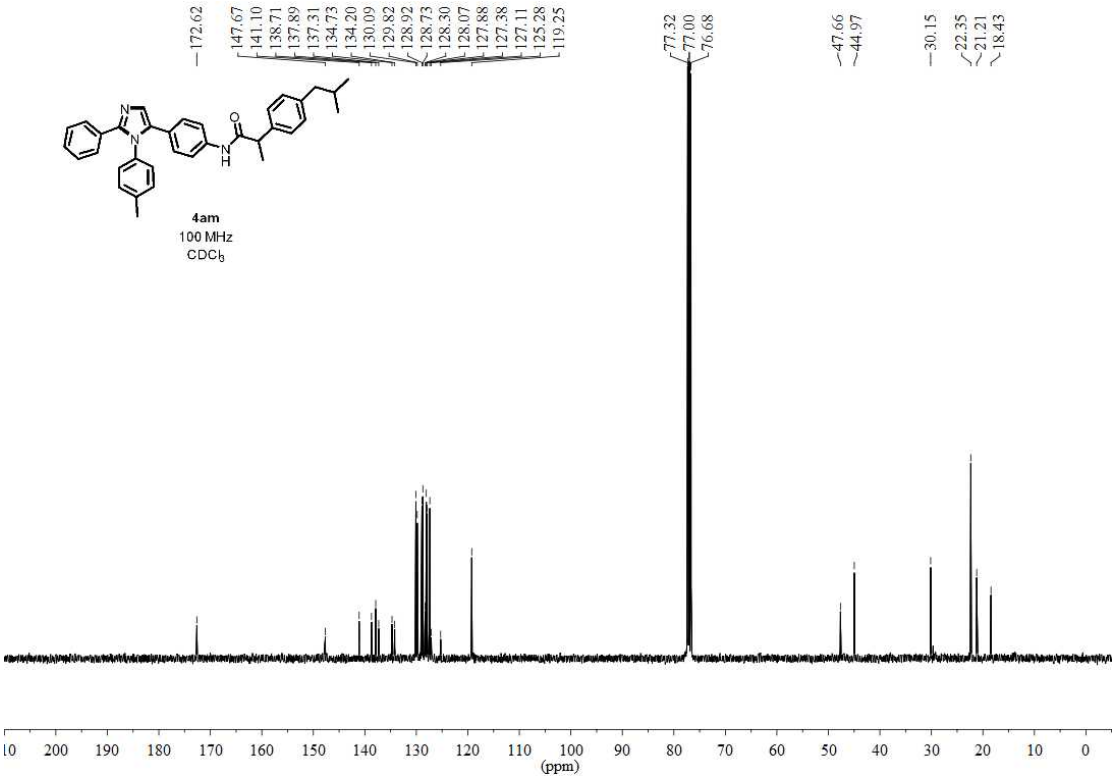
7.342
7.322
7.301
7.281
7.261
7.240
7.234
7.220
7.215
7.139
7.119
7.099
6.978
6.957
6.936
3.702
3.685
3.667
3.649
2.466
2.448
2.361
1.867
1.850
1.833
1.559
1.541
1.255
0.908
0.881
0.000
4am
400 MHz
CDCl3
1.01
2.03
1.02
1.00
1.00
4.01
4.01
4.00
1.00
2.00
3.01
1.06
3.01
1.03
3.01
3.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)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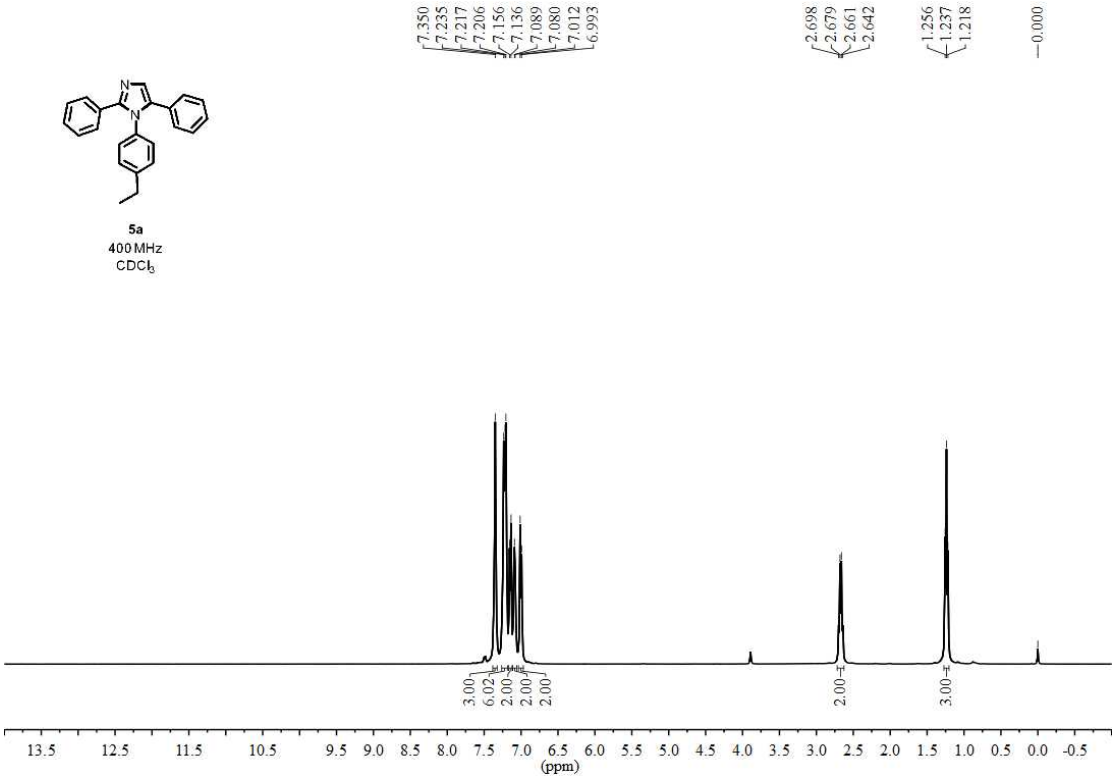
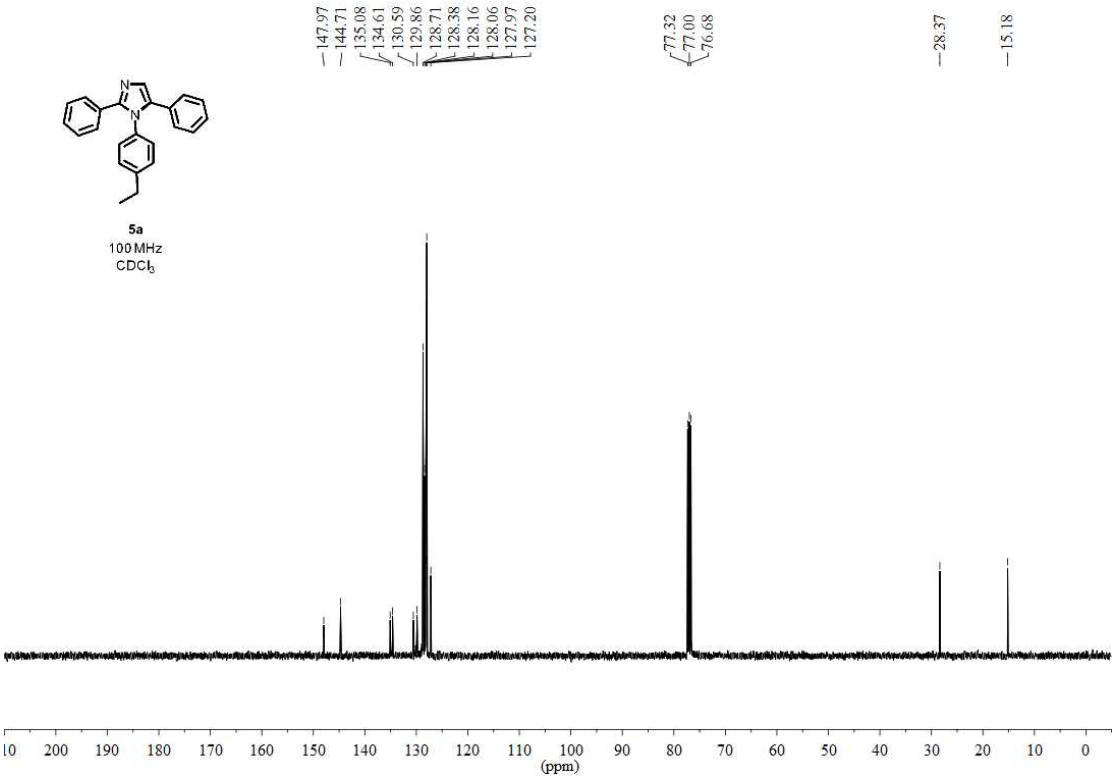
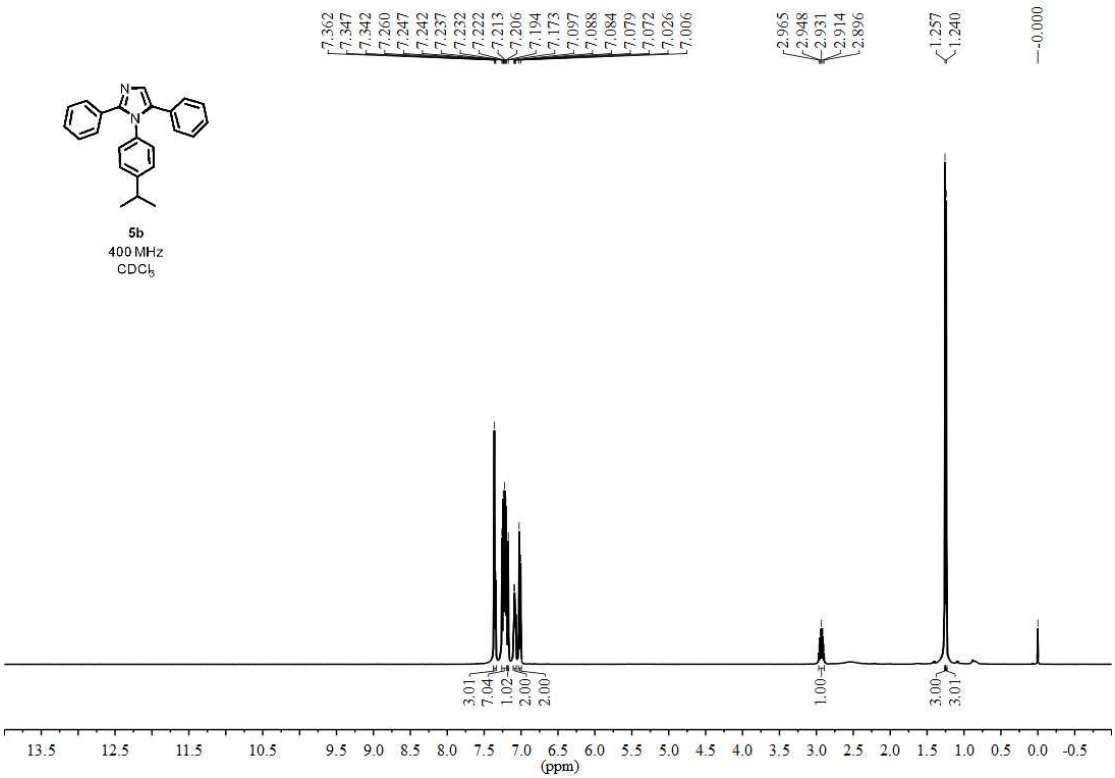
147.67
141.10
138.71
137.89
137.31
134.73
134.20
130.09
129.82
128.92
128.73
128.30
128.07
127.88
127.38
127.11
125.28
119.25
77.32
77.00
76.68
47.66
44.97
30.15
22.35
21.21
18.43
4am
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.350
7.235
7.217
7.206
7.156
7.136
7.089
7.080
7.012
6.993
2.698
2.679
2.661
2.642
1.256
1.237
1.218
0.000
5a
400 MHz
CDCl3
3.00
6.02
2.00
2.00
2.00
2.00
3.00
(ppm)


147.97
144.71
135.08
134.61
130.59
129.86
128.71
128.38
128.16
128.06
127.97
127.20
77.32
77.00
76.68
28.37
15.18
5a
100 MHz
CDCl3
(ppm)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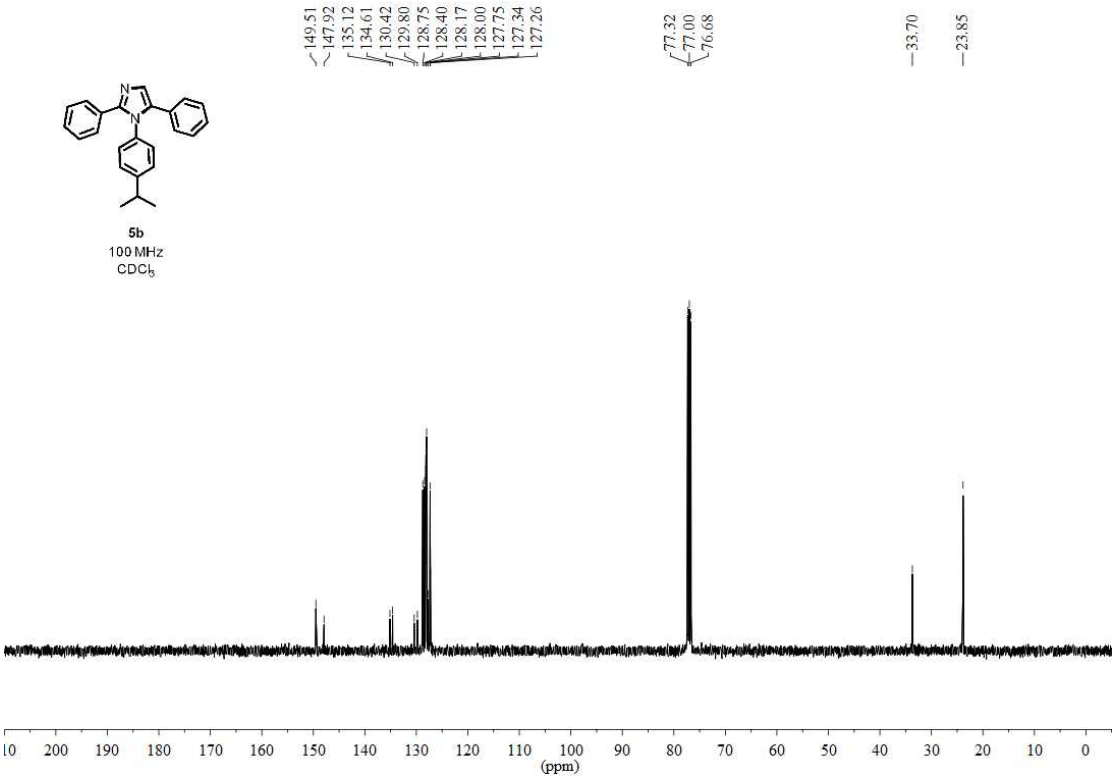
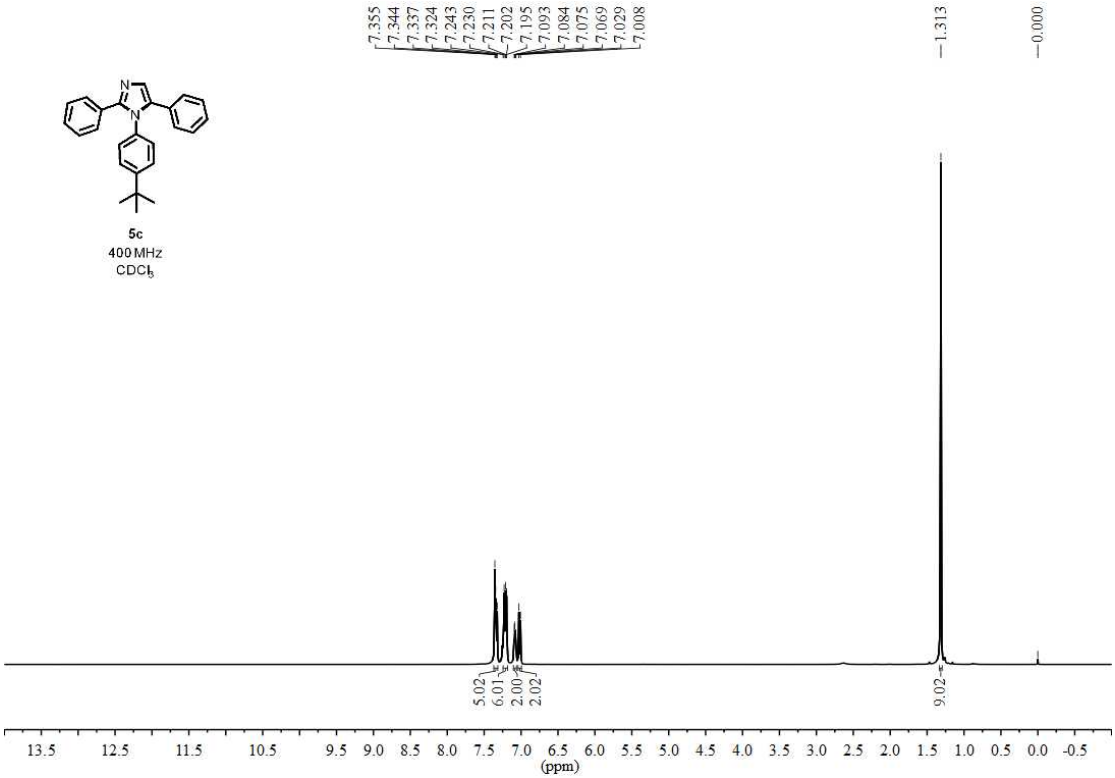
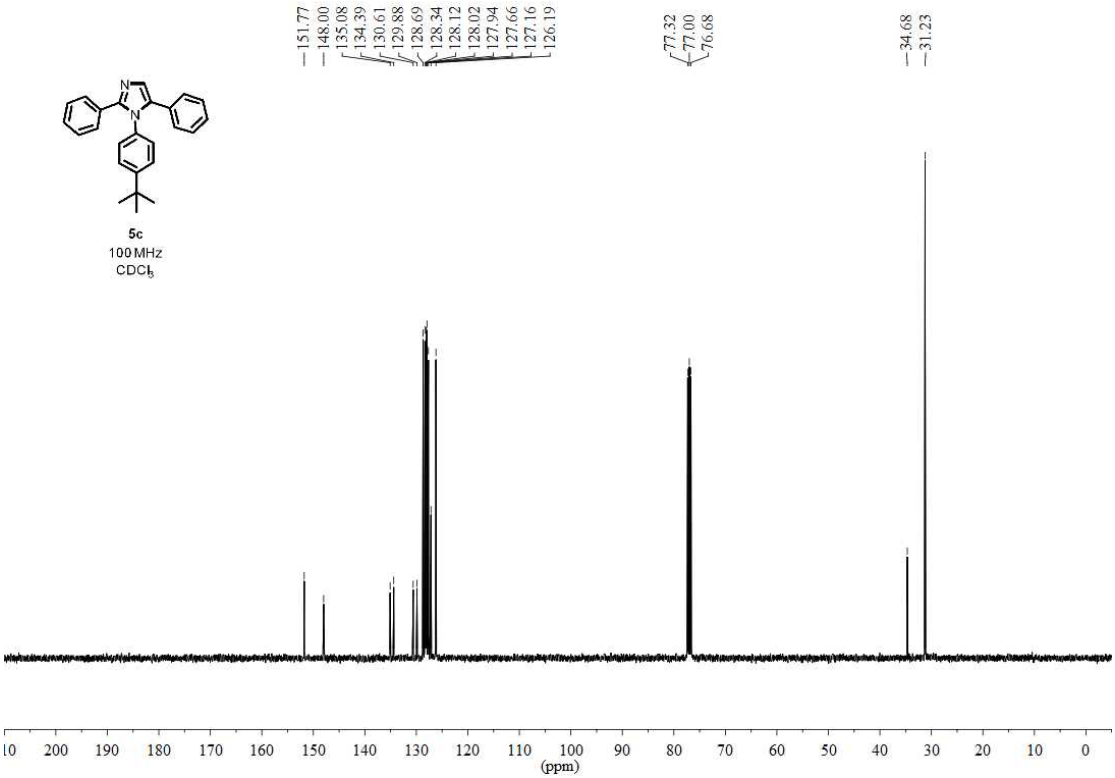
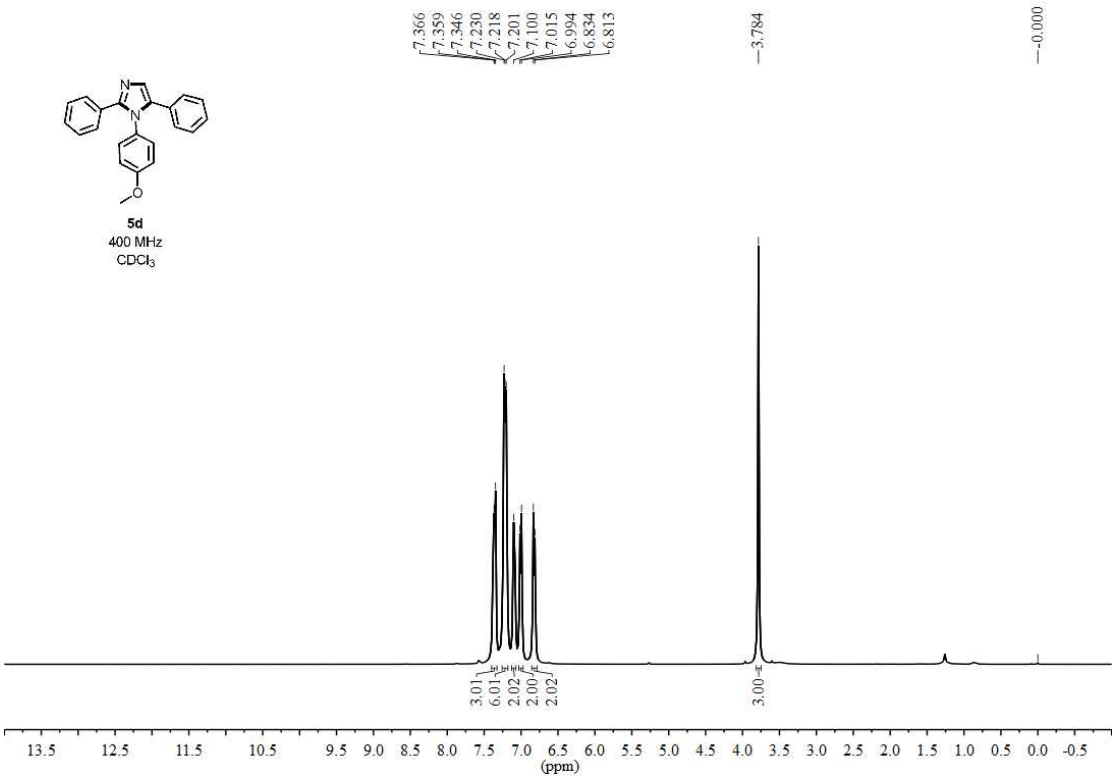
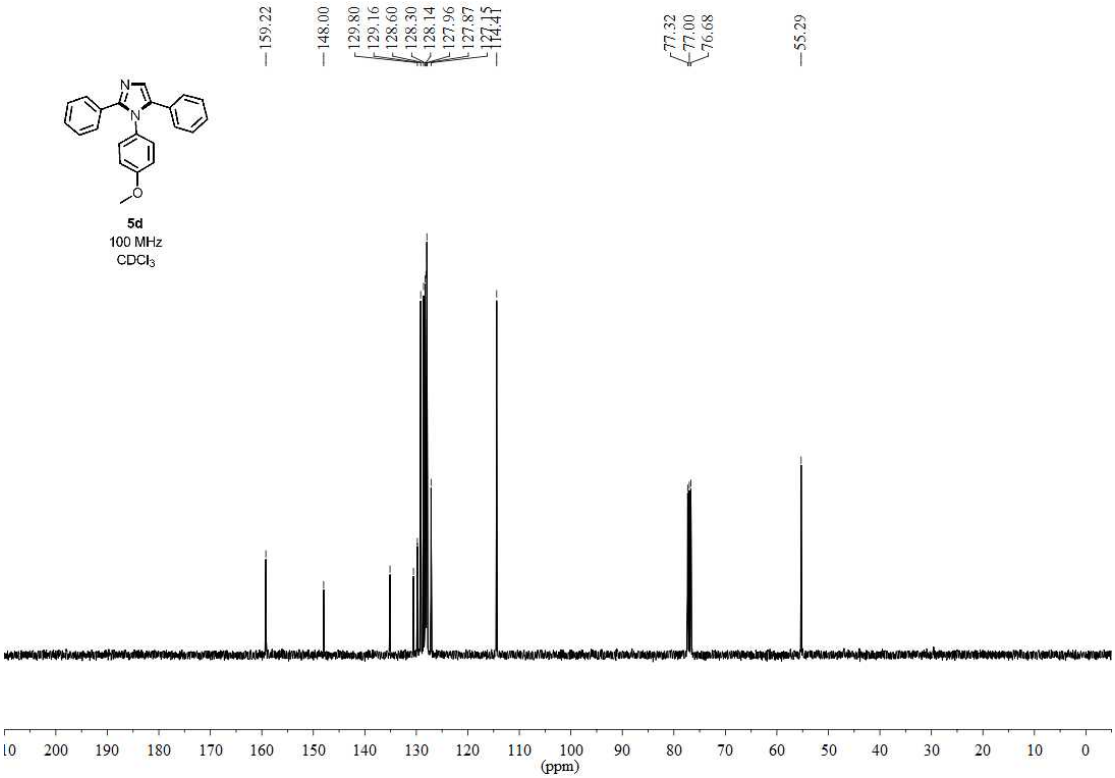
7.347
7.342
7.260
7.247
7.242
7.237
7.232
7.222
7.213
7.206
7.194
7.173
7.097
7.088
7.084
7.079
7.072
7.026
7.006
2.965
2.948
2.931
2.914
2.896
1.257
1.240
-0.000
5b
400 MHz
CDCl3
3.01
7.04
1.02
2.00
2.00
1.00
3.00
3.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

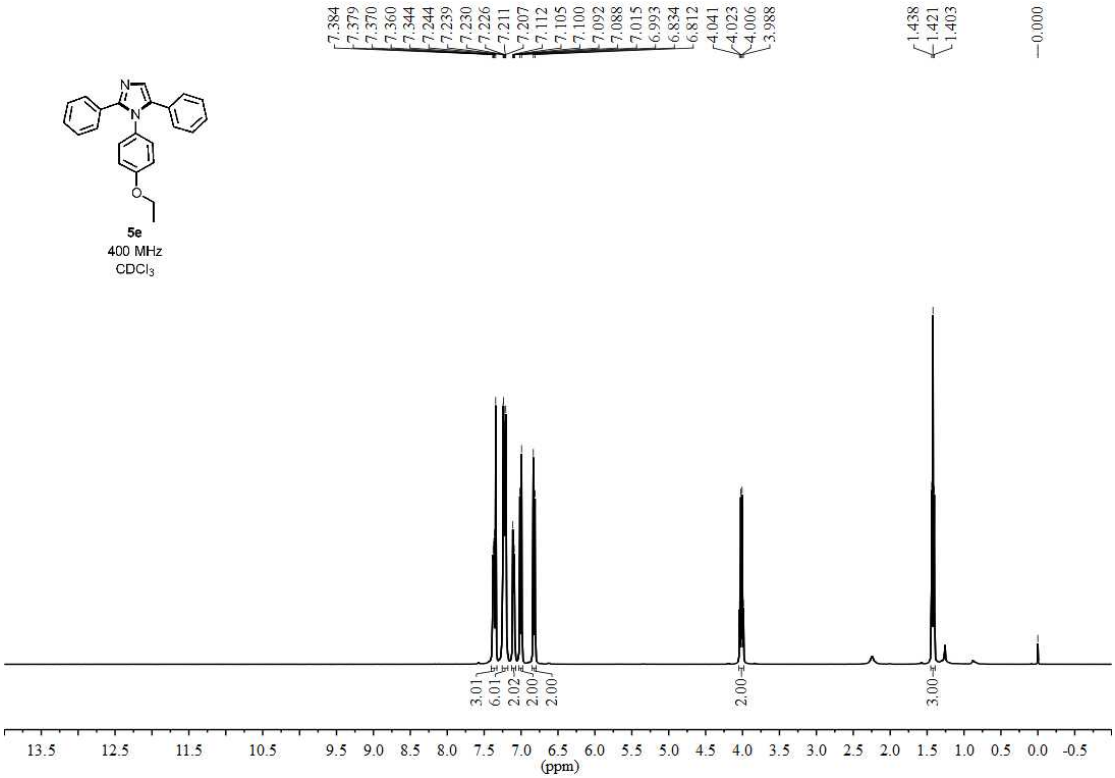

149.51
147.92
135.12
134.61
130.42
129.80
128.75
128.40
128.17
128.00
127.75
127.34
127.26
77.32
77.00
76.68
33.70
23.85
5b
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

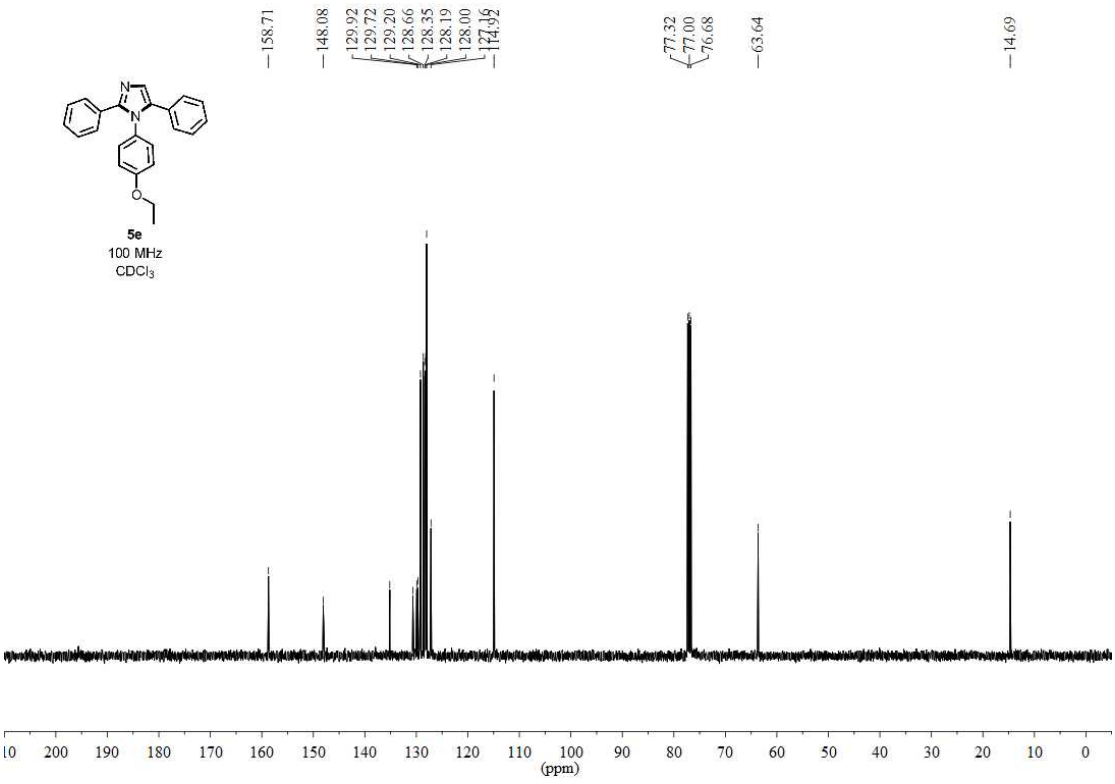

7.355
7.344
7.337
7.324
7.243
7.230
7.211
7.202
7.195
7.093
7.084
7.075
7.069
7.029
7.008
1.313
0.000
5c
400 MHz
CDCl3
5.02
6.01
2.00
2.02
9.02
(ppm)

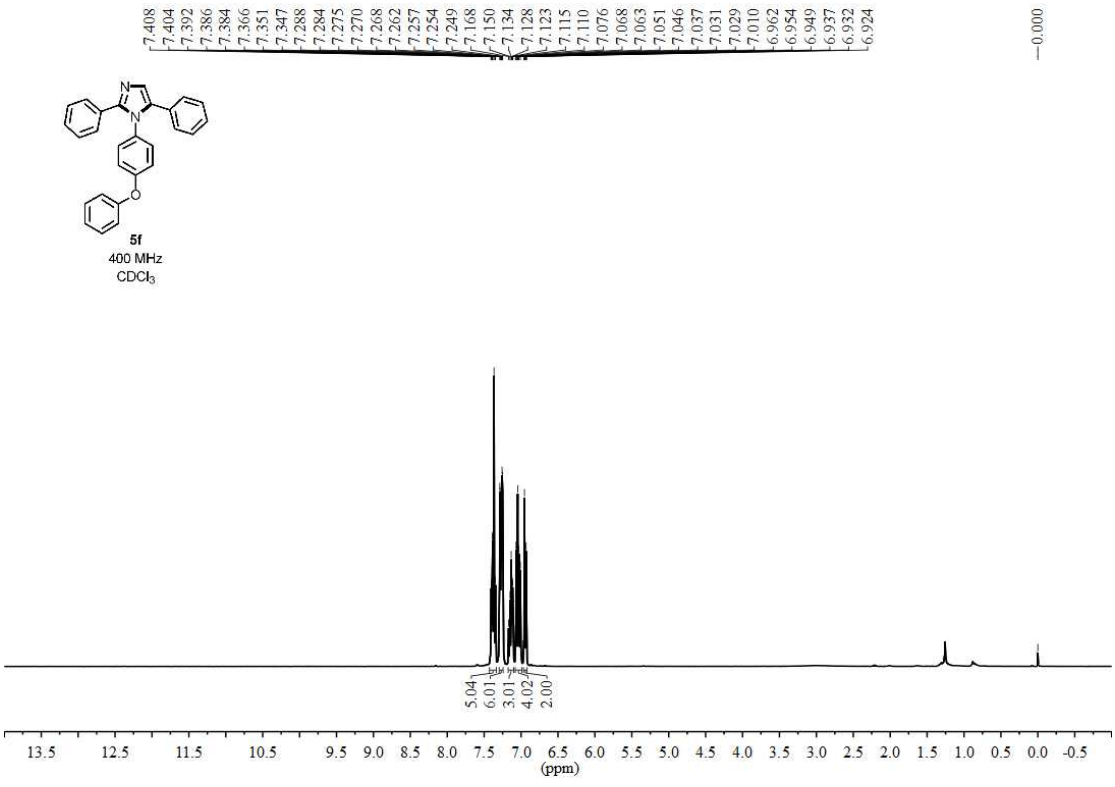

151.77
148.00
135.08
134.39
130.61
129.88
128.69
128.34
128.12
128.02
127.94
127.66
127.16
126.19
77.32
77.00
76.68
34.68
31.23
5c
100 MHz
CDCl3
(ppm)

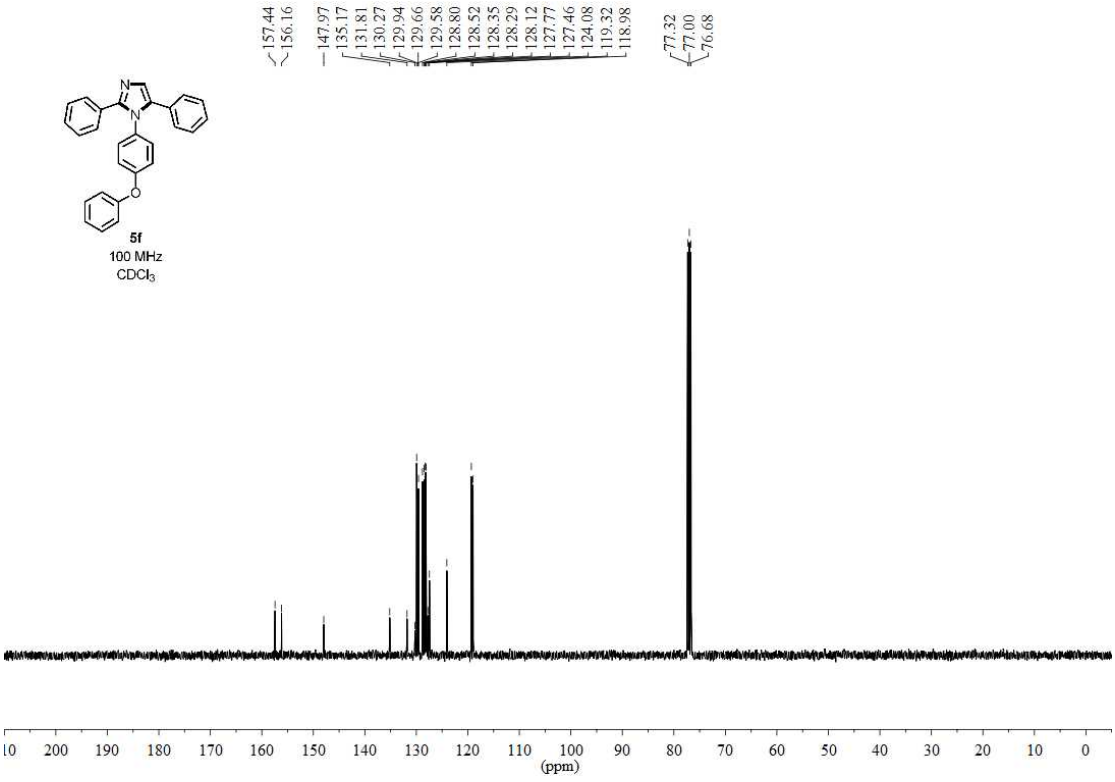

7.366
7.359
7.346
7.230
7.218
7.201
7.100
7.015
6.994
6.834
6.813
3.784
0.000
5d
400 MHz
CDCl3
3.01
6.01
2.02
2.00
2.02
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

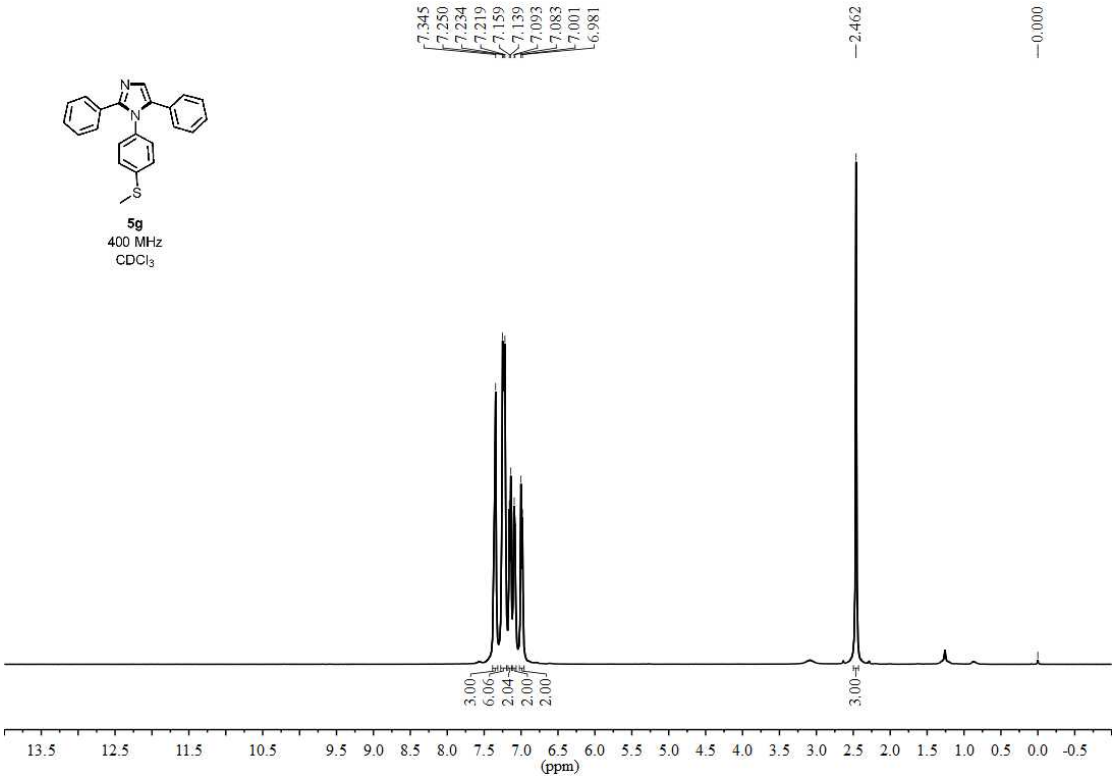

159.22
148.00
129.80
129.16
128.60
128.30
128.14
127.96
127.87
127.15
114.41
77.32
77.00
76.68
55.29
5d
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

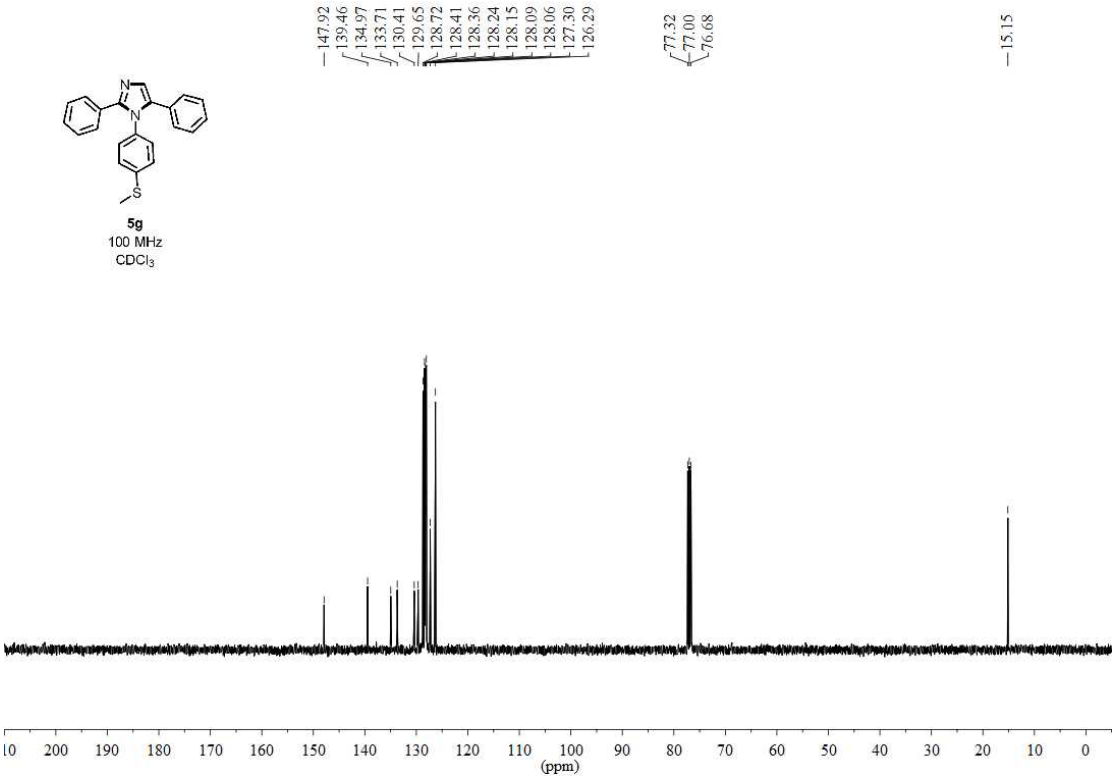

7.384
7.379
7.370
7.360
7.344
7.244
7.239
7.230
7.226
7.211
7.207
7.112
7.105
7.100
7.092
7.088
7.015
6.993
6.834
6.812
4.041
4.023
4.006
3.988
1.438
1.421
1.403
0.000
5e
400 MHz
CDCl3
3.01
6.01
2.02
2.00
2.00
2.00
3.00
(ppm)

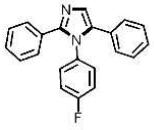

158.71
148.08
129.92
129.72
129.20
128.66
128.35
128.19
128.00
127.18
114.92
77.32
77.00
76.68
63.64
14.69
5e
100 MHz
CDCl3
(ppm)


7.408
7.404
7.392
7.386
7.384
7.366
7.351
7.347
7.288
7.284
7.275
7.270
7.268
7.262
7.257
7.254
7.249
7.168
7.150
7.134
7.128
7.123
7.115
7.110
7.076
7.068
7.063
7.051
7.046
7.037
7.031
7.029
7.010
6.962
6.954
6.949
6.937
6.932
6.924
0.000
5f
400 MHz
CDCl3
5.04
6.01
3.01
4.02
2.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

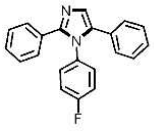

157.44
156.16
147.97
135.17
131.81
130.27
129.94
129.66
129.58
128.80
128.52
128.35
128.29
128.12
127.77
127.46
124.08
119.32
118.98
77.32
77.00
76.68
5f
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.345
7.250
7.234
7.219
7.159
7.139
7.093
7.083
7.001
6.981
2.462
0.000
5g
400 MHz
CDCl3
3.00
6.06
2.04
2.00
2.00
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)

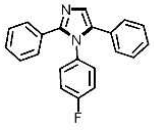

147.92
139.46
134.97
133.71
130.41
129.65
128.72
128.41
128.36
128.24
128.15
128.09
128.06
127.30
126.29
77.32
77.00
76.68
15.15
5g
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)



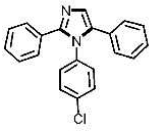
5h
400 MHz
$CDCl_3 + CF_3CO_2D$



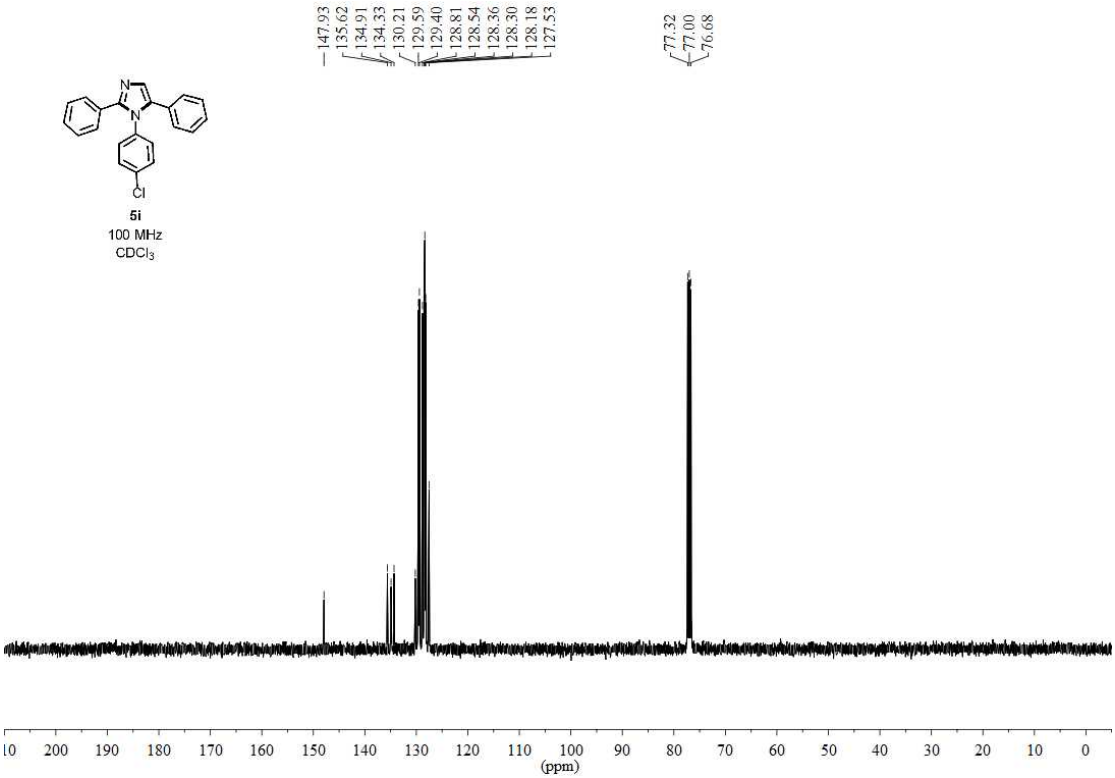
5h
100 MHz
$CDCl_3 + CF_3CO_2D$

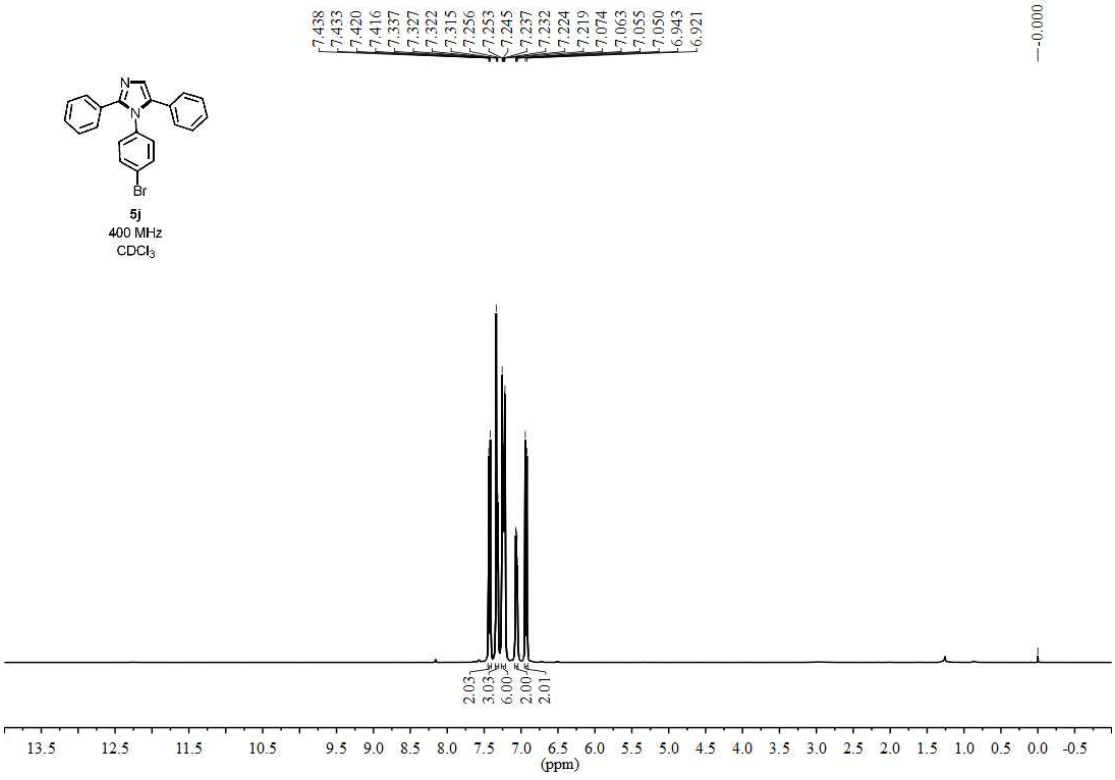


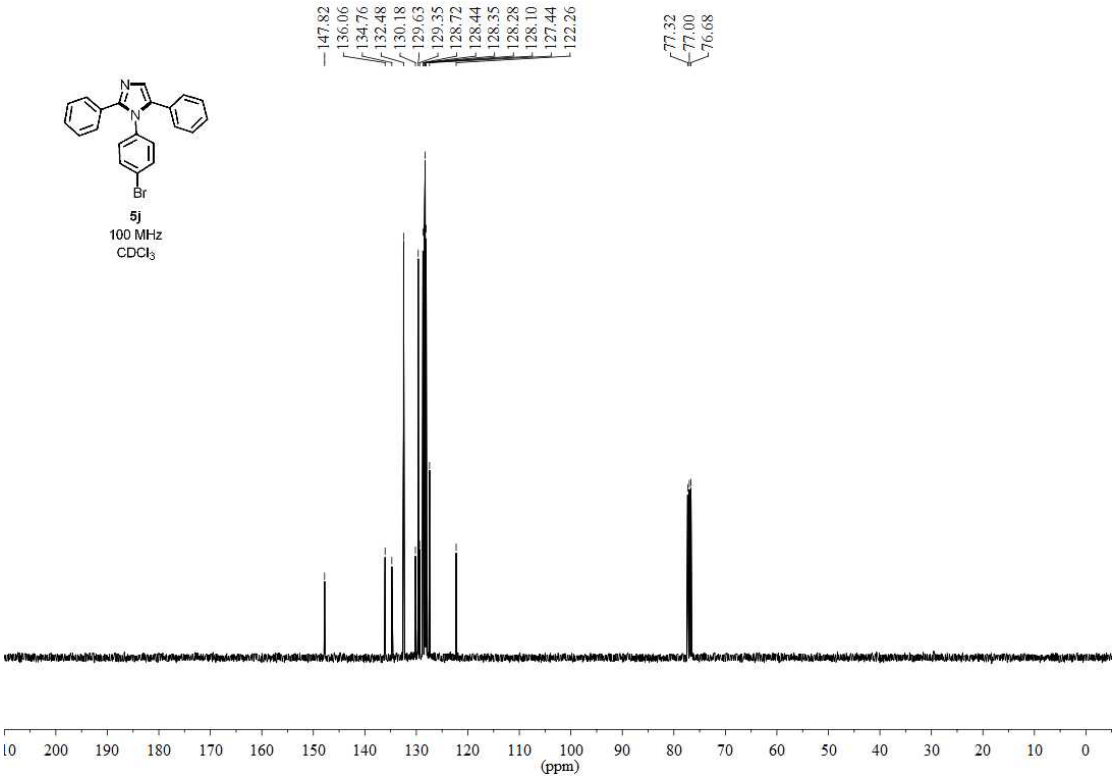
5h
376 MHz
$CDCl_3 + CF_3CO_2D$

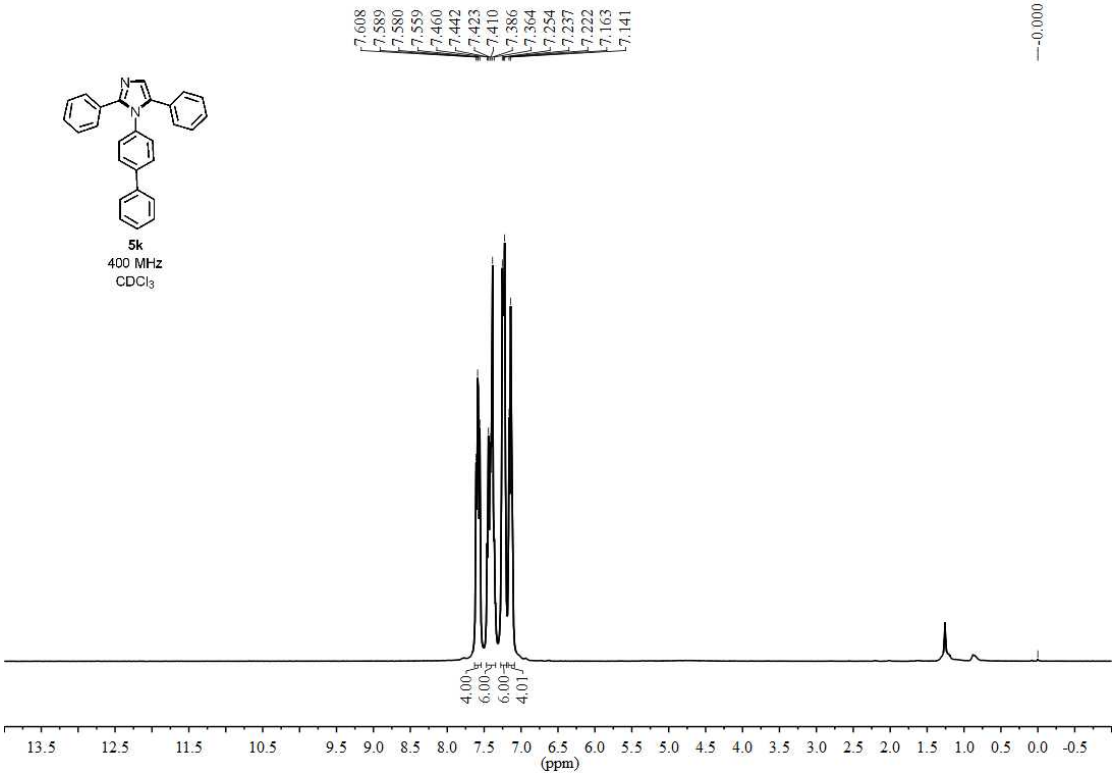


5i
400 MHz
$CDCl_3$


147.93
135.62
134.91
134.33
130.21
129.59
129.40
128.81
128.54
128.36
128.30
128.18
127.53
77.32
77.00
76.68
Cl
5i
100 MHz
CDCl3
(ppm)


7.438
7.433
7.420
7.416
7.337
7.327
7.322
7.315
7.256
7.253
7.245
7.237
7.232
7.224
7.219
7.074
7.063
7.055
7.050
6.943
6.921
-0.000
Br
5j
400 MHz
CDCl3
2.03
3.03
6.00
2.00
2.01
(ppm)


147.82
136.06
134.76
132.48
130.18
129.63
129.35
128.72
128.44
128.35
128.28
128.10
127.44
122.26
77.32
77.00
76.68
Br
5j
100 MHz
CDCl3
(ppm)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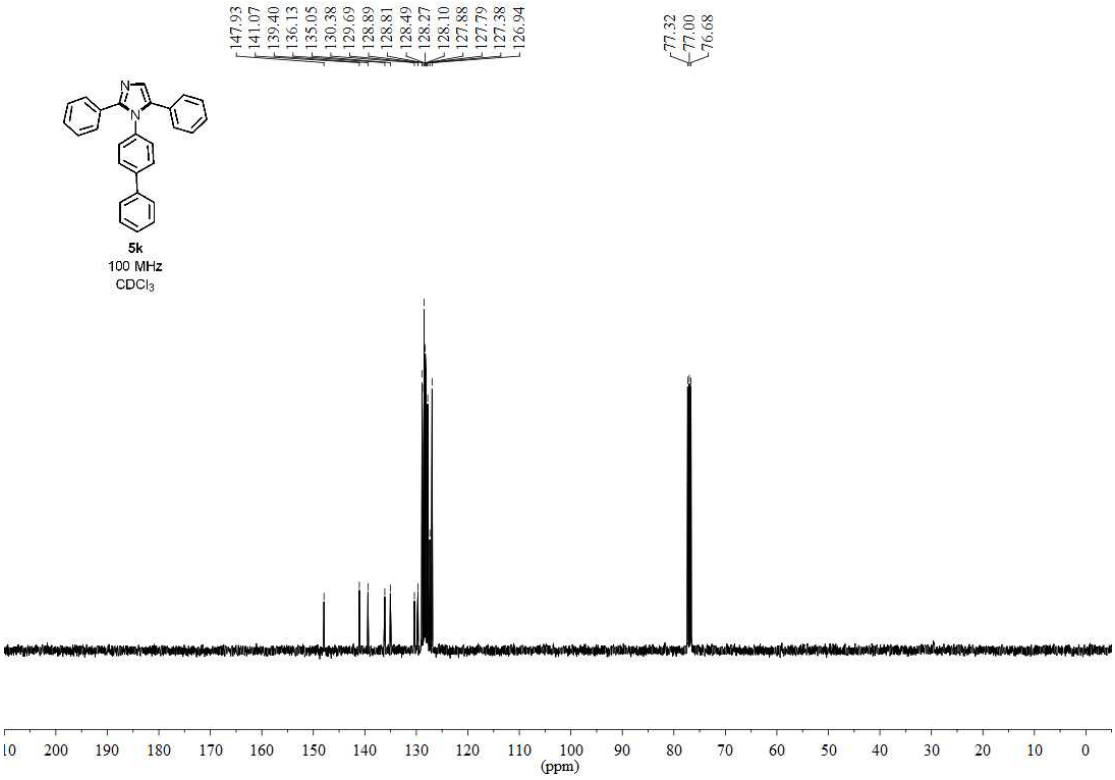
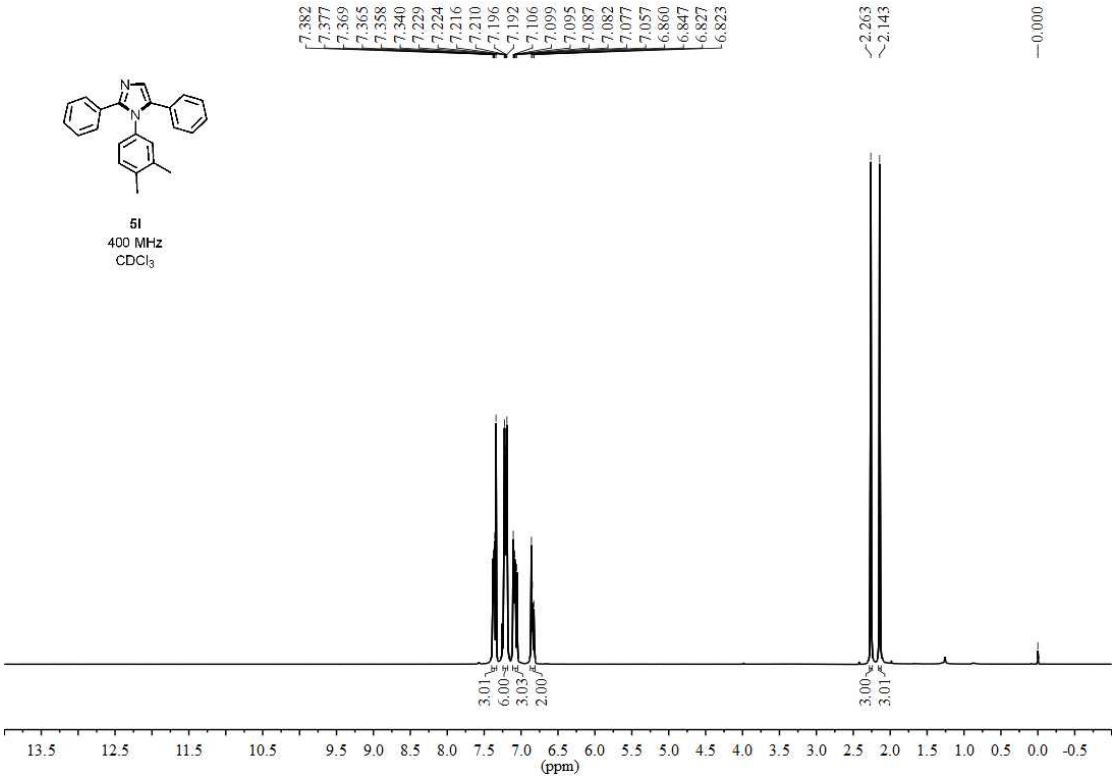
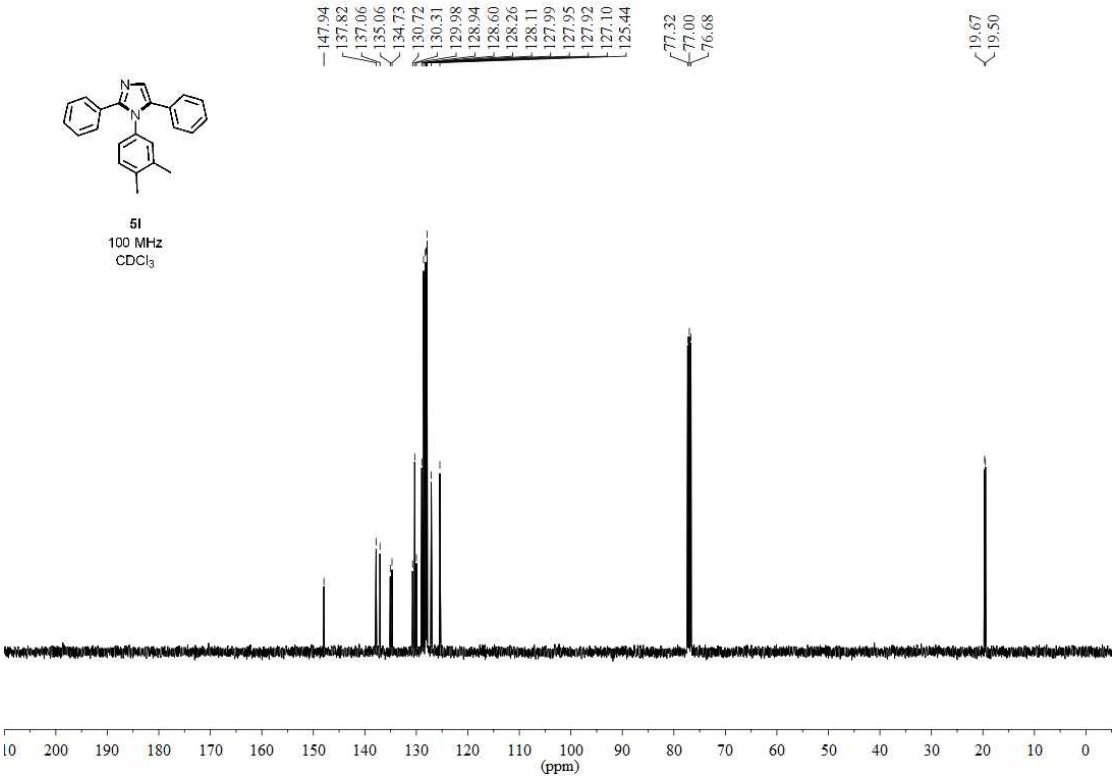
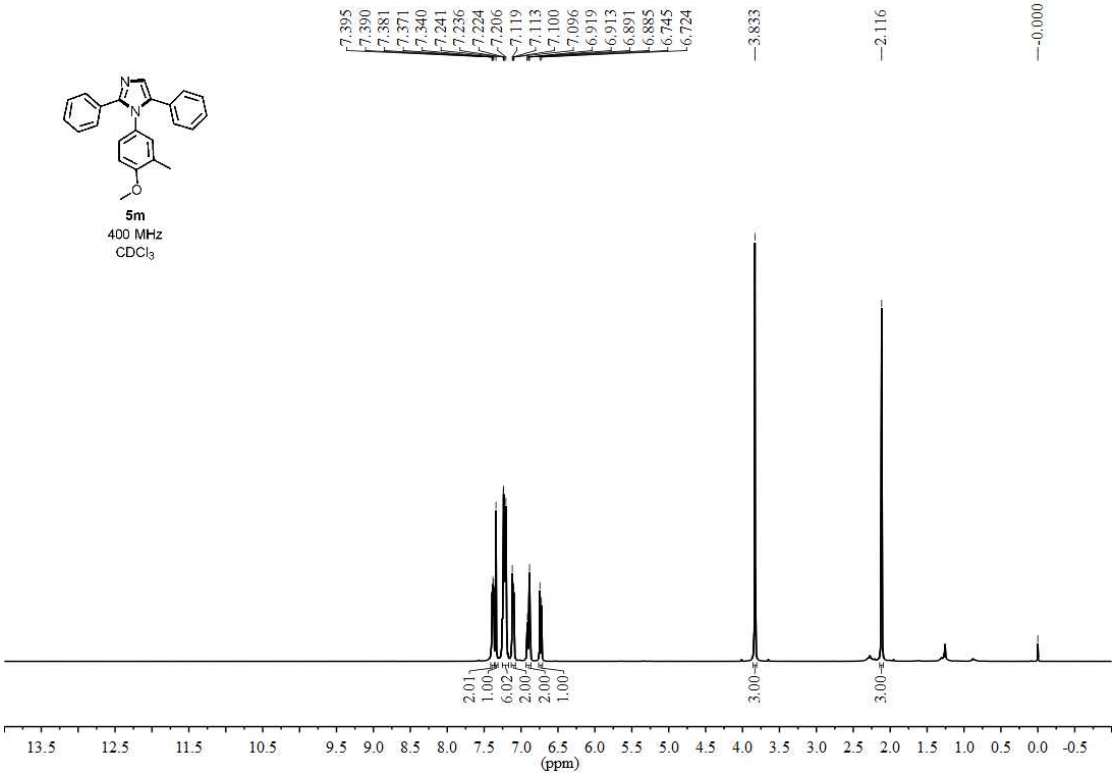
7.589
7.580
7.559
7.460
7.442
7.423
7.410
7.386
7.364
7.254
7.237
7.222
7.163
7.141
-0.000
4.00
6.00
6.00
4.01
5k
400 MHz
CDCl3
(ppm)


147.93
141.07
139.40
136.13
135.05
130.38
129.69
128.89
128.81
128.49
128.27
128.10
127.88
127.79
127.38
126.94
77.32
77.00
76.68
5k
100 MHz
CDCl3
(ppm)


7.382
7.377
7.369
7.365
7.358
7.340
7.229
7.224
7.216
7.210
7.196
7.192
7.106
7.099
7.095
7.087
7.082
7.077
7.057
6.860
6.847
6.827
6.823
2.263
2.143
0.000
5l
400 MHz
CDCl3
3.01
6.00
3.03
2.00
3.00
3.01
(ppm)


147.94
137.82
137.06
135.06
134.73
130.72
130.31
129.98
128.94
128.60
128.26
128.11
127.99
127.95
127.92
127.10
125.44
77.32
77.00
76.68
19.67
19.50
5l
100 MHz
CDCl3
(ppm)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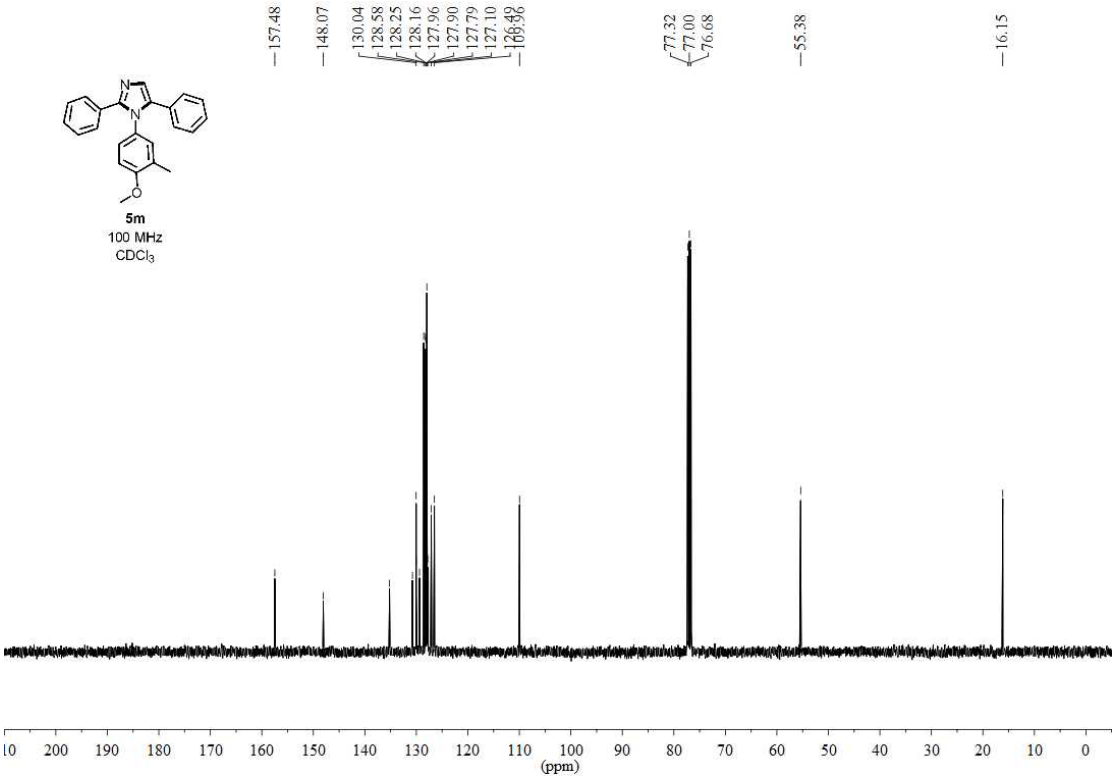
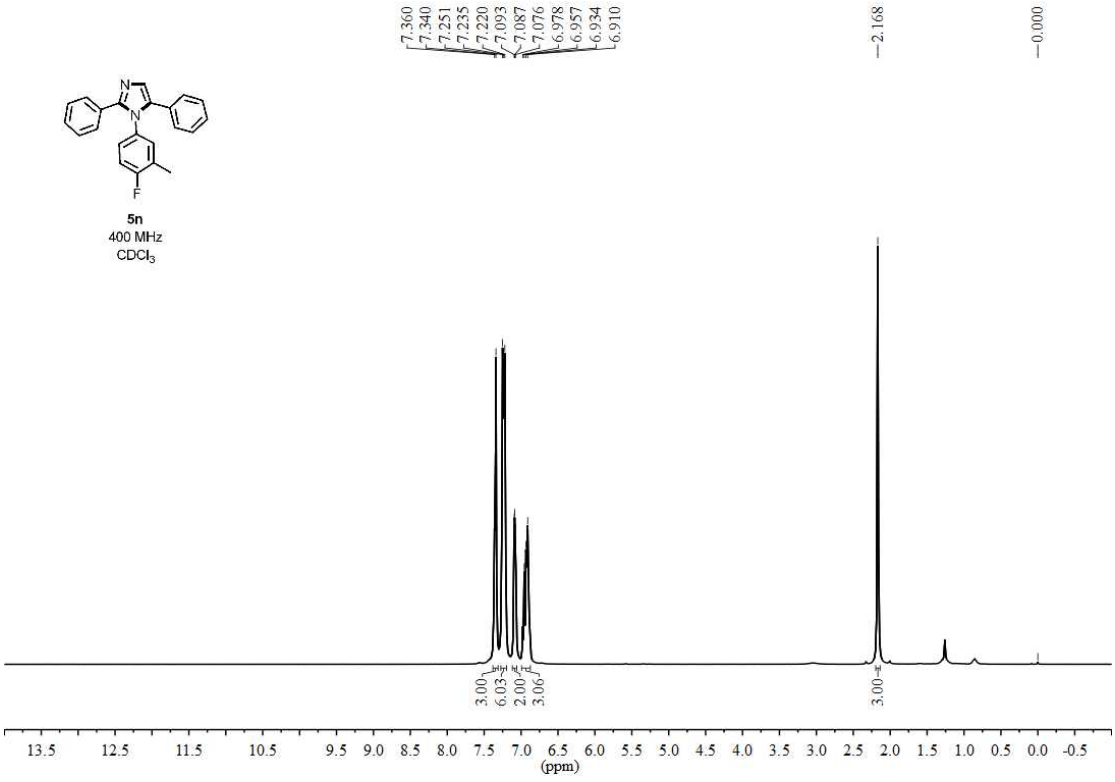
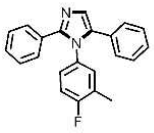
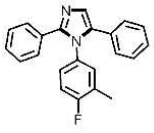
7.390
7.381
7.371
7.340
7.241
7.236
7.224
7.206
7.119
7.113
7.100
7.096
6.919
6.913
6.891
6.885
6.745
6.724
3.833
2.116
-0.000
5m
400 MHz
CDCl3
2.01
1.00
6.02
2.00
2.00
1.00
3.00
3.00
(ppm)


157.48
148.07
130.04
128.58
128.25
128.16
127.96
127.90
127.79
127.10
77.32
77.00
76.68
55.38
16.15
5m
100 MHz
CDCl3
(ppm)

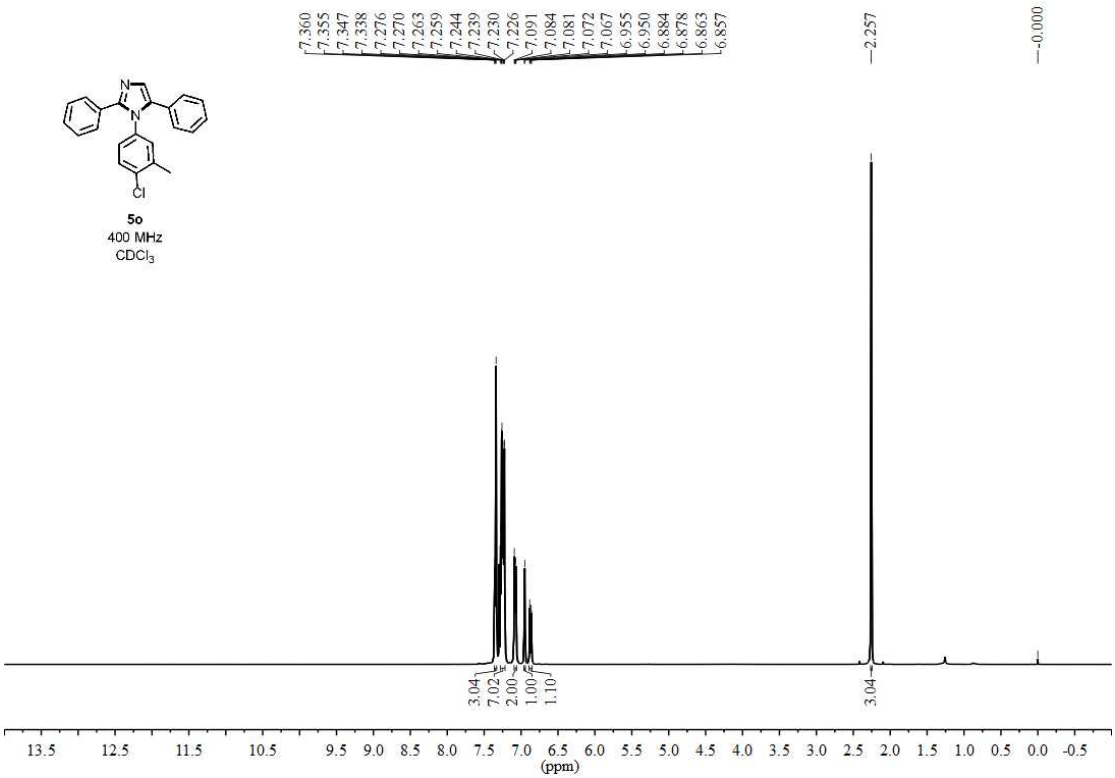

7.360
7.340
7.251
7.235
7.220
7.093
7.087
7.076
6.978
6.957
6.934
6.910
2.168
0.000
3.00
6.03
2.00
3.06
3.00
5n
400 MHz
CDCl3
(ppm)

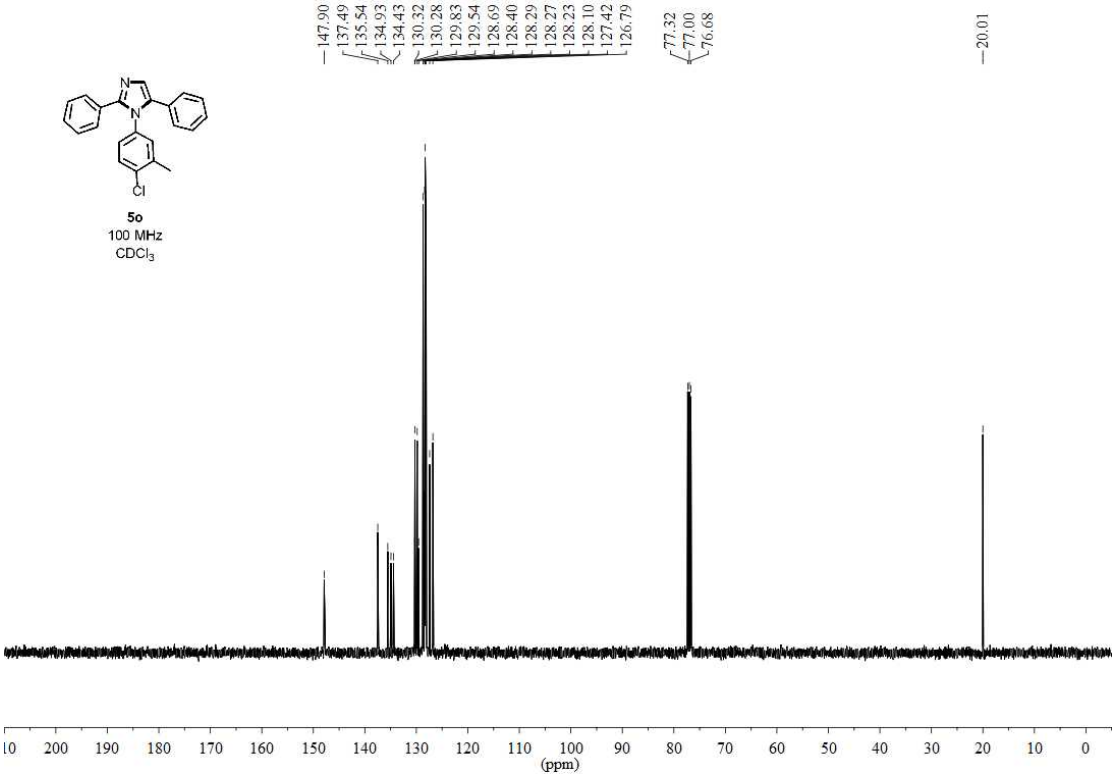


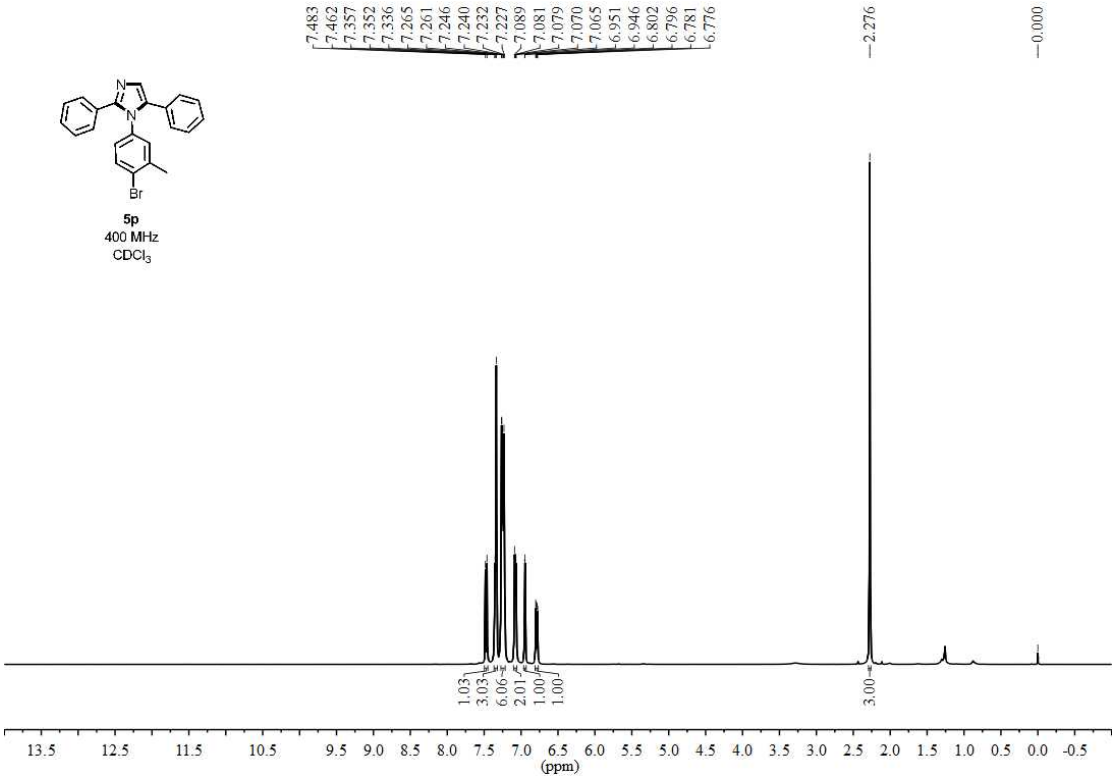
5n
100 MHz
$CDCl_3$

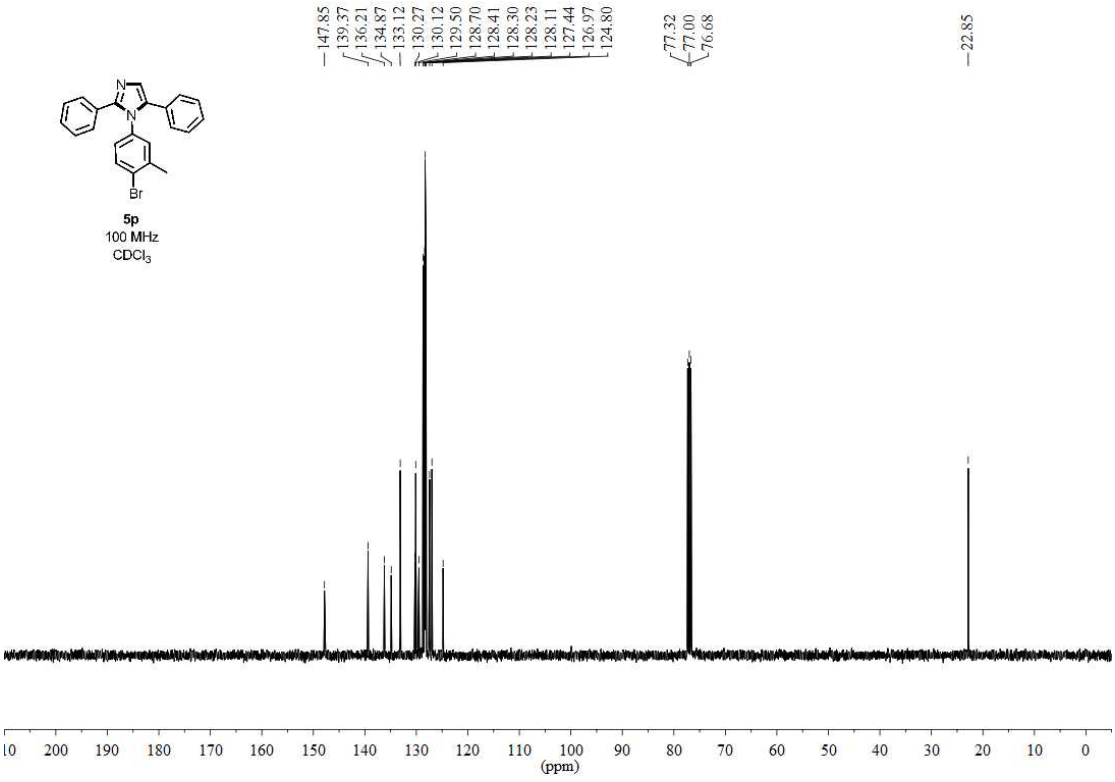


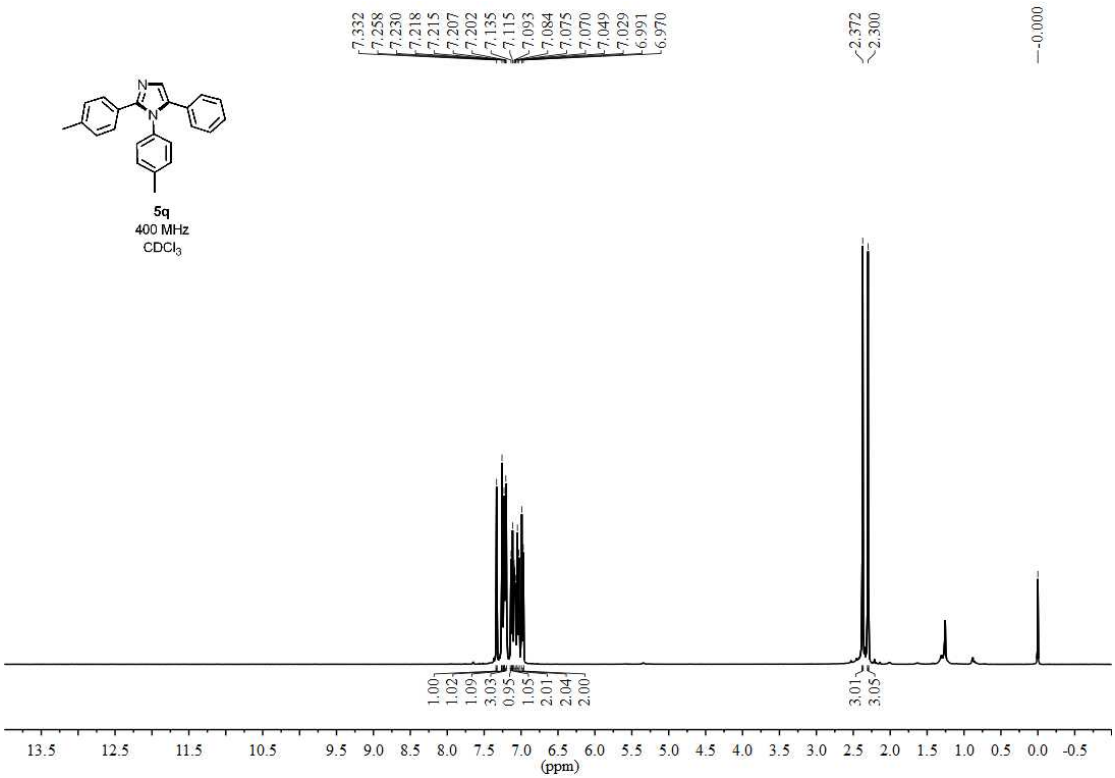
5n
376 MHz
$CDCl_3$

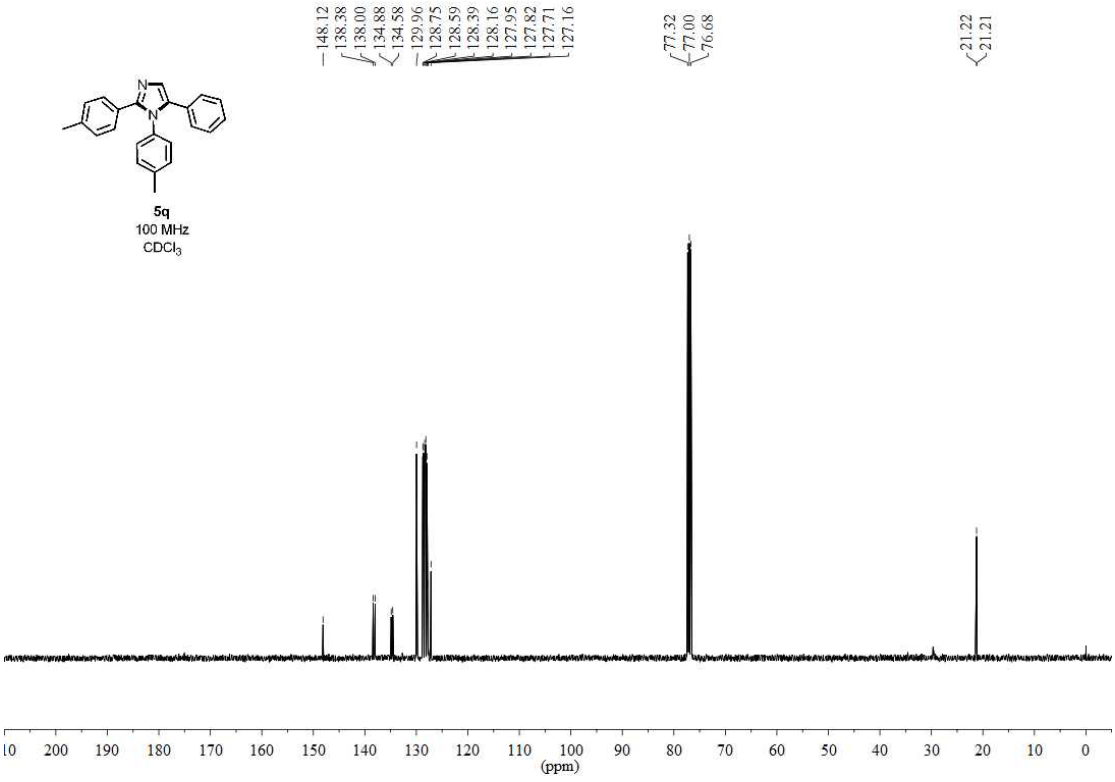

7.360
7.355
7.347
7.338
7.276
7.270
7.263
7.259
7.244
7.239
7.230
7.226
7.091
7.084
7.081
7.072
7.067
6.955
6.950
6.884
6.878
6.863
6.857
2.257
0.000
5o
400 MHz
CDCl3
3.04
7.02
2.00
1.00
1.10
3.04
(ppm)

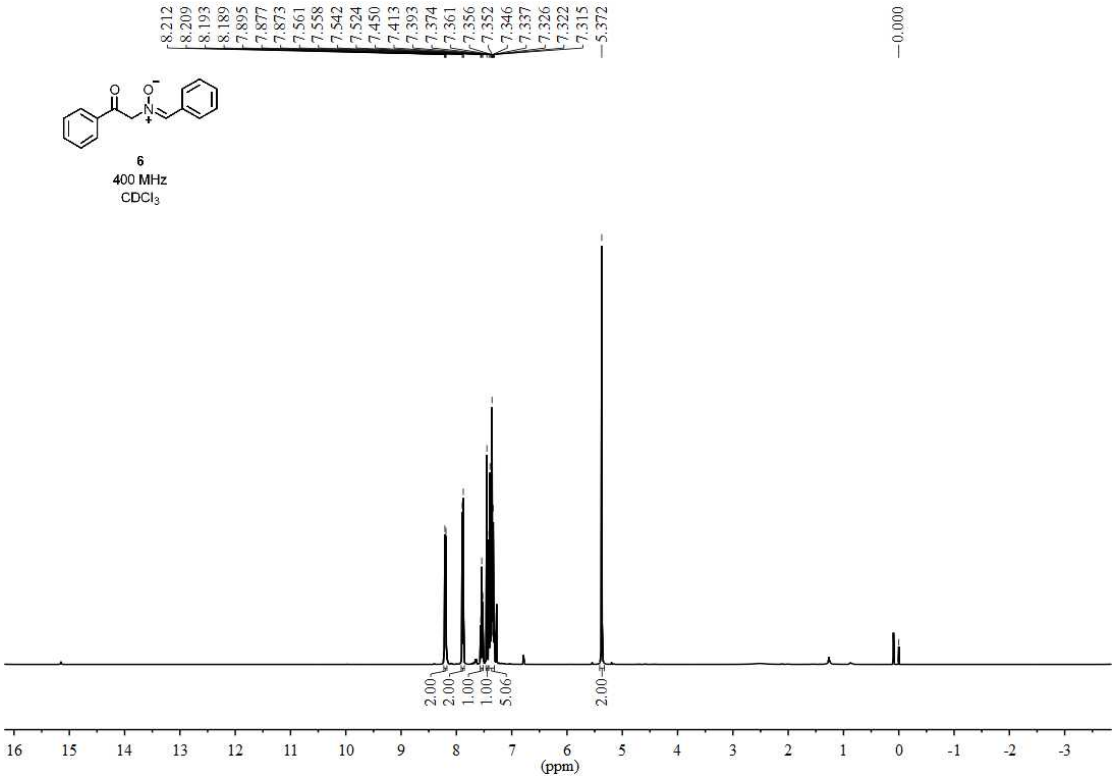

147.90
137.49
135.54
134.93
134.43
130.32
130.28
129.83
129.54
128.69
128.40
128.29
128.27
128.23
128.10
127.42
126.79
77.32
77.00
76.68
20.01
5o
100 MHz
CDCl3
(ppm)

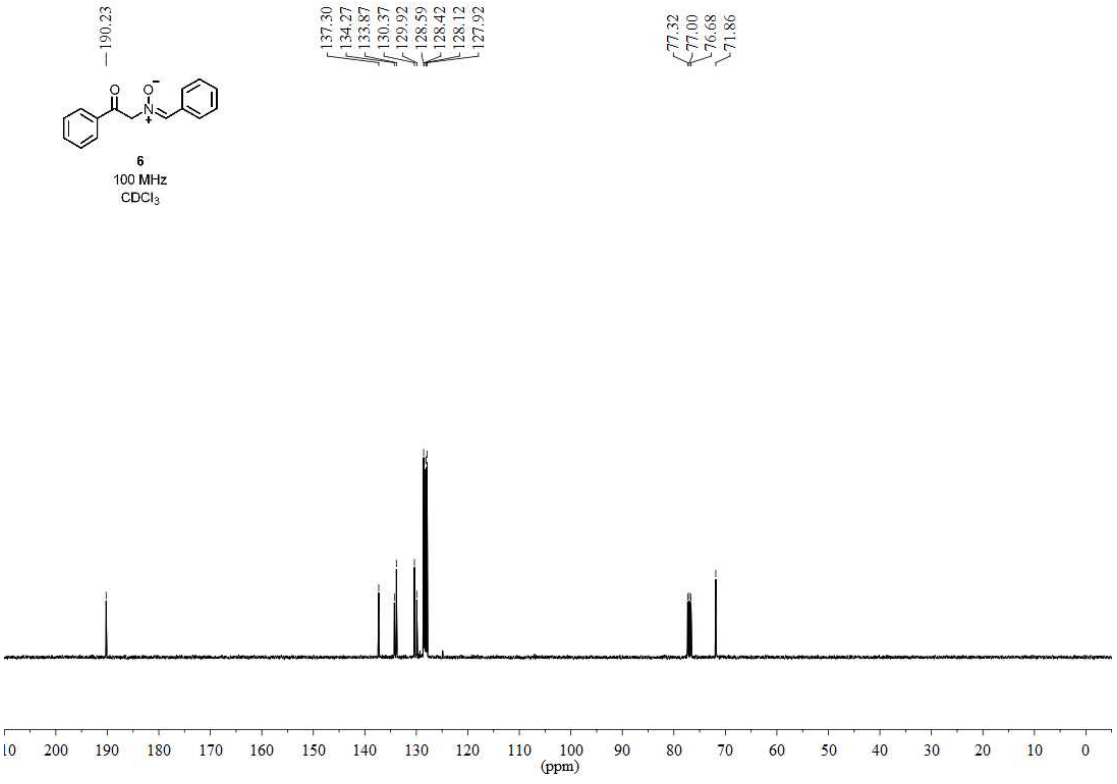

7.483
7.462
7.357
7.352
7.336
7.265
7.261
7.246
7.240
7.232
7.227
7.089
7.081
7.079
7.070
7.065
6.951
6.946
6.802
6.796
6.781
6.776
2.276
0.000
5p
400 MHz
CDCl3
1.03
3.03
6.06
2.01
1.00
1.00
3.00
(ppm)


147.85
139.37
136.21
134.87
133.12
130.27
130.12
129.50
128.70
128.41
128.30
128.23
128.11
127.44
126.97
124.80
77.32
77.00
76.68
22.85
5p
100 MHz
CDCl3
(ppm)


7.332
7.258
7.230
7.218
7.215
7.207
7.202
7.135
7.115
7.093
7.084
7.075
7.070
7.049
7.029
6.991
6.970
2.372
2.300
-0.000
5q
400 MHz
CDCl3
1.00
1.02
1.09
3.03
0.95
1.05
2.01
2.04
2.00
3.01
3.05
(ppm)


148.12
138.38
138.00
134.88
134.58
129.96
128.75
128.59
128.39
128.16
127.95
127.82
127.71
127.16
77.32
77.00
76.68
21.22
21.21
5q
100 MHz
CDCl3
(ppm)


8.212
8.209
8.193
8.189
7.895
7.877
7.873
7.561
7.558
7.542
7.524
7.450
7.413
7.393
7.374
7.361
7.356
7.352
7.346
7.337
7.326
7.322
7.315
5.372
0.000
6
400 MHz
CDCl3
2.00
2.00
1.00
1.00
5.06
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
(ppm)


190.23
137.30
134.27
133.87
130.37
129.92
128.59
128.42
128.12
127.92
77.32
77.00
76.68
71.86
6
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)