Visible-Light-Induced Selectivity Controllable Synthesis of Diamine or Imidazoline Derivatives by Multicomponent Decarboxylative Radical Coupling Reactions

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Contents

I General information:

Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 precoated silica gel plate (0.2 mm thickness). Subsequent to elution, plates were visualized using UV radiation (254 nm) on Spectroline Model ENF-24061/F 254 nm. Further visualization was possible by staining with basic solution of potassium permanganate or acidic solution of ceric molybdate.

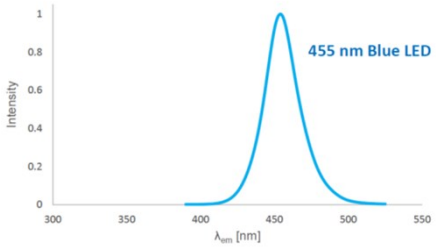
Flash column chromatography was performed using Merck aluminium oxide90 active neutral with freshly distilled solvents. Columns were typically packed as slurry and equilibrated with the appropriate solvent system prior to use.

Proton nuclear magnetic resonance spectra (^{1}H NMR) were recorded on Bruker AMX 500 spectrophotometer ($CDCl_3$ as solvent). Chemical shifts for ^{1}H NMR spectra are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (0.0) and relative to the signal of chloroform-d (7.26, singlet). Multiplicities were given as: s (singlet), d (doublet), t (triplet), dd (doublets of doublet) or m (multiplets). The number of protons (n) for a given resonance is indicated by nH. Coupling constants are reported as a *J* value in Hz. Carbon nuclear magnetic resonance spectra (^{13}C NMR) are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (0.0) and relative to the signal of chloroform-d (77.0, triplet).

Two Blue LEDs (10 W, λ_{max} = 455 nm) were used for irradiation (for emission spectra, see Figure 1). The light source was placed in 3.0 cm distance from the reaction vessel.

The starting materials **1a-1ax, 2a, 2ab-2ai** were all commercial available.

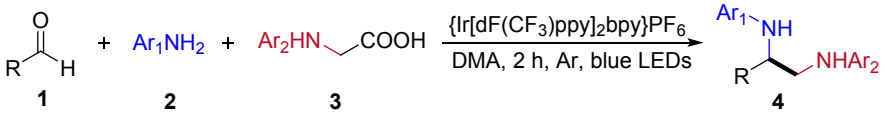
The starting materials **2y-2aa** were prepared according to the literatures reported.[1]



Supplementary Fig. 1. Emission spectra of the used light sources.

II General Procedure

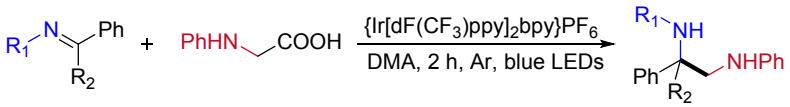
Scheme 1 The general procedure A1 for the production of diamine products.



1 2 3 4

2 (0.2 mmol, 1.0 equiv), **3** (0.6 mmol, 3.0 equiv), $\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$ (0.002 mmol, 1.0 mol%) were added into a 10 mL Schlenk tube. Subsequently, DMA (2 mL) and **1** (0.2 mmol, 1.0 equiv) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere irradiated by blue LEDs (λmax = 455 nm) from a 3.0 cm distance for 2 h at room temperature. The mixture was quenched with water (10 mL) and then extracted with ethyl acetate (5 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 20:1) to afford the desired product **4**.

Scheme 2 The general procedure A2 for the production of **4x**, **4ai**, **4aj**.

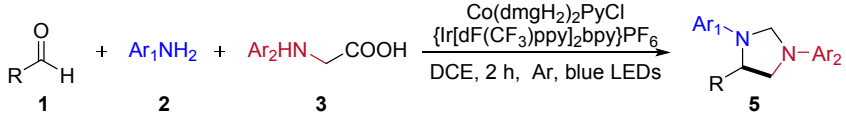


imine **3a** **4**

The starting imines were prepared according to the literature reported.[2]

Corresponding imine (0.2 mmol, 1.0 equiv), **3a** (0.6 mmol, 3.0 equiv), $\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$ (0.002 mmol, 1.0 mol%) were added into a 10 mL Schlenk tube. Subsequently, DMA (2 mL) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere irradiated by blue LEDs (λmax = 455 nm) from a 3.0 cm distance for 2 h at room temperature. The mixture was quenched with water (10 mL) and then extracted with ethyl acetate (5 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 20:1) to afford the desired products **4x, 4ai, 4aj**.

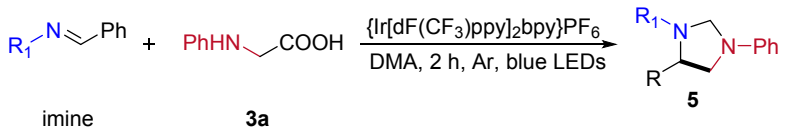
Scheme 3 The general procedure B1 for the production of imidazoline products.



1 2 3 5

2 (0.2 mmol, 1.0 equiv), **3** (0.6 mmol, 3.0 equiv), {Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$ (0.002 mmol, 1.0 mol%), Co(dmgH$_2$)$_2$PyCl (0.03 mmol, 15 mol%) were added into a 10 mL Schlenk tube. Subsequently, DCE (2 mL) and **1** (0.2 mmol, 1.0 equiv) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere irradiated by blue LEDs (λ max = 455 nm) from a 3.0 cm distance for 2 h at room temperature. The mixture was quenched with water (10 mL) and then extracted with ethyl acetate (5 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 50:1) to afford the desired product **5**.

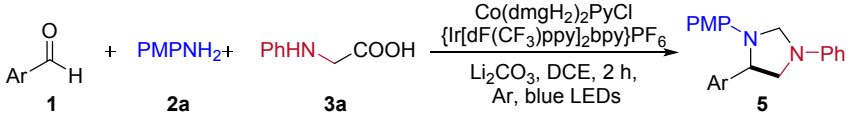
Scheme 4 The general procedure B2 for the production of **5ab**, **5ac**.



The starting imines were prepared according to the literature reported.[2]

Corresponding imine (0.2 mmol, 1.0 equiv), **3a** (0.6 mmol, 3.0 equiv), {Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$ (0.002 mmol, 1.0 mol%), Co(dmgH$_2$)$_2$PyCl (0.03 mmol, 15 mol%) were added into a 10 mL Schlenk tube. Subsequently, DCE (2 mL) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere irradiated by blue LEDs (λ max = 455 nm) from a 3.0 cm distance for 2 h at room temperature. The mixture was quenched with water (10 mL) and then extracted with ethyl acetate (5 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 50:1) to afford the desired product **5ab**, **5ac**.

Scheme 5 The general procedure B3 for the production of **5d**, **5h**, **5j**, **5q**.

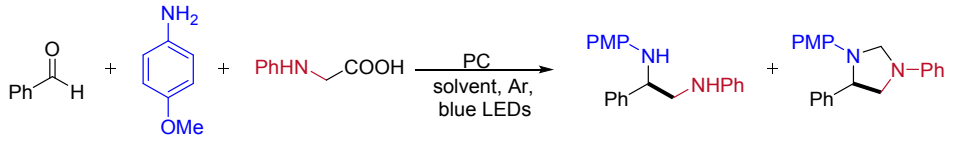


2a (0.2 mmol, 1.0 equiv), **3a** (0.6 mmol, 3.0 equiv), {Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$ (0.002 mmol, 1.0 mol%), Co(dmgH$_2$)$_2$PyCl (0.03 mmol, 15 mol%), Li_2CO_3 (0.04 mmol, 20 mol%) were added into a 10 mL Schlenk tube. Subsequently, DCE (2 mL) and **1** (0.2 mmol, 1.0 equiv) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon

atmosphere irradiated by blue LEDs (λ max = 455 nm) from a 3.0 cm distance for 2 h at room temperature. The mixture was quenched with water (10 mL) and then extracted with ethyl acetate (5 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 50:1) to afford the desired product **5d**, **5h**, **5j**, **5q**.

III Optimization of reaction conditions

Table S1 Reaction condition optimization. [a]

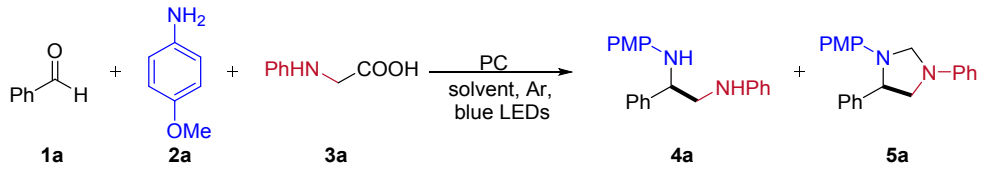


1a **2a** **3a** **4a** **5a**

Entry	PC	Solvent	Yield (%)[b] **4a**/**5a**
1	$Ir(ppy)_3$	DCE	40/22
2	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DCE	49/24
3	$\{Ir[dF(CF_3)ppy]_2dtbbpy\}PF_6$	DCE	30/23
4	$[Ir(ppy)_2dtbbpy]PF_6$	DCE	trace
5	$Ru(bpy)_3(PF_6)_2$	DCE	trace
6	4CzIPN	DCE	42/25
7	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DCM	43/26
8	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	THF	34/22
9	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	MeCN	37/24
10	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	Toluene	16/20
11	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMF	75/13
12	**$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$**	**DMA**	**88/9**
13	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMSO	20/trace
14	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	H_2O	trace
15[c]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	-
16[d]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	72/12
17[e]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	83/14
18[f]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	67/6
19[g]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	81/8
20[h]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	82/16
21[i]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	66/7
22[j]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	83/15
23[k]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	81/17
24[l]	**$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$**	**DMA**	**trace/58**
25	-	DMA	-
26[m]	$\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$	DMA	-

[a]Reaction conditions: **1a** (1.0 equiv, 0.1 mmol), **2a** (1.0 equiv, 0.1 mmol), **3a** (3.0 equiv, 0.3 mmol), PC (1 mol%) in 1 mL solvent, room temperature, 2 h. [b]Yield of isolated product. [c]0 mol% PC. [d]0.5 mol% PC. [e]1.5 mol% PC. [f]1 equiv. **3a**. [g]2 equiv. **3a**. [h]4 equiv. **3a**. [i]30 min. [j]4 h. [k]8 h. [l]under Air. [m]without blue LEDs.

Table S2 Reaction condition optimization. [a]



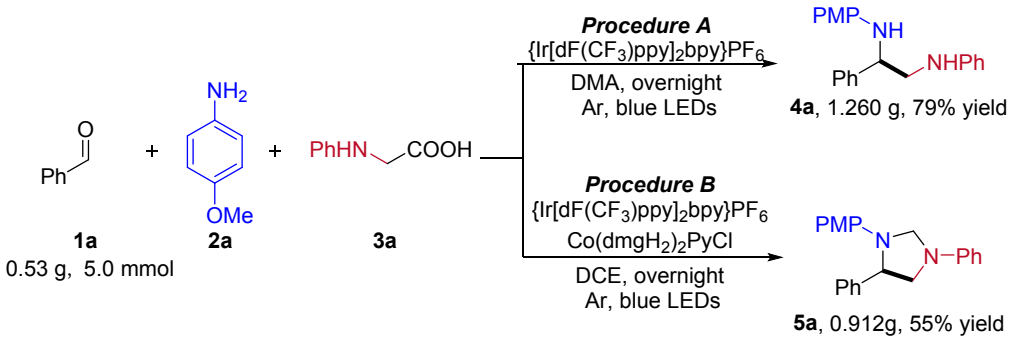
1a **2a** **3a** **4a** **5a**

Entry	PC	Solvent	Additive	Yield (%)[b] **4a**/**5a**
1	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)Cl$_2$	trace/62
2	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$DMAP·Cl	10/68
3	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmg$_3$F$_2$)$_2$(CH$_3$CN)	12/66
4	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	11/70
5	Ir(ppy)$_3$	DCE	Co(dmgH$_2$)$_2$PyCl	17/56
6	{Ir[dF(CF$_3$)ppy]$_2$dtbbpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	15/50
7	[Ir(ppy)$_2$dtbbpy]PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	10/63
8	Ru(bpy)$_3$(PF$_6$)$_2$	DCE	Co(dmgH$_2$)$_2$PyCl	11/52
9	4CzIPN	DCE	Co(dmgH$_2$)$_2$PyCl	14/53
10	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCM	Co(dmgH$_2$)$_2$PyCl	12/68
11	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	THF	Co(dmgH$_2$)$_2$PyCl	9/38
12	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	MeCN	Co(dmgH$_2$)$_2$PyCl	14/44
13	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	Et$_2$O	Co(dmgH$_2$)$_2$PyCl	10/65
14	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	Tolune	Co(dmgH$_2$)$_2$PyCl	trace
15	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DMA	Co(dmgH$_2$)$_2$PyCl	16/44
16	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DMSO	Co(dmgH$_2$)$_2$PyCl	13/36
17[c]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	-
18[d]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	22/32
19[e]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	12/71
20[f]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	18/53
21[g]	**{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$**	**DCE**	**Co(dmgH$_2$)$_2$PyCl**	**trace/74**
22[h]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	trace/74
23[i]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	trace/24
24[j]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	trace/48
25[k]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	trace/76
26[l]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	17/44
27[m]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	trace/74
28[n]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	trace/75
29	-	DCE	Co(dmgH$_2$)$_2$PyCl	-
30[o]	{Ir[dF(CF$_3$)ppy]$_2$bpy}PF$_6$	DCE	Co(dmgH$_2$)$_2$PyCl	-

[a]Reaction conditions: **1a** (1.0 equiv, 0.1 mmol), **2a** (1.0 equiv, 0.1 mmol), **3a** (3.0 equiv, 0.3 mmol), PC (1 mol%), additive (10 mol%) in 1 mL solvent, room temperature, 2 h. [b]Yield of isolated product. [c]0 mol% PC. [d]0.5 mol% PC. [e]1.5 mol% PC. [f]5 mol% [Co]. [g]15 mol% [Co]. [h]20 mol% [Co]. [i]1 equiv. **3a**. [j]2 equiv. **3a**. [k]4 equiv. **3a**. [l]30 min. [m]4 h. [n]8 h. [o]without blue LEDs.

IV Gram-scale reactions and synthetic utility of the reaction.

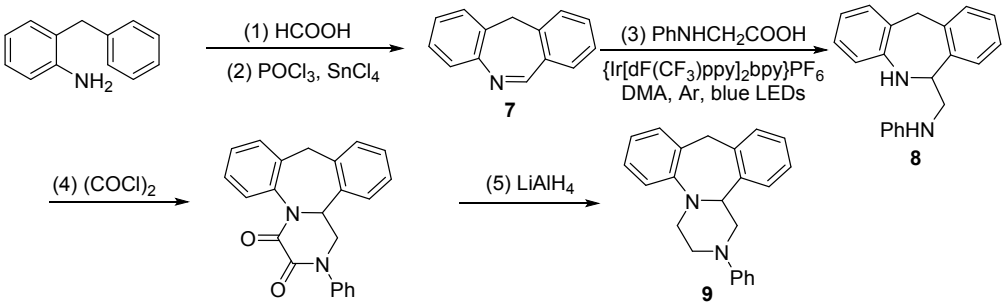
Scheme 6 Gram-scale reactions.



Procedure A : **2a** (5.0 mmol, 1.0 equiv), **3a** (15 mmol, 3.0 equiv), $\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$ (0.005 mmol, 0.1 mol%) were added into a 100 mL round-bottomed flask. Subsequently, DMA (50 mL) and **1a** (5 mmol, 1.0 equiv) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere irradiated by blue LEDs (λmax = 455 nm) from a 3.0 cm distance at room temperature overnight. The mixture was quenched with water (150 mL) and then extracted with ethyl acetate (50 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 20:1) to afford the desired product **4a** (1.260 g, 79% yield).

Procedure B : **2a** (5.0 mmol, 1.0 equiv), **3a** (15 mmol, 3.0 equiv), $\{Ir[dF(CF_3)ppy]_2bpy\}PF_6$ (0.005 mmol, 0.1 mol%), $Co(dmgH_2)_2PyCl$ (0.75 mmol, 15 mol%) were added into a 100 mL round-bottomed flask. Subsequently, DCE (50 mL) and **1a** (5 mmol, 1.0 equiv) was added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere irradiated by blue LEDs (λmax = 455 nm) from a 3.0 cm distance at room temperature overnight. The mixture was quenched with water (150 mL) and then extracted with ethyl acetate (50 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography (PE / EtOAc = 50:1) to afford the desired product **5a** (0.912 g, 55% yield).

Scheme 7 synthetic utility of the reaction.



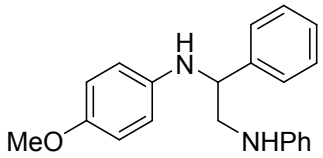
The starting materials **7** were prepared according to the literatures reported.[3,4]

7 (4.0 mmol, 1.0 equiv), {Ir[dF(CF3)ppy]$_2$bpy}PF_6 (0.004 mmol, 0.1 mol%), *N*-phenyl glycine **3a** (8.0 mmol, 3.0 equiv) and DMA (40 mL) were added into a 100 mL round-bottomed flask. The reaction mixture was stirred under an argon atmosphere irradiated by blue LED (λ_{max} = 455 nm) from a 3.0 cm distance overnight at room temperature (The color of reaction solution changed from brown to yellow). The mixture was quenched with water (150 mL), extracted with ethyl acetate (40 mL × 2). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography to afford the desired product **8** as white solid (781.2 mg, 65 % yield).

To a stirred solution of **8** (1.0 mmol, 1.0 equiv) in 5 mL THF was added triethylamine (2.3 mmol) followed by oxalyl chloride (1.1 mmol). After stirring for 30 min at rt, the reaction was diluted with EtOAc and then quenched with 5 mL of sat. aquous $NaHCO_3$. The organic layer was dried over Na_2SO_4 and the solvent removed under reduced pressure. The residue was purified by silica gel column chromatography (PE : EtOAc = 1 : 1) to afford the piperazine-2,3-dione compound as yellow solid (332.9 mg, 94 % yield).

To a stirred solution of LAH (3 mmol) in THF (5 mL) was added the solution of diamide compound (0.5 mmol) in THF (5 mL) dropwise at 0 °C. The resulting suspension was heated on oil bath and refluxed for 5 h. After cooling down to room temperature, the reaction was quenched by the addition of water and 1N NaOH, extracted with ethyl acetate (5 mL × 3). The organic layer was dried over Na_2SO_4 and evaporated in vacuum. The residue was purified by silica gel column chromatography to afford the desired product **9** as white solid.(86.5 mg, 53 % yield).

VI Characterization of products



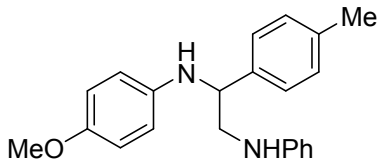
***N*^{1}-(4-methoxyphenyl)-*N*^{2},1-diphenylethane-1,2-diamine (4a)**

Colorless oil, yield (88%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 4H), 7.28 – 7.26 (m, 1H), 7.20 – 7.17 (dd, *J* = 8.3, 7.5 Hz, 2H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.69 – 6.67 (m, 2H), 6.64 (d, *J* = 7.7 Hz, 2H), 6.52 – 6.50 (m, 2H), 4.55 (dd, *J* = 8.1, 4.7 Hz, 1H), 4.05 (s, 2H), 3.68 (s, 3H), 3.48 (dd, *J* = 12.5, 4.7 Hz, 1H), 3.37 (dd, *J* = 12.5, 8.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 147.9, 141.6, 141.2, 129.4, 128.9, 127.6, 126.6, 118.2, 115.1, 114.8, 113.3, 58.4, 55.7, 51.1.

HRMS (ESI+) calcd for $C_{21}H_{23}N_2O$ $(M+H)^+$, m/z 319.1805, found 319.1802.



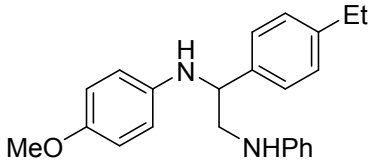
***N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenyl-1-(p-tolyl)ethane-1,2-diamine (4b)**[5]

Colorless oil, yield (75%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.13 (m, 4H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.69 – 6.66 (m, 2H), 6.63 (d, *J* = 7.7 Hz, 2H), 6.52 – 6.47 (m, 2H), 4.51 (dd, *J* = 8.1, 4.7 Hz, 1H), 3.97 (s, 2H), 3.67 (s, 3H), 3.44 (dd, *J* = 12.4, 4.7 Hz, 1H), 3.33 (dd, *J* = 12.4, 8.2 Hz, 1H), 2.32 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 148.0, 141.3, 138.5, 137.2, 129.6, 129.4, 126.5, 118.1, 115.4, 114.8, 113.3, 58.1, 55.8, 51.1, 21.1.

HRMS (ESI+) calcd for $C_{22}H_{25}N_2O$ $(M+H)^+$, m/z 333.1961, found 333.1965.



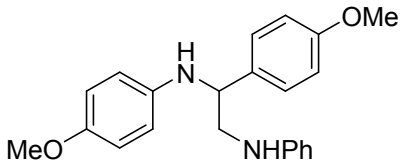
1-(4-ethylphenyl)-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4c)

Colorless oil, yield (80%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.16 (m, 4H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.73 – 6.67 (m, 2H), 6.64 (d, *J* = 7.7 Hz, 2H), 6.52 – 6.49 (m, 2H), 4.53 (dd, *J* = 8.1, 4.7 Hz, 1H), 3.97 (s, 2H), 3.68 (s, 3H), 3.46 (dd, *J* = 12.4, 4.7 Hz, 1H), 3.34 (dd, *J* = 12.4, 8.2 Hz, 1H), 2.63 (q, *J* = 7.6 Hz, 2H), 1.23 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 148.0, 143.5, 141.4, 138.8, 129.4, 128.4, 126.5, 118.1, 115.1, 114.8, 113.3, 58.0, 55.8, 51.1, 28.5, 15.5.

HRMS (ESI+) calcd for $C_{23}H_{27}N_2O$ $(M+H)^+$, m/z 347.2118, found 347.2125.



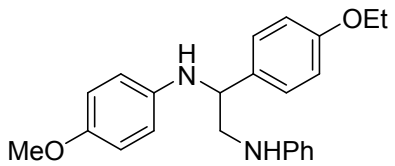
***N*^{1},1-bis(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4d)**

Colorless oil, yield (77%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 2H), 7.19 – 7.16 (m, 2H), 6.89 – 6.86 (m, 2H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.70 – 6.67(m, 2H), 6.63 (d, *J* = 7.7 Hz, 2H), 6.52 – 6.48 (m, 2H), 4.50 (dd, *J* = 8.0, 4.8 Hz, 1H), 3.78 (s, 3H), 3.68 (s, 3H), 3.43 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.34 (dd, *J* = 12.4, 8.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0, 152.3, 148.0, 141.4, 133.5, 129.4, 127.6, 118.1, 115.1, 114.8, 114.3, 113.3, 57.7, 55.8, 55.3, 51.1.

HRMS (ESI+) calcd for $C_{22}H_{25}N_2O_2$ $(M+H)^+$, m/z 349.1911, found 349.1916.



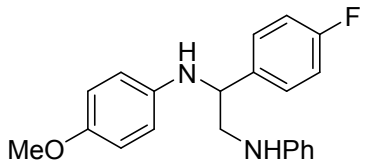
1-(4-ethoxyphenyl)-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4e)

Colorless oil, yield (76%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 2H), 7.19 – 7.16 (m, 2H), 6.88 – 6.85 (m, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.70 – 6.67 (m, 2H), 6.63 (d, *J* = 7.7 Hz, 2H), 6.51 – 6.48 (m, 2H), 4.49 (dd, *J* = 8.0, 4.8 Hz, 1H), 4.00 (q, *J* = 7.0 Hz, 2H), 3.68 (s, 3H), 3.43 (dd, *J* = 12.4, 4.9 Hz, 1H), 3.33 (dd, *J* = 12.4, 8.1 Hz, 1H), 1.39 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 152.3, 148.0, 141.4, 133.4, 129.4, 127.6, 118.1, 115.1, 114.8, 114.8, 113.3, 63.5, 57.7, 55.8, 51.1, 14.9.

HRMS (ESI+) calcd for $C_{23}H_{27}N_2O_2$ $(M+H)^+$, m/z 363.2067, found 363.2062.



1-(4-fluorophenyl)-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4f)

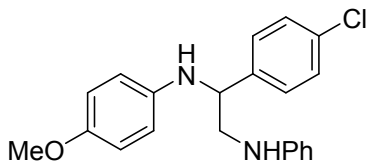
Brown solid, yield (84%), mp. = 109.6 – 110.5 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.19 (dd, *J* = 8.4, 7.5 Hz, 2H), 7.03 (t, *J* = 8.6 Hz, 2H), 6.75 (t, *J* = 7.3 Hz, 1H), 6.70 – 6.67 (m, 2H), 6.64 (d, *J* = 7.7 Hz, 2H), 6.49 – 6.46 (m, 2H), 4.52 (dd, *J* = 8.2, 4.7 Hz, 1H), 3.68 (s, 3H), 3.44 (dd, *J* = 12.6, 4.7 Hz, 1H), 3.34 (dd, *J* = 12.6, 8.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.19 (d, *J* = 244.1 Hz), 152.5, 147.8, 141.0, 137.3 (*J* = 3.0 Hz), 129.4, 128.1 (d, *J* = 8.0 Hz), 118.3, 115.8 (d, *J* = 21.3 Hz), 115.2 114.8, 113.3, 57.8, 55.7, 51.1.

^{19}F NMR (471 MHz, $CDCl_3$) δ -115.03.

HRMS (ESI+) calcd for $C_{21}H_{22}FN_2O$ $(M+H)^+$, m/z 337.1711, found 337.1714.



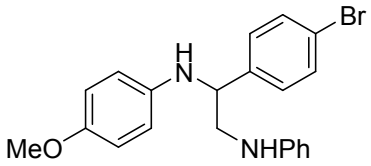
1-(4-chlorophenyl)-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4g)

Yellow oil, yield (57%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 4H), 7.21 – 7.17 (m, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.70 – 6.67 (m, 2H), 6.65 – 6.63 (m, 2H), 6.48 – 6.45 (m, 2H), 4.52 (dd, *J* = 8.2, 4.7 Hz, 1H), 3.69 (s, 3H), 3.45 (dd, *J* = 12.7, 4.7 Hz, 1H), 3.34 (dd, *J* = 12.7, 8.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.4, 146.7, 139.9, 139.2, 132.2, 128.4, 128.0, 126.9, 117.3, 114.1, 113.8, 112.3, 56.7, 54.7, 50.0.

HRMS (ESI+) calcd for $C_{21}H_{22}ClN_2O$ $(M+H)^+$, m/z 353.1415, found 353.1410.



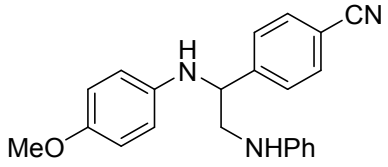
1-(4-bromophenyl)-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4h)

Brown solid, yield (60%), mp. = 118.9 – 119.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ7.47 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.20 – 7.17 (m, 2H), 6.77 – 6.74 (m, 1H), 6.70 – 6.67 (m, 2H), 6.64 (d, *J* = 7.7 Hz, 2H), 6.48 – 6.45 (m, 2H), 4.50 (dd, *J* = 8.1, 4.7 Hz, 1H), 3.69 (s, 3H), 3.44 (dd, *J* = 12.7, 4.7 Hz, 1H), 3.34 (dd, *J* = 12.7, 8.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.5, 147.7, 140.9, 140.8, 132.0, 129.5, 128.3, 121.3, 118.4, 115.2, 114.9, 113.3, 57.9, 55.7, 51.0.

HRMS (ESI+) calcd for $C_{21}H_{22}BrN_2O$ $(M+H)^+$, m/z 397.0910, found 397.0913.



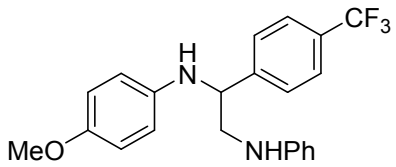
4-(1-((4-methoxyphenyl)amino)-2-(phenylamino)ethyl)benzonitrile (4i)

Yellow oil, yield (81%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.19 (dd, *J* = 8.4, 7.4 Hz, 2H), 6.77 (t, *J* = 7.4 Hz, 1H), 6.70 – 6.67 (m, 2H), 6.67 – 6.62 (m, 2H), 6.45 – 6.41 (m, 2H), 4.58 (dd, *J* = 8.2, 4.7 Hz, 1H), 3.68 (s, 3H), 3.47 (dd, *J* = 12.9, 4.7 Hz, 1H), 3.36 (dd, *J* = 12.9, 8.3 Hz, 1H) .

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.7, 147.627, 147.5, 140.6, 132.7, 129.5, 127.4, 118.8, 118.6, 115.1, 114.9, 113.3, 111.5, 58.2, 55.7, 50.9.

HRMS (ESI+) calcd for $C_{22}H_{22}N_3O$ $(M+H)^+$, m/z 344.1757, found 344.1750.



N^1-(4-methoxyphenyl)-N^2-phenyl-1-(4-(trifluoromethyl)phenyl)ethane-1,2-diamine (4j)

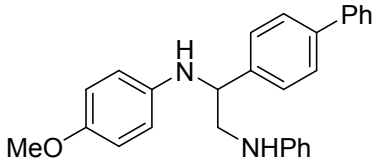
White solid, yield (85%), mp. = 88.7 – 89.2 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.18 (m, 2H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.71 – 6.65 (m, 4H), 6.48 – 6.45 (m, 2H), 4.61 (dd, *J* = 8.2, 4.7 Hz, 1H), 3.69 (s, 3H), 3.49 (dd, *J* = 12.8, 4.7 Hz, 1H), 3.37 (dd, *J* = 12.8, 8.3 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.6, 147.6, 146.0, 140.8, 129.9 (q, *J* = 32.1 Hz),129.5, 127.0, 125.9 (q, *J* = 3.7 Hz), 124.1 (q, *J* = 277.9 Hz), 118.4, 115.1, 114.9, 113.3, 58.1, 55.7, 51.0.

^{19}F NMR (471 MHz, $CDCl_3$) δ -62.42.

HRMS (ESI+) calcd for $C_{22}H_{22}F_3N_2O$ $(M+H)^+$, m/z 387.1679, found 387.1685.



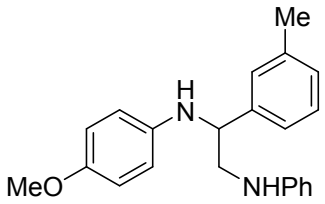
1-([1,1'-biphenyl]-4-yl)-N^1-(4-methoxyphenyl)-N^2-phenylethane-1,2-diamine (4k)

Brown solid, yield (78%), mp. = 62.1 – 63.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 4H), 7.46 – 7.41 (m, 4H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.71 (d, *J* = 8.6 Hz, 2H), 6.67 (d, *J* = 8.3 Hz, 2H), 6.55 – 6.53 (t, *J* = 6.0 Hz, 2H), 4.60 (dd, *J* = 8.1, 4.7 Hz, 1H), 3.69 (s, 3H), 3.52 (dd, *J* = 12.5, 4.7 Hz, 1H), 3.40 (dd, *J* = 12.5, 8.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 147.9, 141.3, 140.8, 140.7, 140.5, 129.4, 128.8, 127.6, 127.4, 127.1, 127.0, 118.2, 115.1, 114.9, 113.4, 58.1, 55.8, 51.1.

HRMS (ESI+) calcd for $C_{27}H_{27}N_2O$ $(M+H)^+$, m/z 395.2118, found 395.2114.



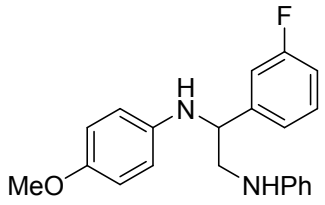
N^1-(4-methoxyphenyl)-N^2-phenyl-1-(m-tolyl)ethane-1,2-diamine (4l)

Colorless oil, yield (62%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (d, *J* = 7.4 Hz, 1H), 7.19 – 7.17 (m, 4H), 7.09 (d, *J* = 7.3 Hz, 1H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.70 (d, *J* = 8.9 Hz, 2H), 6.65 (d, *J* = 7.7 Hz, 2H), 6.52 (d, *J* = 8.9 Hz, 2H), 4.51 (dd, *J* = 7.9, 4.8 Hz, 1H), 4.11 (s, 1H), 3.92 (s, 1H), 3.69 (s, 3H), 3.47 (dd, *J* = 12.4, 4.6 Hz, 1H), 3.36 (dd, *J* = 12.3, 8.3 Hz, 1H), 2.35 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 147.9, 141.4, 138.5, 129.4, 128.7, 128.4, 127.2, 123.6, 118.1, 115.0, 114.8, 113.3, 100.0, 58.4, 55.7, 51.1, 21.6.

HRMS (ESI+) calcd for $C_{22}H_{25}N_2O$ $(M+H)^+$, m/z 333.1961, found 333.1966.



1-(3-fluorophenyl)-N^1-(4-methoxyphenyl)-N^2-phenylethane-1,2-diamine (4m)

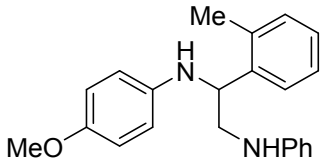
Yellow oil, yield (74%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (td, *J* = 7.9, 5.9 Hz, 1H), 7.20 – 7.16 (m, 3H), 7.12 – 7.09 (m, 1H), 6.97 – 6.93 (m, 1H), 6.77 – 6.74 (m, 1H), 6.70 – 6.67 (m, 2H), 6.65 – 6.63 (m, 2H), 6.49 – 6.46 (m, 2H), 4.52 (dd, *J* = 8.2, 4.6 Hz, 1H), 4.14 (s, 1H), 3.87 (s, 1H), 3.68 (s, 3H), 3.46 (dd, *J* = 12.6, 4.4 Hz, 1H), 3.33 (dd, *J* = 12.5, 8.3 Hz, 1H) .

^{13}C NMR (125 MHz, $CDCl_3$) δ 164.4 (d, *J* = 245.1 Hz), 152.5, 144.8, 144.7 (d, *J* = 6.3 Hz), 141.0, 130.4 (d, *J* = 8.1 Hz), 129.5, 122.2 (d, *J* = 2.7 Hz), 118.4, 115.1, 114.9, 114.62 (d, *J* = 21.1 Hz), 113.5 (d, *J* = 21.7 Hz), 113.4, 58.1~~, 58.1~~, 55.8, 51.0.

^{19}F NMR (471 MHz, $CDCl_3$) δ -112.23.

HRMS (ESI+) calcd for $C_{21}H_{22}FN_2O$ $(M+H)^+$, m/z 337.1711, found 337.1715.



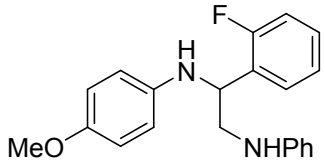
N^1-(4-methoxyphenyl)-N^2-phenyl-1-(o-tolyl)ethane-1,2-diamine (4n)

Colorless oil, yield (61%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.41 (m, 1H), 7.19 – 7.16 (m, 5H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.68 (d, *J* = 8.9 Hz, 2H), 6.64 (d, *J* = 8.4 Hz, 2H), 6.44 (d, *J* = 8.9 Hz, 2H), 4.77 (dd, *J* = 8.4, 4.4 Hz, 1H), 3.68 (s, 3H), 3.44 (dd, *J* = 12.5, 4.4 Hz, 1H), 3.28 (dd, *J* = 12.5, 8.4 Hz, 1H), 2.44 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 148.0, 141.3, 139.2, 135.4, 130.9, 129.4, 127.3, 126.7, 125.5, 118.1, 114.9, 114.8, 113.3, 55.8, 54.8, 49.4, 19.3.

HRMS (ESI+) calcd for $C_{22}H_{25}N_2O$ $(M+H)^+$, m/z 333.1961, found 333.1957.



1-(2-fluorophenyl)-N^1-(4-methoxyphenyl)-N^2-phenylethane-1,2-diamine (4o)

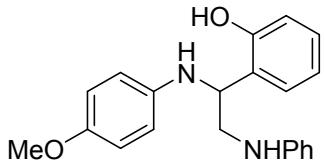
Yellow oil, yield (74%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (td, *J* = 7.7, 1.7 Hz, 1H), 7.24 – 7.21 (m, 1H), 7.19 – 7.16 (m, 2H), 7.09 – 7.05 (m, 2H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.71 – 6.64 (m, 4H), 6.54 – 6.49 (m, 2H), 4.89 (dd, *J* = 8.4, 4.3 Hz, 1H), 4.12 (s, 1H), 3.95 (s, 1H), 3.67 (s, 3H), 3.57 (dd, *J* = 12.6, 4.1 Hz, 1H), 3.34 (dd, *J* = 12.6, 8.5 Hz, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 160.9 (d, *J* = 243.6 Hz), 152.6, 147.9, 141.0, 129.4, 129.0 (d, *J* = 8.3 Hz), 128.3 (d, *J* = 13.2 Hz), 128.2 (d, *J* = 4.6 Hz), 124.6 (d, *J* = 3.3 Hz), 118.16, 115.8 (d, *J* = 21.7 Hz), 114.9, 113.3, 55.7, 52.9, 49.4.

^{19}F NMR (471 MHz, $CDCl_3$) δ -119.25.

HRMS (ESI+) calcd for $C_{21}H_{22}FN_2O$ $(M+H)^+$, m/z 337.1711, found 337.1708.



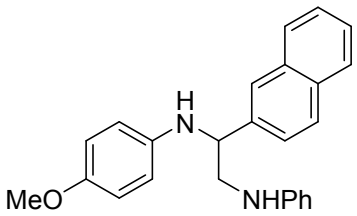
2-(1-((4-methoxyphenyl)amino)-2-(phenylamino)ethyl)phenol (4p)

Colorless oil, yield (72%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 – 7.13 (m, 3H), 7.13 (d, *J* = 7.5 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.79 (t, *J* = 7.3 Hz, 1H), 6.74 – 6.69 (m, 6H), 4.42 (dd, *J* = 9.8, 4.5 Hz, 1H), 3.68 (s, 3H), 3.58 (dd, *J* = 13.5, 10.0 Hz, 1H), 3.45 (dd, *J* = 13.5, 4.6 Hz, 1H) .

^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 154.8, 147.5, 140.0, 129.5, 129.1, 128.2, 124.0, 120.1, 118.9, 118.7, 117.3, 114.7, 113.7, 61.5, 55.6, 49.1.

HRMS (ESI+) calcd for $C_{21}H_{23}N_2O_2$ $(M+H)^+$, m/z 335.1754, found 335.1758.



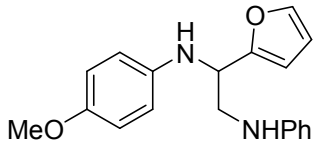
***N*^{1}-(4-methoxyphenyl)-1-(naphthalen-2-yl)-*N*^{2}-phenylethane-1,2-diamine (4q)**

Brown solid, yield (75%), mp. = 68.6 – 70.2 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 – 7.79 (m, 4H), 7.51 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.48 – 7.43 (m, 2H), 7.20 – 7.17 (m, 2H), 6.75 (t, *J* = 7.3 Hz, 1H), 6.67 – 6.64 (m, 4H), 6.55 – 6.52 (m, 2H), 4.70 (dd, *J* = 8.0, 4.8 Hz, 1H), 3.66 (s, 3H), 3.55 (dd, *J* = 12.6, 4.8 Hz, 1H), 3.44 (dd, *J* = 12.6, 8.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 147.9, 141.3, 139.2, 133.5, 133.1, 129.4, 128.8, 127.9, 127.8, 126.3, 125.9, 125.5, 124.6, 118.2, 115.2, 114.9, 113.4, 58.5, 55.7, 51.0.

HRMS (ESI+) calcd for $C_{25}H_{25}N_2O$ $(M+H)^+$, m/z 369.1961, found 369.1966.



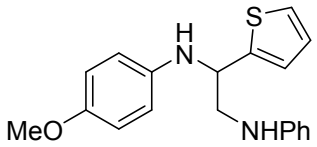
1-(furan-2-yl)-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4r)

Yellow oil, yield (60%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 1.7, 0.7 Hz, 1H), 7.18 (dd, *J* = 8.5, 7.4 Hz, 2H), 6.75 – 6.73 (m, 3H), 6.66 – 6.59 (m, 4H), 6.30 (dd, *J* = 3.2, 1.8 Hz, 1H), 6.21 (d, *J* = 3.2 Hz, 1H), 4.67 (dd, *J* = 7.1, 5.2 Hz, 1H), 3.72 (s, 3H), 3.62 (dd, *J* = 12.6, 5.1 Hz, 1H), 3.46 (dd, *J* = 12.6, 7.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 153.3, 151.8, 146.8, 141.0, 139.9, 128.3, 117.0, 114.6, 113.8, 112.4, 109.3, 106.0, 54.7, 51.8, 46.8.

HRMS (ESI+) calcd for $C_{19}H_{21}N_2O_2$ $(M+H)^+$, m/z 309.1598, found 359.1589.



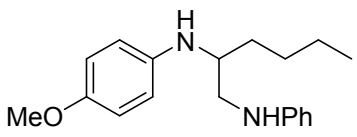
***N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenyl-1-(thiophen-2-yl)ethane-1,2-diamine (4s)**

Yellow oil, yield (62%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 – 7.18 (m, 3H), 7.01 – 7.00 (m, 1H), 6.98 – 6.97 (m, 1H), 6.77 – 6.72 (m, 3H), 6.67 – 6.65 (m, 2H), 6.62 – 6.59 (m, 2H), 4.85 (dd, *J* = 7.2, 5.1 Hz, 1H), 3.72 (s, 3H), 3.58 (dd, *J* = 12.6, 5.1 Hz, 1H), 3.49 (dd, *J* = 12.6, 7.4 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.8, 147.7, 146.5, 140.9, 129.4, 127.1, 124.4, 124.2, 118.2, 115.5, 114.8, 113.4, 55.7, 54.7, 50.9.

HRMS (ESI+) calcd for $C_{19}H_{21}N_2OS$ $(M+H)^+$, m/z 325.1369, found 325.1366.



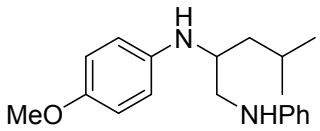
***N*^{2}-(4-methoxyphenyl)-*N*^{1}-phenylhexane-1,2-diamine (4t)**

Colorless oil, yield (51%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (dd, *J* = 8.3, 7.5 Hz, 2H), 6.79 – 6.76 (m, 2H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.62 – 6.59 (m, 4H), 3.75 (s, 3H), 3.51 (dt, *J* = 10.9, 6.5 Hz, 1H), 3.53 – 3.50 (dd, *J* = 12.2, 4.4 Hz, 1H), 3.01 (dd, *J* = 12.2, 7.6 Hz, 1H), 1.61 – 1.55 (m, 2H), 1.39 – 1.30 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H) .

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 148.5, 141.9, 129.3, 117.6, 115.1, 115.0, 113.1, 55.8, 54.3, 48.0, 33.5, 28.3, 22.8, 14.0.

HRMS (ESI+) calcd for $C_{19}H_{27}N_2O$ $(M+H)^+$, m/z 299.2118, found 299.2122.



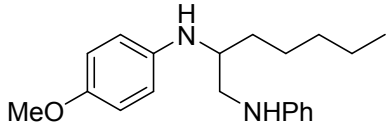
***N*^{2}-(4-methoxyphenyl)-4-methyl-*N*^{1}-phenylpentane-1,2-diamine (4u)**

Colorless oil, yield (54%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (t, *J* = 7.7 Hz, 2H), 6.77 (d, *J* = 8.8 Hz, 2H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.62 – 6.60 (m, 4H), 3.75 (s, 3H), 3.61 – 3.56 (m, 1H), 3.36 (dd, *J* = 12.2, 4.3 Hz, 1H), 2.98 (dd, *J* = 12.2, 7.3 Hz, 1H), 1.79 – 1.73 (m, 1H), 1.53 – 1.36 (m, 1H), 1.42 – 1.36 (m, 1H), 0.95 (d, *J* = 6.6 Hz, 3H), 0.90 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 148.5, 141.9, 129.3, 117.6, 115.0, 115.0, 113.2, 55.8, 52.5, 48.3, 43.5, 25.1, 22.9, 22.8.

HRMS (ESI+) calcd for $C_{19}H_{27}N_2O$ $(M+H)^+$, m/z 299.2118, found 299.2125.



***N*^{2}-(4-methoxyphenyl)-*N*^{1}-phenyloctane-1,2-diamine (4v)**

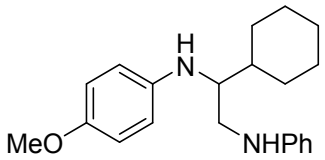
Colorless oil, yield (48%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (t, *J* = 7.9 Hz, 2H), 6.79 – 6.76 (m, 2H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.62 – 6.60 (m, 4H), 3.75 (s, 3H), 3.53 – 3.49 (m, 1H), 3.36 (dd, *J* = 12.2, 4.4 Hz, 1H), 3.01 (dd, *J* = 12.2,

7.6 Hz, 1H), 1.62 – 1.51 (m, 2H), 1.42 – 1.36 (m, 2H), 1.30 – 1.25 (m, 4H), 0.87 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.3, 147.4, 140.9, 128.2, 116.5, 114.1, 114.0, 112.1, 54.8, 53.4, 46.9, 32.7, 30.9, 24.8, 21.6, 13.0.

HRMS (ESI+) calcd for $C_{20}H_{29}N_2O$ $(M+H)^+$, m/z 313.2274, found 313.2270.



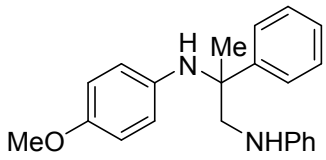
1-cyclohexyl-*N*^{1}-(4-methoxyphenyl)-*N*^{2}-phenylethane-1,2-diamine (4w)

Colorless oil, yield (43%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 – 7.14 (m, 2H), 6.78 – 6.75 (m, 2H), 6.72 – 6.69 (m, 1H), 6.62 – 6.57 (m, 4H), 3.75 (s, 3H), 3.38 (dt, *J* = 8.5, 4.0 Hz, 2H), 2.96 (dd, *J* = 12.8, 9.6 Hz, 1H), 1.83 – 1.73(m, 4H), 1.69 – 1.56 (m, 2H), 1.26 – 1.07 (m, 5H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 148.6, 142.6, 129.2, 117.5, 115.0, 114.9, 113.2, 59.0, 55.8, 45.6, 41.1, 29.7, 29.2, 26.5, 26.4, 26.4.

HRMS (ESI+) calcd for $C_{21}H_{29}N_2O$ $(M+H)^+$, m/z 325.2274, found 325.2270.



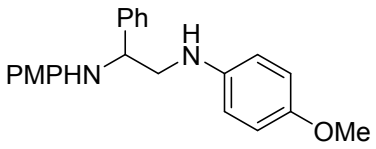
***N*^{2}-(4-methoxyphenyl)-*N*^{1},2-diphenylpropane-1,2-diamine (4x)**

Colorless oil, yield (61%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.52 (m, 2H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.3 Hz, 1H), 7.19 – 7.16 (m, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.66 – 6.61 (m, 4H), 6.39 – 6.35 (m, 2H), 3.68 (s, 3H), 3.43 (d, *J* = 1.6 Hz, 2H), 1.71 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 148.3, 144.8, 139.4, 129.3, 128.7, 127.0, 126.3, 118.0, 117.7, 114.4, 113.4, 59.1, 55.6, 29.7, 24.7.

HRMS (ESI+) calcd for $C_{22}H_{25}N_2S$ $(M+H)^+$, m/z 333.1961, found 333.1966.



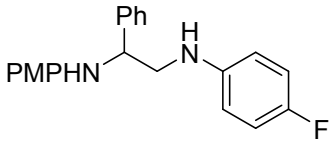
N^1,N^2-bis(4-methoxyphenyl)-1-phenylethane-1,2-diamine (4y)

Colorless oil, yield (62%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 4H), 7.28 – 7.25 (m, 1H), 6.80 – 6.77 (m, 2H), 6.69 – 6.67 (m, 2H), 6.62 – 6.60 (m, 2H), 6.51 – 6.48 (m, 2H), 4.53 (dd, *J* = 8.1, 4.6 Hz, 1H), 3.74 (s, 3H), 3.68 (s, 3H), 3.43 (dd, *J* = 12.4, 4.6 Hz, 1H), 3.31 (dd, *J* = 12.4, 8.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.6, 152.3, 142.0, 141.8, 141.4, 128.9, 127.5, 126.6, 115.1, 115.0, 114.8, 114.8, 58.3, 55.8, 55.7, 52.1.

HRMS (ESI+) calcd for $C_{22}H_{25}N_2O_2$ $(M+H)^+$, m/z 349.1911, found 349.1915.



N^2-(4-fluorophenyl)-N^1-(4-methoxyphenyl)-1-phenylethane-1,2-diamine (4z)

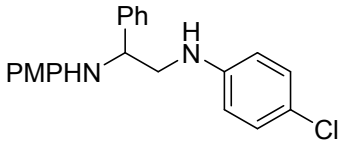
White solid, yield (74%), mp. = 71.7 – 72.8 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.33 (m, 4H), 7.29 – 7.25 (m, 1H), 6.91 – 6.86 (m, 2H), 6.70 – 6.67 (m, 2H), 6.58 – 6.54 (m, 2H), 6.52 – 6.49 (m, 2H), 4.54 (dd, *J* = 8.1, 4.7 Hz, 1H), 4.12 (s, 1H), 3.80 (s, 1H), 3.68 (s, 3H), 3.43 (dd, *J* = 12.4, 4.7 Hz, 1H), 3.30 (dd, *J* = 12.4, 8.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2 (d, *J* = 234.3 Hz), 152.4, 144.2 (d, *J* = 2.0 Hz), 141.5, 141.2, 128.9, 127.6, 126.5, 115.8 (d, *J* = 22.2 Hz), 115.1, 114.8, 114.2 (d, *J* = 7.3 Hz), 58.2, 55.7, 51.7.

^{19}F NMR (471 MHz, $CDCl_3$) δ -127.11.

HRMS (ESI+) calcd for $C_{21}H_{22}FN_2O$ $(M+H)^+$, m/z 337.1711, found 337.1716.



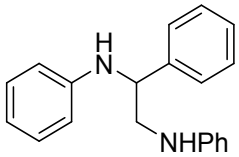
N^2-(4-chlorophenyl)-N^1-(4-methoxyphenyl)-1-phenylethane-1,2-diamine (4aa)

White solid, yield (74%), mp. = 84.4 – 85.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.33 (m, 4H), 7.30 – 7.26 (m, 1H), 7.13 – 7.10 (m, 2H), 6.71 – 6.68 (M, 2H), 6.55 – 6.49 (m, 4H), 4.55 (dd, *J* = 8.1, 4.8 Hz, 1H), 3.95 (s, 2H), 3.69 (s, 3H), 3.44 (dd, *J* = 12.5, 4.8 Hz, 1H), 3.33 (dd, *J* = 12.5, 8.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 146.5, 141.4, 141.1, 129.2, 128.9, 127.7, 126.5, 122.7, 115.1, 114.9, 114.4, 58.2, 55.7, 51.1.

HRMS (ESI+) calcd for $C_{21}H_{22}ClN_2O$ $(M+H)^+$, m/z 353.1415, found 353.1412.



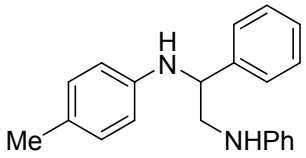
N^1,N^2,1-triphenylethane-1,2-diamine (4ab)

White solid, yield (92%), mp. = 87.4 – 87.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.39 (m, 2H), 7.37 – 7.34 (m, 2H), 7.29 – 7.26 (m, 1H), 7.21 – 7.17 (m, 2H), 7.11 – 7.08 (m, 2H), 6.76 – 6.73 (t, *J* = 7.3 Hz, 1H), 6.69 – 6.64 (m, 3H), 6.55 – 6.54 (dd, *J* = 8.5, 0.9 Hz, 2H), 4.64 (dd, *J* = 7.9, 4.8 Hz, 1H), 4.40 (s, 1H), 3.85 (s, 1H), 3.51 (dd, *J* = 12.5, 4.7 Hz, 1H), 3.39 (dd, *J* = 12.5, 8.0 Hz, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.8, 147.1, 141.4, 129.4, 129.2, 128.9, 127.6, 126.5, 118.2, 117.9, 113.7, 113.3, 57.4, 51.0

HRMS (ESI+) calcd for $C_{20}H_{21}N_2$ $(M+H)^+$, m/z 289.1699, found 289.1696.



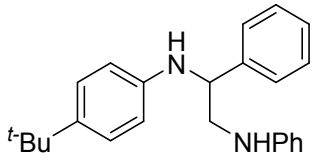
N^2,1-diphenyl-N^1-(p-tolyl)ethane-1,2-diamine (4ac)

White solid, yield (64%), mp. = 75.3 – 77.0 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.32 (m, 4H), 7.28 – 7.25 (m, 1H), 7.22 – 7.16 (m, 2H), 6.90 (d, *J* = 8.1 Hz, 2H), 6.75 – 6.72 (m, 1H), 6.63 (d, *J* = 8.4 Hz, 2H), 6.46 (d, *J* = 8.1 Hz, 2H), 4.60 (dd, *J* = 8.0, 4.7 Hz, 1H), 4.21 (s, 1H), 3.91 (s, 1H), 3.48 (dd, *J* = 12.5, 4.6 Hz, 1H), 3.36 (dd, *J* = 12.4, 8.1 Hz, 1H), 2.18 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.9, 144.9, 141.6, 129.7, 129.4, 128.9, 127.6, 127.1, 126.5, 118.2, 113.9, 113.3, 57.7, 51.0, 20.4.

HRMS (ESI+) calcd for $C_{21}H_{23}N_2$ $(M+H)^+$, m/z 303.1856, found 303.1848.



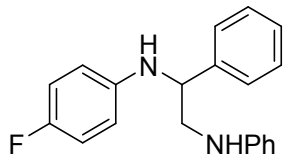
***N*^{1}-(4-(tert-butyl)phenyl)-*N*^{2},1-diphenylethane-1,2-diamine (4ad)**

Colorless oil, yield (66%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 2H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 7.17 (t, *J* = 7.9 Hz, 2H), 7.13 – 7.11 (m, 2H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.63 – 6.61 (m, 2H), 6.51 – 6.49 (m, 2H), 4.59 (dd, *J* = 8.2, 4.7 Hz, 1H), 3.46 (dd, *J* = 12.5, 4.7 Hz, 1H), 3.36 (dd, *J* = 12.5, 8.3 Hz, 1H), 1.23 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.9, 144.9, 141.7, 140.7, 129.4, 128.9, 127.6, 126.6, 126.0, 118.2, 113.5, 113.3, 57.8, 51.1, 33.9, 31.6.

HRMS (ESI+) calcd for $C_{24}H_{29}N_2$ $(M+H)^+$, m/z 345.2325, found 345.2328.



***N*^{1}-(4-fluorophenyl)-*N*^{2},1-diphenylethane-1,2-diamine (4ae)**

Brown solid, yield (62%), mp. = 75.3 – 77.0 °C;

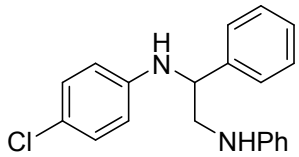
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 4H), 7.23 – 7.19 (m, 1H), 7.13 – 7.10 (m, 2H), 6.73 – 6.66

(m, 3H), 6.57 (d, *J* = 7.7 Hz, 2H), 6.39 – 6.37 (m, 2H), 4.48 (dd, *J* = 8.0, 4.7 Hz, 1H), 3.42 (dd, *J* = 12.6, 4.7 Hz, 1H), 3.30 (dd, *J* = 12.6, 8.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9 (d, *J* = 234.2 Hz), 147.8, 143.5 (d, *J* = 1.8 Hz), 141.2, 129.4, 129.0, 127.7, 126.5, 118.3, 115.7 (d, *J* = 22.2 Hz), 114.7 (d, *J* = 7.4 Hz), 113.4, 58.1, 51.0.

^{19}F NMR (471 MHz, $CDCl_3$) δ -127.46.

HRMS (ESI+) calcd for $C_{20}H_{20}FN_2$ $(M+H)^+$, m/z 307.1605, found 307.1606.



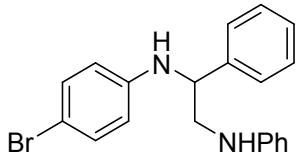
***N*^{1}-(4-chlorophenyl)-*N*^{2},1-diphenylethane-1,2-diamine (4af)**

Brown solid, yield (50%), mp. = 81.1 – 82.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.36 (m, 4H), 7.31 – 7.28 (m, 1H), 7.21 – 7.18 (m, 2H), 7.04 – 7.01 (m, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.65 (d, *J* = 7.8 Hz, 2H), 6.46 – 6.43 (m, 2H), 4.59 (dd, *J* = 7.6, 4.8 Hz, 1H), 4.45 (s, 1H), 3.80 (s, 1H), 3.52 (dd, *J* = 12.6, 4.7 Hz, 1H), 3.40 (dd, *J* = 12.6, 7.8 Hz, 1H) .

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.7, 145.7, 140.8, 129.4, 129.0, 127.8, 126.4, 122.5, 118.4, 114.9, 113.4, 57.6, 50.9.

HRMS (ESI+) calcd for $C_{20}H_{20}ClN_2$ $(M+H)^+$, m/z 323.1310, found 323.1316.



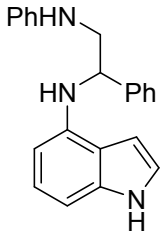
***N*^{1}-(4-bromophenyl)-*N*^{2},1-diphenylethane-1,2-diamine (4ag)**

White solid, yield (36%), mp. = 88.7 – 90.1 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 4.5 Hz, 4H), 7.31 – 7.27 (m, 1H), 7.21 – 7.15 (m, 4H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 2H), 6.41 (d, *J* = 8.8 Hz, 2H), 4.58 (dd, *J* = 7.6, 4.8 Hz, 1H), 3.53 (dd, *J* = 12.6, 4.7 Hz, 1H), 3.40 (dd, *J* = 12.6, 7.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.7, 146.1, 140.7, 131.9, 129.4, 129.0, 127.8, 126.4, 118.4, 115.3, 113.4, 109.5, 57.5, 50.9.

HRMS (ESI+) calcd for $C_{20}H_{20}BrN_2$ $(M+H)^+$, m/z 367.0804, found 367.0808.



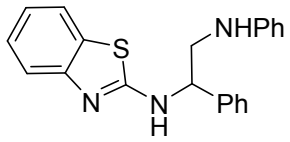
***N*^{1}-(1H-indol-4-yl)-*N*^{2},1-diphenylethane-1,2-diamine (4ah)**

White solid, yield (80%), mp. = 67.8 – 69.6 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.45 – 7.44 (m, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 – 7.25 (m, 1H), 7.21 – 7.18 (m, 2H), 7.08 – 7.07 (m, 1H), 6.92 – 6.89 (m, 1H), 6.78 – 6.74 (m, 2H), 6.67 (d, *J* = 8.4 Hz, 2H), 6.47 – 6.47 (m, 1H), 6.06 (d, *J* = 7.7 Hz, 1H), 4.82 (dd, *J* = 7.9, 4.7 Hz, 1H), 3.60 (dd, *J* = 12.5, 4.7 Hz, 1H), 3.50 (dd, *J* = 12.5, 8.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.0, 141.6, 140.1, 136.4, 129.4, 128.9, 127.5, 126.5, 123.4, 122.1, 118.1, 117.0, 113.4, 101.7, 101.1, 98.7, 57.7, 51.1.

HRMS (ESI+) calcd for $C_{22}H_{22}N_3$ $(M+H)^+$, m/z 328.1808, found 328.1804.



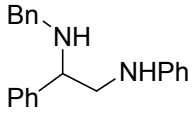
***N*^{1}-(benzo[d]thiazol-2-yl)-*N*^{2},1-diphenylethane-1,2-diamine (4ai)**

Yellow oil, yield (93%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.50 (m, 2H), 7.45 – 7.39 (m, 4H), 7.36 – 7.33 (m, 1H), 7.25 – 7.23 (m, 1H), 7.20 – 7.17 (m, 2H), 7.08 – 7.05 (m, 1H), 6.75 (t, *J* = 7.4 Hz, 1H), 6.67 – 6.65 (m, 2H), 5.01 – 4.99 (m, 1H), 3.63 – 3.62 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 167.5, 151.8, 147.4, 139.5, 130.7, 129.4, 129.0, 128.2, 126.7, 126.0, 121.8, 120.9, 119.0, 118.3, 113.3, 59.0, 50.1.

HRMS (ESI+) calcd for $C_{21}H_{20}N_3S$ $(M+H)^+$, m/z 346.1372, found 346.1380.



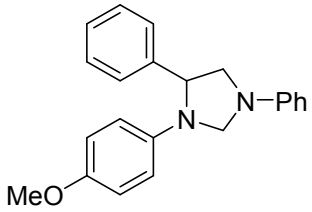
N^1-benzyl-N^2,1-diphenylethane-1,2-diamine (4aj)[6]

Colorless oil, yield (43%);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 5H), 7.32 – 7.21 (m, 5H), 7.14 (t, *J* = 7.6 Hz, 2H), 6.69 (t, *J* = 7.3 Hz, 1H), 6.62 (d, *J* = 8.0 Hz, 2H), 4.25 (s, 2H), 3.99 (dd, *J* = 8.4, 4.8 Hz, 1H), 3.86 (d, *J* = 13.2 Hz, 1H), 3.63 – 3.51 (m, 2H), 3.41 (dd, *J* = 13.4, 4.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 148.1, 141.8, 140.2, 129.3, 128.8, 128.4, 128.2, 127.7, 127.3, 127.0, 117.7, 113.2, 61.4, 51.3, 50.7.

HRMS (ESI+) calcd for $C_{21}H_{23}N_2$ $(M+H)^+$, m/z 303.1856, found 303.1860.



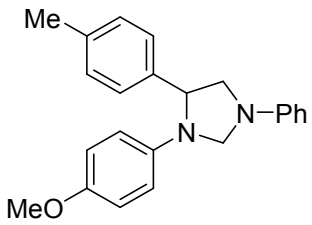
3-(4-methoxyphenyl)-1,4-diphenylimidazolidine (5a)

White solid, yield (74%), mp. = 102.8 – 104.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.35 (m, 2H), 7.33 – 7.23 (m, 5H), 6.82 – 6.76 (m, 3H), 6.68 – 6.65 (m, 2H), 6.57 – 6.54 (m, 2H), 5.16 (d, *J* = 3.1 Hz, 1H), 4.90 (dd, *J* = 7.3, 5.0 Hz, 1H), 4.69 (d, *J* = 3.1 Hz, 1H), 3.93 (dd, *J* = 8.6, 7.3 Hz, 1H), 3.71 (s, 3H), 3.49 (dd, *J* = 8.7, 5.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.2, 146.4, 142.3, 140.1, 129.3, 128.8, 127.5, 126.2, 118.0, 114.8, 114.3, 112.9, 68.5, 62.4, 56.3, 55.7.

HRMS (ESI+) calcd for $C_{22}H_{23}N_2O$ $(M+H)^+$, m/z 331.1805, found 331.1806.



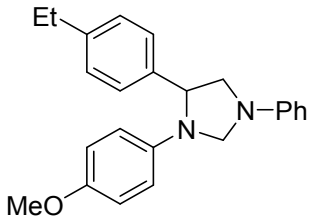
3-(5-methoxyphenyl)-1-phenyl-4-(m-tolyl)imidazolidine (5b)

White solid, yield (57%), mp. = 66.8 – 68.6 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 4H), 7.13 – 7.12 (d, *J* = 7.9 Hz, 2H), 6.82 – 6.76 (m, 3H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.58 – 6.55 (dd, *J* = 9.7, 2.8 Hz, 2H), 5.15 (d, *J* = 3.1 Hz, 1H), 4.87 (dd, *J* = 7.0, 5.2 Hz, 1H), 4.68 (d, *J* = 3.1 Hz, 1H), 3.91 (dd, *J* = 8.4, 7.5 Hz, 1H), 3.71 (s, 3H), 3.46 (dd, *J* = 8.6, 5.1 Hz, 1H), 2.32 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 146.5, 140.2, 139.3, 137.1, 129.5, 129.3, 126.2, 117.9, 114.8, 114.3, 112.9, 68.5, 62.2, 56.4, 55.7, 21.1.

HRMS (ESI+) calcd for $C_{23}H_{25}N_2O$ $(M+H)^+$, m/z 345.1961, found 345.1956.



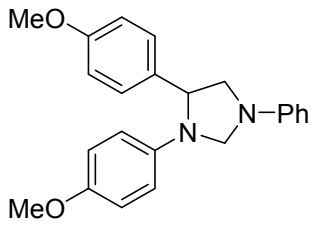
4-(4-ethylphenyl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5c)

White solid, yield (52%), mp. = 75.7 – 77.6 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.25 (m, 4H), 7.14 (d, *J* = 7.9 Hz, 2H), 6.81 – 6.77 (m, 3H), 6.66 – 6.65 (m, 2H), 6.58 – 6.56 (m, 2H), 5.15 (d, *J* = 3.1 Hz, 1H), 4.87 (dd, *J* = 7.0, 5.2 Hz, 1H), 4.68 (d, *J* = 3.1 Hz, 1H), 3.92 – 3.89 (m, 1H), 3.71 (s, 3H), 3.48 (dd, *J* = 8.6, 5.0 Hz, 1H), 2.62 (q, *J* = 7.6 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 146.5, 143.5, 140.3, 139.5, 129.3, ~~129.0,~~ 128.3, 126.2, 117.9, 114.8, 114.3, 112.9, 68.5, 62.2, 56.4, 55.7, 28.5, 15.5.

HRMS (ESI+) calcd for $C_{24}H_{27}N_2O$ $(M+H)^+$, m/z 359.2118, found 359.2110



3,4-bis(4-methoxyphenyl)-1-phenylimidazolidine (5d)

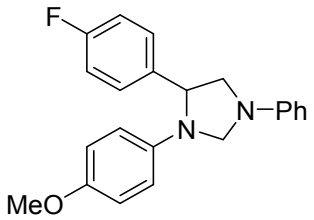
White solid, yield (75%), mp. = 104.6 – 106.5 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 4H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.82 – 6.76 (m, 3H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.59 – 6.55 (m, 2H), 5.15 (d, *J* = 3.1 Hz, 1H), 4.86 (dd, *J* = 7.2, 5.1 Hz, 1H), 4.68 (d, *J* = 3.1 Hz, 1H), 3.91 (dd, *J* = 8.5, 7.3 Hz, 1H), 3.78 (s, 3H), 3.72 (s, 3H), 3.46 (dd, *J* = 8.7, 5.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 152.1, 146.4, 140.2, 134.26, 129.3, 127.3, 117.9, 114.8, 114.37, 114.2, 112.8, 68.4, 61.9, 56.4, 55.7, 55.3.

HRMS (ESI+) calcd for $C_{23}H_{25}N_2O_2$ $(M+H)^+$, m/z 361.1911, found 361.1916.

~~HRMS (ESI+) calcd for $C_{22}H_{22}FN_2O$ $(M+H)^+$, m/z 349.1711, found 349.1717.~~



4-(4-fluorophenyl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5e)

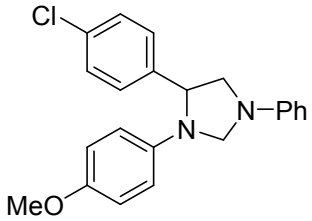
White solid, yield (58%), mp. = 89.9 – 91.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.32 (m, 2H), 7.29 – 7.26 (m, 2H), 7.01 – 6.98 (t, *J* = 8.6 Hz, 2H), 6.83– 6.77 (m, 3H), 6.66 (d, *J* = 7.9 Hz, 2H), 6.54 (d, *J* = 9.0 Hz, 2H), 5.15 (d, *J* = 3.1 Hz, 1H), 4.87 (dd, *J* = 7.0, 5.1 Hz, 1H), 4.66 (d, *J* = 3.1 Hz, 1H), 3.94 – 3.82 (m, 1H), 3.71 (s, 3H), 3.44 (dd, *J* = 8.7, 4.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2 (d, *J* = 244.0 Hz), 152.3, 146.4, 139.9, 138.0 (d, *J* = 3.0 Hz), 129.4, 127.8 (d, *J* = 8.0 Hz), 118.2, 115.8 (d, *J* = 21.3 Hz), 114.9, 114.4, 113.0, 68.5, 61.8, 56.3, 55.7.

^{19}F NMR (470 MHz, $CDCl_3$) δ -115.07.

HRMS (ESI+) calcd for $C_{22}H_{22}FN_2O$ $(M+H)^+$, m/z 349.1711, found 349.1714.



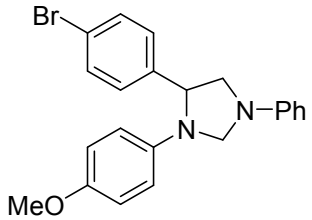
4-(4-chlorophenyl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5f)

White solid, yield (55%), mp. = 129.9 – 130.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 6H), 6.83 – 6.77 (m, 3H), 6.66 (d, *J* = 8.1 Hz, 2H), 6.54 – 6.51 (m, 2H), 5.14 (d, *J* = 3.1 Hz, 1H), 4.85 (dd, *J* = 7.2, 4.9 Hz, 1H), 4.66 (d, *J* = 3.1 Hz, 1H), 3.91 – 3.88 (m, 1H), 3.71 (s, 3H), 3.44 (dd, *J* = 8.7, 4.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 146.3, 140.9, 139.8, 133.2, 129.4, 129.0, 127.7, 118.3, 114.9, 114.4, 113.0, 68.5, 61.8, 56.2, 55.8.

HRMS (ESI+) calcd for $C_{22}H_{22}ClN_2O$ $(M+H)^+$, m/z 365.1415, found 365.1411.



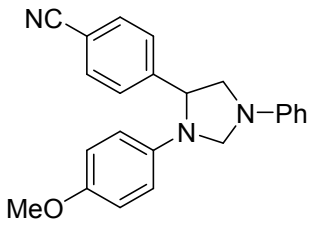
4-(4-bromophenyl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5g)

White solid, yield (53%), mp. = 138.4 – 140.6 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 – 7.43 (m, 2H), 7.30 – 7.25 (m, 4H), 6.84 – 6.77 (m, 3H), 6.66 (d, *J* = 8.2 Hz, 2H), 6.55 – 6.51 (m, 2H), 5.15 (d, *J* = 3.1 Hz, 1H), 4.85 (dd, *J* = 7.2, 4.9 Hz, 1H), 4.67 (d, *J* = 3.1 Hz, 1H), 3.92 – 3.89 (m, 1H), 3.72 (s, 3H), 3.45 (dd, *J* = 8.7, 4.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 146.3, 141.5, 139.8, 132.0, 129.4, 128.0, 121.3, 118.3, 114.9, 114.3, 113.0, 68.4, 61.9, 56.1, 55.7.

HRMS (ESI+) calcd for $C_{22}H_{22}BrN_2O$ (M+H)+, m/z 409.0910, found 409.1913.



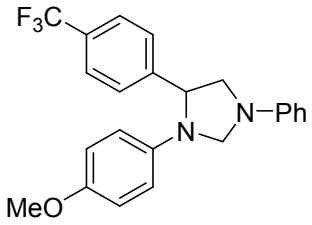
4-(3-(4-methoxyphenyl)-1-phenylimidazolidin-4-yl)benzonitrile (5h)

White solid, yield (74%), mp. = 142.0 – 142.4;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 6.86 – 6.79 (m, 3H), 6.68 (d, *J* = 8.5 Hz, 2H), 6.50 (d, *J* = 8.7 Hz, 2H), 5.18 (d, *J* = 2.8 Hz, 1H), 4.95 (dd, *J* = 7.2, 4.6 Hz, 1H), 4.68 (d, *J* = 2.8 Hz, 1H), 3.94 (t, *J* = 8.0 Hz, 1H), 3.73 (s, 3H), 3.48 (dd, *J* = 8.6, 4.5 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.6, 148.1, 146.2, 139.4, 132.8, 129.4, 127.1, 118.7, 118.6, 115.0, 114.2, 113.1, 111.5, 68.4, 62.0, 55.8, 55.7.

HRMS (ESI+) calcd for $C_{23}H_{22}N_3O$ $(M+H)^+$, m/z 356.1757, found 356.1755.



3-(4-methoxyphenyl)-1-phenyl-4-(4-(trifluoromethyl)phenyl)imidazolidine (5i)

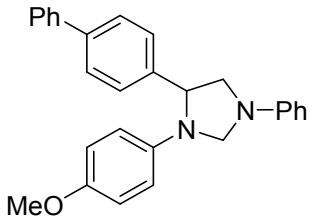
White solid, yield (52%), mp. = 105.7 – 117.1 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.29 (t, *J* = 7.9 Hz, 2H), 6.85 – 6.78 (m, 3H), 6.67 (d, *J* = 8.1 Hz, 2H), 6.54 – 6.51 (m, 2H), 5.19 (d, *J* = 3.1 Hz, 1H), 4.96 (dd, *J* = 7.2, 4.8 Hz, 1H), 4.69 (d, *J* = 3.1 Hz, 1H), 3.94 (dd, *J* = 8.5, 7.6 Hz, 1H), 3.72 (s, 3H), 3.48 (dd, *J* = 8.7, 4.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.4, 145.5, 145.2, 138.6, 128.8 (q, *J* = 32.2 Hz), 128.4, 125.6, 124.8 (q, *J* = 3.8 Hz), 123.1 (q, *J* = 270.4 Hz), 117.4, 113.9, 113.2, 112.0, 67.4, 60.9, 55.0, 54.7.

^{19}F NMR (471 MHz, $CDCl_3$) δ -62.43.

HRMS (ESI+) calcd for $C_{23}H_{21}F_3N_2O$ $(M+H)^+$, m/z 399.1679, found 399.1674.



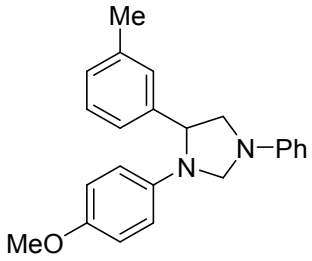
4-([1,1'-biphenyl]-4-yl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5j)

White solid, yield (76%), mp. = 132.9 – 134.1 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.53 (m, 4H), 7.44 – 7.39 (m, 4H), 7.33 – 7.26 (m, 3H), 6.83 – 6.78 (m, 3H), 6.67 (d, *J* = 8.0 Hz, 2H), 6.61 – 6.57 (m, 2H), 5.18 (d, *J* = 3.1 Hz, 1H), 4.93 (dd, *J* = 7.1, 5.1 Hz, 1H), 4.70 (d, *J* = 3.1 Hz, 1H), 3.96 – 3.92 (m, 1H), 3.71 (s, 3H), 3.52 (dd, *J* = 8.7, 5.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.2, 146.5, 141.5, 140.8, 140.5, 140.2, 129.4, 128.8, 127.6, 127.3, 127.1, 126.7, 118.1, 114.9, 114.4, 113.0, 68.5, 62.2, 56.3, 55.8.

HRMS (ESI+) calcd for $C_{28}H_{27}N_2O$ $(M+H)^+$, m/z 407.2118, found 407.2110.



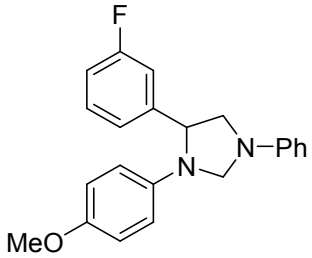
3-(4-methoxyphenyl)-1-phenyl-4-(m-tolyl)imidazolidine (5k)

White solid, yield (55%), mp. = 96.6 – 97.5 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.26 (m, 2H), 7.22 – 7.16 (m, 3H), 7.07 – 7.06 (m, 1H), 6.82 – 6.77 (m, 3H), 6.66 (d, *J* = 7.8 Hz, 2H), 6.58 – 6.55 (m, 2H), 5.16 (d, *J* = 3.1 Hz, 1H), 4.85 (dd, *J* = 7.3, 5.2 Hz, 1H), 4.68 (d, *J* = 3.1 Hz, 1H), 3.91 (dd, *J* = 8.5, 7.5 Hz, 1H), 3.72 (s, 3H), 3.48 (dd, *J* = 8.7, 5.1 Hz, 1H), 2.32 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 146.5, 142.4, 140.3, 138.5, 129.3, 128.7, 128.3, 126.8, 123.3, 118.0, 114.8, 114.3, 112.9, 68.5, 62.5, 56.4, 55.8, 21.6.

HRMS (ESI+) calcd for $C_{23}H_{25}N_2O$ $(M+H)^+$, m/z 345.1961, found345.1964.



4-(3-fluorophenyl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5l)

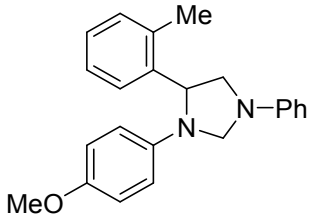
White solid, yield (38%), mp. = 99.8 – 101.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 3H), 7.16 (d, *J* = 7.7 Hz, 1H), 7.10 – 7.07 (m, 1H), 6.96 – 6.92 (m, 1H), 6.84 – 6.78 (m, 3H), 6.67 (d, *J* = 7.8 Hz, 2H), 6.56 – 6.53 (m, 2H), 5.17 (d, *J* = 3.1 Hz, 1H), 4.89 (dd, *J* = 7.3, 4.8 Hz, 1H), 4.67 (d, *J* = 3.1 Hz, 1H), 3.92 (dd, *J* = 8.6, 7.5 Hz, 1H), 3.73 (s, 3H), 3.49 (dd, *J* = 8.7, 4.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 163.3 (d, *J* = 245.0 Hz), 152.3, 146.3, 145.32 (d, *J* = 6.3 Hz), 139.8, 130.4 (d, *J* = 8.1 Hz), 129.4, 121.8, 118.3, 114.9, 114.5 (d, *J* = 21.1 Hz), 114.2, 113.2 (d, *J* = 21.8 Hz), 113.0, 68.4, 61.9, 56.1, 55.7.

^{19}F NMR (471 MHz, $CDCl_3$) δ -112.37.

HRMS (ESI+) calcd for $C_{22}H_{22}FN_2O$ $(M+H)^+$, m/z 349.1711, found 349.1714.



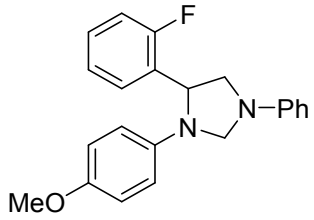
3-(4-methoxyphenyl)-1-phenyl-4-(o-tolyl)imidazolidine (5m)

White solid, yield (55%), mp. = 147.7 – 148.6 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 3H), 7.20 – 7.19 (m, 1H), 7.16 – 7.13 (m, 1H), 7.11 – 7.08 (m, 1H), 6.81 – 6.76 (m, 3H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.48 – 6.44 (m, 2H), 5.19 (d, *J* = 3.1 Hz, 1H), 5.08 (dd, *J* = 7.4, 5.0 Hz, 1H), 4.69 (d, *J* = 3.1 Hz, 1H), 3.97 – 3.94 (m, 1H), 3.71 (s, 3H), 3.42 (dd, *J* = 8.5, 4.9 Hz, 1H), 2.48 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 146.5, 140.1, 139.8, 134.3, 130.7, 129.3, 127.2, 126.7, 125.8, 118.0, 114.9, 114.0, 112.9, 68.3, 59.4, 55.8, 54.8, 19.5.

HRMS (ESI+) calcd for $C_{23}H_{25}N_2O$ $(M+H)^+$, m/z 345.1961, found 345.1968.



4-(2-fluorophenyl)-3-(4-methoxyphenyl)-1-phenylimidazolidine (5n)

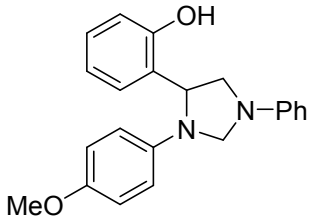
White solid, yield (56%), mp. = 86.7 – 88.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 – 7.13 (m, 4H), 7.03 – 6.99 (dd, *J* = 9.8, 8.9 Hz, 1H), 6.96 – 6.93 (m, 1H), 6.76 – 6.72 (m, 3H), 6.61 (d, *J* = 7.9 Hz, 2H), 6.49 – 6.45 (m, 2H), 5.20 (dd, *J* = 7.3, 3.8 Hz, 1H), 5.09 (d, *J* = 3.1 Hz, 1H), 4.59 (d, *J* = 3.1 Hz, 1H), 3.89 – 3.86 (m, 1H), 3.66 (s, 3H), 3.49 (dd, *J* = 8.7, 3.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 159.3 (d, *J* = 243.3 Hz), 151.2, 145.4, 138.6, 128.3, 128.0 (d, *J* = 12.8 Hz), 127.9 (d, *J* = 8.0 Hz), 126.8 (*J* = 4.2 Hz), 123.4 (d, *J* = 3.4 Hz), 117.2, 114.3 (d, *J* = 21.0 Hz), 113.9, 112.7, 112.0, 66.7, 54.7, 54.5, 53.8.

^{19}F NMR (471 MHz, $CDCl_3$) δ -119.45.

HRMS (ESI+) calcd for $C_{22}H_{22}FN_2O$ $(M+H)^+$, m/z 349.1711, found 349.1717.



2-(3-(4-methoxyphenyl)-1-phenylimidazolidin-4-yl)phenol (5o)

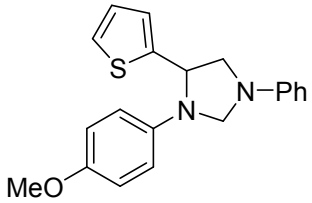
White solid, yield (65%), mp. = 138.2 – 140.0 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.39 (s, 1H), 7.30 – 7.27 (m, 2H), 7.22 – 7.17 (m, 2H), 6.96 – 6.93 (m, 2H), 6.88 (td, *J* = 7.5, 0.6 Hz, 1H), 6.84 – 6.79 (m, 4H), 6.62 (d, *J* = 8.0 Hz, 2H), 5.13 (d, *J* = 3.9 Hz, 1H), 4.84 – 4.81 (m, 1H), 4.48 (d, *J* = 3.9 Hz, 1H), 3.91 (dd, *J* = 8.8, 7.6 Hz, 1H), 3.73 (s, 3H), 3.70 –

3.66 (m, 1H)..

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 154.2, 144.6, 138.6, 128.4, 128.4, 127.5, 121.8, 118.8, 117.9, 117.2, 116.2, 113.7, 111.6, 69.7, 63.7, 54.5, 52.9.

HRMS (ESI+) calcd for $C_{22}H_{23}N_2O_2$ $(M+H)^+$, m/z 347.1754, found 347.1755.



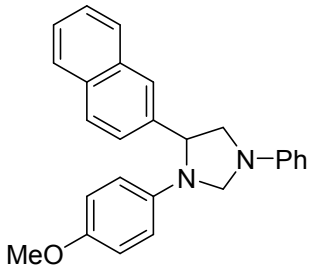
3-(4-methoxyphenyl)-1-phenyl-4-(thiophen-2-yl)imidazolidine (5p)

Yellow solid, yield (57%), mp. = 117.8 – 119.0 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.26 (m, 2H), 7.14 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.02 (d, *J* = 3.4 Hz, 1H), 6.91 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.83 – 6.79 (m, 3H), 6.67 – 6.64 (m, 4H), 5.22 (dd, *J* = 6.8, 3.9 Hz, 1H), 5.04 (d, *J* = 3.2 Hz, 1H), 4.61 (d, *J* = 3.2 Hz, 1H), 3.86 (dd, *J* = 8.6, 6.9 Hz, 1H), 3.72 (s, 3H), 3.63 (dd, *J* = 8.6, 3.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.5, 146.5, 146.3, 139.7, 129.4, 126.7, 124.7, 124.3, 118.1, 114.8, 114.6, 112.9, 67.4, 58.1, 56.1, 55.7.

HRMS (ESI+) calcd for $C_{20}H_{21}N_2OS$ $(M+H)^+$, m/z 337.1369, found 337.1366.



3-(4-methoxyphenyl)-4-(naphthalen-2-yl)-1-phenylimidazolidine (5q)

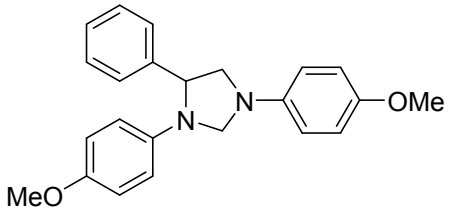
White solid, yield (70%), mp. = 148.0 – 150.0 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.78 (m, 4H), 7.51 – 7.49 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.47 – 7.42 (m, 2H), 7.28 (t, *J* = 7.9 Hz, 2H), 6.81 (t, *J* = 7.3 Hz, 1H), 6.76 – 6.74 (m, 2H), 6.67 (d, *J* = 8.3 Hz, 2H), 6.61 (d, *J* = 9.0 Hz, 2H), 5.24 (d, *J* = 3.1 Hz, 1H), 5.04 (dd, *J* = 7.2, 5.4 Hz, 1H), 4.73 (d, *J* = 3.1 Hz, 1H),

4.00 – 3.97 (m, 1H), 3.68 (s, 3H), 3.55 (dd, *J* = 8.7, 5.2 Hz, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.2, 146.4, 140.3, 140.0, 133.5, 133.1, 129.4, 128.9, 127.9, 127.8, 126.2, 125.8, 125.1, 124.3, 118.1, 114.8, 114.4, 113.0, 68.6, 62.7, 56.3, 55.7.

HRMS (ESI+) calcd for $C_{26}H_{25}N_2O$ $(M+H)^+$, m/z 381.1961, found 381.1964.



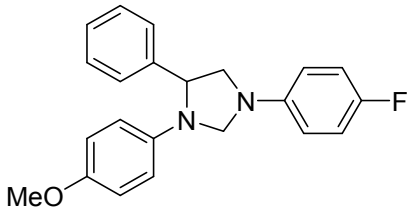
1,3-bis(4-methoxyphenyl)-4-phenylimidazolidine (5r)[7]

White solid, yield (77%), mp. = 113.7 – 115.5 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.37 (m, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.23 (m, 1H), 6.88 – 6.85 (m, 2H), 6.78 – 6.77 (m, 2H), 6.65 – 6.64 (m, 2H), 6.55 – 6.52 (m, 2H), 5.10 (d, *J* = 3.0 Hz, 1H), 4.88 (dd, *J* = 7.1, 4.9 Hz, 1H), 4.64 (d, *J* = 3.0 Hz, 1H), 3.84 (dd, *J* = 8.3, 7.5 Hz, 1H), 3.76 (s, 3H), 3.71 (s, 3H), 3.44 (dd, *J* = 8.5, 4.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.6, 152.0, 142.5, 141.3, 140.3, 128.8, 127.4, 126.3, 114.9, 114.8, 114.3, 114.0, 69.2, 62.6, 57.2, 55.8, 55.8.

HRMS (ESI+) calcd for $C_{23}H_{25}N_2O_2$ $(M+H)^+$, m/z 361.1911, found 361.1919.



1-(4-fluorophenyl)-3-(4-methoxyphenyl)-4-phenylimidazolidine (5s)

Yellow oil, yield (40%);

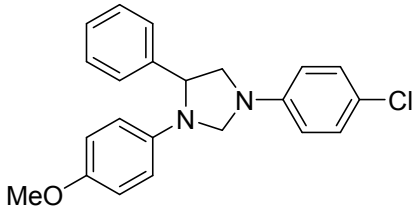
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.36 (m, 2H), 7.34 – 7.31 (M, 2H), 7.27 –7.24 (M, 1H), 7.00 – 6.96 (m, 2H), 6.79 – 6.76 (m, 2H), 6.61 – 6.59 (m, 2H), 6.56 – 6.53 (m, 2H), 5.11 (d, *J* = 3.0 Hz, 1H), 4.90 (dd, *J* = 7.2, 5.0 Hz, 1H), 4.65 (d, *J* = 3.0 Hz, 1H), 3.87 (dd, *J* = 8.4, 7.5 Hz, 1H), 3.71 (s, 3H), 3.44 (dd,

J = 8.5, 5.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2 (d, J = 3.0 Hz), 152.2, 143.2, 142.2, 140.1, 128.9, 127.5, 126.2, 115.8 (d, J = 22.2 Hz), 114.8, 114.2, 113.8 (d, J = 7.4 Hz), 69.0, 62.5, 56.9, 55.7.

^{19}F NMR (471 MHz, $CDCl_3$) δ -127.3.

HRMS (ESI+) calcd for $C_{22}H_{22}FN_2O$ $(M+H)^+$, m/z 349.1711, found 349.1705.



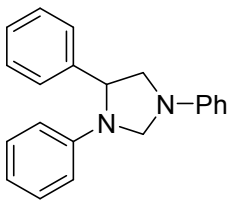
1-(4-chlorophenyl)-3-(4-methoxyphenyl)-4-phenylimidazolidine (5t)

White solid, yield (36%), mp. = 119.9 – 121.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 4H), 7.26 – 7.20 (m, 3H), 6.79 – 6.76 (m, 2H), 6.58 – 6.54 (m, 4H), 5.12 (d, J = 3.1 Hz, 1H), 4.90 (dd, J = 7.2, 5.2 Hz, 1H), 4.66 (d, J = 3.1 Hz, 1H), 3.92 – 3.89 (m, 1H), 3.72 (s, 3H), 3.45 (dd, J = 8.6, 5.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 144.9, 142.0, 140.0, 129.2, 128.9, 127.6, 126.2, 122.9, 114.8, 114.4, 113.9, 68.5, 62.4, 56.4, 55.7.

HRMS (ESI+) calcd for $C_{22}H_{22}ClN_2O$ $(M+H)^+$, m/z 365.1415, found 365.1411.



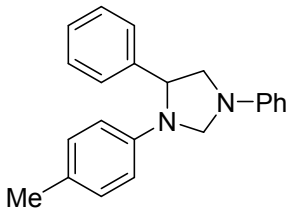
1,3,4-triphenylimidazolidine (5u)

White solid, yield (76%), mp. = 110.8 – 112.1 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.24 (m, 7H), 7.20 – 7.17 (m, 2H), 6.82 (t, J = 7.3 Hz, 1H), 6.73 (t, J = 7.3 Hz, 1H), 6.69 (d, J = 7.9 Hz, 2H), 6.59 (d, J = 8.0 Hz, 2H), 5.19 (d, J = 3.3 Hz, 1H), 4.99 (dd, J = 7.3, 4.0 Hz, 1H), 4.74 (d, J = 3.3 Hz, 1H), 3.92 – 3.89 (m, 1H), 3.55 (dd, J = 8.7, 4.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 145.3, 142.4, 129.4, 129.2, 128.9, 127.5, 126.2, 118.3, 117.5, 113.2, 112.8, 67.5, 61.8, 56.2.

HRMS (ESI+) calcd for $C_{21}H_{21}N_2$ $(M+H)^+$, m/z 301.1699, found 301.1699.



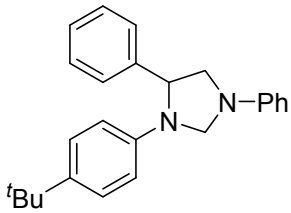
1,4-diphenyl-3-(p-tolyl)imidazolidine (5v)

White solid, yield (75%), mp. = 120.1 – 121.7 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 7H), 6.99 (d, *J* = 8.2 Hz, 2H), 6.81 (t, *J* = 7.3 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 2H), 6.52 – 6.50 (m, 2H), 5.18 (d, *J* = 3.2 Hz, 1H), 4.95 (dd, *J* = 7.3, 4.4 Hz, 1H), 4.72 (d, *J* = 3.2 Hz, 1H), 3.92 (dd, *J* = 8.6, 7.5 Hz, 1H), 3.52 (dd, *J* = 8.7, 4.4 Hz, 1H), 2.22 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 143.3, 142.5, 129.7, 129.3, 128.8, 127.5, 126.7, 126.2, 118.1, 113.0, 113.0, 67.9, 61.9, 56.2, 20.3.

HRMS (ESI+) calcd for $C_{22}H_{23}N_2$ $(M+H)^+$, m/z 315.1856, found 315.1862.



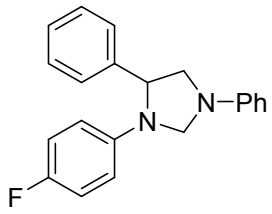
3-(4-(tert-butyl)phenyl)-1,4-diphenylimidazolidine (5w)

White solid, yield (87%), mp. = 148.4 – 150.3 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.38 (m, 2H), 7.35 – 7.26 (m, 5H), 7.24 – 7.21 (m, 2H), 6.82 (t, *J* = 7.3 Hz, 1H), 6.69 (d, *J* = 7.8 Hz, 2H), 6.57 – 6.55 (m, 2H), 5.21 (d, *J* = 3.2 Hz, 1H), 4.96 (dd, *J* = 7.4, 4.3 Hz, 1H), 4.73 (d, *J* = 3.2 Hz, 1H), 3.90 (dd, *J* = 8.6, 7.6 Hz, 1H), 3.54 (dd, *J* = 8.7, 4.3 Hz, 1H), 1.26 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 143.2, 142.7, 140.2, 129.3, 128.8, 127.5, 126.2, 126.0, 118.2, 113.1, 112.5, 67.8, 62.1, 56.3, 33.8, 31.5.

HRMS (ESI+) calcd for $C_{25}H_{29}N_2$ $(M+H)^+$, m/z 357.2325, found 357.2323.



3-(4-fluorophenyl)-1,4-diphenylimidazolidine (5x)

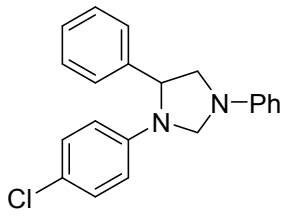
White solid, yield (52%), mp. = 89.8 – 91.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 6H), 7.21 – 7.18 (m, 2H), 6.83 (t, *J* = 7.3 Hz, 1H), 6.75 – 6.69 (m, 3H), 6.59 (d, *J* = 7.9 Hz, 2H), 5.20 (d, *J* = 3.3 Hz, 1H), 5.01 (dd, *J* = 7.3, 3.9 Hz, 1H), 4.75 (d, *J* = 3.3 Hz, 1H), 3.92 (dd, *J* = 8.6, 7.5 Hz, 1H), 3.56 (dd, *J* = 8.7, 4.0 Hz, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.9 (d, *J* = 234.6 Hz), 146.3, 142.0, 142.0, 129.4, 128.9, 127.6, 126.2, 118.3, 115.6 (d, *J* = 22.1 Hz), 113.7 (d, *J* = 7.3 Hz), 113.1, 68.1, 62.2, 56.3.

^{19}F NMR (471 MHz, $CDCl_3$) δ -127.89.

HRMS (ESI+) calcd for $C_{21}H_{20}FN_2$ $(M+H)^+$, m/z 319.1605, found 319.1600.



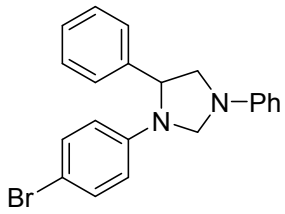
3-(4-chlorophenyl)-1,4-diphenylimidazolidine (5y)

White solid, yield (43%), mp. = 112.3 – 113.5 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 7H), 7.14 – 7.11 (m, 2H), 6.83 (t, *J* = 7.3 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 2H), 6.51 – 6.48 (m, 2H), 5.15 (d, *J* = 3.3 Hz, 1H), 4.96 (dd, *J* = 7.3, 4.1 Hz, 1H), 4.72 (d, *J* = 3.3 Hz, 1H), 3.93 (dd, *J* = 8.6, 7.4 Hz, 1H), 3.54 (dd, *J* = 8.7, 4.1 Hz, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.3, 143.8, 141.9, 129.4, 129.0, 128.9, 127.7, 126.1, 122.5, 118.5, 113.9, 113.2, 67.6, 61.9, 56.2.

HRMS (ESI+) calcd for $C_{21}H_{20}ClN_2$ $(M+H)^+$, m/z 335.1310, found 335.1314.



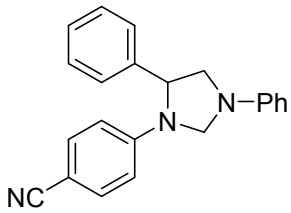
3-(4-bromophenyl)-1,4-diphenylimidazolidine (5z)

White solid, yield (43%), mp. = 100.0 – 101.8 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.26 (m, 7H), 7.21 – 7.17 (m, 2H), 6.83 (t, *J* = 7.3 Hz, 1H), 6.75 – 6.69 (m, 3H), 6.59 (d, *J* = 7.9 Hz, 2H), 5.20 (d, *J* = 3.3 Hz, 1H), 5.01 (dd, *J* = 7.3, 3.9 Hz, 1H), 4.75 (d, *J* = 3.3 Hz, 1H), 3.92 (dd, *J* = 8.5, 7.5 Hz, 1H), 3.56 (dd, *J* = 8.7, 4.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.3, 144.1, 141.8, 131.9, 129.4, 128.9, 127.7, 126.1, 118.5, 114.4, 113.2, 109.6, 67.4, 61.8, 56.1.

HRMS (ESI+) calcd for $C_{21}H_{20}BrN_2$ $(M+H)^+$, m/z 379.0804, found 379.0806.



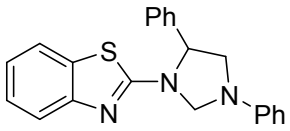
4-(3,5-diphenylimidazolidin-1-yl)benzonitrile (5aa)

White solid, yield (52%), mp. = 123.8 – 124.9 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.23 (m, 2H), 7.31 – 7.24 (m, 4H), 7.20 – 7.17 (m, 2H), 6.82 (t, *J* = 7.3 Hz, 1H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.69 (d, *J* = 8.3 Hz, 2H), 6.59 (d, *J* = 8.3 Hz, 2H), 5.20 (d, *J* = 3.3 Hz, 1H), 5.00 (dd, *J* = 7.3, 4.0 Hz, 1H), 4.75 (d, *J* = 3.3 Hz, 1H), 3.93 – 3.90 (m, 1H), 3.55 (dd, *J* = 8.7, 4.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 145.3, 142.4, 129.4, 129.2, 128.8, 127.5, 126.1, 118.3, 117.5, 113.2, 112.8, 67.5, 61.8, 56.2.

HRMS (ESI+) calcd for $C_{22}H_{20}N_3$ $(M+H)^+$, m/z 326.1652, found 326.1657.



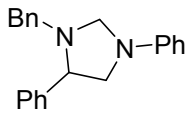
2-(3,5-diphenylimidazolidin-1-yl)benzo[d]thiazole (5ab)

White solid, yield (31%), mp. = 110.9 – 112.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.27 (m, 6H), 7.20 – 7.17 (m, 2H), 6.82 (t, *J* = 7.3 Hz, 1H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.69 (d, *J* = 7.9 Hz, 2H), 6.59 (d, *J* = 7.9 Hz, 2H), 5.20 (d, *J* = 3.3 Hz, 1H), 5.00 (dd, *J* = 7.3, 4.0 Hz, 1H), 4.75 (d, *J* = 3.3 Hz, 1H), 3.92 (dd, *J* = 8.5, 7.5 Hz, 1H), 3.55 (dd, *J* = 8.7, 4.0 Hz, 1H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 145.3, 142.4, 129.4, 129.2, 128.8, 127.5, 126.1, 118.3, 117.5, 113.2, 112.8, 67.5, 61.8, 56.2.

HRMS (ESI+) calcd for $C_{22}H_{20}N_3S$ $(M+H)^+$, m/z 358.1372, found 358.1378.



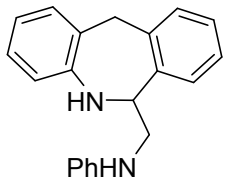
3-benzyl-1,4-diphenylimidazolidine (5ac)

White solid, yield (63%), mp. = 86.7 – 88.4 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.55 (m, 2H), 7.41 – 7.29 (m, 7H), 7.26 – 7.23 (m, 1H), 7.19 – 7.16 (m, 2H), 6.67 (t, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 7.6 Hz, 2H), 4.40 (d, *J* = 4.2 Hz, 1H), 3.97 – 3.92 (m, 2H), 3.81 (d, *J* = 4.2 Hz, 1H), 3.73 (dd, *J* = 8.6, 6.8 Hz, 1H), 3.35 (t, *J* = 8.8 Hz, 1H), 3.28 (d, *J* = 13.3 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 146.2, 139.5, 138.6, 129.2, 128.8, 128.4, 128.4, 128.1, 128.0, 127.2, 116.4, 111.4, 70.5, 68.1, 56.3, 55.7.

HRMS (ESI+) calcd for $C_{22}H_{23}N_2$ $(M+H)^+$, m/z 315.1856, found 315.1855.



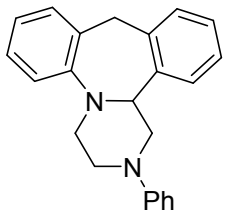
N-((6,11-dihydro-5H-dibenzo[b,e]azepin-6-yl)methyl)aniline (**8**)

White solid, yield (65%), mp. = 98.7 – 100.2 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.21 (m, 5H), 7.17 – 7.16 (m, 1H), 7.06 (dd, J = 7.6, 1.5 Hz, 1H), 7.00 (td, J = 7.6, 1.5 Hz, 1H), 6.78 – 6.70 (m, 4H), 6.59 (dd, J = 7.8, 1.1 Hz, 1H), 4.99 (dd, J = 8.8, 4.7 Hz, 1H), 4.35 (d, J = 14.9 Hz, 1H), 4.04 (s, 2H), 3.95 (d, J = 14.9 Hz, 1H), 3.66 – 3.57 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 147.8, 145.3, 139.5, 137.3, 129.8, 129.5, 128.8, 127.9, 127.6, 127.0, 126.7, 126.0, 119.6, 118.7, 118.1, 113.2, 56.0, 49.2, 40.0.

HRMS (ESI+) calcd for $C_{21}H_{21}N_2$ $(M+H)^+$, m/z 301.1699, found 301.1698.



2-phenyl-1,2,3,4,10,14b-hexahydrodibenzo[c,f]pyrazino[1,2-a]azepine (**9**)

White solid, yield (53%), mp. = 201.8 – 202.3 °C;

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 2H), 7.20 – 7.10 (m, 5H), 7.07 – 7.03 (m, 2H), 6.99 – 6.97 (m, 2H), 6.90 – 6.86 (m, 2H), 4.84 (d, J = 12.7 Hz, 1H), 4.19 (dd, J = 10.4, 2.5 Hz, 1H), 3.80 – 3.76 (m, 1H), 3.63 (dt, J = 11.7, 2.3 Hz, 1H), 3.50 – 3.39 (m, 2H), 3.34 (d, J = 12.7 Hz, 1H), 3.13 – 3.03 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 147.4, 138.7, 138.6, 136.0, 128.5, 128.1, 127.2, 126.3, 126.2, 125.6, 121.4, 118.9, 117.9, 115.1, 65.5, 57.3, 50.2, 48.9, 37.8.

HRMS (ESI+) calcd for $C_{23}H_{23}N_2$ $(M+H)^+$, m/z 327.1856, found 327.1859.

V References

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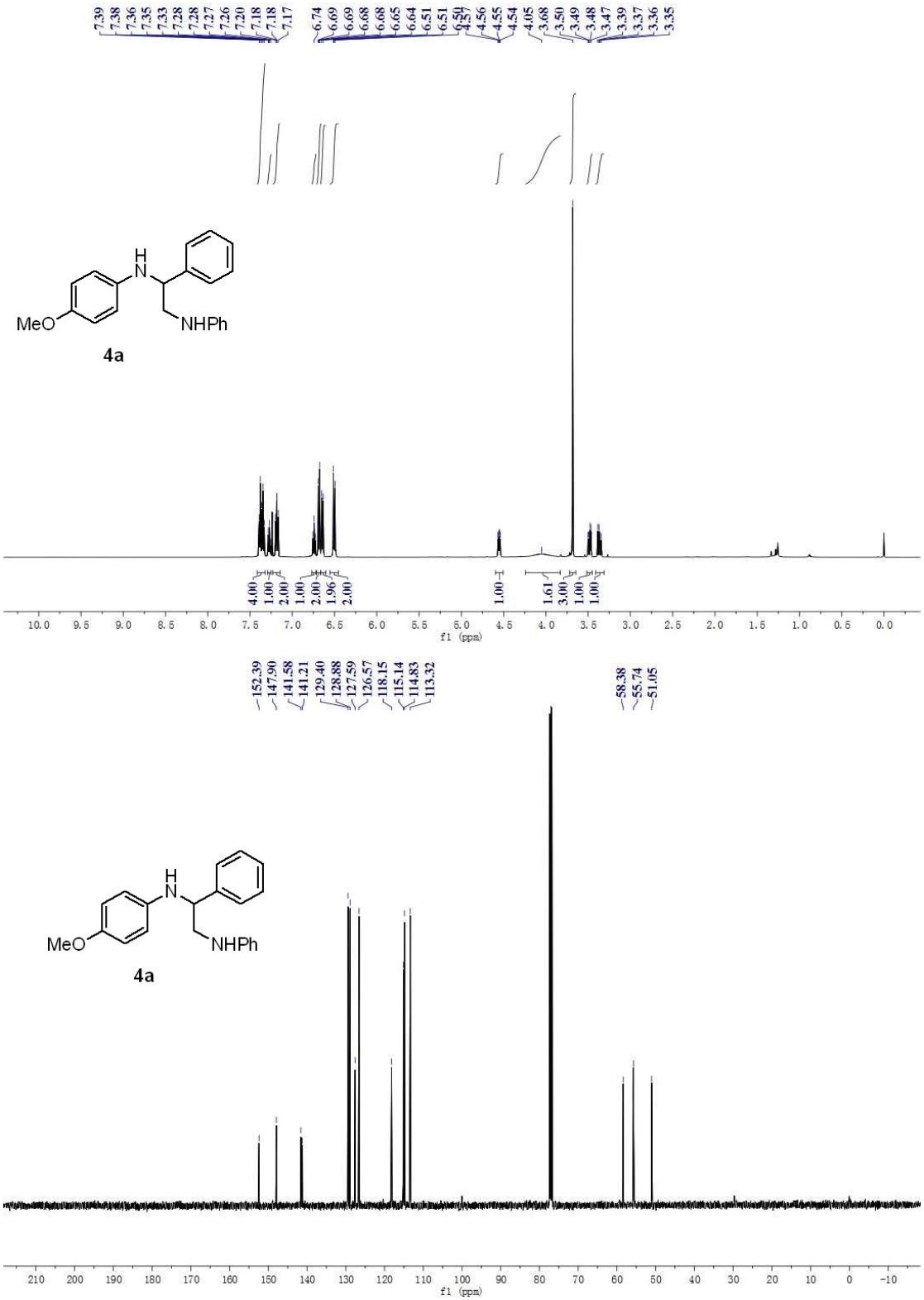
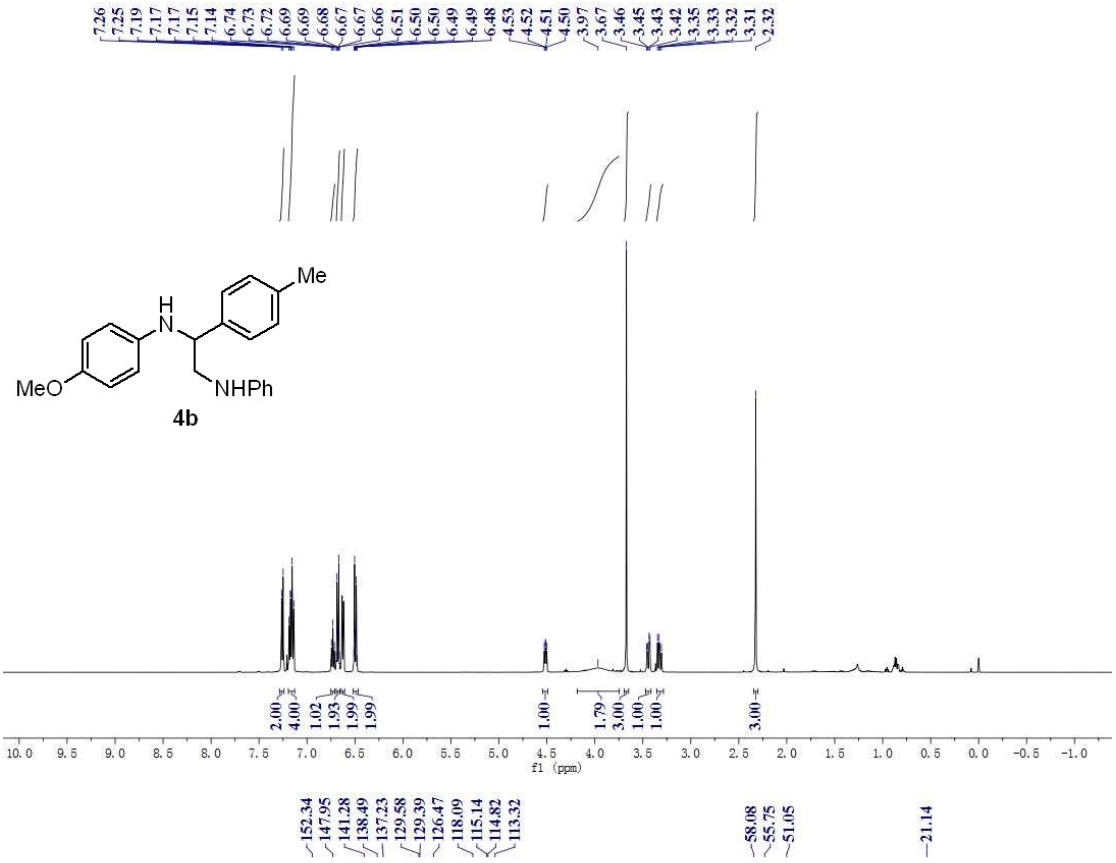
VII NMR Spectra of all products

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3.00
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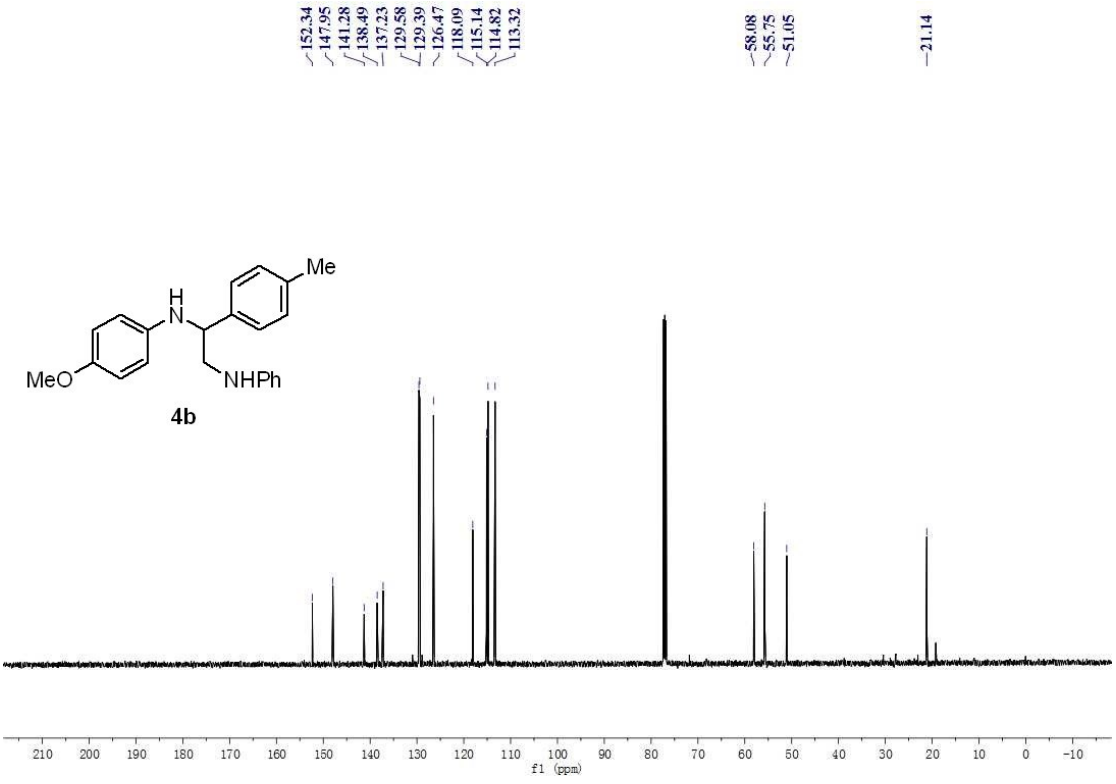
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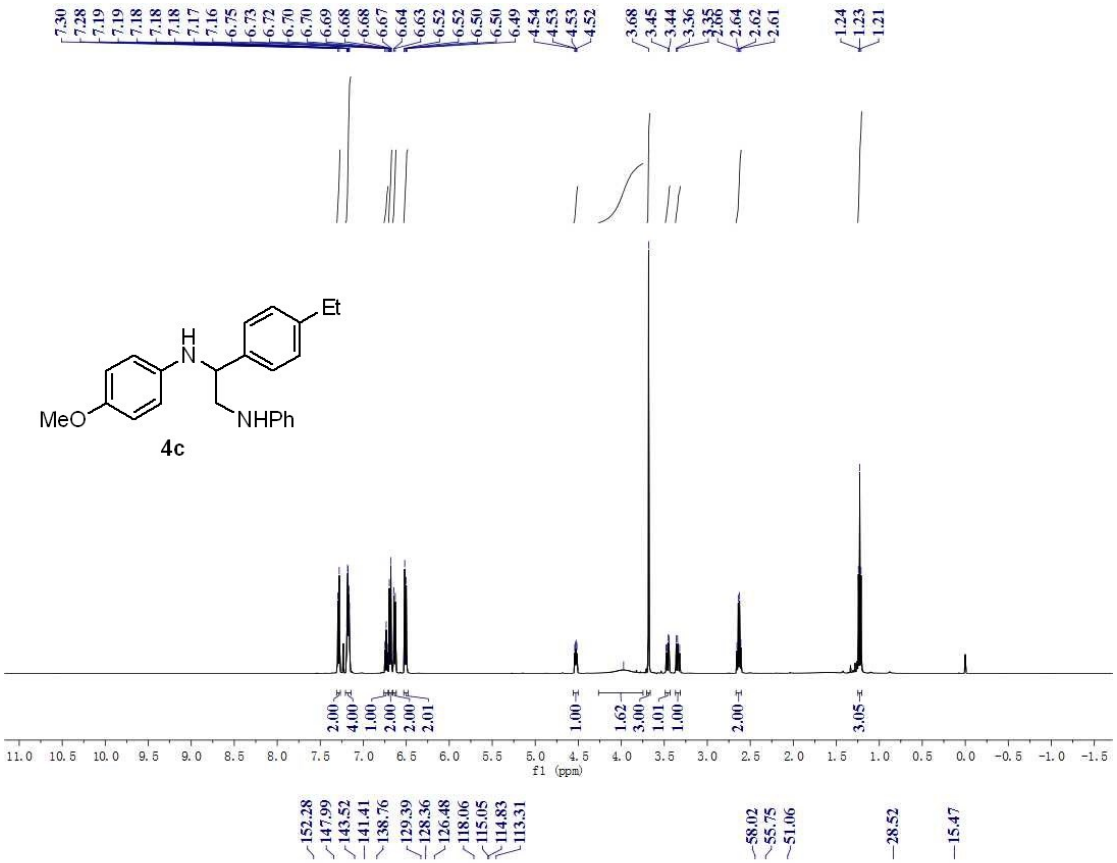
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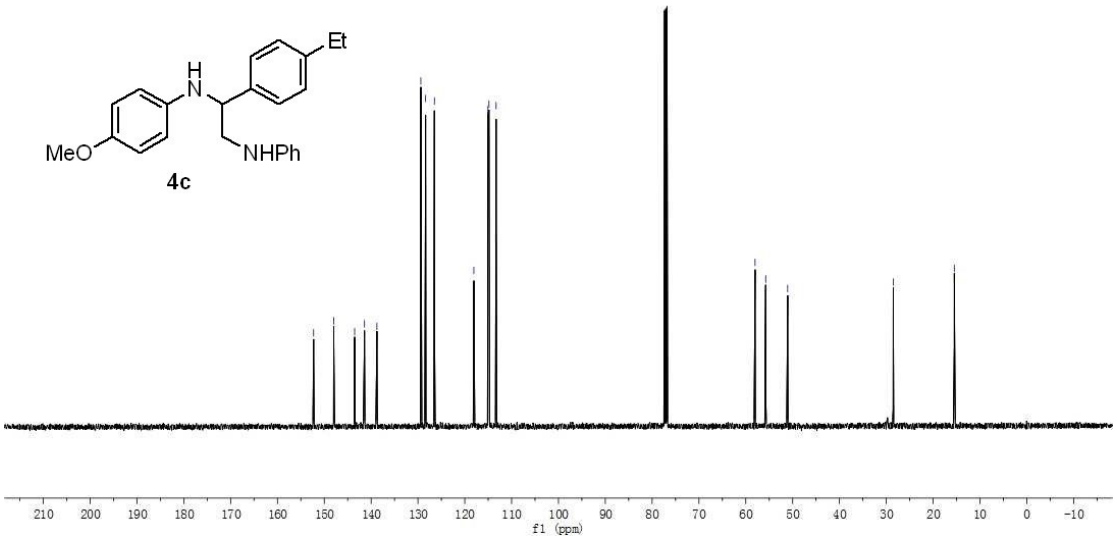
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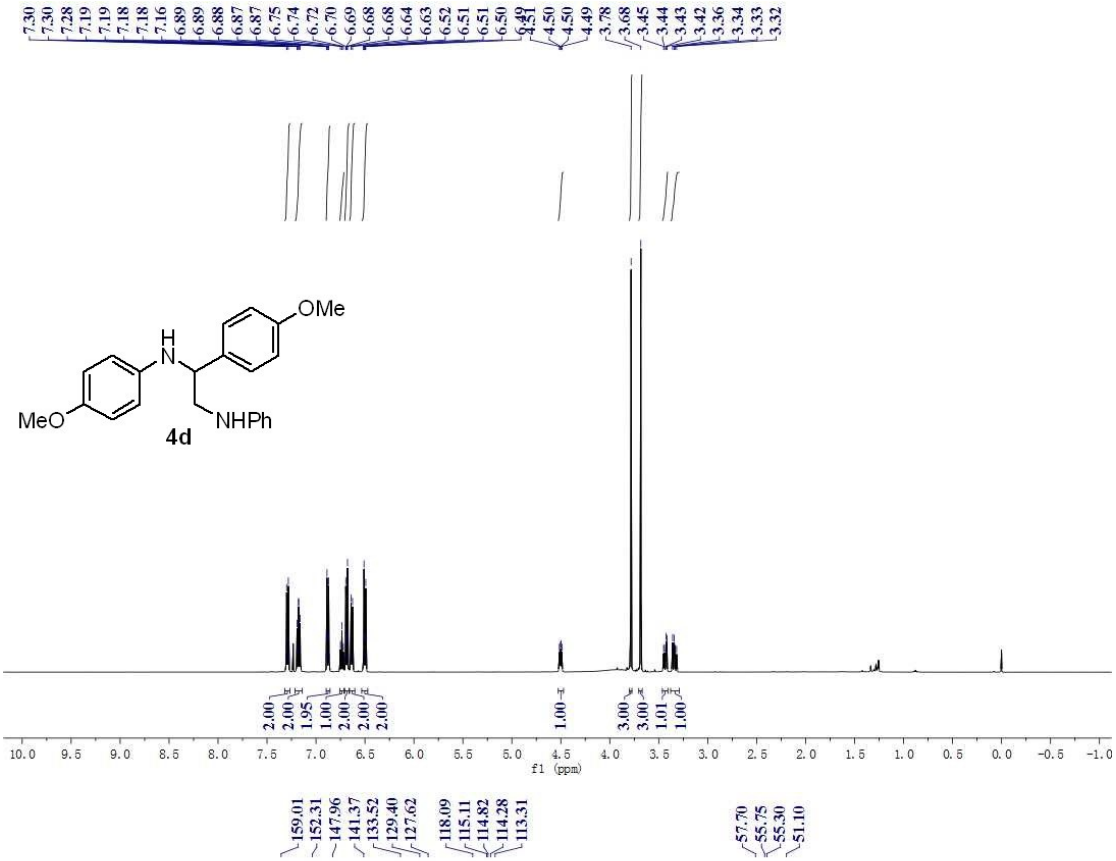
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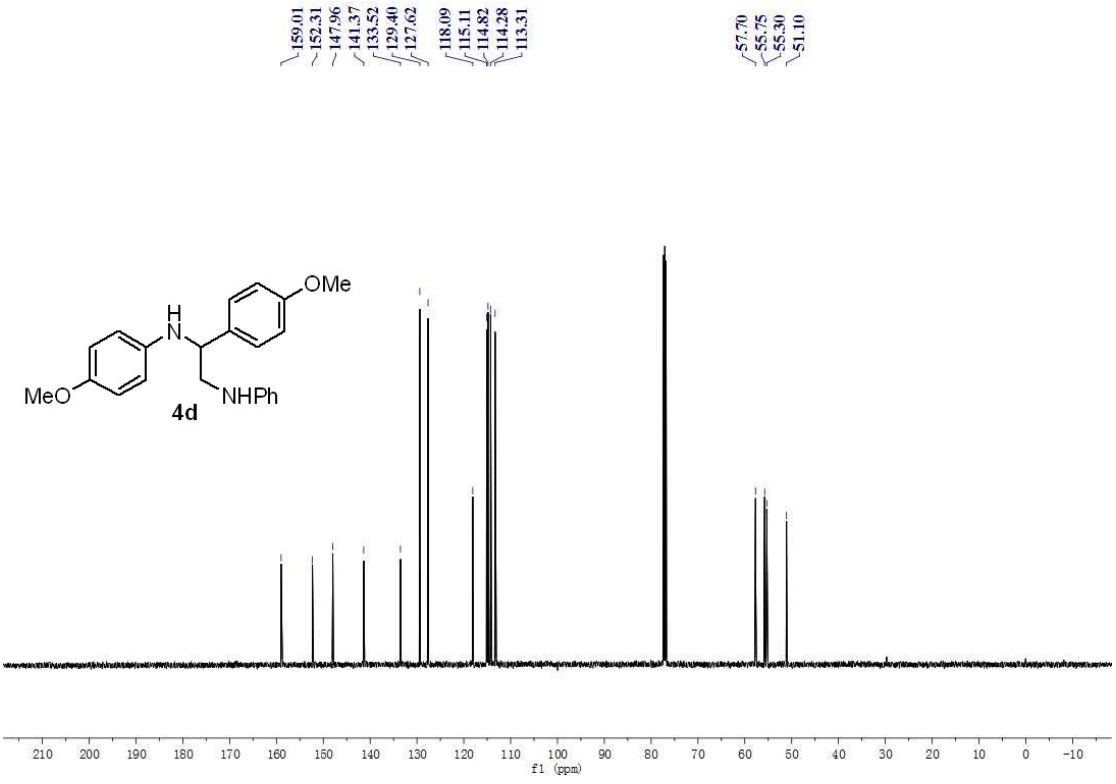
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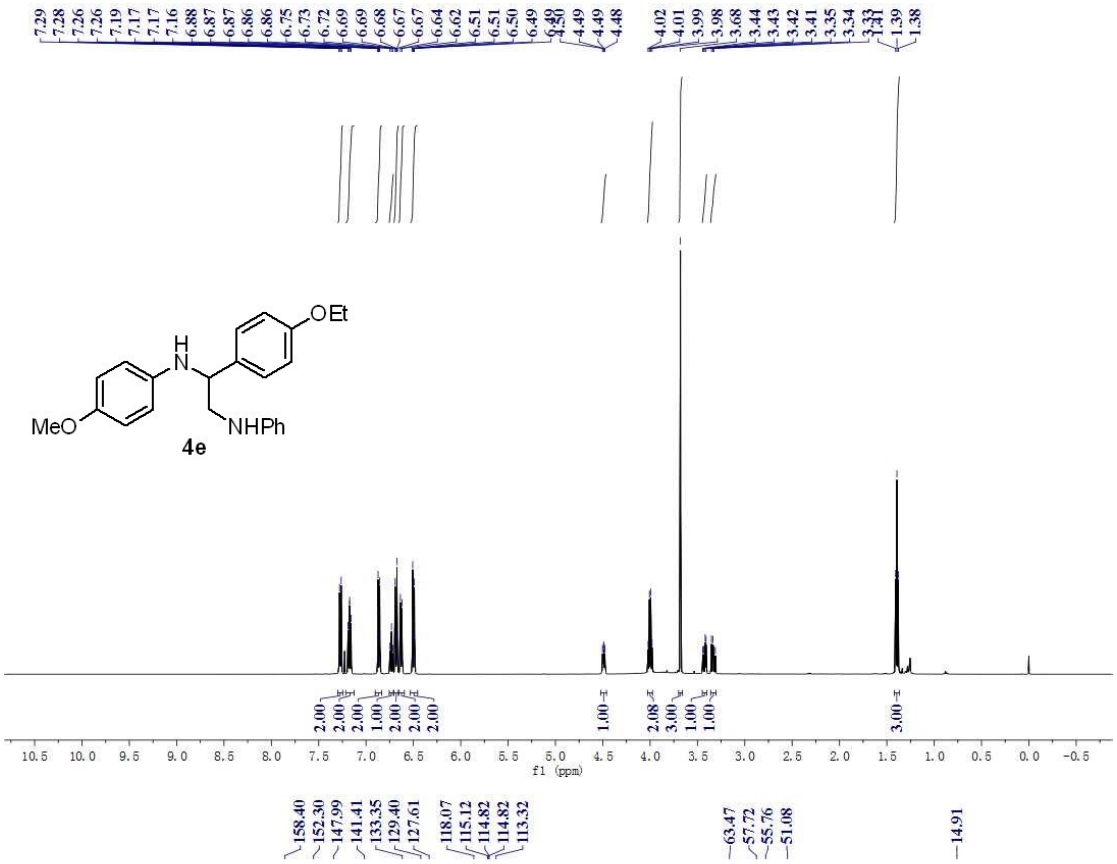
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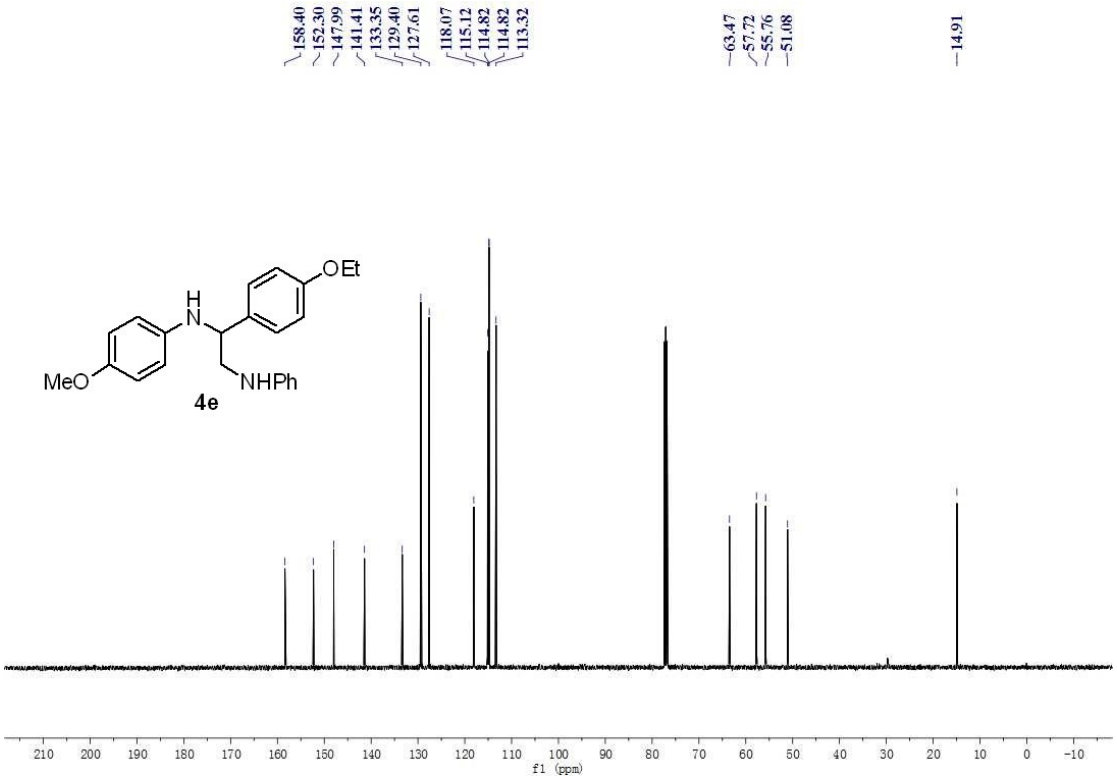
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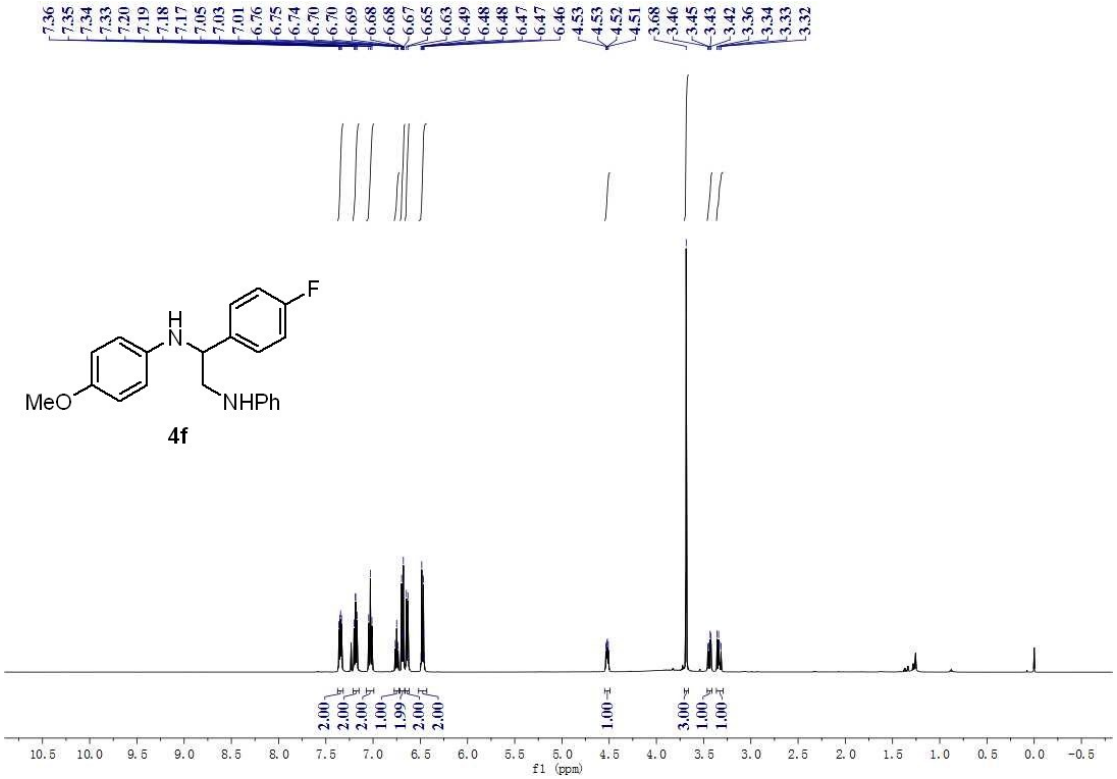
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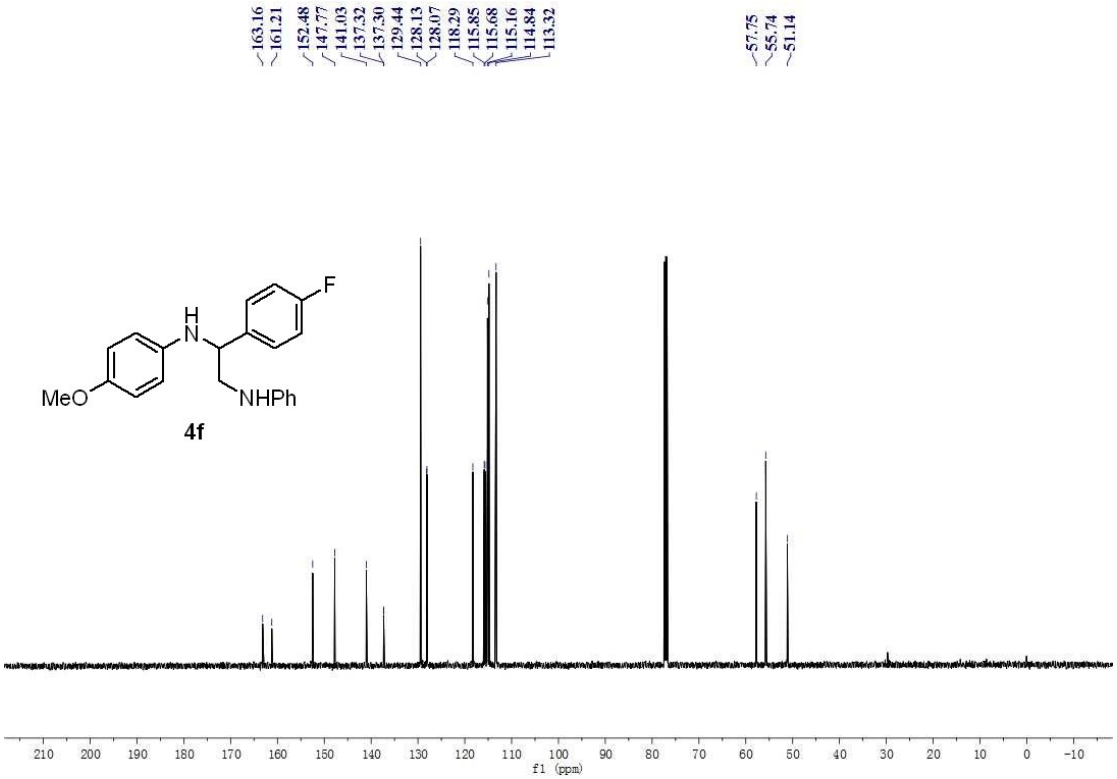
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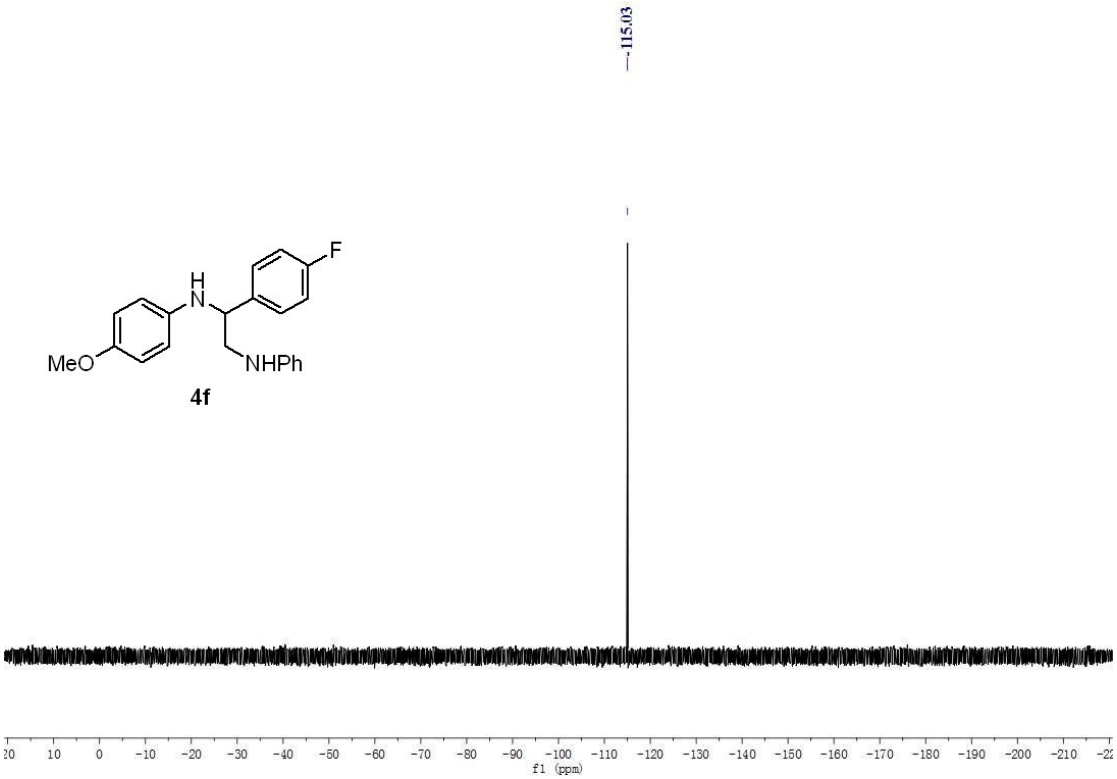
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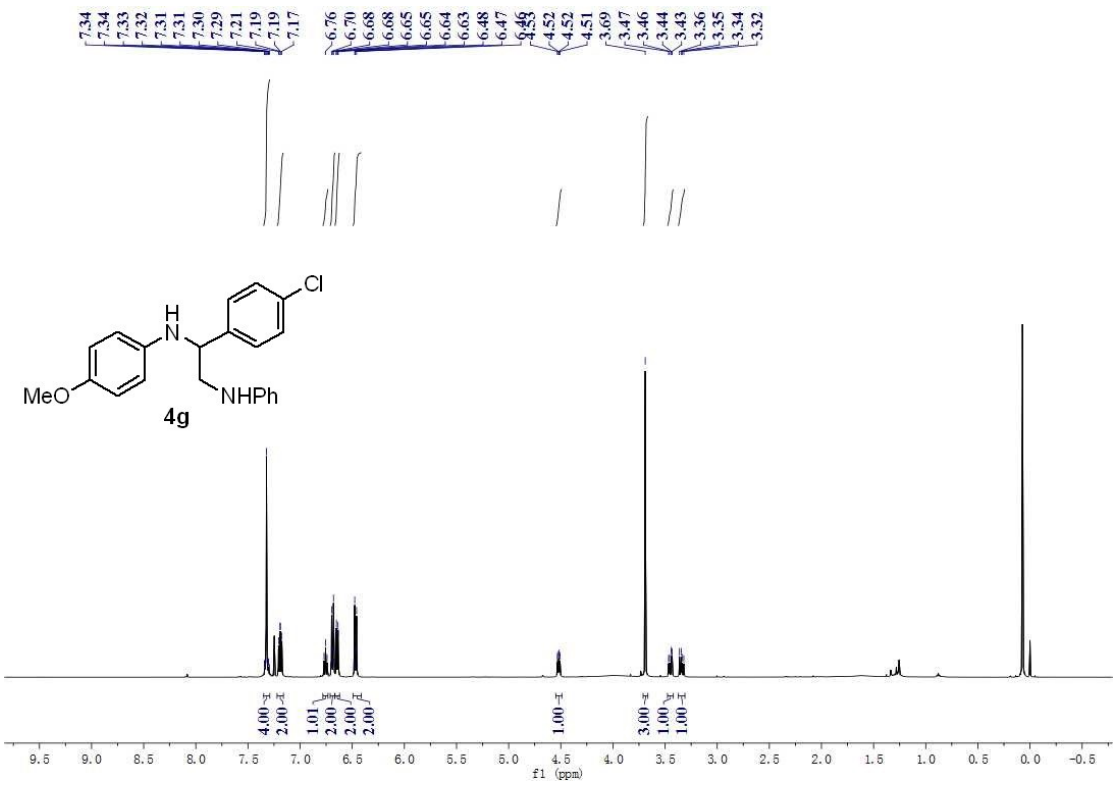
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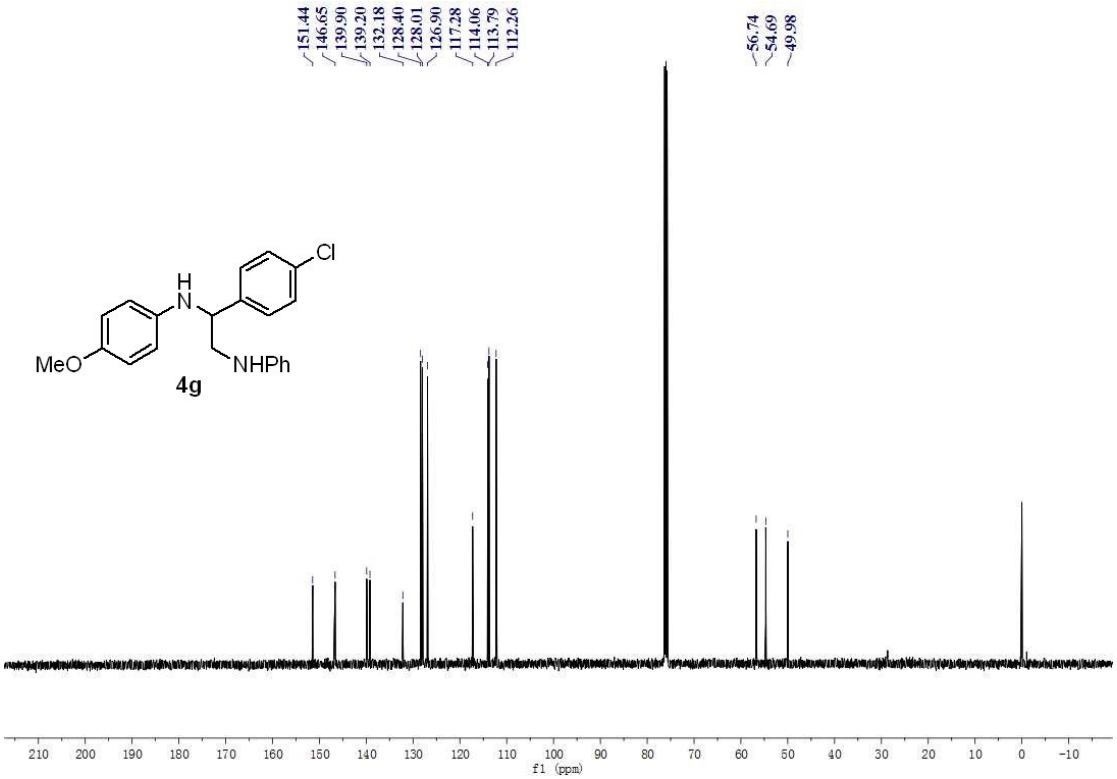
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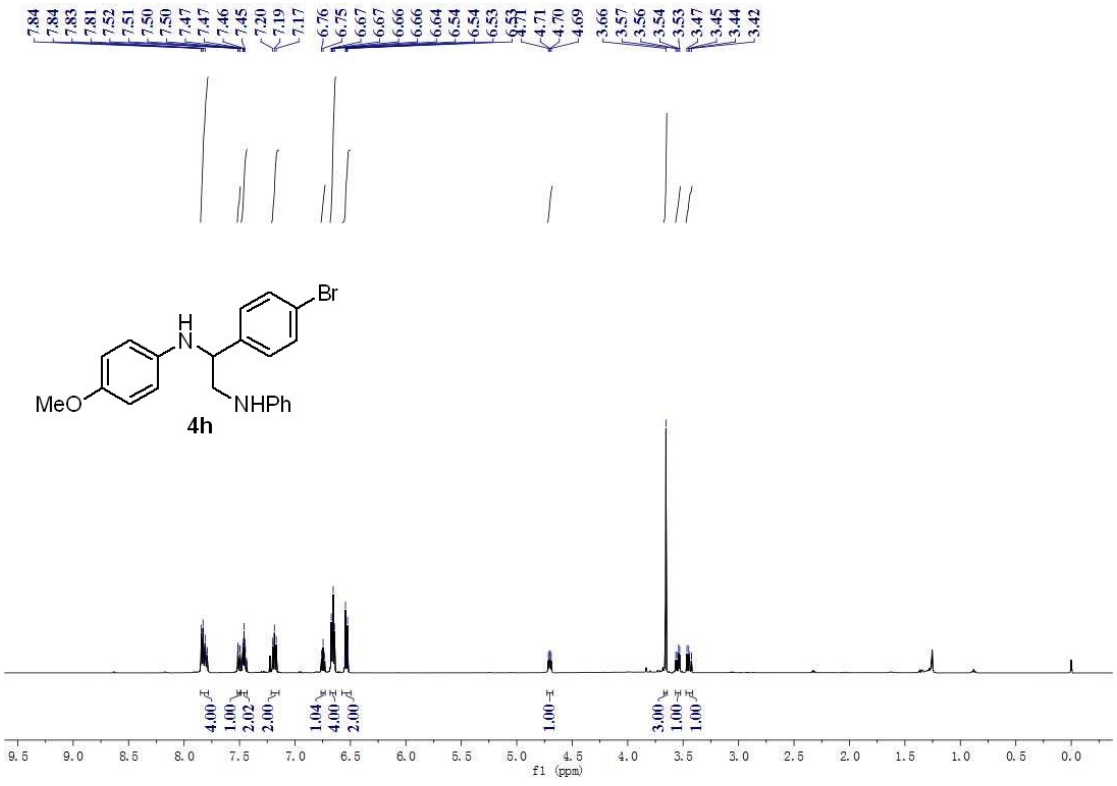
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3.44
3.42
Br
H
N
MeO
NHPh
4h
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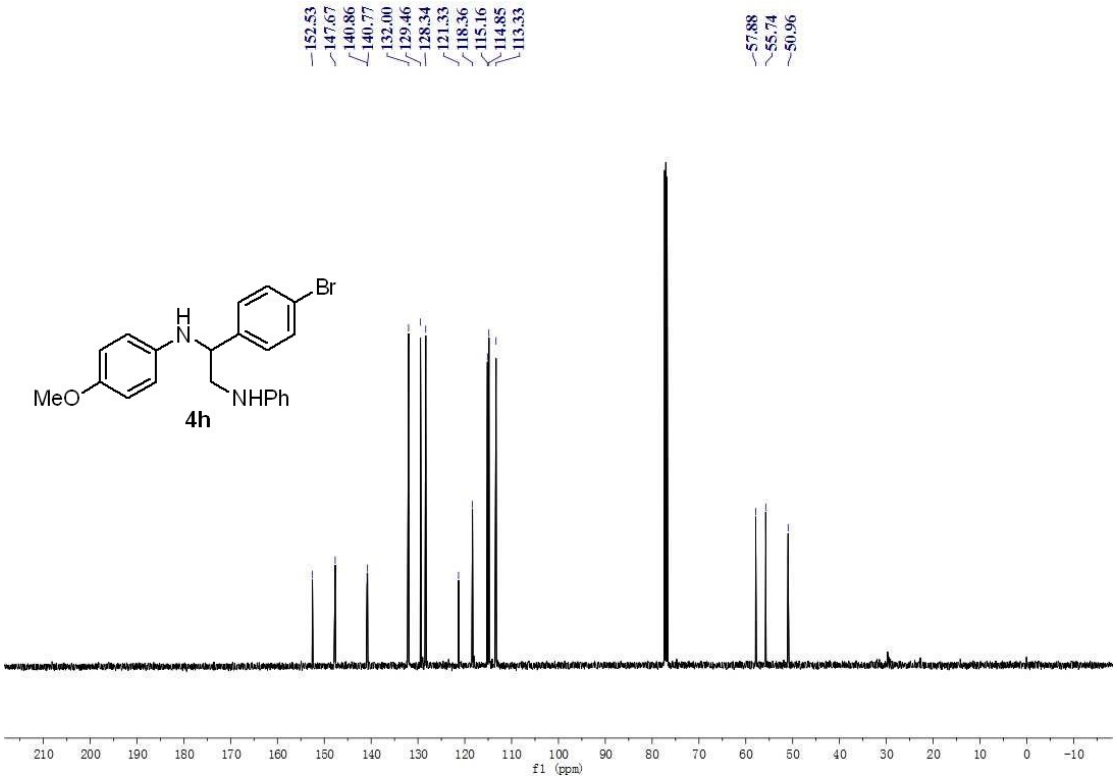
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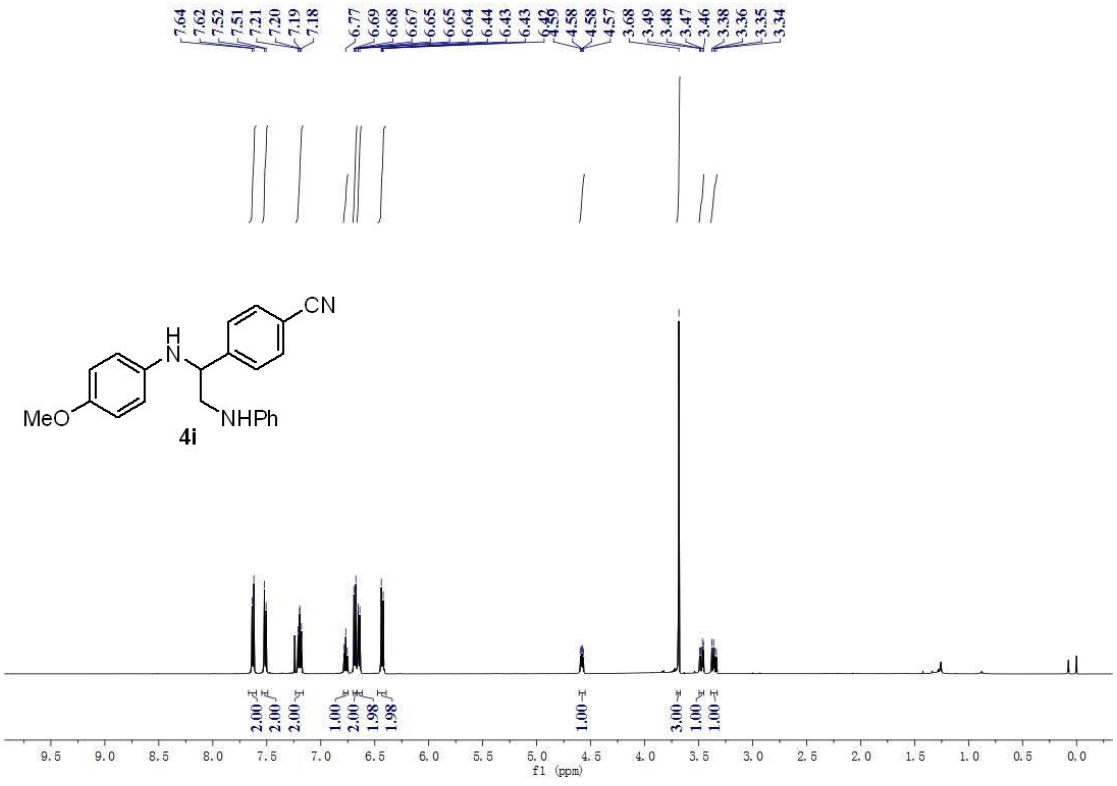
MeO
NHPh
4h
f1 (ppm)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4.57
3.68
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3.48
3.47
3.46
3.38
3.36
3.35
3.34
CN
H
N
MeO
NHPh
4i
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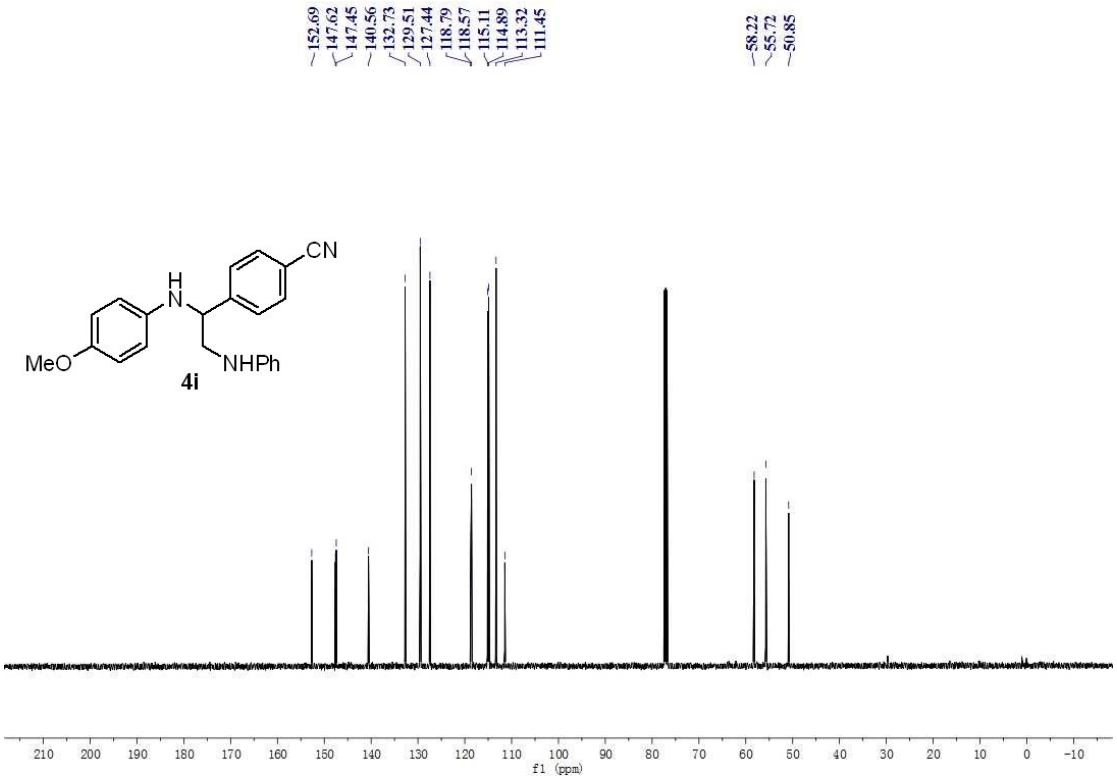
1.00
f1 (ppm)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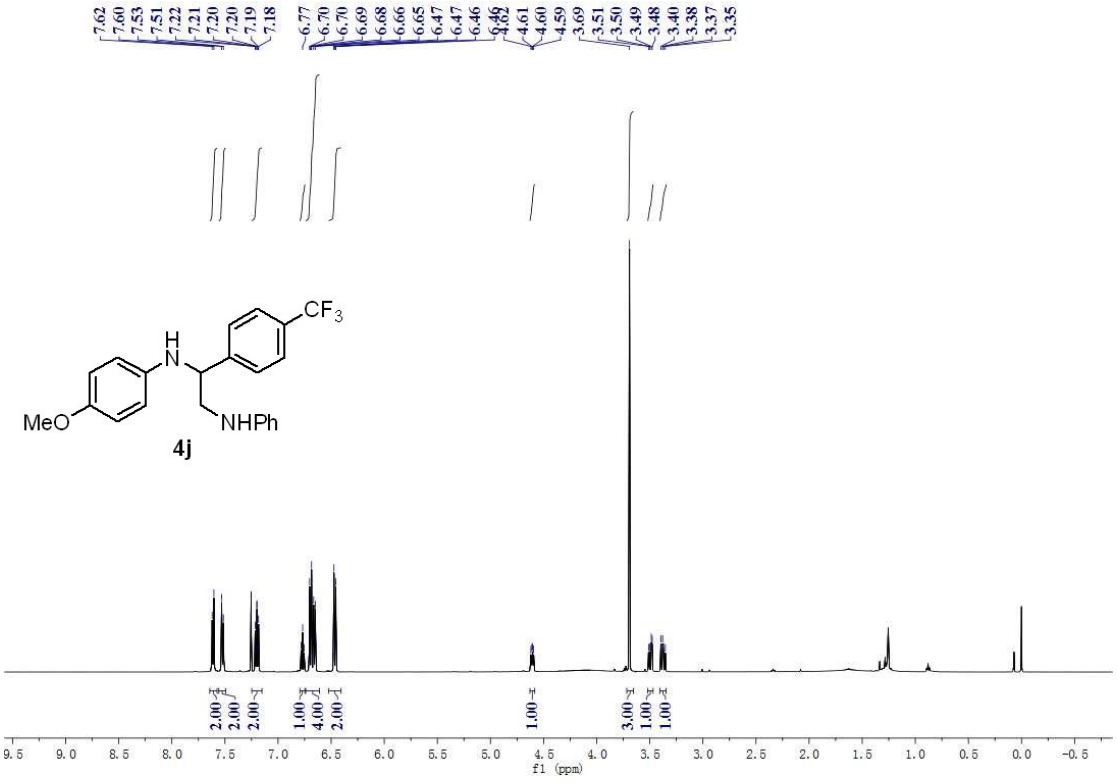
N
MeO
NHPh
4i
f1 (ppm)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4.60
4.59
3.69
3.51
3.50
3.49
3.48
3.40
3.38
3.37
3.35
CF3
H
N
MeO
NHPh
4j
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2.00
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2.00
1.00
3.00
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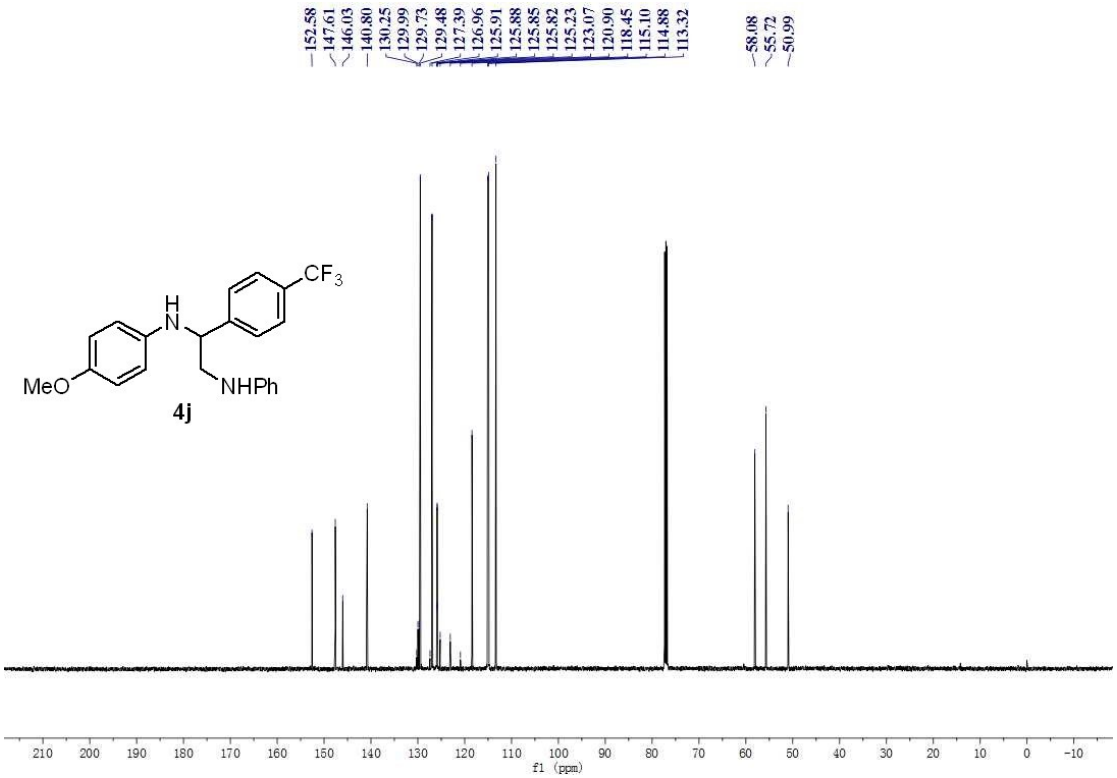
1.00
f1 (ppm)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125.23
123.07
120.90
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58.08
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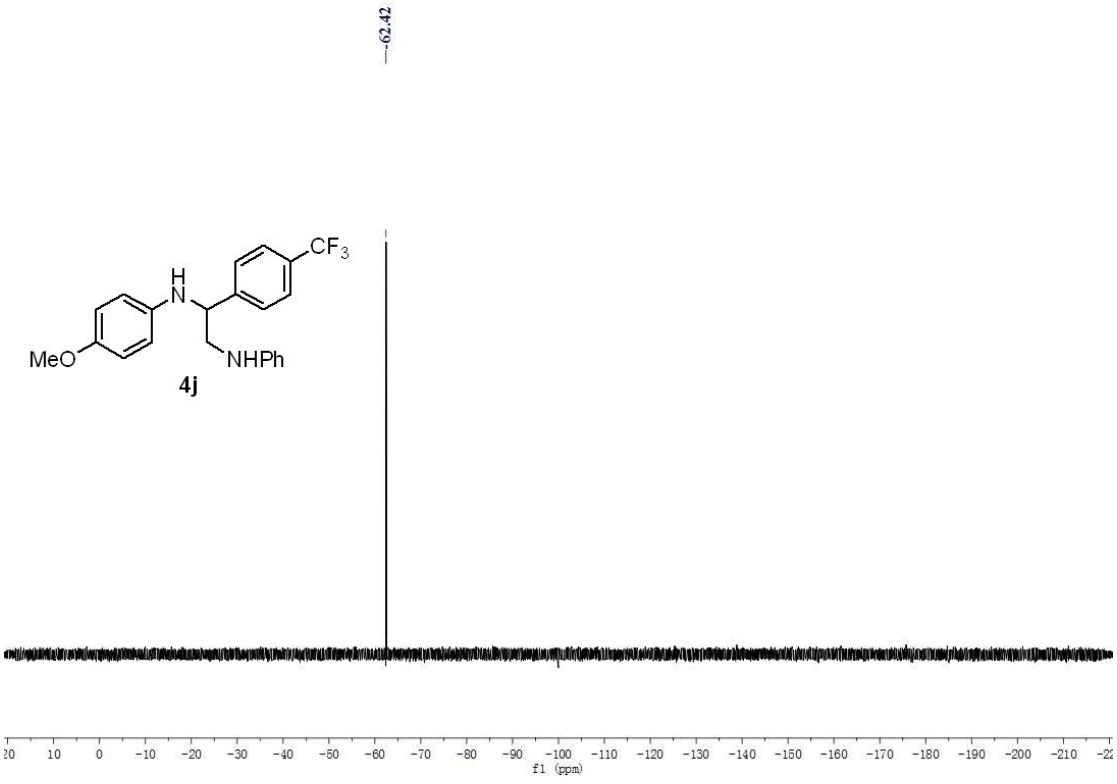
50.99
CF3
H
N
MeO
NHPh
4j
f1 (ppm)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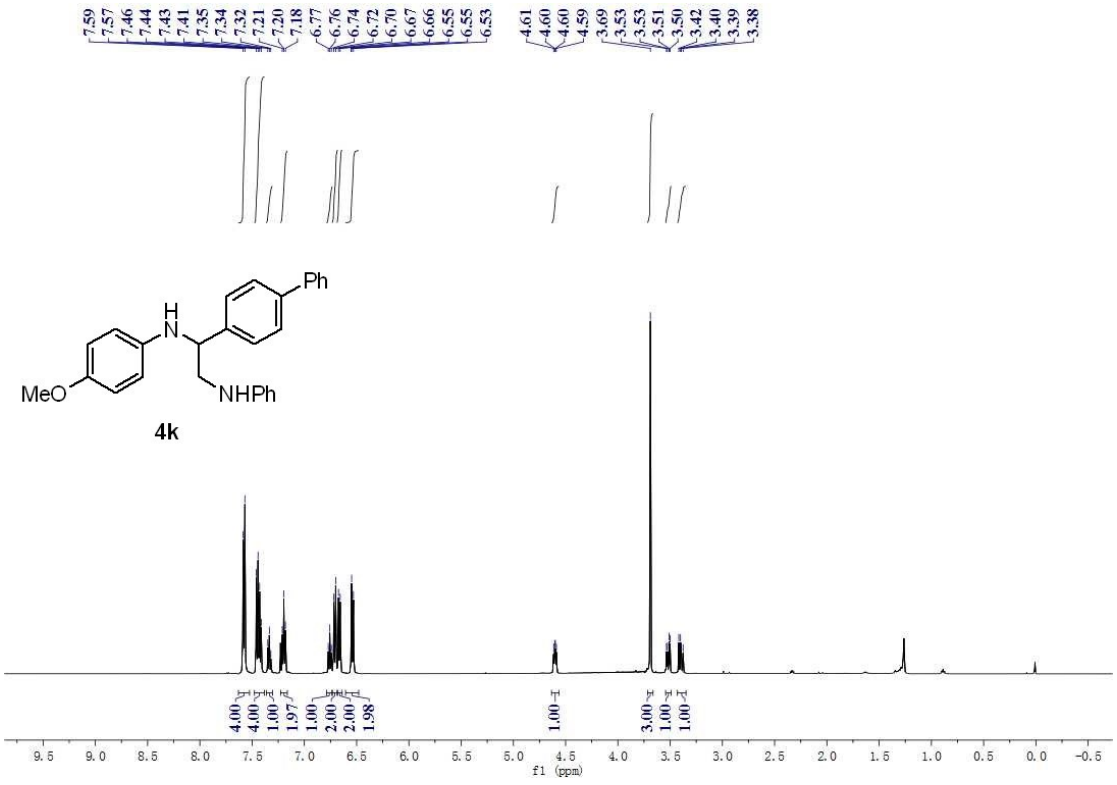
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6.55
6.55
6.53
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4.60
4.60
4.59
3.69
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3.53
3.51
3.50
3.42
3.40
3.39
3.38
Ph
H
N
MeO
NHPh
4k
4.00
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1.00
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3.00
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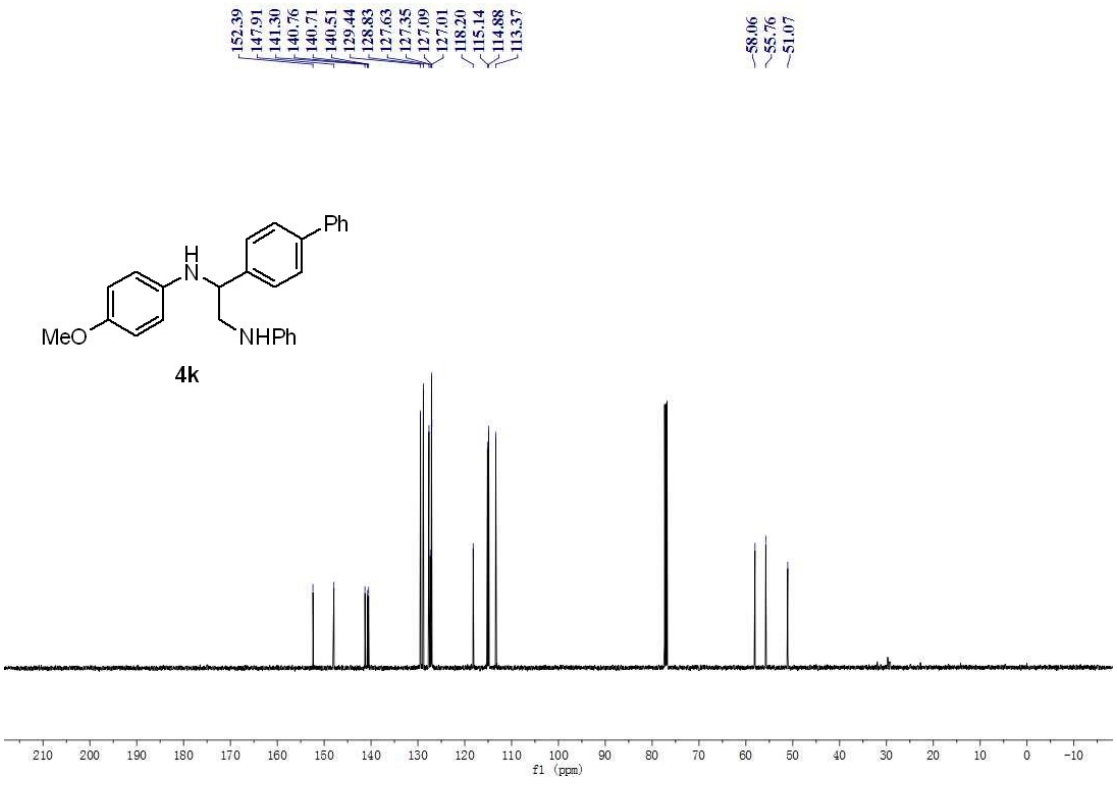
1.00
f1 (ppm)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127.01
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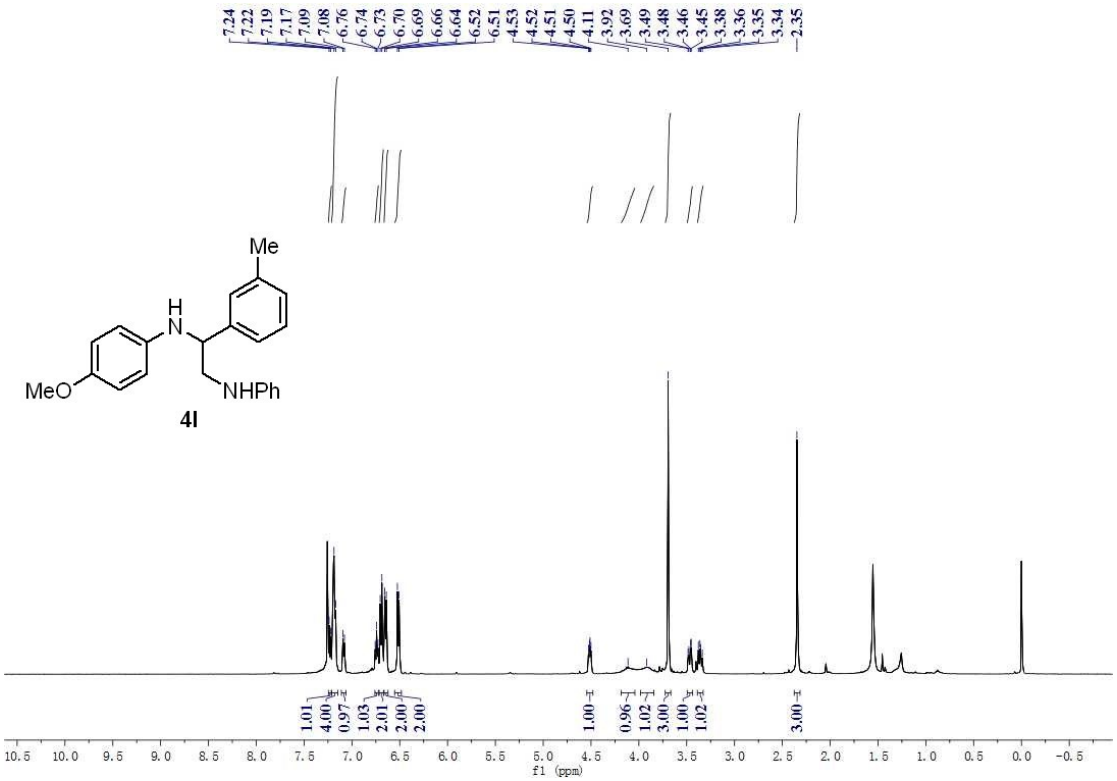
113.37
58.06
55.76
51.07
Ph
H
N
MeO
NHPh
4k
f1 (ppm)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6.52
6.51
4.53
4.52
4.51
4.50
4.11
3.92
3.69
3.49
3.48
3.46
3.45
3.38
3.36
3.35
3.34
2.35
Me
H
N
MeO
NHPh
4l
1.01
4.00
0.97
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2.00
2.00
1.00
0.96
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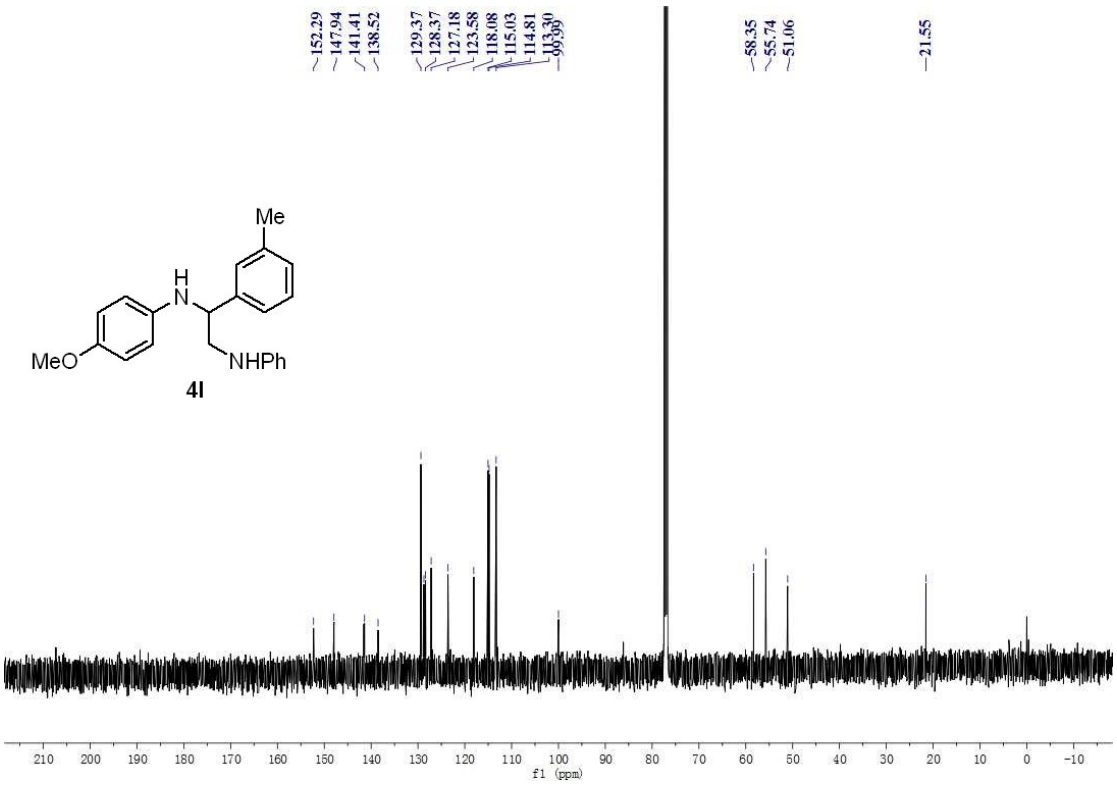
1.00
1.02
3.00
f1 (ppm)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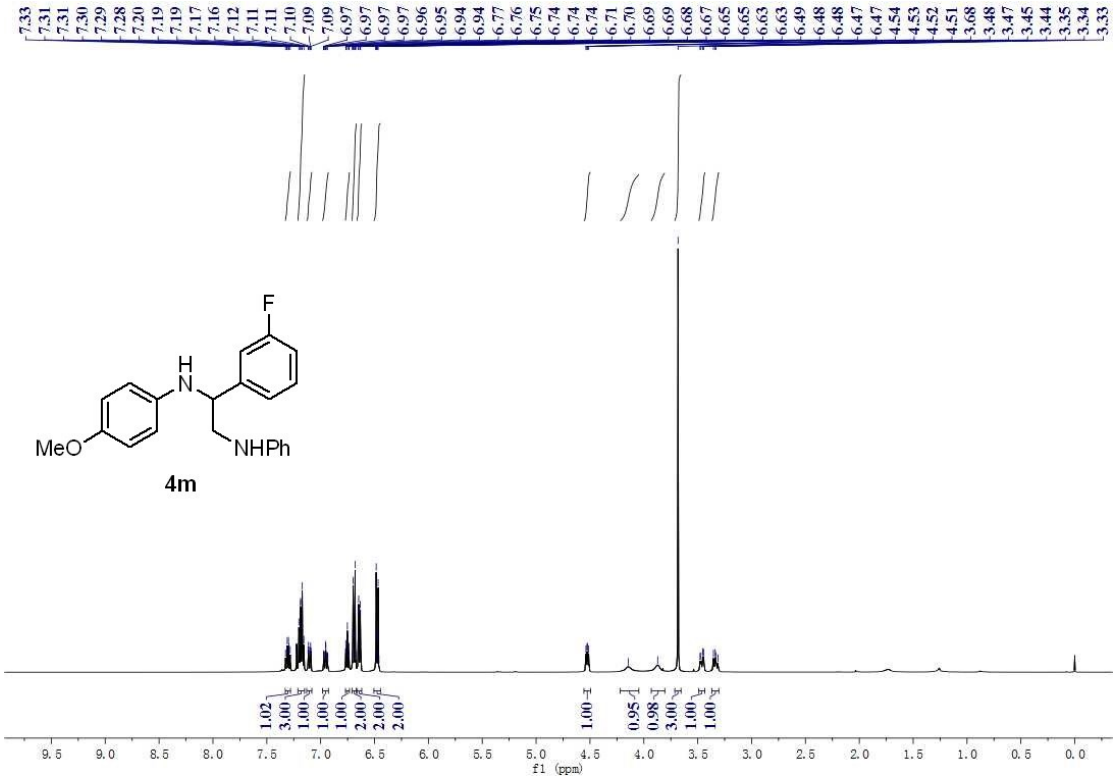
N
MeO
NHPh
4l
f1 (ppm)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6.63
6.63
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6.48
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6.47
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4.52
4.51
3.68
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3.45
3.44
3.35
3.34
3.33
F
H
N
MeO
NHPh
4m
1.02
3.00
1.00
1.00
1.00
2.00
2.00
2.00
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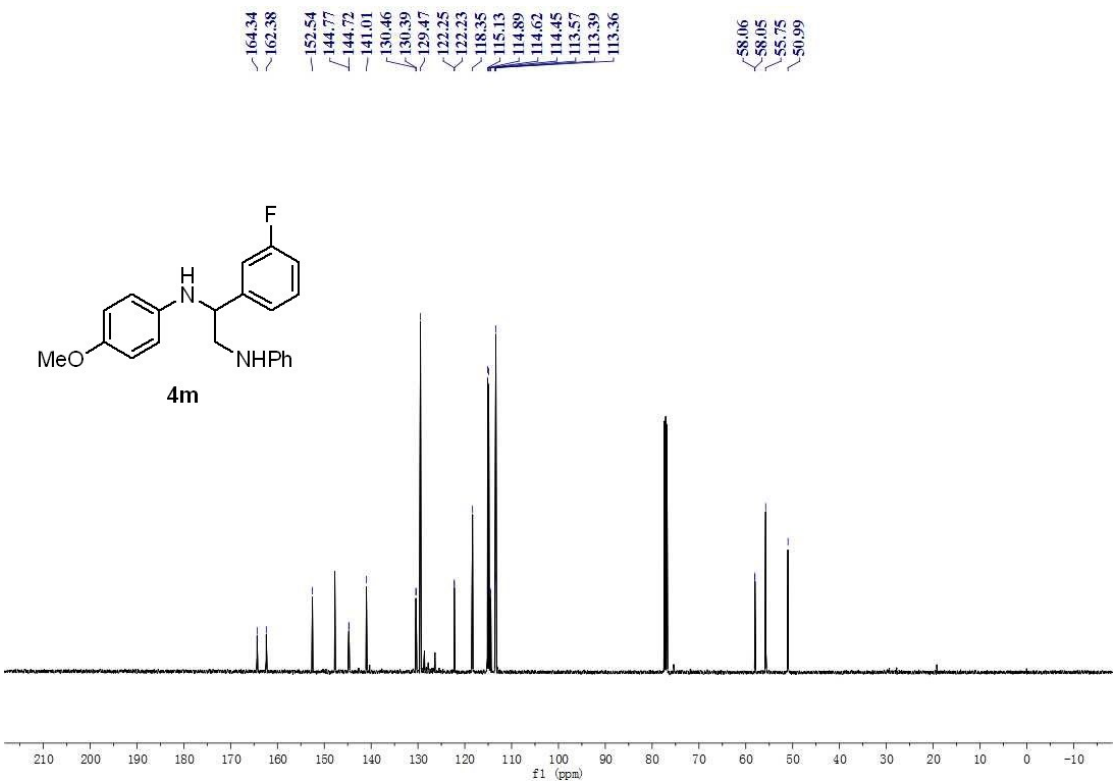
0.98
3.00
1.00
1.00
f1 (ppm)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122.23
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114.89
114.62
114.45
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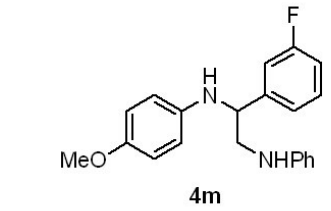
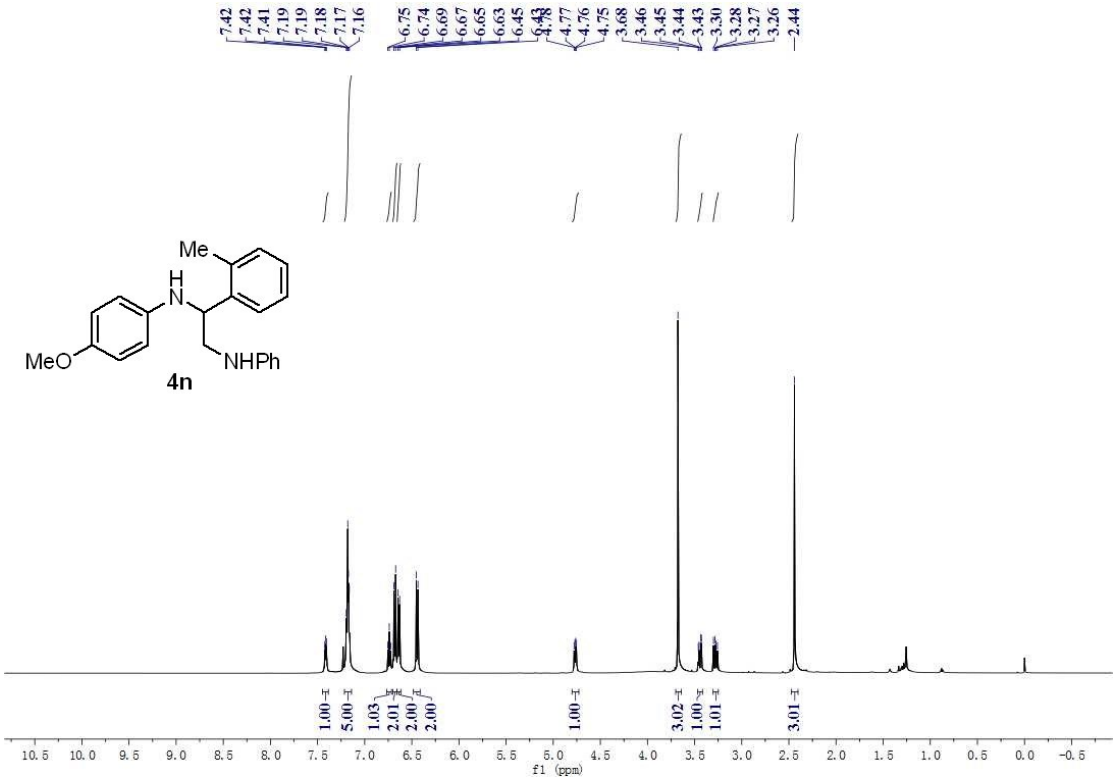
58.05
55.75
50.99
F
H
N
MeO
NHPh
4m
f1 (ppm)


F
H
N
MeO
NHPh

4m

-112.27
f1 (ppm)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6.74
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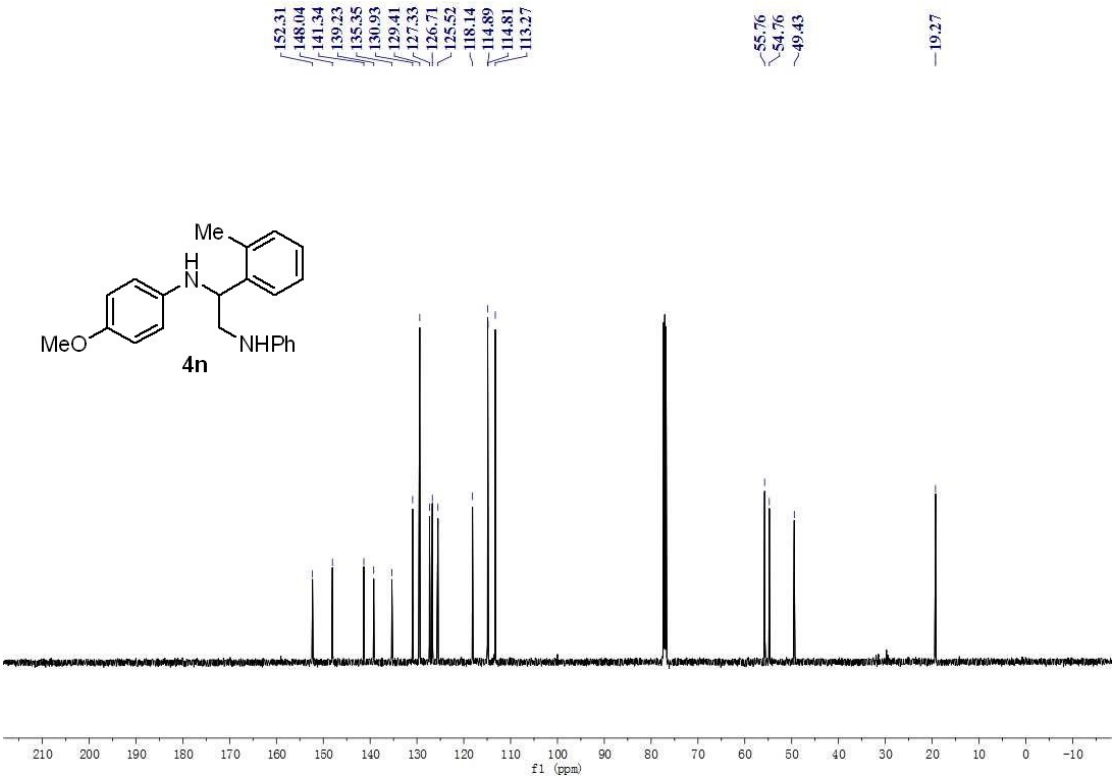
6.63
6.45
4.77
4.76
4.75
3.68
3.46
3.45
3.44
3.43
3.30
3.28
3.27
3.26
2.44
1.00
5.00
1.03
2.01
2.00
2.00
1.00
3.02
1.00
1.01
3.01
f1 (ppm)

Me
H
N
MeO
NHPh

4n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125.52
118.14
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54.76
49.43
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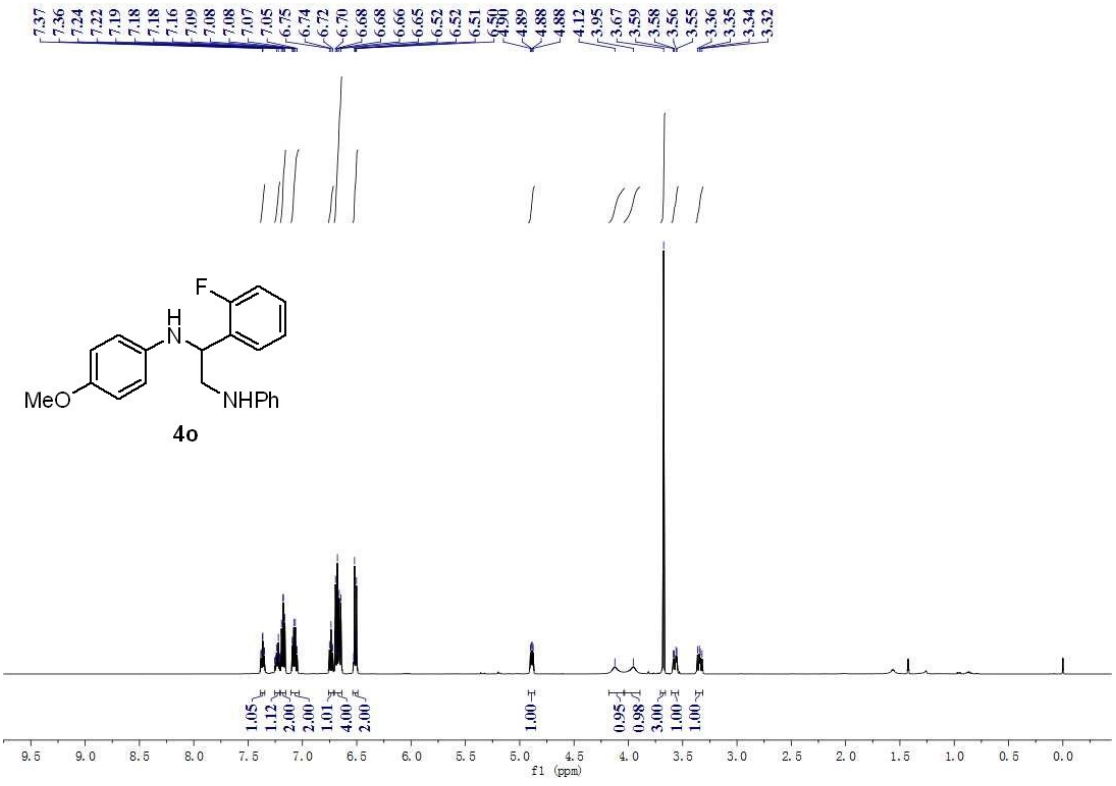
Me
H
N
MeO
NHPh
4n
f1 (ppm)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6.70
6.68
6.68
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6.65
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6.52
6.51
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4.88
4.12
3.95
3.67
3.59
3.58
3.56
3.55
3.36
3.35
3.34
3.32
F
H
N
MeO
NHPh
4o
1.05
1.12
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2.00
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4.00
2.00
1.00
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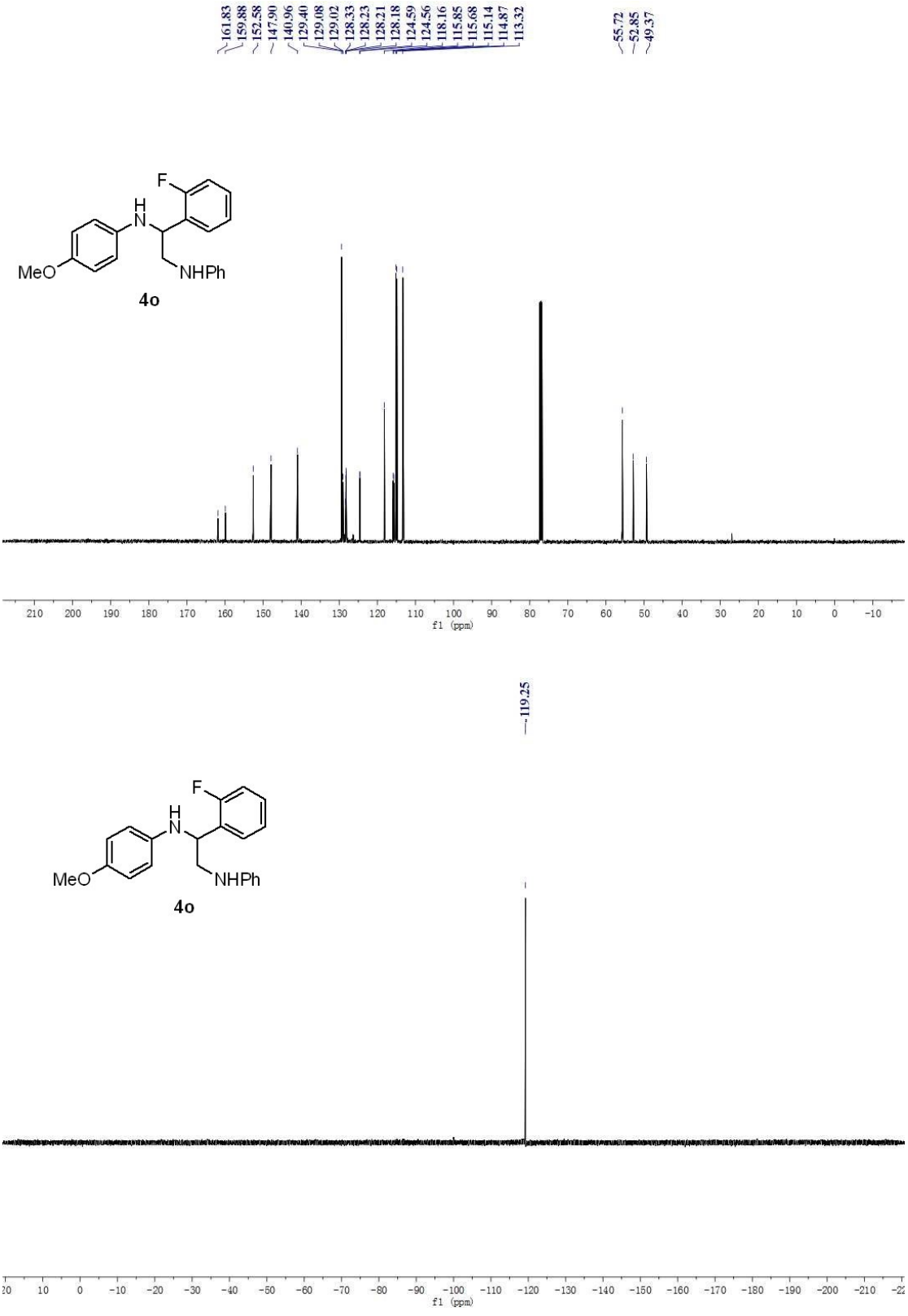
0.98
3.00
1.00
1.00
f1 (ppm)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124.56
118.16
115.85
115.68
115.14
114.87
113.32
55.72
52.85
49.37
F
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NHPh
4o
f1 (ppm)
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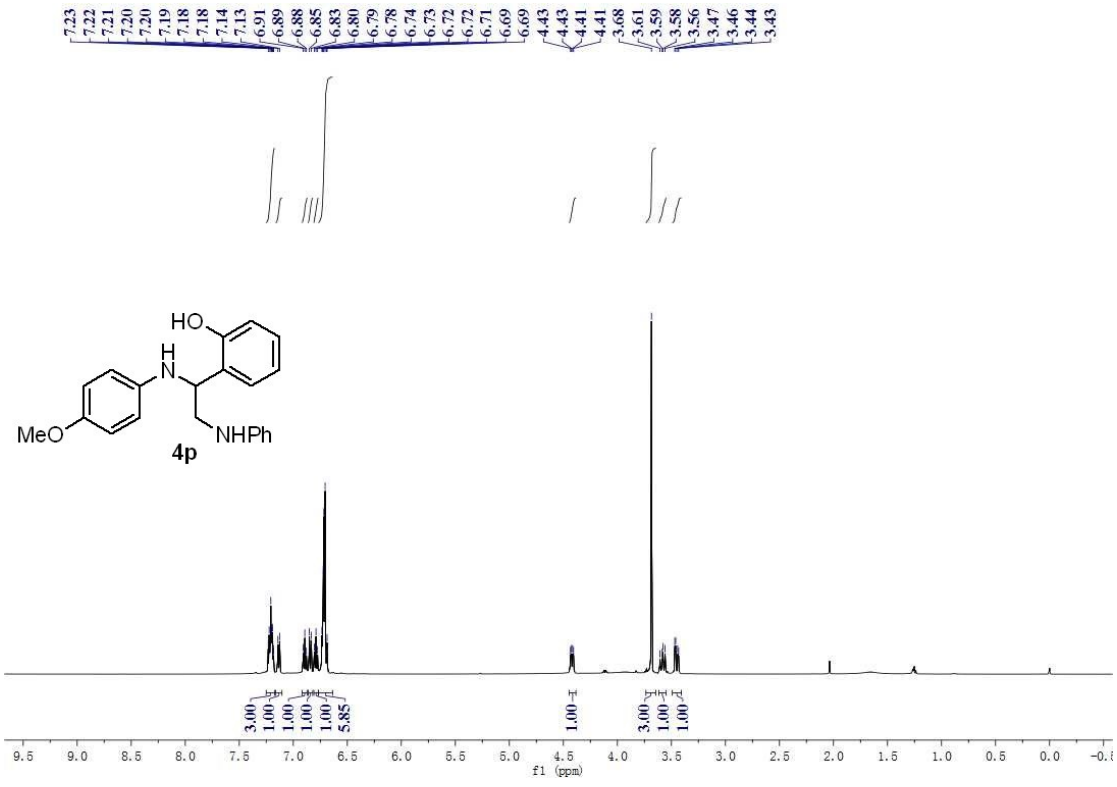
H
N
MeO
NHPh
4o
f1 (ppm)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4.41
4.41
3.68
3.61
3.59
3.58
3.56
3.47
3.46
3.44
3.43
HO
H
N
MeO
NHPh
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3.00
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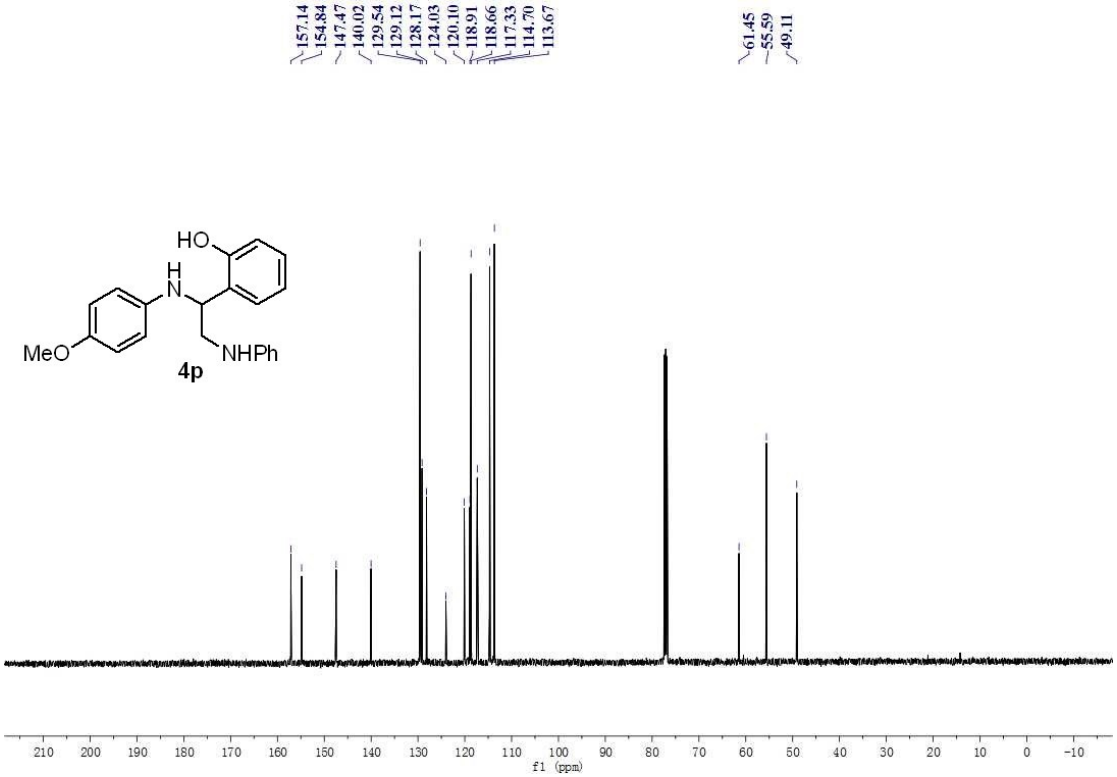
1.00
f1 (ppm)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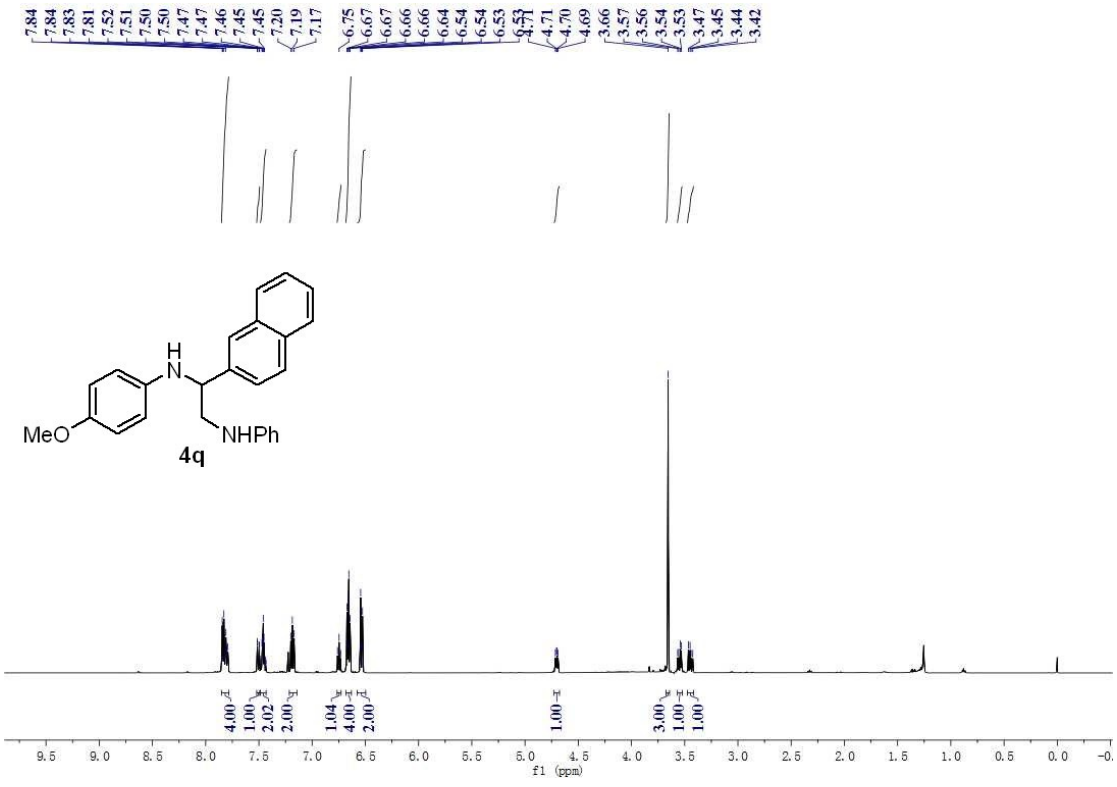
113.67
61.45
55.59
49.11
HO
H
N
MeO
NHPh
4p
f1 (ppm)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7.45
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6.67
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6.66
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6.54
6.53
6.53
4.71
4.71
4.70
4.69
3.66
3.57
3.56
3.54
3.53
3.47
3.45
3.44
3.42
H
N
MeO
NHPh
4q
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2.00
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4.00
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1.00
3.00
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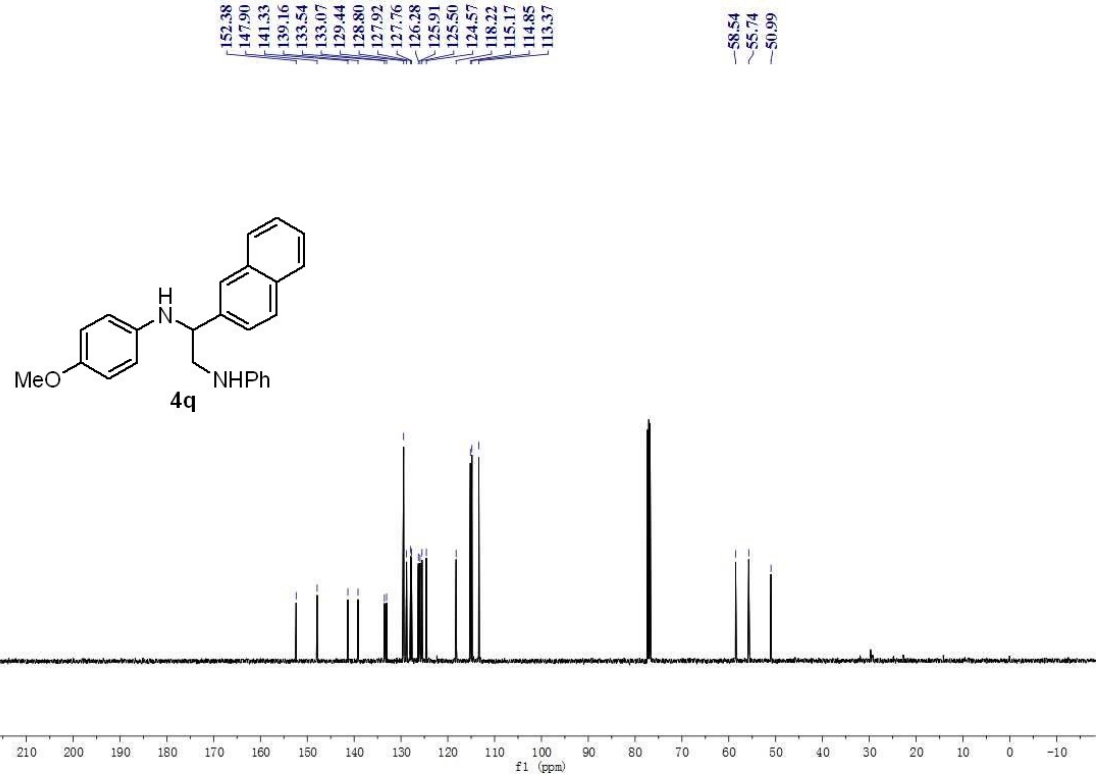
1.00
f1 (ppm)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125.50
124.57
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113.37
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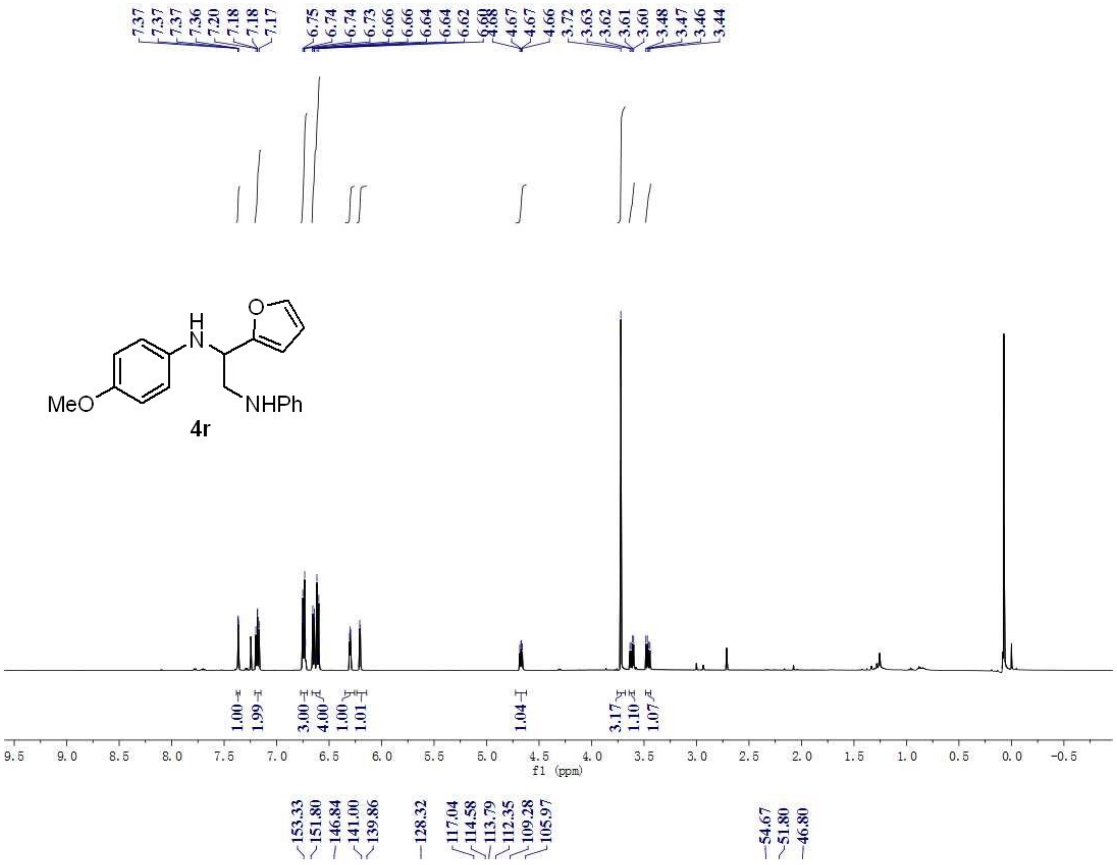
H
N
MeO
NHPh
4q
f1 (ppm)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6.62
4.67
4.67
4.66
3.72
3.63
3.62
3.61
3.60
3.48
3.47
3.46
3.44
MeO
NHPh
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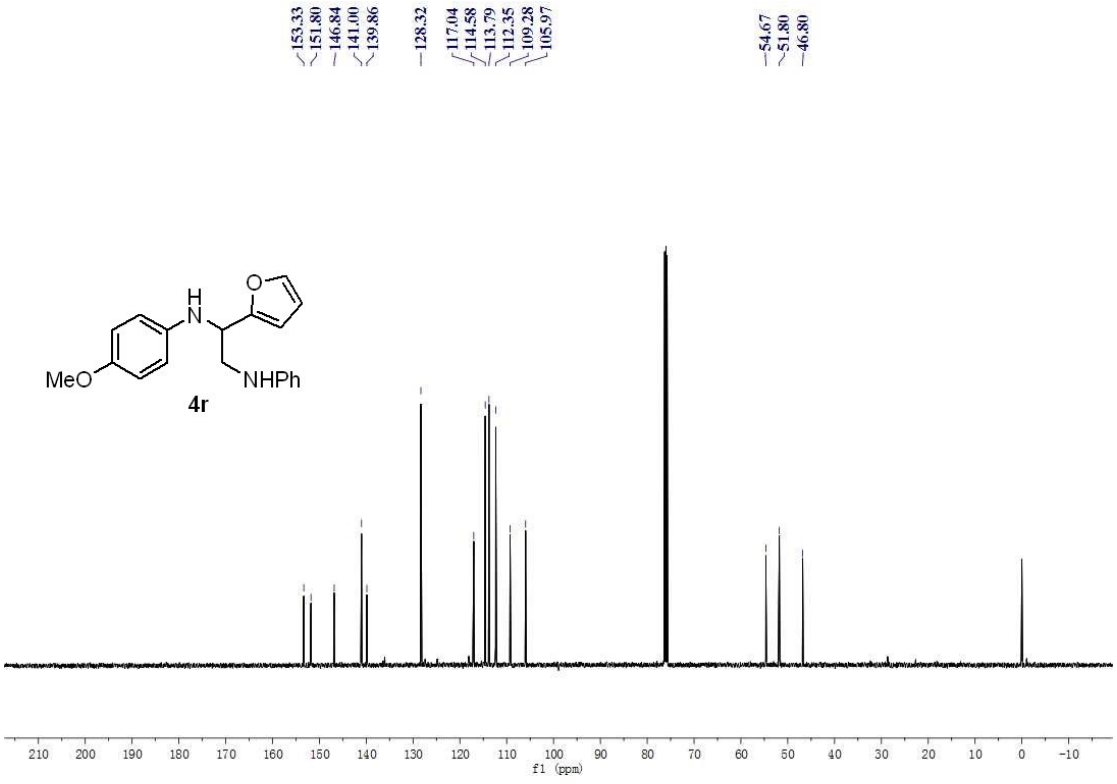
3.00
4.00
1.00
1.01
1.04
3.17
1.10
1.07
f1 (ppm)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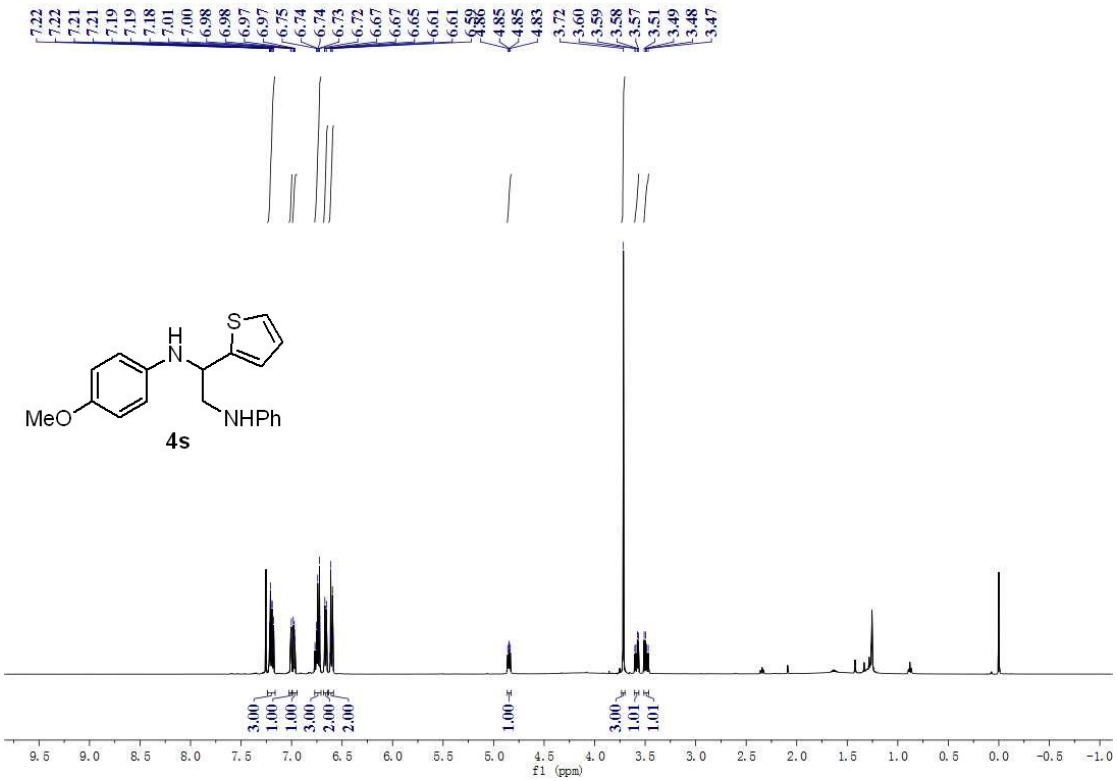
46.80
MeO
NHPh
4r
f1 (ppm)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3.57
3.51
3.49
3.48
3.47
H
N
S
MeO
NHPh
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1.00
3.00
2.00
2.00
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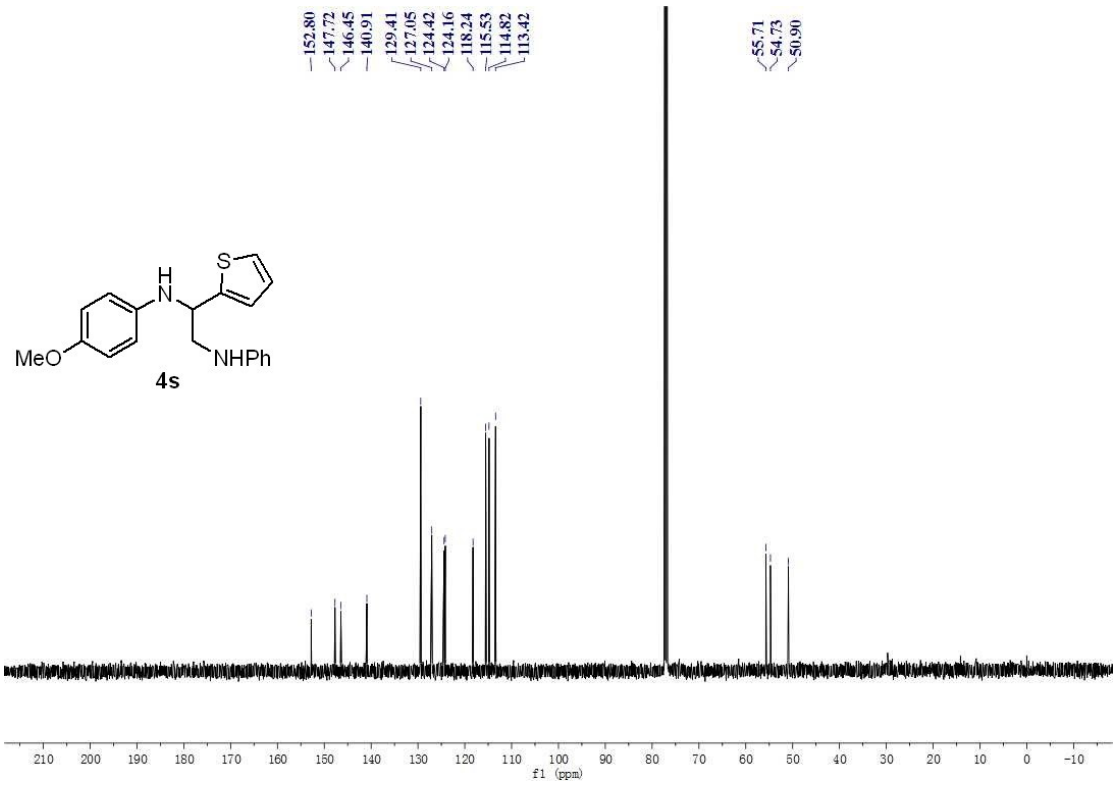
3.00
1.01
1.01
f1 (ppm)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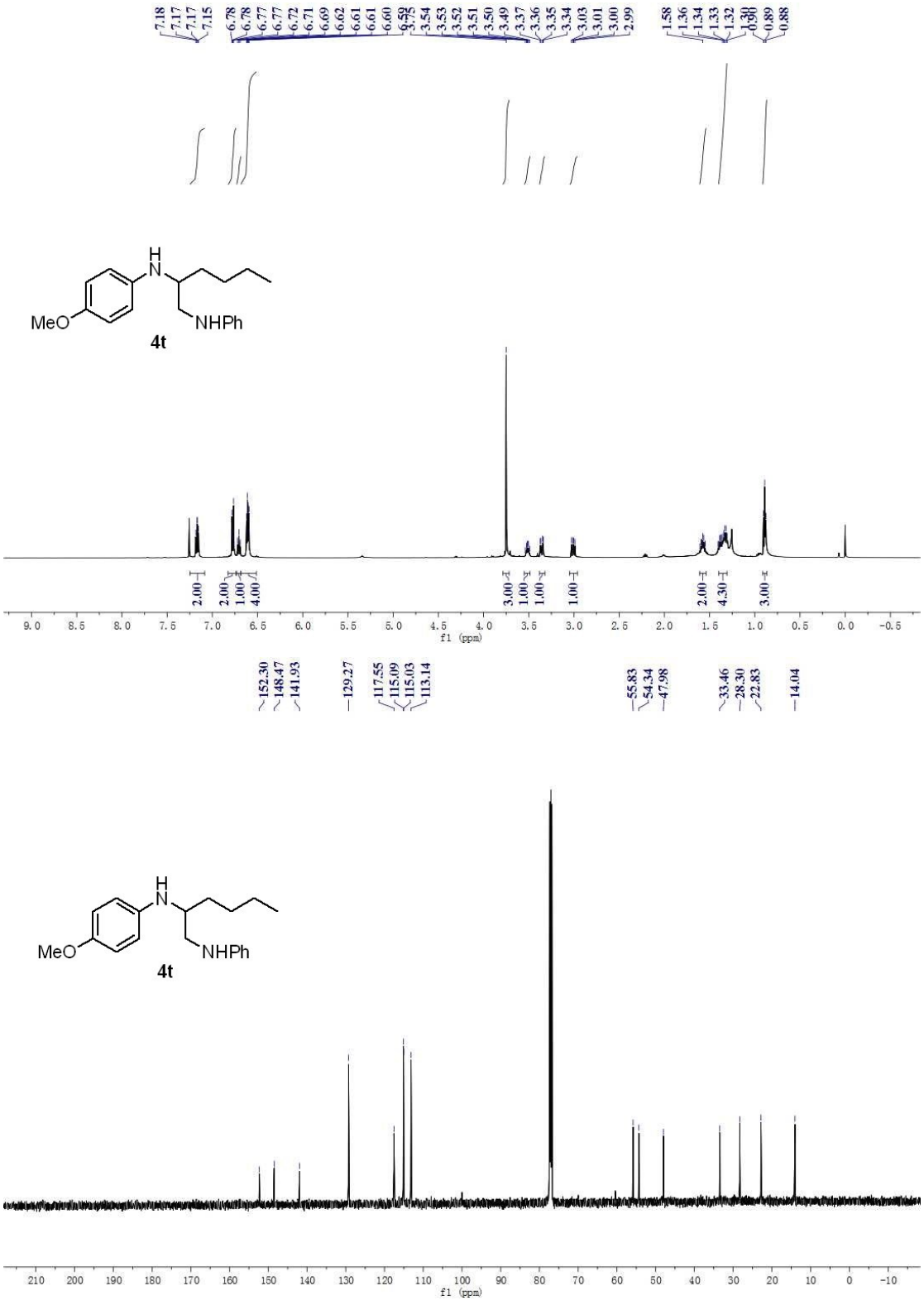
N
S
MeO
NHPh
4s
f1 (ppm)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1.31
0.90
0.89
0.88
H
N
MeO
NHPh
4t
2.00
2.00
1.00
4.00
3.00
1.00
1.00
1.00
2.00
4.30
3.00
f1 (ppm)
152.30
148.47
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129.27
117.55
115.09
115.03
113.14
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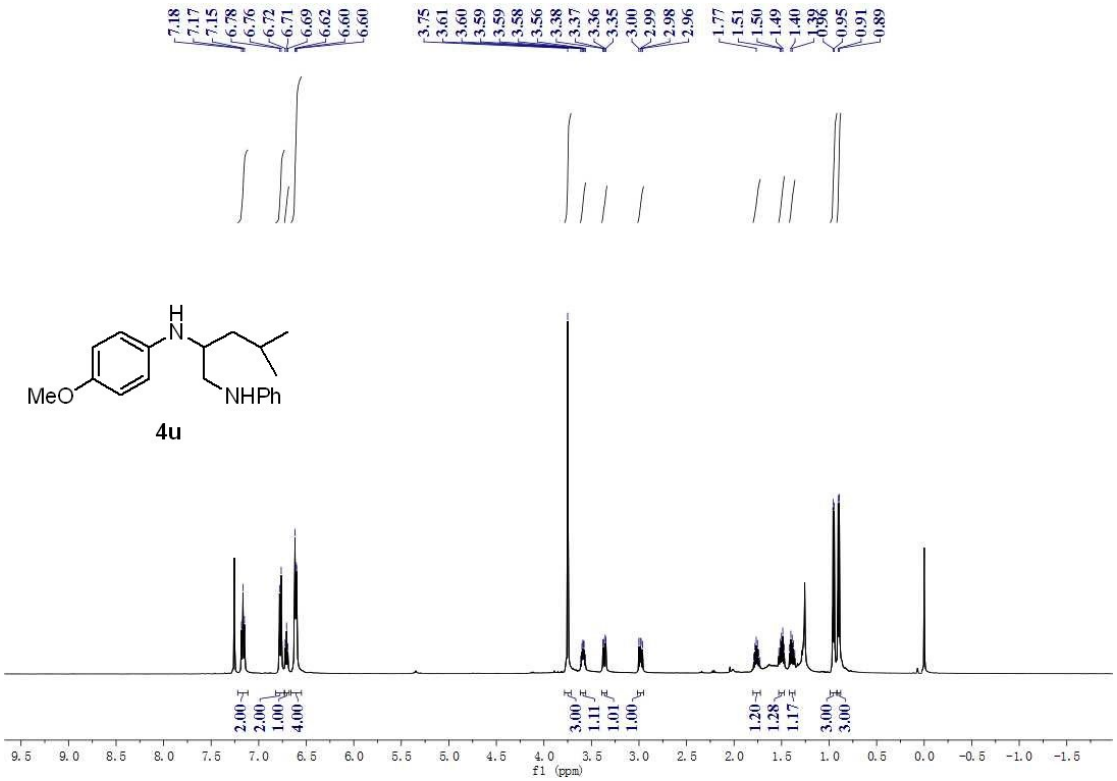
MeO
NHPh
4t
f1 (ppm)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2.98
2.96
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1.50
1.49
1.40
1.39
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0.95
0.91
0.89
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N
MeO
NHPh
4u
2.00
2.00
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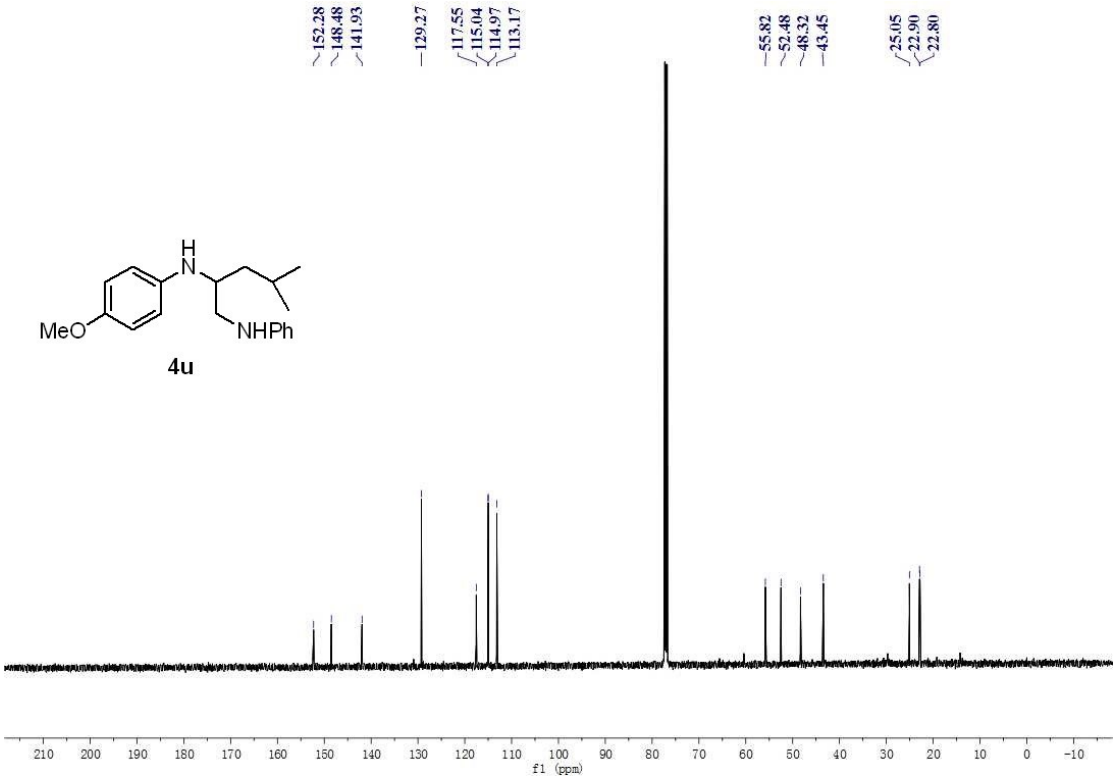
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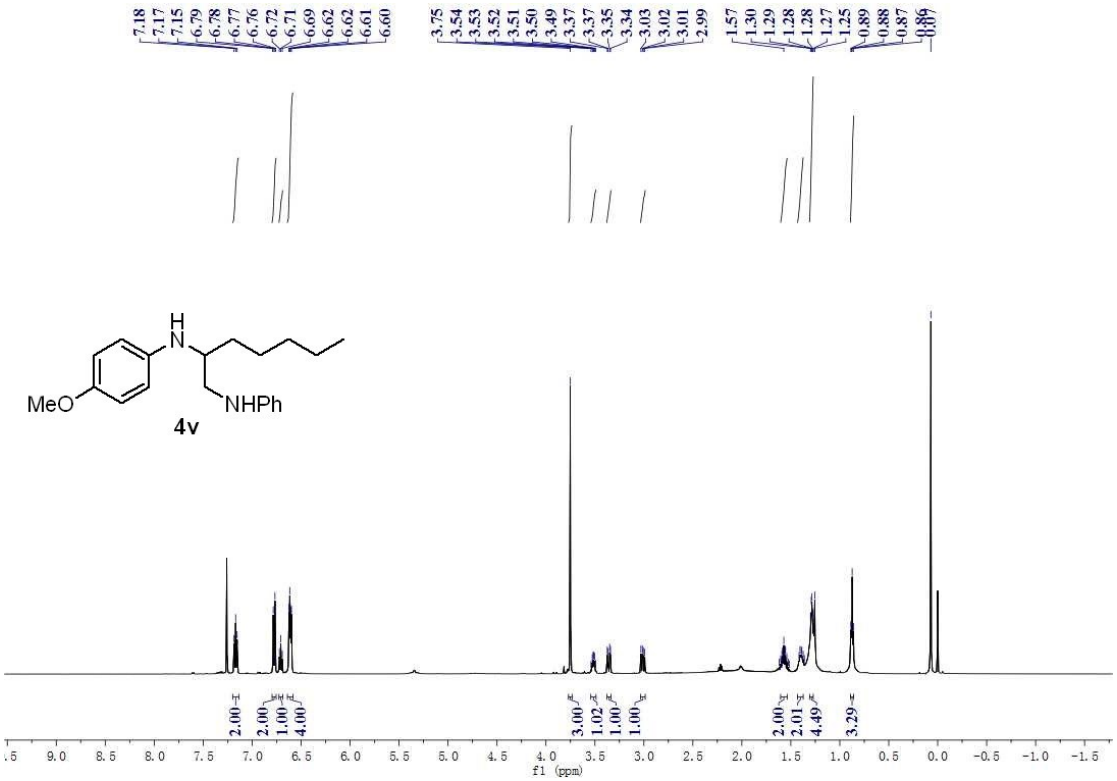
N
MeO
NHPh
4u
f1 (ppm)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6.62
6.61
6.60
3.75
3.54
3.53
3.52
3.51
3.50
3.49
3.37
3.37
3.35
3.34
3.03
3.02
3.01
2.99
1.57
1.30
1.29
1.28
1.28
1.27
1.25
0.89
0.88
0.87
0.86
0.00
H
N
MeO
NHPh
4v
2.00
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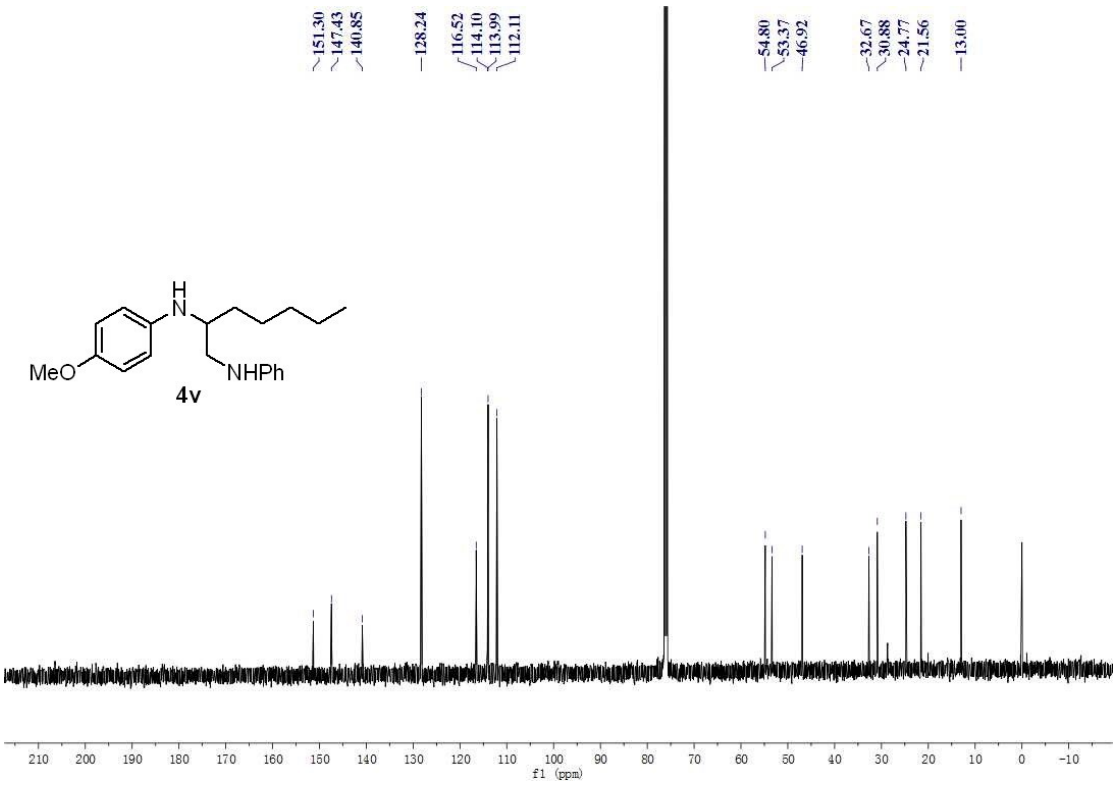
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H
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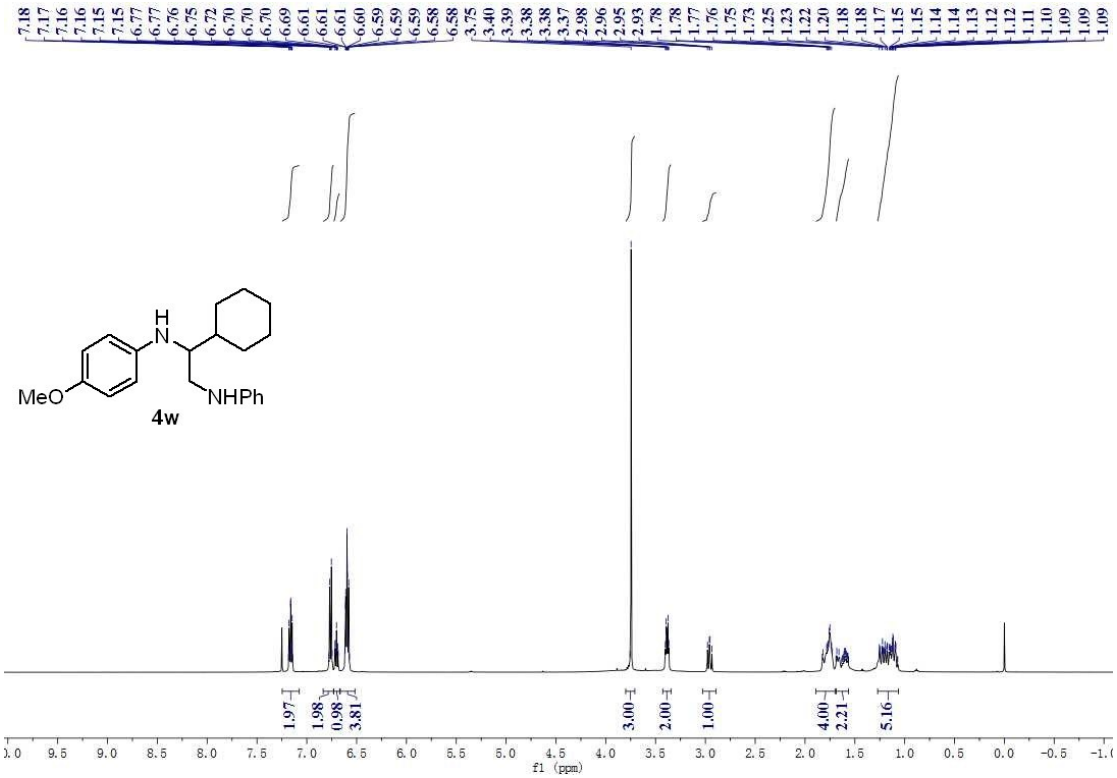
MeO
NHPh
4v
f1 (ppm)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3.75 3.40 3.39 3.38 3.38 3.37 2.98 2.96 2.95 2.93 1.78 1.78 1.77 1.76 1.75 1.73 1.25 1.23 1.22 1.20 1.18 1.18 1.17 1.15 1.15 1.14 1.14 1.13 1.12 1.12 1.11 1.10 1.09 1.09 1.09
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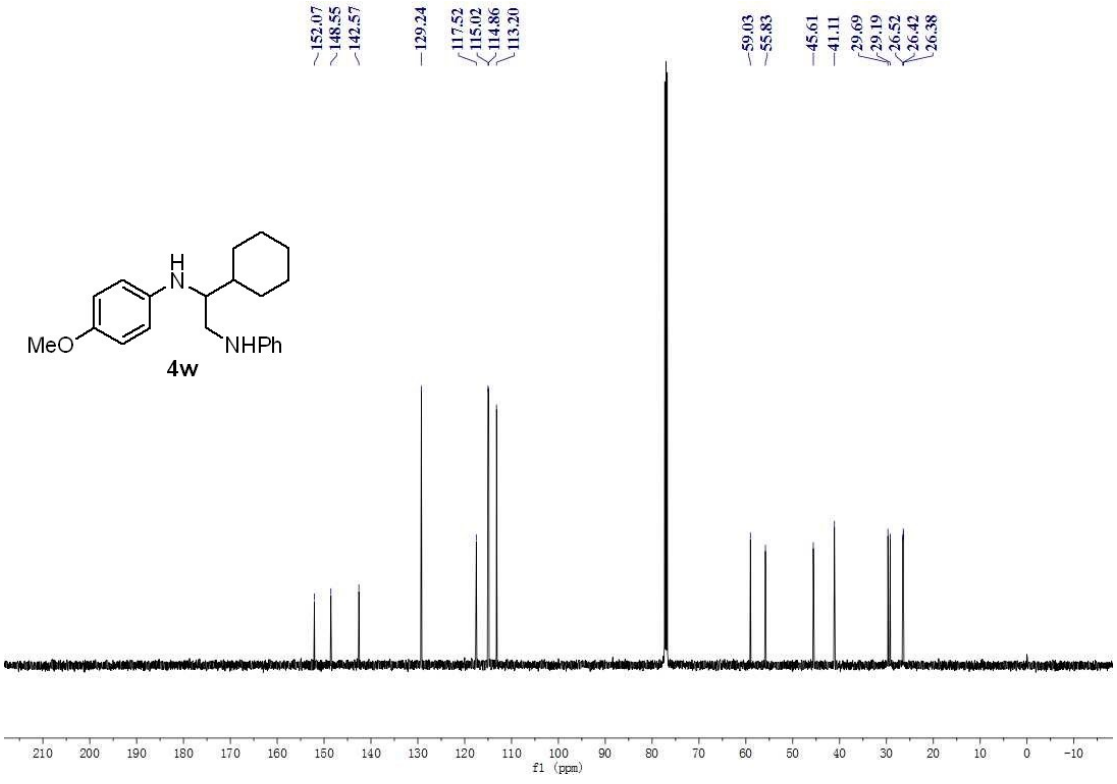
MeO
NHPh
4w
1.97 1.98 0.98 3.81 3.00 2.00 1.00 4.00 2.21 5.16
f1 (ppm)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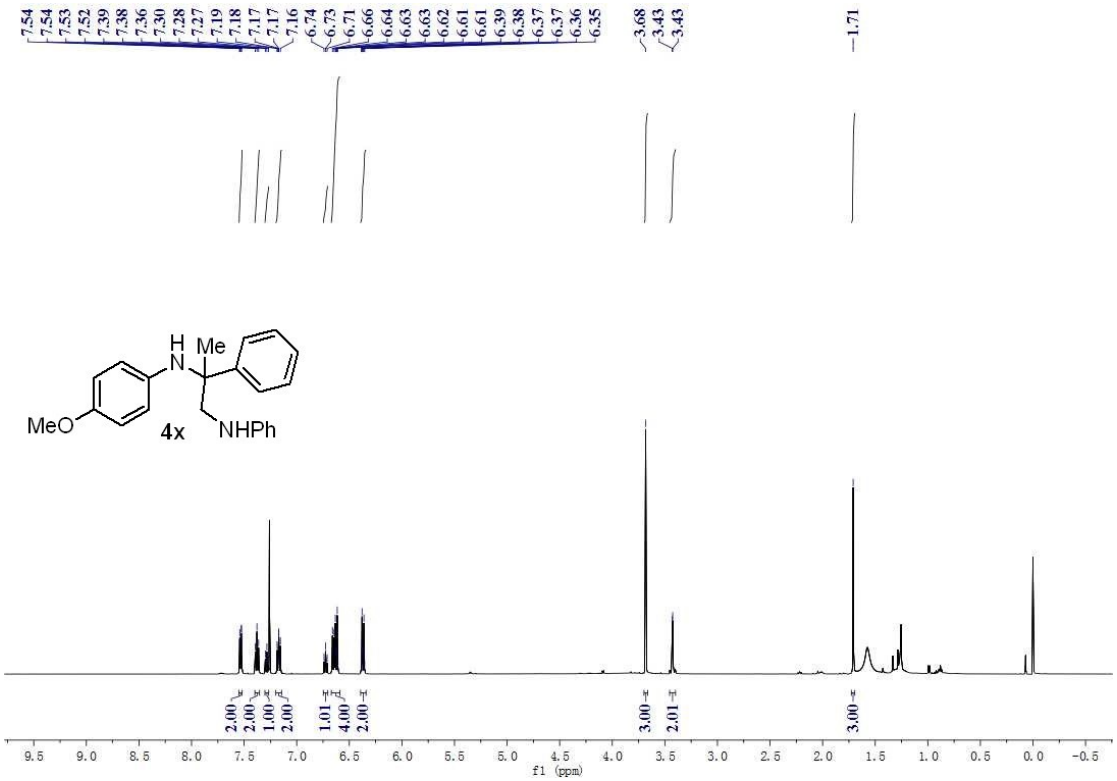
H
N
MeO
NHPh
4w
f1 (ppm)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7.19
7.18
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7.16
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6.64
6.63
6.63
6.62
6.61
6.61
6.39
6.38
6.37
6.37
6.36
6.35
3.68
3.43
3.43
1.71
H
N
Me
MeO
4x
NHPh
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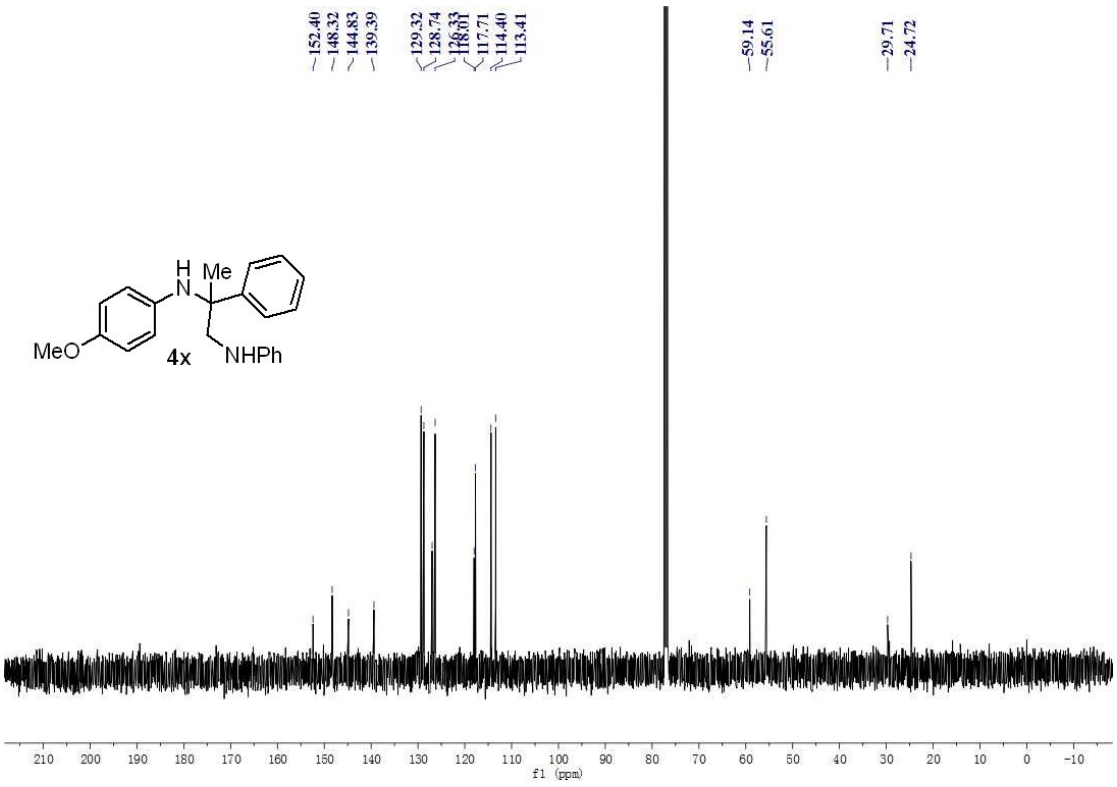
1.00
2.00
1.01
4.00
2.00
3.00
2.01
3.00
f1 (ppm)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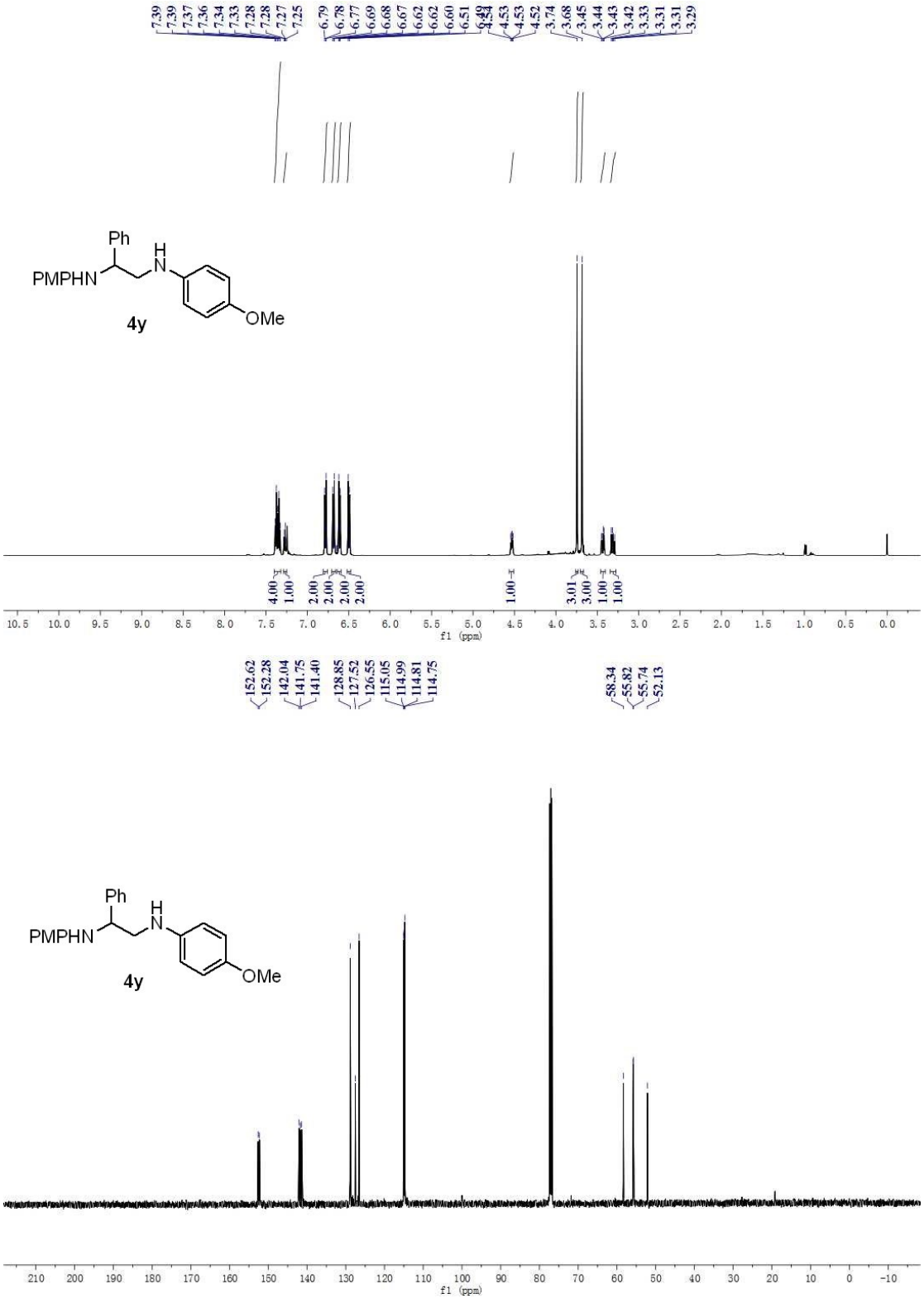
N
Me
MeO
4x
NHPh
f1 (ppm)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4.53
4.53
4.52
3.74
3.68
3.45
3.44
3.43
3.42
3.33
3.31
3.31
3.29
Ph
H
N
PMPHN
OMe
4y
4.00
1.00
2.00
2.00
2.00
2.00
1.00
3.01
3.00
1.00
1.00
f1 (ppm)
152.62
152.28
142.04
141.75
141.40
128.85
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126.55
115.05
114.99
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58.34
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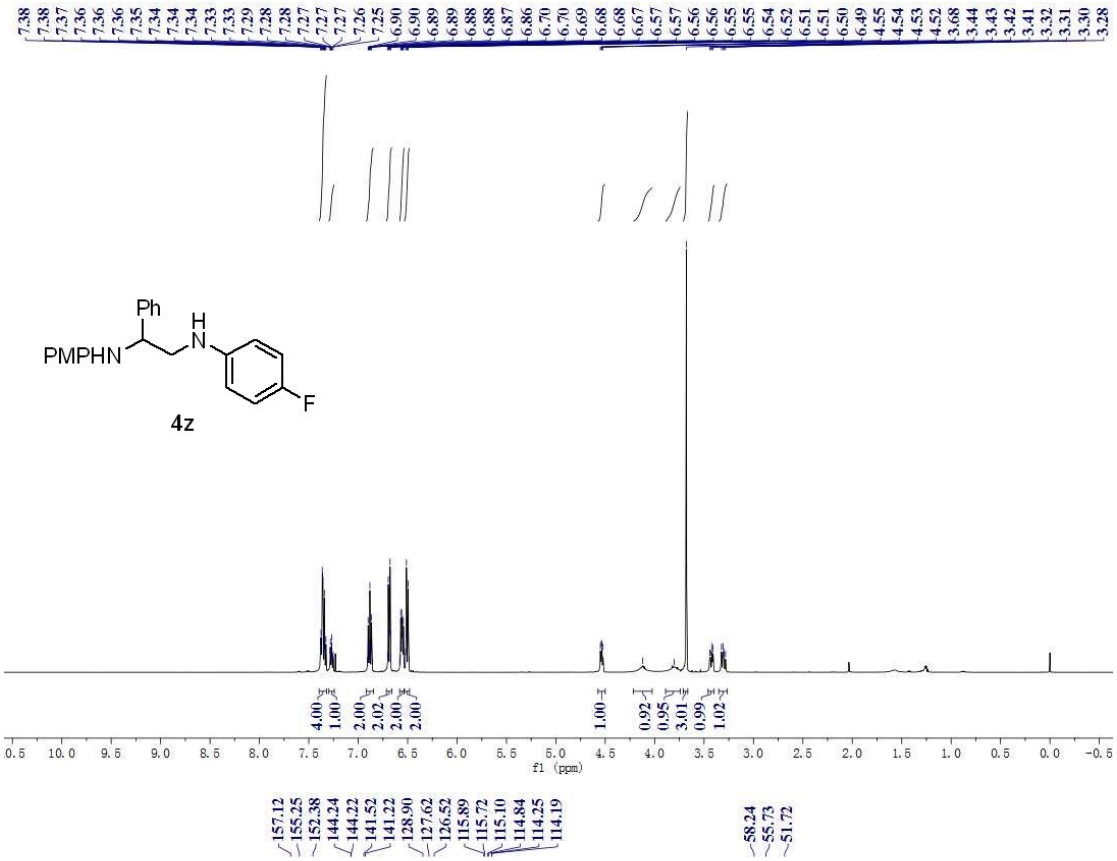
Ph
H
N
PMPHN
OMe
4y
f1 (ppm)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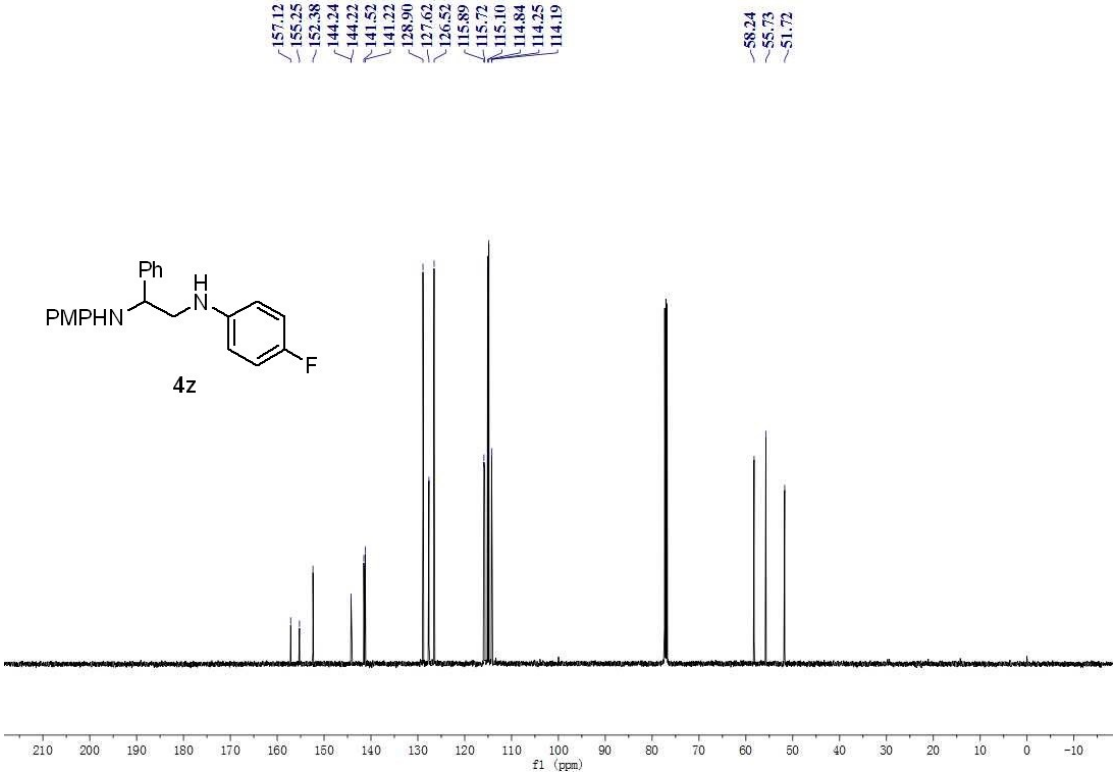
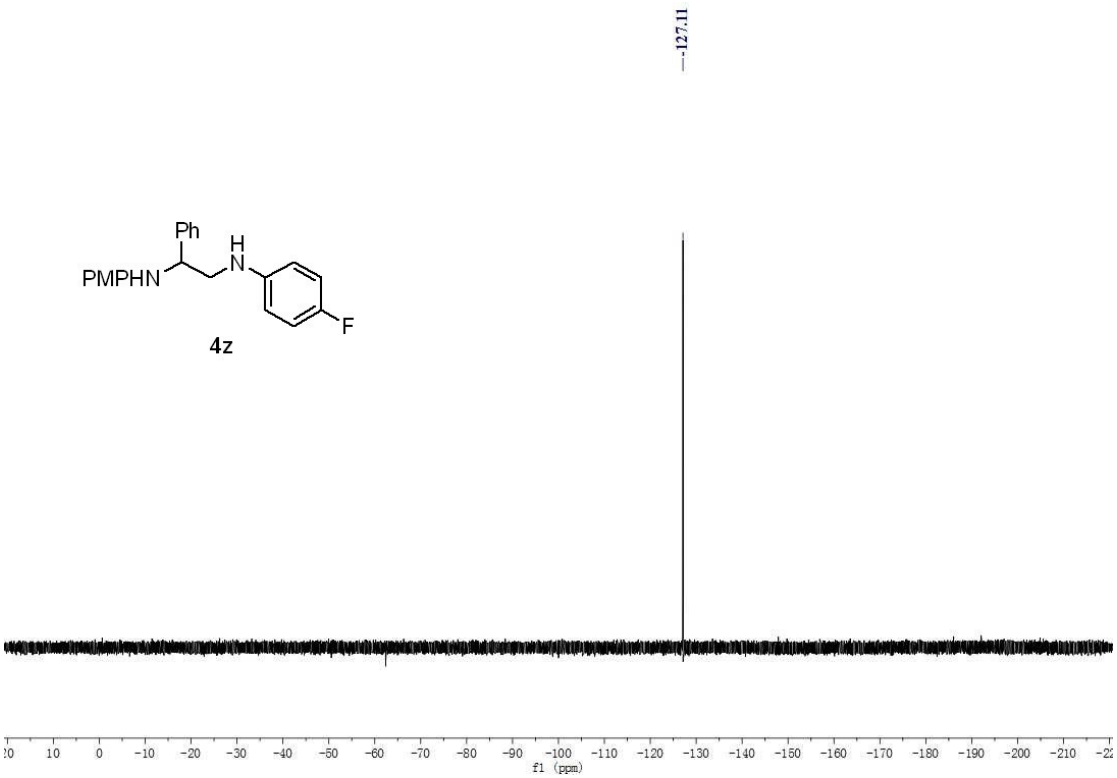
Ph
PMPHN
H
N
F
4z
4.00 1.00 2.00 2.02 2.00 2.00 1.00 0.92 0.95 3.01 0.99 1.02
f1 (ppm)


157.12 155.25 152.38 144.24 144.22 141.52 141.22 128.90 127.62 126.52 115.89 115.72 115.10 114.84 114.25 114.19 58.24 55.73 51.72
Ph
PMPHN
H
N
F
4z
f1 (ppm)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Ph
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F
4z
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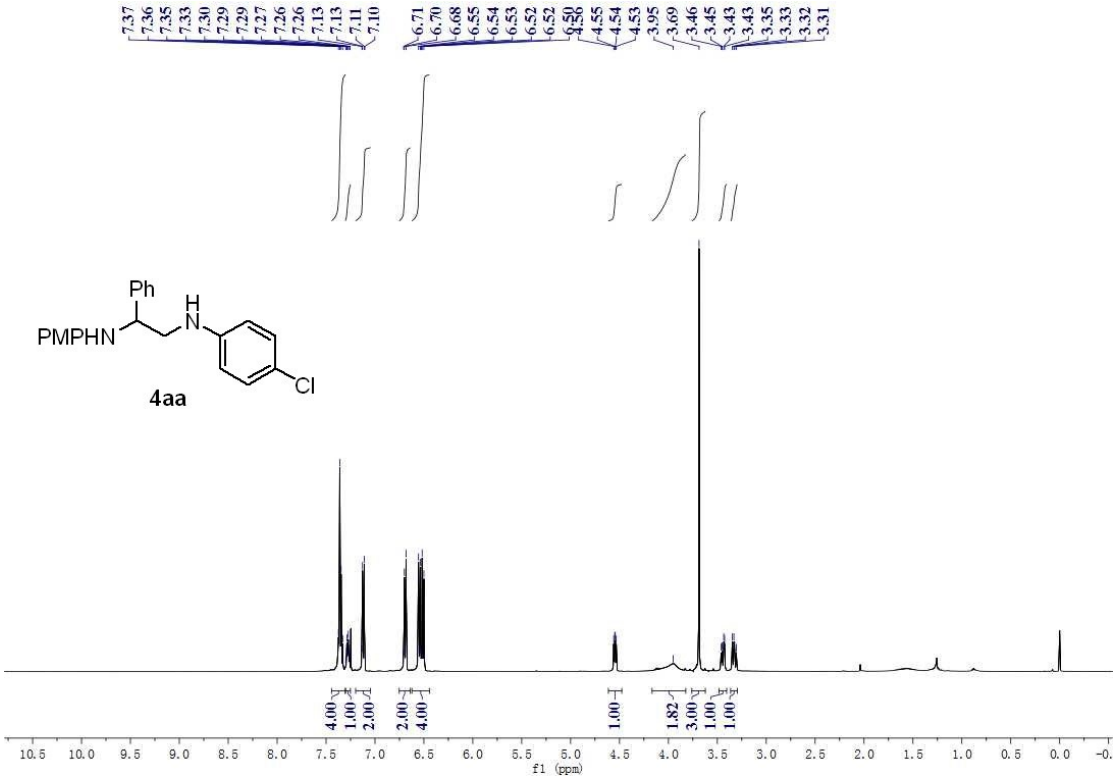
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4.53
3.95
3.69
3.46
3.45
3.43
3.43
3.35
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3.32
3.31
Ph
H
N
PMPHN
Cl
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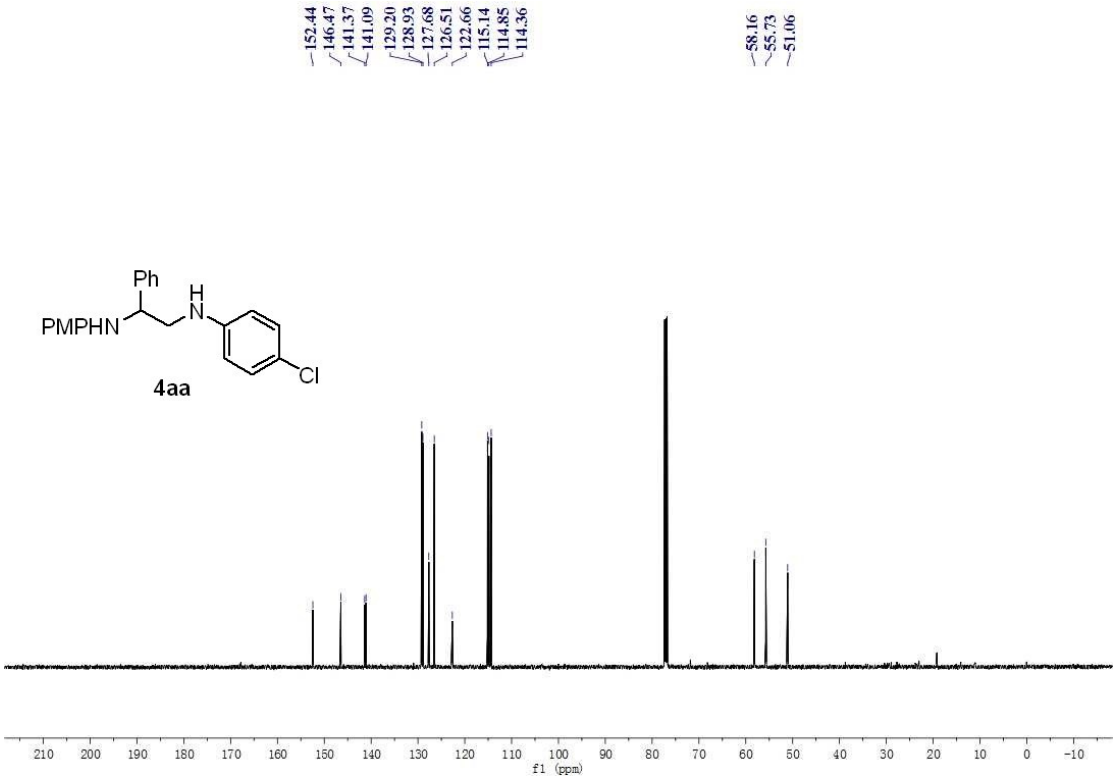
1.00
f1 (ppm)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126.51
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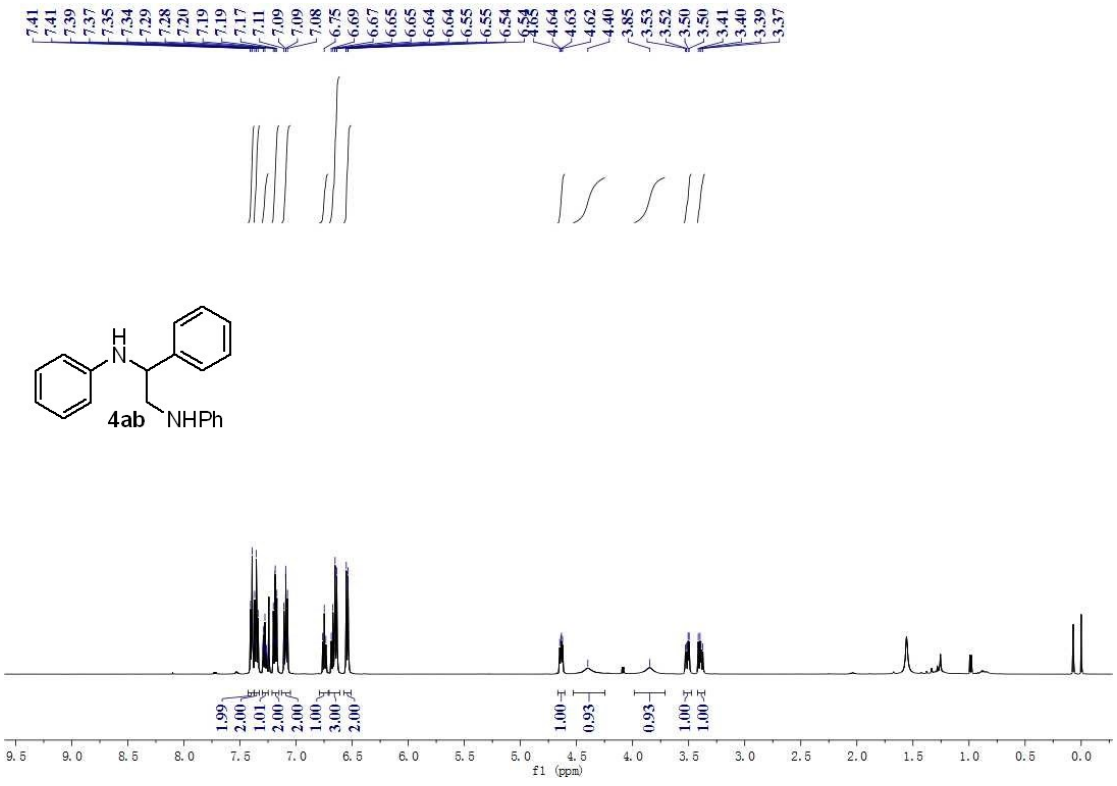
58.16
55.73
51.06
Ph
H
N
PMPHN
Cl
4aa
f1 (ppm)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7.09
7.08
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6.69
6.67
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6.64
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4.63
4.62
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3.85
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3.52
3.50
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3.39
3.37
H
N
4ab
NHPh
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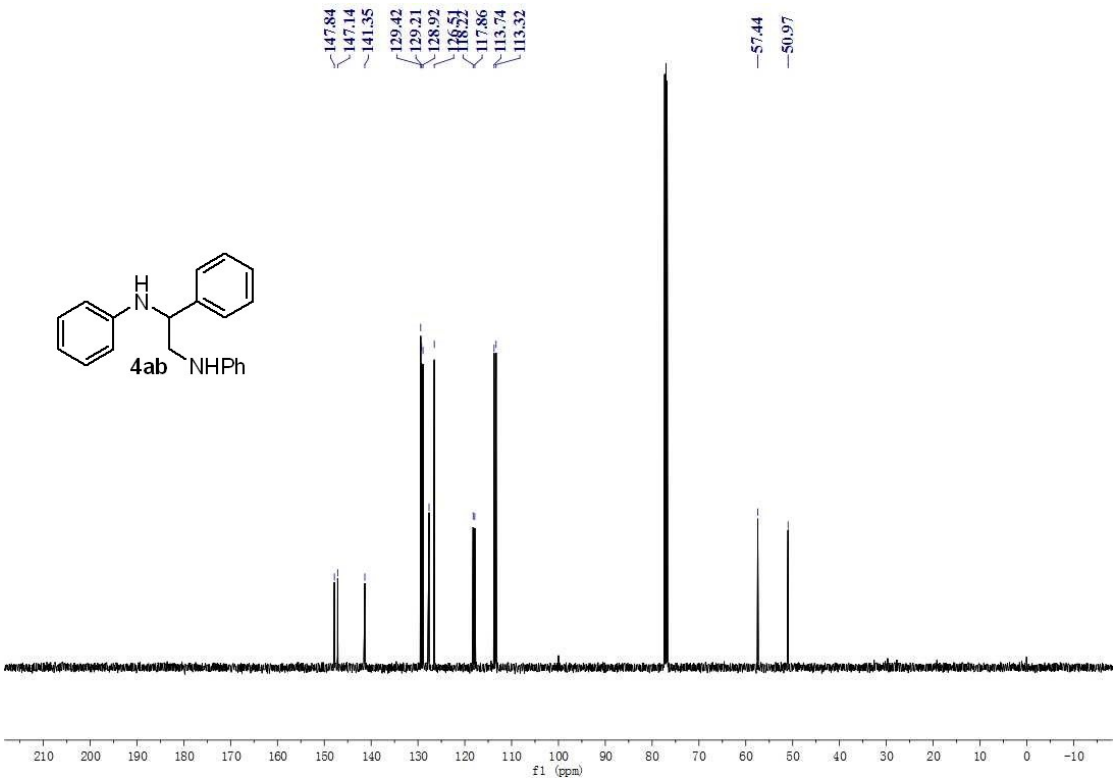
1.00
f1 (ppm)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57.44
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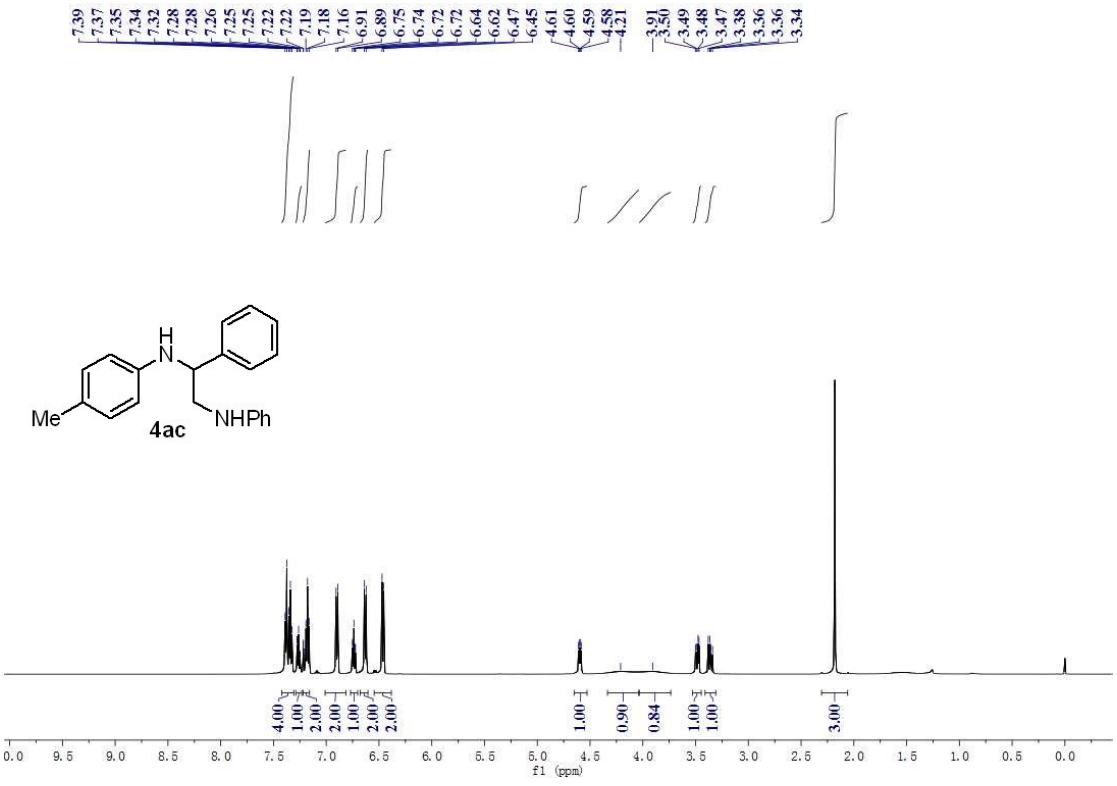
NHPh
f1 (ppm)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Me
4ac
NHPh
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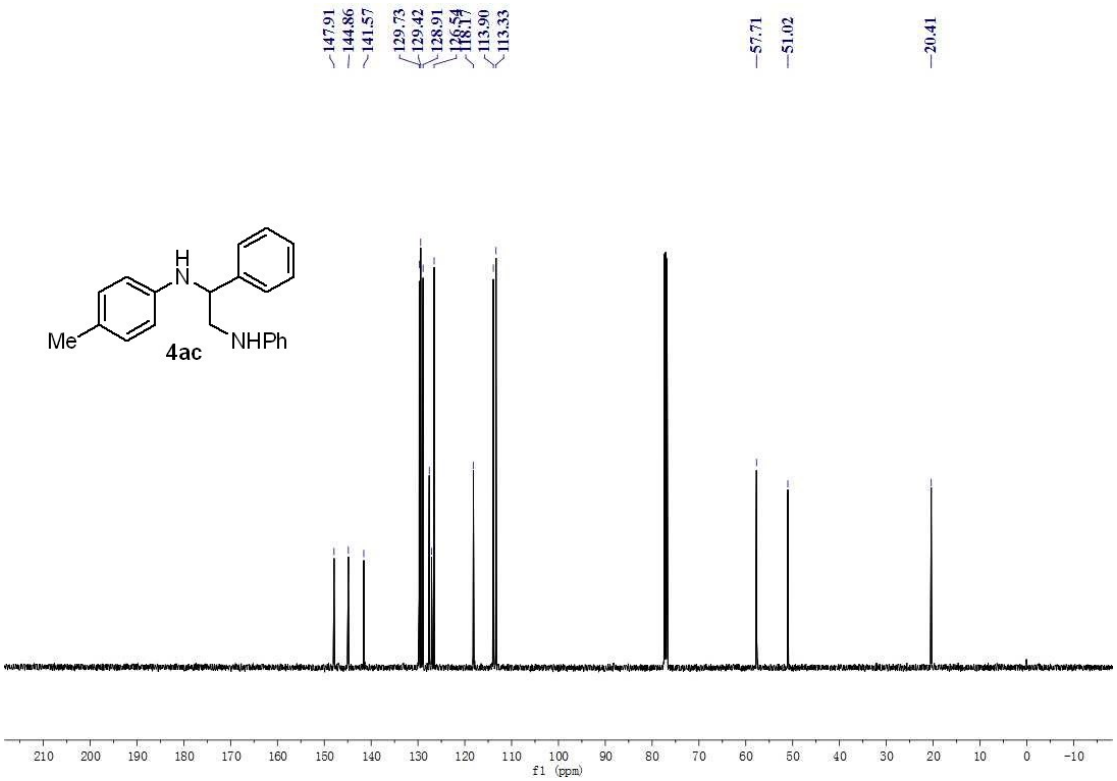
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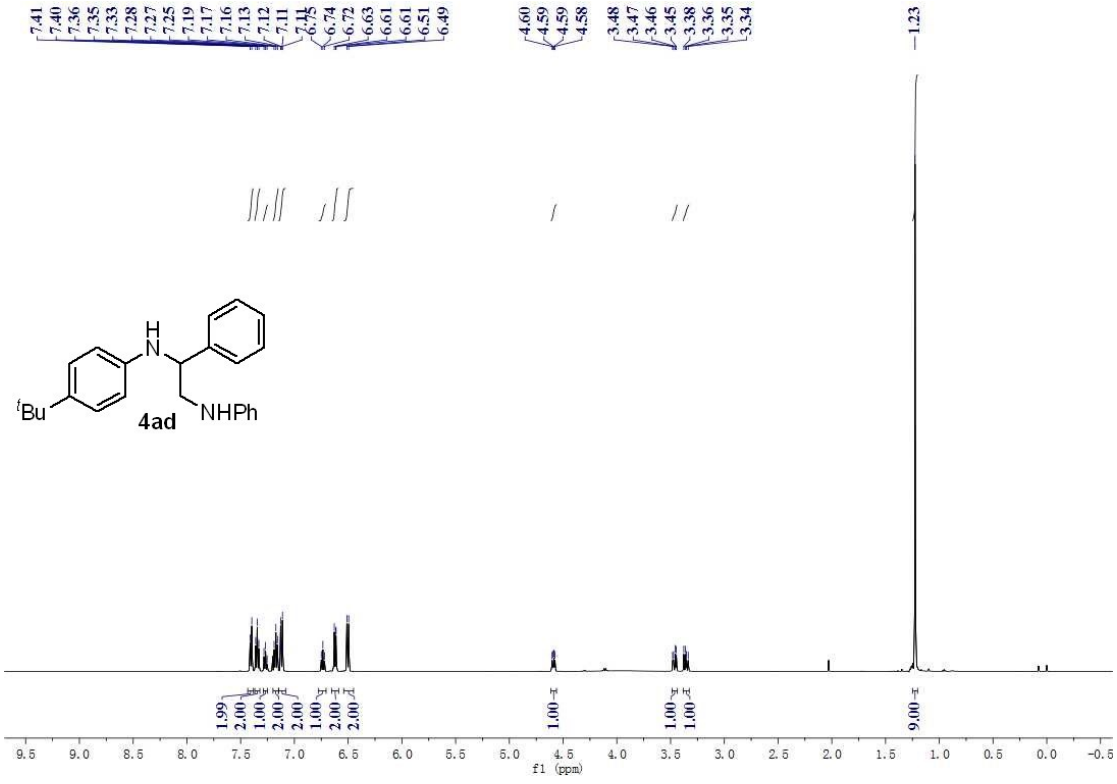
NHPh
4ac
f1 (ppm)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tBu
H
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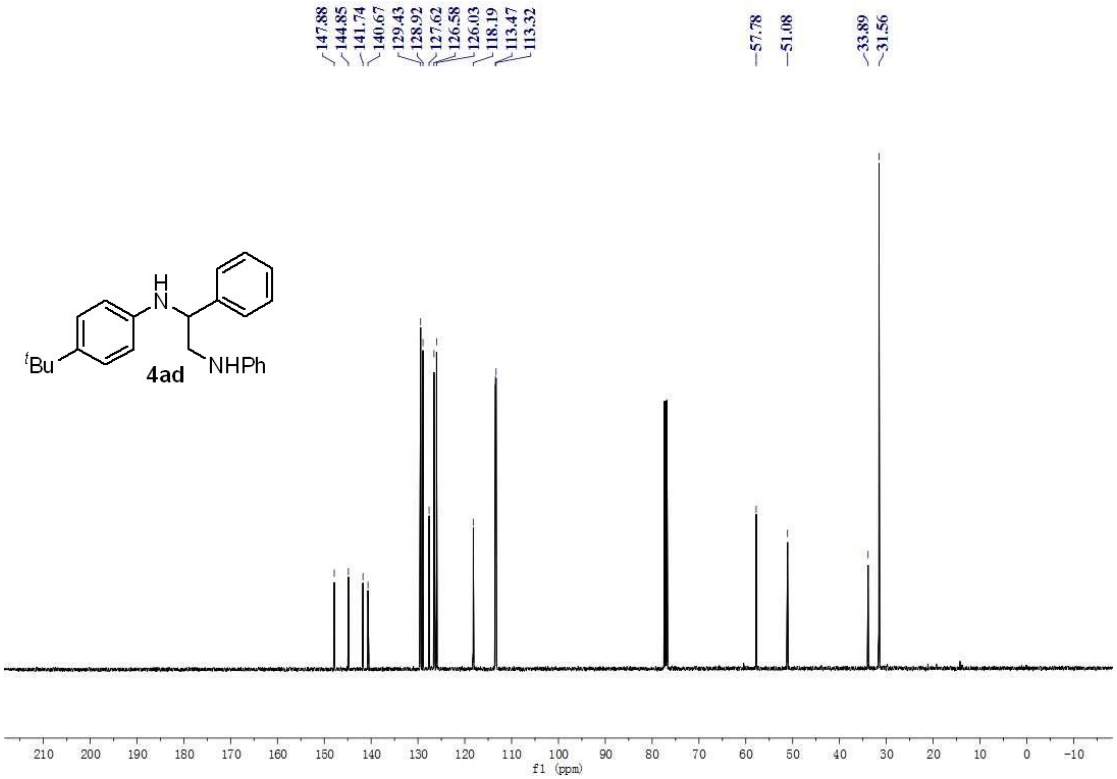
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tBu
H
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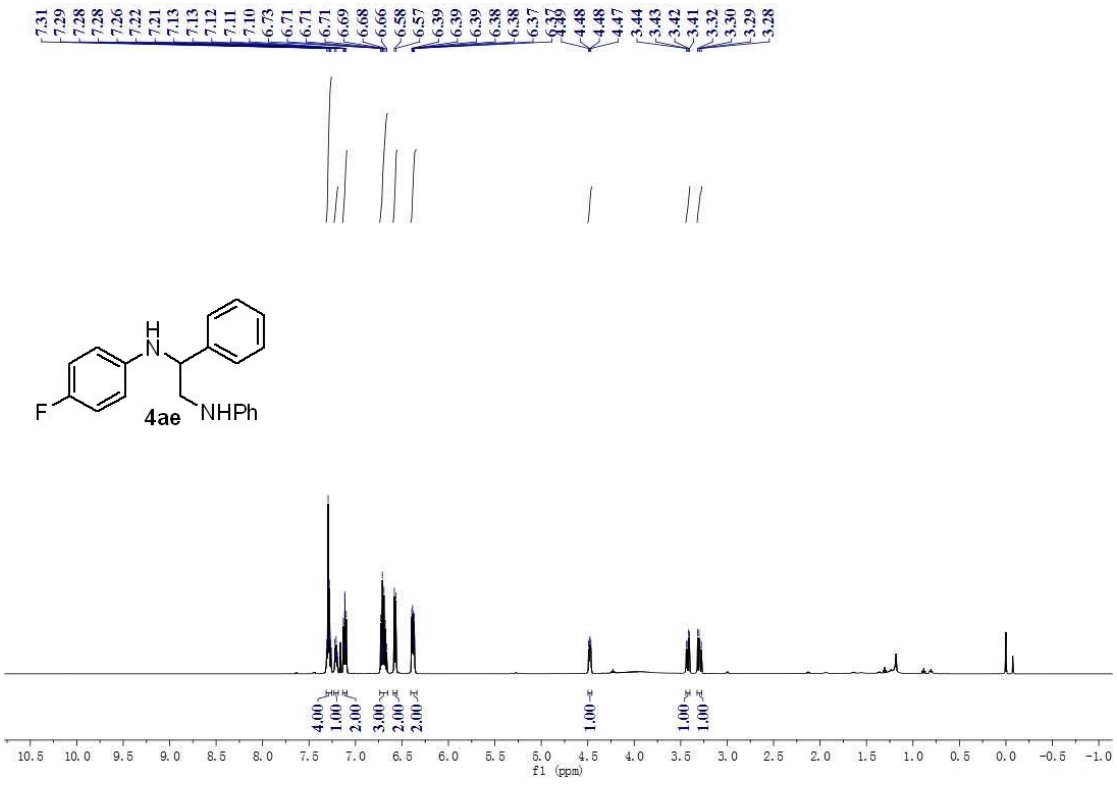
NHPh
4ad
f1 (ppm)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3.32
3.30
3.29
3.28
F
H
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1.00
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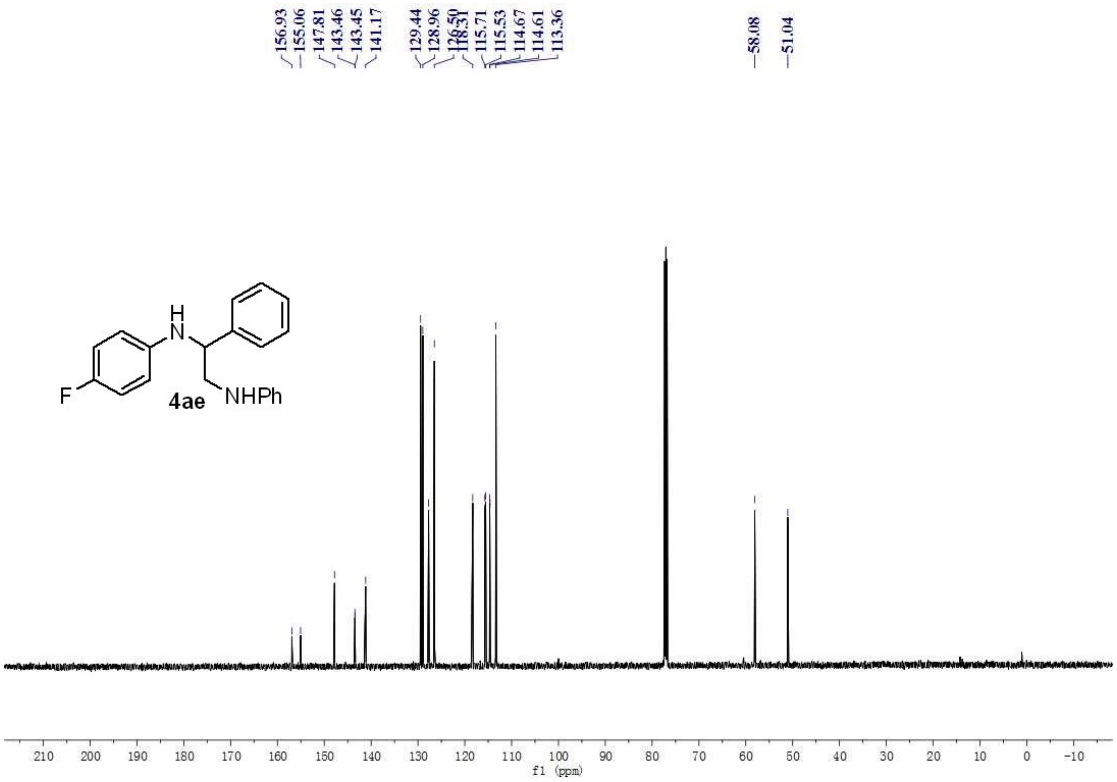
1.00
f1 (ppm)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114.67
114.61
113.36
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N
F
4ae
NHPh
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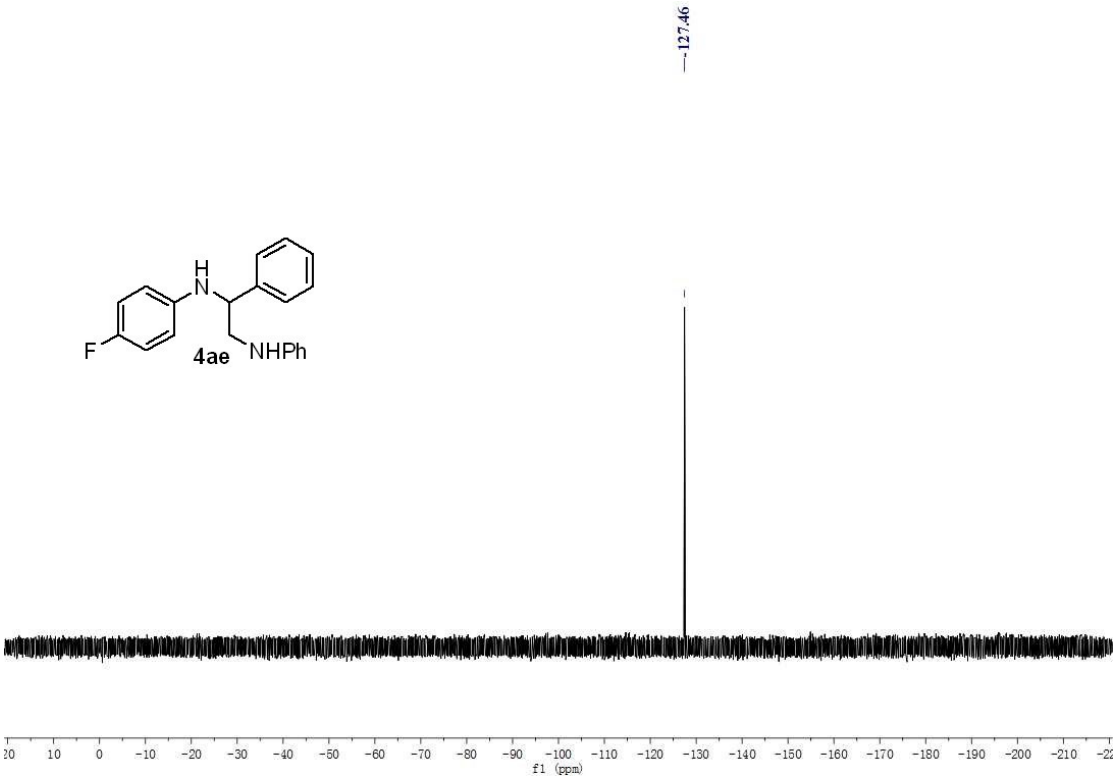
f1 (ppm)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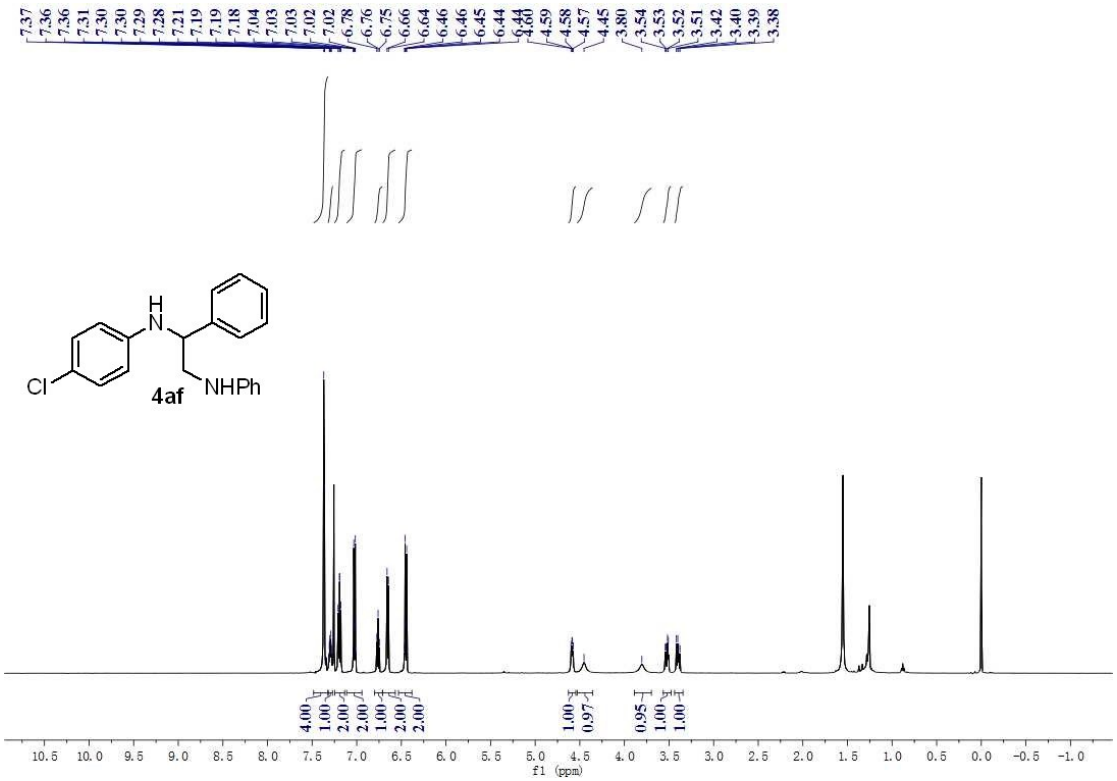
f1 (ppm)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3.38
Cl
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4af
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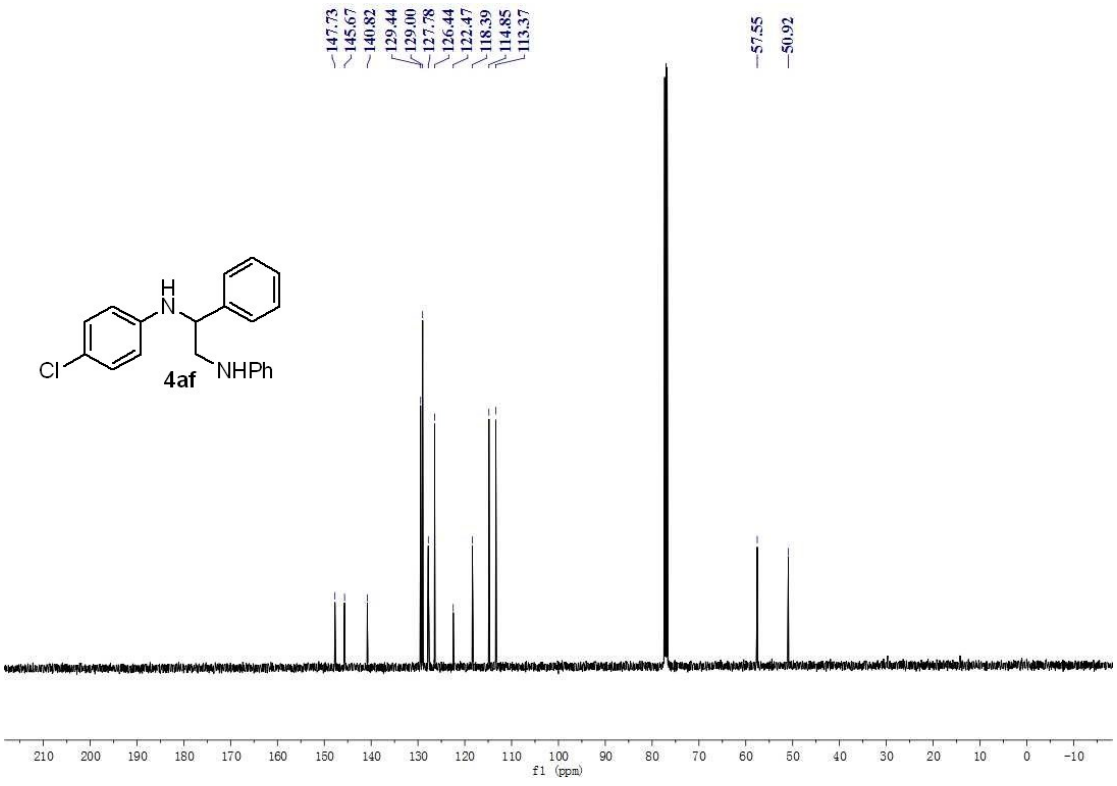
1.00
f1 (ppm)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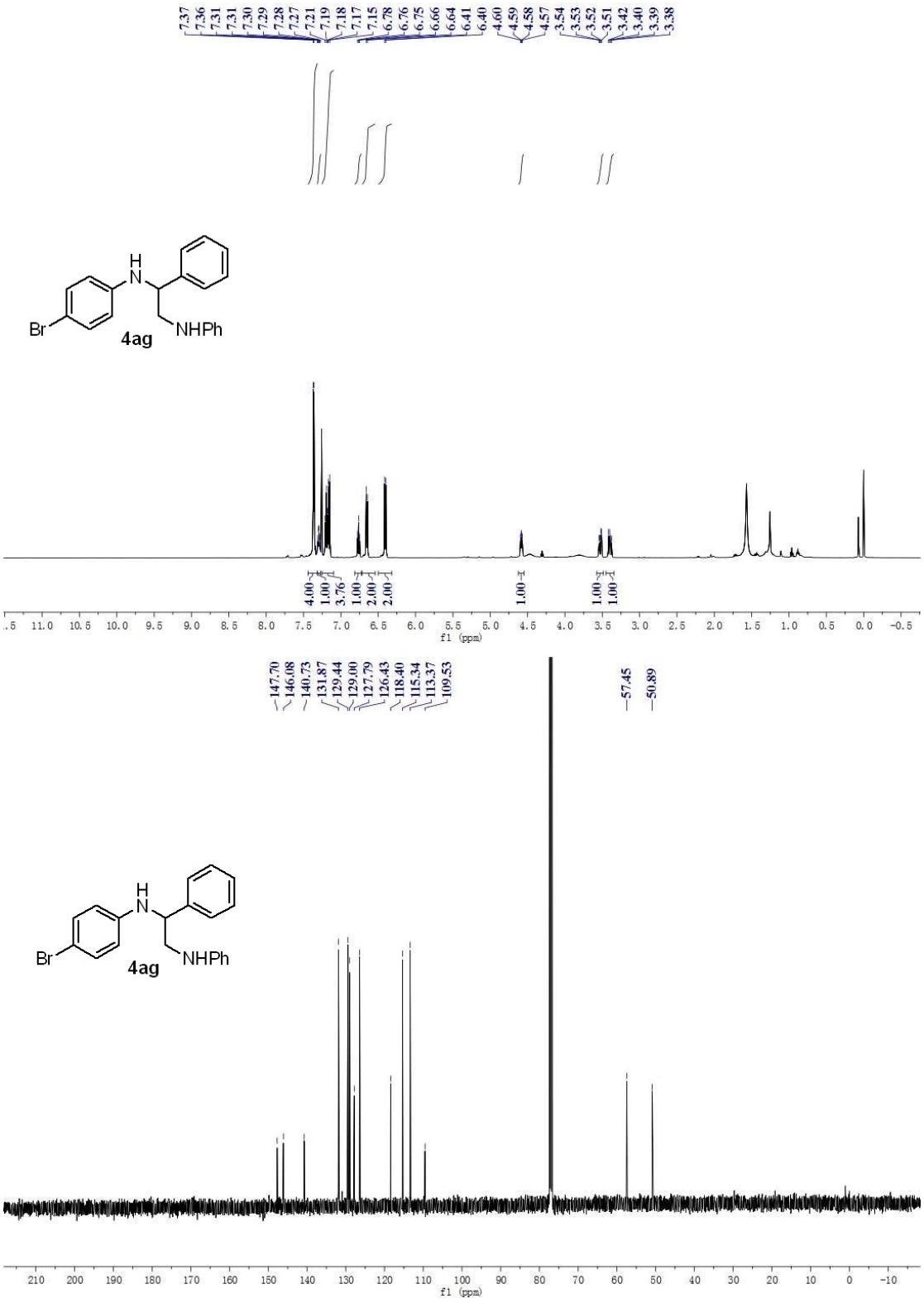
Cl
N
H
NHPh
4af
f1 (ppm)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4.57
3.54
3.53
3.52
3.51
3.42
3.40
3.39
3.38
H
N
Br
NHPh
4ag
4.00
1.00
3.76
1.00
2.00
2.00
1.00
1.00
1.00
f1 (ppm)
147.70
146.08
140.73
131.87
129.44
129.00
127.79
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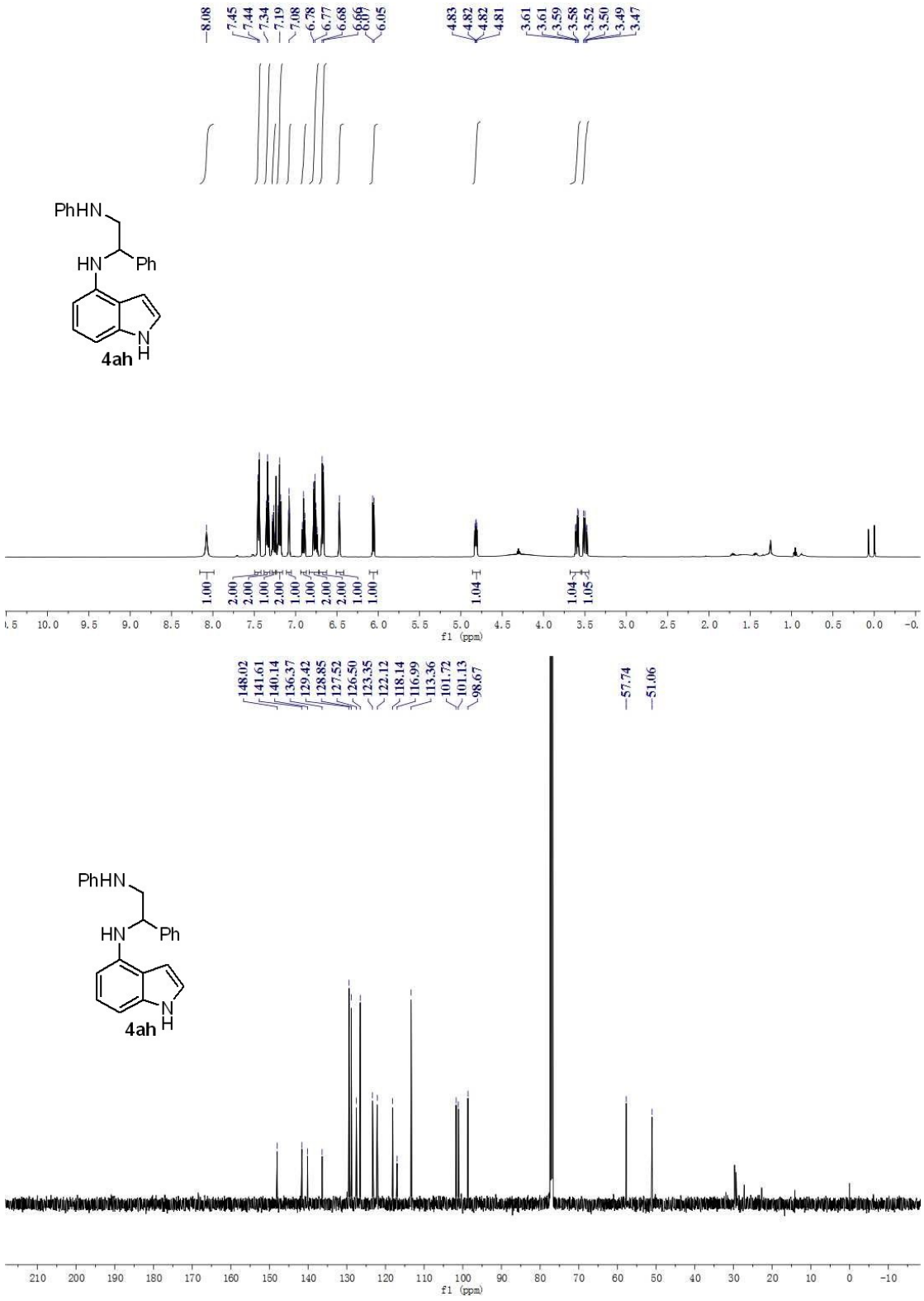
115.34
113.37
109.53
57.45
50.89
H
N
Br
NHPh
4ag
f1 (ppm)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7.08
6.78
6.77
6.68
6.66
6.07
6.05
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4.82
4.82
4.81
3.61
3.61
3.59
3.58
3.52
3.50
3.49
3.47
PhHN
HN
Ph
N
H
4ah
1.00
2.00
2.00
1.00
2.00
1.00
1.00
2.00
2.00
1.00
1.00
1.04
1.04
1.05
f1 (ppm)
148.02
141.61
140.14
136.37
129.42
128.85
127.52
126.50
123.35
122.12
118.14
116.99
113.36
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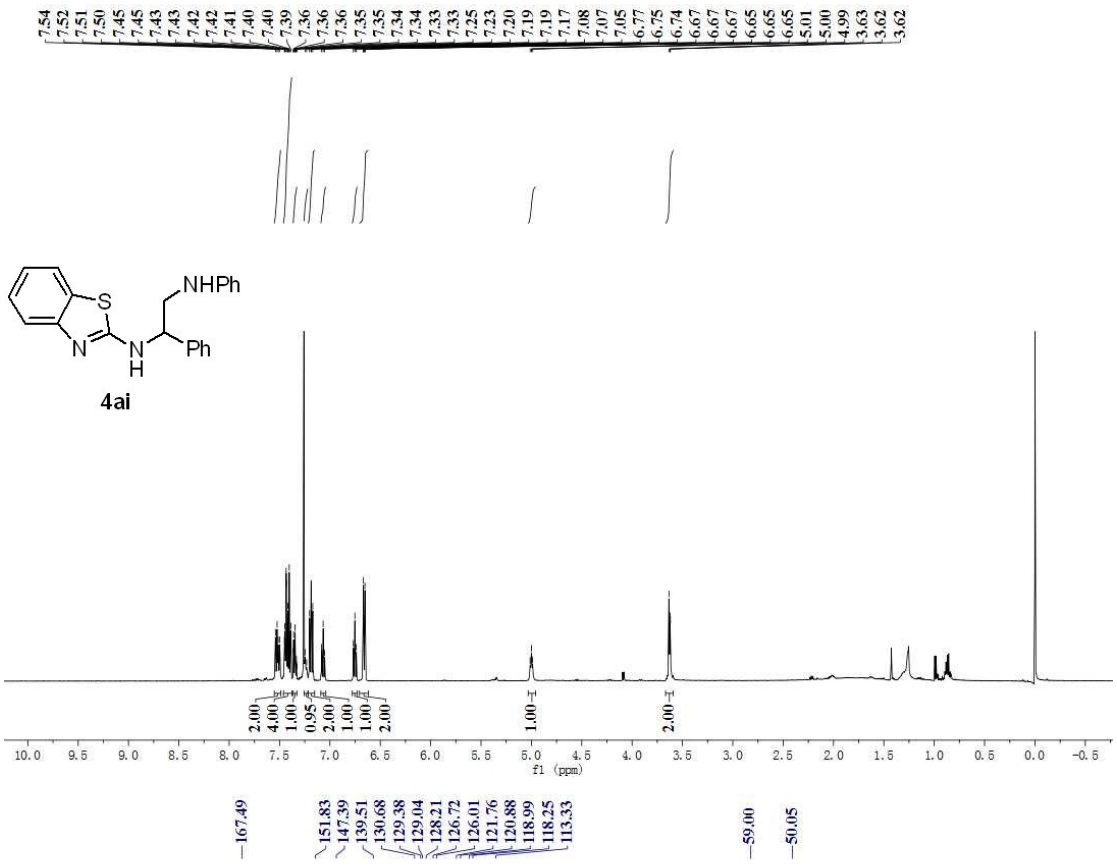
101.13
98.67
57.74
51.06
PhHN
HN
Ph
N
H
4ah
f1 (ppm)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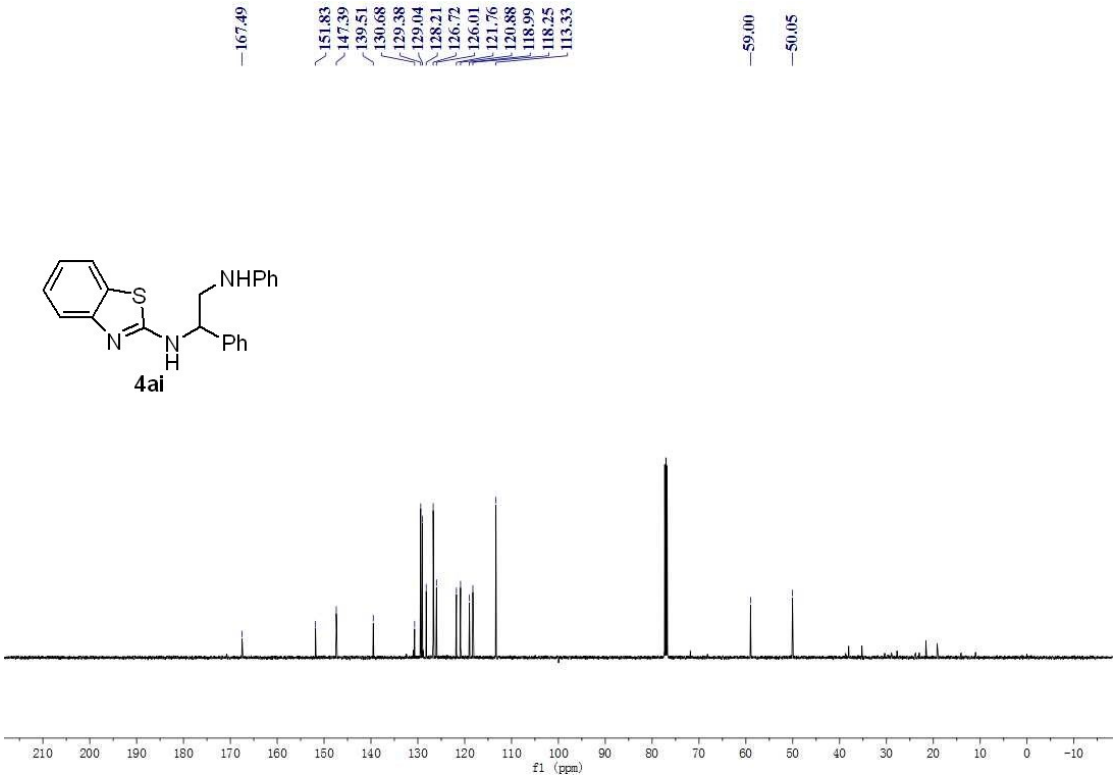
7.39
7.36
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.25
7.23
7.20
7.19
7.19
7.17
7.08
7.07
7.05
6.77
6.75
6.74
6.67
6.67
6.67
6.65
6.65
6.65
5.01
5.00
4.99
3.63
3.62
3.62
NHPh
S
N
N
H
Ph
4ai
2.00
4.00
1.00
0.95
2.00
1.00
1.00
2.00
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.21
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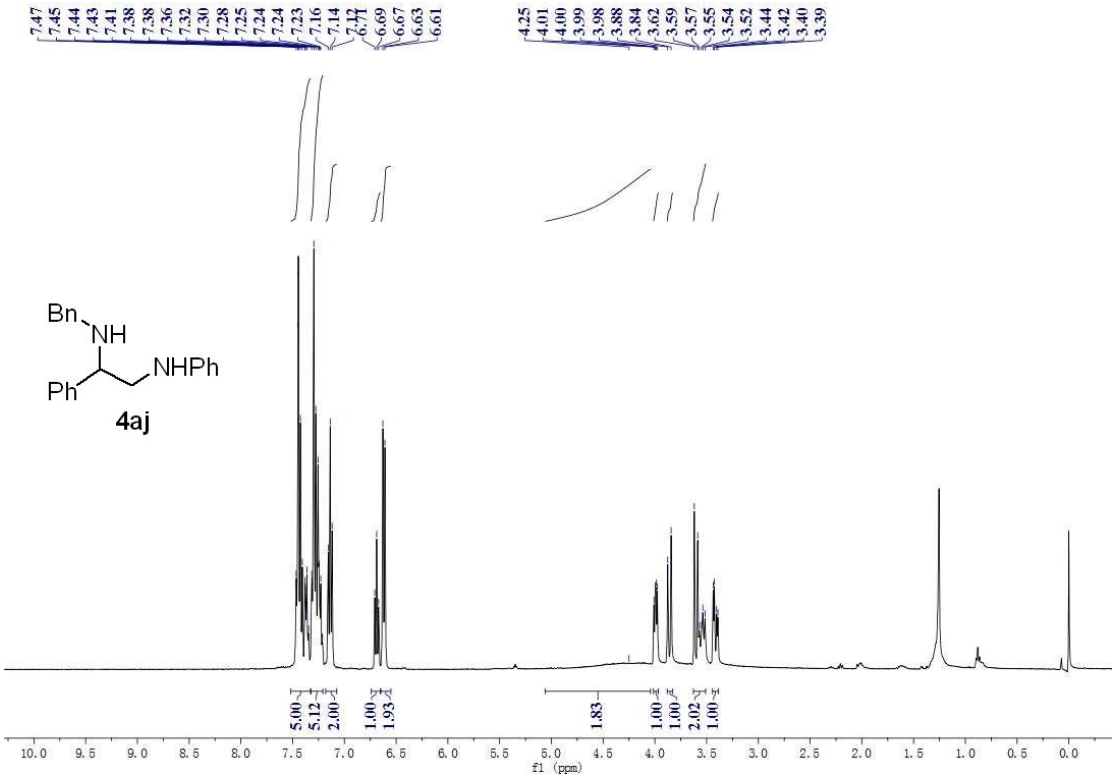
126.01
121.76
120.88
118.99
118.25
113.33
59.00
50.05
NHPh
S
N
N
H
Ph
4ai
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.36
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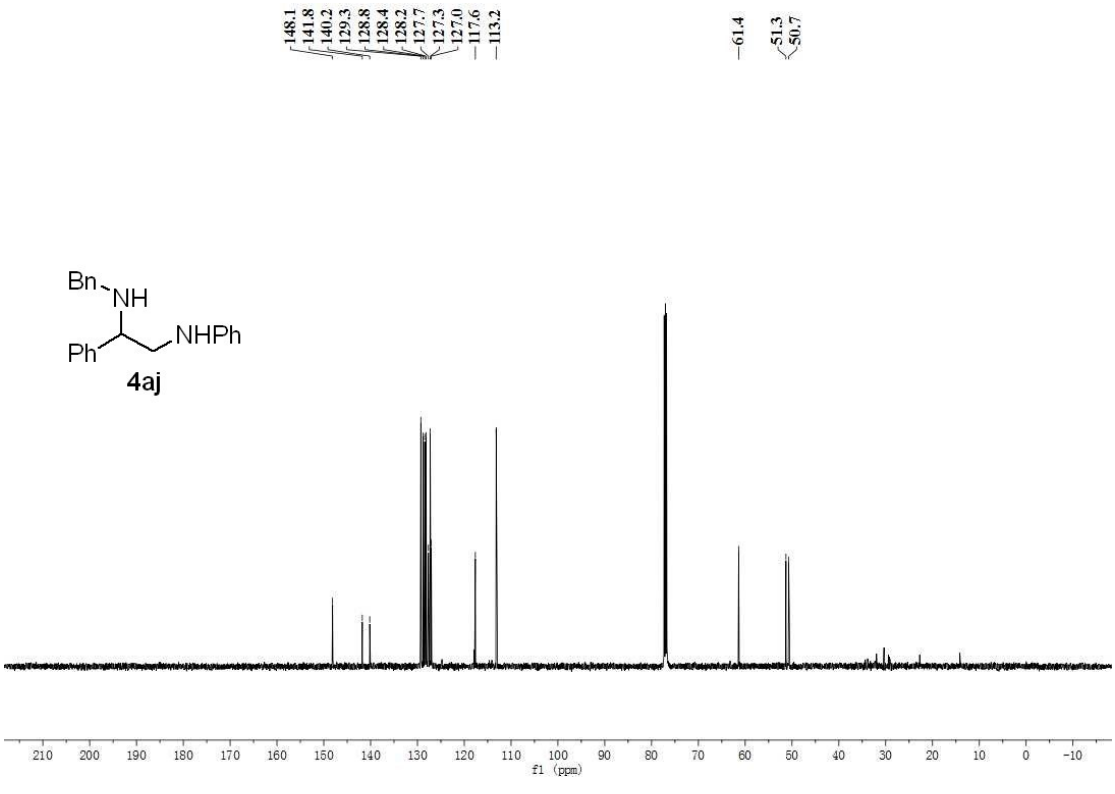
7.28
7.25
7.24
7.24
7.23
7.16
7.14
7.11
6.69
6.67
6.63
6.61
4.25
4.01
4.00
3.99
3.98
3.88
3.84
3.62
3.59
3.57
3.55
3.54
3.52
3.44
3.42
3.40
3.39
Bn
NH
NHPh
Ph
4aj
5.00
5.12
2.00
1.00
1.93
1.83
1.00
1.00
2.02
1.00
f1 (ppm)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141.8
140.2
129.3
128.8
128.4
128.2
127.7
127.3
127.0
117.6
113.2
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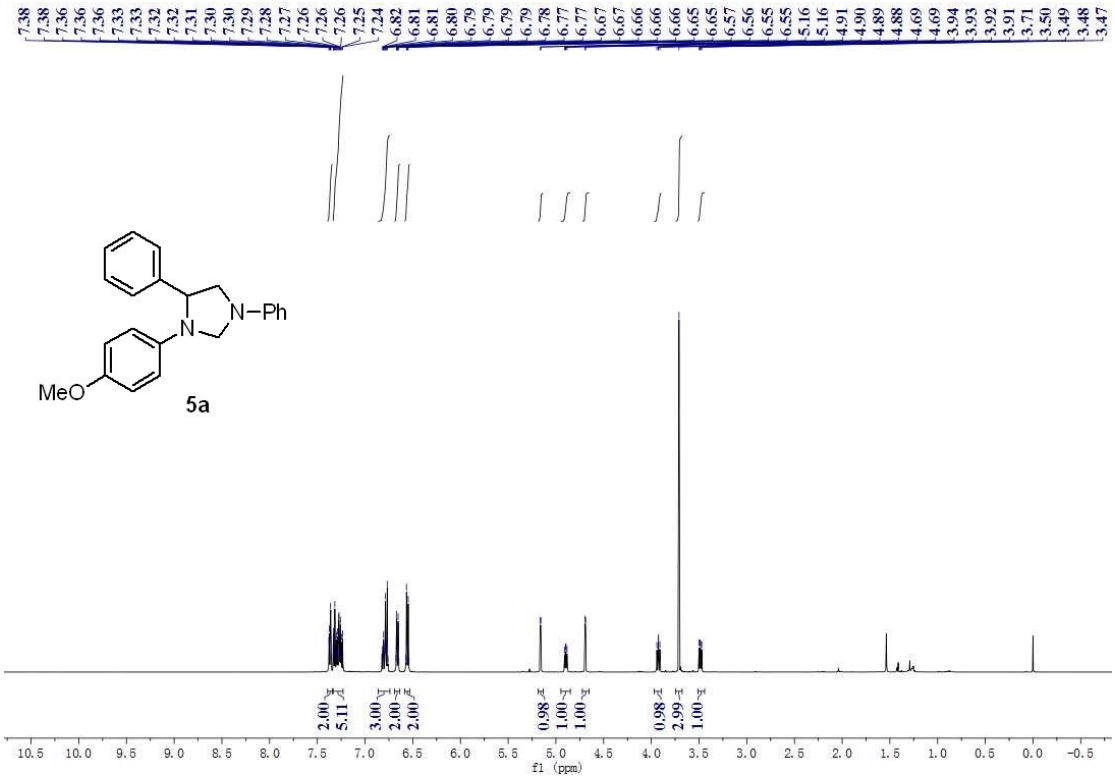
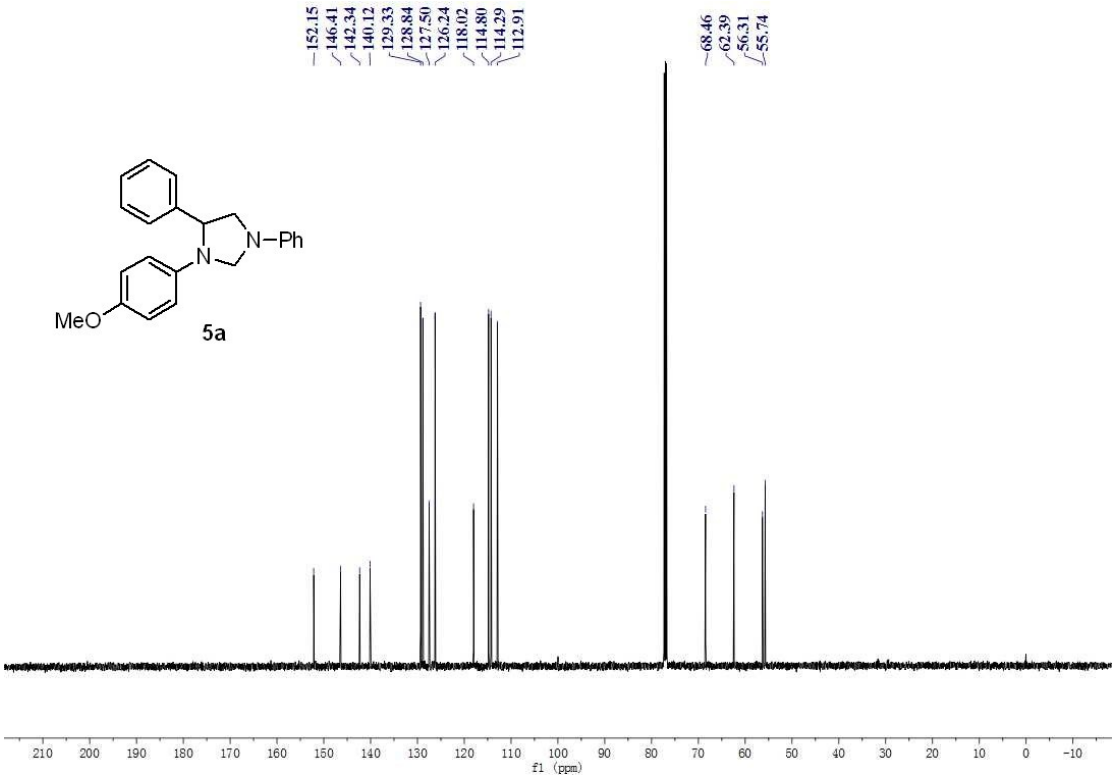
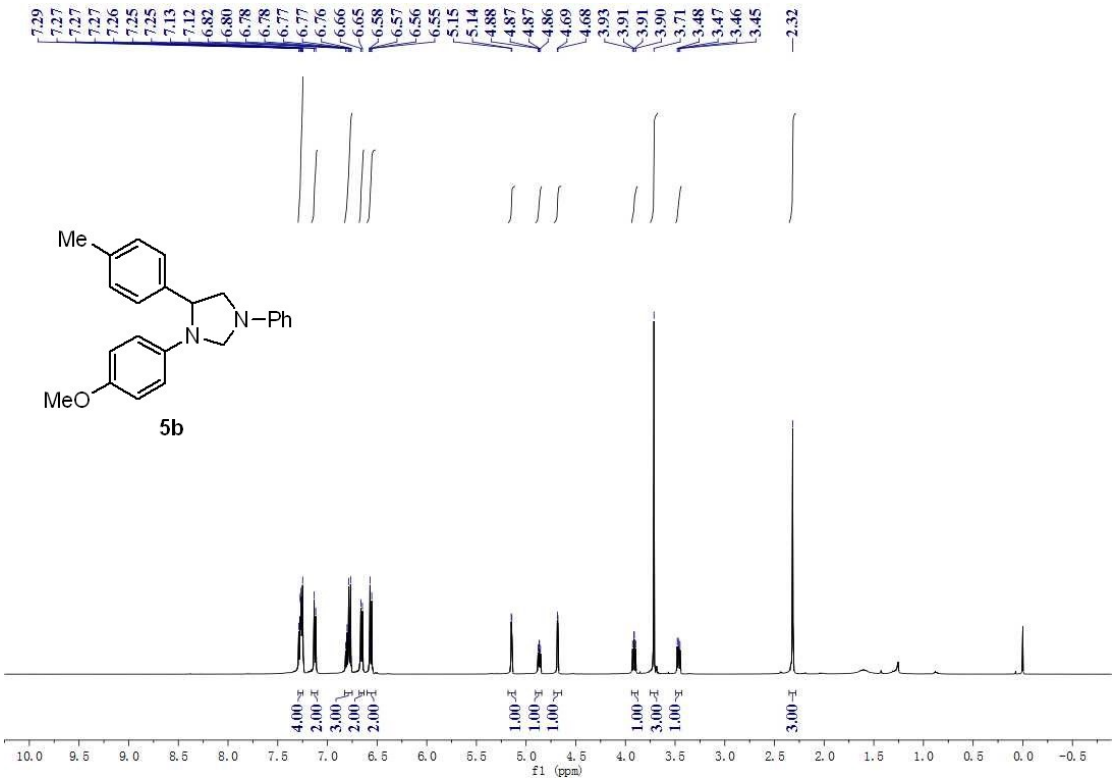
50.7
Bn
NH
NHPh
Ph
4aj
f1 (ppm)


7.38 7.38 7.36 7.36 7.36 7.33 7.33 7.32 7.32 7.31 7.30 7.30 7.29 7.28 7.27 7.26 7.26 7.26 7.25 7.24 6.82 6.81 6.81 6.80 6.79 6.79 6.79 6.79 6.78 6.77 6.77 6.67 6.67 6.66 6.66 6.66 6.65 6.65 6.57 6.56 6.55 6.55 5.16 4.91 4.90 4.89 4.88 4.69 4.69 3.94 3.93 3.92 3.91 3.71 3.50 3.49 3.48 3.47
N–Ph
N
N
MeO
5a
2.00 5.11 3.00 2.00 2.00 0.98 1.00 1.00 0.98 2.99 1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


152.15 146.41 142.34 140.12 129.33 128.84 127.50 126.24 118.02 114.80 114.29 112.91
68.46 62.39 56.31 55.74
N–Ph
N
N
MeO
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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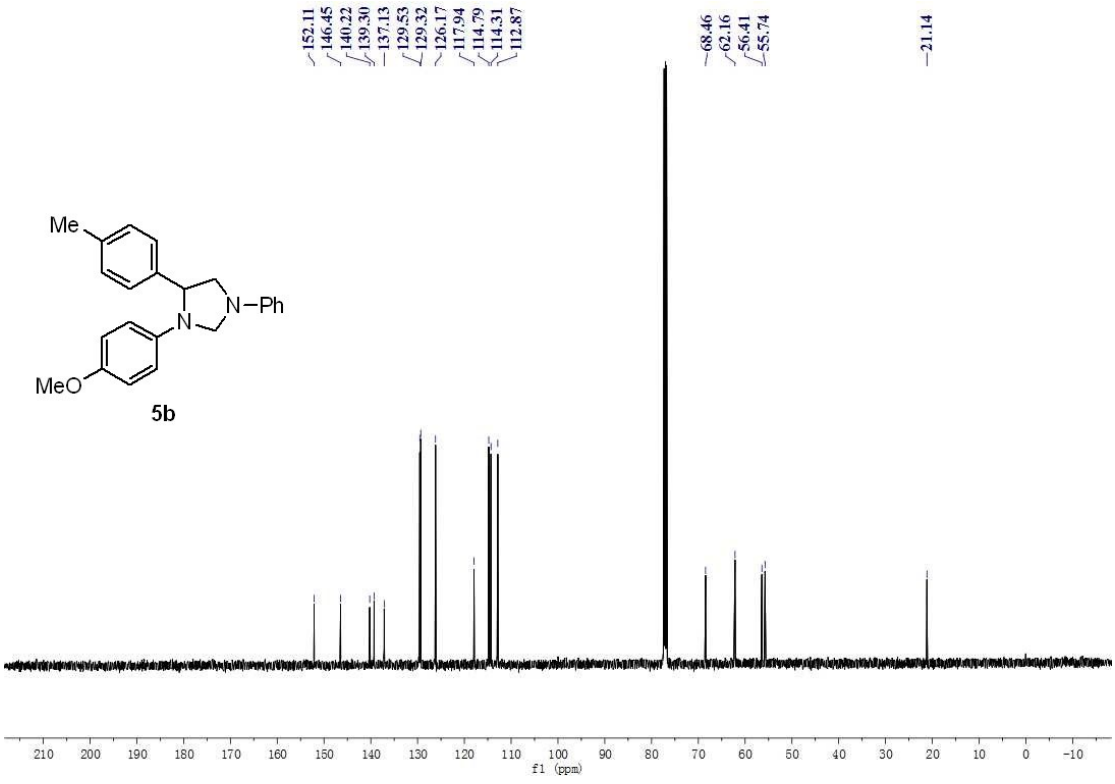
7.13
7.12
6.82
6.80
6.78
6.78
6.77
6.77
6.76
6.66
6.65
6.58
6.57
6.56
6.55
5.15
5.14
4.88
4.87
4.87
4.86
4.69
4.68
3.93
3.91
3.91
3.90
3.71
3.48
3.47
3.46
3.45
2.32
Me
N
N–Ph
MeO
5b
4.00
2.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
3.00
f1 (ppm)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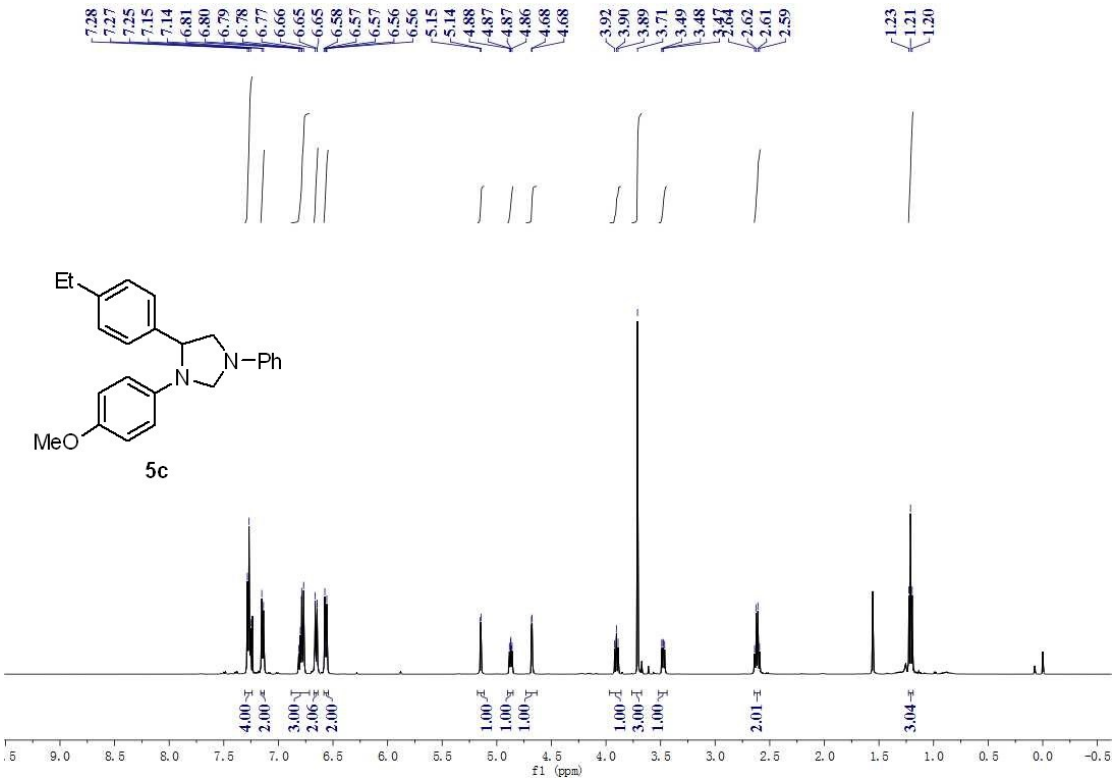
146.45
140.22
139.30
137.13
129.53
129.32
126.17
117.94
114.79
114.31
112.87
68.46
62.16
56.41
55.74
21.14
Me
N
N–Ph
MeO
5b
f1 (ppm)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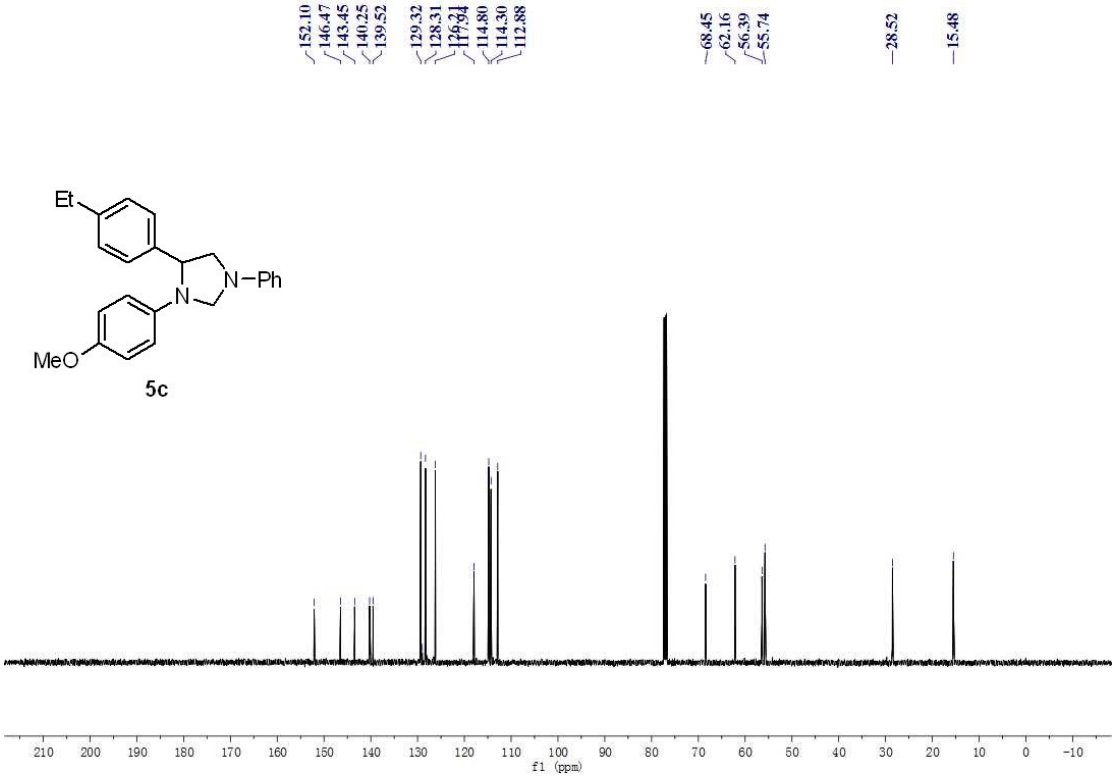
6.79
6.78
6.77
6.66
6.65
6.65
6.58
6.57
6.57
6.56
6.56
5.15
5.14
4.88
4.87
4.87
4.86
4.68
4.68
3.92
3.90
3.89
3.71
3.49
3.48
3.47
2.64
2.62
2.61
2.59
1.23
1.21
1.20
Et
N–Ph
N
MeO
5c
4.00
2.00
3.00
2.06
2.00
1.00
1.00
1.00
1.00
3.00
1.00
2.01
3.04
f1 (ppm)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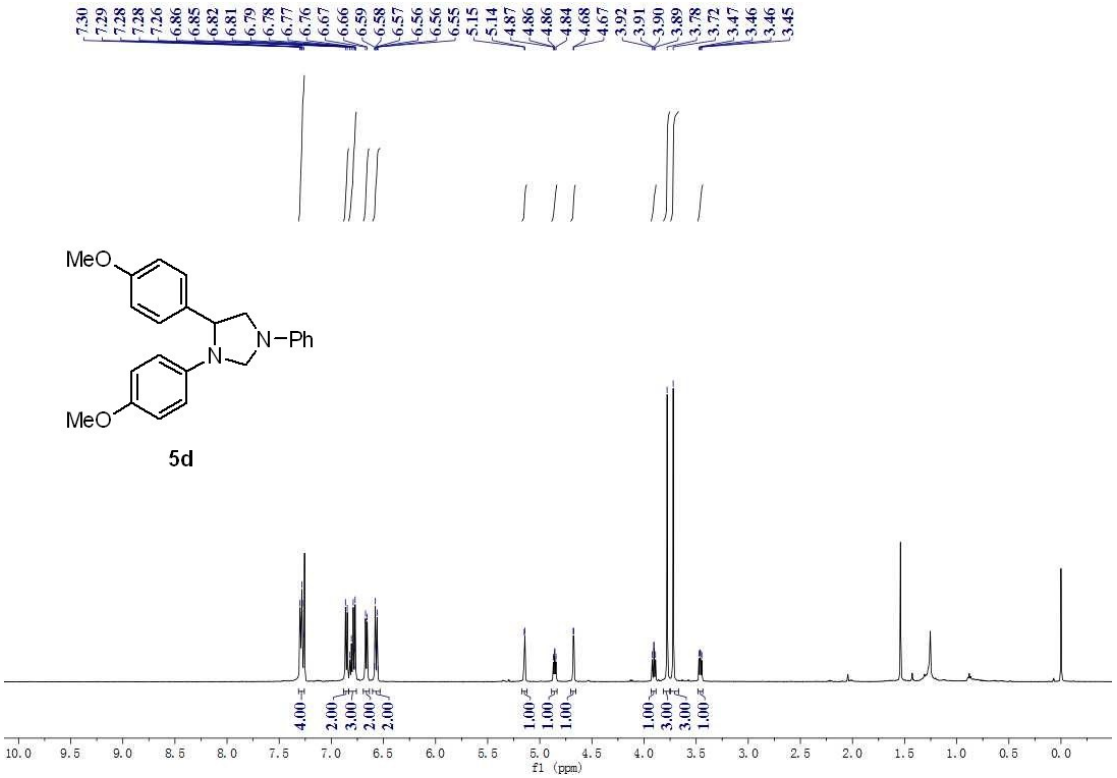
139.52
129.32
128.31
114.80
114.30
112.88
68.45
62.16
56.39
55.74
28.52
15.48
Et
N–Ph
N
MeO
5c
f1 (ppm)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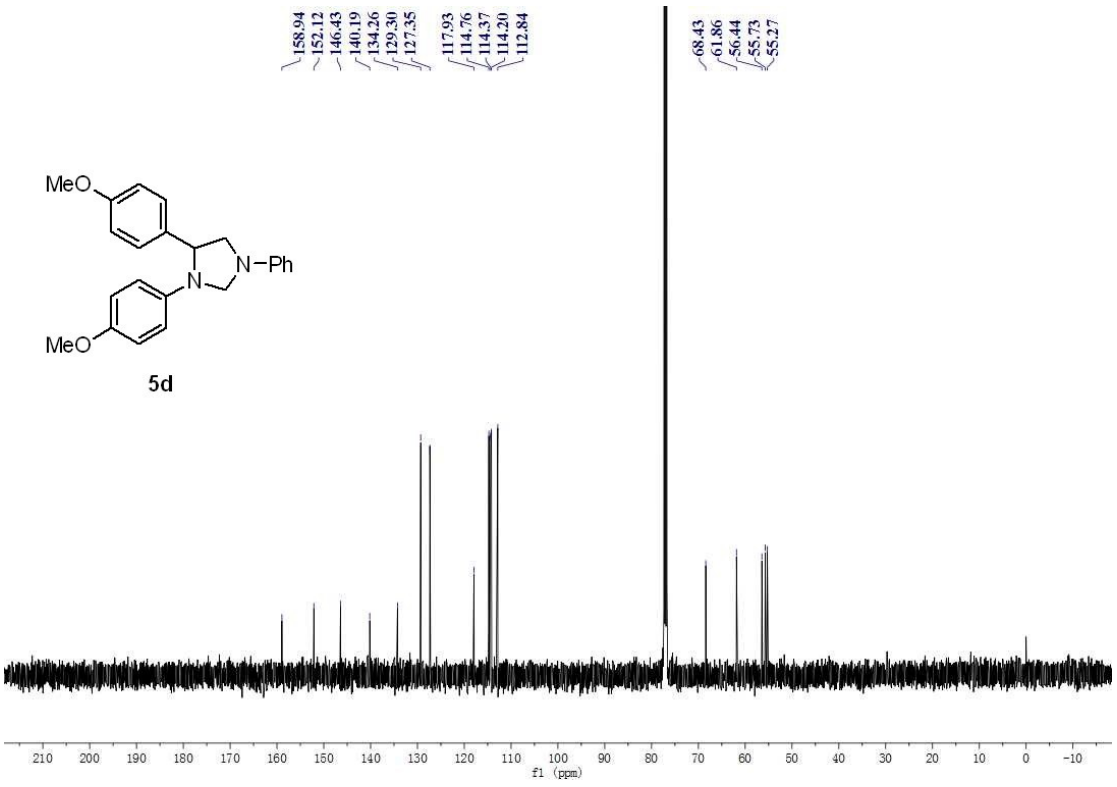
6.85
6.82
6.81
6.79
6.78
6.77
6.76
6.67
6.66
6.59
6.58
6.57
6.56
6.56
6.55
5.15
5.14
4.87
4.86
4.86
4.84
4.68
4.67
3.92
3.91
3.90
3.89
3.78
3.72
3.47
3.46
3.46
3.45
MeO
N–Ph
MeO
5d
4.00
2.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
3.00
1.00
f1 (ppm)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127.35
117.93
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114.37
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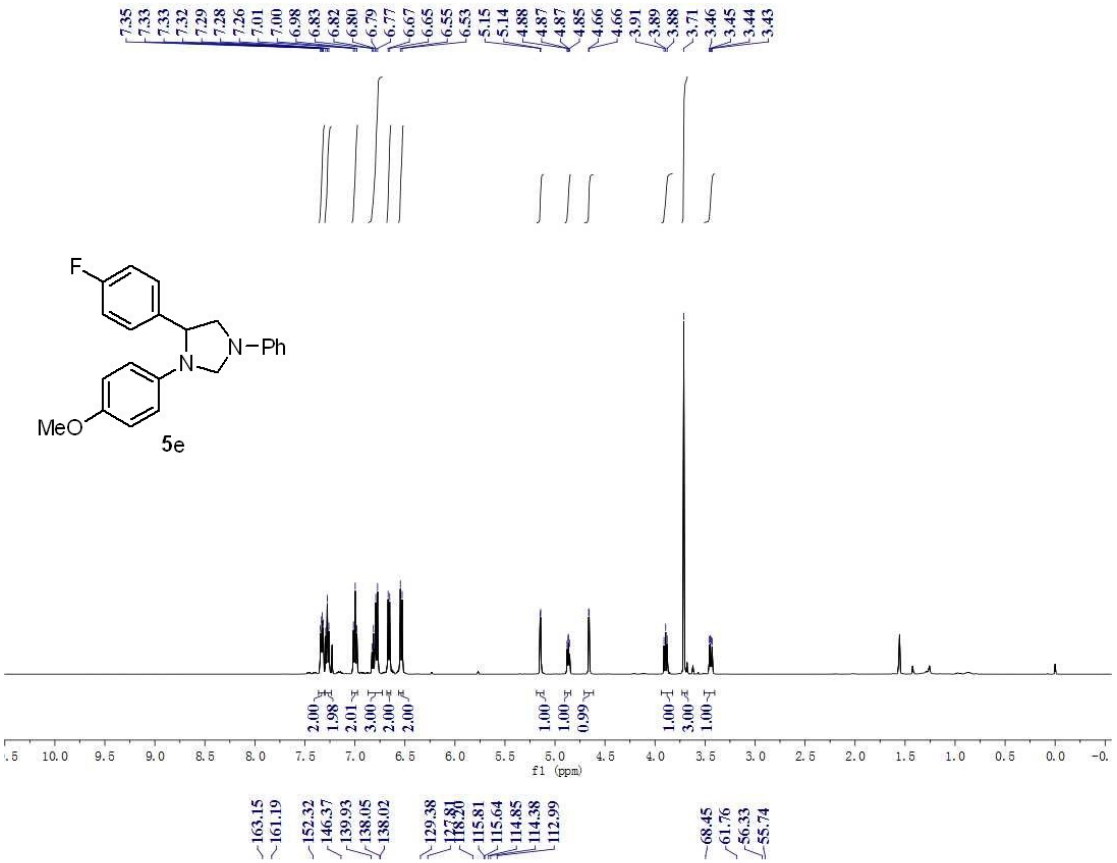
61.86
56.44
55.73
55.27
MeO
N–Ph
MeO
5d
f1 (ppm)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7.00
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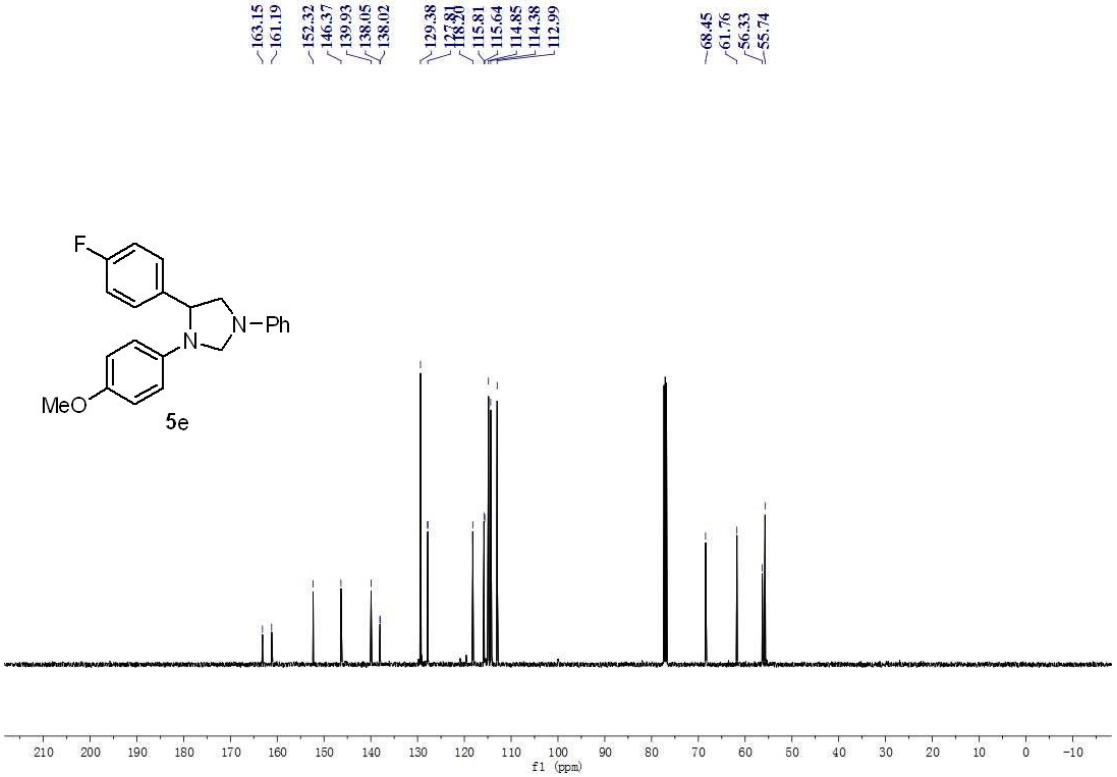
6.82
6.80
6.79
6.77
6.67
6.65
6.55
6.53
5.15
5.14
4.88
4.87
4.87
4.85
4.66
4.66
3.91
3.89
3.88
3.71
3.46
3.45
3.44
3.43
F
N
N–Ph
MeO
5e
2.00
1.98
2.01
3.00
2.00
2.00
1.00
1.00
0.99
1.00
3.00
1.00
f1 (ppm)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161.19
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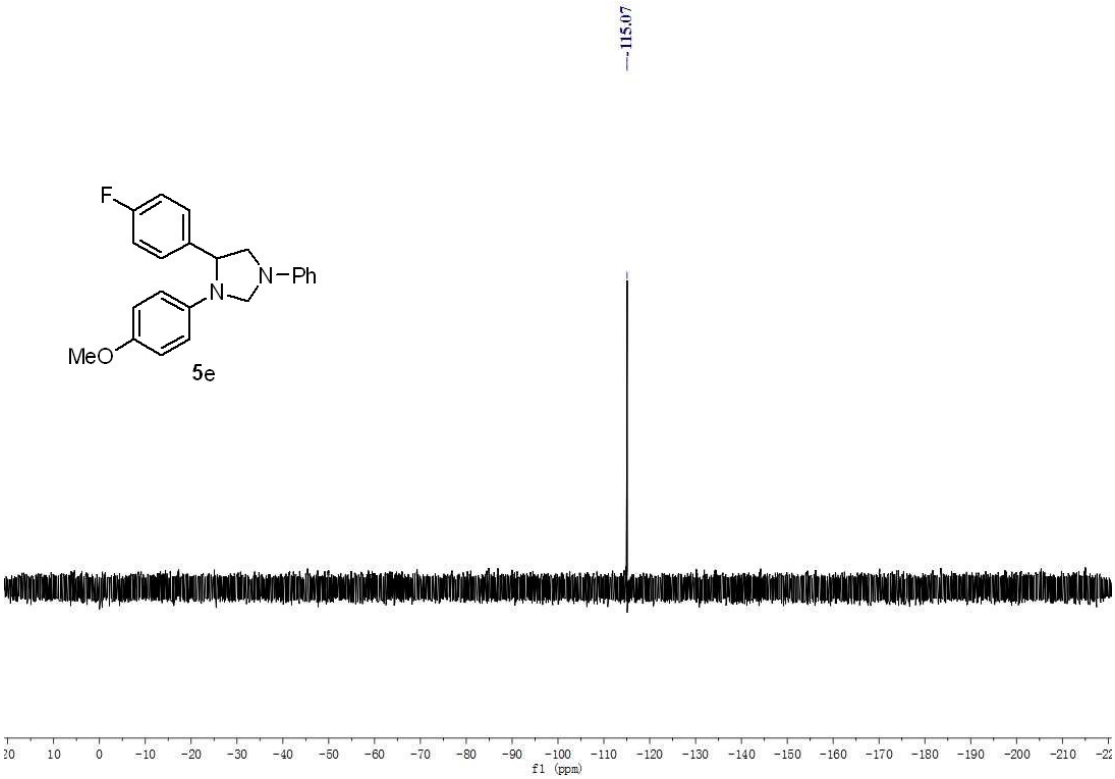
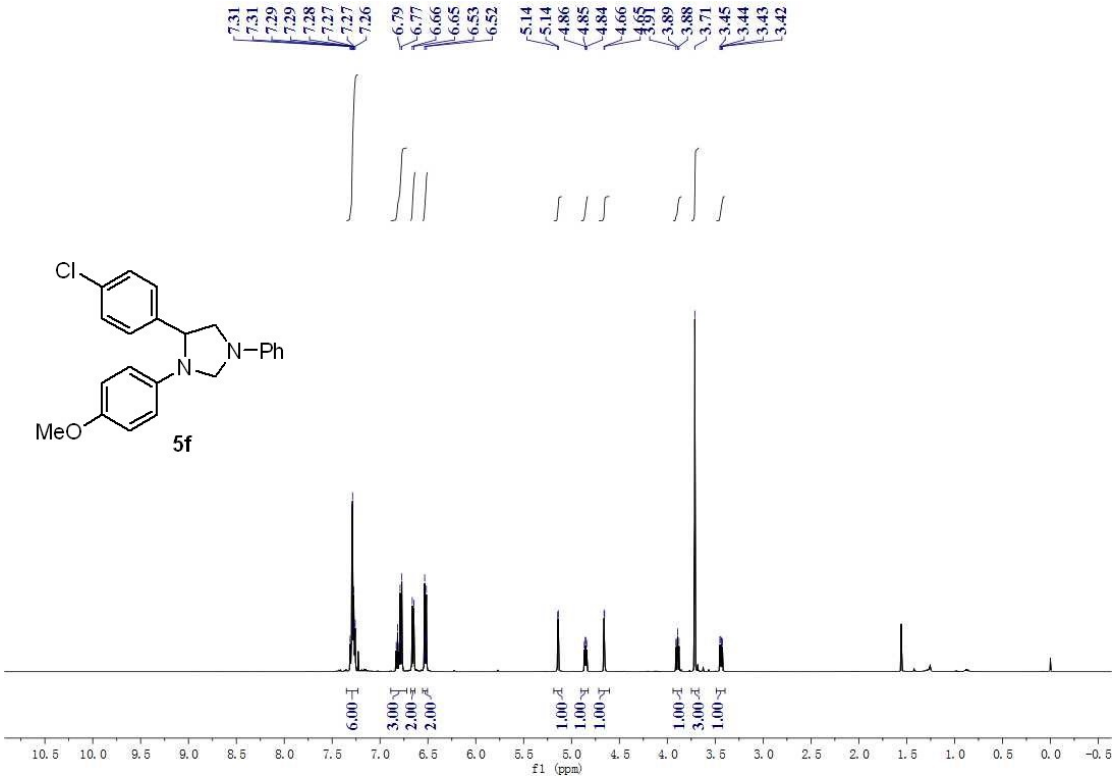
146.37
139.93
138.05
138.02
129.38
115.81
115.64
114.85
114.38
112.99
68.45
61.76
56.33
55.74
F
N
N–Ph
MeO
5e
f1 (ppm)


-115.07
F
N
N
Ph
MeO
5e
f1 (ppm)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6.65
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6.52
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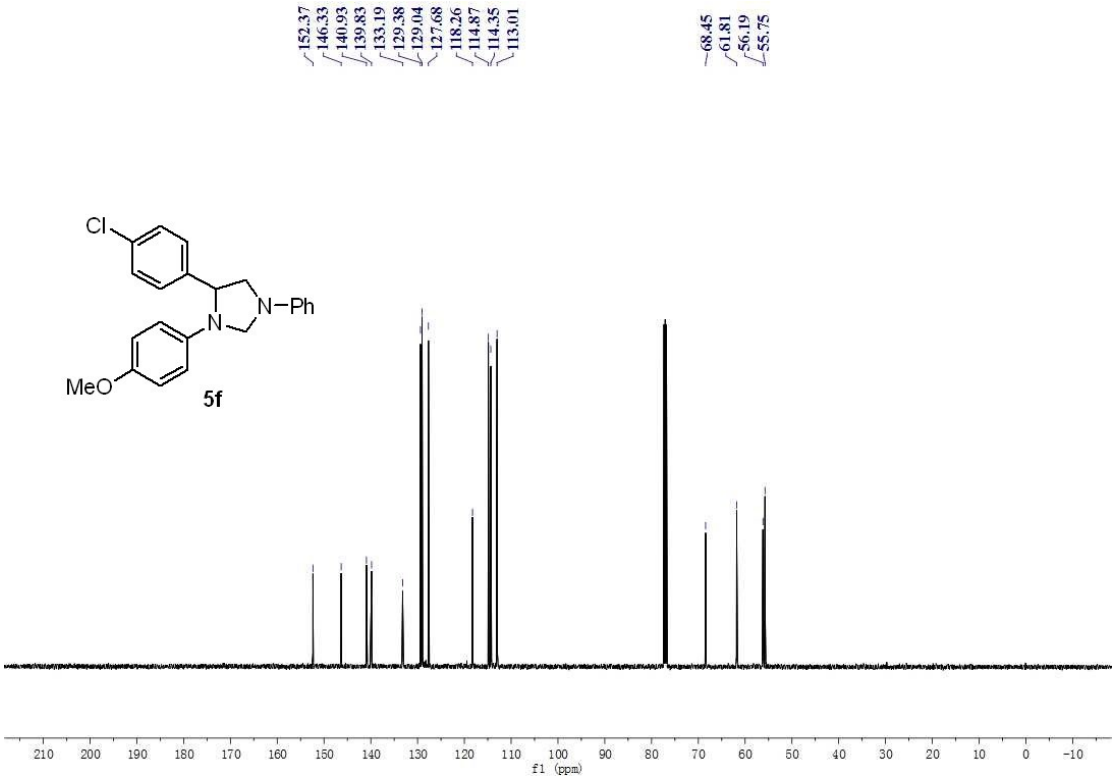
4.85
4.84
4.66
3.91
3.89
3.88
3.71
3.45
3.44
3.43
3.42
Cl
N
N
Ph
MeO
5f
6.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
f1 (ppm)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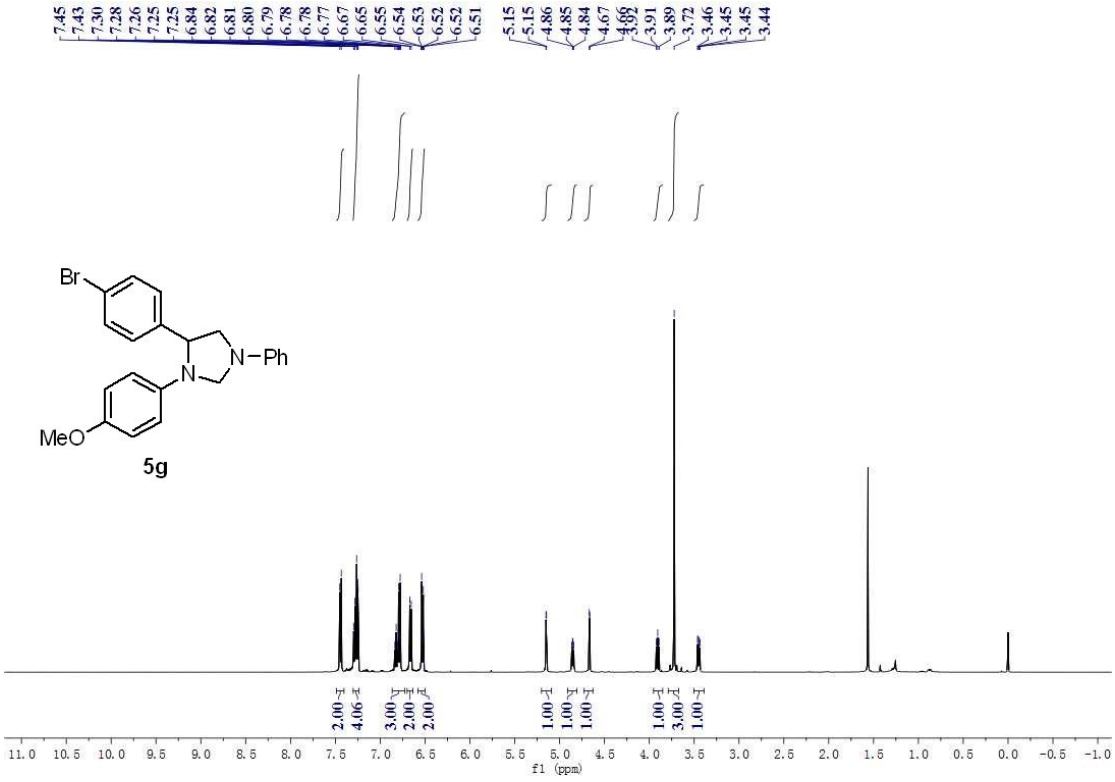
113.01
68.45
61.81
56.19
55.75
Cl
N−Ph
N
MeO
5f
f1 (ppm)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6.82
6.81
6.80
6.79
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6.52
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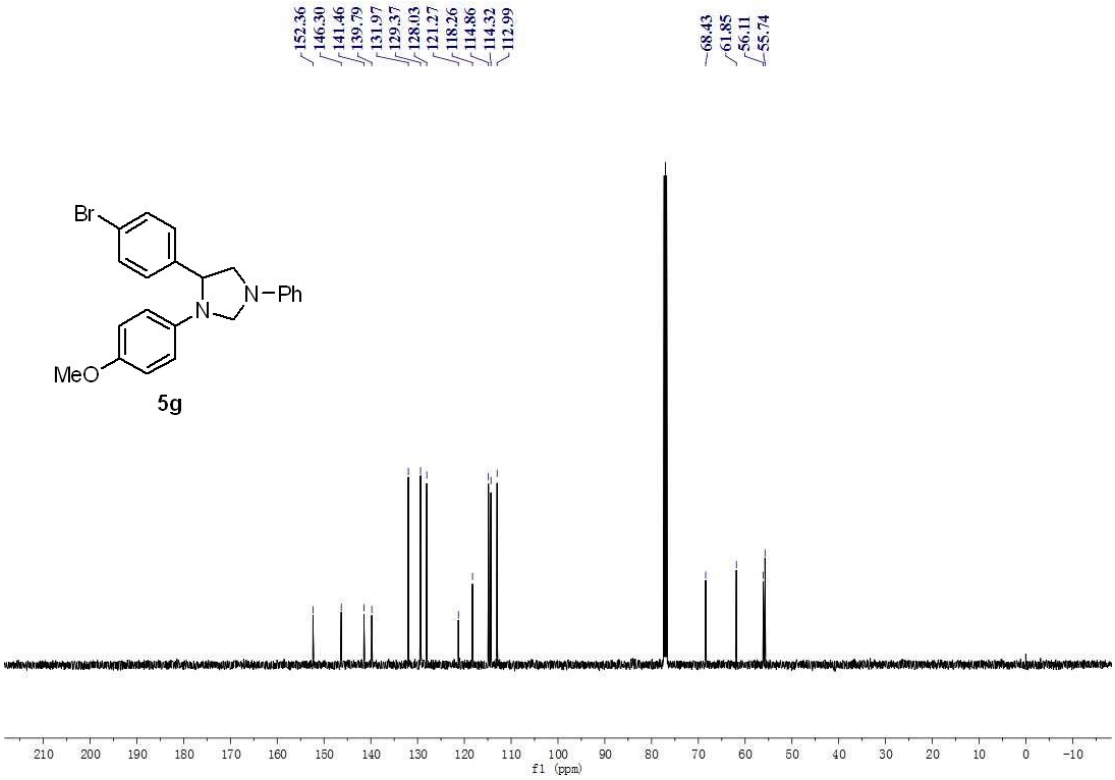
5.15
5.15
4.86
4.85
4.84
4.67
3.91
3.89
3.72
3.46
3.45
3.45
3.44
Br
N−Ph
N
MeO
5g
2.00
4.06
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
f1 (ppm)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121.27
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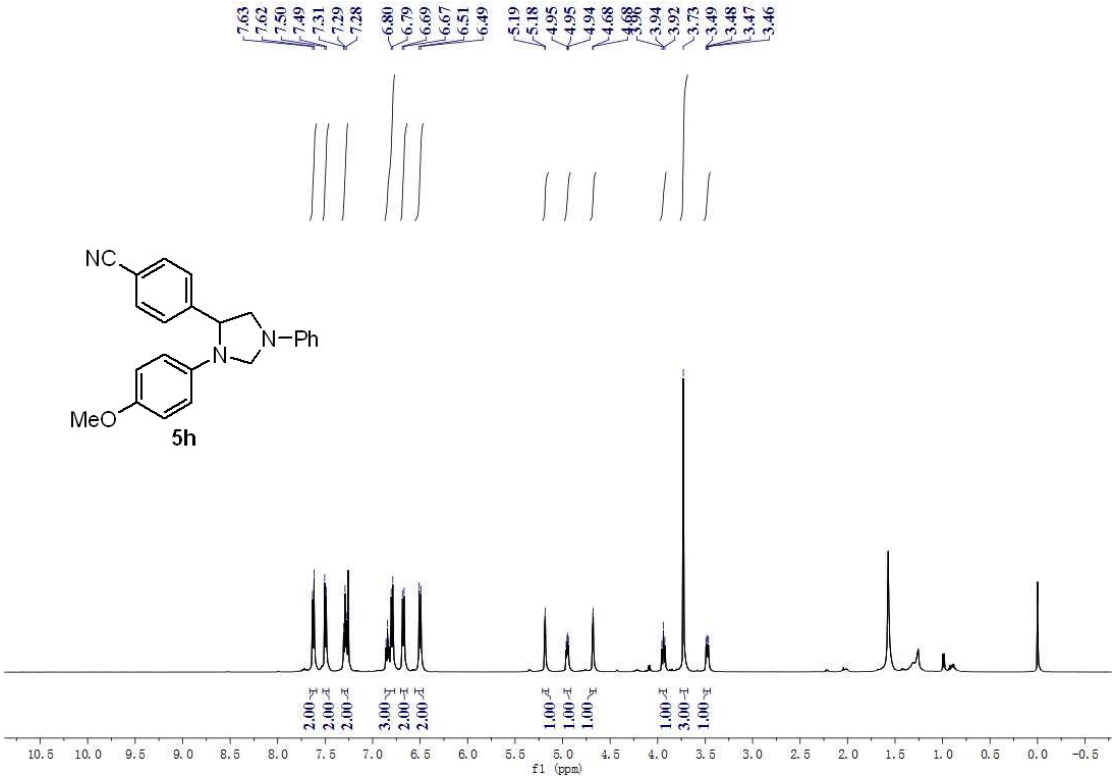
68.43
61.85
56.11
55.74
Br
N
N
Ph
MeO
5g
f1 (ppm)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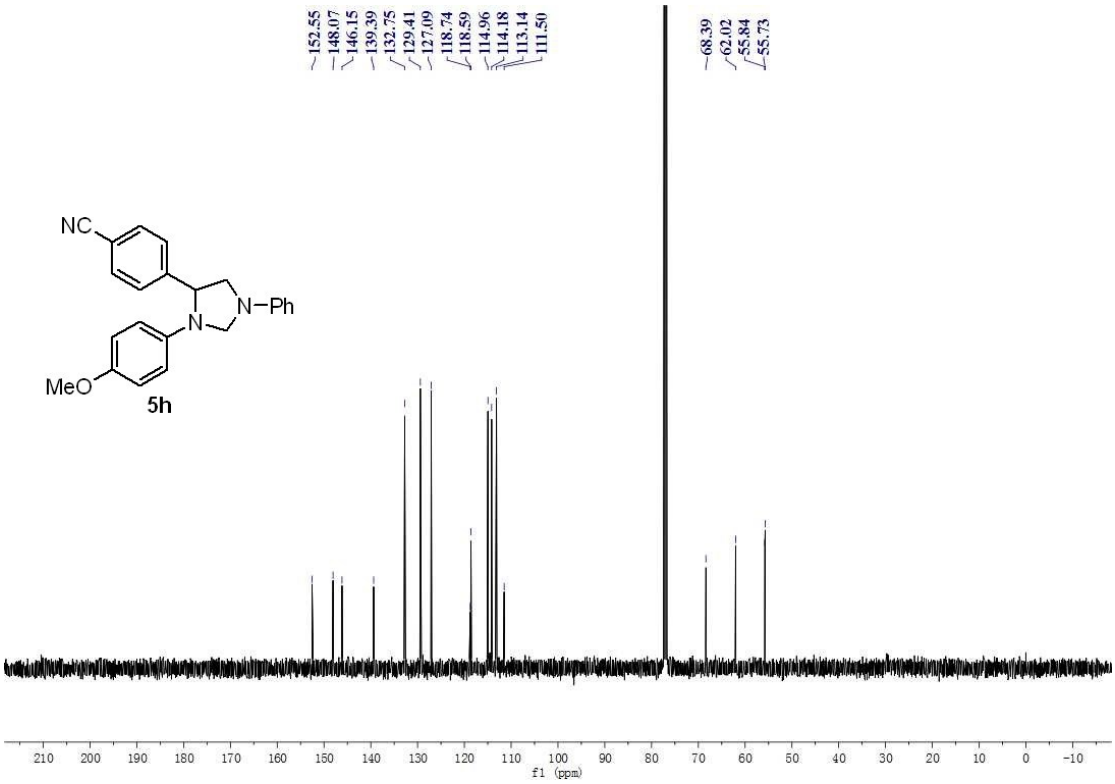
5.18
4.95
4.95
4.94
4.68
3.94
3.92
3.73
3.49
3.48
3.47
3.46
NC
N
N
Ph
MeO
5h
2.00
2.00
2.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
f1 (ppm)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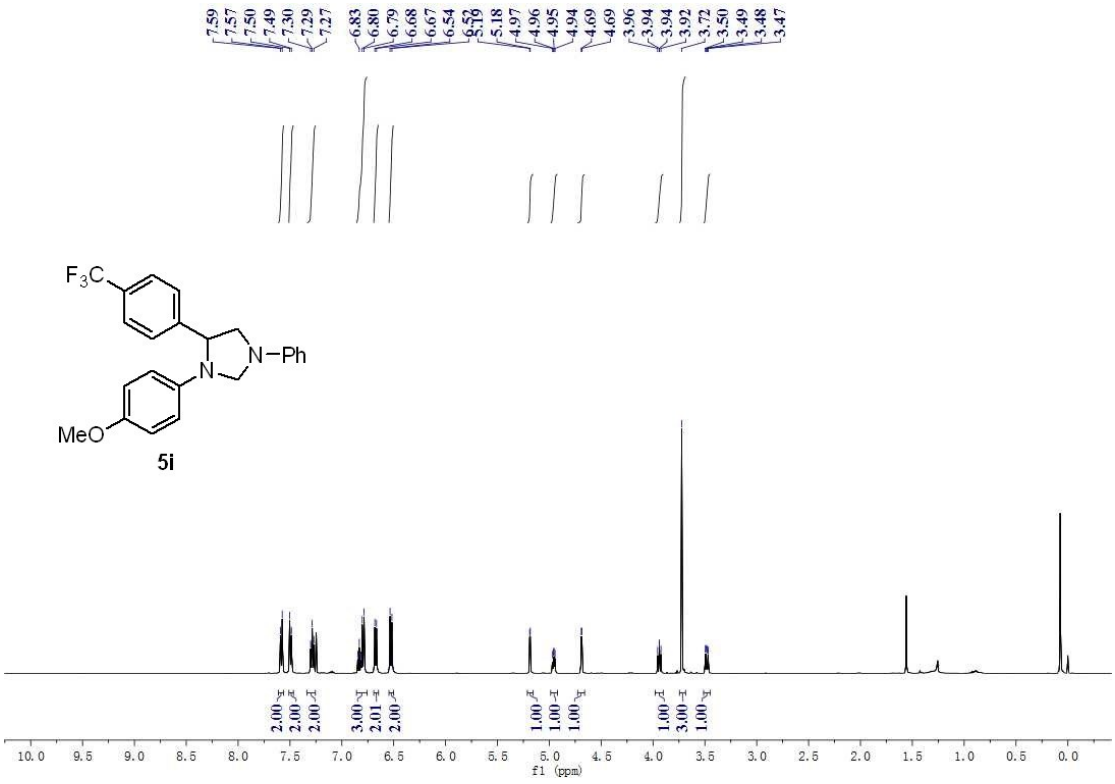
68.39
62.02
55.84
55.73
NC
N–Ph
N
MeO
5h
f1 (ppm)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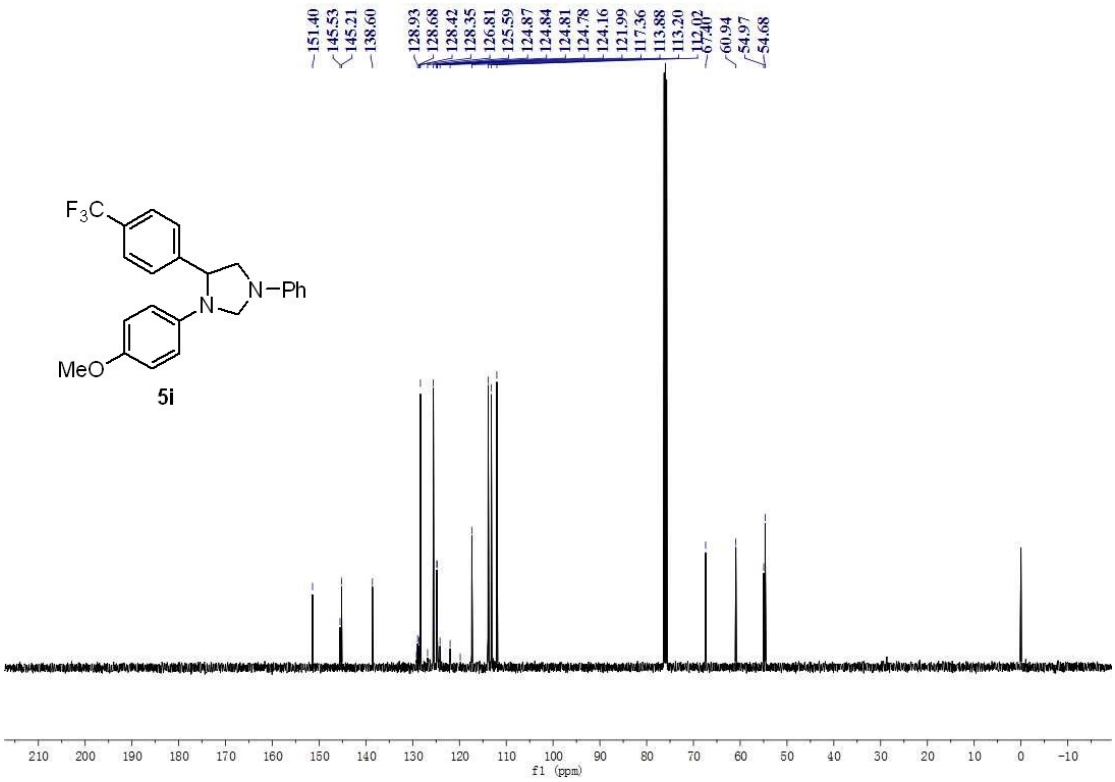
5.18
4.97
4.96
4.95
4.94
4.69
3.96
3.94
3.92
3.72
3.50
3.49
3.48
3.47
F3C
N–Ph
N
MeO
5i
2.00
2.00
2.00
3.00
2.01
2.00
1.00
1.00
1.00
1.00
3.00
1.00
f1 (ppm)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125.59
124.87
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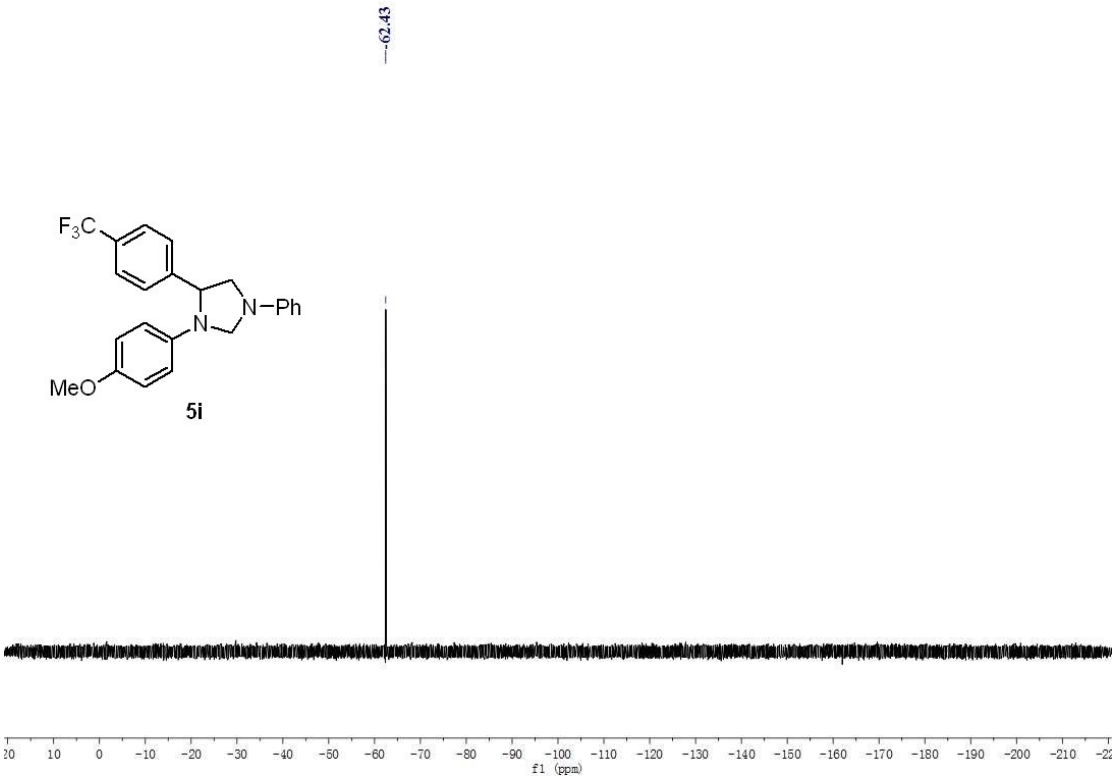
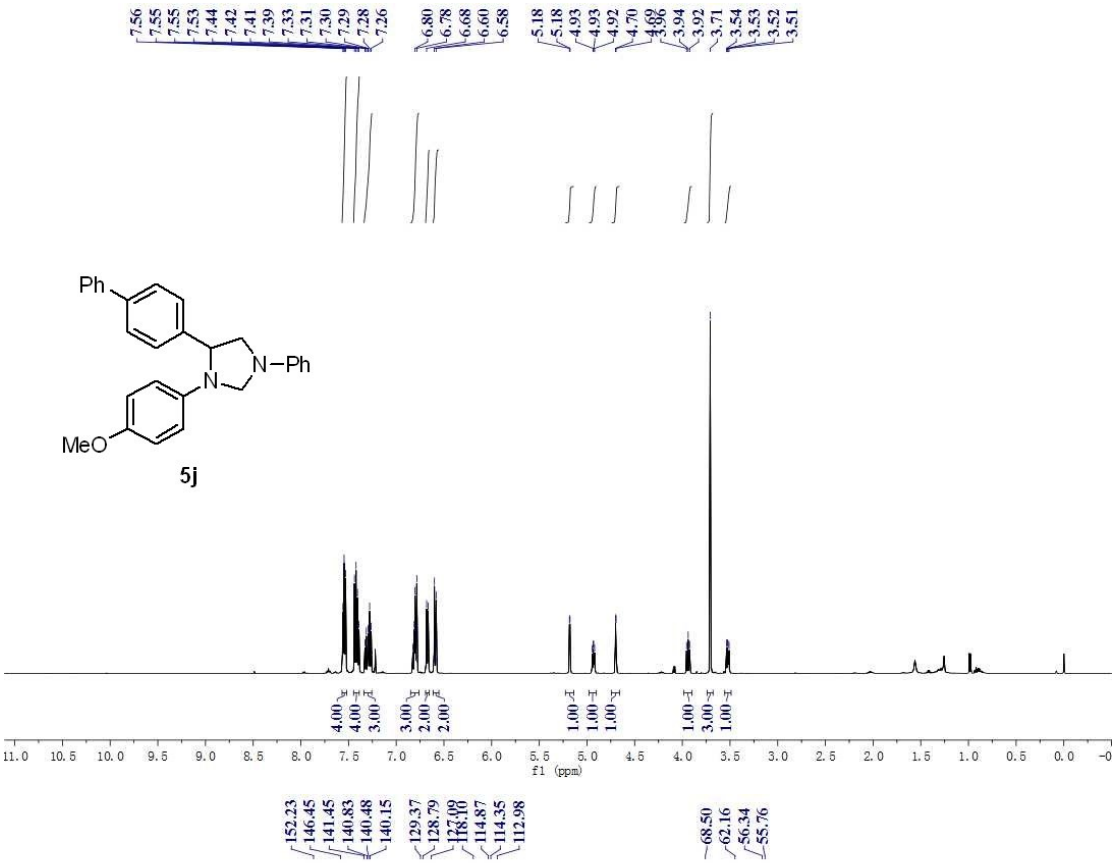
124.78
124.16
121.99
117.36
113.88
113.20
112.02
67.40
60.94
54.97
54.68
F3C
N
N–Ph
MeO
5i
f1 (ppm)


-62.43
F3C
N
N–Ph
MeO
5i
f1 (ppm)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7.31
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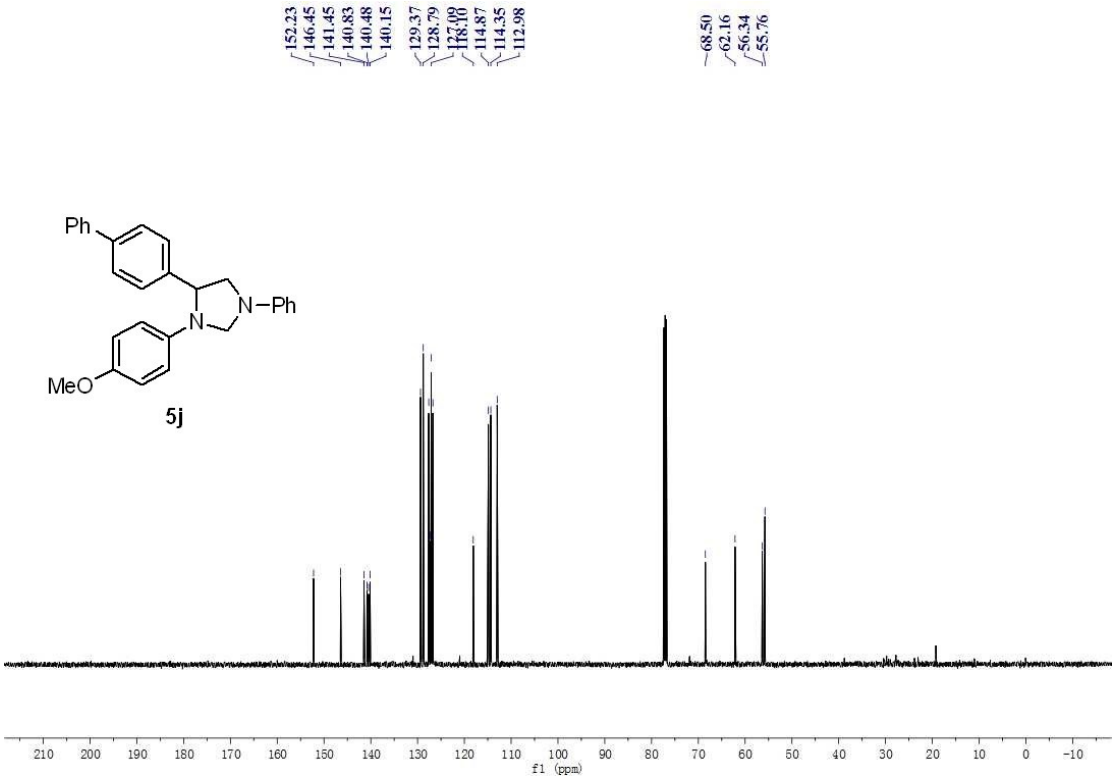
7.29
7.28
7.26
6.80
6.78
6.68
6.60
6.58
5.18
5.18
4.93
4.93
4.92
4.70
3.94
3.92
3.71
3.54
3.53
3.52
3.51
Ph
N–Ph
N
MeO
5j
4.00
4.00
3.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
f1 (ppm)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128.79
118.10
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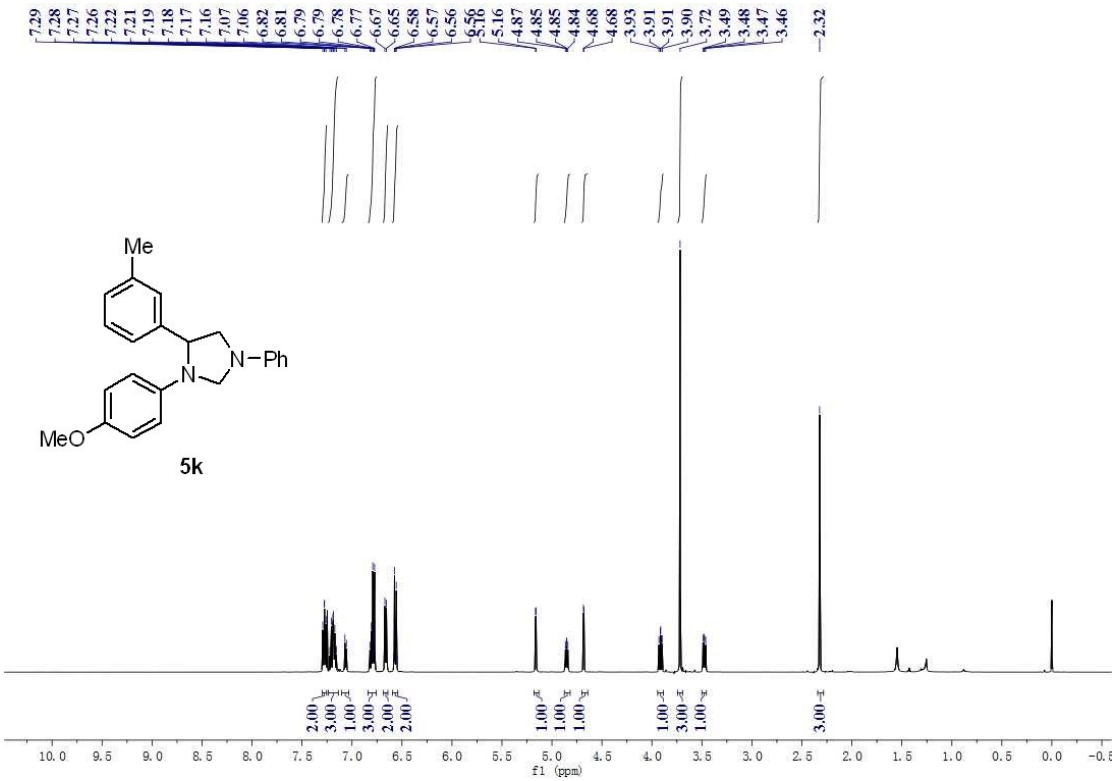
62.16
56.34
55.76
Ph
N–Ph
N
MeO
5j
f1 (ppm)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6.77
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6.57
6.56
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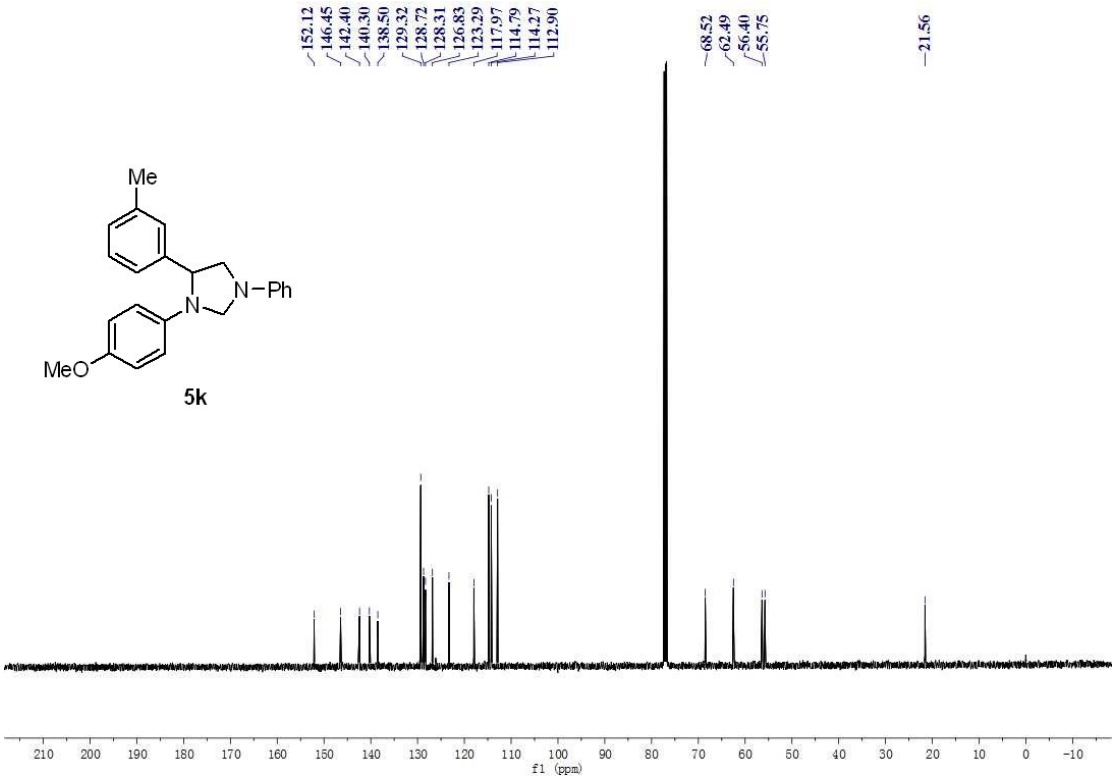
4.85
4.84
4.68
3.93
3.91
3.91
3.90
3.72
3.49
3.48
3.47
3.46
2.32
Me
N
N−Ph
MeO
5k
2.00
3.00
1.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.29
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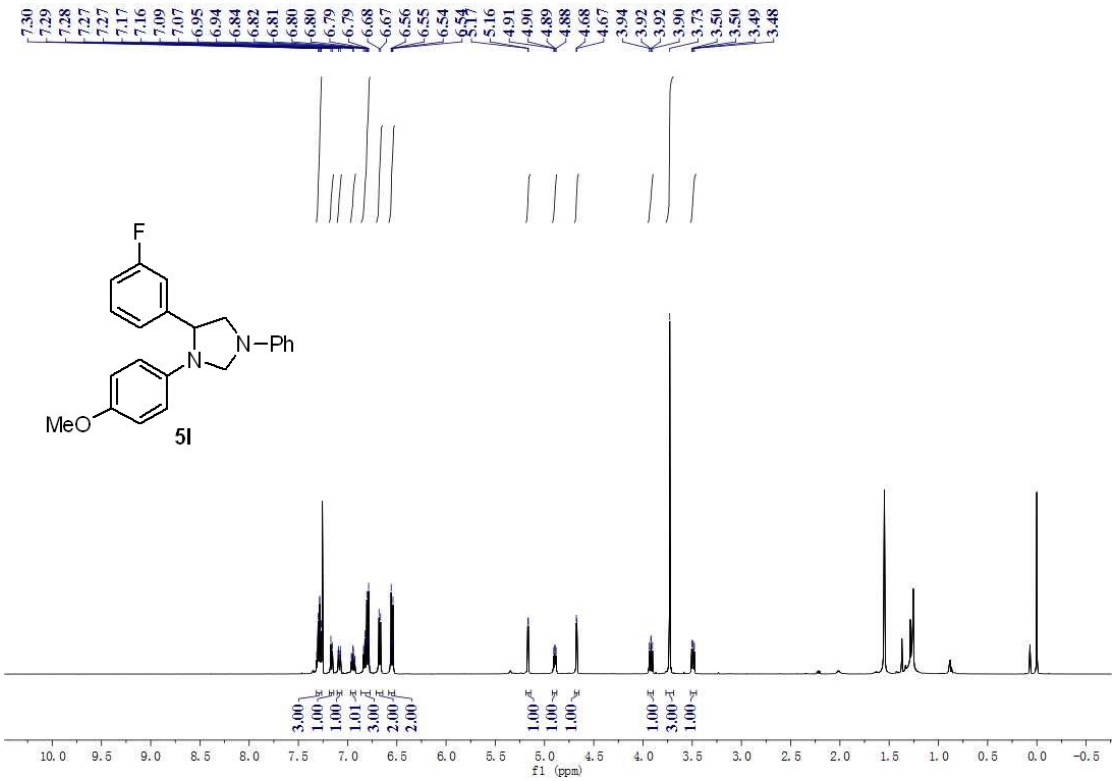
114.79
114.27
112.90
68.52
62.49
56.40
55.75
21.56
Me
N
N−Ph
MeO
5k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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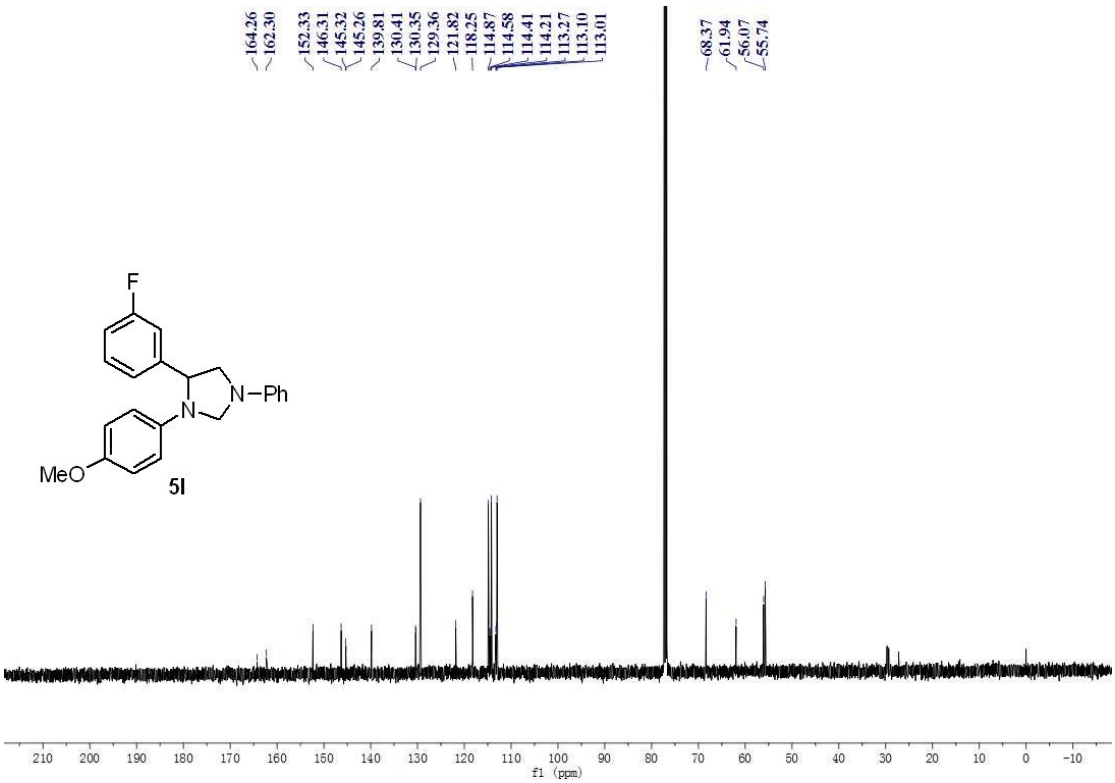
N–Ph
N
MeO
5l
f1 (ppm)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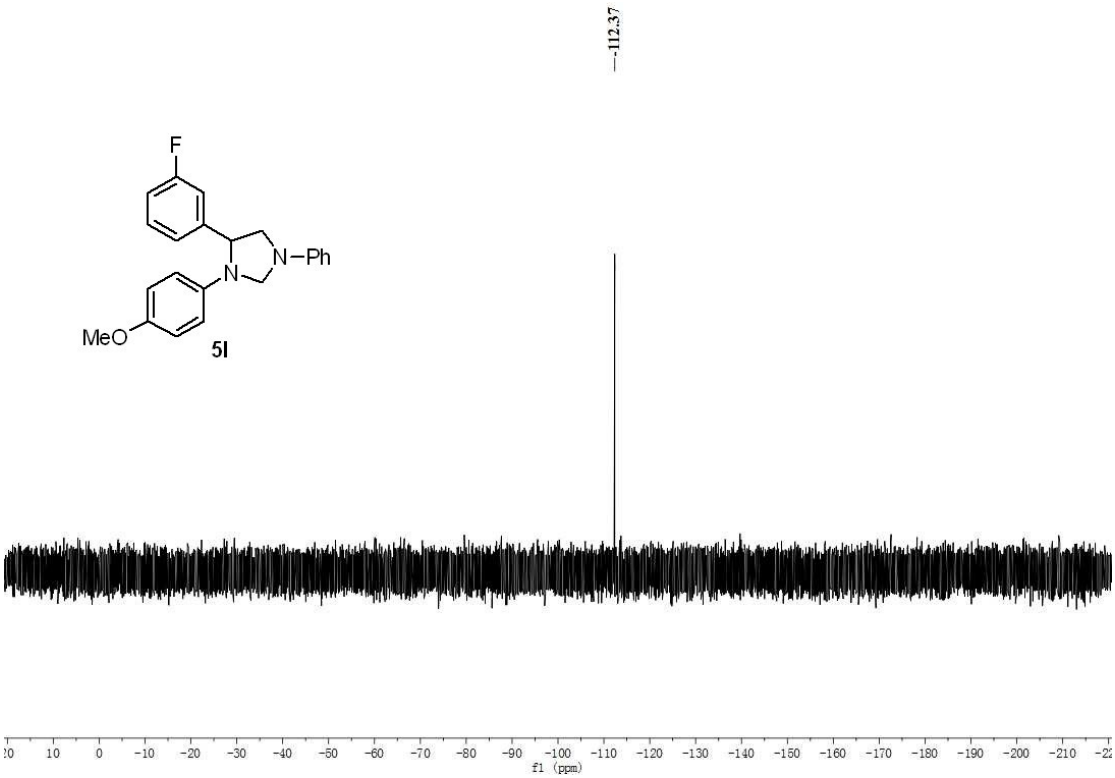
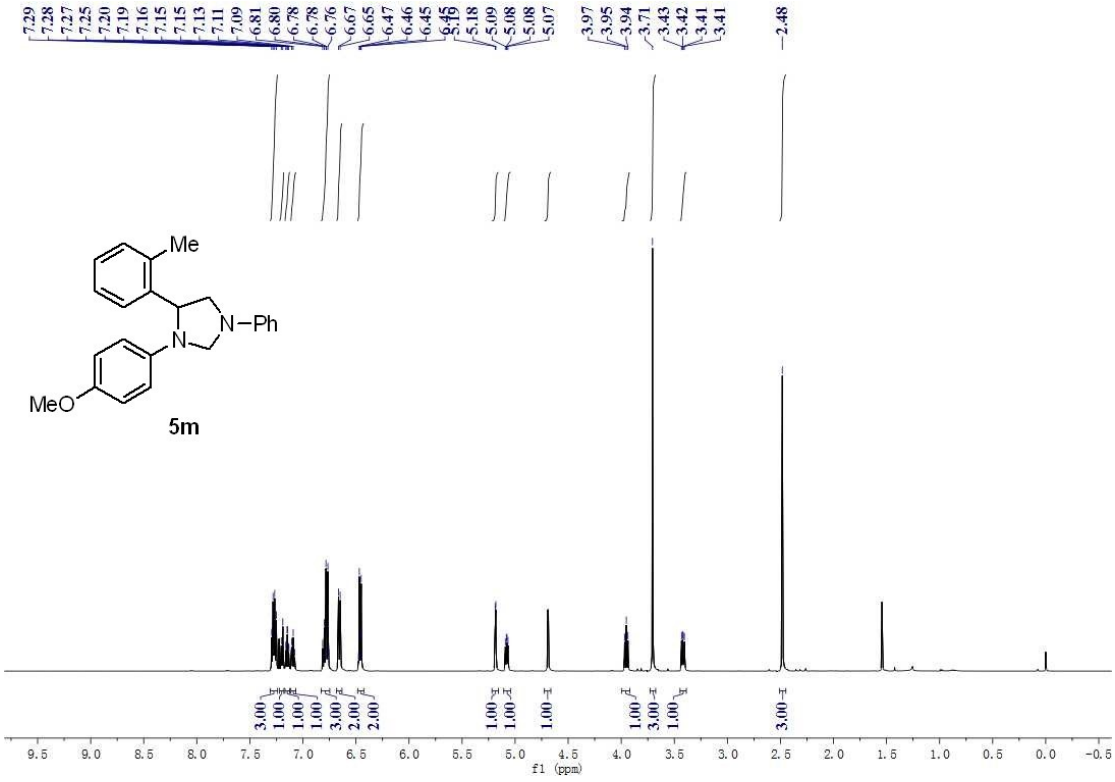
N–Ph
N
MeO
5l
f1 (ppm)


-112.37
F
N
N–Ph
MeO
5l
f1 (ppm)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7.11
7.09
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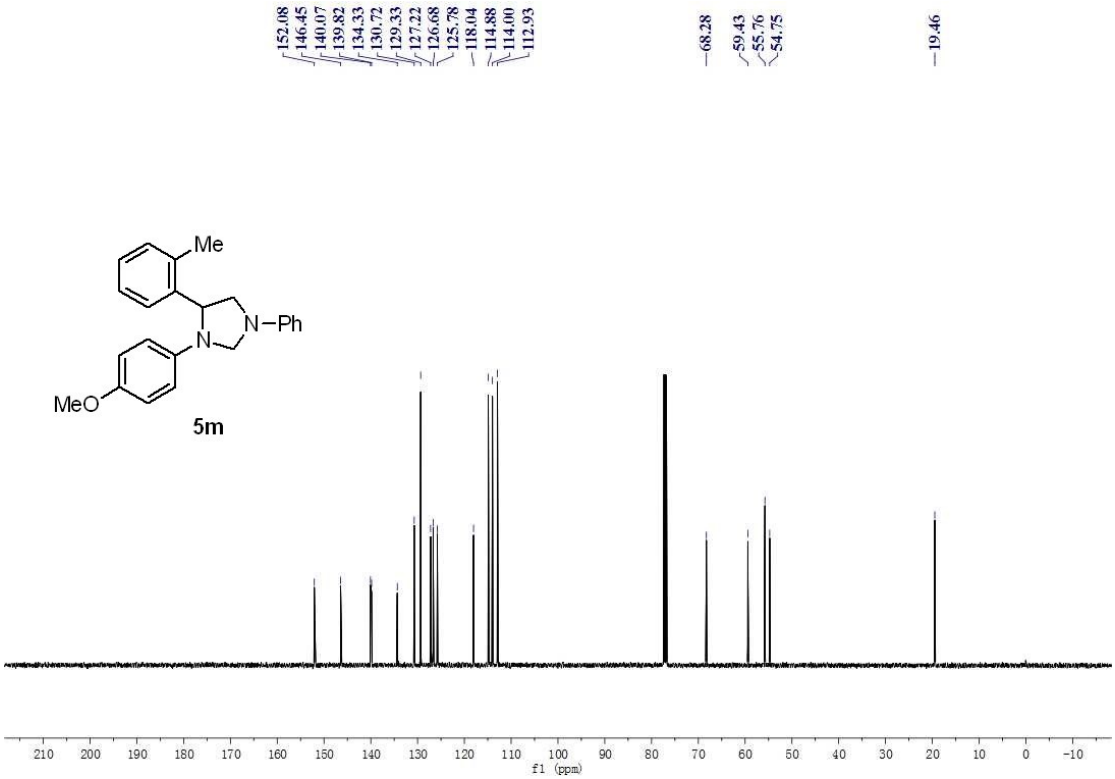
6.80
6.78
6.78
6.76
6.67
6.65
6.47
6.46
6.45
6.45
5.19
5.18
5.09
5.08
5.08
5.07
3.97
3.95
3.94
3.71
3.43
3.42
3.41
3.41
2.48
Me
N
N–Ph
MeO
5m
3.00
1.00
1.00
1.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
3.00
f1 (ppm)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127.22
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125.78
118.04
114.88
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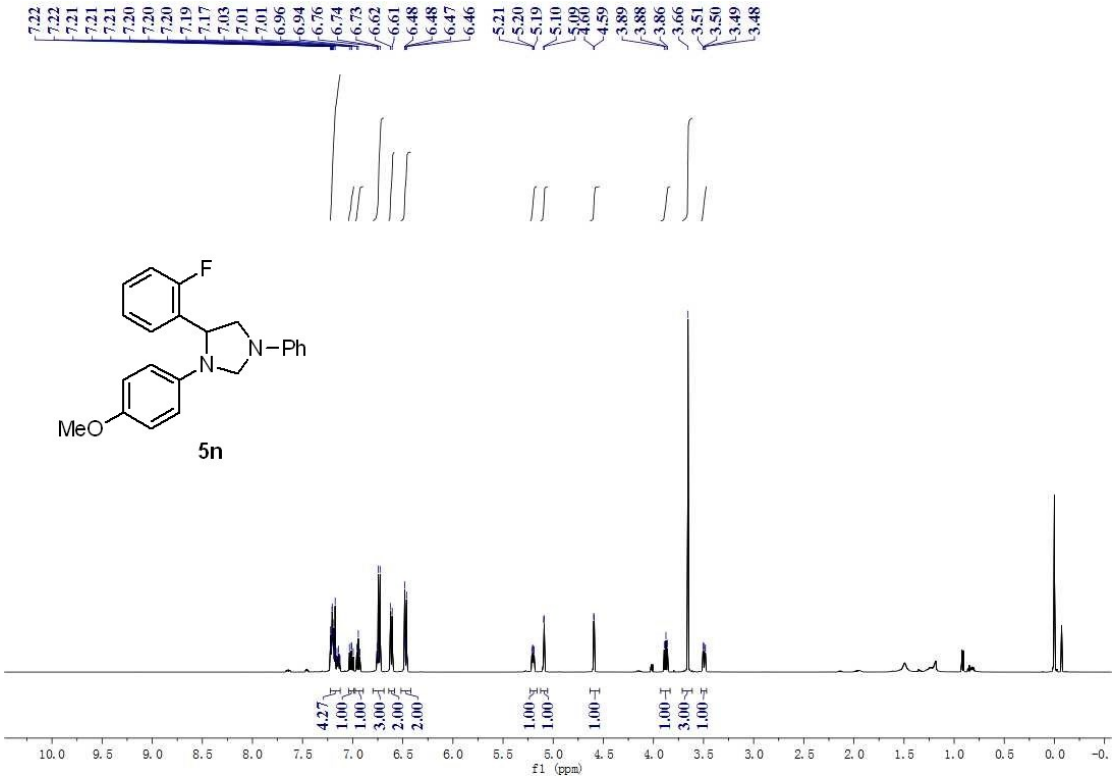
68.28
59.43
55.76
54.75
19.46
Me
N
N–Ph
MeO
5m
f1 (ppm)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7.17
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7.01
7.01
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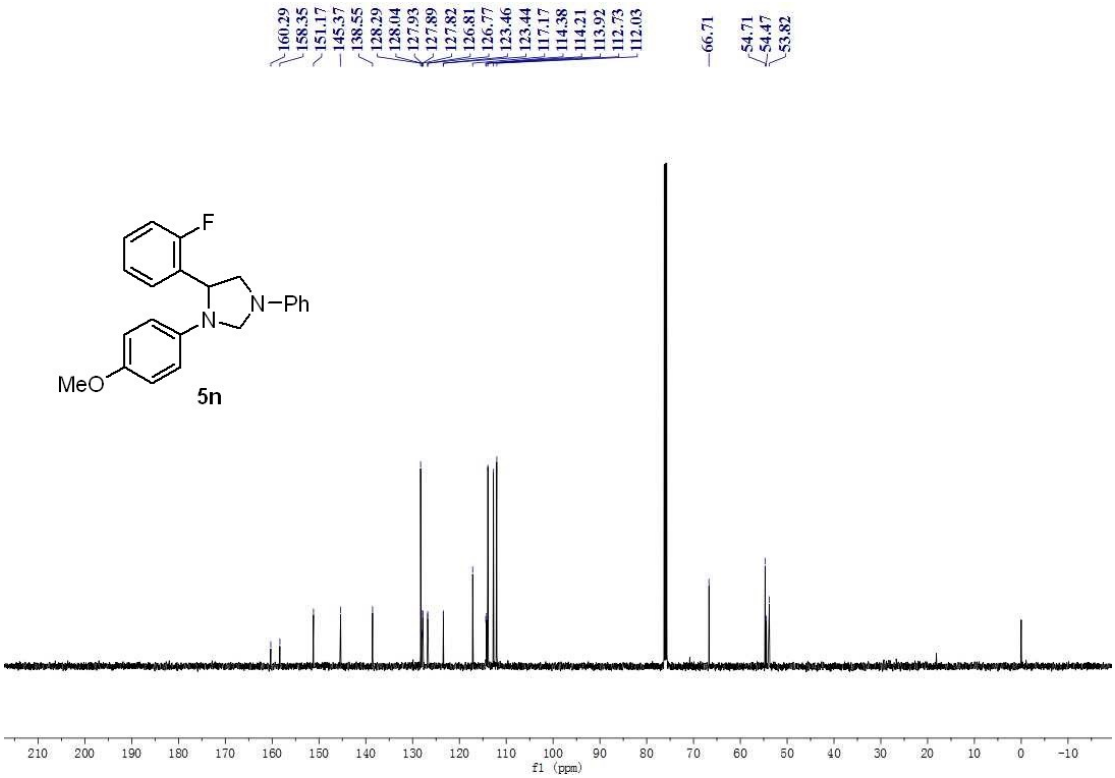
6.94
6.76
6.74
6.73
6.62
6.61
6.48
6.47
6.46
5.21
5.20
5.19
5.10
5.09
4.60
4.59
3.89
3.88
3.86
3.66
3.51
3.50
3.49
3.48
F
N
N–Ph
MeO
5n
4.27
1.00
1.00
3.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
f1 (ppm)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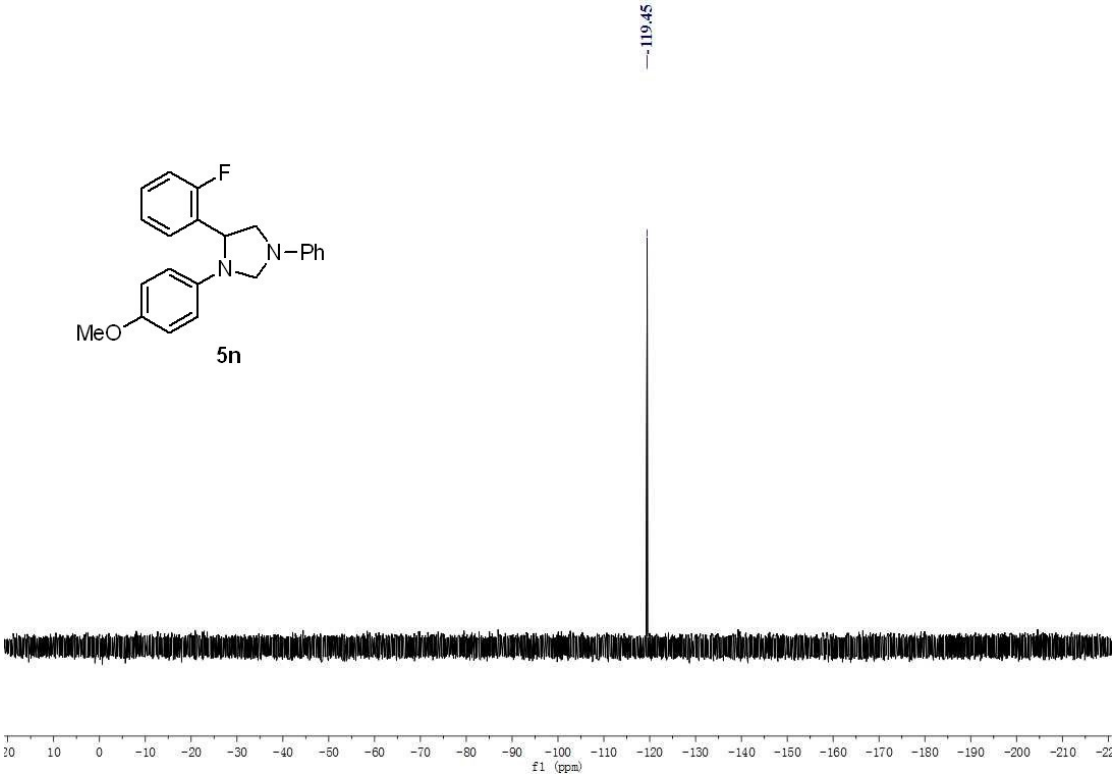
128.29
128.04
127.93
127.89
127.82
126.81
126.77
123.46
123.44
117.17
114.38
114.21
113.92
112.73
112.03
66.71
54.71
54.47
53.82
F
N
N–Ph
MeO
5n
f1 (ppm)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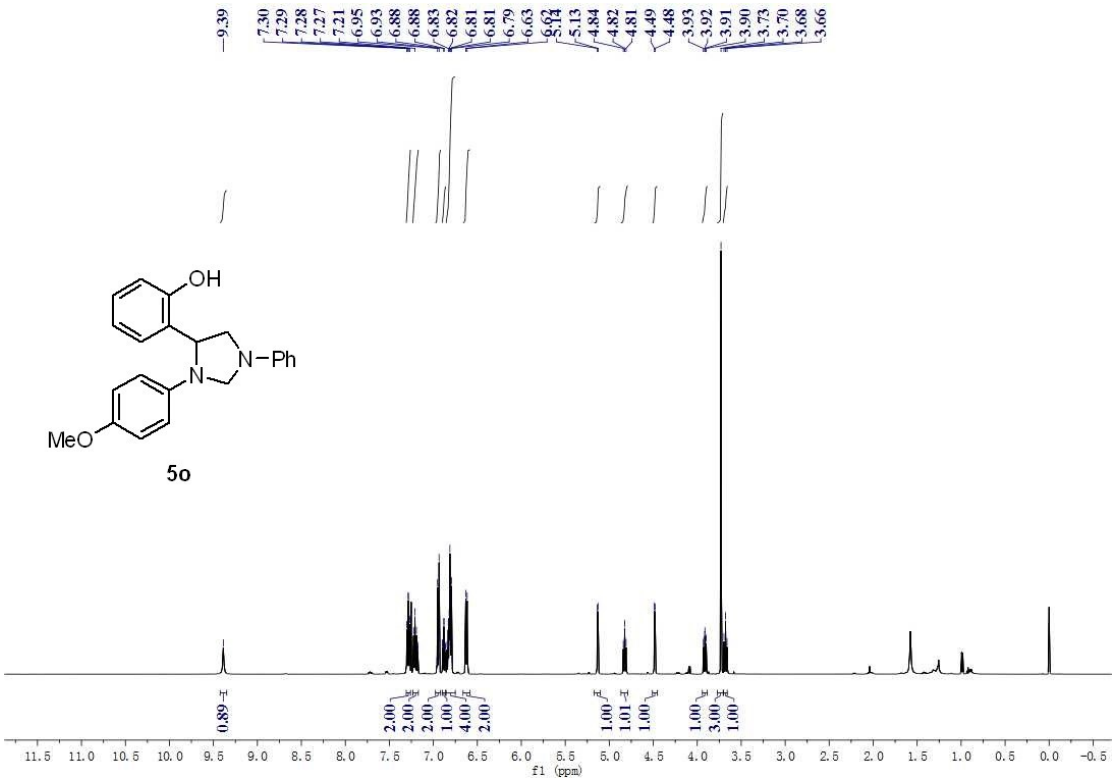
F
N
N–Ph
MeO
5n
f1 (ppm)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6.88
6.88
6.83
6.82
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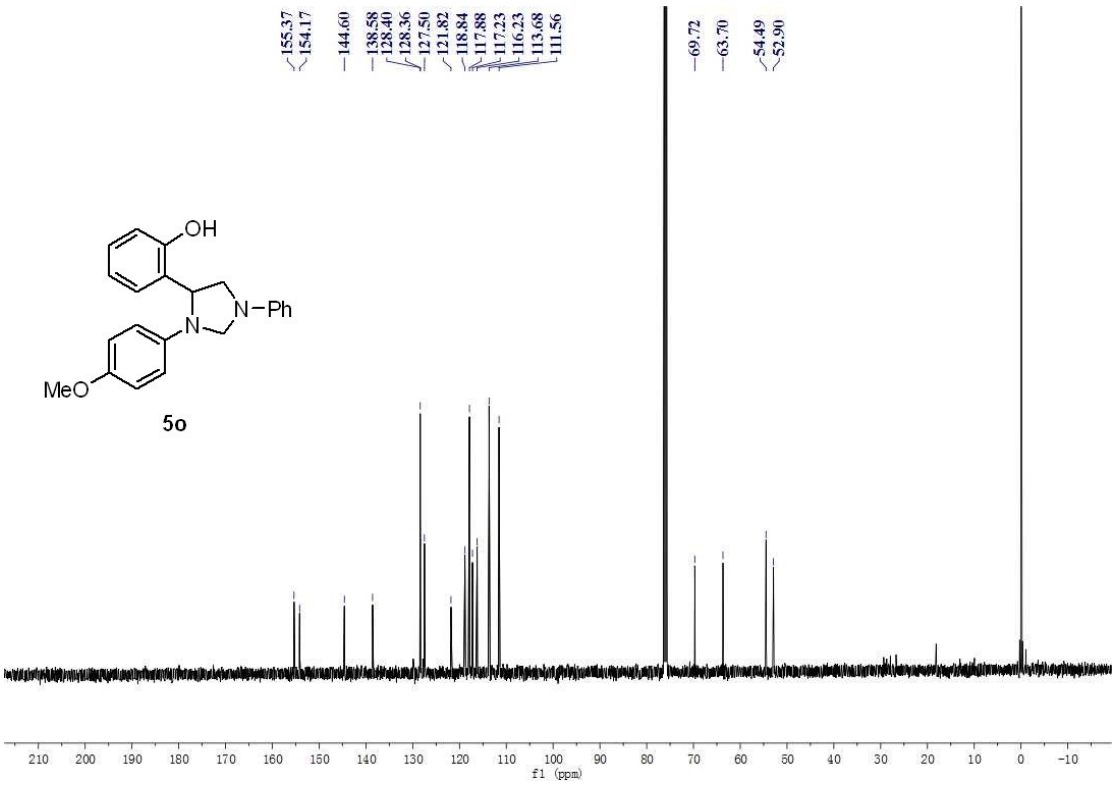
6.81
6.79
6.63
6.62
5.14
5.13
4.84
4.82
4.81
4.49
4.48
3.93
3.92
3.91
3.90
3.73
3.70
3.68
3.66
OH
N
N–Ph
MeO
5o
0.89
2.00
2.00
2.00
1.00
1.00
4.00
2.00
1.00
1.01
1.00
1.00
3.00
1.00
f1 (ppm)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118.84
117.88
117.23
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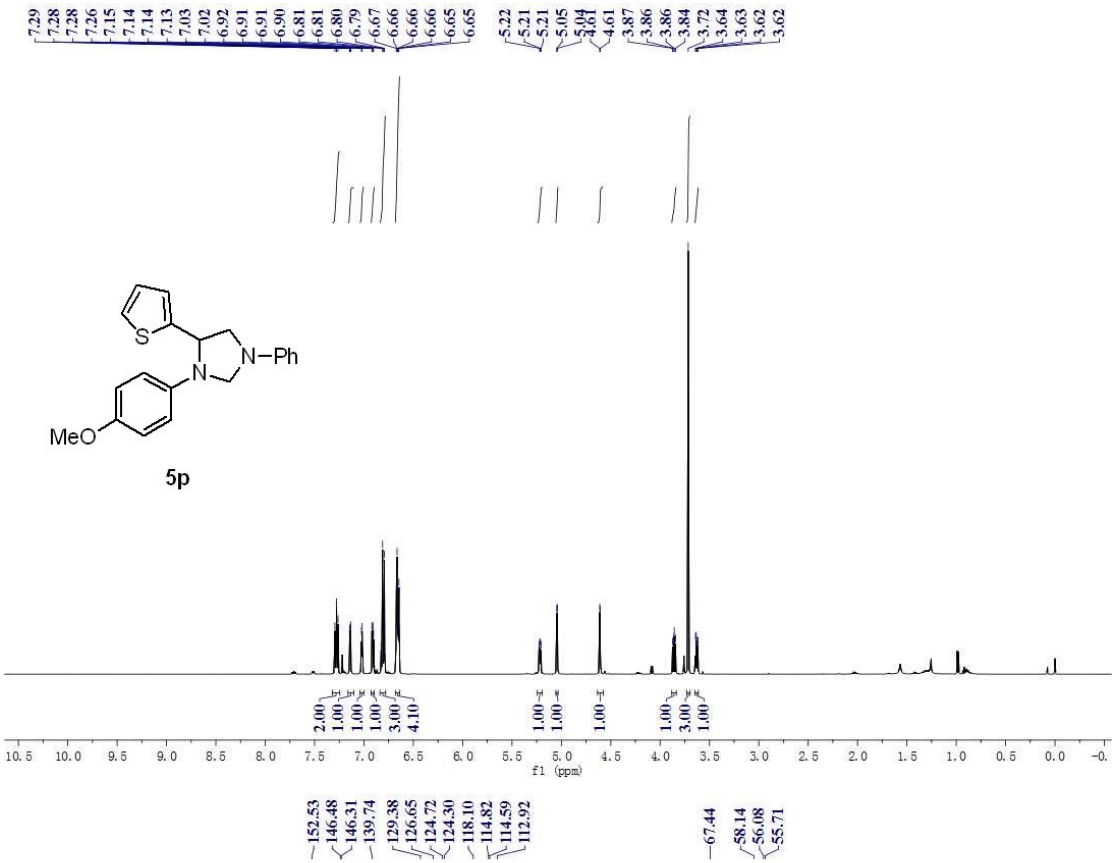
111.56
69.72
63.70
54.49
52.90
OH
N
N–Ph
MeO
5o
f1 (ppm)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7.02
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6.81
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6.66
6.65
6.65
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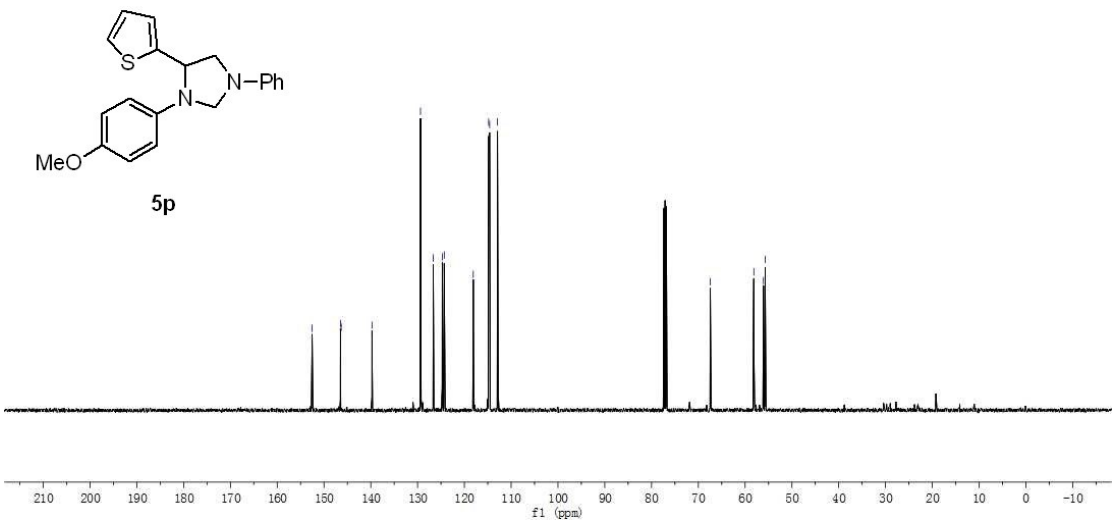
5.21
5.05
5.04
4.61
4.61
3.87
3.86
3.86
3.84
3.72
3.64
3.63
3.62
3.62
S
N
N–Ph
MeO
5p
2.00
1.00
1.00
1.00
3.00
4.10
1.00
1.00
1.00
1.00
3.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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118.10
114.82
114.59
112.92
67.44
58.14
56.08
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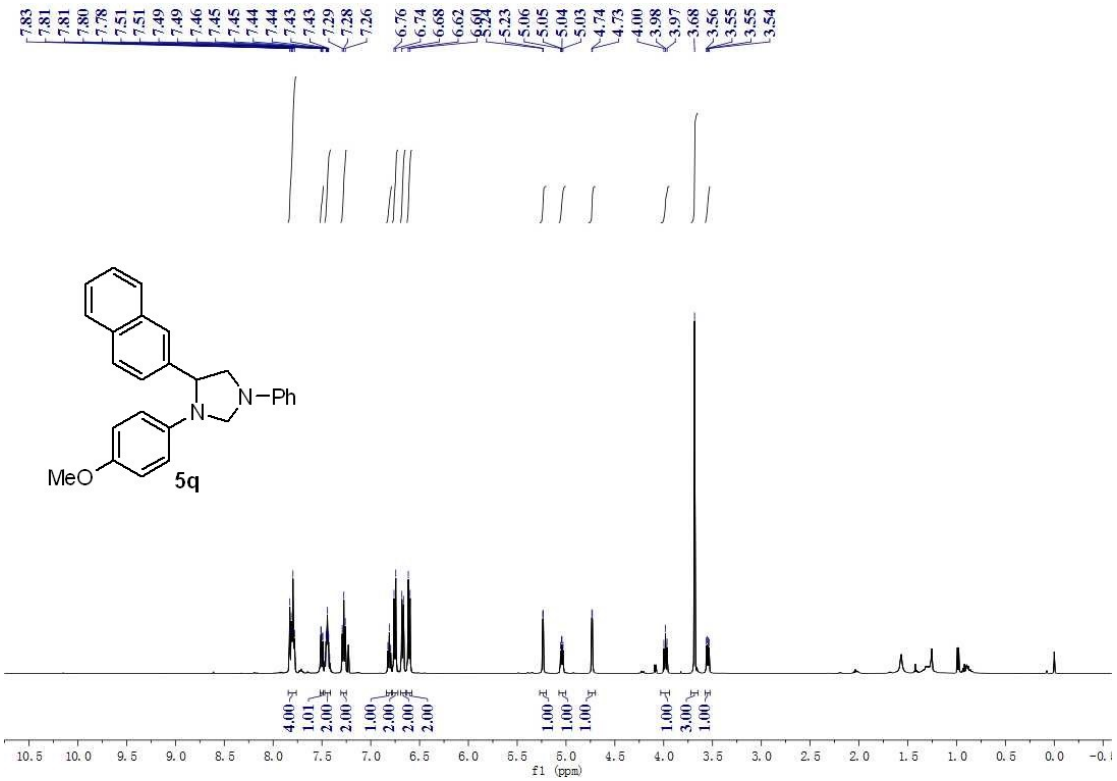
S
N
N–Ph
MeO
5p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.43
7.29
7.28
7.26
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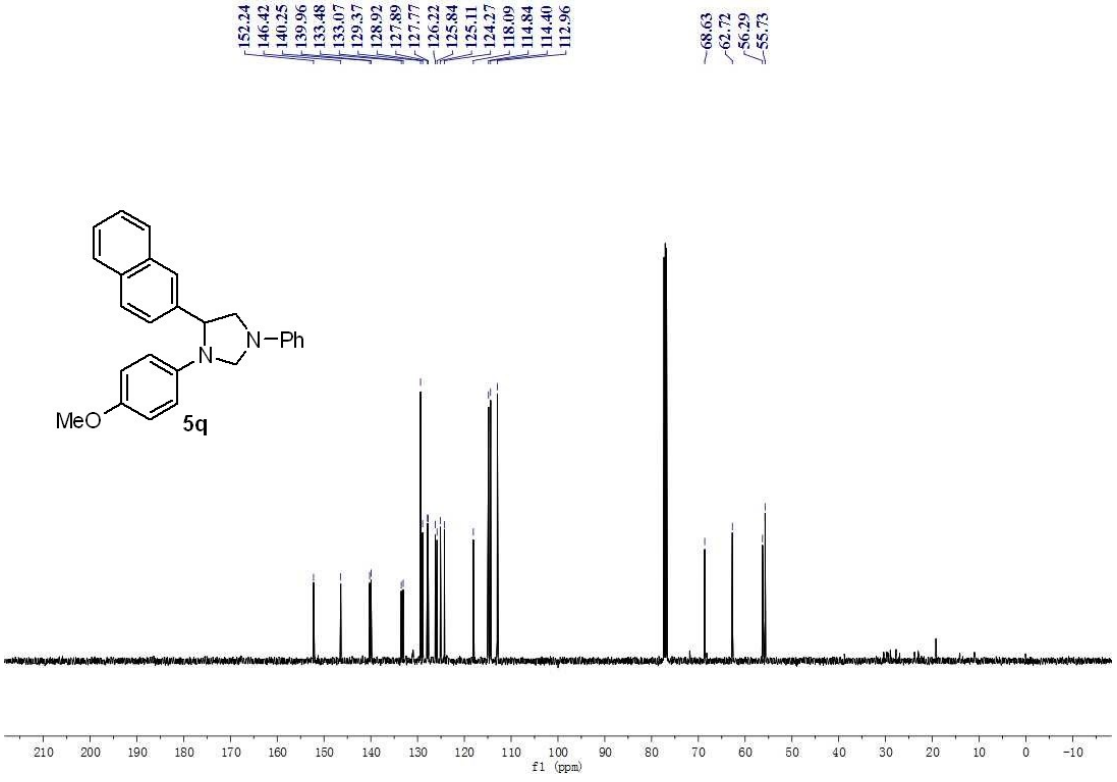
6.74
6.68
6.62
6.60
5.23
5.06
5.05
5.04
5.03
4.74
4.73
4.00
3.98
3.97
3.68
3.56
3.55
3.55
3.54
N–Ph
N
N
MeO
5q
4.00
1.01
2.00
2.00
1.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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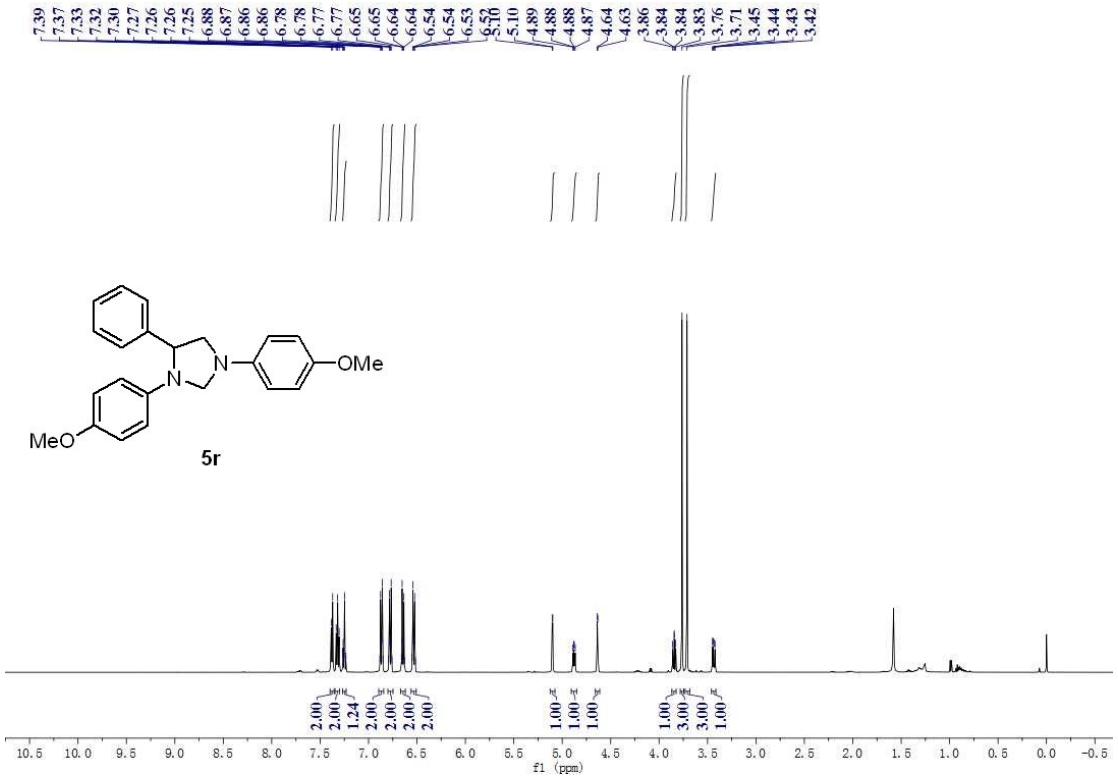
125.11
124.27
118.09
114.84
114.40
112.96
68.63
62.72
56.29
55.73
N–Ph
N
N
MeO
5q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.78
6.77
6.77
6.65
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6.64
6.64
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6.54
6.53
6.52
5.10
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4.88
4.87
4.64
4.63
3.86
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3.84
3.83
3.76
3.71
3.45
3.44
3.43
3.42
OMe
MeO
5r
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2.00
1.24
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2.00
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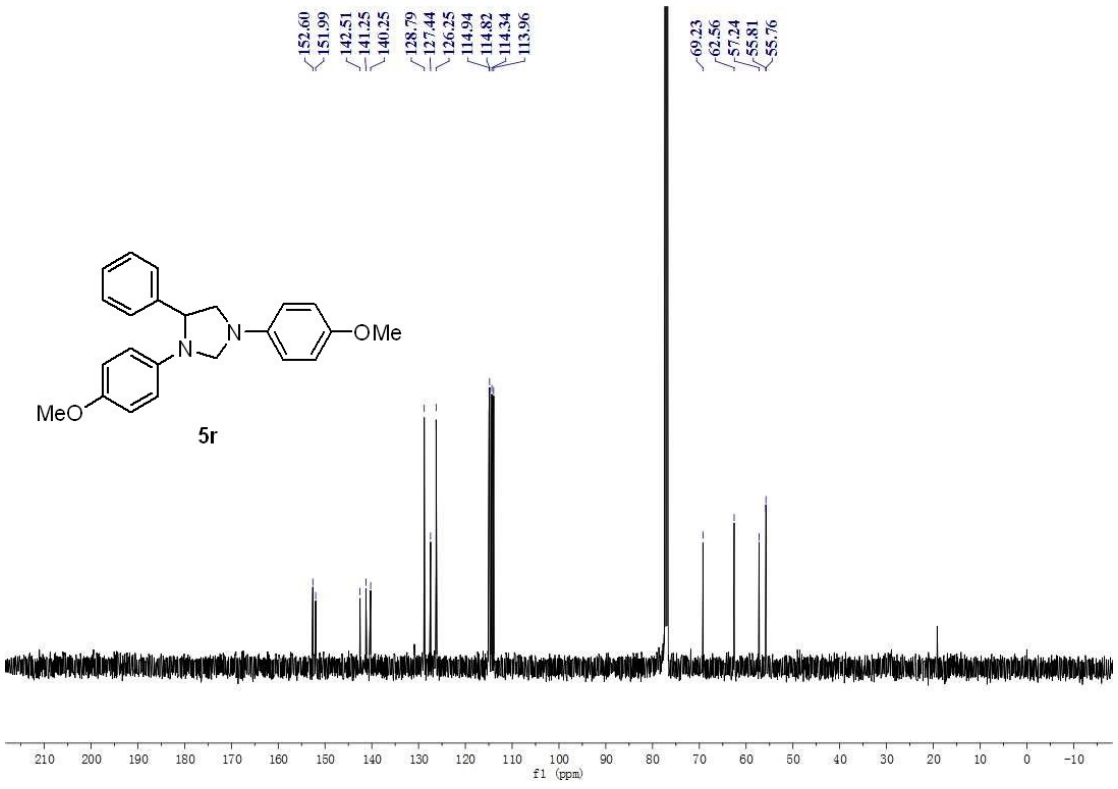
2.00
1.00
1.00
1.00
1.00
3.00
3.00
1.00
f1 (ppm)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126.25
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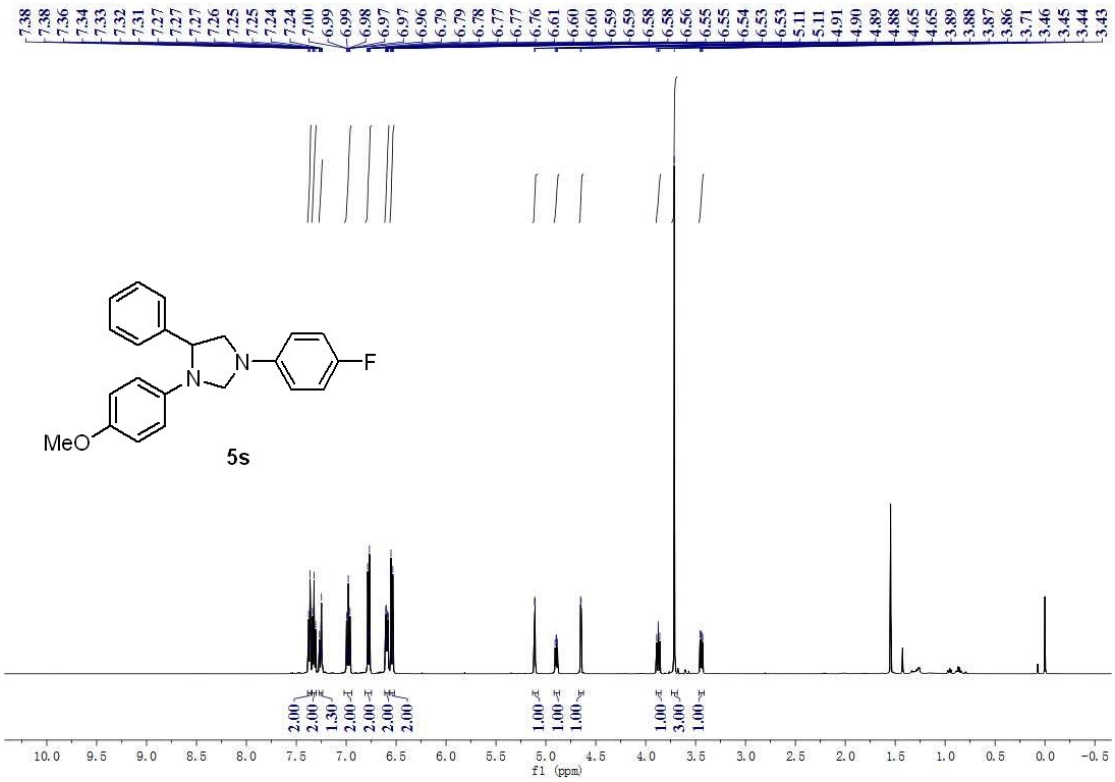
113.96
69.23
62.56
57.24
55.81
55.76
OMe
MeO
5r
f1 (ppm)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3.86
3.71
3.46
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3.43
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F
MeO
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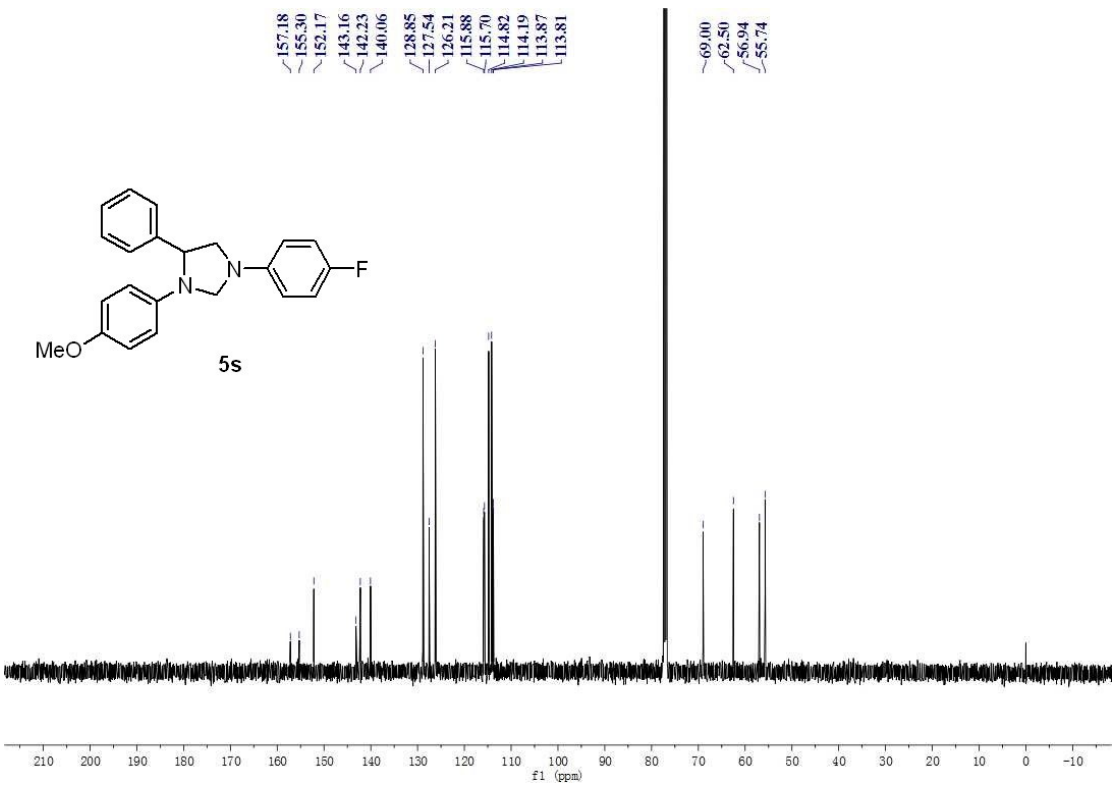
1.30
2.00
2.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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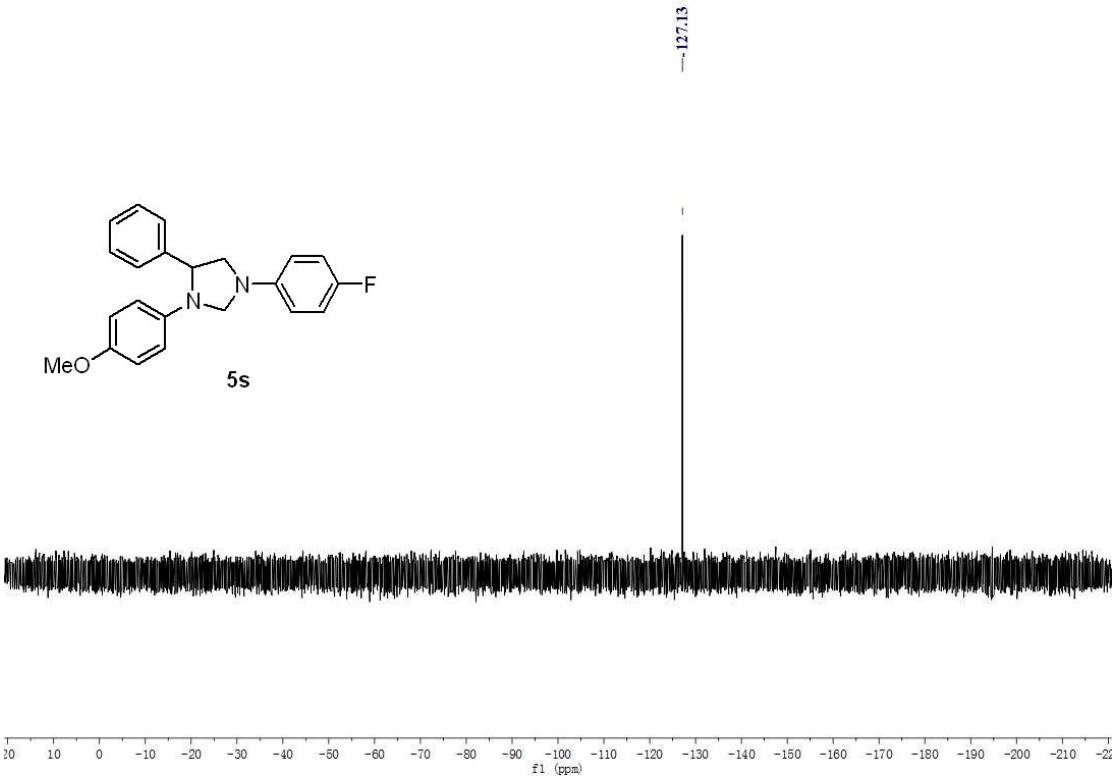
127.54
126.21
115.88
115.70
114.82
114.19
113.87
113.81
69.00
62.50
56.94
55.74
N
N
F
MeO
5s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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F
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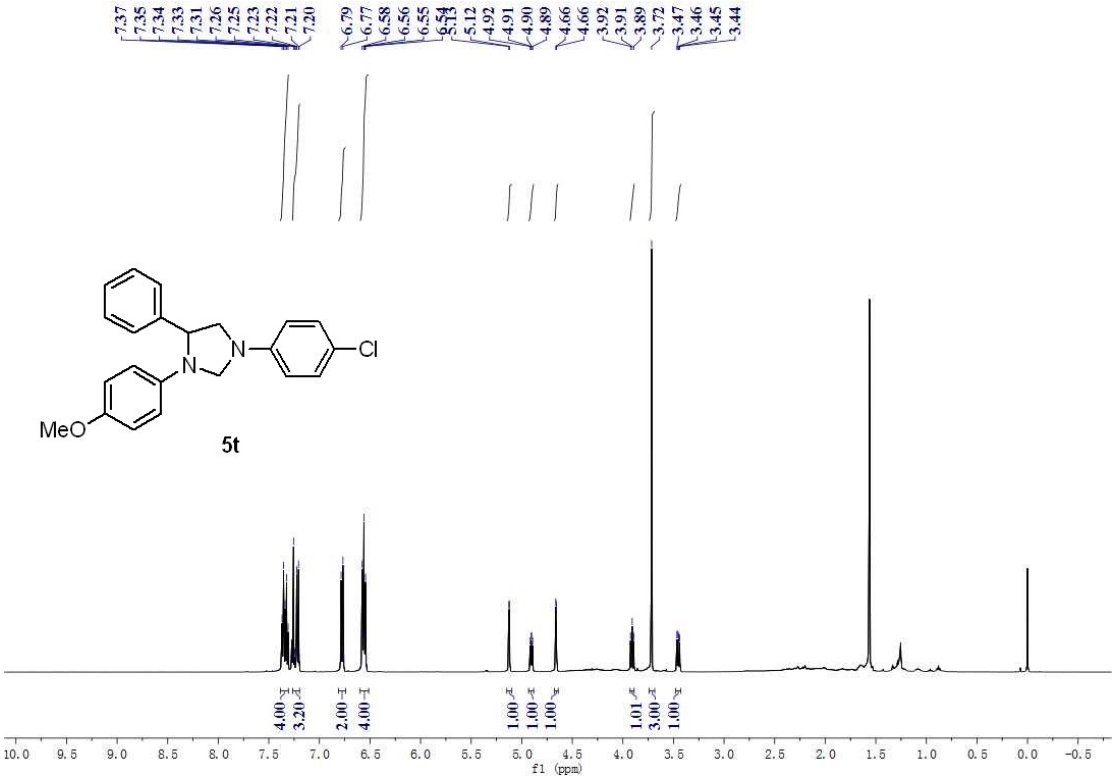
N
MeO
5s
f1 (ppm)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7.33
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7.21
7.20
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6.77
6.58
6.56
6.55
5.12
4.92
4.91
4.90
4.89
4.66
4.66
3.92
3.91
3.89
3.72
3.47
3.46
3.45
3.44
Cl
N
N
MeO
5t
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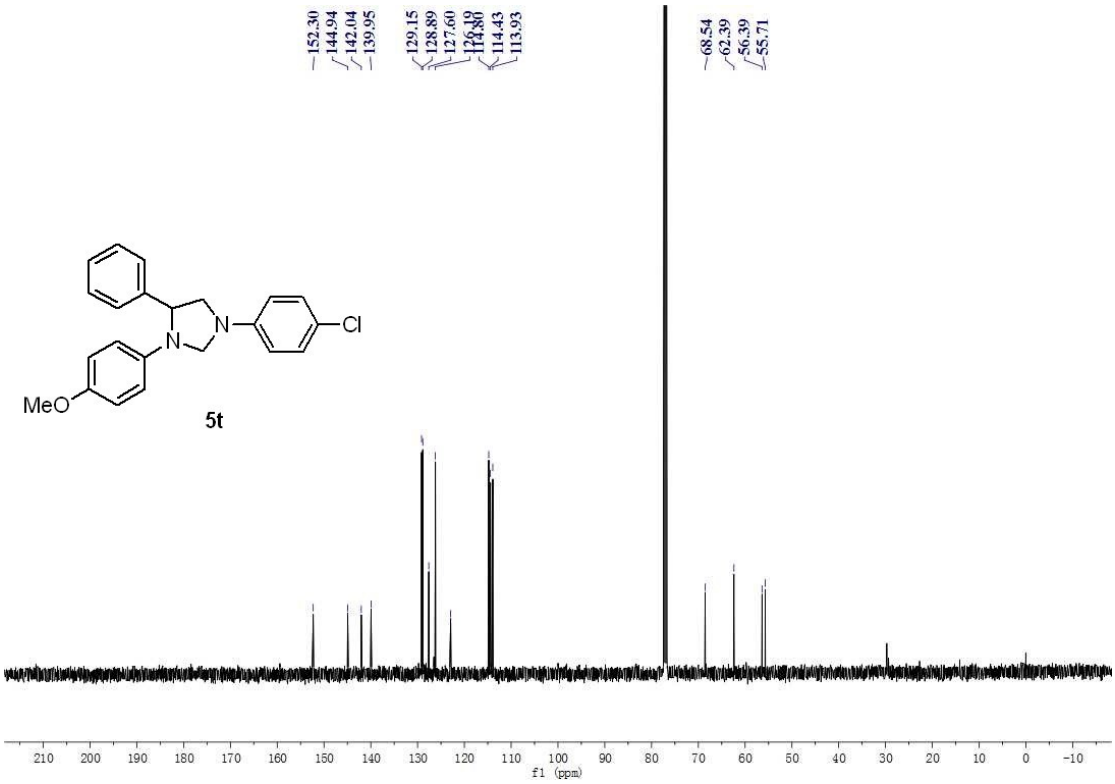
2.00
4.00
1.00
1.00
1.00
1.01
3.00
1.00
f1 (ppm)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128.89
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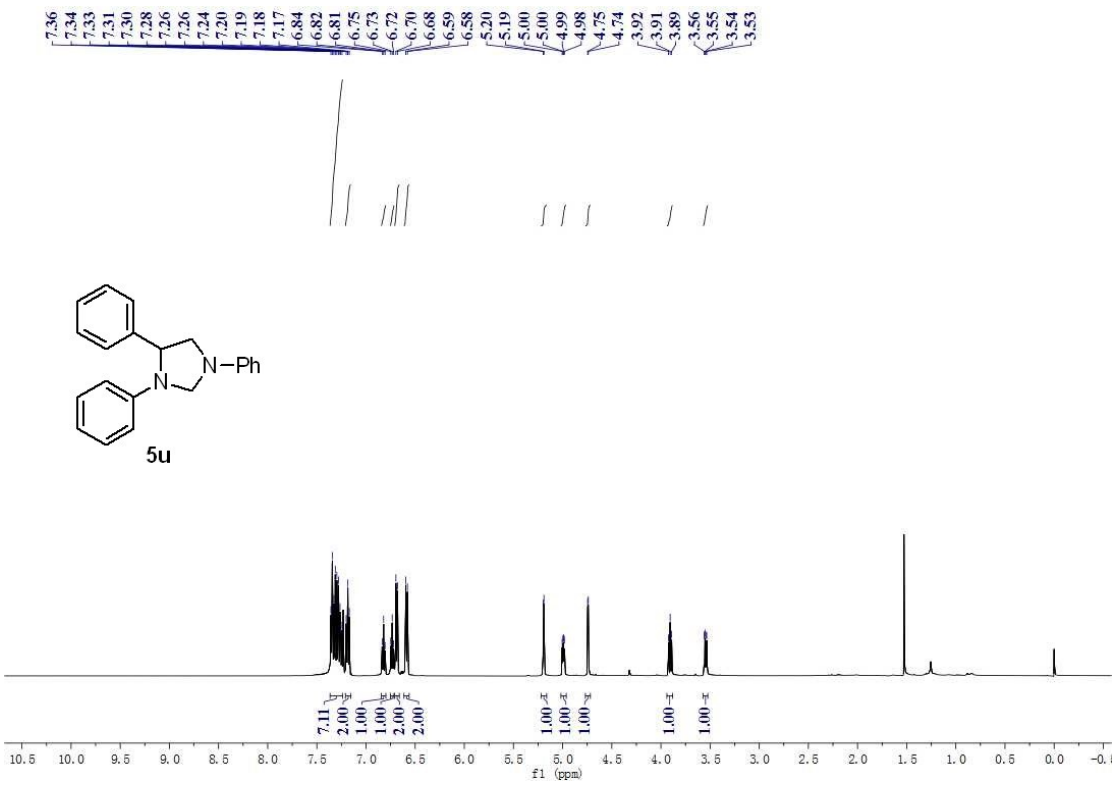
113.93
68.54
62.39
56.39
55.71
Cl
N
N
MeO
5t
f1 (ppm)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7.19
7.18
7.17
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6.82
6.81
6.75
6.73
6.72
6.70
6.68
6.59
6.58
5.20
5.19
5.00
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4.99
4.98
4.75
4.74
3.92
3.91
3.89
3.56
3.55
3.54
3.53
N
N–Ph
5u
7.11
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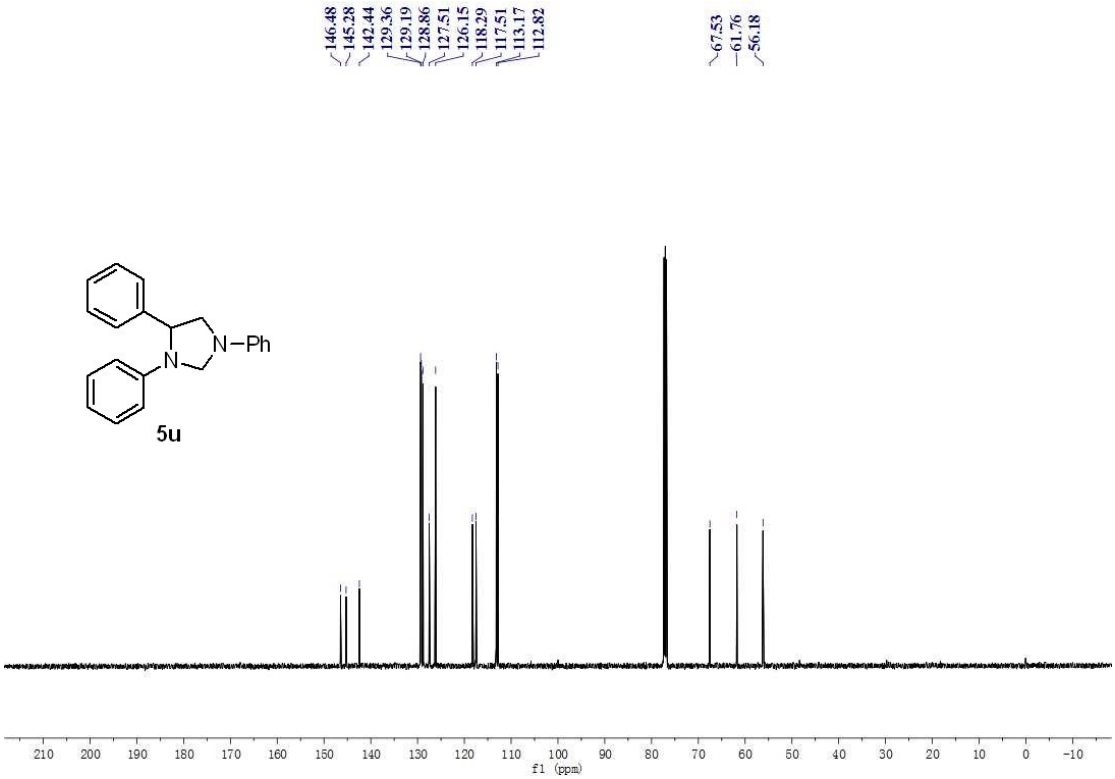
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
f1 (ppm)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145.28
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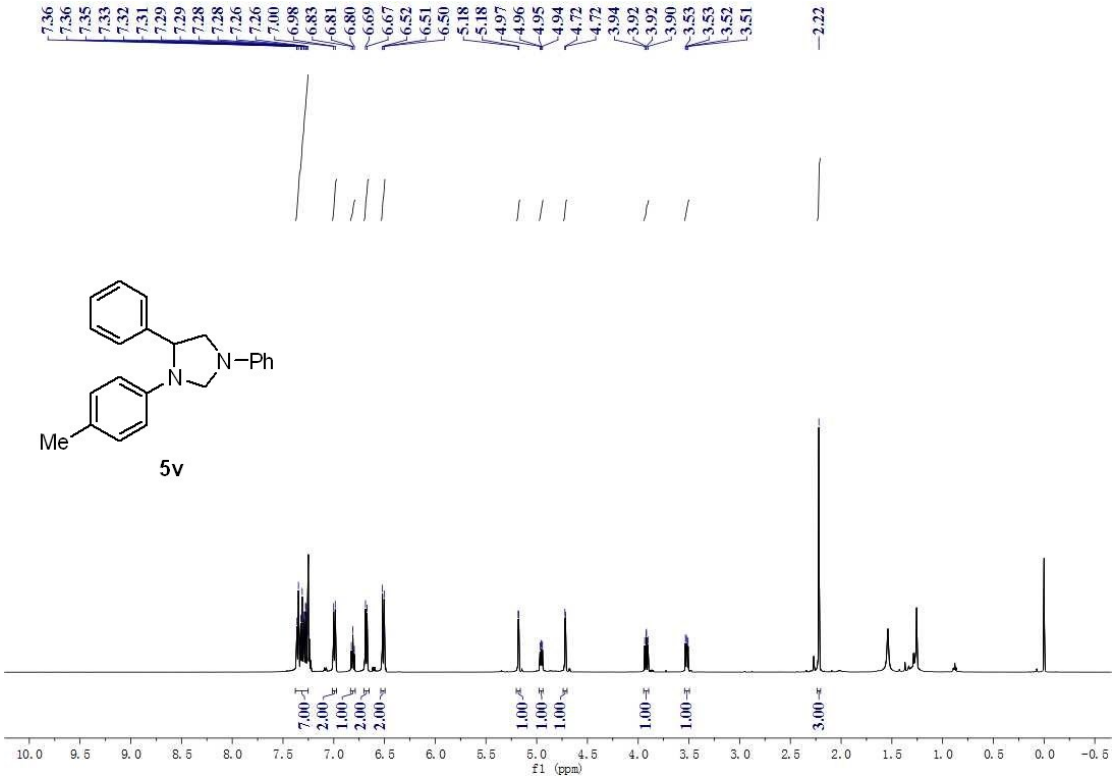
117.51
113.17
112.82
67.53
61.76
56.18
N–Ph
5u
f1 (ppm)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7.29
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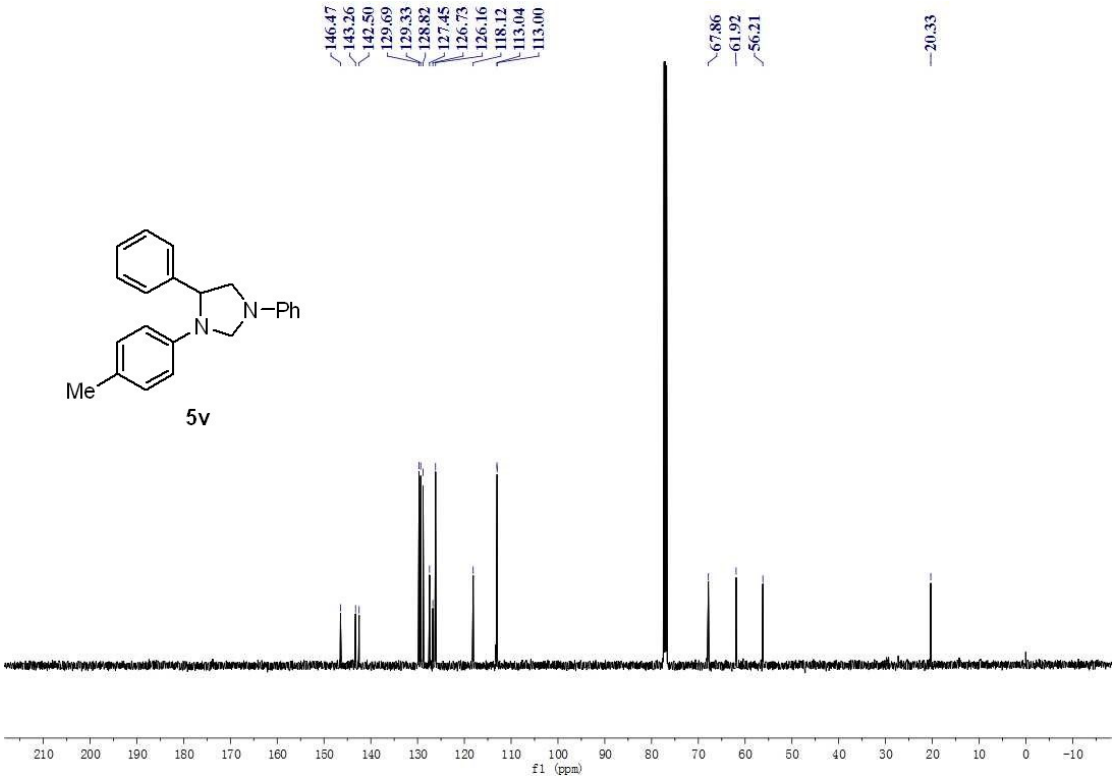
7.26
7.00
6.98
6.83
6.81
6.80
6.69
6.67
6.52
6.51
6.50
5.18
5.18
4.97
4.96
4.95
4.94
4.72
4.72
3.94
3.92
3.92
3.90
3.53
3.53
3.52
3.51
2.22
N–Ph
Me
5v
7.00
2.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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143.26
142.50
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129.33
128.82
127.45
126.73
126.16
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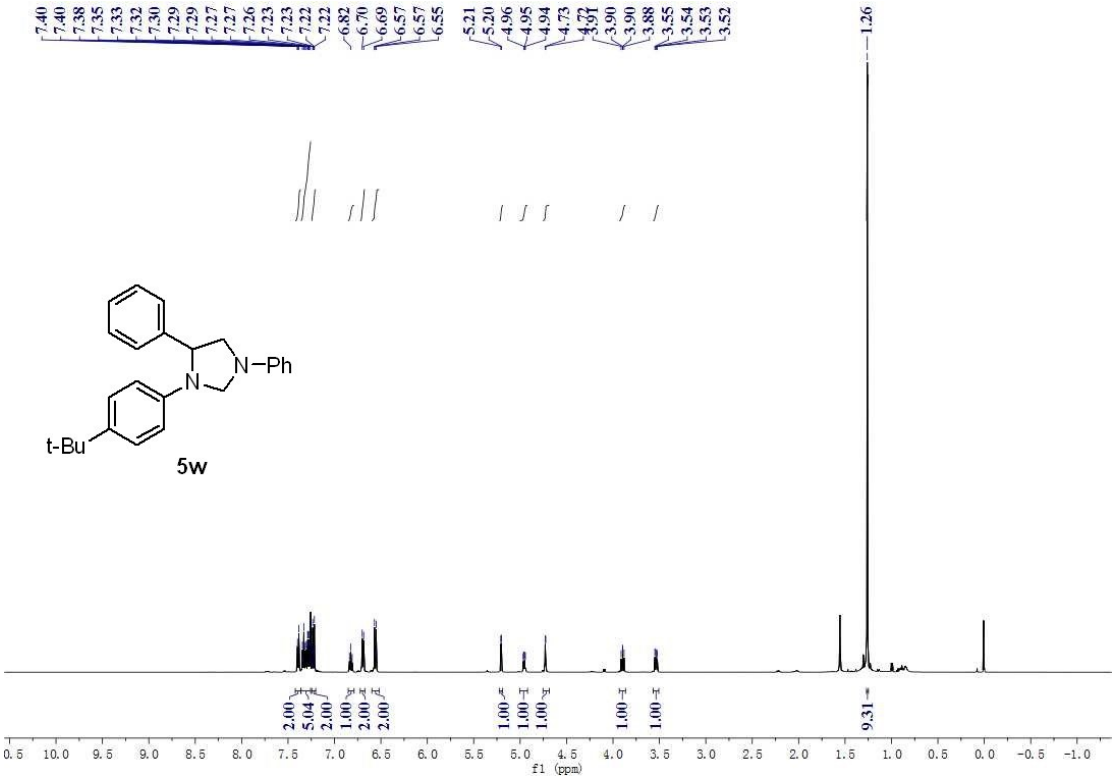
113.04
113.00
67.86
61.92
56.21
20.33
N–Ph
N
N
Me
5v
f1 (ppm)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7.29
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7.27
7.27
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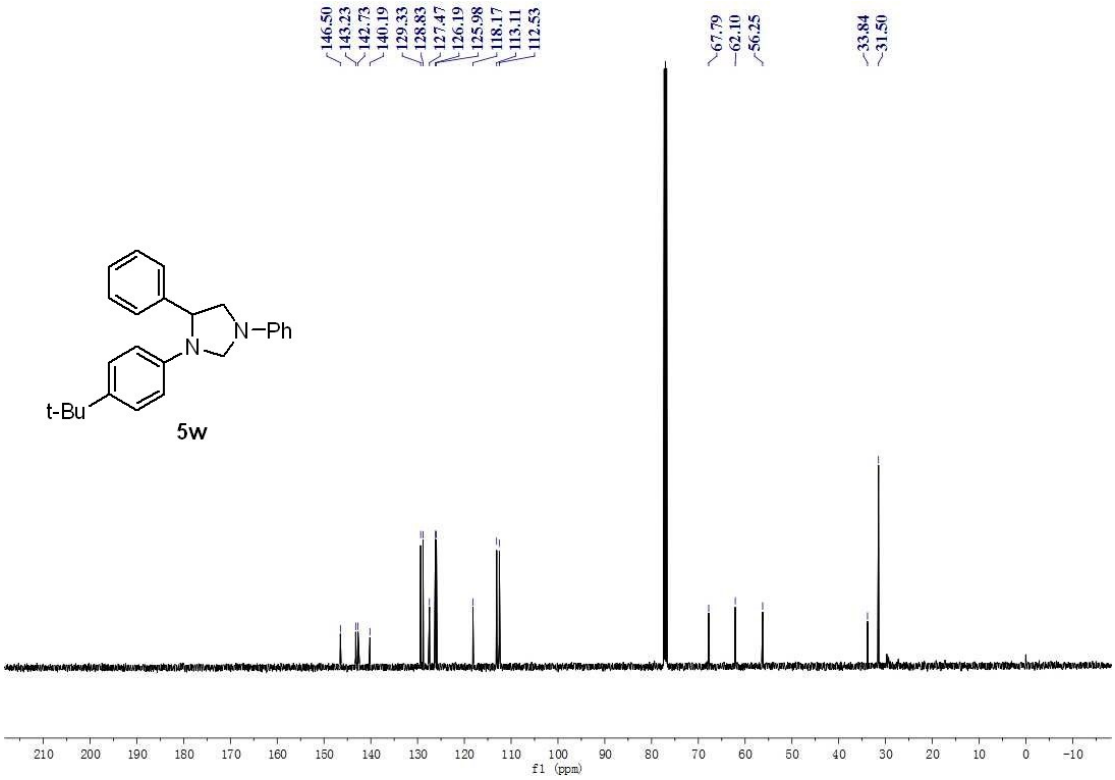
7.23
7.23
7.22
7.22
6.82
6.70
6.69
6.57
6.57
6.55
5.21
5.20
4.96
4.95
4.94
4.73
3.90
3.90
3.88
3.55
3.54
3.53
3.52
1.26
N–Ph
N
N
t-Bu
5w
2.00
5.04
2.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
9.31
f1 (ppm)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140.19
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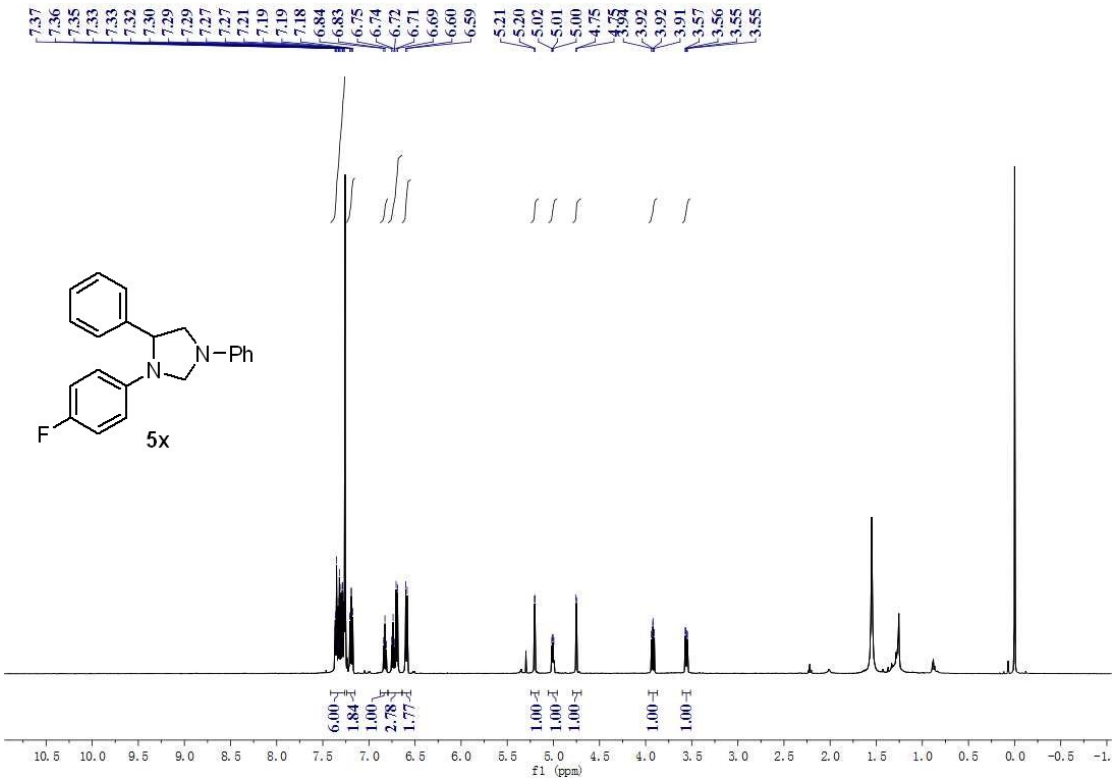
128.83
127.47
126.19
125.98
118.17
113.11
112.53
67.79
62.10
56.25
33.84
31.50
N–Ph
t-Bu
5w
f1 (ppm)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7.36
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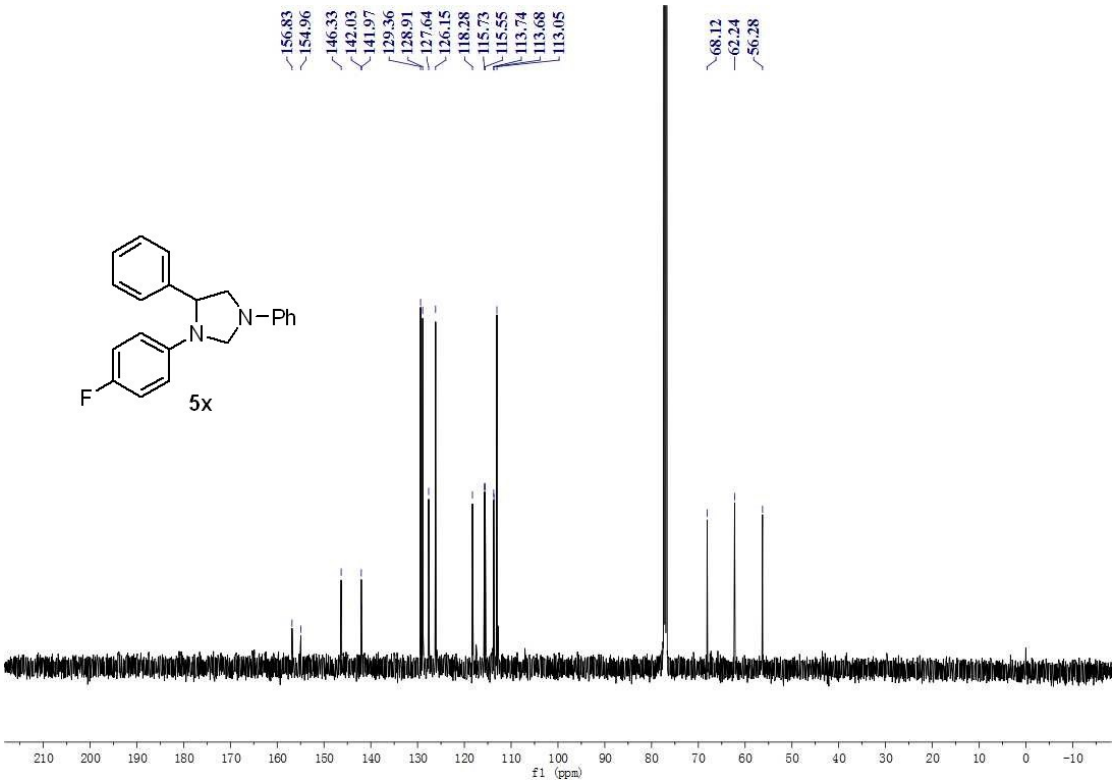
7.27
7.27
7.21
7.19
7.19
7.18
6.84
6.83
6.75
6.74
6.72
6.71
6.69
6.60
6.59
5.21
5.20
5.02
5.01
5.00
4.75
3.94
3.92
3.92
3.91
3.57
3.56
3.55
3.55
N–Ph
F
5x
6.00
1.84
1.00
2.78
1.77
1.00
1.00
1.00
1.00
1.00
f1 (ppm)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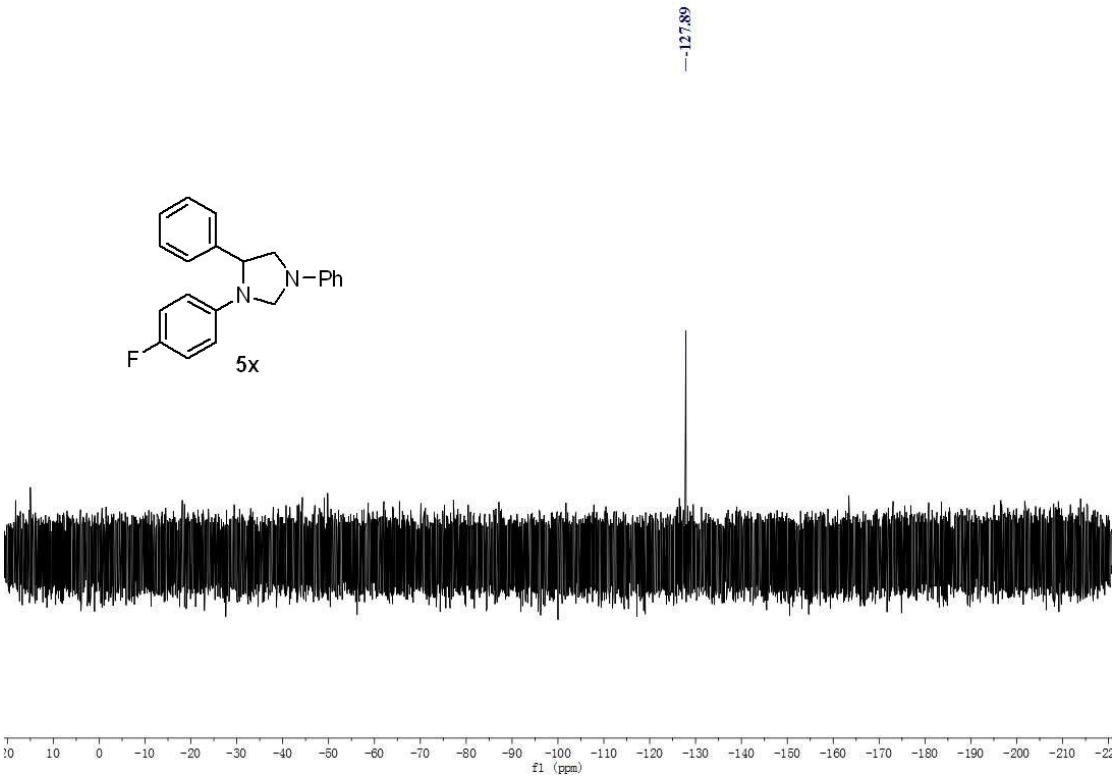
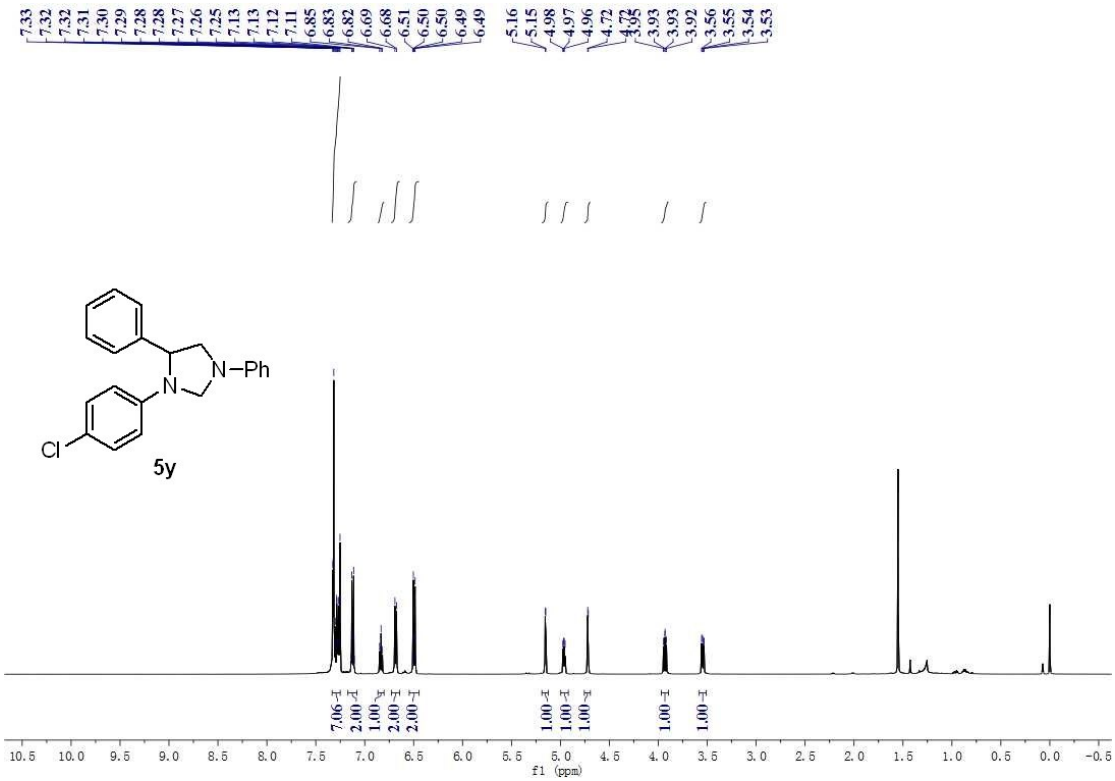
154.96
146.33
142.03
141.97
129.36
128.91
127.64
126.15
118.28
115.73
115.55
113.74
113.68
113.05
68.12
62.24
56.28
N–Ph
N
F
5x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-127.89
N–Ph
N
F
5x
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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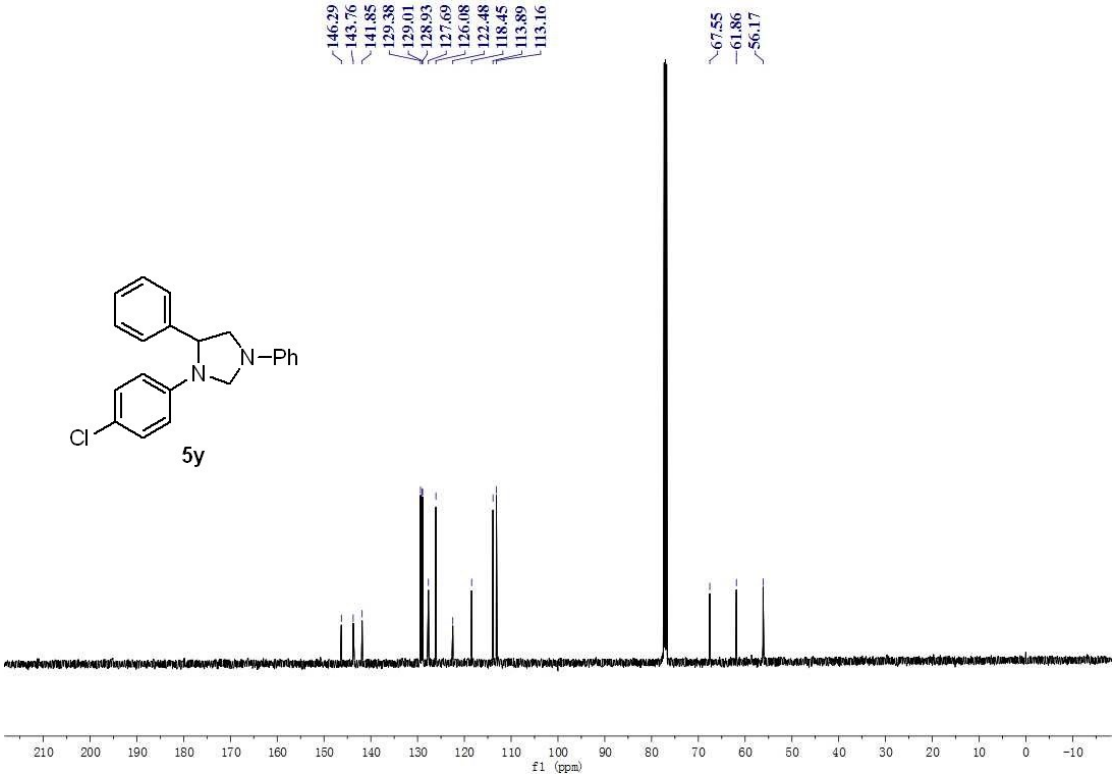
7.30
7.29
7.28
7.28
7.27
7.26
7.25
7.13
7.13
7.12
7.11
6.85
6.83
6.82
6.69
6.68
6.51
6.50
6.50
6.49
6.49
5.16
5.15
4.98
4.97
4.96
4.72
4.72
3.95
3.93
3.93
3.92
3.56
3.55
3.54
3.53
N–Ph
N
N
Cl
5y
7.06
2.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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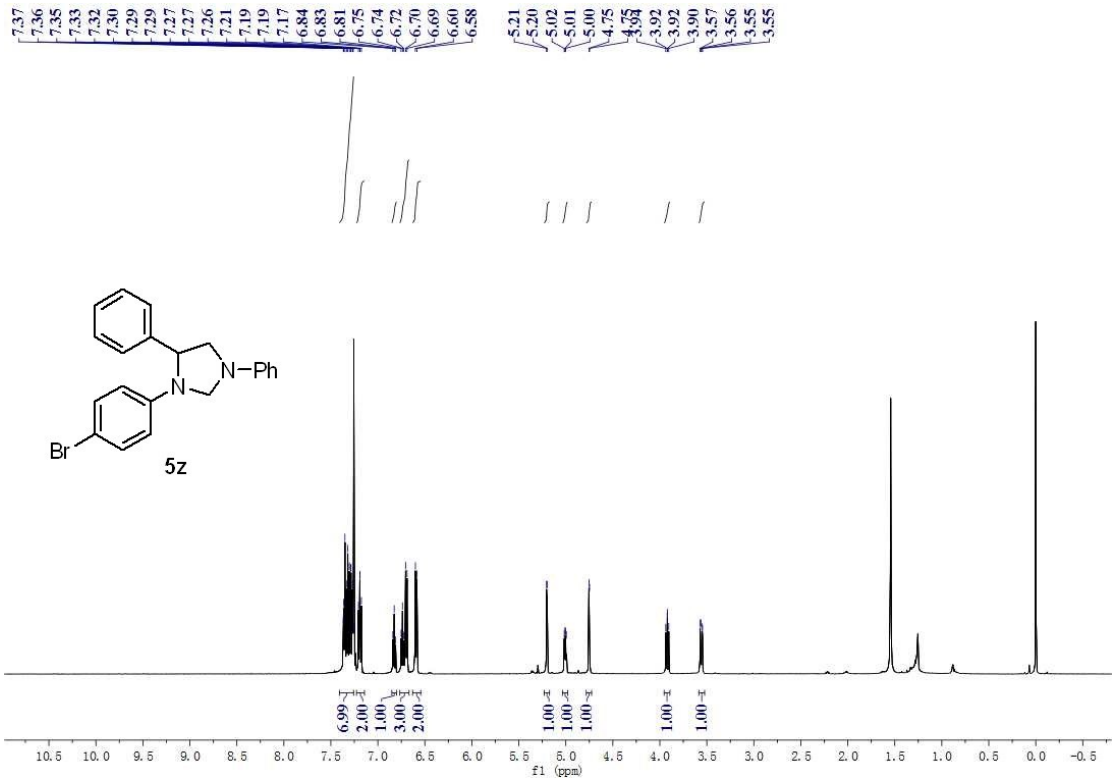
128.93
127.69
126.08
122.48
118.45
113.89
113.16
67.55
61.86
56.17
N–Ph
N
N
Cl
5y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.36
7.35
7.33
7.32
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7.29
7.27
7.27
7.26
7.21
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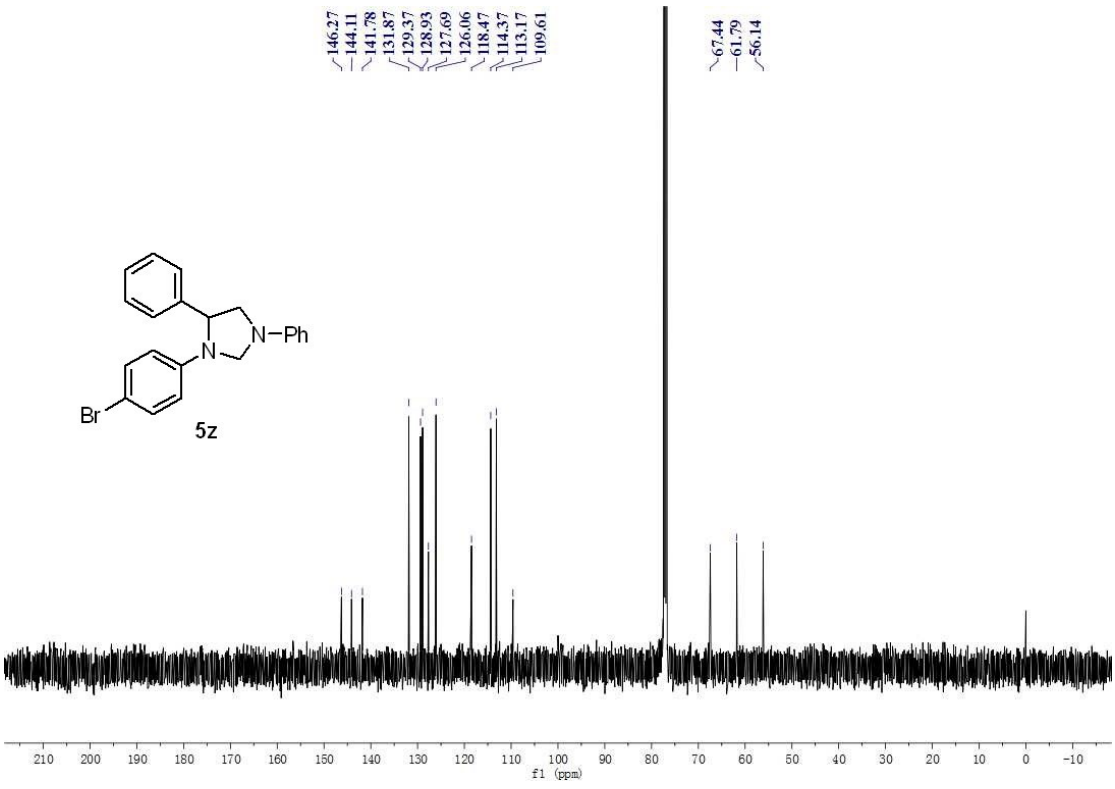
7.19
7.17
6.84
6.83
6.81
6.75
6.74
6.72
6.70
6.69
6.60
6.58
5.21
5.20
5.02
5.01
5.00
4.75
3.94
3.92
3.92
3.90
3.57
3.56
3.55
3.55
N–Ph
N
N
Br
5z
6.99
2.00
1.00
3.00
2.00
1.00
1.00
1.00
1.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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144.11
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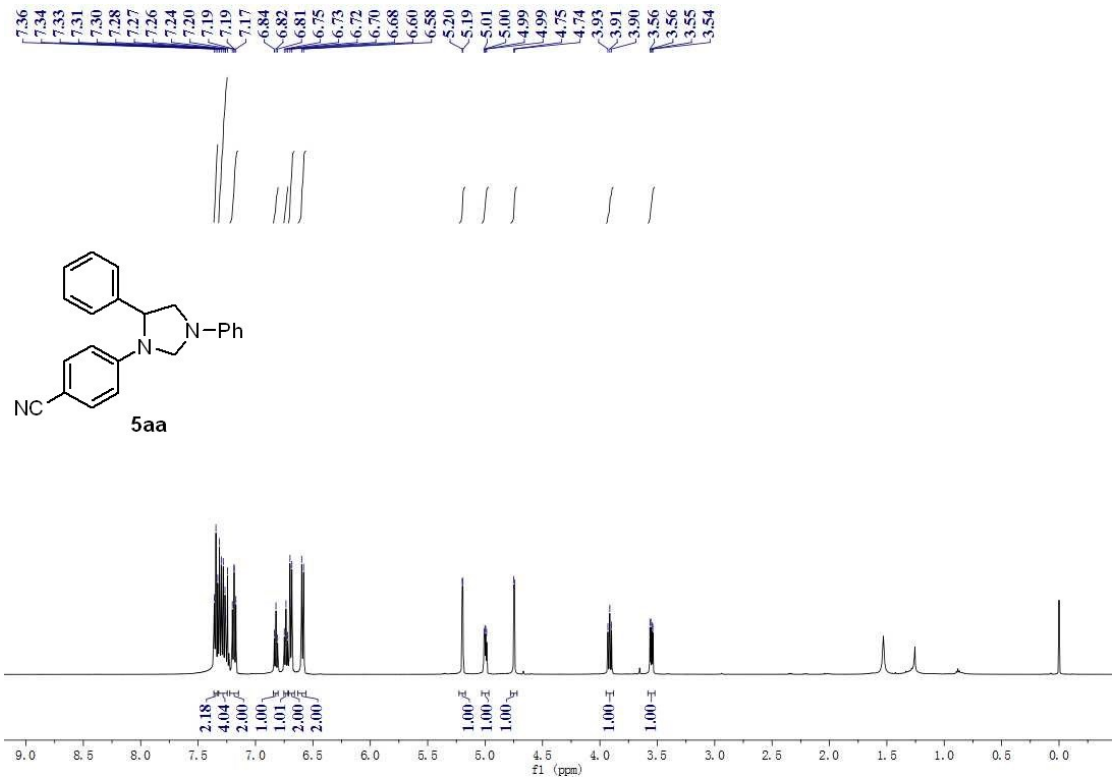
129.37
128.93
127.69
126.06
118.47
114.37
113.17
109.61
67.44
61.79
56.14
N–Ph
N
N
Br
5z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.34
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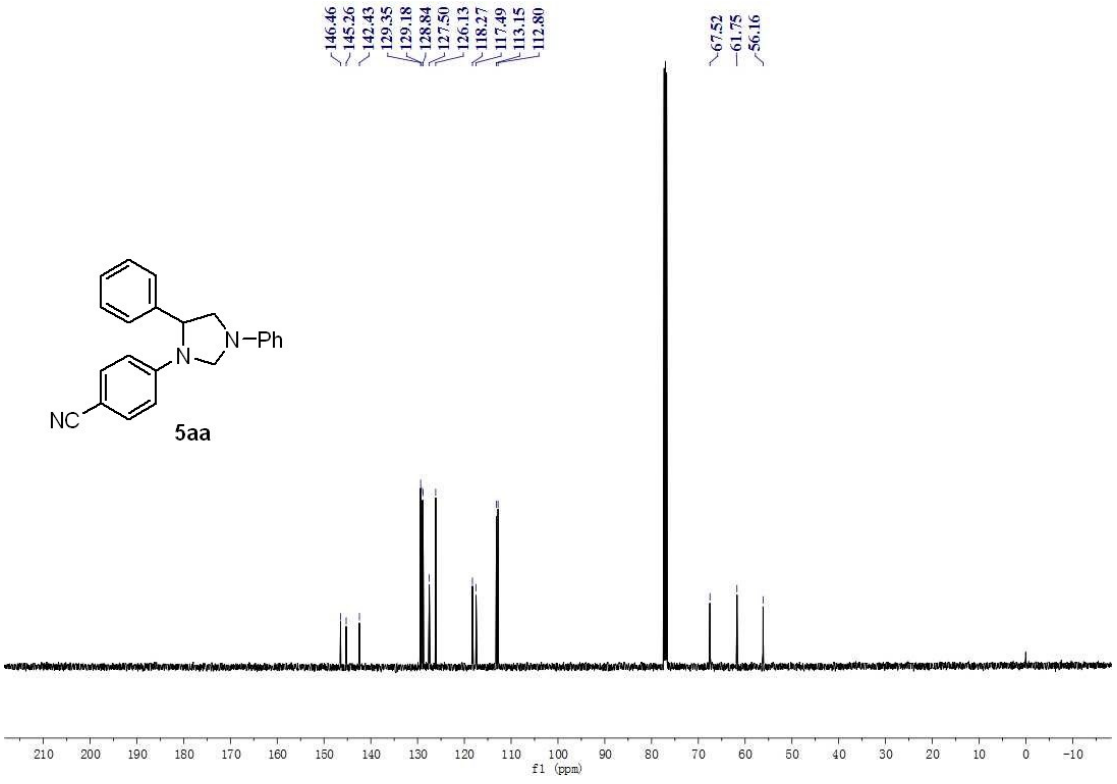
7.27
7.26
7.24
7.20
7.19
7.19
7.17
6.84
6.82
6.81
6.75
6.73
6.72
6.70
6.68
6.60
6.58
5.20
5.19
5.01
5.00
4.99
4.99
4.75
4.74
3.93
3.91
3.90
3.56
3.56
3.55
3.54
N–Ph
N
NC
5aa
2.18
4.04
2.00
1.00
1.01
2.00
2.00
1.00
1.00
1.00
1.00
1.00
f1 (ppm)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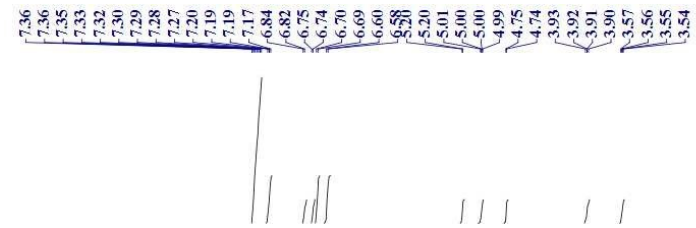
129.18
128.84
127.50
126.13
118.27
117.49
113.15
112.80
67.52
61.75
56.16
N–Ph
N
NC
5aa
f1 (ppm)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7.36
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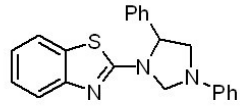
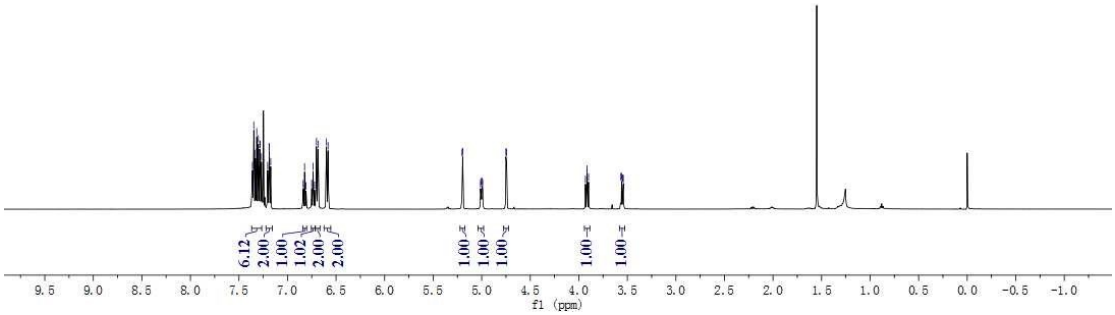
7.33
7.32
7.30
7.29
7.28
7.27
7.20
7.19
7.19
7.17
6.84
6.82
6.75
6.74
6.70
6.69
6.60
6.58
5.20
5.01
5.00
5.00
4.99
4.75
4.74
3.93
3.92
3.91
3.90
3.57
3.56
3.55
3.54


Ph
S
N
N
N
Ph

5ab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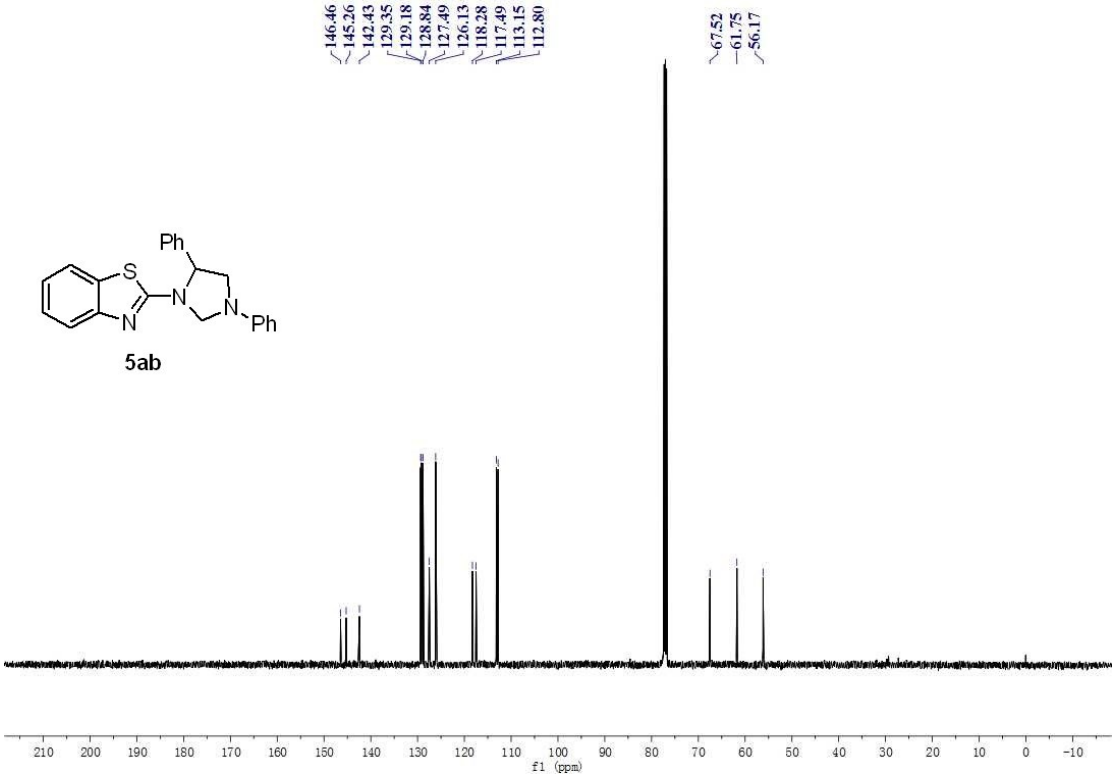
1.00
1.02
2.00
2.00
1.00
1.00
1.00
1.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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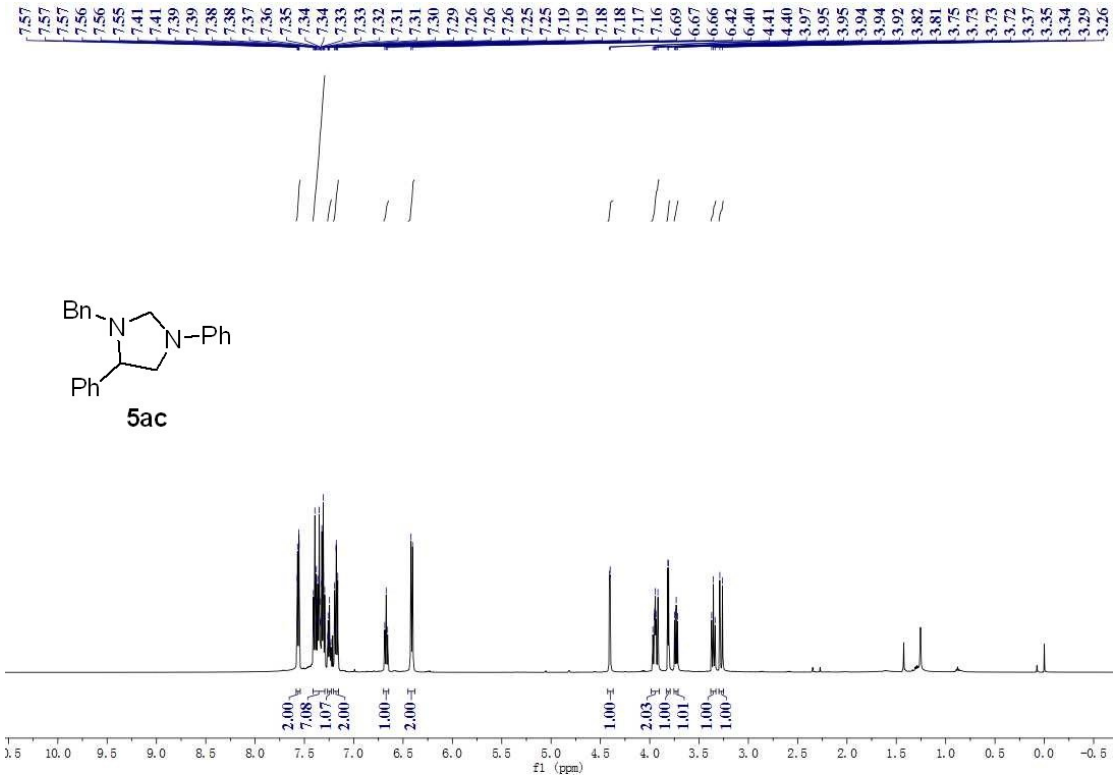
145.26
142.43
129.35
129.18
128.84
127.49
126.13
118.28
117.49
113.15
112.80
67.52
61.75
56.17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Ph
S
N
N
N
Ph

5ab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7.37
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.31
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7.26
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7.19
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7.18
7.17
7.16
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6.67
6.66
6.42
6.40
4.41
4.40
3.97
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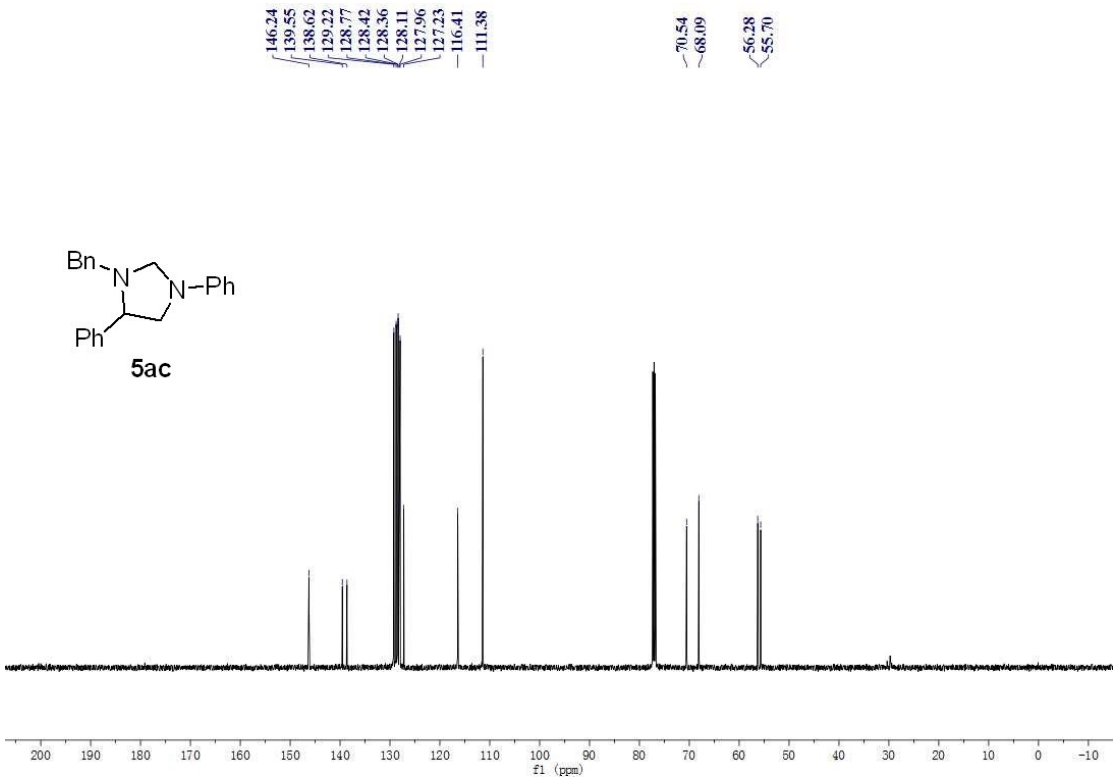
3.94
3.94
3.92
3.82
3.81
3.75
3.73
3.73
3.72
3.37
3.35
3.34
3.29
3.26
Bn
N
N–Ph
Ph
5ac
2.00
7.08
1.07
2.00
1.00
2.00
1.00
2.03
1.00
1.01
1.00
1.00
f1 (ppm)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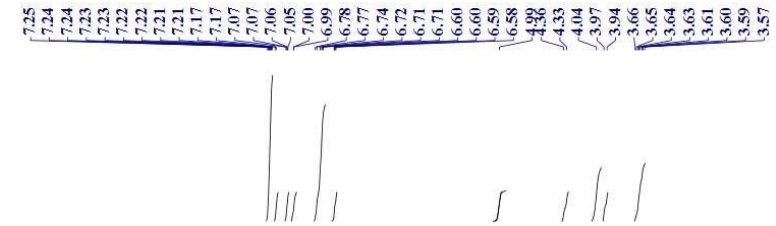
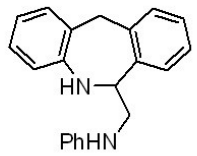
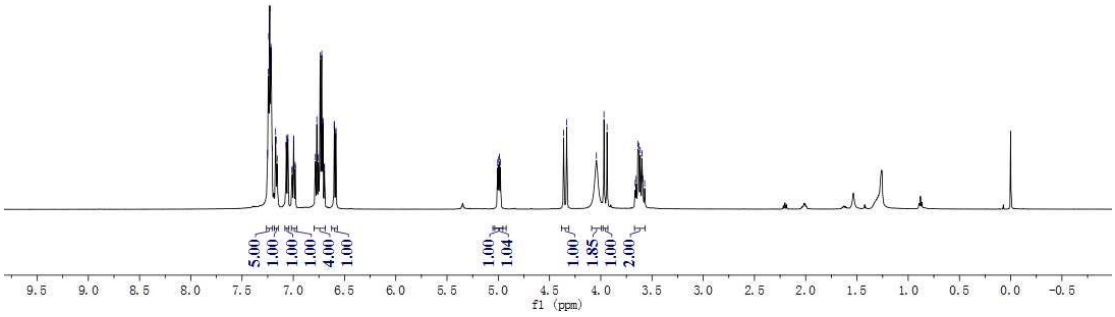
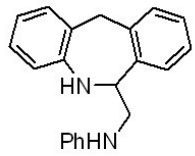
129.22
128.77
128.42
128.36
128.11
127.96
127.23
116.41
111.38
70.54
68.09
56.28
55.70
Bn
N
N–Ph
Ph
5ac
f1 (ppm)




HN
PhHN

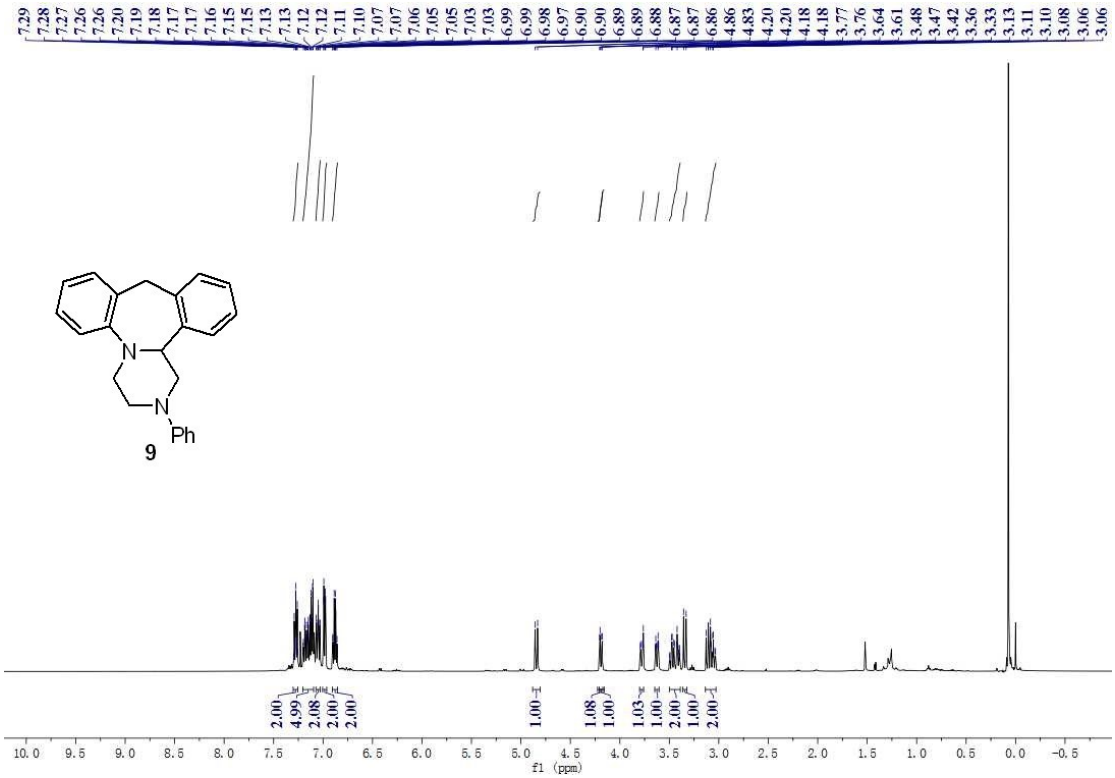
8

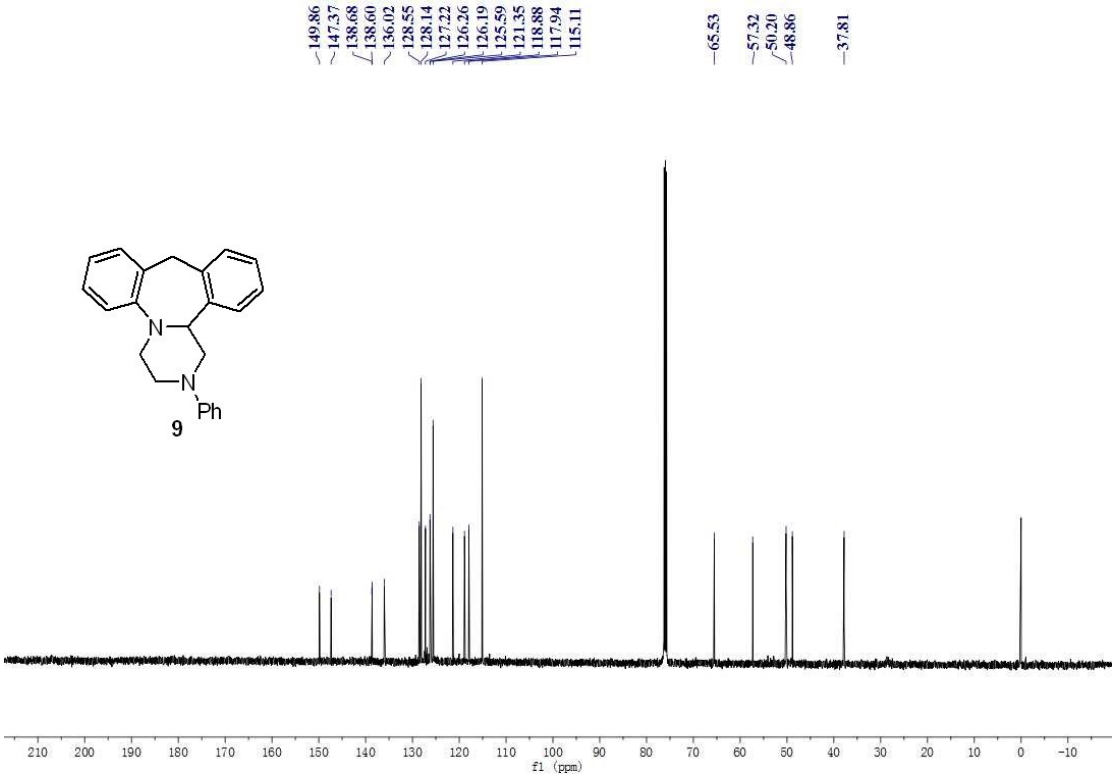

5.00
1.00
1.00
1.00
4.00
1.00
1.00
1.04
1.00
1.85
1.00
2.00
f1 (ppm)


HN
PhHN

8

f1 (ppm)


7.29 7.28 7.27 7.26 7.26 7.20 7.19 7.18 7.17 7.17 7.16 7.15 7.15 7.13 7.13 7.12 7.12 7.11 7.10 7.07 7.07 7.06 7.05 7.05 7.03 7.03 6.99 6.99 6.98 6.97 6.90 6.90 6.89 6.89 6.88 6.87 6.87 6.86 4.86 4.83 4.20 4.20 4.18 4.18 3.77 3.76 3.64 3.61 3.48 3.47 3.42 3.36 3.33 3.13 3.11 3.10 3.08 3.06 3.06
N
N
Ph
9
2.00 4.99 2.08 2.00 2.00 1.00 1.08 1.00 1.03 1.00 2.00 1.00 2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


149.86 147.37 138.68 138.60 136.02 128.55 128.14 127.22 126.26 126.19 125.59 121.35 118.88 117.94 115.11
65.53 57.32 50.20 48.86 37.81
N
N
Ph
9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)