Suzuki-type Cross-Coupling of Alkyl Trifluoroborates with Acid Fluoride Enabled by NHC/Photoredox Dual Catalysis†

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Supplementary Information

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1. General Information

General Procedures. All reactions were performed in oven-dried or flame-dried reaction vessels, modified Schlenk flasks, or round-bottom flasks. The flasks were fitted with Teflon screw caps and reactions were conducted under an atmosphere of argon if needed. Gas-tight syringes with stainless steel needles were used to transfer air- and moisture-sensitive liquids. All moisture and/or air sensitive solid compounds were manipulated inside normal desiccators. Flash column chromatography was performed over silica gel (40 – 45 μm, 300 – 400 mesh).

Analytical thin layer chromatography (TLC) was performed on silica gel $HSGF_{254}$ glass plates (purchased from Jiangyou silica gel development Co., Ltd, Yantai, China) containing a 254 nm fluorescent indicator. TLC plates were visualized by exposure to short wave ultraviolet light (254 nm) or I_2 and to a solution of $KMnO_4$ (1 g of $KMnO_4$, 6 g of K_2CO_3 and 0.1 g of KOH in 100 mL of H_2O) or vanillin (2 g of vanillin and 4 mL of concentrated H_2SO_4 in 100 mL of EtOH) followed by heating.

Organic solutions were concentrated at 30 – 40 °C on rotary evaporators at ~80 mbar followed by drying on vacuum pump below 1 mbar. Reaction temperatures are reported as the temperature of the bath surrounding the vessel unless otherwise stated.

Materials. Commercial reagents and solvents were obtained from Adamas-beta, Aldrich Chemical Co., Alfa Aesar, Macklin, Energy Chemical and Leyan. Acetone were purified by refluxing under positive argon pressure followed by distillation. The benzylic trifluoroborates were synthesized according to the reported literature procedures[1]. The benzoyl fluoride were synthesized according to literature procedures[2]. $Ir(ppy)_2(dtbbpy)(PF_6)$[3] and triazolium salt NHC **1** [4] were synthesized according to the literature procedures. The substituted carbazoles were synthesized according to the reported literature procedures[5].

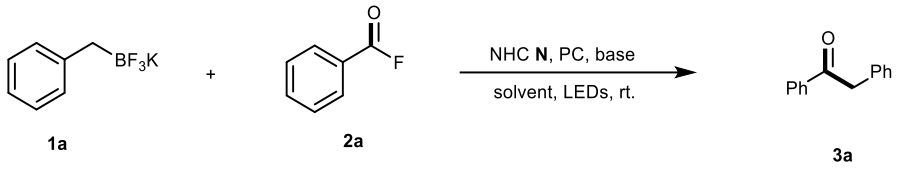
Instrumentation.

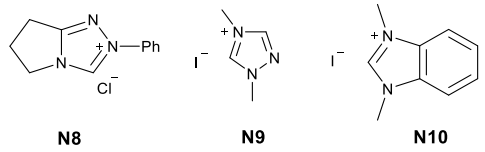
- Proton nuclear magnetic resonance (^{1}H NMR) spectra were measured on a JEOL JNM-ECZ600R/S1 spectrometer at ambient temperature for ^{1}H at 600 MHz. Proton chemical shifts are reported in parts per million (δ scale), and are referenced using tetramethylsilane (TMS) as an internal standard or residual protium in the NMR solvent ($CDCl_3$: δ 7.26 ($CHCl_3$) or DMSO-d_6: δ 2.50 (CD_2HSOCD_3)). Data are reported as follows: chemical shift [multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, td = triplet of doublets, brs = broad singlet), coupling constant(s) (Hz), integration].

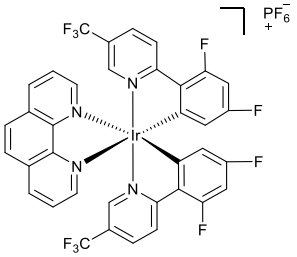
- Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra measured on a JEOL JNM-ECZ600R/S1 spectrometer at ambient temperature for ^{13}C at 151 MHz.. Carbon chemical shifts are reported in parts per million (δ scale), and are referenced using the carbon resonances of the solvent (δ 77.00 ($CDCl_3$) or δ 39.52 (DMSO-d_6)). Data are reported as follows: chemical shift [multiplicity (if not singlet), assignment (C_q = fully substituted carbon)].
- High resolution mass spectra (HRMS) were performed on an Agilent 6230 time-of-flight (TOF) LC/MS instrument or a Waters SYNAPT G2 mass spectrometer by using an electrospray ionization (ESI) ionization source analyzed by quadrupole time-of-flight (Q-TOF). Melting points were determined on a SGW X-4 digital melting point apparatus and temperatures were not corrected.

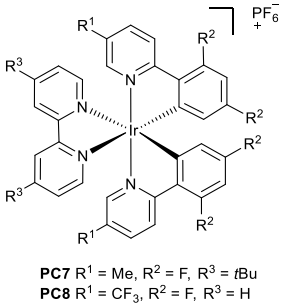
2. Further Optimization Studies

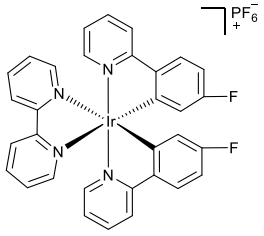
Table 1. Optimization of the benzylic trifluoroborate **1a** and benzoyl fluoride **2a** [a]

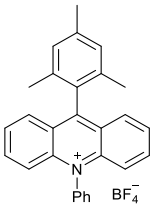


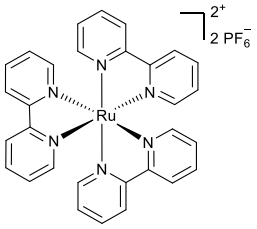


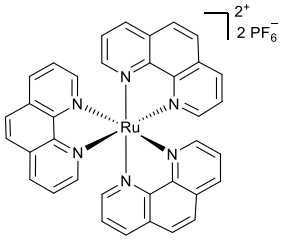


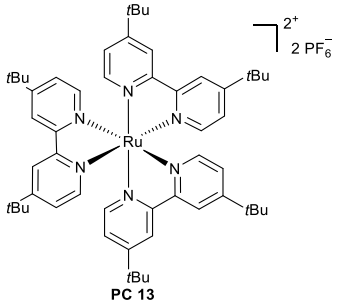


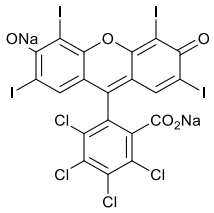


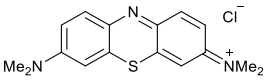












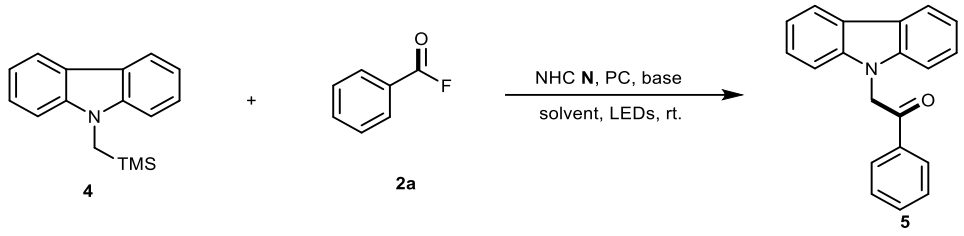
entry	NHC	PC	solvent	base	Yield[%][b]
1	**N1**	PC 4	o-Xylene	Cs_2CO_3	36%
2	**N1**	PC 4	m-Xylene	Cs_2CO_3	20%
3	**N1**	PC 4	p-Xylene	Cs_2CO_3	20%
4	**N1**	PC 4	DCE	Cs_2CO_3	38%
5	**N1**	PC 4	$CHCl_3$	Cs_2CO_3	44%
6	**N1**	PC 4	1,4-Dioxane	Cs_2CO_3	36%
7	**N1**	PC 4	acetone	Cs_2CO_3	56%
8	**N1**	PC 4	DMSO	Cs_2CO_3	41%
9	**N8**	PC 4	acetone	Cs_2CO_3	N.R.[c]

continued

10	**N9**	PC 4	acetone	Cs_2CO_3	5%
11	**N10**	PC 4	acetone	Cs_2CO_3	<5%
12	**N1**	PC 4	acetone	K_3PO_4	38%
13	**N1**	PC 4	acetone	$CsHCO_3$	37%
14	**N1**	PC 6	acetone	Cs_2CO_3	46%
15	**N1**	PC 7	acetone	Cs_2CO_3	60%
16	**N1**	PC 8	acetone	Cs_2CO_3	56%
17	**N1**	PC 9	acetone	Cs_2CO_3	61%
18	**N1**	PC 10	acetone	Cs_2CO_3	N.R.[c]
19	**N1**	PC 11	acetone	Cs_2CO_3	44%
20	**N1**	PC 12	acetone	Cs_2CO_3	12%
21	**N1**	PC 13	acetone	Cs_2CO_3	10%
22	**N1**	PC 14	acetone	Cs_2CO_3	N.R.[c]
23	**N1**	PC 15	acetone	Cs_2CO_3	N.R.[c]
24[d]	**N1**	PC 4	acetone	Cs_2CO_3	39%
25[e]	**N1**	PC 4	acetone/H_2O	Cs_2CO_3	58%
26[f]	**N1**	PC 4	acetone/THF	Cs_2CO_3	34%
27[g]	**N1**	PC 4	acetone/Et_2O	Cs_2CO_3	51%
28[h]	**N1**	PC 4	acetone	Cs_2CO_3	52%
29	**N1**	-	acetone	Cs_2CO_3	N.R.[c]
30	**-**	PC 4	acetone	Cs_2CO_3	N.R.[c]
31[i]	**N1**	PC 4	acetone	Cs_2CO_3	N.R.[c]

[a] Reactions condition: 1a (0.10 mmol, 1.0 equiv.), 2a (0.20 mmol, 2.0 equiv.), base (0.10 mmol, 1.0 equiv.), PC (2% mmol) and NHC (0.02 mmol, 0.2 equiv.) in solvent (1.0 mL), irradiation with blue LEDs at room temperature. [b] Isolated yield of **3a**. [c] no reaction. [d] 1.5 mL solvent. [e] acetone/H_2O = 200/1. [f] acetone/THF = 3/1. [g] acetone/Et_2O = 3/1. [h] 0 °C temperature. [i] no blue LEDs.

Table 2. Optimization of reaction conditions for product **5** [a]



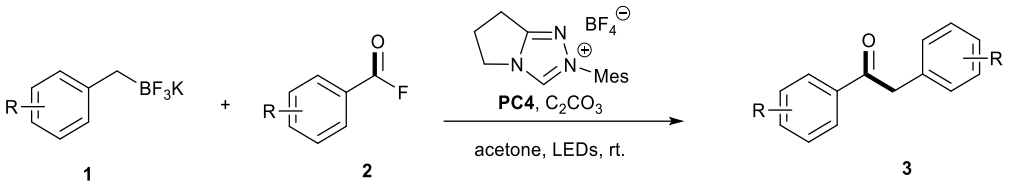
entry	NHC	PC	solvent	base	Yield[%] [b]
1	**N1**	PC 4	acetone	Cs_2CO_3	57%
2	**N1**	PC 5	acetone	Cs_2CO_3	39%
3	**N1**	PC 6	acetone	Cs_2CO_3	<5%
4	**N1**	PC 7	acetone	Cs_2CO_3	39%

continued

5	**N1**	PC 8	acetone	Cs_2CO_3	28%
6	**N1**	PC 9	acetone	Cs_2CO_3	35%
7	**N1**	PC 4	Tol	Cs_2CO_3	77%
8	**N1**	PC 4	THF	Cs_2CO_3	48%
9	**N1**	**PC 4**	**MeCN**	**Cs_2CO_3**	**81%**
10	**N1**	PC 4	DCM	Cs_2CO_3	46%
11 [c]	**N1**	PC 4	MeCN	Cs_2CO_3	N.R. [d]
12	**N1**	-	MeCN	Cs_2CO_3	N.R. [d]

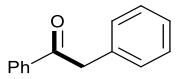
[a] Reactions condition: **4** (0.10 mmol, 1.0 equiv.), **2a** (0.20 mmol, 2.0 equiv.), base (0.10 mmol, 1.0 equiv.), PC (2% mmol) and NHC (0.02 mmol, 0.2 equiv.) in 1.0 mL of solvent. [b] Isolated yield of **5a**. [c] no blue LEDs. [d] no reaction.

3. General Procedure for the 3.



To a flame-dried Schlenk tube were added trifluoroborate **1** (0.10 mmol, 1.0 equiv.), **N1** (0.20 mmol, 0.2 equiv.), photocatalyst **4** (2% mmol) and Cs_2CO_3 (0.10 mmol, 1.0 equiv.), after which the tube was evacuated and back-filled with argon three times. Subsequently, under the protection of Ar, aroyl fluoride **2** (0.20 mmol, 2.0 equiv.) and acetone (2.0 mL) were added via syringe. The resulting mixture was stirred at ambient temperature for 0.5 - 3 h until the reaction was completed (monitored by TLC), after which the reaction mixture was concentrated under reduced pressure and the resulting crude material was purified by column chromatography on silica gel with petroleum ether and ethyl acetate (100:1 to 80:1) as eluents to afford the desired products. All products were dried under vacuum and further analyzed by ^{1}H NMR, ^{13}C NMR, HRMS analysis, *etc*.

1,2-diphenylethan-1-one 3a



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (13.9 mg, 71% yield) as a white solid, m.p. = 49 – 51 °C.

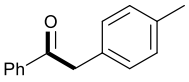
*NMR and HRMS data for the product **3a***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.02 (d, *J* = 8.4 Hz, 2H), 7.56 (tt, *J* = 7.8, *J* = 1.2 Hz, 1H), 7.46 (t, *J* = 8.4 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.28 – 7.25 (m, 3H), 4.30 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.6, 136.6, 134.5, 133.1, 129.4, 128.7, 128.6, 128.6, 126.9, 45.5.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{12}ONa^+$ 219.0781; Found: 219.0775.

1-phenyl-2-(p-tolyl)ethan-1-one 3b



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (13.9 mg, 66% yield) as a white solid, m.p. = 88 – 93 °C.

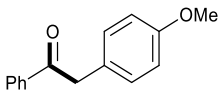
*NMR and HRMS data for the product **3b***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.02 (d, *J* = 7.8 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.17 – 7.13 (m, 4H), 4.25 (s, 2H), 2.32 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.8, 136.6, 136.5, 133.1, 131.4, 129.4, 129.3, 128.6, 45.1, 21.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}ONa^+$ 233.0937; Found: 233.0934.

2-(4-methoxyphenyl)-1-phenylethan-1-one 3c

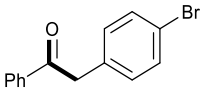


Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (12.7 mg, 56% yield) as a white solid, m.p. = 80 – 84 °C.

*NMR and HRMS data for the product **3c***:

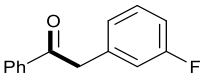
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.01 (d, *J* = 6.6 Hz, 2H), 7.55 (t, *J* = 8.4 Hz, 1H), 7.46. (t, *J* = 7.8 Hz, 2H), 7.19 (d, *J* = 9.0 Hz, 2H), 6.87 (d, *J* = 9.0 Hz, 2H), 4.23 (s, 2H), 3.79 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.9, 158.5, 136.6, 133.1, 130.4, 128.6, 128.6, 126.5, 114.1, 55.2, 44.6.
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}O_2Na^+$ 249.0886; Found: 249.0881.

2-(4-bromophenyl)-1-phenylethan-1-one 3d



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (17.1 mg, 62% yield) as a white solid, m.p. = 137 – 141 ºC.
*NMR and HRMS data for the product **3d***:
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 6.6 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.49 – 7.45 (m, 4H), 7.14 (d, *J* = 8.4 Hz, 2H), 4.25 (s, 2H).
^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.0, 136.4, 133.4, 133.4, 131.7, 131.2, 128.7, 128.5, 120.9, 44.7.
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{11}BrONa^+$ 296.9885 (^{79}Br), 298.9865 (^{81}Br); Found: 296.9877, 298.9866.

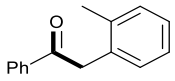
2-(3-fluorophenyl)-1-phenylethan-1-one 3e



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (14.6 mg, 68% yield) as semisolid.
*NMR and HRMS data for the product **3e***:
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.01 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 8.4 Hz, 2H), 7.31 – 7.28 (m, 1H), 7.04 (d, *J* = 7.8 Hz, 1H), 7.00 – 6.94 (m, 2H), 4.29 (s, 2H).
^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.9, 162.9 (C-F, $^1J_{C\text{-}F}$ = 244.5 Hz), 136.8 (C-F, $^3J_{C\text{-}F}$ = 9.0 Hz), 136.4, 133.4, 130.0 (C-F, $^3J_{C\text{-}F}$ = 7.5 Hz), 128.7, 128.5, 125.2, 116.5 (C-F, $^2J_{C\text{-}F}$ = 21.0 Hz), 113.9 (C-F, $^2J_{C\text{-}F}$ = 22.5 Hz), 45.0.
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{11}FONa^+$ 237.0687; Found: 237.0693.

^{19}F NMR (564 MHz, $CDCl_3$) δ (ppm): -113.47 (s, 1F).

1-phenyl-2-(o-tolyl)ethan-1-one 3f



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (12.6 mg, 60% yield) as a white solid, m.p. = 59 – 64 °C.

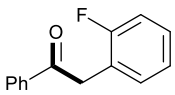
*NMR and HRMS data for the product **3f***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.04 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.23 – 7.13 (m, 4H), 4.32 (s, 2H), 2.27 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.5, 136.9, 133.4, 133.1, 130.3, 130.3, 128.7, 128.3, 127.2, 126.1, 43.5, 19.8.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}ONa^+$ 233.0937; Found: 233.0941.

2-(2-fluorophenyl)-1-phenylethan-1-one 3g



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (10.7 mg, 50% yield) as a white solid, m.p. = 66 – 70 °C.

*NMR and HRMS data for the product **3g***:

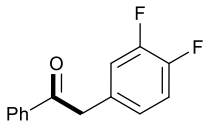
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.04 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 8.4 Hz, 2H), 7.29 – 7.23 (m, 2H), 7.13 – 7.07 (m, 2H), 4.34 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.3, 160.9 (C-F, $^{1}J_{C\text{-}F}$ = 244.5 Hz), 136.4, 133.3, 131.6, 128.9 (C-F, $^{3}J_{C\text{-}F}$ = 7.5 Hz), 128.7, 128.4, 124.1, 121.8 (d, $^{2}J_{C\text{-}F}$ = 16.5 Hz), 115.4 (C-F, $^{2}J_{C\text{-}F}$ = 21.0 Hz), 38.6.

HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{11}FOH^+$ 215.0867; Found: 215.0865.

^{19}F NMR (564 MHz, $CDCl_3$) δ (ppm): -117.57 – -117.61 (m, 1F).

2-(3,4-difluorophenyl)-1-phenylethan-1-one 3h



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (13.5 mg, 58% yield) as a white solid, m.p. = 74 – 78 °C.

*NMR and HRMS data for the product **3h***:

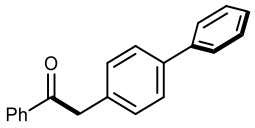
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.2, 1H), 7.49 (t, *J* = 8.4, 2H), 7.14 – 7.07 (m, 2H), 6.98 – 6.96 (m, 1H), 4.25 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.7, 150.2 (C-F, $^{1}J_{C\text{-}F}$ = 246.8, $^{2}J_{C\text{-}F}$ = 13.5 Hz), 149.5 (C-F, $^{1}J_{C\text{-}F}$ = 245.3, $^{2}J_{C\text{-}F}$ = 12.0 Hz), 136.2, 133.5, 131.2 (C-F, $^{3}J_{C\text{-}F}$ = 6.0 Hz), 128.8, 128.4, 125.6 (C-F, $^{3}J_{C\text{-}F}$ = 4.5 Hz), 118.6 (C-F, $^{2}J_{C\text{-}F}$ = 16.5 Hz), 117.3 (C-F, $^{2}J_{C\text{-}F}$ = 18.0 Hz), 44.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{10}F_2ONa^+$ 255.0592; Found: 255.0596.

^{19}F NMR (564 MHz, $CDCl_3$) δ (ppm): -137.99 – -138.07 (m, 1F), -140.84 – -140.91 (m, 1F).

2-([1,1'-biphenyl]-4-yl)-1-phenylethan-1-one 3i



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (13.6 mg, 50% yield) as a white solid, m.p. = 142 – 146 °C.

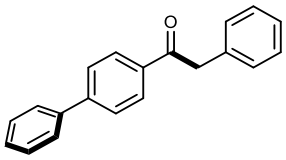
*NMR and HRMS data for the product **3i***:

^{11}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.05 (d, *J* = 7.2 Hz, 2H), 7.59 – 7.56 (m, 5H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.36 – 7.33 (m, 3H), 4.34 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.6, 140.8, 139.9, 136.6, 133.5, 133.2, 129.9, 128.7, 128.7, 128.6, 127.4, 127.2, 127.1, 45.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{16}ONa^+$ 295.1093; Found: 295.1099.

1-([1,1'-biphenyl]-4-yl)-2-phenylethan-1-one 3j



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (22.1 mg, 81% yield) as a white solid, m.p. = 132 – 136 ºC.

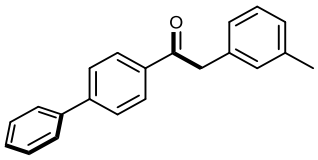
*NMR and HRMS data for the product **3j***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.10 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 6.6 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 6.6 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 1H), 4.33 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.2, 145.8, 139.8, 135.2, 134.6, 129.4, 129.2, 128.9, 128.7, 128.2, 127.3, 127.3, 126.9, 45.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{16}ONa^+$ 295.1093; Found: 295.1098.

1-([1,1'-biphenyl]-4-yl)-2-(m-tolyl)ethan-1-one 3k



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (20.0 mg, 70% yield) as a white solid, m.p. = 81 – 84 ºC.

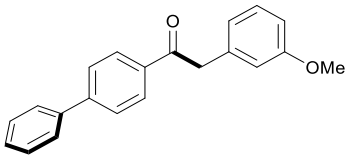
*NMR and HRMS data for the product **3k***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.10 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.2 Hz, 1H), 7.13 – 7.08 (m, 3H), 4.29 (s, 2H), 2.35 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.3, 145.8, 139.8, 138.3, 135.3, 134.5, 130.1, 129.2, 128.9, 128.6, 128.2, 127.7, 127.2, 126.4, 45.5, 21.4.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{18}ONa^+$ 309.1250; Found: 309.1254.

1-([1,1'-biphenyl]-4-yl)-2-(3-methoxyphenyl)ethan-1-one 3l



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (19.4 mg, 64% yield) as a white solid, m.p. = 57 – 59 ºC.

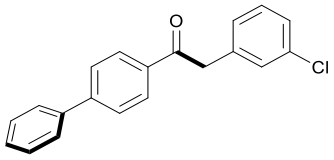
*NMR and HRMS data for the product **3l***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.08 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 9.0 Hz, 2H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.47 – 7.45 (m, 2H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.25 – 7.23 (m, 1H), 6.88 (d, *J* = 7.2 Hz, 1H), 6.84 (s, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 4.28 (s, 2H), 3.79 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.1, 159.8, 145.8, 139.8, 136.1, 135.2, 129.7, 129.2, 128.9, 128.2, 127.3, 127.2, 121.8, 115.1, 112.4, 55.2, 45.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{18}O_2Na^+$ 325.1199; Found: 325.1196.

1-([1,1'-biphenyl]-4-yl)-2-(3-chlorophenyl)ethan-1-one 3m



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (20.0 mg, 65% yield) as a white solid, m.p. = 107 – 110 ºC.

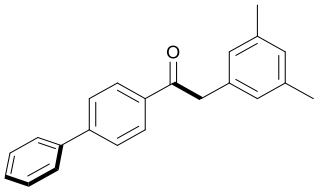
*NMR and HRMS data for the product **3m***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.08 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.18 (d, *J* = 7.2 Hz, 1H), 4.29 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.4, 146.1, 139.7, 136.4, 135.0, 134.4, 129.84, 129.6, 129.1, 129.0, 128.3, 127.7, 127.4, 127.3, 127.2, 44.9.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{15}ClONa^+$ 329.0704 (^{35}Cl), 331.0674 (^{37}Cl); Found: 329.0702, 331.0681.

1-([1,1'-biphenyl]-4-yl)-2-(3,5-dimethylphenyl)ethan-1-one 3n



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (21.1 mg, 70% yield) as a white solid, m.p. = 62 – 63 ºC.

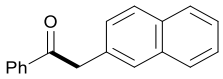
*NMR and HRMS data for the product **3n***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.10 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 9.0 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.42 – 7.40 (m, 1H), 6.93 (s, 2H), 6.91 (s, 1H), 4.24 (s, 2H), 2.31 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.5, 145.7, 139.8, 138.2, 135.3, 134.4, 129.3, 128.9, 128.6, 128.2, 127.2, 127.2, 45.5, 21.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{22}H_{20}ONa^+$ 323.1406; Found: 323.1408.

2-(naphthalen-2-yl)-1-phenylethan-1-one 3o



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (10.6 mg, 43% yield) as a white solid, m.p. = 113 – 118 ºC.

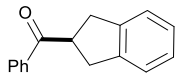
*NMR and HRMS data for the product **3o***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.06 (d, *J* = 7.2 Hz, 2H), 7.82 – 7.78 (m, 3H), 7.73 (s, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.48 – 7.43 (m, 4H), 7.41 – 7.40 (m, 1H), 4.46 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.7, 136.6, 133.6, 133.2, 132.4, 132.1, 128.7, 128.3, 128.1, 127.6, 127.6, 127.6, 126.1, 125.7, 45.7.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{14}ONa^+$ 269.0937; Found: 269.0941.

(2,3-dihydro-1H-inden-2-yl)(phenyl)methanone 3p



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (4.9 mg, 22% yield) as a white solid, m.p. = 59 – 63 ºC.

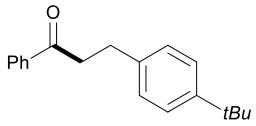
*NMR and HRMS data for the product **3p***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.03 (d, *J* = 6.6 Hz, 2H), 7.61 – 7.59 (m, 1H), 7.52 – 7.50 (m, 2H), 7.27 – 7.18 (m, 4H), 7.34 – 7.29 (m, 1H), 3.42 – 3.38 (m, 2H), 3.30 – 3.26 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 200.9, 141.6, 136.4, 133.0, 128.7, 128.5, 126.6, 124.4, 46.3, 36.2.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{16}H_{14}ONa^+$ 245.0937; Found: 245.0935.

3-(4-(tert-butyl)phenyl)-1-phenylpropan-1-one 3q



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 200:1) to afford (6.1 mg, 23% yield) as colorless oil.

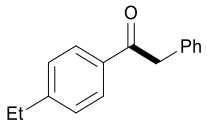
*NMR and HRMS data for the product **3q***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.04 (d, *J* = 7.8 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.47 – 7.43 (m, 2H), 7.36 – 7.32 (m, 2H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 4.52 (t, *J* = 7.2 Hz, 1H), 3.31 (t, *J* = 7.8 Hz, 1H), 3.07 – 3.03 (m, 2H), 1.32 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 199.4, 133.0, 129.6, 128.6, 128.6, 128.3, 128.1, 128.0, 125.4, 40.5, 34.7, 31.4, 29.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{19}H_{22}ONa^+$ 289.1563; Found: 289.11564.

1-(4-ethylphenyl)-2-phenylethan-1-one 3r



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (14.6 mg, 65% yield) as a white solid, m.p. = 54 – 57 °C.

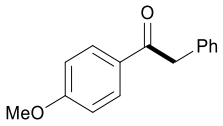
*NMR and HRMS data for the product **3r***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.95 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 2H), 7.29 – 7.24 (m, 5H), 4.27 (s, 2H), 2.70 (q, *J* = 7.8 Hz, 2H), 1.26 (t, *J* = 7.8 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.3, 150.1, 134.8, 134.3, 129.4, 128.9, 128.6, 128.1, 126.8, 45.4, 28.9, 15.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{16}H_{16}ONa^+$ 247.1093; Found: 247.1093.

1-(4-methoxyphenyl)-2-phenylethan-1-one 3s



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (12.0 mg, 53% yield) as a white solid, m.p. = 62 – 64 °C.

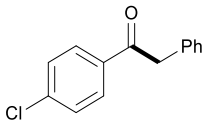
*NMR and HRMS data for the product **3s***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 9.0 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 2H), 7.28 – 7.23 (m, 3H), 6.93 (d, *J* = 9.0 Hz, 2H), 4.24 (s, 2H), 3.86 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.2, 163.5, 135.0, 130.9, 129.6, 129.4, 128.6, 126.8, 113.8, 55.5, 45.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}O_2Na^+$ 249.0886; Found: 249.0881.

1-(4-chlorophenyl)-2-phenylethan-1-one 3t



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (15.3 mg, 66% yield) as a white solid, m.p. = 97 – 100 ºC.

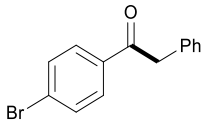
*NMR and HRMS data for the product **3t***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.95 (d, *J* = 9.0 Hz, 2H), 7.43 (d, *J* = 9.0 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.27 – 7.25 (m, 3H), 4.26 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.4, 139.6, 134.9, 134.2, 130.0, 129.4 129.0, 128.8, 127.0, 45.5.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{11}ClONa^+$ 253.0391 (^{35}Cl), 255.0361 (^{37}Cl); Found: 253.0391, 255.0359.

1-(4-bromophenyl)-2-phenylethan-1-one 3u



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (14.1 mg, 51% yield) as a white solid, m.p. = 105 – 107 ºC.

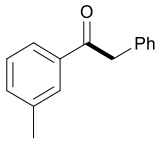
*NMR and HRMS data for the product **3u***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.87 (d, *J* = 9.0 Hz, 2H), 7.59 (d, *J* = 9.0 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.27 – 7.24 (m, 3H), 4.25 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.6, 135.2, 134.1, 132.0, 130.1, 129.4, 128.8, 128.4, 127.0, 45.5.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{11}BrONa^+$ 296.9885 (^{79}Br), 298.9865 (^{81}Br); Found: 296.9884, 296.9864.

2-phenyl-1-(m-tolyl)ethan-1-one 3v



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (13.5 mg, 64% yield) as a white solid, m.p. = 35 – 40 °C.

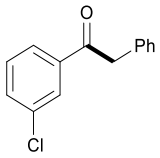
*NMR and HRMS data for the product **3v***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.83 – 7.81 (m, 2H), 7.38 – 7.32 (m, 4H), 7.27 – 7.24 (m, 3H), 4.28 (s, 2H), 2.41 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.8, 138.4, 136.6, 134.6, 133.9, 129.5, 129.1, 128.6, 128.5, 126.8, 125.9, 45.5, 21.4.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}OH^+$ 211.1117; Found: 211.1121.

1-(3-chlorophenyl)-2-phenylethan-1-one 3w



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (11.6 mg, 50% yield) as a white solid, m.p. = 50 – 53 °C.

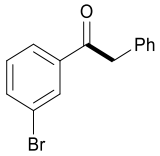
*NMR and HRMS data for the product **3w***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.98 (s, 1H), 7.88 (d, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 8.4 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 2H), 7.28 – 7.25 (m, 3H), 4.26 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.3, 138.1, 135.0, 133.9, 133.1, 130.0, 129.4, 128.8, 128.7, 127.1, 126.7, 45.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{11}ClONa^+$ 253.0391 (^{35}Cl), 255.0361 (^{37}Cl); Found: 253.0398, 255.0371.

1-(3-bromophenyl)-2-phenylethan-1-one 3x



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (14.6 mg, 53% yield) as colorless oil.

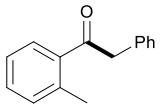
*NMR and HRMS data for the product **3x***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.77 (d, *J* = 4.2 Hz, 1H), 7.64 (d, *J* = 4.2 Hz, 1H), 7.34 – 7.31 (m, 4H), 7.28 – 7.25 (m, 2H), 7.13 – 7.12 (m, 1H), 4.20 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 190.4, 143.9, 134.3, 134.0, 132.6, 129.4, 128.7, 128.2, 127.0, 46.4.

HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{11}BrOH^+$ 275.0066 (^{79}Br), 277.0046 (^{81}Br); Found: 275.0065, 277.0045.

2-phenyl-1-(o-tolyl)ethan-1-one 3y



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (9.7 mg, 46% yield) as colorless oil.

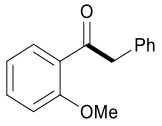
*NMR and HRMS data for the product **3y***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.72 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.33 – 7.31 (m, 2H), 7.27 – 7.23 (m, 5H), 4.22 (s, 2H), 2.45 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 201.4, 138.5, 137.6, 134.4, 132.0, 131.3, 129.5, 128.6, 126.9, 125.6, 48.4, 21.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}OH^+$ 211.1117; Found: 211.1116.

1-(2-methoxyphenyl)-2-phenylethan-1-one 3z



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (13.8 mg, 61% yield) as colorless oil.

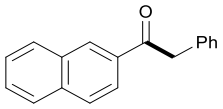
*NMR and HRMS data for the product **3z***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.67 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 8.4 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.23 – 7.21 (m, 3H), 6.99 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 7.8 Hz, 1H), 4.30 (s, 2H), 3.92 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 200.1, 158.4, 135.2, 133.5, 130.6, 129.7, 128.3, 128.2, 126.5, 120.7, 111.5, 55.4, 50.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{14}O_2Na^+$ 249.0886; Found: 249.0886.

1-(naphthalen-2-yl)-2-phenylethan-1-one 3aa



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (17.8 mg, 72% yield) as a white solid, m.p. = 91 – 95 °C.

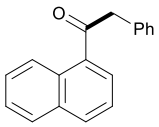
*NMR and HRMS data for the product **3aa***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.56 (s, 1H), 8.07 (dd, *J* = 9.0, *J* = 2.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.36 – 7.33 (m, 4H), 7.28 – 7.25 (m, 1H), 4.43 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 197.6, 135.6, 134.7, 133.9, 132.5, 130.4, 129.6, 129.5, 128.7, 128.5, 128.5, 127.8, 126.9, 126.8, 124.2, 45.5.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{14}ONa^+$ 269.0937; Found: 269.0933.

1-(naphthalen-1-yl)-2-phenylethan-1-one 3ab



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (15.0 mg, 61% yield) as a white solid, m.p. = 52 – 56 ºC.

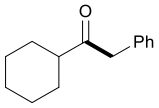
*NMR and HRMS data for the product **3ab***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.58 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.57 (t, *J* = 8.4 Hz, 1H), 7.54 – 749 (m, 2H), 7.34 – 7.30 (m, 4H), 7.27 – 7.24 (m, 1H), 4.38 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 201.5, 135.6, 134.5, 134.0, 132.7, 130.4, 129.5, 128.7, 128.4, 128.0, 127.9, 126.9, 126.5, 125.8, 124.3, 48.9.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{14}ONa^+$ 269.0937; Found: 269.0938.

1-cyclohexyl-2-phenylethan-1-one 3ac



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (10.5 mg, 52% yield) as colorless.

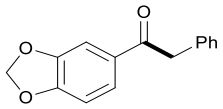
*NMR and HRMS data for the product **3ac***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.34 (t, *J* = 7.2Hz, 2H), 7.28 (d, *J* = 7.2Hz, 1H), 7.21 (d, *J* = 7.2Hz, 2H), 3.75 (s, 2H), 2.48 (tt, *J* = 10.8, *J* = 3.6 Hz, 1H), 1.85 – 1.78 (m, 4H), 1.69 – 1.66 (m, 1H), 1.42 – 1.35 (m, 2H), 1.31 – 1.20 (m, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 211.3, 134.4, 129.4, 128.6, 126.8, 50.1, 47.8, 28.5, 25.8, 25.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{18}ONa^+$ 225.1250; Found: 225.1257.

1-(benzo[d][1,3]dioxol-5-yl)-2-phenylethan-1-one 3ad



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (12.0 mg, 50% yield) as a white solid, m.p. = 81 – 85 °C.

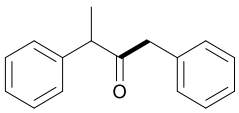
*NMR and HRMS data for the product **3ad***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.63 (dd, *J* = 7.8, *J* = 1.8 Hz, 1H), 7.48 (s, 1H), 7.34 – 7.31 (m, 2H), 7.26 – 7.24 (m, 3H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.03 (s, 2H), 4.21 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 195.7, 151.8, 148.2, 134.8, 131.4, 129.3, 128.7, 126.8, 125.0, 108.4, 107.9, 101.8, 45.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{12}O_3Na^+$ 263.0679; Found: 263.0680.

1,3-diphenylbutan-2-one 3ae



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 150:1 to 100:1) to afford (8.1 mg, 36% yield) as colorless oil.

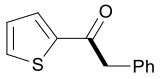
*NMR and HRMS data for the product **3ae***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 – 7.26 (m, 3H), 7.24 – 7.22 (m, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.05 (d, *J* = 7.2 Hz, 2H), 3.86 (q, *J* = 6.6 Hz, 1H), 3.62 (s, 2H), 1.37 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 208.0, 140.4, 134.3, 129.4, 129.0, 128.5, 128.1, 127.2, 126.8, 52.1, 48.0, 17.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{16}H_{16}ONa^+$ 247.1093; Found: 247.1099.

2-phenyl-1-(thiophen-2-yl)ethan-1-one 3af



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (4.9 mg, 24% yield) as colorless oil.

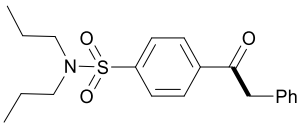
*NMR and HRMS data for the product **3af***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.77 (d, *J* = 3.6 Hz, 1H), 7.64 (d, *J* = 4.8 Hz, 1H), 7.35 – 7.31 (m, 4H), 7.27 – 7.25 (m, 1H), 7.12 (t, *J* = 4.2 Hz, 1H), 4.20 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 190.4, 143.9, 134.3, 134.0, 132.6, 129.4, 128.7, 128.1, 127.0, 46.4.

HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{10}OSH^+$ 203.0526; Found: 203.0523.

4-(2-phenylacetyl)-N,N-dipropylbenzenesulfonamide 3ag



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1 to 80:1) to afford (12.6 mg, 35% yield) as a white solid, m.p. = 58 – 61 °C.

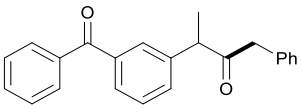
*NMR and HRMS data for the product **3ag***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.10 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.8 Hz, 2H), 7.29 – 7.25 (m, 3H), 4.31 (s, 2H), 3.09 (t, *J* = 7.2 Hz, 4H), 1.58 – 1.51 (m, 4H), 0.86 (t, *J* = 7.2 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.5, 144.2, 139.2, 133.7, 129.4, 129.1, 128.8, 127.3, 127.2, 50.0, 45.8, 22.0, 11.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{25}NO_3SNa^+$ 382.1447; Found: 382.1448.

3-(3-benzoylphenyl)-1-phenylbutan-2-one 3ah



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 150:1 to 100:1) to afford (9.9 mg, 30% yield) as colorless oil.

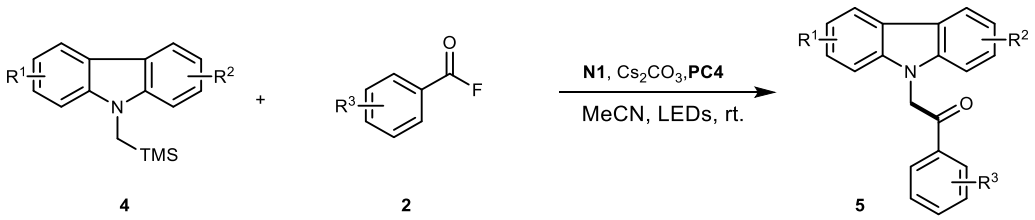
*NMR and HRMS data for the product **3ah***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 7.77 (d, *J* = 6.6 Hz, 2H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.63 (s, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.50 – 7.48 (m, 2H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.28 – 7.21 (m, 3H), 7.06 (d, *J* = 7.8 Hz, 2H), 3.95 (q, *J* = 7.2 Hz, 1H), 3.67 (s, 2H), 1.41 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 207.5, 196.4, 140.6, 138.2, 137.4, 133.9, 132.6, 131.8, 130.0, 129.7, 129.4, 129.1, 128.9, 128.6, 128.3, 127.0, 51.8, 48.4, 17.8.

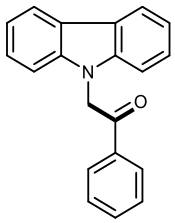
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{23}H_{20}O_2Na^+$ 351.1356; Found: 351.1362.

4. General Procedure for the 5.



To a flame-dried Schlenk tube were added α-silyl carbazole **4** (0.10 mmol, 1.0 equiv.), **N1** (0.20 mmol, 0.2 equiv.), photocatalyst **4** (2% mmol) and Cs_2CO_3 (0.10 mmol, 1.0 equiv.), after which the tube was evacuated and back-filled with argon three times. Subsequently, under the protection of Ar, aroyl fluoride **2** (0.20 mmol, 2.0 equiv.) and MeCN (1.0 mL) were added via syringe. Then, the resulting suspension was stirred at room temperature for 1.0 h, after which the reaction mixture was concentrated under reduced pressure and the resulting crude material was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, 50/1 to 20/1) to afford the corresponding products **5**, which were dried under vacuum and further analyzed by ^{1}H NMR, ^{13}C NMR, HRMS, *etc*.

2-(9H-carbazol-9-yl)-1-phenylethan-1-one 5a



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (23.1 mg, 81% yield) as a white solid, m.p. = 208 – 211 °C.

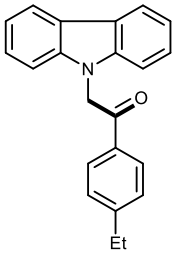
*NMR and HRMS data for the product **5a***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.13 (d, *J* = 7.8 Hz, 2H), 8.08 (d, *J* = 7.8 Hz, 2H), 7.67 – 7.65 (m, 1H), 7.55 – 7.52 (m, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.24 (m, 4H), 5.67 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 193.0, 140.8, 134.9, 134.0, 129.0, 128.0, 125.9, 123.3, 120.5, 119.5, 108.3, 49.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{15}NONa^+$ 308.1046; Found: 308.1048.

2-(9H-carbazol-9-yl)-1-(4-ethylphenyl)ethan-1-one 5b



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (20.4 mg, 65% yield) as a white solid, m.p. = 167 – 172 ºC.

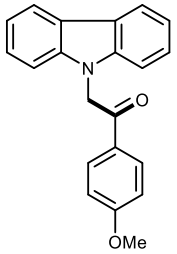
*NMR and HRMS data for the product **5b***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.10 (d, *J* = 7.2 Hz, 2H), 7.95 (d, *J* = 7.8 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.25 – 7.19 (m, 4H), 5.55 (s, 2H), 2.72 (q, *J* = 7.8 Hz, 2H), 1.26 (t, *J* = 7.8 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 192.6, 151.1, 140.8, 132.6, 128.5, 128.2, 125.8, 123.3, 120.5, 119.4, 108.3, 49.2, 29.0, 15.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{22}H_{19}NONa^+$ 336.1359; Found: 336.1361.

2-(9H-carbazol-9-yl)-1-(4-methoxyphenyl)ethan-1-one 5c



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (28.4 mg, 90% yield) as a white solid, m.p. = 201 – 206 ºC.

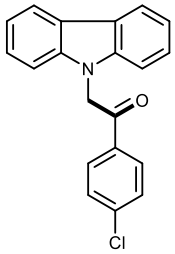
*NMR and HRMS data for the product **5c***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.12 (d, *J* = 7.8 Hz, 2H), 8.05 (d, *J* = 9.0 Hz, 2H), 7.42 (t, *J* = 7.2 Hz, 2H), 7.26 – 7.23 (m, 4H), 6.98 (d, *J* = 9.0 Hz, 2H), 5.61 (s, 2H), 3.89 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 191.5, 164.2, 140.9, 130.4, 127.9, 125.9, 123.3, 120.5, 119.4, 114.2, 108.4, 55.6, 49.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{17}NO_2Na^+$ 338.1151; Found: 338.1141.

2-(9H-carbazol-9-yl)-1-(4-chlorophenyl)ethan-1-one 5d



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (21.8 mg, 68% yield) as a white solid, m.p. = 167 – 169 ºC.

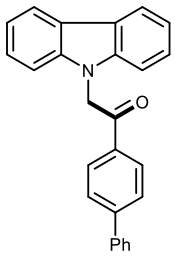
*NMR and HRMS data for the product **5d***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.11 (d, *J* = 7.8 Hz, 2H), 7.95 (d, *J* = 9.0 Hz, 2H), 7.46 – 7.44 (m, 2H), 7.41 (t, *J* = 8.4 Hz, 2H), 7.25 – 7.23 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 5.55 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 192.1, 140.7, 140.6, 133.1, 129.4, 129.3, 126.0, 123.3, 120.6, 119.6, 108.2, 49.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{14}ClNONa^+$ 342.0656 (^{35}Cl), 344.0627 (^{37}Cl); Found: 342.0652, 344.0638.

1-([1,1'-biphenyl]-4-yl)-2-(9H-carbazol-9-yl)ethan-1-one 5e



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (31.1 mg, 86% yield) as a white solid, m.p. = 178 – 181 ºC.

*NMR and HRMS data for the product **5e***:

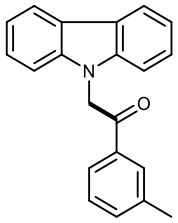
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.13 (d, *J* = 7.8 Hz, 4H), 7.73 (d, *J* = 9.0 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.49 (t, *J* = 7.2 Hz, 2H), 7.45 – 7.42 (m, 3H), 7.27 – 7.25 (m, 4H), 5.67 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 192.6, 146.7, 140.8, 139.6, 133.5, 129.0, 128.7, 128.5,

127.6, 127.3, 125.9, 123.3, 120.5, 119.5, 108.3, 49.4.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{19}NONa^+$ 384.1359; Found: 384.1366.

2-(9H-carbazol-9-yl)-1-(m-tolyl)ethan-1-one 5f



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (18.9 mg, 63% yield) as a white solid, m.p. = 133 – 137 °C.

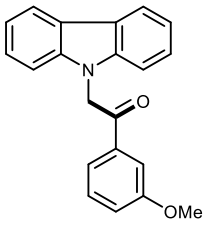
*NMR and HRMS data for the product **5f***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.14 (d, *J* = 7.8 Hz, 2H), 7.88 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.41 (m, 3H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 5.60 (s, 2H), 2.45 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 193.1, 140.8, 138.9, 134.8, 134.8, 128.8, 128.5, 125.8, 125.2, 123.3, 120.5, 119.4, 108.3, 49.3, 21.3.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{17}NONa^+$ 322.1202; Found: 322.1204.

2-(9H-carbazol-9-yl)-1-(3-methoxyphenyl)ethan-1-one 5g



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (15.8 mg, 50% yield) as a white solid, m.p. = 146 – 148 °C.

*NMR and HRMS data for the product **5g***:

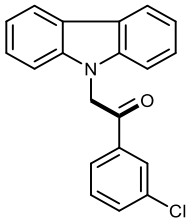
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.13 (d, *J* = 6.6 Hz, 2H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.54 (s, 1H), 7.45 – 7.42 (m, 3H), 7.27 – 7.25 (m, 4H), 7.19 (dd, *J* = 7.8, *J* = 2.4 Hz, 1H), 5.66 (s, 2H), 3.81 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 193.0, 160.0, 140.8, 136.1, 130.0, 125.9, 123.3, 120.7,

120.5, 120.5, 119.5, 112.2, 108.3, 55.5, 49.5.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{17}NO_2Na^+$ 338.1151; Found: 338.1150.

2-(9H-carbazol-9-yl)-1-(3-chlorophenyl)ethan-1-one 5h



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (17.6 mg, 55% yield) as a white solid, m.p. = 163 – 167 °C.

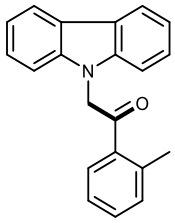
*NMR and HRMS data for the product **5h***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.13 (d, *J* = 7.2 Hz, 2H), 8.03 (s, 1H), 7.91 (d, *J* = 7.2 Hz, 1H), 7.62 (d, *J* = 6.6 Hz, 1H), 7.46 – 7.42 (m, 3H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 5.57 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 192.0, 140.6, 136.2, 135.4, 133.9, 130.3, 128.2, 126.0, 126.0, 123.3, 120.6, 119.7, 108.2, 49.4.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{14}ClNONa^+$ 342.0656 (^{35}Cl), 344.0627 (^{37}Cl); Found: 342.0652, 344.0637.

2-(9H-carbazol-9-yl)-1-(o-tolyl)ethan-1-one 5i



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (16.2 mg, 54% yield) as a white solid, m.p. = 144 – 147 °C.

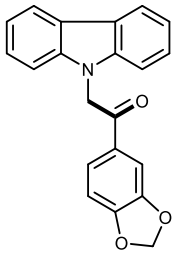
*NMR and HRMS data for the product **5i***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.11 (d, *J* = 7.8 Hz, 2H), 7.87 (d, *J* = 7.2 Hz, 1H), 7.45 – 7.42 (m, 3H),7.32 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.26 – 7.24 (m, 4H), 5.55 (s, 2H), 2.49 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 196.5, 140.8, 139.5, 134.9, 132.5, 132.3, 128.2, 125.9, 125.9, 123.3, 120.5, 119.5, 108.2, 51.0, 21.4.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{17}NONa^+$ 322.1202; Found: 322.1201.

1-(benzo[d][1,3]dioxol-5-yl)-2-(9H-carbazol-9-yl)ethan-1-one 5j



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (21.4 mg, 65% yield) as a white solid, m.p. = 168 – 173 °C.

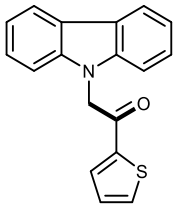
*NMR and HRMS data for the product **5j***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.12 (d, *J* = 7.8 Hz, 2H), 7.69 (dd, *J* = 8.4, *J* = 1.8 Hz, 1H), 7.50 (s, 1H), 7.43 (t, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.07 (s, 2H), 5.56 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 191.0, 152.5, 148.5, 140.8, 129.6, 125.9, 124.3, 123.3, 120.5, 119.5, 108.3, 108.2, 107.9, 102.0, 49.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{15}NO_3Na^+$ 352.0944; Found: 352.0949.

2-(9H-carbazol-9-yl)-1-(thiophen-2-yl)ethan-1-one 5k



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (8.0 mg, 27% yield) as a white solid, m.p. = 169 – 173 °C.

*NMR and HRMS data for the product **5k***:

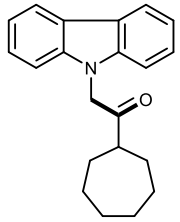
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.12 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 4.2 Hz, 1H), 7.66 (d, *J* = 4.2 Hz, 1H), 7.45 – 7.42 (m, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.10

(t, *J* = 4.8 Hz, 1H), 5.49 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 186.9, 141.0, 140.7, 134.7, 132.4, 128.4, 126.1, 123.3, 120.5, 119.7, 108.5, 50.1.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{15}NO_3Na^+$ 352.0944; Found: 352.0949.

2-(9H-carbazol-9-yl)-1-cycloheptylethan-1-one 5l



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (16.5 mg, 54% yield) as a white solid, m.p. = 124 – 127 ºC.

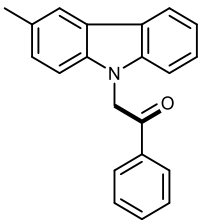
*NMR and HRMS data for the product **5l***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.12 (d, *J* = 7.8 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 5.03 (s, 2H), 2.61 – 2.56 (m, 1H), 1.85 – 1.80 (m, 2H), 1.70 – 1.62 (m, 4H), 1.48 – 1.46 (m, 4H), 1.35 – 1.29 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 209.2, 140.6, 126.0, 123.2, 120.5, 119.6, 108.2, 50.9, 48.5, 29.9, 28.2, 26.4.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{23}NONa^+$ 328.1672; Found: 328.1676.

2-(3-methyl-9H-carbazol-9-yl)-1-phenylethan-1-one 5m



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (26.9 mg, 90% yield) as a white solid, m.p. = 216 – 219 ºC.

*NMR and HRMS data for the product **5m***:

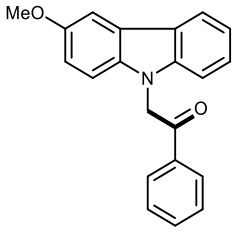
^{1}H NMR (600 MHz, DMSO-*d_6*) δ (ppm): 8.14 (d, *J* = 8.4 Hz, 2H), 8.10 (d, *J* = 7.8 Hz, 1H), 7.94 (s, 1H), 7.72 (t, *J* = 6.6 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.38 –

7.34 (m, 2H), 7.22 – 7.16 (m, 2H), 6.03 (s, 2H), 2.48 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d_6) δ (ppm): 194.1, 140.9, 139.0, 134.9, 133.5, 128.6, 127.9, 127.5, 126.6, 125.2, 122.3, 122.0, 119.7, 119.7, 118.5, 109.0, 108.8, 49.1, 20.7.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{15}NONa^+$ 322.1203; Found: 322.1200.

2-(3-methoxy-9H-carbazol-9-yl)-1-phenylethan-1-one 5n



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (17.7 mg, 56% yield) as a white solid, m.p. = 192 – 194 ºC.

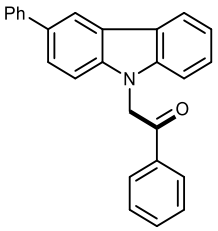
*NMR and HRMS data for the product **5m***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.08 – 8.05 (m, 3H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 2.4 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.24 – 7.21 (m, 2H), 7.16 (d, *J* = 9.0 Hz, 1H), 7.07 (dd, *J* = 9.0, *J* = 2.4 Hz, 1H), 5.62 (s, 2H), 3.93 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 193.2, 154.2, 141.5, 135.9, 135.1, 133.9, 129.0, 128.0, 125.9, 123.8, 123.3, 120.5, 119.1, 115.0, 109.0, 108.4, 103.9, 56.2, 49.6.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{17}NO_2Na^+$ 338.1152; Found: 338.1151.

1-phenyl-2-(3-phenyl-9H-carbazol-9-yl)ethan-1-one 5o



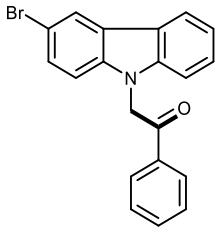
Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1 to 20:1) to afford (25.7 mg, 71% yield) as a white solid, m.p. = 112 – 115 ºC.

*NMR and HRMS data for the product **5o***:

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.32 (s, 1H), 8.16 (d, *J* = 7.2 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 7.2 Hz, 2H), 7.66 – 7.63 (m, 2H), 7.52 (t, *J* = 8.4 Hz, 2H), 7.47 (t, *J* = 7.2

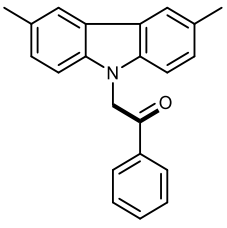
Hz, 2H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.28 – 7.22 (m, 3H), 5.63 (s, 2H).
^{13}C NMR (151 MHz, $CDCl_3$) δ (ppm): 192.8, 142.0, 141.2, 140.3, 134.7, 134.1, 133.0, 129.0, 128.7, 128.0, 127.3, 126.4, 126.1, 125.5, 123.7, 123.4, 120.6, 119.6, 119.1, 108.5, 108.4, 49.3.
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{19}NONa^+$ 384.1359; Found: 384.1358.

2-(3-bromo-9H-carbazol-9-yl)-1-phenylethan-1-on 5p



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (31.0 mg, 85% yield) as a white solid, m.p. = 197 – 202 °C.
*NMR and HRMS data for the product **5p***:
^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 8.44 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 8.16 (d, *J* = 7.2 Hz, 2H), 7.75 (t, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 2H), 7.56 – 7.52 (m, 3H), 7.43 (t, *J* = 8.4 Hz, 1H), 7.24 (t, *J* = 7.2 Hz, 1H), 6.18 (s, 2H).
^{13}C NMR (151 MHz, DMSO-d_6) δ (ppm): 194.1, 141.2, 139.7, 134.8, 134.0, 128.9, 128.4, 128.0, 126.5, 124.3, 122.8, 121.4, 120.8, 119.5, 111.6, 111.2, 109.8, 49.5.
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for Calcd for $C_{20}H_{14}BrNONa^+$ 386.0151 (^{79}Br), 388.0131 (^{81}Br); Found: 386.0159, 388.0139.

2-(3,6-dimethyl-9H-carbazol-9-yl)-1-phenylethan-1-one 5q



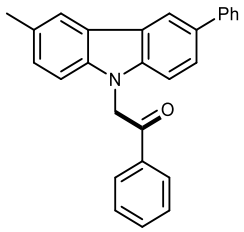
Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (17.6 mg, 56% yield) as a white solid, m.p. = 220 – 225 °C.
*NMR and HRMS data for the product **5q***:
^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 8.15 (d, *J* = 7.8 Hz, 2H), 7.91 (s, 2H), 7.73 (t, *J* =

7.2 Hz, 1H), 7.62 (t, *J* = 7.2 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 6.04 (s, 2H), 2.47 (s, 6H).

^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ (ppm): 194.2, 139.2, 134.9, 133.5, 128.6, 127.9, 127.2, 126.5, 122.2, 119.6, 108.8, 49.2, 20.7.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{22}H_{19}NOH^+$ 314.1540; Found: 314.1533.

2-(3-methyl-6-phenyl-9H-carbazol-9-yl)-1-phenylethan-1-one 5r



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (33.8 mg, 90% yield) as a white solid, m.p. = 198 – 202 ºC.

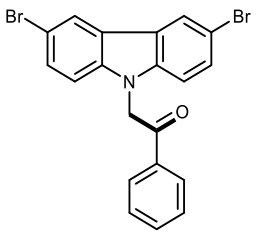
*NMR and HRMS data for the product **5r***:

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ (ppm): 8.41 (s, 1H), 8.15 (d, *J* = 7.8 Hz, 2H), 8.05 (s, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.72 (t, *J* = 7.2 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 6.02 (s, 2H), 2.51 (s, 3H).

^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ (ppm): 194.2, 141.1, 140.6, 139.6, 134.9, 133.7, 131.2, 128.7, 128.1, 127.8, 127.0, 126.5, 126.2, 124.4, 122.8, 122.6, 120.1, 118.0, 109.6, 109.1, 49.3, 20.9.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{27}H_{21}NONa^+$ 398.1516; Found: 398.1510.

2-(3,6-dibromo-9H-carbazol-9-yl)-1-phenylethan-1-one 5s



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (39.0 mg, 88% yield) as a white solid, m.p. = 162 – 167 ºC.

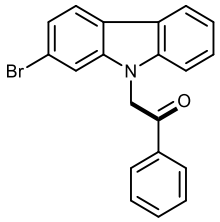
*NMR and HRMS data for the product **5s***:

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ (ppm): 8.51 (s, 2H), 8.14 (d, *J* = 7.2 Hz, 2H), 7.75 (t, *J* = 7.8 Hz, 1H), 7.63 (t, *J* = 8.4 Hz, 2H), 7.56 (s, 4H), 6.19 (s, 2H).

^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ (ppm): 193.8, 140.1, 134.7, 134.1, 128.9, 128.8, 128.4, 123.4, 123.3, 112.0, 111.6, 49.7.

HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for Calcd for $C_{20}H_{13}Br_2NONa^+$ 463.9257 (^{79}Br), 467.9216 (^{81}Br); Found: 463.9257, 467.9220.

2-(2-bromo-9H-carbazol-9-yl)-1-phenylethan-1-one 5t



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 100:1, 50:1 to 20:1) to afford (25.1 mg, 69% yield) as a white solid, m.p. = 170 – 173 ºC.

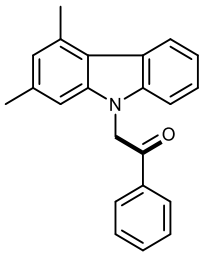
*NMR and HRMS data for the product **5t***:

^{1}H NMR (600 MHz, CDCl$_3$) δ (ppm): 8.06 (t, *J* = 7.8 Hz, 3H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.35 – 7.33 (m, 2H), 7.27 – 7.24 (m, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 5.56 (s, 2H).

^{13}C NMR (151 MHz, CDCl$_3$) δ (ppm): 192.2, 141.6, 140.9, 134.5, 134.2, 129.1, 128.0, 126.3, 122.7, 122.7, 122.2, 121.6, 120.5, 120.0, 119.4, 111.5, 108.4, 49.1.

HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for Calcd for $C_{20}H_{14}BrNONa^+$ 386.0151 (^{79}Br), 388.0131 (^{81}Br); Found: 386.0147, 388.0125.

2-(2,4-dimethyl-9H-carbazol-9-yl)-1-phenylethan-1-one 5u



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (24.1 mg, 77% yield) as a white solid, m.p. = 231 – 234 ºC.

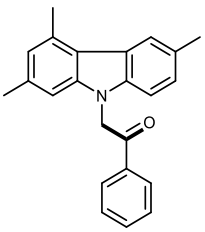
*NMR and HRMS data for the product **5u***:

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ (ppm): 8.17 (d, *J* = 6.6 Hz, 2H), 8.11 (d, *J* = 7.2 Hz, 1H), 7.75 (t, *J* = 7.2 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 2H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 7.17 (s, 1H), 6.84 (s, 1H), 6.08 (s, 2H), 2.79 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ (ppm): 194.0, 141.2, 140.6, 134.9, 134.7, 133.5, 131.9, 128.6, 127.9, 124.2, 122.8, 121.9, 121.4, 118.7, 118.5, 108.7, 106.7, 49.0, 21.3, 19.9.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{22}H_{19}NONa^+$ 336.1359; Found: 336.1361.

1-phenyl-2-(2,4,6-trimethyl-9H-carbazol-9-yl)ethan-1-one 5v



Prepared according to ***General Procedure***. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 50:1, 20:1 to 5:1) to afford (28.5 mg, 87% yield) as a white solid, m.p. = 197 – 199 ºC.

*NMR and HRMS data for the product **5v***:

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ (ppm): 8.16 (d, *J* = 8.4 Hz, 2H), 7.91 (s, 1H), 7.73 (t, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.11 (s, 1H), 6.81 (s, 1H), 6.01 (s, 2H), 2.79 (s, 3H), 2.49 (s, 3H), 2.40 (s, 3H),.

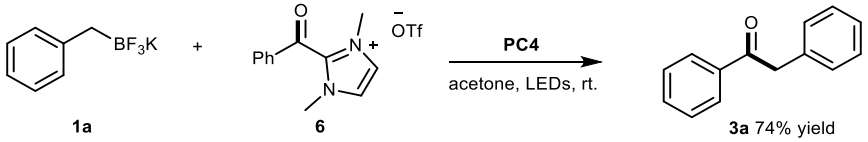
^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ (ppm): 194.1, 141.4, 139.0, 134.9, 134.5, 133.5, 131.8, 128.6, 127.9, 127.3, 125.4, 123.0, 121.7, 121.4, 118.3, 108.4, 106.6, 49.1, 21.3, 20.9, 20.0.

HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{23}H_{21}NONa^+$ 350.1516; Found: 350.1524.

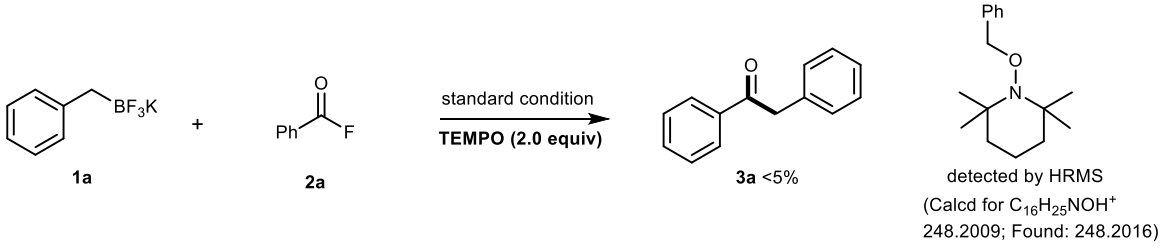
5. Mechanistic Studies.

5.1 Control experiments

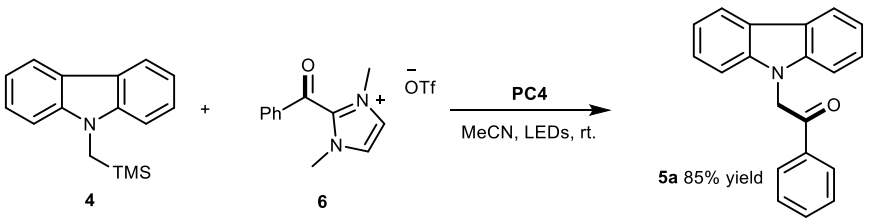
Severe control experiments revealed that all of the reaction parameters were crucial for this transformation.



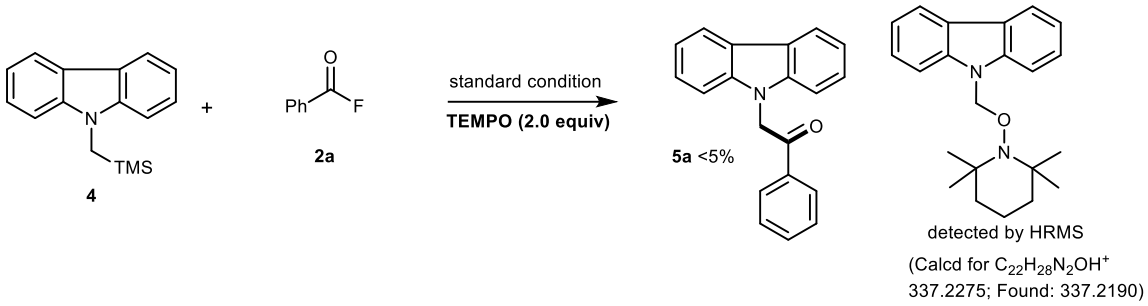
According to the ***General Procedure***, to a flame-dried Schlenk tube were added alkyl trifluoroborates **1a** (0.10 mmol, 1.0 equiv.), photocatalyst **4** (2% mmol), and 2-benzoyl-1,3-dimethyl-1H-imidazol-3-ium trifluoromethanesulfonate **6** (0.20 mmol, 2.0 equiv.). Then, the reaction tube was evacuated and back-filled with argon three times. Subsequently, acetone (2.0 mL) was added via syringe. The resulting mixture was stirred at ambient temperature for about 3 h (monitored by TLC). After the reaction mixture was concentrated, the resulting crude material was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1 to 80/1) to afford **3a** (14.5 mg, 74%).



To a flame-dried Schlenk tube were added trifluoroborate **1a** (0.10 mmol, 1.0 equiv.), NHC **N1** (0.20 mmol, 0.2 equiv.), photocatalyst **4** (2% mmol), Cs_2CO_3 (0.10 mmol, 1.0 equiv.), and 2,2,6,6-tetramethyl piperidine-N-oxyl (TEMPO, 0.20 mmol, 2.0 equiv.). Then, the tube was evacuated and back-filled with argon three times. Subsequently, under the protection of Ar, aroyl fluoride **2** (0.20 mmol, 2.0 equiv.) and acetone (2.0 mL) were added via syringe. The resulting mixture was stirred at ambient temperature for about 3 h. The reaction was found to be suppressed upon addition of TEMPO, and less than 5% yield of **3a** was obtained.



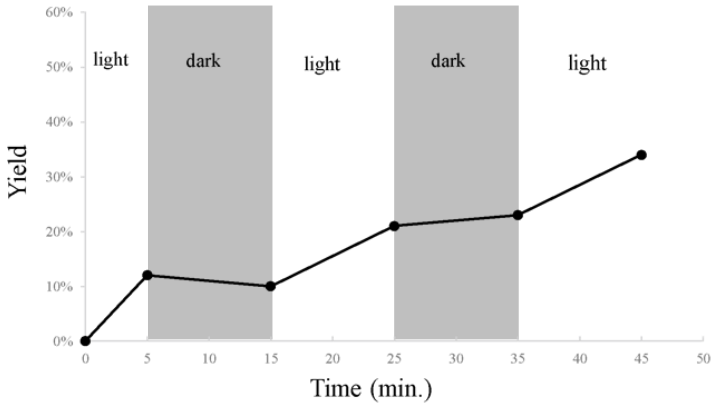
To a flame-dried Schlenk tube were added α-silyl carbazole **4** (0.10 mmol, 1.0 equiv.), photocatalyst **PC4** (2% mmol) and 2-benzoyl-1,3-dimethyl-1H-imidazol-3-ium trifluoromethanesulfonate **6** (0.20 mmol, 2.0 equiv.). Then, the tube was evacuated and back-filled with argon three times. Subsequently, under the protection of Ar, MeCN (1.0 mL) was added via syringe. Then, the resulting suspension was stirred at room temperature for 1.0 h. The reaction mixture was concentrated under reduced pressure, and the resulting crude material was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, 50/1 to 20/1) to afford **5a** (24.3 mg, 85%).

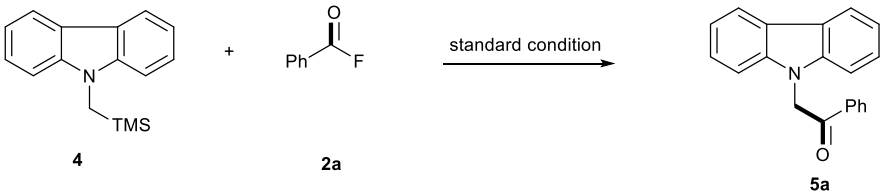


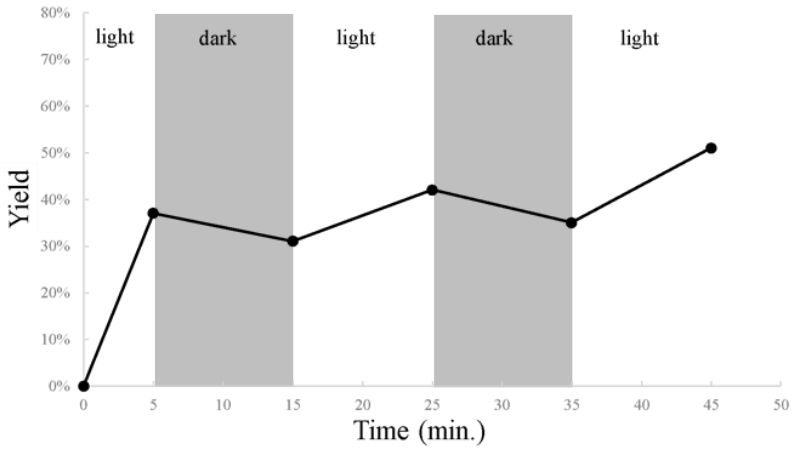
To a flame-dried Schlenk tube were added α-silyl carbazole **4** (0.10 mmol, 1.0 equiv.), NHC **N1** (0.20 mmol, 0.2 equiv.), photocatalyst **PC4** (2% mmol), Cs_2CO_3 (0.10 mmol, 1.0 equiv.) and 2,2,6,6-tetramethyl piperidine-N-oxyl (TEMPO, 0.20 mmol, 2.0 equiv.). Then, the tube was evacuated and back-filled with argon three times. Subsequently, under the protection of Ar, aroyl fluoride **2** (0.20 mmol, 2.0 equiv.) and MeCN (1.0 mL) were added via syringe. The resulting mixture was stirred at ambient temperature for 1.0 h. The reaction was found to be suppressed upon addition of TEMPO, and less than 5% yield of **5a** was obtained.

5.2 Light on-off experiments

The light-on experiments were performed according to the general procedure and set up five reactions in parallel. The corresponding yields were calculated by ^{1}H NMR with CH_2Br_2 as internal standard. The light on−off results indicated the reaction underwent a catalytic radical reaction rather than a radical chain pathway.







5.3 Quantum Yield Measurement for the reaction with alkyl trifluoroborates 1a and benzoyl fluoride 2a

The photon flux of the spectrophotometer was determined by ferrioxalate actinometry. A ferrioxalate actinometer solution was prepared according to literature procedures[6]. The ferrioxalate actinometer solution measures the decomposition of ferric ions to ferrous ions, which are complexed by 1,10-phenanthroline and monitored by UV/Vis absorbance at 510 nm. The moles of iron-phenanthroline complex formed are related to moles of photons absorbed. The solutions were prepared and stored in a dark laboratory (red light):

1. Potassium ferrioxalate solution: 59 mg of potassium ferrioxalate and 27.8 μL of sulfuric acid (96%) were added to a 10 mL volumetric flask, and filled to the mark with water (HPLC grade).
2. Phenantroline solution: 0.2% by weight of 1,10-phenanthroline in water (20 mg in 10 mL volumetric flask).
3. Buffer solution: to a 10 mL volumetric flask, 494 mg of NaOAc and 100 μL of sulfuric acid (96%) were added and filled to the mark with water (HPLC grade).

To determine the photon flux of the spectrophotometer, 1.0 mL of the ferrioxalate solution was placed in a flame-dried Schlenk tube and irradiated for 30.0 seconds at λ = 450 nm. The ferrioxalate solution was irradiated with five 30 W Blue LEDs which same light intensity as model reaction without stirring. After irradiation, the actinometer solution was removed and placed in a 10 mL volumetric flask containing 0.18 mL of 1,10-phenanthroline solution and 1 mL of buffer solution. This flask was filled to the mark with water (HPLC grade). The flask was then allowed to rest for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance of the solution was measured at 510 nm. A non-irradiated sample was also prepared and the absorbance at 510 nm measured. Conversion was calculated using eq 1 .

$$moles\ Fe^{2+} = \frac{V1 \cdot V3 \cdot \Delta A(510\ nm)}{10^3 \cdot V2 \cdot l \cdot \varepsilon(510\ nm)} \qquad \text{eq 1}$$

where V1 is the irradiated volume (1 mL), V2 is the aliquot of the irradiated solution taken for the determination of the ferrous ions (1 mL), V3 is the final volume after complexation with phenanthroline (10 mL), l is the optical path-length of the irradiation cell (1 cm), ΔA(510 nm) the optical difference in absorbance between the irradiated solution and the one stored in the dark, ε (510 nm) is that of the complex $Fe(phen)_3^{2+}$ (11100 L $mol^{-1}.cm^{-1}$)

$$q^0_{n,p} = \frac{\text{moles Fe}^{2+}}{\Phi \cdot t \cdot [1\text{-}10^{-A(\lambda)}]} \qquad \text{eq 2}$$

Where Φ is the quantum yield for the ferrioxalate actinometer (0.9 for a 0.011 M solution at λ = 450 nm)[6b], t is the time (30.0 s), and f is the fraction of light absorbed at λ = 450 nm. The photon flux ($q^0_{n,p}$) was calculated (average of three experiments) to be 3.22×10^{-8} einstein s^{-1}.

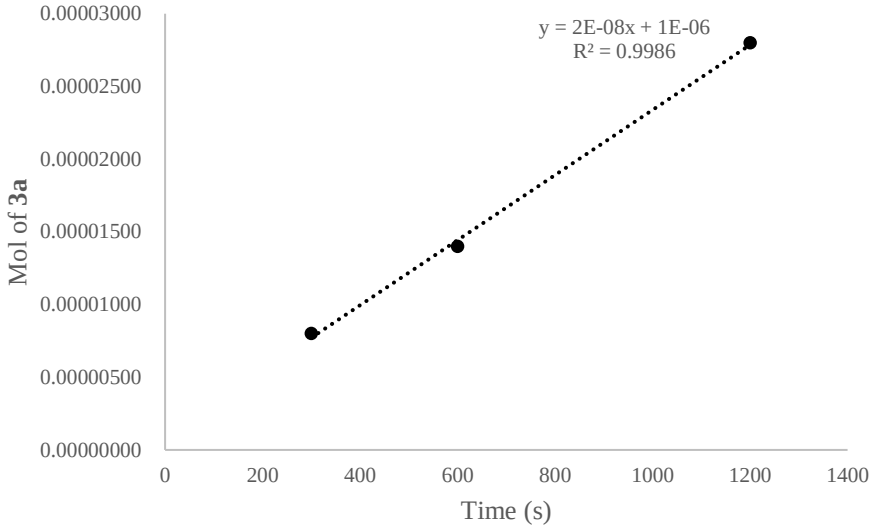
Sample calculation: $moles\ Fe^{2+} = \frac{1\ mL \cdot 10\ mL \cdot 0.482}{10^3 \cdot 1\ mL \cdot 1\ cm \cdot 11100\ L\ mol^{-1}.cm^{-1}} = 4.3 \times 10^{-7}$ mol

$$q^0_{n,p} = \frac{4.3 \times 10^{-7}\ \text{moL}}{0.9 \cdot 30s \cdot [1\text{-}10^{-0.276}]} = 3.39 \times 10^{-8}\ \text{einstein}\ s^{-1}$$

The measurements for the reaction in this study were performed as follows: To a flame-dried Schlenk tube were added trifluoroborate **1a** (0.10 mmol, 1.0 equiv.), **N1** (0.20 mmol, 0.2 equiv.), photocatalyst **4** (2% mmol) and Cs_2CO_3 (0.10 mmol, 1.0 equiv.), after which the tube was evacuated and back-filled with argon three times. Subsequently, under the protection of argon, aroyl fluoride **2a** (0.20 mmol, 2.0 equiv.) and acetone (2.0 mL) were added via syringe. The resulting mixture was stirred and irradiated (λ = 450 nm) at ambient temperature. The product 3a was determined calculated by 1H NMR with CH2Br2 as internal standard. The moles of product per unit of time are related to the number of photons absorbed. The moles of **3a** formed (x) are plotted as a function of time (t). The slope of this line was correlated to the moles of incident photons by unit of time by the use of the following eq 3.

$$\Phi(\lambda) = \frac{dx/dt}{q^0_{n,p}[1\text{-}10^{-A(\lambda)}]} \qquad \text{eq 3}$$

According to eq 3, the moles of **3a** formed (x) were plotted as a function of time (t): Φ was the quantum yield to be determined and A(450 nm) was the absorption of the reaction under study. A(450 nm) was measured using a SHIMADZU UV-2450 UV/Vis spectrometer in 1 cm path quartz to carry out the measurements, obtaining an absorbance of 0.957.

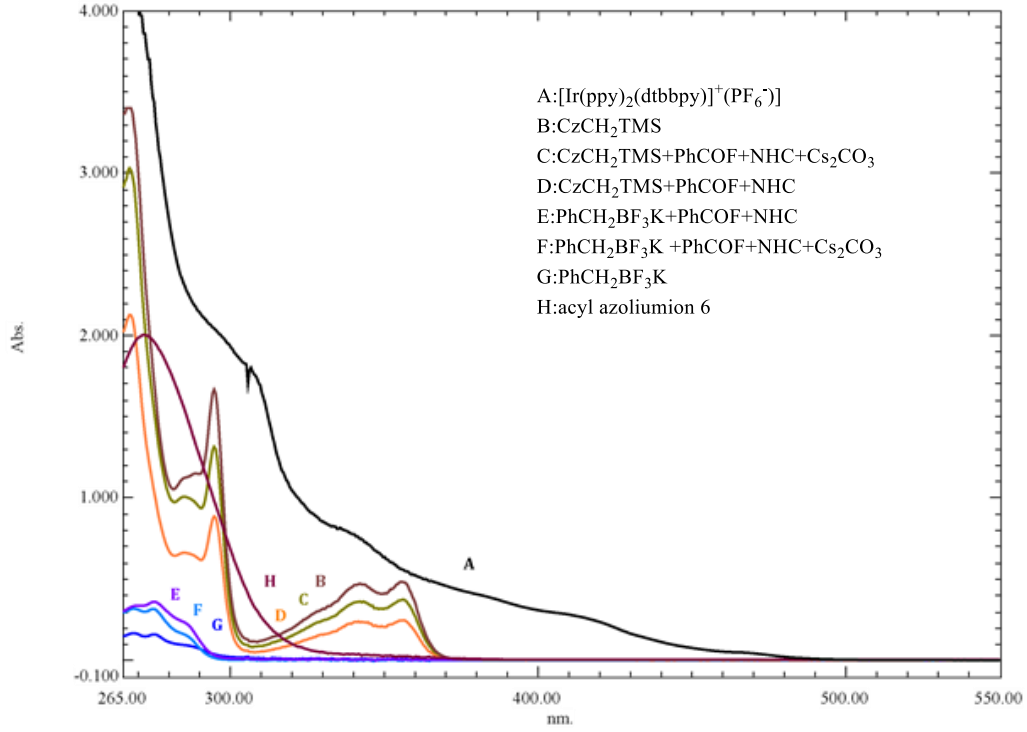


The quantum yield (Φ) of the reation of alkyl trifluoroborates **1a** and benzoyl fluoride **2a** was calculated to be 0.69.

5.4 UV-vis Absorption

The UV-Vis absorption spectrum of **PC4** (10^{-4} M in MeCN, A line), benzylic trifluoroborates **1a** (10^{-4} M in MeCN, G line), α-silyl carbazole **4** (10^{-4} M in MeCN, B line) or

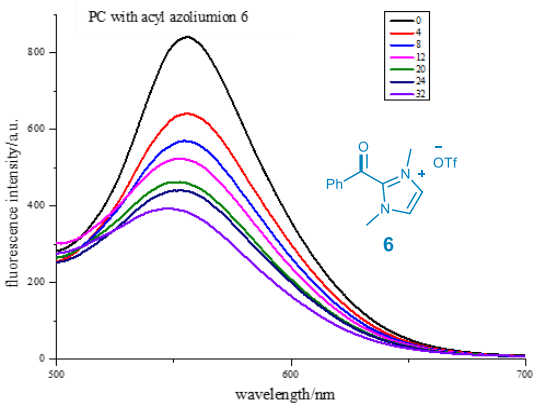
acyl azolium **6** (10^{-4} M in MeCN, H line) were respectively measured by SHIMADZU UV-2450 UV/Vis spectrometer. And the absorption spectrum of different combination of the reagents were also measured in MeCN using the same method. As shown in the following figure, the absorption spectrum of **PC4** revealed a significant absorption of visible light. By contrast, other compounds have little absorptions at the visible light region.

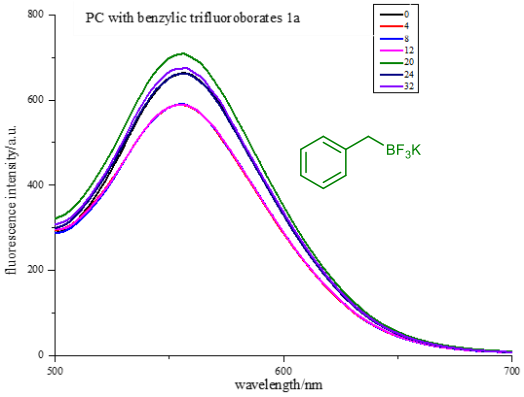


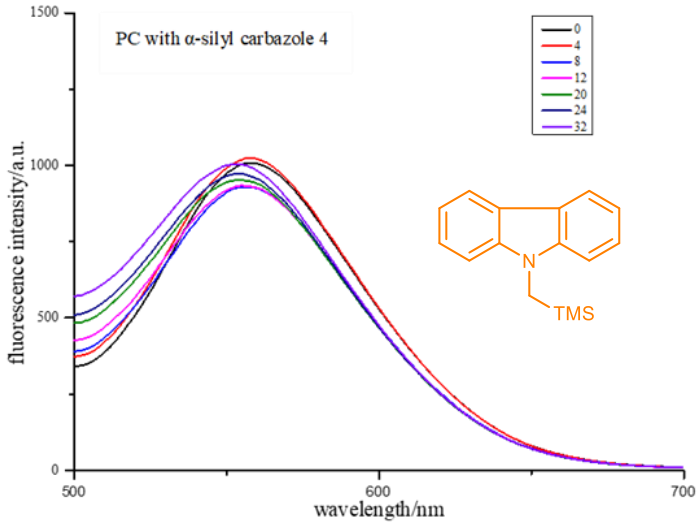
5.5 Luminescence quenching experiments

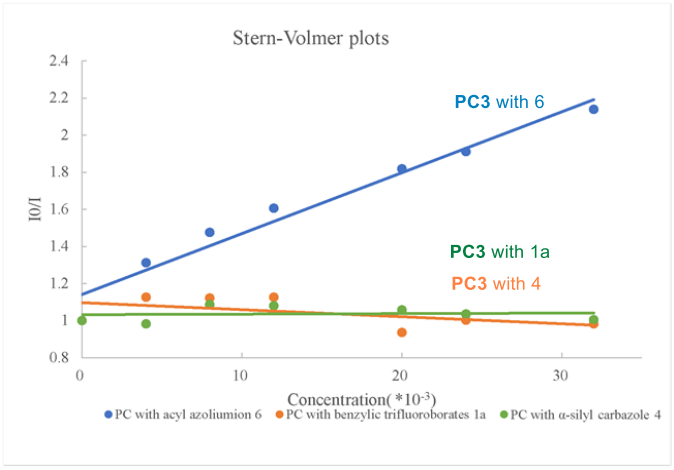
The fluoresence intensity was measured by HITACHI F-7000 spectrofluorometer. The sample was prepared by adding 100 μL of 10^{-4} M solution of **PC4** and degassed MeCN solution of benzylic trifluoroborates **1a,** α-silyl carbazole **4** or acyl azolium **6** (quencher) in different concentrations (4×10^{-3} , 8×10^{-3}, 12×10^{-3}, 20×10^{-3}, 24×10^{-3}, or 32×10^{-3} M, respectively) , and mixed. All **PC4** solutions were excited at 460 nm and the emission intensity was collected at 500-700 nm.

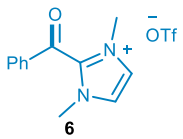
The Stern-Volmer fluorescence quenching experiments revealed that only acyl azolium **6** could quench the excited state of Ir*(Ⅲ), while no significant quenching phenomenon was observed with benzylic trifluoroborates **1a** or α-silyl carbazole **4**.


PC with acyl azoliumion 6
fluorescence intensity/a.u.
wavelength/nm
0
4
8
12
20
24
32
Ph
O
N
N
OTf
6

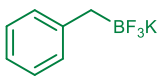

PC with benzylic trifluoroborates 1a
fluorescence intensity/a.u.
wavelength/nm
0
4
8
12
20
24
32
BF3K


PC with α-silyl carbazole 4
fluorescence intensity/a.u.
wavelength/nm
0
4
8
12
20
24
32
N
TMS

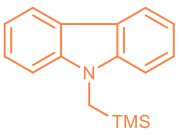

Stern-Volmer plots
I0/I
Concentration(*10-3)
PC3 with 6
PC3 with 1a
PC3 with 4
PC with acyl azoliumion 6
PC with benzylic trifluoroborates 1a
PC with α-silyl carbazole 4


Ph
O
N
N
OTf

6


BF3K

1a

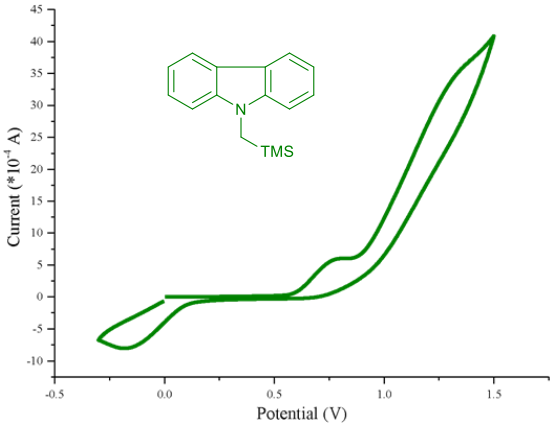

N
TMS

4

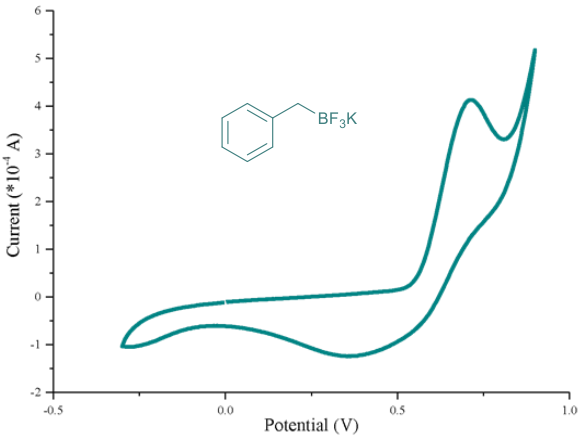
5.6 Cyclic Voltammograms

Electrochemical measurements were recorded by a Metrohm Autolab analyzer. Cyclic voltammetry (CV) experiments were conducted by using a 10 mL glass vial which fitted with a platinum sheet as working electrode, calomel electrode as reference electrode, and a platinum sheet as counter electrode. The electrolyte of nBu$_4$NPF$_6$ (0.05 M) was dissolved in dry MeCN as blank control experiment. (Sweep rate: 100 mV/s)

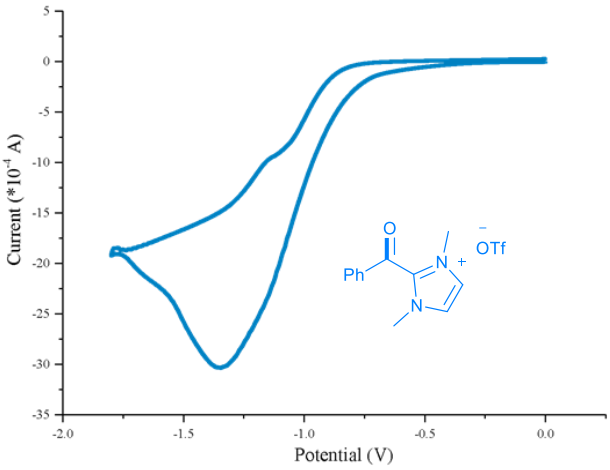
The redox potential of α-silyl carbazole **4** was determined by cyclic voltammetry (α-silyl carbazole 4 (0.01M) in [0.05 M] nBu4NPF6 in MeCN). The Cyclic voltammogram of α-silyl carbazole **4** feature irreversible peak at $E_{ox} = E_{pa} = + 0.78$ V vs SCE. E_{pa} is the anodic peak potential, while E_{ox} value describes the electrochemical properties of α-silyl carbazole **4**.



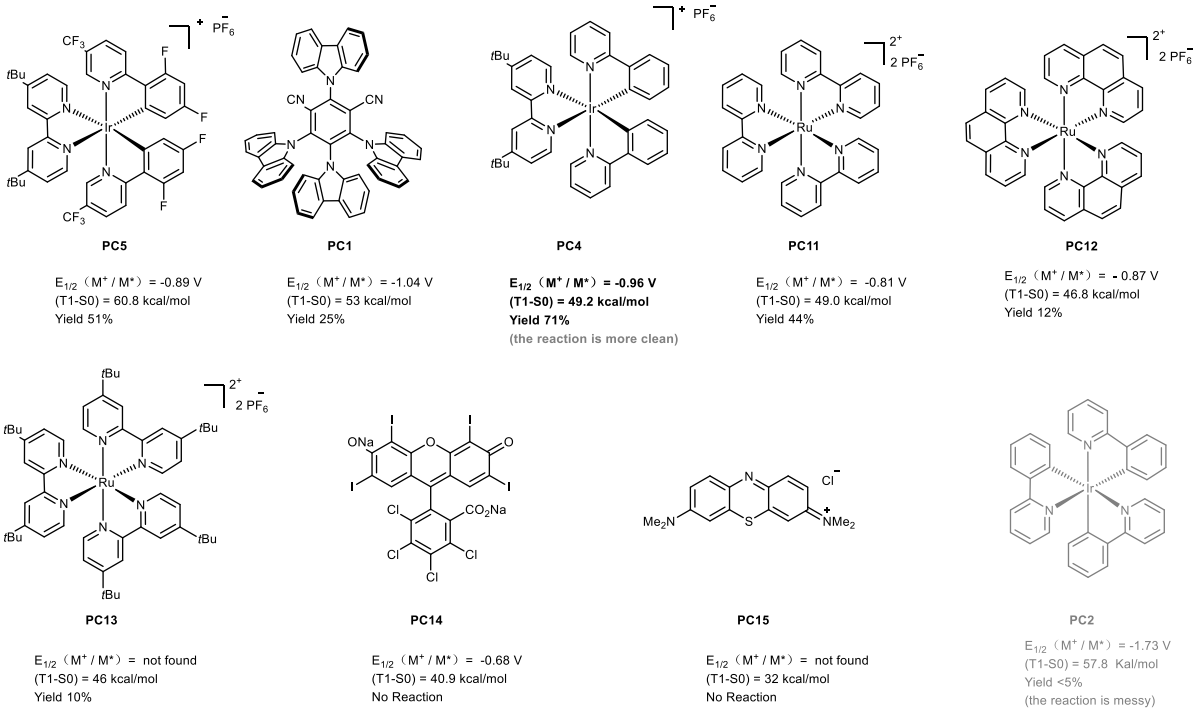
Cyclic voltammogram of benzylic trifluoroborates **1a** solutions feature irreversible peak at $E_{ox} = E_{pa} = + 0.72$ V vs SCE. E_{pa} is the anodic peak potential, while E_{ox} value describes the electrochemical properties of benzylic trifluoroborates **1a**.



Cyclic voltammogram of acyl azoliums **6** solutions feature irreversible peak at $E_{red} = E_{pc}$ = - 1.31 V vs SCE. E_{pc} is the cathodic peak potential,, while E_{red} value describes the electrochemical properties of acyl azoliums **6**.

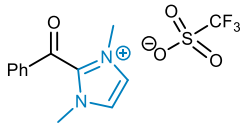


- We have checked and compared the excited-state triplet energy ($\Delta G_{(T1\text{-}S0)}$) of the photocatalysts[7] screened in the catalytic reaction. And the oxidation potential ($E_{1/2}$ M^+/M^*) of the photocatalysts as well as the isolated yields of the target products were also listed, respectively. As shown in the following figure, we can recognize that when the excited-state triplet energy of a photocatalyst is greater than (or similar to) **PC4**, such as **PC5**, **PC1**, and **PC11**, the catalytic reaction could proceed smoothy. Accordingly, if the excited-state triplet energy of a photocatalyst is slightly lower than **PC4**, such as **PC12** and **PC13**, the reaction efficiency decreased. And no reaction was observed when the triplet energy of photocatalyst (such as **PC15**) is significantly lower than **PC4**. On the other hand, the oxidation potential of these photocatalysts (generally higher than the reduction potential of the substrates E_{red} = –1.31 V vs. SCE) did not match the reaction outcome of the photocatalytic system. Based on the above comparison, we may suggest that a single-electron transfer between the excited photocatalyst and acyl acylium is unlikely, but an energy transfer (EnT) process might be feasible. (It should be noted that the reaction with **PC2** is messy, therefore the reaction results of **PC2** did not match neither of the SET pathway nor EnT pathway.).



5.7 DFT Calculations

Computational details：Density functional theory (DFT) calculations were performed with the Gaussian 09 program package.[8] The SMD continuum solvation model[9] was employed to simulate the solvent effect of acetone solution. Full geometry optimizations were operated to locate all of the stationary points, using (U)B3LYP[10] and (U)M06-2X[11] density functional theory methods with the LANL2DZ basis set and effective core potential for Ir atom, as well as the 6-31G(d,p) basis set[12] for all other atoms, where the spin-restricted DFT method for closed-shell species (acyl azoliumion **6**, triazolium salt **7**, and **PC4**) and the spin-unrestricted DFT method with the "guess(mix, always)" keyword for open-shell triplet species (**6-T$_1$**, **7-T$_1$**, and **PC4-T$_1$**). In the meantime, the stability of the density function theory (DFT) wave-function of the auxiliary Kohn–Sham determinant was examined.[13] Harmonic vibrational frequency calculations were conducted to characterize all stationary point. Herein, minima have zero imaginary frequencies. Unless mentioned otherwise, the triplet-singlet energy gap [$\Delta G(T_1\text{-}S_0)$] were obtained at the levels of (U)B3LYP/6-31G(d,p),LANL2DZ + SMD(acetone) and (U)M06-2X/6-31G(d,p),LANL2DZ + SMD(acetone), under experimental temperature and pressure (298.15 K and 1 atm).



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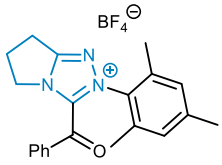

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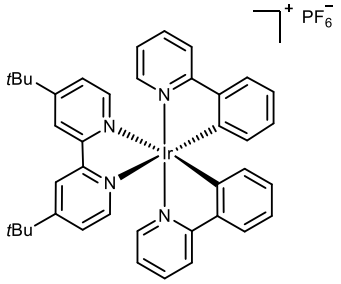


PC4

DFT Calculation level	ΔG(T1-S0)/kcal mol^{-1}		
	6	**7**	**PC4** [a]
(U)B3LYP/6-31G(d,p),LANL2DZ + SMD(acetone)	**39.5**	**27.1**	**49.7**
(U)M06-2X/6-31G(d,p),LANL2DZ + SMD(acetone)	50.9	29.9	59.2

[a] The experimentally determined triplet-singlet energy gap ΔG(T1-S0) of **PC4** is 49.2 kcal/mol.[7]

As shown in Table S1, the calculated triplet-singlet energy gap [$\Delta G(T_1\text{-}S_0)$] of **PC4** is 49.7 kcal/mol at the (U)B3LYP/6-31G(d,p),LANL2DZ + SMD(acetone) level, which is in close proximity to experimentally determined result (49.2 kcal/mol). For comparison, we also performed DFT calculation at (U)M06-2X/6-31G(d,p),LANL2DZ + SMD(acetone) level. The result indicted that the [$\Delta G(T_1\text{-}S_0)$] of **PC4** is 59.2kcal/mol, which is dramatically higher than the experimentally [$\Delta G(T_1\text{-}S_0)$] of 49.2 kcal/mol. Thus, the calculated triplet-singlet energy gaps [$\Delta G(T_1\text{-}S_0)$] of acyl azoliumion **6** and triazolium salt **7** by using (U)B3LYP functional are discussed in the manuscript. Moreover, the calculated [$\Delta G(T_1\text{-}S_0)$] of **6** and **7** are 39.5 and 27.1 kcal/mol, which are below the theoretical and experimental [$\Delta G(T_1\text{-}S_0)$] values of **PC4** (49.7 and 49.2 kcal/mol). These results corroborate well with experimentally observed phenomenon.

6. References and Notes.

1. (a) E. E. Stache, T. Rovis and A. G. Doyle, *Angew.Chem. Int.Ed*., 2017, **56**, 3679-3683; (b) J. Luo, B. Hu, W. D. Wu, M. W. Hu and T. L. Liu, *Angew.Chem. Int.Ed.*, 2021, **60**, 6107-6116.

2. F.-F. Pan, P. Guo, C.-L. Li, P. Su and X.-Z. Shu, *Org. Lett.*, 2019, **21**, 3701-3705.

3. W. Guo, H. Ding, C. Gu, Y. Liu, X. Jiang, B. Su and Y. Shao, *J. Am. Chem. Soc.*, 2018, **140**, 15904-15915.

4. K. B. Ling and A. D. Smith, *Chem. Commun.*, 2011, **47**, 373-375.

5. (a) B. A. Dalvi and P. D. Lokhande, *Tetrahedron Lett.*, 2018, **59**, 2145-2149; (b) M.-L. Louillat, A. Biafora, F. Legros and F. W. Patureau, *Angew. Chem. Int. Ed.,* 2014, **53**, 3505-3509; (c) W. Qu, Z. Gao, W. Li, X. Fan, Y. Shi, Y. Miao, G. Yu, H. Zhou, J. Huang and H. Wang, *Dyes Pigments*, 2021, **196**, 109808.

6. (a) A. Bahamonde and P. Melchiorre, *J. Am. Chem. Soc.,* 2016, **138**, 8019-8030; (b) M. A. Cismesia and T. P. Yoon, *Chem. Sci.,* 2015, **6**, 5426-5434.

7. (a) M. Teders, C. Henkel, L. Anhäuser, F. Strieth-Kalthoff, A. Gómez-Suárez, R. Kleinmans, A. Kahnt, A. Rentmeister, D. Guldi and F. Glorius. *Nat. Chem.,* 2018, **10**, 981-988; (b) F. Strieth-Kalthoff, M. J. James, M. Teders, L. Pitzera and F. Glorius, *Chem. Soc. Rev.*, 2018, **47**, 7190-7202.

8. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

9. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.* 2009, **113**, 6378-6396.

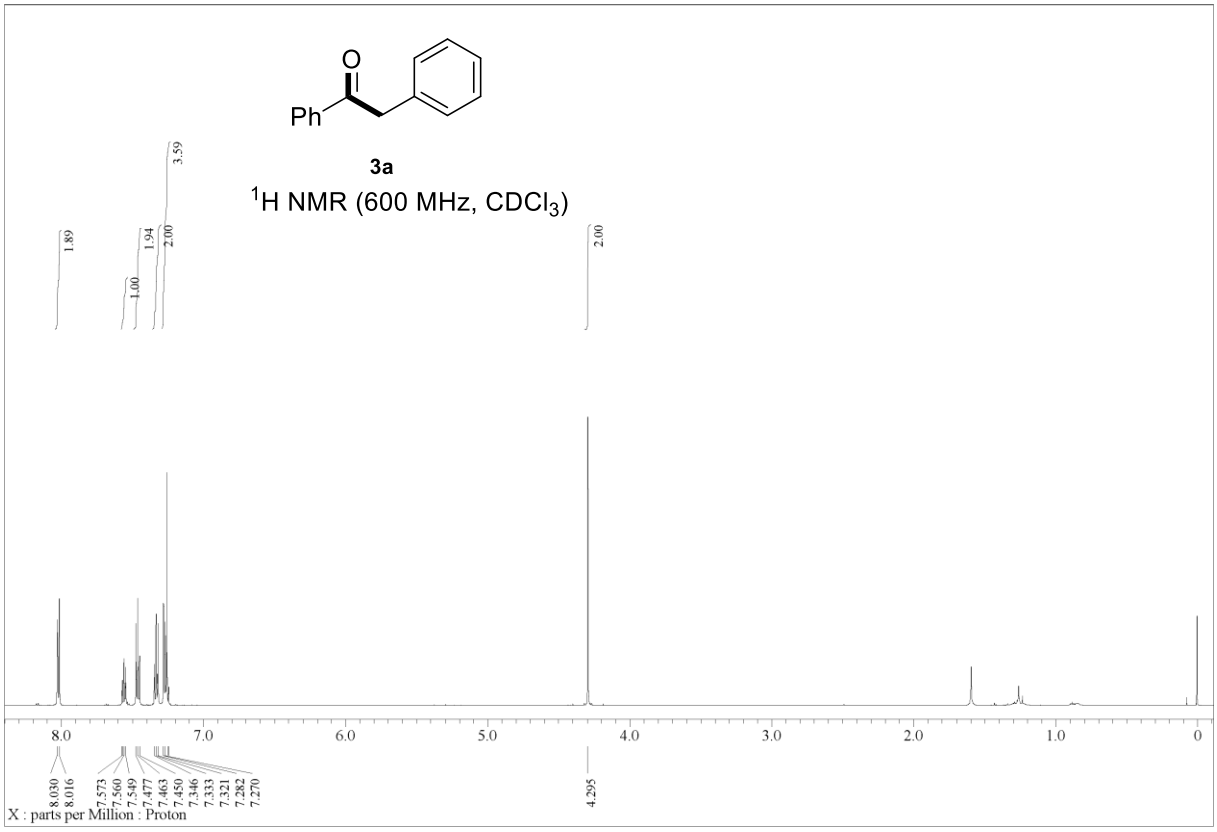
10. (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.

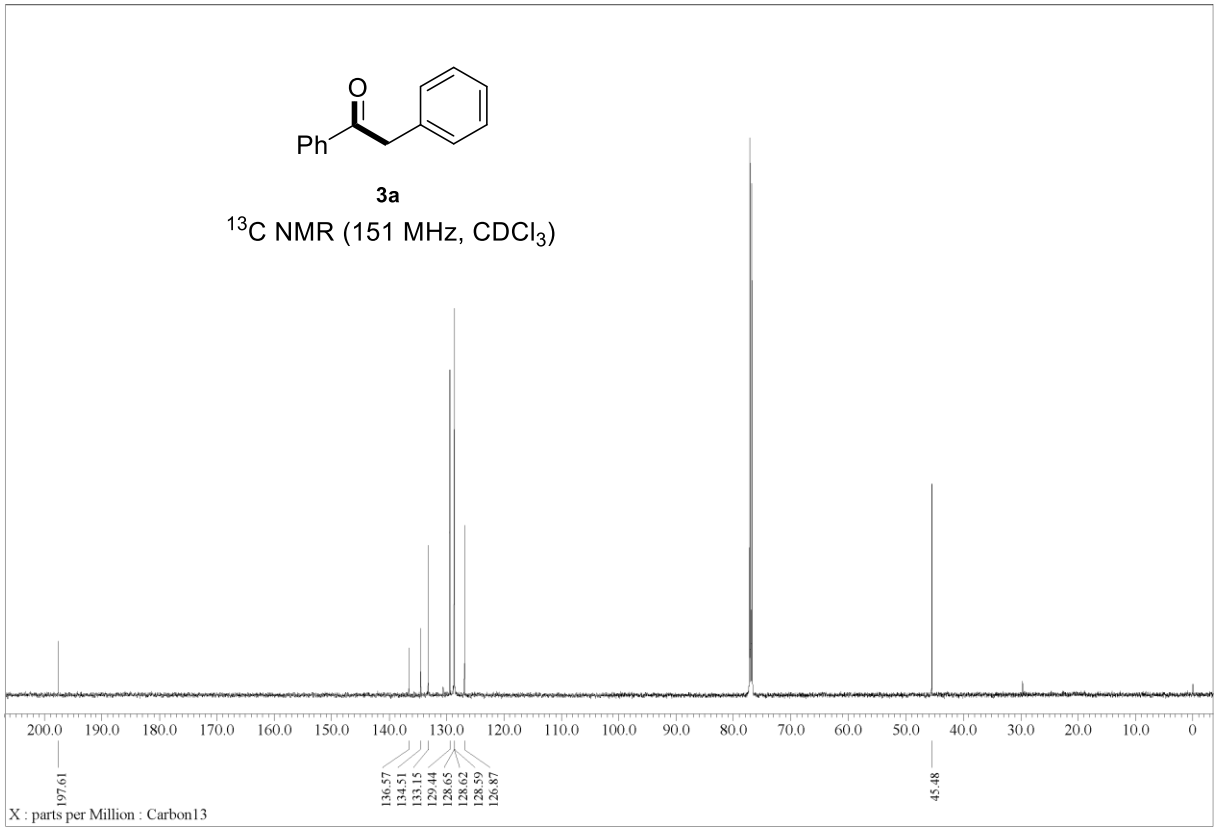
11. (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241; (b) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157-167.

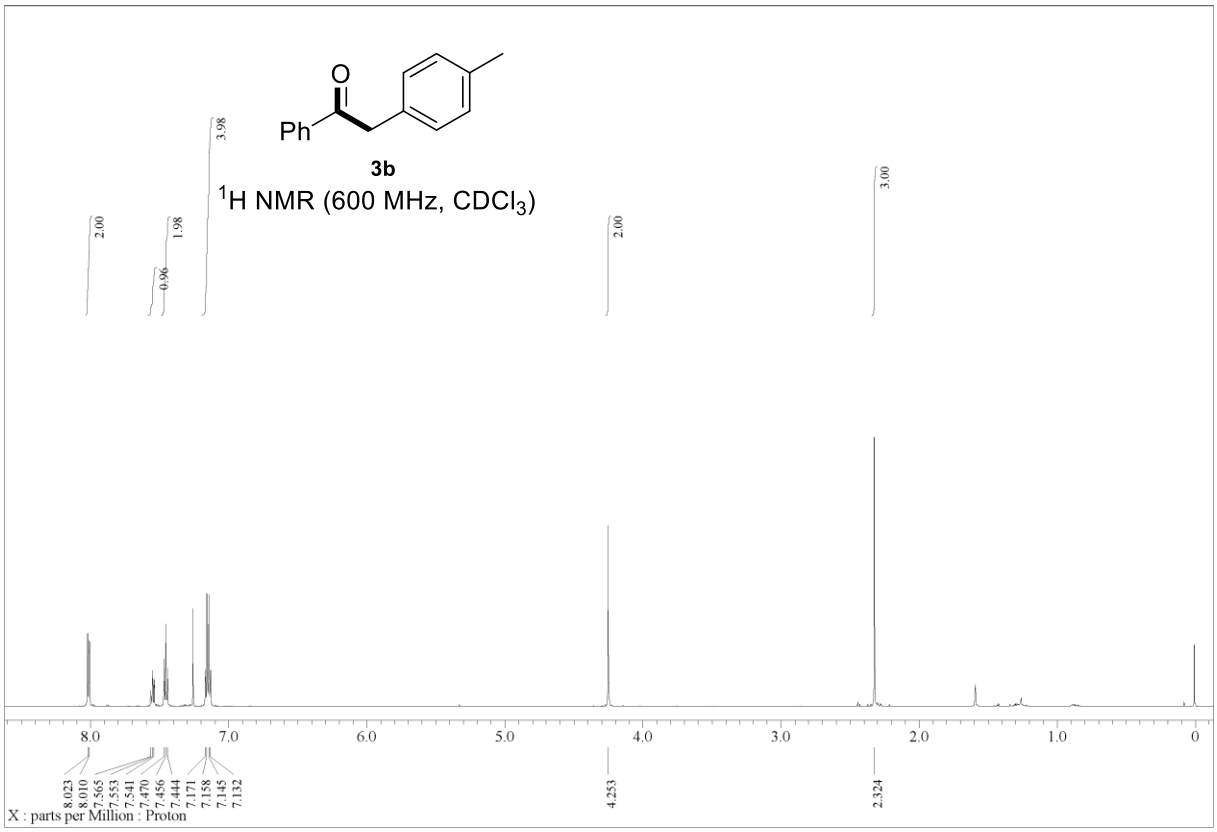
12. (a) R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Phys. Chem.*, 1980, **72**, 650-654; (b) A. D. McLean and G.S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639-5648.

13. R. Bauernschmitt and R. Ahlrichs, *J. Chem. Phys.*, 1996, **104**, 9047-9052.

7. Copies of ^{1}H, ^{13}C NMR Spectra



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Ph
3b
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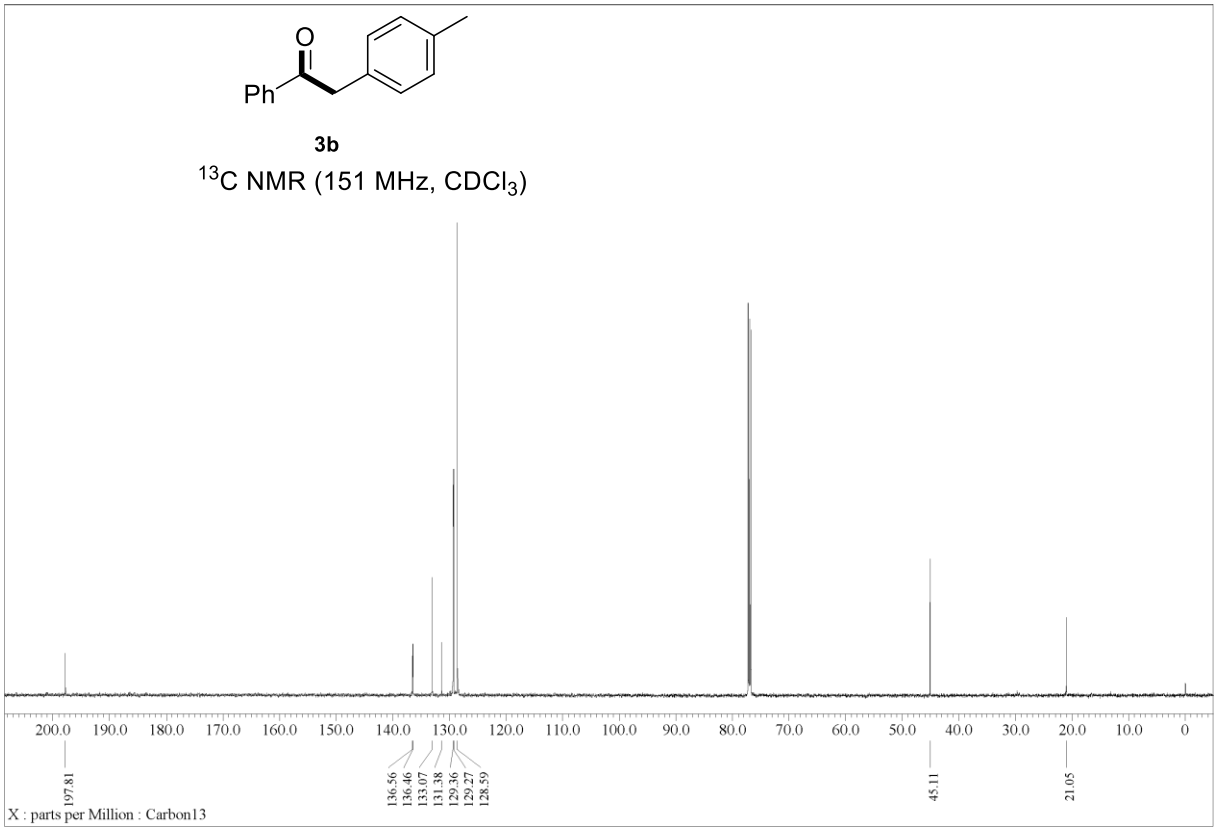
1.98
0.96
3.98
2.00
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.023
8.010
7.565
7.553
7.541
7.470
7.456
7.444
7.171
7.158
7.145
7.132
4.253
2.324
X : parts per Million : Proton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Ph
3b
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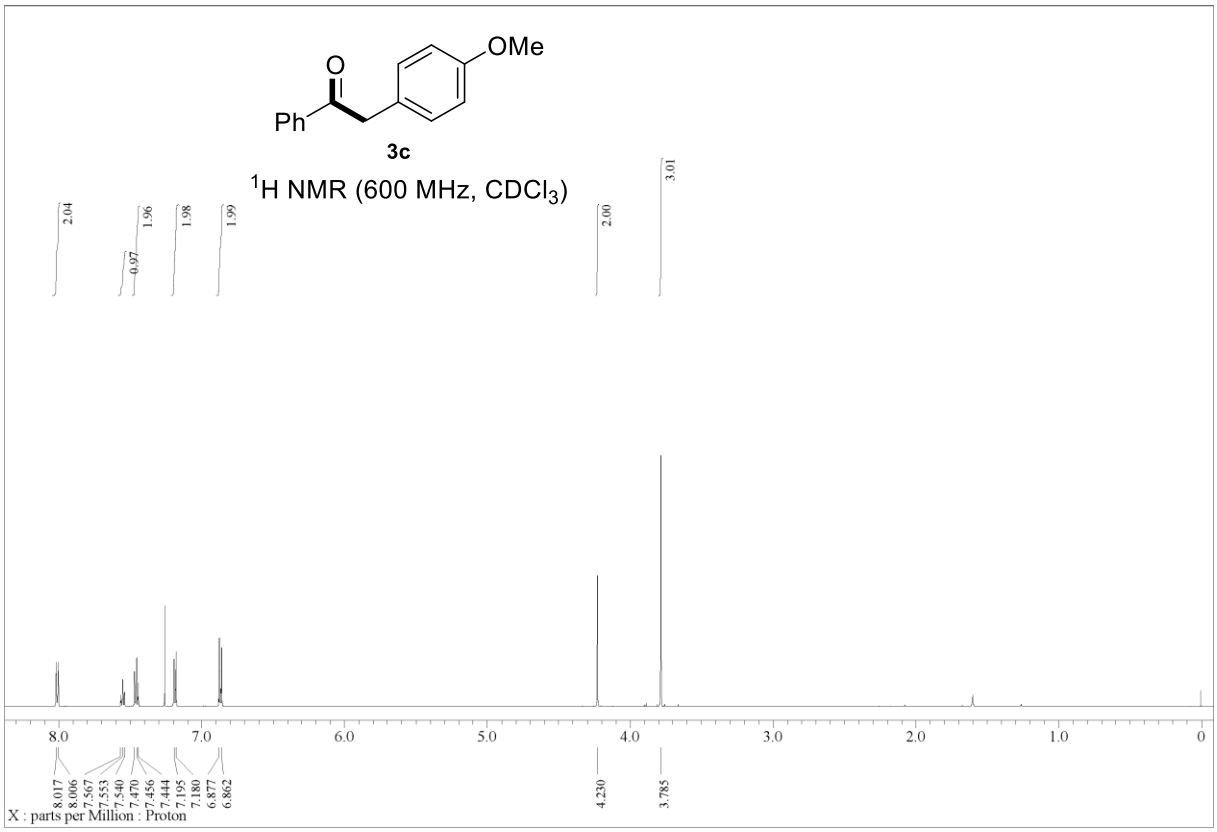
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.81
136.56
136.46
133.07
131.38
129.36
129.27
128.59
45.11
21.05
X : parts per Million : Carbon13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O
Ph
3c
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1.98
1.99
2.00
3.01
8.017
8.006
7.567
7.553
7.540
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7.444
7.195
7.180
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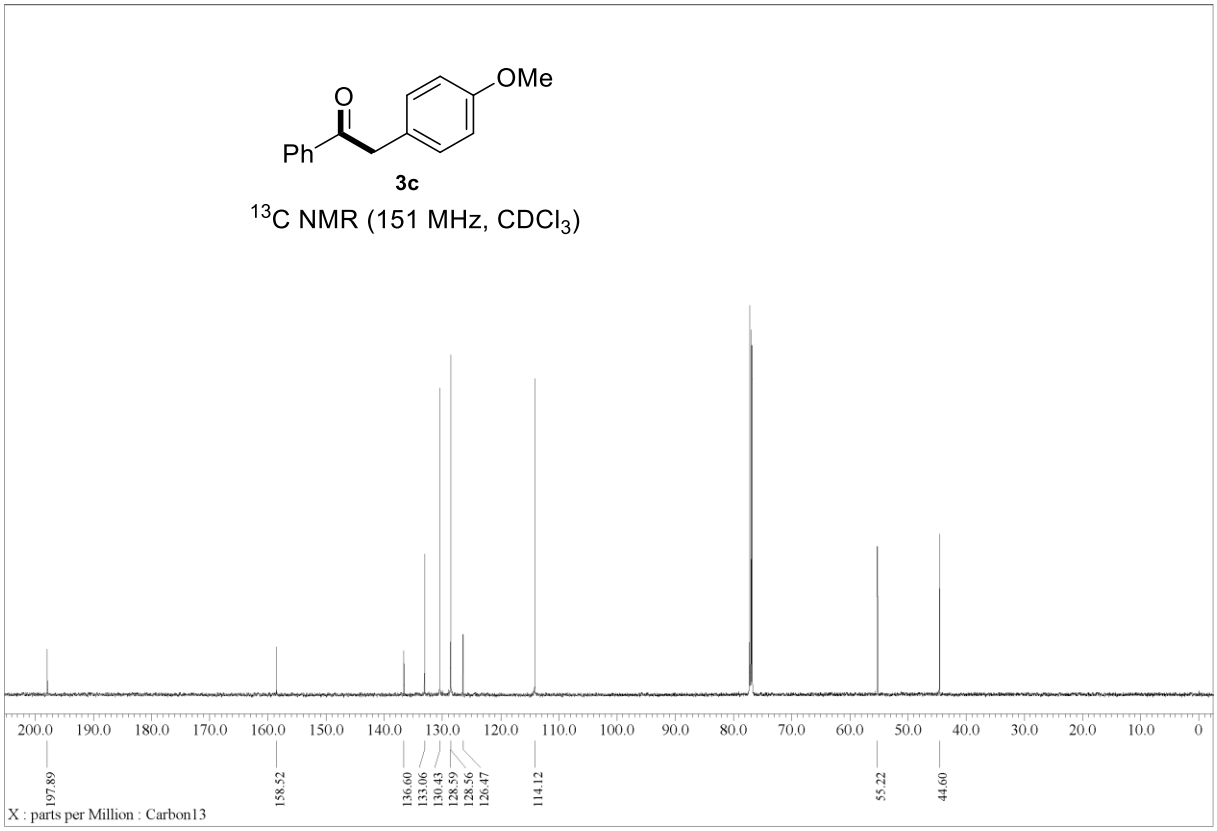
4.220
3.785
X : parts per Million : Proton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O
Ph
3c
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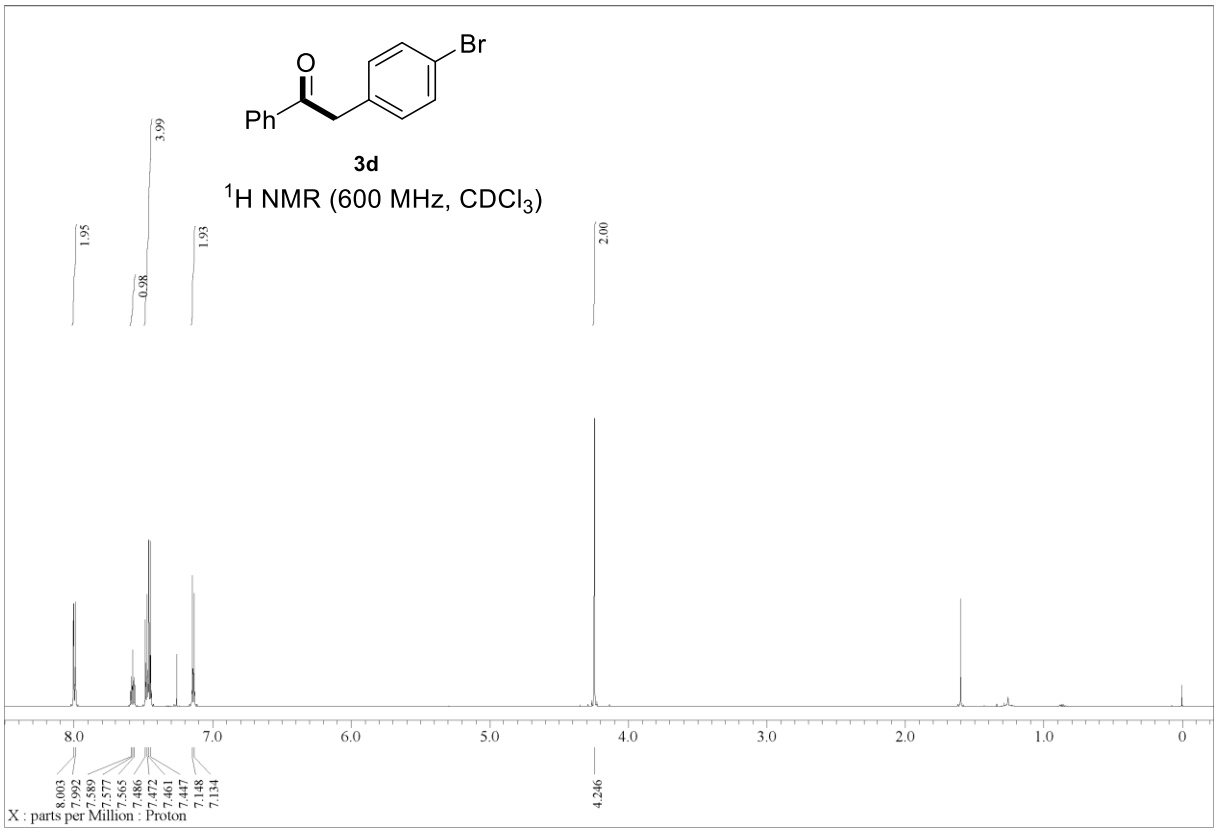
114.12
55.22
44.60
X : parts per Million : Carbon13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O
Ph
3d
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0.98
1.93
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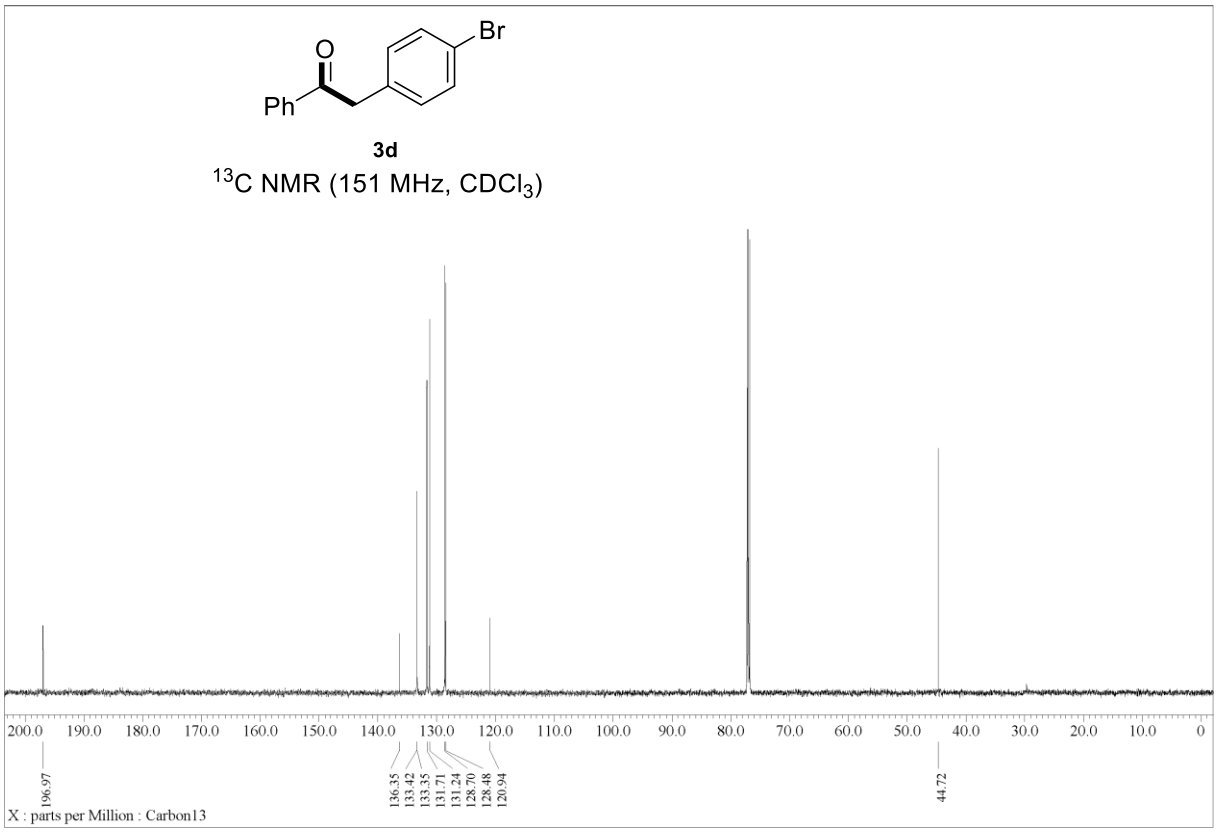
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.003
7.992
7.589
7.577
7.565
7.486
7.472
7.461
7.447
7.148
7.134
4.246
X : parts per Million : Proton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O
Ph
3d
13C NMR (151 MHz, CDCl3)
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190.0
180.0
170.0
160.0
150.0
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130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.97
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133.42
133.35
131.71
131.24
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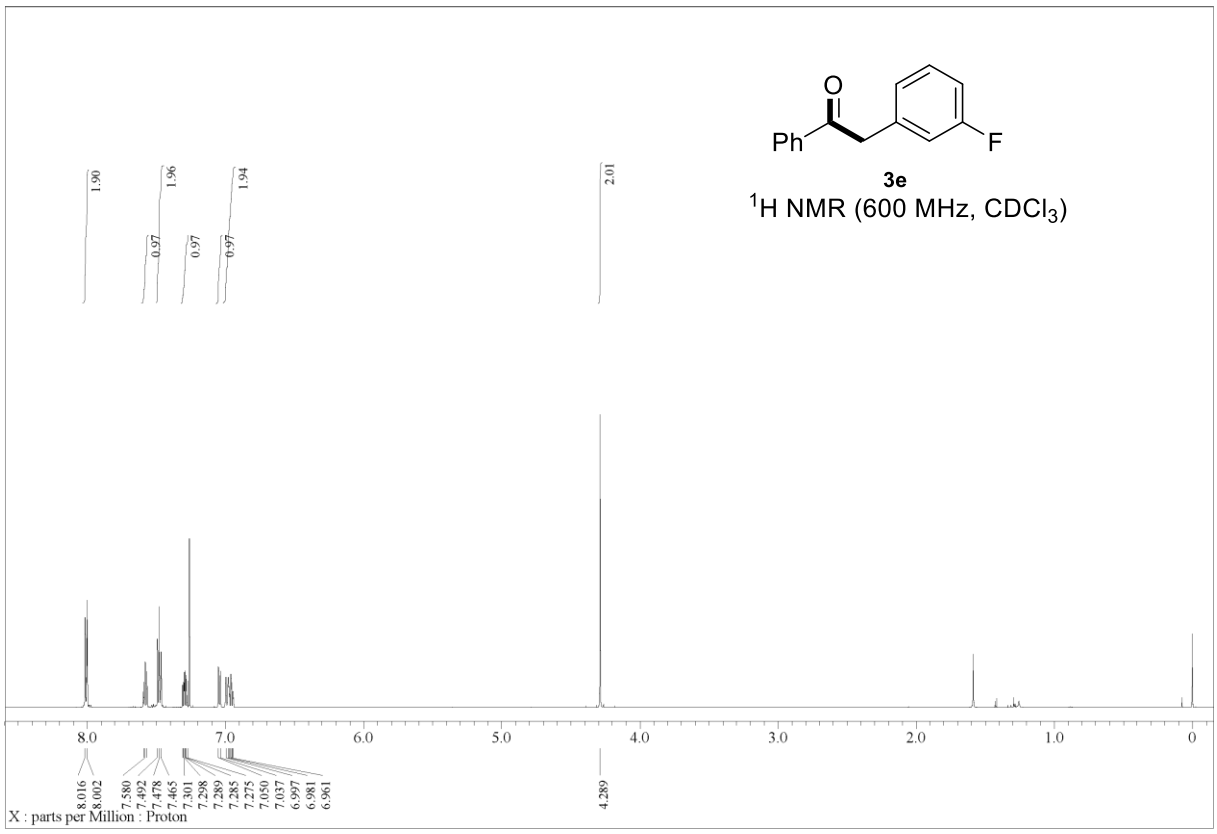
128.48
120.94
44.72
X : parts per Million : Carbon13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Ph
F
3e
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1.96
1.94
0.97
0.97
0.97
2.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.016
8.002
7.580
7.492
7.478
7.465
7.301
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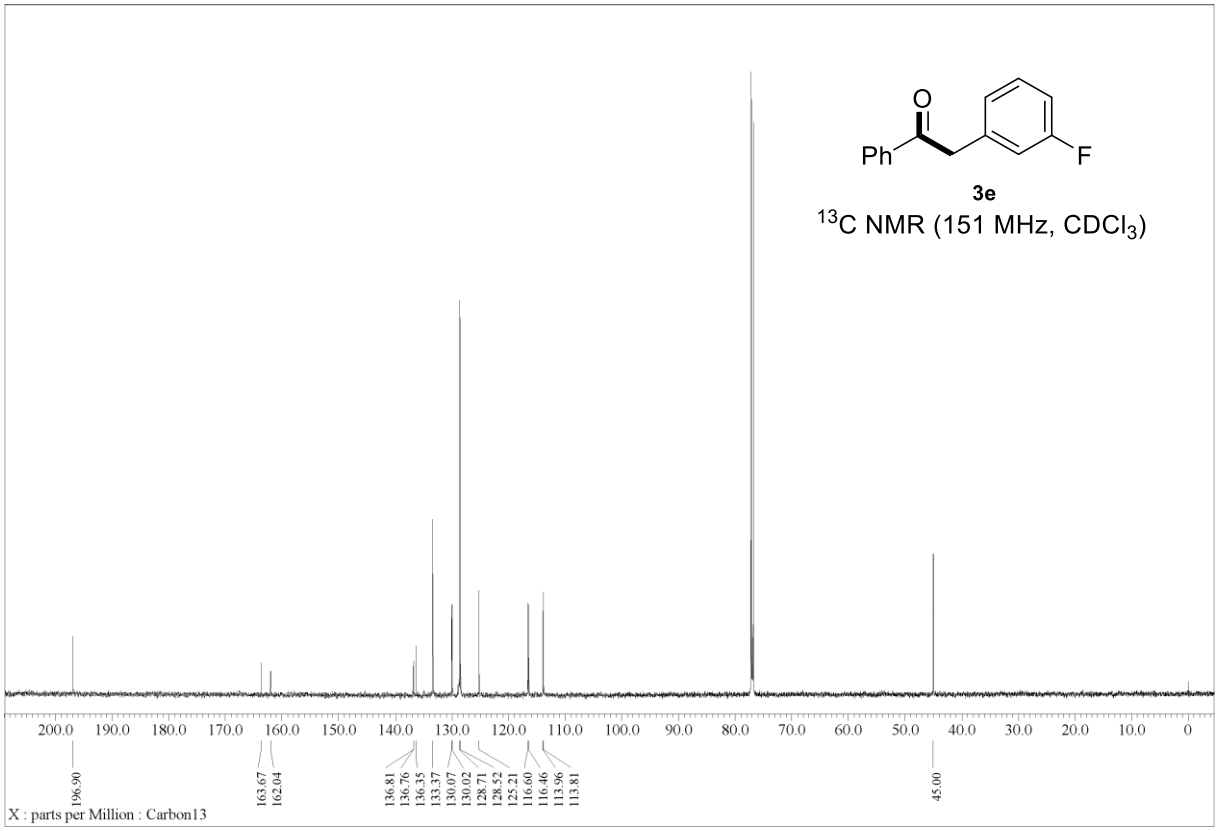
X : parts per Million : Proton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Ph
F
3e
13C NMR (151 MHz, CDCl3)
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120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.90
163.67
162.04
136.81
136.76
136.35
133.37
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130.02
128.71
128.52
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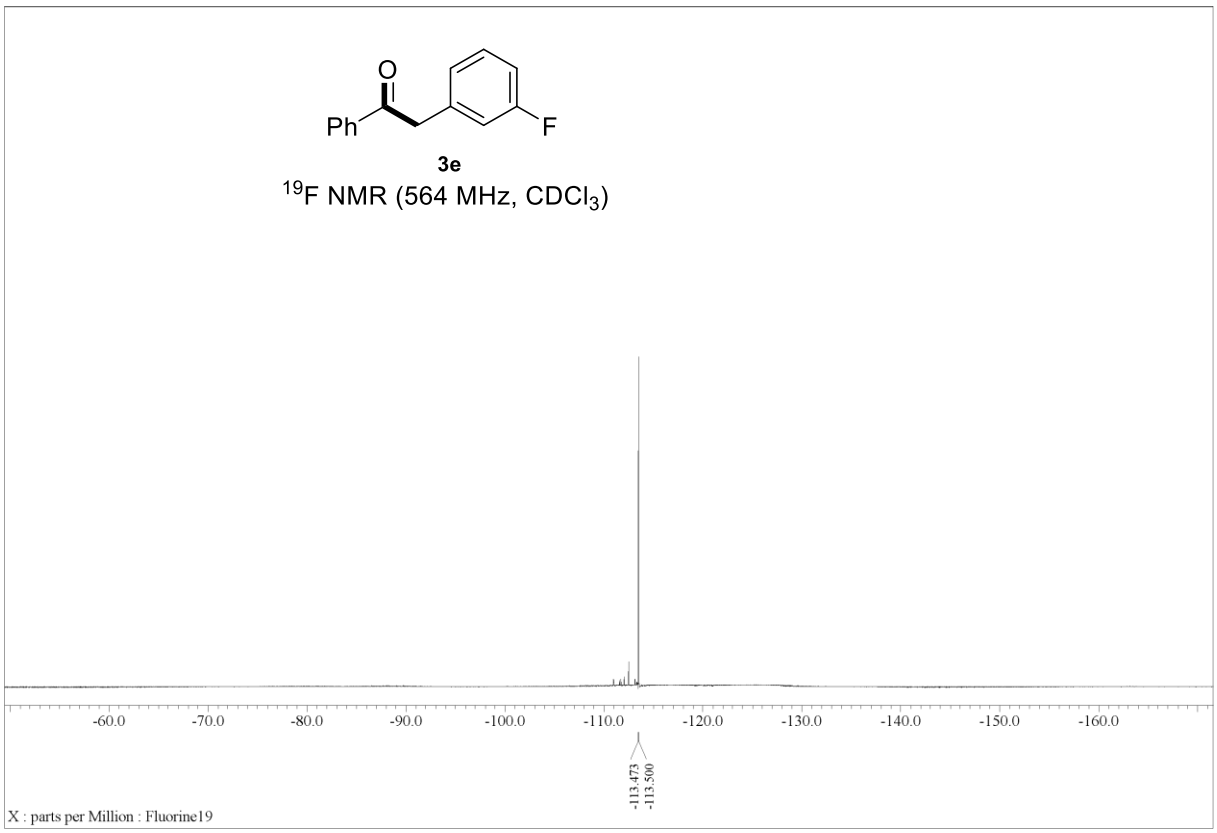
116.60
116.46
113.96
113.81
45.00
X : parts per Million : Carbon13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Ph
F
3e
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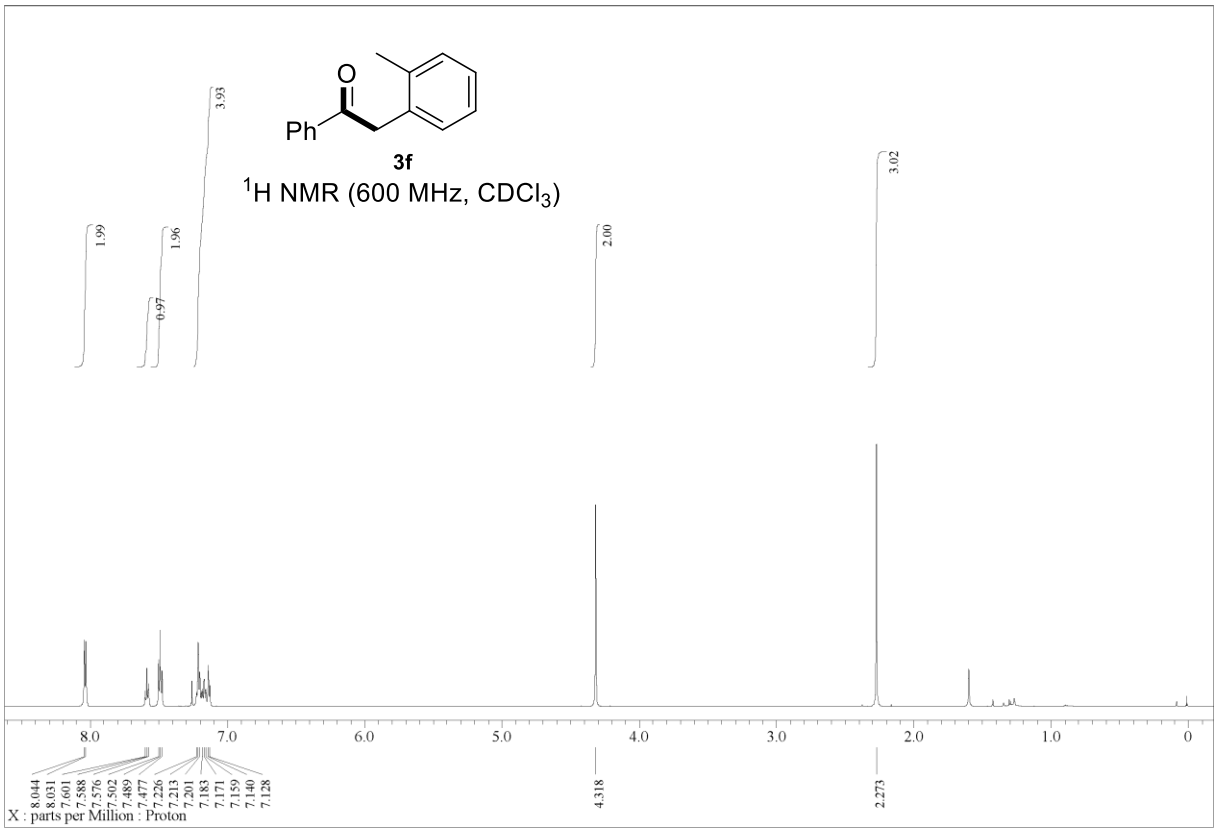
-113.473
-113.500
X : parts per Million : Fluorine19



3f

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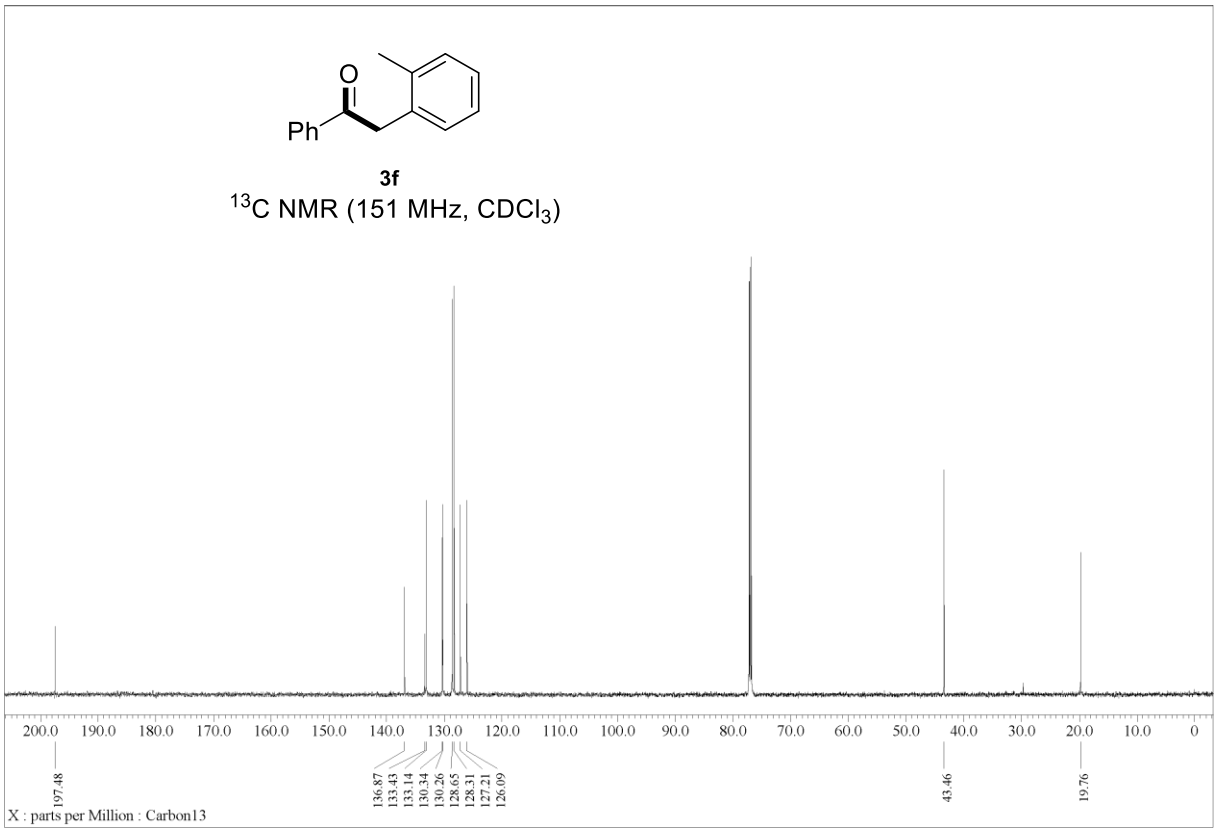

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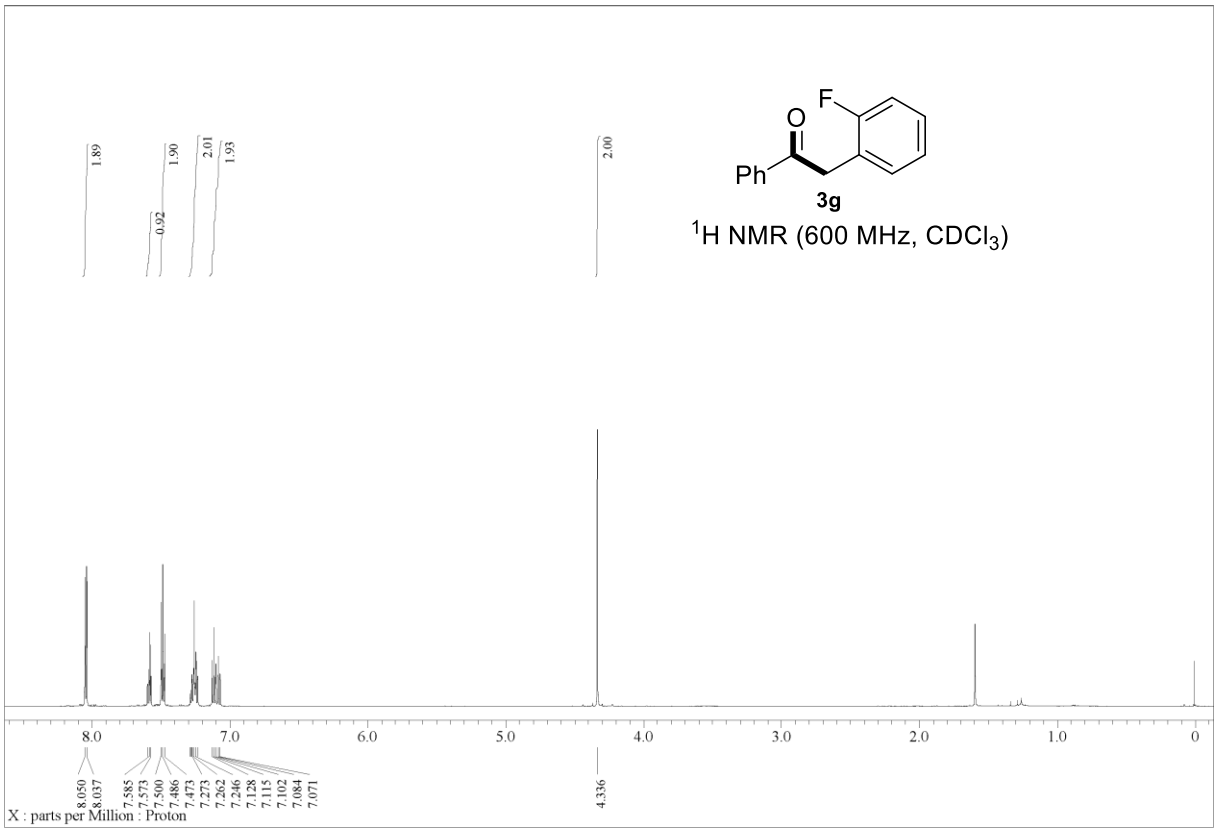
^{13}C NMR (151 MHz, $CDCl_3$)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O
Ph
3g
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1.90
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2.00
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8.037
7.585
7.573
7.500
7.486
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7.262
7.246
7.128
7.115
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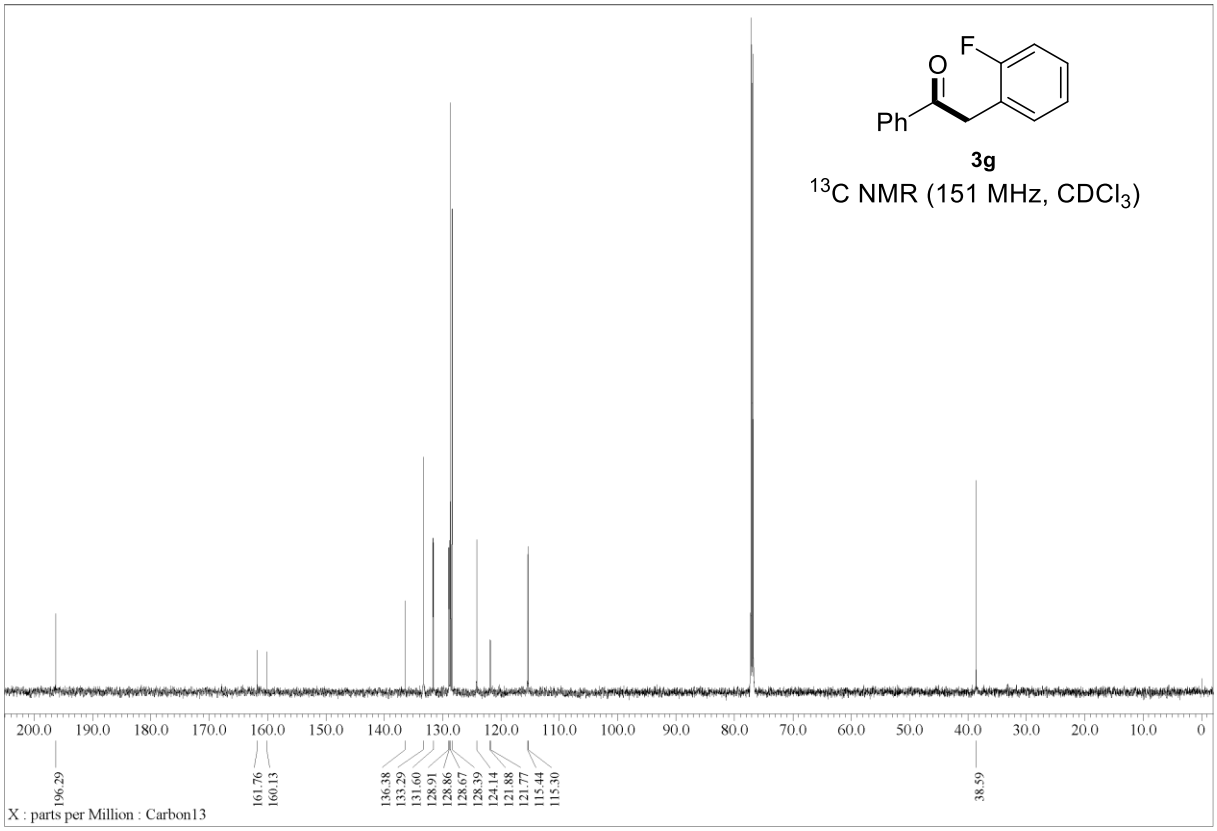
7.084
7.071
4.336
X : parts per Million : Proton


F
O
Ph
3g
13C NMR (151 MHz, CDCl3)
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136.38
133.29
131.60
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128.39
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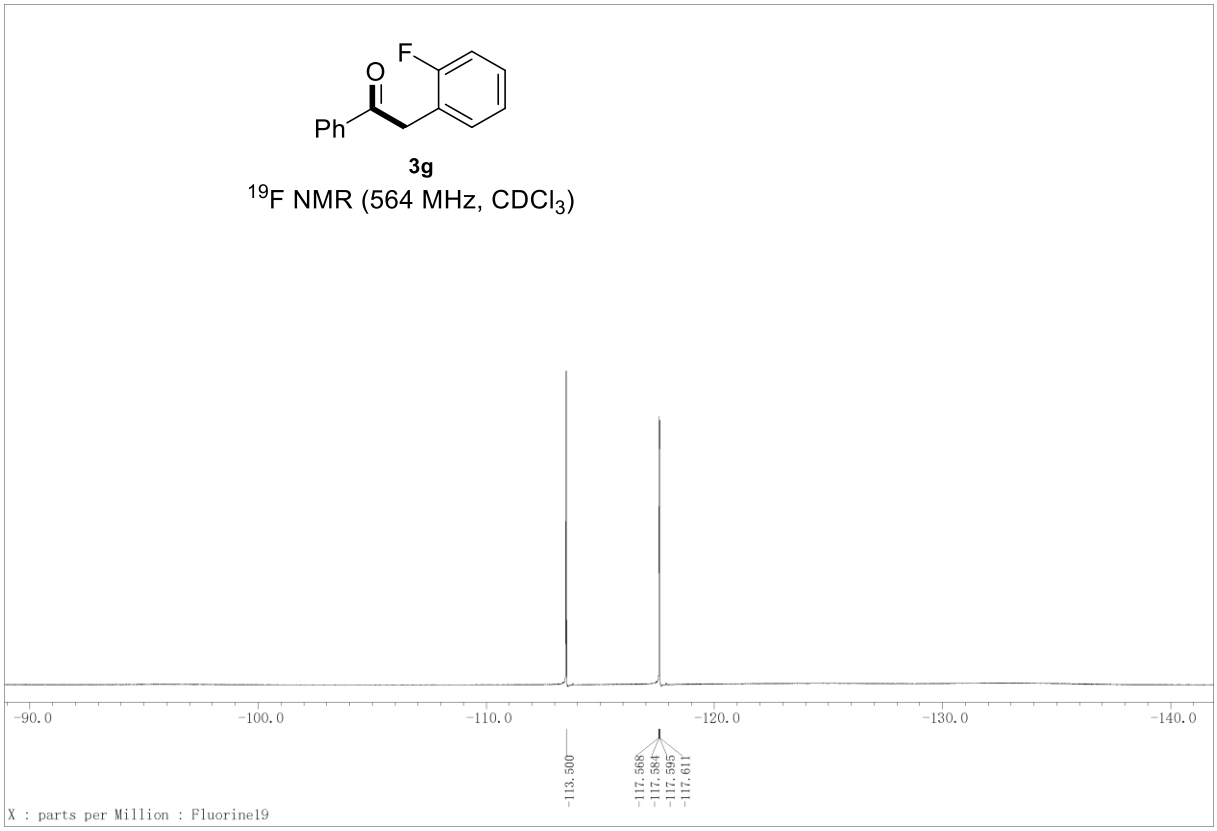
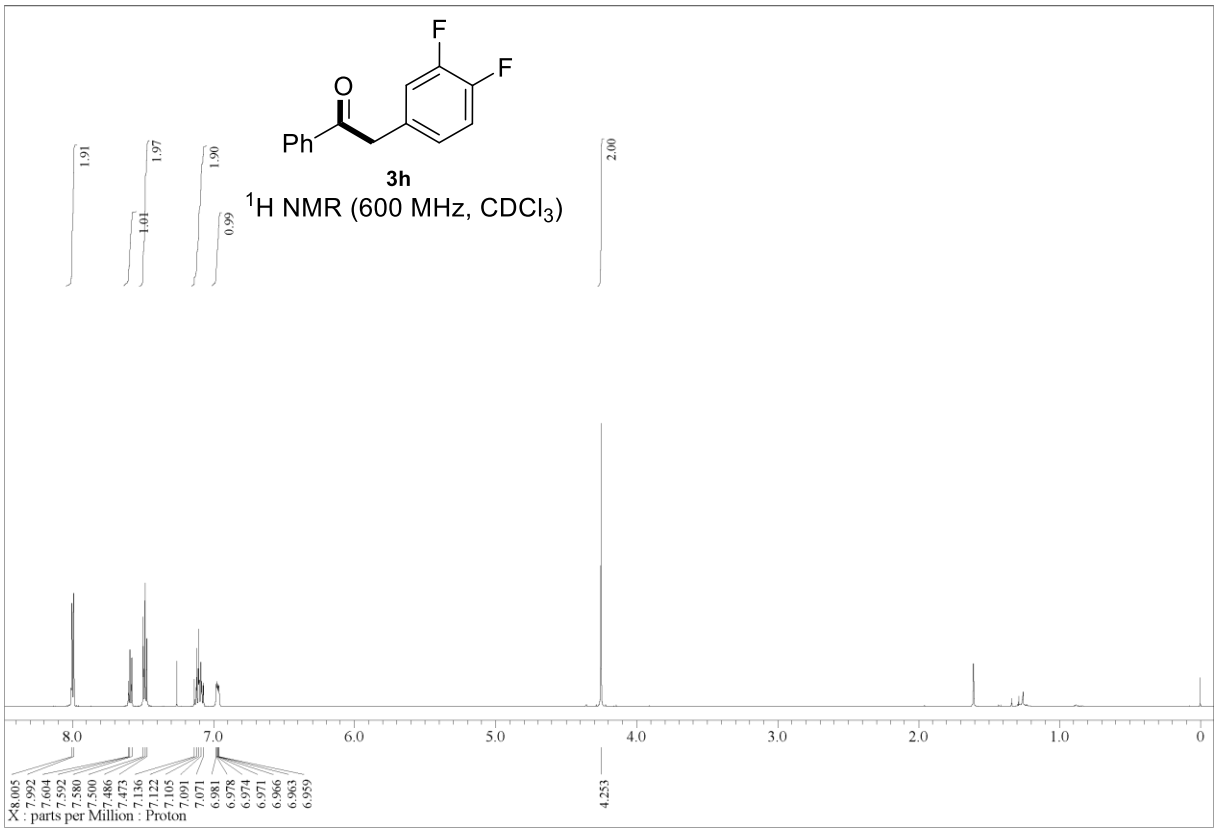
115.30
38.59
X : parts per Million : Carbon13



3g

^{19}F NMR (564 MHz, $CDCl_3$)


F
F
O
Ph
3h
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1.90
0.99
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.005
7.992
7.604
7.592
7.580
7.500
7.486
7.473
7.136
7.122
7.105
7.091
7.071
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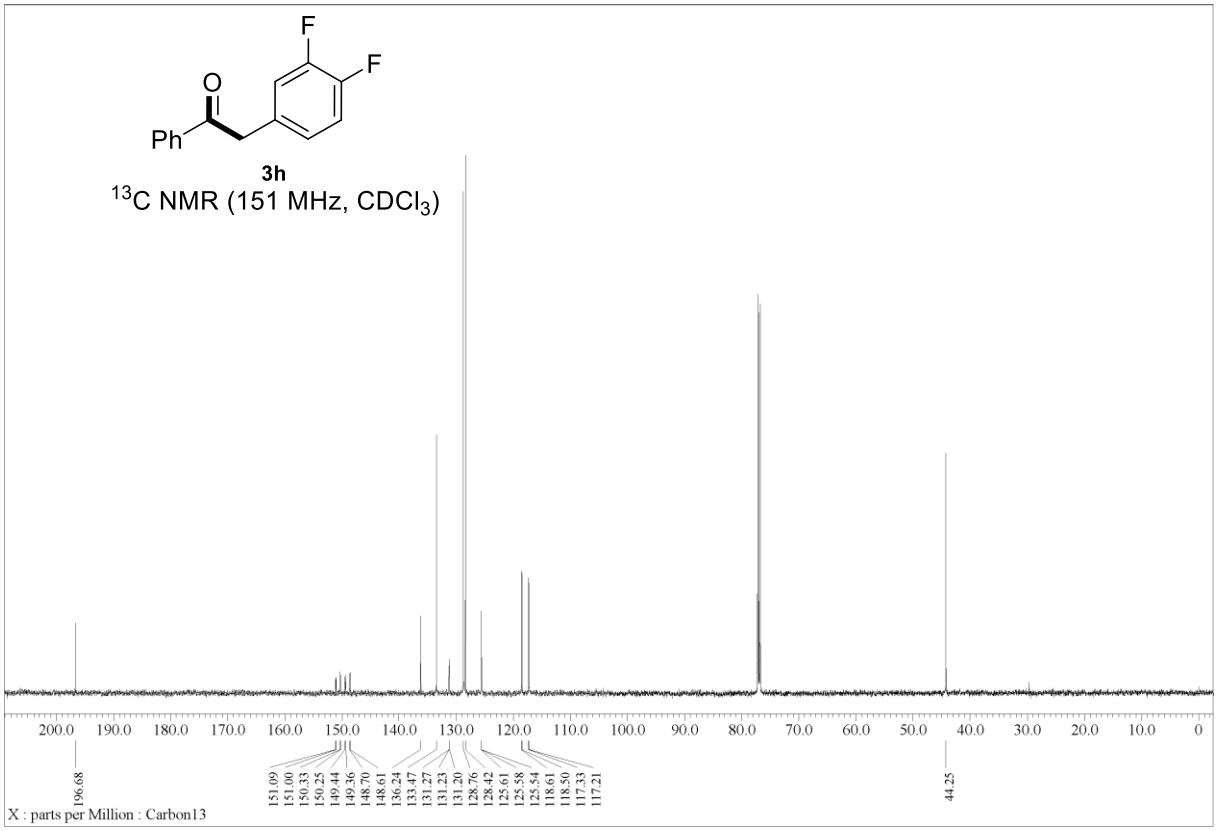
6.978
6.974
6.971
6.966
6.963
6.959
4.253
X : parts per Million : Proton


F
F
O
Ph
3h
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180.0
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160.0
150.0
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130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.68
151.09
151.00
150.33
150.25
149.44
149.36
148.70
148.61
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131.27
131.23
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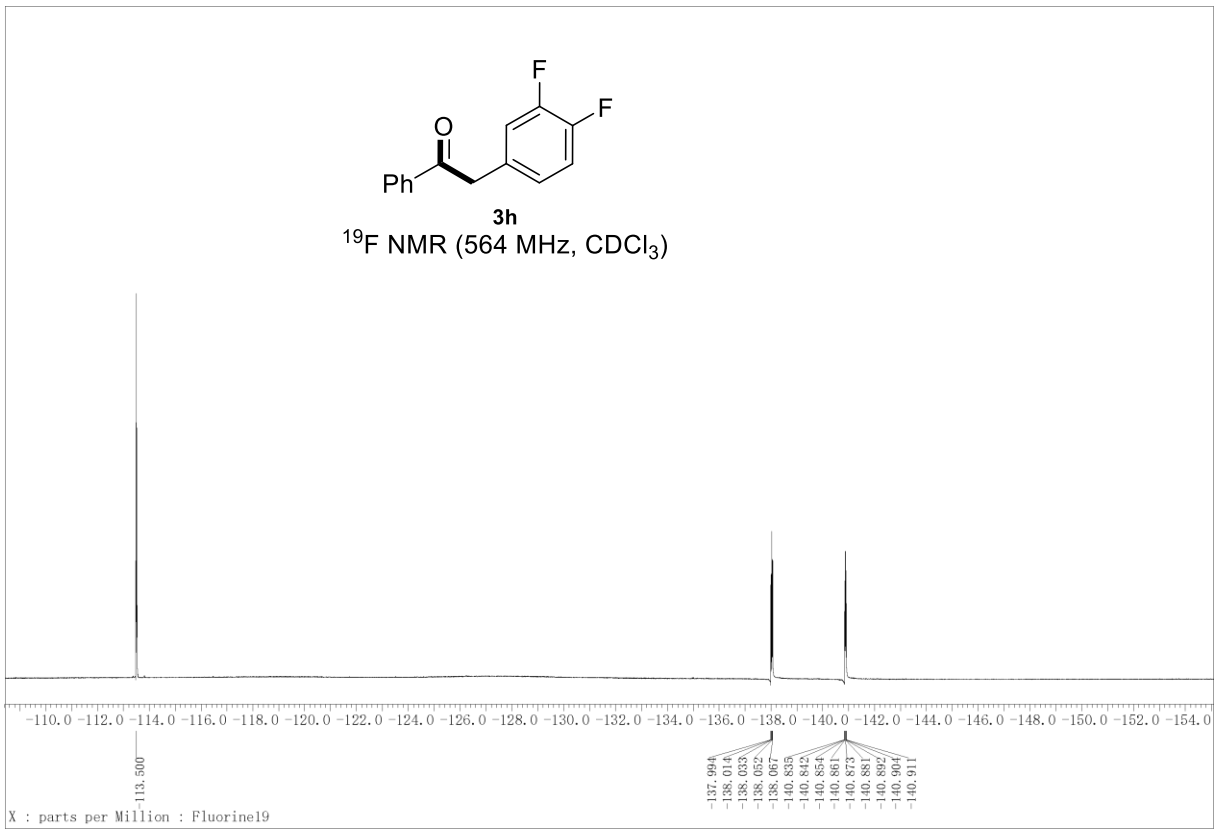
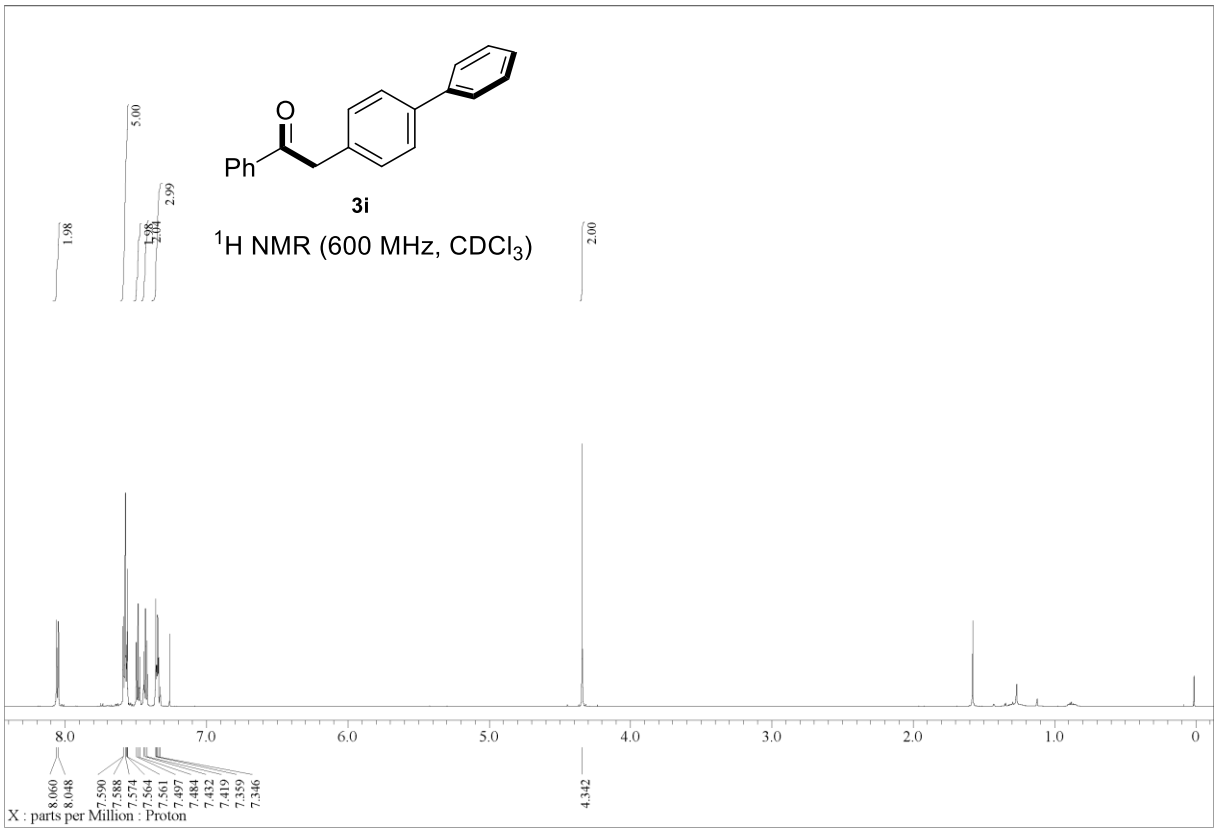


3h

^{19}F NMR (564 MHz, $CDCl_3$)


O
Ph
3i
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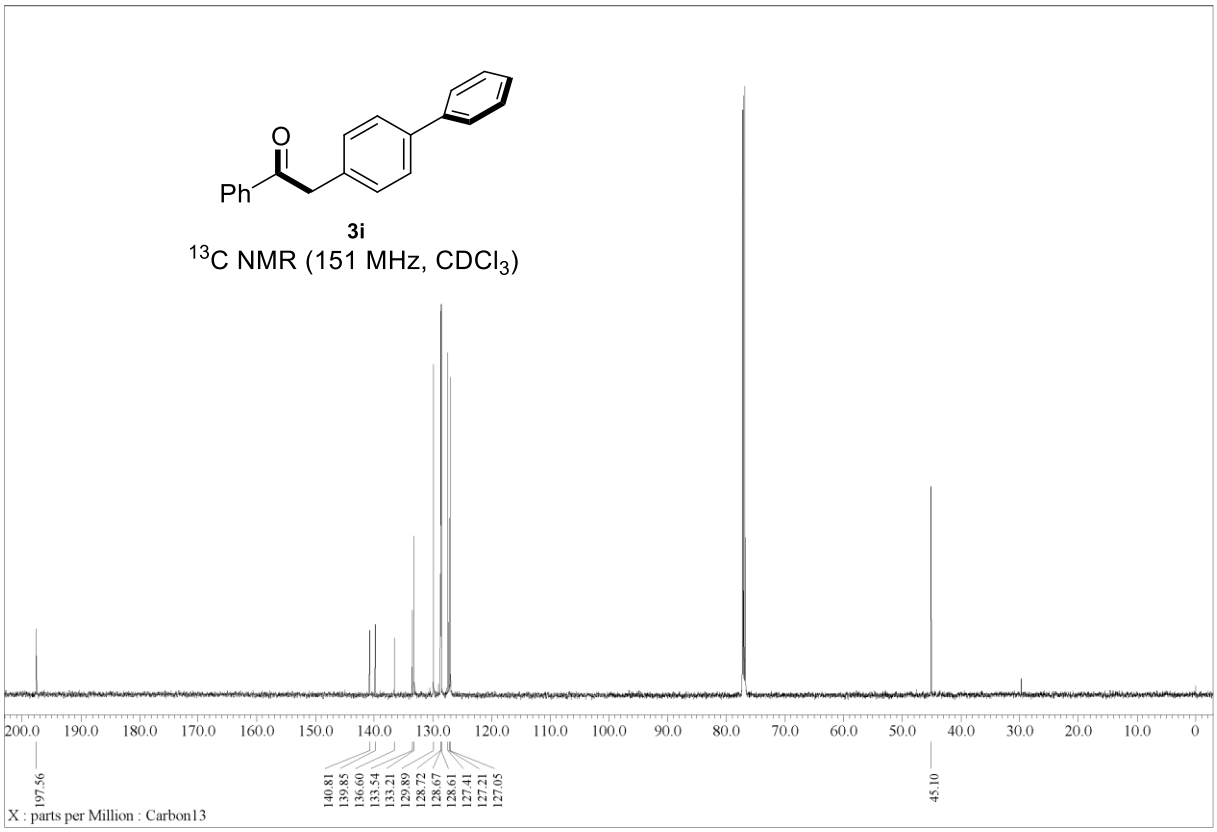
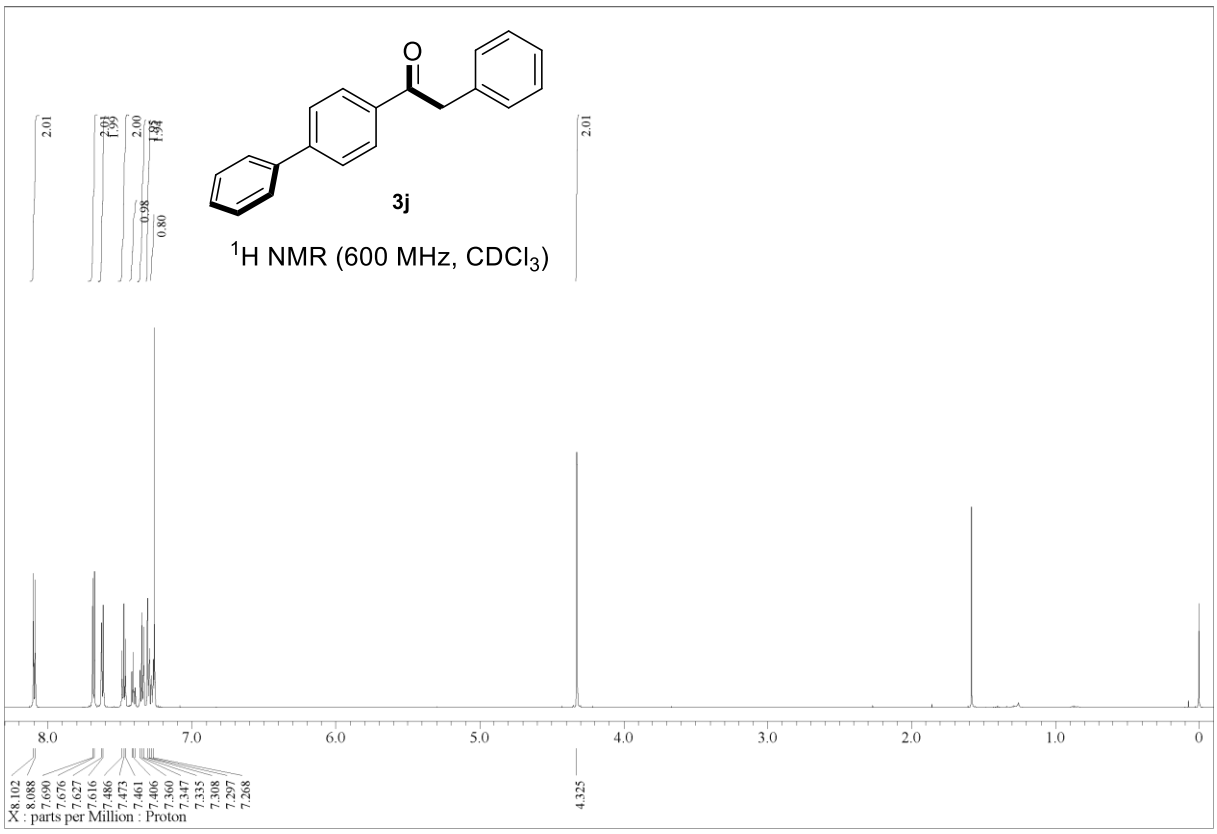
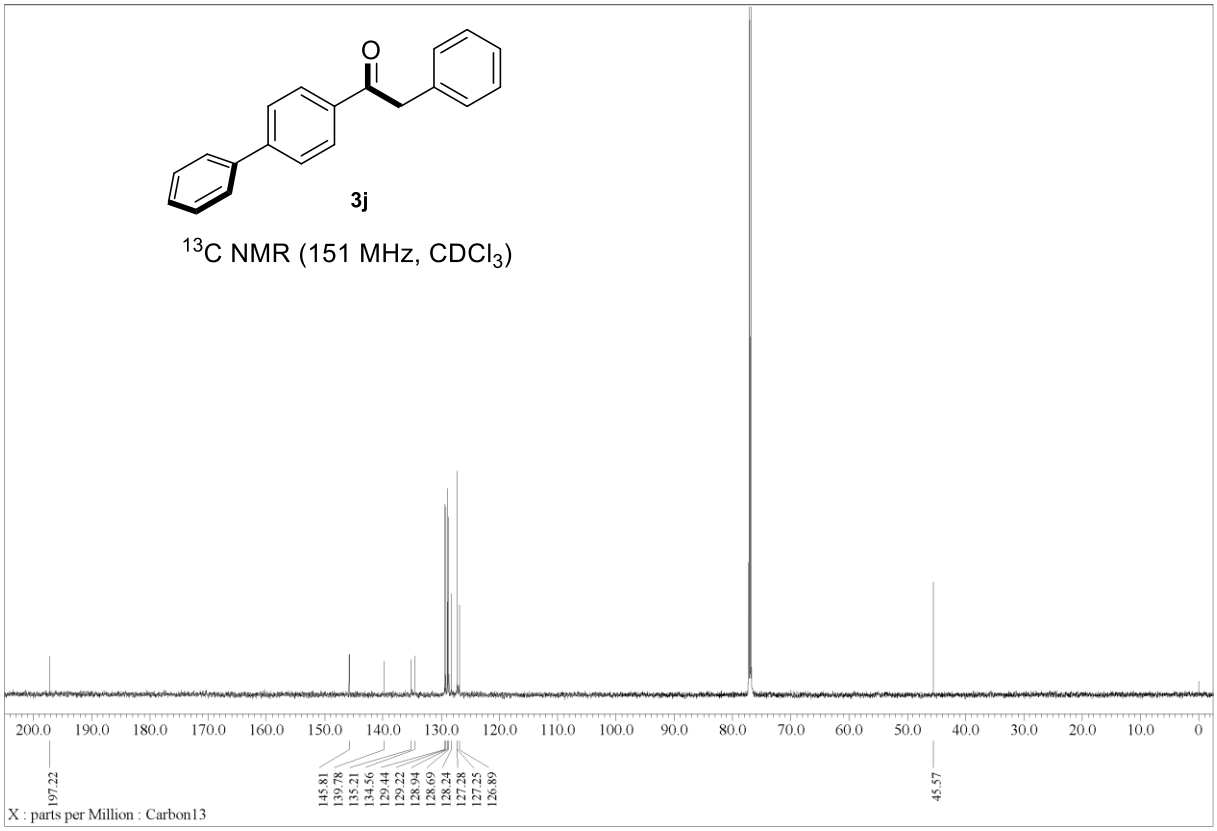
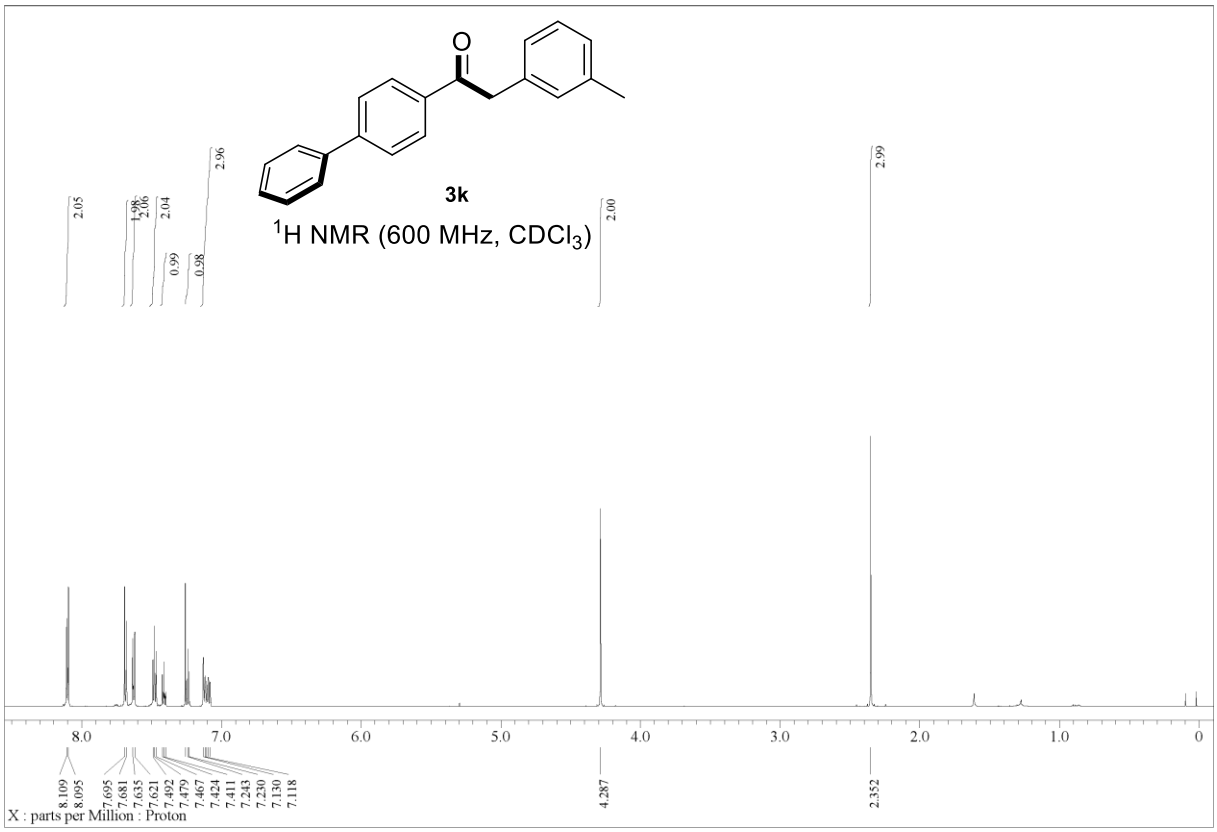
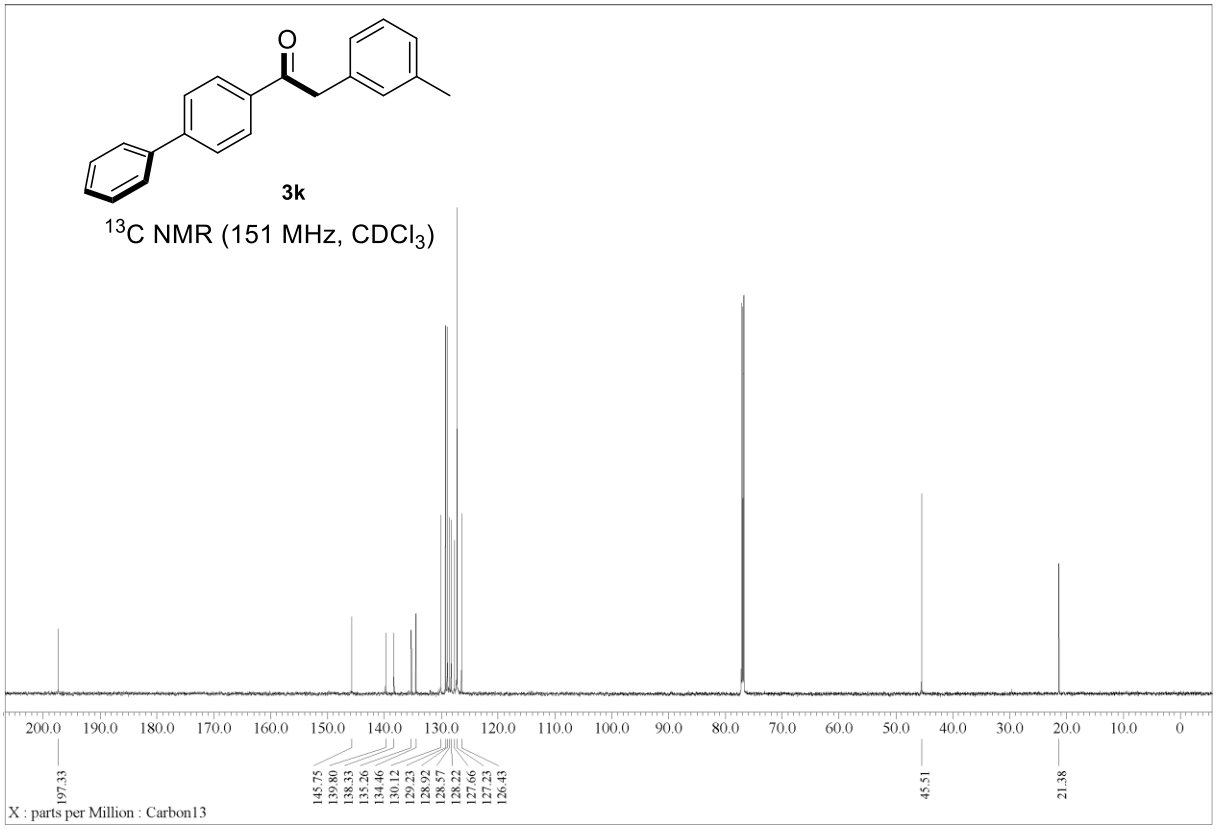
5.00
2.99
1.98
1.98
2.04
2.00
8.060
8.048
7.590
7.588
7.574
7.564
7.561
7.497
7.484
7.432
7.419
7.359
7.346
4.342
X : parts per Million : Proton

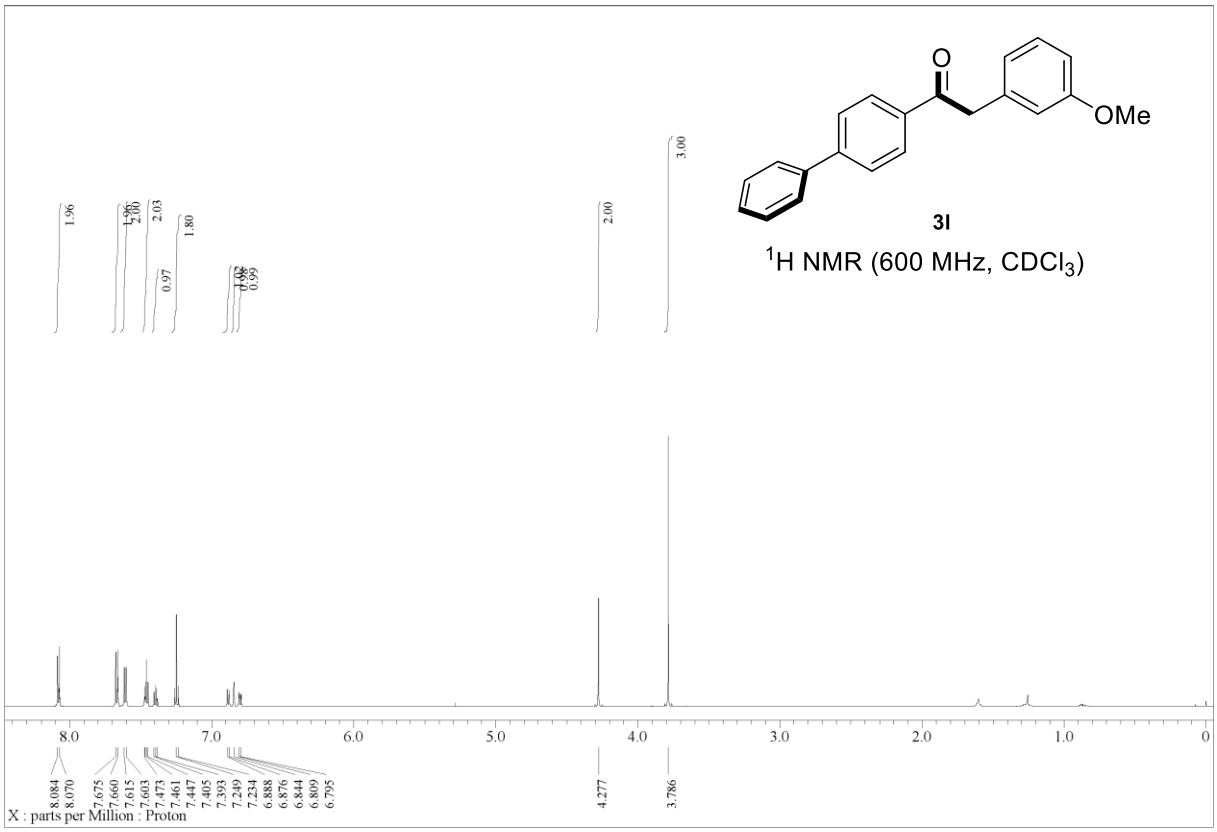

O
Ph
3i
13C NMR (151 MHz, CDCl3)
197.56
140.81
139.85
136.60
133.54
133.21
129.89
128.72
128.67
128.61
127.41
127.21
127.05
45.10
X : parts per Million : Carbon13

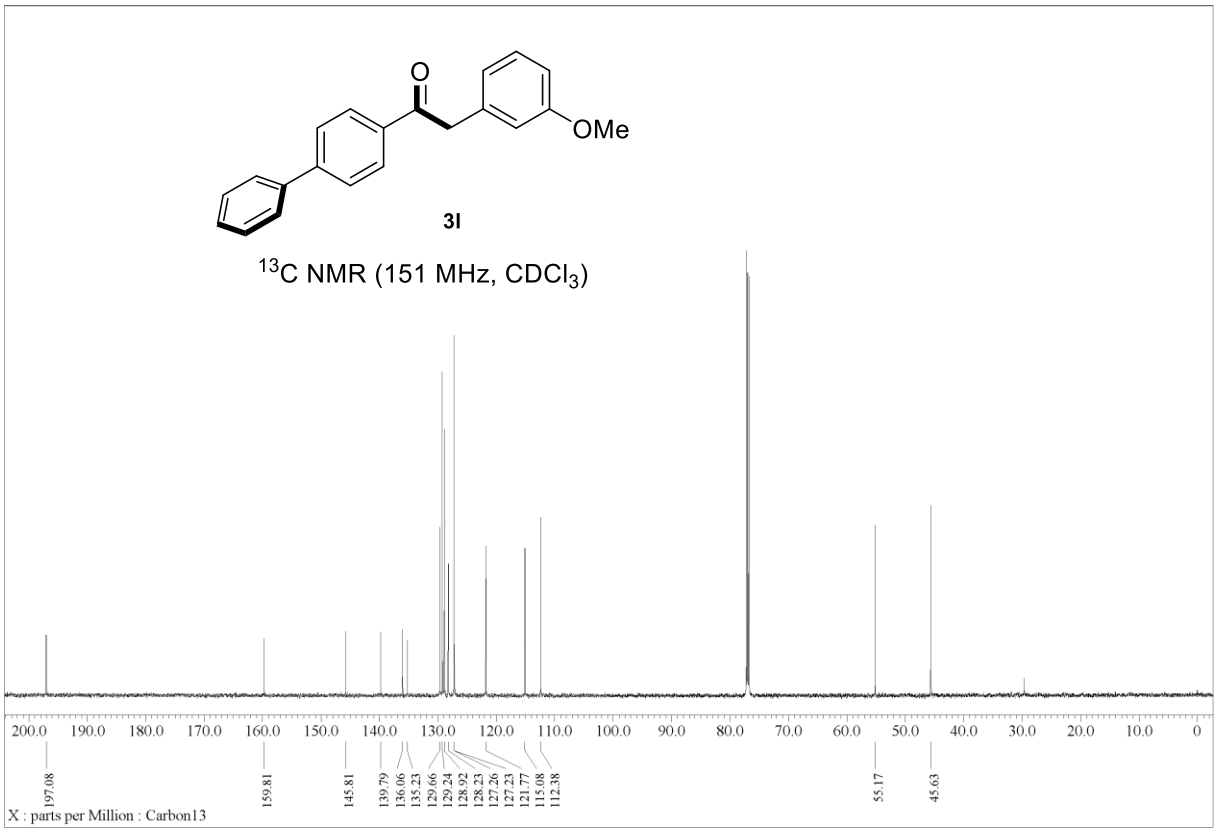

O
3j
^{1}H NMR (600 MHz, $CDCl_3$)
2.01
2.01
1.99
2.00
1.93
1.92
0.98
0.80
2.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.102
8.088
7.690
7.676
7.627
7.616
7.486
7.473
7.461
7.406
7.360
7.347
7.335
7.308
7.297
7.268
4.325
X : parts per Million : Proton

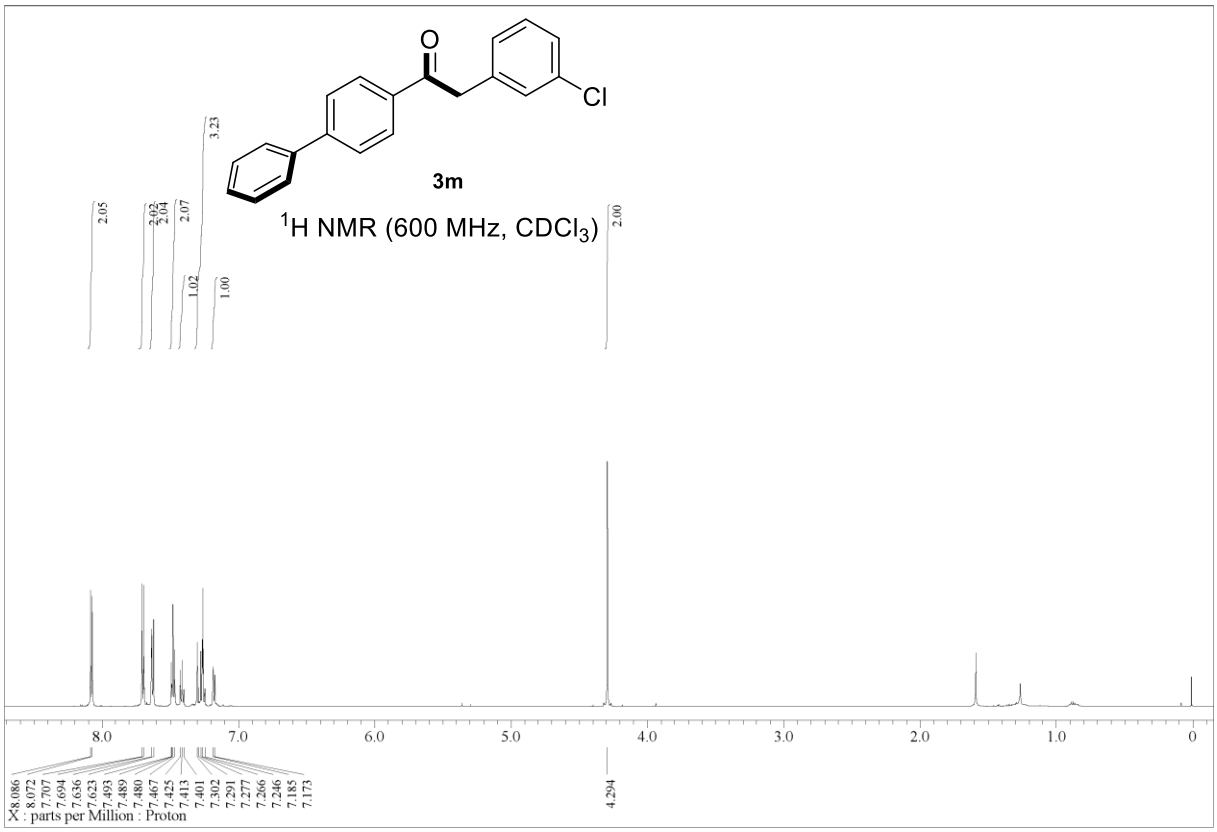

O
3j
^{13}C NMR (151 MHz, $CDCl_3$)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.22
145.81
139.78
135.21
134.56
129.44
129.22
128.94
128.69
128.24
127.28
127.25
126.89
45.57
X : parts per Million : Carbon13

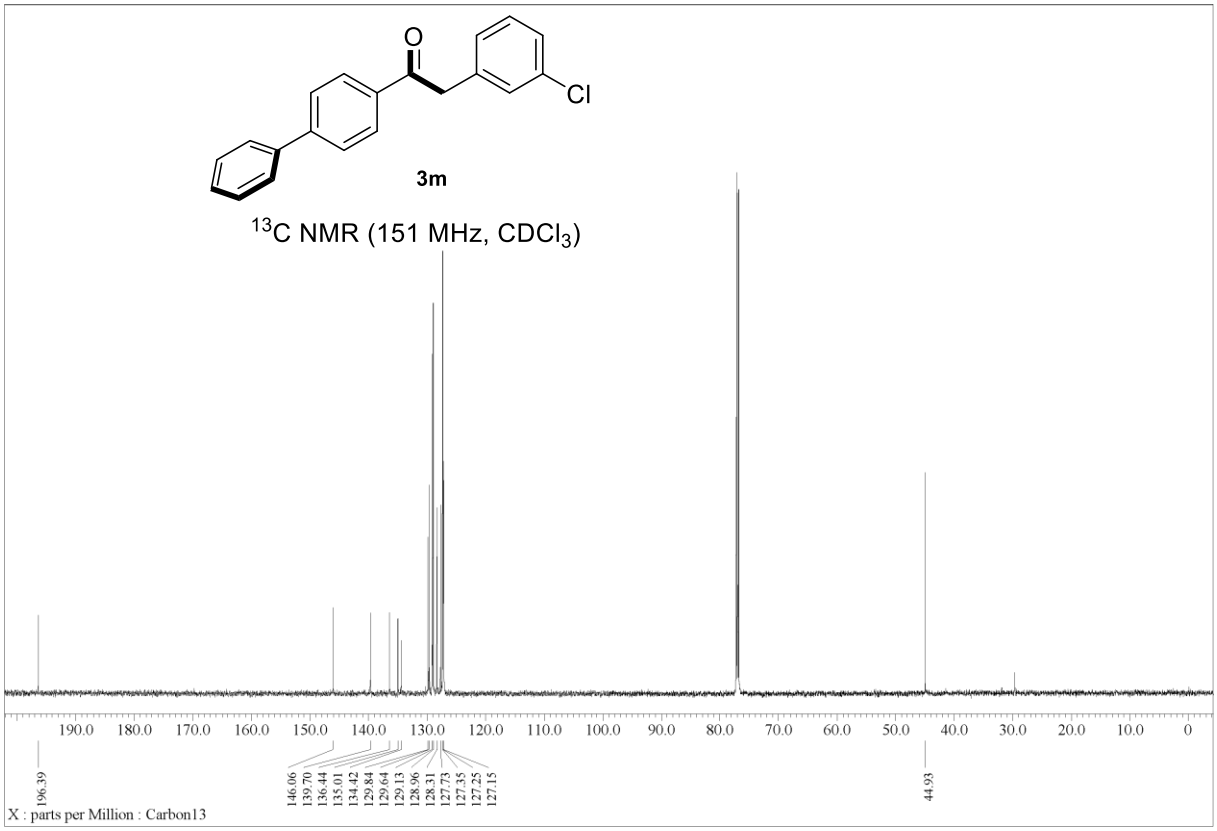

3k
^{1}H NMR (600 MHz, $CDCl_3$)
2.05
1.98
2.06
2.04
2.96
0.99
0.98
2.00
2.99
8.109
8.095
7.695
7.681
7.635
7.621
7.492
7.479
7.467
7.424
7.411
7.243
7.230
7.130
7.118
4.287
2.352
X : parts per Million : Proton

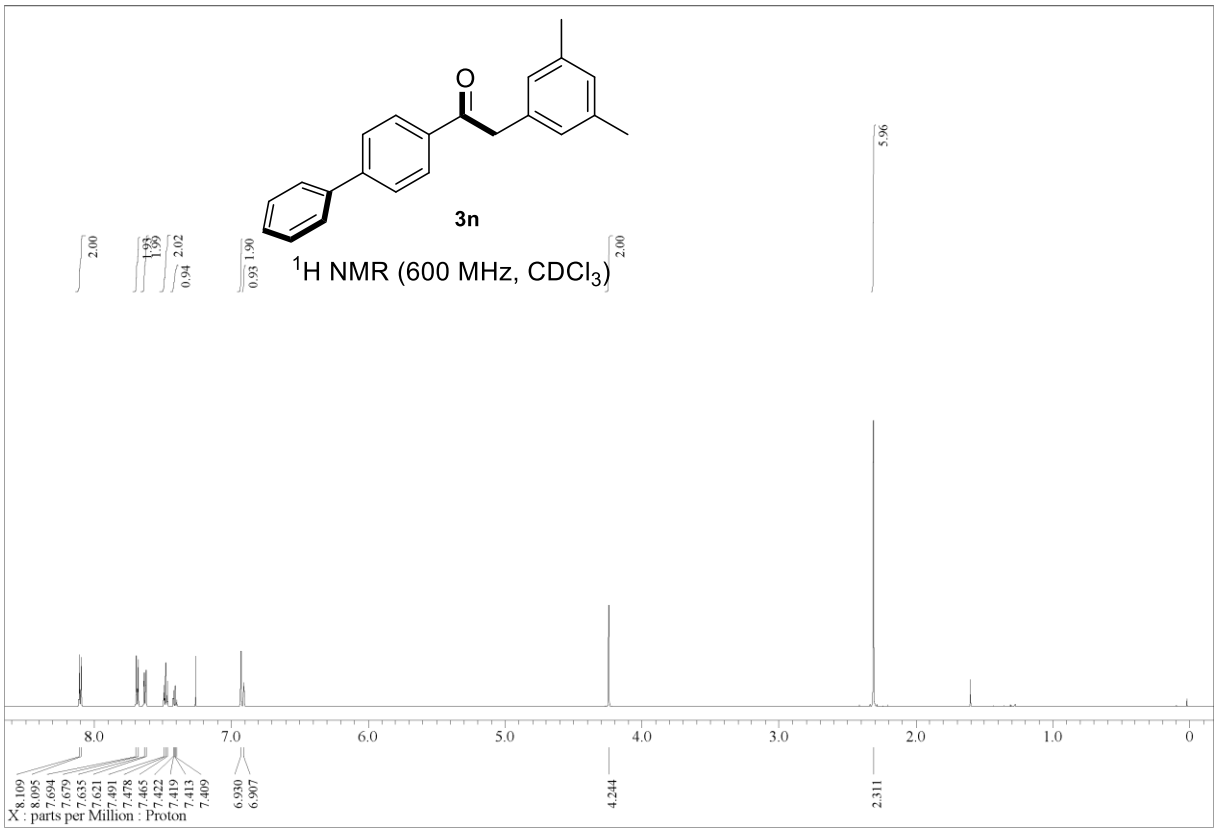

3k
^{13}C NMR (151 MHz, $CDCl_3$)
197.33
145.75
139.80
138.33
135.26
134.46
130.12
129.23
128.92
128.57
128.22
127.66
127.23
126.43
45.51
21.38
X : parts per Million : Carbon13

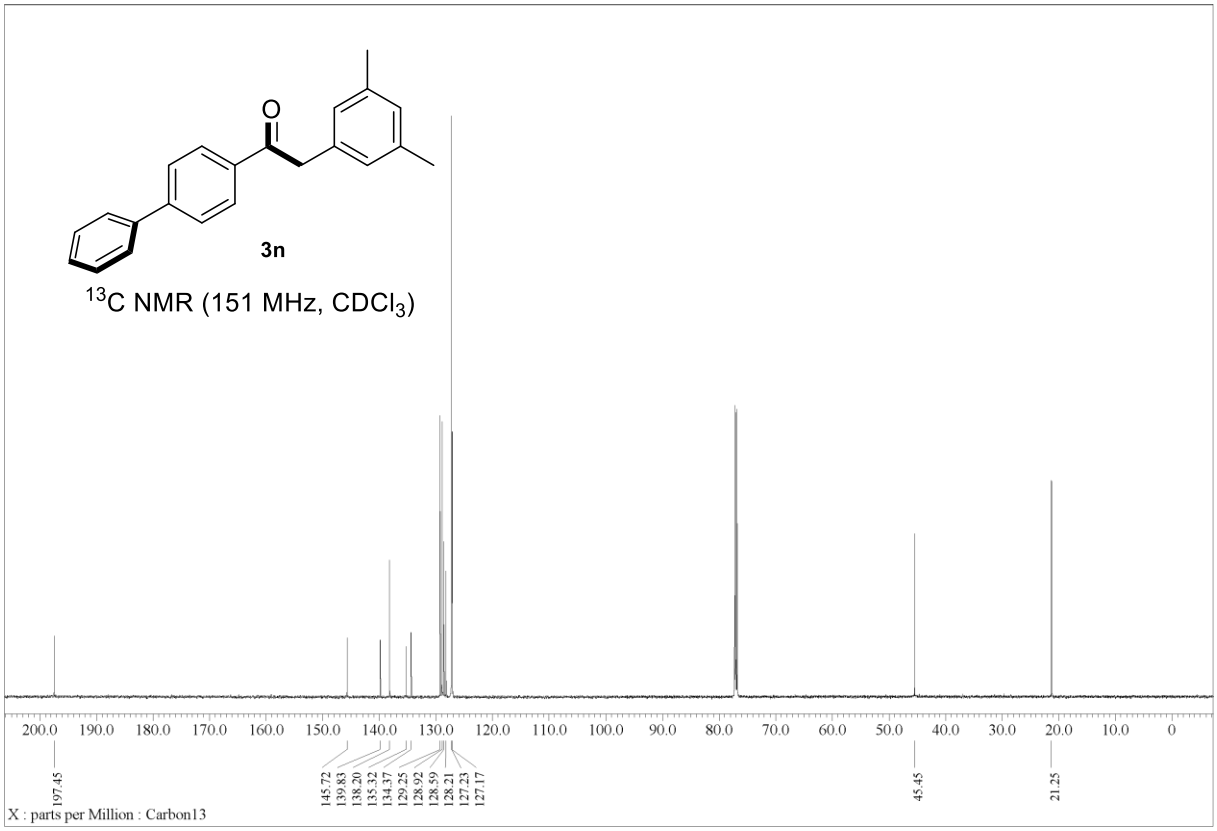

O
OMe
3I
1H NMR (600 MHz, CDCl3)
1.96
1.96
2.00
2.03
1.80
0.97
0.98
0.98
0.99
2.00
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.084
8.070
7.675
7.660
7.615
7.603
7.473
7.461
7.447
7.405
7.393
7.249
7.234
6.888
6.876
6.844
6.809
6.795
4.277
3.786
X : parts per Million : Proton

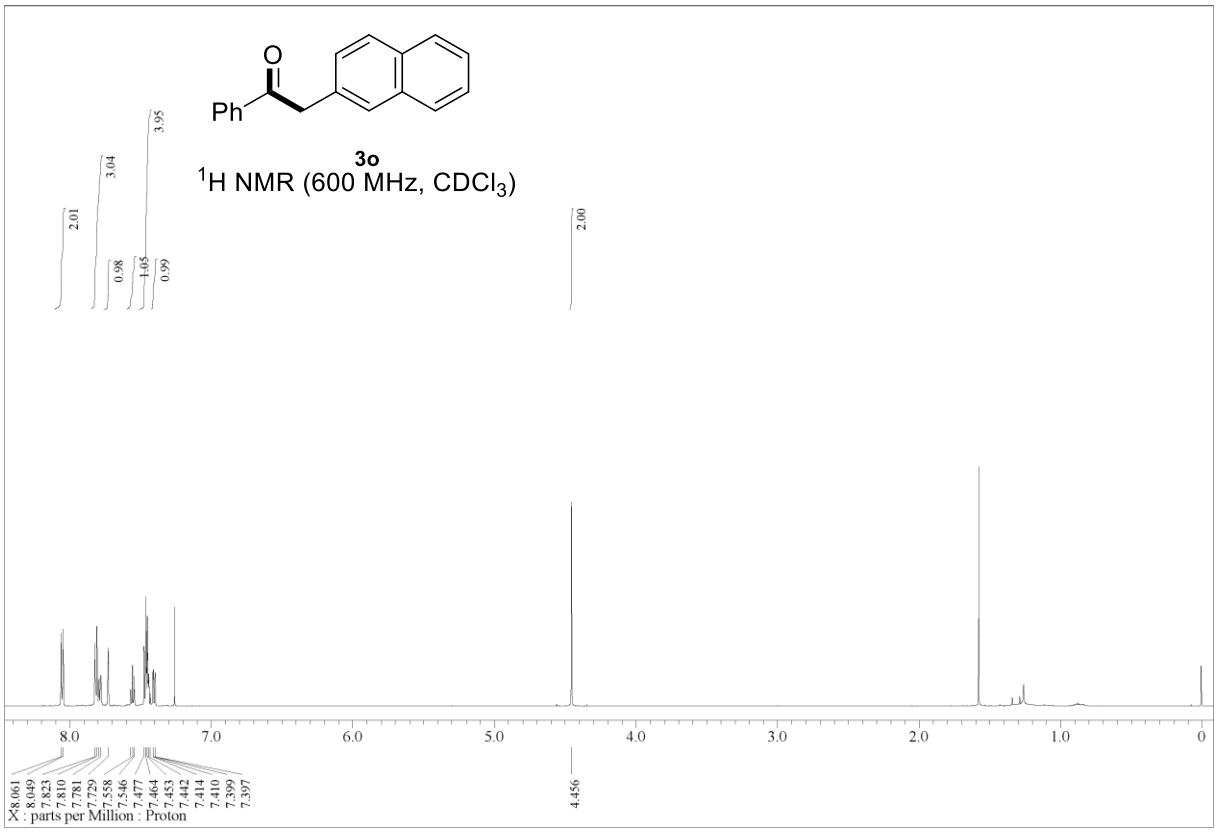

O
OMe
3I
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.08
159.81
145.81
139.79
136.06
135.23
129.66
129.24
128.92
128.23
127.26
127.23
121.77
115.08
112.38
55.17
45.63
X : parts per Million : Carbon13

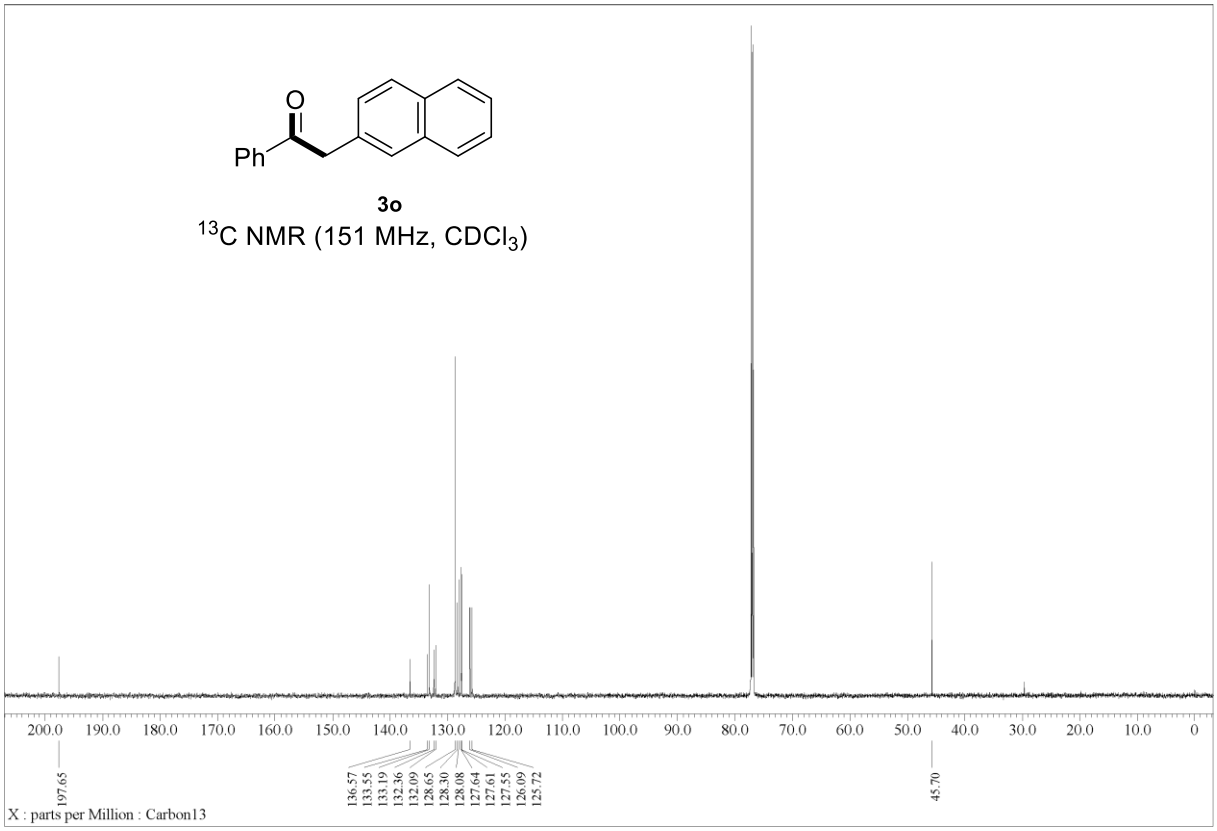

O
Cl
3m
^{1}H NMR (600 MHz, $CDCl_3$)
2.05
2.02
2.04
2.07
3.23
1.02
1.00
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.086
8.072
7.707
7.694
7.636
7.623
7.493
7.489
7.480
7.467
7.425
7.413
7.401
7.302
7.291
7.277
7.266
7.246
7.185
7.173
4.294
X : parts per Million : Proton

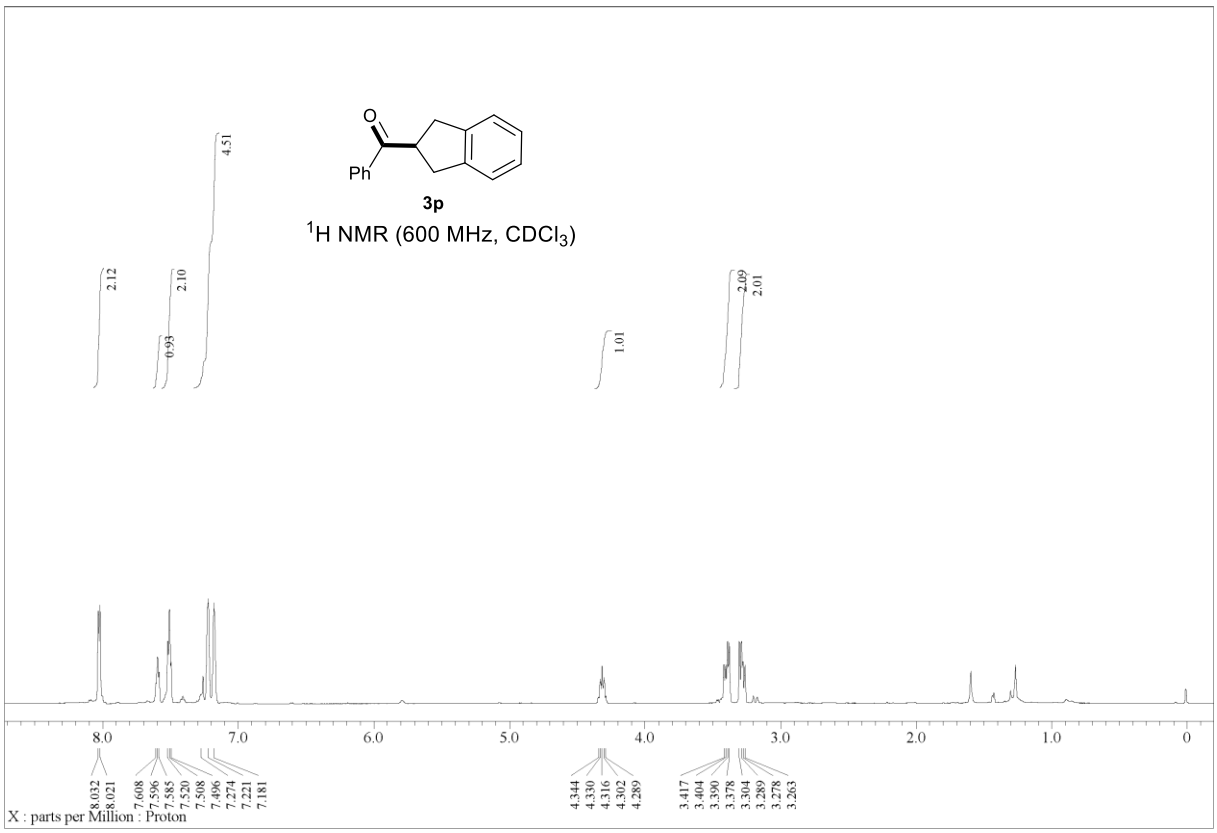

O
Cl
3m
^{13}C NMR (151 MHz, $CDCl_3$)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.39
146.06
139.70
136.44
135.01
134.42
129.84
129.64
129.13
128.96
128.31
127.73
127.35
127.25
127.15
44.93
X : parts per Million : Carbon13

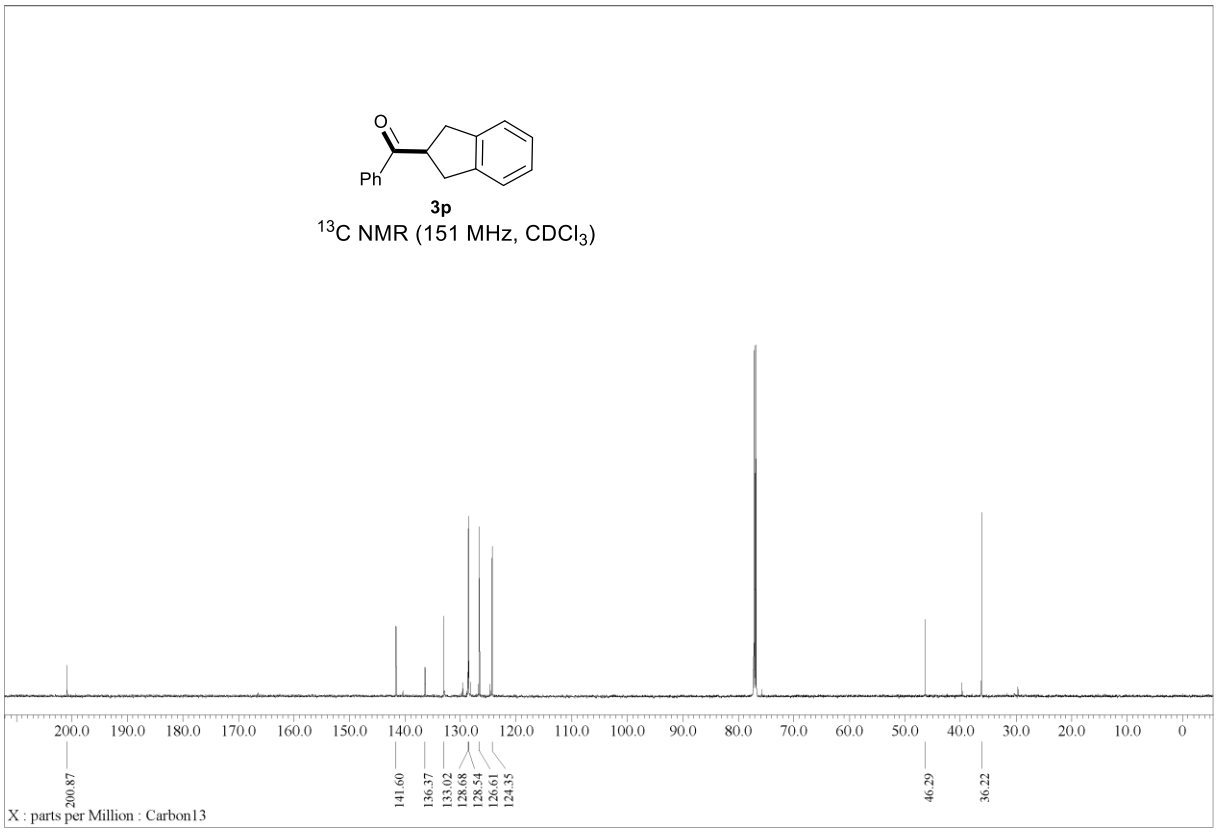

3n
^{1}H NMR (600 MHz, $CDCl_3$)
X : parts per Million : Proton

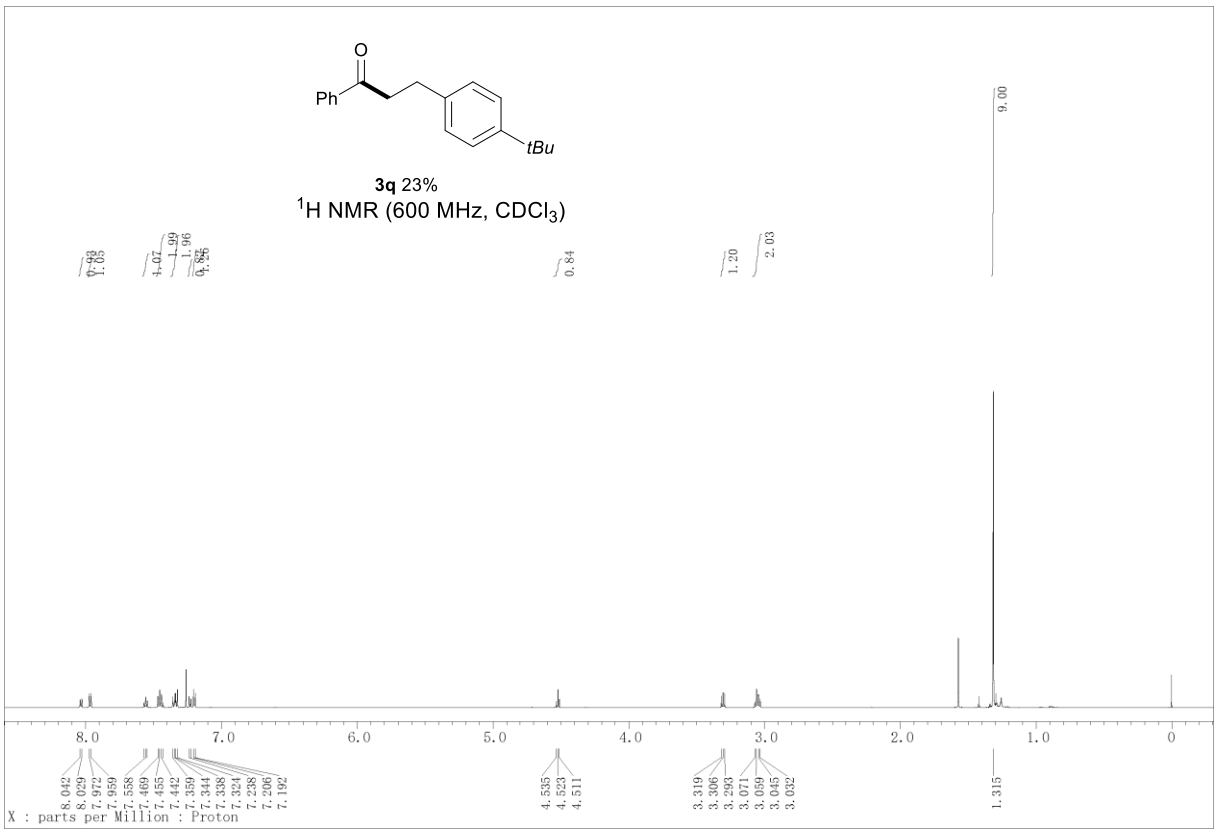

3n
^{13}C NMR (151 MHz, $CDCl_3$)
X : parts per Million : Carbon13


O
Ph
3o
1H NMR (600 MHz, CDCl3)
2.01
3.04
0.98
1.05
3.95
0.99
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.061
8.049
7.823
7.810
7.781
7.729
7.558
7.546
7.477
7.464
7.453
7.442
7.414
7.410
7.399
7.397
4.456
X : parts per Million : Proton


O
Ph
3o
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.65
136.57
133.55
133.19
132.36
132.09
128.65
128.30
128.08
127.64
127.61
127.55
126.09
125.72
45.70
X : parts per Million : Carbon13

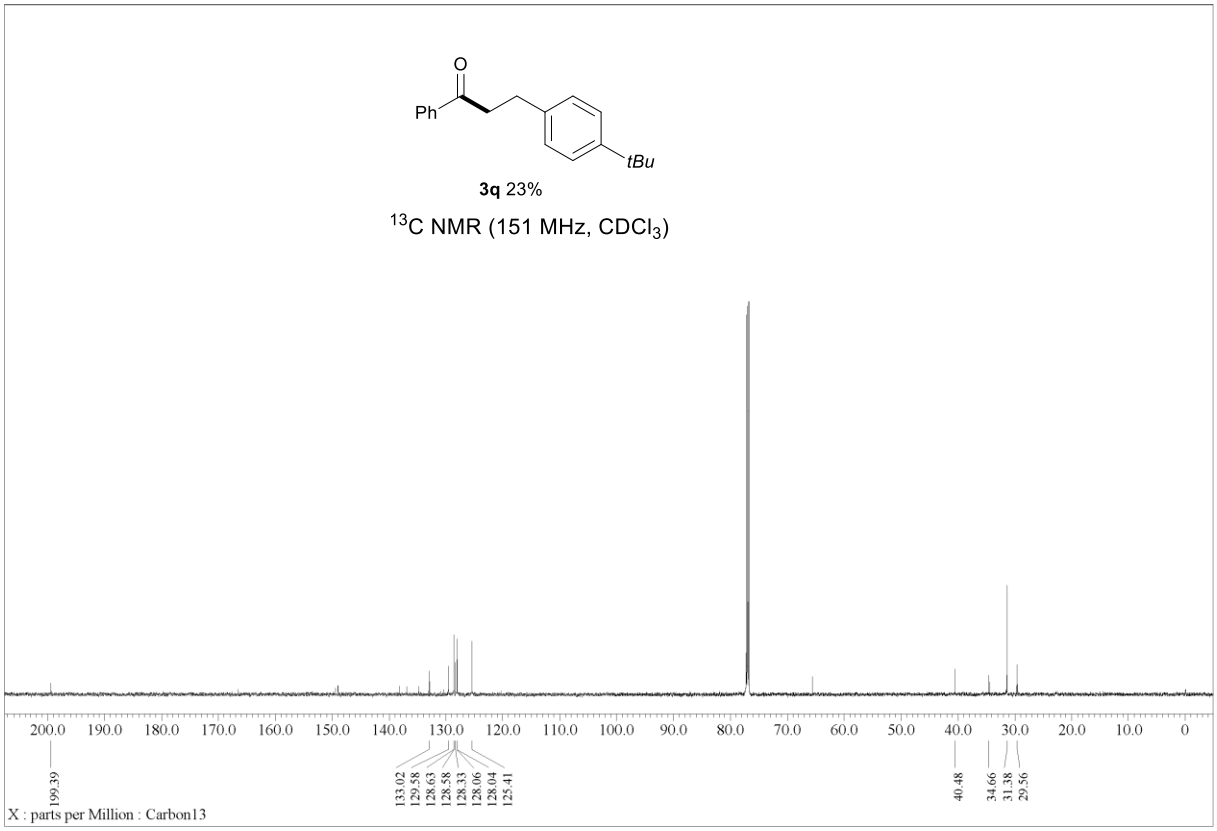

O
Ph
3p
1H NMR (600 MHz, CDCl3)
2.12
2.10
0.93
4.51
1.01
2.09
2.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.032
8.021
7.608
7.596
7.585
7.520
7.508
7.496
7.274
7.221
7.181
4.344
4.330
4.316
4.302
4.289
3.417
3.404
3.390
3.378
3.304
3.289
3.278
3.263
X : parts per Million : Proton


O
Ph
3p
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.87
141.60
136.37
133.02
128.68
128.54
126.61
124.35
46.29
36.22
X : parts per Million : Carbon13



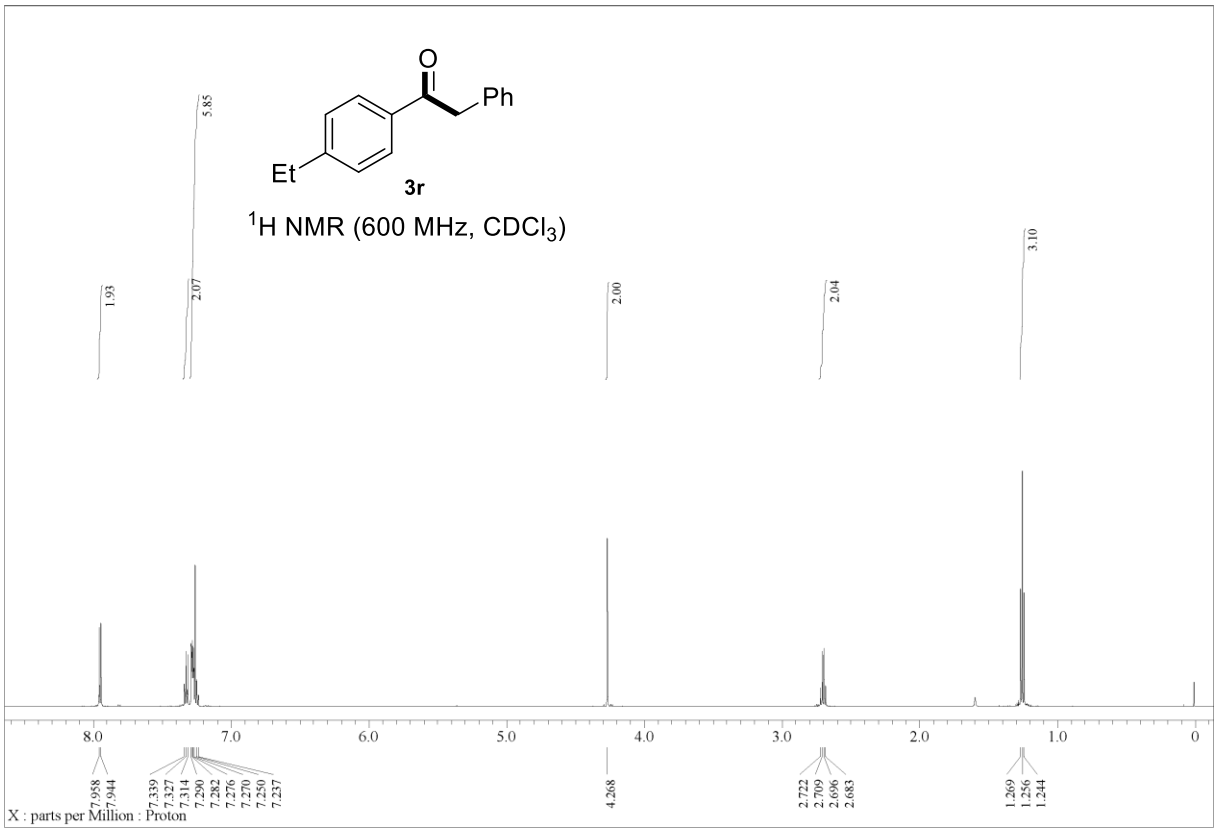
3q 23%

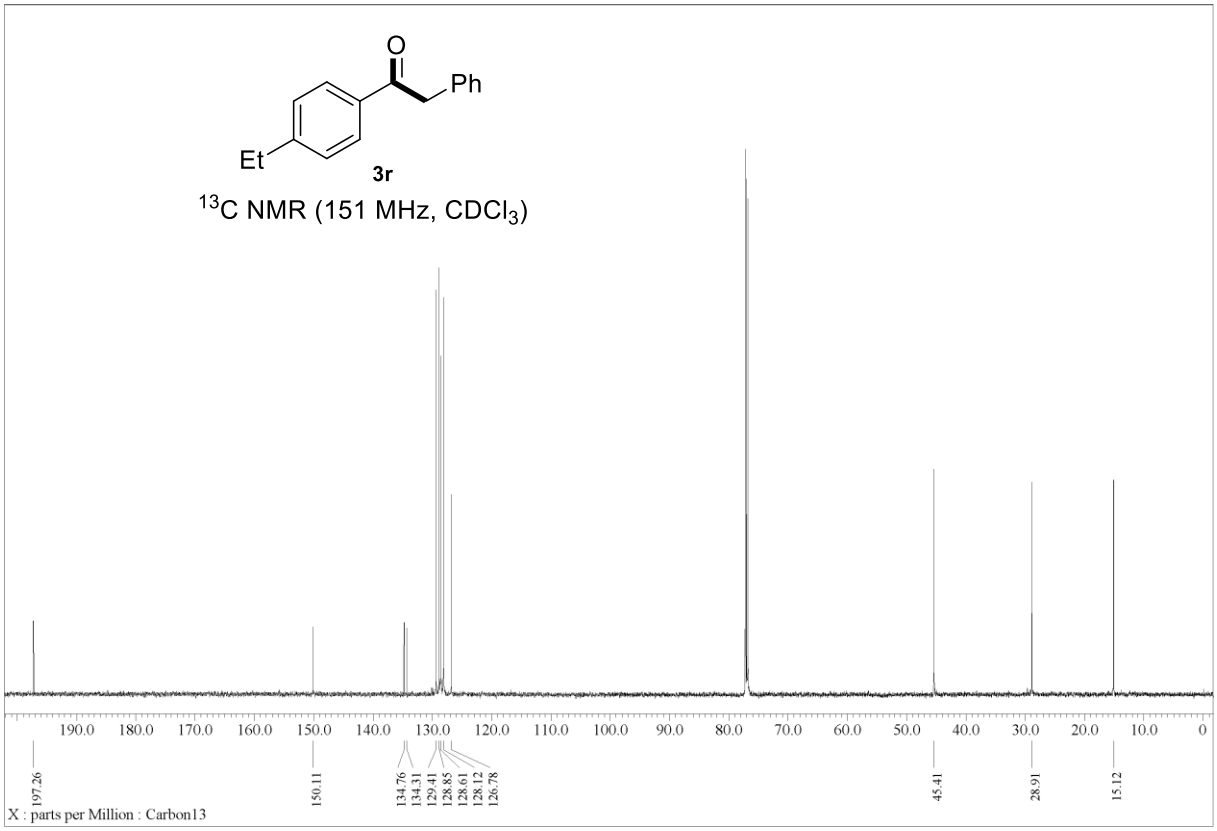
^{1}H NMR (600 MHz, $CDCl_3$)

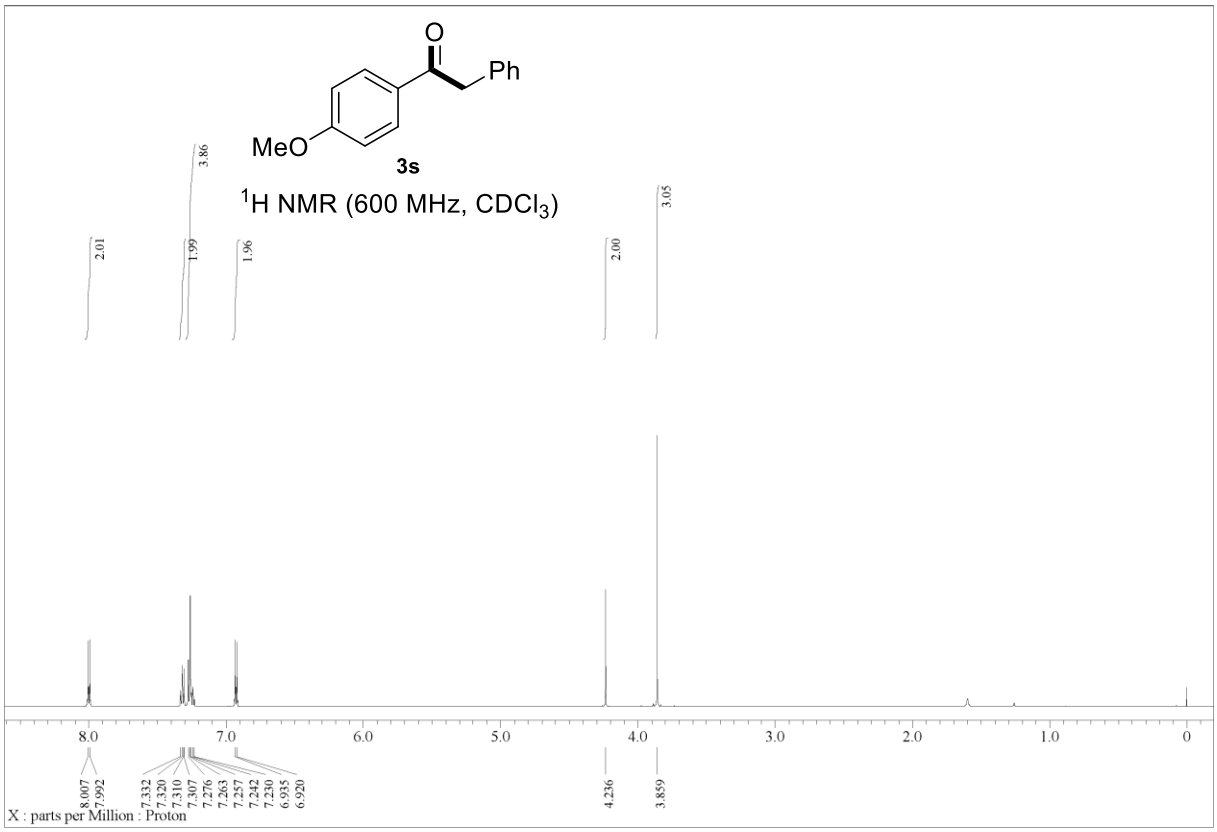


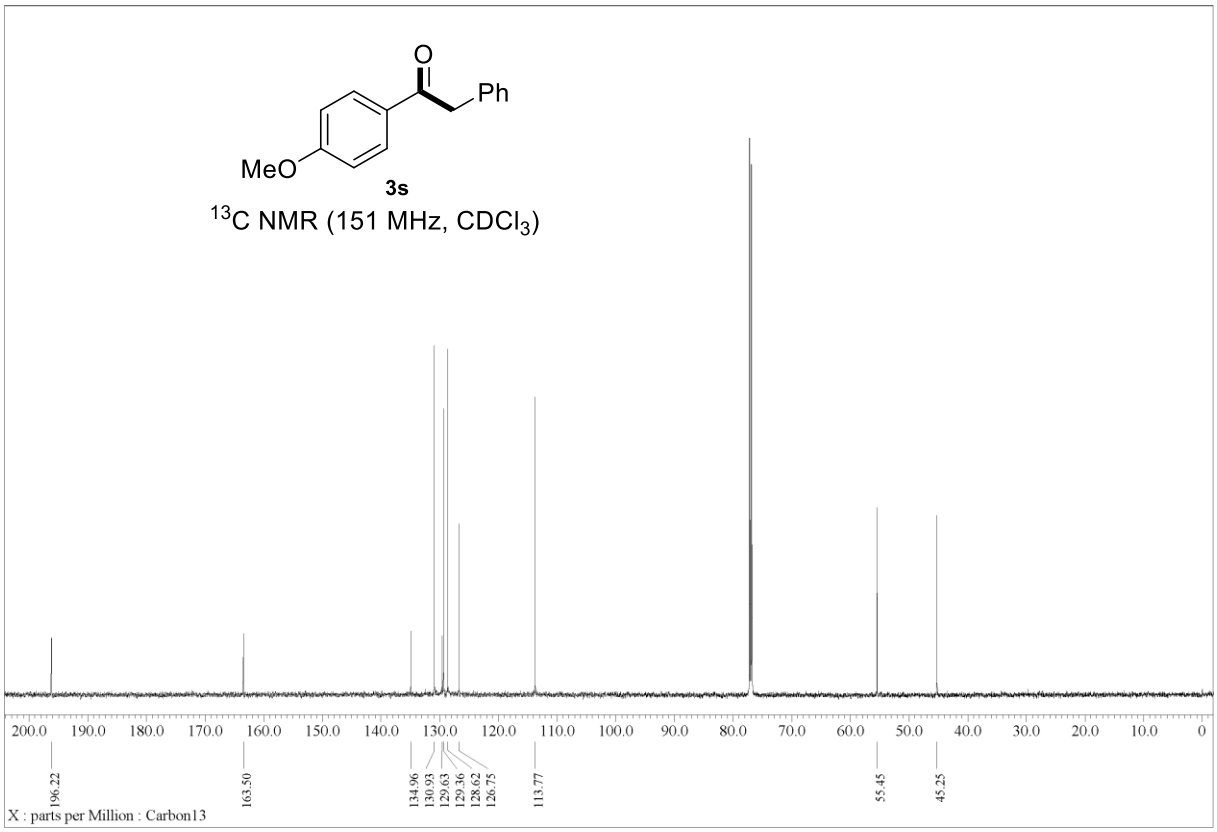
3q 23%

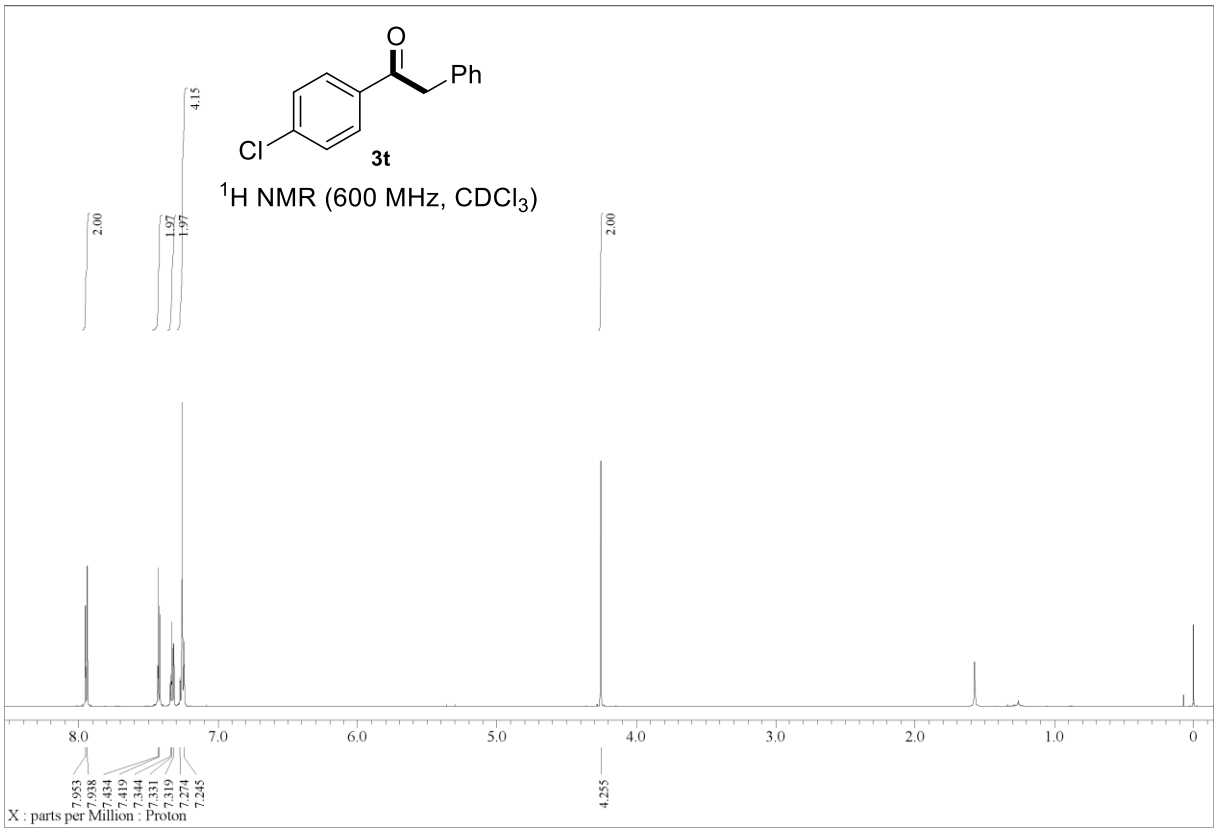
^{13}C NMR (151 MHz, $CDCl_3$)

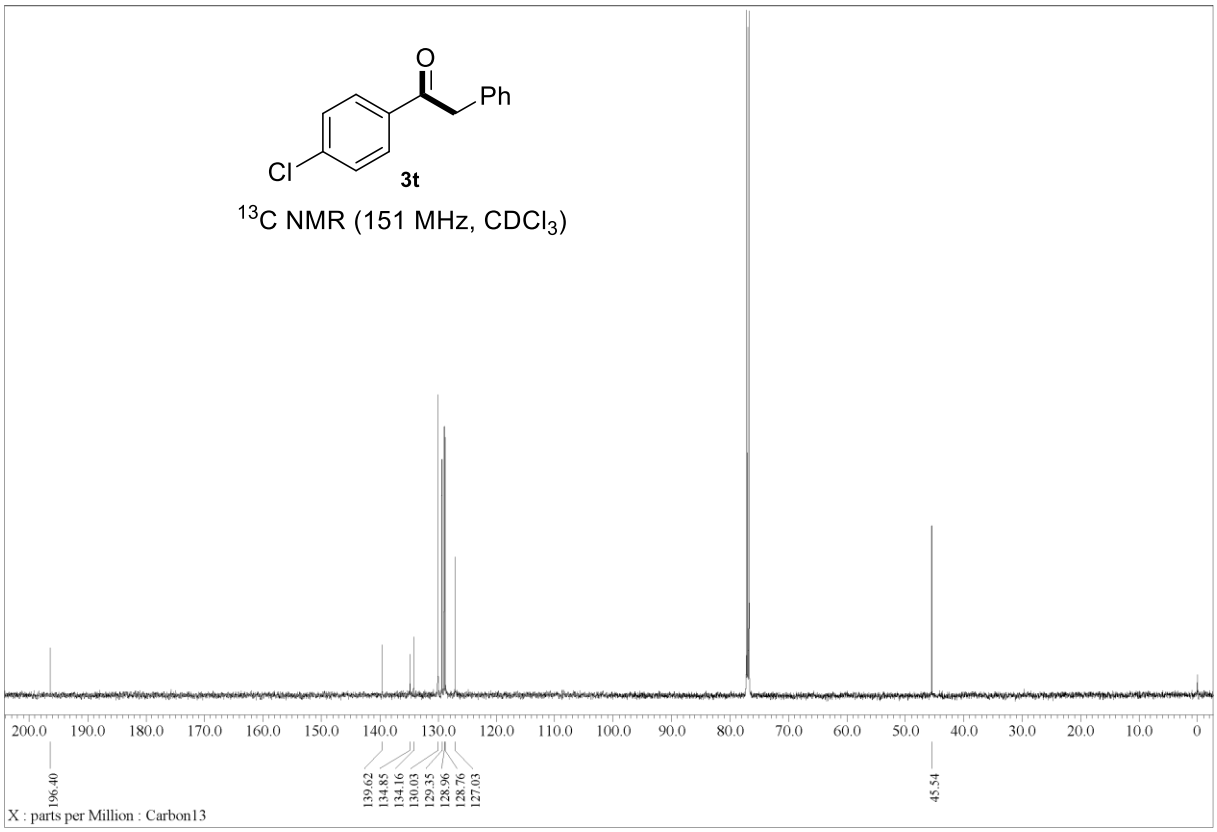

O
Ph
Et
3r
^{1}H NMR (600 MHz, CDCl$_3$)
5.85
1.93
2.07
2.00
2.04
3.10
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.958
7.944
7.339
7.327
7.314
7.290
7.282
7.276
7.270
7.250
7.237
4.268
2.722
2.709
2.696
2.683
1.269
1.256
1.244
X : parts per Million : Proton

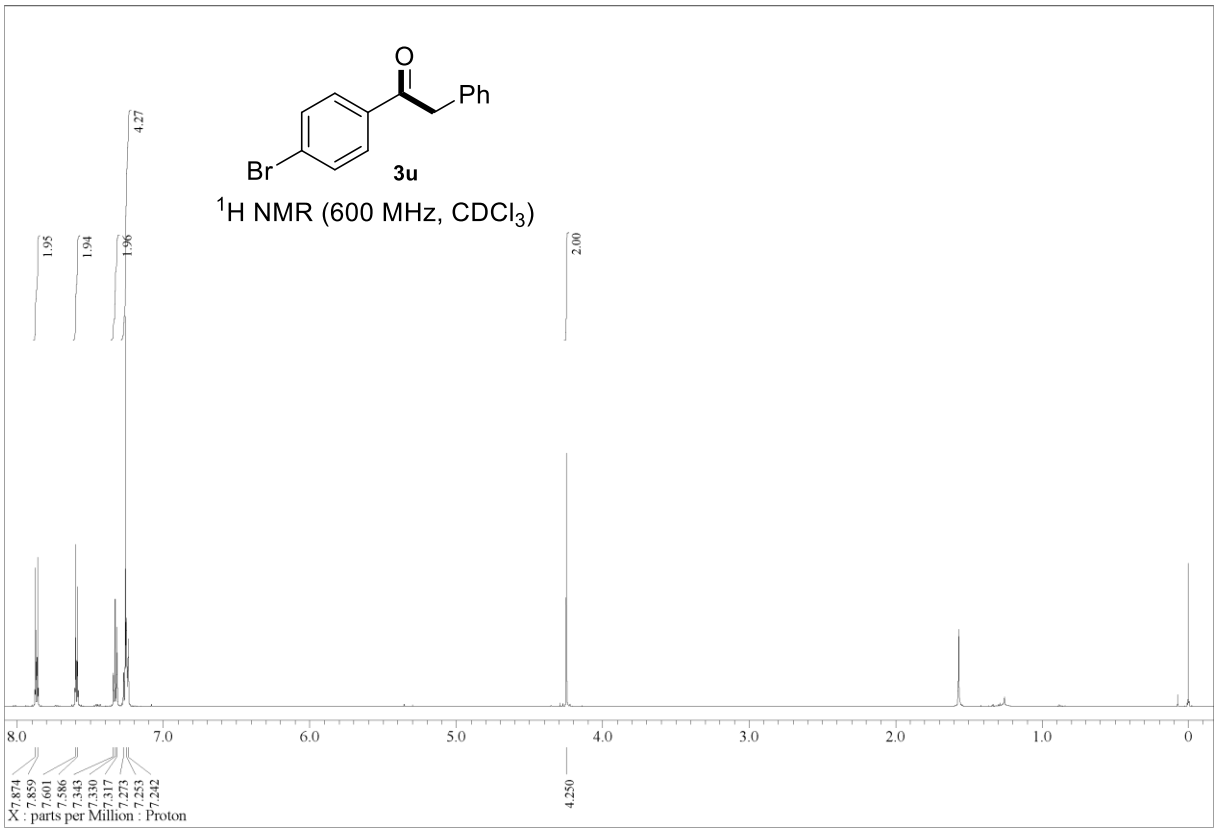

O
Ph
Et
3r
^{13}C NMR (151 MHz, CDCl$_3$)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.26
150.11
134.76
134.31
129.41
128.85
128.61
128.12
126.78
45.41
28.91
15.12
X : parts per Million : Carbon13

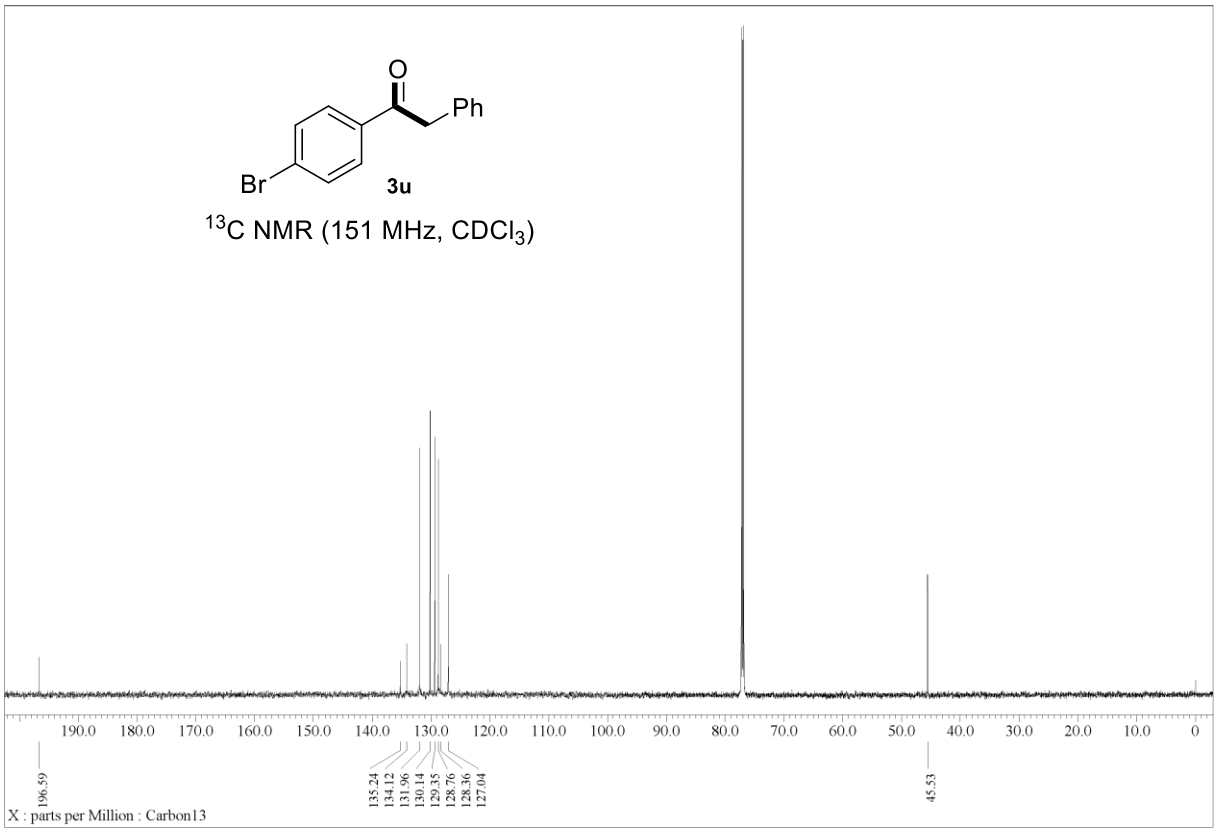

O
Ph
MeO
3s
^{1}H NMR (600 MHz, $CDCl_3$)
3.86
3.05
2.01
1.99
1.96
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.007
7.992
7.332
7.320
7.310
7.307
7.276
7.263
7.257
7.242
7.230
6.935
6.920
4.236
3.859
X : parts per Million : Proton

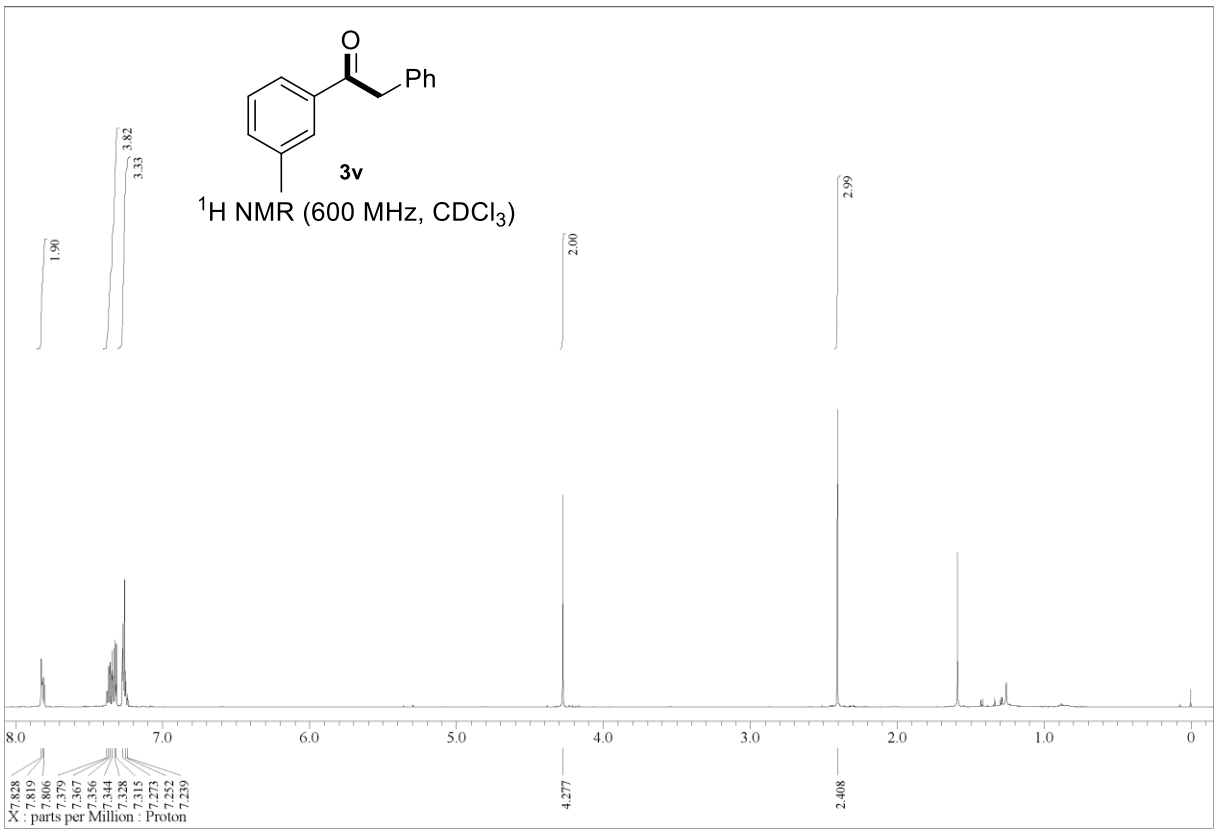

O
Ph
MeO
3s
^{13}C NMR (151 MHz, $CDCl_3$)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.22
163.50
134.96
130.93
129.63
129.36
128.62
126.75
113.77
55.45
45.25
X : parts per Million : Carbon13

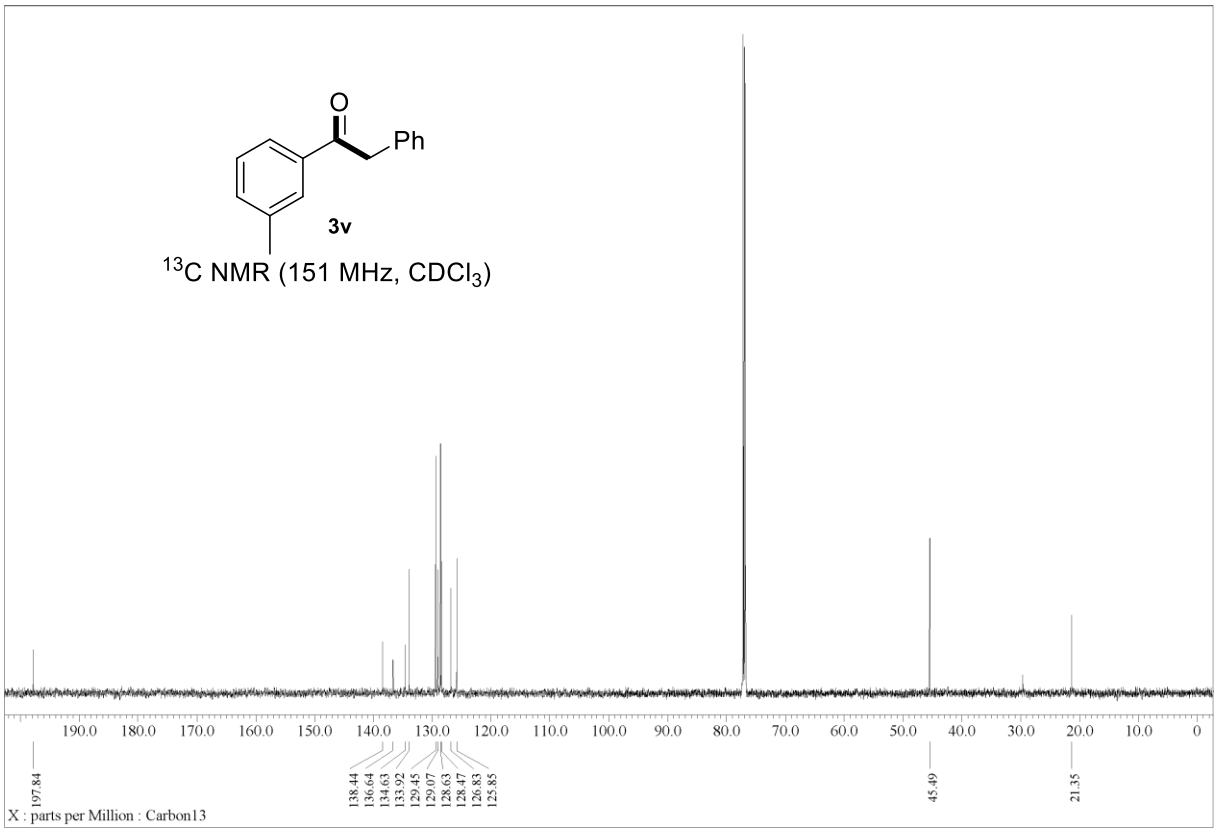

O
Ph
Cl
3t
^{1}H NMR (600 MHz, $CDCl_3$)
4.15
2.00
1.97
1.97
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.953
7.938
7.434
7.419
7.344
7.331
7.319
7.274
7.245
4.255
X : parts per Million : Proton

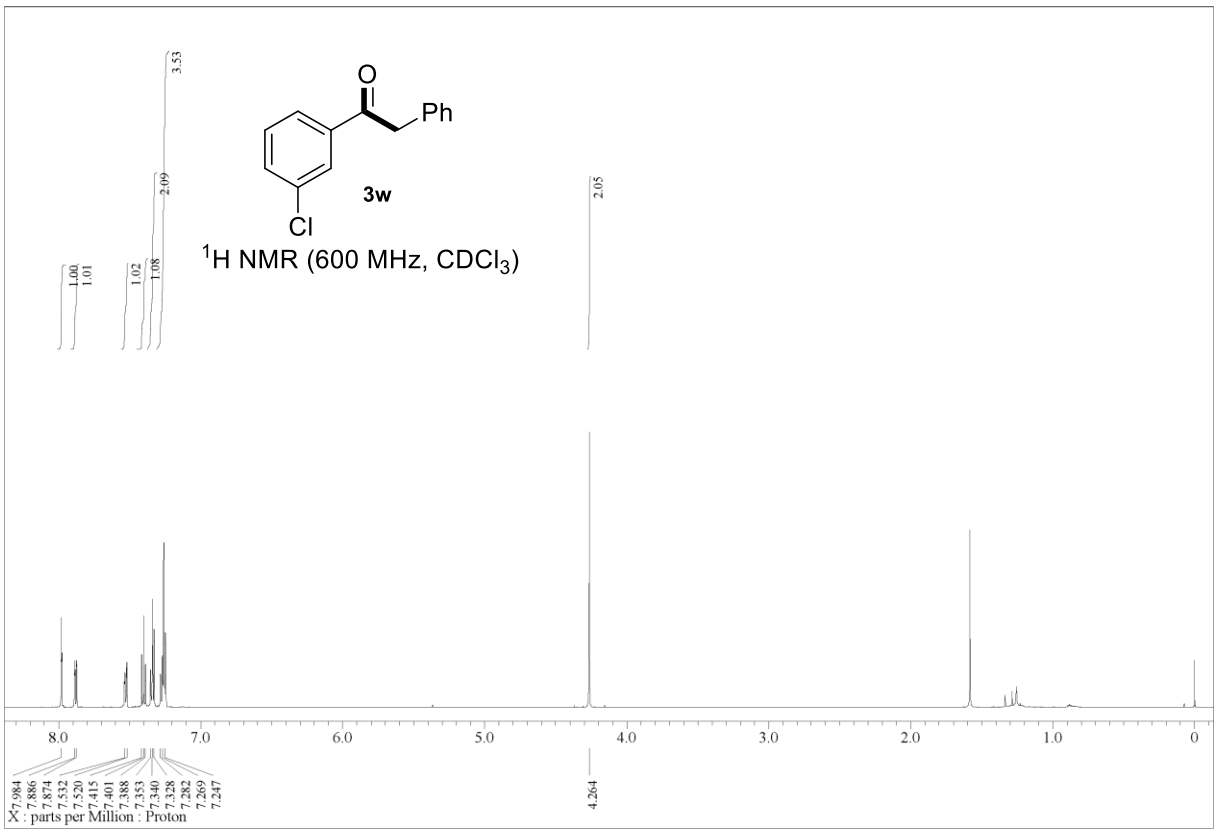

O
Ph
Cl
3t
^{13}C NMR (151 MHz, $CDCl_3$)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.40
139.62
134.85
134.16
130.03
129.35
128.96
128.76
127.03
45.54
X : parts per Million : Carbon13

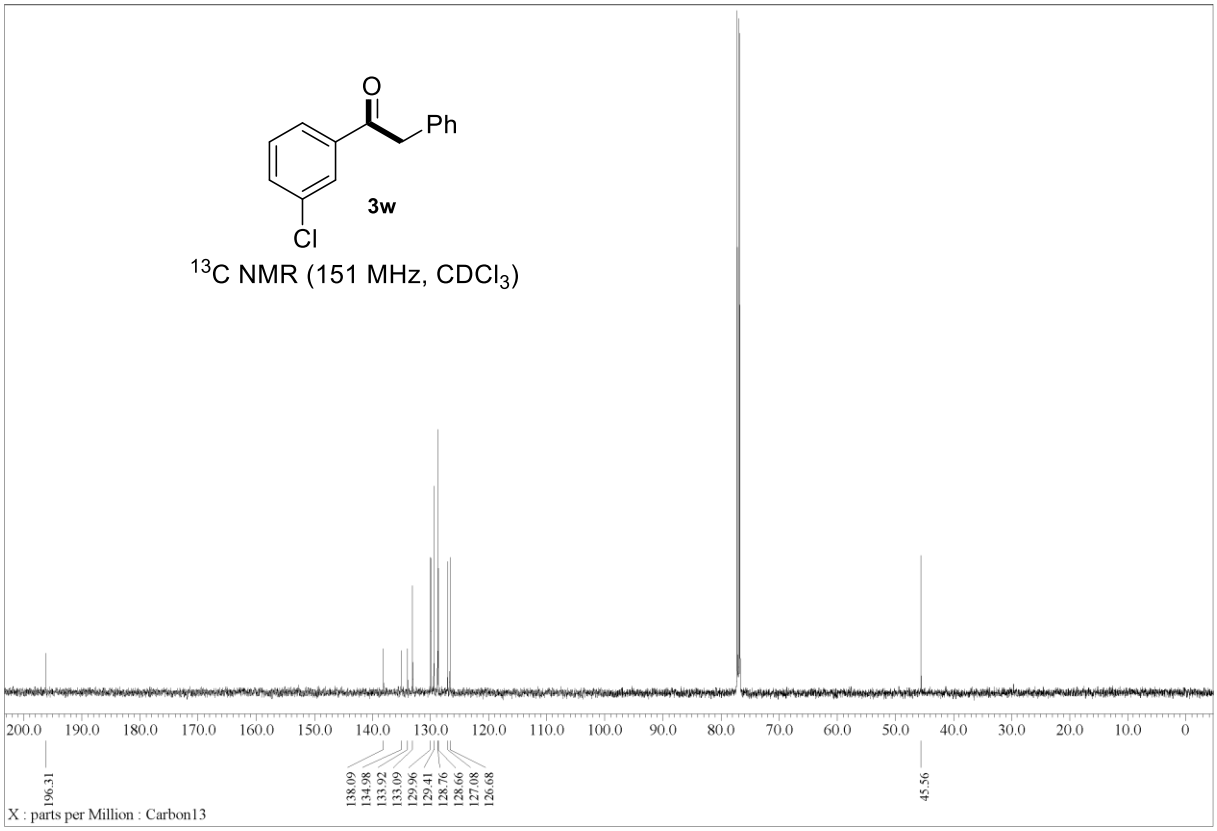

O
Ph
Br
3u
^{1}H NMR (600 MHz, $CDCl_3$)
4.27
1.95
1.94
1.96
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.874
7.859
7.601
7.586
7.343
7.330
7.317
7.273
7.253
7.242
4.250
X : parts per Million : Proton

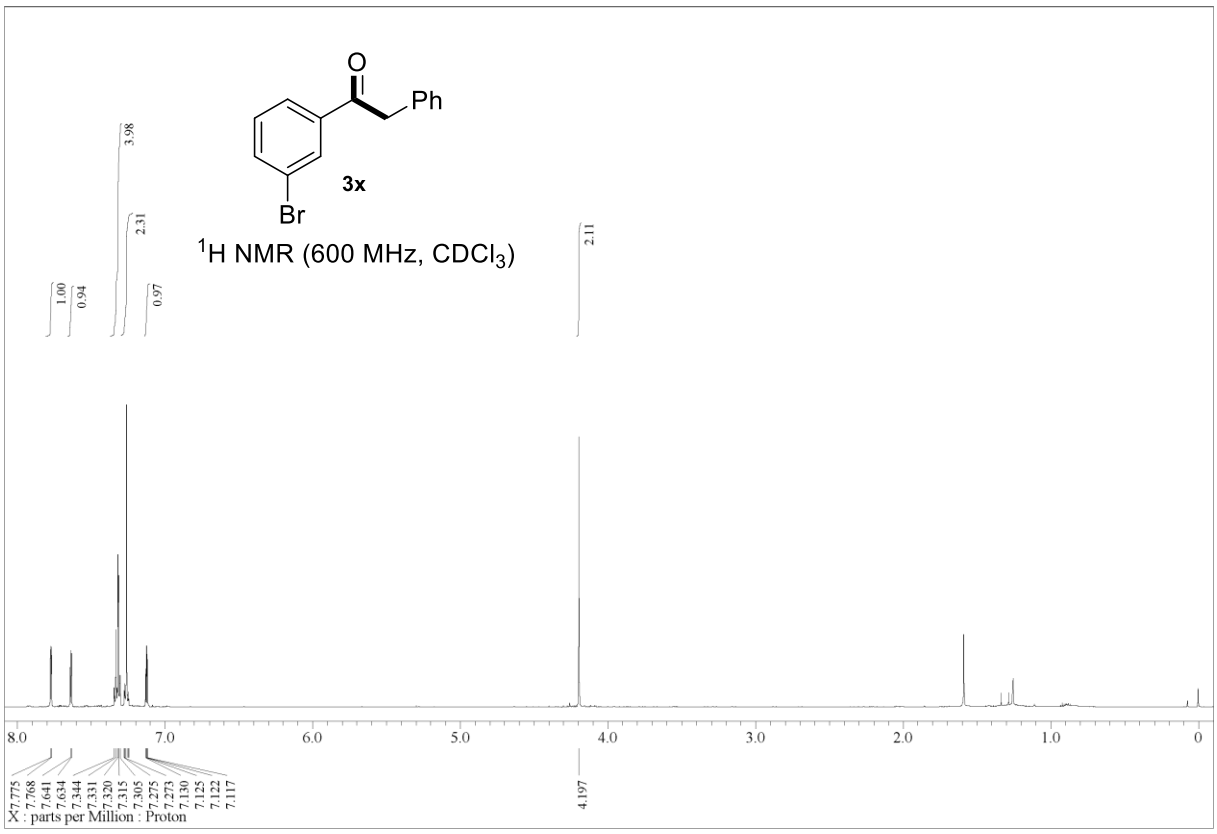

O
Ph
Br
3u
^{13}C NMR (151 MHz, $CDCl_3$)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.59
135.24
134.12
131.96
130.14
129.35
128.76
128.36
127.04
45.53
X : parts per Million : Carbon13

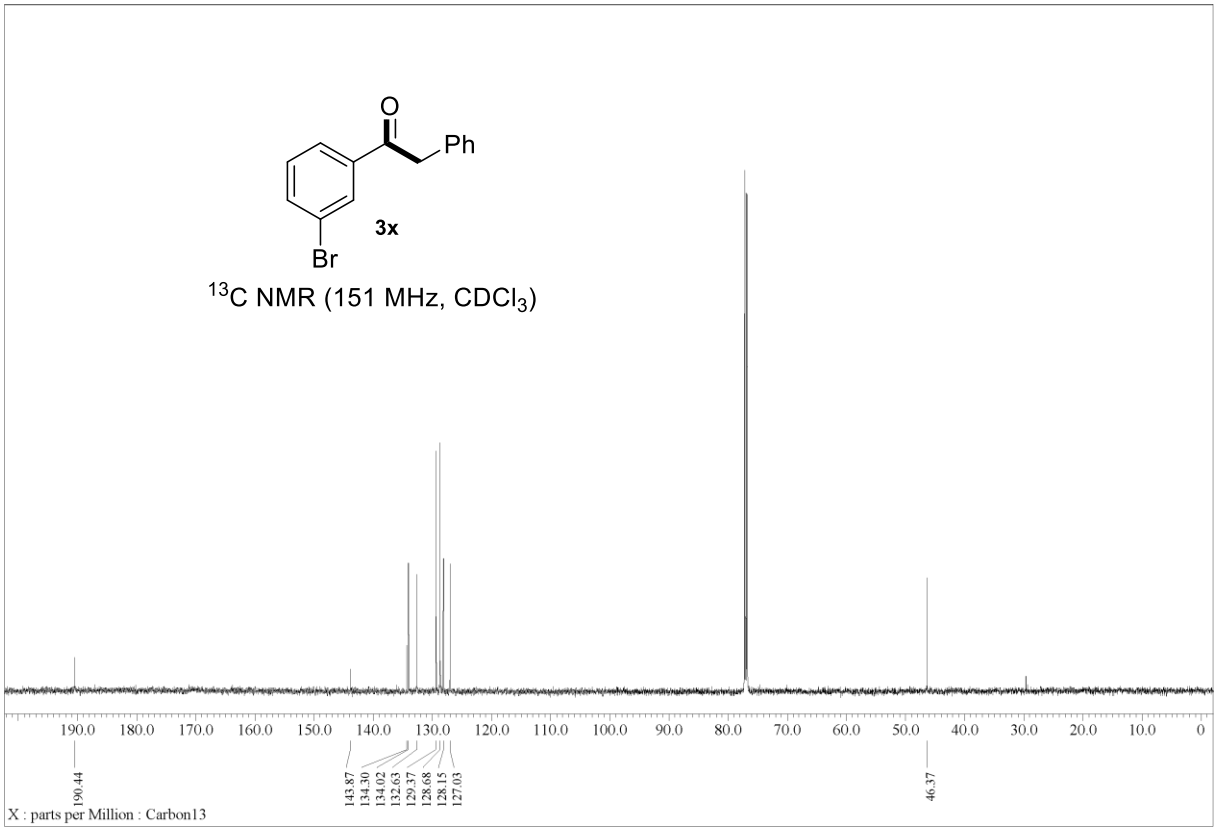

O
Ph
3v
^{1}H NMR (600 MHz, $CDCl_3$)
1.90
3.82
3.33
2.00
2.99
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.828
7.819
7.806
7.379
7.367
7.356
7.344
7.328
7.315
7.273
7.252
7.239
4.277
2.408
X : parts per Million : Proton

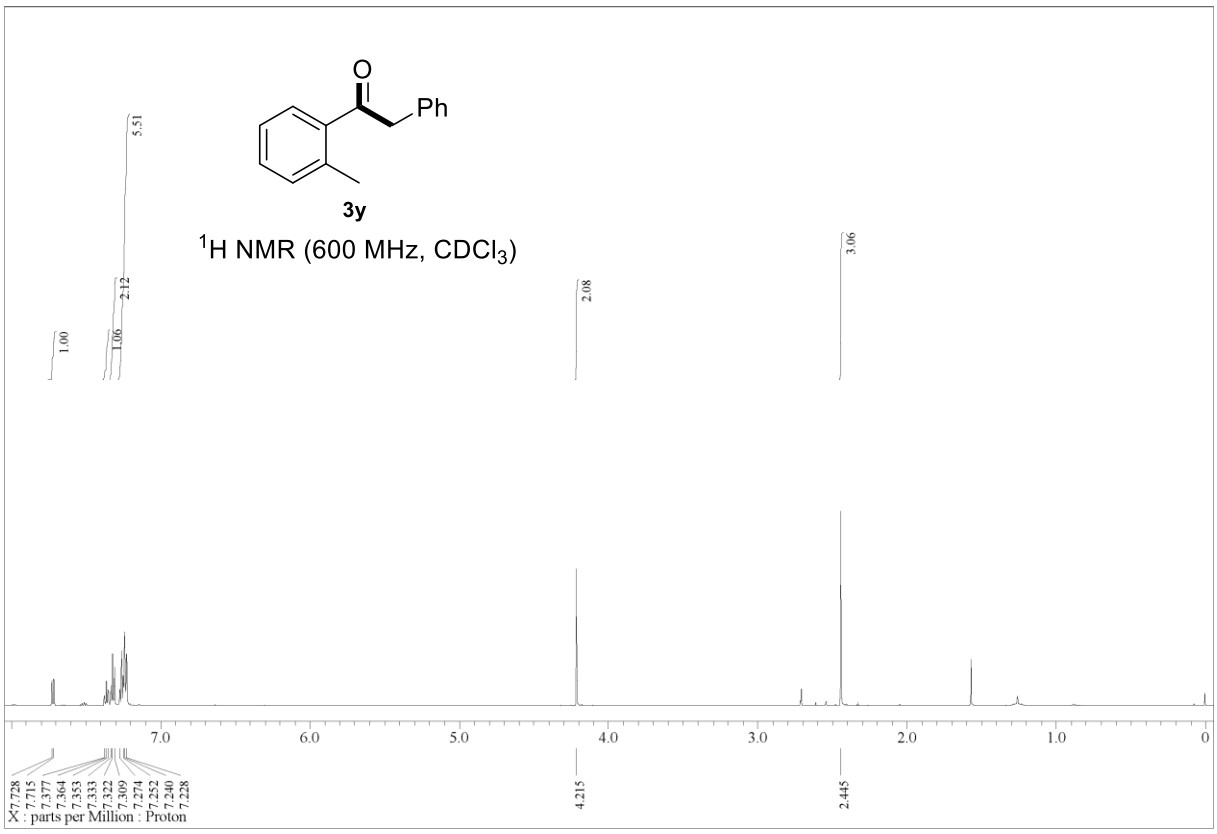

O
Ph
3v
^{13}C NMR (151 MHz, $CDCl_3$)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.84
138.44
136.64
134.63
133.92
129.45
129.07
128.63
128.47
126.83
125.85
45.49
21.35
X : parts per Million : Carbon13

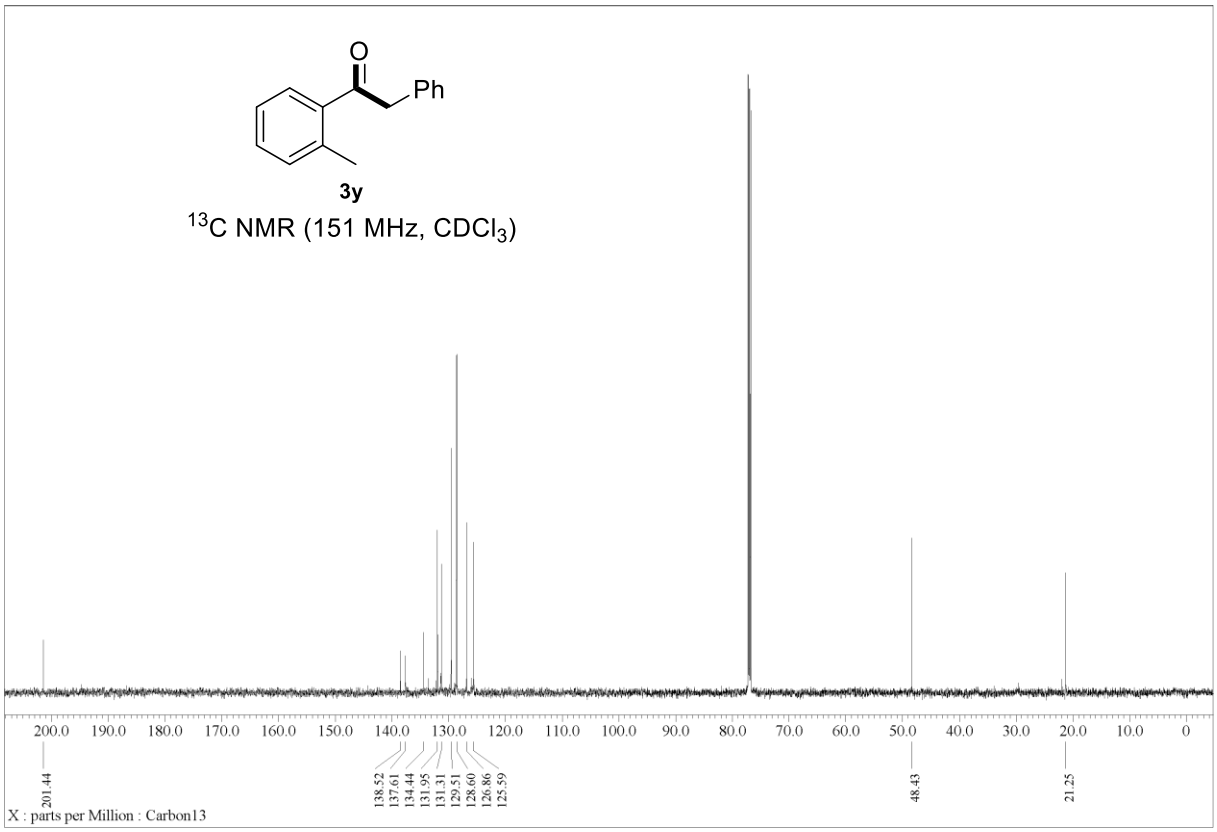

O
Ph
Cl
3w
^{1}H NMR (600 MHz, $CDCl_3$)
3.53
2.09
2.05
1.08
1.02
1.01
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.984
7.886
7.874
7.532
7.520
7.415
7.401
7.388
7.353
7.340
7.328
7.282
7.269
7.247
4.264
X : parts per Million : Proton

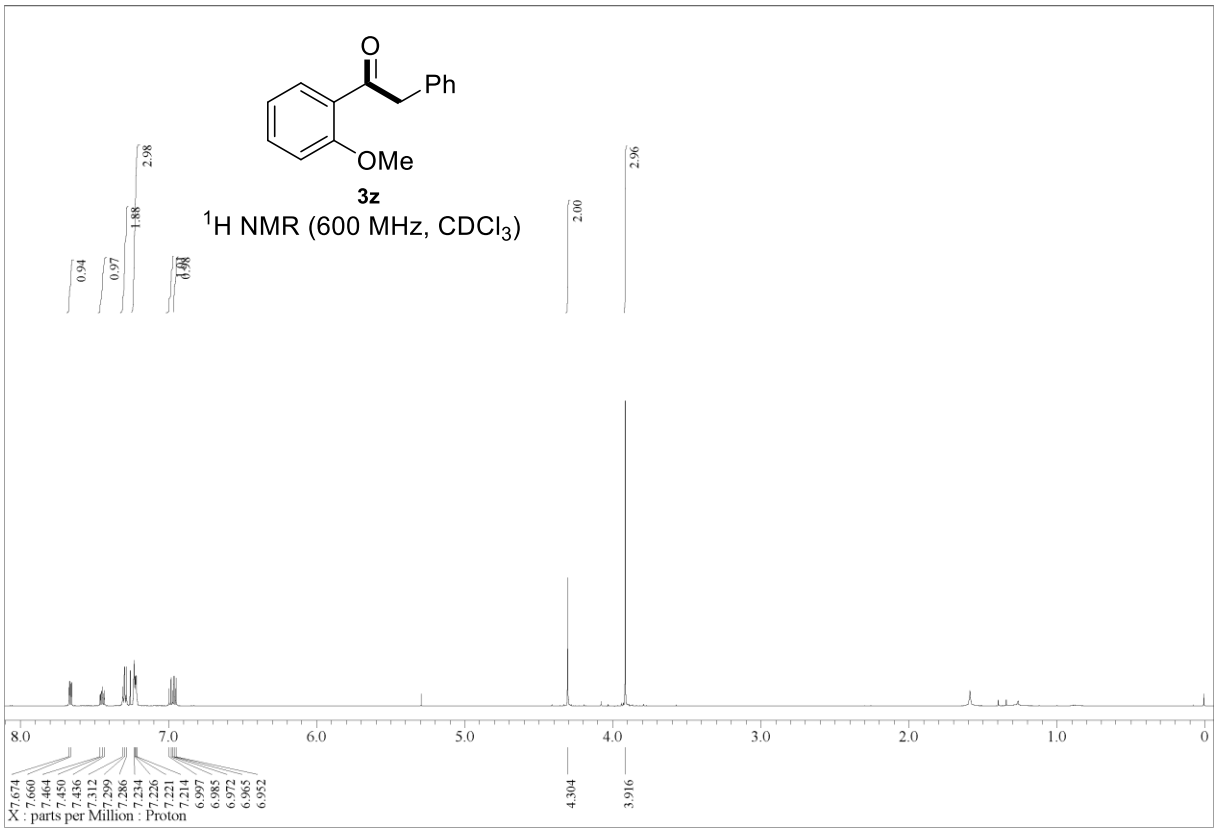

O
Ph
Cl
3w
^{13}C NMR (151 MHz, $CDCl_3$)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.31
138.09
134.98
133.92
133.09
129.96
129.41
128.76
128.66
127.08
126.68
45.56
X : parts per Million : Carbon13

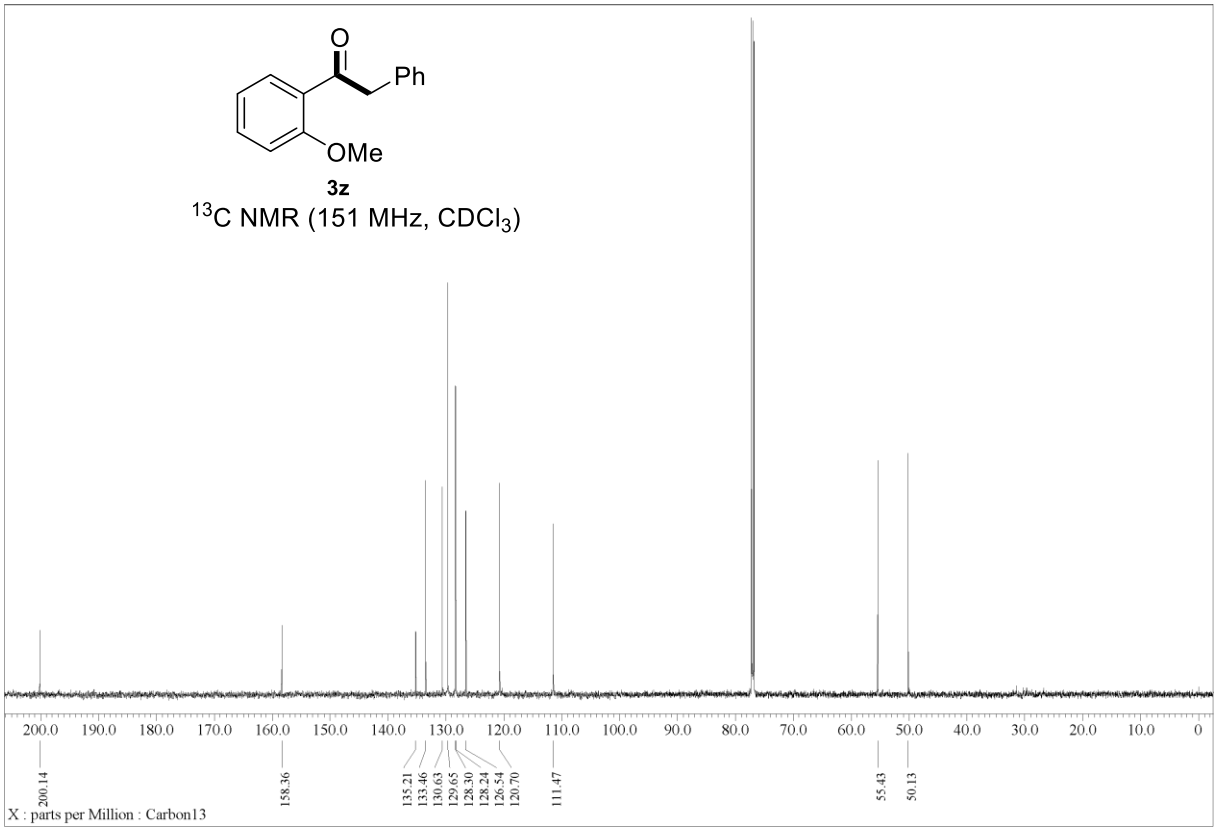

O
Ph
Br
3x
^{1}H NMR (600 MHz, $CDCl_3$)
3.98
2.31
0.97
1.00
0.94
2.11
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.775
7.768
7.641
7.634
7.344
7.331
7.320
7.315
7.305
7.275
7.273
7.130
7.125
7.122
7.117
4.197
X : parts per Million : Proton

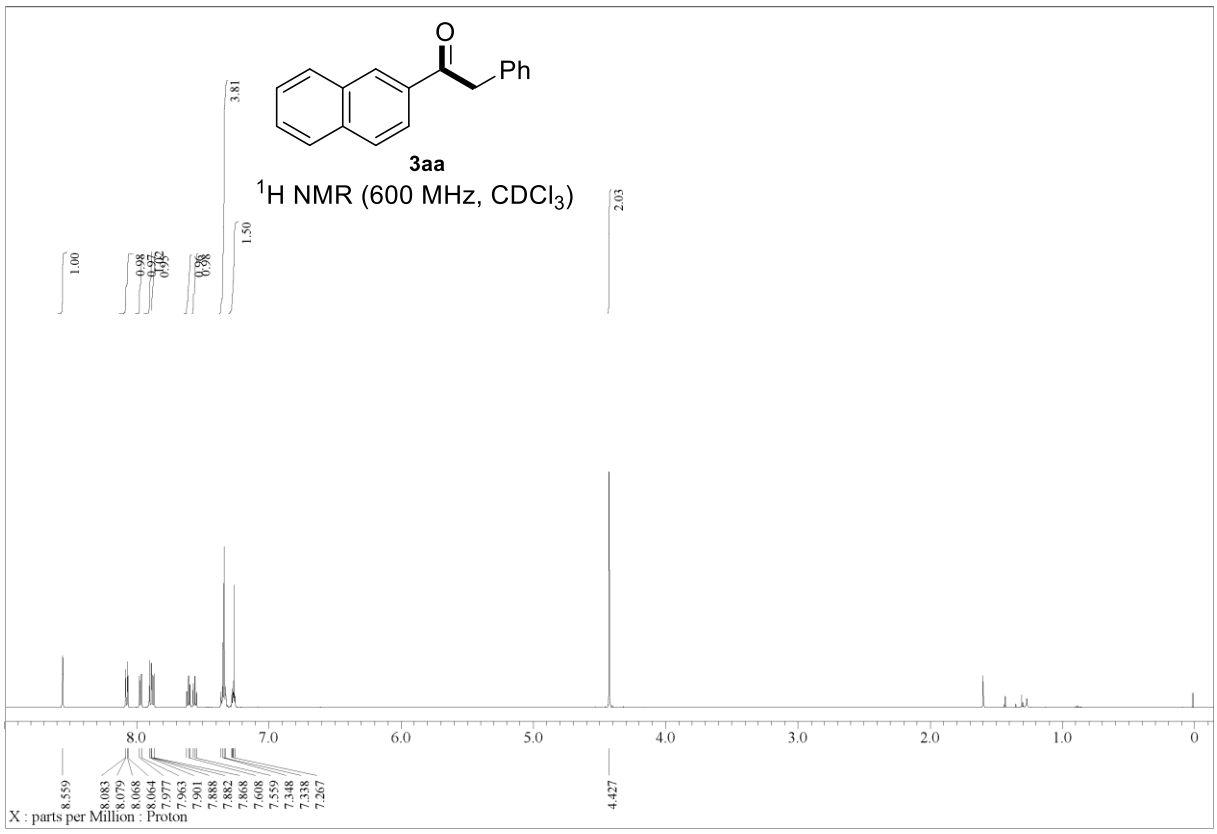

O
Ph
Br
3x
^{13}C NMR (151 MHz, $CDCl_3$)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
190.44
143.87
134.30
134.02
132.63
129.37
128.68
128.15
127.03
46.37
X : parts per Million : Carbon13

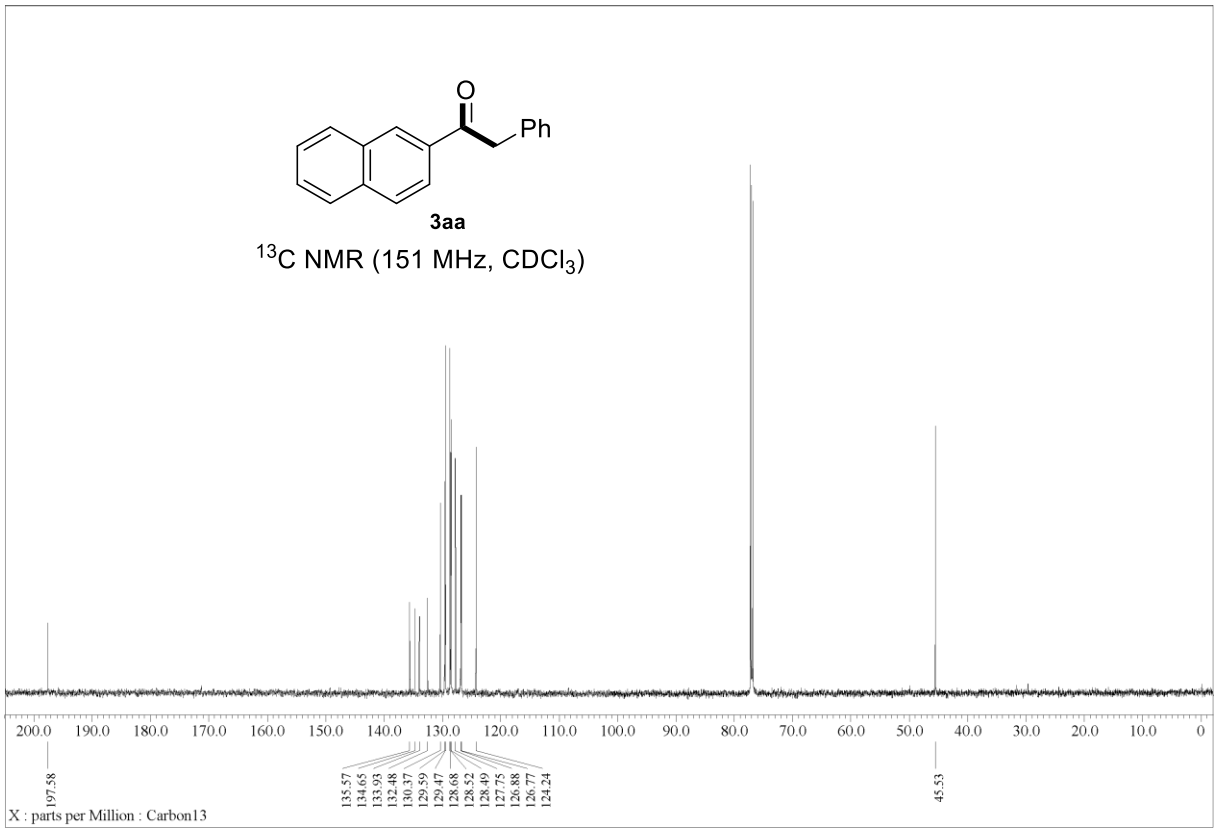

O
Ph
3y
1H NMR (600 MHz, CDCl3)
5.51
2.12
1.06
1.00
2.08
3.06
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.728
7.715
7.377
7.364
7.353
7.333
7.322
7.309
7.274
7.252
7.240
7.228
4.215
2.445
X : parts per Million : Proton

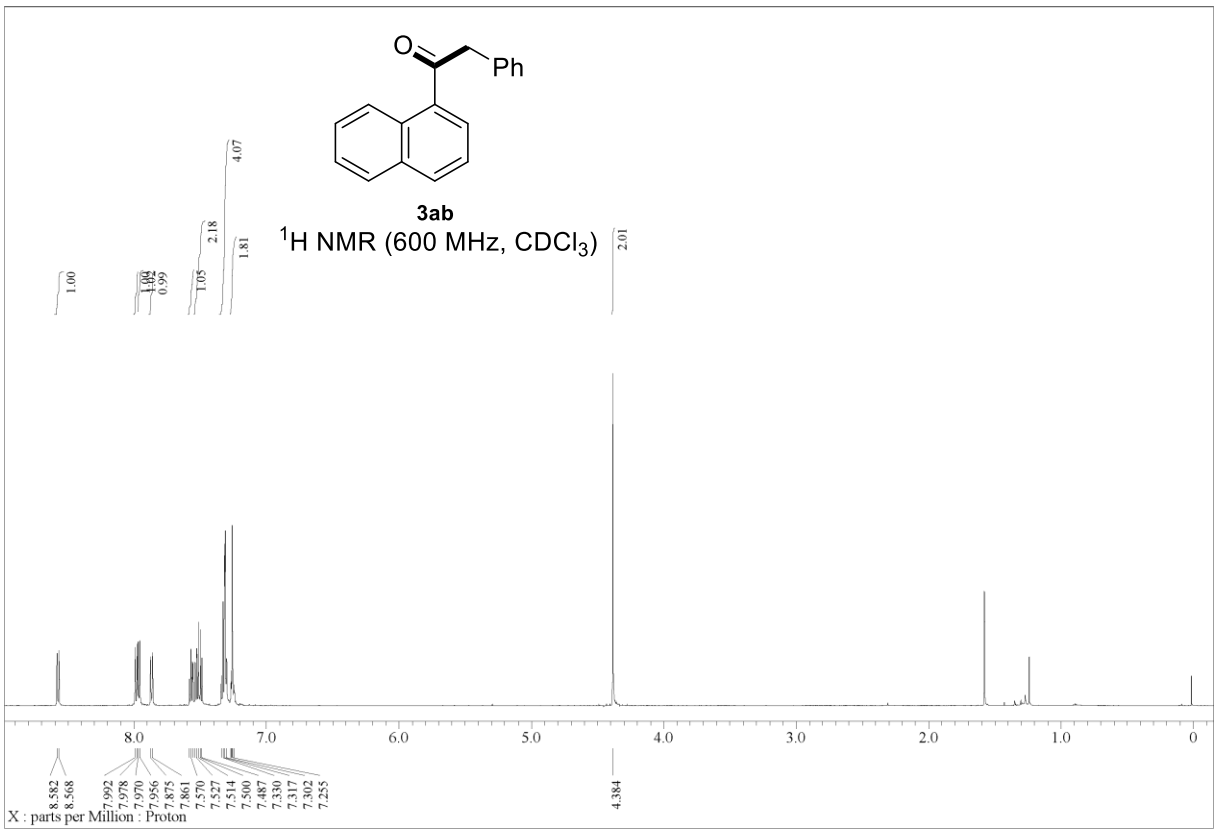

O
Ph
3y
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
201.44
138.52
137.61
134.44
131.95
131.31
129.51
128.60
126.86
125.59
48.43
21.25
X : parts per Million : Carbon13

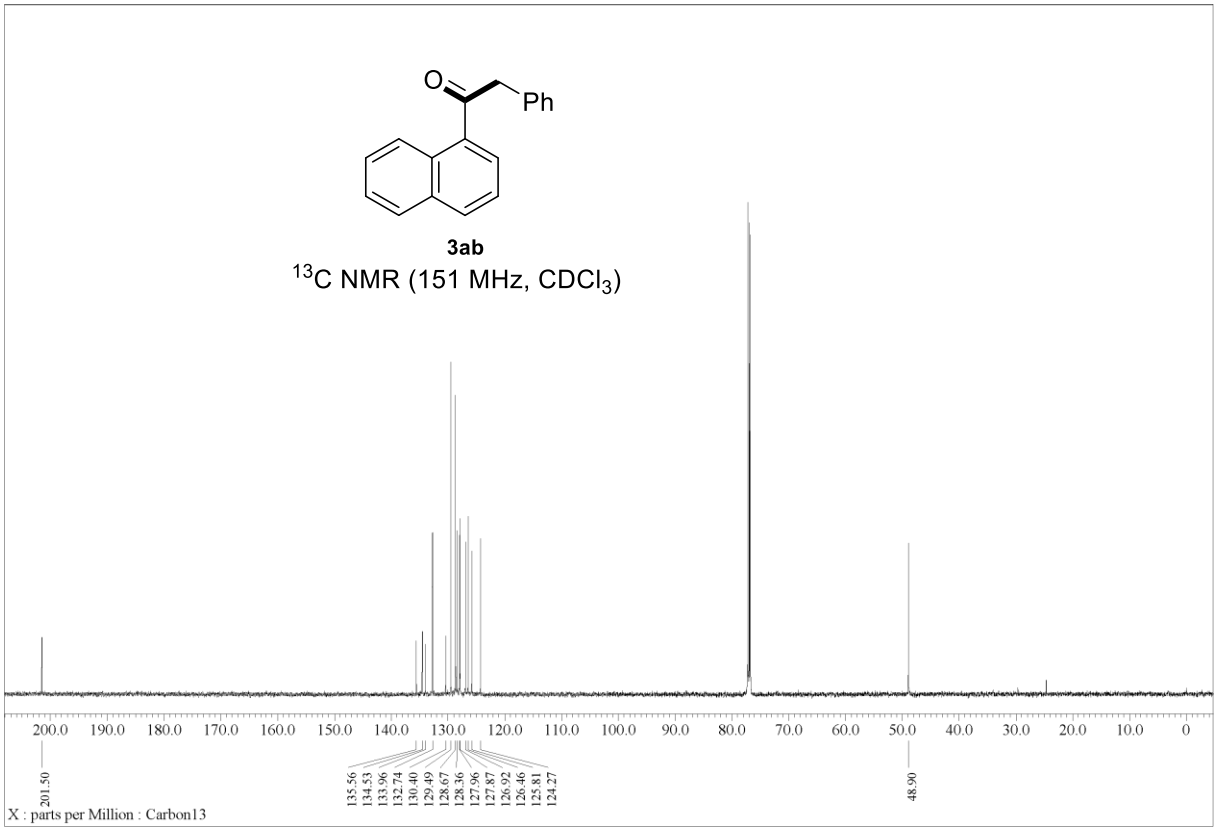

O
Ph
OMe
3z
1H NMR (600 MHz, CDCl3)
0.94
0.97
1.88
2.98
2.00
2.96
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.674
7.660
7.464
7.450
7.436
7.312
7.299
7.286
7.234
7.226
7.221
7.214
6.997
6.985
6.972
6.965
6.952
4.304
3.916
X : parts per Million : Proton

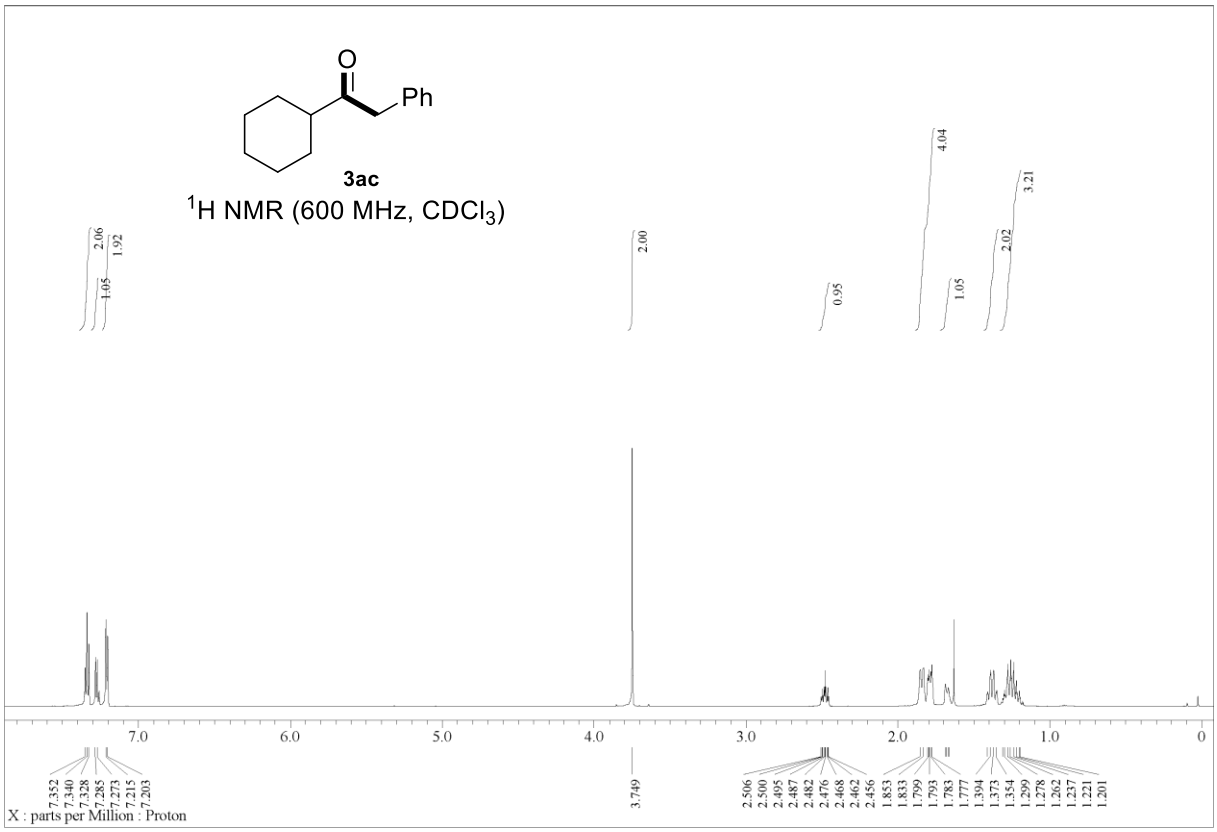

O
Ph
OMe
3z
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.14
158.36
135.21
133.46
130.63
129.65
128.30
128.24
126.54
120.70
111.47
55.43
50.13
X : parts per Million : Carbon13

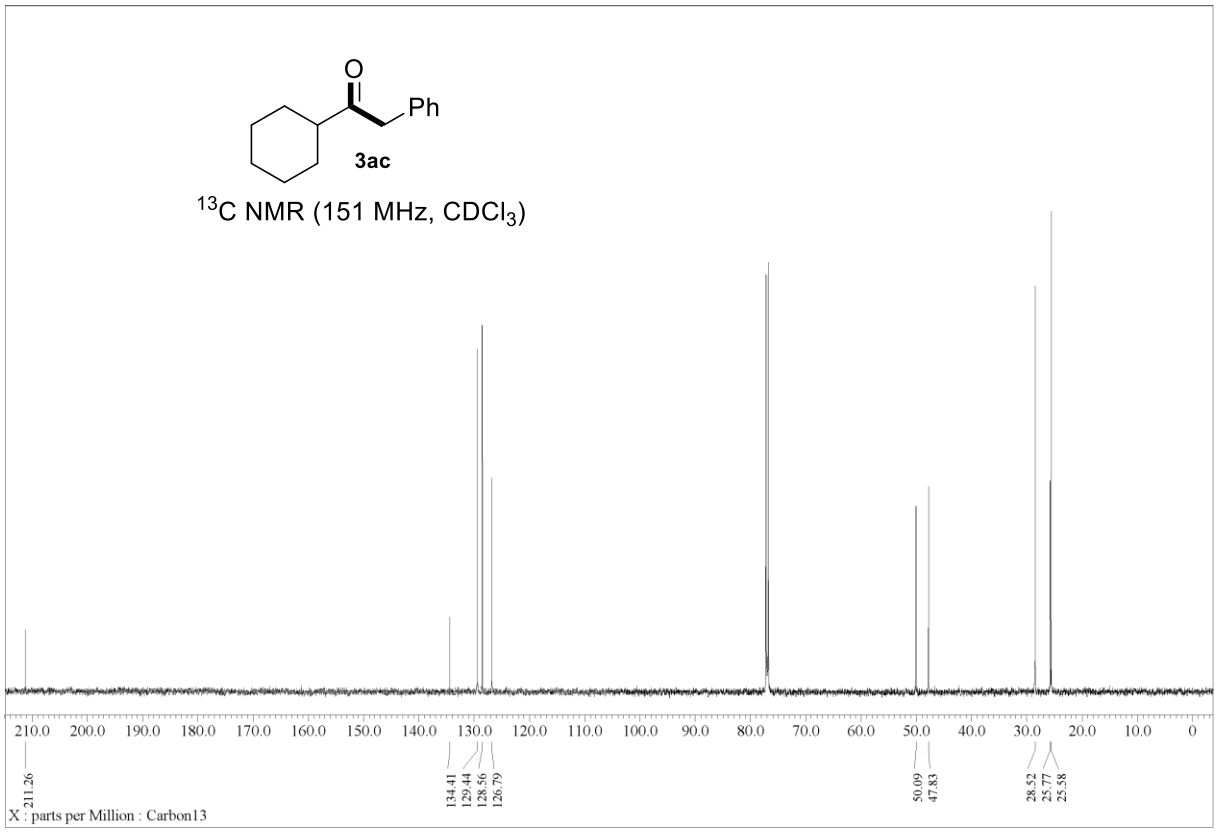

O
Ph
3aa
1H NMR (600 MHz, CDCl3)
3.81
2.03
1.50
1.00
0.98
0.96
8.559
8.083
8.079
8.068
8.064
7.977
7.963
7.901
7.888
7.882
7.868
7.608
7.559
7.348
7.338
7.267
4.427
X : parts per Million : Proton

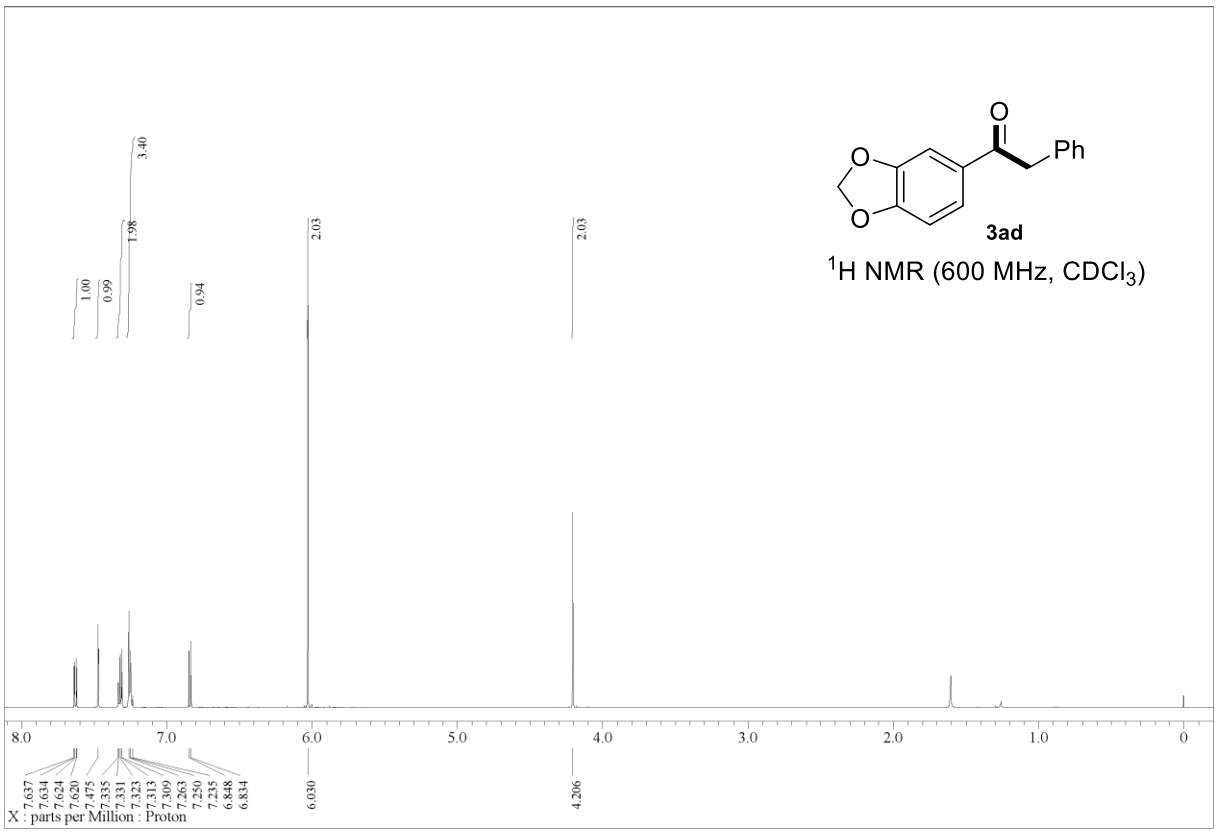

O
Ph
3aa
13C NMR (151 MHz, CDCl3)
197.58
135.57
134.65
133.93
132.48
130.37
129.59
129.47
128.68
128.52
128.49
127.75
126.88
126.77
124.24
45.53
X : parts per Million : Carbon13

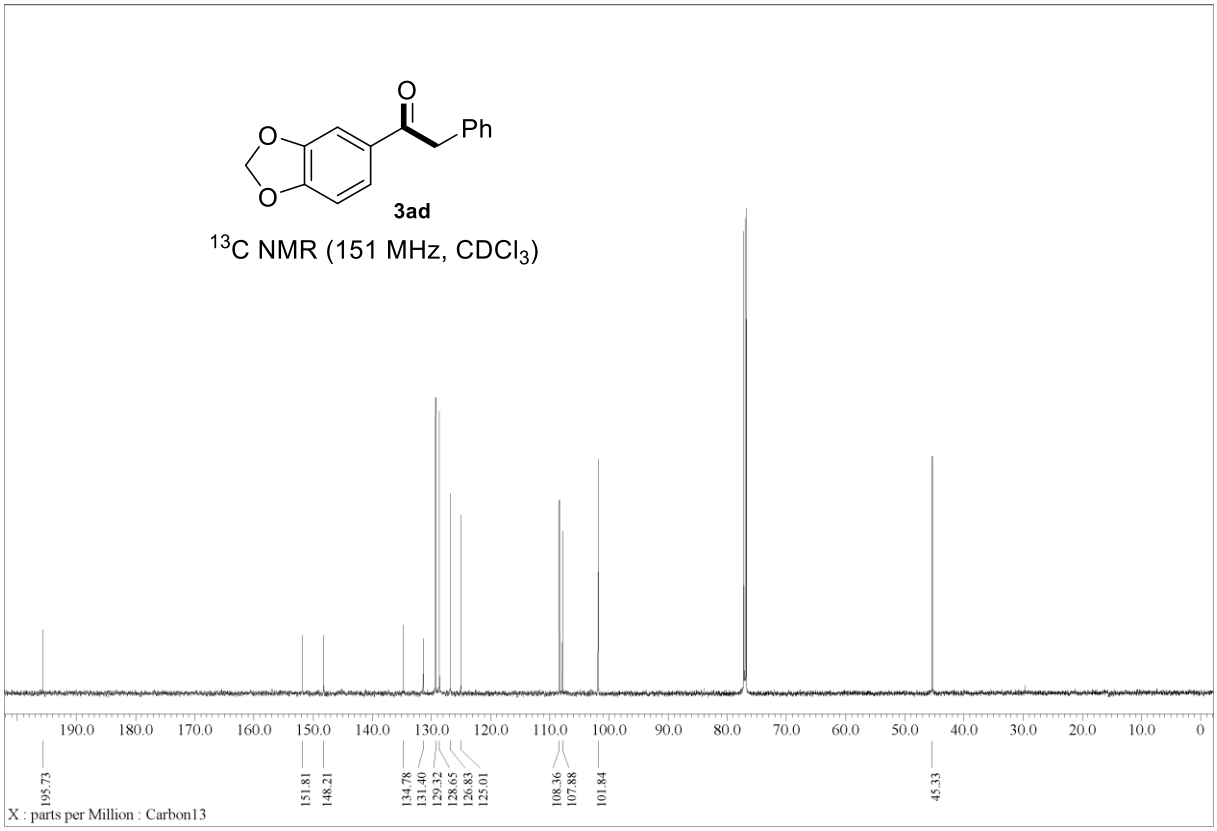

O
Ph
3ab
1H NMR (600 MHz, CDCl3)
1.00
1.04
1.02
0.99
1.05
2.18
4.07
1.81
2.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.582
8.568
7.992
7.978
7.970
7.956
7.875
7.861
7.570
7.527
7.514
7.500
7.487
7.330
7.317
7.302
7.255
4.384
X : parts per Million : Proton

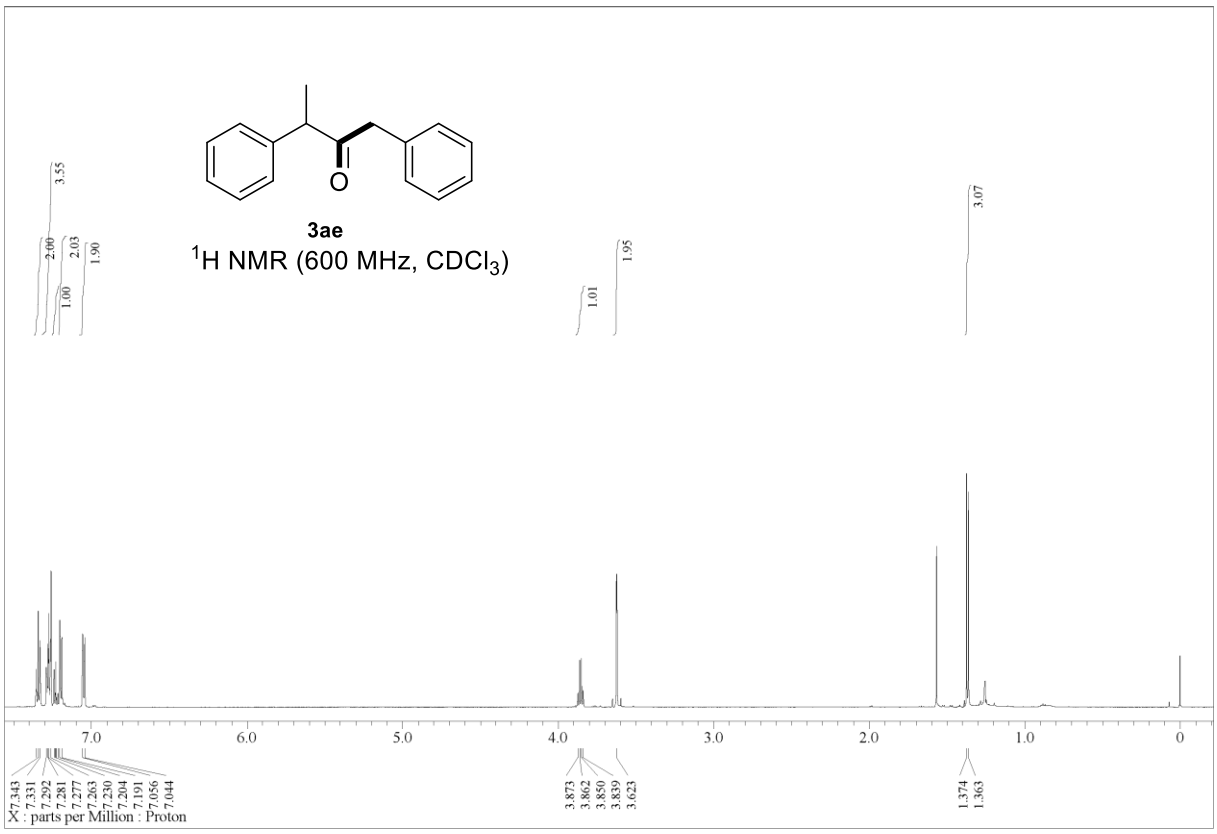

O
Ph
3ab
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
201.50
135.56
134.53
133.96
132.74
130.40
129.49
128.67
128.36
127.96
127.87
126.92
126.46
125.81
124.27
48.90
X : parts per Million : Carbon13

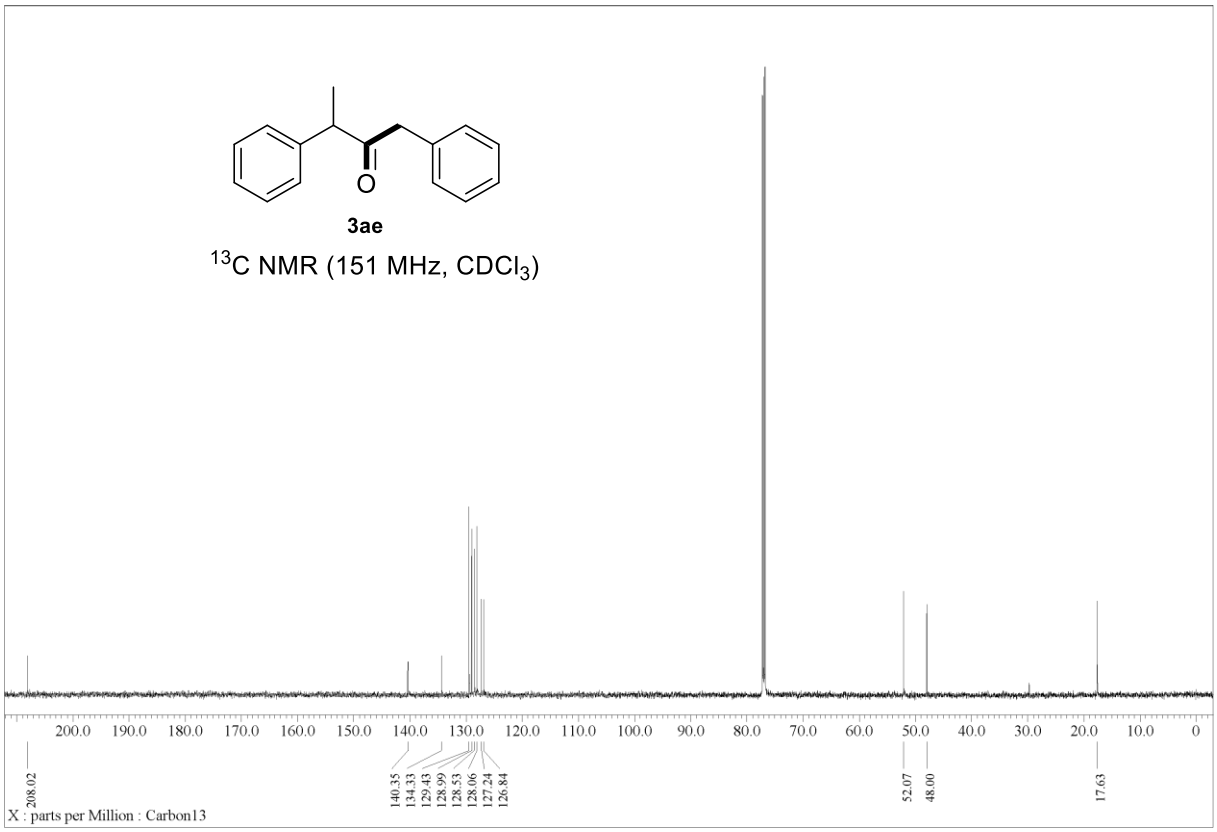

O
Ph
3ac
1H NMR (600 MHz, CDCl3)
2.06
1.92
1.05
2.00
0.95
4.04
1.05
2.02
3.21
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.352
7.340
7.328
7.285
7.273
7.215
7.203
3.749
2.506
2.500
2.495
2.487
2.482
2.476
2.468
2.462
2.456
1.853
1.833
1.799
1.793
1.783
1.777
1.394
1.373
1.354
1.299
1.278
1.262
1.237
1.221
1.201
X : parts per Million : Proton

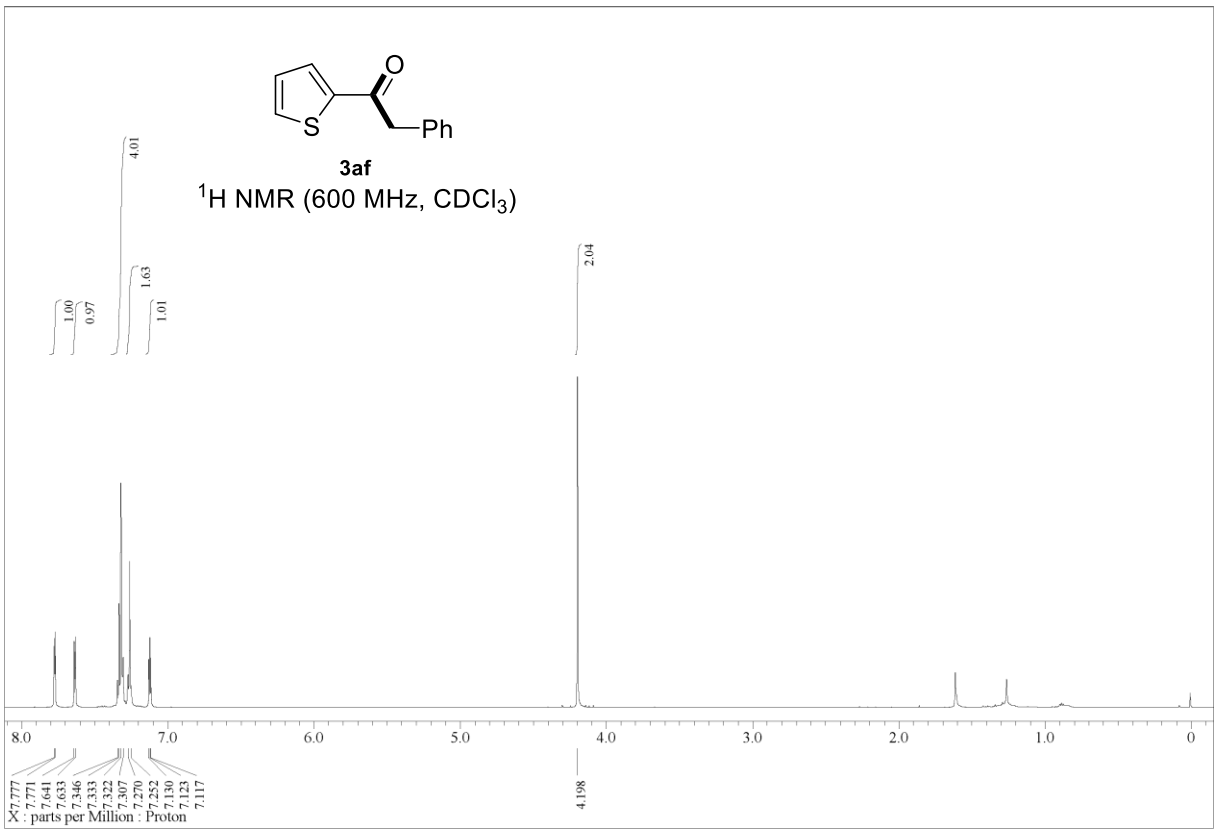

O
Ph
3ac
13C NMR (151 MHz, CDCl3)
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
211.26
134.41
129.44
128.56
126.79
50.09
47.83
28.52
25.77
25.58
X : parts per Million : Carbon13

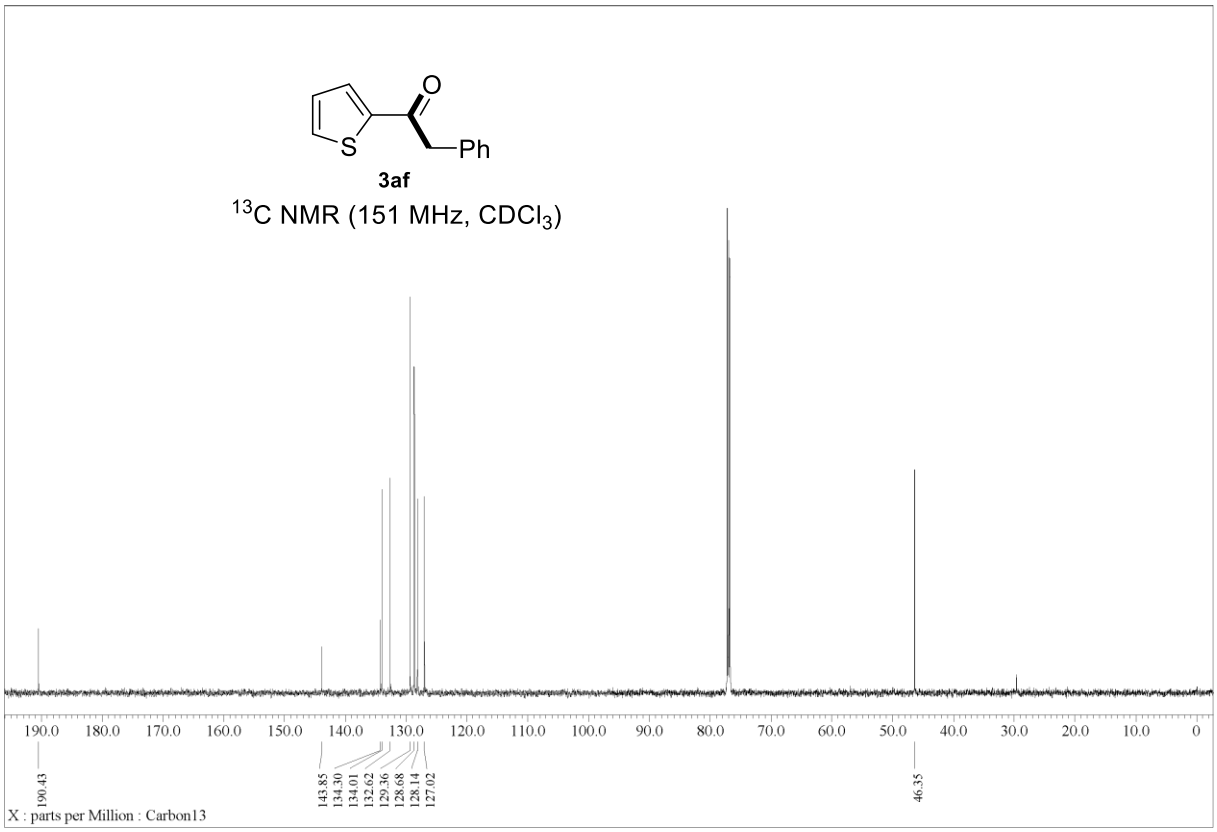

3ad
1H NMR (600 MHz, CDCl3)
3.40
1.98
2.03
2.03
1.00
0.99
0.94
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.637
7.634
7.624
7.620
7.475
7.335
7.331
7.323
7.313
7.309
7.263
7.250
7.235
6.848
6.834
6.030
4.206
X : parts per Million : Proton

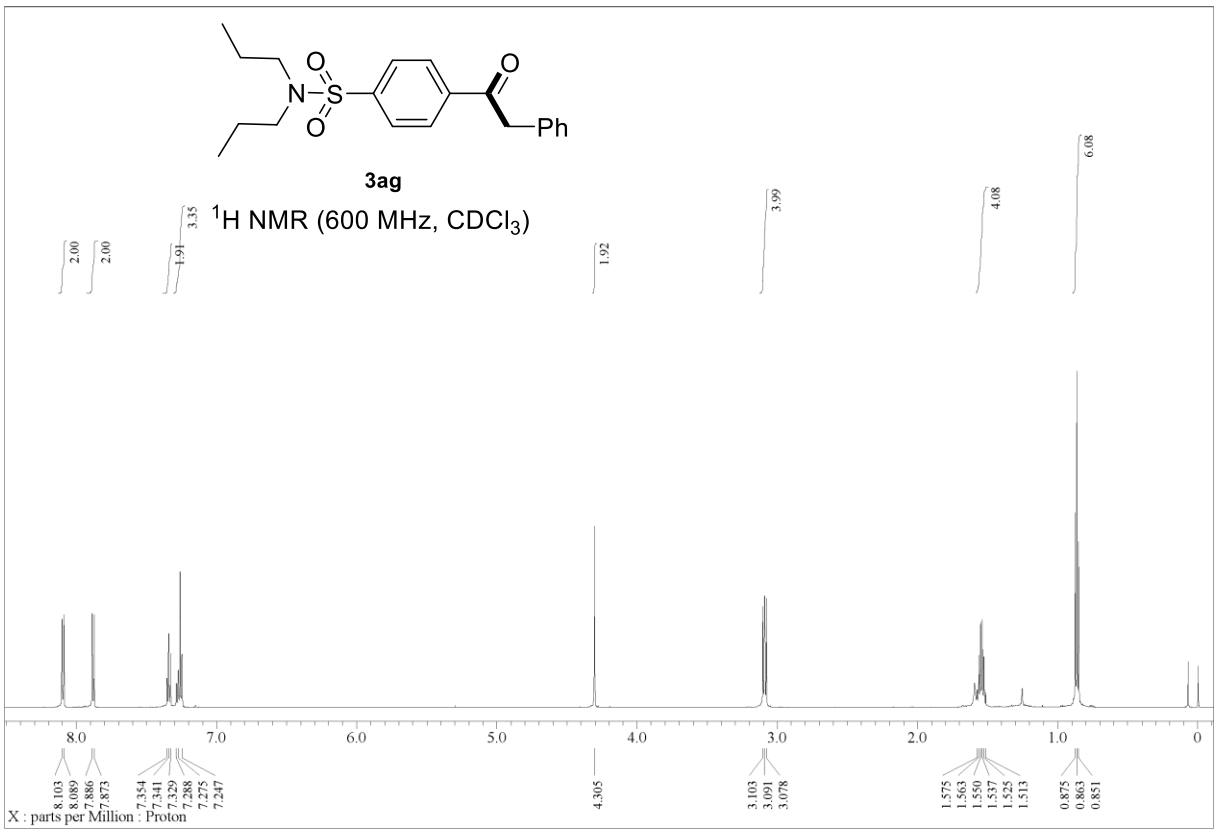

3ad
13C NMR (151 MHz, CDCl3)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
195.73
151.81
148.21
134.78
131.40
129.32
128.65
126.83
125.01
108.36
107.88
101.84
45.33
X : parts per Million : Carbon13

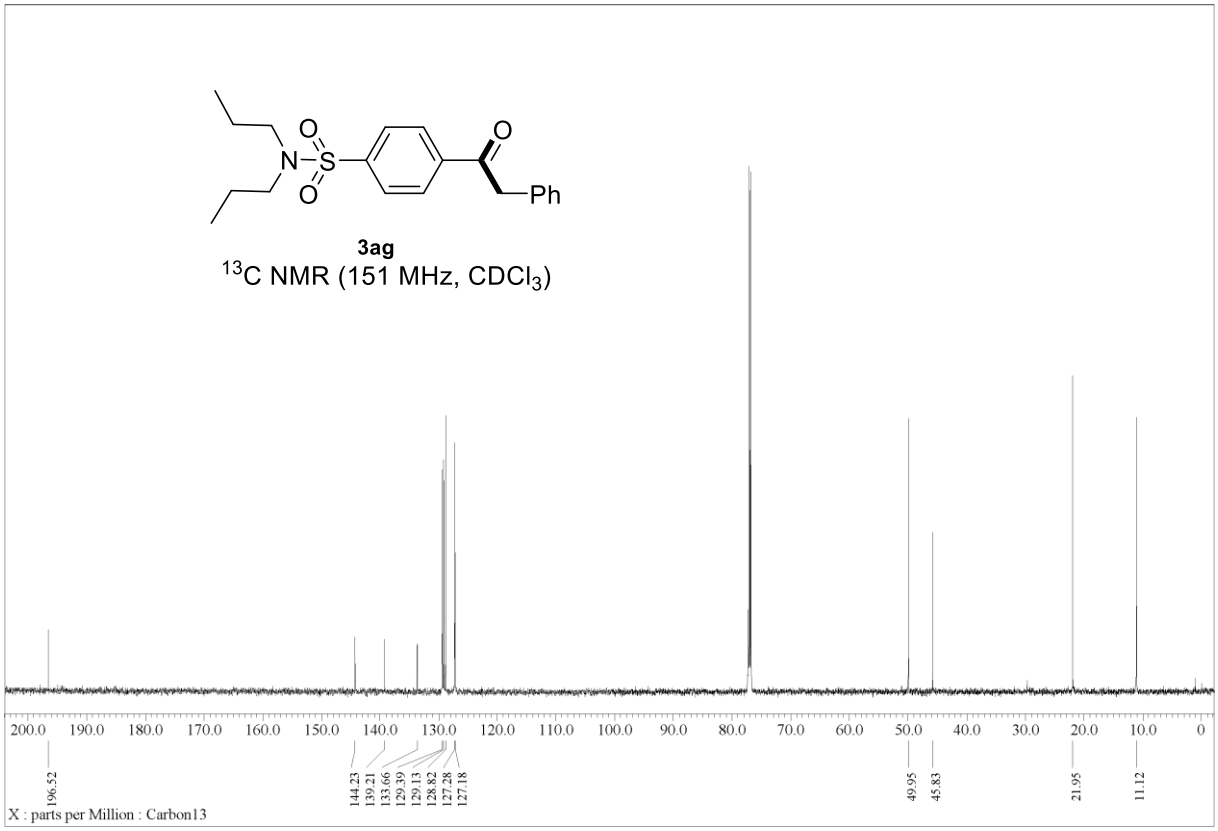

3ae
1H NMR (600 MHz, CDCl3)
3.55
2.00
2.03
1.90
1.00
1.01
1.95
3.07
7.343
7.331
7.292
7.281
7.277
7.263
7.230
7.204
7.191
7.056
7.044
3.873
3.862
3.850
3.839
3.623
1.374
1.363
X : parts per Million : Proton

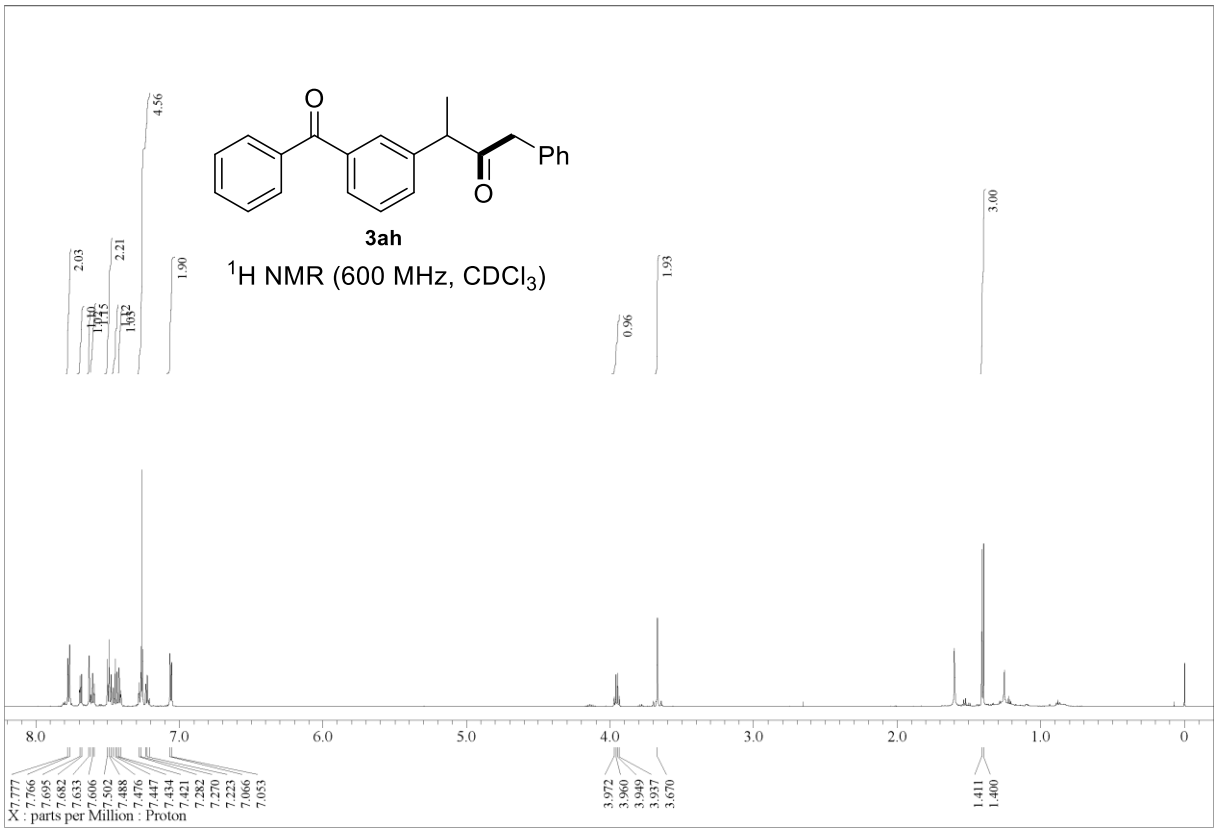

3ae
13C NMR (151 MHz, CDCl3)
208.02
140.35
134.33
129.43
128.99
128.53
128.06
127.24
126.84
52.07
48.00
17.63
X : parts per Million : Carbon13

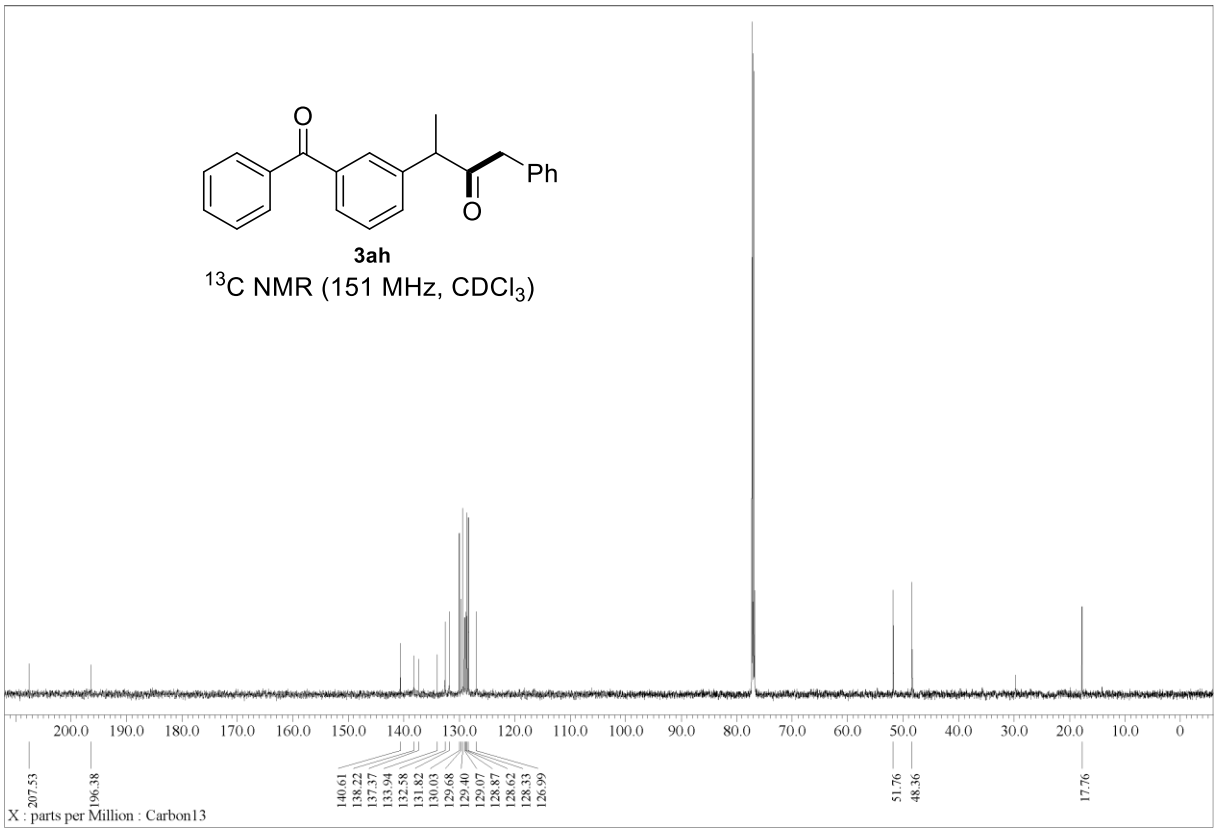

O
S
Ph
3af
1H NMR (600 MHz, CDCl3)
4.01
1.63
1.01
1.00
0.97
2.04
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.777
7.771
7.641
7.633
7.346
7.333
7.322
7.307
7.270
7.252
7.130
7.123
7.117
4.198
X : parts per Million : Proton

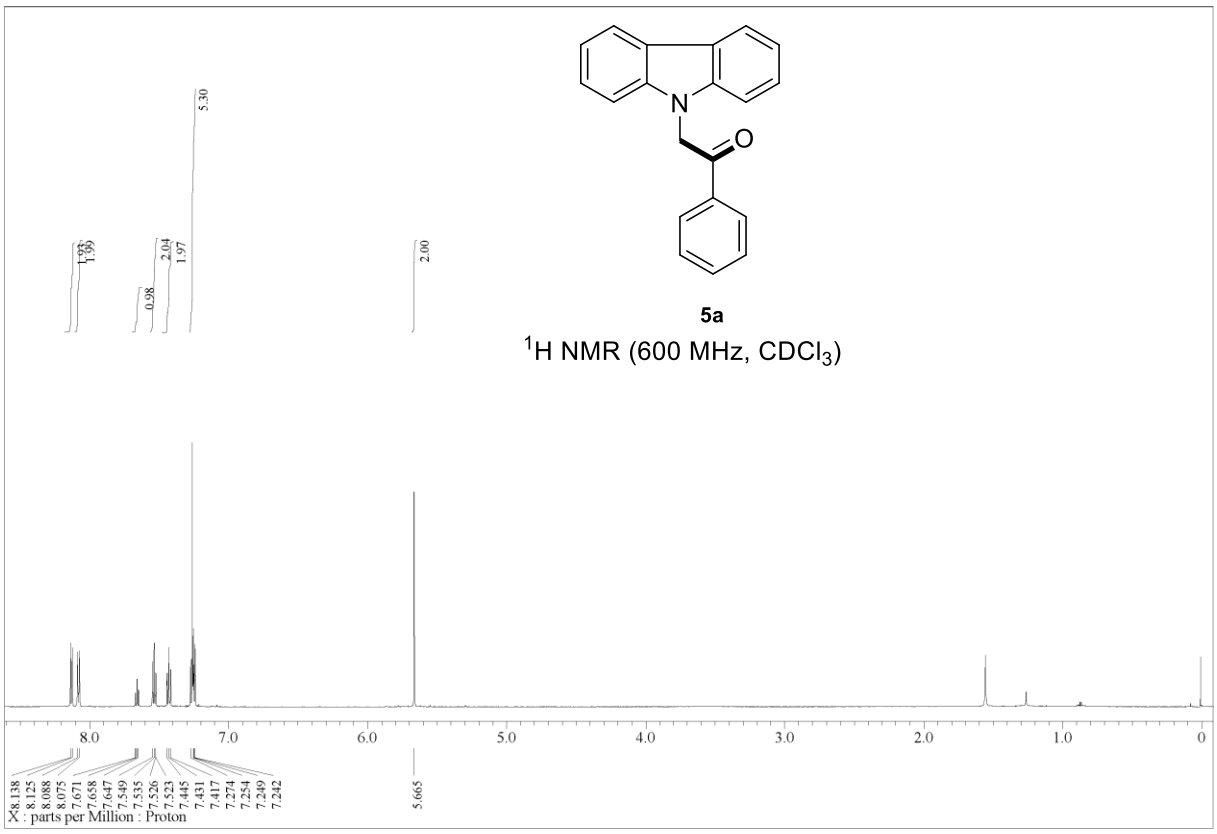

O
S
Ph
3af
13C NMR (151 MHz, CDCl3)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
190.43
143.85
134.30
134.01
132.62
129.36
128.68
128.14
127.02
46.35
X : parts per Million : Carbon13


3ag
^{1}H NMR (600 MHz, $CDCl_3$)
X : parts per Million : Proton


3ag
^{13}C NMR (151 MHz, $CDCl_3$)
X : parts per Million : Carbon13

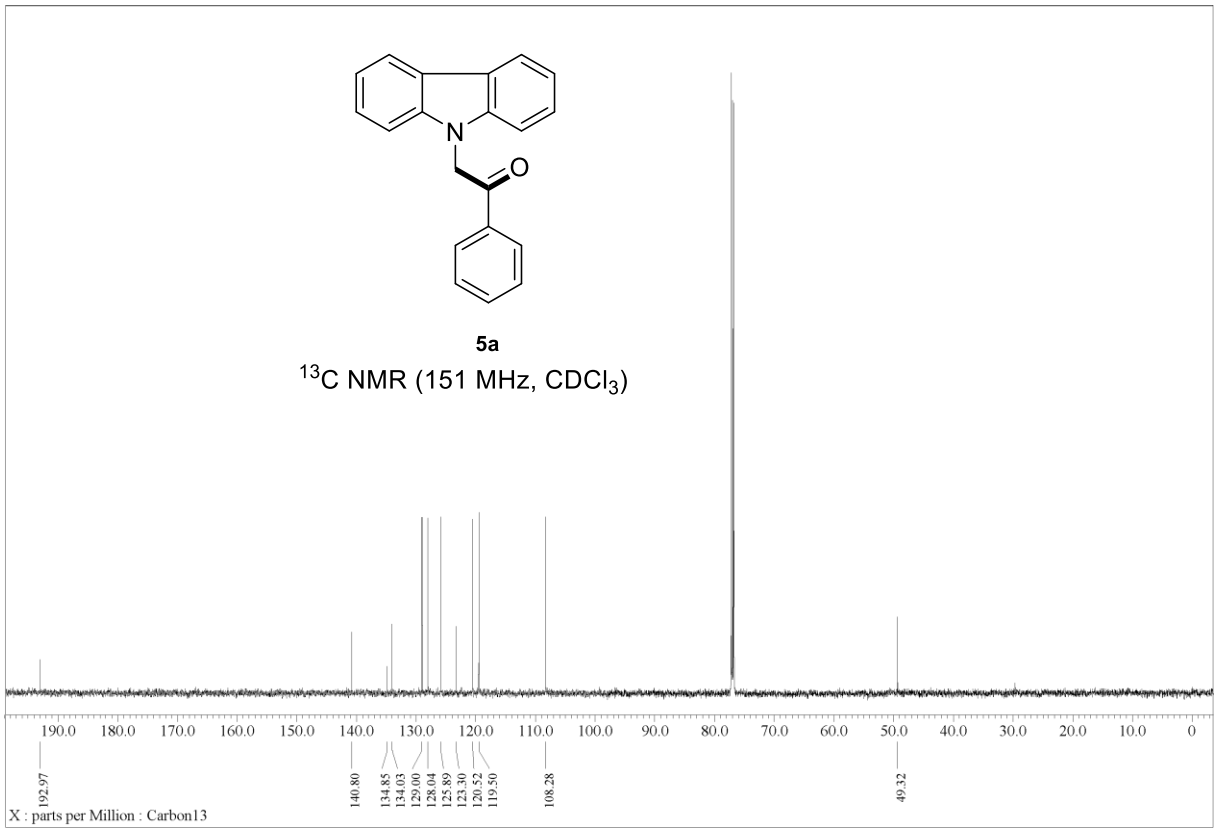

O
Ph
O
3ah
^{1}H NMR (600 MHz, $CDCl_3$)
4.56
2.03
2.21
1.90
1.93
0.96
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.777
7.766
7.695
7.682
7.633
7.606
7.502
7.488
7.476
7.447
7.434
7.421
7.282
7.270
7.223
7.066
7.053
3.972
3.960
3.949
3.937
3.670
1.411
1.400
X : parts per Million : Proton


O
Ph
O
3ah
^{13}C NMR (151 MHz, $CDCl_3$)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
207.53
196.38
140.61
138.22
137.37
133.94
132.58
131.82
130.03
129.68
129.40
129.07
128.87
128.62
128.33
126.99
51.76
48.36
17.76
X : parts per Million : Carbon13



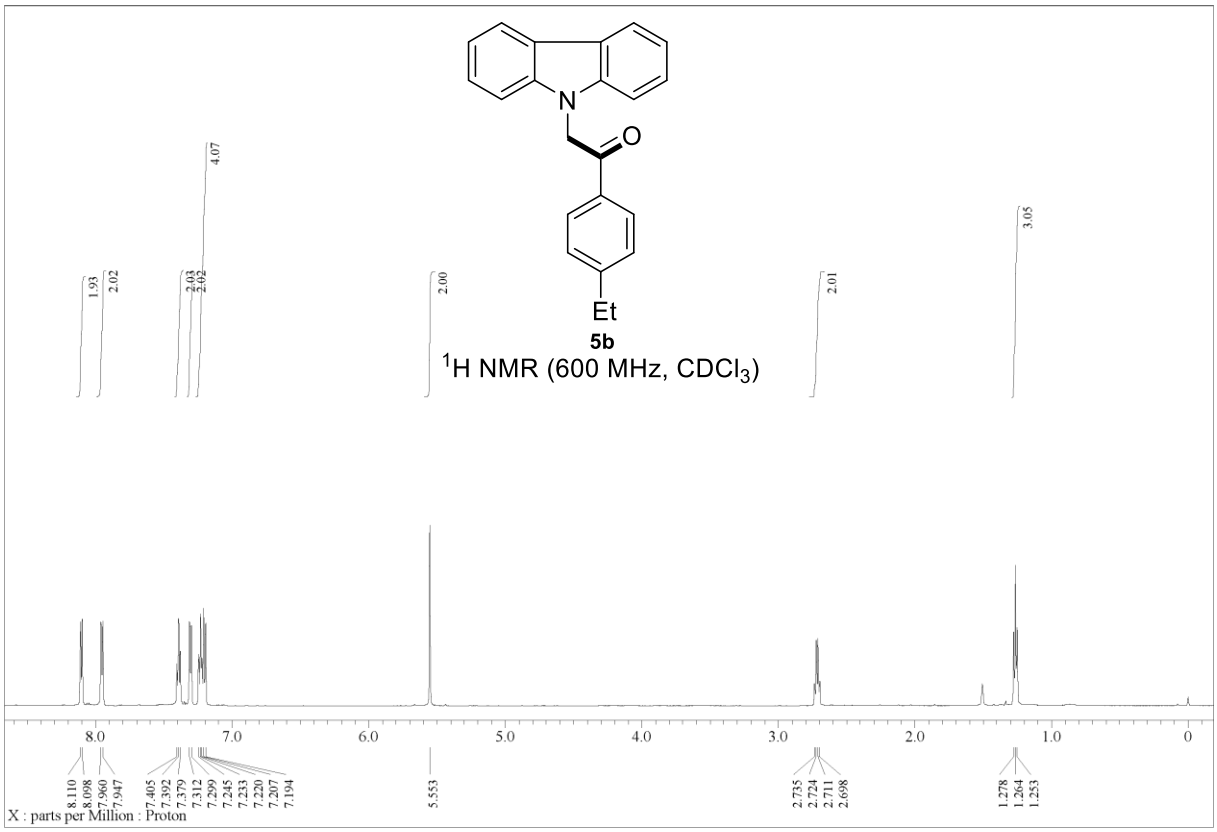
5a

^{1}H NMR (600 MHz, $CDCl_3$)



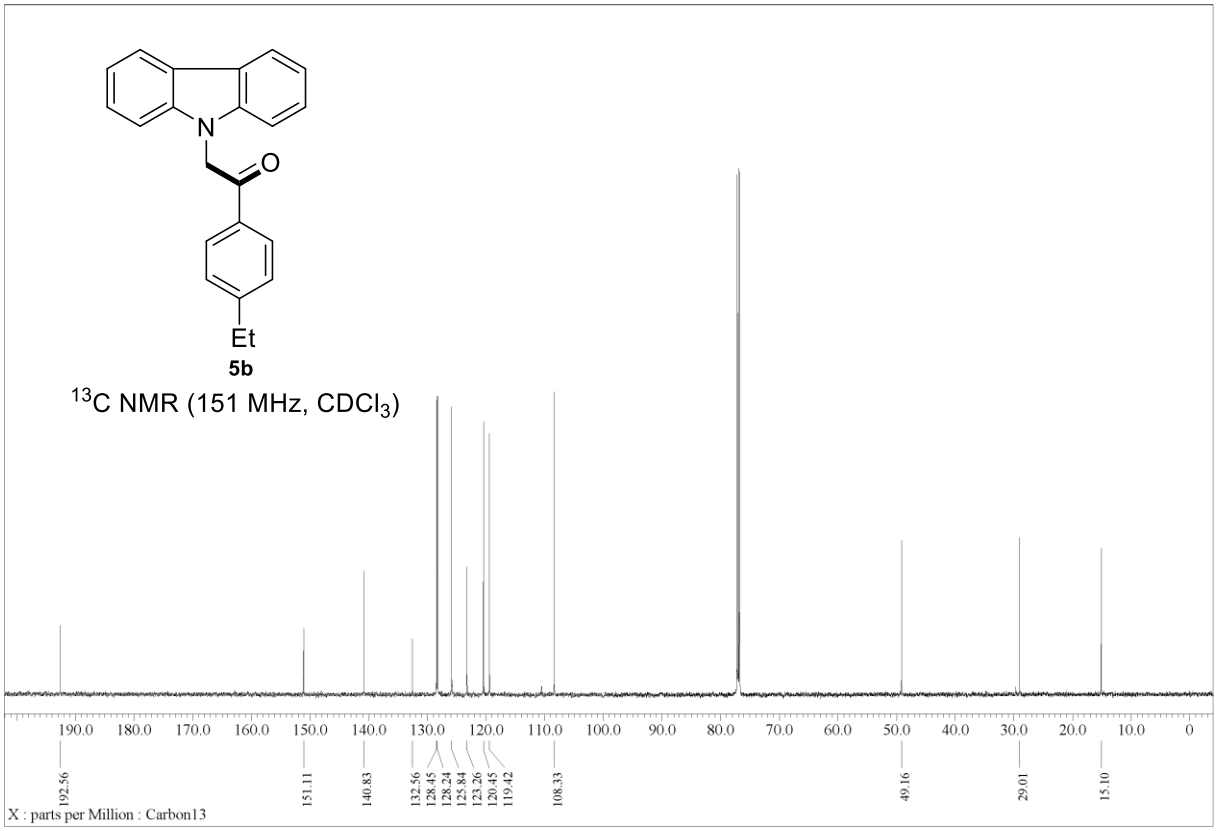
5a

^{13}C NMR (151 MHz, $CDCl_3$)



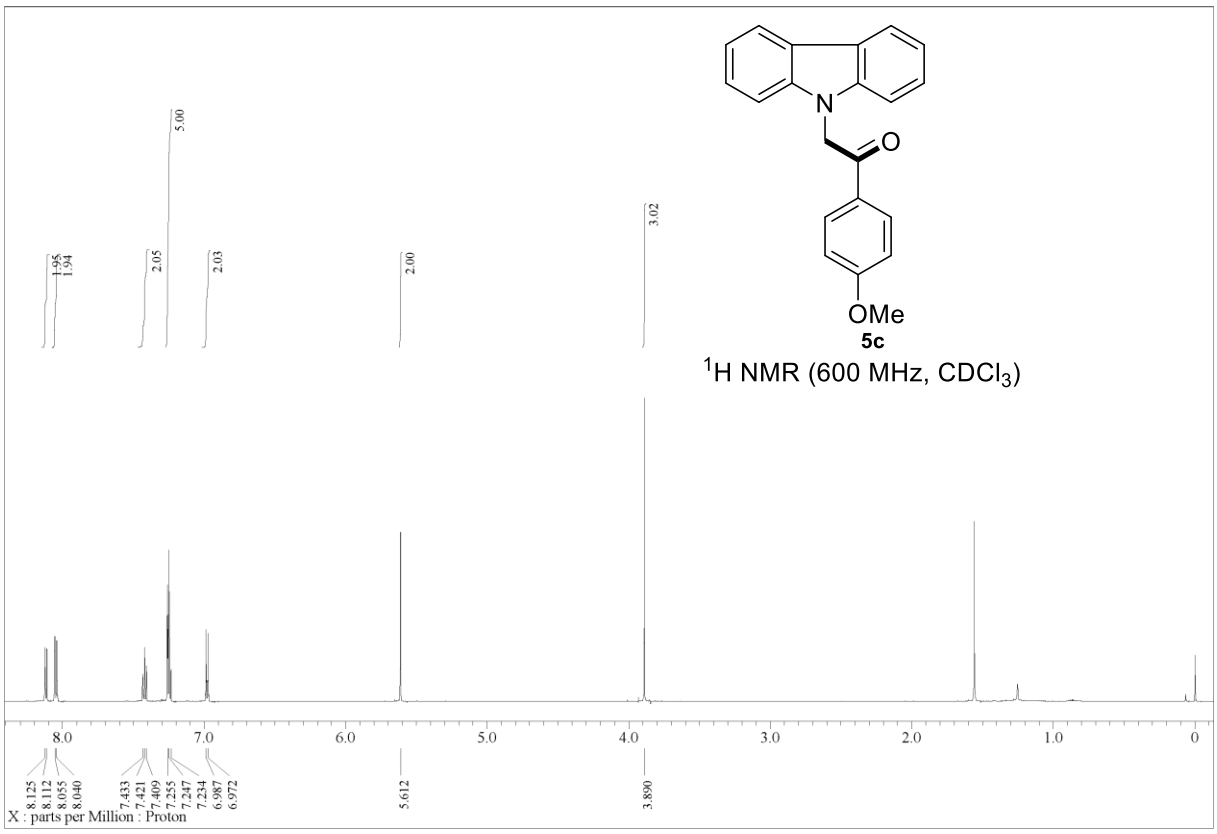
5b

^{1}H NMR (600 MHz, $CDCl_3$)



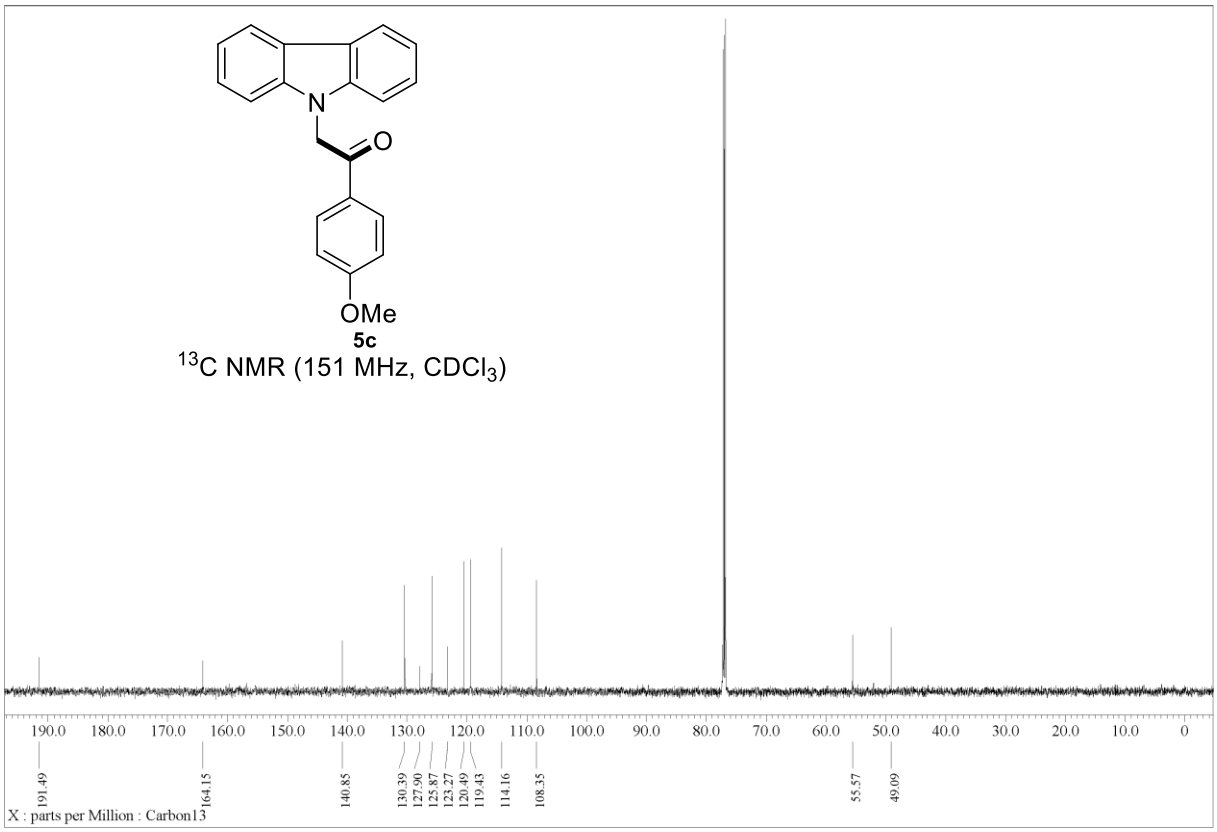
5b

^{13}C NMR (151 MHz, $CDCl_3$)



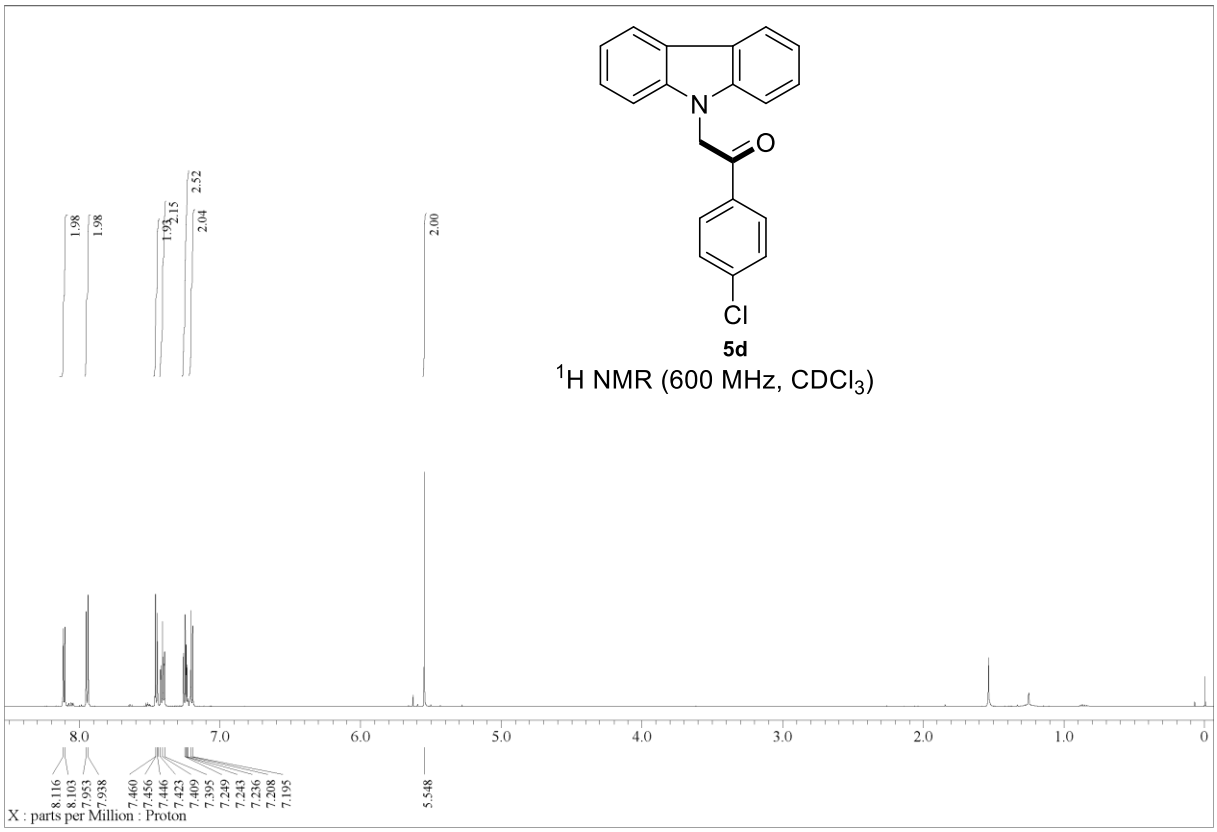
5c

^{1}H NMR (600 MHz, $CDCl_3$)



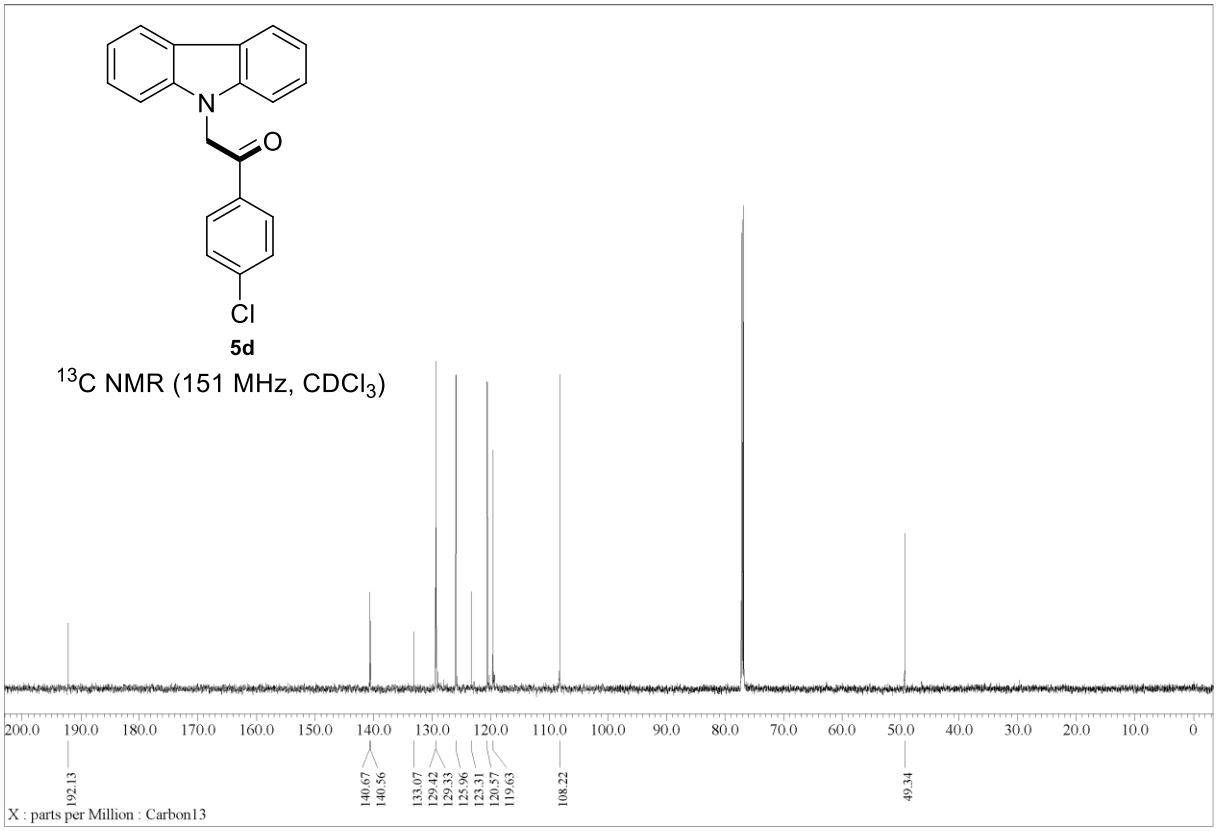
5c

^{13}C NMR (151 MHz, $CDCl_3$)



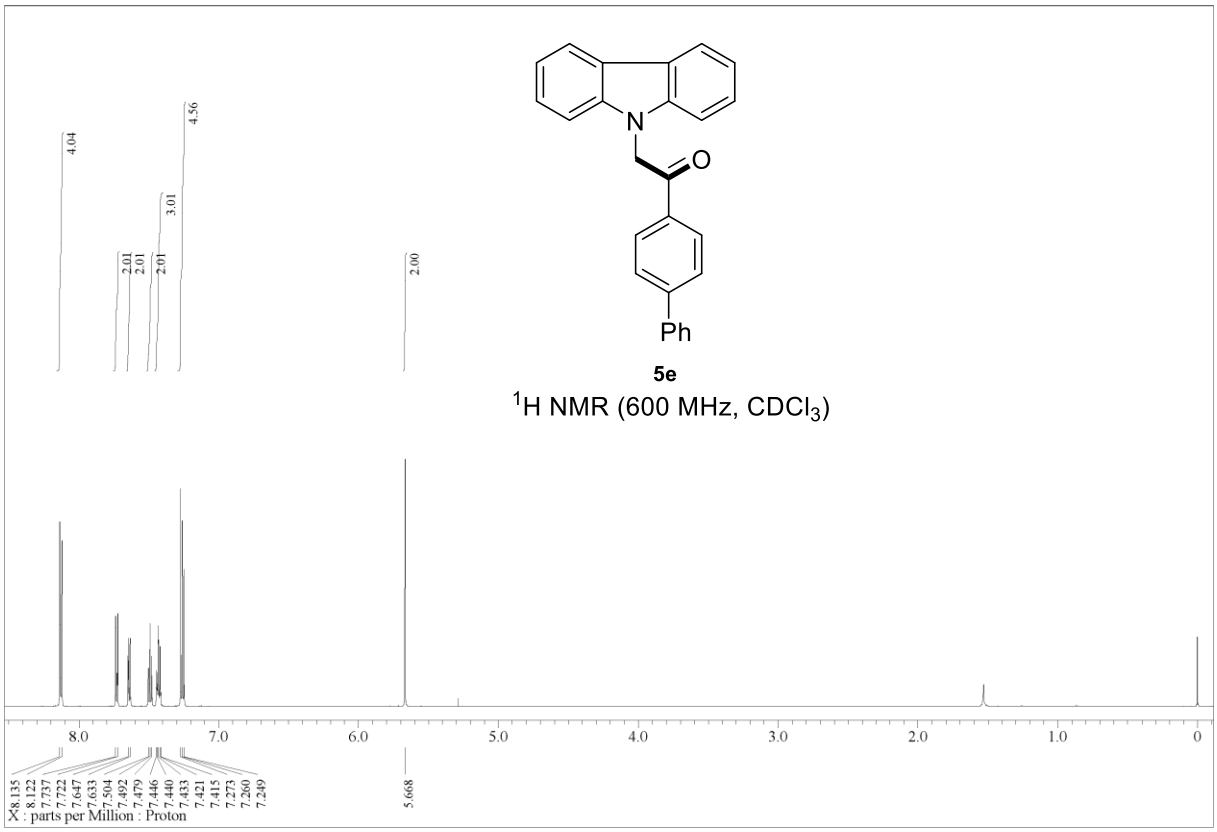
5d

^{1}H NMR (600 MHz, $CDCl_3$)



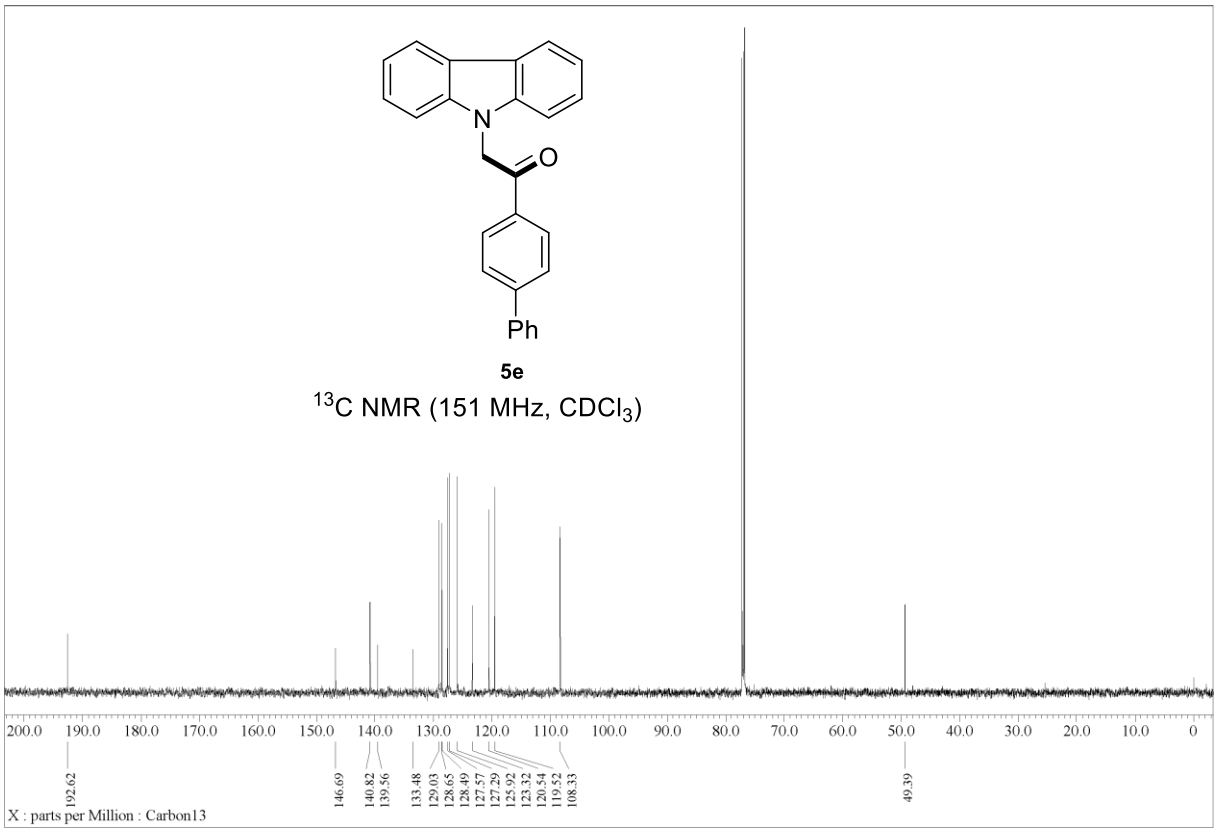
5d

^{13}C NMR (151 MHz, $CDCl_3$)



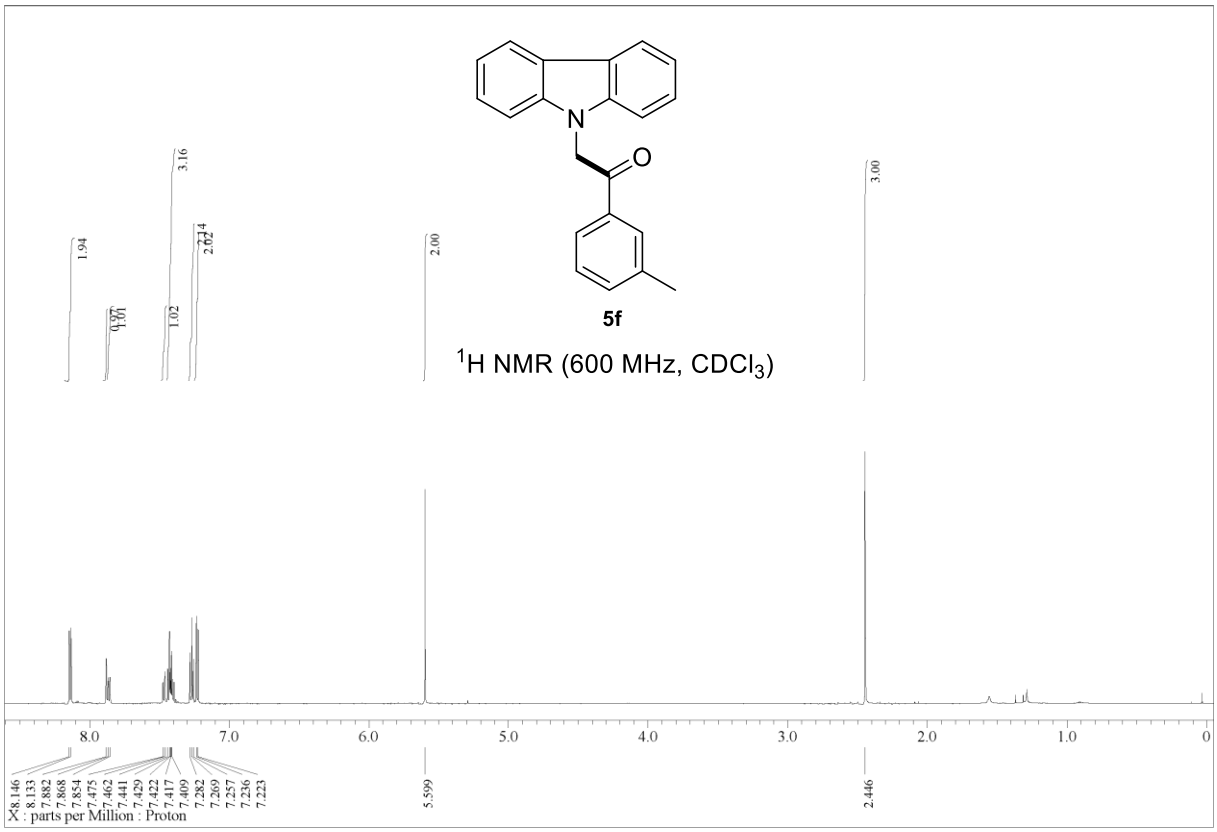
5e

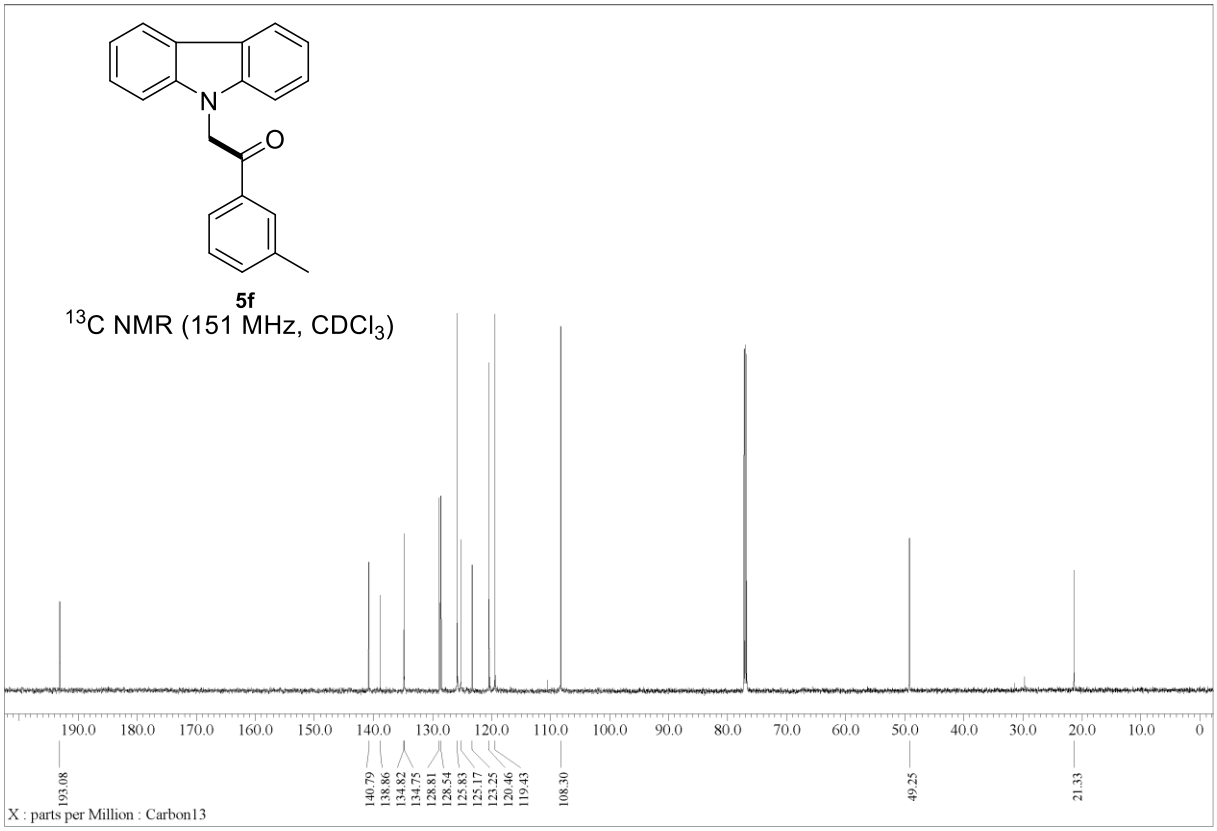
^{1}H NMR (600 MHz, $CDCl_3$)

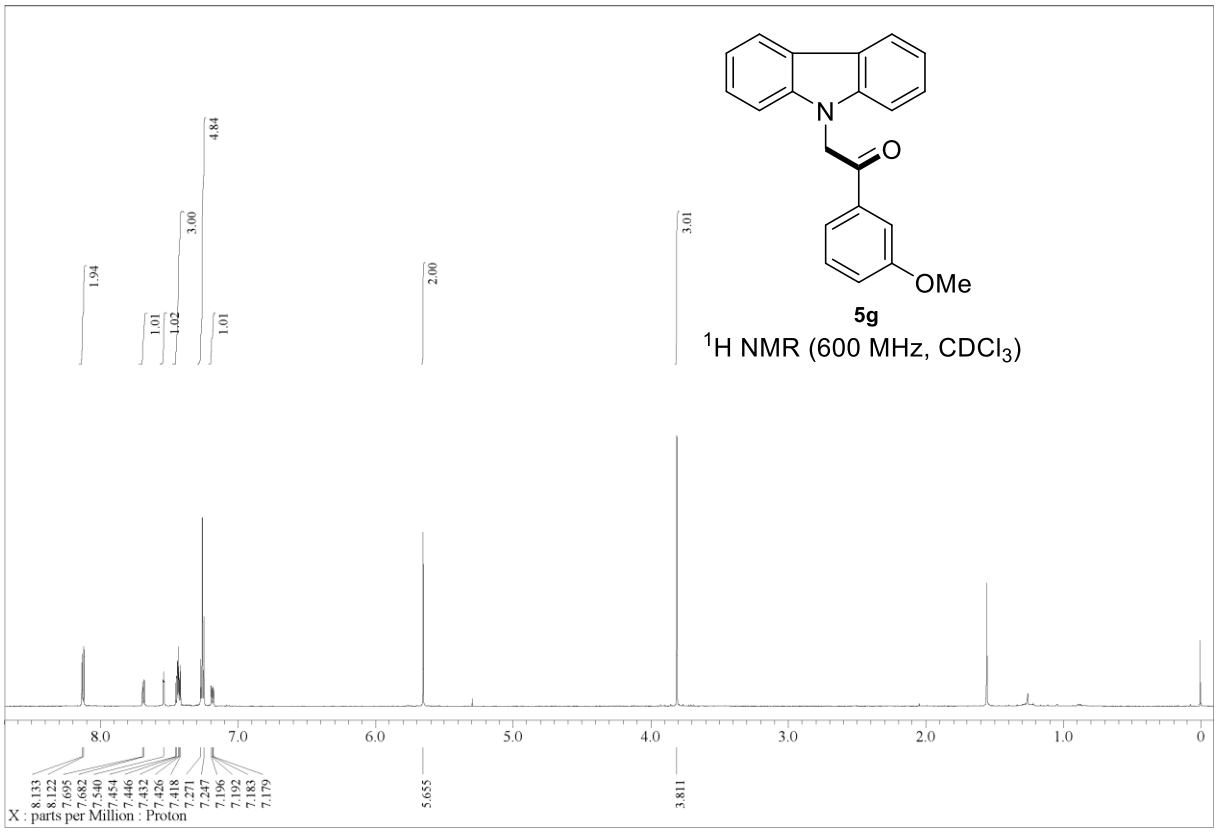


5e

^{13}C NMR (151 MHz, $CDCl_3$)

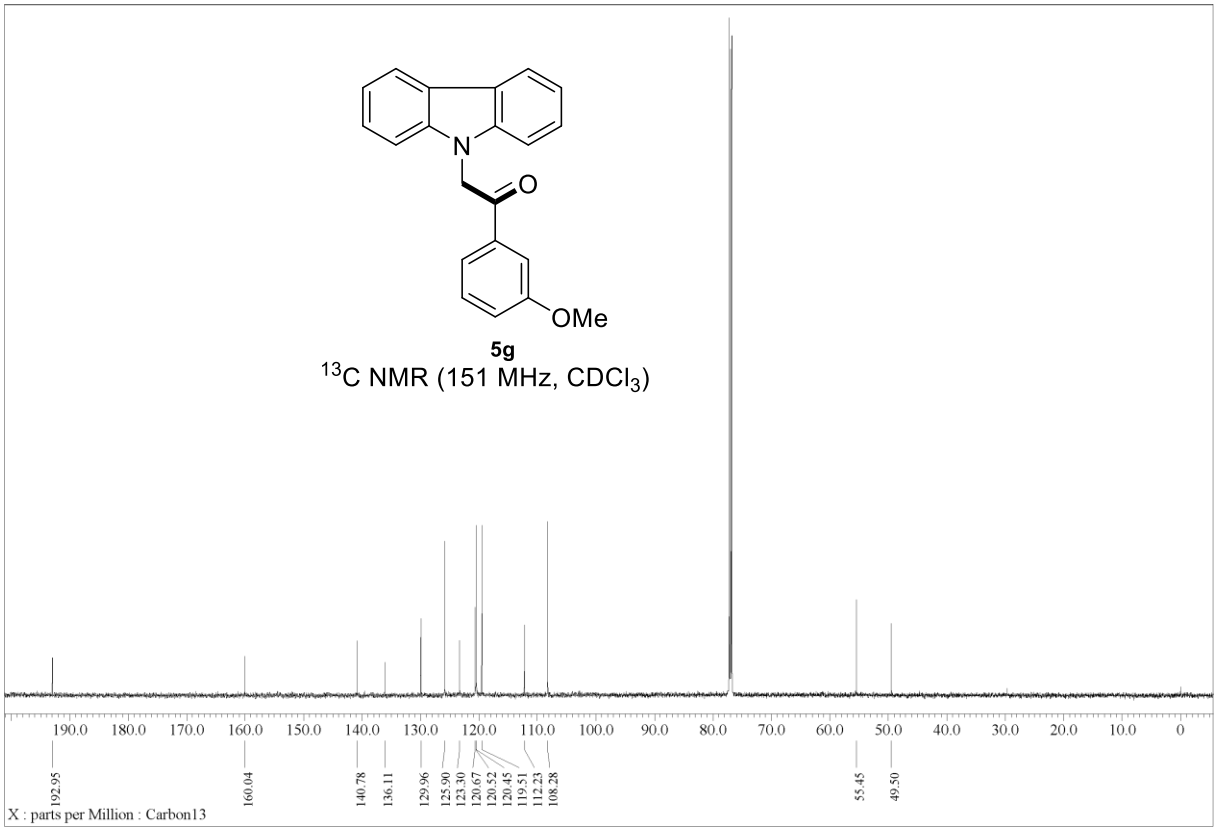

N
O
5f
1H NMR (600 MHz, CDCl3)
1.94
0.97
1.01
3.16
1.02
2.02
2.14
2.00
3.00
8.146
8.133
7.882
7.868
7.854
7.475
7.462
7.441
7.429
7.422
7.417
7.409
7.282
7.269
7.257
7.236
7.223
5.599
2.446
X : parts per Million : Proton


N
O
5f
13C NMR (151 MHz, CDCl3)
193.08
140.79
138.86
134.82
134.75
128.81
128.54
125.83
125.17
123.25
120.46
119.43
108.30
49.25
21.33
X : parts per Million : Carbon13



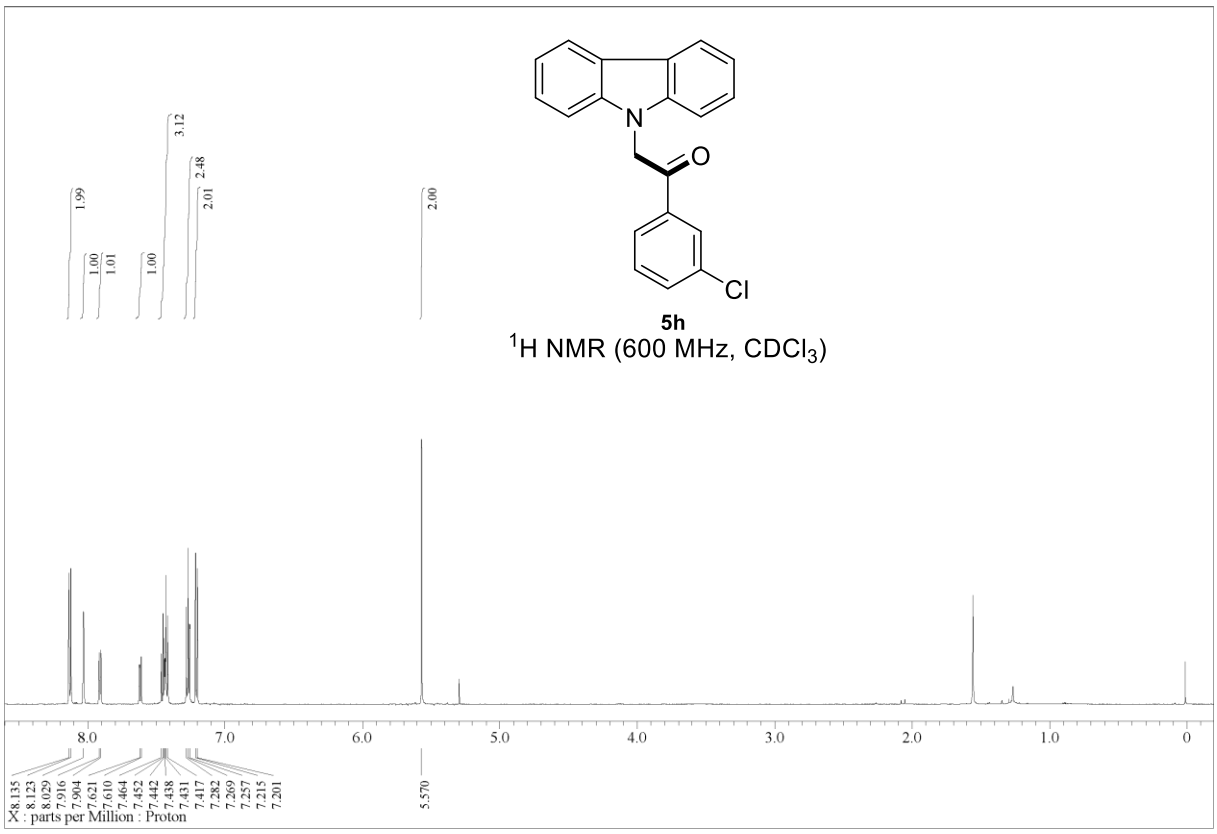
5g

^{1}H NMR (600 MHz, $CDCl_3$)



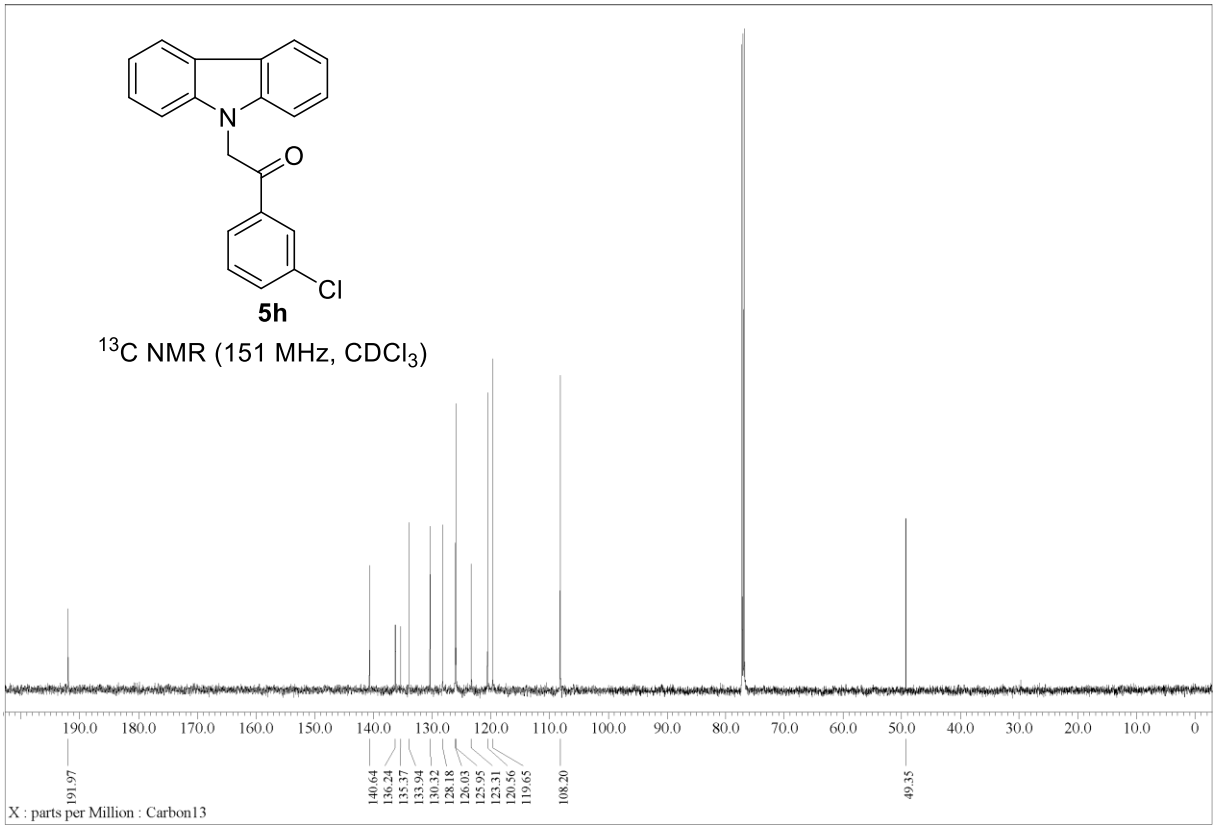
5g

^{13}C NMR (151 MHz, $CDCl_3$)



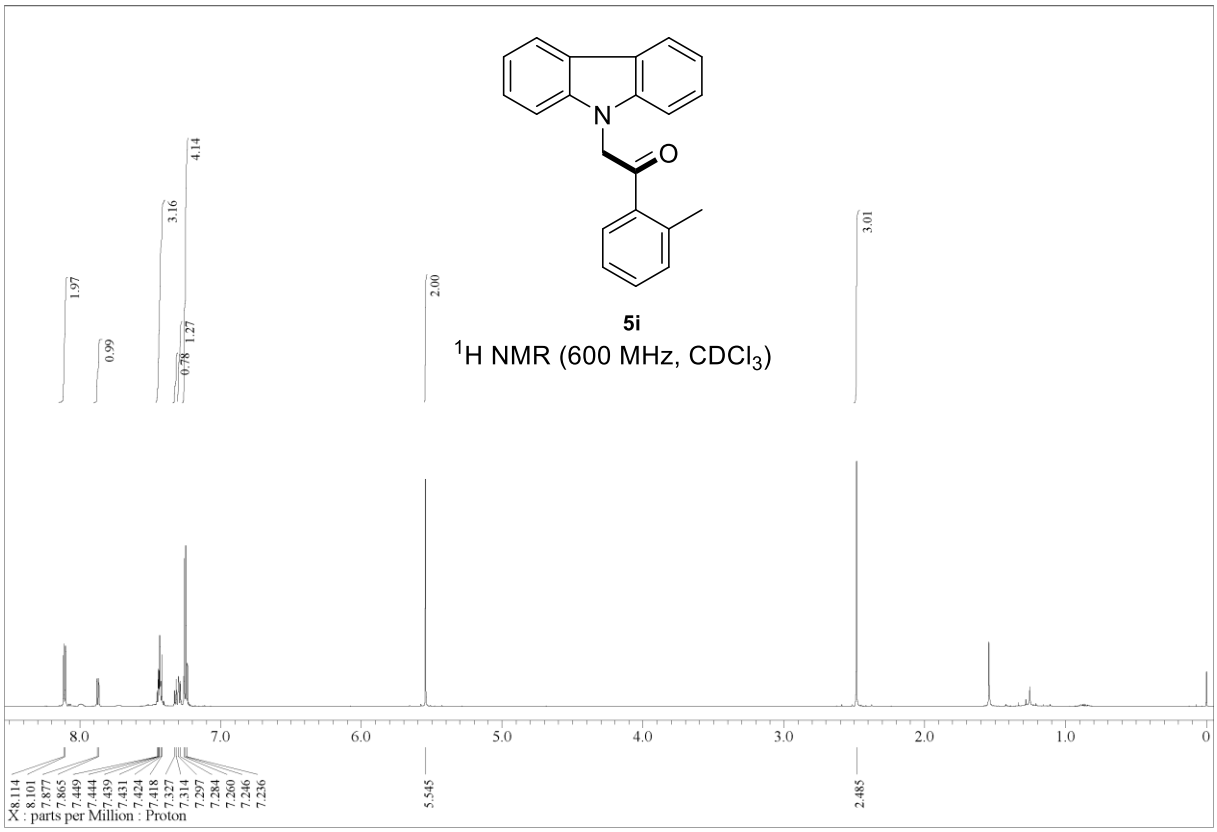
5h

^{1}H NMR (600 MHz, $CDCl_3$)



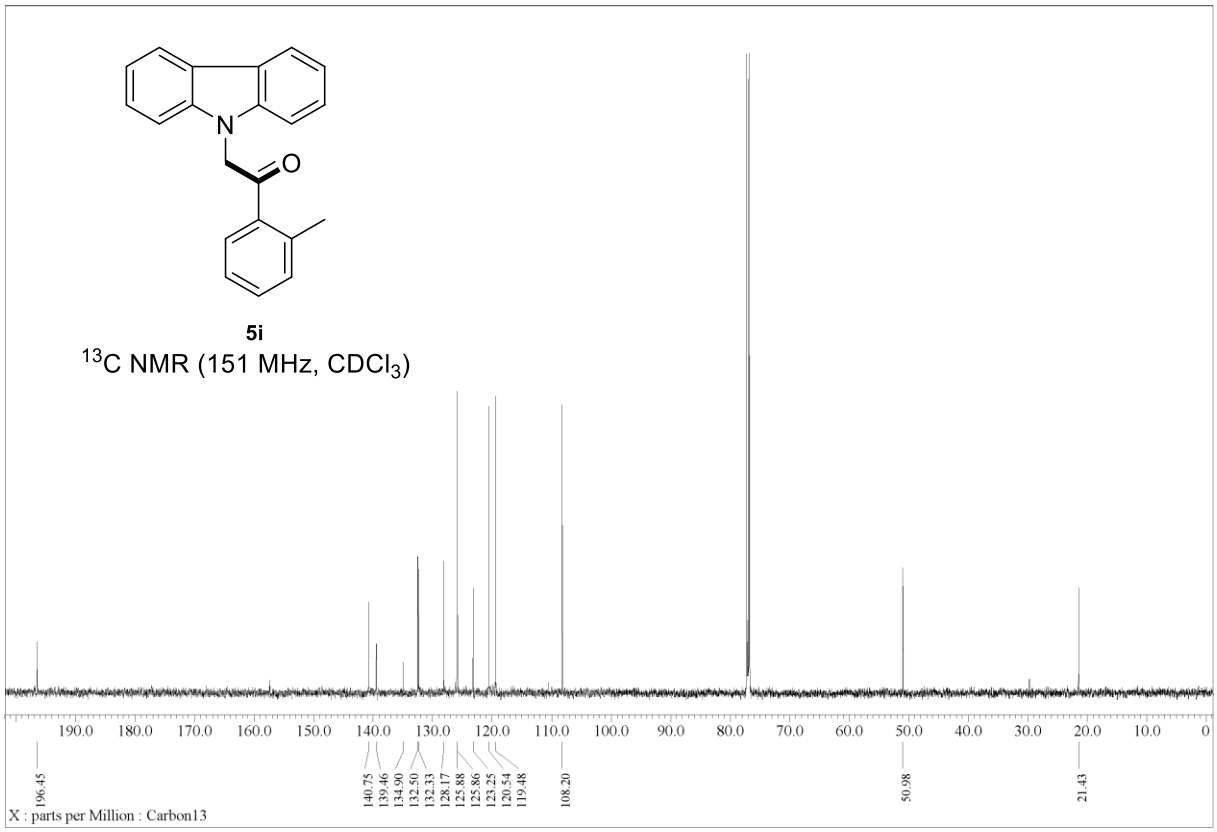
5h

^{13}C NMR (151 MHz, $CDCl_3$)



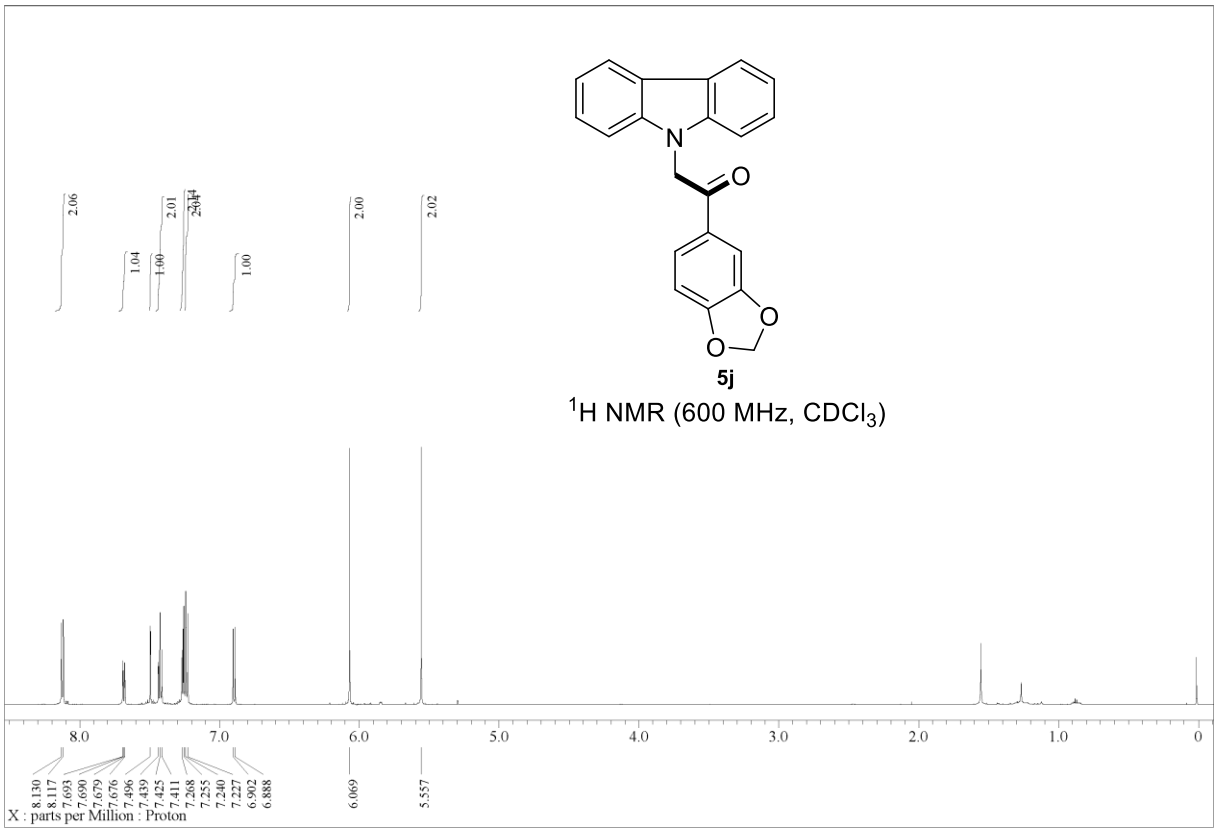
5i

^{1}H NMR (600 MHz, $CDCl_3$)



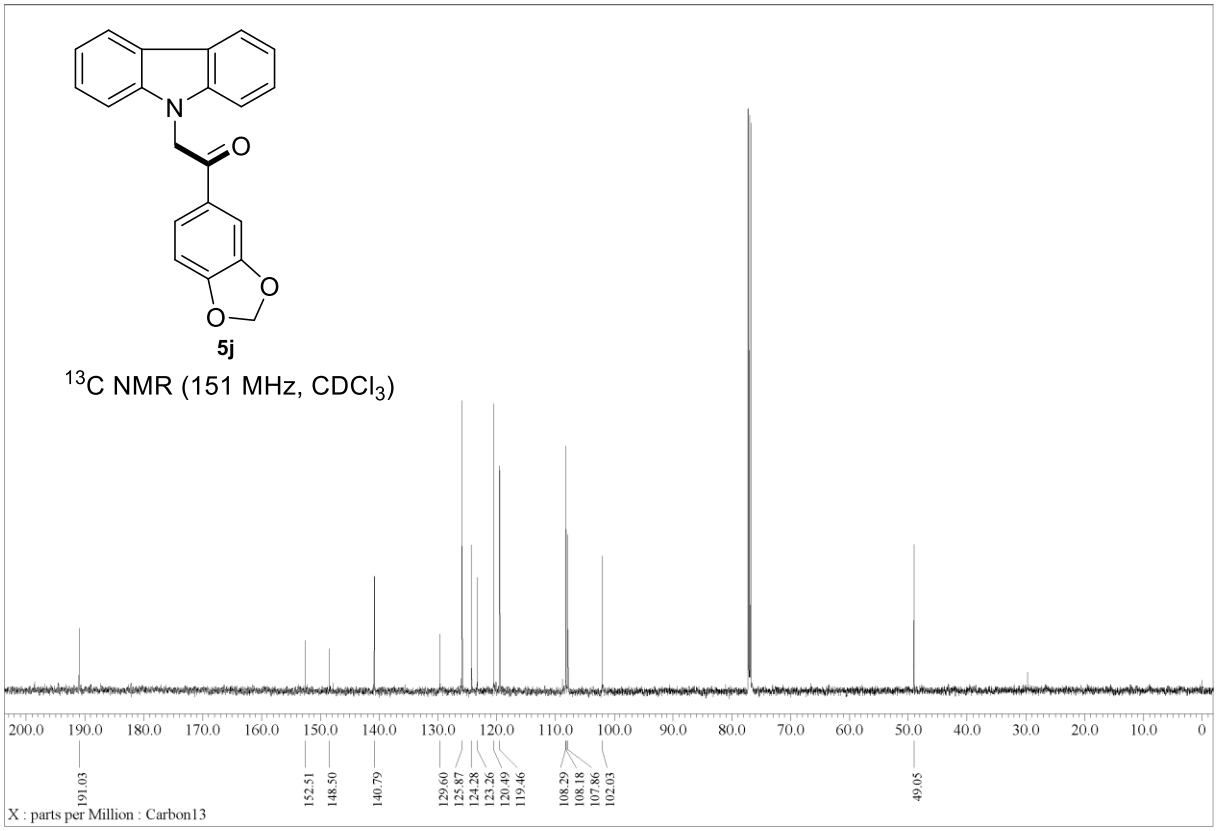
5i

^{13}C NMR (151 MHz, $CDCl_3$)



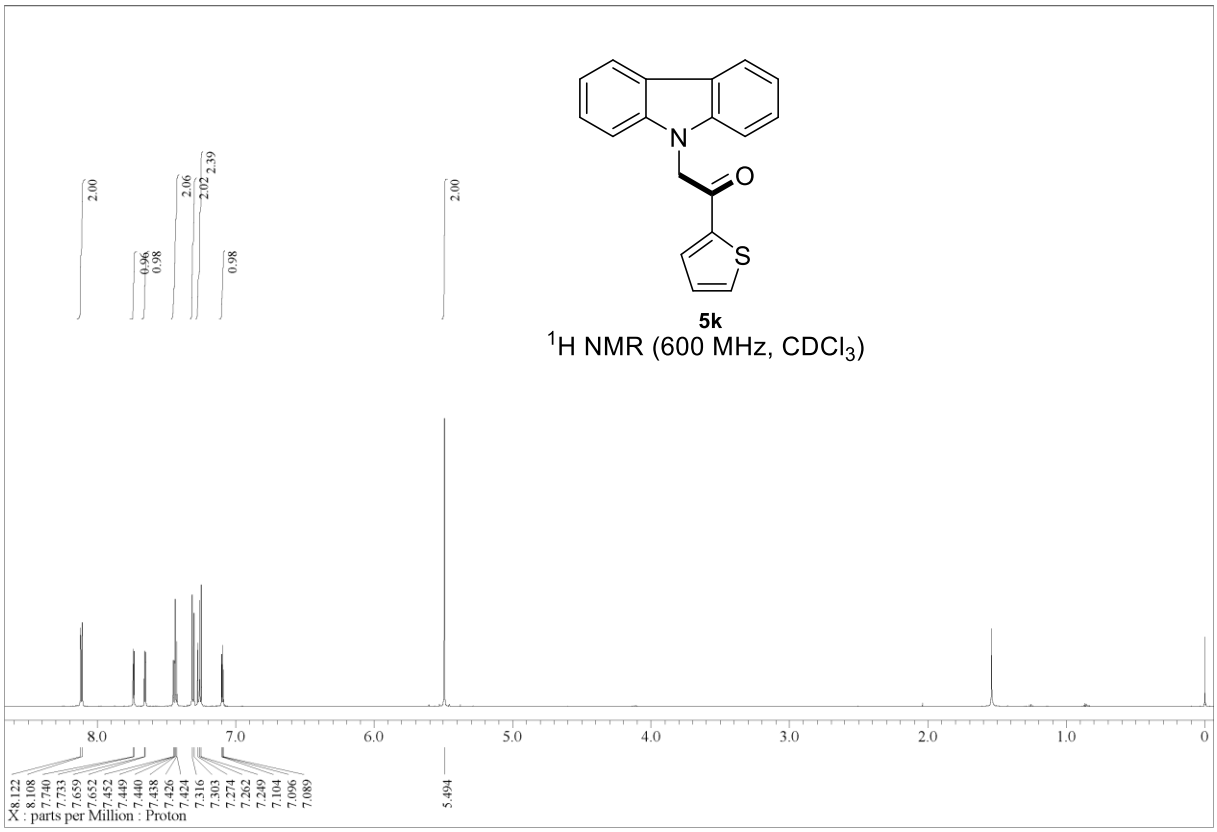
5j

^{1}H NMR (600 MHz, $CDCl_3$)



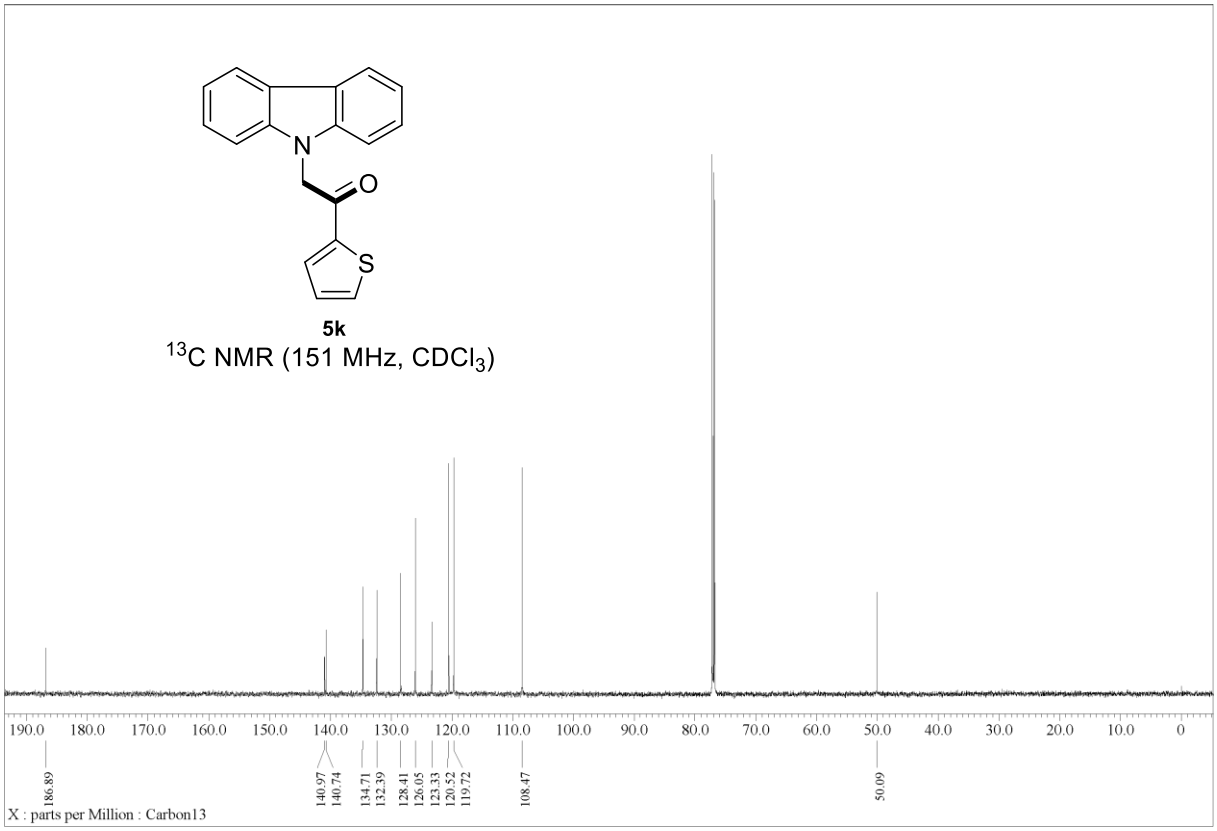
5j

^{13}C NMR (151 MHz, $CDCl_3$)



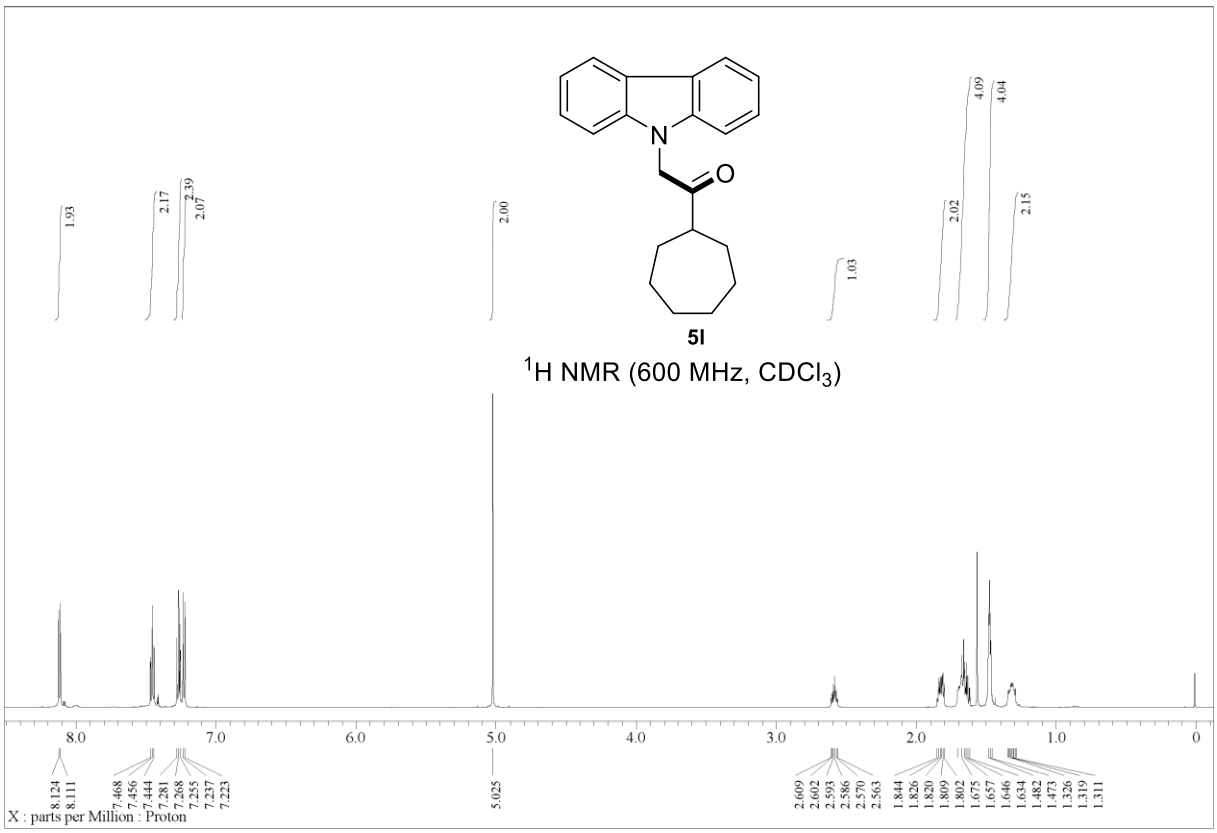
5k

^{1}H NMR (600 MHz, $CDCl_3$)



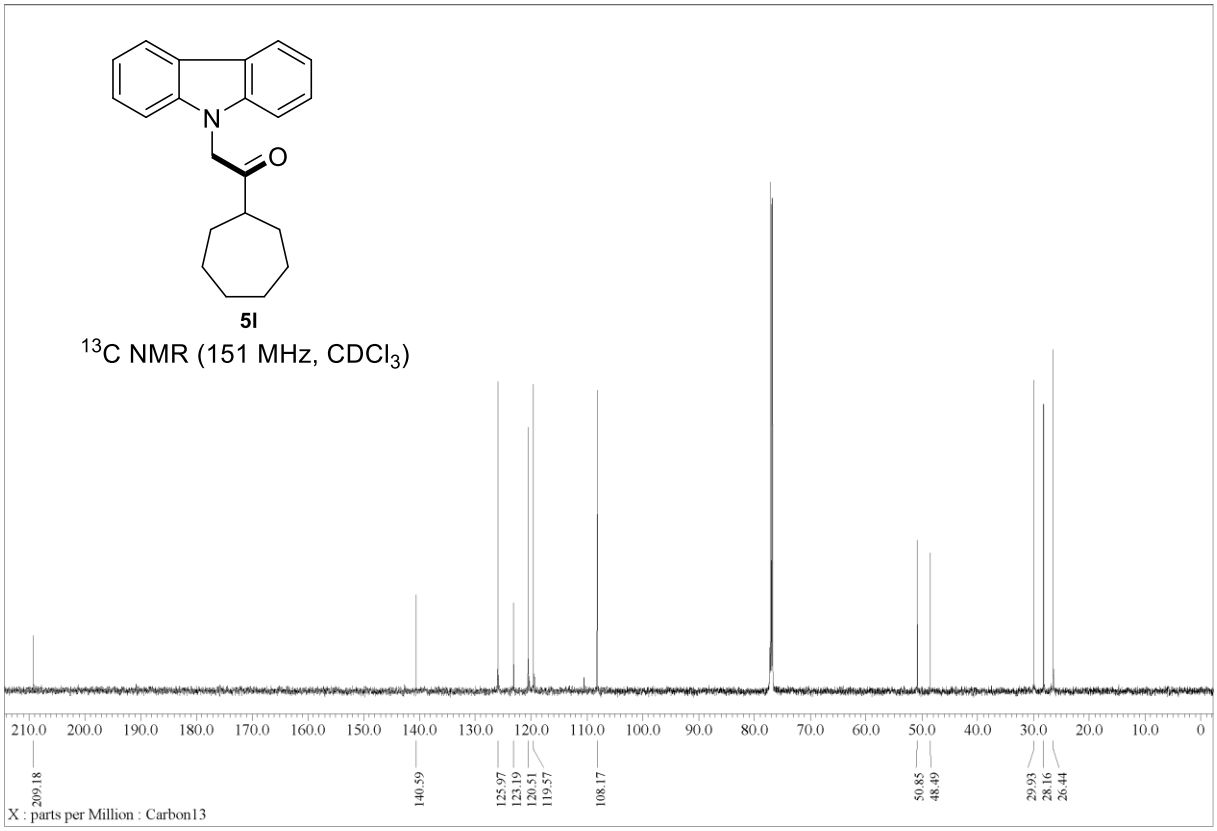
5k

^{13}C NMR (151 MHz, $CDCl_3$)



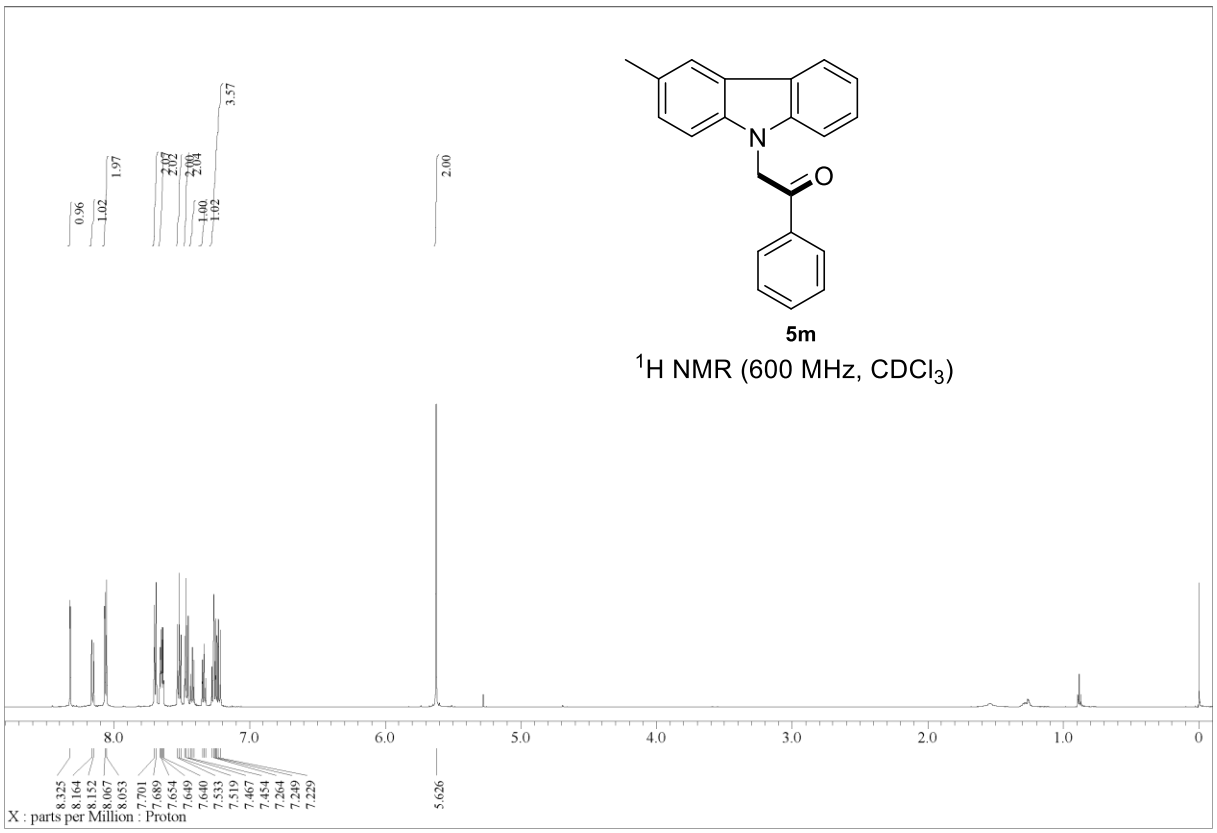
5l

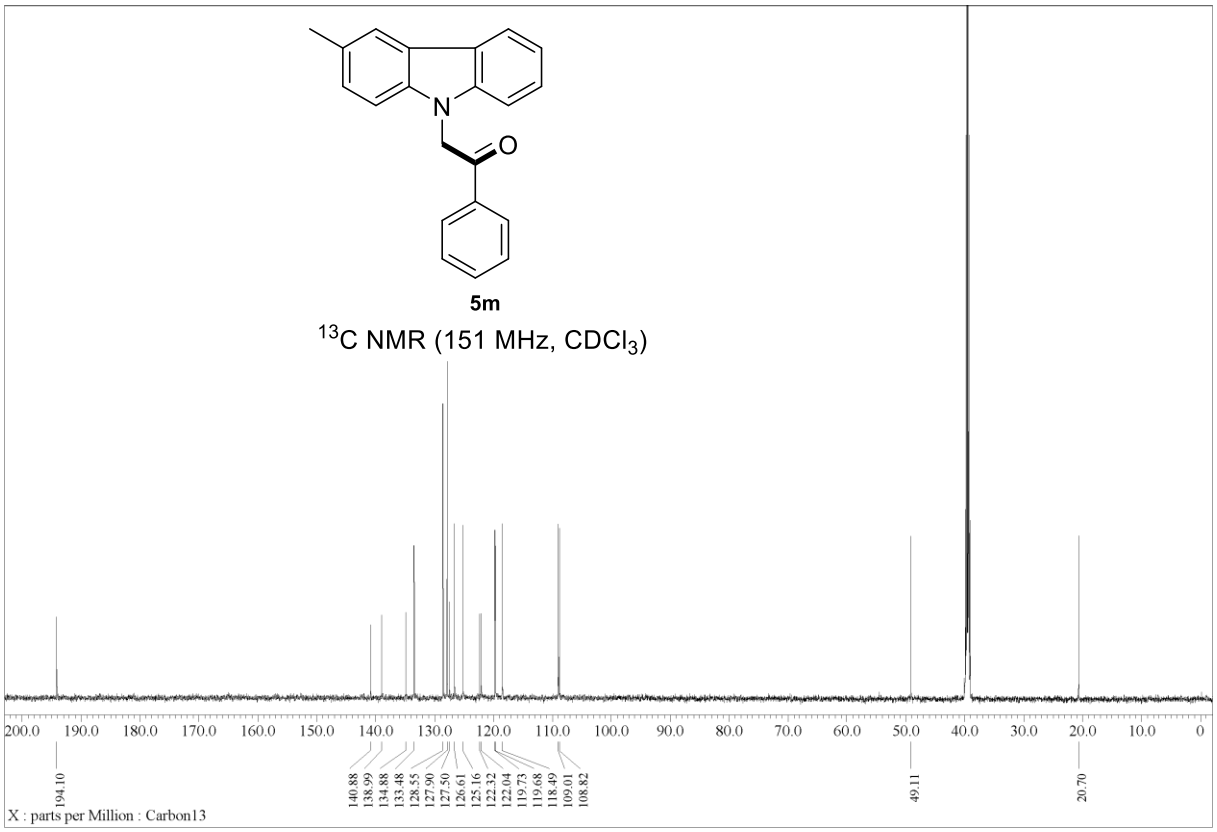
^{1}H NMR (600 MHz, $CDCl_3$)

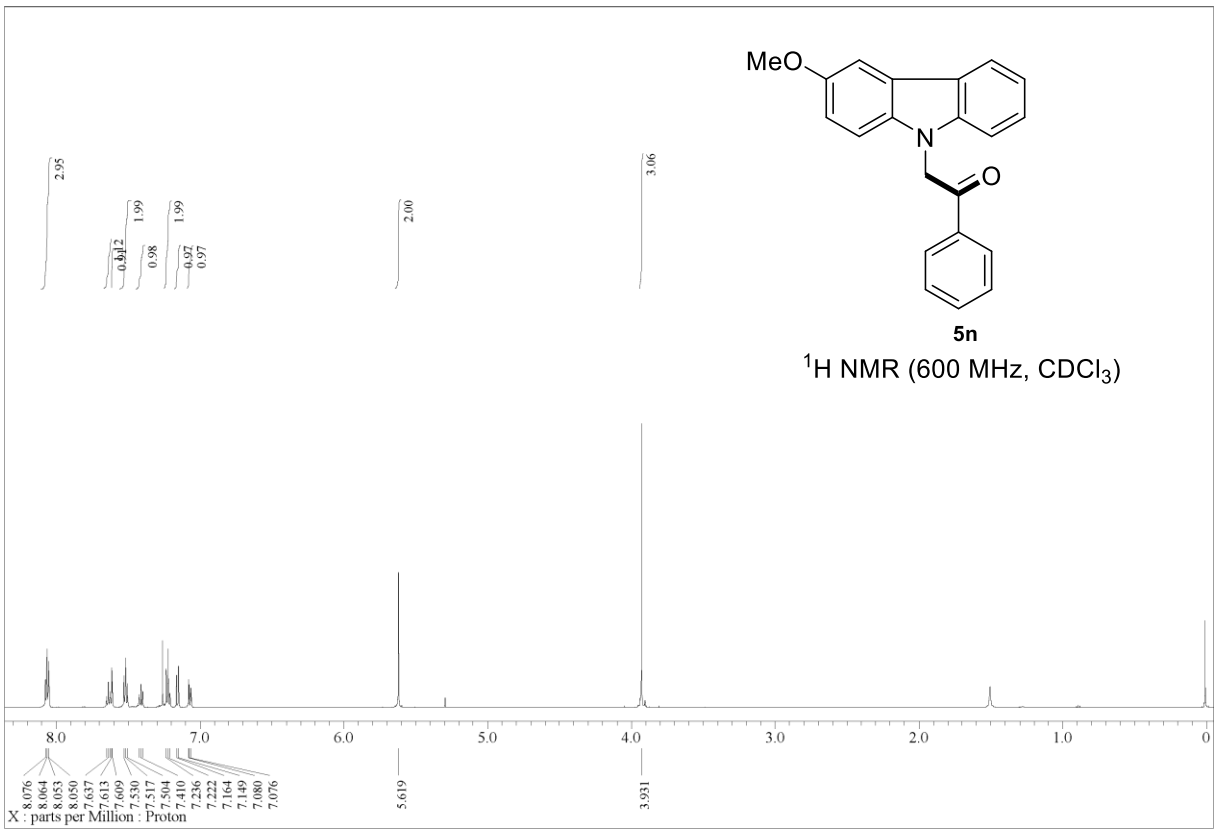


5l

^{13}C NMR (151 MHz, $CDCl_3$)

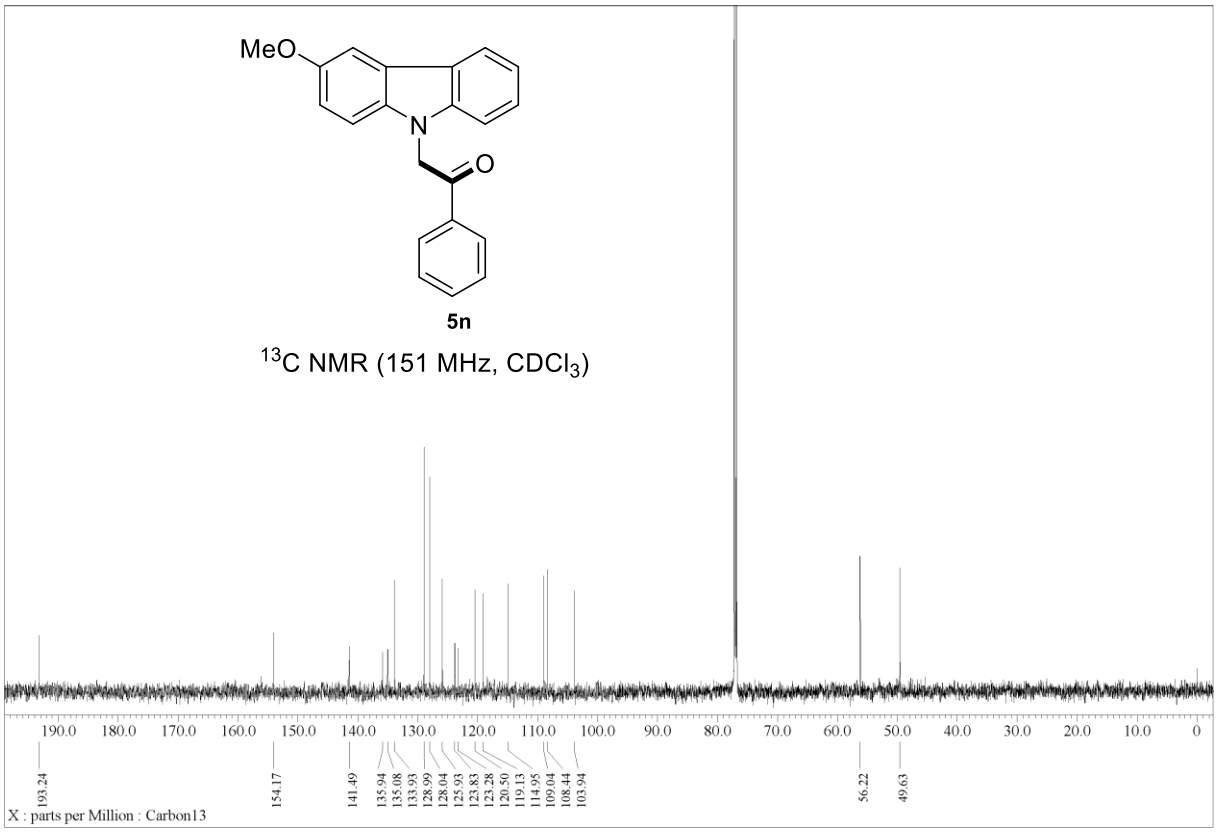

N
O
5m
1H NMR (600 MHz, CDCl3)
0.96
1.02
1.97
2.02
2.02
2.00
2.04
2.00
1.00
1.02
3.57
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.325
8.164
8.152
8.067
8.053
7.701
7.689
7.654
7.649
7.640
7.533
7.519
7.467
7.454
7.264
7.249
7.229
5.626
X : parts per Million : Proton


N
O
5m
13C NMR (151 MHz, CDCl3)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
194.10
140.88
138.99
134.88
133.48
128.55
127.90
127.50
126.61
125.16
122.32
122.04
119.73
119.68
118.49
109.01
108.82
49.11
20.70
X : parts per Million : Carbon13



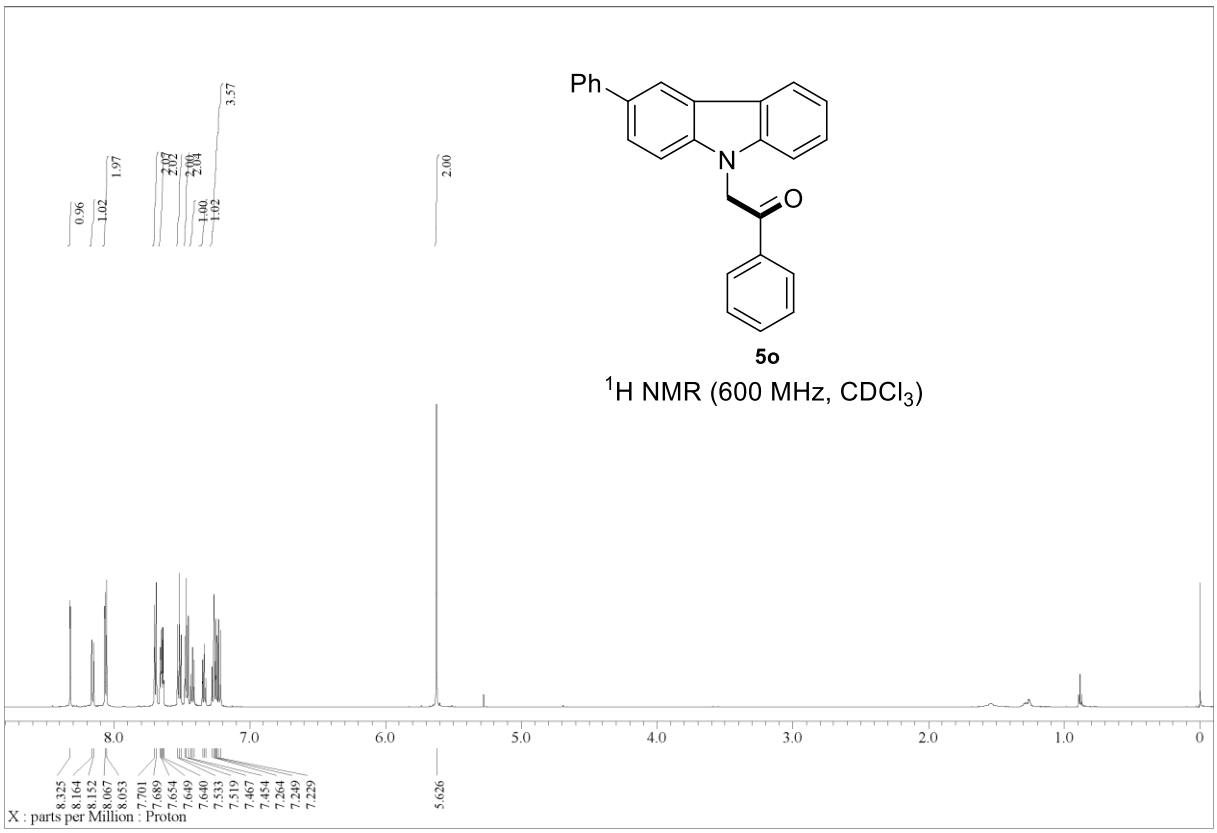
5n

^{1}H NMR (600 MHz, $CDCl_3$)



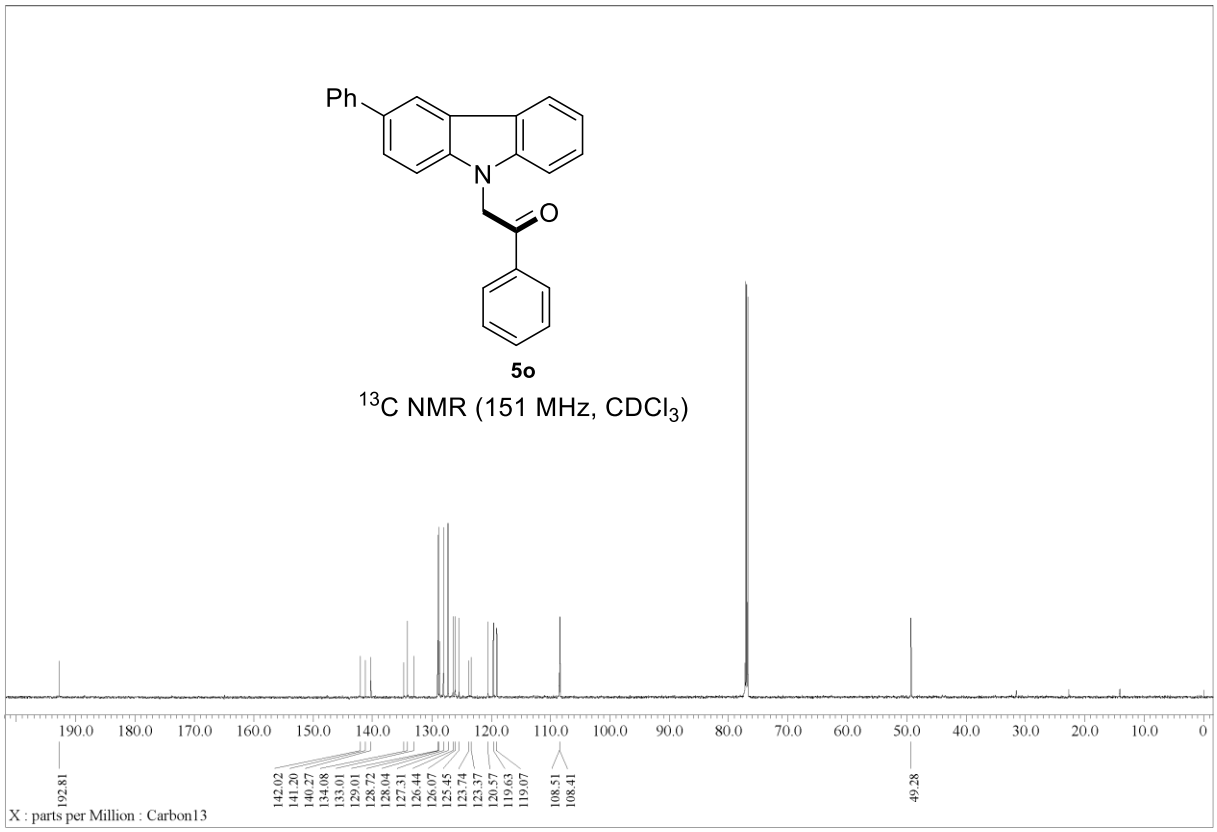
5n

^{13}C NMR (151 MHz, $CDCl_3$)



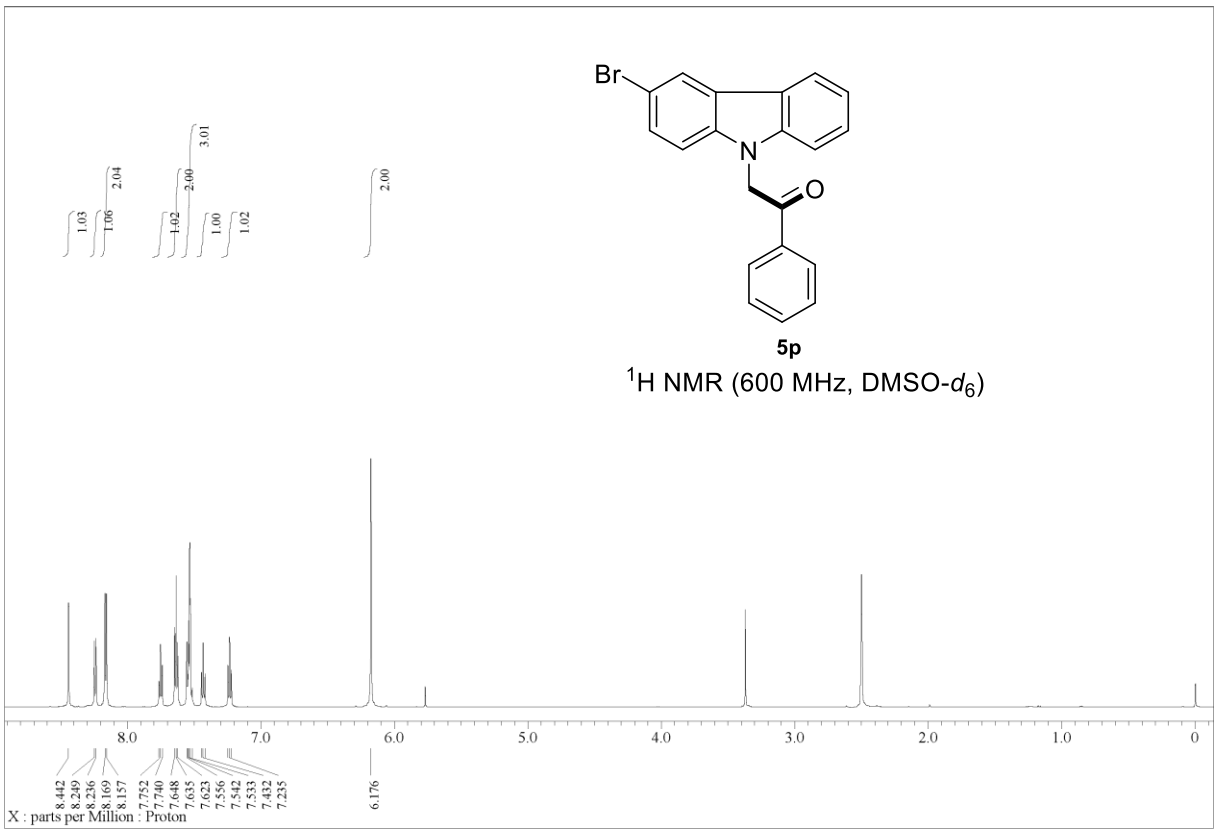
5o

^{1}H NMR (600 MHz, $CDCl_3$)



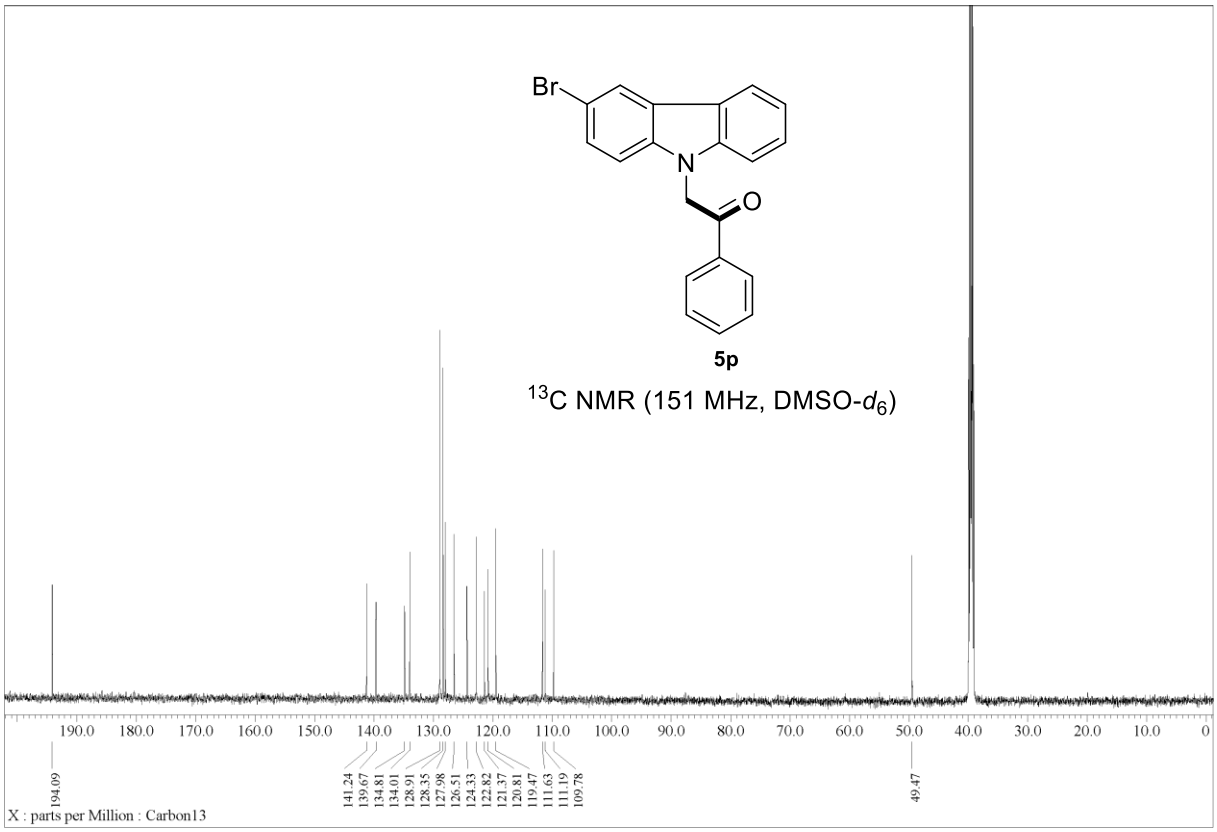
5o

^{13}C NMR (151 MHz, $CDCl_3$)



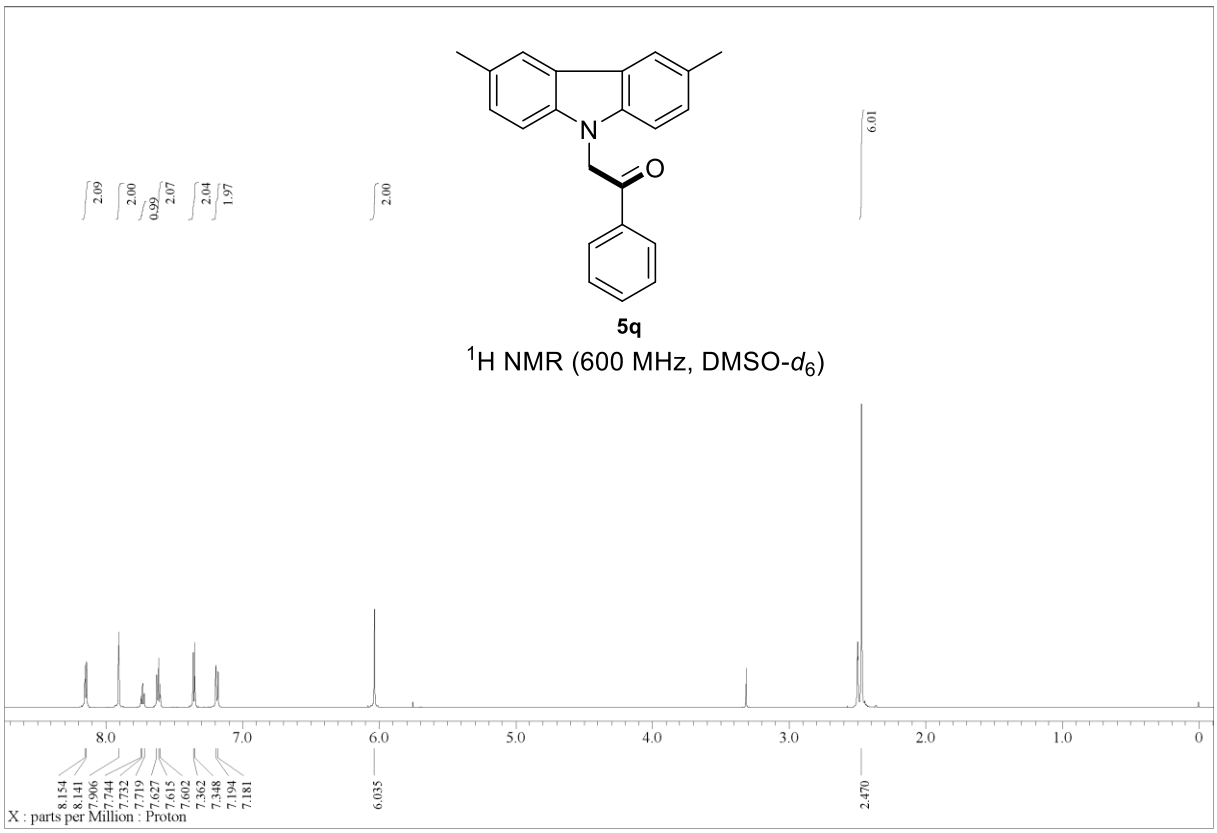
5p

^{1}H NMR (600 MHz, DMSO-d_6)



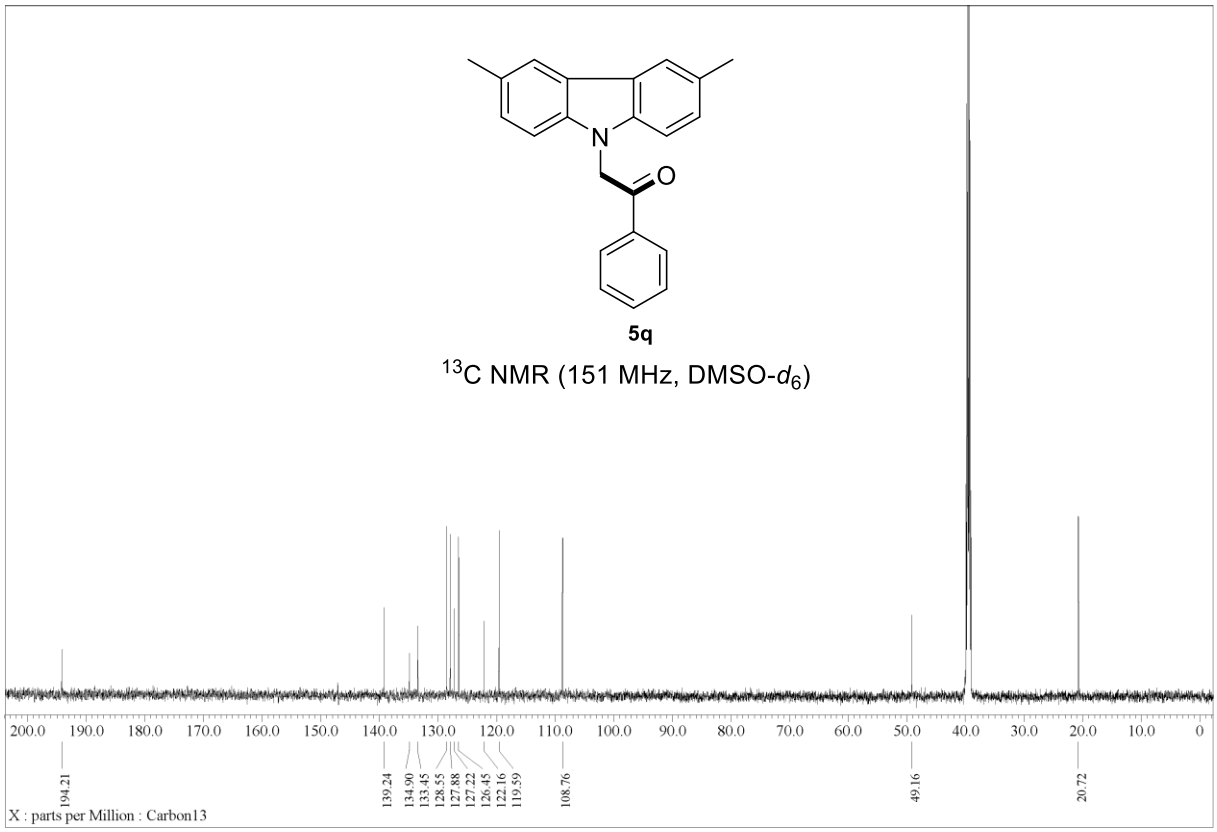
5p

^{13}C NMR (151 MHz, DMSO-d_6)



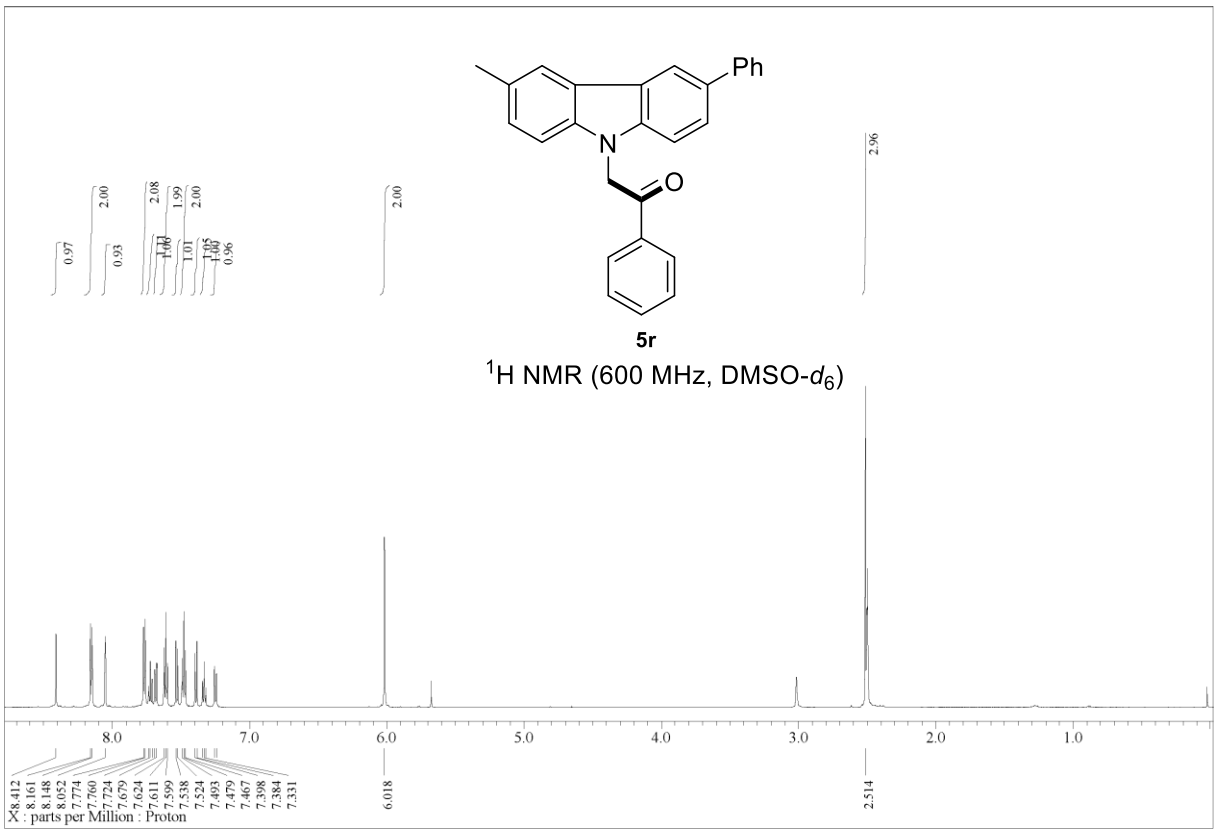
5q

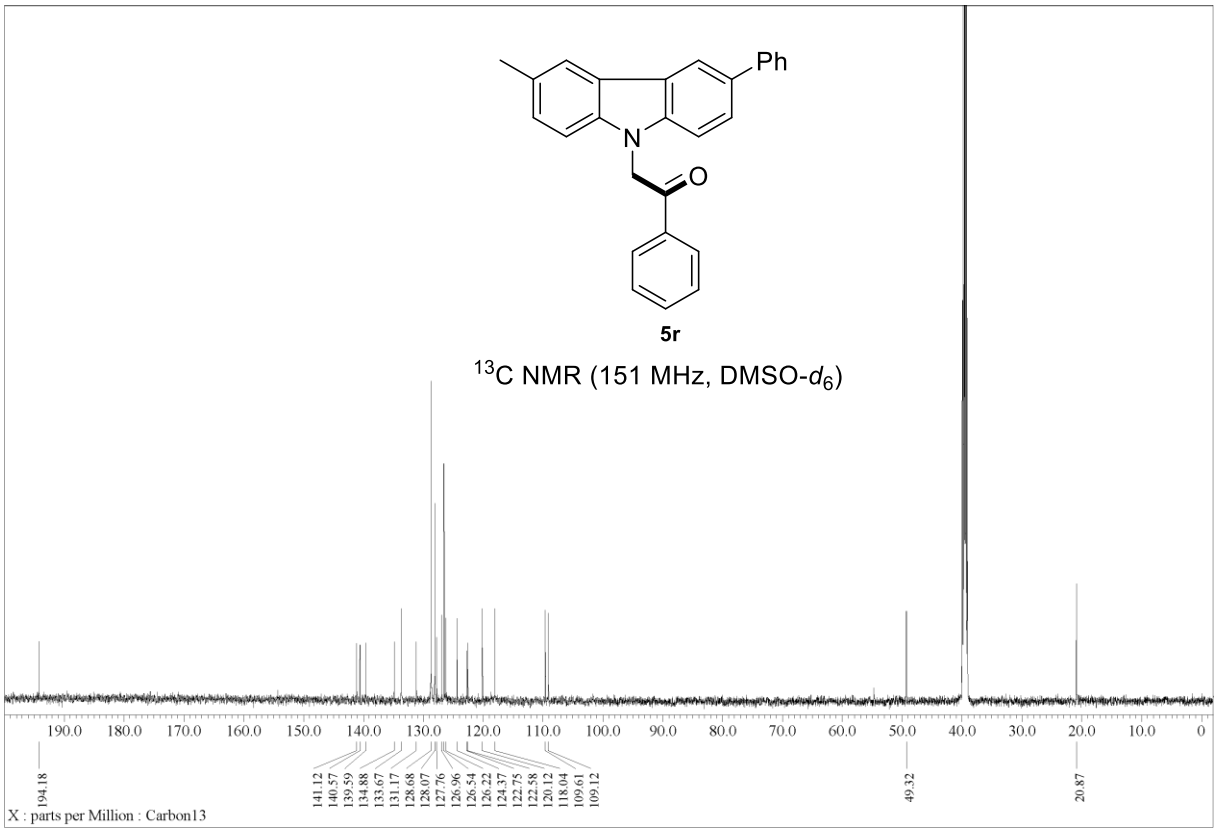
^{1}H NMR (600 MHz, DMSO-d_6)

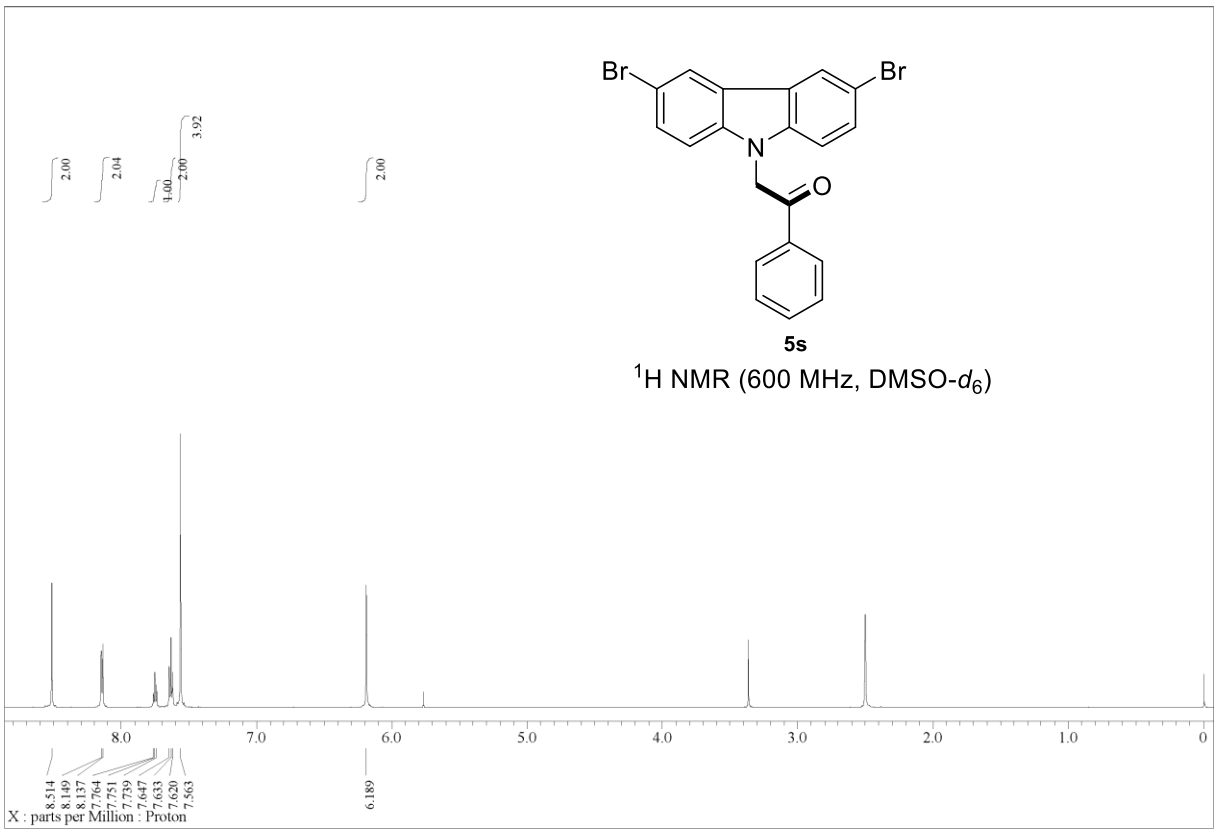


5q

^{13}C NMR (151 MHz, DMSO-d_6)

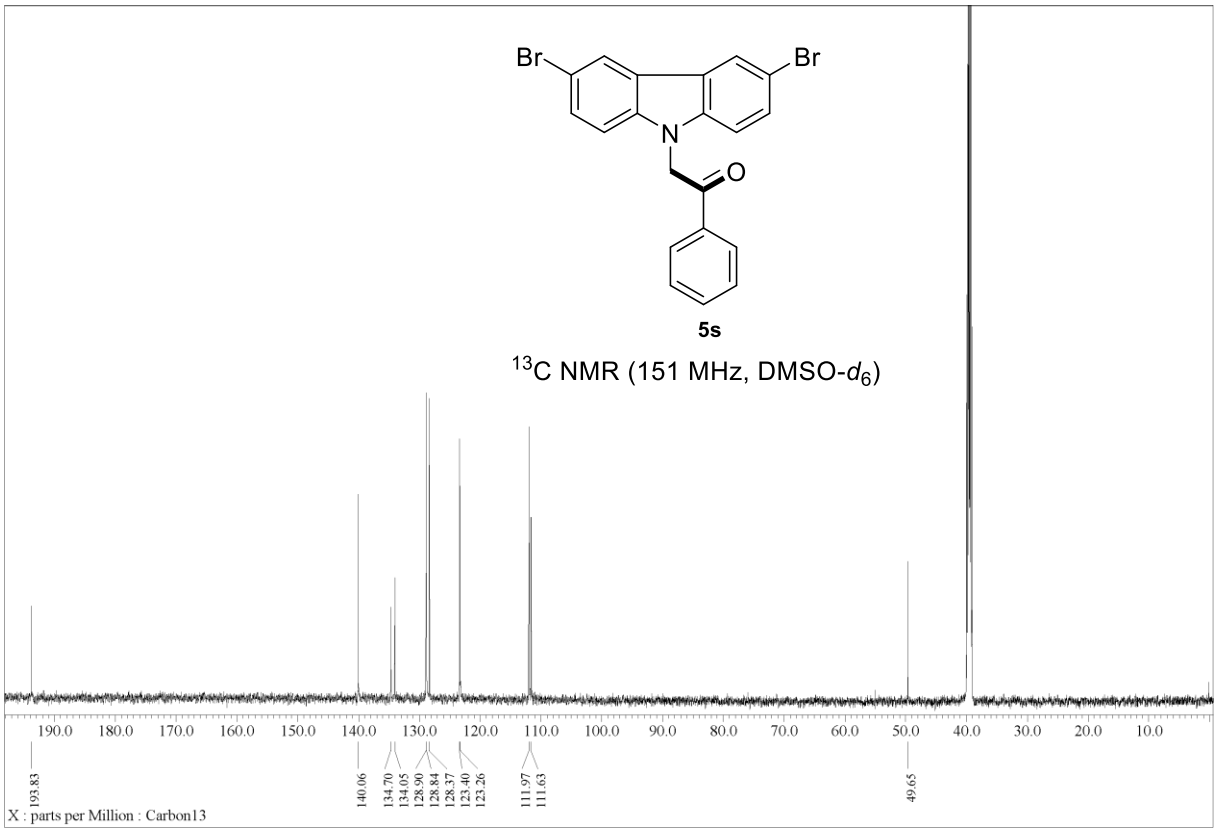

Ph
N
O
5r
^{1}H NMR (600 MHz, DMSO-d_6)
X : parts per Million : Proton


Ph
N
O
5r
^{13}C NMR (151 MHz, DMSO-d_6)
X : parts per Million : Carbon13



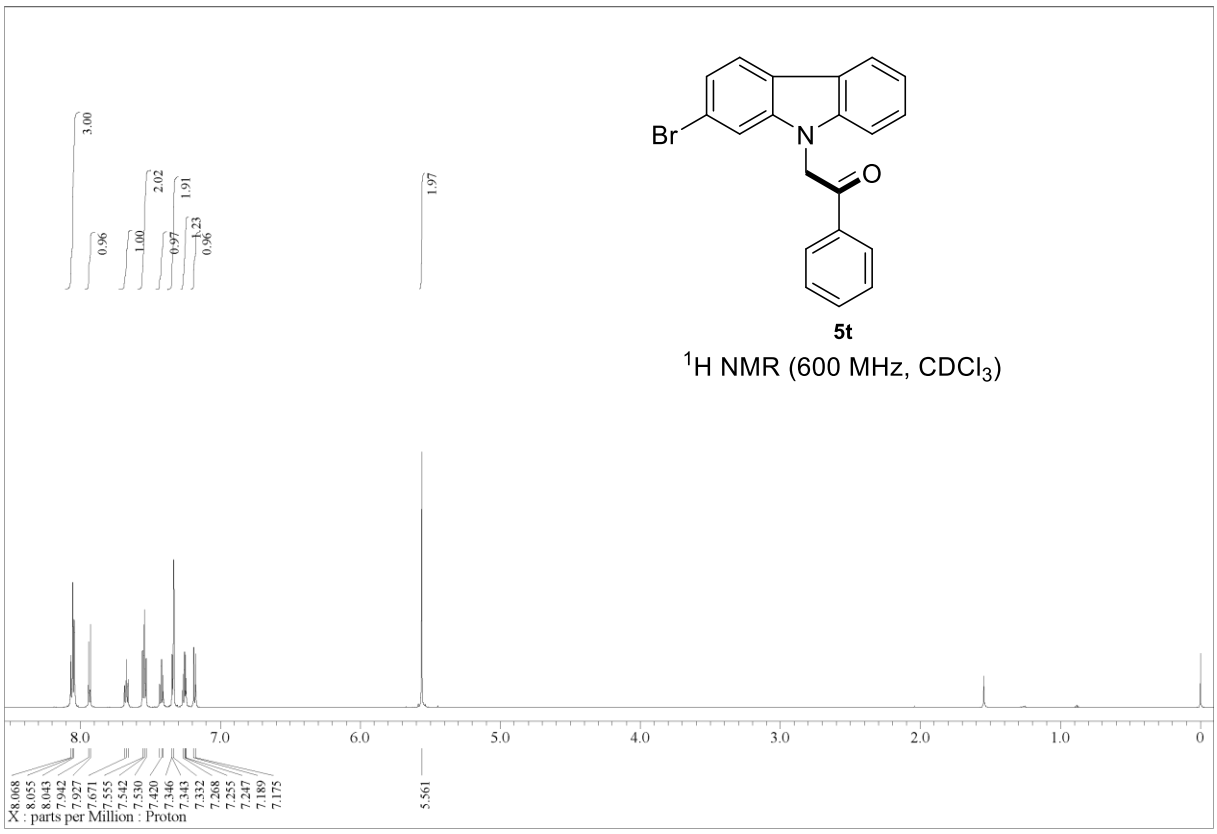
5s

^{1}H NMR (600 MHz, DMSO-d_6)



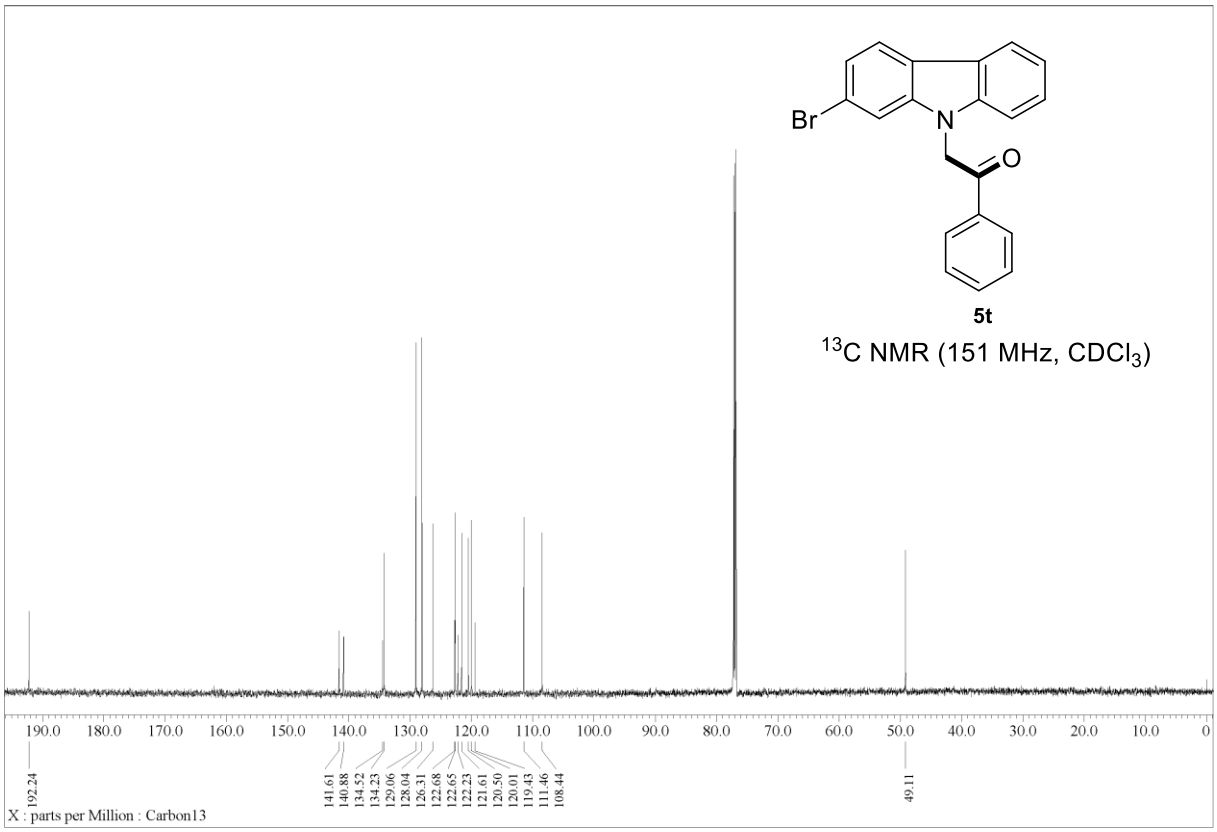
5s

^{13}C NMR (151 MHz, DMSO-d_6)



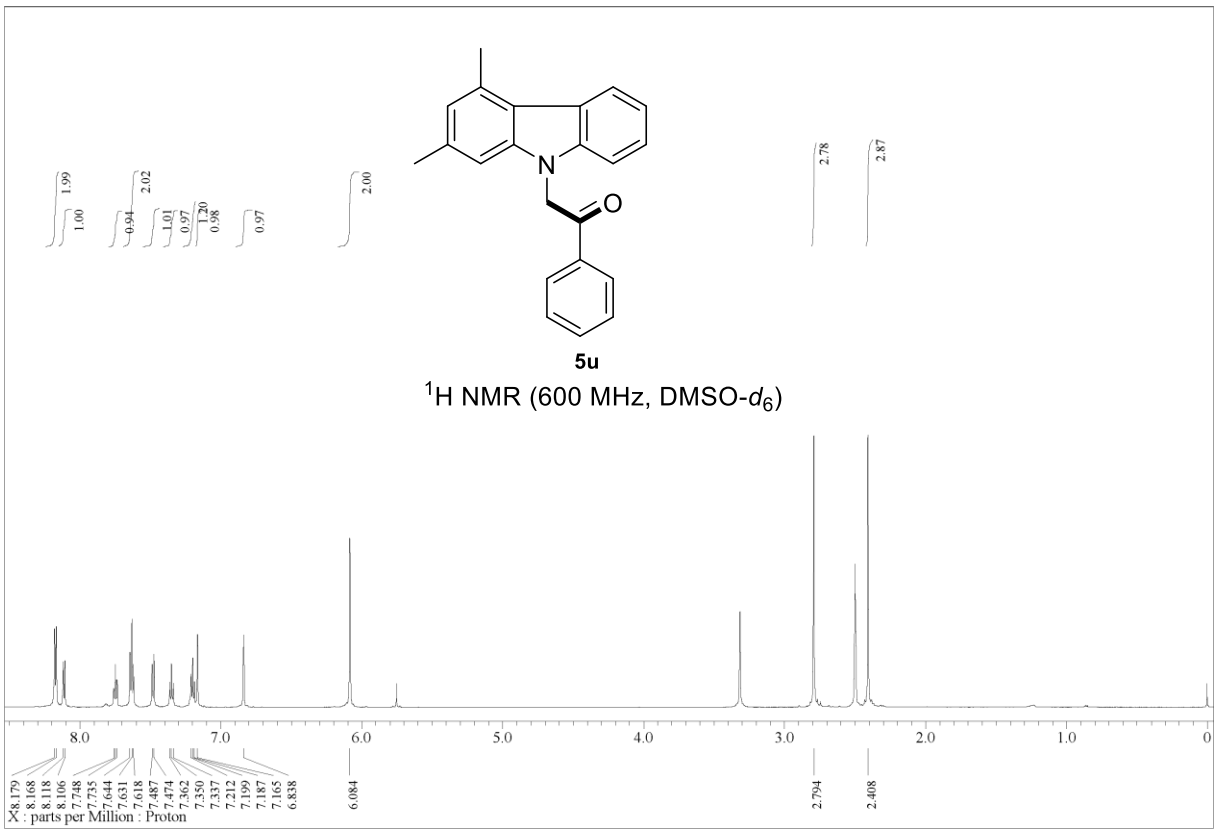
5t

^{1}H NMR (600 MHz, $CDCl_3$)



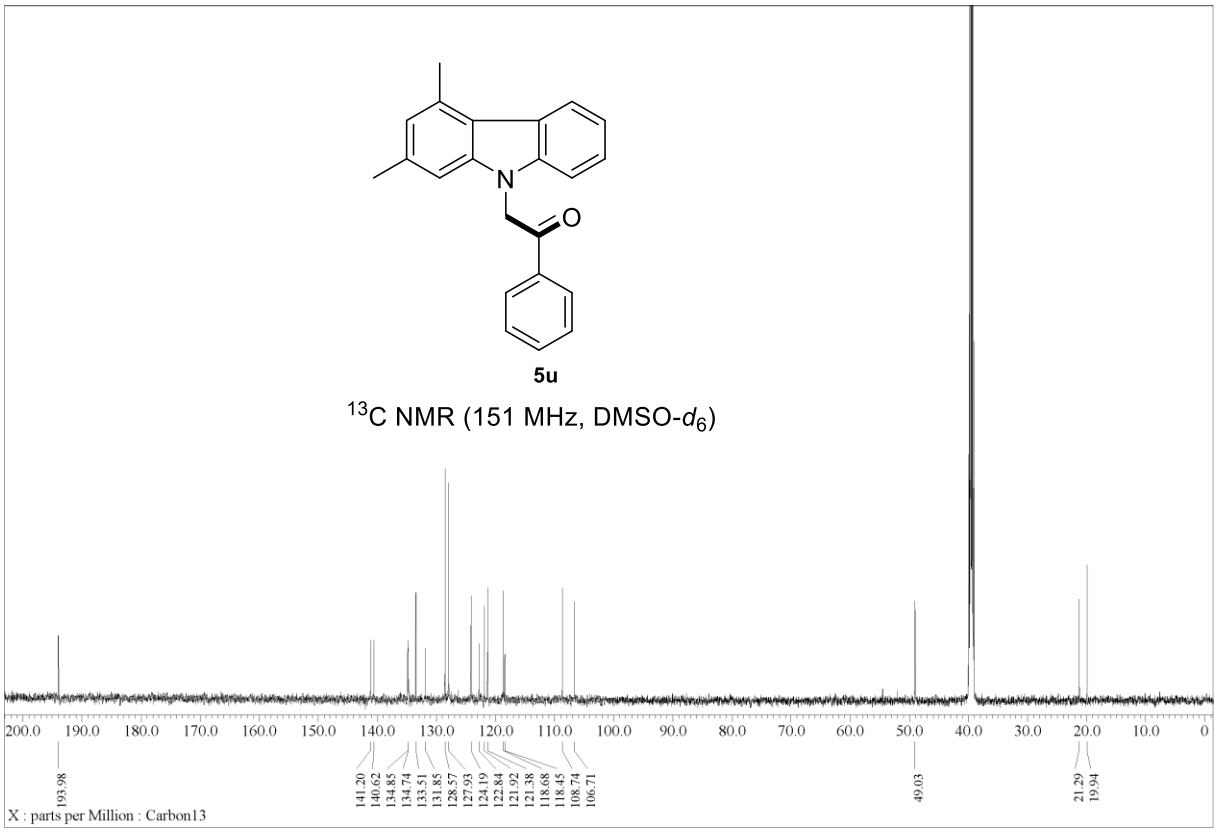
5t

^{13}C NMR (151 MHz, $CDCl_3$)



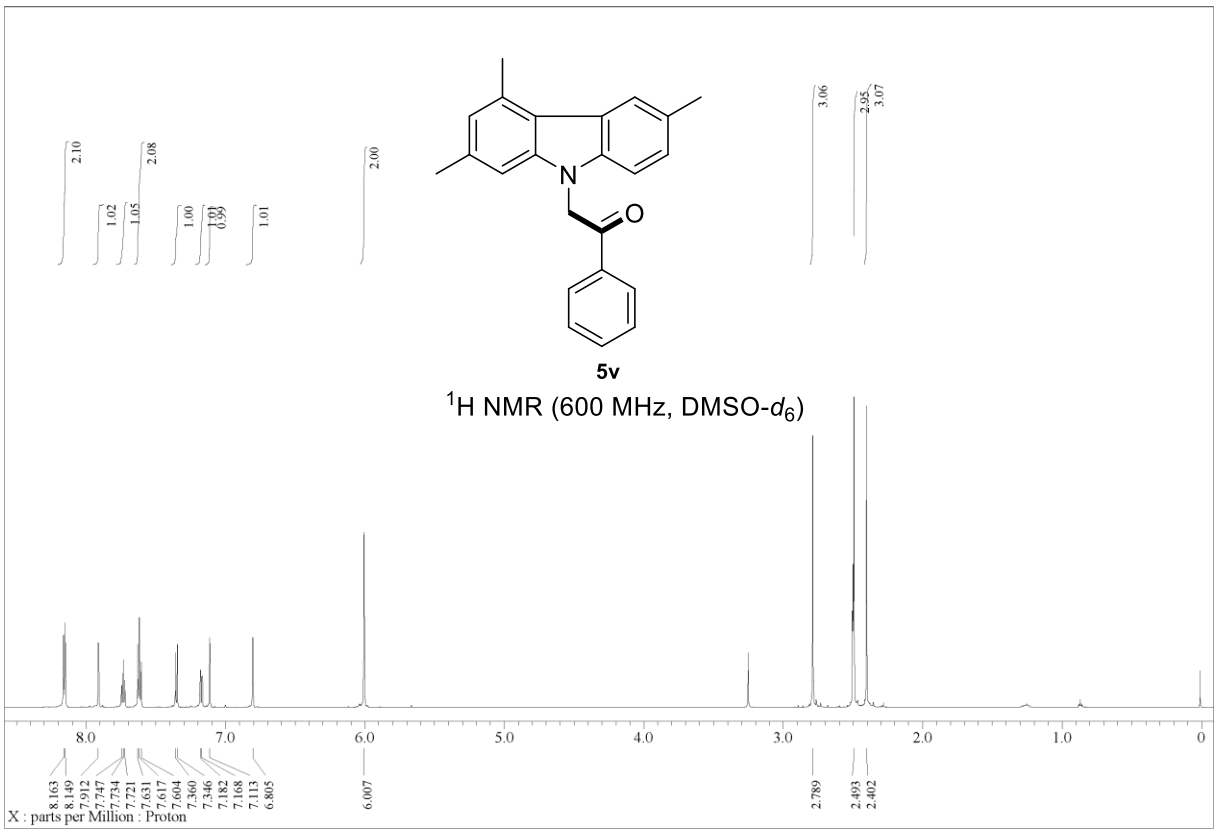
5u

^{1}H NMR (600 MHz, DMSO-d_6)



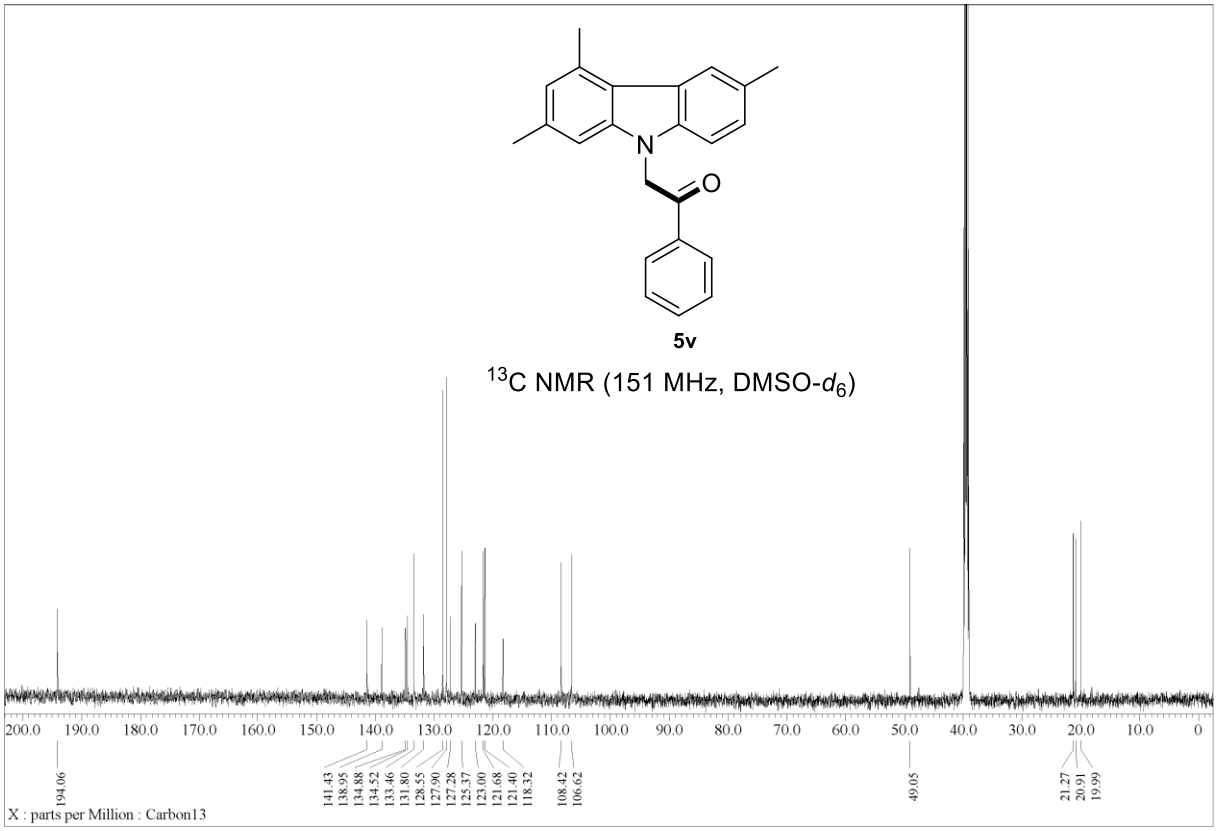
5u

^{13}C NMR (151 MHz, DMSO-d_6)



5v

^{1}H NMR (600 MHz, DMSO-d_6)



5v

^{13}C NMR (151 MHz, DMSO-d_6)

Cartesian coordinates and energies and of all optimized structures

PC4 (M06-2X functional)

Zero-point correction =	0.734859 (Hartree/Particle)
Thermal correction to Energy =	0.782542
Thermal correction to Enthalpy =	0.783487
Thermal correction to Gibbs Free Energy =	0.651255
Sum of electronic and zero-point Energies =	-2811.052475
Sum of electronic and thermal Energies =	-2811.004791
Sum of electronic and thermal Enthalpies =	-2811.003847
Sum of electronic and thermal Free Energies =	-2811.136079
SCF Done =	-2811.78733378

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.041613	-0.029301	-0.109937
2	6	0	-2.096962	1.943709	0.861627
3	6	0	-0.004433	2.975363	0.975235
4	6	0	-0.543155	4.139471	1.502270
5	6	0	-1.919429	4.188794	1.711915
6	6	0	-2.701347	3.087875	1.391808
7	1	0	1.061546	2.874040	0.789591
8	1	0	0.100150	4.977714	1.742020
9	1	0	-2.380634	5.079935	2.125596
10	1	0	-3.771751	3.115417	1.556534
11	6	0	-2.807203	0.703601	0.483977
12	6	0	-4.197118	0.583730	0.609978
13	6	0	-2.017009	-0.370681	-0.000983
14	6	0	-4.833915	-0.600445	0.260538
15	6	0	-2.692649	-1.550092	-0.347132
16	6	0	-4.075878	-1.668471	-0.218274
17	1	0	-5.911149	-0.689187	0.359793

18	1	0	-2.126458	-2.400058	-0.719365
19	7	0	-0.759720	1.915519	0.664589
20	6	0	2.626235	0.215910	1.255351
21	6	0	2.865360	0.987120	-0.910692
22	6	0	4.214334	1.260496	-0.713874
23	6	0	4.798649	0.991164	0.524878
24	6	0	3.967521	0.458870	1.516771
25	1	0	2.385630	1.177934	-1.866824
26	6	0	1.692707	-0.345506	2.262864
27	6	0	2.089034	-0.657093	3.555300
28	6	0	1.188643	-1.212455	4.469905
29	6	0	-0.457166	-1.082515	2.715719
30	6	0	-0.112540	-1.426242	4.016481
31	1	0	-1.462579	-1.238890	2.340608
32	7	0	2.089351	0.477946	0.046696
33	6	0	0.367699	-1.871230	-2.303099
34	6	0	0.810877	-2.970652	-0.211953
35	6	0	1.102990	-4.147002	-0.901429
36	6	0	1.027353	-4.192102	-2.294965
37	6	0	0.660492	-3.050546	-2.997429
38	1	0	0.872543	-2.969343	0.874284
39	1	0	1.254029	-5.109769	-2.828143
40	6	0	-0.035306	-0.624202	-2.968450
41	6	0	-0.160496	-0.435334	-4.346517
42	6	0	-0.546626	0.801946	-4.839294
43	1	0	0.046239	-1.255907	-5.023180
44	6	0	-0.666551	1.599548	-2.592613
45	6	0	-0.805997	1.842002	-3.949185
46	1	0	-0.645455	0.955530	-5.909025
47	1	0	-0.853087	2.369480	-1.851624
48	1	0	-1.112335	2.823188	-4.291182
49	1	0	4.783623	1.675477	-1.536799
50	1	0	4.380808	0.230406	2.491221
51	6	0	0.432231	-1.804411	-0.890733
52	7	0	-0.289875	0.403077	-2.117888

53	1	0	-4.790748	1.413863	0.981170
54	1	0	-4.565604	-2.598986	-0.492853
55	1	0	-0.876780	-1.856424	4.652009
56	1	0	3.111031	-0.469282	3.861680
57	1	0	0.601142	-3.085221	-4.081716
58	1	0	1.389679	-5.037546	-0.348499
59	7	0	0.417434	-0.553456	1.851669
60	6	0	6.272958	1.227137	0.836987
61	6	0	6.389806	2.131395	2.075577
62	6	0	6.926771	-0.132154	1.140878
63	6	0	7.001274	1.886806	-0.335077
64	1	0	5.887470	3.090374	1.910346
65	1	0	5.967158	1.659459	2.965737
66	1	0	7.446596	2.330751	2.281542
67	1	0	6.836604	-0.810974	0.286548
68	1	0	7.990776	0.013453	1.354624
69	1	0	6.472910	-0.604697	2.016342
70	1	0	8.048052	2.051959	-0.063318
71	1	0	6.984290	1.257443	-1.230791
72	1	0	6.562382	2.858438	-0.585680
73	6	0	1.658086	-1.534910	5.884445
74	6	0	2.879006	-2.469091	5.815557
75	6	0	2.064885	-0.219688	6.570472
76	6	0	0.557362	-2.210022	6.704620
77	1	0	2.632505	-3.399081	5.292986
78	1	0	3.726711	-1.995905	5.313267
79	1	0	3.197780	-2.721777	6.832173
80	1	0	1.219379	0.474274	6.619062
81	1	0	2.398573	-0.428102	7.592333
82	1	0	2.890445	0.267244	6.044236
83	1	0	0.938741	-2.434845	7.705022
84	1	0	-0.318427	-1.562907	6.819243
85	1	0	0.234681	-3.151669	6.247896
86	15	0	6.383197	-0.152040	5.506915
87	9	0	5.219751	-0.343003	4.365715

88	9	0	5.264662	-0.363860	6.661105
89	9	0	6.086348	1.442126	5.515223
90	9	0	7.528596	0.036528	6.631517
91	9	0	7.480516	0.059278	4.333234
92	9	0	6.650219	-1.748723	5.473983

PC4-T1 (UM06-2X functional)

Zero-point correction = 0.729929 (Hartree/Particle)

Thermal correction to Energy = 0.778362

Thermal correction to Enthalpy = 0.779306

Thermal correction to Gibbs Free Energy = 0.643754

Sum of electronic and zero-point Energies = -2810.940457

Sum of electronic and thermal Energies = -2810.892024

Sum of electronic and thermal Enthalpies = -2810.891079

Sum of electronic and thermal Free Energies = -2811.026631

SCF Done = -2811.67038572

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.016848	-0.058683	-0.160983
2	6	0	-2.035328	1.906059	0.869370
3	6	0	0.053499	2.954355	0.909095
4	6	0	-0.468608	4.111935	1.467202
5	6	0	-1.836129	4.152070	1.729693
6	6	0	-2.621467	3.055343	1.425651
7	1	0	1.110202	2.871376	0.667593
8	1	0	0.176828	4.953861	1.684942
9	1	0	-2.284197	5.045770	2.151309
10	1	0	-3.690857	3.082154	1.598693
11	6	0	-2.762799	0.715336	0.447701
12	6	0	-4.152020	0.574071	0.645036

13	6	0	-1.984358	-0.385377	-0.055159
14	6	0	-4.784572	-0.616317	0.354990
15	6	0	-2.660112	-1.597609	-0.264001
16	6	0	-4.035195	-1.709520	-0.108693
17	1	0	-5.854923	-0.717439	0.506914
18	1	0	-2.096591	-2.459217	-0.613086
19	7	0	-0.694518	1.881312	0.643395
20	6	0	2.643215	0.224403	1.246901
21	6	0	2.903063	1.002632	-0.915563
22	6	0	4.247363	1.287212	-0.702221
23	6	0	4.816203	1.026447	0.545593
24	6	0	3.978180	0.483676	1.526725
25	1	0	2.431100	1.185851	-1.877297
26	6	0	1.703143	-0.351427	2.243209
27	6	0	2.089033	-0.658902	3.540439
28	6	0	1.185686	-1.226597	4.444903
29	6	0	-0.434032	-1.141628	2.665629
30	6	0	-0.102323	-1.474684	3.972630
31	1	0	-1.428249	-1.329284	2.274121
32	7	0	2.123061	0.480767	0.030517
33	6	0	0.244354	-1.877884	-2.384870
34	6	0	0.796261	-2.976869	-0.233102
35	6	0	1.006407	-4.167330	-0.914167
36	6	0	0.822456	-4.221698	-2.335973
37	6	0	0.446952	-3.116888	-3.061062
38	1	0	0.914164	-2.954992	0.847544
39	1	0	0.976880	-5.164291	-2.853020
40	6	0	-0.088868	-0.657079	-3.021988
41	6	0	-0.261344	-0.454416	-4.420079
42	6	0	-0.570327	0.792484	-4.899315
43	1	0	-0.135154	-1.288070	-5.102147
44	6	0	-0.567984	1.627272	-2.628420
45	6	0	-0.734749	1.867429	-3.983851
46	1	0	-0.697647	0.951599	-5.964941
47	1	0	-0.692834	2.413724	-1.891062

48	1	0	-0.990493	2.864731	-4.320237
49	1	0	4.824003	1.708159	-1.516940
50	1	0	4.382679	0.257283	2.505481
51	6	0	0.424195	-1.805891	-0.915069
52	7	0	-0.223847	0.426444	-2.148186
53	1	0	-4.729515	1.396085	1.056979
54	1	0	-4.538648	-2.644025	-0.336670
55	1	0	-0.864389	-1.925508	4.596517
56	1	0	3.105221	-0.459902	3.859172
57	1	0	0.316049	-3.191734	-4.135433
58	1	0	1.291015	-5.064067	-0.373380
59	7	0	0.436759	-0.580331	1.818670
60	6	0	6.282974	1.281117	0.877795
61	6	0	6.372679	2.179043	2.123021
62	6	0	6.950391	-0.071623	1.181575
63	6	0	7.017489	1.957318	-0.280773
64	1	0	5.859505	3.132142	1.957295
65	1	0	5.946538	1.696835	3.005848
66	1	0	7.424367	2.391153	2.342128
67	1	0	6.880558	-0.745984	0.321803
68	1	0	8.009365	0.086462	1.410766
69	1	0	6.490071	-0.555441	2.047518
70	1	0	8.061151	2.124407	0.001732
71	1	0	7.011611	1.337956	-1.183488
72	1	0	6.575675	2.929454	-0.524191
73	6	0	1.642532	-1.540521	5.865300
74	6	0	2.871293	-2.465298	5.811157
75	6	0	2.032240	-0.220433	6.552037
76	6	0	0.538365	-2.221003	6.676038
77	1	0	2.637780	-3.398709	5.288737
78	1	0	3.719755	-1.985448	5.316529
79	1	0	3.181774	-2.712059	6.831836
80	1	0	1.181505	0.467844	6.589285
81	1	0	2.355347	-0.424313	7.578205
82	1	0	2.860773	0.271038	6.034725

83	1	0	0.912820	-2.444673	7.679316
84	1	0	-0.341185	-1.577658	6.783667
85	1	0	0.223544	-3.163889	6.216537
86	15	0	6.359523	-0.124826	5.541323
87	9	0	5.208657	-0.319118	4.387636
88	9	0	5.231433	-0.350523	6.683364
89	9	0	6.050607	1.466958	5.553839
90	9	0	7.492322	0.067069	6.677660
91	9	0	7.466521	0.099838	4.379400
92	9	0	6.638799	-1.719303	5.503813

PC4-T1 (UM06-2X, singlet, freq)

Zero-point correction =	0.733357 (Hartree/Particle)
Thermal correction to Energy =	0.780035
Thermal correction to Enthalpy =	0.780979
Thermal correction to Gibbs Free Energy =	0.653052
Sum of electronic and zero-point Energies =	-2811.040647
Sum of electronic and thermal Energies =	-2810.993969
Sum of electronic and thermal Enthalpies =	-2810.993025
Sum of electronic and thermal Free Energies =	-2811.120952
SCF Done =	-2811.77400404

PC4-T1 (UB3LYP functional)

Zero-point correction=	0.723785 (Hartree/Particle)
Thermal correction to Energy=	0.772724
Thermal correction to Enthalpy=	0.773669
Thermal correction to Gibbs Free Energy=	0.637627
Sum of electronic and zero-point Energies=	-2812.065554
Sum of electronic and thermal Energies=	-2812.016614
Sum of electronic and thermal Enthalpies=	-2812.015670
Sum of electronic and thermal Free Energies=	-2812.151712
SCF Done =	-2812.78933840

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.044887	-0.064572	-0.115643
2	6	0	-2.093124	1.948657	0.858763
3	6	0	0.026238	2.943330	0.993389
4	6	0	-0.494218	4.114244	1.529111
5	6	0	-1.873582	4.191051	1.734256
6	6	0	-2.674442	3.105979	1.398475
7	1	0	1.089538	2.832016	0.812127
8	1	0	0.166547	4.937406	1.776886
9	1	0	-2.320495	5.087428	2.153366
10	1	0	-3.745100	3.152993	1.557193
11	6	0	-2.826115	0.732514	0.468263
12	6	0	-4.225832	0.640552	0.570974
13	6	0	-2.057530	-0.362319	-0.021181
14	6	0	-4.888327	-0.524114	0.195592
15	6	0	-2.758661	-1.522940	-0.392941
16	6	0	-4.149203	-1.608188	-0.287344
17	1	0	-5.969600	-0.585851	0.277921
18	1	0	-2.209245	-2.383142	-0.763284
19	7	0	-0.747048	1.893442	0.665940
20	6	0	2.632882	0.191606	1.264958
21	6	0	2.850199	0.970260	-0.916143
22	6	0	4.195494	1.263337	-0.727383
23	6	0	4.799823	1.006872	0.510005
24	6	0	3.979142	0.461409	1.511126
25	1	0	2.363563	1.155416	-1.867610
26	6	0	1.705783	-0.375428	2.273745
27	6	0	2.090360	-0.687779	3.576770
28	6	0	1.184283	-1.242637	4.493956
29	6	0	-0.458377	-1.111059	2.726911
30	6	0	-0.119454	-1.449481	4.030209

31	1	0	-1.462443	-1.266827	2.353503
32	7	0	2.083910	0.446273	0.049046
33	6	0	0.314244	-1.881806	-2.366258
34	6	0	0.776423	-3.018503	-0.215010
35	6	0	1.054733	-4.198564	-0.904991
36	6	0	0.958999	-4.226236	-2.333711
37	6	0	0.602456	-3.112939	-3.050957
38	1	0	0.847686	-3.018669	0.868969
39	1	0	1.176850	-5.153100	-2.858646
40	6	0	-0.037470	-0.680478	-2.994245
41	6	0	-0.183078	-0.461690	-4.402617
42	6	0	-0.550670	0.764199	-4.889905
43	1	0	0.003275	-1.289393	-5.078363
44	6	0	-0.641738	1.593366	-2.608853
45	6	0	-0.793494	1.828944	-3.970248
46	1	0	-0.659634	0.926511	-5.957402
47	1	0	-0.818298	2.383089	-1.887408
48	1	0	-1.091359	2.814556	-4.308823
49	1	0	4.749937	1.683980	-1.556433
50	1	0	4.401886	0.243590	2.482730
51	6	0	0.398977	-1.843956	-0.881247
52	7	0	-0.265639	0.408811	-2.106788
53	1	0	-4.804863	1.480142	0.943241
54	1	0	-4.656825	-2.523378	-0.582365
55	1	0	-0.890199	-1.873012	4.661084
56	1	0	3.109028	-0.501259	3.889785
57	1	0	0.540438	-3.161881	-4.133433
58	1	0	1.340427	-5.098583	-0.369294
59	7	0	0.422469	-0.588215	1.857264
60	6	0	6.282073	1.285233	0.791014
61	6	0	6.404371	2.227610	2.011953
62	6	0	6.988100	-0.056223	1.104782
63	6	0	6.981115	1.944498	-0.410883
64	1	0	5.868015	3.167888	1.842786
65	1	0	6.021285	1.768468	2.925075

66	1	0	7.459071	2.467940	2.184839
67	1	0	6.905835	-0.752881	0.263229
68	1	0	8.052055	0.122345	1.294345
69	1	0	6.569209	-0.536092	1.992623
70	1	0	8.030259	2.131457	-0.161228
71	1	0	6.963775	1.305543	-1.300224
72	1	0	6.526522	2.906765	-0.670516
73	6	0	1.632487	-1.583725	5.920983
74	6	0	2.850320	-2.537966	5.865485
75	6	0	2.035720	-0.274268	6.640776
76	6	0	0.511426	-2.266164	6.725012
77	1	0	2.606551	-3.460391	5.327080
78	1	0	3.716798	-2.076561	5.386578
79	1	0	3.146397	-2.810636	6.884308
80	1	0	1.195192	0.427112	6.683810
81	1	0	2.342526	-0.497921	7.668245
82	1	0	2.874497	0.221282	6.145687
83	1	0	0.877798	-2.503520	7.728700
84	1	0	-0.365738	-1.620499	6.840195
85	1	0	0.188967	-3.204164	6.260031
86	15	0	6.515040	-0.100741	5.649944
87	9	0	5.344813	-0.336656	4.500551
88	9	0	5.378389	-0.253699	6.816586
89	9	0	6.228772	1.507572	5.585786
90	9	0	7.665049	0.132313	6.781522
91	9	0	7.630525	0.051632	4.464573
92	9	0	6.773970	-1.711532	5.690459

PC4-T1 (UB3LYP, singlet, freq)

Zero-point correction=	0.726803 (Hartree/Particle)
Thermal correction to Energy=	0.774115
Thermal correction to Enthalpy=	0.775059
Thermal correction to Gibbs Free Energy=	0.645457
Sum of electronic and zero-point Energies=	-2812.149632
Sum of electronic and thermal Energies=	-2812.102320

Sum of electronic and thermal Enthalpies=	-2812.101376
Sum of electronic and thermal Free Energies=	-2812.230977
SCF Done =	-2812.87643464

Acyl azoliumion **6** (M06-2X functional)

Zero-point correction =	0.263726 (Hartree/Particle)
Thermal correction to Energy =	0.285868
Thermal correction to Enthalpy =	0.286812
Thermal correction to Gibbs Free Energy =	0.208773
Sum of electronic and zero-point Energie s=	-1610.548856
Sum of electronic and thermal Energies =	-1610.526714
Sum of electronic and thermal Enthalpies =	-1610.525770
Sum of electronic and thermal Free Energies =	-1610.603809
SCF Done =	-1610.81258223

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.511499	-0.388056	0.329247
2	6	0	2.148555	0.978951	-0.226008
3	6	0	0.969793	1.628361	-0.444766
4	7	0	-0.030550	0.765199	-0.083708
5	1	0	3.171110	1.298395	-0.354336
6	1	0	0.754909	2.622221	-0.818152
7	7	0	1.845627	-0.270072	0.251451
8	6	0	-1.459402	1.089988	-0.147092
9	1	0	-2.023939	0.188328	-0.377961
10	1	0	-1.779776	1.493906	0.813479
11	1	0	-1.585670	1.825628	-0.940145
12	6	0	2.857602	-1.247791	0.665163
13	1	0	3.160125	-1.852084	-0.190400
14	1	0	3.711985	-0.690916	1.047694

15	1	0	2.455631	-1.880974	1.453905
16	6	0	-0.295195	-1.545506	0.851101
17	8	0	-1.221513	-1.292229	1.594840
18	6	0	0.054117	-2.916315	0.416586
19	6	0	0.743303	-3.149619	-0.778430
20	6	0	-0.370535	-3.987932	1.211270
21	6	0	1.011091	-4.456144	-1.173113
22	1	0	1.049612	-2.318169	-1.408352
23	6	0	-0.086626	-5.288742	0.818993
24	1	0	-0.910179	-3.785295	2.131048
25	6	0	0.603434	-5.521661	-0.372023
26	1	0	1.535267	-4.642711	-2.104451
27	1	0	-0.400796	-6.123117	1.437349
28	1	0	0.822408	-6.540236	-0.677256
29	16	0	-0.777275	4.516149	-2.228690
30	8	0	-0.949100	3.121575	-2.670452
31	8	0	-0.597055	5.499603	-3.298643
32	8	0	0.110747	4.670597	-1.064422
33	6	0	-2.425214	4.927965	-1.540578
34	9	0	-2.748709	4.081754	-0.556009
35	9	0	-3.370583	4.846878	-2.478800
36	9	0	-2.440275	6.165054	-1.040912

6-T1 (UM06-2X functional)

Zero-point correction=	0.260285 (Hartree/Particle)
Thermal correction to Energy=	0.282074
Thermal correction to Enthalpy=	0.283018
Thermal correction to Gibbs Free Energy=	0.205332
Sum of electronic and zero-point Energies=	-1610.445324
Sum of electronic and thermal Energies=	-1610.423535
Sum of electronic and thermal Enthalpies=	-1610.422591
Sum of electronic and thermal Free Energies=	-1610.500277
SCF Done =	-1610.70560916

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.539915	-0.494209	0.107725
2	6	0	2.087217	0.960663	-0.502709
3	6	0	0.874465	1.575741	-0.592795
4	7	0	-0.073316	0.660576	-0.220629
5	1	0	3.082488	1.324242	-0.704886
6	1	0	0.607043	2.574416	-0.899865
7	7	0	1.866998	-0.318592	-0.064146
8	6	0	-1.512379	0.907865	-0.179092
9	1	0	-2.036274	0.040253	-0.581855
10	1	0	-1.806795	1.103798	0.851313
11	1	0	-1.717083	1.778091	-0.801045
12	6	0	2.911512	-1.241916	0.366284
13	1	0	3.051707	-2.037449	-0.366526
14	1	0	3.832913	-0.671040	0.470143
15	1	0	2.629664	-1.658411	1.334273
16	6	0	-0.104598	-1.658160	0.644596
17	8	0	-1.088307	-1.407726	1.504249
18	6	0	0.164055	-3.037206	0.321550
19	6	0	0.798273	-3.382857	-0.889542
20	6	0	-0.250704	-4.058254	1.201991
21	6	0	1.046908	-4.714700	-1.183696
22	1	0	1.077693	-2.607611	-1.597581
23	6	0	-0.012587	-5.387089	0.881100
24	1	0	-0.733385	-3.800229	2.139555
25	6	0	0.641917	-5.722296	-0.304719
26	1	0	1.547001	-4.971251	-2.112195
27	1	0	-0.329676	-6.166578	1.566575
28	1	0	0.833769	-6.762797	-0.545294
29	16	0	0.814120	1.362988	3.185897

30	8	0	-0.425508	1.844625	2.558339
31	8	0	1.875255	2.364902	3.333233
32	8	0	1.262011	0.036544	2.731288
33	6	0	0.293217	1.041184	4.912406
34	9	0	-0.697133	0.146339	4.953612
35	9	0	-0.139640	2.161105	5.497762
36	9	0	1.308276	0.564654	5.637891

6-T1 (UM06-2X, singlet, freq)

Zero-point correction=	0.263051 (Hartree/Particle)
Thermal correction to Energy=	0.283971
Thermal correction to Enthalpy=	0.284915
Thermal correction to Gibbs Free Energy=	0.211169
Sum of electronic and zero-point Energies=	-1610.529508
Sum of electronic and thermal Energies=	-1610.508589
Sum of electronic and thermal Enthalpies=	-1610.507645
Sum of electronic and thermal Free Energies=	-1610.581391
SCF Done =	-1610.79255980

6-T1 (UB3LYP functional)

Zero-point correction=	0.256850 (Hartree/Particle)
Thermal correction to Energy=	0.279722
Thermal correction to Enthalpy=	0.280666
Thermal correction to Gibbs Free Energy=	0.201003
Sum of electronic and zero-point Energies=	-1610.953702
Sum of electronic and thermal Energies=	-1610.93083
Sum of electronic and thermal Enthalpies=	-1610.929886
Sum of electronic and thermal Free Energies=	-1611.009549
SCF Done =	-1611.21055237

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.603266	-0.237221	-0.125797
2	6	0	2.128600	1.008979	-1.179138
3	6	0	0.945262	1.683835	-1.209878
4	7	0	0.009528	0.914593	-0.558380
5	1	0	3.099419	1.270475	-1.568803
6	1	0	0.689610	2.636692	-1.645503
7	7	0	1.917296	-0.170629	-0.499020
8	6	0	-1.401768	1.270869	-0.410970
9	1	0	-2.030289	0.443987	-0.745881
10	1	0	-1.615827	1.501412	0.632162
11	1	0	-1.591466	2.142925	-1.036371
12	6	0	2.982646	-1.083420	-0.084937
13	1	0	2.971041	-1.998277	-0.680206
14	1	0	3.933601	-0.570896	-0.227583
15	1	0	2.853306	-1.322113	0.971602
16	6	0	-0.023378	-1.274238	0.627521
17	8	0	-1.017570	-0.968044	1.445967
18	6	0	0.228406	-2.701925	0.520293
19	6	0	0.617608	-3.309206	-0.698915
20	6	0	-0.002661	-3.523864	1.654482
21	6	0	0.824391	-4.680309	-0.757590
22	1	0	0.744823	-2.702024	-1.589516
23	6	0	0.187679	-4.898247	1.572618
24	1	0	-0.291800	-3.060414	2.590475
25	6	0	0.606373	-5.483443	0.373184
26	1	0	1.140873	-5.134982	-1.691667
27	1	0	0.021714	-5.515687	2.450387
28	1	0	0.760575	-6.556496	0.313930
29	16	0	0.860189	0.799229	3.566915
30	8	0	-0.209659	1.136551	2.578385

31	8	0	1.416505	1.980899	4.258855
32	8	0	1.845417	-0.201398	3.103913
33	6	0	-0.068585	-0.091571	4.912051
34	9	0	-0.644931	-1.217123	4.456962
35	9	0	-1.035387	0.690335	5.421429
36	9	0	0.764232	-0.429638	5.912243

6-T1 (UB3LYP, singlet, freq)

Zero-point correction=	0.259184 (Hartree/Particle)
Thermal correction to Energy=	0.28059
Thermal correction to Enthalpy=	0.281543
Thermal correction to Gibbs Free Energy=	0.206428
Sum of electronic and zero-point Energies=	-1611.019739
Sum of electronic and thermal Energies=	-1610.998324
Sum of electronic and thermal Enthalpies=	-1610.997380
Sum of electronic and thermal Free Energies=	-1611.072495
SCF Done =	-1611.27892306

Triazolium salt **7** (M06-2X functional)

Zero-point correction=	0.410789 (Hartree/Particle)
Thermal correction to Energy=	0.439026
Thermal correction to Enthalpy=	0.439970
Thermal correction to Gibbs Free Energy=	0.350307
Sum of electronic and zero-point Energies=	-1476.492731
Sum of electronic and thermal Energies=	-1476.464495
Sum of electronic and thermal Enthalpies=	-1476.463551
Sum of electronic and thermal Free Energies=	-1476.553214
SCF Done =	-1476.90352059

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.843098	0.359823	-0.610946
2	6	0	-0.679311	2.128664	-0.107655
3	7	0	-0.601571	0.035332	-0.252602
4	7	0	-1.908047	1.688250	-0.511716
5	6	0	-2.842189	2.785855	-0.829970
6	1	0	-3.836246	2.564161	-0.443534
7	1	0	-2.875912	2.891734	-1.916046
8	6	0	-2.890060	-0.627880	-1.071409
9	8	0	-2.553012	-1.446499	-1.898759
10	6	0	-4.239753	-0.534821	-0.480970
11	6	0	-4.472368	0.156877	0.714428
12	6	0	-5.286107	-1.204141	-1.128342
13	6	0	-5.752873	0.177718	1.257127
14	1	0	-3.660351	0.660867	1.233007
15	6	0	-6.562846	-1.168612	-0.586852
16	1	0	-5.083441	-1.738390	-2.051045
17	6	0	-6.795040	-0.479153	0.605130
18	1	0	-5.936373	0.703895	2.187801
19	1	0	-7.378922	-1.677185	-1.089072
20	1	0	-7.794534	-0.455673	1.028140
21	9	0	1.238655	2.484863	-2.335000
22	9	0	2.875609	1.217879	-1.345784
23	9	0	3.404608	3.215206	-2.324972
24	7	0	0.137931	1.126967	0.075678
25	6	0	-0.639032	3.618468	-0.083016
26	1	0	-0.122983	4.011210	0.791882
27	1	0	-0.103534	3.940854	-0.979117
28	6	0	-2.145509	3.969479	-0.127171
29	6	0	-0.028765	-1.283492	-0.159239
30	6	0	0.698818	-1.756045	-1.251008

31	6	0	-0.216324	-1.998873	1.025410
32	6	0	1.273760	-3.021400	-1.120758
33	6	0	0.373459	-3.258107	1.100978
34	6	0	1.124185	-3.778626	0.042199
35	1	0	1.848376	-3.423496	-1.951393
36	1	0	0.248730	-3.843344	2.009075
37	6	0	0.812937	-0.946449	-2.512142
38	1	0	-0.167287	-0.877364	-2.997300
39	1	0	1.162942	0.069270	-2.308740
40	1	0	1.507083	-1.422640	-3.207365
41	6	0	-1.033179	-1.428531	2.152126
42	1	0	-0.677422	-0.431846	2.433338
43	1	0	-2.086523	-1.333897	1.862286
44	1	0	-0.980006	-2.074268	3.030201
45	6	0	1.768176	-5.133537	0.170615
46	1	0	2.597758	-5.098618	0.884569
47	1	0	1.052516	-5.872918	0.541270
48	1	0	2.160210	-5.479720	-0.788018
49	5	0	2.434223	2.522530	-1.591493
50	9	0	2.201800	3.185254	-0.377676
51	1	0	-2.336601	4.903429	-0.654631
52	1	0	-2.532431	4.056855	0.890517

7-T1 (UM06-2X functional)

Zero-point correction=	0.408219 (Hartree/Particle)
Thermal correction to Energy=	0.436660
Thermal correction to Enthalpy=	0.437604
Thermal correction to Gibbs Free Energy=	0.345881
Sum of electronic and zero-point Energies=	-1476.403531
Sum of electronic and thermal Energies=	-1476.375090
Sum of electronic and thermal Enthalpies=	-1476.374146
Sum of electronic and thermal Free Energies=	-1476.465869
SCF Done =	-1476.81175032

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.542101	0.387072	0.096250
2	6	0	-0.185609	2.058734	0.484174
3	7	0	-0.273419	-0.025780	0.335797
4	7	0	-1.491628	1.731902	0.227467
5	6	0	-2.328375	2.896630	-0.091254
6	1	0	-3.288348	2.837689	0.418738
7	1	0	-2.467720	2.922698	-1.172042
8	6	0	-2.475693	-0.607120	-0.261000
9	8	0	-1.969041	-1.804982	-0.375313
10	6	0	-3.902470	-0.397562	-0.530520
11	6	0	-4.657907	0.493721	0.243515
12	6	0	-4.526046	-1.139035	-1.544302
13	6	0	-6.010130	0.675024	-0.027360
14	1	0	-4.196469	1.008467	1.080423
15	6	0	-5.879002	-0.956817	-1.802825
16	1	0	-3.939539	-1.839006	-2.131030
17	6	0	-6.621891	-0.044425	-1.052540
18	1	0	-6.590572	1.366325	0.575420
19	1	0	-6.355988	-1.523379	-2.596379
20	1	0	-7.677701	0.097533	-1.260359
21	9	0	-1.182920	1.473904	-2.543193
22	9	0	0.971361	2.206453	-2.259296
23	9	0	-0.079394	2.484795	-4.276909
24	7	0	0.587381	1.014089	0.571317
25	6	0	0.007112	3.537300	0.461953
26	1	0	0.572475	3.899500	1.321190
27	1	0	0.542958	3.784316	-0.457108
28	6	0	-1.450340	4.055966	0.428556
29	6	0	0.114435	-1.394990	0.269643

30	6	0	0.724908	-1.869588	-0.928943
31	6	0	0.079867	-2.165672	1.470470
32	6	0	1.203168	-3.166777	-0.924486
33	6	0	0.576100	-3.448019	1.413050
34	6	0	1.136901	-3.967485	0.226160
35	1	0	1.644839	-3.572339	-1.829919
36	1	0	0.544651	-4.074368	2.300379
37	6	0	0.780856	-0.990398	-2.134960
38	1	0	-0.227148	-0.682281	-2.432542
39	1	0	1.330276	-0.066853	-1.928737
40	1	0	1.256094	-1.514216	-2.965563
41	6	0	-0.530257	-1.582886	2.707140
42	1	0	-0.049752	-0.635553	2.971720
43	1	0	-1.594932	-1.377227	2.544412
44	1	0	-0.435896	-2.275488	3.544317
45	6	0	1.658249	-5.369600	0.215892
46	1	0	2.422792	-5.495091	0.989708
47	1	0	0.850369	-6.071478	0.449482
48	1	0	2.085849	-5.634287	-0.752034
49	5	0	-0.251658	2.469083	-2.894798
50	9	0	-0.729136	3.716561	-2.457740
51	1	0	-1.551177	4.931208	-0.212286
52	1	0	-1.768254	4.323648	1.438298

7-T1 (UM06-2X, singlet, freq)

Zero-point correction=	0.410171 (Hartree/Particle)
Thermal correction to Energy=	0.437213
Thermal correction to Enthalpy=	0.438157
Thermal correction to Gibbs Free Energy=	0.351552
Sum of electronic and zero-point Energies=	-1476.454855
Sum of electronic and thermal Energies=	-1476.427813
Sum of electronic and thermal Enthalpies=	-1476.426868
Sum of electronic and thermal Free Energies=	-1476.513474
SCF Done =	-1476.86502581

7-T1 (UB3LYP functional)

Zero-point correction=	0.403757 (Hartree/Particle)
Thermal correction to Energy=	0.432918
Thermal correction to Enthalpy=	0.433862
Thermal correction to Gibbs Free Energy=	0.339095
Sum of electronic and zero-point Energies=	-1476.993328
Sum of electronic and thermal Energies=	-1476.964168
Sum of electronic and thermal Enthalpies=	-1476.963224
Sum of electronic and thermal Free Energies=	-1477.057990
SCF Done =	-1477.39708530

Imaginary frequency: 0 (cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.940563	0.348205	0.012272
2	6	0	-0.626422	2.105773	0.228009
3	7	0	-0.624123	-0.001998	0.151102
4	7	0	-1.931878	1.711027	0.072937
5	6	0	-2.842482	2.842627	-0.188198
6	1	0	-3.773284	2.734219	0.365404
7	1	0	-3.062071	2.873082	-1.259234
8	6	0	-2.891215	-0.678250	-0.183389
9	8	0	-2.385686	-1.882542	-0.279932
10	6	0	-4.351678	-0.539540	-0.316563
11	6	0	-5.099725	0.319702	0.509666
12	6	0	-5.024134	-1.352229	-1.250949
13	6	0	-6.484021	0.397473	0.366400
14	1	0	-4.606797	0.896014	1.285278
15	6	0	-6.407502	-1.270804	-1.383155
16	1	0	-4.452751	-2.029720	-1.876578
17	6	0	-7.141814	-0.391964	-0.580986
18	1	0	-7.051015	1.065735	1.007774

19	1	0	-6.913847	-1.892241	-2.115832
20	1	0	-8.220780	-0.329985	-0.686561
21	9	0	1.795478	1.866350	-2.854696
22	9	0	3.817744	1.917011	-1.763296
23	9	0	3.316449	3.516726	-3.332998
24	7	0	0.204935	1.098860	0.281539
25	6	0	-0.504703	3.593278	0.195637
26	1	0	0.109288	3.976622	1.013133
27	1	0	-0.023874	3.888217	-0.740700
28	6	0	-1.988190	4.042998	0.288409
29	6	0	-0.127764	-1.340330	0.077883
30	6	0	0.317531	-1.839152	-1.187750
31	6	0	0.088525	-2.053470	1.297132
32	6	0	0.907289	-3.095194	-1.205228
33	6	0	0.687367	-3.295832	1.210477
34	6	0	1.104152	-3.837268	-0.028243
35	1	0	1.239905	-3.507457	-2.152816
36	1	0	0.853804	-3.868975	2.117947
37	6	0	0.151518	-1.034446	-2.441565
38	1	0	-0.903066	-0.799522	-2.624508
39	1	0	0.692223	-0.083594	-2.384054
40	1	0	0.528397	-1.591667	-3.301687
41	6	0	-0.342506	-1.469560	2.611139
42	1	0	0.108174	-0.484987	2.775308
43	1	0	-1.430079	-1.337657	2.644360
44	1	0	-0.054370	-2.124797	3.435633
45	6	0	1.758650	-5.184840	-0.068263
46	1	0	2.664980	-5.189789	0.549720
47	1	0	1.092054	-5.948815	0.350083
48	1	0	2.028691	-5.475649	-1.085503
49	5	0	2.797429	2.702974	-2.315337
50	9	0	2.229182	3.513632	-1.310104
51	1	0	-2.188695	4.929586	-0.314370
52	1	0	-2.238603	4.272082	1.327287

7-T1 (UB3LYP, singlet, freq)

Zero-point correction=	0.405639 (Hartree/Particle)
Thermal correction to Energy=	0.433405
Thermal correction to Enthalpy=	0.434350
Thermal correction to Gibbs Free Energy=	0.344150
Sum of electronic and zero-point Energies=	-1477.039721
Sum of electronic and thermal Energies=	-1477.011955
Sum of electronic and thermal Enthalpies=	-1477.011011
Sum of electronic and thermal Free Energies=	-1477.101210
SCF Done =	-1477.44536031