Electronic Supplementary Information

Divergent Synthesis of Indoles, Oxindoles, Isocoumarins and Isoquinolinones by General Pd-Catalyzed Retro-Aldol/α-Arylation

Song-Lin Zhang* and Ze-Long Yu

The Key Laboratory of Food Colloids and Biotechnology, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, Wuxi, Jiangsu 214122, China

E-mail: slzhang@jiangnan.edu.cn

Contents

1. Experimental details

1.1 General experimental considerations:

All the reactants and reagents were used as received commercially without further purification except **2c**. **2c** was prepared according to a recent report that uses the nucleophilic addition of PhMgBr to 1-phenylbutane-1,3-dione.[S1] All the reactions were performed under N_2 atmosphere. NMR spectra of the products were recorded in $CDCl_3$ or DMSO-d_6 on a 400 MHz spectrometer. Elemental analyses were performed using Elementar VARIOEL III.

Ref S1: Yuan, R.; Zhao, D.; Zhang, L.-Y.; Pan, X.; Yang, Y.; Wang, P.; Li, H.-F.; Da, C.-S. *Org. Biomol. Chem.* **2016**, *14*, 724.

1.2 Procedure for the two-step synthesis of indoles (4) and oxindoles (5)

Step 1: Procedure for Pd-catalyzed retro-aldol reaction of β-hydroxy carbonyl compounds (2) with various *o*-nitro aryl halides (1) to produce 3:

Cs_2CO_3 (244 mg, 0.75 mmol), $Pd(OAc)_2$ (6.0 mg, 0.025 mmol), PPh_3 (26 mg, 0.10 mmol) and aryl halide (**1**, 0.5 mmol) were added in an oven-dried Schlenk tube. The tube was then sealed, evacuated, and backfilled with nitrogen using standard Schlenk technique. Toluene (3.0 mL) and β-hydroxy carbonyl compound **2a** (348 mg, 3.0 mmol) were sequentially added by syringe at ambient temperature. The resulting mixture was heated at 120°C (oil bath) for 5 hours. After the mixture was cooled to room temperature, water (20 mL) was added. The product was extracted with ethyl acetate (5 mL × 3). The combined organic layer was then washed with brine, dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by column chromatography on silica gel (eluent: V(petroleum ether)/V(ethyl acetate) = 10:1~5:1 to give **3**.

When **2b** was used to react with aryl halides **1** (0.5 mmol), the catalyst system was $Pd(TFA)_2$ (8 mg, 0.025 mmol), PCy_3 (14 mg, 0.05 mmol) in xylene; **2b** was used in 3 equivalents (219 mg, 1.5 mmol). Reaction time was extended to 15 hours.

When **2c** was used to react with aryl halides **1** (0.5 mmol)**,** the catalyst system was $Pd(TFA)_2$ (8 mg, 0.025 mmol)), PPh_3 (13 mg, 0.05 mmol) in xylene; **2c** was used in 2 equivalents (240 mg, 1.0 mmol). Reaction time was extended to 15 hours.

Step 2: Procedure for the synthesis of indoles (4) or oxindoles (5) from 3:

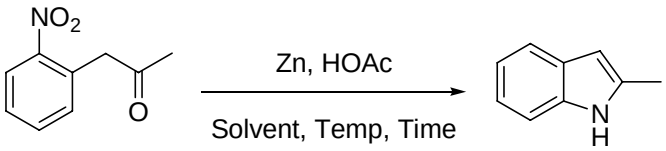
Zinc dust (0.196 g, 3 mmol) and glacial acetic acid (0.360 g, 6 mmol) were added to a reaction tube. Ethanol (2 mL) and **3** (0.5 mmol) were sequentially added by syringe at ambient temperature. The mixture was stirred at 70°C for 4 hours. Water (20 mL) was then added to the reaction mixture, and the resulting mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic layers were then washed with brine, dried over Na_2SO_4, and concentrated in vacuum. The residue was purified by column chromatography on silica gel (eluting with 10:1 (v/v) petroleum ether/ethyl acetate) to provide indoles **4** or oxindoles **5**.

1.3 Procedure for the one-step synthesis of isocoumarins (6) or *N*-arylated isoquinolin-1-one (7):

Cs_2CO_3 (244 mg, 0.75 mmol), $Pd(OAc)_2$ (6.0 mg, 0.025 mmol), PPh_3 (26 mg, 0.10 mmol) (for **7b**, Xantphos 0.05 mmol was used) were added in a reaction flask. The flask was then filled with nitrogen using standard Schlenk technique. Then methyl 2-halobenzoate (0.5 mmol) or 2-bromobenzonitrile (0.5 mmol) and 4-hydroxy-4-methyl-pentan-2-one (**2a**, 348 mg, 3.0 mmol) in toluene (3 mL) were sequentially added at ambient temperature. The resulting mixture was heated at 120°C (oil bath) for 5 hours. After the mixture was cooled to room temperature, water (20 mL) was added. The product was extracted with ethyl acetate (5 mL × 3). The combined organic layer was then washed with brine, dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by column chromatography on silica gel (eluent: V(petroleum ether)/V(ethyl acetate) = 10:1~5:1 to provide isocoumarins **6** or isoquinolin-1-one **7**.

2. Optimization study of reduction/condensation of intermediates 3

Table S1. Reaction conditions optimization for the nitro reduction/condensation of **3a** to produce indole **4a** [a]



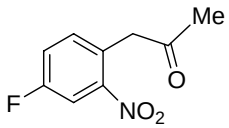
3a **4a**

Entry	Solvent	Temp (℃)	Time (h)	Zn (equiv)	HOAc(equiv)	Yield (%)[b]
1	MeOH	RT	1.5	4	8	45
2	MeOH	70	1.5	4	8	52
3	EtOH	70	1.5	4	8	65
4	EtOH	70	4	4	8	69
5	**EtOH**	**70**	**4**	**6**	**12**	**82**
6	toluene	70	1.5	4	8	10
7	toluene	70	4	4	8	18
8	toluene	70	4	6	8	21
9	toluene	70	4	6	12	36
10	toluene	70	4	8	8	46
11	toluene	120	4	4	8	18
12	THF	70	4	4	8	35

[a] Reaction conditions: **3a** (0.5 mmol), solvent (2 mL). [b] Isolated yield after column chromatography.

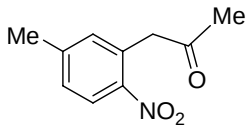
3. Spectroscopic characterization data of the products

For the characterization of **3a-d**,**i**,**j**, see our recent report: Zhang, S.-L.; Yu, Z.-L. *J. Org. Chem.*, **2016**, *81*, 57.



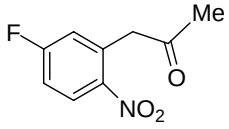
1-(4-Fluoro-2-nitrophenyl)propan-2-one (**3e**; 88 mg, 89%). Brown solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (dd, J = 8.9, 2.7 Hz, 1H), 7.63 (td, J = 8.3, 2.8 Hz, 1H), 7.52 (dd, J = 8.6, 5.8 Hz, 1H), 4.23 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 204.3 (s), 160.9 (d, J = 247.1 Hz), 149.5 (d, J = 8.7 Hz), 135.8 (d, J = 8.1 Hz), 127.2 (d, J = 3.6 Hz), 121.3 (d, J = 21.0 Hz), 112.6 (d, J = 26.9 Hz), 47.3 (s), 30.1 (s).

Anal. Calcd for $C_9H_8FNO_3$: C, 54.83; H, 4.09; N, 7.10. Found: C, 54.89; H, 4.13; N, 7.07.



1-(5-Methyl-2-nitrophenyl)propan-2-one (**3f**; 73 mg, 75%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 1H), 7.26 (dd, J = 8.4, 1.3 Hz, 1H), 7.08 (s, 1H), 4.10 (s, 2H), 2.45 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.8, 144.9, 134.2, 130.5, 129.0, 128.3, 125.5, 48.7, 30.0, 21.4. Anal. Calcd for $C_{10}H_{11}NO_3$: C, 62.17; H, 5.74; N, 7.25. Found: C, 62.10; H, 5.77; N, 7.27.

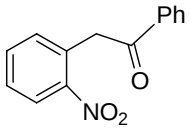
(Reference: Sutherland, R. G.; Chowdhury, R. L.; Pidrko, A.; Lee, C. C. *J. Org. Chem.* **1987**, *52*, 4618.)



1-(5-Fluoro-2-nitrophenyl)propan-2-one (**3g**; 79 mg, 80%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 9.1, 5.1 Hz, 1H), 7.19 – 7.12 (m, 1H), 7.00 (dd, *J* = 8.6, 2.7 Hz, 1H), 4.15 (s, 2H), 2.36 (s, 3H).

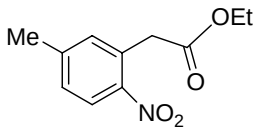
^{13}C NMR (101 MHz, $CDCl_3$) δ 202.8 (s), 164.8 (d, *J* = 257.7 Hz), 144.7 (s), 133.9 (d, *J* = 9.5 Hz), 128.2 (d, *J* = 10.0 Hz), 120.4 (d, *J* = 23.6 Hz), 115.4 (d, *J* = 23.0 Hz), 48.6 (s), 30.0 (s).

Anal. Calcd for $C_9H_8FNO_3$: C, 54.83; H, 4.09; N, 7.10. Found: C, 54.93; H, 4.06; N, 7.05.

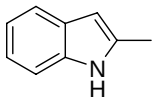


2-(2-Nitrophenyl)-1-phenylethanone (**3h**; 76 mg, 63%). Brown oil; ^{1}H NMR (400 MHz, CDCl3) δ 8.18 (dd, *J* = 8.2, 1.2 Hz, 1H), 8.07 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.66 – 7.61 (m, 2H), 7.53 (t, *J* = 7.6 Hz, 3H), 7.38 (dd, *J* = 7.6, 1.1 Hz, 1H), 4.76 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 149.1, 136.5, 133.7, 133.5, 130.7, 129.1, 128.8, 128.4, 128.3, 125.3, 44.1. Anal. Calcd for $C_{14}H_{11}NO_3$: C, 69.70; H, 4.60; N, 5.81. Found: C, 69.46; H, 4.57; N, 5.97.

(Reference: (a) Hering, T.; Hari, D. P.; König, B. *J. Org. Chem*. **2012**, *77*, 10347. (b) Strazzolini, P.; Giumanini, A. G.; Runcio, A.; Scuccato, M. *J. Org. Chem.* **1998**, *63*, 952.)

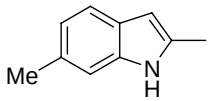


Ethyl 2-(5-methyl-2-nitrophenyl)acetate (**3k**; 61 mg; 54%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.26 (d, *J* = 1.3 Hz, 1H), 7.16 (s, 1H), 4.20 (q, *J* = 7.1 Hz, 2H), 4.00 (s, 2H), 2.45 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 146.5, 144.8, 134.0, 130.0, 129.1, 125.5, 61.2, 40.0, 21.4, 14.1. Anal. Calcd for $C_{11}H_{13}NO_4$: C, 59.19; H, 5.87; N, 6.27. Found: C, 59.16; H, 5.90; N, 6.31.



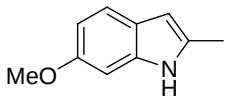
2-Methyl-1*H*-indole (**4a**; 53 mg; 82%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (br s, 1H), 7.58 (d, *J* = 7.4 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), δ 7.21 – 7.10 (m, 2H), 6.27 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.1, 135.1, 129.1, 120.9, 119.7, 110.2 100.4, 13.7. Anal. Calcd for C_9H_9N: C, 82.41; H, 6.92; N, 10.68. Found: C, 82.56; H, 6.94; N, 10.50.

(Reference: Rubio-Marqués, P.; Rivero-Crespo, M. A.; Leyva-Pérez, A.; Corma, A. *J. Am. Chem. Soc.* **2015**, *137*, 11832.)



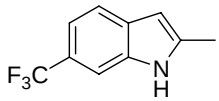
2,6-Dimethyl-1*H*-indole (**4b**; 53 mg; 73%).White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (br s, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.09 (s, 1H), 6.96 (d, *J* = 7.7 Hz, 1H), 6.21 (s, 1H), 2.50 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 134.4, 130.6, 126.8, 121.3, 119.3, 110.3, 100.1, 21.7, 13.7. Anal. Calcd for $C_{10}H_{11}N$: C, 82.72; H, 7.64; N, 9.65. Found: C, 82.85; H, 7.67; N, 9.48.

(Reference: Ferretti, F.; Muto, S.; Hagar, M.; Gallo, E.; Ragaini, F. *Eur. J. Org. Chem.* **2015**, 5712.)



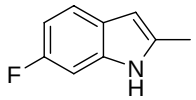
6-Methoxy-2-methyl-1*H*-indole (**4c**; 70 mg; 86%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (br s, 1H), 7.41 (d, *J* = 8.3 Hz, 1H), 6.87 – 6.73 (m, 2H), 6.17 (s, 1H), 3.86 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.7, 136.8, 133.9, 123.3, 120.1, 109.0, 100.0, 94.5, 55.8, 13.7. Anal. Calcd for $C_{10}H_{11}NO$: C, 74.51; H, 6.88; N, 8.69. Found: C, 74.35; H, 6.95; N, 8.77.

(Reference: Ferretti, F.; Muto, S.; Hagar, M.; Gallo, E.; Ragaini, F. *Eur. J. Org. Chem.* **2015**, 5712.)



2-Methyl-6-(trifluoromethyl)-1*H*-indole (**4d**; 53 mg; 53%). Green solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (br s, 1H), 7.64 – 7.54 (m, 2H), 7.33 (d, *J* = 8.2 Hz, 1H), 6.31 (s, 1H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.1, 134.9, 131.5, 125.3 (q, *J* = 272.3 Hz), 123.0 (q, *J* = 31.5 Hz), 119.8, 116.4 (q, *J* = 3.5 Hz), 107.6 (q, *J* = 4.8 Hz), 100.9, 13.8. Anal. Calcd for $C_{10}H_8F_3N$: C, 60.30; H, 4.05; N, 7.03. Found: C, 60.39; H, 4.02; N, 7.01.

(Reference: Shen, M.; Leslie, B. E.; Driver, T. G. *Angew. Chem. Int. Ed.* **2008**, *47*, 5056.)

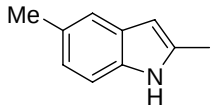


6-Fluoro-2-methyl-1*H*-indole (**4e**; 60 mg; 80%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.43 (dd, *J* = 8.6, 5.4 Hz, 1H), 6.98 (dd, *J* = 9.6, 2.2 Hz, 1H), 6.87 (ddd, *J* = 9.8, 8.6, 2.3 Hz, 1H), 6.22 (s, 1H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3 (d, *J* = 235.9 Hz), 135.9 (d, *J* = 12.3 Hz), 135.4 (d, *J* = 2.5 Hz), 125.5 (s), 120.1 (d, *J* = 9.9 Hz), 108.0 (d, *J* = 24.1 Hz), 100.3 (s), 96.8 (d, *J* = 26.2 Hz), 13.7 (s).

Anal. Calcd for C_9H_8FN: C, 72.47; H, 5.41; N, 9.39. Found: C, 72.35; H, 5.46; N, 9.45.

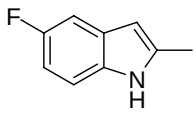
(Reference: Ferretti, F.; Muto, S.; Hagar, M.; Gallo, E.; Ragaini, F. *Eur. J. Org. Chem.* **2015**, 5712.)



2,5-Dimethyl-1*H*-indole (**4f**; 58 mg; 79%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (br s, 1H), 7.34 (s, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.17 (s, 1H), 2.47 (d, *J* = 2.7 Hz, 3H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.1,

134.4, 129.4, 128.8, 122.4, 119.4, 109.9, 100.0, 21.5, 13.8. Anal. Calcd for $C_{10}H_{11}N$: C, 82.72; H, 7.64; N, 9.65. Found: C, 82.87; H, 7.56; N, 9.57.

(Reference: Rodriguez-Dafonte, P.; Terrier, F.; Lakhdar, S.; Kurbatov, S.; Goumont, R. *J. Org. Chem.* **2009**, *74*, 3305.)

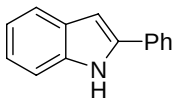


5-Fluoro-2-methyl-1*H*-indole (**4g**; 64 mg; 85%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (br s, 1H), 7.24 – 7.14 (m, 2H), 6.88 (td, *J* = 9.2, 2.3 Hz, 1H), 6.22 (s, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0 (d, *J* = 233.4 Hz), 137.03 (s), 132.53 (s), 129.5 (d, *J* = 10.2 Hz), 110.6 (d, *J* = 9.8 Hz), 109.0 (d, *J* = 26.2 Hz), 104.6 (d, *J* = 23.6 Hz), 100.7 (s), 13.8 (s).

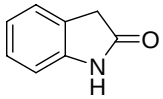
Anal. Calcd for C_9H_8FN: C, 72.47; H, 5.41; N, 9.39. Found: C, 72.38; H, 5.45; N, 9.43.

(Reference: Neumann, J. J.; Rakshit, S.; Drçge, T.; Glorius, F. *Chem. Eur. J.* **2011**, *17*, 7298.)



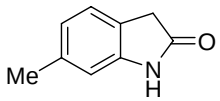
2-phenyl-1*H*-indole (**4h**; 69 mg, 71%). Pale-yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (br s, 1H), 7.75-7.65 (m, 3H), 7.52-7.40 (m, 3H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.23 (t, *J* = 7.1 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 6.86 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.9, 136.8, 132.4, 129.3, 129.0, 127.9, 127.7, 125.2, 122.4, 120.7, 120.3, 110.9, 100.0. Anal. Calcd for $C_{14}H_{11}N$: C, 87.01; H, 5.74; N, 7.25. Found: C, 87.09; H, 5.81; N, 7.10.

(Reference: Shen, M.; Leslie, B. E.; Driver, T. G. *Angew. Chem. Int. Ed.* **2008**, *47*, 5056.)

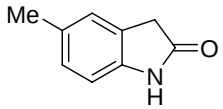


Indolin-2-one (**5a**; 62 mg; 93%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (s, 1H), 7.24 (t, *J* = 7.4 Hz, 2H), 7.04 (t, *J* = 7.7 Hz, 1H), 6.93 (d, *J* = 7.7 Hz, 1H), 3.57 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.0, 142.6, 127.9, 125.3, 124.6, 122.3, 109.8, 36.3. Anal. Calcd for C_8H_7NO: C, 72.17; H, 5.30; N, 10.52. Found: C, 72.05; H, 5.36; N, 10.55.

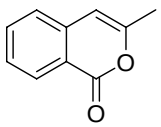
(Reference: Motoyama, Y.; Kamo, K.; Nagashima, H. *Org. Lett.* **2009**, *11*, 1345.)



6-Methylindolin-2-one (**5b**; 62 mg; 84%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (s, 1H), 7.12 (d, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 7.5 Hz, 1H), 6.76 (s, 1H), 3.53 (s, 2H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.4, 142.7, 138.0, 124.3, 122.9, 122.2, 110.7, 36.1, 21.6. Anal. Calcd for C_9H_9NO: C, 73.45; H, 6.16; N, 9.52. Found: C, 73.51; H, 6.27; N, 9.32.



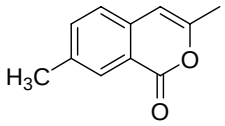
5-Methylindolin-2-one (**5c**; 64 mg; 86%). White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (s, 1H), 7.06 (s, 1H), 7.03 (d, *J* = 7.9 Hz, 1H), 6.81 (d, *J* = 7.9 Hz, 1H), 3.53 (s, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.1, 140.2, 131.8, 128.2, 125.4, 109.5, 36.4, 21.1. Anal. Calcd for C_9H_9NO: C, 73.45; H, 6.16; N, 9.52. Found: C, 73.56; H, 6.21; N, 9.45.



3-Methyl-1*H*-isochromen-1-one (**6a**; 55 mg, 70%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.5 Hz, 1H), δ 7.69 (td, *J* = 7.7, 1.3 Hz, 1H), 7.46 (t, *J* = 8.2 Hz, 1H), 7.35 (d, *J* = 7.9 Hz, 1H), 6.28 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)

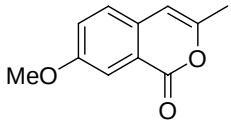
δ 162.9, 137.7, 134.7, 129.5, 127.5, 124.8, 120.0, 103.5, 19.6. Anal. Calcd for $C_{10}H_8O_2$: C, 74.99; H, 5.03. Found: C, 75.06; H, 5.05.

(Reference: Hauser, F. M.; Baghdanov, V. M. *J. Org. Chem.* **1988**, *53*, 4676)



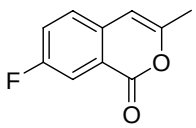
3,7-Dimethyl-1*H*-isochromen-1-one (**6b**; 77 mg; 88%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.50 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 6.24 (s, 1H), 2.46 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 153.6, 137.7, 136.0, 135.2, 129.2, 124.8, 119.8, 103.4, 21.3, 19.6. Anal. Calcd for $C_{11}H_{10}O_2$: C, 75.84; H, 5.79. Found: C, 75.78; H, 5.86.

(Reference: Zhang, M.; Zhang, H.-J.; Han, T.; Ruan, W.; Wen, T.-B. *J. Org. Chem.* **2015**, *80*, 620.)



7-Methoxy-3-methyl-1*H*-isochromen-1-one (**6c**; 73 mg; 77%). Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.29 (s, 2H), 6.24 (s, 1H), 3.91 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 159.1, 152.4, 131.4, 126.4, 124.5, 121.0, 109.9, 103.1, 55.7, 19.4. Anal. Calcd for $C_{11}H_{10}O_3$: C, 69.46; H, 5.30. Found: C, 69.41; H, 5.36.

(Reference: Kavala, V.; Wang, C.-C.; Barange, D. K.; Kuo, C.-W.; Lei, P.-M.; Yao, C.-F. *J. Org. Chem.* **2012**, *77*, 5022.)

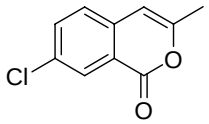


7-Fluoro-3-methyl-1*H*-isochromen-1-one (**6d**; 56 mg; 63%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.5 Hz, 1H), 7.45-7.33 (m, 2H), 6.27 (s, 1H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1 (d, *J* = 3.6 Hz), 161.5 (d, *J* = 248.6 Hz), 153.9 (d, *J* = 2.7 Hz), 134.1 (d, *J* = 2.5 Hz), 127.0 (d, *J* = 7.6 Hz), 123.1 (d, *J* = 23.2 Hz), 121.5 (d, *J* = 8.1 Hz), 114.9 (d, *J* = 23.2 Hz), 102.8 (s), 19.5 (s).

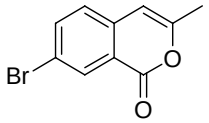
Anal. Calcd for $C_{10}H_7FO_2$: C, 67.42; H, 3.96. Found: C, 67.35; H, 3.99.

(Reference: Liu, L. et al. *Tetrahedron* **2012**, *68*, 5391.)



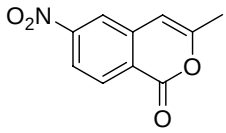
7-Chloro-3-methyl-1*H*-isochromen-1-one (**6e**; 60 mg; 62%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 6.26 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7, 155.0, 136.0, 135.1, 133.2, 129.0, 126.4, 121.1, 102.8, 19.6. Anal. Calcd for $C_{10}H_7ClO_2$: C, 61.72; H, 3.63. Found: C, 61.65; H, 3.51.

(Reference: Kavala, V.; Wang, C.-C.; Barange, D. K.; Kuo, C.-W.; Lei, P.-M.; Yao, C.-F. *J. Org. Chem.* **2012**, *77*, 5022.)



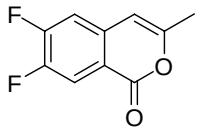
7-Bromo-3-methyl-1*H*-isochromen-1-one (**6f**; 72 mg; 60%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 1.9 Hz, 1H), 7.78 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 6.26 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6, 155.2, 137.8, 136.3, 132.1, 126.5, 121.4, 120.8, 102.9, 19.7. Anal. Calcd for $C_{10}H_7BrO_2$: C, 50.24; H, 2.95. Found: C, 50.39; H, 2.81.

(Reference: Liu, L. et al. *Tetrahedron* **2012**, *68*, 5391.)



3-Methyl-6-nitro-1*H*-isochromen-1-one (**6g**; 79 mg; 77%). Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.3 Hz, 1H), 8.24 (d, *J* = 2.2 Hz, 1H), 8.22 (s, 1H), 6.41 (s, 1H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.1, 157.2, 151.6, 138.7,

131.6, 123.9, 121.5, 120.0, 103.0, 19.8. Anal. Calcd for $C_{10}H_7NO_4$: C, 58.54; H, 3.44; N, 6.83. Found: C, 58.61; H, 3.45; N, 6.71.

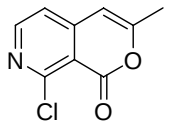


6,7-Difluoro-3-methyl-1*H*-isochromen-1-one (**6h**; 61 mg; 62%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 9.8, 8.0 Hz, 1H), 7.14 (dd, *J* = 10.1, 7.1 Hz, 1H), 6.22 (s, 1H), 2.30 (s, 3H).

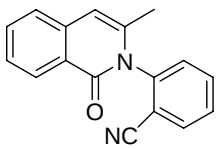
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2 (d, *J* = 2.9 Hz), 155.6 (d, *J* = 2.6 Hz), 155.2 (dd, *J* = 259.4, 14.0 Hz), 149.8 (dd, *J* = 252.2, 13.9 Hz), 135.7 (dd, *J* = 9.0, 3.0 Hz), 118.0 (dd, *J* = 18.9, 2.5 Hz), 116.7 (dd, *J* = 6.2, 2.7 Hz), 112.9 (d, *J* = 18.5 Hz), 102.35 – 102.27 (m), 19.6 (s).

Anal. Calcd for $C_{10}H_6F_2O_2$: C, 61.23; H, 3.08. Found: C, 61.11; H, 3.17.

(Reference: Okuma, K.; Hirano, K.; Tanabe, Y.; Itoyama, R.; Miura, A.; Nagahora, N.; Shioji, K. *Chem. Lett.* **2014**, *43*, 492.)

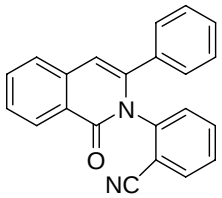


8-Chloro-3-methyl-1*H*-pyrano[3,4-*c*]pyridin-1-one (**6i**; 69 mg; 70%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 5.2 Hz, 1H), 7.14 (d, *J* = 5.2 Hz, 1H), 6.25 (s, 1H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.1, 157.9, 153.7, 152.1, 147.9, 118.0, 102.2, 20.0. Anal. Calcd for $C_9H_6ClNO_2$: C, 55.26; H, 3.09; N, 7.16. Found: C, 55.49; H, 2.99; N, 7.11. ESI-MS m/z: $[M + H]^+$ Calcd 196.0; Found: 196.1.



2-(3-Methyl-1-oxoisoquinolin-2(1H)-yl)benzonitrile (**7a**; 36 mg, 55%). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.0 Hz, 1H), 7.67 (dd, *J* = 7.8, 1.2 Hz, 1H),

7.62 – 7.53 (m, 2H), 7.48 – 7.42 (m, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.17 (td, *J* = 7.7, 1.0 Hz, 1H), 6.14 (s, 1H), 2.14 (d, *J* = 0.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5, 150.3, 134.4, 133.2, 133.1, 132.9 128.1, 127.9, 124.6, 123.4, 123.0, 122.2, 118.0, 106.8, 103.3, 19.1. Anal. Calcd for $C_{17}H_{12}N_2O$: C, 78.44; H, 4.65; N, 10.76. Found: C, 78.31; H, 4.69; N, 10.82. IR (ν_{max}, cm^{-1}): 2219, 1674, 1634, 1160, 1073, 749, 677. ESI-MS m/z: $[M + H]^+$ Calcd 261.1; Found 261.1.



2-(1-Oxo-3-phenylisoquinolin-2(1H)-yl)benzonitrile (**7b**; 51 mg, 63%). Pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 7.9 Hz, 1H), 7.72 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.67- 7.59 (m, 2H), 7.58 – 7.54 (m, 2H), 7.50 (td, *J* = 7.6, 1.1 Hz, 1H), 7.42 (dd, *J* = 7.7, 4.9 Hz, 2H), 7.40 – 7.35 (m, 3H), 7.22 (td, *J* = 7.7, 1.0 Hz, 1H), 6.84 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.1, 151.6, 150.5, 134.2, 133.4, 133.2, 133.0, 132.0, 128.8, 128.6, 128.2, 125.8, 124.6, 123.6, 122.8, 122.7, 117.9, 106.8, 101.8. Anal. Calcd for $C_{22}H_{14}N_2O$: C, 81.97; H, 4.38; N, 8.69. Found: C, 82.10; H, 4.51; N, 8.52. IR (ν_{max}, cm^{-1}): 2225, 1656, 1623, 1153, 1076, 756, 686.

4. ^{1}H and ^{13}C NMR spectra of the products

Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **3e**

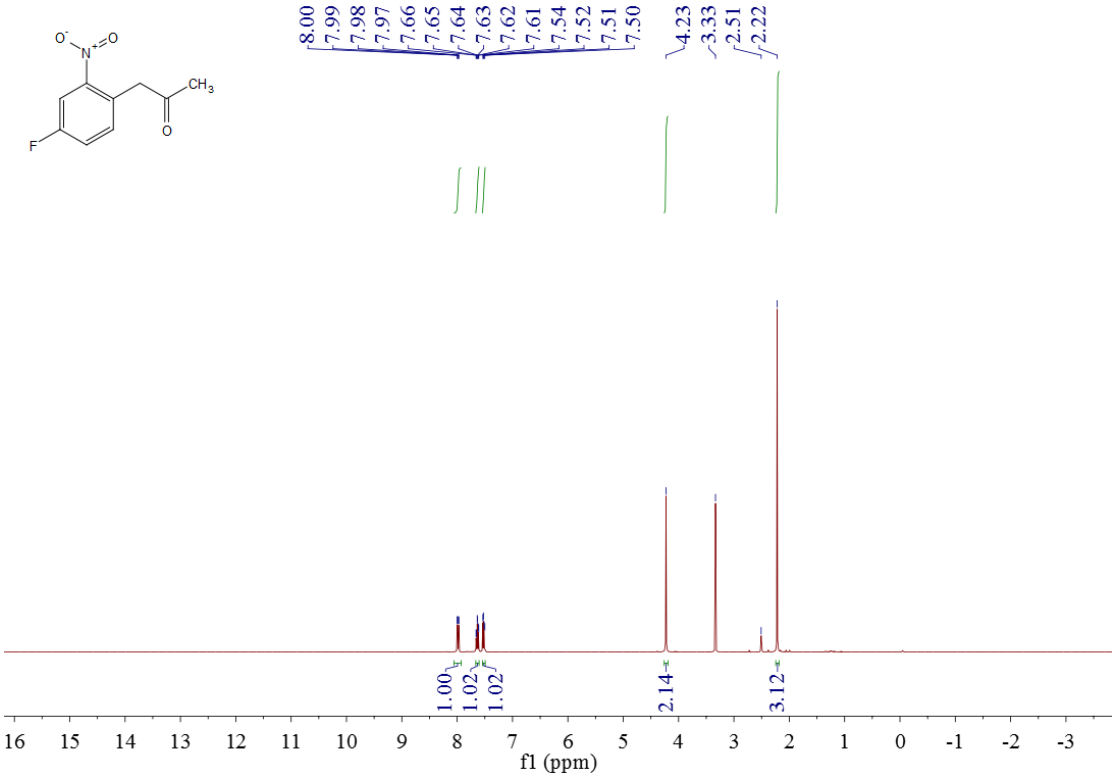


Figure S2. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **3e**

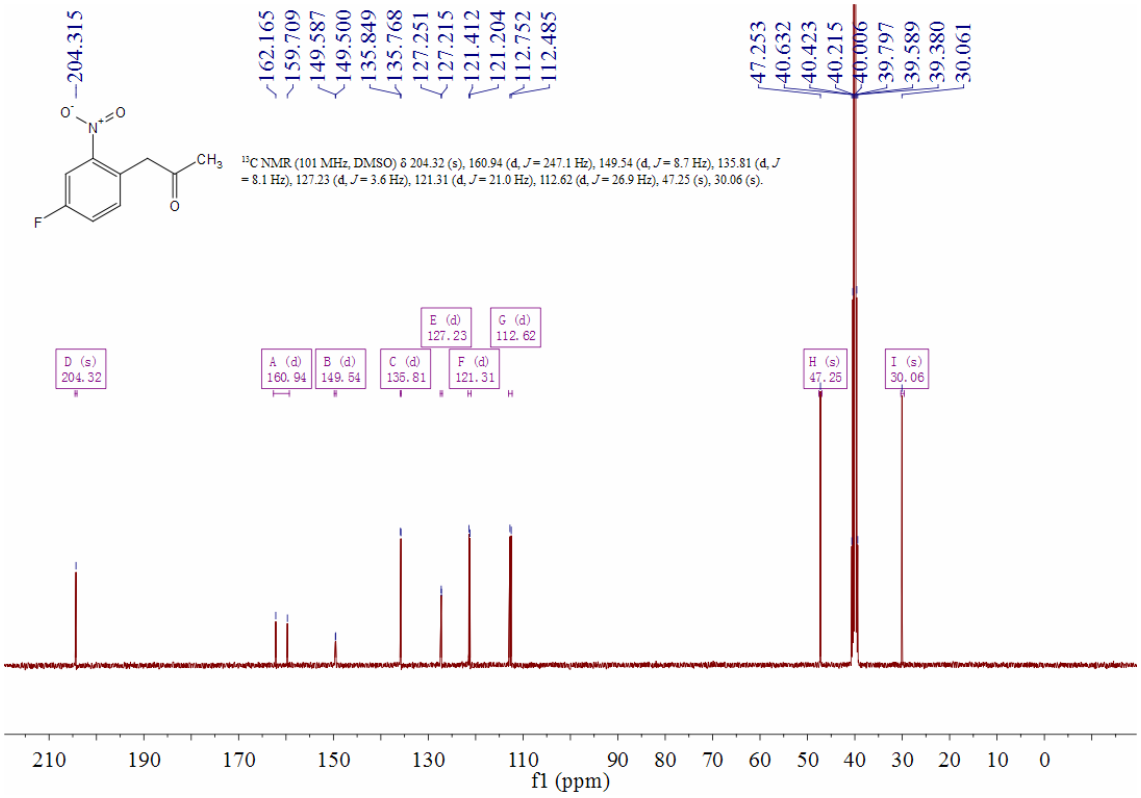


Figure S3. ^{1}H NMR spectrum of **3f**

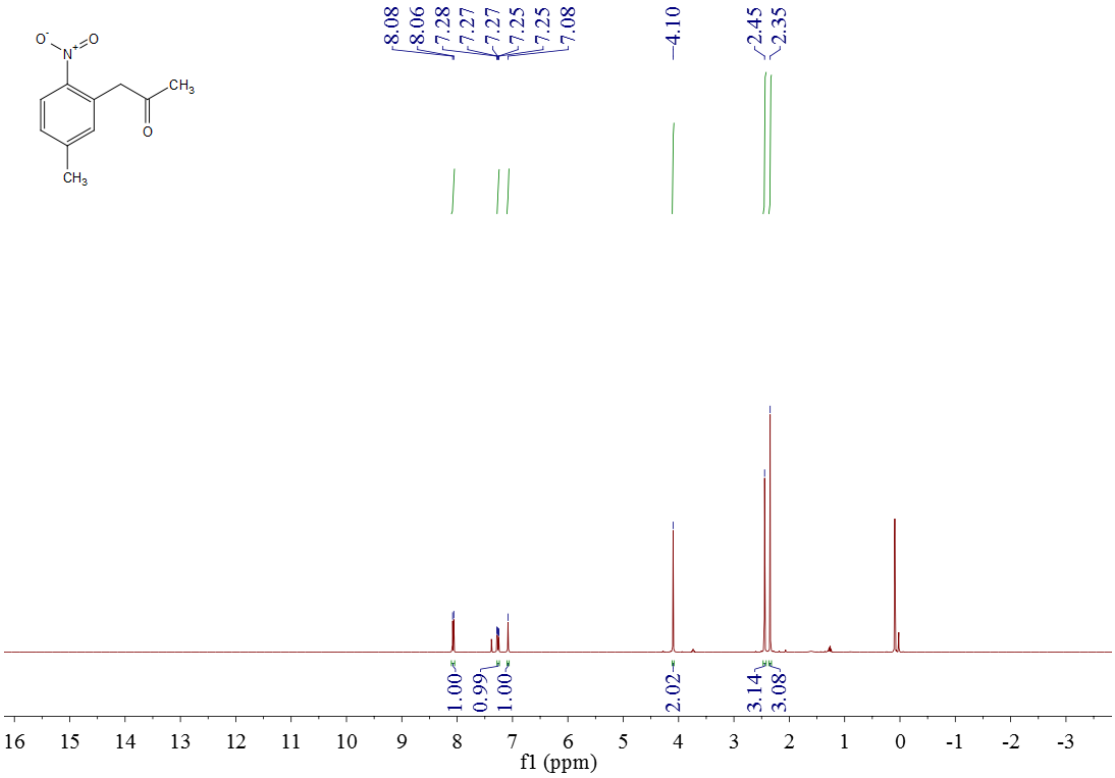


Figure S4. ^{13}C NMR spectrum of **3f**

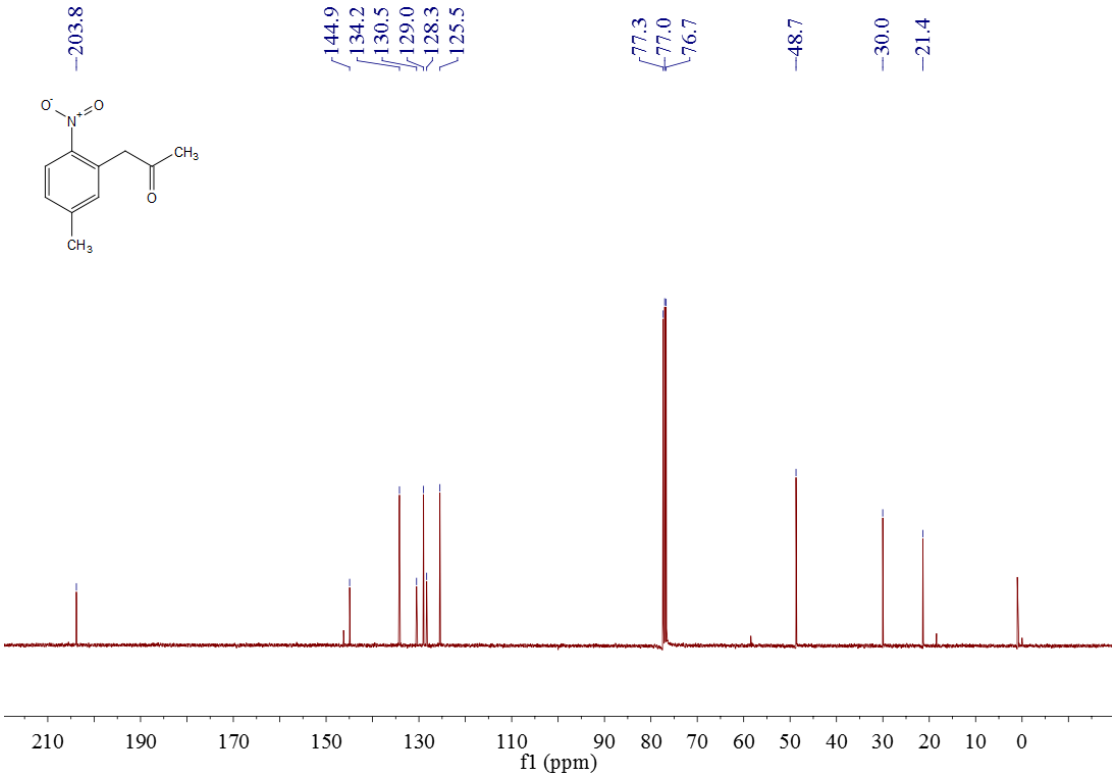


Figure S5. ^{1}H NMR spectrum of **3g**

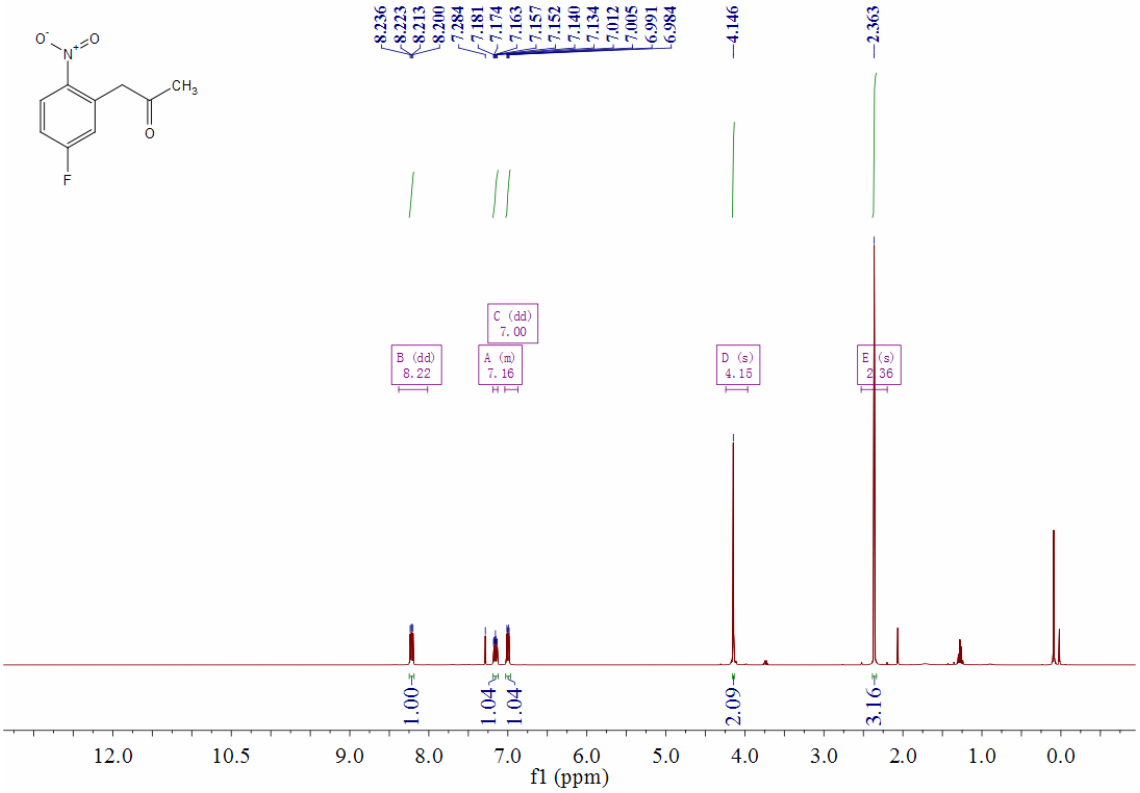


Figure S6. ^{13}C NMR spectrum of **3g**

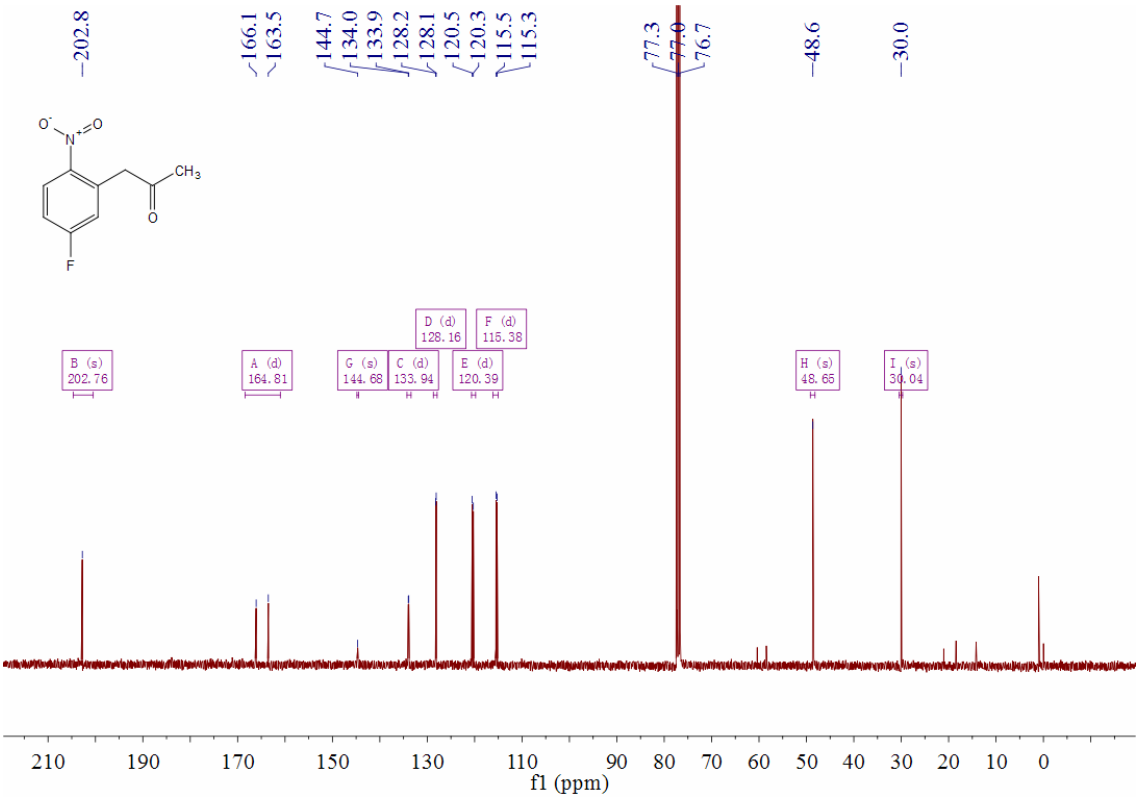


Figure S7. ^{1}H NMR spectrum of **3h**

Figure S8. ^{13}C NMR spectrum of **3h**

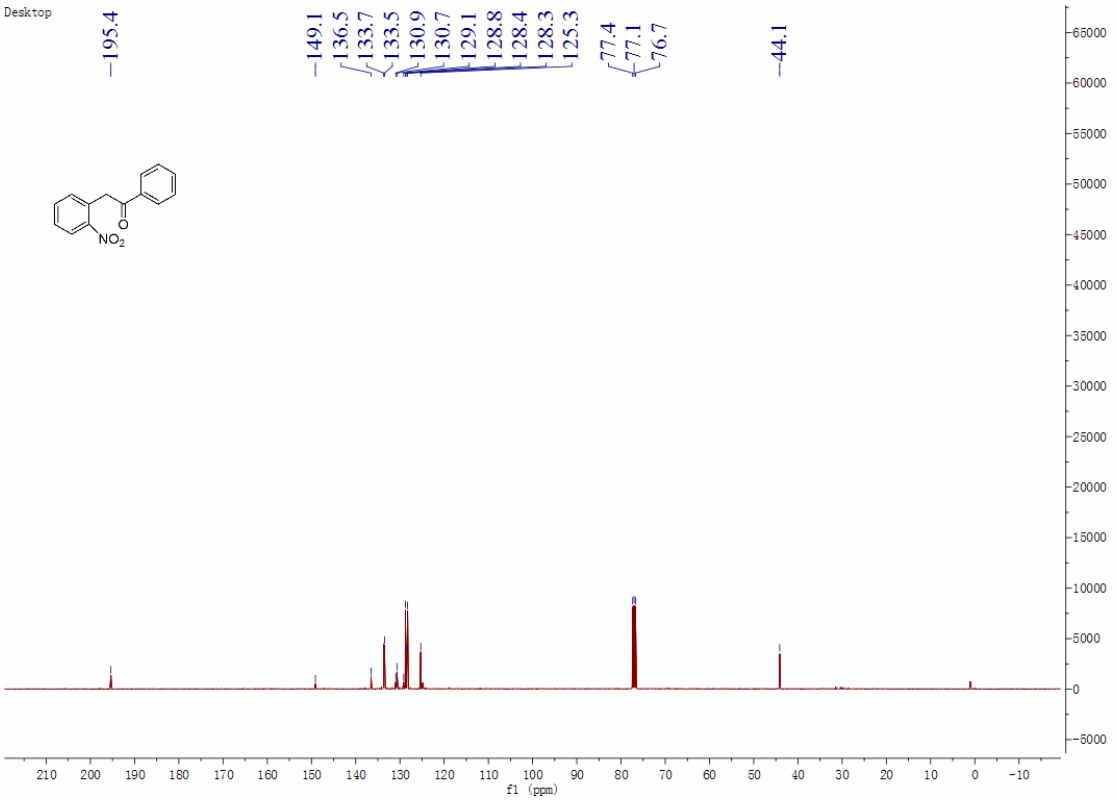


Figure S9. ^{1}H NMR spectrum of **3k**

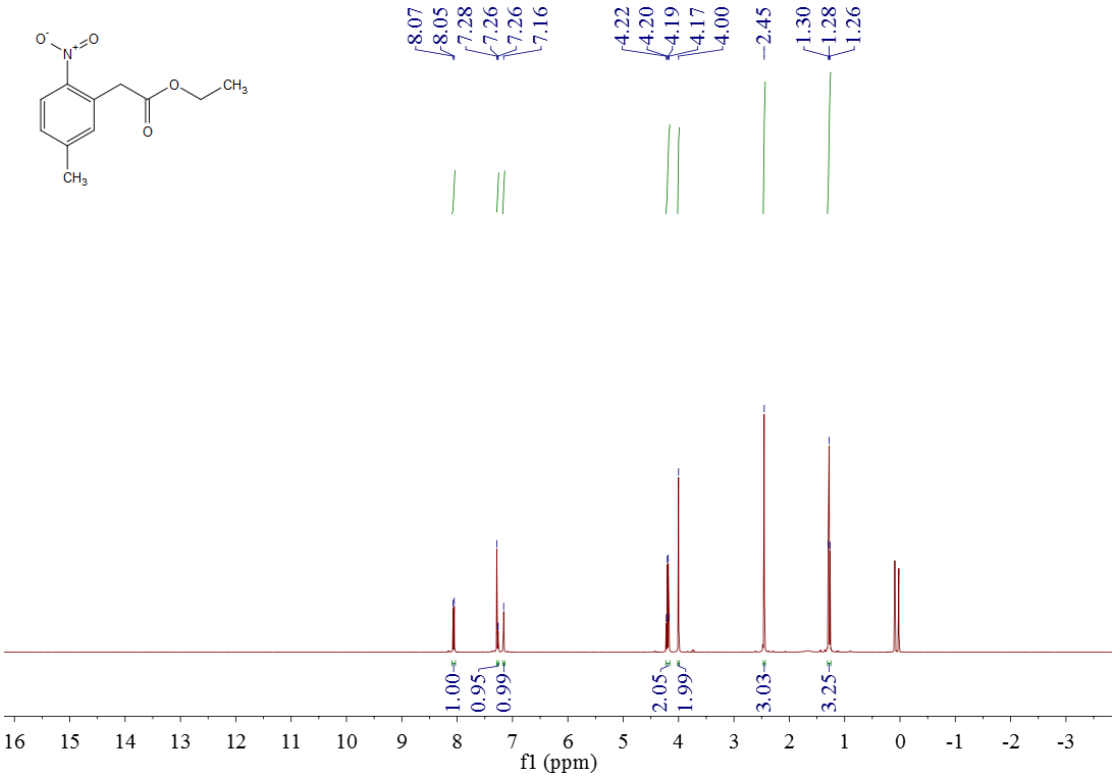


Figure S10. ^{13}C NMR spectrum of **3k**

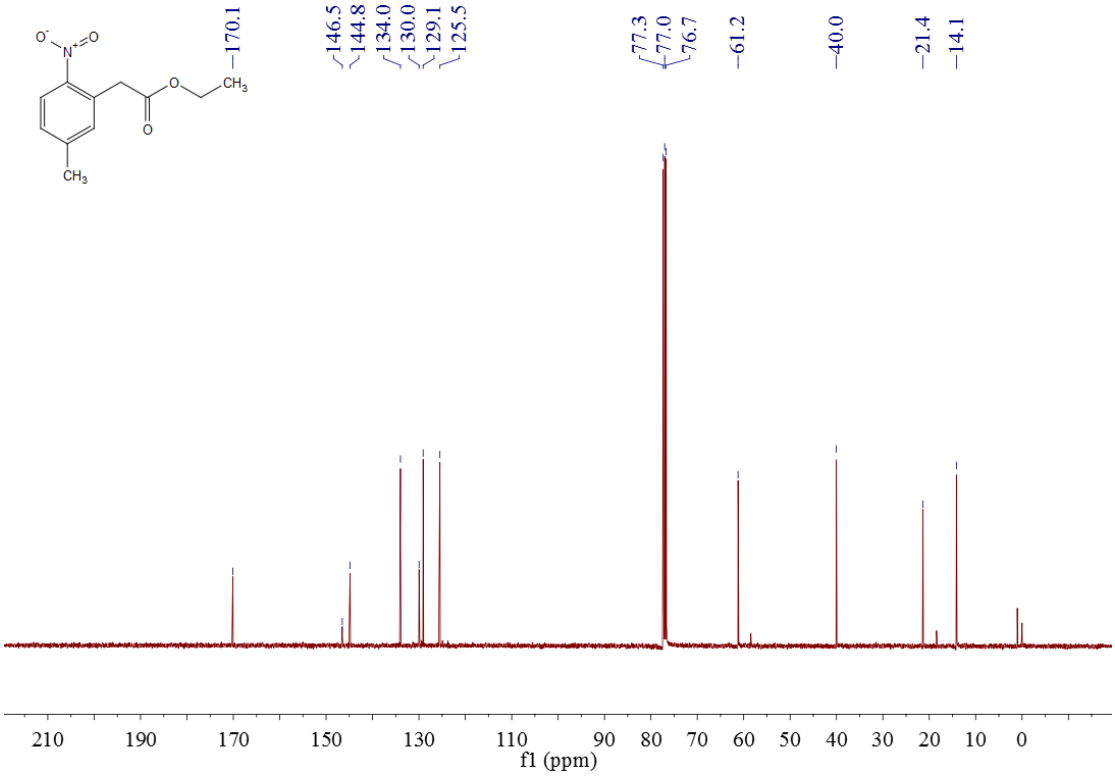


Figure S11. ^{1}H NMR spectrum of **4a**

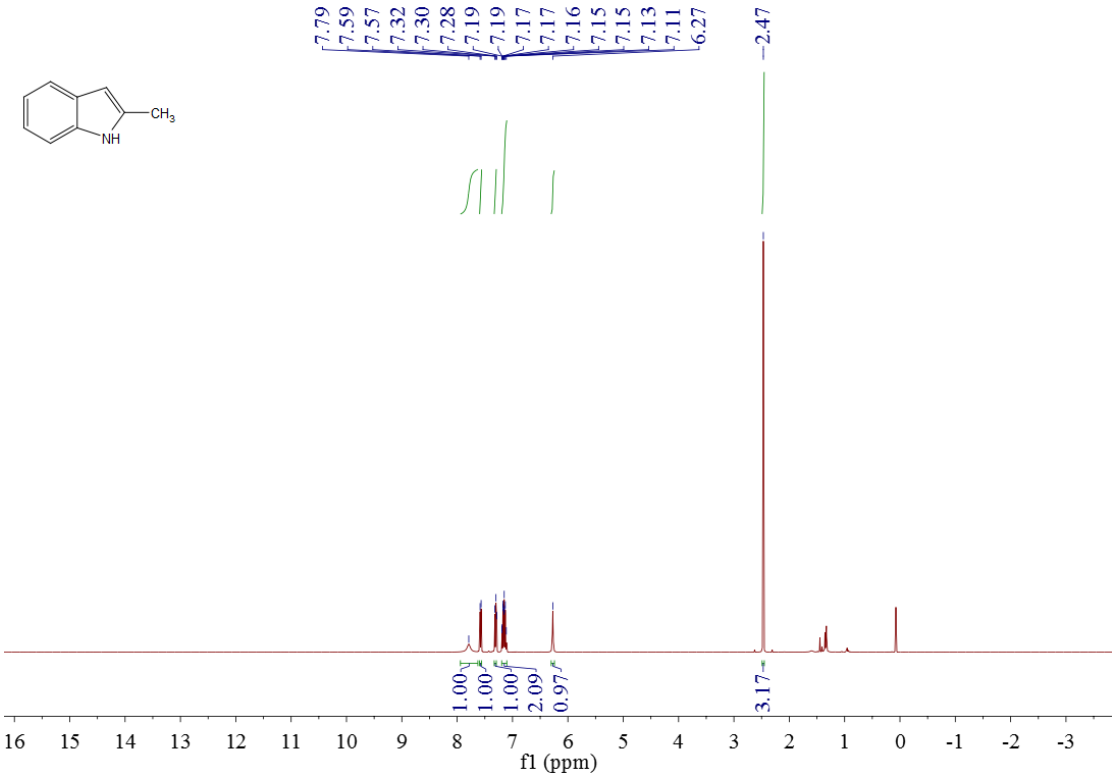


Figure S12. ^{13}C NMR spectrum of **4a**

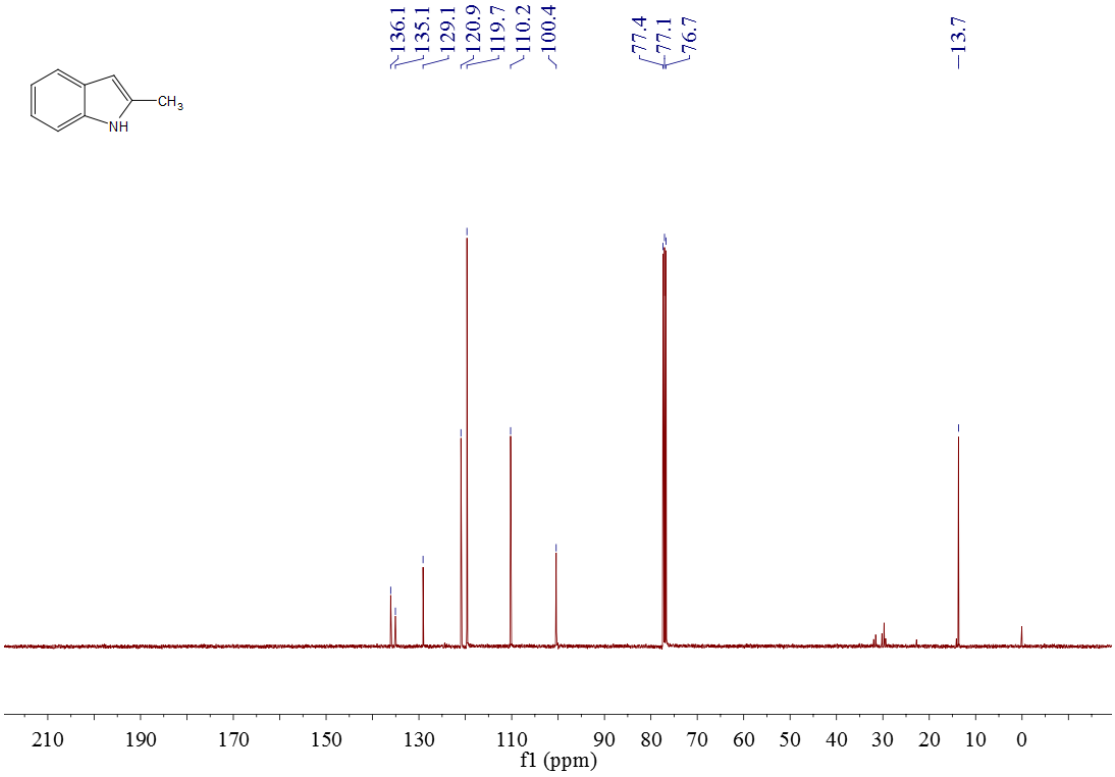


Figure S13. ^{1}H NMR spectrum of **4b**

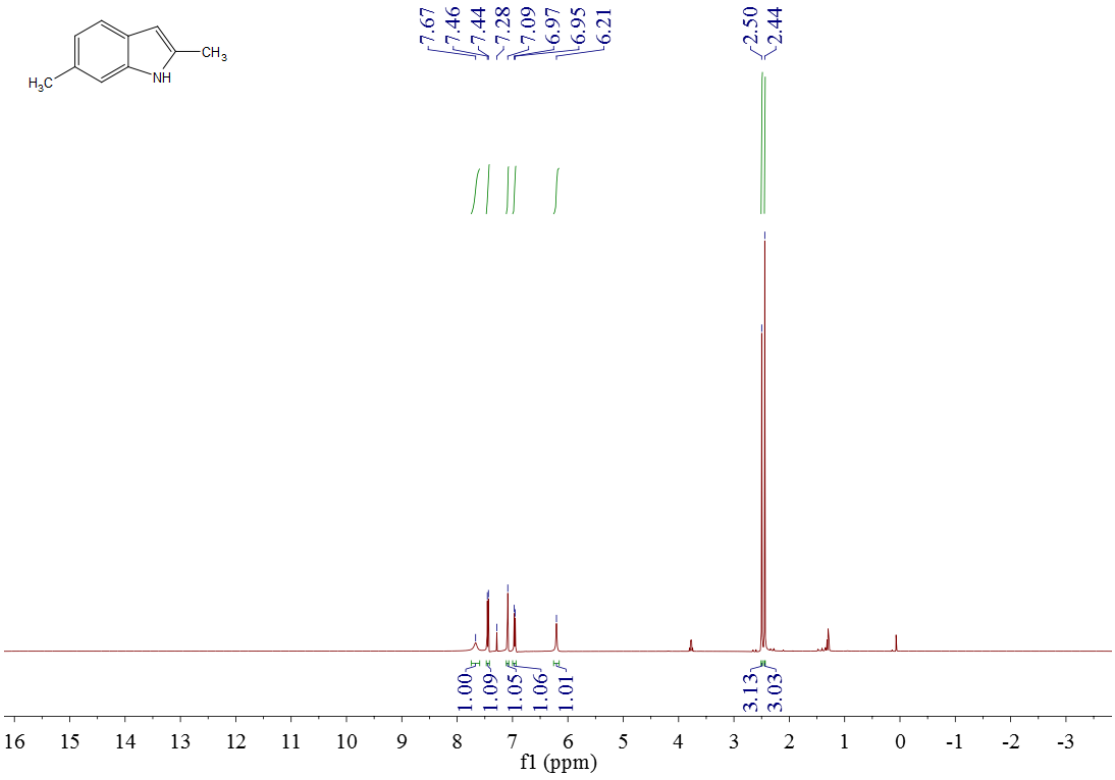


Figure S14. ^{13}C NMR spectrum of **4b**

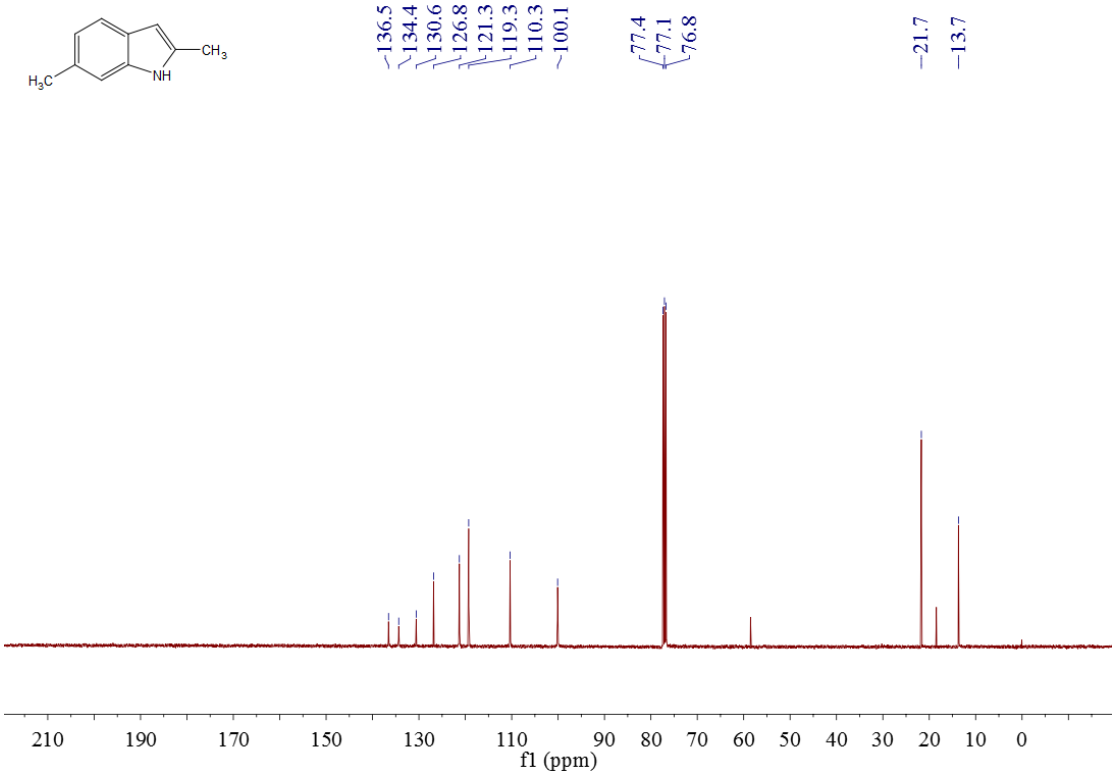


Figure S15. ^{1}H NMR spectrum of **4c**

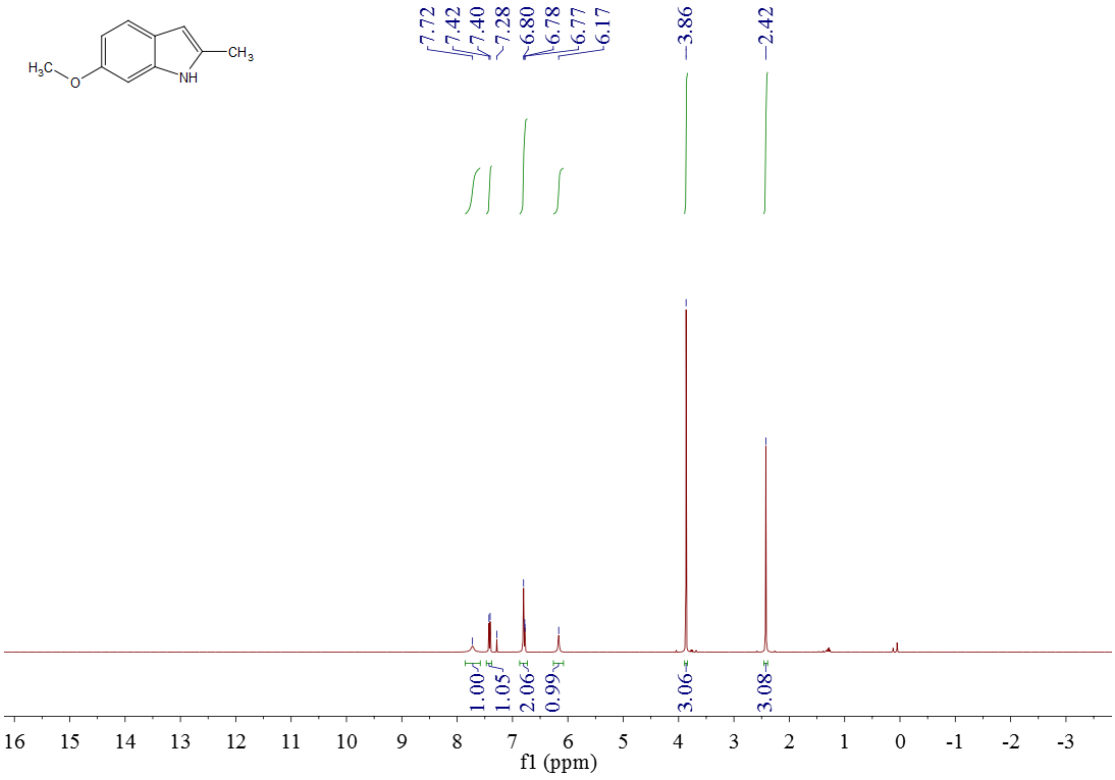


Figure S16. ^{13}C NMR spectrum of **4c**

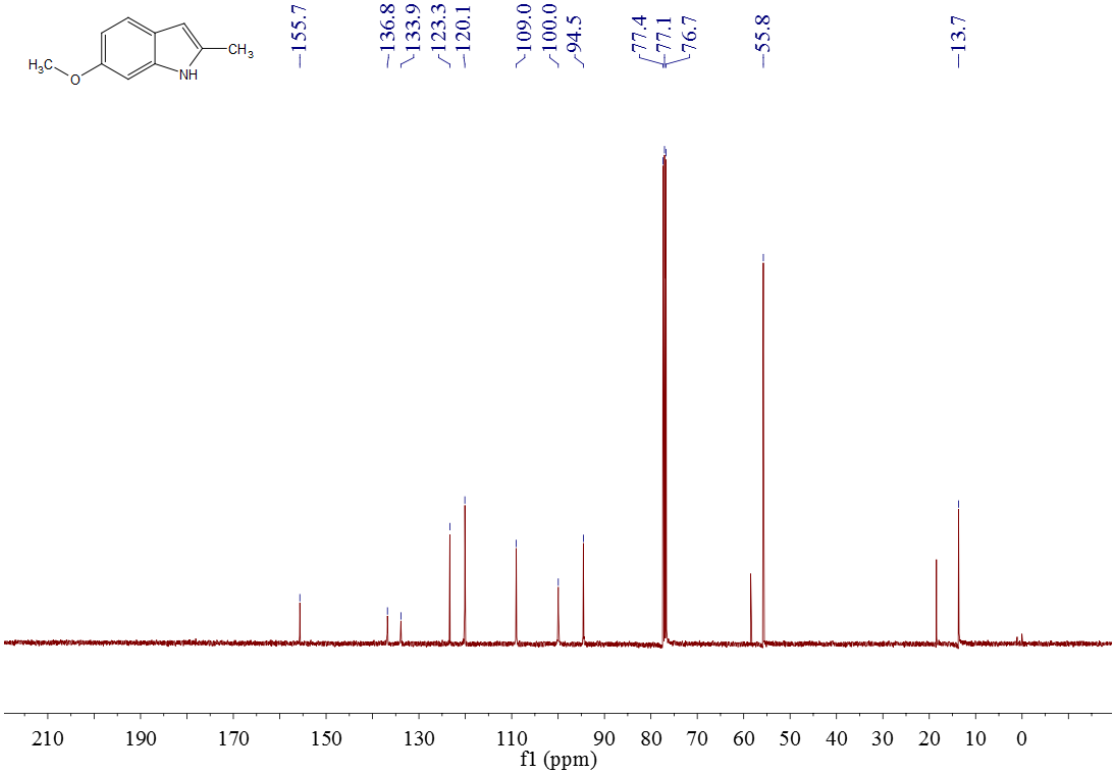


Figure S17. ^{1}H NMR spectrum of **4d**

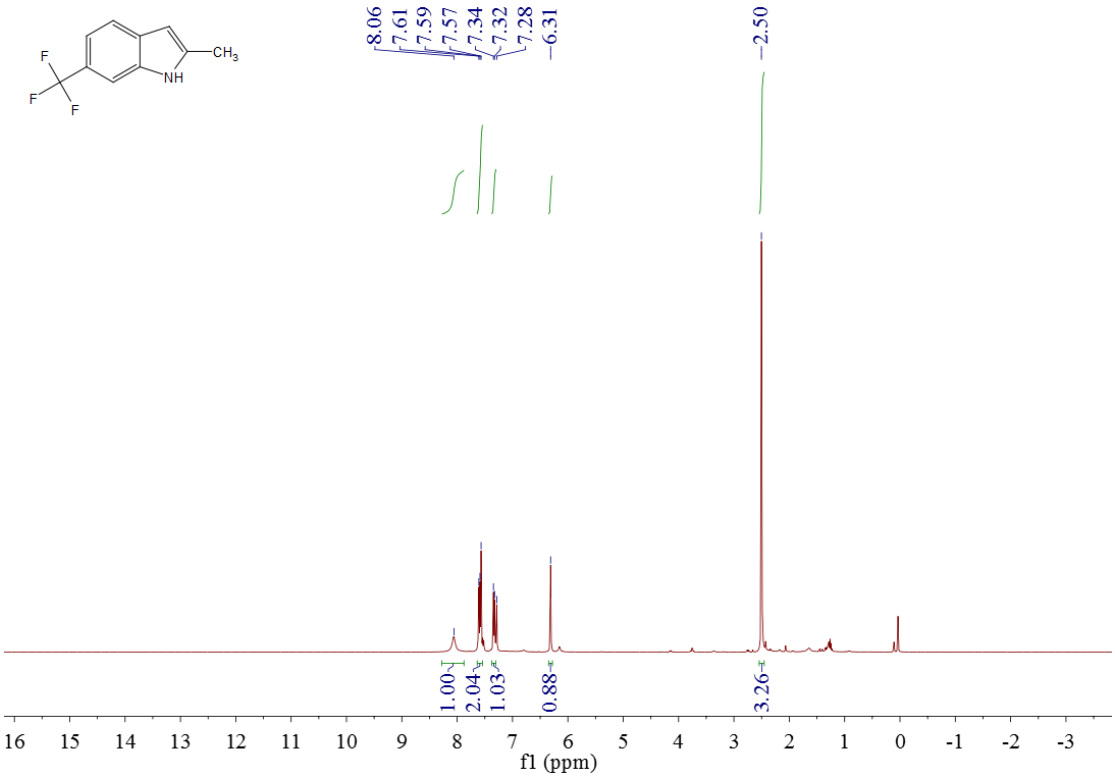


Figure S18. ^{13}C NMR spectrum of **4d**

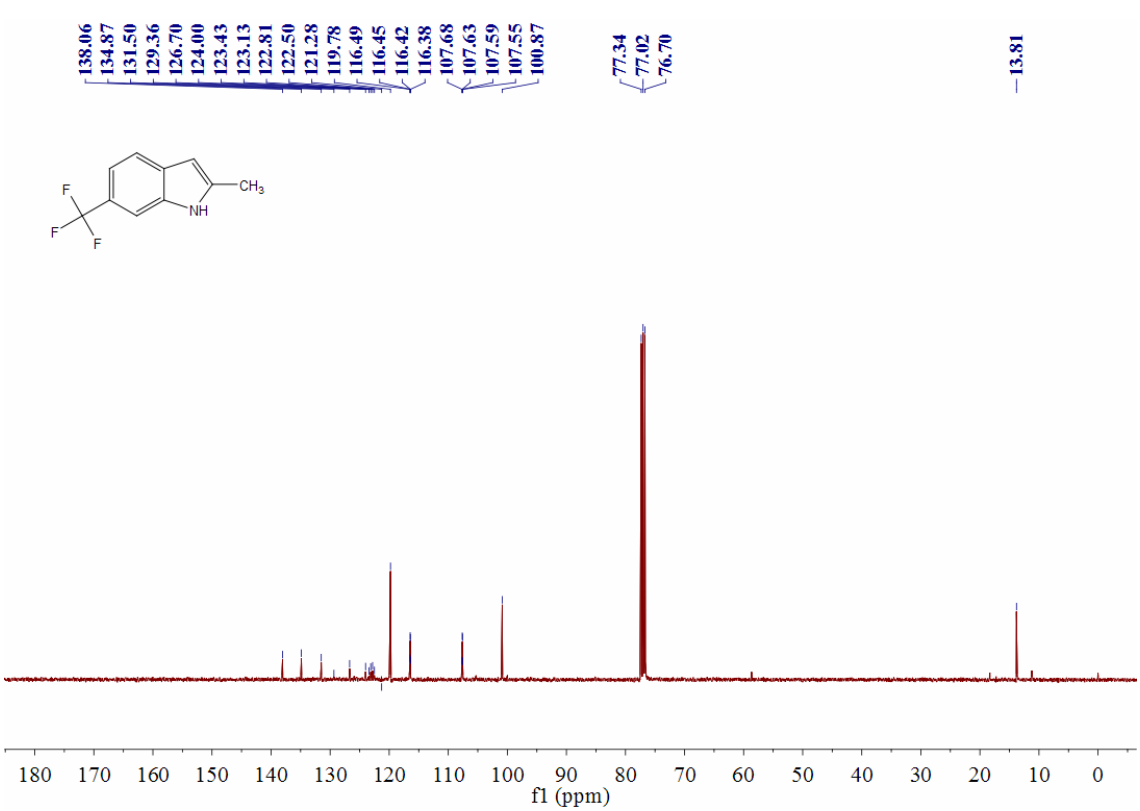


Figure S19. ^{1}H NMR spectrum of **4e**

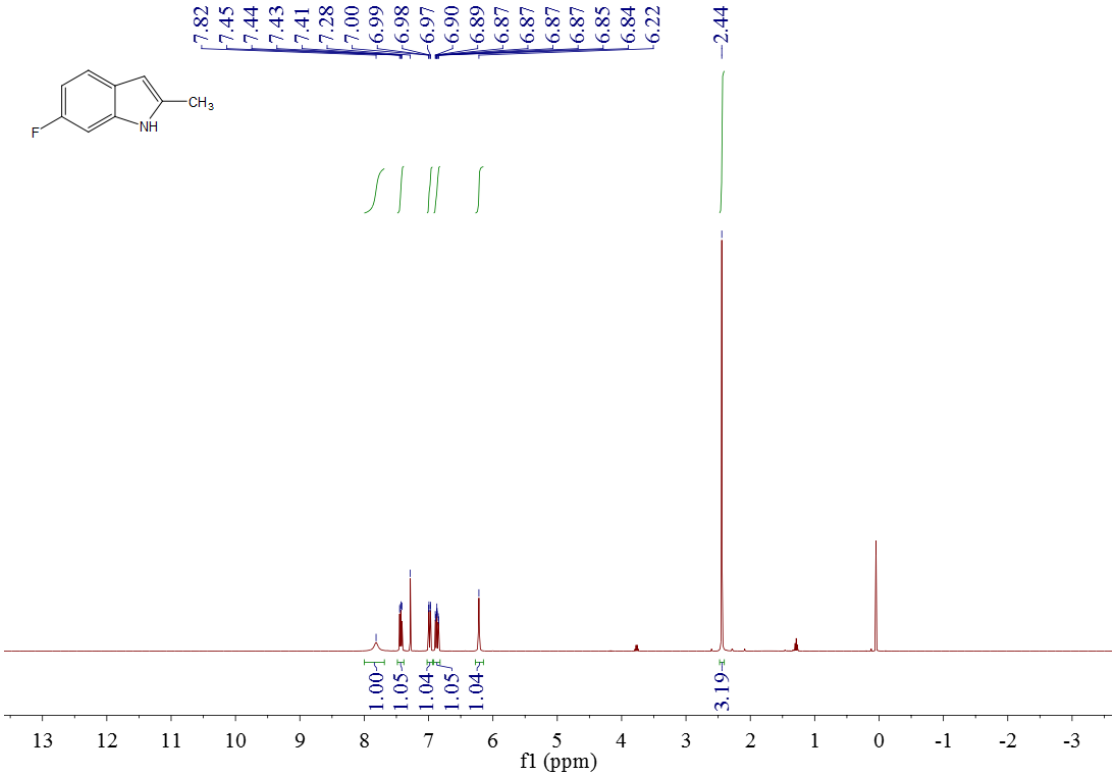


Figure S20. ^{13}C NMR spectrum of **4e**

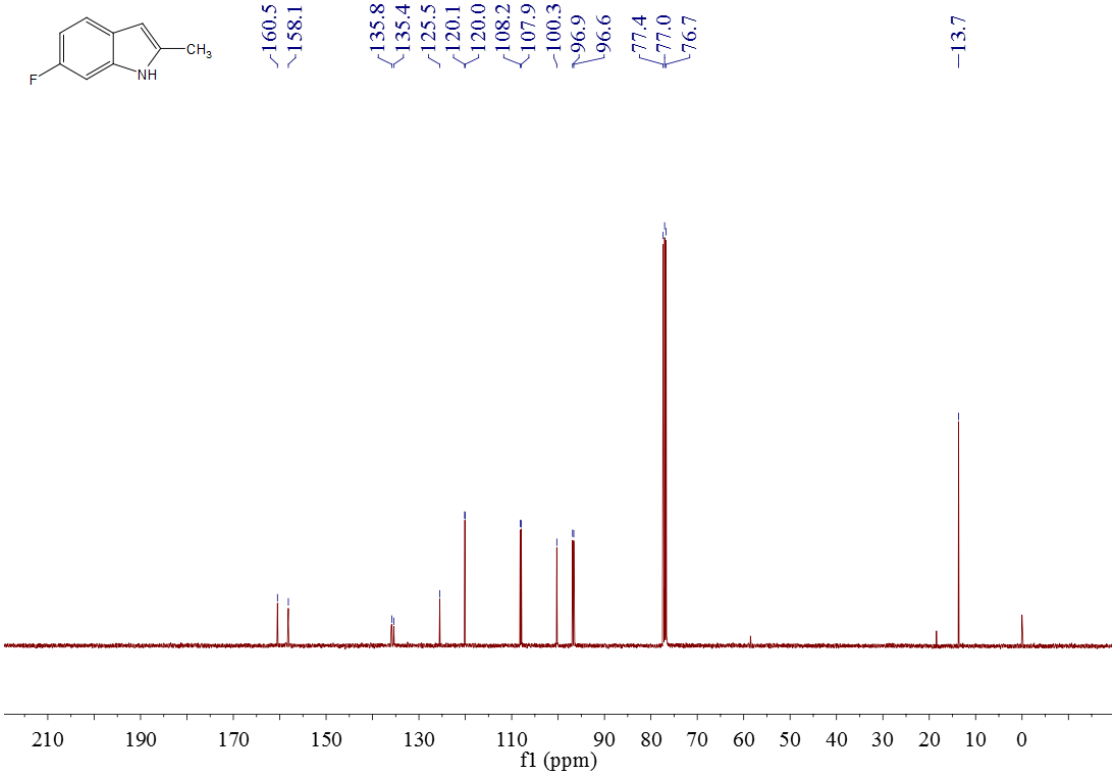


Figure S21. ^{1}H NMR spectrum of **4f**

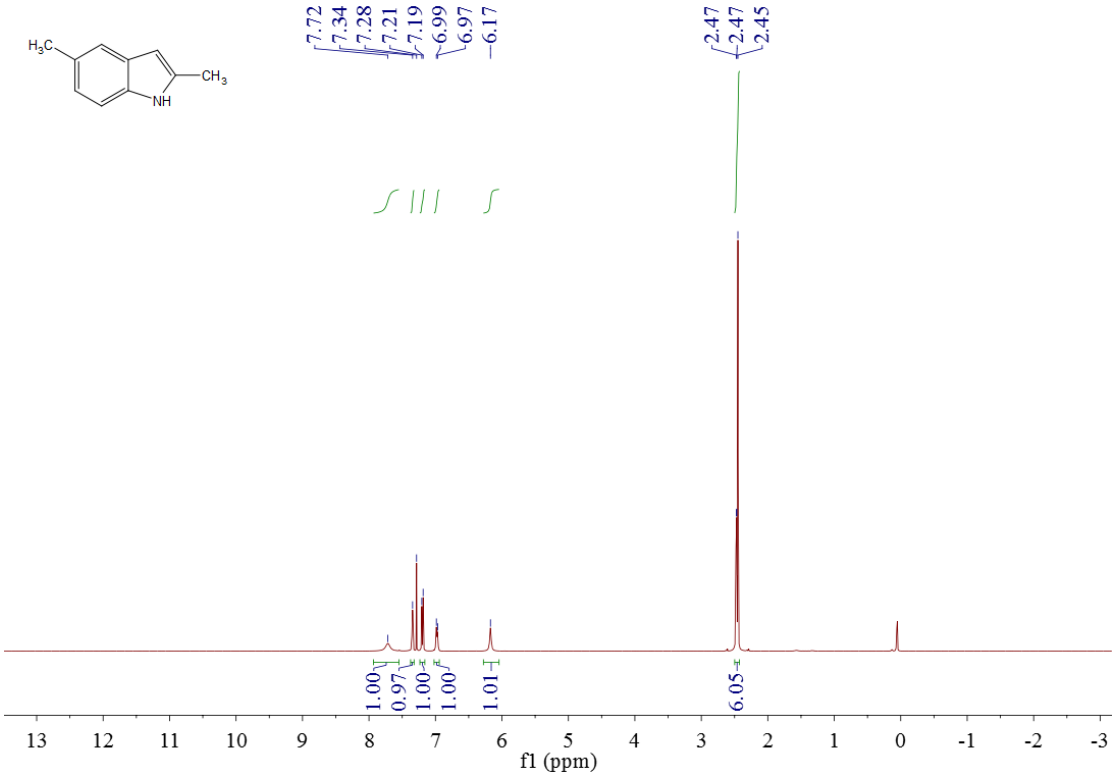


Figure S22. ^{13}C NMR spectrum of **4f**

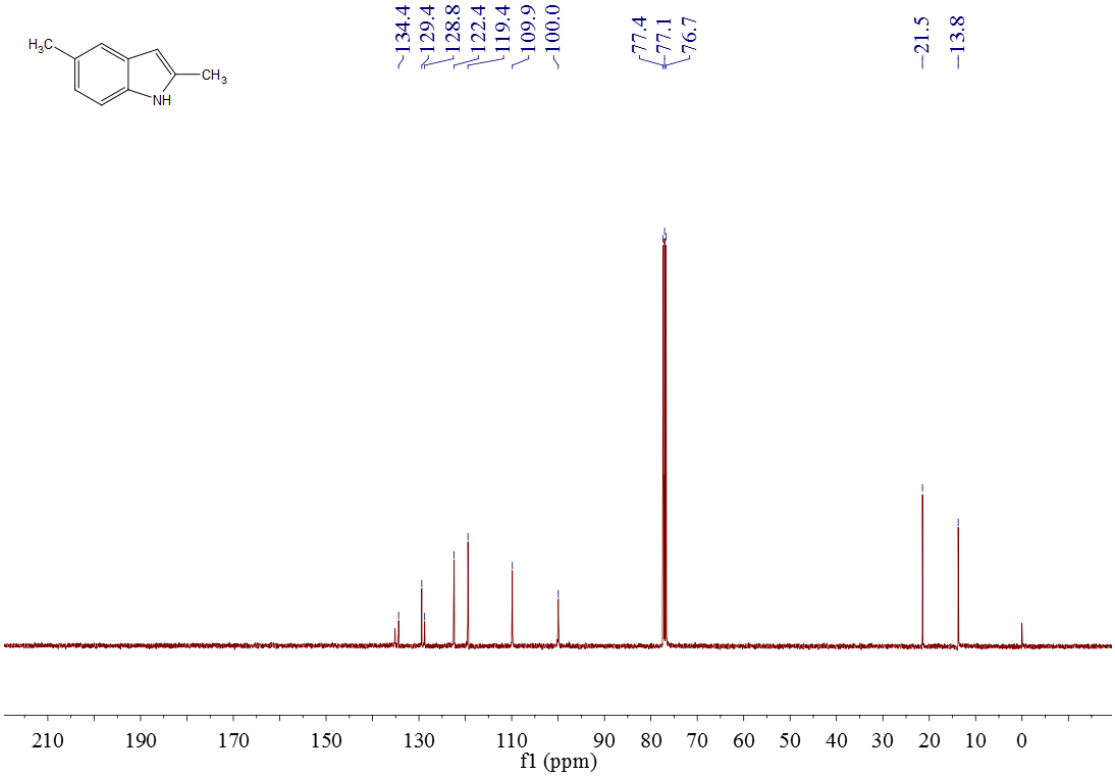


Figure S23. ^{1}H NMR spectrum of **4g**

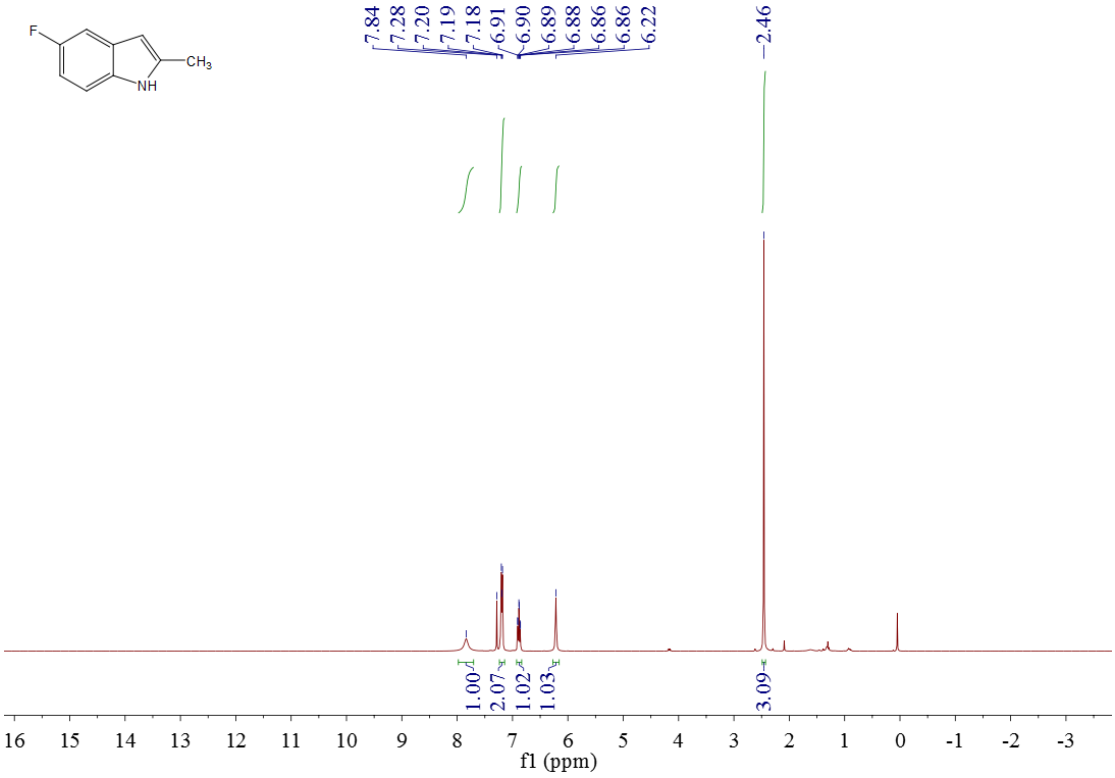


Figure S24. ^{13}C NMR spectrum of **4g**

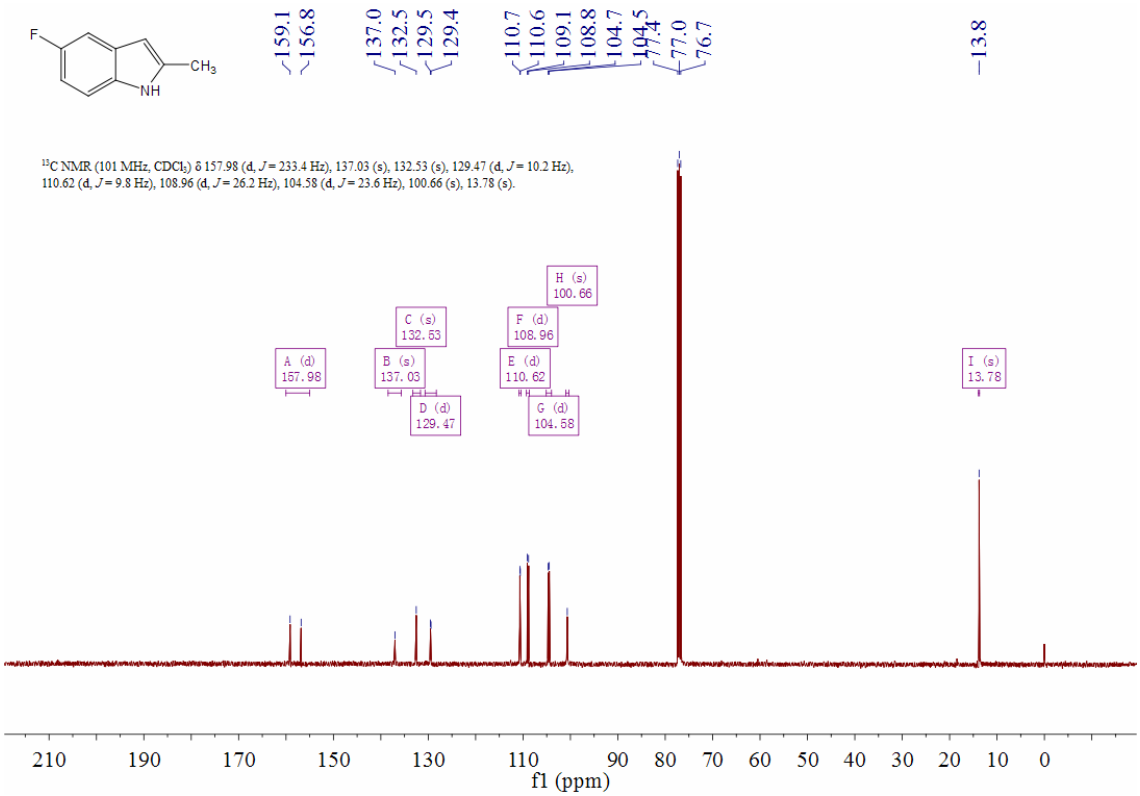


Figure S25. ^{1}H NMR spectrum of **4h**

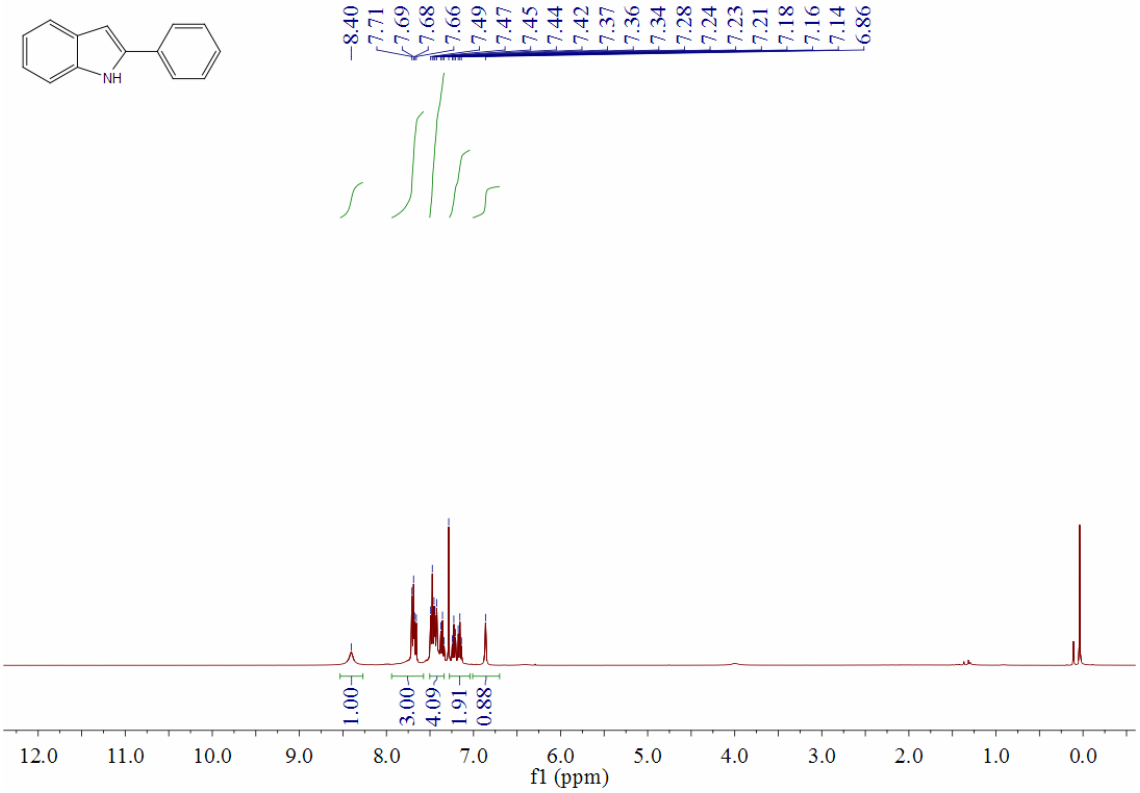


Figure S26. ^{13}C NMR spectrum of **4h**

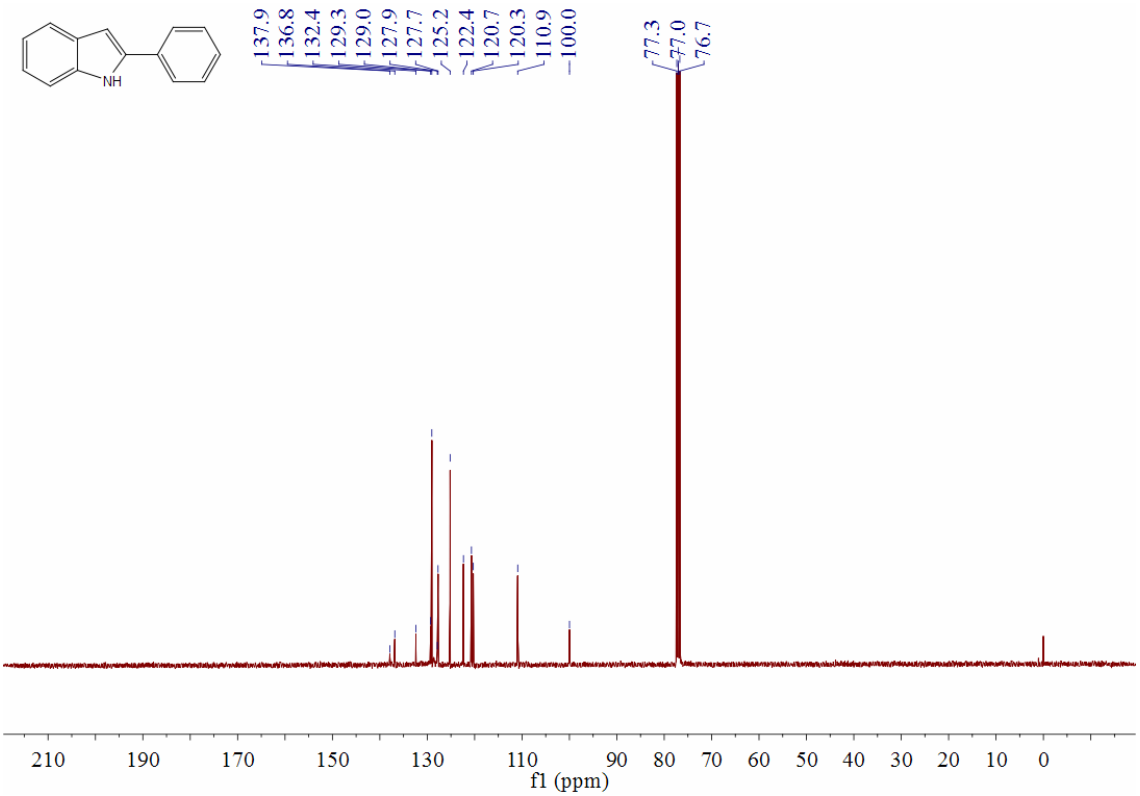


Figure S27. ^{1}H NMR spectrum of **5a**

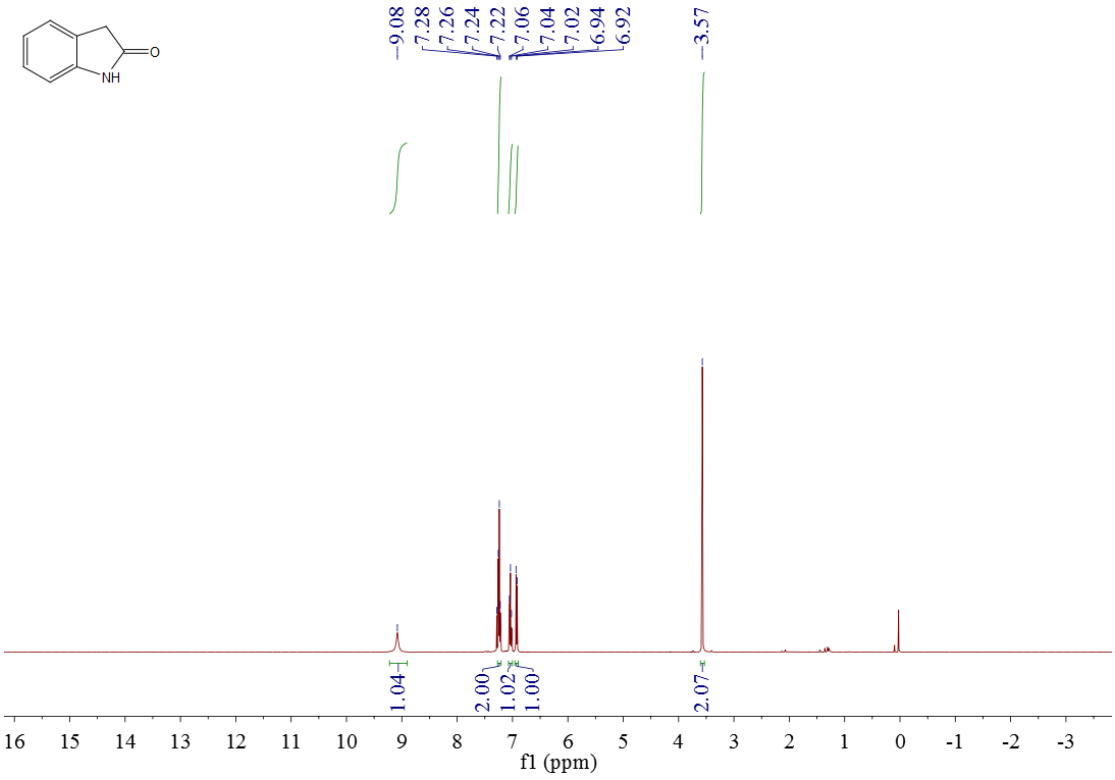


Figure S28. ^{13}C NMR spectrum of **5a**

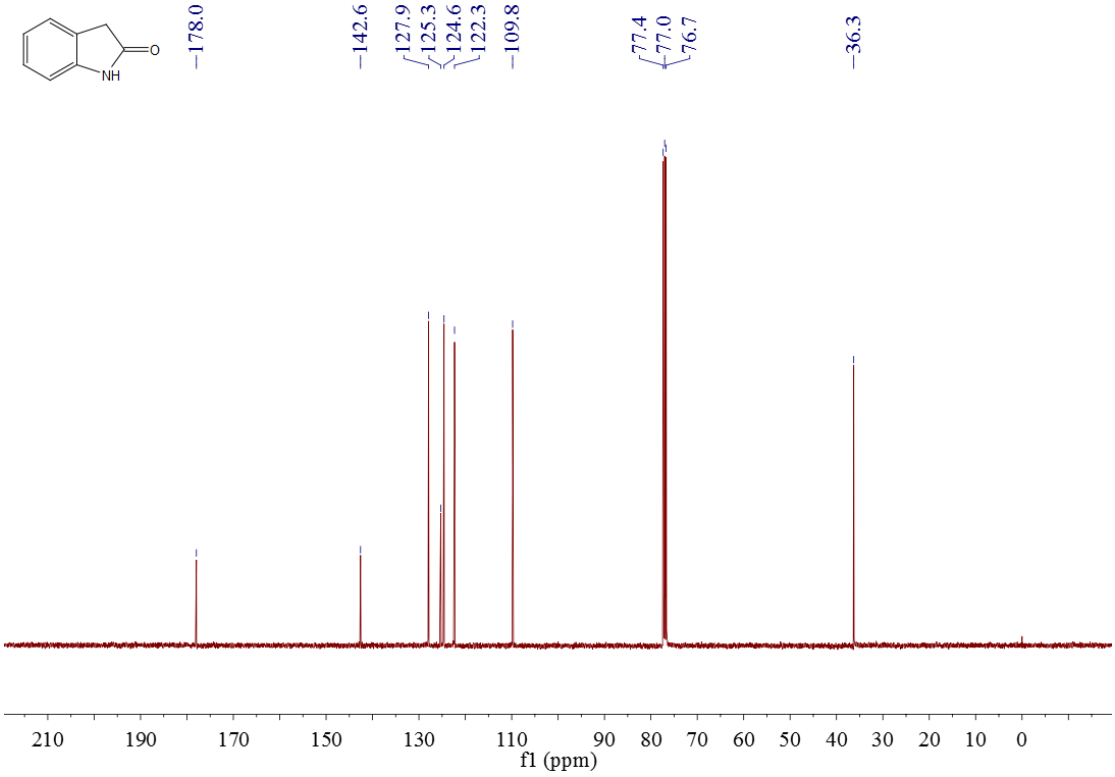


Figure S29. ^{1}H NMR spectrum of **5b**

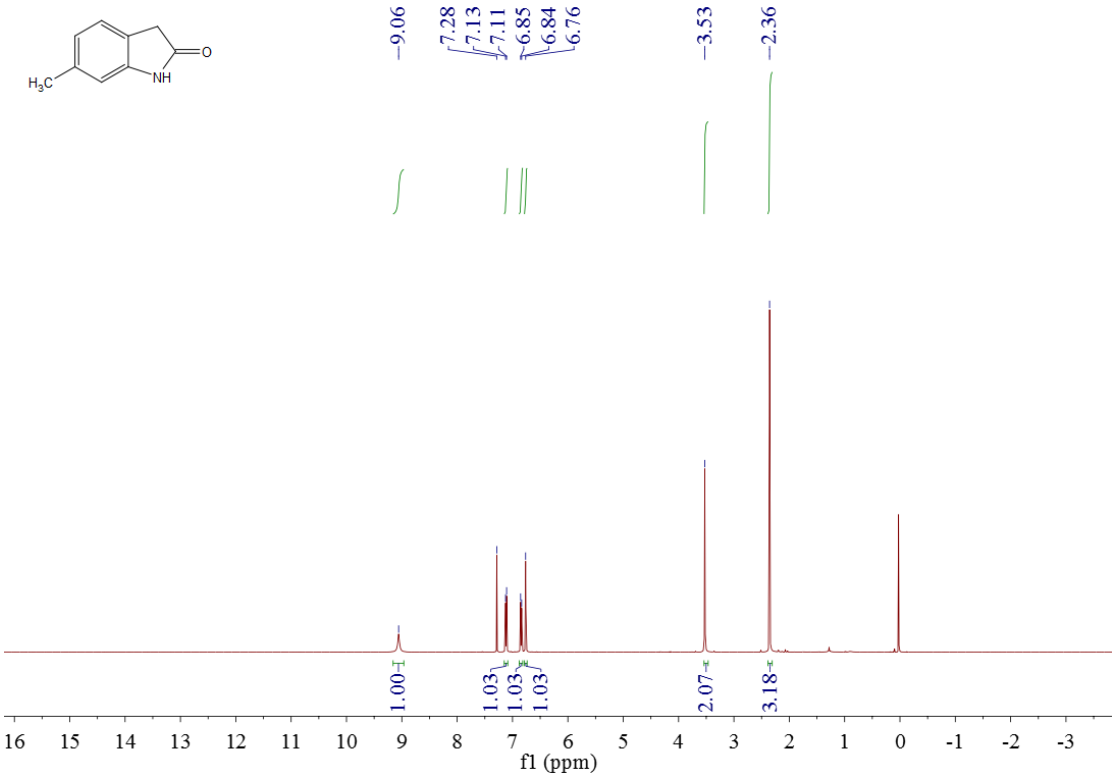


Figure S30. ^{13}C NMR spectrum of **5b**

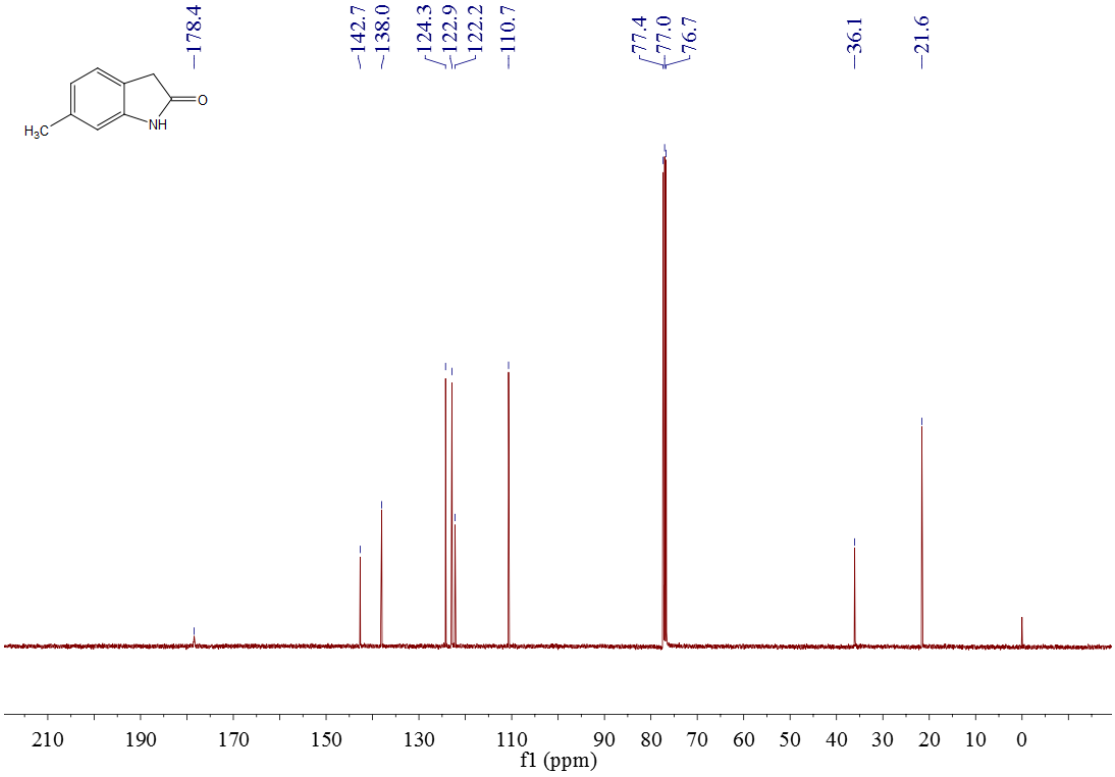


Figure S31. ^{1}H NMR spectrum of **5c**

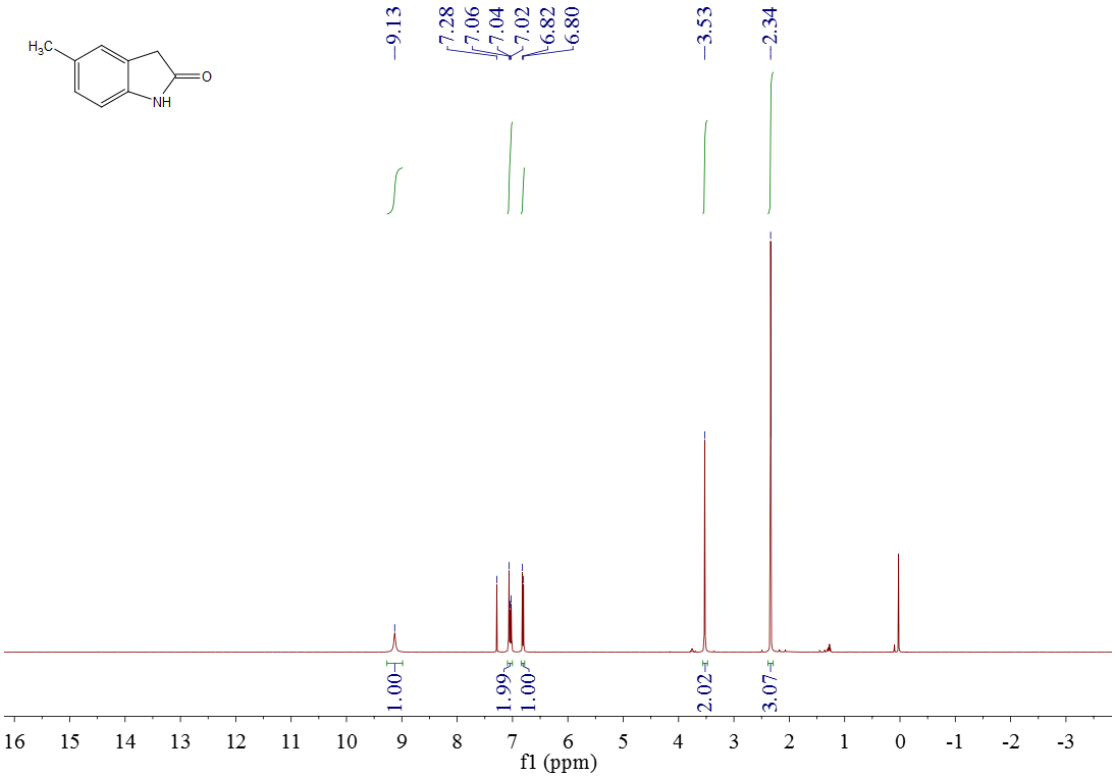


Figure S32. ^{13}C NMR spectrum of **5c**

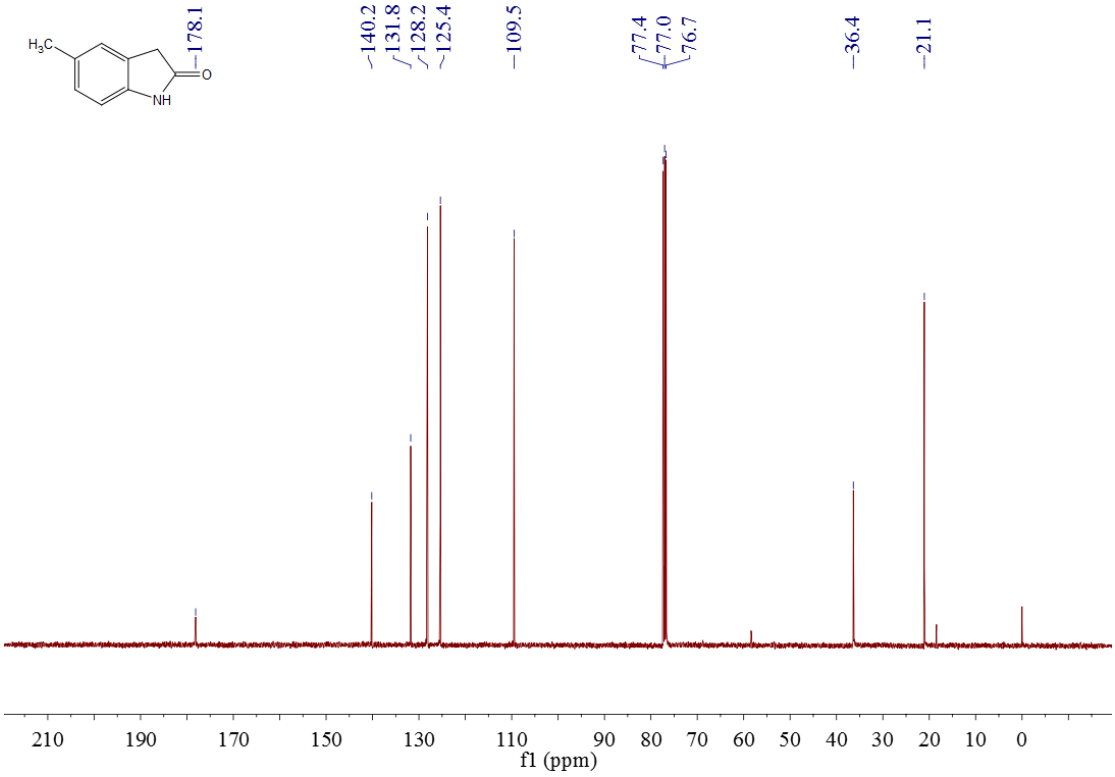


Figure S33. ^{1}H NMR spectrum of **6a**

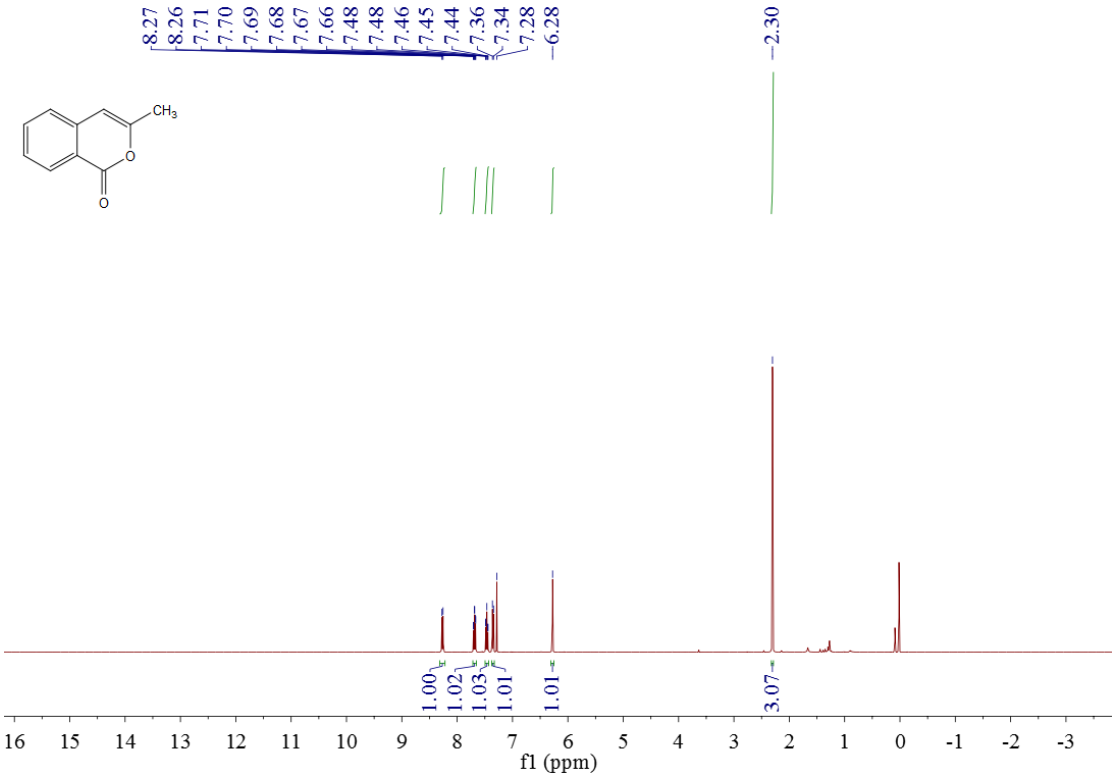


Figure S34. ^{13}C NMR spectrum of **6a**

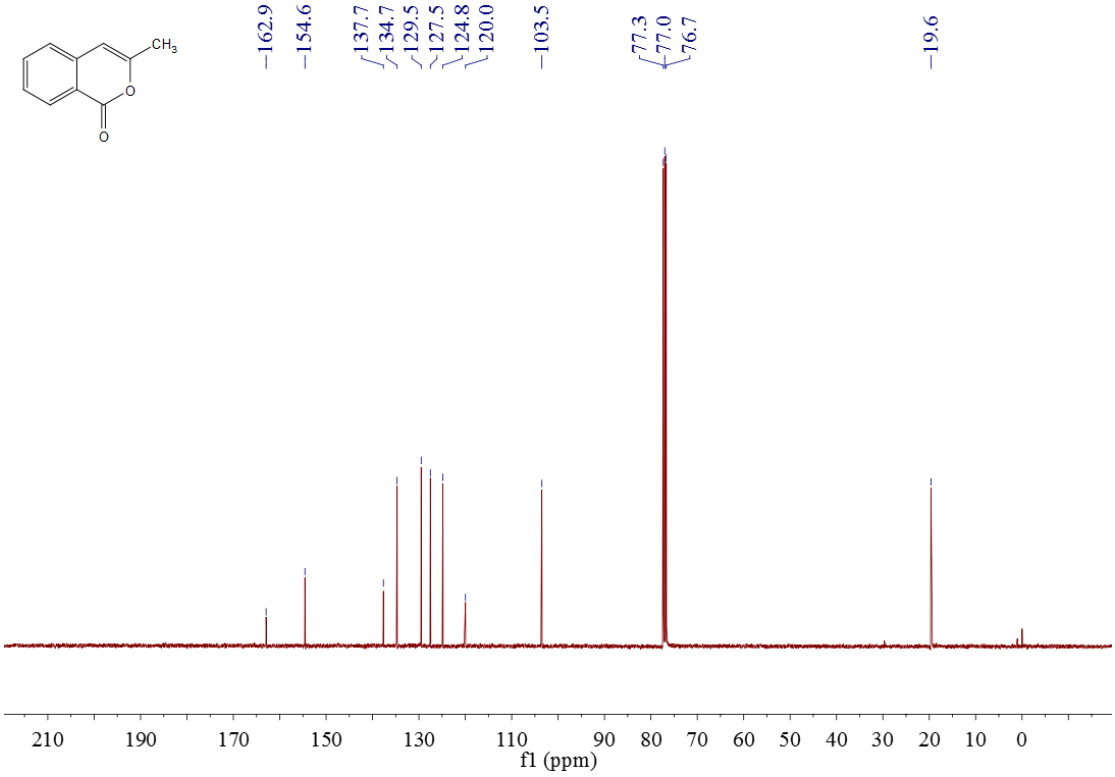


Figure S35. ^{1}H NMR spectrum of **6b**

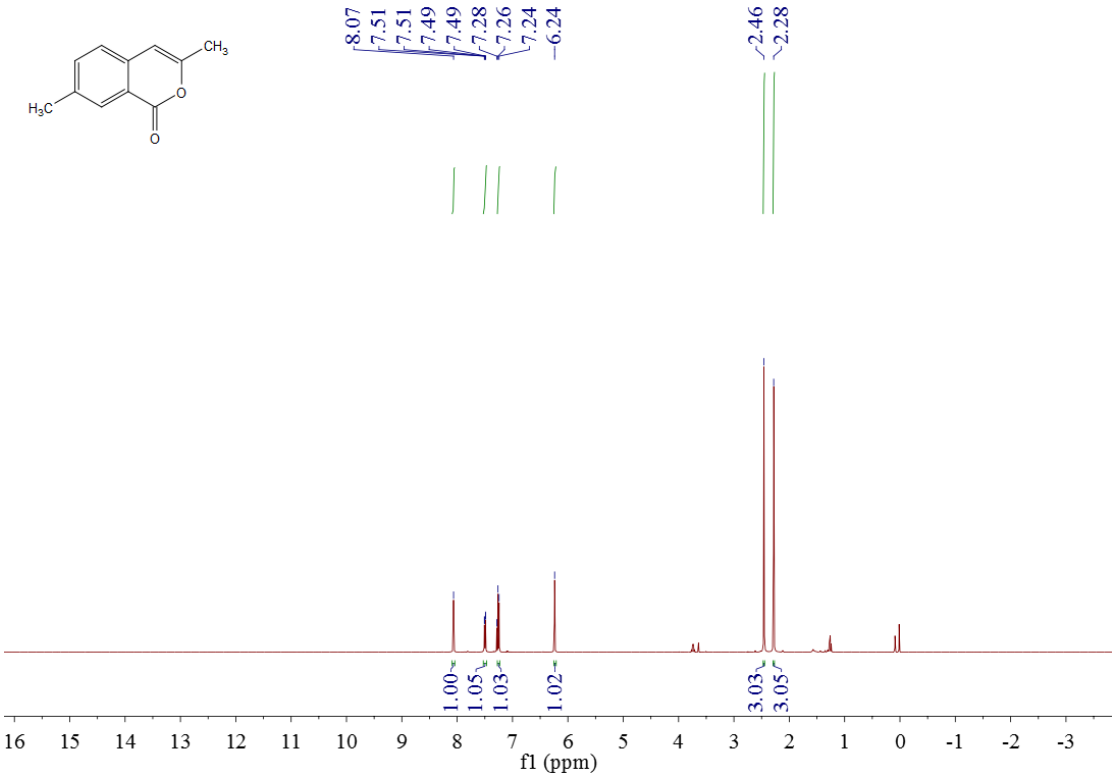


Figure S36. ^{13}C NMR spectrum of **6b**

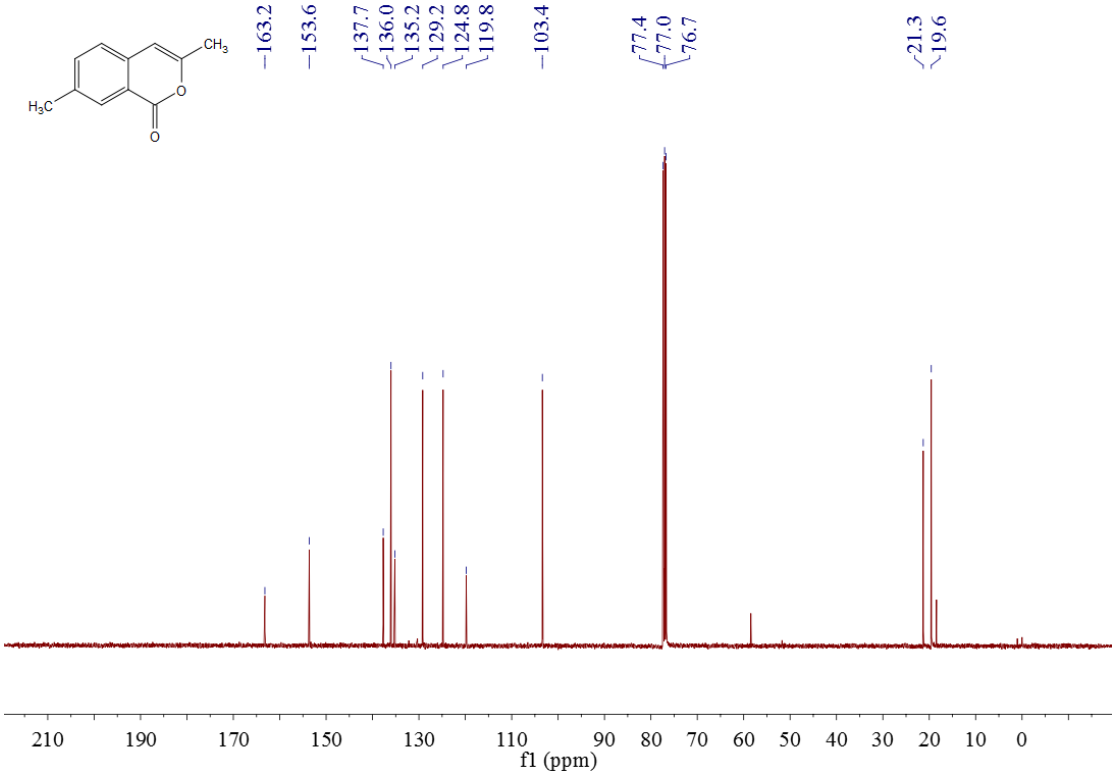


Figure S37. ^{1}H NMR spectrum of **6c**

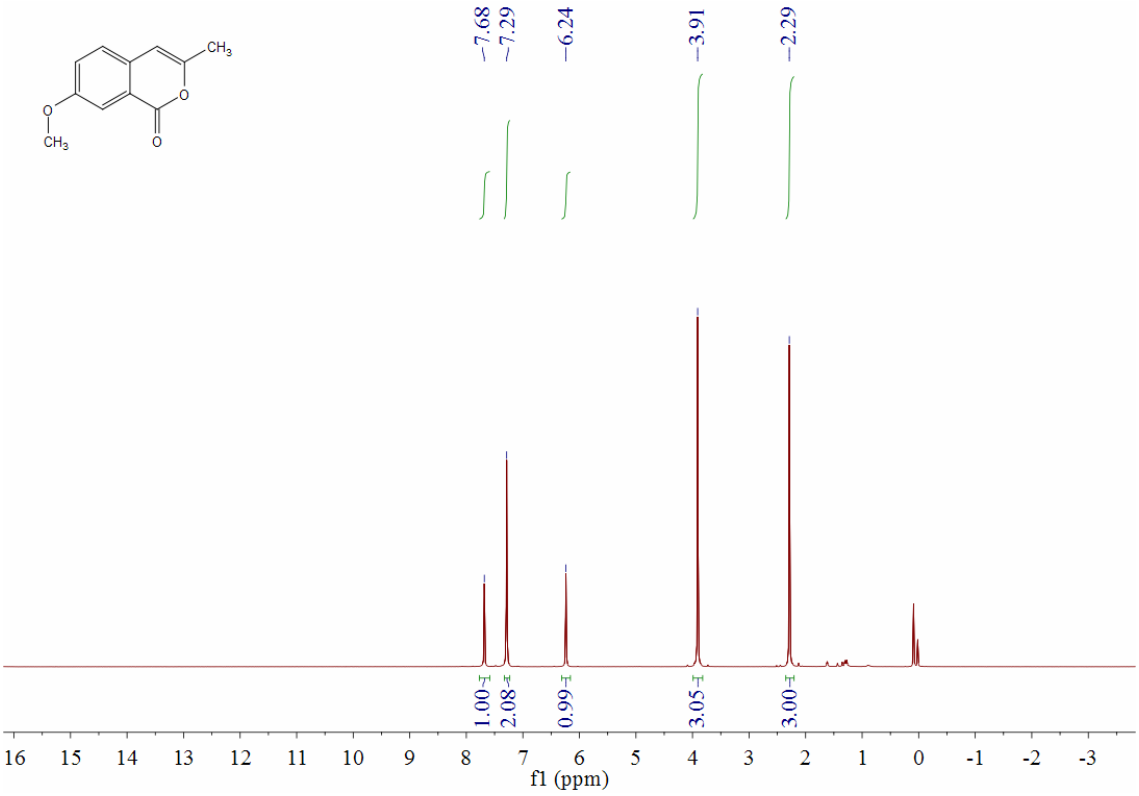


Figure S38. ^{13}C NMR spectrum of **6c**

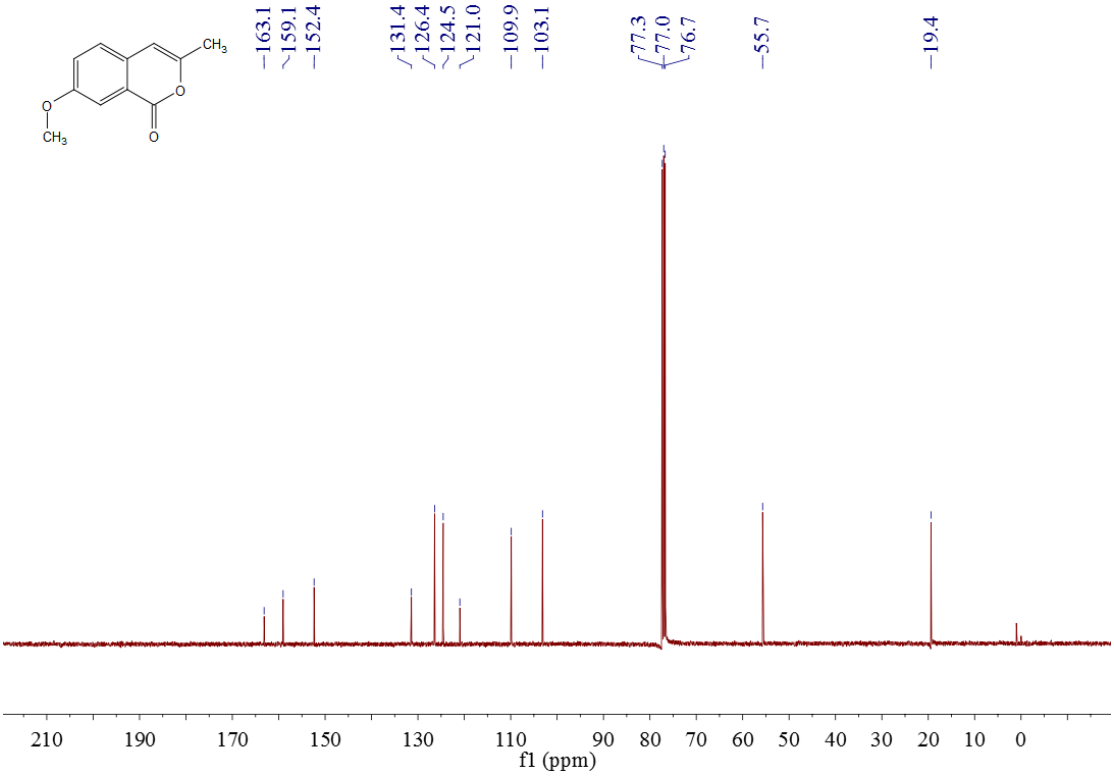


Figure S39. ^{1}H NMR spectrum of **6d**

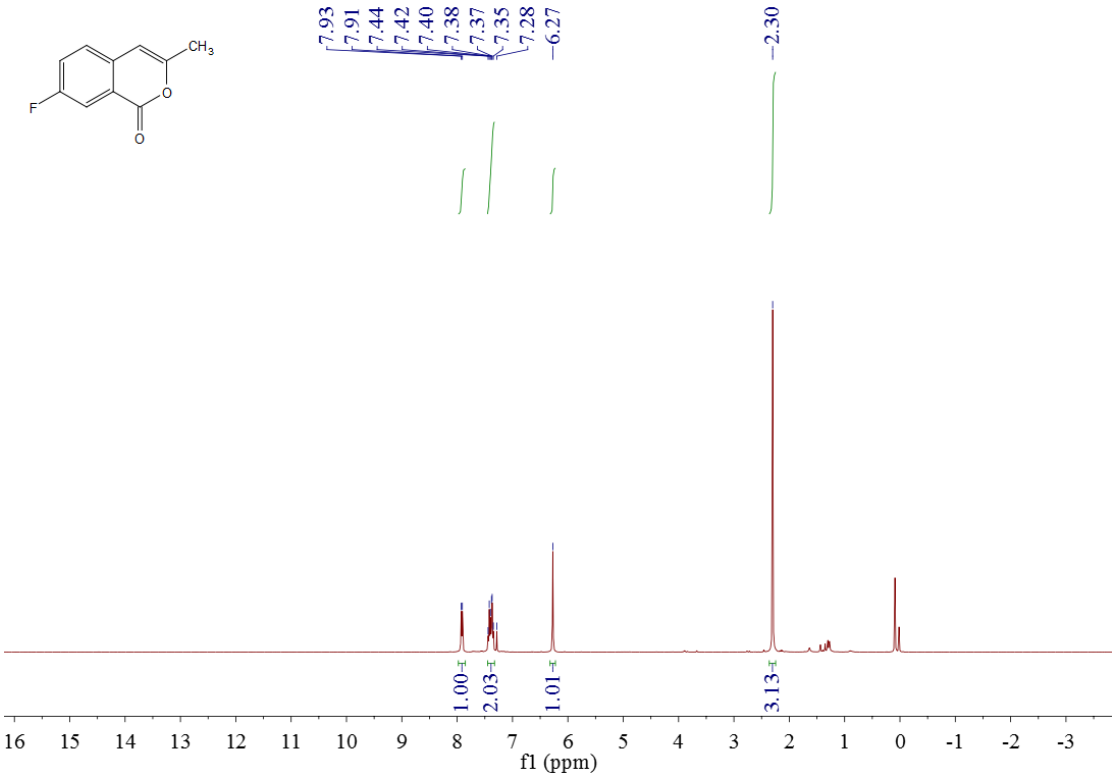


Figure S40. ^{13}C NMR spectrum of **6d**

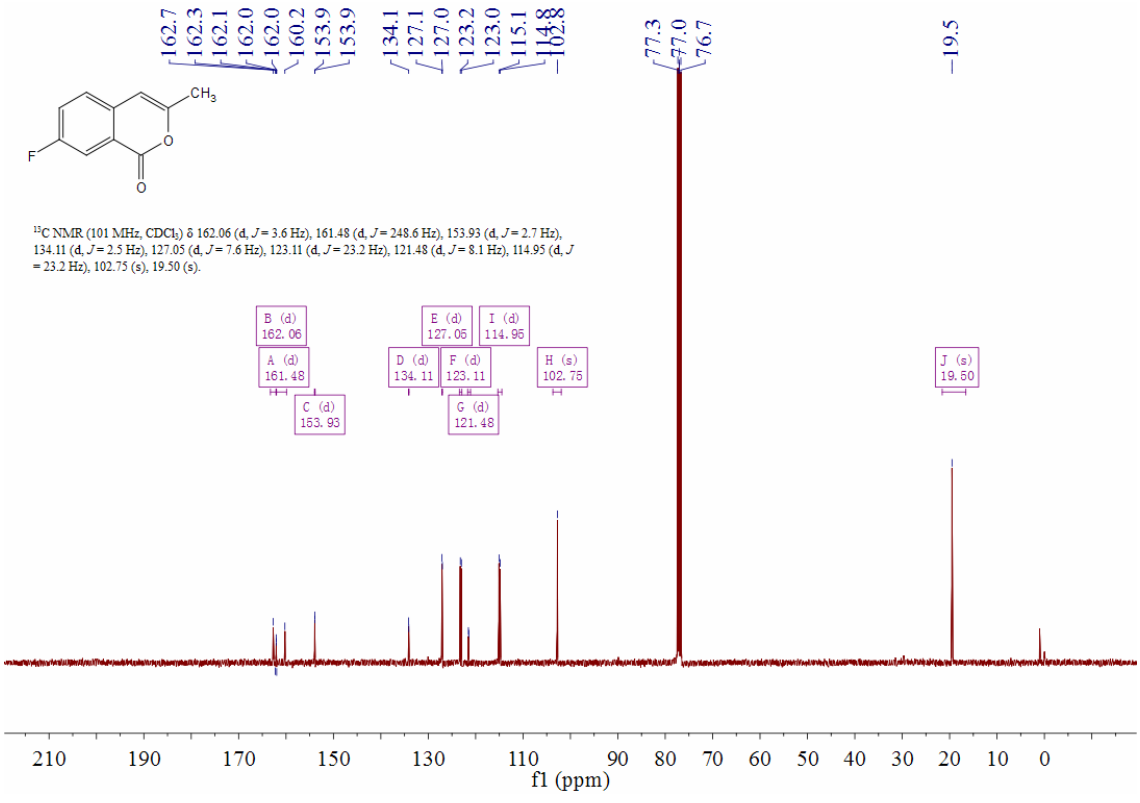


Figure S41. ^{1}H NMR spectrum of **6e**

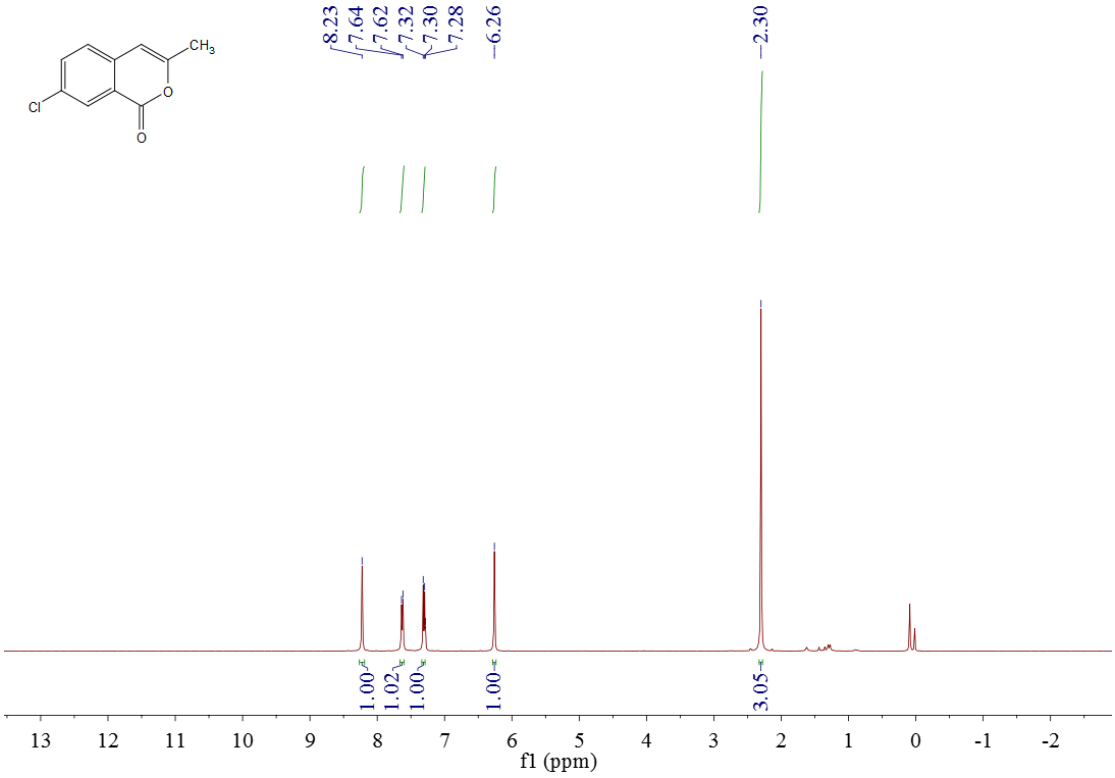


Figure S42. ^{13}C NMR spectrum of **6e**

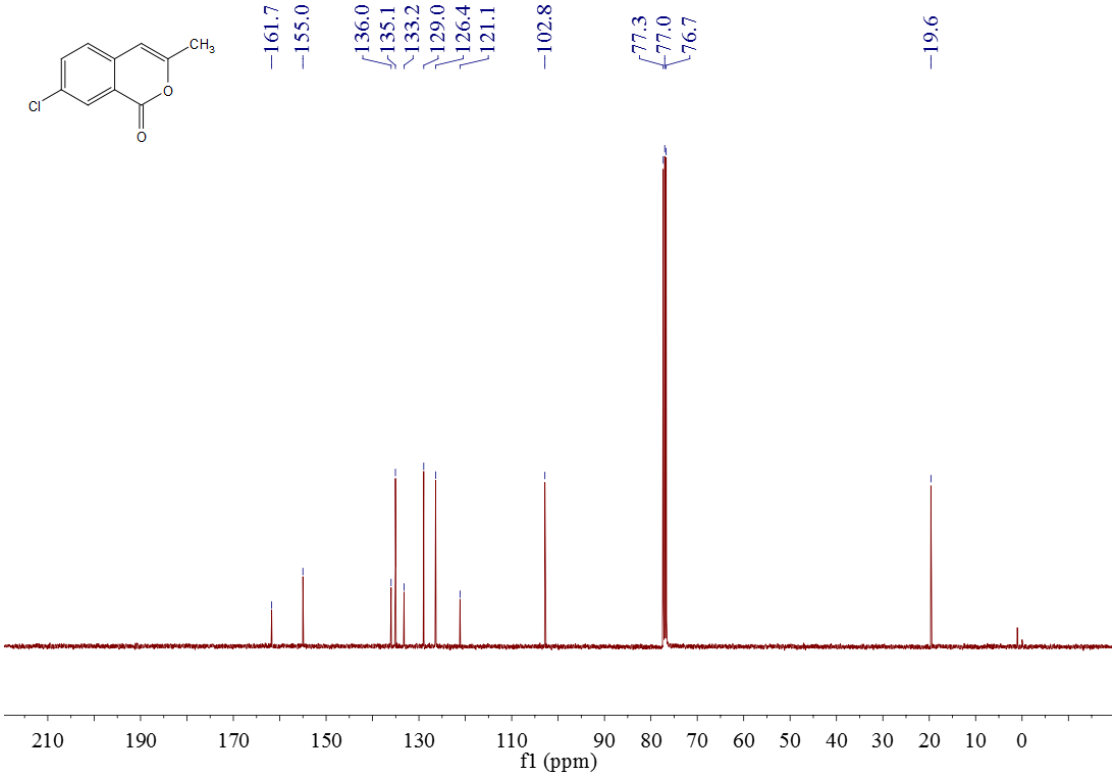


Figure S43. ^{1}H NMR spectrum of **6f**

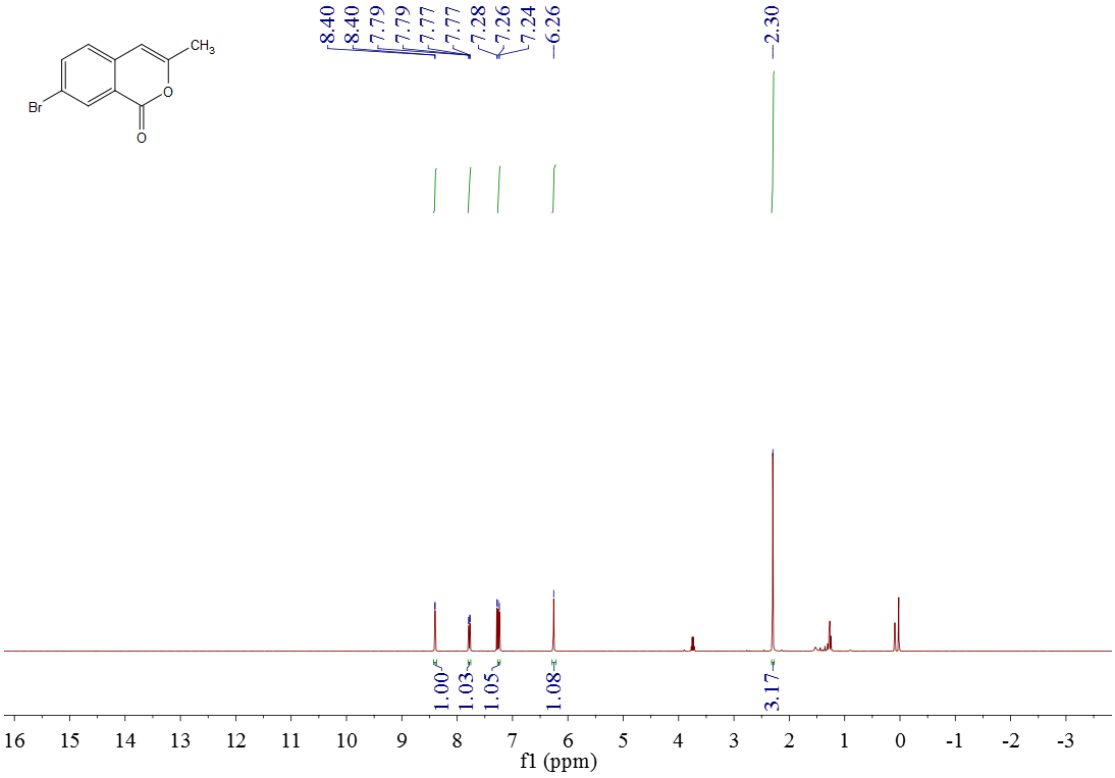


Figure S44. ^{13}C NMR spectrum of **6f**

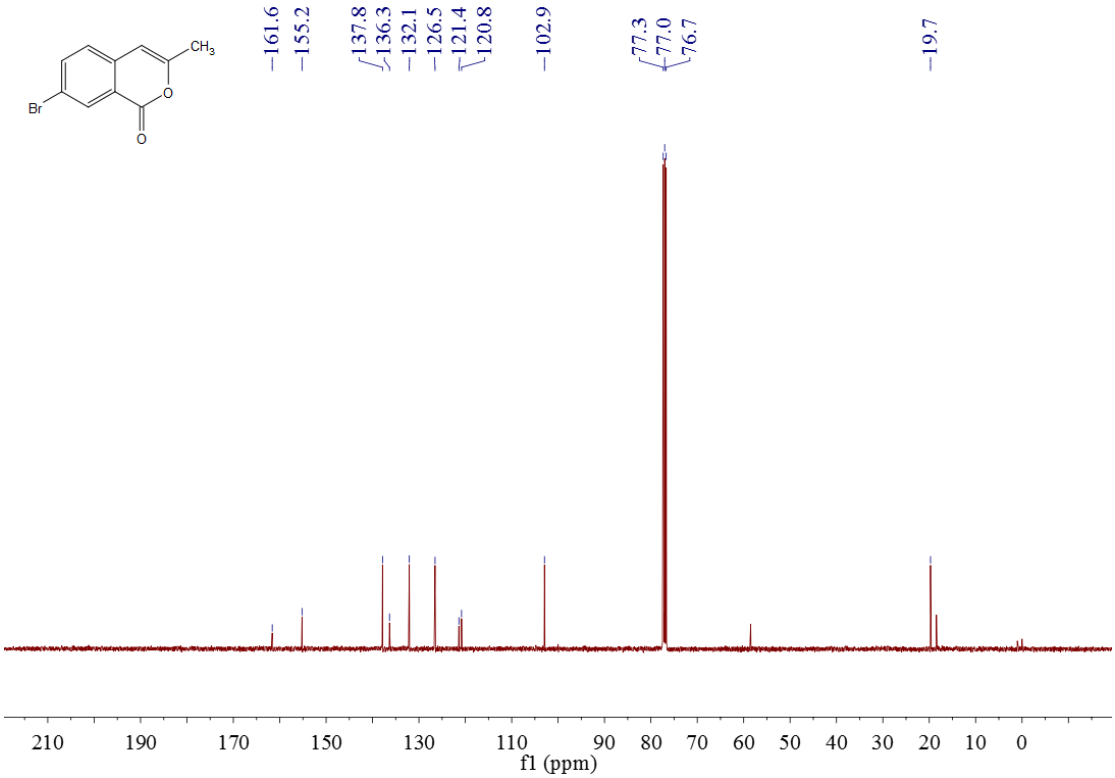


Figure S45. ^{1}H NMR spectrum of **6g**

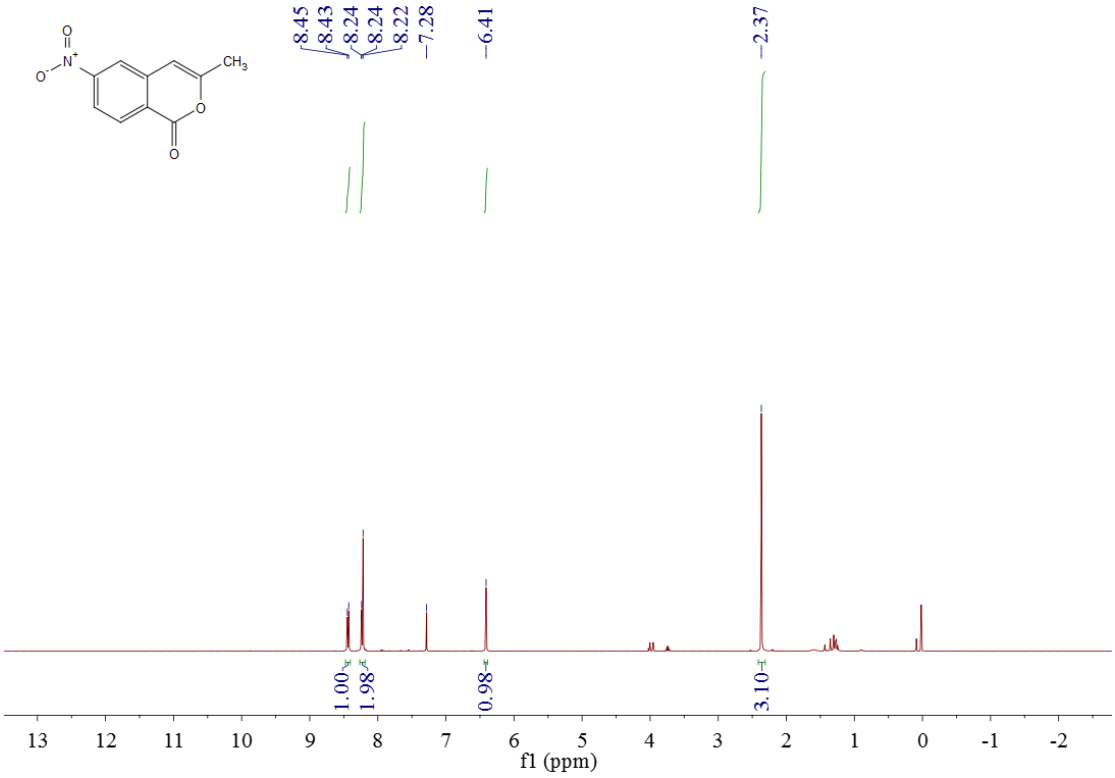


Figure S46. ^{13}C NMR spectrum of **6g**

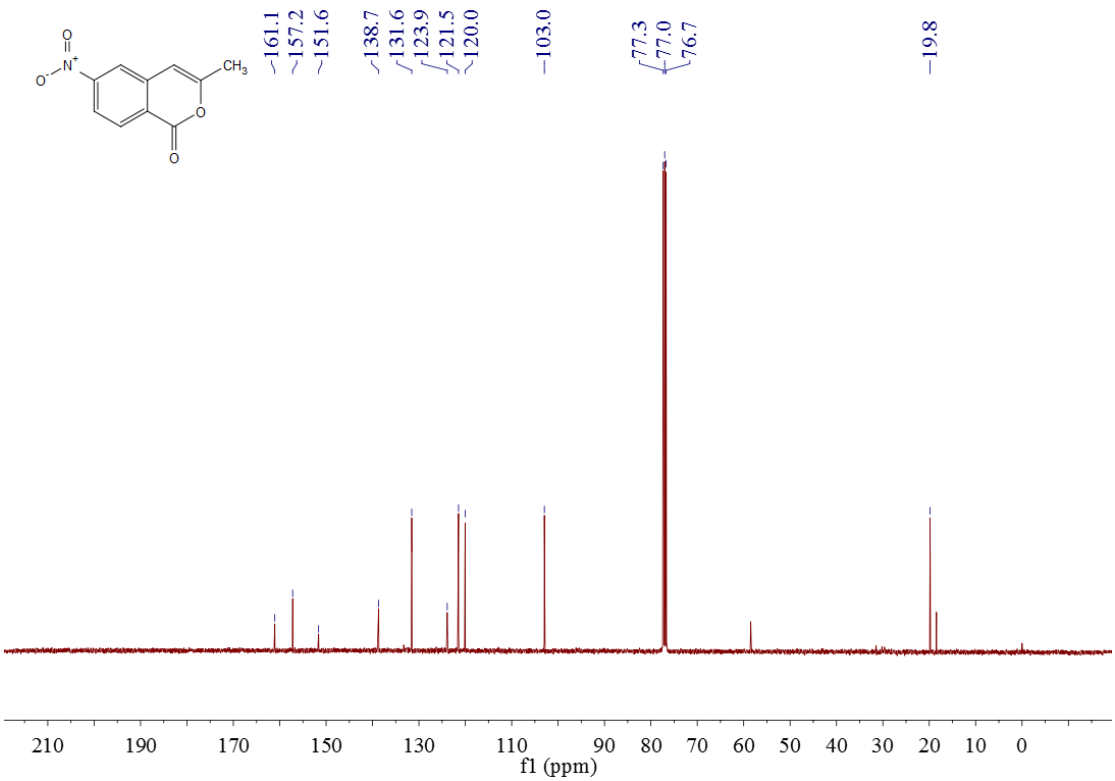


Figure S47. ^{1}H NMR spectrum of **6h**

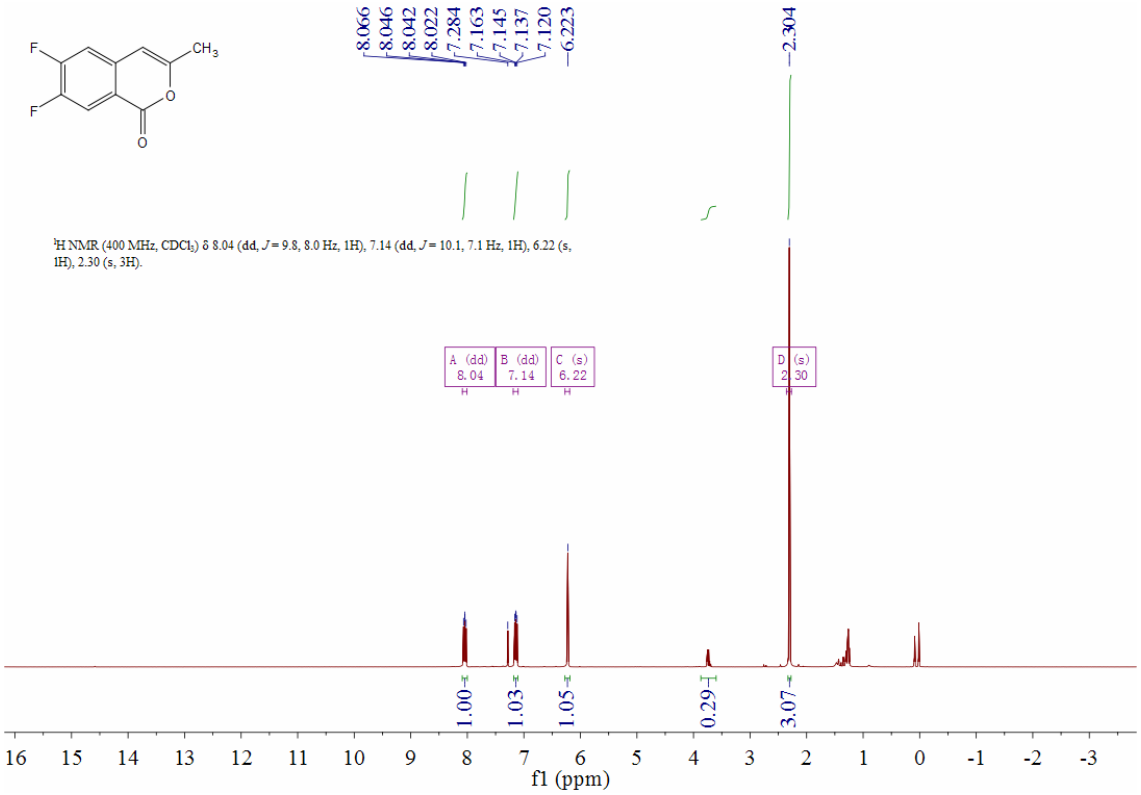


Figure S48. ^{13}C NMR spectrum of **6h**

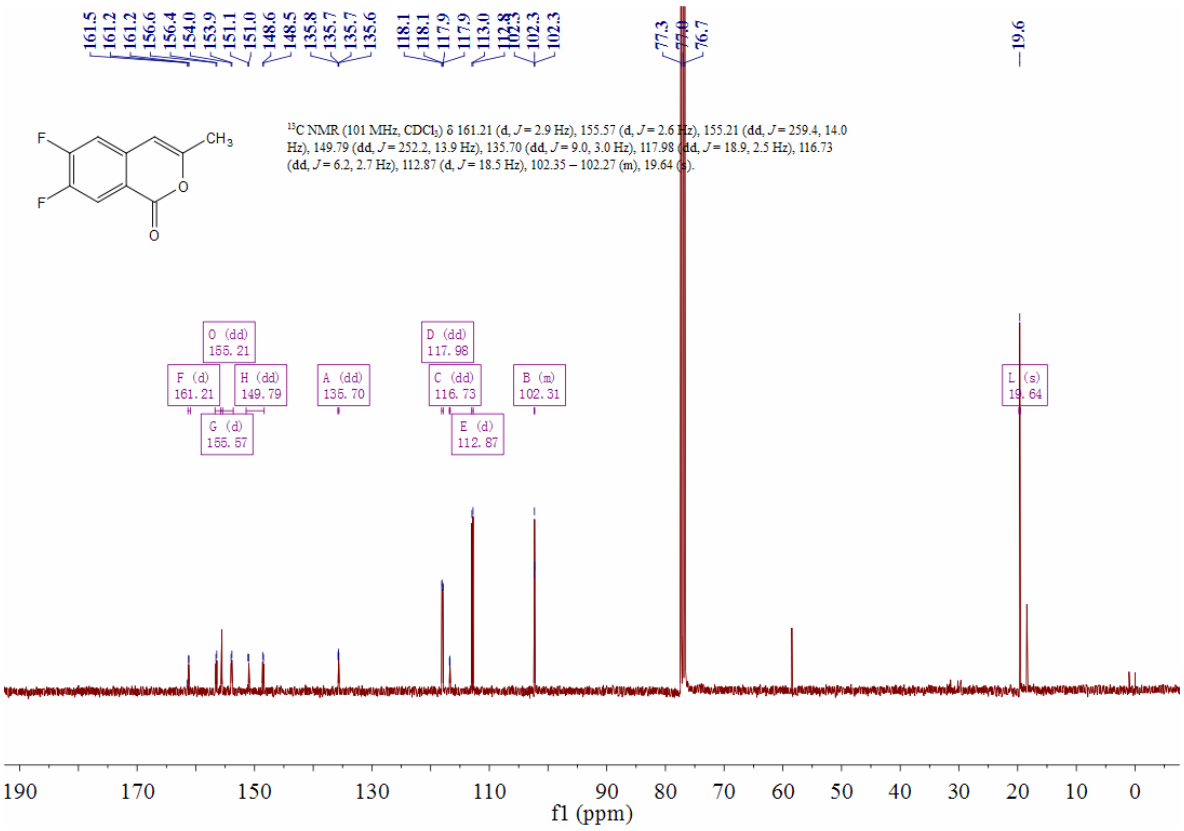


Figure S49. ^{1}H NMR spectrum of **6i**

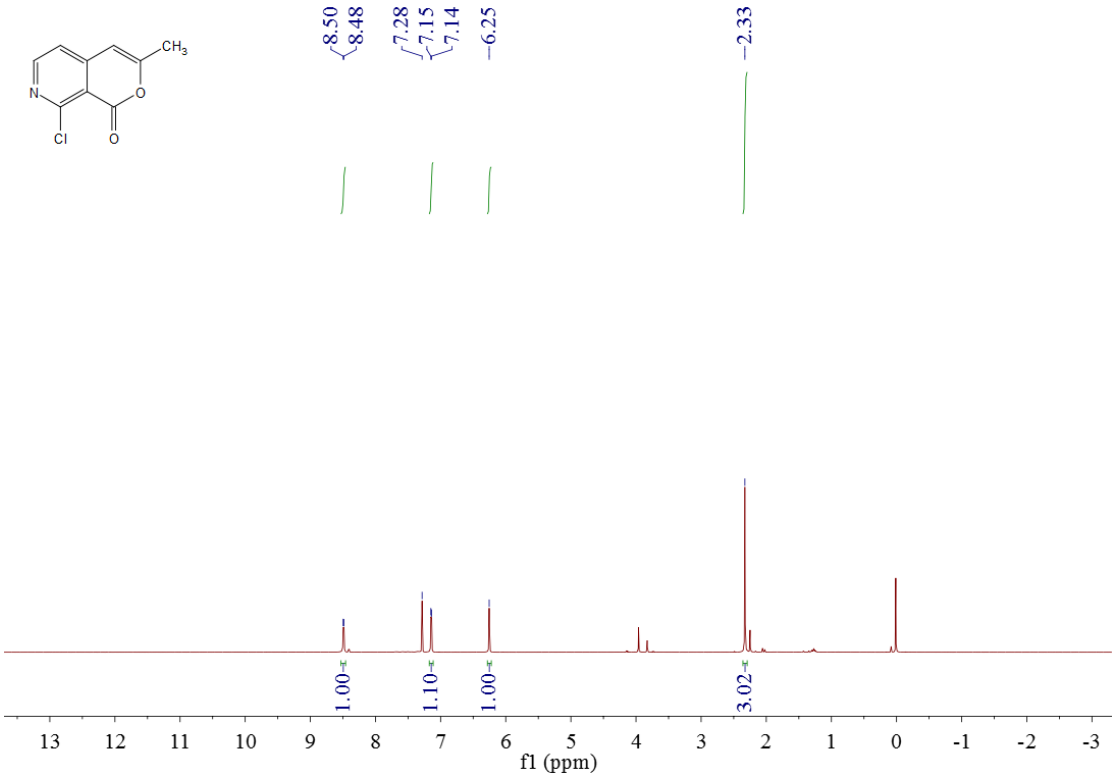


Figure S50. ^{13}C NMR spectrum of **6i**

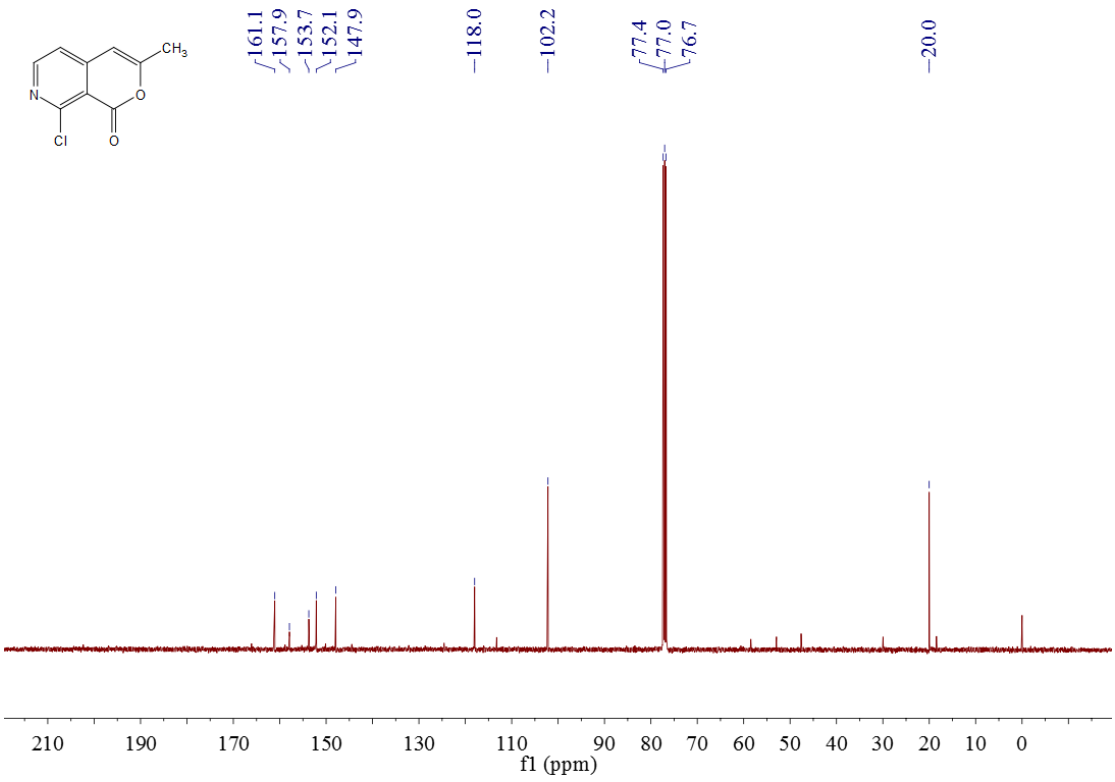


Figure S51. ^{1}H NMR spectrum of **7a**

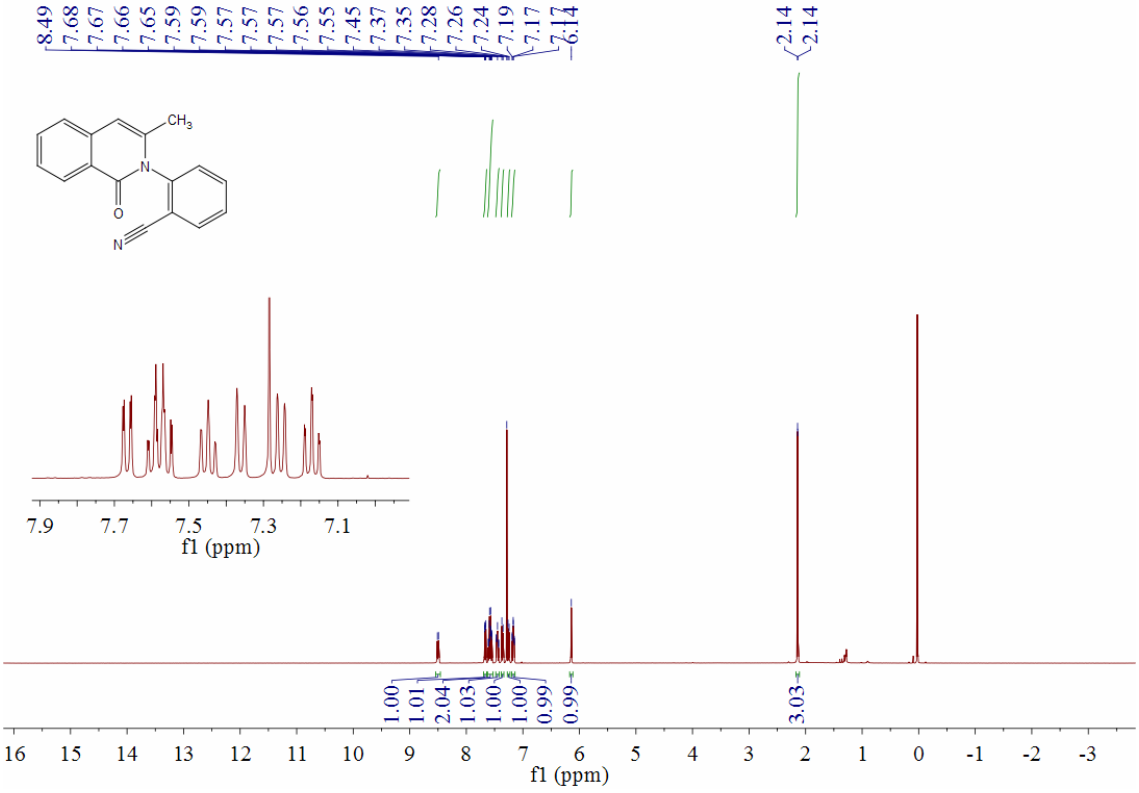


Figure S52. ^{13}C NMR spectrum of **7a**

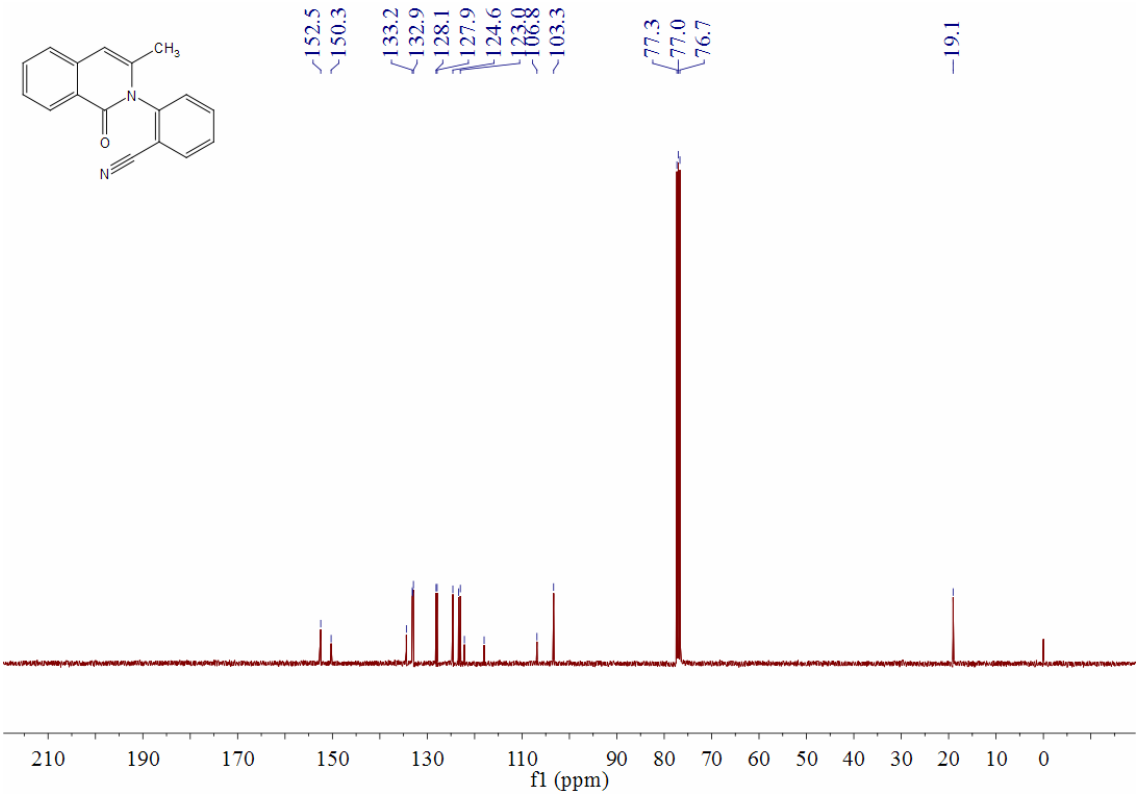


Figure S53. ^{1}H NMR spectrum of **7b**

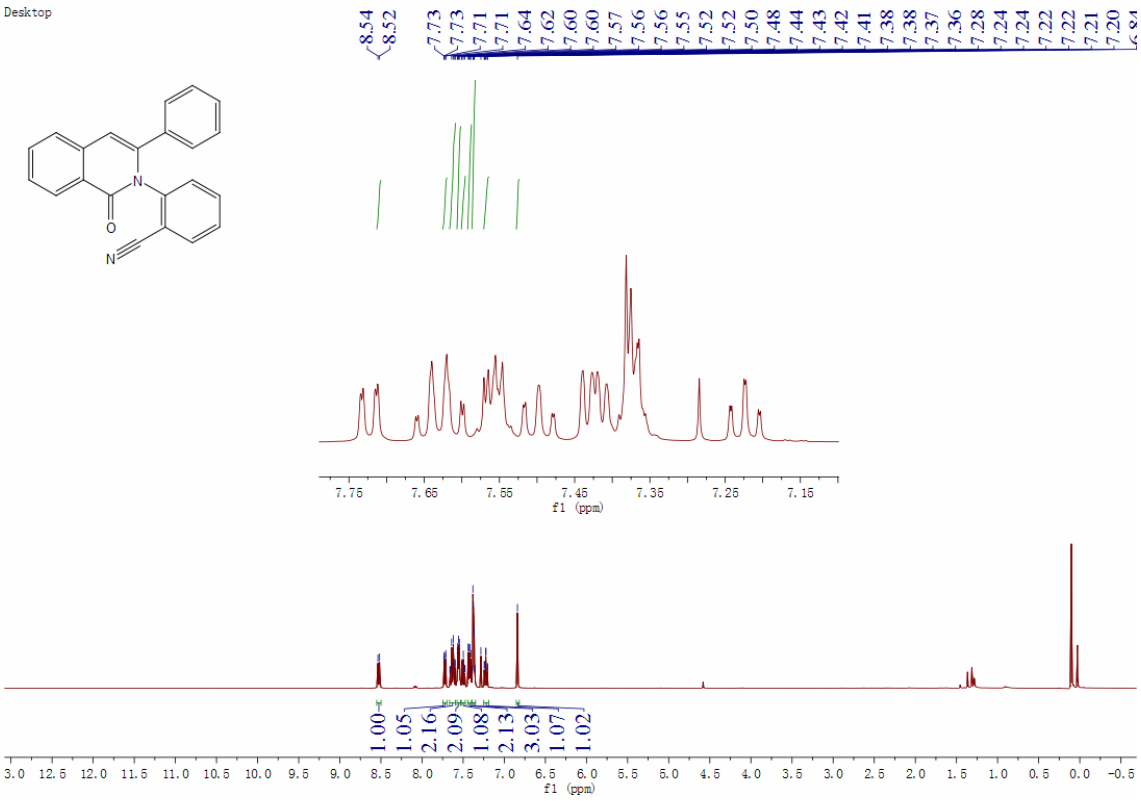
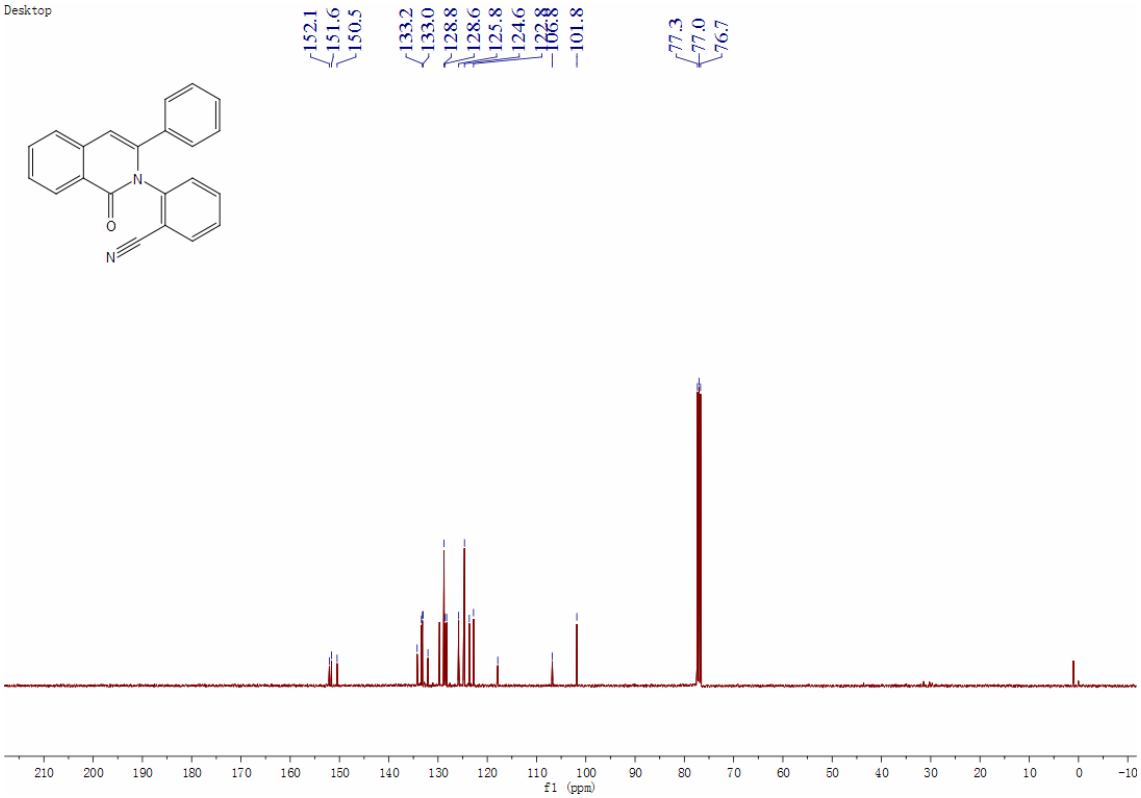


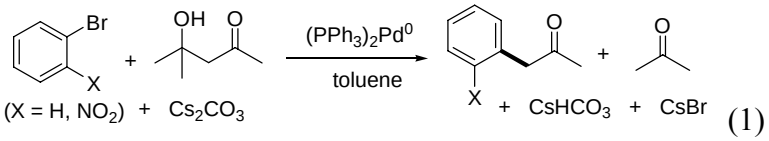
Figure S54. ^{13}C NMR spectrum of **7b**



5. DFT computational studies

5.1 Computational methods and model reactions

All calculations were performed with Gaussian 09.[1] Geometry optimization calculations were done using B3LYP method with LANL2DZ for Pd, P and Cs, and 6-31G(d) for the other elements.[2,3] Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to get the thermodynamic energy corrections. For each saddle point, the intrinsic reaction coordinate (IRC) analysis[4] was carried out to confirm that it connected the correct reactant and product on the potential energy surface. Solution-phase single-point energy calculations were performed on the gas-phase stationary points by using M06[5] with a larger basis set (i.e. SDD[6] for Pd, LANL2DZ for Cs and 6-311+G(d, p) for the other elements). Solvent effect (solvent = toluene) was considered by using self-consistent reaction field (SCRF) method[7] with SMD solvation model.[8] For each stationary point, its energy was calculated by the solution-phase single-point electronic energy corrected by Gibbs free energy correction item. For complexes with several possible isomers, the most stable ones were discussed. The model reactions studied are shown in Eqn 1.



(1)

References:

[1] Frisch, M. J., et al. *Gaussian 09*, revision B.01; Gaussian, Inc.: Wallingford, CT, 2010.

[2] Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

[3] Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

[4] Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.

[5] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

[6] Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. J. Chem. Phys. 1987, 86, 866.

[7] Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669.

[8] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

5.2 Optimized Cartesian coordinates for the stationary points in Scheme 4

For the structures of **CP1 (X = H)**, **CP2 (X=H)**, **CP3 (X=H)**, **CP4 (X=H)**,**$TS^{retro\text{-}aldol}$ (X=H)** and **TSrd (X=H)**, please refer to supporting information in our previous study: *J. Org. Chem.* 2016, 81, 57-65.

CP1 ($X=NO_2$)

SCF Done: E(RB3LYP) = -4537.21323086 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.665498	-1.232127	2.603325
2	6	0	-3.332216	-0.523638	1.597116
3	6	0	-4.637861	-0.062982	1.823167
4	6	0	-5.268690	-0.311888	3.043388
5	6	0	-4.600350	-1.016814	4.046098
6	6	0	-3.301658	-1.475692	3.822160
7	15	0	-2.479661	-0.213653	-0.051332
8	46	0	-0.017361	-0.198251	-0.015420
9	35	0	-0.055209	-2.706445	0.530326
10	6	0	-3.134217	-1.534949	-1.215528
11	6	0	-2.402873	-1.827329	-2.373310
12	6	0	-2.875198	-2.771221	-3.285553
13	6	0	-4.074885	-3.442306	-3.039548
14	6	0	-4.800369	-3.162851	-1.880607
15	6	0	-4.334727	-2.210315	-0.971532
16	6	0	-3.326328	1.354913	-0.655641
17	6	0	-3.955314	1.423367	-1.903243
18	6	0	-4.541344	2.618053	-2.331443
19	6	0	-4.505771	3.749643	-1.517211
20	6	0	-3.878357	3.685239	-0.270179
21	6	0	-3.288830	2.496809	0.158273
22	6	0	0.011044	1.770415	-0.518198
23	6	0	-0.024784	2.153213	-1.870321
24	6	0	0.033200	3.491334	-2.262091
25	6	0	0.150526	4.507527	-1.307283
26	6	0	0.214262	4.169615	0.037508
27	6	0	0.126963	2.820215	0.403328
28	15	0	2.444350	-0.283618	-0.049278
29	6	0	3.223599	-0.465847	1.653320
30	6	0	4.518739	0.004604	1.915509
31	6	0	5.080177	-0.156944	3.183483
32	6	0	4.354134	-0.785732	4.196503
33	6	0	3.066762	-1.257444	3.936142
34	6	0	2.499081	-1.100250	2.670398
35	6	0	3.088107	-1.730872	-1.058647
36	6	0	2.348311	-2.161268	-2.165959
37	6	0	2.827833	-3.193592	-2.972790
38	6	0	4.041438	-3.813398	-2.668509
39	6	0	4.774881	-3.395598	-1.556858
40	6	0	4.302746	-2.354857	-0.754290
41	6	0	3.365530	1.183958	-0.791141
42	6	0	3.961774	1.097310	-2.054840
43	6	0	4.608171	2.205773	-2.607788
44	6	0	4.667976	3.407722	-1.902970
45	6	0	4.073664	3.499499	-0.642264
46	6	0	3.422768	2.396993	-0.088894
47	1	0	1.388854	-1.701421	-2.381321
48	1	0	2.244537	-3.524371	-3.827816
49	1	0	4.409859	-4.624753	-3.290583
50	1	0	5.715258	-3.880685	-1.309110
51	1	0	4.877259	-2.040049	0.111185
52	1	0	1.506557	-1.486770	2.464035
53	1	0	2.495598	-1.748132	4.719387
54	1	0	4.790026	-0.905468	5.184845
55	1	0	6.083316	0.213390	3.377638
56	1	0	5.087481	0.506162	1.139183
57	1	0	3.930098	0.165520	-2.609582

58	1	0	5.069498	2.122830	-3.588391
59	1	0	5.174057	4.268541	-2.331874
60	1	0	4.112339	4.431539	-0.085203
61	1	0	2.965157	2.491463	0.891086
62	1	0	-0.098714	1.387837	-2.638439
63	1	0	-0.008112	3.743351	-3.319023
64	1	0	0.195599	5.549323	-1.610654
65	1	0	0.320494	4.922901	0.810054
66	7	0	0.184304	2.539125	1.843411
67	1	0	-3.995889	0.547652	-2.542748
68	1	0	-5.030055	2.657628	-3.301480
69	1	0	-4.964142	4.677064	-1.850130
70	1	0	-3.845505	4.562202	0.370724
71	1	0	-2.801808	2.453776	1.127741
72	1	0	-5.161433	0.497396	1.055203
73	1	0	-6.280199	0.049711	3.208779
74	1	0	-5.090009	-1.205759	4.997857
75	1	0	-2.774795	-2.024504	4.597958
76	1	0	-1.663956	-1.606965	2.423697
77	1	0	-4.902731	-2.005845	-0.069710
78	1	0	-5.729596	-3.688750	-1.678165
79	1	0	-4.438028	-4.185506	-3.744358
80	1	0	-2.298412	-2.992741	-4.179529
81	1	0	-1.454842	-1.327321	-2.550150
82	8	0	0.844620	3.304043	2.552430
83	8	0	-0.436100	1.563621	2.278020

CP2 (X=NO_2)

SCF Done: E(RB3LYP) = -2351.45209956 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.018971	-0.209468	-2.497849
2	6	0	-3.443641	-0.156307	-1.162671
3	6	0	-4.692566	-0.689259	-0.822138
4	6	0	-5.503742	-1.264095	-1.804595
5	6	0	-5.078743	-1.306244	-3.133718
6	6	0	-3.834754	-0.774405	-3.479451
7	15	0	-2.306897	0.652315	0.102895
8	6	0	-2.729082	2.484781	-0.065341
9	6	0	-3.313657	3.010560	-1.222630
10	6	0	-3.570193	4.380687	-1.322425
11	6	0	-3.247055	5.236075	-0.269325
12	6	0	-2.664353	4.715825	0.888703
13	6	0	-2.406235	3.349073	0.991524
14	46	0	0.097857	0.009064	-0.098437
15	8	0	-0.348966	-1.907247	0.672933
16	6	0	-0.571588	-3.088821	-0.071811
17	6	0	0.436248	-4.165947	0.380920
18	15	0	2.548292	-0.444146	0.057907
19	6	0	3.224181	-1.557578	-1.299240
20	6	0	2.889169	-1.265712	-2.629798
21	6	0	3.371459	-2.059937	-3.670562
22	6	0	4.177766	-3.165731	-3.391219
23	6	0	4.501579	-3.468921	-2.068579
24	6	0	4.031015	-2.667497	-1.025111
25	6	0	0.500308	1.816917	-0.929826
26	6	0	0.499527	1.863117	-2.339036
27	6	0	0.768437	3.031289	-3.052542
28	6	0	1.053468	4.221628	-2.373982
29	6	0	1.060735	4.223547	-0.987050
30	6	0	0.784323	3.035622	-0.294245
31	6	0	3.681762	1.064868	-0.000045
32	6	0	4.451252	1.386837	-1.122685
33	6	0	5.241926	2.539376	-1.126871
34	6	0	5.269768	3.378346	-0.013151
35	6	0	4.505176	3.059061	1.111528

36	6	0	3.718138	1.907964	1.120365
37	6	0	3.086137	-1.239282	1.674695
38	6	0	4.428637	-1.189026	2.082523
39	6	0	4.814351	-1.773997	3.288751
40	6	0	3.863723	-2.403602	4.096752
41	6	0	2.530116	-2.451834	3.690640
42	6	0	2.134157	-1.874364	2.480396
43	6	0	-2.018113	-3.553775	0.264668
44	6	0	-2.593262	-4.806382	-0.383888
45	6	0	-4.088384	-5.018738	-0.165810
46	6	0	-0.437376	-2.872414	-1.590141
47	8	0	-1.949777	-5.605282	-1.042896
48	6	0	-3.055379	0.236952	1.778092
49	6	0	-4.208592	0.893713	2.235667
50	6	0	-4.747194	0.574664	3.482929
51	6	0	-4.135511	-0.394000	4.282266
52	6	0	-2.989042	-1.046041	3.826956
53	6	0	-2.445087	-0.738712	2.576406
54	1	0	2.247016	-0.418010	-2.851180
55	1	0	3.107235	-1.821535	-4.697344
56	1	0	4.544710	-3.791358	-4.200268
57	1	0	5.120568	-4.333027	-1.842804
58	1	0	4.288699	-2.913207	-0.000441
59	1	0	1.104342	-1.932292	2.132927
60	1	0	1.788467	-2.942484	4.315655
61	1	0	4.164851	-2.853279	5.039511
62	1	0	5.855230	-1.732125	3.598772
63	1	0	5.169793	-0.686596	1.468318
64	1	0	4.446574	0.741502	-1.994507
65	1	0	5.838248	2.775663	-2.004367
66	1	0	5.882949	4.275542	-0.019913
67	1	0	4.513738	3.707080	1.983298
68	1	0	3.125245	1.671820	1.998323
69	1	0	0.281414	0.953116	-2.894858
70	1	0	0.755962	3.014852	-4.140160
71	1	0	1.264481	5.135450	-2.921435
72	1	0	1.272972	5.122905	-0.422844
73	7	0	0.802139	3.127347	1.171705
74	1	0	1.459188	-3.840722	0.162945
75	1	0	0.358386	-4.324303	1.463523
76	1	0	0.253203	-5.117403	-0.126888
77	1	0	0.567084	-2.512000	-1.830955
78	1	0	-0.607376	-3.806269	-2.135359
79	1	0	-1.162986	-2.129591	-1.939248
80	1	0	-2.087357	-3.700849	1.353891
81	1	0	-2.709908	-2.728219	0.051336
82	1	0	-4.355665	-4.912858	0.892575
83	1	0	-4.378904	-6.007882	-0.527317
84	1	0	-4.650726	-4.252613	-0.715461
85	1	0	-3.579310	2.358465	-2.047945
86	1	0	-4.028029	4.774761	-2.226000
87	1	0	-3.447547	6.301169	-0.348974
88	1	0	-2.404591	5.372239	1.714548
89	1	0	-1.949765	2.957488	1.894927
90	1	0	-4.679696	1.661657	1.629922
91	1	0	-5.639437	1.088545	3.830920
92	1	0	-4.551554	-0.635873	5.256962
93	1	0	-2.509395	-1.799058	4.447032
94	1	0	-1.570040	-1.261468	2.194375
95	1	0	-5.034788	-0.660165	0.207166
96	1	0	-6.471279	-1.674938	-1.528162
97	1	0	-5.711246	-1.754097	-3.895240
98	1	0	-3.492726	-0.808905	-4.510200
99	1	0	-2.045612	0.189384	-2.768995
100	8	0	1.095538	4.209302	1.685973
101	8	0	0.520106	2.123940	1.838969

CP2-cis (X=H)

SCF Done: E(RB3LYP) = -2146.95262938 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.720405	0.558421	-2.529996
2	6	0	4.596397	-0.092398	-1.292724
3	6	0	4.894309	-1.459492	-1.217240
4	6	0	5.308433	-2.159173	-2.354940
5	6	0	5.436742	-1.500354	-3.579347
6	6	0	5.144000	-0.136671	-3.663799
7	15	0	3.979407	0.936620	0.171215
8	6	0	3.622391	-0.389692	1.466302
9	6	0	4.455947	-0.656825	2.560218
10	6	0	4.093464	-1.625168	3.501062
11	6	0	2.905582	-2.343617	3.352148
12	6	0	2.071704	-2.089344	2.260026
13	6	0	2.424958	-1.108864	1.331175
14	6	0	5.585328	1.708004	0.802850
15	6	0	5.473602	2.850928	1.608146
16	6	0	6.611750	3.483229	2.111412
17	6	0	7.880169	2.987074	1.803288
18	6	0	8.002395	1.854878	0.995323
19	6	0	6.862374	1.216860	0.500622
20	8	0	-0.419065	-2.674998	0.178599
21	6	0	-0.343870	-3.595490	-0.853526
22	6	0	1.076205	-4.206016	-0.837255
23	46	0	-1.660381	-1.054664	-0.019311
24	15	0	-2.849342	1.042805	-0.279353
25	6	0	-1.737363	2.513664	0.085988
26	6	0	-2.243959	3.727283	0.568664
27	6	0	-1.378594	4.793519	0.824622
28	6	0	-0.007241	4.653172	0.602622
29	6	0	0.500735	3.444531	0.121273
30	6	0	-0.360071	2.376375	-0.136443
31	6	0	-2.661219	-1.636335	1.599885
32	6	0	-2.001423	-1.634369	2.836160
33	6	0	-2.658168	-2.078774	3.989187
34	6	0	-3.971892	-2.548977	3.917477
35	6	0	-4.625988	-2.569806	2.684653
36	6	0	-3.977018	-2.110925	1.532351
37	6	0	-1.389729	-4.718964	-0.682024
38	6	0	-0.612444	-2.936146	-2.280147
39	6	0	0.074977	-1.612935	-2.445680
40	6	0	1.234244	-1.485605	-3.400011
41	6	0	-3.336071	1.261137	-2.081638
42	6	0	-3.859278	0.153321	-2.762861
43	6	0	-4.242311	0.263789	-4.100047
44	6	0	-4.095715	1.480451	-4.770950
45	6	0	-3.568839	2.584581	-4.098885
46	6	0	-3.191572	2.477839	-2.757832
47	6	0	-4.421716	1.429823	0.669500
48	6	0	-5.576839	1.897569	0.031150
49	6	0	-6.721010	2.192690	0.777158
50	6	0	-6.716949	2.027568	2.162508
51	6	0	-5.565847	1.561760	2.802292
52	6	0	-4.423678	1.259266	2.061333
53	8	0	-0.293284	-0.627971	-1.794163
54	1	0	-3.307887	3.839927	0.752971
55	1	0	-1.778260	5.731063	1.202387
56	1	0	0.664168	5.482605	0.809332
57	1	0	1.567051	3.316443	-0.043551
58	1	0	0.039132	1.439648	-0.512443
59	1	0	-2.779891	3.339847	-2.242214
60	1	0	-3.448780	3.532234	-4.617225
61	1	0	-4.387754	1.565941	-5.814226
62	1	0	-4.648399	-0.600732	-4.618498
63	1	0	-3.958197	-0.797253	-2.244777

64	1	0	-5.589105	2.034399	-1.045292
65	1	0	-7.612961	2.553526	0.271707
66	1	0	-7.607713	2.256712	2.741462
67	1	0	-5.557304	1.420310	3.879357
68	1	0	-3.542580	0.875299	2.564579
69	1	0	-5.646986	-2.939287	2.614633
70	1	0	-4.478576	-2.899743	4.813264
71	1	0	-2.135289	-2.065766	4.943341
72	1	0	2.019393	-2.204357	-3.135313
73	1	0	0.906336	-1.734418	-4.417503
74	1	0	1.645709	-0.475182	-3.378113
75	1	0	-0.330416	-3.632179	-3.077468
76	1	0	-1.691471	-2.749500	-2.345552
77	1	0	1.214538	-4.952620	-1.629933
78	1	0	1.838980	-3.427226	-0.944853
79	1	0	1.244308	-4.694506	0.127888
80	1	0	-1.347752	-5.461405	-1.490483
81	1	0	-1.213400	-5.229783	0.270375
82	1	0	-2.396862	-4.289462	-0.648560
83	1	0	-4.510102	-2.123578	0.584896
84	1	0	4.488686	3.249571	1.839814
85	1	0	6.507870	4.366253	2.736759
86	1	0	8.768208	3.481963	2.187723
87	1	0	8.986973	1.463956	0.750927
88	1	0	6.968600	0.335381	-0.124482
89	1	0	5.386546	-0.111374	2.683378
90	1	0	4.746742	-1.819781	4.348378
91	1	0	2.630641	-3.098787	4.084395
92	1	0	1.146504	-2.636070	2.103449
93	1	0	1.752251	-0.922861	0.498430
94	1	0	4.799997	-1.981104	-0.269874
95	1	0	5.537312	-3.219388	-2.279924
96	1	0	5.761604	-2.045227	-4.461959
97	1	0	5.239604	0.384470	-4.613043
98	1	0	4.480411	1.616531	-2.606676
99	1	0	-0.970367	-1.298330	2.903097

CP2-cis (X=NO2)

SCF Done: E(RB3LYP) = -2351.44628144 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.070168	-0.641352	-2.060278
2	6	0	3.371755	-0.287739	-0.739216
3	6	0	4.673800	-0.469017	-0.259490
4	6	0	5.665408	-0.991177	-1.093065
5	6	0	5.366841	-1.325718	-2.414937
6	6	0	4.068125	-1.147466	-2.896486
7	15	0	2.017489	0.484229	0.317643
8	6	0	2.657418	0.297239	2.084244
9	6	0	3.555967	1.205841	2.662188
10	6	0	4.000781	1.018112	3.972910
11	6	0	3.553359	-0.076569	4.715111
12	6	0	2.665937	-0.987333	4.139133
13	6	0	2.218684	-0.807184	2.828368
14	46	0	-0.284573	-0.798614	0.138875
15	15	0	-1.652390	1.151677	-0.343913
16	6	0	-1.866612	2.403145	1.038892
17	6	0	-2.690307	3.529333	0.888005
18	6	0	-2.859825	4.421820	1.946787
19	6	0	-2.227175	4.185718	3.170562
20	6	0	-1.431847	3.051205	3.334152
21	6	0	-1.250972	2.160379	2.271841
22	6	0	-1.972484	-1.914613	0.243549
23	6	0	-2.562771	-2.354012	1.438683
24	6	0	-3.709742	-3.161749	1.478788
25	6	0	-4.319049	-3.537071	0.290192

26	6	0	-3.761129	-3.119323	-0.923388
27	6	0	-2.610790	-2.330082	-0.940005
28	7	0	-1.991026	-2.004031	2.749962
29	8	0	-1.281628	-0.997680	2.842474
30	8	0	1.067239	-2.335368	0.332240
31	6	0	1.074068	-3.703134	0.079538
32	6	0	2.567068	-4.109080	0.017287
33	6	0	0.399442	-4.503949	1.216960
34	6	0	0.345027	-4.122137	-1.259642
35	6	0	0.754129	-3.378184	-2.511405
36	6	0	1.781503	-4.036688	-3.419419
37	6	0	-0.906023	2.031824	-1.828528
38	6	0	-0.456764	1.220165	-2.882869
39	6	0	0.061062	1.802117	-4.041626
40	6	0	0.152020	3.191467	-4.150684
41	6	0	-0.271812	3.997764	-3.093849
42	6	0	-0.802790	3.422280	-1.937075
43	6	0	-3.448300	0.893668	-0.860974
44	6	0	-3.860149	0.986358	-2.193939
45	6	0	-5.199046	0.769585	-2.532427
46	6	0	-6.133118	0.460118	-1.544420
47	6	0	-5.724489	0.365633	-0.211492
48	6	0	-4.390176	0.580470	0.129307
49	8	0	0.254922	-2.303570	-2.823099
50	8	0	-2.265025	-2.729345	3.708127
51	6	0	2.286908	2.328738	-0.019943
52	6	0	1.774975	3.281613	0.873874
53	6	0	1.929951	4.646363	0.627873
54	6	0	2.594845	5.082041	-0.520179
55	6	0	3.099128	4.141892	-1.418787
56	6	0	2.948173	2.775336	-1.171165
57	1	0	-3.214669	3.701546	-0.047468
58	1	0	-3.495593	5.294007	1.819648
59	1	0	-2.368206	4.876722	3.997465
60	1	0	-0.957304	2.847001	4.289944
61	1	0	-0.657292	1.263245	2.407732
62	1	0	-1.114859	4.061845	-1.119052
63	1	0	-0.187116	5.078813	-3.163180
64	1	0	0.560543	3.642635	-5.051118
65	1	0	0.399701	1.164598	-4.853884
66	1	0	-0.498832	0.136598	-2.798596
67	1	0	-3.144841	1.229254	-2.972469
68	1	0	-5.507951	0.848084	-3.571536
69	1	0	-7.173791	0.293156	-1.809287
70	1	0	-6.444391	0.122480	0.565229
71	1	0	-4.082988	0.500544	1.167760
72	1	0	-4.222949	-3.413354	-1.863008
73	1	0	-5.215811	-4.149629	0.307699
74	1	0	-4.098342	-3.475464	2.440317
75	1	0	2.696012	-4.279675	-2.867908
76	1	0	1.378504	-4.983849	-3.802105
77	1	0	2.017143	-3.380550	-4.260274
78	1	0	0.505095	-5.197917	-1.404730
79	1	0	-0.723450	-3.952855	-1.114061
80	1	0	2.693837	-5.175980	-0.209053
81	1	0	3.098515	-3.516539	-0.732925
82	1	0	3.036078	-3.905451	0.985658
83	1	0	0.498344	-5.587560	1.070993
84	1	0	0.870296	-4.243504	2.171400
85	1	0	-0.665498	-4.266370	1.287187
86	1	0	-2.179276	-2.045804	-1.894513
87	1	0	1.260949	2.963350	1.774117
88	1	0	1.531752	5.366623	1.337917
89	1	0	2.719875	6.144851	-0.710723
90	1	0	3.619380	4.467922	-2.315741
91	1	0	3.351657	2.060104	-1.879515
92	1	0	3.906491	2.064071	2.098049
93	1	0	4.696282	1.729398	4.411337
94	1	0	3.895700	-0.218496	5.737056

95	1	0	2.313563	-1.842249	4.710063
96	1	0	1.552146	-1.526972	2.363558
97	1	0	4.917386	-0.208513	0.765382
98	1	0	6.671664	-1.133532	-0.707476
99	1	0	6.140430	-1.726369	-3.064998
100	1	0	3.825513	-1.411424	-3.922393
101	1	0	2.056240	-0.541122	-2.432099

CP3 (X=NO_2)

SCF Done: E(RB3LYP) = -1650.03608825 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.307395	2.333881	0.362681
2	6	0	2.439307	1.140443	-0.362429
3	6	0	3.402635	1.055321	-1.373620
4	6	0	4.226102	2.149486	-1.653864
5	6	0	4.097353	3.330771	-0.923835
6	6	0	3.136287	3.420078	0.086961
7	15	0	1.286815	-0.287561	0.023305
8	46	0	-1.052641	-0.006009	-0.331654
9	8	0	-1.190439	-2.057003	0.001476
10	6	0	-2.410050	-2.707801	-0.063808
11	6	0	-2.339389	-3.943310	0.863918
12	6	0	1.944826	-1.715125	-0.996877
13	6	0	1.300642	-2.048575	-2.193234
14	6	0	1.794077	-3.084391	-2.988165
15	6	0	2.924238	-3.799092	-2.586087
16	6	0	3.561827	-3.476201	-1.386286
17	6	0	3.074326	-2.436799	-0.591820
18	6	0	1.681569	-0.748563	1.799885
19	6	0	2.829999	-0.290062	2.456797
20	6	0	3.079970	-0.681235	3.774838
21	6	0	2.190016	-1.529599	4.434994
22	6	0	1.048336	-1.990602	3.774791
23	6	0	0.788013	-1.603603	2.459791
24	6	0	-0.951529	1.990592	-0.620228
25	6	0	-0.464639	2.518199	-1.829719
26	6	0	-0.496765	3.883922	-2.111549
27	6	0	-1.010178	4.788865	-1.174716
28	6	0	-1.496324	4.311832	0.034433
29	6	0	-1.468529	2.932086	0.285510
30	8	0	-3.155071	0.106923	-0.893621
31	6	0	-3.982065	-0.692788	-0.440555
32	6	0	-3.597717	-1.814221	0.478754
33	6	0	-5.425753	-0.546418	-0.849721
34	6	0	-2.713694	-3.175942	-1.507474
35	1	0	-5.762060	-1.465593	-1.346217
36	1	0	-6.052847	-0.419664	0.041683
37	1	0	-5.553797	0.306847	-1.518568
38	1	0	-4.478776	-2.428039	0.696640
39	1	0	-3.250036	-1.369935	1.420444
40	1	0	-3.672124	-3.707615	-1.587555
41	1	0	-2.726843	-2.324540	-2.197490
42	1	0	-1.918344	-3.853343	-1.835351
43	1	0	-3.244571	-4.561479	0.807255
44	1	0	-2.195644	-3.630750	1.904551
45	1	0	-0.047286	1.841397	-2.570732
46	1	0	-0.115655	4.246787	-3.063395
47	1	0	-1.033941	5.853519	-1.388493
48	1	0	-1.905743	4.976921	0.785085
49	7	0	-2.032832	2.500647	1.575990
50	1	0	3.514227	0.138851	-1.943453
51	1	0	4.970175	2.072315	-2.442215
52	1	0	4.739836	4.179761	-1.141433
53	1	0	3.025112	4.338374	0.656835
54	1	0	1.553298	2.418492	1.139290

55	1	0	3.524412	0.374659	1.952835
56	1	0	3.969829	-0.319160	4.283073
57	1	0	2.384705	-1.829020	5.461547
58	1	0	0.353318	-2.651207	4.286472
59	1	0	-0.092145	-1.956419	1.926126
60	1	0	3.568638	-2.196256	0.344852
61	1	0	4.436498	-4.035105	-1.064426
62	1	0	3.303406	-4.610196	-3.202163
63	1	0	1.287544	-3.339834	-3.914994
64	1	0	0.404905	-1.509722	-2.485536
65	1	0	-1.479624	-4.554854	0.571652
66	8	0	-2.304335	3.365599	2.410868
67	8	0	-2.222543	1.293634	1.774034

$TS^{retro\text{-}aldol}$ ($X=NO_2$)

SCF Done: E(RB3LYP) = -1650.01303149 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.216651	-1.766914	-2.476336
2	6	0	1.916988	-1.598722	-1.275374
3	6	0	3.072448	-2.353939	-1.038153
4	6	0	3.525198	-3.261255	-1.997505
5	6	0	2.828643	-3.419896	-3.197730
6	6	0	1.674301	-2.671810	-3.436196
7	15	0	1.277146	-0.349627	-0.028359
8	6	0	1.790029	-1.039337	1.641205
9	6	0	3.030188	-0.727412	2.214343
10	6	0	3.392283	-1.283630	3.443116
11	6	0	2.520005	-2.149657	4.104326
12	6	0	1.284306	-2.459803	3.533126
13	6	0	0.914371	-1.908215	2.305336
14	46	0	-1.101393	-0.045964	-0.308108
15	6	0	-0.947236	1.919731	-0.580971
16	6	0	-0.743864	2.411121	-1.879115
17	6	0	-0.799226	3.776747	-2.162620
18	6	0	-1.076714	4.700782	-1.149663
19	6	0	-1.299256	4.246336	0.143273
20	6	0	-1.220443	2.873330	0.409909
21	8	0	-3.117140	0.220303	-0.799126
22	6	0	-4.067880	-0.385758	-0.170450
23	6	0	-5.416135	-0.281156	-0.858723
24	6	0	-3.915960	-1.161709	0.972318
25	8	0	-1.428608	-2.179918	0.116840
26	6	0	-2.548520	-2.769882	0.019528
27	6	0	-3.160945	-2.957381	-1.354891
28	6	0	-2.861764	-3.839455	1.052390
29	6	0	2.377517	1.151829	-0.248188
30	6	0	3.285934	1.260060	-1.306049
31	6	0	4.064476	2.412735	-1.445241
32	6	0	3.943614	3.456734	-0.528397
33	6	0	3.036865	3.350285	0.529857
34	6	0	2.253283	2.205856	0.669020
35	1	0	-6.185148	-0.875980	-0.358292
36	1	0	-5.733952	0.768002	-0.866697
37	1	0	-5.332321	-0.598887	-1.904554
38	1	0	-4.804942	-1.578012	1.437332
39	1	0	-3.067744	-0.991391	1.624680
40	1	0	-4.207193	-3.270313	-1.306217
41	1	0	-3.070322	-2.042013	-1.944428
42	1	0	-2.588860	-3.746426	-1.865606
43	1	0	-3.920798	-4.108106	1.061861
44	1	0	-2.555361	-3.515293	2.049456
45	1	0	-0.552632	1.711786	-2.687958
46	1	0	-0.633179	4.120706	-3.180680
47	1	0	-1.121814	5.763714	-1.367662
48	1	0	-1.528970	4.927149	0.954450

49	7	0	-1.436155	2.471808	1.807796
50	1	0	3.390710	0.450973	-2.021639
51	1	0	4.767225	2.488800	-2.270740
52	1	0	4.551237	4.351079	-0.637179
53	1	0	2.935218	4.161109	1.245966
54	1	0	1.543669	2.128178	1.487322
55	1	0	3.710252	-0.045495	1.713644
56	1	0	4.354463	-1.034700	3.882851
57	1	0	2.800896	-2.577733	5.062965
58	1	0	0.599860	-3.129383	4.047209
59	1	0	-0.043993	-2.149332	1.855496
60	1	0	3.613733	-2.242371	-0.103502
61	1	0	4.420089	-3.846813	-1.804521
62	1	0	3.181584	-4.128789	-3.941981
63	1	0	1.123541	-2.797042	-4.364517
64	1	0	0.306837	-1.198223	-2.649616
65	1	0	-2.282458	-4.739452	0.795369
66	8	0	-2.056216	3.242475	2.540891
67	8	0	-0.963612	1.394971	2.192411

CP4 (X=NO2)

SCF Done: E(RB3LYP) = -1456.87372800 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.331908	-2.622747	-0.694991
2	6	0	1.778708	-1.411831	-1.127946
3	6	0	1.749356	-1.120206	-2.498796
4	6	0	2.273626	-2.024570	-3.423008
5	6	0	2.824319	-3.231943	-2.986457
6	6	0	2.850698	-3.529427	-1.623209
7	15	0	1.099897	-0.113575	0.049772
8	6	0	2.590400	0.984392	0.381702
9	6	0	2.422691	2.373941	0.412643
10	6	0	3.519487	3.201117	0.673701
11	6	0	4.780007	2.649455	0.901253
12	6	0	4.950179	1.262605	0.863233
13	6	0	3.860666	0.432162	0.603013
14	46	0	-0.877303	1.063296	-0.838767
15	6	0	-2.344648	2.331273	-1.787950
16	6	0	-1.565060	3.297775	-1.063534
17	6	0	-2.187062	4.238438	-0.057994
18	6	0	-2.063461	-0.554671	-0.719529
19	6	0	-3.056502	-0.727656	0.259970
20	6	0	-3.900817	-1.846253	0.307650
21	6	0	-3.759840	-2.847000	-0.643810
22	6	0	-2.785595	-2.710703	-1.639588
23	6	0	-1.960798	-1.585268	-1.673539
24	8	0	-0.296322	3.231860	-1.186270
25	6	0	0.824785	-1.024580	1.667823
26	6	0	-0.018869	-2.145669	1.692120
27	6	0	-0.288112	-2.795210	2.896980
28	6	0	0.268758	-2.326465	4.089181
29	6	0	1.098963	-1.205735	4.070213
30	6	0	1.378395	-0.556567	2.865331
31	1	0	2.350290	-2.865883	0.362888
32	1	0	3.275152	-4.468339	-1.277577
33	1	0	3.227531	-3.938892	-3.706505
34	1	0	2.246760	-1.787935	-4.483259
35	1	0	1.311517	-0.185038	-2.840069
36	1	0	4.003264	-0.643982	0.566059
37	1	0	5.931563	0.827383	1.032423
38	1	0	5.630463	3.295910	1.101377
39	1	0	3.383345	4.278980	0.690612
40	1	0	1.450884	2.813510	0.208286
41	1	0	2.024986	0.314702	2.862907
42	1	0	1.532687	-0.831206	4.993513

43	1	0	0.052464	-2.830123	5.027398
44	1	0	-0.940540	-3.664145	2.902748
45	1	0	-0.467872	-2.512502	0.774374
46	7	0	-3.275055	0.284790	1.308830
47	1	0	-4.646827	-1.908070	1.090567
48	1	0	-4.402344	-3.722044	-0.612760
49	1	0	-2.669071	-3.484472	-2.394915
50	1	0	-1.214221	-1.508861	-2.458350
51	1	0	-2.877244	4.929523	-0.556000
52	1	0	-2.759097	3.664368	0.679260
53	1	0	-1.406336	4.805494	0.454150
54	1	0	-2.045561	2.125404	-2.814543
55	1	0	-3.408653	2.245739	-1.583602
56	8	0	-4.320510	0.222173	1.959361
57	8	0	-2.412340	1.148593	1.500557

TSrd (X=NO_2)

SCF Done: E(RB3LYP) = -1456.83914868 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.143211	2.384649	-1.394174
2	6	0	-1.855262	1.723607	-0.384459
3	6	0	-2.872272	2.401621	0.301098
4	6	0	-3.180593	3.722492	-0.029895
5	6	0	-2.475356	4.374632	-1.043959
6	6	0	-1.456579	3.704919	-1.723989
7	15	0	-1.397232	-0.056144	-0.000381
8	6	0	-1.840644	-0.261827	1.814760
9	6	0	-3.099957	-0.708519	2.234221
10	6	0	-3.383219	-0.832393	3.596695
11	6	0	-2.413792	-0.508811	4.547242
12	6	0	-1.155724	-0.065979	4.132474
13	6	0	-0.866807	0.052255	2.772439
14	46	0	0.867718	-0.695206	-0.673536
15	6	0	2.849152	-1.353743	-1.346035
16	6	0	3.451448	-2.550262	-0.679694
17	6	0	4.968980	-2.624365	-0.640232
18	6	0	2.558095	-0.024221	0.220525
19	6	0	3.033381	1.291409	0.010602
20	6	0	3.727904	2.004130	0.998742
21	6	0	3.974389	1.418189	2.231514
22	6	0	3.527606	0.111214	2.467765
23	6	0	2.852174	-0.598641	1.478901
24	7	0	2.801498	1.996917	-1.254635
25	8	0	3.202129	3.159237	-1.351903
26	8	0	2.757186	-3.427172	-0.184728
27	6	0	-2.688536	-1.093706	-0.893144
28	6	0	-2.460807	-2.475529	-0.980218
29	6	0	-3.374462	-3.299768	-1.636830
30	6	0	-4.517705	-2.750257	-2.222924
31	6	0	-4.744176	-1.375455	-2.146229
32	6	0	-3.834625	-0.547616	-1.482128
33	8	0	2.227209	1.401661	-2.175435
34	1	0	-3.417345	1.905907	1.099079
35	1	0	-3.968532	4.242498	0.508651
36	1	0	-2.713636	5.404405	-1.296586
37	1	0	-0.893817	4.210083	-2.503968
38	1	0	-0.332669	1.875074	-1.908755
39	1	0	-4.017431	0.521030	-1.428985
40	1	0	-5.629272	-0.941976	-2.604357
41	1	0	-5.225513	-3.391106	-2.741719
42	1	0	-3.188498	-4.368620	-1.697502
43	1	0	-1.565718	-2.905459	-0.536018
44	1	0	-3.857893	-0.968057	1.501210
45	1	0	-4.362005	-1.183605	3.912680
46	1	0	-2.635249	-0.607042	5.606599

47	1	0	-0.393896	0.179664	4.867473
48	1	0	0.119907	0.376934	2.454524
49	1	0	3.714654	-0.362348	3.428505
50	1	0	4.511964	1.968023	2.997831
51	1	0	4.053197	3.012297	0.774211
52	1	0	2.541810	-1.620523	1.669566
53	1	0	5.284447	-3.531840	-0.120937
54	1	0	5.380506	-2.620416	-1.657414
55	1	0	5.374386	-1.743595	-0.126669
56	1	0	2.128125	-1.698720	-2.116173
57	1	0	3.556832	-0.687345	-1.832317

$TS^{C\text{-}O}$ (X=H)

SCF Done: E(RB3LYP) = -2146.90204062 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.865830	-2.088318	2.361068
2	6	0	-1.982026	-2.309591	0.973288
3	6	0	-3.168715	-2.865014	0.459922
4	6	0	-4.235741	-3.140054	1.323687
5	6	0	-4.138199	-2.890761	2.692618
6	6	0	-2.943044	-2.358987	3.198649
7	46	0	-1.002248	-0.977722	-0.279672
8	8	0	-0.351838	-2.901778	0.403791
9	6	0	-0.162306	-4.068426	-0.390134
10	6	0	-0.947806	-5.260087	0.193243
11	15	0	-2.086510	1.158941	-0.404570
12	6	0	-1.245611	2.334618	-1.610942
13	6	0	-0.512405	1.777012	-2.667392
14	6	0	0.123959	2.606268	-3.593696
15	6	0	0.041553	3.994052	-3.467942
16	6	0	-0.679809	4.554131	-2.411097
17	6	0	-1.321267	3.728451	-1.485318
18	6	0	-3.889434	1.160708	-0.941659
19	6	0	-4.355449	1.906647	-2.030570
20	6	0	-5.701751	1.844731	-2.401728
21	6	0	-6.591887	1.044159	-1.685510
22	6	0	-6.130485	0.298565	-0.597416
23	6	0	-4.786121	0.349677	-0.229365
24	6	0	-2.117653	2.128047	1.207687
25	6	0	-3.140476	3.029754	1.528173
26	6	0	-3.099224	3.740370	2.730299
27	6	0	-2.037423	3.556754	3.618243
28	6	0	-1.018489	2.654129	3.305543
29	6	0	-1.061389	1.937639	2.108378
30	6	0	-0.584226	-3.879226	-1.889810
31	6	0	0.319782	-2.978822	-2.717942
32	8	0	0.295364	-1.759999	-2.615459
33	6	0	1.346622	-4.363921	-0.279929
34	6	0	1.251518	-3.652720	-3.708706
35	1	0	-3.973951	3.171736	0.846429
36	1	0	-3.899299	4.435292	2.972399
37	1	0	-2.008496	4.109324	4.553772
38	1	0	-0.192873	2.496386	3.994237
39	1	0	-0.280672	1.218404	1.876572
40	1	0	-1.874173	4.171323	-0.662096
41	1	0	-0.743044	5.634138	-2.304802
42	1	0	0.543990	4.637452	-4.185451
43	1	0	0.693634	2.164909	-4.407093
44	1	0	-0.424735	0.697201	-2.755188
45	1	0	-3.672669	2.536737	-2.591429
46	1	0	-6.051696	2.426593	-3.250632
47	1	0	-7.638726	0.998418	-1.974302
48	1	0	-6.815414	-0.331893	-0.036501
49	1	0	-4.434628	-0.249646	0.605002
50	1	0	-5.153994	-3.549121	0.906720

51	1	0	-4.969572	-3.110434	3.356176
52	1	0	-2.846077	-2.157521	4.263360
53	1	0	1.879467	-4.397005	-3.205378
54	1	0	0.661579	-4.190060	-4.462938
55	1	0	1.881104	-2.909584	-4.202036
56	1	0	-0.632058	-4.869872	-2.357526
57	1	0	-1.589745	-3.448834	-1.905402
58	1	0	1.622279	-5.253362	-0.861212
59	1	0	1.941558	-3.512965	-0.625899
60	1	0	1.604796	-4.549279	0.767149
61	1	0	-0.645637	-6.195217	-0.293192
62	1	0	-0.734906	-5.341727	1.263946
63	1	0	-2.026603	-5.140030	0.074269
64	1	0	-3.282892	-3.041596	-0.604029
65	15	0	2.633206	0.448053	0.108515
66	6	0	3.502248	2.121058	-0.052294
67	6	0	2.717541	0.129291	1.972272
68	6	0	3.951226	-0.745358	-0.535597
69	6	0	2.684378	3.261173	-0.044022
70	6	0	3.238119	4.535697	-0.174937
71	6	0	4.617552	4.686878	-0.330899
72	6	0	5.438339	3.557650	-0.352992
73	6	0	4.885022	2.282411	-0.212995
74	1	0	1.607352	3.151059	0.054549
75	1	0	2.589551	5.407880	-0.166820
76	1	0	5.049873	5.678129	-0.441232
77	1	0	6.512685	3.667388	-0.479244
78	1	0	5.533638	1.411869	-0.235275
79	6	0	3.382848	0.963781	2.879523
80	6	0	3.358417	0.684269	4.249613
81	6	0	2.675842	-0.435331	4.726794
82	6	0	2.009769	-1.272680	3.827589
83	6	0	2.021324	-0.989663	2.460542
84	1	0	3.920581	1.836143	2.520726
85	1	0	3.878954	1.341973	4.941594
86	1	0	2.659321	-0.652933	5.791672
87	1	0	1.472189	-2.145464	4.189855
88	1	0	1.477315	-1.636217	1.775303
89	6	0	4.996606	-1.255068	0.246511
90	6	0	5.932439	-2.132739	-0.306401
91	6	0	5.835277	-2.509233	-1.647564
92	6	0	4.792396	-2.012082	-2.432232
93	6	0	3.851853	-1.140883	-1.877922
94	1	0	5.076630	-0.969797	1.291430
95	1	0	6.737943	-2.521688	0.311592
96	1	0	6.564758	-3.191245	-2.076897
97	1	0	4.707484	-2.307029	-3.475317
98	1	0	3.023287	-0.778805	-2.481262
99	1	0	-0.940508	-1.690264	2.763729

$TS^{C\text{-}O}$ (X=NO_2)

SCF Done: E(RB3LYP) = -2351.41223163 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.359048	-2.393868	1.537123
2	6	0	-1.719736	-2.139082	0.279345
3	6	0	-2.491610	-2.460244	-0.881449
4	6	0	-3.712619	-3.095718	-0.782262
5	6	0	-4.267412	-3.441593	0.472252
6	6	0	-3.592808	-3.072103	1.617654
7	46	0	-0.293189	-0.702077	0.127512
8	8	0	-0.068355	-2.863510	0.334291
9	6	0	0.368528	-4.005134	-0.393365
10	6	0	-0.322408	-5.233378	0.235030
11	15	0	-1.656139	1.259036	-0.327489
12	6	0	-0.820229	2.330212	-1.625470

13	6	0	-0.486916	1.710000	-2.841509
14	6	0	0.124945	2.444561	-3.858469
15	6	0	0.434187	3.793690	-3.664292
16	6	0	0.132897	4.402603	-2.446384
17	6	0	-0.496255	3.676777	-1.430732
18	6	0	-3.403835	1.034025	-1.005950
19	6	0	-3.818737	1.553044	-2.237446
20	6	0	-5.138825	1.381197	-2.664200
21	6	0	-6.052582	0.694220	-1.865002
22	6	0	-5.640758	0.172238	-0.636663
23	6	0	-4.323433	0.336434	-0.210699
24	6	0	-2.020855	2.360141	1.153488
25	6	0	-2.770840	3.538610	1.020708
26	6	0	-3.066392	4.314031	2.141909
27	6	0	-2.634952	3.908175	3.408006
28	6	0	-1.915212	2.721552	3.548578
29	6	0	-1.606957	1.947084	2.425493
30	6	0	0.055740	-4.038216	-1.931402
31	6	0	0.632024	-2.924911	-2.790070
32	8	0	0.103827	-1.824033	-2.862033
33	6	0	1.889456	-4.086727	-0.167973
34	6	0	1.867241	-3.253165	-3.609804
35	1	0	-3.137532	3.845098	0.045105
36	1	0	-3.644200	5.227565	2.028304
37	1	0	-2.873817	4.508398	4.282068
38	1	0	-1.598513	2.385123	4.532018
39	1	0	-1.073050	1.008005	2.545989
40	1	0	-0.715990	4.161372	-0.486049
41	1	0	0.387648	5.445479	-2.278786
42	1	0	0.916127	4.362495	-4.455107
43	1	0	0.366383	1.957782	-4.799905
44	1	0	-0.688743	0.651732	-2.987352
45	1	0	-3.122158	2.095630	-2.867400
46	1	0	-5.449720	1.791619	-3.621533
47	1	0	-7.079068	0.563520	-2.197467
48	1	0	-6.340373	-0.373924	-0.010174
49	1	0	-4.013521	-0.087357	0.739642
50	1	0	-4.267142	-3.313264	-1.692935
51	1	0	-5.220259	-3.957765	0.534341
52	1	0	-3.990062	-3.271831	2.606089
53	7	0	-1.759675	-1.972752	2.760283
54	1	0	2.677704	-3.612838	-2.965421
55	1	0	1.635164	-4.064111	-4.313111
56	1	0	2.202849	-2.373280	-4.160061
57	1	0	0.431623	-5.000686	-2.298134
58	1	0	-1.028055	-4.036220	-2.058697
59	1	0	2.318540	-4.964509	-0.668384
60	1	0	2.391204	-3.189224	-0.544423
61	1	0	2.103608	-4.164419	0.902132
62	1	0	0.036227	-6.168816	-0.211962
63	1	0	-0.112348	-5.258242	1.308922
64	1	0	-1.406997	-5.176883	0.101464
65	1	0	-2.096187	-2.175290	-1.849075
66	8	0	-2.300669	-2.261957	3.838098
67	8	0	-0.697219	-1.305769	2.714474
68	15	0	2.133294	0.359859	0.338804
69	6	0	2.427071	2.220721	0.513240
70	6	0	2.950744	-0.284343	1.911555
71	6	0	3.354098	-0.124928	-1.017391
72	6	0	1.773185	2.882698	1.562902
73	6	0	1.931846	4.256348	1.743688
74	6	0	2.744656	4.988882	0.874474
75	6	0	3.396914	4.336582	-0.171803
76	6	0	3.241709	2.958791	-0.352165
77	1	0	1.138784	2.325241	2.244924
78	1	0	1.417566	4.751942	2.562834
79	1	0	2.869275	6.059557	1.014189
80	1	0	4.035180	4.896379	-0.850797
81	1	0	3.758467	2.466566	-1.169037

82	6	0	4.067450	0.352471	2.474611
83	6	0	4.657323	-0.155629	3.632509
84	6	0	4.134369	-1.300362	4.239950
85	6	0	3.020253	-1.931656	3.686839
86	6	0	2.426529	-1.428319	2.525736
87	1	0	4.472557	1.248550	2.013472
88	1	0	5.521057	0.345598	4.061949
89	1	0	4.589966	-1.691662	5.145961
90	1	0	2.597173	-2.811436	4.163853
91	1	0	1.545707	-1.913052	2.118297
92	6	0	4.572902	-0.761716	-0.751135
93	6	0	5.443615	-1.086466	-1.795306
94	6	0	5.113902	-0.764872	-3.112440
95	6	0	3.897527	-0.133753	-3.384621
96	6	0	3.015119	0.169596	-2.346511
97	1	0	4.848370	-1.002172	0.270102
98	1	0	6.384902	-1.582872	-1.573807
99	1	0	5.797088	-1.007619	-3.922138
100	1	0	3.628674	0.116024	-4.407948
101	1	0	2.061440	0.636326	-2.571278

$TS^{protonation}$ (X=H)

SCF Done: E(RB3LYP) = -1638.66281631 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.585812	-0.742889	-2.352249
2	6	0	-2.585884	-0.947913	-0.965081
3	6	0	-3.801227	-1.097708	-0.291657
4	6	0	-5.005362	-1.041748	-0.999013
5	6	0	-5.002513	-0.838687	-2.378793
6	6	0	-3.788701	-0.691121	-3.054992
7	15	0	-0.928664	-0.990376	-0.079828
8	46	0	0.269976	1.062176	0.148934
9	8	0	2.461252	0.580288	0.193383
10	6	0	3.244721	0.151326	1.303473
11	6	0	3.159495	1.162018	2.464384
12	6	0	-1.284642	-1.755987	1.597776
13	6	0	-1.861762	-0.948924	2.589587
14	6	0	-2.141846	-1.478781	3.849577
15	6	0	-1.833196	-2.810861	4.135248
16	6	0	-1.246366	-3.611451	3.154809
17	6	0	-0.974015	-3.089327	1.887912
18	6	0	0.003808	-2.285693	-1.062811
19	6	0	-0.657040	-3.432906	-1.531512
20	6	0	0.053476	-4.405590	-2.234449
21	6	0	1.422028	-4.241725	-2.469672
22	6	0	2.077882	-3.099747	-2.010369
23	6	0	1.368980	-2.114801	-1.314780
24	6	0	-1.448785	2.082313	0.157306
25	6	0	-1.859634	2.626166	1.382717
26	6	0	-2.952591	3.498926	1.440057
27	6	0	-3.641687	3.839450	0.274683
28	6	0	-3.231783	3.303906	-0.947927
29	6	0	-2.144763	2.423907	-1.007293
30	8	0	1.639023	2.813413	0.183027
31	6	0	1.759666	3.764607	-0.798054
32	6	0	2.670624	3.687364	-1.778616
33	6	0	0.812089	4.914794	-0.609911
34	6	0	2.779369	-1.225085	1.803274
35	1	0	0.968889	5.682569	-1.372765
36	1	0	-0.227169	4.572232	-0.660401
37	1	0	0.956385	5.364962	0.380158
38	1	0	2.765793	4.488180	-2.502980
39	1	0	3.346157	2.843580	-1.871728
40	1	0	3.346927	-1.526015	2.692261
41	1	0	1.719692	-1.176747	2.077905

42	1	0	2.916188	-1.997619	1.044448
43	1	0	2.130117	1.218602	2.837928
44	1	0	3.455158	2.165396	2.139974
45	1	0	-1.315409	2.395481	2.296016
46	1	0	-3.256577	3.917211	2.397061
47	1	0	-4.489123	4.518648	0.318490
48	1	0	-3.758510	3.567112	-1.862430
49	1	0	-1.845095	2.015513	-1.967927
50	1	0	-3.817387	-1.261781	0.780553
51	1	0	-5.944937	-1.160790	-0.466326
52	1	0	-5.940122	-0.796823	-2.926320
53	1	0	-3.777071	-0.535152	-4.130320
54	1	0	-1.645873	-0.631211	-2.886103
55	1	0	-1.720736	-3.564703	-1.355957
56	1	0	-0.462013	-5.291382	-2.596201
57	1	0	1.974036	-5.006099	-3.010323
58	1	0	3.144925	-2.969701	-2.163088
59	1	0	1.877216	-1.221956	-0.961405
60	1	0	-0.513280	-3.719738	1.135080
61	1	0	-0.995273	-4.645960	3.372507
62	1	0	-2.043801	-3.220055	5.119537
63	1	0	-2.593077	-0.846950	4.609772
64	1	0	-2.090540	0.091208	2.377326
65	1	0	3.807758	0.864870	3.297536
66	1	0	2.311152	1.924898	0.118829
67	6	0	4.734147	0.080814	0.821307
68	1	0	5.342191	-0.407837	1.591603
69	6	0	4.888609	-0.698778	-0.478547
70	1	0	5.102989	1.104763	0.689544
71	8	0	4.853542	-1.919789	-0.498959
72	6	0	5.055470	0.106842	-1.750773
73	1	0	5.899653	0.802596	-1.667764
74	1	0	5.204729	-0.556871	-2.605726
75	1	0	4.150052	0.707554	-1.895582

$TS^{protonation}$ ($X=NO_2$)

SCF Done: E(RB3LYP) = -1843.16543567 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.768011	-2.208659	-1.590508
2	6	0	1.490266	-1.861698	-0.258739
3	6	0	2.393783	-2.330854	0.706869
4	6	0	3.530541	-3.085170	0.386174
5	6	0	3.772948	-3.413316	-0.940551
6	6	0	2.882556	-2.978216	-1.928840
7	46	0	-0.241126	-0.958408	0.148305
8	8	0	-1.527977	-2.806036	0.098762
9	6	0	-1.622995	-3.578031	-1.034161
10	6	0	-0.974440	-4.920977	-0.856920
11	15	0	0.694505	1.224189	-0.212955
12	6	0	-0.326360	2.199847	-1.449470
13	6	0	0.224997	3.269686	-2.171503
14	6	0	-0.580200	4.012761	-3.036424
15	6	0	-1.934656	3.699348	-3.178730
16	6	0	-2.482532	2.634470	-2.462385
17	6	0	-1.680240	1.876827	-1.604962
18	6	0	2.445978	1.320841	-0.883027
19	6	0	2.684859	1.038099	-2.235197
20	6	0	3.984227	1.070180	-2.740652
21	6	0	5.057555	1.373859	-1.899870
22	6	0	4.824501	1.648051	-0.552058
23	6	0	3.523512	1.624584	-0.043515
24	6	0	0.754628	2.274789	1.345446
25	6	0	0.949863	1.650104	2.584350
26	6	0	1.039583	2.419591	3.747019
27	6	0	0.924289	3.808807	3.681262

28	6	0	0.718576	4.431072	2.448064
29	6	0	0.634942	3.669018	1.282062
30	8	0	-2.389541	-0.591825	0.334369
31	6	0	-3.150879	-0.218573	1.482697
32	6	0	-4.649793	-0.485080	1.134033
33	6	0	-5.058875	0.039398	-0.241592
34	6	0	-5.564744	-0.991042	-1.233297
35	6	0	-2.764433	-1.081652	2.697439
36	6	0	-2.932006	1.265563	1.808154
37	6	0	-2.239884	-3.169134	-2.152596
38	8	0	-5.005106	1.223607	-0.530543
39	1	0	-1.071391	-5.533002	-1.757936
40	1	0	0.091029	-4.798138	-0.627492
41	1	0	-1.426752	-5.454659	-0.012143
42	1	0	-2.328637	-3.831446	-3.006354
43	1	0	-2.661829	-2.173002	-2.239450
44	1	0	-3.506215	1.554316	2.697363
45	1	0	-1.873933	1.448107	2.017872
46	1	0	-3.250938	1.899465	0.978813
47	1	0	-1.715043	-0.911284	2.962784
48	1	0	-2.884195	-2.148007	2.475141
49	7	0	2.168376	-2.062057	2.129615
50	1	0	4.188941	-3.408755	1.183556
51	1	0	4.642757	-4.007900	-1.203176
52	1	0	3.059338	-3.237160	-2.970004
53	1	0	1.091488	-1.884536	-2.376767
54	1	0	3.353592	1.847926	1.004830
55	1	0	5.653359	1.886339	0.108842
56	1	0	6.069701	1.396707	-2.294408
57	1	0	4.157117	0.856216	-3.791914
58	1	0	1.856925	0.802773	-2.897394
59	1	0	1.276755	3.519216	-2.069181
60	1	0	-0.147707	4.838115	-3.595930
61	1	0	-2.559347	4.286207	-3.847084
62	1	0	-3.536505	2.386330	-2.546152
63	1	0	-2.110225	1.044530	-1.054170
64	1	0	0.464298	4.161641	0.330458
65	1	0	0.618279	5.511583	2.391173
66	1	0	0.987132	4.404618	4.587850
67	1	0	1.189856	1.926135	4.703136
68	1	0	1.015413	0.568450	2.650126
69	1	0	-3.382074	-0.840765	3.571418
70	1	0	-2.207962	-1.939261	0.152987
71	1	0	-5.288094	-0.003087	1.886214
72	1	0	-4.840062	-1.563657	1.184322
73	1	0	-6.453707	-1.494467	-0.830041
74	1	0	-5.815556	-0.513020	-2.183059
75	1	0	-4.806620	-1.767683	-1.390707
76	8	0	3.102117	-2.231860	2.913026
77	8	0	1.043626	-1.681069	2.486886

CP5 (X=H)

SCF Done: E(RB3LYP) = -1953.78498049 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.464143	-0.845547	2.598329
2	6	0	-2.712696	0.103434	1.897417
3	6	0	-2.025117	1.107249	2.600826
4	6	0	-2.112170	1.163797	3.991617
5	6	0	-2.866513	0.216892	4.691339
6	6	0	-3.537492	-0.787328	3.993845
7	15	0	-2.480208	0.056737	0.033042
8	6	0	-3.314725	1.626429	-0.581775
9	6	0	-3.195082	1.948090	-1.939524
10	6	0	-3.861412	3.059041	-2.457798
11	6	0	-4.644526	3.861120	-1.625816

12	6	0	-4.759099	3.548278	-0.270489
13	6	0	-4.098172	2.433584	0.251384
14	46	0	-0.025979	-0.023581	-0.145811
15	8	0	-0.183222	2.081914	0.048376
16	6	0	-0.058458	2.853060	-1.020830
17	6	0	-0.186156	4.330539	-0.702946
18	6	0	0.013768	-2.054581	-0.258826
19	6	0	0.483359	-2.695806	-1.417334
20	6	0	0.447075	-4.090580	-1.540014
21	6	0	-0.053427	-4.878136	-0.501335
22	6	0	-0.519366	-4.257926	0.659886
23	6	0	-0.488883	-2.863761	0.776426
24	15	0	2.436896	0.078693	-0.008246
25	6	0	-3.679685	-1.249016	-0.600794
26	6	0	-3.224147	-2.338445	-1.350678
27	6	0	-4.134737	-3.270448	-1.857668
28	6	0	-5.500476	-3.123352	-1.618881
29	6	0	-5.961403	-2.032562	-0.876549
30	6	0	-5.057188	-1.096638	-0.375946
31	6	0	0.146589	2.431703	-2.296658
32	1	0	-3.991842	-1.628791	2.063842
33	1	0	-4.122141	-1.529172	4.531661
34	1	0	-2.927028	0.261232	5.775602
35	1	0	-1.583919	1.945759	4.530975
36	1	0	-1.424350	1.827075	2.049262
37	1	0	-4.194487	2.200073	1.306628
38	1	0	-5.363886	4.169274	0.385318
39	1	0	-5.159762	4.728064	-2.031073
40	1	0	-3.757017	3.302468	-3.511554
41	1	0	-2.569371	1.345921	-2.588921
42	1	0	-5.425866	-0.239629	0.180231
43	1	0	-7.025209	-1.904941	-0.694149
44	1	0	-6.205680	-3.850473	-2.013011
45	1	0	-3.767617	-4.111908	-2.438815
46	1	0	-2.165025	-2.463444	-1.540093
47	1	0	0.815751	-4.559076	-2.450325
48	1	0	-0.080052	-5.960920	-0.595401
49	1	0	-0.916536	-4.857911	1.476289
50	1	0	-0.873771	-2.407245	1.686520
51	1	0	-0.078976	4.953818	-1.596003
52	1	0	-1.166399	4.529109	-0.251764
53	1	0	0.575558	4.627524	0.027819
54	1	0	0.224442	3.139300	-3.115488
55	1	0	0.178523	1.372690	-2.540775
56	6	0	3.137210	1.807655	0.232144
57	6	0	3.299705	-0.842972	1.395614
58	6	0	3.280077	-0.560032	-1.561351
59	6	0	4.617733	-0.513765	1.747987
60	6	0	5.261138	-1.192937	2.782384
61	6	0	4.594912	-2.204279	3.479150
62	6	0	3.284331	-2.532667	3.134256
63	6	0	2.637065	-1.855086	2.097080
64	1	0	5.140876	0.279146	1.222879
65	1	0	6.281540	-0.927687	3.046319
66	1	0	5.095869	-2.730483	4.287544
67	1	0	2.756996	-3.316828	3.670897
68	1	0	1.622444	-2.121885	1.829482
69	6	0	2.569858	2.609709	1.231022
70	6	0	3.115676	3.862351	1.514414
71	6	0	4.221638	4.327815	0.799539
72	6	0	4.781815	3.535021	-0.202542
73	6	0	4.244333	2.276506	-0.484872
74	1	0	1.686731	2.268627	1.758019
75	1	0	2.668935	4.478911	2.289946
76	1	0	4.641604	5.305697	1.020064
77	1	0	5.640030	3.891006	-0.766501
78	1	0	4.690582	1.666101	-1.263124
79	6	0	4.088774	-1.701759	-1.545480
80	6	0	4.654871	-2.176978	-2.731482

81	6	0	4.420670	-1.515009	-3.936914
82	6	0	3.611786	-0.375561	-3.955967
83	6	0	3.036802	0.098858	-2.776365
84	1	0	4.277161	-2.224234	-0.613533
85	1	0	5.279542	-3.066038	-2.708416
86	1	0	4.863164	-1.885320	-4.857927
87	1	0	3.422835	0.144849	-4.891193
88	1	0	2.400264	0.980291	-2.796619
89	1	0	0.881881	-2.108761	-2.241197

CP5 (X=NO2)

SCF Done: E(RB3LYP) = -2158.29054231 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.008648	0.914945	2.545401
2	6	0	-2.903853	1.250867	1.753218
3	6	0	-2.109417	2.355676	2.097358
4	6	0	-2.420358	3.104113	3.233938
5	6	0	-3.515483	2.761384	4.030995
6	6	0	-4.310026	1.668290	3.683319
7	15	0	-2.447601	0.288005	0.201852
8	6	0	-3.284805	1.213989	-1.196015
9	6	0	-2.828286	1.018356	-2.505598
10	6	0	-3.473939	1.655113	-3.568248
11	6	0	-4.561965	2.495328	-3.329664
12	6	0	-5.010038	2.699981	-2.022239
13	6	0	-4.375848	2.059910	-0.956824
14	46	0	-0.000700	0.181638	-0.036160
15	8	0	-0.168800	2.249836	-0.361633
16	6	0	-0.002408	2.791245	-1.570094
17	6	0	-0.347492	4.267462	-1.586226
18	6	0	0.049339	-1.812546	0.361763
19	6	0	-0.116657	-2.810092	-0.616098
20	6	0	-0.103371	-4.183342	-0.335972
21	6	0	0.092158	-4.609119	0.970156
22	6	0	0.260509	-3.653631	1.978166
23	6	0	0.233981	-2.291640	1.673374
24	7	0	-0.327085	-2.450100	-2.027350
25	8	0	-0.206839	-1.264376	-2.363321
26	15	0	2.467296	0.203752	0.074503
27	6	0	-3.431771	-1.309250	0.329934
28	6	0	-3.259093	-2.143053	1.445246
29	6	0	-3.945916	-3.353270	1.535473
30	6	0	-4.805390	-3.751750	0.508815
31	6	0	-4.975657	-2.930843	-0.605547
32	6	0	-4.295748	-1.713473	-0.694994
33	6	0	0.424541	2.159807	-2.687513
34	8	0	-0.614356	-3.344659	-2.823149
35	1	0	-4.633268	0.067669	2.282107
36	1	0	-5.167825	1.398798	4.294059
37	1	0	-3.750526	3.345765	4.916857
38	1	0	-1.803309	3.959870	3.495822
39	1	0	-1.272363	2.628406	1.459257
40	1	0	-4.729201	2.221826	0.056779
41	1	0	-5.853653	3.357656	-1.829623
42	1	0	-5.057059	2.994538	-4.158587
43	1	0	-3.111578	1.502025	-4.580863
44	1	0	-1.971267	0.381759	-2.695928
45	1	0	-4.440606	-1.082842	-1.565529
46	1	0	-5.640523	-3.232382	-1.410450
47	1	0	-5.336005	-4.697632	0.577210
48	1	0	-3.802795	-3.987721	2.406027
49	1	0	-2.585107	-1.852232	2.244444
50	1	0	-0.242943	-4.885786	-1.148361
51	1	0	0.112194	-5.670281	1.200799
52	1	0	0.413170	-3.970399	3.007589

53	1	0	0.368940	-1.579837	2.480925
54	1	0	-0.214159	4.707426	-2.578977
55	1	0	-1.389174	4.411943	-1.273185
56	1	0	0.280930	4.818417	-0.873681
57	1	0	0.526261	2.702496	-3.621459
58	1	0	0.631150	1.094630	-2.701755
59	6	0	3.424436	1.794014	-0.249689
60	6	0	3.121950	-0.204555	1.793999
61	6	0	3.209612	-1.054746	-1.096109
62	6	0	4.393778	-0.751115	2.006036
63	6	0	4.870499	-0.940233	3.304674
64	6	0	4.089332	-0.570062	4.401301
65	6	0	2.828084	-0.008643	4.195309
66	6	0	2.345472	0.171084	2.897374
67	1	0	5.016828	-1.030173	1.161954
68	1	0	5.856661	-1.370703	3.457606
69	1	0	4.464195	-0.714557	5.411021
70	1	0	2.216430	0.288646	5.042993
71	1	0	1.361999	0.606728	2.738021
72	6	0	2.826402	3.012887	0.089948
73	6	0	3.554290	4.199036	-0.025587
74	6	0	4.872387	4.177131	-0.483567
75	6	0	5.467679	2.961157	-0.824849
76	6	0	4.749551	1.770369	-0.702632
77	1	0	1.787872	3.026451	0.404528
78	1	0	3.082642	5.143379	0.233276
79	1	0	5.433856	5.103104	-0.576885
80	1	0	6.493520	2.935539	-1.183245
81	1	0	5.223506	0.830513	-0.967900
82	6	0	3.440209	-2.378823	-0.700105
83	6	0	3.894909	-3.319691	-1.626947
84	6	0	4.111384	-2.951357	-2.955368
85	6	0	3.862364	-1.637743	-3.358342
86	6	0	3.408491	-0.693753	-2.436923
87	1	0	3.258478	-2.683426	0.325566
88	1	0	4.073077	-4.342871	-1.307175
89	1	0	4.462149	-3.685757	-3.675261
90	1	0	4.012914	-1.345677	-4.393941
91	1	0	3.199791	0.320803	-2.763624
