Supporting Information

For

Synthesis of Cyclohepta[b]indoles Via Gold Mediated Energy Transfer Photocatalysis

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1.General information

Unless otherwise noted all reactions were performed in anhydrous/dried over molecular sieves and degassed solvents. All organic reagents were purchased and used as received without further purification unless otherwise stated. ^{1}H, ^{13}C and ^{19}F nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance 300, 400 or 500 MHz spectrometers at 298 K. Chemical shifts (ppm) in ^{1}H and ^{13}C are referenced to the residual solvent peak ($CDCl_3$: δH = 7.26 ppm, δC = 77.16 ppm). Coupling constants (J) are given in hertz. Abbreviations used in the designation of the signals: s = singlet, br s = broad singlet, d = doublet, br d = broad doublet, dd = doublet of doublets, dt = doublet of triplets, ddt = doublet of doublet of triplets, m = multiplet, q = quadruplet, br q = broad quadruplet, dq = doublet of quadruplets.

Both [Au(SIPr)(Cbz)] and [Au(IPr)(Cbz)] were synthesized according to previously reported procedures.[1] Photocatalytic experiments were performed in EvoluChemTM PhotoRedOx Box by HepatoChem, equipped with an EvoluChemTM LED. 365PF (365 nm, 30 W, 9 mW/cm²) lamps were used.

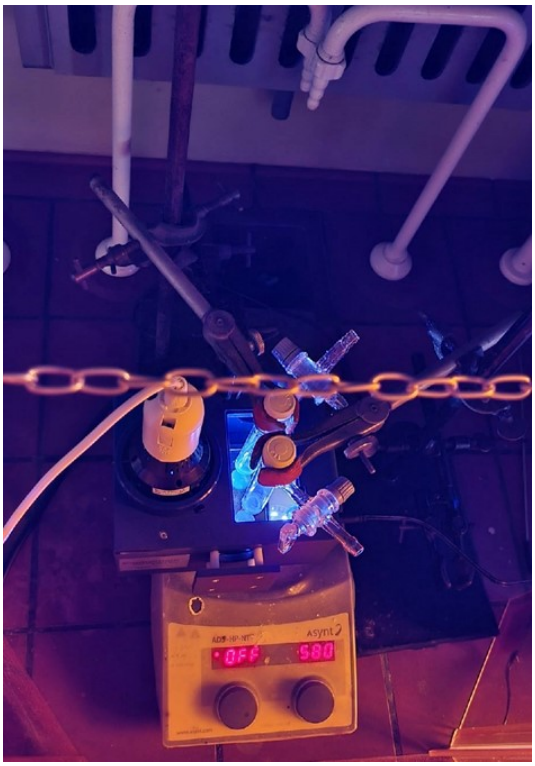


Figure S1. The photocatalytic setup in Nolan group

2.Photophysical properties of gold complexes

The absorption, excitation and emission spectra were previously reported.[1]

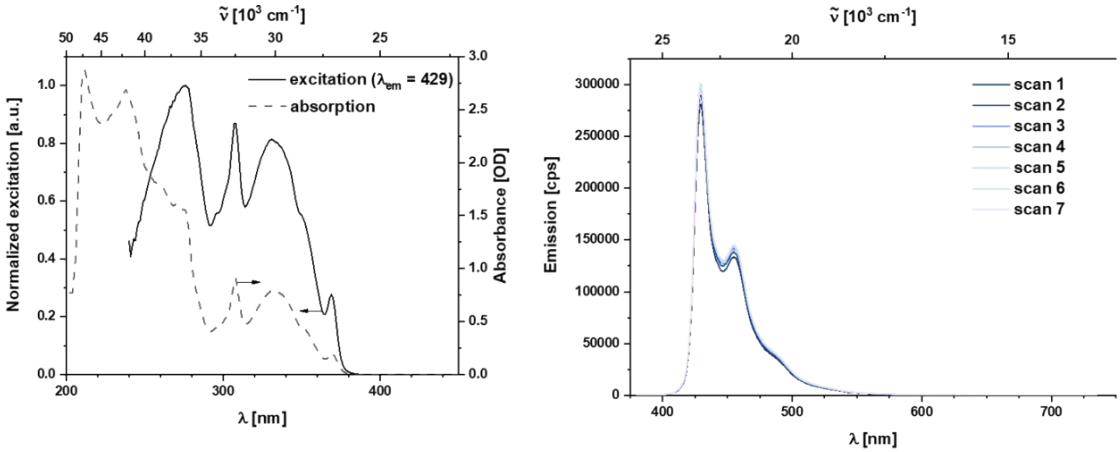


Figure S2. PL spectra of [Au(SIPr)Cbz] (PhotAu I)

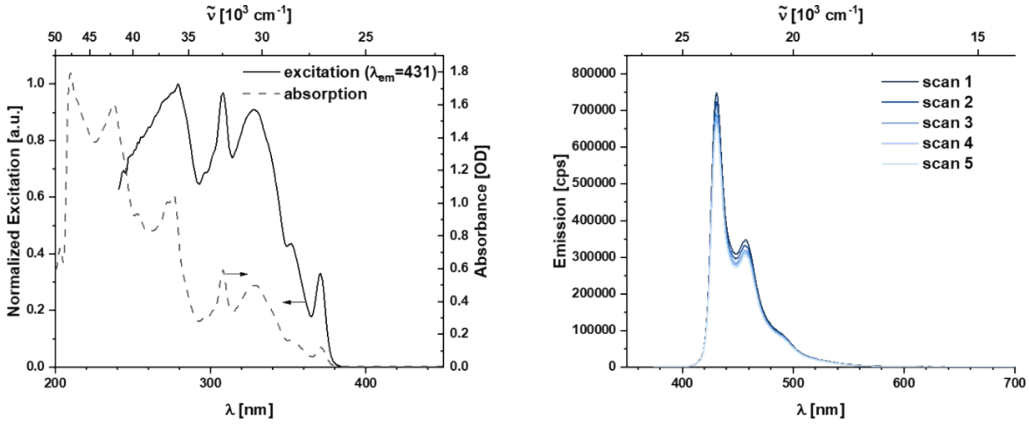
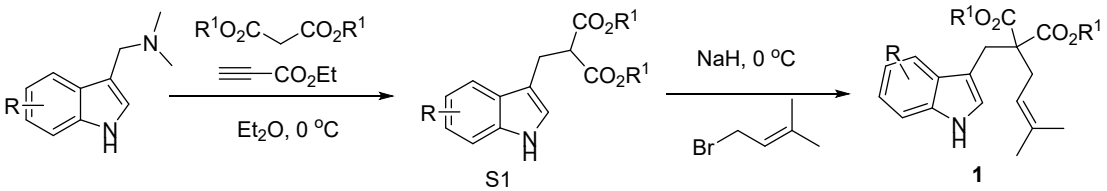


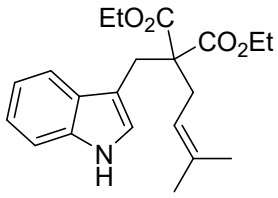
Figure S3. PL spectra of [Au(IPr)(Cbz)] (PhotAu II)

3. General procedures for the preparation of indoles 12, 3 (GP 1)



In a round bottom flask, the gramine (1.0 equiv.) was suspended into reagent grade Et_2O (0.5 mL/mmol). After the addition of dialkyl malonate (1.1 equiv.), the mixture was cooled to 0°C in ice bath. Ethylpropriolate (1.1 equiv.) was added at once, the reaction mixture was allowed to stir for 10 minutes before removing the ice bath. The reaction mixture was left stirring for 16-20 hours at room temperature. After the reaction was complete (monitored by TLC), it was quenched with water (1mL/mmol). The aqueous layer was extracted with EtOAc (3x). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Then the residue was purified by silica gel column chromatography (PE/EtOAc) to afford the desired product S1. To a solution of S1 (1.0 equiv.) in THF (0.5 mL/mmol) NaH (60% in oil) (1.2 equiv.) was added, the reaction mixture was allowed to stir for 30 minutes at ambient temperature. After it was cooled down to 0°C in ice bath followed by the dropwise addition of alkenyl bromide (1.2 equiv.). Then the reaction was allowed to stir at ambient temperature for 16-20 hours. After the reaction was complete (monitored by TLC), it was quenched with water (20 mL). The aqueous layer was extracted with EtOAc (3x). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Then the residue was purified by silica gel column chromatography (PE/EtOAc) to afford the desired products **1**.

Diethyl 2-((1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (**1a**)



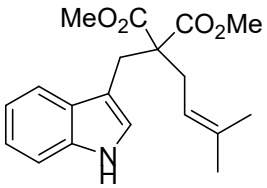
1a was prepared according to GP 1 as a yellow oil. Eluent: PE/EtOAc= 10/1; R_f = 0.2. Yield: 70%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.16 (br s, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 – 7.05 (m, 2H), 6.95 (d, *J* = 2.4 Hz, 1H), 5.26 – 5.12 (m, 1H), 4.12 (qq, *J* = 10.8, 7.1 Hz, 4H), 3.43 (s, 2H), 2.64 (d, *J* = 7.1 Hz, 2H), 1.73 (s, 3H), 1.53 (s,

3H), 1.20 (t, *J* = 7.1 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.8, 135.4, 123.1, 121.8, 119.2, 118.9, 118.1, 111.0, 110.2, 61.2, 58.7, 31.2, 27.2, 26.1, 18.1, 14.0 ppm.

HRMS (ESI): calculated for $C_{21}H_{28}NO_4^+[M+H]^+$: 358.2012, found 358.2004.

Dimethyl 2-((1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1b)

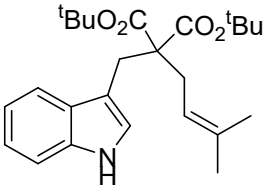


1b was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 6/1; R_f = 0.2. Yield: 72%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.10 (br s, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.12 (dtd, *J* = 16.0, 7.1, 1.0 Hz, 2H), 6.94 (d, *J* = 2.4 Hz, 1H), 5.26 – 5.09 (m, 1H), 3.66 (s, 6H), 3.43 (s, 2H), 2.64 (d, *J* = 7.1 Hz, 2H), 1.74 (s, 3H), 1.54 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.1, 135.7, 128.1, 123.2, 121.9 , 119.4 , 118.8, 118.0, 111.1, 110.1, 58.9, 52.4, 31.3, 27.9, 26.1, 18.0 ppm.

HRMS (ESI): calculated for $C_{19}H_{24}NO_4^+[M+H]^+$: 330.1700, found: 330.1693.

Di-tert-butyl 2-((1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1c)

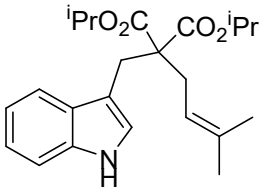


1c was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 51%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.11 (br s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.18 – 6.97 (m, 3H), 5.23 – 5.13 (m, 1H), 3.35 (s, 2H), 2.58 (d, *J* = 6.9 Hz, 2H), 1.71 (s, 3H), 1.46 (s, 3H), 1.41 (s, 18H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.1, 135.6 , 134.7, 128.6, 122.7, 121.8, 119.2, 118.6, 110.8, 81.2,59.3, 31.1, 27.9, 27.0, 26.1, 18.1 ppm.

HRMS (ESI): calculated for $C_{25}H_{36}NO_4^+[M+H]^+$: 414.2639, found：414.2632.

Diisopropyl 2-((1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1d)

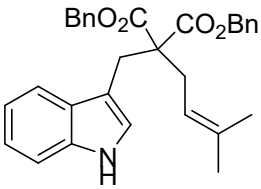


1d was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 10/1; R_f = 0.3. Yield: 71%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (brs, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.19 – 7.03 (m, 2H), 6.97 (d, *J* = 2.3 Hz, 1H), 5.25 – 5.13 (m, 1H), 5.09 – 4.91 (m, 2H), 3.41 (s, 2H), 2.62 (d, *J* = 7.0 Hz, 2H), 1.71 (d, *J* = 0.9 Hz, 3H), 1.48 (s, 3H), 1.17 (dd, *J* = 6.3, 3.4 Hz, 12H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.4, 135.7, 135.1, 128.5, 122.9, 121.8, 119.2, 119.0, 118.3, 110.9, 110.5, 68.7, 58.6, 34.2, 31.3, 27.6, 26.1, 22.4, 21.6, 18.1, 14.1 ppm.

HRMS (ESI): calculated for $C_{23}H_{32}NO_4^+[M+H]^+$: 386.2326, found: 386.2317.

Dibenzyl 2-((1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1e)



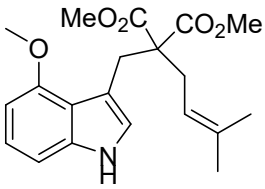
1e was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 6/1; R_f = 0.4. Yield: 46%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94 (s, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.36 – 6.97 (m, 13H), 6.74 (d, *J* = 2.1 Hz, 1H), 5.20 – 4.91 (m, 5H), 3.43 (s, 2H), 2.64 (d, *J* = 7.0 Hz, 2H), 1.65 (s, 3H), 1.41 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.4, 135.7, 135.5, 128.5, 128.3, 123.3, 121.9, 119.4, 118.9, 117.9, 111.0, 110.0, 67.0, 59.0, 31.3, 27.9, 26.1, 18.0 ppm.

HRMS (ESI): calculated for $C_{31}H_{32}NO_4^+[M+H]^+$: 482.2326, found: 482.2315.

Dimethyl 2-((4-methoxy-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-

yl)malonate (1f)

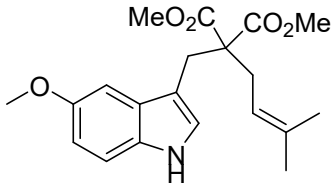


1f was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 10/1; R_f = 0.3. Yield: 42%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.03 (br s, 1H), 7.05 (t, *J* = 8.0 Hz, 1H), 6.99 – 6.89 (m, 1H), 6.81 (d, *J* = 2.3 Hz, 1H), 6.46 (d, *J* = 7.7 Hz, 1H), 5.30 – 5.13 (m, 1H), 3.90 (s, 3H), 3.65 (d, *J* = 15.0 Hz, 8H), 2.63 (d, *J* = 7.4 Hz, 2H), 1.69 (s, 3H), 1.55 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.3, 154.7, 137.3, 134.5, 122.6, 121. 8, 118.9, 118.1, 110.8, 104.4, 99.3, 59.8, 54.8, 52.1, 31.5, 29.3, 26.1, 17.7 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_5^+[M+H]^+$: 360.1805, found: 360.1798.

Dimethyl 2-((5-methoxy-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1yl)malonate (1g)

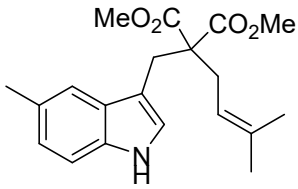


1g was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 10/1; R_f = 0.3. Yield: 60%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.99 (br s, 1H), 7.27 – 7.14 (m, 1H), 7.08 – 6.74 (m, 3H), 5.16 (ddd, *J* = 7.1, 4.3, 1.3 Hz, 1H), 3.84 (s, 3H), 3.66 (s, 6H), 3.39 (s, 2H), 2.64 (d, *J* = 7.1 Hz, 2H), 1.73 (s, 3H), 1.54 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.1, 154.0, 135.7, 130.9, 128.6, 123.8, 118.0, 112.4, 111.8, 109.9, 100.5, 58.8, 55.8, 52.4, 31.2, 27.9, 26.1, 18.0 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_5^+[M+H]^+$: 360.1805, found 360.1797.

Dimethyl 2-((5-methyl-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1h)

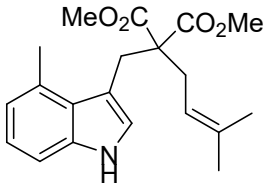


1h was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 6/1; R_f = 0.3. Yield: 25%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.96 (br s, 1H), 7.30 (s, 1H), 7.20 (d, *J* = 8.3 Hz, 1H), 6.90 (d, *J* = 2.4 Hz, 2H), 5.24 – 5.01 (m, 1H), 3.66 (s, 6H), 3.39 (s, 2H), 2.62 (d, *J* = 7.0 Hz, 2H), 2.43 (s, 3H), 1.74 (s, 3H), 1.52 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.1, 135.6, 134.1, 128.4, 123.5, 123.2, 118.6, 118.0, 110.7, 109.6, 58.8, 52.3, 31.2, 27.8, 26.1, 21.6, 18.0 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_4^+$[M+H]$^+$: 344.1856, found: 344.1849.

Dimethyl 2-((4-methyl-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1i)

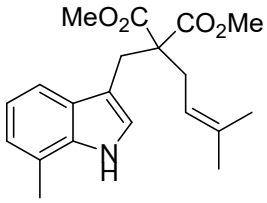


1i was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 51%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.17 (br s, 1H), 7.17 (d, *J* = 8.1 Hz, 1H), 7.08 – 6.95 (m, 2H), 6.83 (d, *J* = 7.1 Hz, 1H), 5.08 (t, *J* = 7.4 Hz, 1H), 3.69 (s, 2H), 3.64 (s, 6H), 2.79 (d, *J* = 7.4 Hz, 2H), 2.74 (s, 3H), 1.69 (s, 3H), 1.47 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.3, 136.1, 135.8, 130.8, 126.4, 122.2, 121.9, 121.6, 117.9, 111.2, 109.2, 58.9, 52.4, 31.8 29.4, 26.1, 20.8, 17.8 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_4^+$[M+H]$^+$: 344.1856, found: 344.1849.

Dimethyl 2-((7-methyl-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1j)

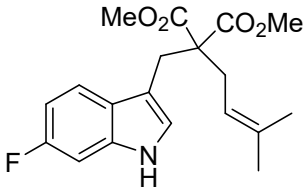


1j was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 25%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.04 (br s, 1H), 7.38 (d, *J* = 7.9 Hz, 1H), 7.05 – 6.92 (m, 3H), 5.25 – 5.10 (m, 1H), 3.66 (s, 6H), 3.42 (s, 2H), 2.65 (d, *J* = 7.1 Hz, 2H), 2.41 (s, 3H), 1.75 (d, *J* = 1.0 Hz, 3H), 1.56 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.7, 135.2, 133.7, 128.0, 123.1, 122.8, 118.2, 117.6, 110.3, 109.2, 58.4, 51.9, 30.8, 27.4, 25.7, 21.2, 17.6 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_4^+[M+H]^+$: 344.1856, found: 344.1850.

Dimethyl 2-((6-fluoro-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1k)

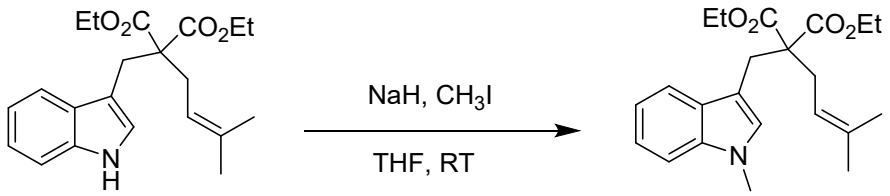


1k was prepared according to GP 1 as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 20%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.08 (br s, 1H), 7.42 (dd, *J* = 8.7, 5.3 Hz, 1H), 7.07 – 6.77 (m, 3H), 5.19 – 5.05 (m, 1H), 3.65 (s, 6H), 3.38 (s, 2H), 2.62 (d, *J* = 7.1 Hz, 2H), 1.73 (s, 3H), 1.52 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.0, 161.1, 158.7, 135.8, 135.7, 135.5, 124.7, 123.4, 117.8, 110.3, 108.3, 97.4, 97.2, 58.8, 52.4, 31.30, 27.8, 26.1, 18.0; **^{19}F NMR** (471 MHz, $CDCl_3$) δ = -121.5 ppm.

HRMS (ESI): calculated for $C_{19}H_{23}FNO_4^+[M+H]^+$: 348.1606, found: 348.1599.

Dimethyl 2-((1-methyl-1H-indol-3-yl)methyl)-2-(3-methylbut-2-en-1-yl)malonate (1l)



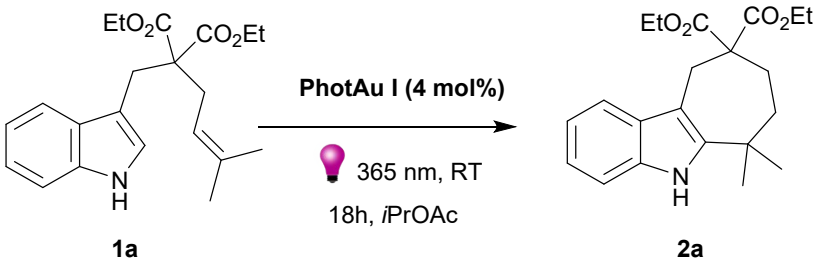
The reported procedure was followed with some modifications.[4] To a solution of **1a** (1.5 mmol, 1.0 equiv.) in THF (0.5 mL/mmol) NaH (60% in oil) (2 equiv.) was added, the reaction mixure was allowed to stir for 30 minutes at ambient temperature. After it was cooled down to 0°C in ice bath followed by the dropwise addition of methyl iodide (2 equiv.). Then the reaction was allowed to stir at ambient temperature for 16-20 hours. After the reaction was complete (monitored by TLC), it was quenched with water (20 mL). The aqueous layer was extracted with EtOAc (3x). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Then the residue was purified by silica gel column chromatography (PE/EtOAc= 15/1; R_f = 0.4) gave **1l** as a white solid (340 mg, 70% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.57 – 7.49 (m, 1H), 7.26 – 7.13 (m, 2H), 7.06 (ddd, *J* = 8.0, 6.9, 1.2 Hz, 1H), 6.80 (s, 1H), 5.24 – 5.13 (m, 1H), 4.26 – 4.03 (m, 4H), 3.73 (s, 3H), 3.40 (s, 2H), 2.62 (d, *J* = 7.1 Hz, 2H), 1.73 (d, *J* = 1.1 Hz, 3H), 1.53 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.7, 136.5, 135.3, 128.8, 127.9, 121.4, 119.0, 118.7, 118.2, 109.0, 108.6, 61.1, 58.7, 32.7, 31.05 (s), 27.5, 26.1, 18.1, 14.0 ppm.

HRMS (ESI): calculated for $C_{22}H_{30}NO_4^+$ $[M+H]^+$: 372.2169, found: 372.2161.

4. Optimization of Catalytic Reaction Conditions

Table S1 Optimization of reaction conditions.[a]

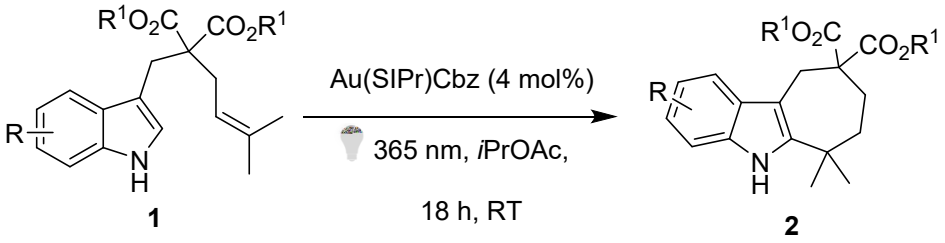


1a **2a**

Entry	Deviations from standard conditions	NMR yield(%)[b]
1	**PhotAuCat III** instead of **PhotAuCat I**, EtOAc	64[c]
2	EtOAc	74
3	None	84
4	Et_2O	75
5	MTBE	73
6	2-MeTHF	78
7	MeCN	15
8	MeOH	53
9	Acetone	57
10	THF	8
11	**PhotAuCat II** instead of **PhotAuCat I**	61
12[d]	**PC I** instead of **PhotAuCat I**	NR
13[d]	**PC II** instead of **PhotAuCat I**	NR
14	2 mol% **PhotAuCat I**	37
15	Without **PhotAuCat I**	NR
16	Without LED	NR

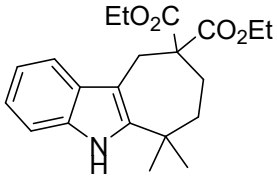
[a] Unless otherwise noted, the reaction was conducted with **1a** (0.10 mmol) and catalyst (0.004 mmol, 4 mol%) in solvent (2 mL) using 365 nm LEDs. [b] NMR yields were determined using 1,3,5-trimethoxybenzene as internal standard. [c] Previously reported value.[27] [d] Using 405 nm LEDs.

5.General procedures for the photocatalytic cycloaddition of indoles



Indole **1** (0.1 mmol) and 4 mol% of [Au(SIPr)(Cbz)] were weighted and transferred into 4 mL vial, *i*PrOAc (2 mL) was added in reaction mixtures, the reaction mixture was then degassed by sparging with N_2 or Ar for 3 min. The reaction mixtures were stirred at room temperature and irradiated at 365 nm for 18 hours (Parallel set up three reactions), after that, the solvent was removed under reduced pressure and the crude product was purified *via* column chromatography on silica gel to give the corresponding product **2**.

Diethyl 6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H) dicarboxylate (2a)



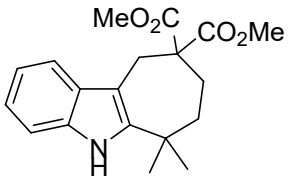
2a was prepared according to GP 2 from **1a** as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 78%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 (br s, 1H), 7.54 (dd, *J* = 6.2, 2.9 Hz, 1H), 7.24 (dt, *J* = 4.8, 2.3 Hz, 1H), 7.16 – 6.99 (m, 2H), 4.19 – 3.97 (m, 4H), 3.47 (s, 2H), 2.40 (dd, *J* = 7.2, 4.5 Hz, 2H), 1.93 (dd, *J* = 7.3, 3.6 Hz, 2H), 1.39 (s, 6H), 1.14 (t, *J* = 7.1 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.9, 142.5, 134.1, 129.2, 120.9, 119.2, 118.0, 110.3, 106.0, 61.2, 56.7, 36.8, 35.5, 30.6, 28.0, 14.0 ppm.

HRMS (ESI): calculated for $C_{21}H_{28}NO_4^+[M+H]^+$: 358.2013, found: 358.2000.

Dimethyl 6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-

dicarboxylate (2b)

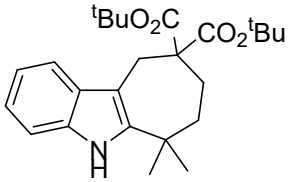


2b was prepared according to GP 2 from **1b** as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 80%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.90 (br s, 1H), 7.53 (dd, *J* = 5.6, 3.3 Hz, 1H), 7.30 – 7.19 (m, 1H), 7.15 – 7.03 (m, 2H), 3.61 (s, 6H), 3.47 (s, 2H), 2.46 – 2.34 (m, 2H), 1.99 – 1.84 (m, 2H), 1.38 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.4, 142.5, 134.2, 129.1, 120.9, 119.4, 117.8, 110.3, 105.8, 56.8, 52.5, 36.8, 35.5, 30.6, 28.1 ppm.

HRMS (ESI): calculated for $C_{19}H_{23}NO_4^+$[M+H]$^+$: 331.1733, found 331.1730.

Di-tert-butyl 6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H) dicarboxylate (2c)

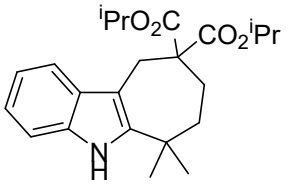


2c was prepared according to GP 2 from **1c** as a white solid. Eluent: PE/EtOAc= 10/1; R_f = 0.2. Yield: 95%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.86 (br s, 1H), 7.54 (dd, *J* = 6.2, 2.7 Hz, 1H), 7.29 – 7.21 (m, 1H), 7.12 – 7.02 (m, 2H), 3.39 (s, 2H), 2.38 – 2.28 (m, 2H), 1.95 (s, 2H), 1.39 (s, 6H), 1.31 (s, 18H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 171.2, 142.5, 134.1, 129.3, 120.8, 119.0, 118.2, 110.2, 106.1, 81.0, 57.6, 36.7, 35.5, 30.6, 27.7 ppm.

HRMS (ESI): calculated for $C_{25}H_{36}NO_4^+$[M+H]$^+$: 414.2639, found 414.2639.

Diisopropyl 6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2d)

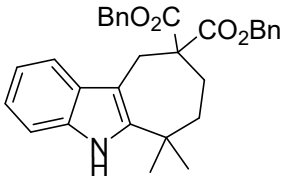


2d was prepared according to GP 2 from **1d** as a white solid. Eluent: PE/EtOAc = 8/1; R_f = 0.33. Yield: 85%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.86 (br s, 1H), 7.64 – 7.46 (m, 1H), 7.26 – 7.22 (m, 1H), 7.17 – 6.95 (m, 2H), 4.92 (dt, *J* = 12.5, 6.3 Hz, 2H), 3.43 (s, 2H), 2.38 (dd, *J* = 6.7, 5.0 Hz, 2H), 1.99 – 1.86 (m, 2H), 1.39 (s, 6H), 1.19 (d, *J* = 6.3 Hz, 6H), 1.02 (d, *J* = 6.3 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.4, 142.5, 134.1, 129.3, 120.8, 119.1, 118.3, 110.2, 106.1, 68.6, 56.6, 36.8, 35.5, 30.7, 28.0, 21.5 ppm.

HRMS (ESI): calculated for $C_{23}H_{32}NO_4^+$[M+H]$^+$: 386.2326, found: 386.2317.

Dibenzyl 6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2e)

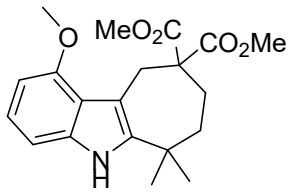


2e was prepared according to GP 2 from **1e** as a white solid. Eluent: PE/EtOAc= 10/1; R_f = 0.2. Yield: 60%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.88 (br s, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.37 –7.24 (m, 8H), 7.23 – 6.99 (m, 6H), 5.05 (d, *J* = 12.3 Hz, 2H), 4.93 (d, *J* = 12.3 Hz, 2H), 3.51 (s, 2H), 2.44 (dd, *J* = 7.0, 4.3 Hz, 2H), 2.02 – 1.85 (m, 2H), 1.38 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.6, 142.5, 135.5, 134.1, 129.1, 128.5, 128.2, 121.0, 119.4, 118.1, 110.3, 105.8, 67.0, 57.0, 36.7, 35.5 30.7, 28.1, 22.4, 14.1 ppm.

HRMS (ESI): calculated for $C_{31}H_{32}NO_4^+$[M+H]$^+$: 482.2326, found: 482.2327.

Dimethyl 1-methoxy-6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole 9,9(5H)-dicarboxylate (2f)

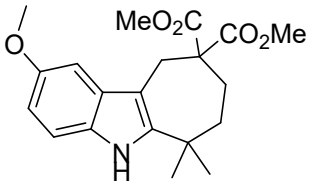


2f was prepared according to GP 2 from **1f** as a white solid. Eluent: PE/EtOAc= 10/1; R_f = 0.35. Yield: 80%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84 (br s, 1H), 7.08 – 6.77 (m, 2H), 6.45 (d, *J* = 7.9 Hz, 1H), 3.99 – 3.81 (m, 4H), 3.61 (s, 6H), 2.43 – 2.28 (m, 2H), 1.95 – 1.79 (m, 2H), 1.37 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.3, 154.1, 143.5, 129.6, 129.2, 111.1, 105.8, 99.8, 56.7, 52.5, 36.9, 35.5, 30.7, 28.4, 27.9 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_5^+[M+H]^+$: 360.1805, found: 360.1797.

Dimethyl 2-methoxy-6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2g)

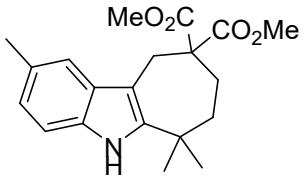


2g was prepared according to GP 2 from **1g** as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 81%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.76 (br s, 1H), 7.13 (d, *J* = 8.7 Hz, 1H), 6.99 (d, *J* = 2.4 Hz, 1H), 6.74 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.85 (d, *J* = 6.0 Hz, 3H), 3.64 (d, *J* = 16.4 Hz, 6H), 3.43 (s, 2H), 2.40 (dd, *J* = 7.1, 4.5 Hz, 2H), 1.90 (dd, *J* = 7.4, 3.8 Hz, 2H), 1.38 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.2, 154.2, 143.50, 129.5, 129.2, 111.0, 105.8, 99.7, 56.7, 56.0, 52.5, 36.8, 35.5, 30.7, 28.4, 27.9 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_5^+[M+H]^+$: 360.1805, found: 360.1798.

Dimethyl 2,6,6-trimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2h)

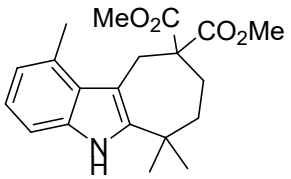


2h was prepared according to GP 2 from **1h** as a white solid. Eluent: PE/EtOAc= 6/1; R_f = 0.3. Yield: 80%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (br s, 1H), 7.30 (d, *J* = 28.2 Hz, 1H), 7.14 (d, *J* = 8.2 Hz, 1H), 6.91 (dd, *J* = 8.2, 1.2 Hz, 1H), 3.62 (s, 6H), 3.44 (s, 2H), 2.44 (s, 3H), 2.44 – 2.37 (m, 4H), 1.97 – 1.82 (m, 2H), 1.38 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.3, 142.6, 132.5, 129.4, 128.5, 122.4, 117.6, 109.9, 105.4, 56.8, 52.5, 36.9, 35.5, 30.6, 28.1, 21.6 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_4^+[M+H]^+$: 344.1856, found 344.1857.

Dimethyl 1,6,6-trimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2i)

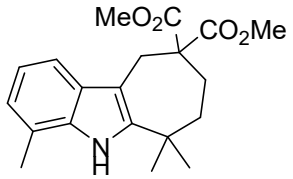


2i was prepared according to GP 2 from **1i** as a white solid. Eluent: PE/EtOAc= 6/1; R_f = 0.3. Yield: 78%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (br s, 1H), 7.33 (s, 1H), 7.14 (d, *J* = 8.2 Hz, 1H), 6.92 (d, *J* = 1.2 Hz, 1H), 3.62 (s, 6H), 3.44 (s, 2H), 2.44 (s, 3H), 2.43 – 2.36 (m, 2H), 1.98 – 1.84 (m, 2H), 1.38 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 172.3, 142.6, 132.5, 129.4, 128.5, 122.4, 117.6, 109.9, 105.4, 56.8, 52.5, 36.9, 35.5, 30.6, 28.1, 21.6 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_4^+[M+H]^+$: 344.1856, found: 344.1849.

Dimethyl 4,6,6-trimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2j)

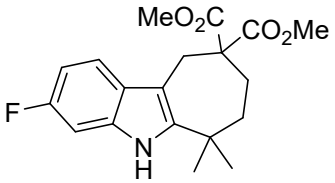


2j was prepared according to GP 2 from **1j** as a white solid. Eluent: PE/EtOAc= 6/1; R_f = 0.3. Yield: 62%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.70 (br s, 1H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.00 (d, *J* = 7.7 Hz, 1H), 6.90 (d, *J* = 7.1 Hz, 1H), 3.62 (s, 6H), 3.47 (s, 2H), 2.46 (s, 3H), 2.41 (dd, *J* = 7.0, 4.5 Hz, 2H), 1.92 (dd, *J* = 7.5, 3.7 Hz, 2H), 1.42 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 172.4, 142.1, 133.6, 128.7, 121.6, 119.5, 115.6, 106.4, 56.8, 52.5, 36.9, 35.6, 30.6, 28.2, 16.6 ppm.

HRMS (ESI): calculated for $C_{20}H_{26}NO_4^+[M+H]^+$: 344.1856, found: 344.1848.

Dimethyl 3-fluoro-6,6-dimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2k)

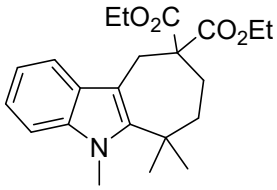


2k was prepared according to GP 2 from **1k** as a white solid. Eluent: PE/EtOAc= 8/1; R_f = 0.3. Yield: 33%.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.86 (s, 1H), 7.42 (dd, *J* = 8.7, 5.3 Hz, 1H), 7.03 – 6.76 (m, 2H), 3.62 (d, *J* = 3.7 Hz, 6H), 3.42 (s, 2H), 2.39 (dd, *J* = 6.7, 4.9 Hz, 2H), 1.89 (dd, *J* = 7.5, 3.8 Hz, 2H), 1.38 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 172.2, 160.5, 158.2, 142.7, 133.9, 125.7, 118.5, 108.0, 107.8, 105.9, 96.9, 96.7, 56.7, 52.5, 36.8, 35.5, 30.5, 28.1; **^{19}F NMR** (471 MHz, $CDCl_3$) δ = -122.8 ppm.

HRMS (ESI): calculated for $C_{19}H_{23}FNO_4^+[M+H]^+$: 348.1606, found 348.1603.

Diethyl 5,6,6-trimethyl-6,7,8,10-tetrahydrocyclohepta[b]indole-9,9(5H)-dicarboxylate (2l)



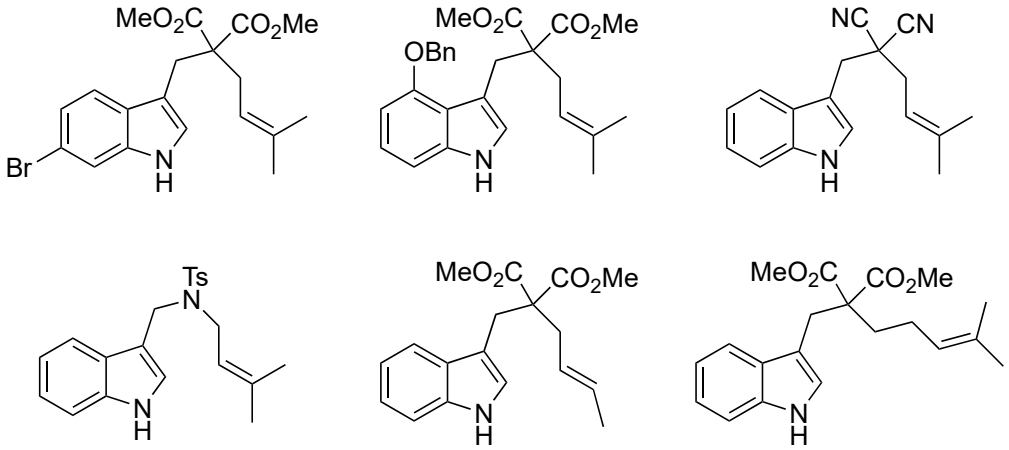
2l was prepared according to GP 2 from **1l** as a white solid. Eluent: PE/EtOAc= 15/1; R_f = 0.5. Yield: 75%.

^{1}H NMR (300 MHz, $CDCl_3$)) δ = 7.56 (d, *J* = 7.6 Hz, 1H), 7.24 – 7.01 (m, 3H), 4.07 (s, 4H), 3.80 (s, 3H), 3.51 (s, 2H), 2.33 (s, 2H), 1.55 (s, 3H), 1.49 (s, 6H), 1.20 (s, 6H)；

^{13}C NMR (126 MHz, $CDCl_3$) δ = 141.9, 137.3, 128.1, 127.8, 120.6, 118.6, 117.8, 107.9, 105.5, 60.8, 57.2, 39.4, 36.9, 32.3, 27.1, 26.0, 13.6 ppm.

HRMS (ESI): calculated for $C_{22}H_{30}NO_4^+[M+H]^+$: 372.2169, found: 372.2160.

Incompatible Substrates



6. Reaction with TEMPO

Indole **1** (0.1 mmol), 4 mol% of [Au(SIPr)(Cbz)] and (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) (1 equiv.) were weighted and transferred into 4 mL vial, *i*PrOAc (2 mL) was added in reaction mixtures, the reaction mixture was then degassed by sparging with N_2 or Ar for 3 min. The reaction mixtures were stirred at room

temperature and irradiated at 365 nm for 18 hours. After that time, solvent was evaporated and ^{1}H NMR, HRMS of reaction mixture was recorded. No traces of product were observed.

7. Absorption spectroscopy studies

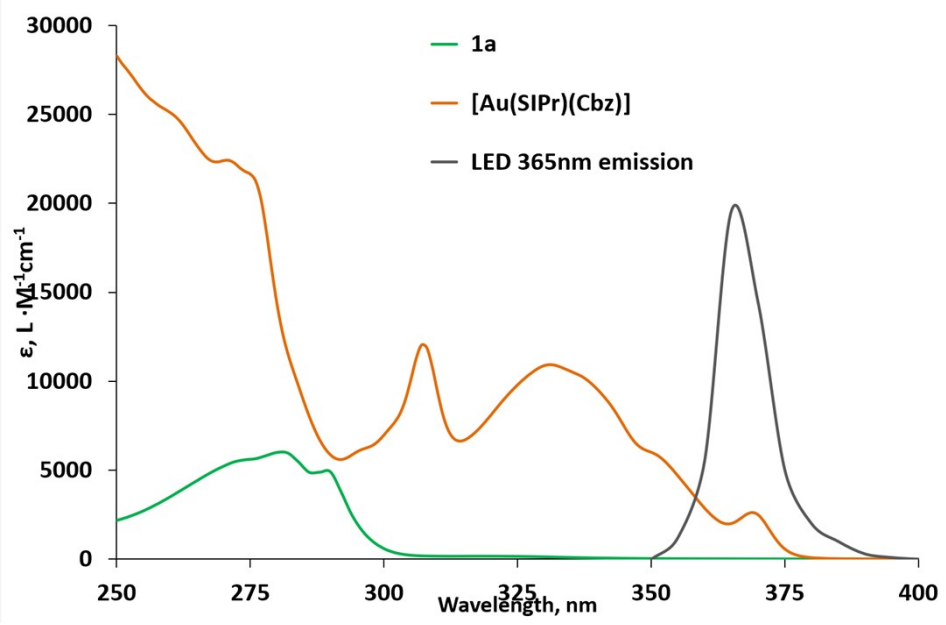


Figure S4. Absorption spectra of 1a and [Au(SIPr)(Cbz)]

8. DFT calculations

All the geometries were optimized with Gaussian 16 program package,[5] using long-range dispersion corrected hybrid density functional, ωB97X-D.[6] All atoms were treated with the Ahlrichs split-valance polarization basis function def2-SVP.[7] The geometries were optimized without any symmetry constraints. Harmonic force constants were computed at the optimized geometries to characterize the stationary points as minima or saddle points. All transition states were located using the linear synchronous transit (LST) method in which the reaction coordinate was kept fixed at different distances while all other degrees of freedom were relaxed.[8] After the linear transit search the transition states were optimized using the default Berny algorithm implemented in the Gaussian 16 codes.[5] For further validation of energetics, single-point calculations were performed on the optimized geometries employing a valence triple-ζ-type of basis set (def2-TZVPP) for all atoms.[9] The solvent effects (EtOAc: ε = 5.9867) were evaluated implicitly by a self-consistent reaction field (SCRF) approach for all the intermediates and transitions states, using the SMD continuum solvation model for geometry optimization and single point calculations.[10] Unless specified otherwise, the ΔG was used throughout the text. The ΔG value was obtained by augmenting the ΔE_e^S energy terms at ωB97X-D(SMD-EtOAc)/def2-TZVPP with the respective free energy corrections at the ωB97X-D/def2-SVP level of theory.

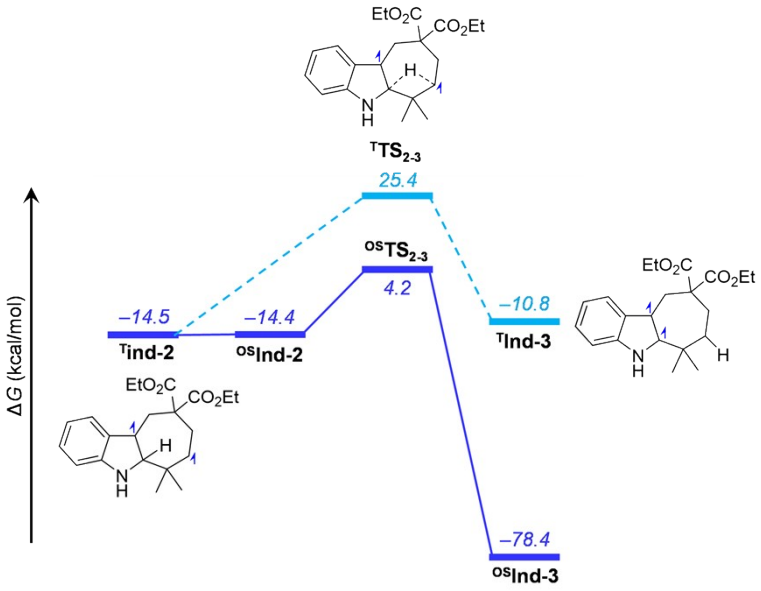


Figure S5. Open-shell singlet surface vs. triplet surface of H-atom transfer step. Energy values (in kcal/mol) are reported at ωB97X-D(SMD-EtOAc)/def2-TZVPP//ωB97X-D/def2-SVP level of theory.

Cartesian coordinates (Å) of the optimized structures of all intermediates and transition states at ωB97X-D/def2-SVP level of theory. E_e^S represents the absolute electronic energy in Hartree at ωB97X-D(SMD-EtOAc)/def2-TZVPP level of theory.

PC

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E_e^S: -1812.92651915

C	-0.353263	3.420167	0.667983
N	0.030100	4.704724	0.822379
N	-1.149480	3.419550	-0.423857
C	-0.523081	5.506722	-0.159479
C	-1.268622	4.692036	-0.949556
H	-0.332276	6.574357	-0.204206
H	-1.868541	4.897209	-1.830599
C	0.889685	5.138558	1.885632
C	2.273191	5.171730	1.649619
C	0.313480	5.444677	3.127962

C	3.094132	5.556582	2.712110
C	1.178913	5.825540	4.156946
C	2.552900	5.884091	3.951415
H	4.176831	5.585822	2.573763
H	0.770202	6.067398	5.140567
C	-1.776843	2.228051	-0.921903
C	-1.069910	1.436506	-1.840568
C	-3.031521	1.868052	-0.405246
C	-1.683953	0.260265	-2.277970
C	-3.602106	0.683097	-0.876505
C	-2.939241	-0.109633	-1.807123
H	-1.162160	-0.387862	-2.985367
H	-4.573277	0.364367	-0.491896
C	-1.181662	5.337665	3.382087
H	-1.663008	5.014318	2.447388
C	2.872342	4.731406	0.323102
H	2.055798	4.664521	-0.411583
C	-3.734145	2.684552	0.667206
H	-3.107031	3.560172	0.891680
C	0.335289	1.787591	-2.302096
H	0.601536	2.763564	-1.869622
Au	0.026651	1.822428	1.809628
C	-1.784800	6.695444	3.756230
H	-1.587156	7.450020	2.979793
H	-2.874960	6.610155	3.881417
H	-1.370333	7.072870	4.704197
C	-1.487247	4.267275	4.435939
H	-1.064400	3.292584	4.148884
H	-1.071636	4.538912	5.418720
H	-2.574613	4.145576	4.553916

C	3.478822	3.328455	0.453779
H	3.864270	2.981561	-0.517227
H	4.313568	3.325037	1.172076
H	2.731069	2.601994	0.805995
C	3.886940	5.738206	-0.225308
H	3.451187	6.745309	-0.307570
H	4.780488	5.808242	0.414028
H	4.226323	5.428994	-1.225411
C	0.417101	1.929883	-3.824888
H	-0.298398	2.678681	-4.197108
H	1.428262	2.242355	-4.127015
H	0.200579	0.977050	-4.332584
C	1.348140	0.767884	-1.767837
H	1.164736	-0.234621	-2.184593
H	2.372740	1.063968	-2.039714
H	1.292092	0.689561	-0.671492
C	-5.088575	3.208885	0.180392
H	-4.981056	3.808977	-0.735974
H	-5.784337	2.383808	-0.038552
H	-5.555704	3.840843	0.950990
C	-3.864952	1.881322	1.966631
H	-4.300270	2.506380	2.761112
H	-4.516694	1.003992	1.833908
H	-2.884750	1.519479	2.312255
H	3.212339	6.176763	4.771108
H	-3.397687	-1.037704	-2.154550
C	0.937149	-0.023757	4.098382
C	-0.321114	-1.070895	2.606848
C	1.682798	0.921822	4.820175
C	0.797425	-1.353912	4.578488

C	-1.117669	-1.406356	1.499325
C	-0.025013	-2.037636	3.604266
C	2.278326	0.523643	6.009180
H	1.788338	1.944969	4.447764
C	1.408122	-1.731672	5.779989
C	-1.605560	-2.702432	1.407175
H	-1.346918	-0.662926	0.730145
C	-0.527868	-3.338913	3.487957
C	2.145863	-0.792655	6.490738
H	2.863074	1.246974	6.583365
H	1.304826	-2.753369	6.154565
C	-1.316030	-3.666845	2.391171
H	-2.227116	-2.978830	0.551254
H	-0.303734	-4.087843	4.251952
H	2.627491	-1.074480	7.429682
H	-1.714712	-4.678642	2.289199
N	0.263103	0.140282	2.909264

^{T}PC

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E_e^S: -1812.80983918

C	-0.416301	3.431867	0.702158
N	-0.006145	4.708523	0.843607
N	-1.182796	3.426762	-0.409528
C	-0.509113	5.502445	-0.170304
C	-1.254842	4.690192	-0.963609
H	-0.290714	6.563982	-0.230855
H	-1.825484	4.891903	-1.864684
C	0.837688	5.138630	1.921438
C	2.228268	5.049070	1.754857

C	0.230204	5.559403	3.114641
C	3.026764	5.429944	2.836204
C	1.073966	5.928289	4.165221
C	2.456772	5.868009	4.026935
H	4.113795	5.367533	2.750730
H	0.641746	6.253068	5.114146
C	-1.814364	2.236560	-0.906875
C	-1.096986	1.424937	-1.799722
C	-3.083221	1.897984	-0.411176
C	-1.713912	0.248141	-2.231315
C	-3.655611	0.711123	-0.875476
C	-2.981605	-0.102648	-1.779577
H	-1.184439	-0.416252	-2.917492
H	-4.637656	0.407736	-0.506411
C	-1.279050	5.560481	3.299526
H	-1.740897	5.326438	2.328709
C	2.860117	4.507945	0.482188
H	2.056614	4.335348	-0.249324
C	-3.799384	2.738438	0.633542
H	-3.174146	3.617782	0.848988
C	0.319396	1.756730	-2.241076
H	0.588369	2.734556	-1.814365
Au	-0.028839	1.832205	1.839991
C	-1.803477	6.934400	3.727352
H	-1.504042	7.718377	3.015468
H	-2.902531	6.923488	3.782849
H	-1.427198	7.221313	4.721508
C	-1.704517	4.458320	4.277096
H	-1.352313	3.470917	3.942100
H	-1.293957	4.636741	5.283104

H	-2.801269	4.420349	4.361458
C	3.529481	3.153247	0.742358
H	3.927650	2.734334	-0.194279
H	4.366321	3.250047	1.451394
H	2.814909	2.430306	1.164216
C	3.831845	5.512660	-0.144205
H	3.339794	6.476652	-0.343456
H	4.694890	5.705153	0.511928
H	4.222705	5.124044	-1.096772
C	0.426156	1.883323	-3.763771
H	-0.276144	2.635202	-4.154473
H	1.444893	2.182835	-4.053150
H	0.208001	0.927527	-4.265074
C	1.314441	0.732962	-1.681687
H	1.127401	-0.272438	-2.089433
H	2.345454	1.016409	-1.942532
H	1.243151	0.666172	-0.585490
C	-5.146192	3.254612	0.117726
H	-5.025348	3.834035	-0.810146
H	-5.841373	2.426688	-0.091768
H	-5.621553	3.904423	0.868137
C	-3.949847	1.961676	1.946798
H	-4.397511	2.601496	2.722348
H	-4.598455	1.081031	1.821151
H	-2.974852	1.607374	2.314247
H	3.098550	6.153460	4.862965
H	-3.441432	-1.032287	-2.120706
C	1.010507	-0.054157	4.030870
C	-0.271287	-1.096913	2.558578
C	1.746242	0.962308	4.722752

C	0.967029	-1.394042	4.460132
C	-1.098089	-1.412562	1.477926
C	0.142350	-2.076314	3.517499
C	2.471807	0.543608	5.927025
H	1.760878	1.994320	4.366232
C	1.680637	-1.785055	5.636650
C	-1.526534	-2.730202	1.343176
H	-1.398224	-0.643137	0.759830
C	-0.306886	-3.403418	3.355755
C	2.431344	-0.748060	6.342752
H	3.045471	1.286307	6.484988
H	1.674212	-2.811111	6.003838
C	-1.128827	-3.708469	2.278791
H	-2.173820	-3.008664	0.508631
H	-0.012920	-4.178948	4.066446
H	2.981303	-1.034100	7.243941
H	-1.479267	-4.736123	2.150010
N	0.275049	0.125655	2.900142

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E_e^S: -1172.27773788

C	-0.519285	-1.648330	1.027872
C	-1.251309	-2.859592	1.034265
C	-1.800670	-3.315052	2.243365
C	-1.609948	-2.568171	3.395349
C	-0.875135	-1.364672	3.367368
C	-0.321928	-0.889088	2.188175
C	-0.533532	-2.469557	-1.056853
C	-1.238555	-3.379191	-0.310187

H	-2.363474	-4.250828	2.277539
H	-2.032302	-2.913741	4.341433
H	-0.739908	-0.797271	4.290707
H	0.248662	0.041858	2.166933
H	0.443943	-0.646048	-0.576735
N	-0.092969	-1.438462	-0.259263
C	-0.894734	-5.769544	-1.254673
C	0.006533	-6.357295	-0.137781
C	0.882703	-5.363144	0.565904
C	-1.868943	-4.665280	-0.762679
C	1.012094	-5.182874	1.887479
H	-0.651906	-6.877819	0.571024
H	-0.305586	-2.479061	-2.119655
H	-2.449360	-5.092663	0.066075
H	0.641920	-7.124326	-0.612080
H	1.479943	-4.728799	-0.095532
H	-2.587838	-4.464107	-1.570971
C	-1.700345	-6.945024	-1.817294
C	-0.040889	-5.279694	-2.426848
O	-1.456130	-7.512702	-2.849694
O	-2.689468	-7.303887	-0.998696
O	-0.787658	-4.642258	-3.332873
O	1.142798	-5.443738	-2.545563
C	-0.135050	-4.241151	-4.535150
H	0.290313	-5.133085	-5.020347
H	0.708318	-3.577612	-4.283448
C	-1.155970	-3.553450	-5.410923
H	-0.689003	-3.235383	-6.353969
H	-1.986119	-4.234241	-5.646781
H	-1.569443	-2.664667	-4.911986

C	-3.478029	-8.428889	-1.389649
H	-3.921818	-8.227228	-2.376850
H	-2.818862	-9.303395	-1.504555
C	-4.531713	-8.649765	-0.330242
H	-5.179641	-7.767012	-0.231742
H	-5.158936	-9.511154	-0.600552
H	-4.069512	-8.851601	0.646716
C	1.906229	-4.098940	2.426279
H	1.300624	-3.341979	2.954464
H	2.631768	-4.499306	3.154389
H	2.461608	-3.591549	1.625018
C	0.297015	-5.978921	2.945922
H	1.019194	-6.580377	3.523838
H	-0.198459	-5.302630	3.660508
H	-0.460724	-6.664225	2.544239

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E_e^S: -1172.17269900

C	-1.191111	-1.304759	0.883378
C	-1.746353	-2.607449	0.881448
C	-2.266268	-3.126899	2.078441
C	-2.208067	-2.357003	3.229195
C	-1.637401	-1.067957	3.212498
C	-1.123672	-0.524723	2.044255
C	-1.060094	-2.115684	-1.201512
C	-1.646171	-3.112641	-0.465563
H	-2.705587	-4.127255	2.103374
H	-2.605627	-2.752231	4.166277
H	-1.601006	-0.485831	4.135815

H	-0.686159	0.475852	2.030957
H	-0.340320	-0.180914	-0.704379
N	-0.785865	-1.032833	-0.399819
C	-1.089857	-5.567339	-1.120684
C	-0.407414	-5.997181	0.227726
C	0.907251	-5.389826	0.608281
C	-2.143090	-4.438280	-0.953774
C	1.128410	-4.007750	1.040280
H	-1.155991	-5.810990	1.018478
H	-0.817974	-2.103330	-2.261270
H	-2.901377	-4.815065	-0.253226
H	-0.265405	-7.087344	0.197488
H	1.770955	-6.069609	0.605905
H	-2.649320	-4.305508	-1.920544
C	-1.837160	-6.790682	-1.660702
C	-0.052050	-5.246042	-2.197104
O	-1.615054	-7.333139	-2.711645
O	-2.777435	-7.199184	-0.808055
O	-0.576392	-4.523292	-3.190920
O	1.090850	-5.614191	-2.186806
C	0.266480	-4.277831	-4.314000
H	0.618159	-5.242840	-4.709601
H	1.156703	-3.720190	-3.981276
C	-0.534757	-3.507925	-5.337770
H	0.081861	-3.310910	-6.226326
H	-1.419473	-4.081114	-5.649288
H	-0.874228	-2.542308	-4.934334
C	-3.534978	-8.350910	-1.181185
H	-4.032613	-8.154818	-2.143656
H	-2.845688	-9.194756	-1.340285

C	-4.527805	-8.632340	-0.078223
H	-5.209588	-7.781341	0.062505
H	-5.127665	-9.517951	-0.331885
H	-4.011822	-8.824407	0.873384
C	1.103318	-3.698267	2.507447
H	2.095359	-3.870178	2.974582
H	0.836957	-2.643327	2.688063
H	0.376538	-4.325089	3.045006
C	1.869022	-3.062664	0.144363
H	1.630766	-2.014140	0.386421
H	2.965983	-3.180537	0.264945
H	1.646212	-3.242176	-0.916789

^{T}TS$_{1\text{-}2}$

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E_e^S: -1172.15545101

C	-1.034089	-1.397811	1.150649
C	-1.907384	-2.503454	0.965700
C	-3.083018	-2.579514	1.734709
C	-3.349601	-1.579569	2.659776
C	-2.464937	-0.498846	2.834467
C	-1.297346	-0.394448	2.084801
C	-0.092204	-2.776493	-0.371324
C	-1.330372	-3.340835	-0.040308
H	-3.775088	-3.415261	1.606672
H	-4.258010	-1.629371	3.263925
H	-2.698942	0.272767	3.571118
H	-0.612452	0.445167	2.221818
H	0.836368	-0.967367	0.254623
N	0.015238	-1.552284	0.278523

C	-0.978106	-5.637447	-1.146736
C	-0.047094	-6.209462	-0.039386
C	1.213761	-5.486000	0.305911
C	-1.957172	-4.569852	-0.612583
C	1.413638	-4.065556	0.672062
H	-0.683683	-6.331432	0.859698
H	0.475734	-2.928961	-1.287653
H	-2.572890	-5.055286	0.158782
H	0.245231	-7.229585	-0.332292
H	2.051913	-6.145524	0.575565
H	-2.646701	-4.292874	-1.428002
C	-1.797616	-6.816257	-1.684060
C	-0.169929	-5.145048	-2.350257
O	-1.687354	-7.287920	-2.785284
O	-2.634420	-7.290608	-0.761867
O	-0.921442	-4.410033	-3.167377
O	0.991801	-5.381527	-2.549941
C	-0.311497	-3.955872	-4.373114
H	0.033865	-4.830366	-4.945837
H	0.580278	-3.359470	-4.121499
C	-1.334563	-3.146462	-5.134426
H	-0.898391	-2.777714	-6.073778
H	-2.213359	-3.760561	-5.377279
H	-1.667944	-2.281791	-4.542618
C	-3.422886	-8.425424	-1.124913
H	-4.021048	-8.173871	-2.014339
H	-2.750487	-9.249338	-1.410479
C	-4.290652	-8.787078	0.057187
H	-4.957161	-7.954389	0.323935
H	-4.910381	-9.661350	-0.187791

H	-3.675382	-9.033555	0.934321
C	1.159369	-3.757970	2.127308
H	1.866103	-4.313735	2.772731
H	1.284979	-2.686519	2.347390
H	0.139599	-4.047411	2.424624
C	2.663820	-3.460306	0.086317
H	2.733250	-2.379031	0.292682
H	3.565995	-3.925163	0.528386
H	2.716653	-3.627031	-1.000644

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E_e^S: -1172.20091316

C	-0.779106	-1.371739	0.969677
C	-1.727878	-2.364763	0.576134
C	-3.106300	-2.087661	0.697523
C	-3.507237	-0.839837	1.165665
C	-2.559818	0.130807	1.520210
C	-1.183730	-0.125440	1.428233
C	0.458124	-3.186502	0.168324
C	-1.022236	-3.488817	0.108696
H	-3.846819	-2.839186	0.414861
H	-4.571198	-0.610906	1.255126
H	-2.897087	1.105072	1.880781
H	-0.452505	0.631539	1.719248
H	1.277635	-1.272349	0.691376
N	0.487746	-1.886686	0.828164
C	-0.842651	-5.725297	-1.178994
C	0.348783	-6.367259	-0.402078
C	1.464210	-5.443090	-0.051677

C	-1.673485	-4.768250	-0.300337
C	1.342631	-4.266015	0.880760
H	-0.087785	-6.829066	0.499678
H	0.869689	-3.091871	-0.861819
H	-1.987482	-5.338367	0.592372
H	0.753085	-7.181855	-1.020587
H	2.344926	-5.471678	-0.698756
H	-2.603543	-4.521083	-0.837033
C	-1.737070	-6.870869	-1.654773
C	-0.345474	-5.030232	-2.449340
O	-1.846063	-7.228481	-2.798055
O	-2.362488	-7.459444	-0.635545
O	-1.284468	-4.237290	-2.956574
O	0.748461	-5.166060	-2.928804
C	-0.971780	-3.541711	-4.161744
H	-0.802955	-4.279512	-4.961574
H	-0.028853	-2.990578	-4.021425
C	-2.125321	-2.617872	-4.473949
H	-1.918436	-2.057071	-5.396604
H	-3.054620	-3.187842	-4.615732
H	-2.279936	-1.899413	-3.655985
C	-3.200000	-8.575036	-0.946125
H	-3.970229	-8.252708	-1.663777
H	-2.594224	-9.346063	-1.447006
C	-3.803207	-9.078253	0.343798
H	-4.404691	-8.295255	0.827382
H	-4.455462	-9.939343	0.140110
H	-3.019109	-9.396560	1.045632
C	0.724747	-4.641399	2.234919
H	1.393847	-5.315697	2.790572

H	0.563922	-3.734887	2.837984
H	-0.246750	-5.143620	2.125689
C	2.743581	-3.681397	1.107319
H	2.715553	-2.850188	1.827148
H	3.418267	-4.452664	1.507896
H	3.178776	-3.315354	0.162909

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E_e^S: -1172.20155703

C	-0.774904	-1.371386	0.988700
C	-1.721824	-2.365202	0.593740
C	-3.099600	-2.108250	0.756717
C	-3.502766	-0.877886	1.267044
C	-2.557591	0.094069	1.624760
C	-1.181745	-0.143490	1.493885
C	0.461364	-3.164473	0.137777
C	-1.015067	-3.471206	0.084708
H	-3.838277	-2.861452	0.473669
H	-4.566651	-0.663859	1.388520
H	-2.896900	1.054657	2.018606
H	-0.452029	0.613649	1.788185
H	1.278224	-1.247911	0.665976
N	0.491613	-1.866999	0.796768
C	-0.835526	-5.720123	-1.185183
C	0.347841	-6.359616	-0.394985
C	1.465715	-5.435818	-0.049335
C	-1.667737	-4.752614	-0.319101
C	1.344827	-4.254309	0.867071
H	-0.096589	-6.809842	0.508968

H	0.885467	-3.072917	-0.884892
H	-1.987096	-5.313841	0.577758
H	0.752054	-7.182462	-1.002734
H	2.336580	-5.459711	-0.709907
H	-2.595385	-4.507064	-0.860994
C	-1.728653	-6.868722	-1.657899
C	-0.330355	-5.036128	-2.458314
O	-1.817108	-7.245598	-2.796754
O	-2.376172	-7.436977	-0.641181
O	-1.271680	-4.259495	-2.986153
O	0.770153	-5.166253	-2.924297
C	-0.953838	-3.581364	-4.199955
H	-0.761721	-4.331069	-4.983248
H	-0.022196	-3.011888	-4.057381
C	-2.117899	-2.683073	-4.545721
H	-1.907679	-2.137448	-5.476676
H	-3.035760	-3.271103	-4.688223
H	-2.295162	-1.950936	-3.744693
C	-3.211451	-8.555155	-0.948591
H	-3.966337	-8.242964	-1.686728
H	-2.598739	-9.336756	-1.424011
C	-3.841533	-9.033683	0.337874
H	-4.449572	-8.240374	0.795757
H	-4.492702	-9.896150	0.136559
H	-3.072429	-9.342034	1.060432
C	0.713825	-4.607131	2.220505
H	1.377898	-5.271623	2.793840
H	0.547161	-3.690637	2.806882
H	-0.256023	-5.112174	2.110887
C	2.744364	-3.666816	1.095709

H	2.710975	-2.825913	1.803990
H	3.416169	-4.432237	1.511769
H	3.186456	-3.313347	0.149794

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E_e^S: -1172.16986552

C	-0.662822	-1.340562	0.661817
C	-1.660468	-2.283371	0.279112
C	-2.946563	-1.819469	-0.062899
C	-3.201693	-0.454958	-0.033656
C	-2.196645	0.460620	0.326765
C	-0.915367	0.030021	0.672528
C	0.346739	-3.397396	0.604872
C	-1.072841	-3.571015	0.317107
H	-3.726065	-2.523995	-0.360611
H	-4.193655	-0.083876	-0.299953
H	-2.422470	1.529100	0.337655
H	-0.138082	0.744635	0.951264
H	1.381369	-1.581650	1.057568
N	0.480913	-2.030532	0.976464
C	-0.903542	-5.641841	-1.153724
C	0.431385	-6.225461	-0.609125
C	1.445819	-5.260590	-0.064573
C	-1.713299	-4.852976	-0.092835
C	1.227443	-4.478155	1.239709
H	0.160035	-6.967143	0.163361
H	0.908919	-3.712187	-0.496829
H	-1.868150	-5.524795	0.765665
H	0.895173	-6.780457	-1.436476

H	2.484786	-5.491193	-0.325598
H	-2.710270	-4.637607	-0.500455
C	-1.758299	-6.812159	-1.636600
C	-0.625602	-4.785924	-2.396642
O	-2.065342	-7.019423	-2.780789
O	-2.127051	-7.597784	-0.622590
O	-1.637527	-3.962627	-2.654732
O	0.374772	-4.848637	-3.058542
C	-1.505026	-3.107382	-3.788891
H	-1.473595	-3.729798	-4.696979
H	-0.542849	-2.576697	-3.722691
C	-2.675383	-2.152524	-3.792754
H	-2.610521	-1.485991	-4.664832
H	-3.626843	-2.701293	-3.847560
H	-2.678901	-1.537792	-2.880948
C	-2.923627	-8.739088	-0.944531
H	-3.841427	-8.401772	-1.450665
H	-2.372464	-9.367487	-1.661210
C	-3.223863	-9.475369	0.339613
H	-3.775707	-8.832771	1.040585
H	-3.837541	-10.362343	0.127188
H	-2.296195	-9.805805	0.828556
C	0.616401	-5.239510	2.417141
H	1.302749	-6.029030	2.761659
H	0.429316	-4.559021	3.261962
H	-0.338230	-5.716483	2.159335
C	2.567240	-3.871703	1.663412
H	2.448371	-3.196291	2.524568
H	3.265450	-4.670894	1.954703
H	3.035036	-3.314652	0.834970

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E_e^S: -1172.31072912

C	-0.667823	-1.355648	0.722522
C	-1.627127	-2.297377	0.281791
C	-2.881662	-1.838184	-0.153456
C	-3.141311	-0.476036	-0.141204
C	-2.169827	0.445817	0.300185
C	-0.924110	0.020532	0.737691
C	0.251162	-3.408572	0.876642
C	-1.023185	-3.598824	0.392340
H	-3.638355	-2.544530	-0.502532
H	-4.112770	-0.107190	-0.477817
H	-2.402625	1.512872	0.298242
H	-0.171288	0.734341	1.079371
H	1.315002	-1.648248	1.407438
N	0.454412	-2.059364	1.080443
C	-0.864640	-5.651298	-1.091834
C	0.450201	-6.266420	-0.558238
C	1.557878	-5.325413	-0.074818
C	-1.657570	-4.896789	-0.001119
C	1.317786	-4.444554	1.173875
H	0.176445	-6.973663	0.240040
H	1.860217	-4.677054	-0.909718
H	-1.774924	-5.573393	0.858654
H	0.883365	-6.866944	-1.373043
H	2.426661	-5.968317	0.147728
H	-2.671165	-4.696878	-0.373634
C	-1.700622	-6.812290	-1.632624

C	-0.591861	-4.733630	-2.288285
O	-1.854530	-7.067854	-2.797728
O	-2.221576	-7.543478	-0.645218
O	-1.670206	-4.024541	-2.606513
O	0.456087	-4.654060	-2.873241
C	-1.545801	-3.123317	-3.706124
H	-1.285145	-3.700827	-4.606639
H	-0.711714	-2.433496	-3.504739
C	-2.855584	-2.388029	-3.862770
H	-2.799342	-1.707963	-4.724923
H	-3.681504	-3.093979	-4.032461
H	-3.076606	-1.792822	-2.965439
C	-2.994142	-8.683560	-1.023380
H	-3.827249	-8.353634	-1.663186
H	-2.366972	-9.354055	-1.631385
C	-3.482261	-9.355180	0.238459
H	-4.107113	-8.670902	0.830159
H	-4.083342	-10.239507	-0.016822
H	-2.637057	-9.679783	0.862270
C	0.885068	-5.291774	2.383943
H	1.625888	-6.082483	2.584837
H	0.798953	-4.664412	3.283846
H	-0.089048	-5.773605	2.225206
C	2.654060	-3.765490	1.511548
H	2.575431	-3.132473	2.410163
H	3.419685	-4.526239	1.722504
H	3.020089	-3.152204	0.673155

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E_e^S: -1172.31072911

C	-0.667823	-1.355648	0.722522
C	-1.627127	-2.297377	0.281791
C	-2.881662	-1.838184	-0.153457
C	-3.141311	-0.476036	-0.141204
C	-2.169828	0.445817	0.300185
C	-0.924110	0.020532	0.737690
C	0.251162	-3.408572	0.876642
C	-1.023185	-3.598824	0.392340
H	-3.638355	-2.544530	-0.502532
H	-4.112770	-0.107190	-0.477817
H	-2.402625	1.512872	0.298242
H	-0.171288	0.734341	1.079371
H	1.315002	-1.648248	1.407438
N	0.454412	-2.059364	1.080443
C	-0.864640	-5.651298	-1.091834
C	0.450201	-6.266420	-0.558238
C	1.557878	-5.325412	-0.074818
C	-1.657570	-4.896789	-0.001119
C	1.317786	-4.444554	1.173875
H	0.176445	-6.973663	0.240040
H	1.860217	-4.677054	-0.909718
H	-1.774924	-5.573393	0.858654
H	0.883365	-6.866944	-1.373043
H	2.426661	-5.968317	0.147729
H	-2.671165	-4.696878	-0.373634
C	-1.700622	-6.812291	-1.632624
C	-0.591861	-4.733630	-2.288285
O	-1.854530	-7.067854	-2.797728
O	-2.221576	-7.543478	-0.645218

O	-1.670206	-4.024541	-2.606514
O	0.456088	-4.654060	-2.873241
C	-1.545801	-3.123317	-3.706124
H	-1.285144	-3.700827	-4.606639
H	-0.711714	-2.433496	-3.504739
C	-2.855584	-2.388030	-3.862770
H	-2.799342	-1.707963	-4.724923
H	-3.681504	-3.093979	-4.032461
H	-3.076606	-1.792822	-2.965439
C	-2.994141	-8.683560	-1.023380
H	-3.827249	-8.353635	-1.663186
H	-2.366972	-9.354055	-1.631385
C	-3.482261	-9.355181	0.238459
H	-4.107113	-8.670903	0.830159
H	-4.083342	-10.239507	-0.016823
H	-2.637057	-9.679783	0.862270
C	0.885068	-5.291774	2.383943
H	1.625888	-6.082483	2.584837
H	0.798953	-4.664412	3.283846
H	-0.089048	-5.773605	2.225206
C	2.654060	-3.765490	1.511548
H	2.575431	-3.132473	2.410163
H	3.419685	-4.526239	1.722504
H	3.020089	-3.152204	0.673155

^{OS}TS$_{2-4}$

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E_e^S: -1172.16711377

C	-0.963399	-1.567672	1.343318
C	-1.165492	-2.063772	0.028527

C	-2.039934	-1.408365	-0.835480
C	-2.670660	-0.236595	-0.415072
C	-2.450321	0.255115	0.875150
C	-1.607978	-0.407565	1.770594
C	0.555632	-3.187445	1.040842
C	-0.480730	-3.371855	-0.037127
H	-2.214980	-1.816244	-1.833006
H	-3.339075	0.298034	-1.092992
H	-2.948555	1.173802	1.193785
H	-1.458554	-0.025694	2.783075
H	0.491436	-1.925668	2.742412
N	-0.110376	-2.402101	2.078812
C	-0.832989	-5.521038	-1.349904
C	0.551842	-5.989213	-0.848394
C	1.292778	-4.821930	-0.283149
C	-1.400556	-4.555902	-0.290905
C	1.348662	-4.495665	1.202317
H	0.391009	-6.766047	-0.086992
H	1.296263	-2.512795	0.561110
H	-1.602055	-5.125741	0.627702
H	1.103295	-6.431046	-1.690074
H	2.049963	-4.350198	-0.915898
H	-2.370335	-4.173124	-0.634497
C	-1.744403	-6.720721	-1.593137
C	-0.664922	-4.801415	-2.693240
O	-2.070811	-7.131402	-2.675532
O	-2.113418	-7.293807	-0.445824
O	-1.770471	-4.139105	-3.030783
O	0.328231	-4.828340	-3.368457
C	-1.775046	-3.500927	-4.307453

H	-1.459477	-4.230024	-5.068869
H	-1.029241	-2.689996	-4.301724
C	-3.171266	-2.985355	-4.567050
H	-3.212345	-2.497354	-5.551298
H	-3.896525	-3.811300	-4.557393
H	-3.474485	-2.250555	-3.806841
C	-2.936175	-8.457943	-0.537014
H	-3.852172	-8.204035	-1.092530
H	-2.405679	-9.224961	-1.122609
C	-3.237454	-8.925718	0.867210
H	-3.767870	-8.147235	1.434088
H	-3.871582	-9.823093	0.834747
H	-2.311427	-9.175856	1.404653
C	0.696974	-5.507990	2.146050
H	1.279848	-6.441811	2.176832
H	0.670379	-5.091717	3.163876
H	-0.333396	-5.765773	1.876533
C	2.781391	-4.229752	1.683061
H	2.782486	-3.821146	2.706841
H	3.371892	-5.158819	1.693298
H	3.296059	-3.510228	1.028302

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E_e^S: -1172.21904805

C	-1.179883	-1.709198	0.998567
C	-0.672557	-2.127030	-0.266615
C	-0.880424	-1.357827	-1.397501
C	-1.585399	-0.151267	-1.281992
C	-2.088271	0.250899	-0.046014

C	-1.892933	-0.520412	1.106679
C	0.282085	-3.307516	1.427832
C	-0.172997	-3.524938	0.011805
H	-0.487262	-1.688153	-2.362043
H	-1.739229	0.476405	-2.162299
H	-2.637992	1.191803	0.032103
H	-2.284655	-0.187134	2.070514
H	-0.701863	-2.184044	2.937976
N	-0.854935	-2.626384	2.037184
C	-0.843731	-5.395398	-1.383589
C	0.644050	-5.654424	-1.041412
C	1.062597	-4.468553	-0.165418
C	-1.354166	-4.504529	-0.231673
C	1.092229	-4.646859	1.428352
H	0.751966	-6.607262	-0.504645
H	1.097615	-2.559110	1.345886
H	-1.591797	-5.114534	0.642714
H	1.233510	-5.714341	-1.964322
H	1.981134	-3.981124	-0.518132
H	-2.273871	-3.978219	-0.510254
C	-1.600086	-6.702200	-1.562683
C	-0.947761	-4.606856	-2.695935
O	-1.875664	-7.196721	-2.623530
O	-1.875483	-7.277824	-0.389246
O	-2.200876	-4.216507	-2.908564
O	-0.022519	-4.328442	-3.412178
C	-2.483369	-3.435511	-4.068526
H	-2.638364	-4.123600	-4.914659
H	-1.608137	-2.813217	-4.304959
C	-3.711076	-2.601475	-3.784233

H	-3.973068	-2.005403	-4.670383
H	-4.569531	-3.239508	-3.529967
H	-3.523481	-1.916139	-2.944341
C	-2.511520	-8.555362	-0.425297
H	-3.470276	-8.461305	-0.958311
H	-1.885715	-9.250262	-1.006846
C	-2.699474	-9.020509	0.999569
H	-3.323113	-8.312258	1.563758
H	-3.193951	-10.002288	1.011032
H	-1.731340	-9.115022	1.512429
C	0.464284	-5.911791	2.010493
H	1.161008	-6.758799	1.904698
H	0.286385	-5.767783	3.087480
H	-0.481210	-6.217964	1.553068
C	2.489079	-4.492476	2.028911
H	2.444209	-4.444100	3.129010
H	3.122661	-5.351667	1.757489
H	2.989158	-3.580954	1.667910

^{S}Ind-4

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E_e^S: -1172.21904598

C	-1.179466	-1.709057	0.998157
C	-0.672269	-2.127074	-0.267021
C	-0.880068	-1.357920	-1.397942
C	-1.584861	-0.151240	-1.282492
C	-2.087620	0.251091	-0.046530
C	-1.892334	-0.520165	1.106218
C	0.282333	-3.307527	1.427481
C	-0.172893	-3.525025	0.011515

H	-0.487009	-1.688357	-2.362489
H	-1.738632	0.476380	-2.162846
H	-2.637197	1.192082	0.031549
H	-2.283949	-0.186746	2.070047
H	-0.701355	-2.183768	2.937567
N	-0.854565	-2.626196	2.036840
C	-0.844134	-5.395543	-1.383558
C	0.643676	-5.654734	-1.041602
C	1.062511	-4.468851	-0.165752
C	-1.354264	-4.504443	-0.231687
C	1.092283	-4.647015	1.428037
H	0.751607	-6.607553	-0.504809
H	1.097971	-2.559253	1.345427
H	-1.591895	-5.114283	0.642814
H	1.232953	-5.714764	-1.964622
H	1.981105	-3.981624	-0.518601
H	-2.273911	-3.978025	-0.510249
C	-1.600753	-6.702235	-1.562300
C	-0.948306	-4.607242	-2.696043
O	-1.876942	-7.196702	-2.623014
O	-1.875672	-7.277820	-0.388728
O	-2.201330	-4.216473	-2.908336
O	-0.023184	-4.329333	-3.412645
C	-2.483965	-3.435600	-4.068347
H	-2.639748	-4.123795	-4.914249
H	-1.608502	-2.813861	-4.305370
C	-3.711061	-2.600805	-3.783611
H	-3.973239	-2.004864	-4.669795
H	-4.569709	-3.238306	-3.528664
H	-3.522592	-1.915324	-2.944033

C	-2.511893	-8.555259	-0.424458
H	-3.470966	-8.461057	-0.956878
H	-1.886545	-9.250218	-1.006428
C	-2.699039	-9.020464	1.000497
H	-3.322259	-8.312178	1.565104
H	-3.193614	-10.002191	1.012205
H	-1.730604	-9.115108	1.512764
C	0.464219	-5.911787	2.010407
H	1.160924	-6.758844	1.904869
H	0.286238	-5.767525	3.087345
H	-0.481231	-6.218044	1.552951
C	2.489220	-4.492760	2.028419
H	2.444500	-4.444385	3.128523
H	3.122679	-5.352016	1.756910
H	2.989346	-3.581291	1.667350

$^{T}TS_{2\text{-}3}$

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E_e^S: -1172.13219466

C	-0.691313	-1.365725	0.546482
C	-1.697663	-2.347530	0.261748
C	-3.031372	-1.926247	0.067649
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53

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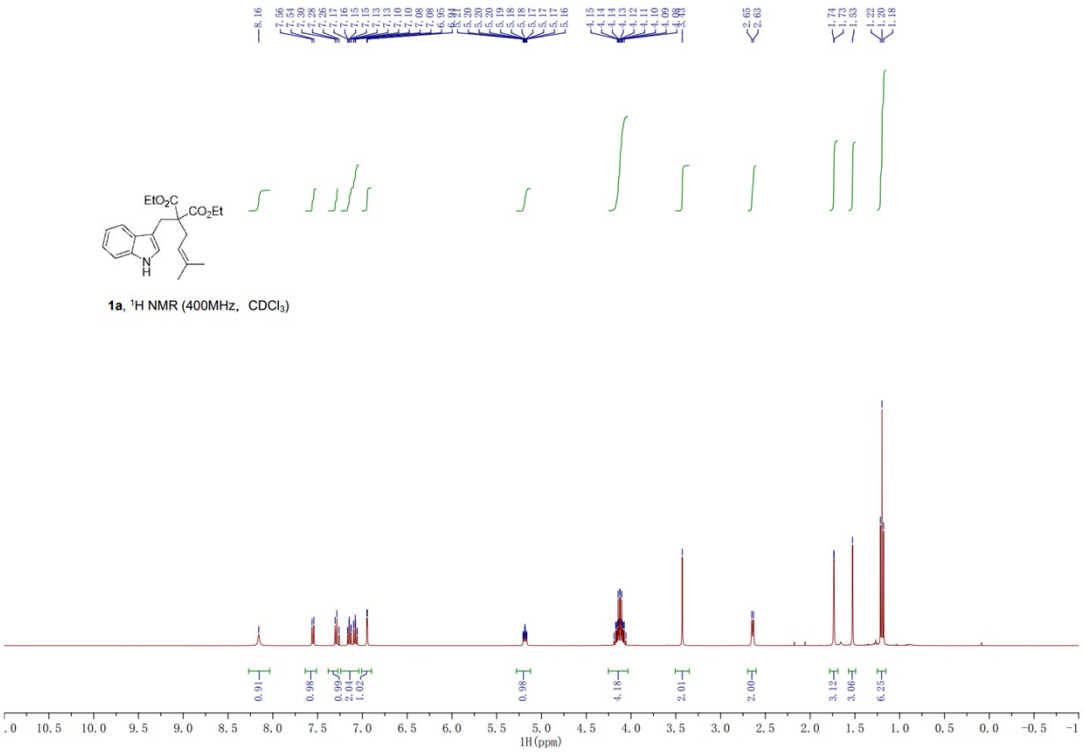
10. NMR spectra



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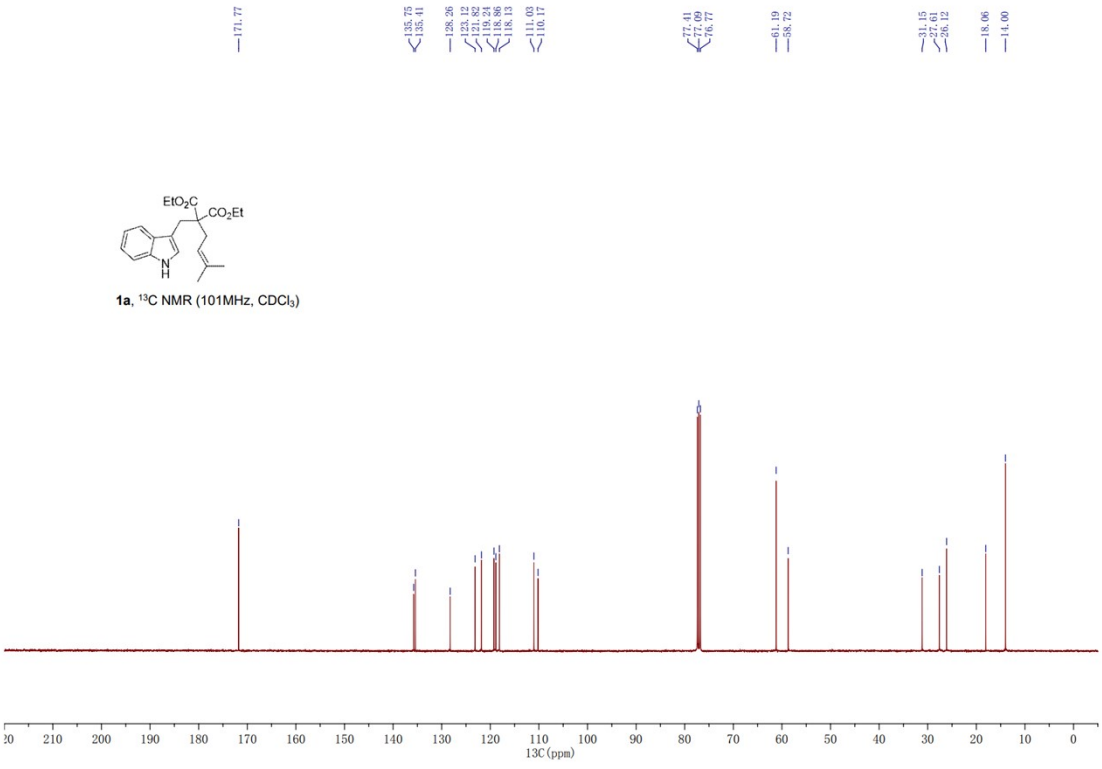

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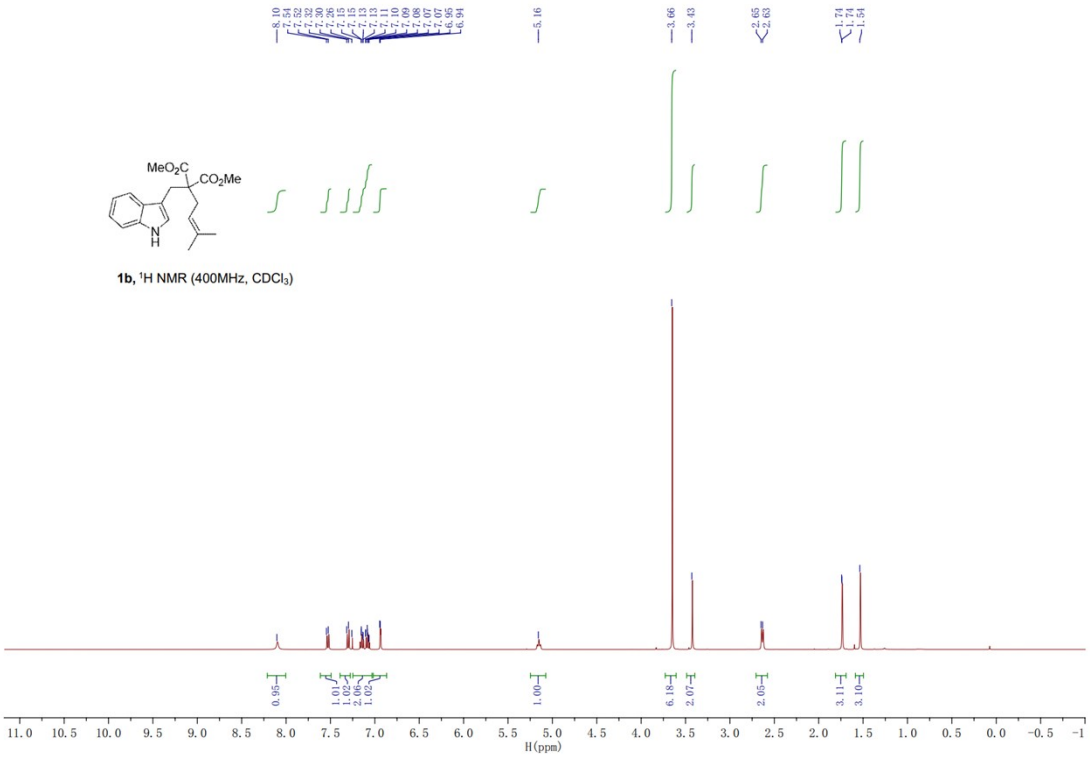

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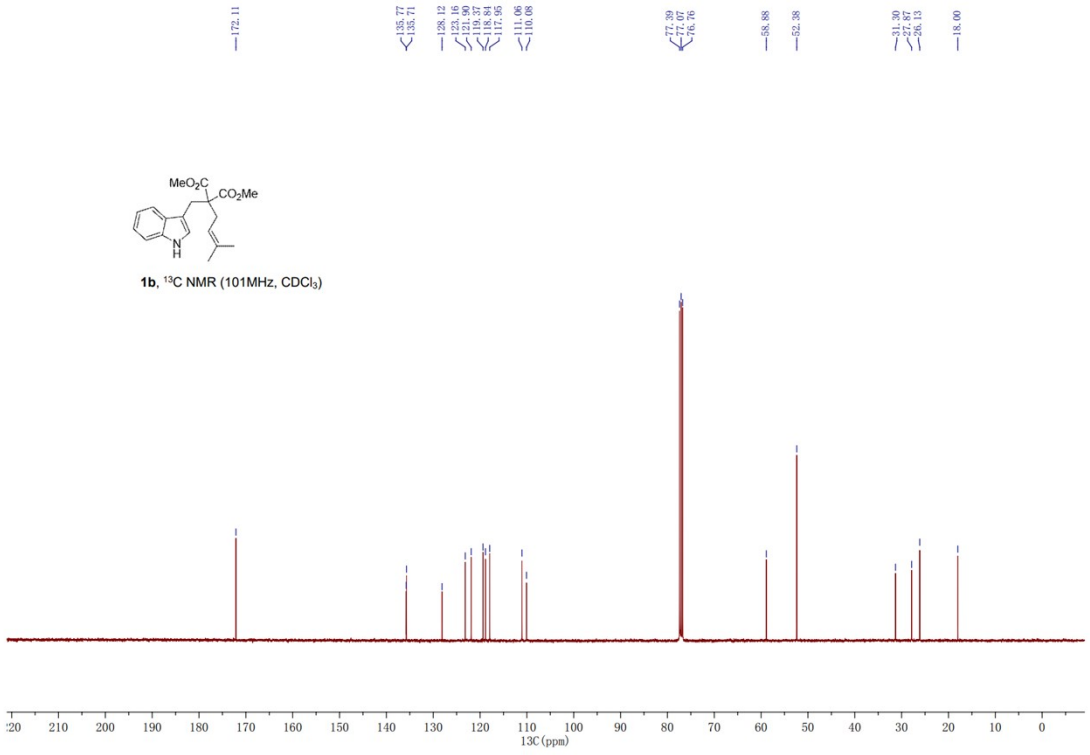

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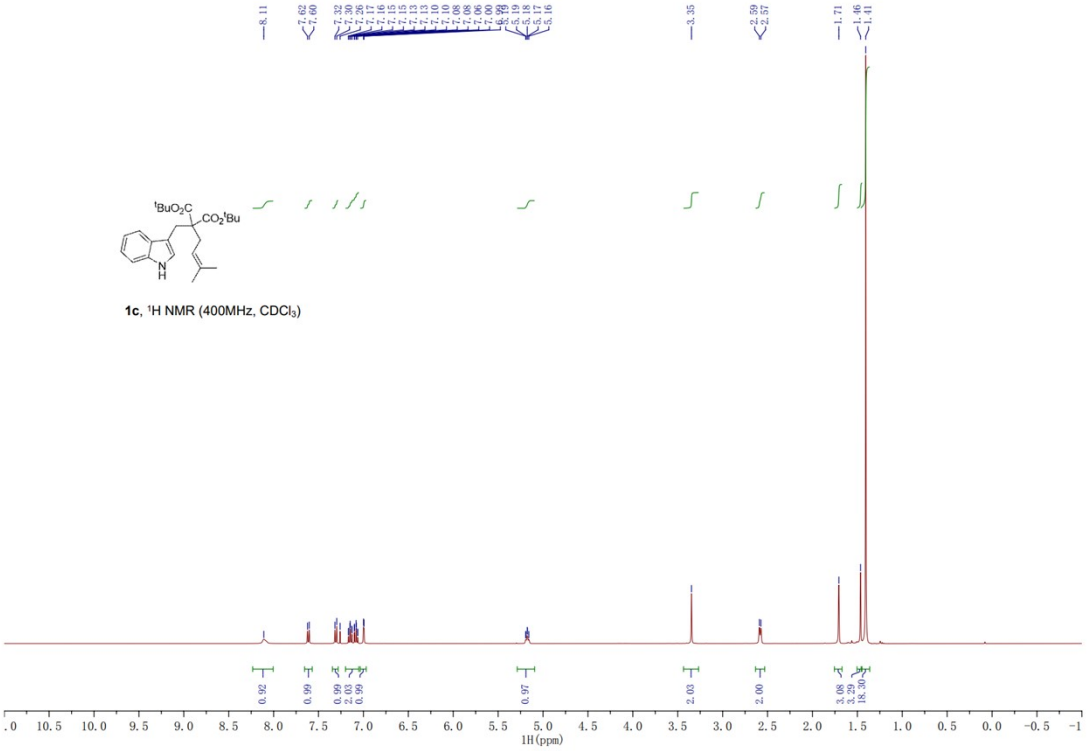

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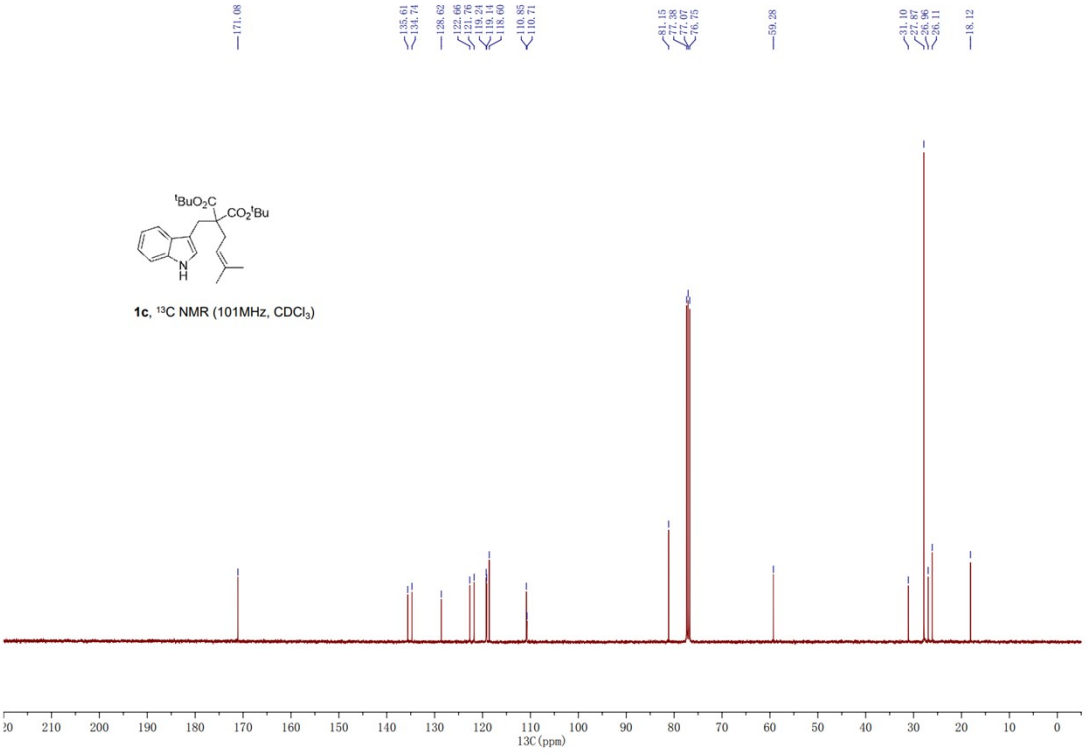

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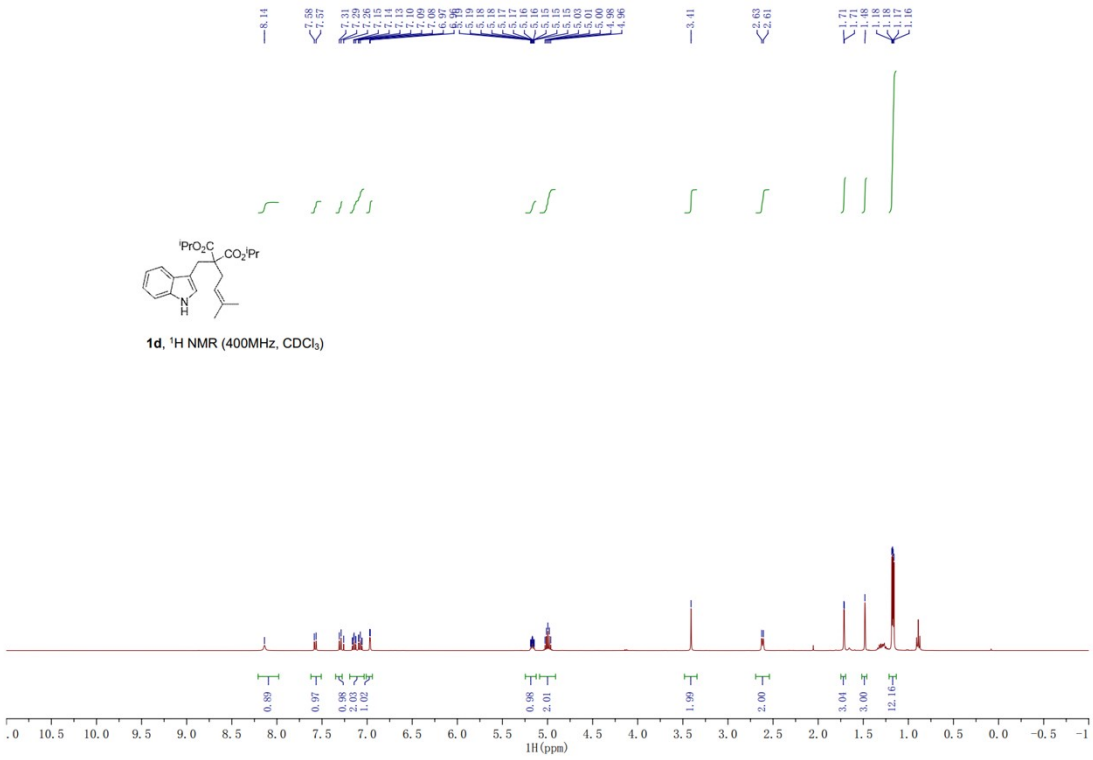

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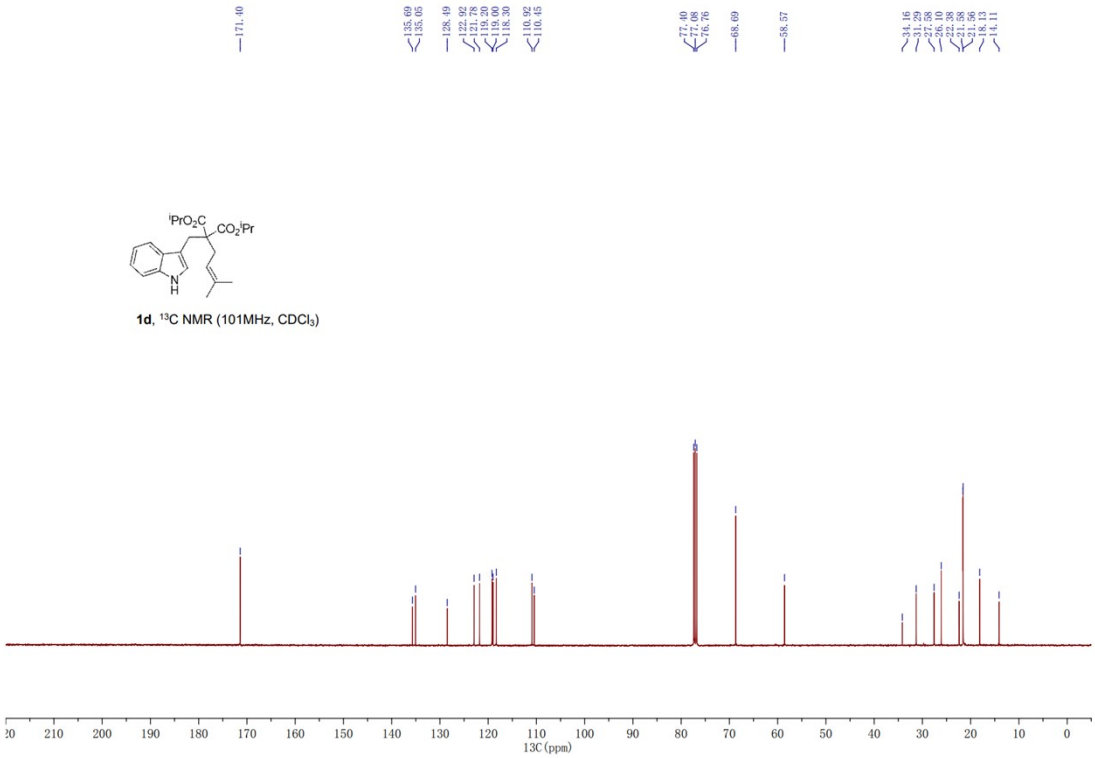

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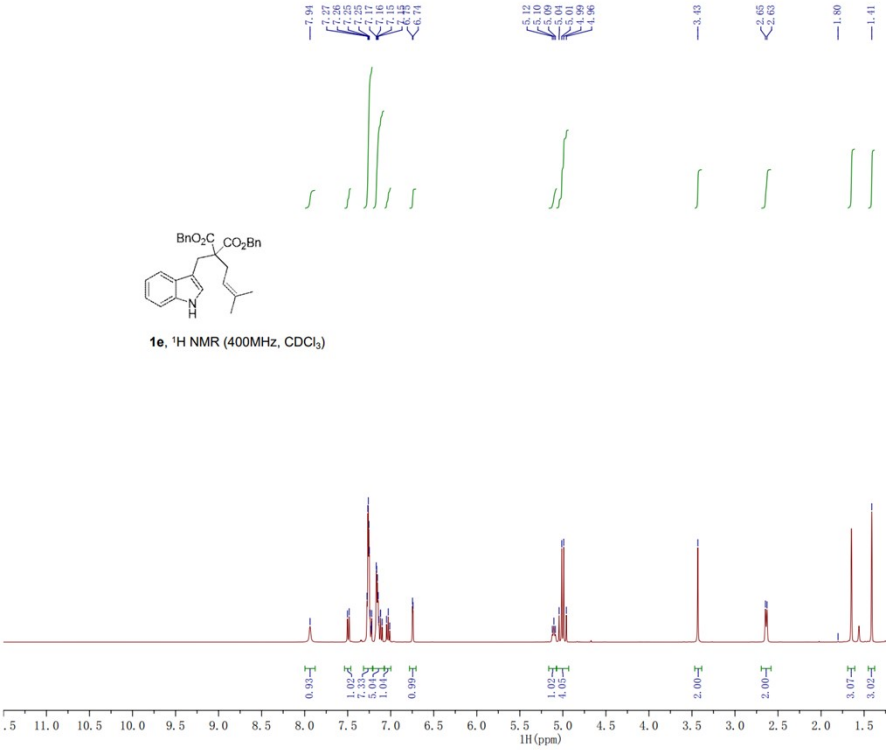

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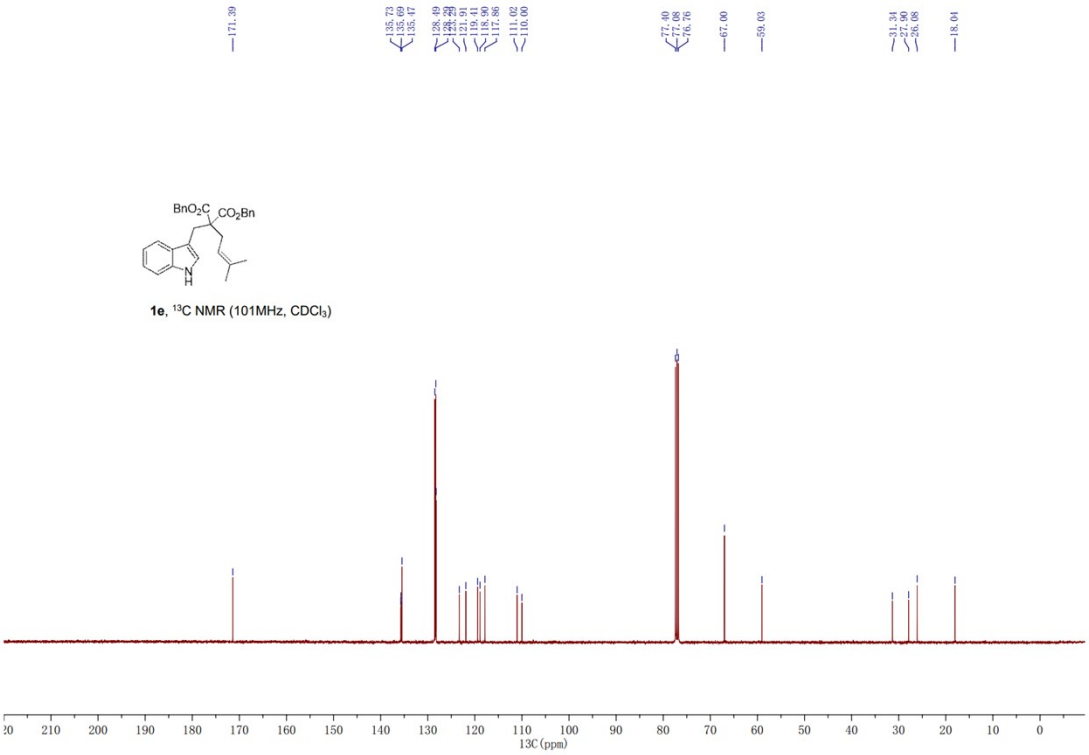

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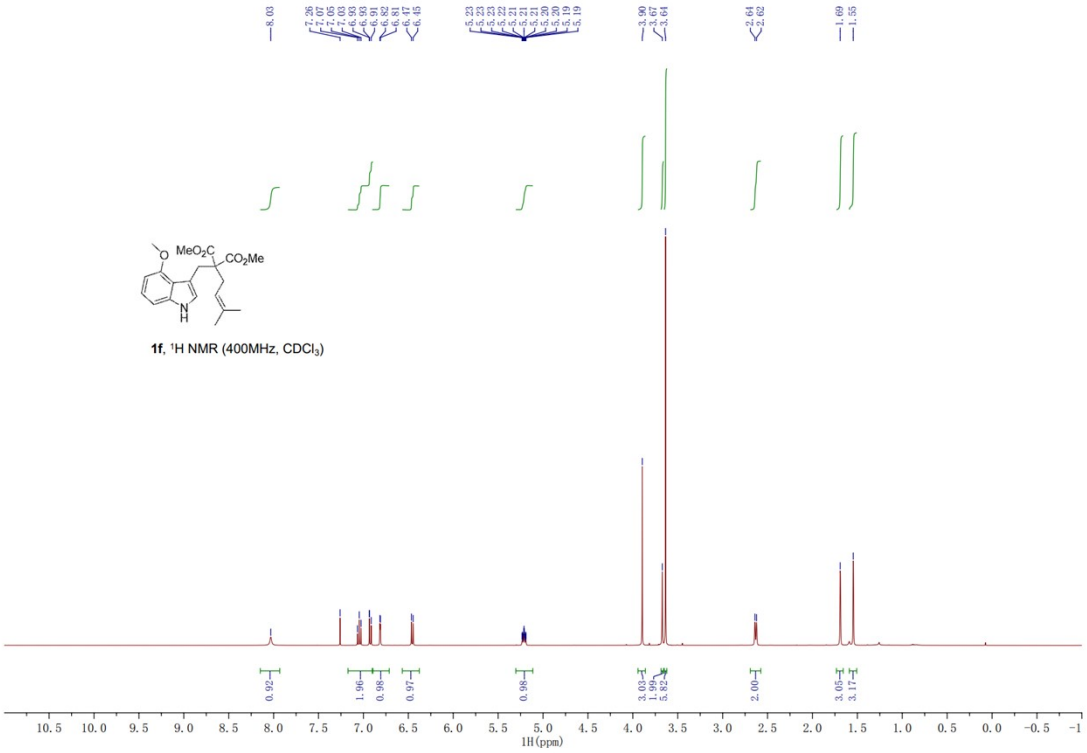

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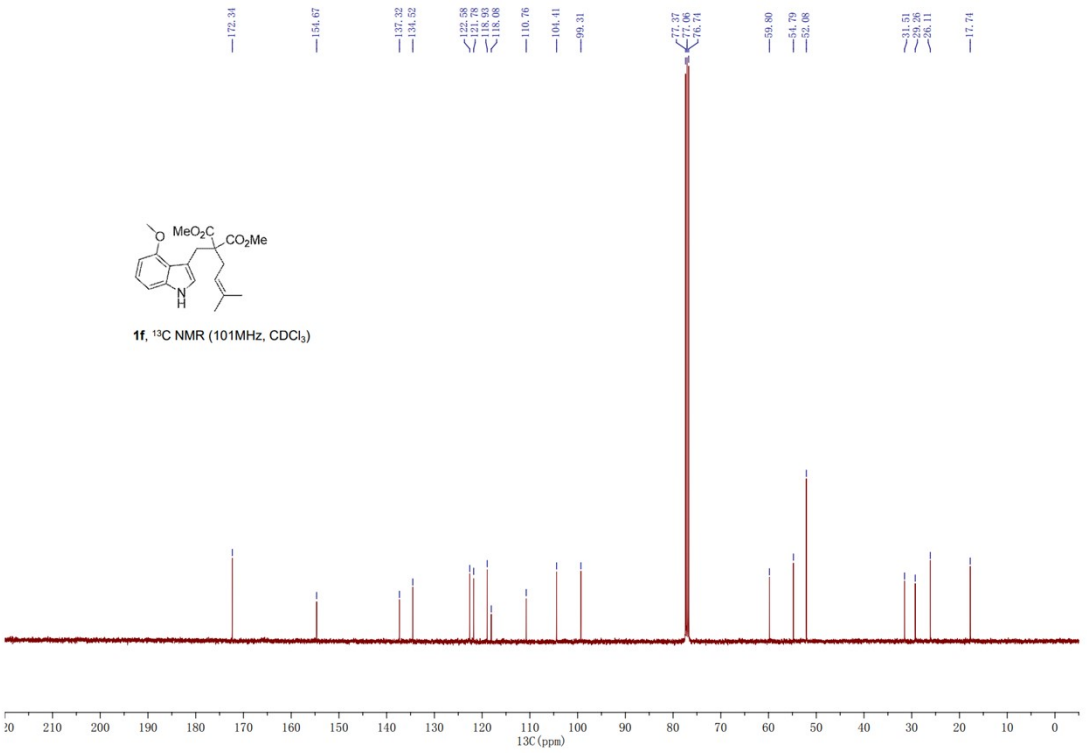

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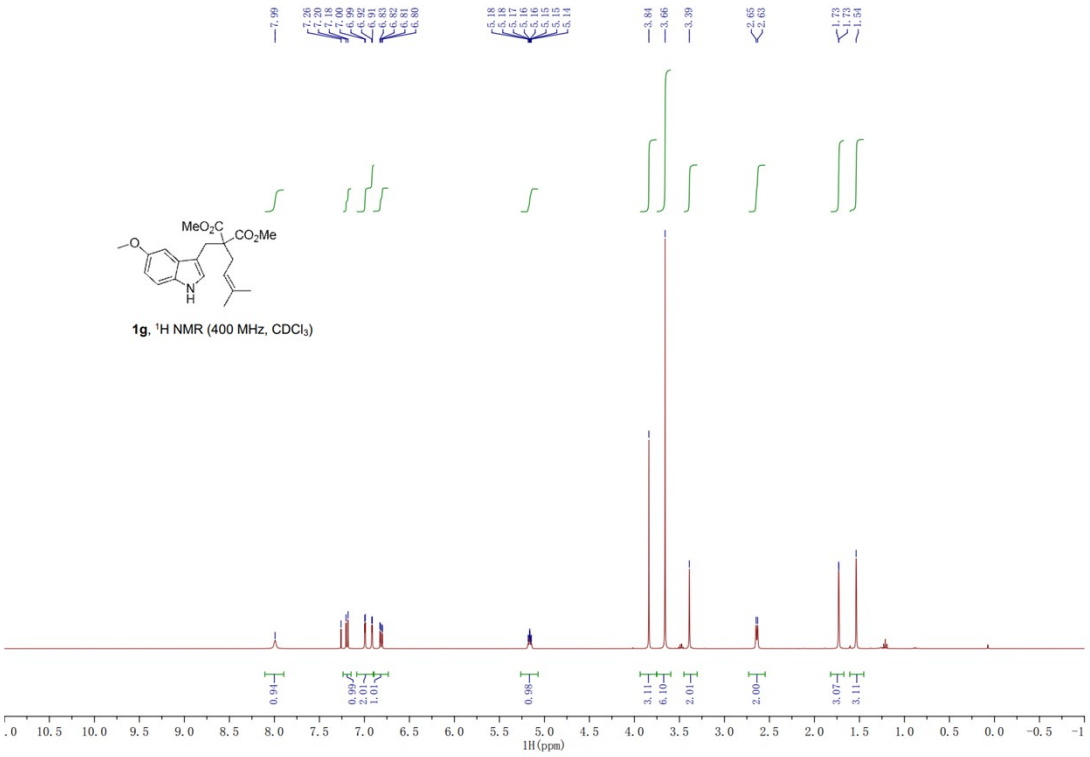

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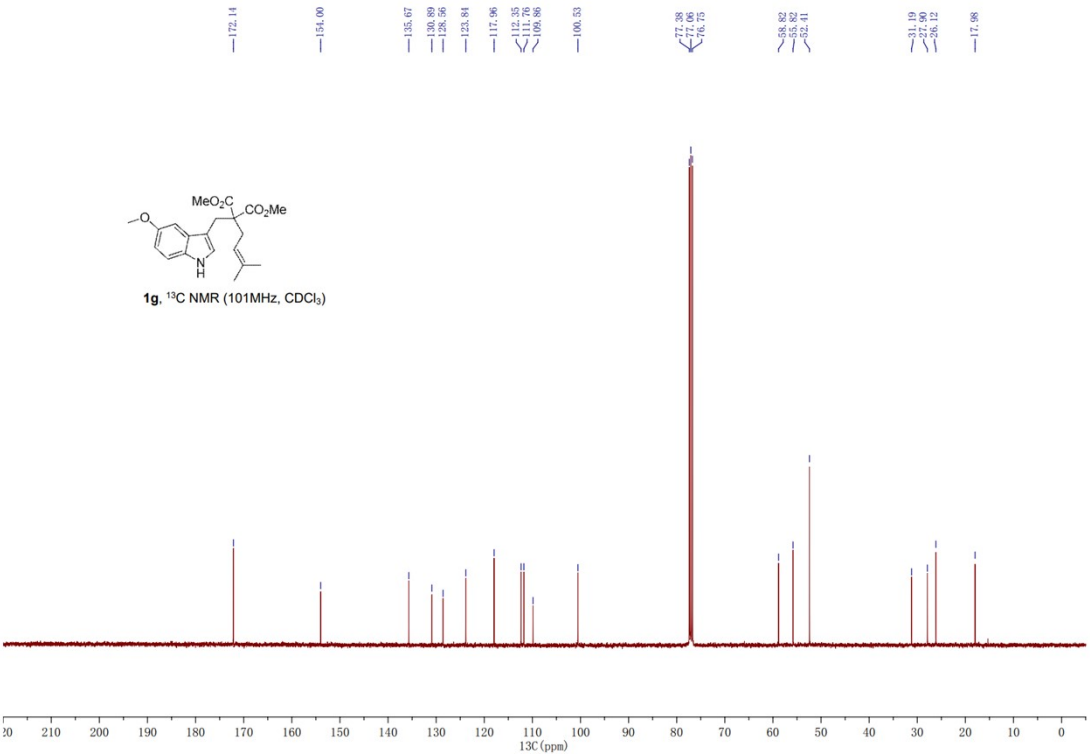

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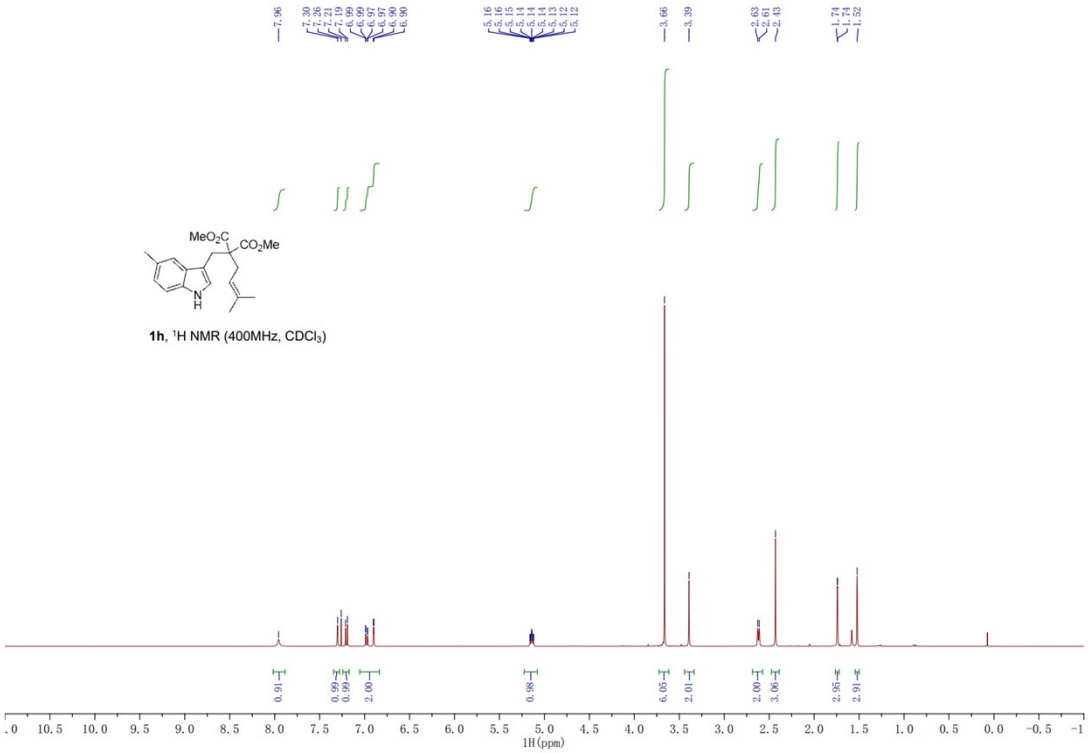

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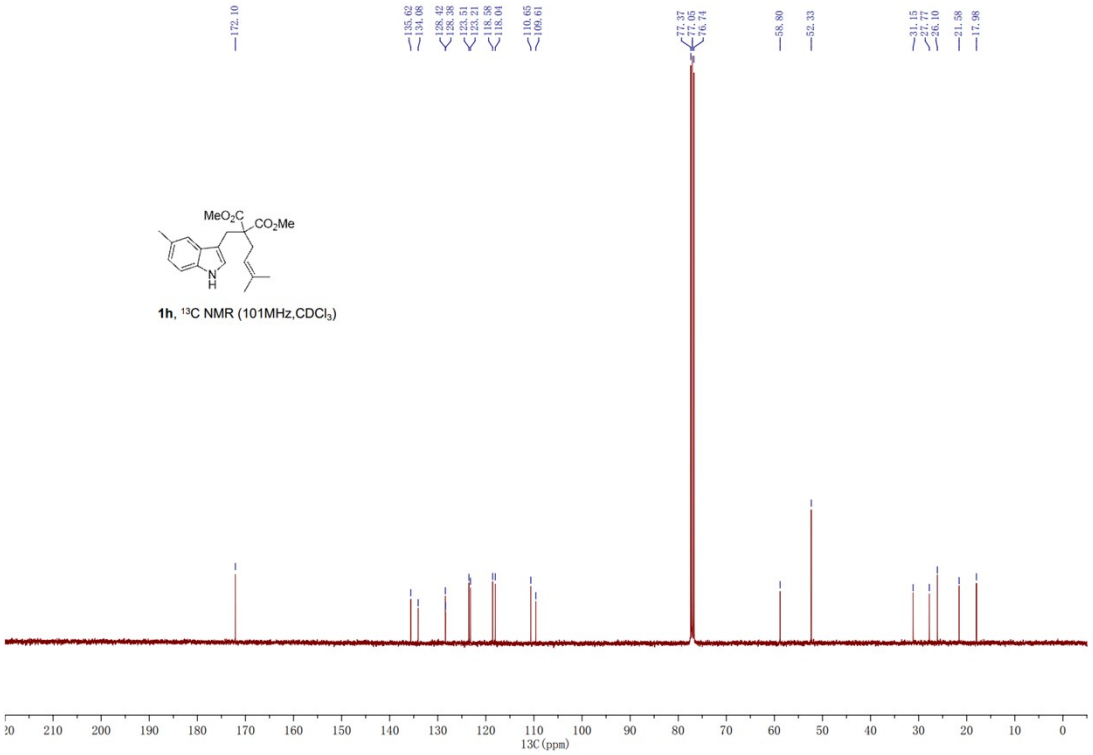

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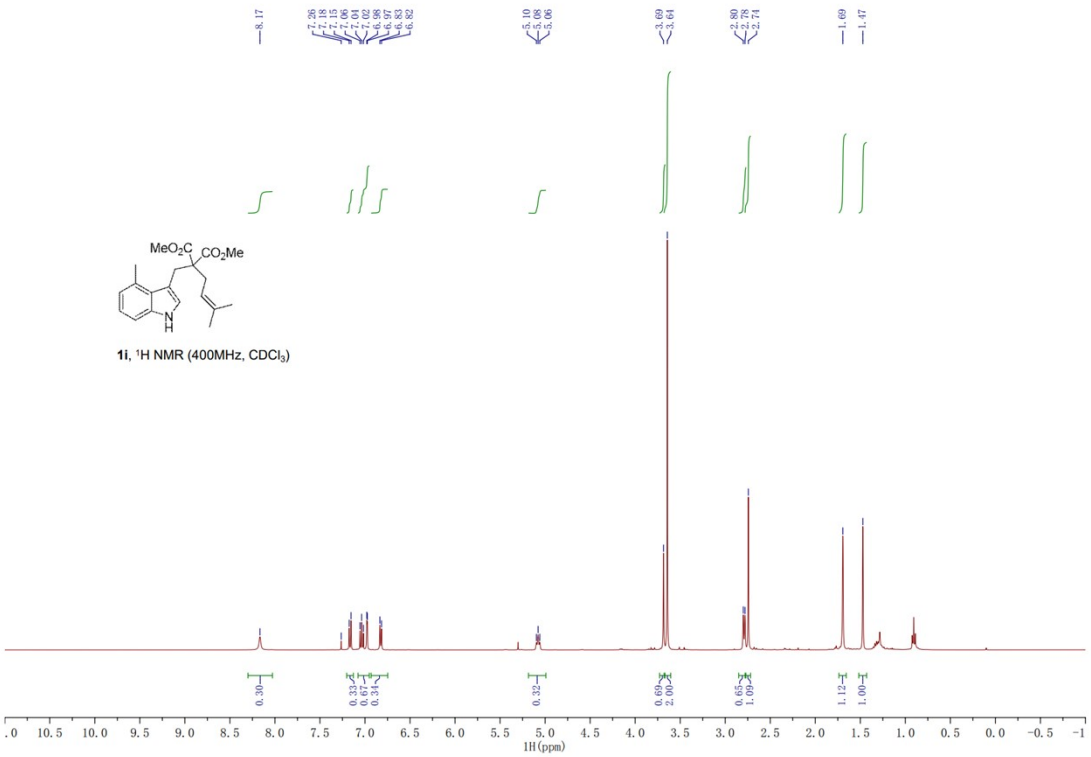

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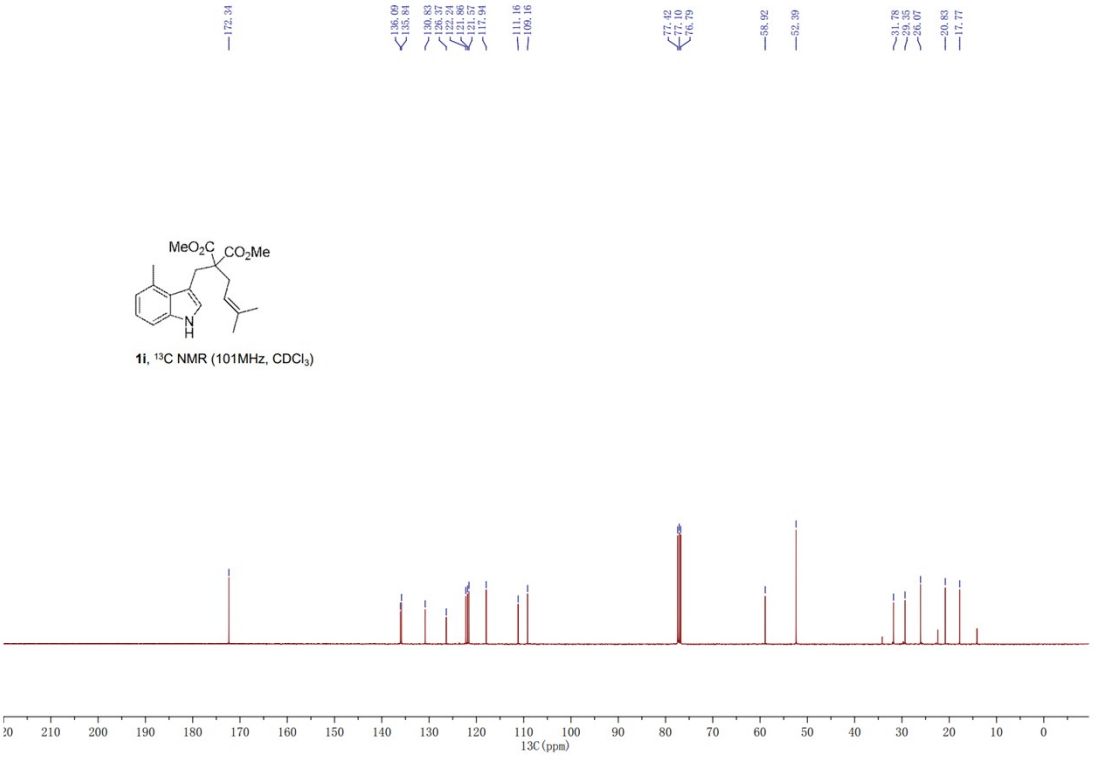

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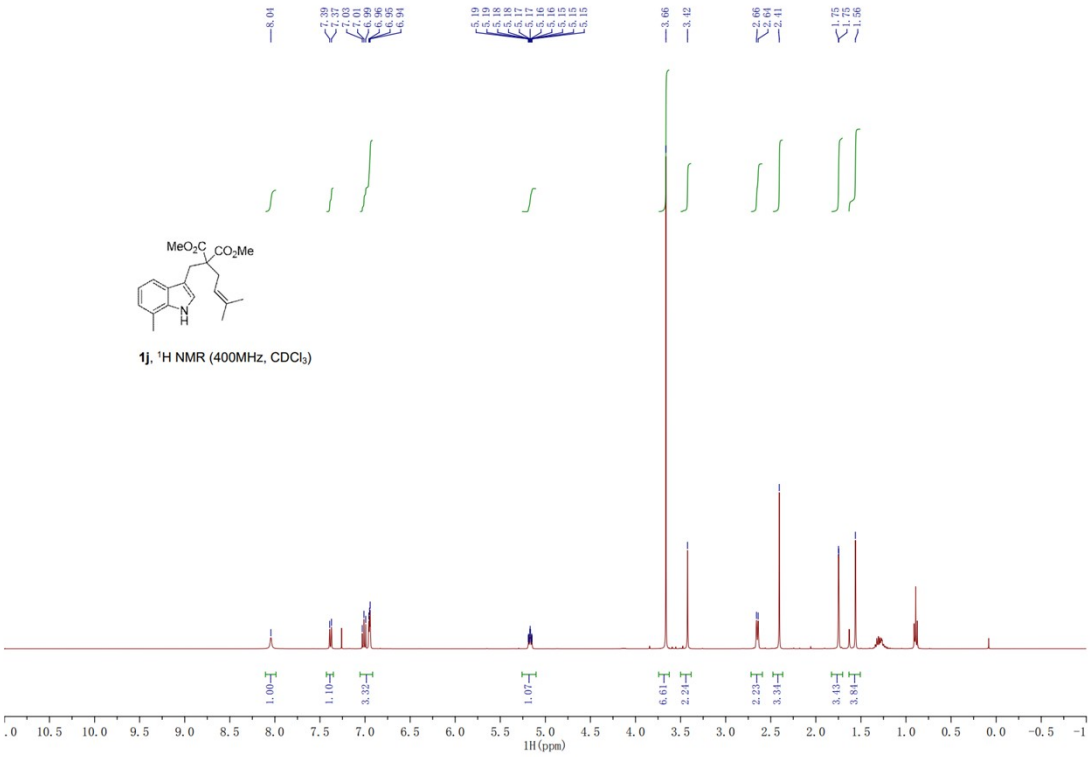

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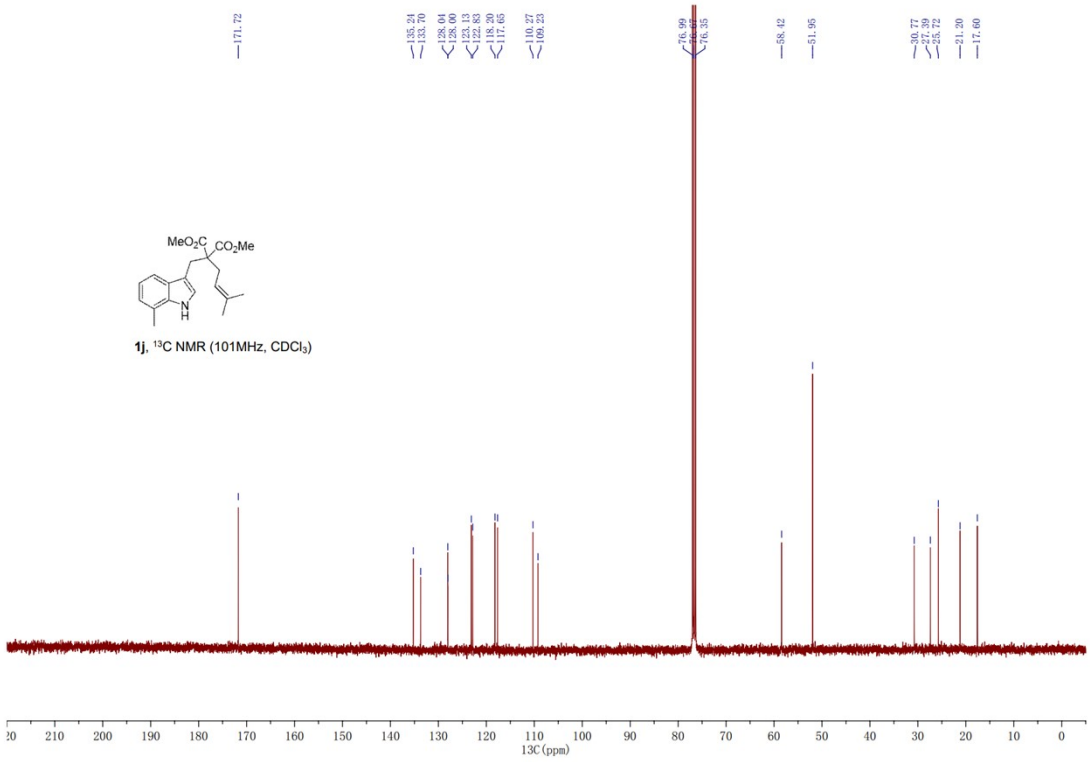

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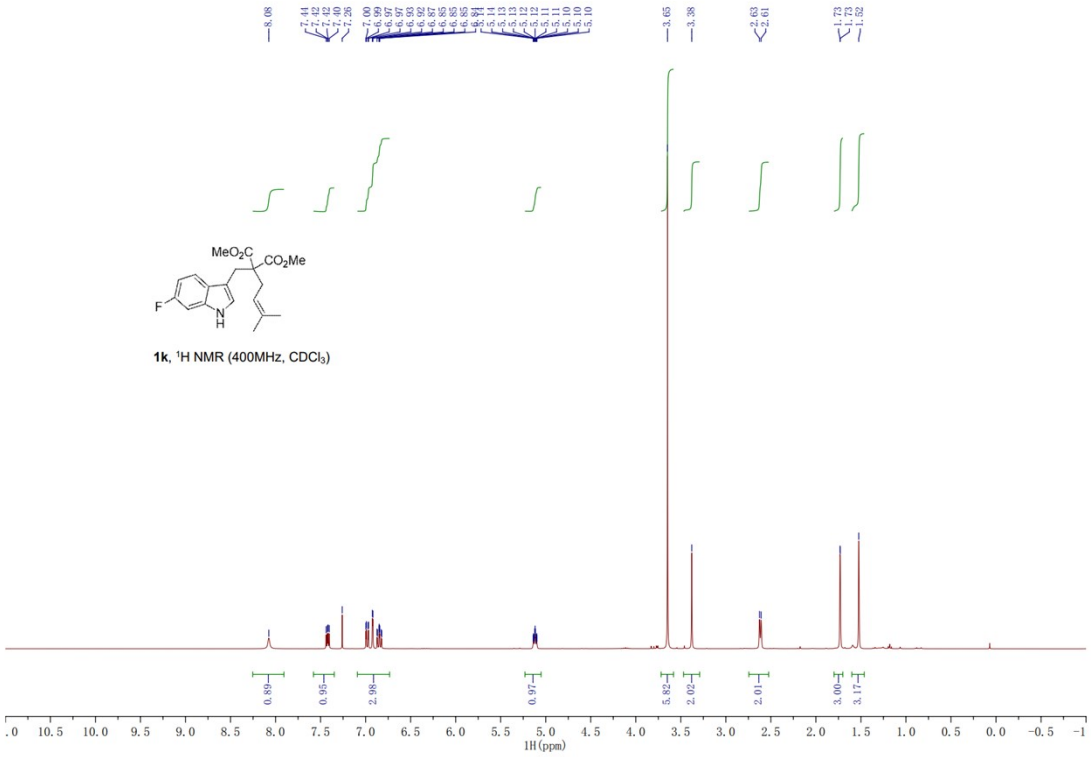

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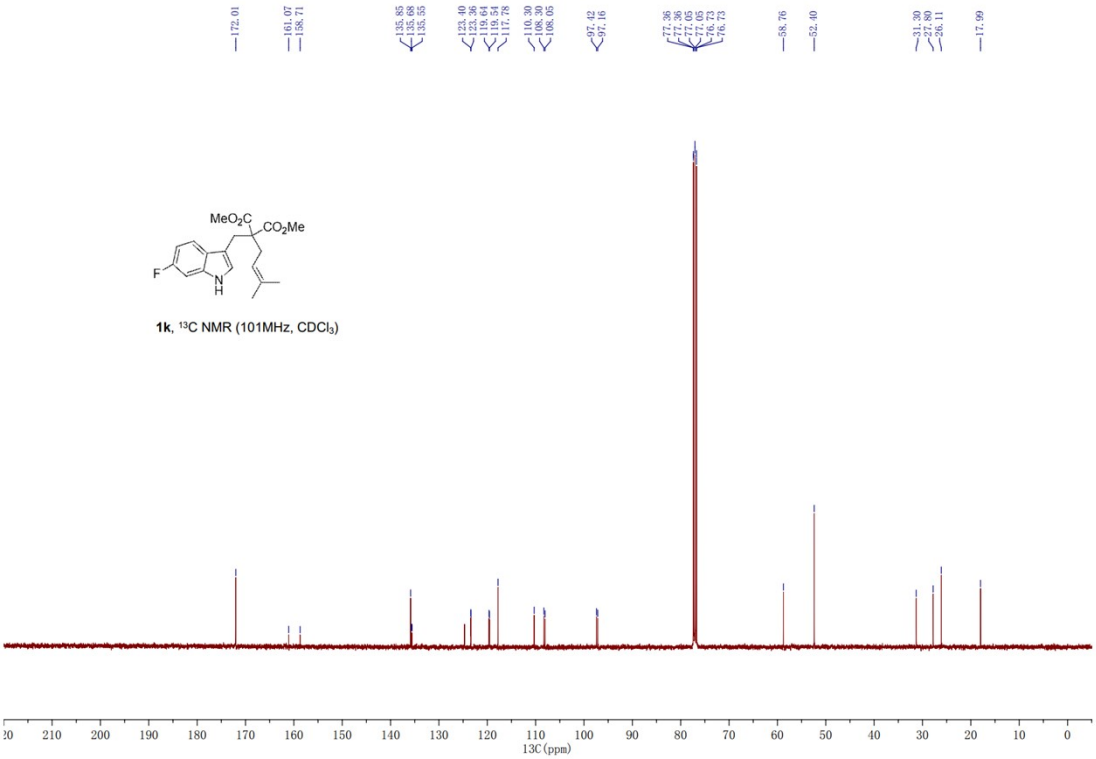

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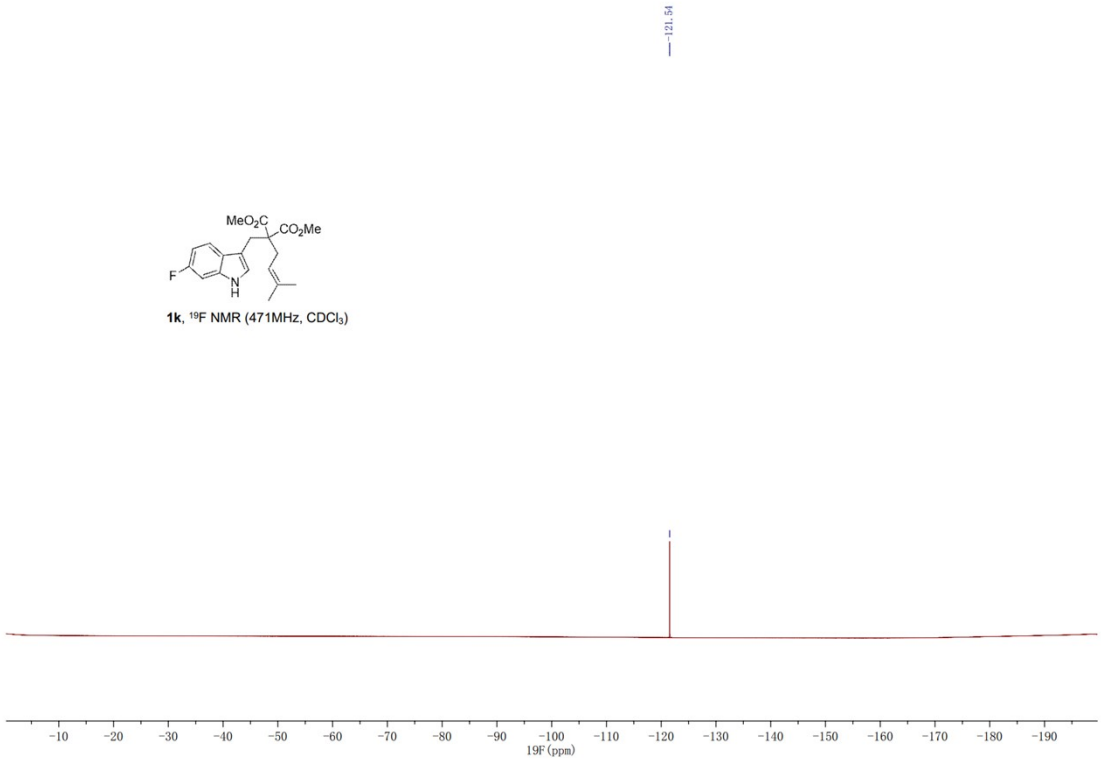

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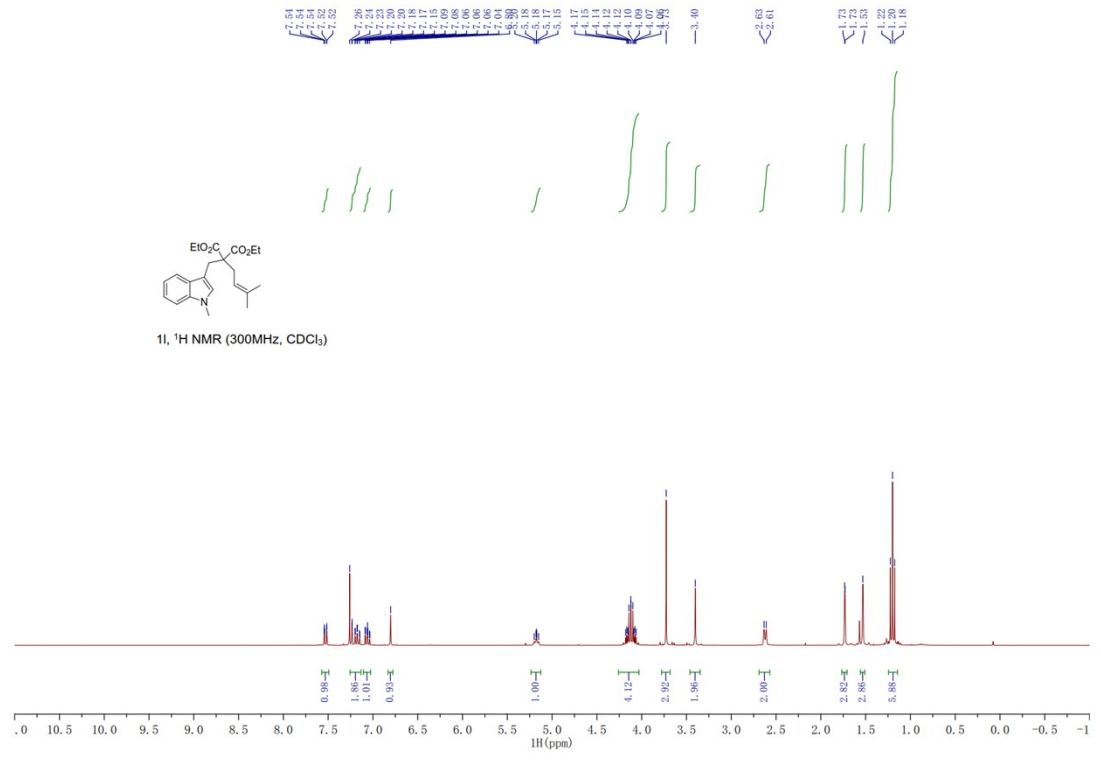

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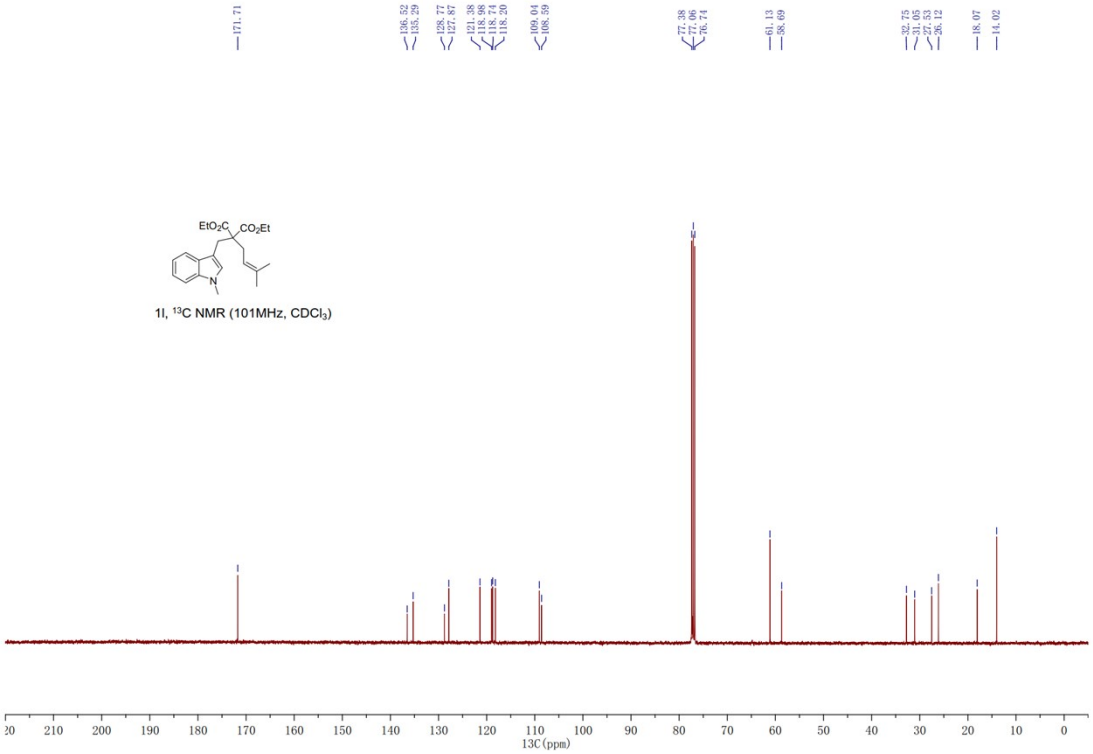

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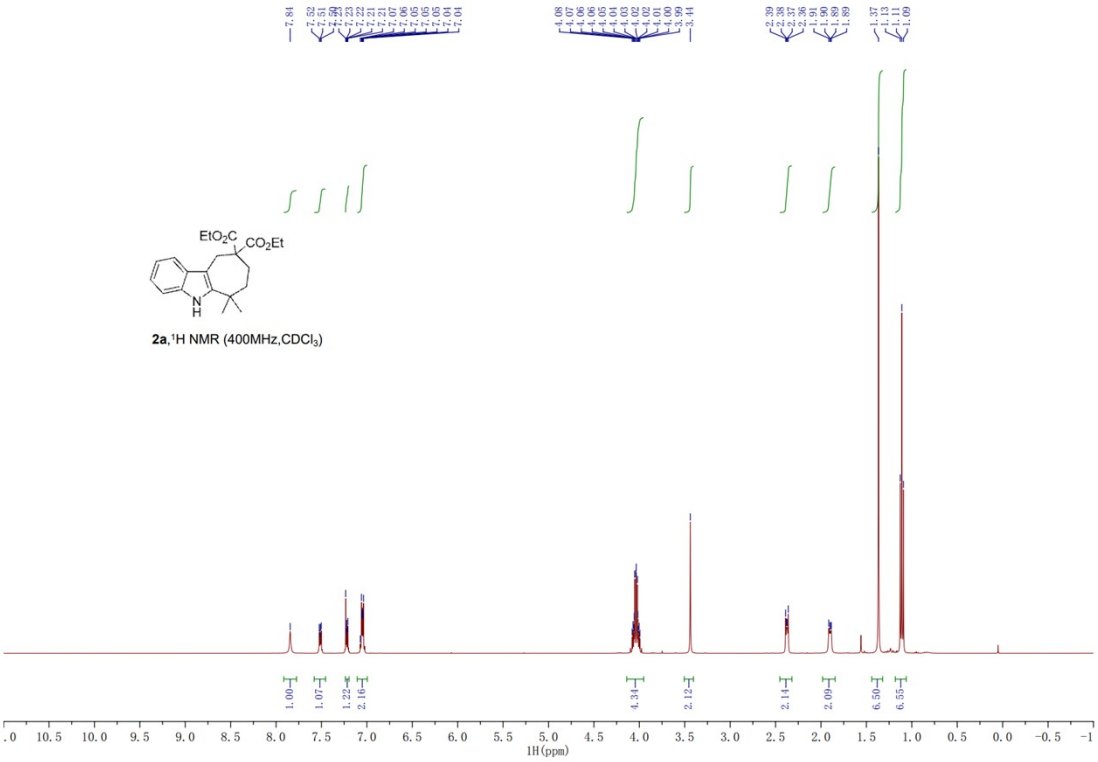

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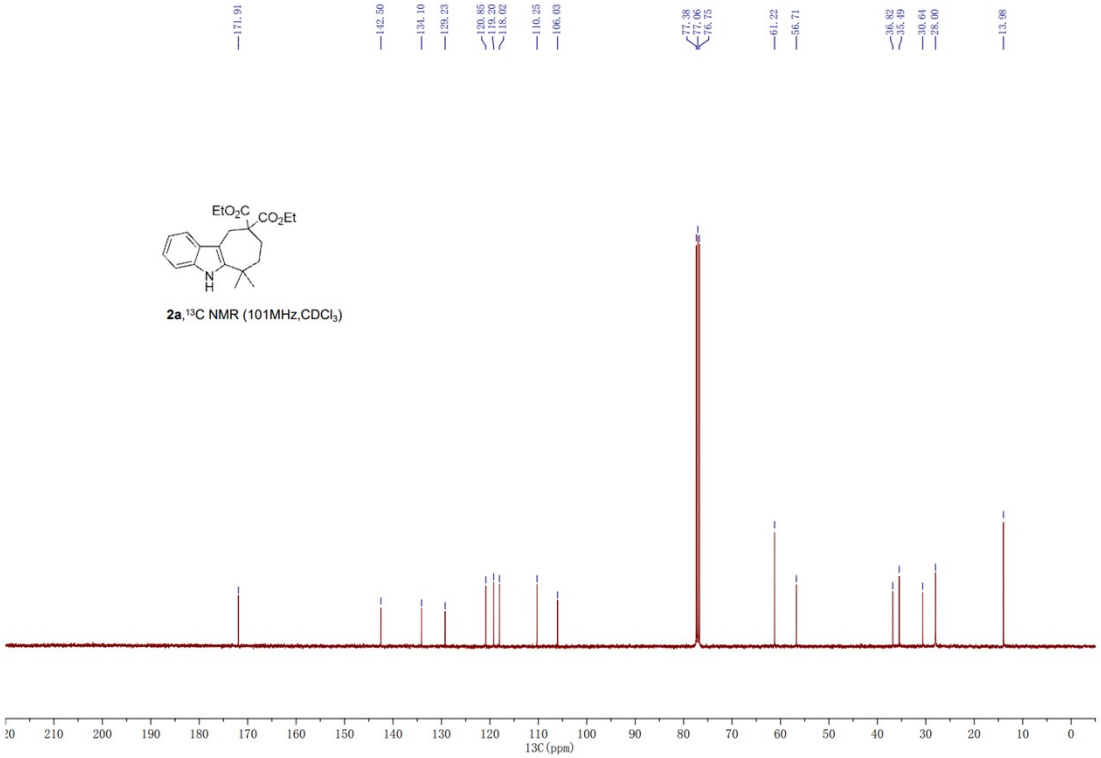

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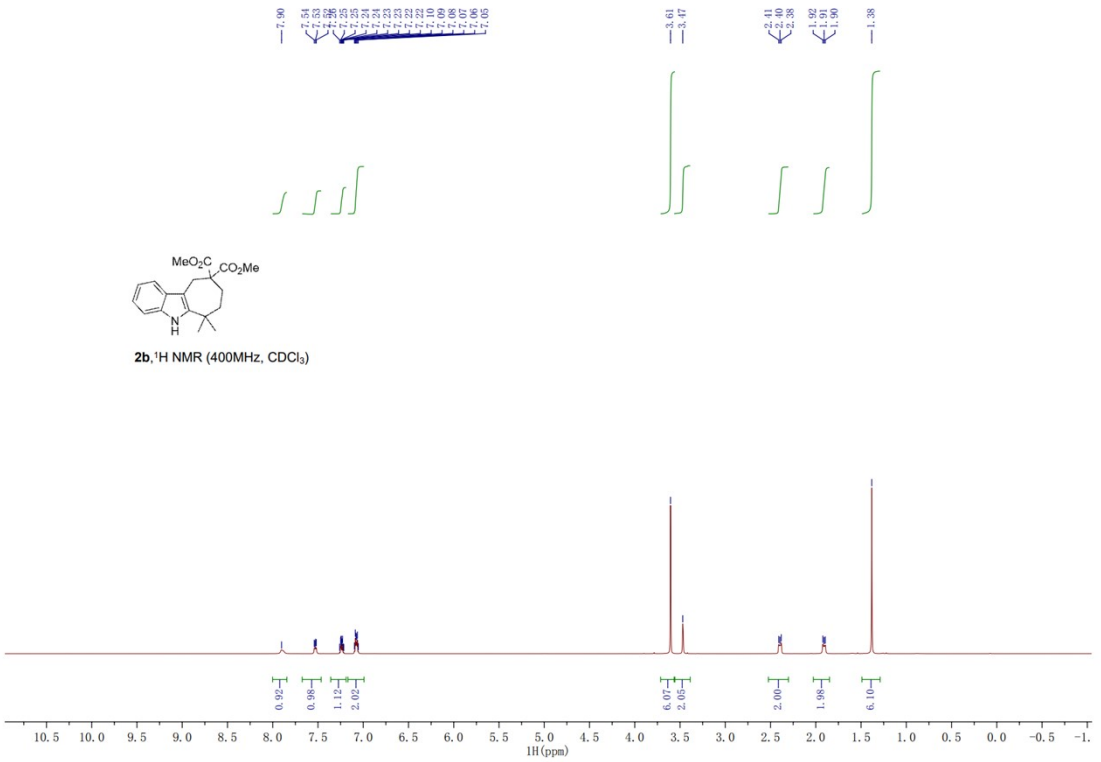

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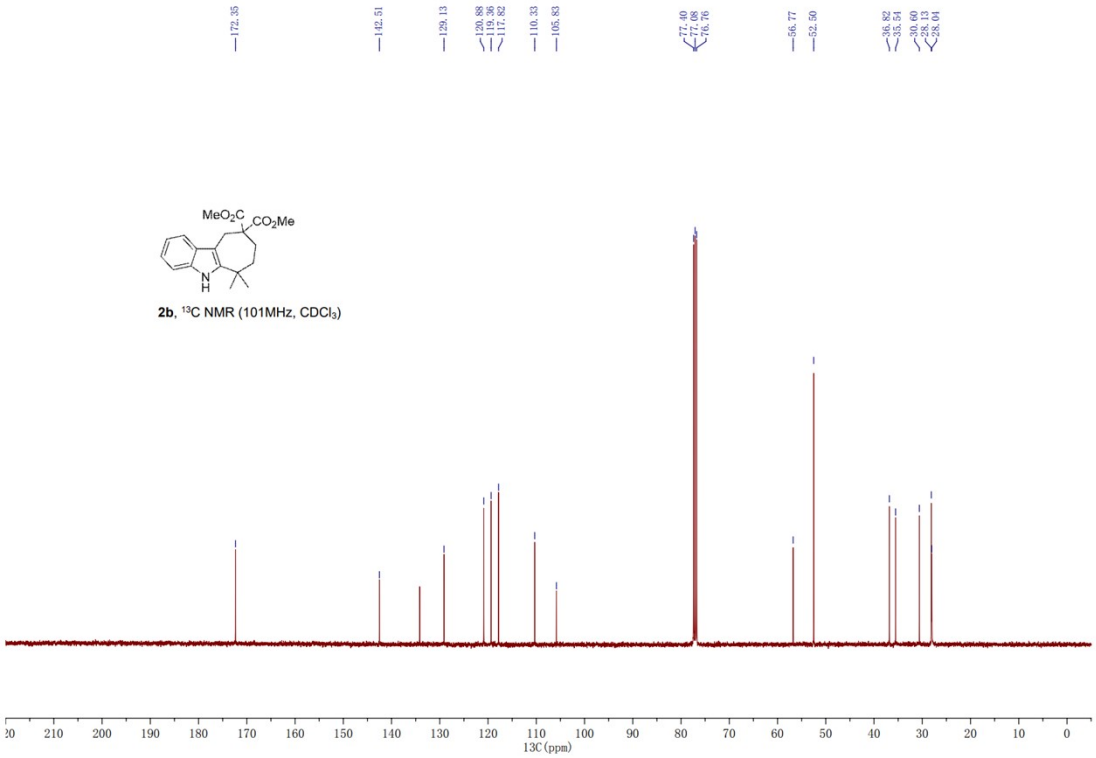

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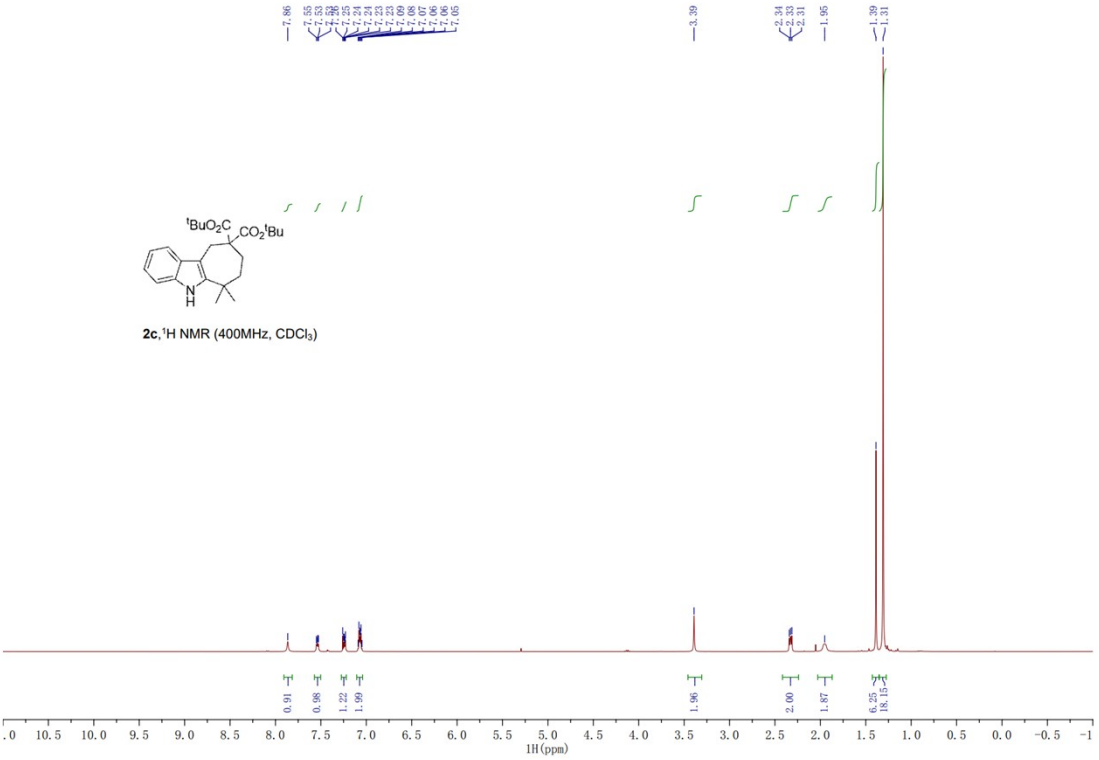

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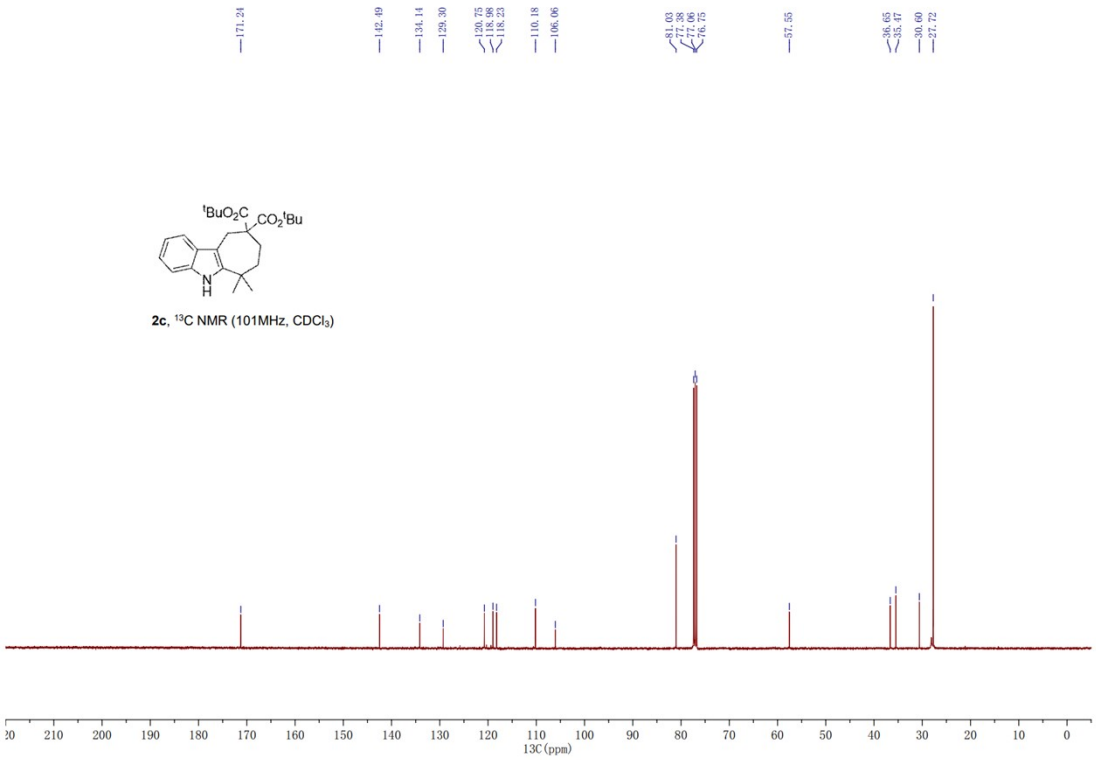

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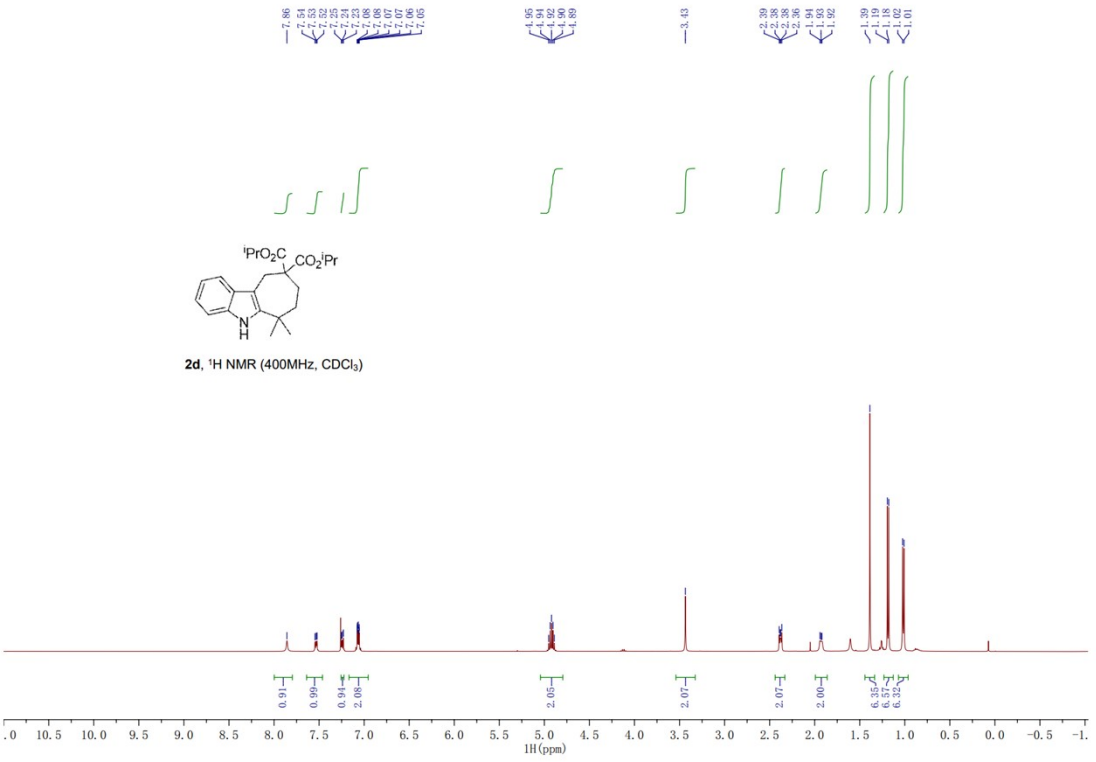

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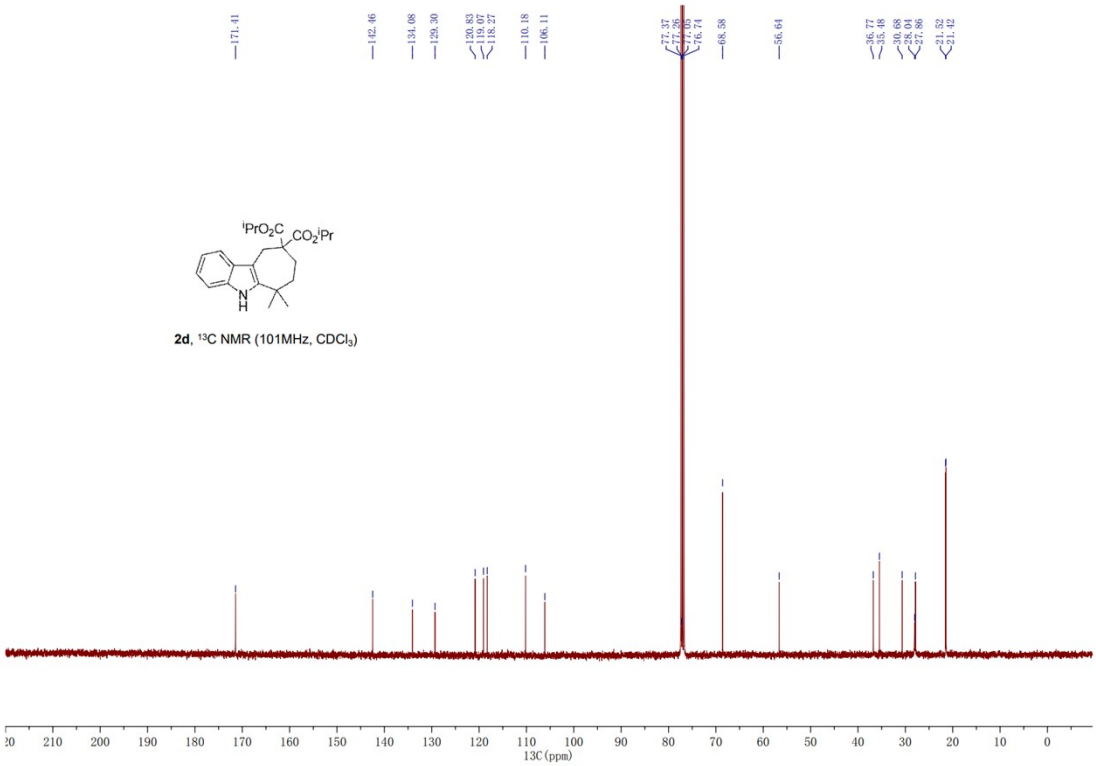

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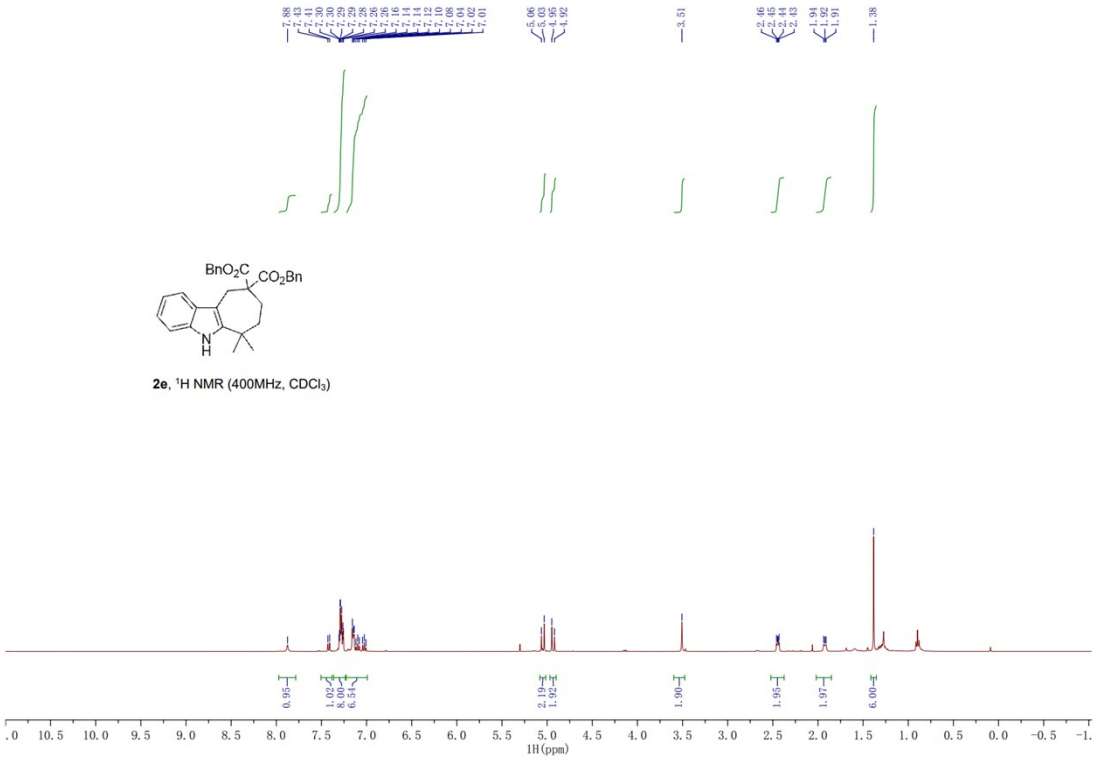
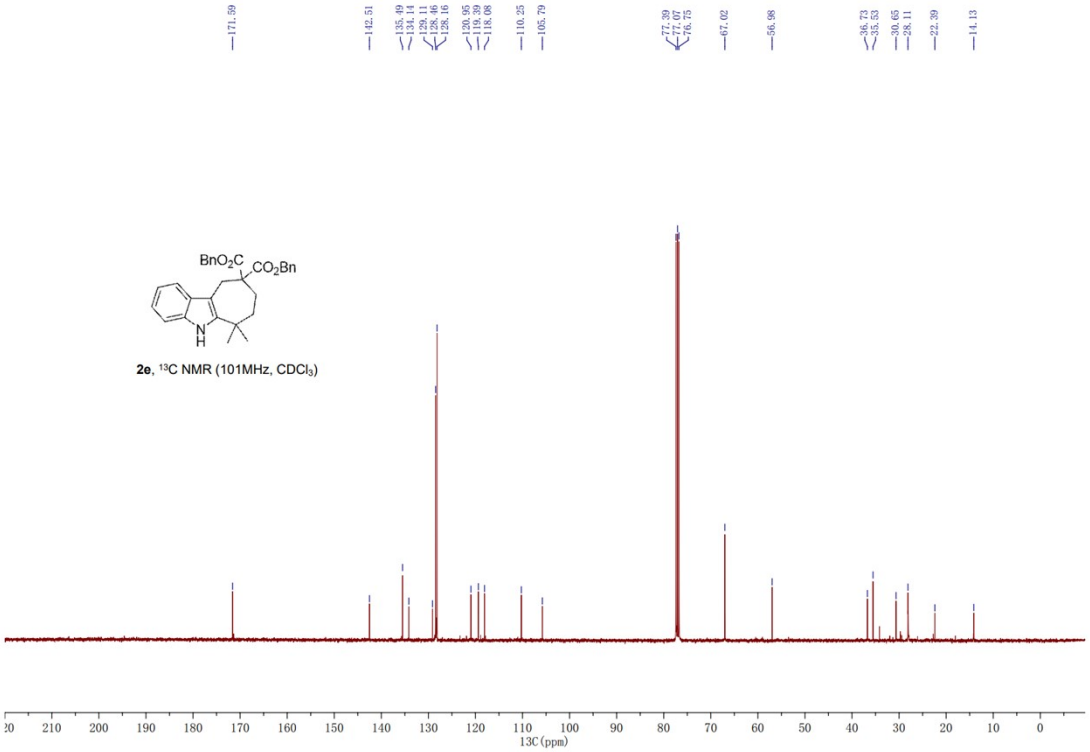
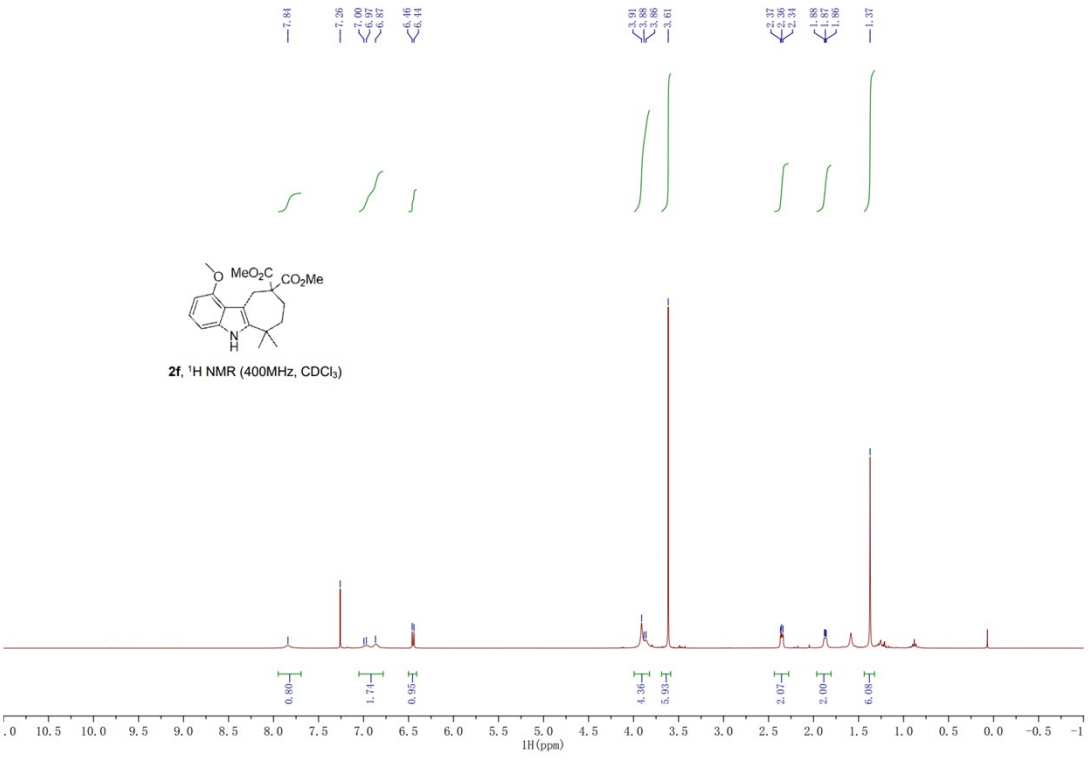


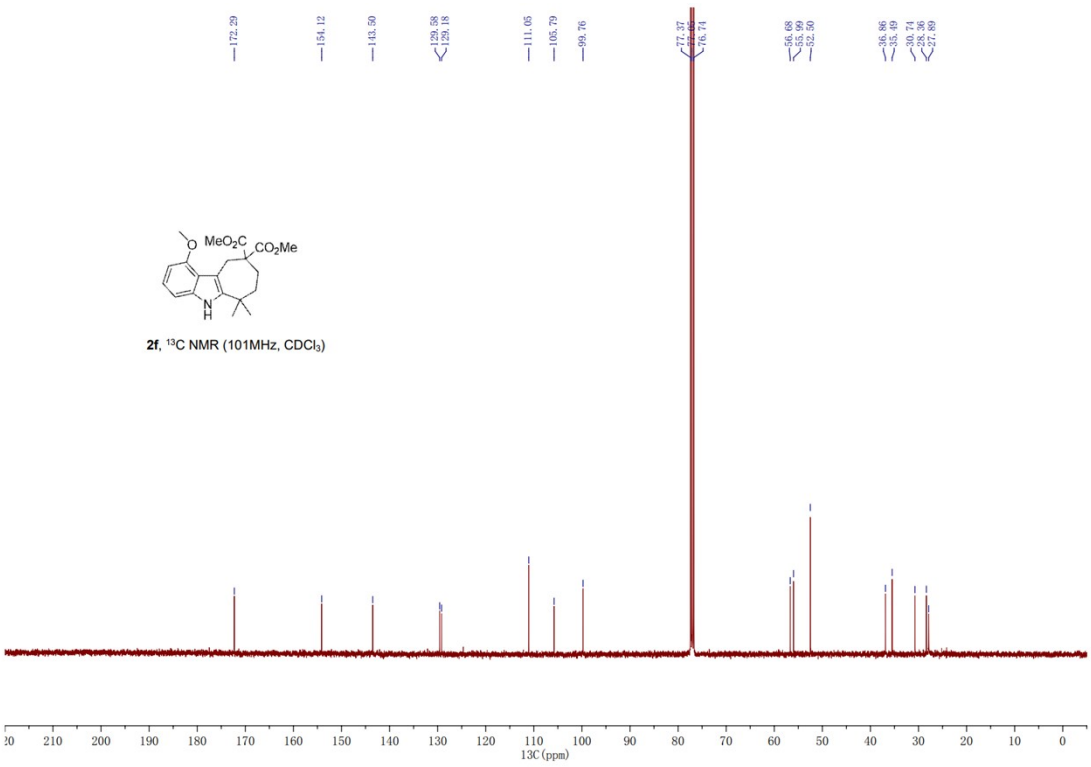
^{1}H NMR of 2e



^{13}C NMR of 2e

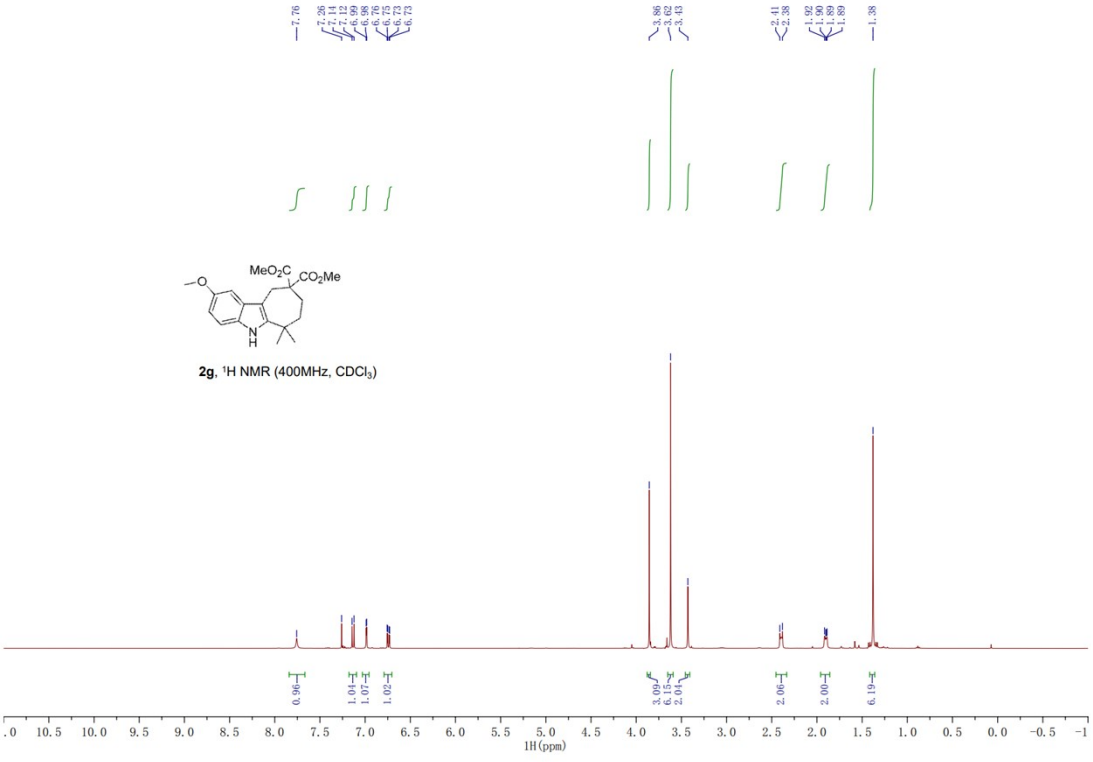


^{1}H NMR of 2f



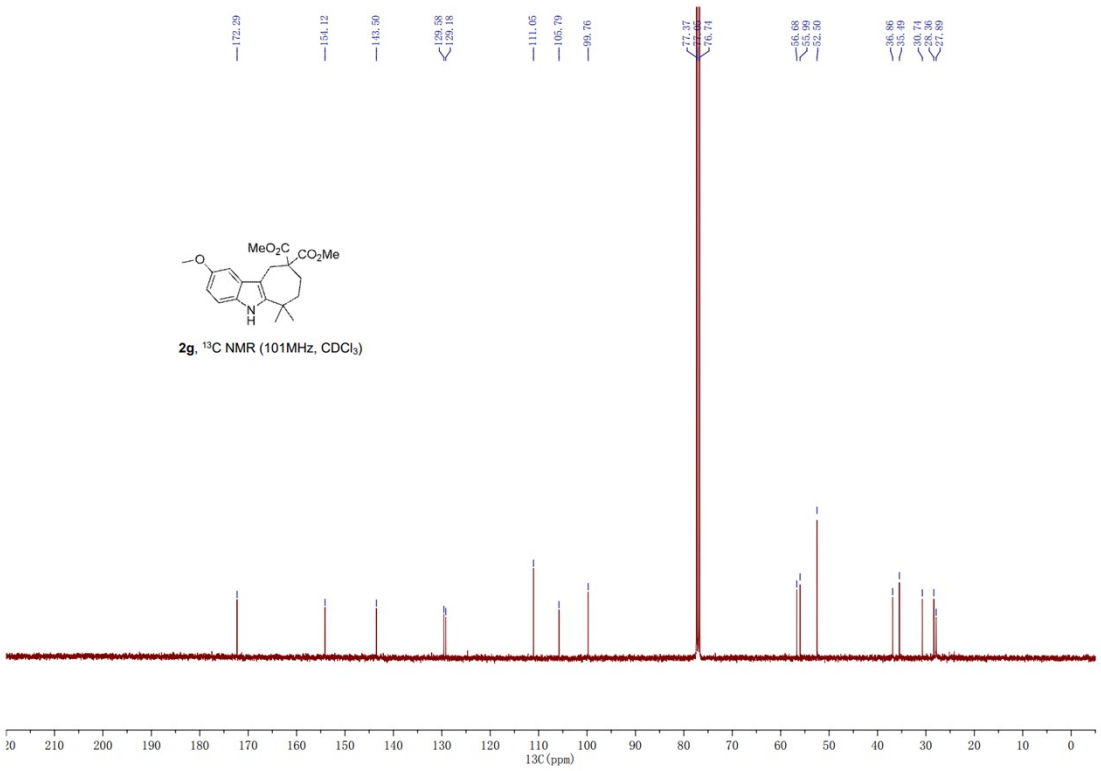
2f, ^{13}C NMR (101MHz, $CDCl_3$)

^{13}C NMR of 2f

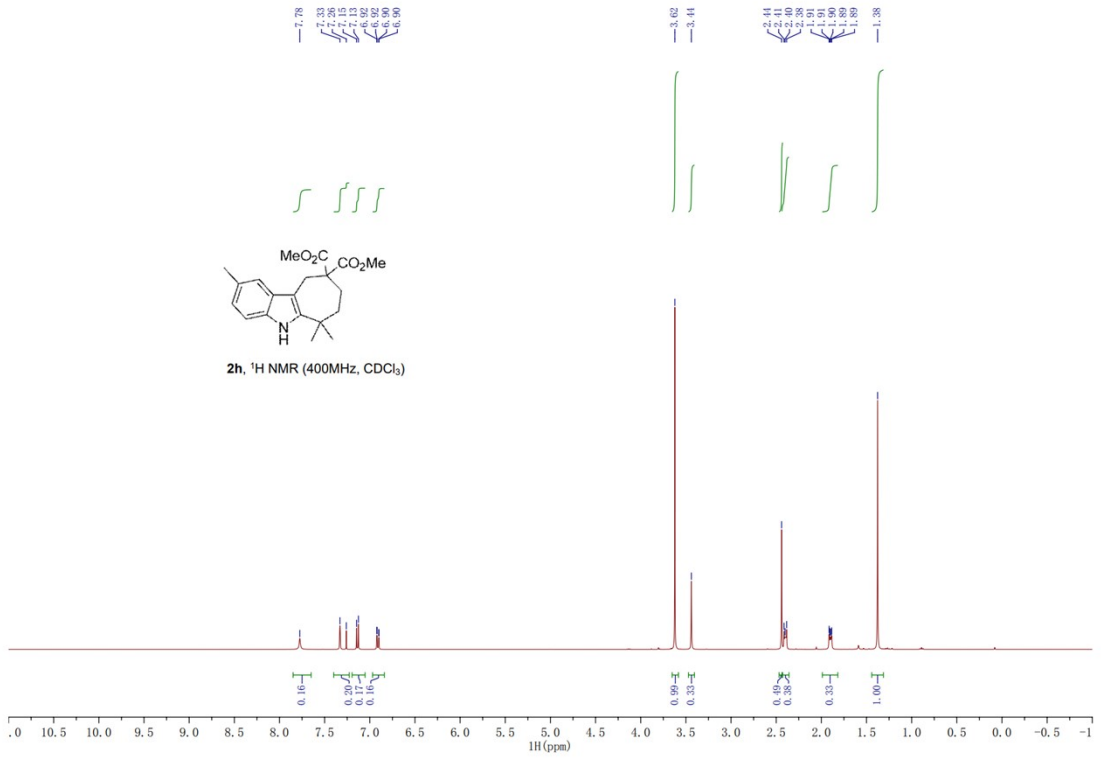


2g, ^{1}H NMR (400MHz, $CDCl_3$)

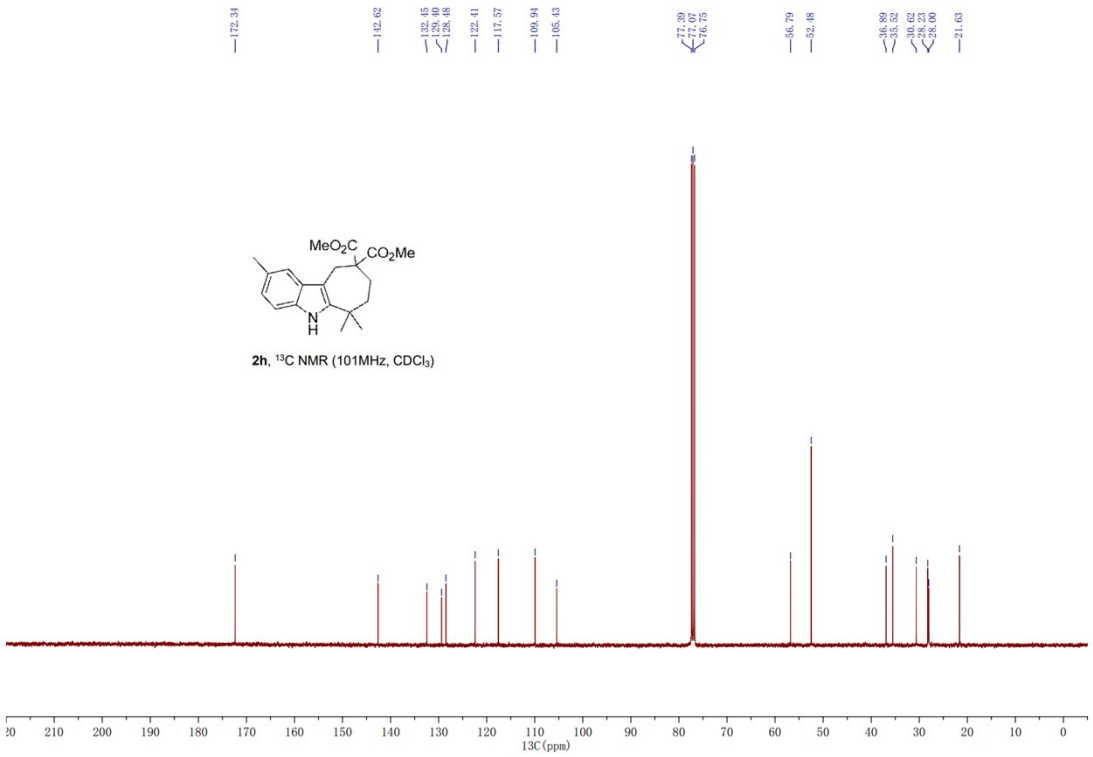
^{1}H NMR of 2g



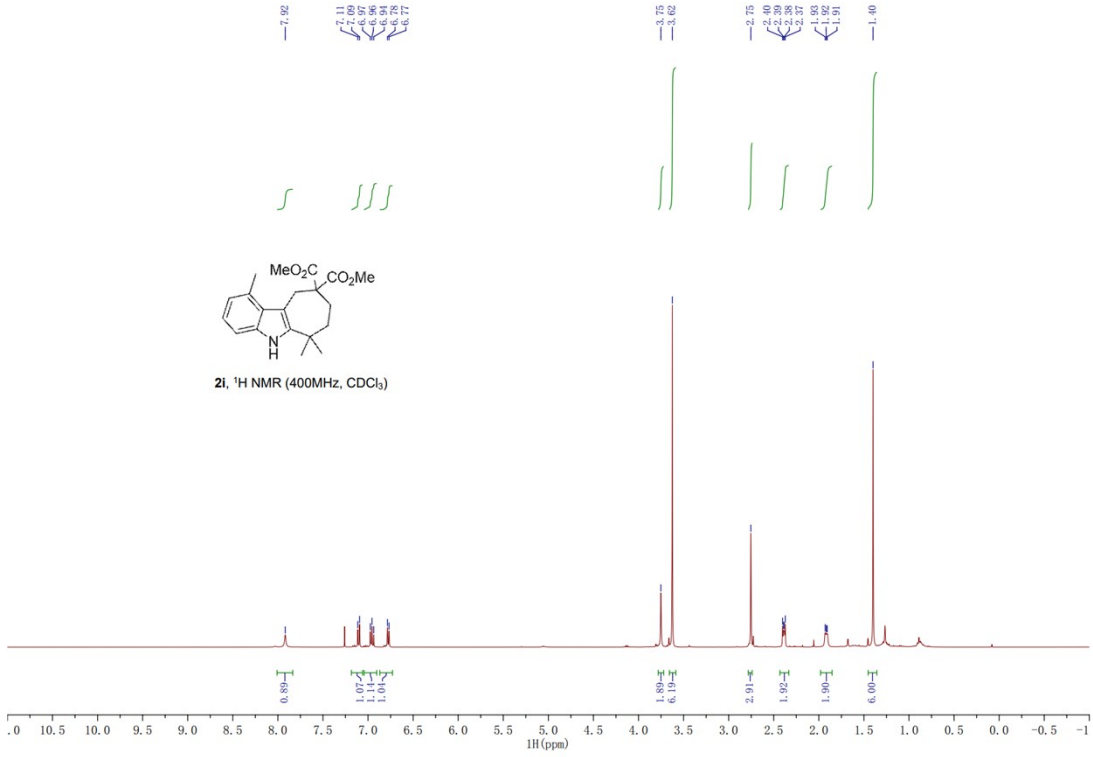
^{13}C NMR of 2g



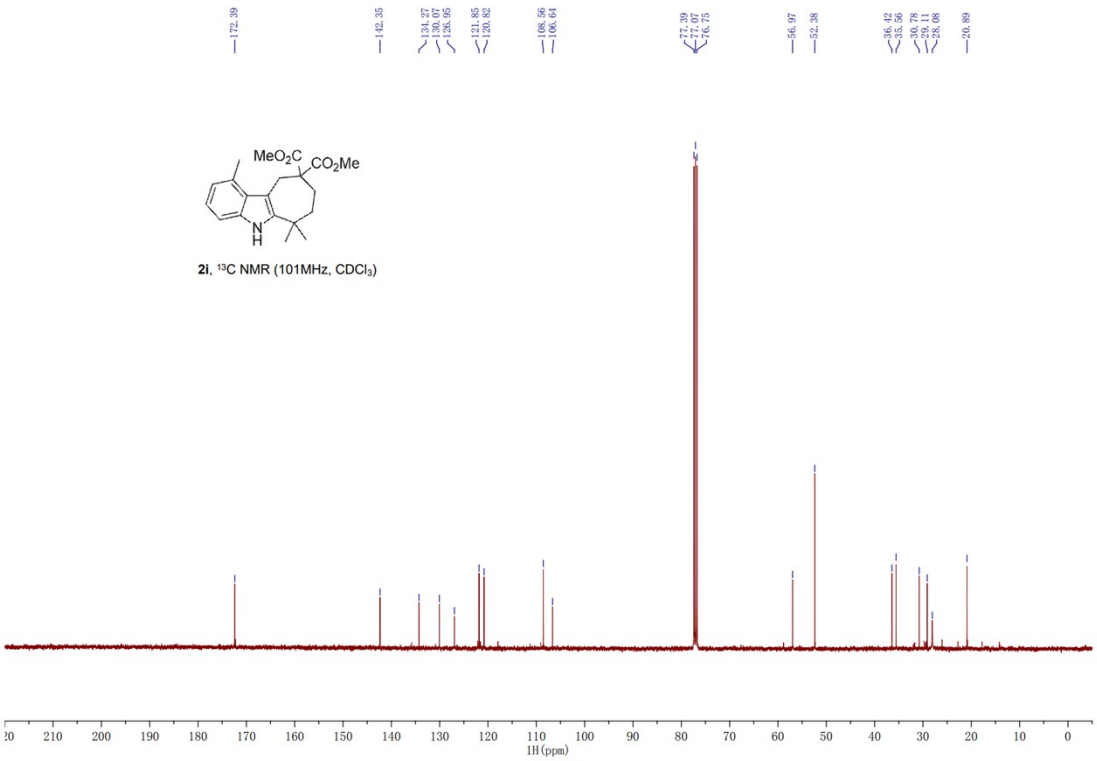
^{1}H NMR of 2h



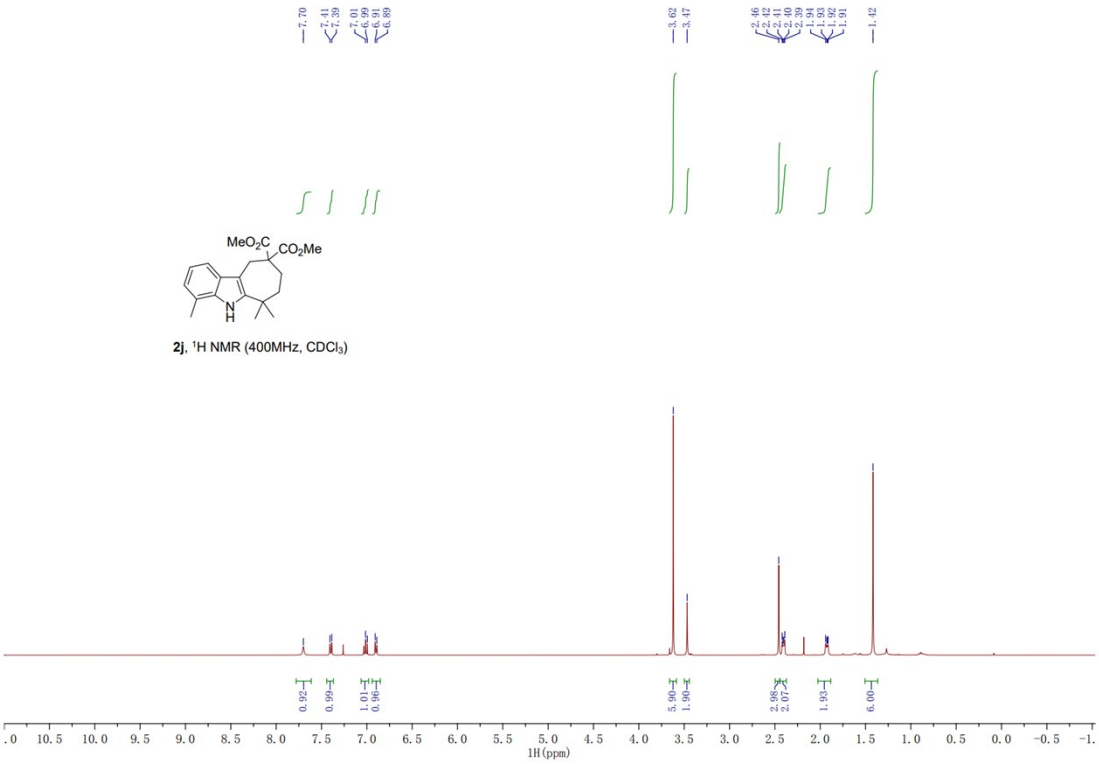
^{13}C NMR of 2h



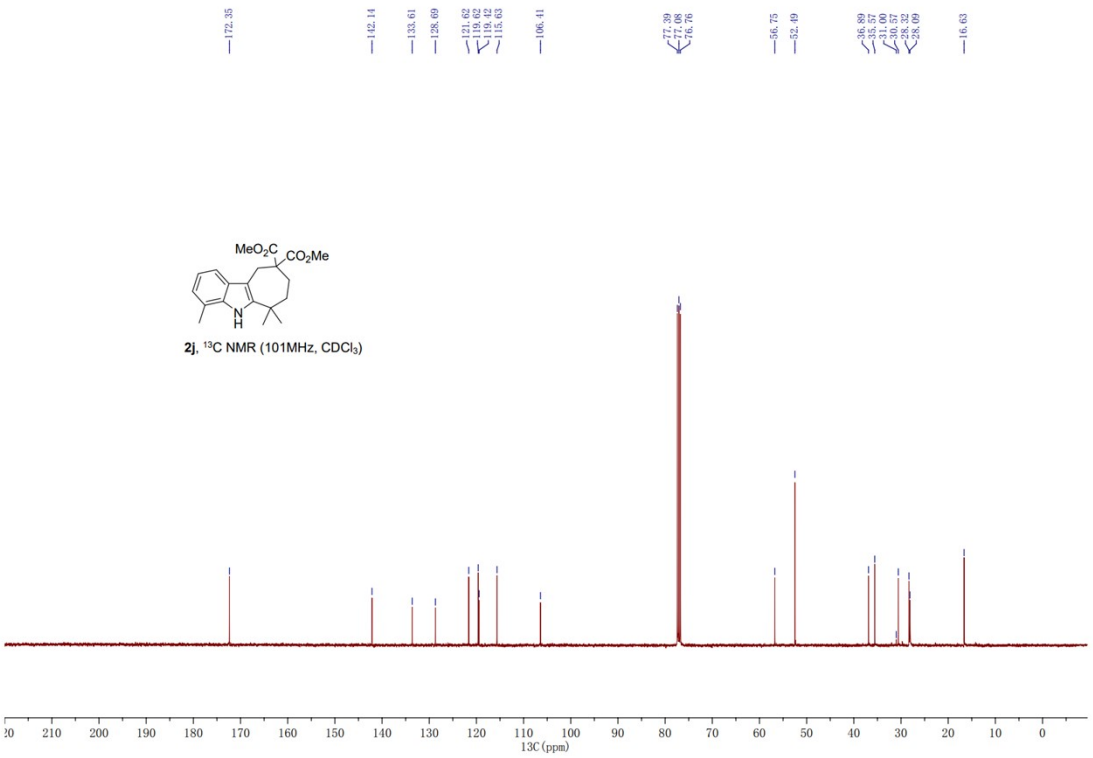
^{1}H NMR of 2l



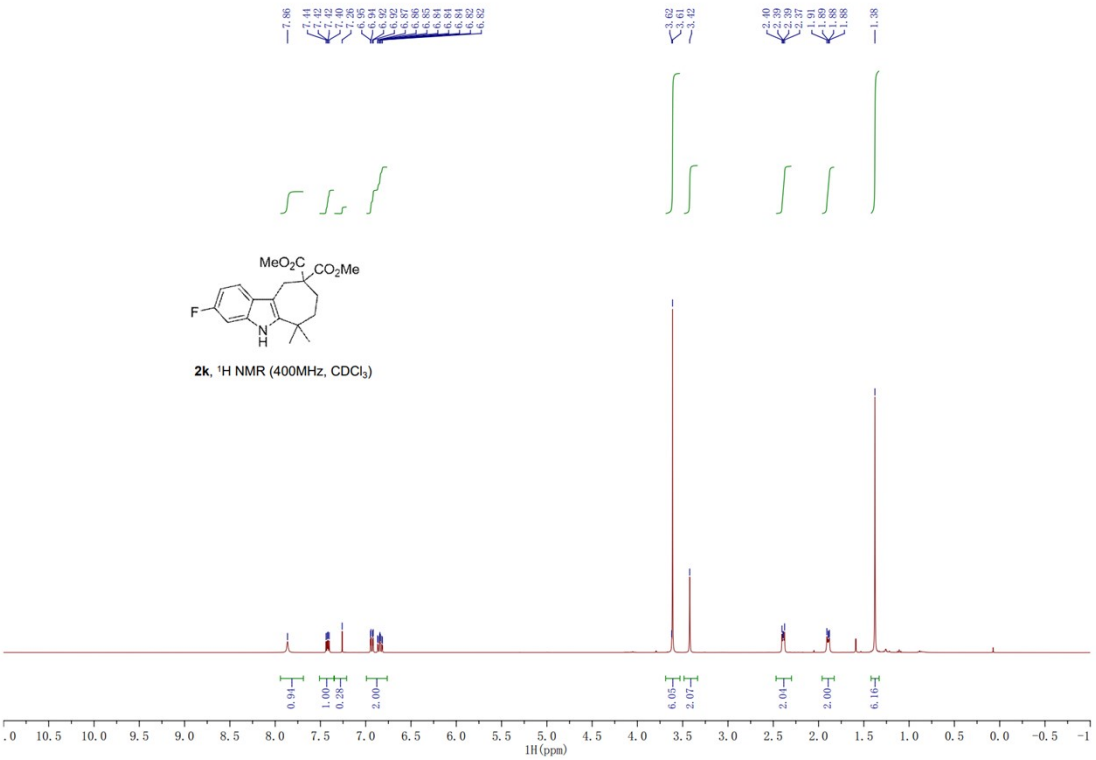
^{13}C NMR of 2l



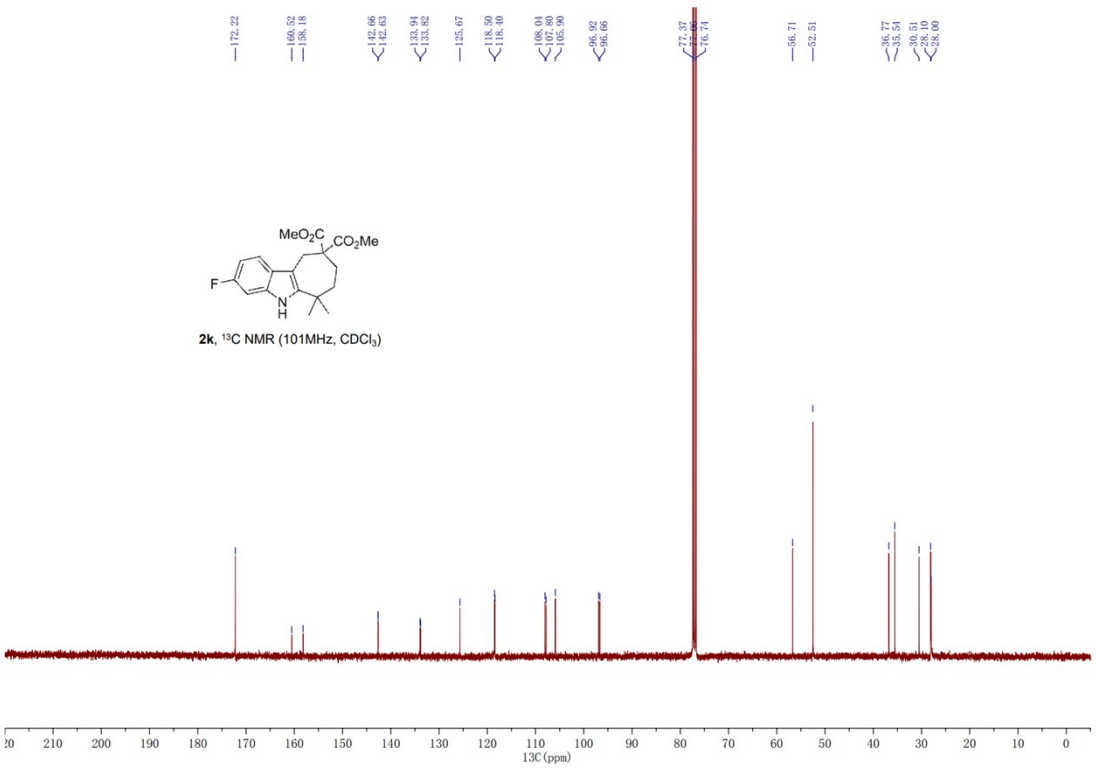
^{1}H NMR of 2j



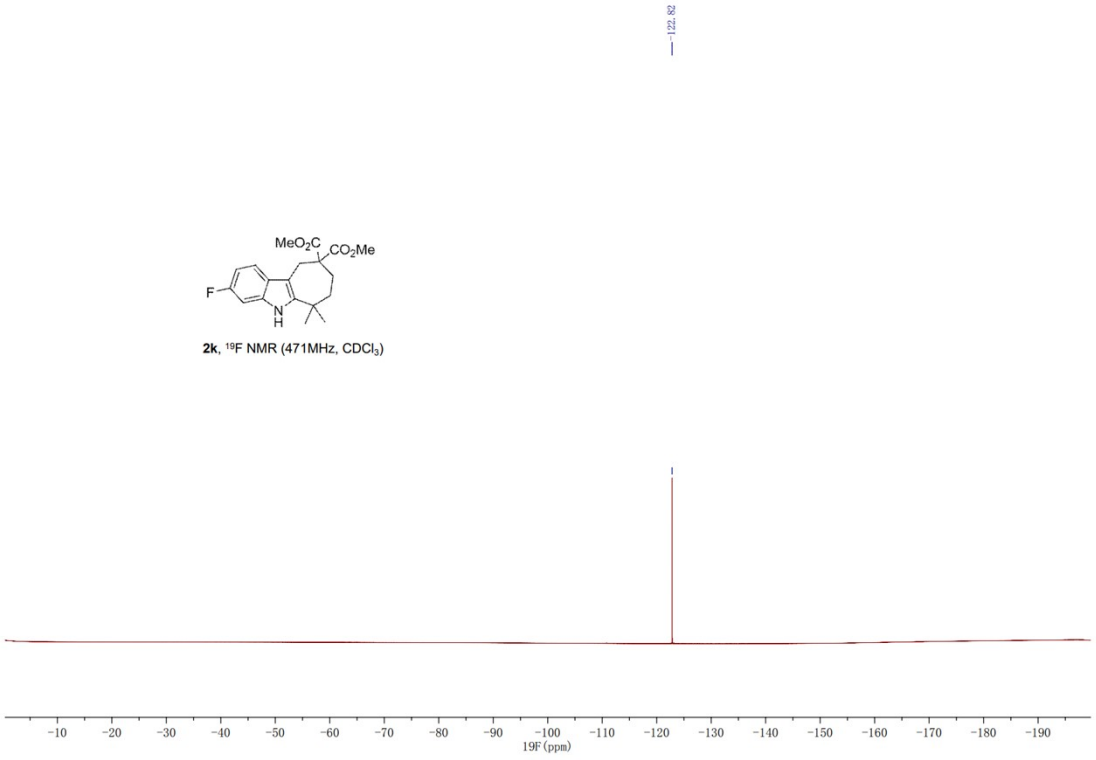
^{13}C NMR of 2j



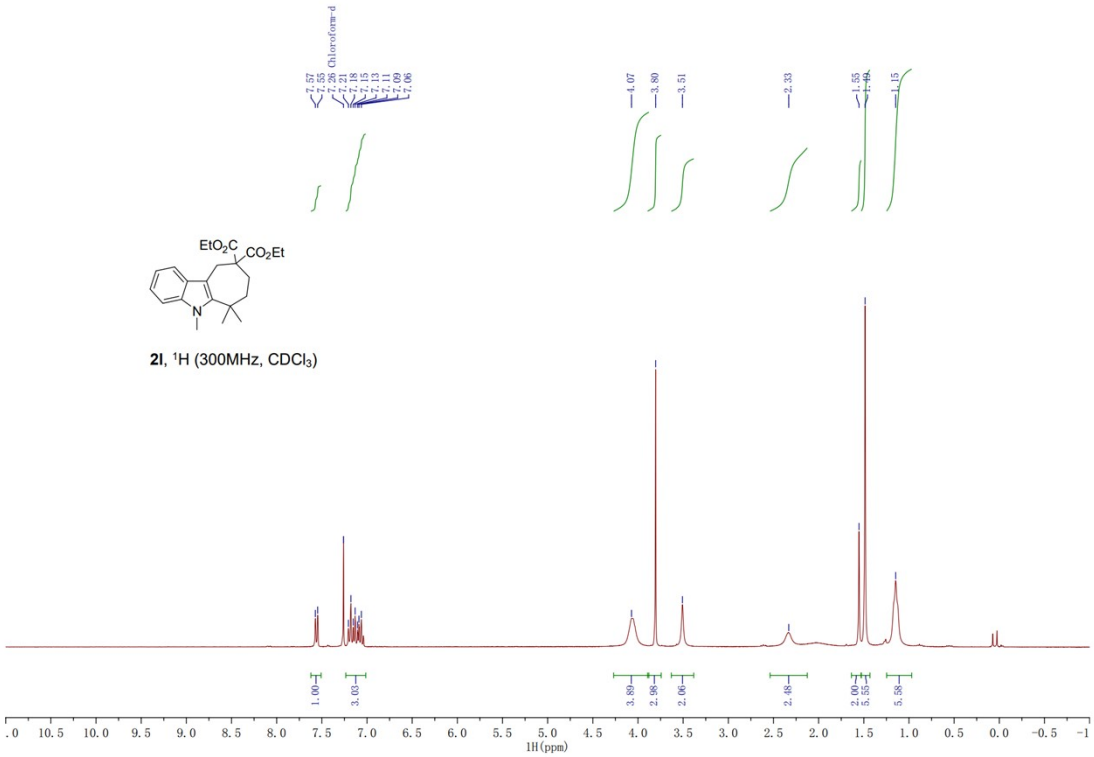
^{1}H NMR of 2k



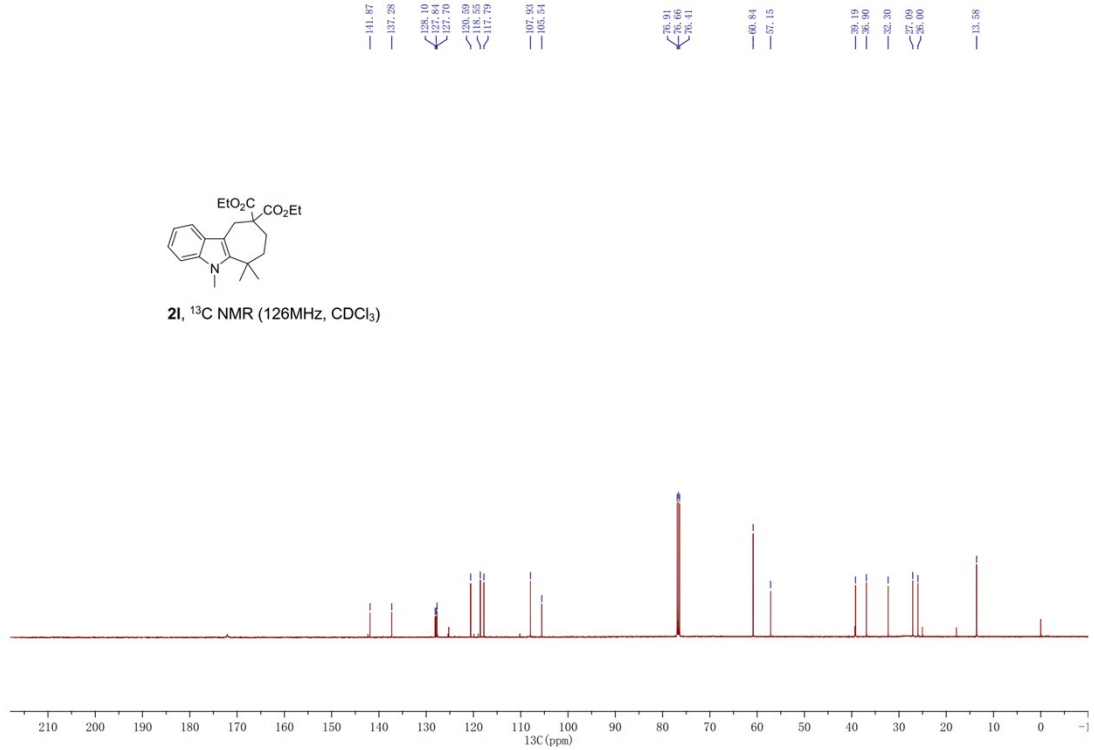
^{13}C NMR of 2k



^{19}F NMR of 2k



^{1}H NMR of 2l



^{13}CNMR of 2l