

Electronic Supporting Information for
Catalytic photoinduced deoxygenation via B(C₆F₅)₃-enabled OAT for aromatic C–H amination of alkylarenes

Zhentao Pan^{1*}, Huanyi Qiu^{2,3}, Lei Wang², Renhua Zheng¹, Yongmin Ma^{2*}

¹School of Pharmaceutical and Chemical Engineering, Taizhou University, Jiaojiang, Zhejiang
318000, P. R. China

²Institute of Advanced Studies and School of Pharmaceutical Sciences, Taizhou University,
Jiaojiang, Zhejiang 318000, P. R. China

³School of Pharmaceutical Science, Zhejiang Chinese Medical University, Hangzhou, Zhejiang,
310053, P. R. China

*Corresponding authors: panzt@tzc.edu.cn; yongmin.ma@tzc.edu.cn

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1 General Information

The reactions were carried out under an inert atmosphere of argon via standard Schlenk techniques or in a glovebox. All visible light-induced reactions were conducted in borosilicate glass tubes with Teflon-coated magnetic stirring bars in a circulating cooling device and placed 5 cm from a commercial blue LEDs. Reactions were monitored by HPLC, ^1H NMR, and/or by TLC on 254 nm silica gel plates (0.2 mm thickness). Thin layer chromatography was performed using hexanes/EtOAc as the eluents and visualized using UV light. Commercial reagents were used without further purification unless otherwise indicated. Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator using a water bath. Flash column chromatography was performed on silica gel (200–300 mesh). All mixed solvent eluents are reported as v/v solutions. Column chromatography was performed. Arenes, *N*-hydroxyphthalimides, boranes, photocatalyst, bases, and solvents were purchased from Energy Chemical (shanghai, china). Commercially available materials purchased from Energy Chemical were used as received. The photoreaction instrument was purchased from 3s-technology co., China, model: 021-AM2410-229, 0~100 W, λ = 460–470 nm, URL: <https://www.3s-tech.net/products/ilmt.html#am>.

NMR spectra data were obtained on Avance (III) HD 400 MHz instruments. ^1H NMR and ^{13}C NMR spectra were referenced to residual protic solvent peaks or TMS signal (0 ppm). ^{19}F NMR chemical shifts were externally referenced to CCl_3F (0 ppm). Data for ^1H NMR are recorded as follows: chemical shift (δ , ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant (J) in Hz, integration). Data for ^{13}C and ^{19}F NMR are reported in terms of chemical shift (δ , ppm). Liquid chromatography (LC) analysis was performed on an Agilent 1200 Infinity II LC system. High resolution mass spectrometer analysis (HRMS) was performed on Waters Q-TOF Premier (ESI) mass spectrometers. Melting point (m.p.): melting points were measured on a Beijing Tech Instrument X-4 digital display micro melting point apparatus and are uncorrected. Visible light luminescence intensities were recorded using Shimadzu UV-2600i UV-Vis spectrofluorometer. Cyclic voltammograms were recorded using a CHI 660E potentiostat and a Pt working electrode, a Ag/AgCl reference electrode and a Pt sheet auxiliary electrode.

Photochemical Setup

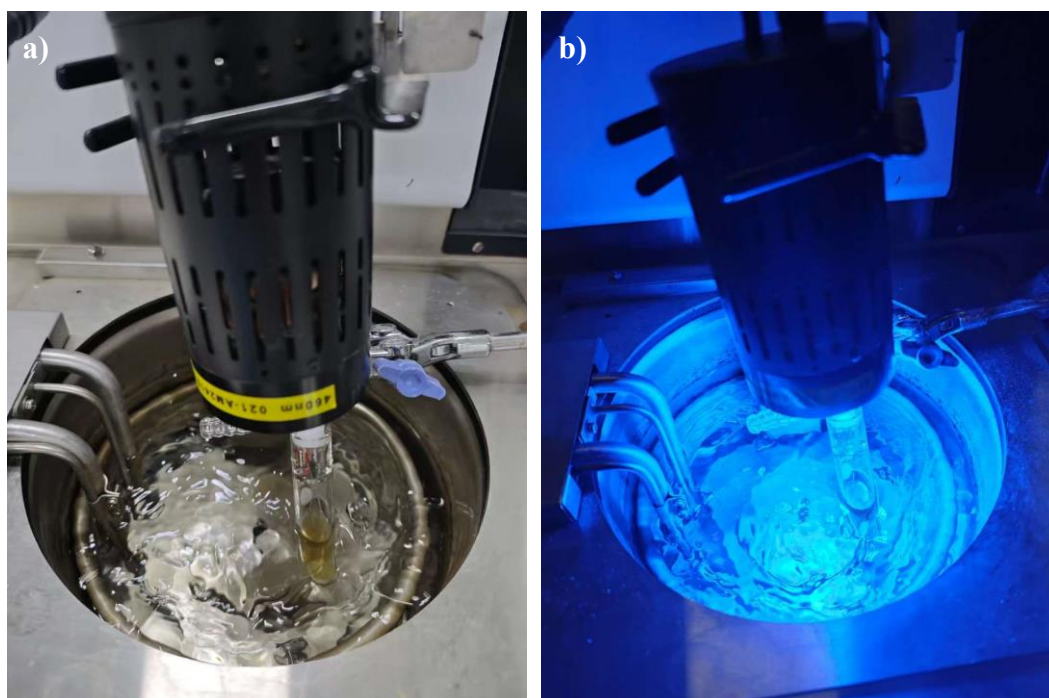


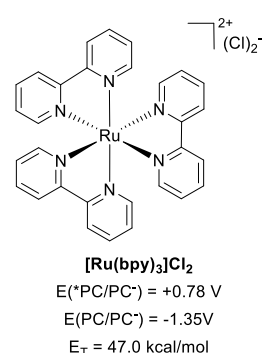
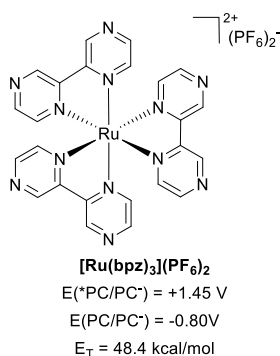
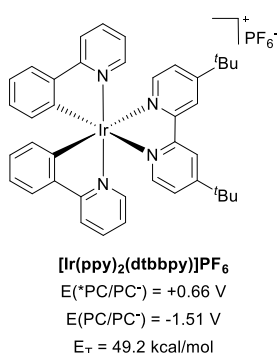
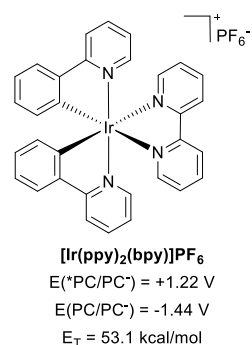
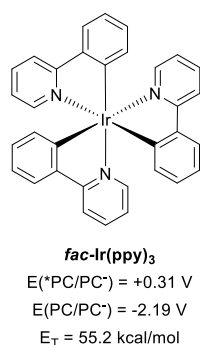
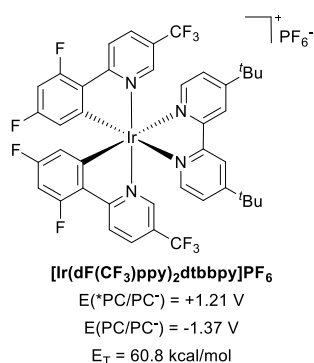
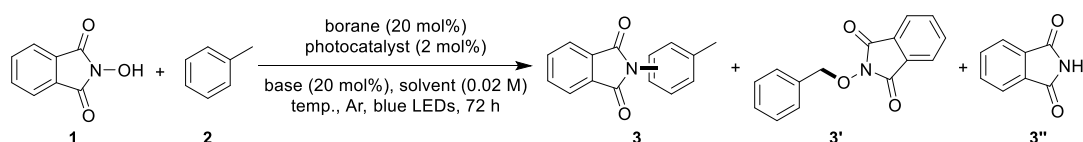
Figure S1. General reaction setup

2 Reaction Optimization

General Procedure for the Reaction Optimization

To a dry Schlenk tube equipped with a magnetic stir bar was added NHPI (**1**) (16.3 mg, 0.1 mmol, 1 equiv.), borane (0.02 mmol, 20 mol%), photocatalyst (0.002 mmol, 2 mol%) and base (0.02 mmol, 20 mol%) and the Schlenk tube was evacuated and backfilled with Ar (three times). After addition of a solution of solvent (5.0 mL, 0.02 M) containing toluene (**2**) (46 mg, 0.5 mmol, 5 equiv.) by syringe under Ar, the Schlenk tube was positioned approximately 5 cm away from a 25 W blue LEDs lamp. Then the reaction mixture was stirred at the corresponding temperature for 72 h. After completion, the reaction mixture was concentrated to dryness. The yield was determined by ^1H NMR analysis of the crude product using 1,3,5-trimethoxybenzene (16.8 mg, 0.1 mmol, 1.0 equiv.) as the internal standard.

Table S1. Reaction optimization

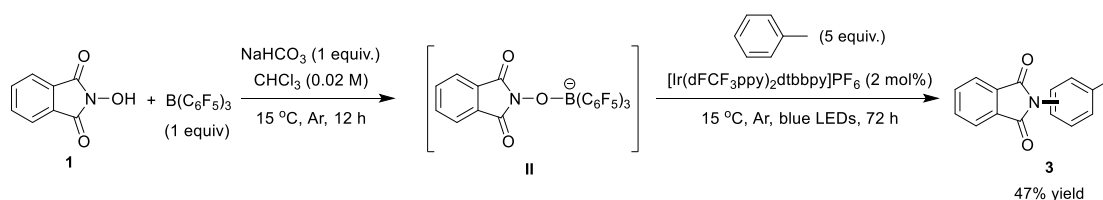


entry	boron	photocatalyst	base	solvent	temp. (°C)	yield (%) (3a/3a'/3a'')
1	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	68/<1/17
2	B(3,4,5-F ₃ C ₆ H ₂) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	30/43/8
3	Ph ₃ B	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	11/62/3
4	BCl ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	<1/70/<1
5	B(C ₆ F ₅) ₃	<i>fac</i> -Ir(ppy) ₃	NaHCO ₃	CHCl ₃	15	47/<1/11
6	B(C ₆ F ₅) ₃	[Ir(ppy) ₂ (bpy)]PF ₆	NaHCO ₃	CHCl ₃	15	35/<1/9
7	B(C ₆ F ₅) ₃	[Ir(ppy) ₂ (dtbbpy)]PF ₆	NaHCO ₃	CHCl ₃	15	18/<1/4
8	B(C ₆ F ₅) ₃	[Ru(bpz) ₃](PF ₆) ₂	NaHCO ₃	CHCl ₃	15	<1/<1/<1
9	B(C ₆ F ₅) ₃	[Ru(bpy) ₃]Cl ₂	NaHCO ₃	CHCl ₃	15	<1/<1/<1
10	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	Na ₂ CO ₃	CHCl ₃	15	57/<1/13
11	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	K ₂ HPO ₄	CHCl ₃	15	32/<1/9
12	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	Et ₃ N	CHCl ₃	15	<1/<1/<1
13	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	DBU	CHCl ₃	15	<1/<1/<1
14	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CH ₂ Cl ₂	15	56/<1/14
15	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CH ₃ CN	15	34/<1/9
16	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	MeOH	15	<1/<1/<1
17	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	EtOAc	15	27/<1/7
18	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	MTBE	15	<1/<1/<1
19	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	30	48/<1/37
20	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	0	11/<1/<1
21 ^a	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	38/<1/16
22 ^b	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	68/<1/16
23 ^c	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	49/<1/13
24	-	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	<1/73/<1
25	B(C ₆ F ₅) ₃	-	NaHCO ₃	CHCl ₃	15	<1/<1/<1
26	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	-	CHCl ₃	15	27/<1/9
27 ^d	B(C ₆ F ₅) ₃	[Ir(dFCF ₃ ppy) ₂ dtbbpy]PF ₆	NaHCO ₃	CHCl ₃	15	<1/<1/<1

^a Reaction performed in 1 mL of CHCl₃. ^b Reaction performed with 10 equiv. of **2**. ^c Reaction performed with 2.5 equiv. of **2**. ^d Reaction performed in the dark.

3 Mechanistic Investigations

3.1 Two-Step Experiment



Step 1: To a dry Schlenk tube equipped with a magnetic stir bar was added *N*-hydroxyphthalimide (**1**) (16.3 mg, 0.1 mmol, 1 equiv.), $\text{B}(\text{C}_6\text{F}_5)_3$ (51.2 mg, 0.1 mmol, 1 equiv.), NaHCO_3 (8.4 mg, 0.1 mmol, 1 equiv.) and 5 mL CHCl_3 , the Schlenk tube was evacuated and backfilled with Ar (three times). Then the reaction mixture was stirred at the 15 °C for 12 h and a red suspension was obtained. The red solid $\text{Phth-O-B}(\text{C}_6\text{F}_5)_3$ anion (**II**) could be further separated by filtration and characterized by ^1H (Figure S1), ^{19}F NMR (Figure S2) and HRMS (Figure S3).

Step 2: Add toluene (**2**) (46 mg, 0.5 mmol, 5 equiv.) and $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ (2.2 mg, 0.002 mmol, 2.0 mol%) into the red suspension in a argon-filled glovebox. Then the Schlenk tube was positioned approximately 5 cm away from a 25 W blue LEDs lamp. The reaction mixture was stirred at 15 °C for 72 h. After completion, the reaction mixture was concentrated to dryness. The yield was determined by ^1H NMR analysis of the crude product using 1,3,5-trimethoxybenzene (16.8 mg, 0.1 mmol, 1.0 equiv.) as the internal standard.

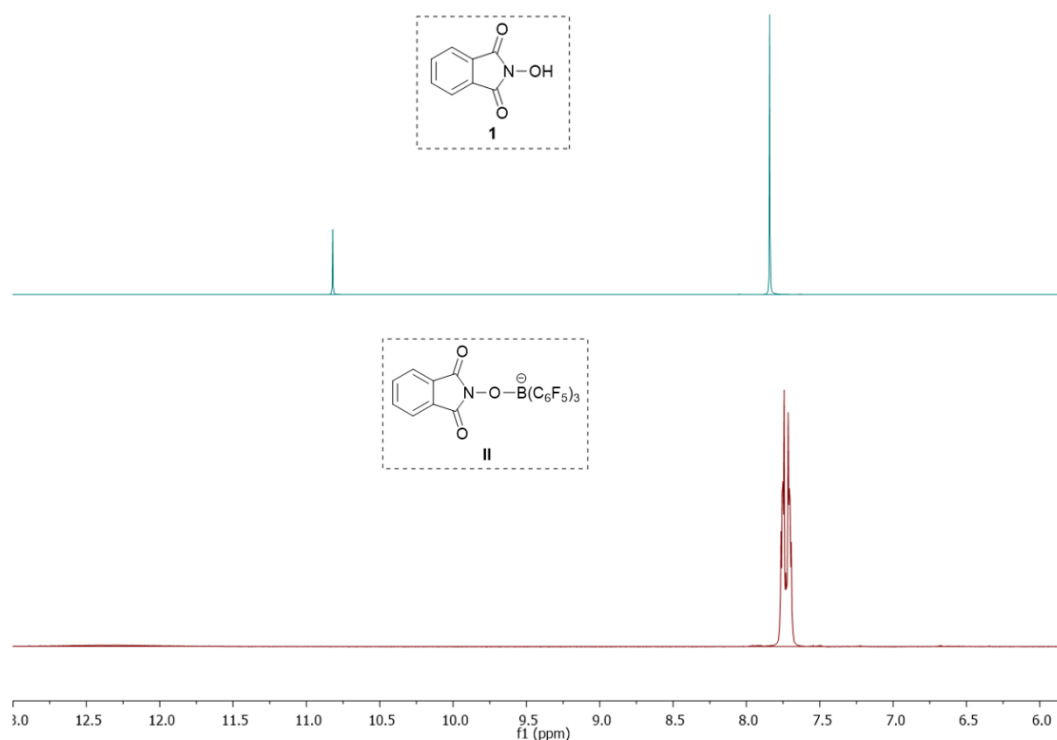


Figure S2. ^1H NMR of NHPI (**1**) and $\text{PhthN-O-B}(\text{C}_6\text{F}_5)_3$ anion (**II**)

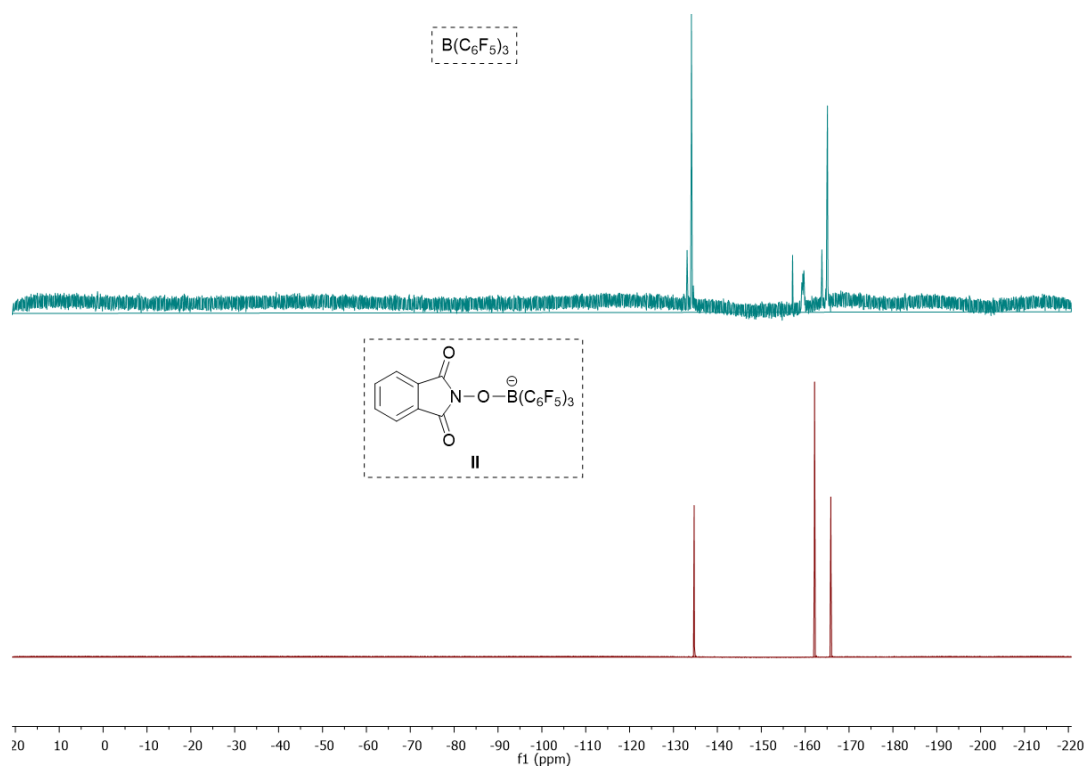


Figure S3. ^{19}F NMR of $\text{B}(\text{C}_6\text{F}_5)_3$ and PhthN-O-B(C₆F₅)₃ anion (II)

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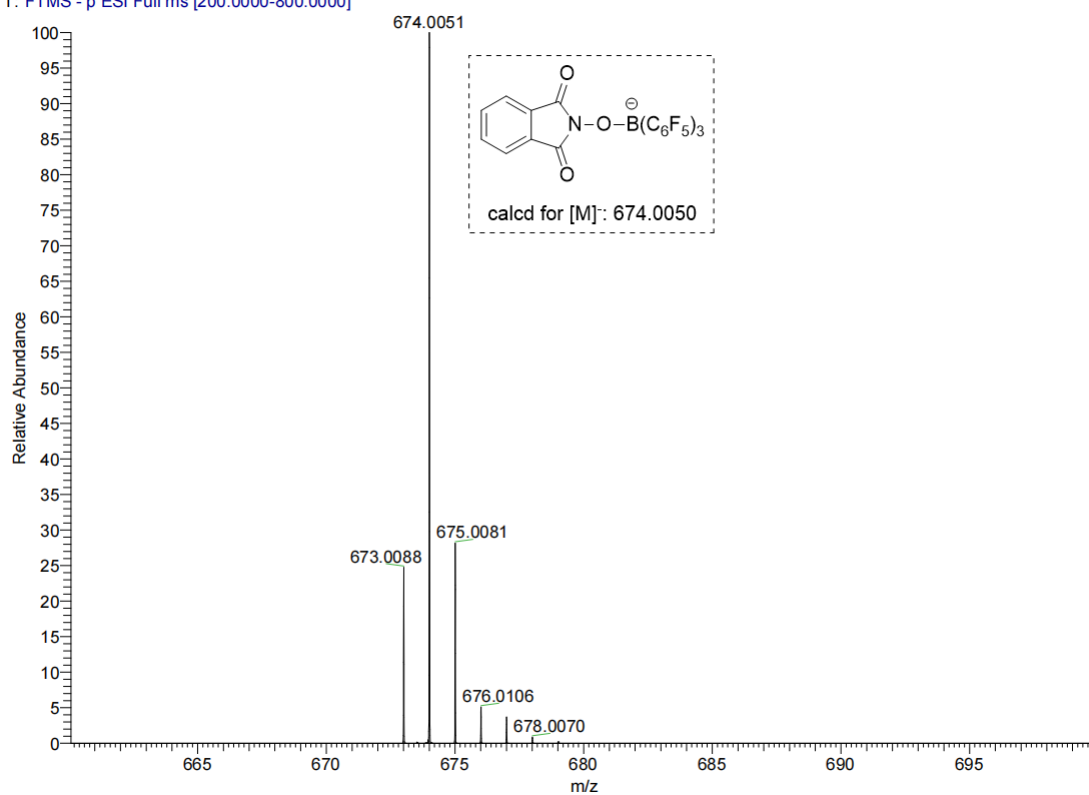


Figure S4. HRMS spectrum of PhthN-O-B(C₆F₅)₃ anion (II)

3.2 Stern–Volmer Luminescence Quenching Studies

Visible light luminescence intensities were recorded using a Shimadzu UV-Vis (UV-2600i) spectrofluorometer. All luminescence measurements were recorded using a screw-top quartz cuvette (Hellma fluorescence quartz cuvette, 10 x 10 mm, 3.5 mL). A stock solution of $[\text{Ir}(\text{dF}(\text{CF}_3)\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ in CHCl_3 with concentration $2\ \mu\text{M}$ was prepared. $3\ \text{mM}$ solution of $\text{PhthN-O-B}(\text{C}_6\text{F}_5)_3$ (**II**), *N*-hydroxyphthalimide (**1**) and $\text{B}(\text{C}_6\text{F}_5)_3$ were prepared in CHCl_3 . For each quenching experiment, $50\ \mu\text{L}$ of quencher solution was added to $3\ \text{mL}$ of $[\text{Ir}(\text{dF}(\text{CF}_3)\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ solution. Addition of $50\ \mu\text{L}$ of quencher solution leads to an increase of $50\ \mu\text{M}$ quencher concentration in the solution. Samples were excited at $430\ \text{nm}$ and the emission was measured at $600\ \text{nm}$. The Stern–Volmer analysis was conducted according to the following relationship:

$$I_0/I = 1 + K_{\text{sv}}[Q]$$

Where, I_0 is the luminescence intensity of the catalyst solution without the quencher, and I is the intensity in presence of the quencher. $[Q]$ is concentration of quencher and K_{sv} is quenching rate constant.

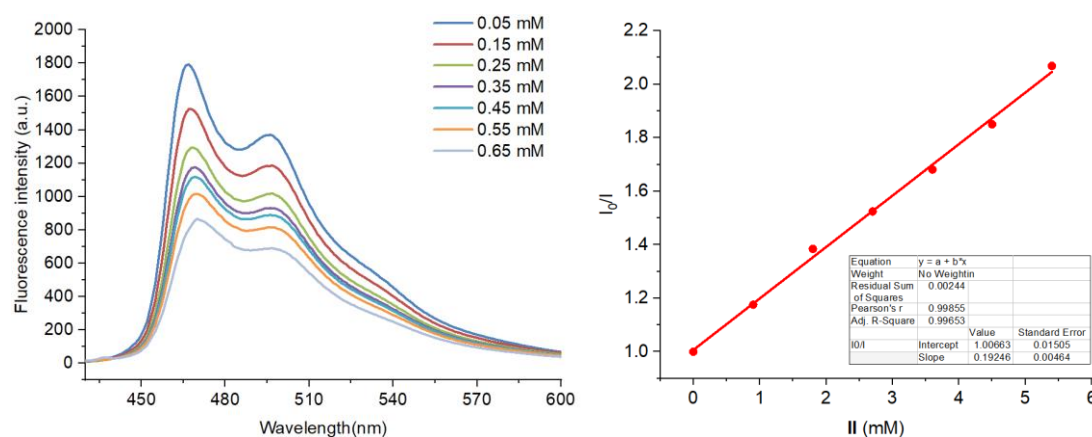


Figure S5. Emission spectra for $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ luminescence quenching by $\text{PhthN-O-B}(\text{C}_6\text{F}_5)_3$ anion (**II**) as additive (left) and Stern-Volmer plot (right).

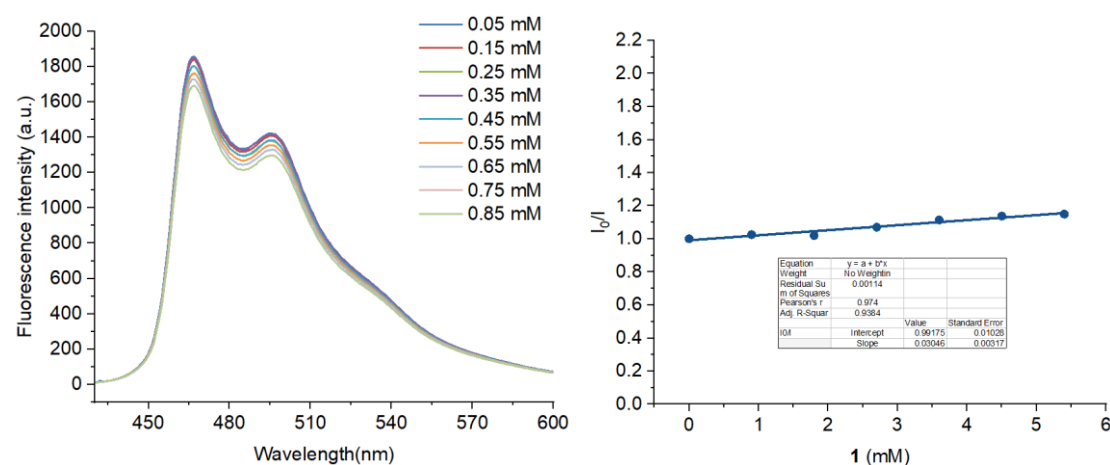


Figure S6. Emission spectra for $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ luminescence quenching by *N*-hydroxyphthalimide (**1**) as additive (left) and Stern-Volmer plot (right).

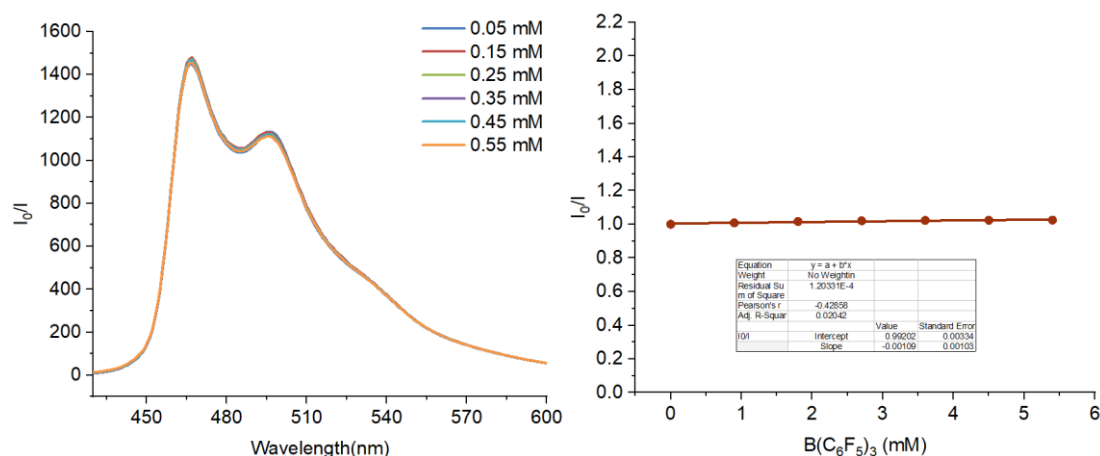


Figure S7. Emission spectra for $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ luminescence quenching by $\text{B}(\text{C}_6\text{F}_5)_3$ as additive (left) and Stern-Volmer plot (right).

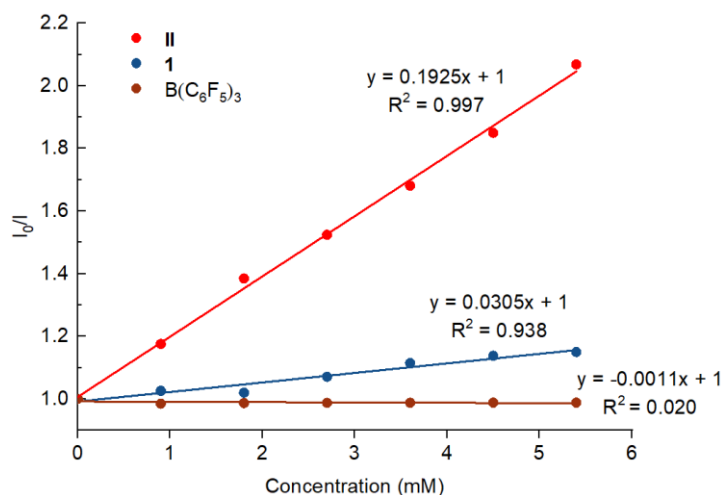


Figure S8. Stern–Volmer fluorescence quenching plot of $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ with various quenchers.

3.3 Cyclic Voltammograms Studies

Cyclic voltammograms were recorded using a CHI 660E potentiostat and a Pt working electrode, a Ag/AgCl reference electrode and a Pt sheet auxiliary electrode. The voltammograms were recorded at room temperature in 0.1 M tetrabutylammonium hexafluorophosphate in CHCl_3 (3 mL) containing $\text{PhthN-O-B}(\text{C}_6\text{F}_5)_3$ anion (**II**) (3.4 mg, 0.005 mmol). The scan rate was 10 mV/s.

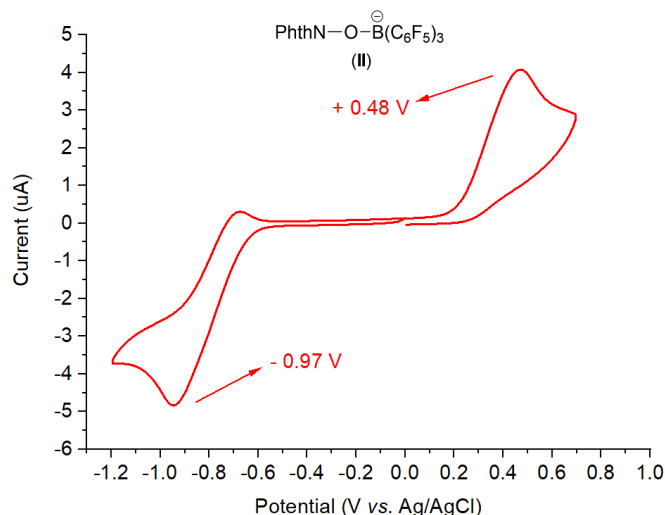


Figure S9. Cyclic Voltammetry for reduction and oxidation of PhthN–O–B(C₆F₅)₃ (**II**) in CHCl₃. An oxidation peak at E_{ox} = + 0.48 V and reduction peak at E_{red} = – 0.97 V are observed.

3.4 UV-Vis Absorption Spectrum

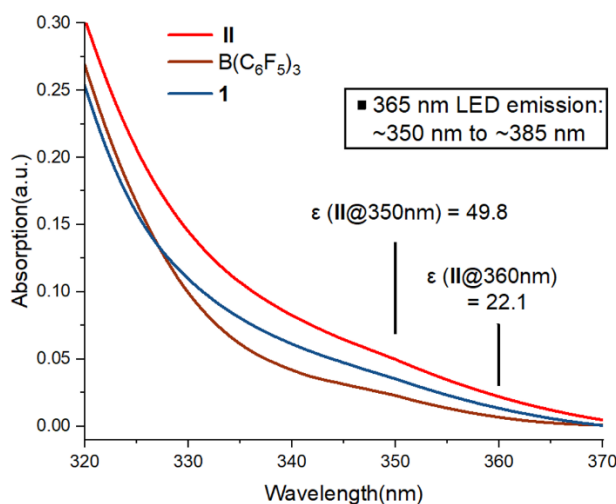
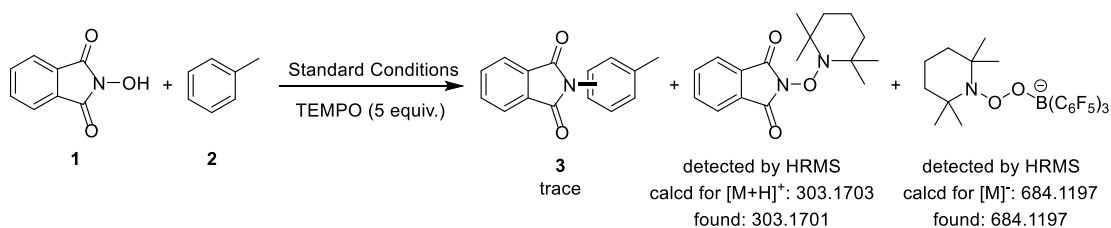


Figure S10. UV-vis absorption spectrum of PhthN–O–B(C₆F₅)₃ anion (**II**) in CHCl₃.

3.5 TEMPO-Trapping experiment



To a dry Schlenk tube equipped with a magnetic stir bar was added NHPI (**1**) (16.3 mg, 0.1 mmol, 1 equiv.), B(C₆F₅)₃ (10.2 mg, 0.02 mmol, 20 mol%), [Ir(dF(CF₃)ppy)₂dtbbpy]PF₆ (2.2 mg, 0.002 mmol, 2 mol%), NaHCO₃ (1.7 mg, 0.02 mmol, 20 mol%) and TEMPO (7.8 mg, 0.5 mmol, 5 equiv.).

and the Schlenk tube was evacuated and backfilled with Ar (three times). After addition of a solution of CHCl_3 (5.0 mL, 0.02 M) containing toluene (**2**) (46 mg, 0.5 mmol, 5 equiv.) by syringe under Ar, the Schlenk tube was positioned approximately 5 cm away from a 25 W blue LEDs lamp. Then the reaction mixture was stirred at the corresponding temperature for 72 h. After completion of the reaction, no **3** was detected and the adduct **TEMPO-NPhth** and **TEMPO-B(C₆F₅)₃** were detected by ESI-HRMS shown in Figure S11 and S12.

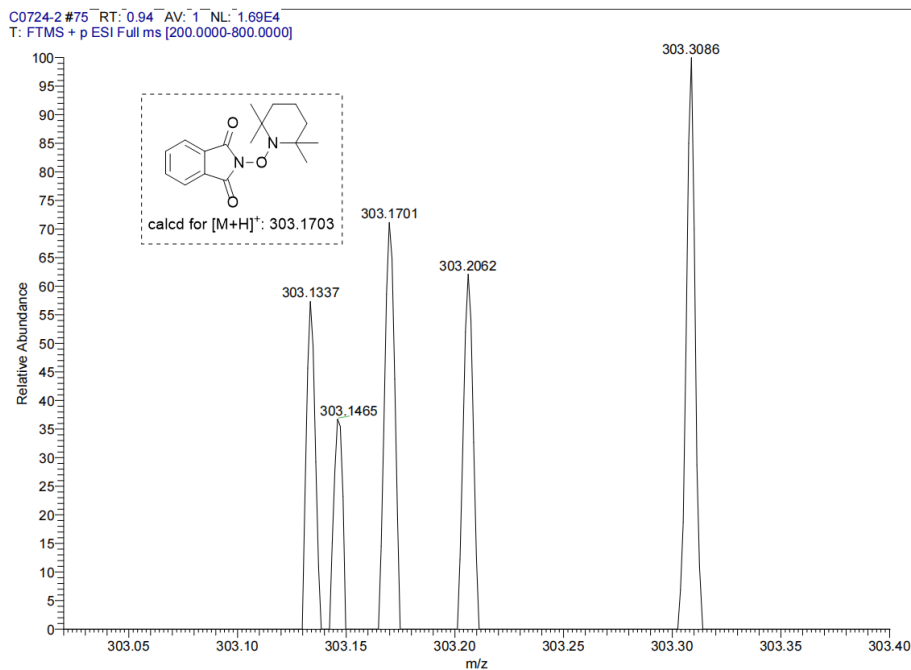


Figure S11. HRMS spectrum of **TEMPO-NPhth**

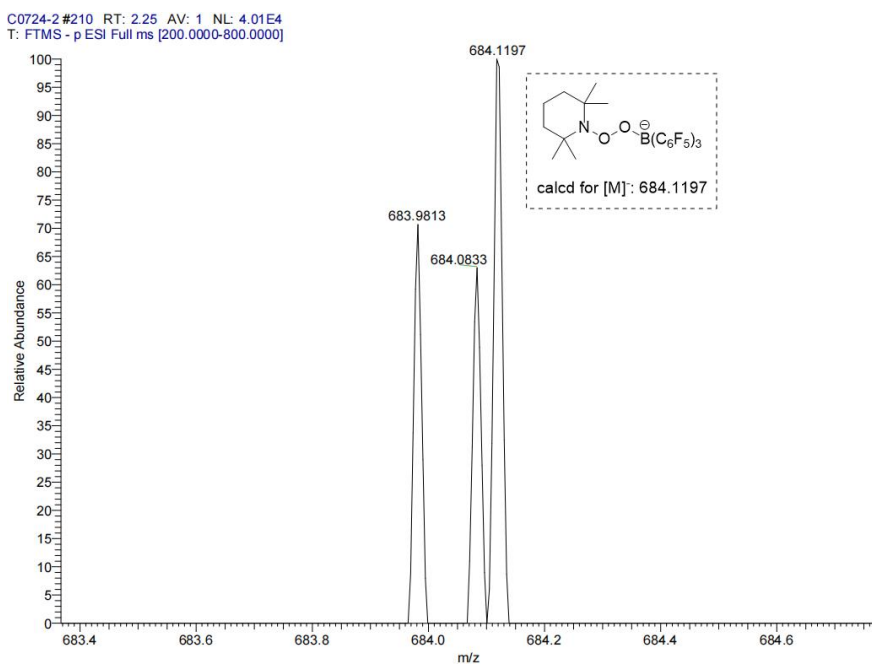


Figure S12. HRMS spectrum of **TEMPO-B(C₆F₅)₃**

4 DFT Calculation Details

Computational Methods

Density Functional Theory (DFT) calculations were carried out with the Gaussian 16 software.

The M06-2X functional¹ was adopted for all calculations. For geometry optimization and frequency calculations, the def2-SVP basis set² was used. The single point energy calculations were performed with a larger basis set def2-TZVP basis set.

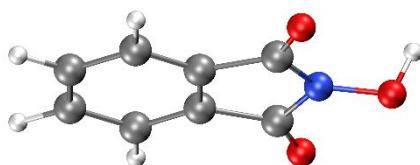
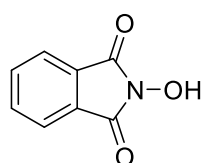
The DFT-D3 dispersion correction was applied to correct the weak interaction to improve the calculation accuracy.

The SMD implicit solvation model³ was used to account for the solvation effect (eps=2.22092).

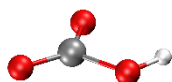
Finally, the single point energy of each compound was added to the free energy correction terms calculated before to obtain the Gibbs free energy.

Calculated Coordinates (without counterions) (B3LYP):

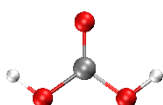
NHPI (1)



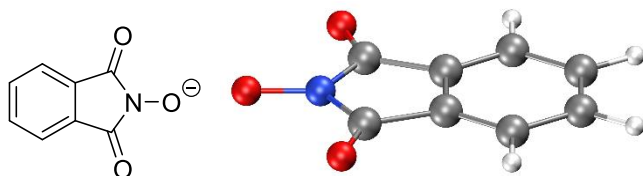
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C	-0.50370100	0.69750200	-0.00075600
C	-0.50373300	-0.69802200	-0.00089500
C	-1.68328300	-1.42374700	0.00227000
C	0.91388000	1.17714300	0.00206700
N	1.67190600	0.00037200	0.05123800
C	0.91367600	-1.17725300	0.00241500
O	1.35481500	-2.29113800	-0.02065900
O	1.35374200	2.29171800	-0.02083600
O	3.01259900	0.00004800	-0.11106300
H	-3.83297100	-1.23316000	0.00167400
H	-3.83280300	1.23317100	0.00193800
H	-1.67222800	2.51400900	0.00362700
H	-1.67283100	-2.51430400	0.00306300
H	3.39922500	-0.00121900	0.77873500



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O	-1.20564300	-0.56373000	-0.00000200
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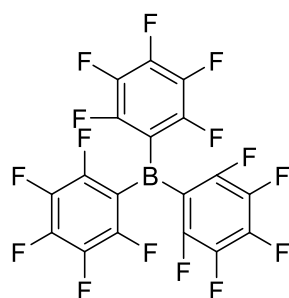
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O	1.08155300	-0.67299000	-0.00003400
H	1.85670400	-0.09258000	0.00012800
H	-1.85657800	-0.09210700	-0.00036800



C	2.84733600	-0.69647500	0.00051500
C	2.84738100	0.69637400	0.00052000
C	1.63920800	1.42010100	0.00000600
C	0.46329800	0.69710500	-0.00046800
C	0.46325400	-0.69707500	-0.00049600
C	1.63911700	-1.42013100	0.00002100
C	-0.96866300	1.15017400	-0.00031800
N	-1.74751100	-0.00000400	0.00079200
C	-0.96871200	-1.15010600	-0.00039900
O	-1.37375100	-2.29436600	-0.00102800
O	-1.37366500	2.29440800	-0.00106100
O	-3.05116200	0.00000900	0.00163300

H	3.79750500	-1.23332900	0.00097000
H	3.79757800	1.23317800	0.00096900
H	1.62648900	2.51122300	-0.00004900
H	1.62631800	-2.51124900	-0.00007200

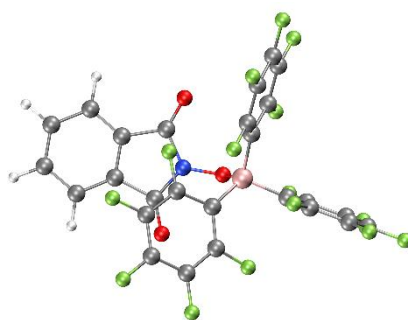
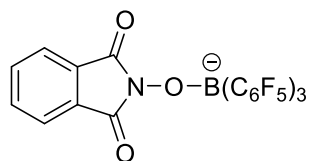
B(C₆F₅)₃



F	0.96759200	5.63425400	0.00004600
C	0.74485500	4.33695200	0.00021200
C	1.62112500	3.48061700	-0.66097100
F	2.67310700	3.97199300	-1.29257800
C	1.37451600	2.11316200	-0.64247700
F	2.24103900	1.34335900	-1.28788100
C	0.26613600	1.54889300	0.00056900
C	-0.59059000	2.45071400	0.64335000
F	-1.66435900	2.01430200	1.28874400
C	-0.36675500	3.82209300	0.66167100
F	-1.19465200	4.63638400	1.29298900
B	0.00012800	-0.00022000	0.00040000
C	-1.47456700	-0.54407900	0.00018900
C	-1.82780600	-1.73611900	0.64419200
F	-0.91346600	-2.44715100	1.29104900
C	-3.12747100	-2.22766700	0.66239800
F	-3.41944200	-3.35097200	1.29484900
C	-4.12861800	-1.52286500	-0.00037700
F	-5.36353300	-1.97847900	-0.00094000
C	-3.82456400	-0.33660300	-0.66264800
F	-4.77568300	0.32818000	-1.29547200
C	-2.51694300	0.13334700	-0.64402000

F	-2.28300200	1.26787800	-1.29064500
C	1.20850300	-1.00522900	0.00033800
C	2.41818300	-0.71401100	0.64250500
F	2.57732500	0.43420400	1.28765400
C	3.49397600	-1.59344500	0.66047700
F	4.61333100	-1.28348200	1.29133100
C	3.38375800	-2.81382200	-0.00047700
F	4.39599000	-3.65521900	-0.00091200
C	2.20372400	-3.14473900	-0.66101900
F	2.10291300	-4.30159500	-1.29231400
C	1.14271500	-2.24751900	-0.64225100
F	0.04265200	-2.61332100	-1.28724900

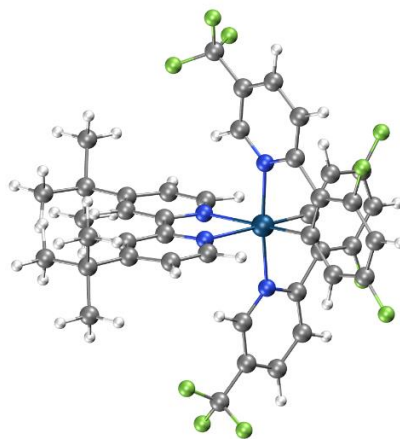
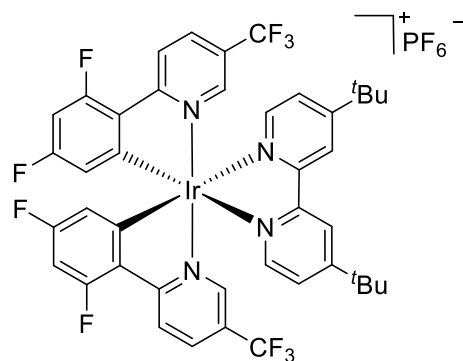
II



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C	-6.06298700	0.27490700	-1.45076500
C	-5.00026700	-0.63122200	-1.56392000
C	-3.72042800	-0.10452100	-1.60621600
C	-3.49056300	1.26838100	-1.53754400
C	-4.53269000	2.17310400	-1.43116600
C	-2.39894600	-0.80121000	-1.71224700
N	-1.45531400	0.22354600	-1.63107600
C	-2.01085700	1.50294000	-1.57968200
O	-1.40702700	2.54121100	-1.56949400
O	-2.16848700	-1.97589900	-1.82799300
O	-0.13305800	-0.00980300	-1.65309000
H	-6.68187000	2.33193600	-1.29959800
H	-7.08702700	-0.09855500	-1.41018300
H	-5.16644900	-1.70813400	-1.61567400
H	-4.34210600	3.24570000	-1.37763500

F	1.85229300	5.13356800	1.79547500
C	1.52910600	3.92890300	1.34103700
C	1.70672100	3.61423700	-0.00146900
F	2.21615900	4.52126100	-0.82991800
C	1.36840600	2.34206700	-0.45171400
F	1.61899100	2.08584700	-1.73329000
C	0.81822000	1.35560300	0.36681100
C	0.68827400	1.70677100	1.70759400
F	0.23166500	0.83796500	2.61272500
C	1.01883300	2.96784400	2.20316000
F	0.86093600	3.25507700	3.49254100
B	0.51506800	-0.12773400	-0.29602900
C	-0.48272300	-1.07000900	0.61948000
C	-0.36033700	-2.45276900	0.70983600
F	0.70355700	-3.08601000	0.21344500
C	-1.33520600	-3.27524100	1.27357300
F	-1.16319700	-4.59116100	1.32846200
C	-2.50375300	-2.71322000	1.76869600
F	-3.44706200	-3.48148800	2.29660000
C	-2.67749300	-1.33571700	1.69843400
F	-3.79831000	-0.78433800	2.15042300
C	-1.66628500	-0.55485400	1.14841500
F	-1.92026900	0.75972000	1.09510700
C	2.00461100	-0.76657500	-0.54319800
C	2.76391800	-1.10525000	0.57551400
F	2.22538200	-0.97570900	1.79234100
C	4.06450600	-1.58851000	0.51567700
F	4.73328300	-1.90567500	1.61974200
C	4.66902900	-1.73477900	-0.72920300
F	5.91241100	-2.19046600	-0.82013700
C	3.95837800	-1.39888800	-1.87247600
F	4.53225200	-1.53142200	-3.06452300
C	2.64915400	-0.92031400	-1.76760000
F	2.06157600	-0.61891700	-2.92174800

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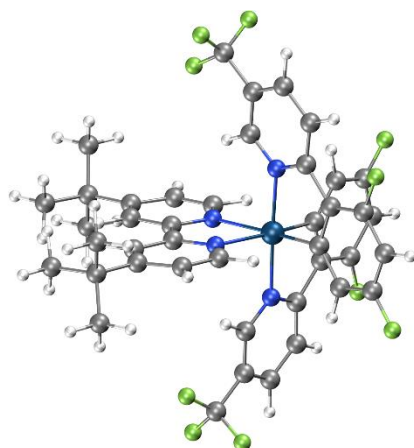


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C	3.25464400	-1.01722200	-2.76472800
C	1.97529600	-1.11918100	-3.32987000
C	0.85714200	-0.82632300	-2.56403000
H	4.28665000	-0.51238500	-0.94035000
C	-1.42956000	-4.31833200	2.00551000
C	-2.15554200	-3.21377400	2.41878500
C	-1.93558900	-1.96825200	1.80670800
C	-0.31066200	-2.92470900	0.41321500
C	-0.48877300	-4.17381000	0.98372000
C	-2.60962500	-0.70574200	2.12091800
C	-3.57245300	-0.53093500	3.12489200
C	-4.16708500	0.69303100	3.37999500
C	-3.77009400	1.76789400	2.59193700
C	-2.81911400	1.65471100	1.58396900
C	-2.22429900	0.41483300	1.33460400
H	-2.89131000	-3.30446000	3.21163600
H	0.41105900	-2.76592200	-0.38896400
H	-4.91329600	0.80167300	4.16492300
H	-2.56736300	2.54847700	1.01135100
C	-0.94394100	4.43692900	-2.00917800
C	-1.77228900	3.41125600	-2.44108300
C	-1.69461800	2.15022900	-1.83202200
C	-0.00030900	2.92600600	-0.41057000
C	-0.04345900	4.19342400	-0.97465100
C	-2.49975800	0.96853100	-2.15239300
C	-3.47194500	0.90188900	-3.16053000

C	-4.20237800	-0.24624600	-3.41480200
C	-3.93809700	-1.35583100	-2.61924100
C	-2.98636100	-1.34806800	-1.60603900
C	-2.24976000	-0.18559100	-1.36026400
H	-2.48191000	3.58151000	-3.24429500
H	0.69733700	2.68884100	0.39588700
H	-4.95129500	-0.27146900	-4.20409500
H	-2.84693700	-2.26053600	-1.02472300
Ir	-0.81069000	0.03453700	-0.00804500
H	-1.58798700	-5.28912700	2.47786700
C	2.17365300	0.12018600	0.70985900
C	3.35737500	0.32034500	1.42335200
C	3.32147200	0.71202200	2.76457900
H	4.31236800	0.17270600	0.92684500
C	0.91611800	0.68560100	2.56970100
C	2.05336300	0.88779100	3.33652700
H	-0.08331900	0.82926300	2.98744500
H	1.93706100	1.18540500	4.37853900
H	1.83430000	-1.43142200	-4.36460800
H	-0.99569600	5.42125900	-2.47502900
H	-0.15139000	-0.90626300	-2.97716500
F	-4.32690300	2.95304000	2.81891500
F	-3.94475900	-1.56386900	3.88202800
F	-4.62973400	-2.46854100	-2.84246400
F	-3.72010100	1.96877900	-3.92217700
C	0.86454200	5.26604600	-0.43472300
C	0.29210800	-5.36105600	0.48972400
F	0.96418100	6.28890100	-1.27796400
F	0.42024900	5.74350500	0.72876000
F	2.09169400	4.78824500	-0.21556000
F	1.31322500	-4.98881800	-0.28313400
F	-0.47340200	-6.18511500	-0.22525400
F	0.78303800	-6.06593100	1.50781500
C	4.58060500	0.93951500	3.59607200
C	4.57242900	2.38577000	4.12037800
H	3.69676500	2.58775600	4.75351000
H	5.47312600	2.56220400	4.72587300

H	4.57006900	3.10421700	3.28754300
C	4.56945000	-0.04423600	4.77903800
H	3.69311500	0.10592100	5.42506100
H	4.56326000	-1.08500000	4.42380200
H	5.47012100	0.10616100	5.39157200
C	5.85288500	0.71574300	2.77560300
H	5.92029100	-0.31727600	2.40366700
H	5.90862400	1.40392600	1.91955100
H	6.73097100	0.89945100	3.40973600
C	4.49254400	-1.35456300	-3.59084400
C	4.53316700	-0.43055700	-4.82010900
H	5.42024600	-0.66428800	-5.42635400
H	3.64694000	-0.55842500	-5.45749000
H	4.59134800	0.62470000	-4.51546100
C	4.39238200	-2.82181200	-4.04350800
H	5.27693600	-3.08427300	-4.64149200
H	4.34821200	-3.49743600	-3.17685100
H	3.50181800	-2.99717900	-4.66318000
C	5.78287200	-1.16867500	-2.78889200
H	5.90287500	-0.12941800	-2.44908900
H	5.81712100	-1.83305100	-1.91289700
H	6.64402900	-1.41371900	-3.42566600
N	0.94458500	-0.43876500	-1.28674800
N	0.97430000	0.31762500	1.28485300
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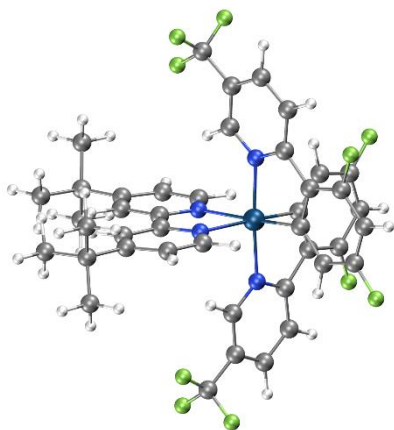


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C	2.00071100	-0.31169200	-3.40011600
C	0.88310500	-0.41826300	-2.61201500
H	4.07710200	0.97000000	-1.03982100
C	0.53616900	-4.38876400	2.09180900
C	-0.52452300	-3.64297400	2.58766600
C	-0.90188400	-2.46600800	1.92994800
C	0.79395700	-2.77738100	0.33657000
C	1.20567100	-3.95099300	0.95022600
C	-1.97468600	-1.54269900	2.32581200
C	-2.82971200	-1.71669400	3.41748600
C	-3.80976200	-0.78754100	3.74377100
C	-3.93300100	0.34523000	2.94645400
C	-3.11220400	0.57223100	1.84658300
C	-2.13772100	-0.37656400	1.52588800
H	-1.05331400	-3.96213800	3.48033600
H	1.29280800	-2.38569900	-0.55203800
H	-4.46018300	-0.94935200	4.60250100
H	-3.25772900	1.48171300	1.26260800
C	-2.49356000	3.77377200	-2.04688900
C	-2.90598100	2.51988100	-2.47556000
C	-2.41203800	1.37873200	-1.83161000
C	-1.13765800	2.71252200	-0.37941900
C	-1.59397700	3.87277600	-0.98588500
C	-2.71180600	-0.01994700	-2.16784900
C	-3.58165000	-0.44100800	-3.17691800
C	-3.79475200	-1.78562400	-3.45478100
C	-3.11644400	-2.73005900	-2.69190400
C	-2.24250500	-2.37123600	-1.67119900
C	-2.04383400	-1.01455600	-1.39788100
H	-3.59800400	2.42064000	-3.30605800
H	-0.42914000	2.73470700	0.45085200
H	-4.47692200	-2.08361300	-4.25012300
H	-1.74134400	-3.16019300	-1.10911700
Ir	-0.85696300	-0.26952900	0.00922500

H	0.84705500	-5.30424200	2.59782700
C	1.90338400	0.84246600	0.63648300
C	2.97701700	1.41703500	1.38053100
C	2.83125400	1.77366200	2.69936000
H	3.92584500	1.57357900	0.87394800
C	0.54568300	0.98743300	2.55336300
C	1.55473700	1.53882900	3.30203400
H	-0.43573000	0.81140400	2.99852100
H	1.35921600	1.79141500	4.34308500
H	1.94162700	-0.62565000	-4.44106500
H	-2.86694900	4.67130800	-2.54313600
H	-0.04632300	-0.81619300	-3.02460700
F	-4.86527000	1.23395300	3.25046600
F	-2.72505500	-2.79304200	4.18835900
F	-3.31451000	-4.01242400	-2.95198100
F	-4.23842600	0.44809600	-3.91289800
C	-1.12957900	5.22309200	-0.50300700
C	2.34686400	-4.75011600	0.37464400
F	-0.64671800	5.94631500	-1.51061600
F	-2.13681400	5.91166000	0.03090500
F	-0.17730800	5.11036600	0.41918500
F	3.03888500	-4.03932900	-0.51233800
F	1.90245300	-5.84493800	-0.24063700
F	3.18072400	-5.14488900	1.33316900
C	3.94852500	2.40030000	3.52753000
C	3.48181300	3.77786300	4.02812000
H	2.57981600	3.69998100	4.65168300
H	4.27296400	4.24314800	4.63480300
H	3.25782300	4.44406100	3.18179500
C	4.24666200	1.48941900	4.73046600
H	3.36171000	1.35646200	5.36900700
H	4.57999700	0.49657900	4.39373800
H	5.04416800	1.93149400	5.34615600
C	5.23307000	2.58129900	2.71596300
H	5.61870500	1.61817300	2.35048300
H	5.07454600	3.24408500	1.85245000
H	6.00755900	3.03484100	3.35050600

C	4.46373000	0.29180500	-3.70646500
C	4.16781000	1.20195100	-4.91053500
H	5.05688700	1.27020500	-5.55502100
H	3.33871800	0.81535100	-5.52011700
H	3.90488300	2.21651200	-4.57623200
C	4.82633500	-1.11856800	-4.20255800
H	5.72644800	-1.07376700	-4.83365300
H	5.03129400	-1.78834500	-3.35415000
H	4.01624200	-1.56007700	-4.80042900
C	5.65628300	0.86523900	-2.93820500
H	5.44986600	1.88252900	-2.57426800
H	5.92337000	0.23381600	-2.07810100
H	6.53064700	0.91627700	-3.60233300
N	0.85707700	-0.06422200	-1.30719100
N	0.68371400	0.64756800	1.25236100
N	-1.54869700	1.51059600	-0.79282600
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PC²⁻

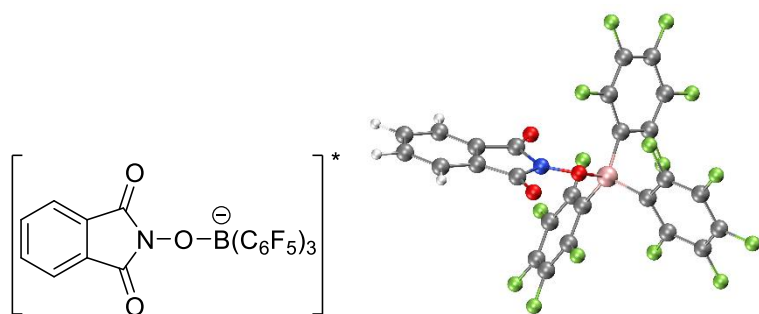


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C	3.30943800	0.31093500	1.45641500
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C	1.97855300	0.88386100	3.36633000
C	0.85537500	0.69232400	2.59027900
H	4.26706600	0.15556400	0.96580900
C	-0.91980200	4.47763100	-1.89558200
C	-1.76187600	3.47793400	-2.35223100
C	-1.70381200	2.19986500	-1.76944900

C	-0.00546300	2.92108500	-0.32060100
C	-0.02263400	4.19583200	-0.86284700
C	-2.51391100	1.03203600	-2.12962000
C	-3.48202100	1.00227300	-3.14249900
C	-4.21166800	-0.13548600	-3.44199400
C	-3.94846300	-1.27367300	-2.68550600
C	-3.00192400	-1.30200900	-1.67023100
C	-2.26334100	-0.14934700	-1.37506000
H	-2.46499600	3.67446100	-3.15526700
H	0.67421500	2.64741800	0.48826600
H	-4.95742600	-0.13225800	-4.23460700
H	-2.85776600	-2.23536700	-1.12273600
C	-1.28818300	-4.38558700	1.87617700
C	-2.05326200	-3.32384100	2.32832100
C	-1.88636300	-2.05182300	1.75346300
C	-0.23363700	-2.89986700	0.32069100
C	-0.35838000	-4.17148300	0.85616100
C	-2.60375400	-0.82437000	2.11186500
C	-3.57440700	-0.72053800	3.11750300
C	-4.21069500	0.47173800	3.41790500
C	-3.84880600	1.58846500	2.67026600
C	-2.89551600	1.54414600	1.66194400
C	-2.25193900	0.33621100	1.36538200
H	-2.77949800	-3.46737800	3.12183500
H	0.47567900	-2.67817000	-0.47856700
H	-4.96053600	0.52568700	4.20482800
H	-2.67069700	2.46527400	1.12106100
Ir	-0.83005000	0.03828200	-0.00109200
H	-0.95830000	5.47382400	-2.33993400
C	2.10398100	-0.27502200	-0.68000900
C	3.28221800	-0.56533200	-1.43594200
C	3.21620300	-0.94601300	-2.75595000
H	4.24640500	-0.48723200	-0.93986400
C	0.81172100	-0.74909800	-2.58355100
C	1.92010600	-1.03322600	-3.35246600
H	-0.19460200	-0.81530600	-3.00826000
H	1.78645600	-1.32342800	-4.39361100

H	1.86264200	1.18130100	4.40756200
H	-1.41173800	-5.37741400	2.31463000
H	-0.14470700	0.83900100	3.00958000
F	-4.64103100	-2.37935400	-2.95586300
F	-3.73180500	2.09760600	-3.86745100
F	-4.45008700	2.74589100	2.94260500
F	-3.91923700	-1.79513100	3.83443900
C	0.48990900	-5.30553300	0.35397400
C	0.90759900	5.26167900	-0.35648400
F	1.25305800	-5.80839500	1.32687800
F	-0.26502400	-6.30866200	-0.10053800
F	1.29506000	-4.92390900	-0.63542400
F	1.66106800	4.82653700	0.65141200
F	0.23017100	6.32877000	0.07364500
F	1.72654500	5.68851700	-1.32026300
C	4.44994900	-1.28204700	-3.59096500
C	4.33855100	-2.73675900	-4.07803200
H	3.44148600	-2.88921400	-4.69479800
H	5.21766000	-3.00005500	-4.68578700
H	4.28732200	-3.42869700	-3.22407400
C	4.50771000	-0.33784300	-4.80345200
H	3.61157400	-0.43163300	-5.43313600
H	4.58760500	0.70952900	-4.47616100
H	5.38507300	-0.57450200	-5.42451400

II*

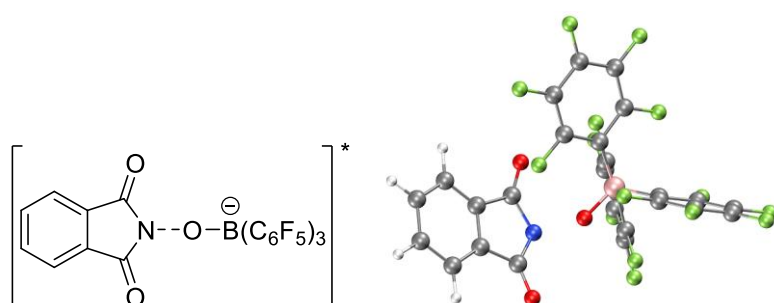


C	-6.17803300	-0.72234300	-2.41327800
C	-6.19787200	-1.29448600	-1.10059800
C	-5.05028900	-1.39105600	-0.34894800
C	-3.83656800	-0.90892900	-0.89416800

C	-3.81592600	-0.34149500	-2.21138600
C	-5.00848100	-0.25233900	-2.96505400
C	-2.53802200	-0.90765200	-0.30788900
N	-1.71651100	-0.26885400	-1.35836600
C	-2.49464100	0.06530000	-2.56736900
O	-1.96532900	0.58041400	-3.53440200
O	-2.05613900	-1.31297600	0.73904500
O	-0.47587900	-0.03866700	-1.34667500
H	-7.10842300	-0.66194000	-2.97967300
H	-7.14335100	-1.65824400	-0.69560800
H	-5.06044000	-1.82619100	0.65173400
H	-4.98717000	0.18282700	-3.96569300
F	5.21190100	2.25799400	-2.53818500
C	4.11928100	1.77901300	-1.96217500
C	3.50509700	0.63765600	-2.46625000
F	4.01903400	0.02092300	-3.52257300
C	2.36221100	0.15217100	-1.83839500
F	1.83150000	-0.96260500	-2.34162900
C	1.77693900	0.76178400	-0.72848400
C	2.43134300	1.89386100	-0.25216400
F	1.98806000	2.55003400	0.81966700
C	3.58049300	2.41116200	-0.84855900
F	4.16657800	3.49713900	-0.35958500
B	0.44884900	0.06784800	-0.07048100
C	-0.35860500	1.01591600	0.97571900
C	-0.70020400	0.68830400	2.28575800
F	-0.34519100	-0.46864500	2.83143500
C	-1.43302800	1.54317100	3.10777100
F	-1.73511100	1.18859700	4.35127200
C	-1.86604300	2.76900900	2.61817400
F	-2.56788100	3.58582600	3.38975200
C	-1.55178200	3.13504500	1.31435100
F	-1.95387200	4.30633600	0.83740400
C	-0.81409300	2.25533300	0.52967200
F	-0.52760900	2.65532100	-0.71164100
C	0.89441500	-1.40003900	0.46024100
C	1.83265900	-1.45909200	1.48545500

F	2.26445600	-0.32182100	2.03862500
C	2.34015600	-2.64884800	1.99371300
F	3.22265600	-2.65122400	2.98587400
C	1.91255600	-3.85149300	1.44010800
F	2.38381900	-5.00218400	1.90096800
C	0.98931300	-3.83913900	0.40159800
F	0.58524800	-4.98513000	-0.13370800
C	0.50296400	-2.62194300	-0.07264300
F	-0.36287200	-2.68579700	-1.08375900

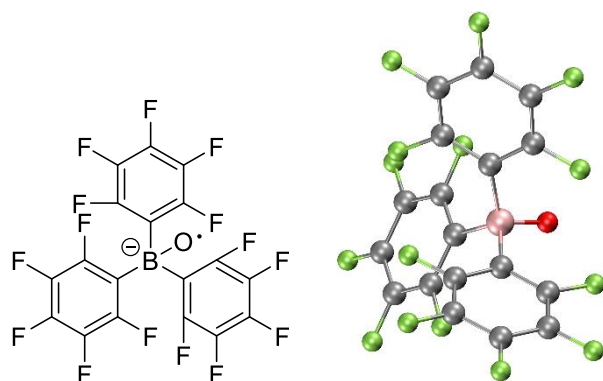
TS



C	-5.76931100	-0.71046000	-2.61254400
C	-5.88973900	-1.07040900	-1.26119400
C	-4.98287600	-0.60694200	-0.30562800
C	-3.96242600	0.22201300	-0.75254500
C	-3.83768800	0.57359200	-2.09140100
C	-4.73622700	0.12171700	-3.04995800
C	-2.82159100	0.85549700	-0.01612100
N	-2.12065500	1.68452000	-0.91610900
C	-2.62648900	1.44958900	-2.21395300
O	-2.16178100	1.91461200	-3.22190400
O	-2.53663300	0.70913600	1.14597000
O	-0.47806400	0.10749100	-1.28247400
H	-6.49451300	-1.09464900	-3.33137400
H	-6.70512300	-1.72852800	-0.95738600
H	-5.05993000	-0.88874300	0.74546200
H	-4.62857900	0.40178700	-4.09860900
F	5.39759900	-1.98036100	-2.57767100
C	4.29315700	-1.50232000	-2.02021500
C	3.07252800	-2.13464600	-2.22912400

F	3.01419800	-3.22628800	-2.98389600
C	1.92890800	-1.61509200	-1.62906300
F	0.79349800	-2.28198300	-1.84341900
C	1.93101100	-0.47308400	-0.82852900
C	3.17561700	0.11917100	-0.63895000
F	3.31802000	1.20095800	0.12775800
C	4.34600300	-0.36788900	-1.22028100
F	5.51039300	0.23657500	-1.01073600
B	0.48993100	0.02382400	-0.18203600
C	0.55326500	1.50086500	0.52816000
C	0.21631300	1.83652800	1.83306400
F	-0.10890300	0.91499500	2.73836200
C	0.18696000	3.15657400	2.28700400
F	-0.14039300	3.43088400	3.54675300
C	0.49541100	4.19163900	1.41614000
F	0.47138100	5.45069400	1.83612800
C	0.83420100	3.89977600	0.09803200
F	1.12872400	4.88579000	-0.74374600
C	0.84765700	2.57356400	-0.30957200
F	1.15910400	2.33715700	-1.58739000
C	0.00127200	-1.18127100	0.82018000
C	0.80830600	-1.50920900	1.90539700
F	1.91493200	-0.80096000	2.13784000
C	0.50878000	-2.53366300	2.79526100
F	1.30215000	-2.80210100	3.82614000
C	-0.64216900	-3.29002400	2.59146300
F	-0.94837200	-4.27452500	3.42613600
C	-1.46859400	-3.00483800	1.51231300
F	-2.56741700	-3.72448900	1.31181700
C	-1.12547600	-1.97111600	0.64182300
F	-1.94779200	-1.76944800	-0.38923600

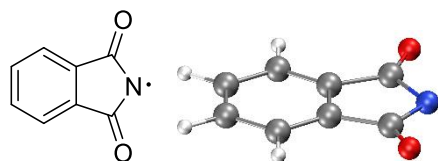
III



O	0.20081900	-0.04712100	2.37692000
F	-2.22432400	4.93510000	-0.99086000
C	-1.66843200	3.80646900	-0.56698400
C	-2.22671800	3.10640300	0.49709200
F	-3.32686900	3.56464900	1.08597100
C	-1.62214000	1.92454400	0.91653100
F	-2.21576600	1.27118400	1.92000500
C	-0.46875700	1.39934200	0.34074600
C	0.04533800	2.12637300	-0.72691500
F	1.13860900	1.71907400	-1.37717300
C	-0.52396700	3.31473900	-1.18331300
F	0.01159900	3.98065800	-2.20205200
B	0.07937900	-0.04566400	0.95036900
C	1.65721500	-0.35492700	0.55909100
C	2.15121300	-1.59249200	0.15726800
F	1.34630900	-2.64369500	-0.00311900
C	3.50052000	-1.82129500	-0.11211300
F	3.91974400	-3.01838200	-0.50830800
C	4.41596900	-0.79064300	0.05502200
F	5.70383500	-0.99303800	-0.18724100
C	3.96963300	0.45793100	0.47439600
F	4.83951900	1.44884500	0.63691900
C	2.61494400	0.64375000	0.72990400
F	2.25319400	1.86167200	1.13248500
C	-0.98614200	-1.16332500	0.36717500
C	-1.03836300	-1.44326500	-0.99482200
F	-0.15087400	-0.86919300	-1.81468600
C	-1.96087500	-2.30821400	-1.57055700

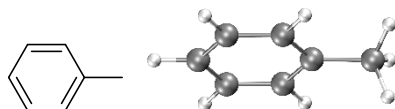
F	-1.95841600	-2.55221300	-2.87754900
C	-2.90484600	-2.92365000	-0.75273300
F	-3.80235900	-3.75126200	-1.27499000
C	-2.90013500	-2.66547000	0.61150800
F	-3.80399800	-3.24789900	1.39399200
C	-1.94982100	-1.79249000	1.14633700
F	-2.02256500	-1.58743100	2.46071600

IV



C	-2.52032400	0.70226900	-0.00019500
C	-2.52031100	-0.70229700	0.00004500
C	-1.32740100	-1.42747300	-0.00200000
C	-0.14501900	-0.69681300	-0.00428800
C	-0.14503600	0.69679600	-0.00409400
C	-1.32742100	1.42745600	-0.00233700
C	1.27640700	-1.14784800	-0.00560000
N	2.12443100	0.00002300	-0.06368700
C	1.27636500	1.14779500	-0.00268500
O	1.70671400	2.26963000	0.03528600
O	1.70676800	-2.26955700	0.03622300
H	-3.47334500	1.23259300	0.00201400
H	-3.47332400	-1.23263400	0.00219900
H	-1.31786900	-2.51784300	-0.00182400
H	-1.31790700	2.51782500	-0.00172900

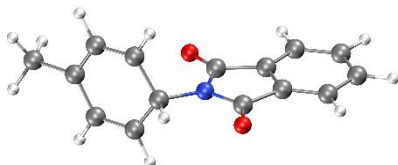
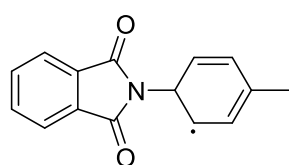
2



C	-1.19962100	1.20448000	0.00202100
C	0.19510400	1.20191700	-0.00921700
C	0.91427500	0.00035300	-0.01168700
C	0.19554200	-1.20164200	-0.00921600

C	-1.19903600	-1.20481000	0.00202000
C	-1.90270500	-0.00025700	0.00866000
H	-1.73985700	2.15281000	0.00211600
H	0.73822300	2.14994500	-0.01867700
H	0.73913400	-2.14941800	-0.01869100
H	-1.73892900	-2.15333600	0.00211500
H	-2.99376500	-0.00052500	0.01485300
C	2.42095000	0.00013200	0.00917300
H	2.79583500	-0.01336400	1.04456300
H	2.82611500	-0.88489100	-0.49976700
H	2.82618800	0.89773300	-0.47703300

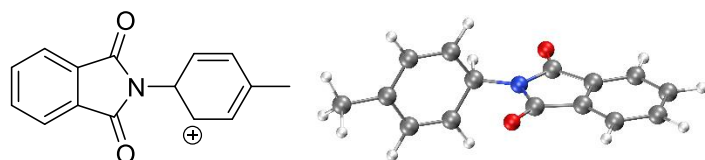
V



C	4.61740900	-0.29565900	-0.00037400
C	4.13385400	-1.60864900	-0.00020400
C	2.75900400	-1.87470700	0.00000700
C	1.90410600	-0.78442400	0.00004900
C	2.38537000	0.52174600	-0.00011200
C	3.74318100	0.79824100	-0.00032700
C	0.40616700	-0.73020700	0.00028100
N	0.07921900	0.63048700	0.00028000
C	1.21036800	1.44950200	0.00000800
O	1.20124700	2.65277500	-0.00007800
O	-0.37909500	-1.63925800	0.00042800
H	5.69449100	-0.12380300	-0.00054300
H	4.84245900	-2.43787700	-0.00023500
H	2.37196300	-2.89440800	0.00014500
H	4.10964300	1.82547200	-0.00046000
C	-2.02543000	0.74300500	-1.25141200
C	-3.18486000	0.03262400	-1.22068100
C	-3.80349600	-0.36471300	0.00023600
C	-3.18498400	0.03188600	1.22104300
C	-2.02541900	0.74247400	1.25207200

C	-1.29888000	1.14545000	0.00042700
H	-1.57321900	1.03725600	-2.20075600
H	-3.66501100	-0.24423700	-2.16274700
H	-3.66501400	-0.24549200	2.16299700
H	-1.57322600	1.03628800	2.20154900
H	-1.14562700	2.24130200	0.00060700
C	-5.04175700	-1.20637600	-0.00099100
H	-4.78742800	-2.28018900	-0.01994700
H	-5.64622600	-1.03184200	0.89982000
H	-5.66236000	-1.00517700	-0.88533300

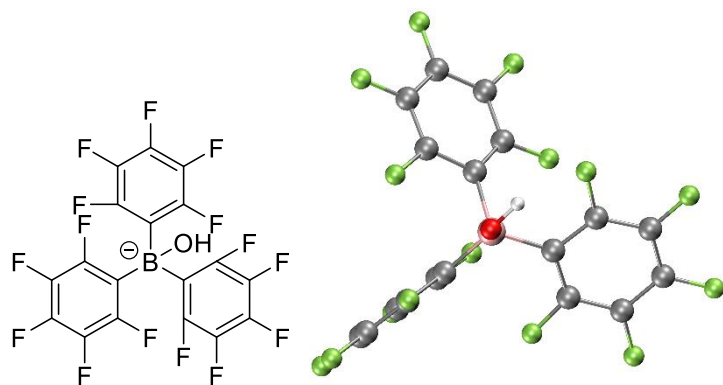
VI



C	4.70614800	0.05476300	-0.03149500
C	4.38581200	-1.30652700	-0.04193100
C	3.05401400	-1.73951000	-0.02795200
C	2.07281400	-0.76196500	-0.00377600
C	2.39268800	0.59841800	0.00527400
C	3.70701600	1.03597200	-0.00750700
C	0.58752900	-0.89809800	0.01583800
N	0.10201400	0.41982100	0.03653700
C	1.12533600	1.38517600	0.02814100
O	0.93049000	2.56831200	0.03739000
O	-0.12227000	-1.86537700	0.01654300
H	5.75396100	0.35638900	-0.04226700
H	5.18948100	-2.04330000	-0.06119200
H	2.79638900	-2.79898800	-0.03574000
H	3.94843900	2.09924100	0.00024200
C	-2.00149000	0.43868500	-1.22892300
C	-3.30334500	0.04807700	-1.23956500
C	-3.98753300	-0.20574400	-0.01487300
C	-3.31874300	-0.06174400	1.23248200
C	-2.01418200	0.32570700	1.26991500
C	-1.29671400	0.72551100	0.04049400

H	-1.45165300	0.61214300	-2.15699500
H	-3.82926600	-0.10659200	-2.18208600
H	-3.85383300	-0.29921500	2.15183600
H	-1.47313000	0.41072300	2.21548400
H	-1.33764100	1.85128900	0.09072700
C	-5.39151800	-0.67144200	-0.05819000
H	-5.38879600	-1.70826400	-0.44025400
H	-5.86914200	-0.65905600	0.92613600
H	-5.97166600	-0.08028300	-0.78070600

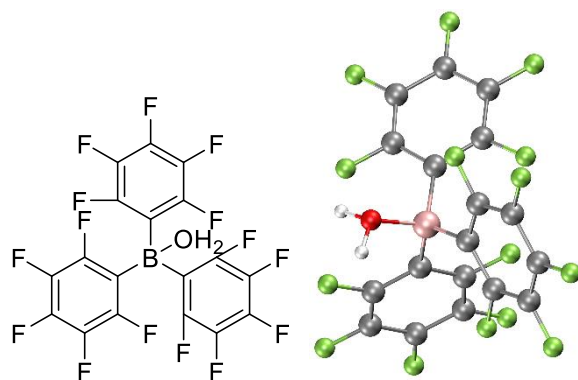
VII



O	-0.05420400	-0.00307900	-2.44463500
F	1.71305600	5.13315000	1.00364000
C	1.28084300	3.95255600	0.57623900
C	2.01416300	3.23203900	-0.35933200
F	3.16101000	3.72377900	-0.81989500
C	1.54005000	1.99439600	-0.78784300
F	2.31382500	1.34604900	-1.66060900
C	0.34384600	1.42636700	-0.34685400
C	-0.34414000	2.17995400	0.59925200
F	-1.48840600	1.74555100	1.13635900
C	0.09133400	3.42303400	1.05856800
F	-0.61543100	4.10231700	1.95782400
B	-0.07418100	-0.06082600	-0.99487600
C	-1.60006700	-0.52902200	-0.50428600
C	-1.97350900	-1.69176300	0.15985500
F	-1.07124800	-2.59027400	0.56663700
C	-3.30097600	-2.01878100	0.44859400
F	-3.59611400	-3.14616200	1.08902000

C	-4.32137800	-1.16712400	0.05133700
F	-5.58824900	-1.46639700	0.31206900
C	-4.00141700	0.00488000	-0.62776600
F	-4.96785500	0.83145600	-1.01520500
C	-2.66610200	0.28127100	-0.88920700
F	-2.41475900	1.42763400	-1.54307000
C	1.09355300	-1.08256500	-0.43914100
C	1.26931300	-1.21387700	0.93751500
F	0.42176300	-0.59404200	1.76708200
C	2.26651200	-1.97924700	1.52796300
F	2.37538200	-2.07229700	2.85051500
C	3.16405300	-2.65737600	0.70850500
F	4.13072700	-3.39645800	1.24120100
C	3.03324300	-2.55870100	-0.66912900
F	3.88725500	-3.20707500	-1.45749400
C	2.01182200	-1.77802500	-1.21859200
F	1.97406400	-1.74925800	-2.54851500
H	-0.71748100	0.62891200	-2.73865800

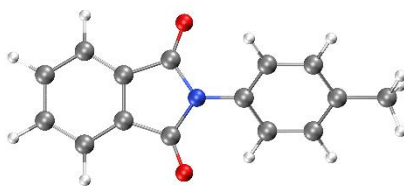
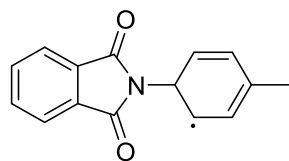
VIII



O	-0.07092600	0.06598900	-2.40461200
F	1.91070300	5.05794100	1.01958700
C	1.42887700	3.90056700	0.60312700
C	2.04614700	3.22345800	-0.44442500
F	3.12071800	3.73032000	-1.02639600
C	1.51131300	2.00798300	-0.85203800
F	2.14661500	1.36721200	-1.85459900
C	0.38079500	1.42404400	-0.28903700
C	-0.19921900	2.13293500	0.75960200

F	-1.27392600	1.66706600	1.38737700
C	0.30184000	3.35396700	1.20787200
F	-0.28417300	3.99670600	2.20514300
B	-0.08739000	-0.04695900	-0.80107800
C	-1.62444900	-0.44996100	-0.49370600
C	-2.05551300	-1.67132900	0.02022000
F	-1.19366500	-2.64355300	0.30893800
C	-3.39922600	-1.95937300	0.26001600
F	-3.75755800	-3.13579100	0.75117200
C	-4.36640300	-1.00686700	-0.03360900
F	-5.64328600	-1.26772800	0.17987500
C	-3.98323800	0.22471900	-0.55820300
F	-4.89965300	1.13770100	-0.84016900
C	-2.63412700	0.47243400	-0.77746200
F	-2.31427400	1.66720200	-1.27164600
C	1.04994400	-1.11318400	-0.33681700
C	1.18120100	-1.35645200	1.02897100
F	0.31986000	-0.78220600	1.86901700
C	2.15534100	-2.18646700	1.56643300
F	2.23212200	-2.39723700	2.87051100
C	3.06752500	-2.79962800	0.70863100
F	4.00631600	-3.59126600	1.19702000
C	2.98329600	-2.57721300	-0.65981900
F	3.84739600	-3.15298300	-1.48113800
C	1.98318200	-1.73925800	-1.15120500
F	1.96006100	-1.55475200	-2.48208000
H	-0.36898600	-0.74744700	-2.84717800
H	0.81432600	0.28438900	-2.75534500

3

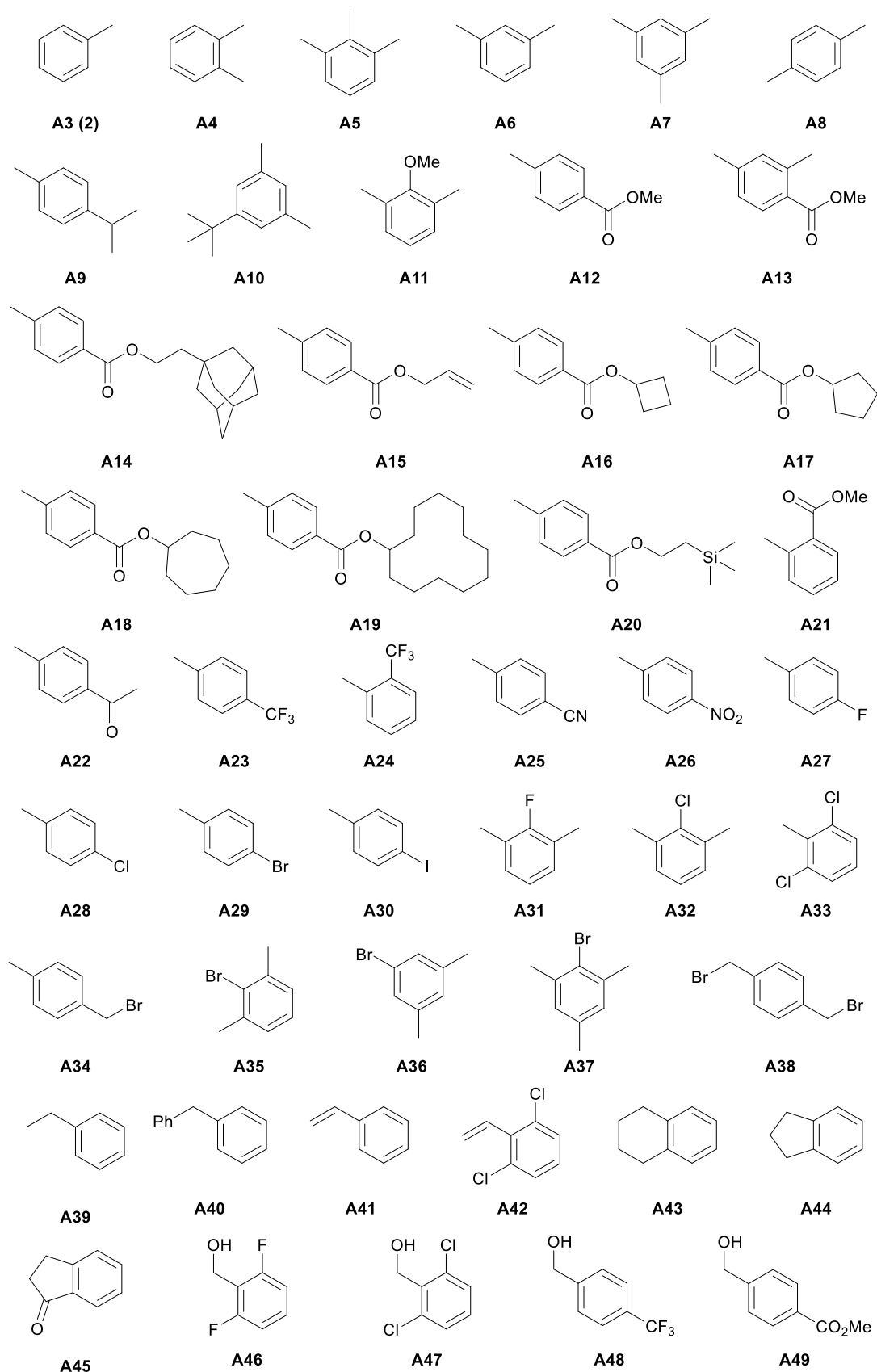


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C	-4.66620400	0.69135400	-0.12007500
C	-3.46804800	1.40584400	-0.23737700

C	-2.28992800	0.68617900	-0.11499500
C	-2.29068900	-0.68521600	0.11342200
C	-3.46959200	-1.40422800	0.23195500
C	-0.87146600	1.14968200	-0.18909500
N	-0.08131600	-0.00030500	0.00262400
C	-0.87272000	-1.14952400	0.19226000
O	-0.46104200	-2.26187900	0.37842300
O	-0.45835400	2.26173200	-0.37347400
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H	-3.45562500	2.48149800	-0.41659700
H	-3.45832400	-2.47988000	0.41126100
C	2.04030600	-1.00501500	-0.67018400
C	3.43130700	-1.00268600	-0.65621800
C	4.15281400	-0.00133000	0.00634700
C	3.43200700	0.99699200	0.66993800
C	2.03900700	1.00108900	0.68010700
C	1.33991500	-0.00043100	0.00395900
H	1.49442900	-1.78944500	-1.19285800
H	3.97000100	-1.79640500	-1.17849400
H	3.96992500	1.78606200	1.19948600
H	1.49338300	1.78321100	1.20647400
C	5.65841200	0.00533900	-0.01751600
H	6.03048400	0.36324100	-0.98974700
H	6.06600300	0.66379100	0.76029000
H	6.06121200	-1.00534300	0.13554000

5 Synthesis of Starting Materials

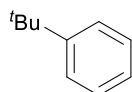
Commercially Available Alkylarenes



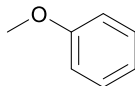
Commercially Available Arenes



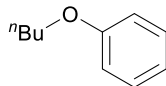
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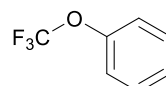
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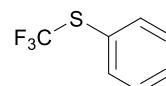
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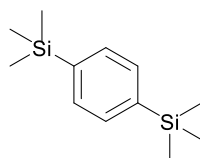
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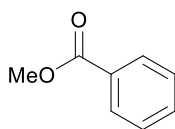
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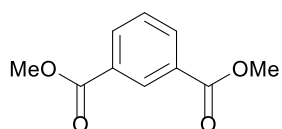
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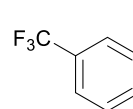
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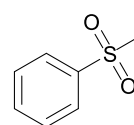
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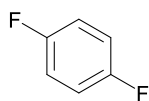
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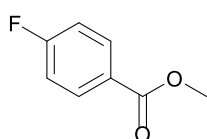
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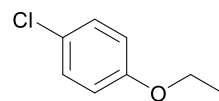
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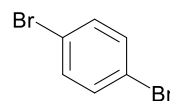
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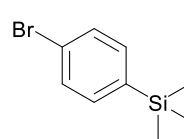
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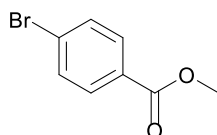
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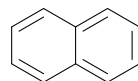
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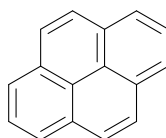
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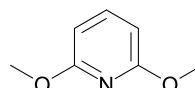
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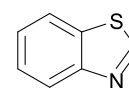
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A68



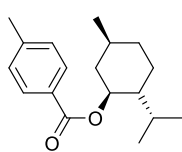
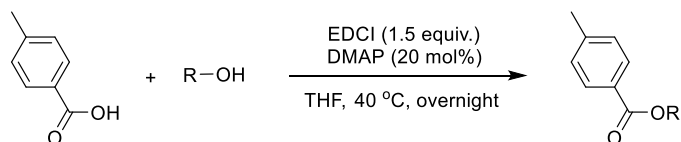
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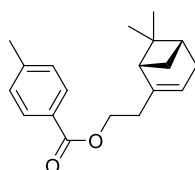
A70

General Procedure for the Synthesis of Biomolecule and Drug Derived Alkylarenes

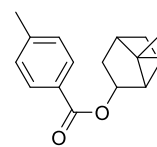
To a solution of 4-methylbenzoic acid (272 mg, 2 mmol, 1.0 equiv.) and the corresponding alcohol (2.4 mmol, 1.2 equiv) in THF (2 mL, 1 M) were added EDCI (576 mg, 3 mmol, 1.5 equiv) and the resulting mixture was stirred at 40 °C overnight. After completion, the reaction mixture was concentrated to dryness and the residue was purified by flash column chromatography (hexane : ethyl acetate = 40:1) to afford the products **A71-A82**.



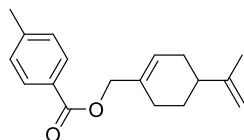
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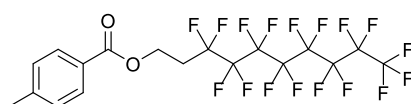
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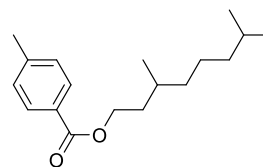
A73



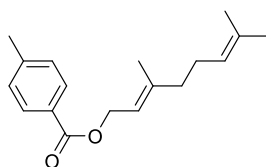
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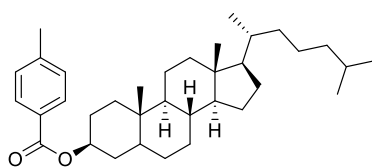
A75



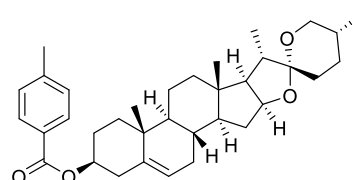
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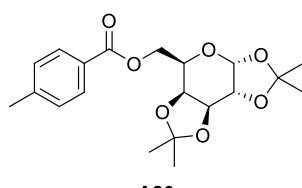
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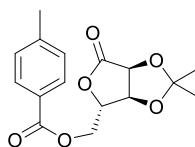
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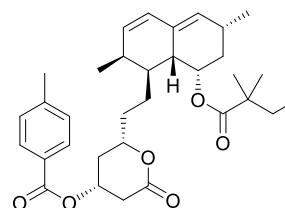
A79



A80



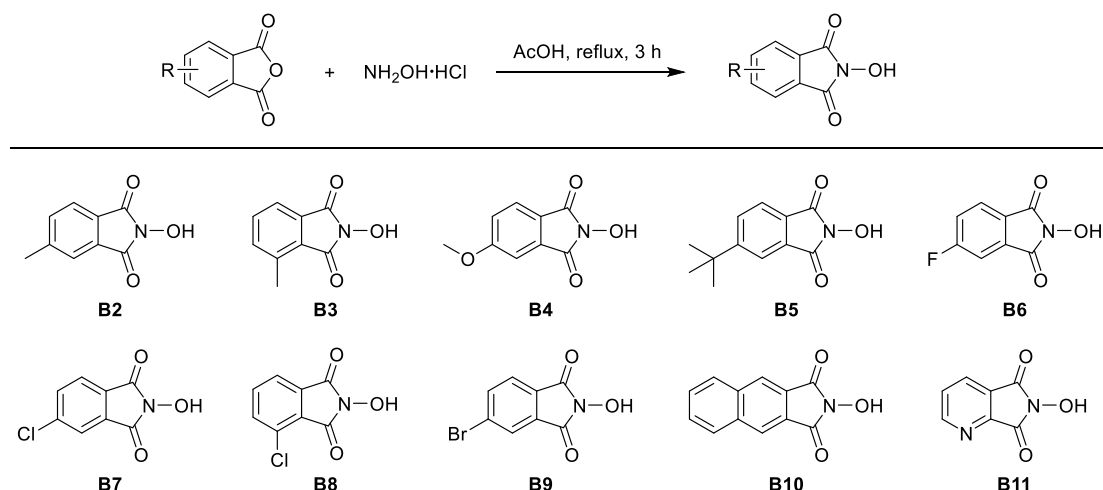
A81



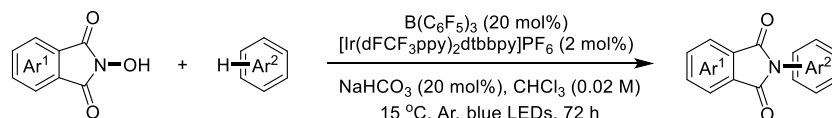
A82

General Procedure for the Synthesis of *N*-Hydroxyphthalimides

To a solution of hydroxylamine hydrochloride (166 mg, 2.4 mmol, 1.2 equiv) in acetic acid (2 mL, 1 M) were added the corresponding phthalic anhydride derivate (2 mmol, 1.0 equiv) and the resulting mixture was reflux for 3 h. After completion, the reaction mixture was poured into ice cold water. The precipitate was collected by filtration, washed with cold water, dried under high vacuum for 1 hour, and then used without purification.



6 Aromatic C–H Amidation of Arenes



General procedure: To a dry Schlenk tube equipped with a magnetic stir bar was added *N*-hydroxyphthalimide (**B**) (0.2 mmol, 1 equiv.), $\text{B}(\text{C}_6\text{F}_5)_3$ (20.4 mg, 0.04 mmol, 20 mol%), $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ (4.4 mg, 0.004 mmol, 2 mol%) and NaHCO_3 (3.4 mg, 0.04 mmol, 20 mol%) and the Schlenk tube was evacuated and backfilled with Ar (three times). After addition of a solution of CHCl_3 (10 mL, 0.02 M) containing arene (**A**) (1.0 mmol, 5 equiv.) by syringe under Ar, the Schlenk tube was positioned approximately 5 cm away from a 25 W blue LEDs lamp. Then the reaction mixture was stirred at the corresponding temperature for 72 h. After completion, the reaction mixture was concentrated to dryness and the residue was purified by flash column chromatography to afford the products.

7 Synthesis of Methyl 3-Amino-4-Methylbenzoate (93)

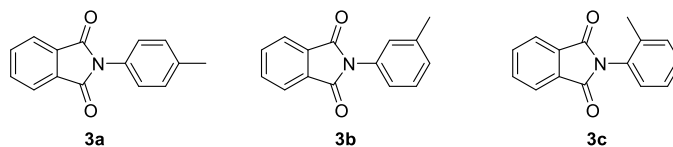
To a dry Schlenk tube equipped with a magnetic stir bar was added NHPI (**B1**) (32.6 mg, 0.2 mmol, 1 equiv.), $\text{B}(\text{C}_6\text{F}_5)_3$ (20.4 mg, 0.04 mmol, 20 mol%), $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbbpy}]\text{PF}_6$ (4.4 mg, 0.004 mmol, 2 mol%) and NaHCO_3 (3.4 mg, 0.04 mmol, 20 mol%) and the Schlenk tube was evacuated

and backfilled with Ar (three times). After addition of a solution of CHCl_3 (10 mL, 0.02 M) containing 4-methylbenzoate (**A12**) (150.2 mg, 1 mmol, 5 equiv.) by syringe under Ar, the Schlenk tube was positioned approximately 5 cm away from a 25 W blue LEDs lamp. Then the reaction mixture was stirred at the corresponding temperature for 72 h.

Subsequently, a solution of ethanol (10 mL) containing hydrazine monohydrate (98%, 0.1 mL, 2 mmol, 10 equiv.) was added to the reaction by syringe. After stirring at room temperature for 6 h, the resulting suspension was filtered through a short pad of silica with diethyl ether. The filtrate was washed with 2 M NaOH aqueous solution, dried over anhydrous magnesium sulfate, filtered and concentrated carefully under reduced pressure to afford the crude mixture which was purified by flash column chromatography (silica gel, hexane : ethyl acetate = 5:1) to furnish methyl 3-amino-4-methylbenzoate (**93**) as a white solid (17.5 mg, 53%).

8 Experimental Details and Characterization Data

2-(*p*-Tolyl)isoindoline-1,3-dione (3a), 2-(*m*-Tolyl)isoindoline-1,3-dione (3b), and 2-(*o*-Tolyl)isoindoline-1,3-dione (3c)



A3 (92.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **3a**, **3b**, and **3c** as a white solid (32.2 mg, 68%); **3a/3b/3c** = 4.7:1:4.4 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.51 (hexane : ethyl acetate = 4:1).

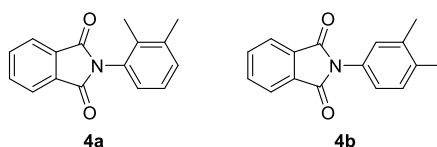
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dt, J = 5.2, 2.4 Hz, 2H), 7.80 (dt, J = 5.2, 2.4 Hz, 2H), 7.39–7.20 (m, 4H), 2.43, 2.41, and 2.22 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.5, 167.4, 167.4, 138.2, 136.6, 134.4, 132.0, 132.0, 131.8, 131.19, 129.8, 129.5, 129.0, 128.8, 127.8, 126.9, 126.5, 123.8, 123.7, 21.4, 21.3, 18.1.

Melting point 168–169 °C.

Analytic data match the literature⁴.

2-(2,3-Dimethylphenyl)isoindoline-1,3-dione (4a), 2-(3,4-Dimethylphenyl)isoindoline-1,3-dione (4b)



A4 (106.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **4a** and **4b** as a white solid (31.2 mg, 62%); **4a/4b** = 4.0:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.53 (hexane : ethyl acetate = 4:1).

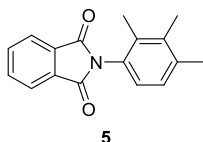
^1H NMR (400 MHz, CDCl_3) δ 7.95 (dt, J = 5.2, 2.4 Hz, 2H), 7.79 (dt, J = 5.2, 2.4 Hz, 2H), 7.27 (d, J = 7.2 Hz, 1H), 7.28 – 7.05 (m, 3H), 2.36 and 2.31 (s, 3H), 2.32 and 2.08 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.6, 138.5, 137.7, 137.1, 135.2, 134.3, 132.1, 131.9, 131.0, 130.5, 130.3, 129.1, 127.8, 126.3, 126.3, 124.2, 123.8, 123.7, 20.5, 19.9, 19.6, 14.7.

Melting point 177–179 °C.

Analytic data match the literature⁴.

2-(2,3,4-Trimethylphenyl)isoindoline-1,3-dione (5)



A5 (120.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **5** as a white solid (25.4 mg, 48%).

R_f = 0.56 (hexane : ethyl acetate = 4:1).

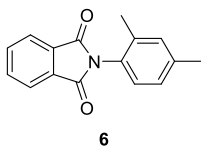
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dt, J = 5.2, 2.4 Hz, 2H), 7.79 (dt, J = 5.2, 2.4 Hz, 2H), 7.14 (d, J = 8.0 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1H), 2.34 (s, 3H), 2.25 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.8, 138.2, 136.8, 134.7, 134.3, 132.1, 128.2, 128.2, 125.6, 123.8, 20.9, 16.2, 15.2.

Melting point 181–182 °C.

Analytic data match the literature⁴.

2-(2,4-Dimethylphenyl)isoindoline-1,3-dione (6)



A6 (106.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **6** as a white solid (30.2 mg, 60%).

R_f = 0.53 (hexane : ethyl acetate = 4:1).

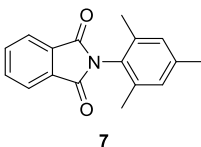
^1H NMR (400 MHz, CDCl_3) δ 7.95 (dt, J = 5.2, 2.4 Hz, 2H), 7.79 (dt, J = 5.2, 2.4 Hz, 2H), 7.18 (s, 1H), 7.14 (d, J = 8.4 Hz, 1H), 7.08 (d, J = 8.0 Hz, 1H), 2.38 (s, 3H), 2.17 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.6, 139.5, 136.2, 134.3, 132.1, 131.9, 128.5, 127.9, 127.7, 123.7, 21.2, 17.9.

Melting point 173–174 °C.

Analytic data match the literature⁴.

2-Mesitylisoindoline-1,3-dione (**7**)



A7 (120.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **7** as a white solid (27.0 mg, 51%).

R_f = 0.53 (hexane : ethyl acetate = 4:1).

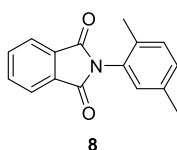
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dt, J = 5.2, 2.4 Hz, 2H), 7.80 (dt, J = 5.2, 2.4 Hz, 2H), 7.01 (s, 2H), 2.33 (s, 3H), 2.12 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.5, 139.4, 136.5, 134.3, 132.0, 129.3, 127.0, 123.8, 21.2, 18.0.

Melting point 183–184 °C.

Analytic data match the literature⁴.

2-(2,5-Dimethylphenyl)isoindoline-1,3-dione (**8**)



A8 (106.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **8** as a white solid (28.2 mg, 56%).

R_f = 0.52 (hexane : ethyl acetate = 4:1).

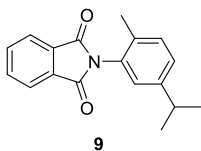
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97 (dt, J = 5.2, 2.4 Hz, 2H), 7.80 (dt, J = 5.2, 2.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 1H), 7.22 – 7.17 (m, 1H), 7.02 (s, 1H), 2.37 (s, 3H), 2.16 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.5, 136.7, 134.3, 133.3, 132.1, 131.0, 130.4, 130.3, 129.2, 123.8, 20.8, 17.6.

Melting point 178–179 °C.

Analytic data match the literature⁴.

2-(5-Isopropyl-2-methylphenyl)isoindoline-1,3-dione (**9**)



A9 (134.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **9** as a white solid (35.7 mg, 64%).

R_f = 0.58 (hexane : ethyl acetate = 4:1).

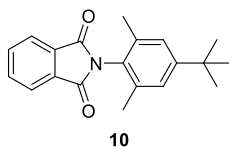
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.96 (dd, J = 5.6, 3.2 Hz, 2H), 7.80 (dd, J = 5.6, 3.2 Hz, 2H), 7.29 (d, J = 8.0 Hz, 1H), 7.24 (dd, J = 8.0, 1.6 Hz, 1H), 7.05 (d, J = 1.2 Hz, 1H), 2.92 (hept, J = 6.8 Hz, 1H), 2.17 (s, 3H), 1.26 (d, J = 6.8 Hz, 6H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.5, 147.7, 134.3, 133.6, 132.1, 131.0, 130.4, 127.7, 126.7, 123.7, 33.5, 26.9, 23.9, 17.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{18}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 280.1332, found: 280.1333.

Melting point 174–176 °C.

2-(4-(Tert-butyl)-2,6-dimethylphenyl)isoindoline-1,3-dione (**10**)



A10 (162.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **10** as a yellow solid (24.6 mg, 40%).

R_f = 0.54 (hexane : ethyl acetate = 4:1).

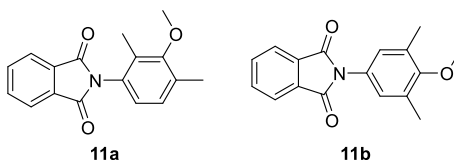
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (td, J = 5.2, 2.0 Hz, 2H), 7.80 (td, J = 5.2, 2.0 Hz, 2H), 7.18 (s, 2H), 2.15 (s, 6H), 1.33 (s, 9H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.5, 152.2, 135.9, 134.3, 132.1, 127.0, 125.7, 123.8, 34.5, 31.3, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{20}\text{H}_{22}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 308.1645, found: 308.1642.

Melting point 175–177 °C.

2-(3-Methoxy-2,4-dimethylphenyl)isoindoline-1,3-dione (11a), 2-(4-Methoxy-3,5-dimethylphenyl)isoindoline-1,3-dione (11b)



A11 (136.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **11a** and **11b** as a white solid (26.4 mg, 47%); **11a/11b** = 1:1 (the isomer ratio was determined by $^1\text{H NMR}$); the isolated product was an inseparable mixture of isomers.

R_f = 0.43 (hexane : ethyl acetate = 4:1).

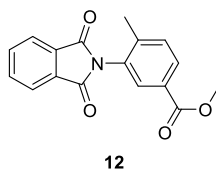
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (td, J = 4.8, 3.2 Hz, 2H), 7.79 (td, J = 5.6, 3.2 Hz, 2H), 7.15 and 6.91 (d, J = 8.0 Hz, 1H), 7.05 (s, 1H), 3.77 and 3.76 (s, 3H), 2.35 and 2.12 (s, 3H), 2.33 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.6, 167.5, 157.6, 156.9, 134.3, 132.5, 132.0, 132.0, 131.8, 130.1, 129.5, 128.9, 127.2, 126.8, 124.2, 123.8, 123.7, 60.0, 59.7, 16.3, 16.3, 11.5.

Melting point 183–185 °C.

Analytic data match the literature⁵.

Methyl 3-(1,3-dioxoisoindolin-2-yl)-4-methylbenzoate (12)



A12 (150.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 5:1) to afford **12** as a white solid (42.5 mg, 72%).

R_f = 0.31 (hexane : ethyl acetate = 4:1).

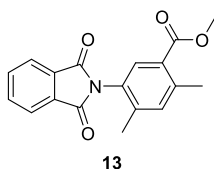
^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dd, J = 5.4, 3.2 Hz, 2H), 7.91 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.4, 3.2 Hz, 2H), 7.45 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.1, 166.1, 142.2, 134.5, 131.9, 131.3, 130.9, 130.5, 130.3, 129.3, 123.9, 52.2, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 296.0917, found: 296.0924.

Melting point 189–192 °C.

Methyl 2-(1,3-dioxoisindolin-2-yl)-3,5-dimethylbenzoate (**13**)



A13 (164.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **13** as a white solid (35.2 mg, 57%).

R_f = 0.40 (hexane : ethyl acetate = 4:1).

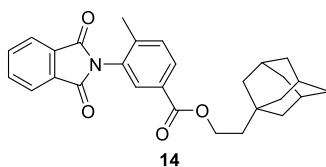
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dd, J = 5.6, 3.2 Hz, 2H), 7.82 (s, 1H), 7.79 (dd, J = 5.6, 3.2 Hz, 2H), 7.38 (s, 1H), 3.69 (s, 3H), 2.42 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.8, 165.4, 139.5, 138.7, 136.0, 134.2, 132.5, 130.3, 128.4, 127.9, 123.8, 52.3, 21.1, 17.9.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{15}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 310.1074, found: 310.1069.

Melting point 185–186 °C.

2-((1s,3s)-Adamantan-1-yl)ethyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**14**)



A14 (298.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 5:1) to afford **14** as a white solid (54.0 mg, 61%).

R_f = 0.35 (hexane : ethyl acetate = 4:1).

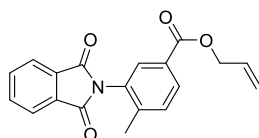
¹H NMR (400 MHz, CDCl₃) δ 8.04 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dt, J = 6.8, 3.4 Hz, 2H), 7.89 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.1 Hz, 2H), 7.45 (d, J = 8.0 Hz, 1H), 4.36 (t, J = 7.6 Hz, 2H), 2.27 (s, 3H), 1.96 (s, 3H), 1.72 (s, 1H), 1.65 – 1.61 (m, 3H), 1.58 – 1.52 (m, 8H).

¹³C NMR (100 MHz, CDCl₃) δ 167.1, 165.7, 142.0, 134.5, 131.9, 131.3, 130.8, 130.5, 130.2, 129.7, 123.9, 61.7, 42.5, 42.5, 37.0, 31.8, 28.6, 18.4.

HRMS (ESI-TOF) m/z calcd for C₂₈H₂₉NO₄ [M+H]⁺: 444.2169, found: 444.2167.

Melting point 162–164 °C.

Allyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**15**)



15

A15 (176.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **15** as a white solid (40.4 mg, 63%).

R_f = 0.35 (hexane : ethyl acetate = 4:1).

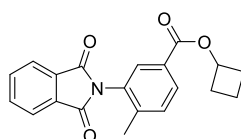
¹H NMR (400 MHz, CDCl₃) δ 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.91 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.46 (d, J = 8.0 Hz, 1H), 4.42 (t, J = 6.8 Hz, 2H), 2.65 (td, J = 6.8, 2.8 Hz, 2H), 2.28 (s, 3H), 2.01 (t, J = 2.8 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 167.1, 165.3, 142.5, 134.5, 131.9, 131.4, 130.9, 130.6, 130.3, 129.1, 124.0, 70.1, 62.8, 19.1, 18.4.

HRMS (ESI-TOF) m/z calcd for C₁₉H₁₅NO₄ [M+H]⁺: 322.1074, found: 322.1066.

Melting point 172–173 °C.

Cyclobutyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**16**)



16

A16 (190.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **16** as a white solid (41.5 mg, 62%).

R_f = 0.43 (hexane : ethyl acetate = 4:1).

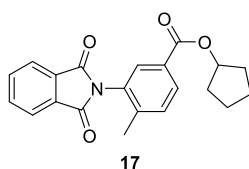
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dd, J = 5.2, 3.2 Hz, 2H), 7.90 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.2, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.24 – 5.16 (m, 1H), 2.47 – 2.40 (m, 2H), 2.27 (s, 3H), 2.24 – 2.14 (m, 2H), 1.88 – 1.80 (m, 1H), 1.71 – 1.64 (m, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.1, 164.9, 142.1, 134.5, 131.9, 131.3, 130.8, 130.5, 130.2, 129.5, 123.9, 69.5, 30.4, 18.4, 13.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{20}\text{H}_{17}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 336.1230, found: 336.1238.

Melting point 161–162 °C.

Cyclopentyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**17**)



A17 (204.3 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **17** as a white solid (47.5 mg, 68%).

R_f = 0.39 (hexane : ethyl acetate = 4:1).

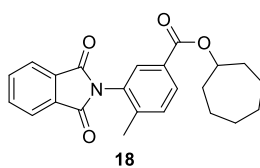
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.03 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.86 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.39 (tt, J = 6.0, 2.8 Hz, 1H), 2.27 (s, 3H), 1.98 – 1.93 (m, 2H), 1.84 – 1.76 (m, 4H), 1.63 (t, J = 6.8 Hz, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.2, 165.3, 142.0, 134.5, 132.0, 131.2, 130.8, 130.5, 130.1, 130.1, 123.9, 32.8, 23.8, 18.3.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{21}\text{H}_{19}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 350.1387, found: 350.1393.

Melting point 165–167 °C.

Cycloheptyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**18**)



A18 (232.3 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **18** as a white solid (38.5 mg, 51%).

R_f = 0.36 (hexane : ethyl acetate = 4:1).

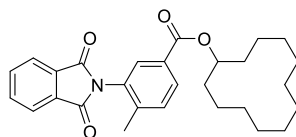
^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.88 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.18 (dt, J = 8.0, 4.0 Hz, 1H), 2.27 (s, 3H), 2.00 (dddd, J = 13.2, 7.6, 4.4, 2.8 Hz, 2H), 1.83 – 1.75 (m, 2H), 1.61 – 1.58 (m, 5H), 1.54 – 1.51 (m, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.2, 164.9, 141.9, 134.5, 132.0, 131.2, 130.8, 130.5, 130.2, 130.1, 123.9, 76.0, 72.8, 37.6, 33.8, 28.3, 28.1, 22.9, 22.6, 18.3.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{23}\text{H}_{23}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 378.1700, found: 378.1691.

Melting point 162–163 °C.

Cyclododecyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**19**)



19

A19 (302.5 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **19** as a yellow solid (51.9 mg, 58%).

R_f = 0.52 (hexane : ethyl acetate = 4:1).

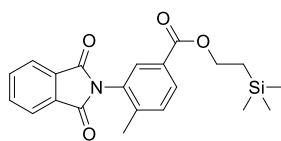
^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.87 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.25 (ddd, J = 7.2, 4.8, 2.8 Hz, 1H), 2.26 (s, 3H), 1.81 (dd, J = 14.0, 6.8 Hz, 2H), 1.66 – 1.59 (m, 2H), 1.46 – 1.29 (m, 18H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.2, 165.2, 141.9, 134.5, 132.0, 131.2, 130.8, 130.6, 130.1, 130.1, 123.9, 73.3, 29.1, 24.2, 24.0, 23.4, 23.2, 20.9, 18.3.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{28}\text{H}_{33}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 448.2482, found: 448.2488.

Melting point 173–174 °C.

(Trimethylsilyl)methyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**20**)



20

A20 (236.4 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **20** as a yellow solid (39.6 mg, 52%).

R_f = 0.57 (hexane : ethyl acetate = 4:1).

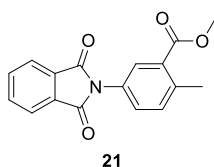
^1H NMR (400 MHz, CDCl_3) δ 7.97 (dd, J = 8.0, 1.8 Hz, 1H), 7.90 (dd, J = 5.5, 3.0 Hz, 2H), 7.83 (d, J = 1.9 Hz, 1H), 7.74 (dd, J = 5.5, 3.1 Hz, 2H), 7.37 (d, J = 8.0 Hz, 1H), 4.37 – 4.28 (m, 2H), 2.20 (s, 3H), 1.08 – 1.00 (m, 2H), 0.00 (s, 9H).

^{13}C NMR (100 MHz, CDCl_3) δ 168.6, 167.2, 143.4, 136.0, 133.4, 132.7, 132.3, 131.9, 131.6, 131.3, 125.4, 64.9, 19.8, 18.9, 2.5.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{20}\text{H}_{21}\text{NO}_4\text{Si}$ $[\text{M}+\text{H}]^+$: 382.1469, found: 382.1473.

Melting point 177–179 °C.

Methyl 5-(1,3-dioxoisindolin-2-yl)-2-methylbenzoate (**21**)



A21 (150.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 5:1) to afford **21** as a white solid (39.6 mg, 67%).

R_f = 0.35 (hexane : ethyl acetate = 4:1).

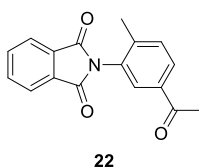
^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, J = 2.4 Hz, 1H), 7.96 (dd, J = 5.6, 3.2 Hz, 2H), 7.80 (dd, J = 5.6, 3.2 Hz, 2H), 7.49 (dd, J = 8.4, 2.4 Hz, 1H), 7.40 (d, J = 8.4 Hz, 1H), 3.89 (s, 3H), 2.67 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.1, 167.0, 140.6, 134.5, 132.5, 131.7, 130.2, 129.9, 129.4, 128.8, 123.8, 52.0, 21.5.

Melting point 187–188 °C.

Analytic data match the literature⁴.

2-(5-Acetyl-2-methylphenyl)isoindoline-1,3-dione (**22**)



A22 (134.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 5:1) to afford **22** as a white solid (33.6 mg, 60%).

R_f = 0.34 (hexane : ethyl acetate = 4:1).

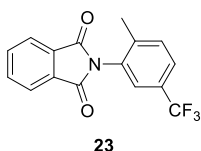
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dt, J = 6.4, 3.1 Hz, 3H), 7.86 – 7.80 (m, 3H), 7.48 (d, J = 8.0 Hz, 1H), 2.60 (s, 3H), 2.28 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 196.6, 167.1, 142.5, 136.2, 134.6, 131.9, 131.5, 131.1, 129.2, 129.1, 124.0, 26.6, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 280.0968, found: 280.0962.

Melting point 157–158 °C.

2-(2-Methyl-5-(trifluoromethyl)phenyl)isoindoline-1,3-dione (**23**)



A23 (160.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **23** as a white solid (33.0 mg, 54%).

R_f = 0.48 (hexane : ethyl acetate = 4:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dt, J = 7.2, 3.5 Hz, 2H), 7.87 – 7.80 (m, 2H), 7.63 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 7.6 Hz, 2H), 2.28 (s, 3H).

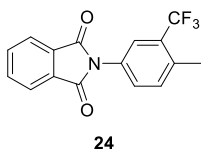
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.9, 141.0, 134.6, 131.8, 131.8, 131.1, 129.5 (q, J = 124.1 Hz), 126.2, 126.2, 126.2 (q, J = 3.6 Hz), 126.05 (q, J = 3.6 Hz), 125.0, 124.0, 122.3, 18.3.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -62.38.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{10}\text{F}_3\text{NO}_2$ $[\text{M}+\text{H}]^+$: 306.0736, found: 306.0745.

Melting point 210–212 °C.

2-(4-Methyl-3-(trifluoromethyl)phenyl)isoindoline-1,3-dione (**24**)



A24 (160.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **24** as a white solid (36.6 mg, 60%).

$R_f = 0.47$ (hexane : ethyl acetate = 4:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.96 (tt, $J = 5.2, 2.4$ Hz, 2H), 7.82 (td, $J = 5.2, 2.0$ Hz, 2H), 7.72 (d, $J = 2.0$ Hz, 1H), 7.53 (dd, $J = 8.4, 2.0$ Hz, 1H), 7.43 (d, $J = 8.4$ Hz, 1H), 2.56 – 2.52 (m, 3H).

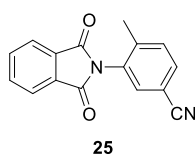
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.0, 136.7 (q, $J = 6.0$ Hz), 134.6, 132.7, 131.6, 129.8 (q, $J = 112.8$ Hz), 129.5, 125.3, 124.2 (q, $J = 21.8$ Hz), 123.9, 122.6, 19.1, 19.1.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -61.98.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{10}\text{F}_3\text{NO}_2$ $[\text{M}+\text{H}]^+$: 306.0736, found: 306.0745.

Melting point 208–210 °C.

3-(1,3-Dioxoisindolin-2-yl)-4-methylbenzonitrile (**25**)



A25 (117.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 5:1) to afford **25** as a yellow solid (33.6 mg, 64%).

$R_f = 0.37$ (hexane : ethyl acetate = 4:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dt, $J = 7.2, 3.6$ Hz, 2H), 7.84 (dd, $J = 5.6, 3.2$ Hz, 2H), 7.67 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.56 – 7.52 (m, 1H), 7.49 (d, $J = 8.0$ Hz, 1H), 2.29 (s, 3H).

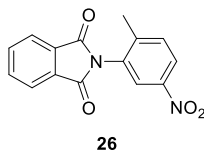
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.7, 142.9, 134.8, 132.7, 132.6, 132.2, 131.7, 124.1, 117.9, 111.0, 18.7.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{10}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 263.0815, found: 263.0818.

Melting point 196–199 °C.

Analytic data match the literature⁶.

2-(2-Methyl-5-nitrophenyl)isoindoline-1,3-dione (**26**)



A26 (137.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 5:1) to afford **26** as a yellow solid (23.8 mg, 42%).

$R_f = 0.31$ (hexane : ethyl acetate = 4:1).

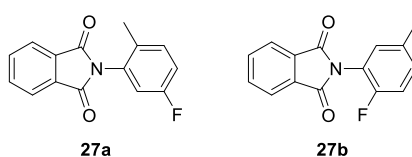
¹H NMR (400 MHz, CDCl₃) δ 8.25 (dd, J = 8.4, 2.4 Hz, 1H), 8.14 (d, J = 2.4 Hz, 1H), 7.99 (dd, J = 5.6, 3.2 Hz, 2H), 7.85 (dd, J = 5.6, 3.2 Hz, 2H), 7.55 (d, J = 8.4 Hz, 1H), 2.33 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 166.6, 146.7, 144.8, 134.8, 131.9, 131.7, 131.6, 124.5, 124.2, 124.1, 18.6.

HRMS (ESI-TOF) m/z calcd for C₁₅H₁₀N₂O₄ [M+H]⁺: 283.0713, found: 283.0714.

Melting point 229–231 °C.

2-(5-Fluoro-2-methylphenyl)isoindoline-1,3-dione (27a), 2-(2-Fluoro-5-methylphenyl)isoindoline-1,3-dione (27b)



A27 (110.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **27a** and **27b** as a white solid (26.6 mg, 52%); **27a/27b** = 4:1 (the isomer ratio was determined by ¹H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.57 (hexane : ethyl acetate = 4:1).

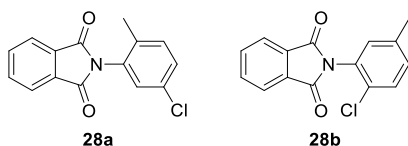
¹H NMR (400 MHz, CDCl₃) δ 7.96 (dt, J = 7.2, 3.6 Hz, 2H), 7.85 – 7.78 (m, 2H), 7.34 – 6.95 (m, 3H), 2.38 and 2.17 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 167.0, 166.7, 161.0, 159.8, 134.5, 134.4, 132.4, 132.4, 132.1, 132.0, 132.0, 131.9, 131.5, 131.4, 131.3, 131.2, 130.1, 123.9, 116.6, 116.4, 116.2, 116.1, 115.9, 20.7, 17.5.

Melting point 159–160 °C.

Analytic data match the literature⁴.

2-(5-Chloro-2-methylphenyl)isoindoline-1,3-dione (28a), 2-(2-Chloro-5-methylphenyl)isoindoline-1,3-dione (28b)



A28 (126.6 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **28a** and **28b** as a white solid (34.2 mg, 63%); **28a/28b** = 1.8:1 (the

isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.58 (hexane : ethyl acetate = 4:1).

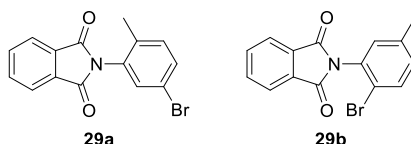
^1H NMR (400 MHz, CDCl_3) δ 7.97 (dt, J = 5.6, 2.8 Hz, 2H), 7.81 (dq, J = 5.6, 3.2, 2.8 Hz, 2H), 7.45 – 7.16 (m, 3H), 2.39 and 2.18 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 165.9, 165.8, 137.0, 134.2, 133.5, 133.4, 131.1, 130.9, 130.9, 130.8, 130.6, 130.5, 130.1, 129.0, 128.9, 128.6, 127.9, 122.9, 19.8, 16.6.

Melting point 165–167 °C.

Analytic data match the literature⁴.

2-(5-Bromo-2-methylphenyl)isoindoline-1,3-dione (29a), 2-(2-Bromo-5-methylphenyl)isoindoline-1,3-dione (29b)



A29 (171.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **29a** and **29b** as a yellow solid (44.0 mg, 70%); **29a/29b** = 11.5:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.60 (hexane : ethyl acetate = 4:1).

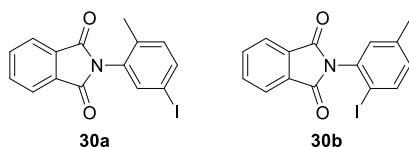
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dt, J = 7.2, 3.6 Hz, 2H), 7.81 (dq, J = 6.8, 3.6 Hz, 2H), 7.62 – 7.16 (m, 3H), 2.37 and 2.16 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 166.9, 135.8, 134.6, 134.5, 132.5, 132.4, 131.8, 131.7, 123.9, 119.5, 17.8.

Melting point 175–177 °C.

Analytic data match the literature⁴.

2-(5-Iodo-2-methylphenyl)isoindoline-1,3-dione (30a), 2-(2-Iodo-5-methylphenyl)isoindoline-1,3-dione (30b)



A30 (218.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **30a** and **30b** as a white solid (45.0 mg, 62%); **30a/30b** = 11.7:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.51 (hexane : ethyl acetate = 4:1).

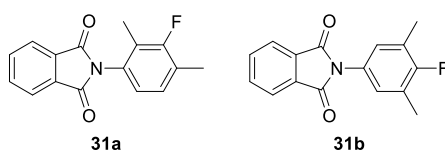
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dt, J = 7.2, 3.6 Hz, 2H), 7.81 (dq, J = 6.8, 3.6 Hz, 2H), 7.70 – 7.02 (m, 2H), 2.37 and 2.16 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 138.4, 137.4, 136.5, 134.5, 132.7, 132.0, 131.8, 123.9, 90.2, 17.8.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_{10}\text{INO}_2$ $[\text{M}+\text{H}]^+$: 363.9829, found: 363.9825.

Melting point 180–182 °C.

2-(3-Fluoro-2,4-dimethylphenyl)isoindoline-1,3-dione (31a), **2-(4-Fluoro-3,5-dimethylphenyl)isoindoline-1,3-dione (31b)**



A31 (124.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **31a** and **31b** as a white solid (28.2 mg, 53%); **31a/31b** = 1:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.57 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 7.96 (dd, J = 5.6, 3.2 Hz, 2H), 7.81 (dd, J = 5.6, 3.2 Hz, 2H), 7.17 – 6.92 (m, 2H), 2.32 (d, J = 2.4 Hz, 3H), 2.10 (d, J = 2.4 Hz, 3H).

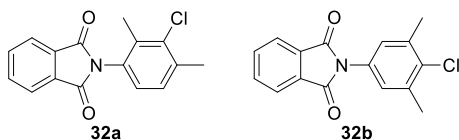
^{13}C NMR (100 MHz, CDCl_3) δ 167.3, 161.2, 158.8, 134.5, 131.9, 129.5, 129.4, 128.7, 128.7, 126.2, 126.0, 124.1, 123.9, 123.8, 123.7, 14.8, 14.8, 10.5, 10.4.

^{19}F NMR (376 MHz, CDCl_3) δ -117.42.

Melting point 171–172 °C.

Analytic data match the literature⁵.

2-(3-Chloro-2,4-dimethylphenyl)isoindoline-1,3-dione (32a), **2-(4-Chloro-3,5-dimethylphenyl)isoindoline-1,3-dione (32b)**



A32 (140.6 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **32a** and **32b** as a white solid (38.2 mg, 67%); **32a/32b** = 9:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.60 (hexane : ethyl acetate = 4:1).

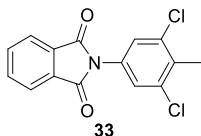
^1H NMR (400 MHz, CDCl_3) δ 7.99 – 7.94 (m, 2H), 7.84 – 7.78 (m, 2H), 7.24 – 7.03 (m, 2H), 2.44, 2.43, and 2.23 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.3, 138.0, 135.9, 135.2, 134.5, 131.9, 129.3, 128.5, 126.6, 123.9, 21.1, 16.2.

Melting point 175–176 °C.

Analytic data match the literature⁵.

2-(3,5-Dichloro-4-methylphenyl)isoindoline-1,3-dione (**33**)



A33 (161.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **33** as a white solid (42.7 mg, 70%).

R_f = 0.55 (hexane : ethyl acetate = 4:1).

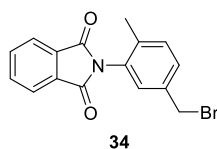
^1H NMR (400 MHz, CDCl_3) δ 7.96 (dt, J = 7.2, 3.6 Hz, 2H), 7.82 (dq, J = 6.8, 4.0 Hz, 2H), 7.45 (s, 2H), 2.51 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 166.6, 135.6, 134.7, 134.5, 131.5, 130.3, 125.6, 124.0, 17.3.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_9\text{Cl}_2\text{NO}_2$ $[\text{M}+\text{H}]^+$: 306.0083, found: 306.0079.

Melting point 219–220 °C.

2-(5-(Bromomethyl)-2-methylphenyl)isoindoline-1,3-dione (**34**)



34 (185.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **34** as a yellow solid (40.2 mg, 61%).

R_f = 0.61 (hexane : ethyl acetate = 4:1).

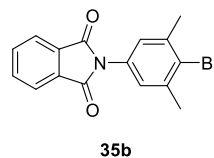
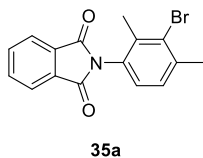
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.96 (dt, J = 7.2, 3.6 Hz, 2H), 7.81 (dd, J = 5.6, 3.2 Hz, 2H), 7.41 (dd, J = 8.0, 1.6 Hz, 1H), 7.35 (d, J = 8.0 Hz, 1H), 7.25 (d, J = 1.6 Hz, 1H), 4.50 (s, 2H), 2.21 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.2, 136.9, 136.6, 134.5, 132.0, 131.6, 130.8, 130.1, 129.3, 123.9, 32.4, 18.0.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{13}\text{BrNO}_2$ $[\text{M}+\text{H}]^+$: 330.0124, found: 330.0128.

Melting point 193–195 °C.

2-(3-Bromo-2,4-dimethylphenyl)isoindoline-1,3-dione (35a), **2-(4-Bromo-3,5-dimethylphenyl)isoindoline-1,3-dione (35b)**



A35 (185.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **35** as a white solid (46.1 mg, 70%).

R_f = 0.37 (hexane : ethyl acetate = 4:1).

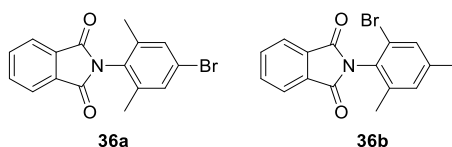
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.81 (dd, J = 5.6, 3.2 Hz, 2H), 7.26 – 7.07 (m, 2H), 2.48 (s, 2H), 2.47 (s, 1H), 2.28 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.2, 139.5, 134.5, 131.7, 126.2, 123.8, 24.1.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{12}\text{BrNO}_2$ $[\text{M}+\text{H}]^+$: 330.0124, found: 330.0128.

Melting point 187–188 °C.

2-(4-Bromo-2,6-dimethylphenyl)isoindoline-1,3-dione (36a), **2-(2-Bromo-4,6-dimethylphenyl)isoindoline-1,3-dione (36b)**



A36 (185.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **36a** and **36b** as a white solid (47.4 mg, 72%); **36a/36b** = 1.4:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

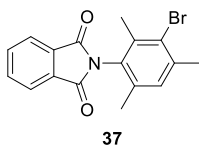
R_f = 0.57 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 8.01 – 7.93 (m, 2H), 7.82 (dt, J = 5.6, 2.8 Hz, 2H), 7.39, 7.35, and 7.11 (s, 3H), 2.36, 2.20, and 2.14 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 166.7, 141.3, 139.1, 139.0, 134.5, 134.4, 132.0, 131.9, 131.4, 131.4, 130.8, 129.0, 127.6, 123.9, 123.9, 123.5, 123.4, 21.0, 18.6, 18.0.

Melting point 183–184 °C.

2-(3-Bromo-2,4,6-trimethylphenyl)isoindoline-1,3-dione (**37**)



A37 (189.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **37** as a yellow solid (43.9 mg, 64%).

R_f = 0.45 (hexane : ethyl acetate = 4:1).

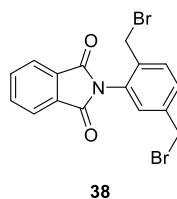
^1H NMR (400 MHz, CDCl_3) δ 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.12 (s, 1H), 2.44 (s, 3H), 2.25 (s, 3H), 2.09 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.2, 139.9, 137.1, 135.5, 134.5, 131.9, 130.2, 128.1, 125.5, 123.9, 24.1, 19.3, 17.9.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{14}\text{BrNO}_2$ $[\text{M}+\text{H}]^+$: 344.0281, found: 344.0291.

Melting point 191–192 °C.

2-(2,5-Bis(bromomethyl)phenyl)isoindoline-1,3-dione (**38**)



A38 (264.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **38** as a white solid (40.7 mg, 50%).

R_f = 0.50 (hexane : ethyl acetate = 4:1).

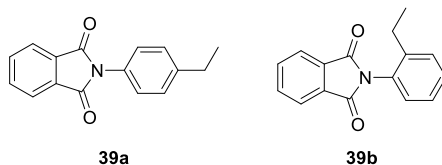
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.99 (dd, J = 5.6, 3.2 Hz, 2H), 7.84 (dd, J = 5.6, 3.2 Hz, 2H), 7.55 – 7.48 (m, 2H), 7.31 (s, 1H), 4.50 (s, 2H), 4.41 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.1, 139.6, 136.0, 134.7, 131.8, 131.6, 131.1, 130.4, 130.3, 124.1, 31.6, 29.0.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{Br}_2\text{NO}_2$ $[\text{M}+\text{H}]^+$: 407.9229, found: 407.9232.

Melting point 181–182 °C.

2-(4-Ethylphenyl)isoindoline-1,3-dione (**39a**), 2-(2-Ethylphenyl)isoindoline-1,3-dione (**39b**)



A39 (106.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **39a** and **39b** as a white solid (31.6 mg, 63%); **39a/39b** = 5.7:1 (the isomer ratio was determined by $^1\text{H NMR}$); the isolated product was an inseparable mixture of isomers.

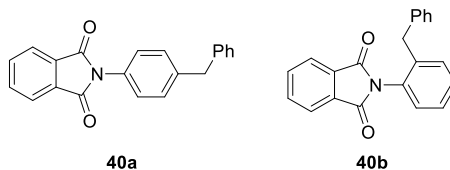
R_f = 0.55 (hexane : ethyl acetate = 4:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 – 7.92 (m, 2H), 7.78 (dp, J = 6.8, 3.2 Hz, 2H), 7.44 – 7.17 (m, 4H), 2.74 – 2.50 (m, 2H), 1.29 – 1.15 (m, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.5, 144.4, 134.3, 132.0, 131.9, 129.8, 129.3, 129.1, 129.0, 128.6, 126.9, 126.5, 123.8, 123.7, 28.6, 24.4, 15.4, 14.3.

Melting point 171–173 °C.

2-(4-Benzylphenyl)isoindoline-1,3-dione (**40a**), 2-(2-Benzylphenyl)isoindoline-1,3-dione (**40b**)



A40 (168.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **40a** and **40b** as a white solid (38.2 mg, 61%); **40a/40b** > 20:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.58 (hexane : ethyl acetate = 4:1).

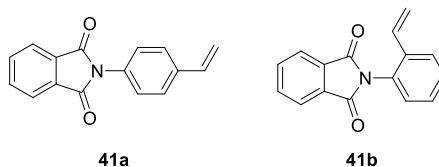
^1H NMR (400 MHz, CDCl_3) δ 7.94 (dt, J = 7.2, 3.6 Hz, 2H), 7.79 (td, J = 5.2, 2.0 Hz, 2H), 7.58 – 7.12 (m, 4H), 2.66 – 2.45 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.4, 141.3, 140.4, 134.4, 131.8, 129.6, 129.1, 128.6, 126.6, 126.3, 123.8, 41.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{21}\text{H}_{15}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 314.1176, found: 314.1180.

Melting point 125–126 °C.

2-(4-Vinylphenyl)isoindoline-1,3-dione (**41a**), 2-(3-Vinylphenyl)isoindoline-1,3-dione (**41b**)



A41 (104.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **41a** and **41b** as a white solid (31.4 mg, 63%); **41a/41b** = 18:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.51 (hexane : ethyl acetate = 4:1).

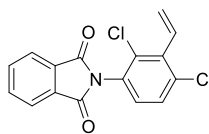
^1H NMR (400 MHz, CDCl_3) δ 7.95 (dt, J = 6.8, 3.2 Hz, 2H), 7.83 – 7.76 (m, 2H), 7.55 – 7.33 (m, 4H), 6.79 – 6.72 (m, 1H), 5.82 – 5.77 (m, 1H), 5.33 – 5.30 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.3, 137.4, 136.0, 134.5, 131.8, 131.0, 126.9, 126.6, 123.8, 115.0.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 250.0863, found: 250.0862.

Melting point 193–195 °C.

2-(2,4-Dichloro-3-vinylphenyl)isoindoline-1,3-dione (42)



42

A42 (173.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **42** as a white solid (32.3 mg, 51%).

R_f = 0.45 (hexane : ethyl acetate = 4:1).

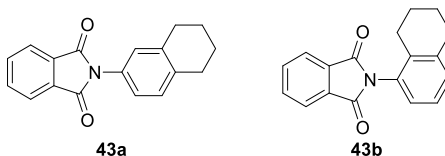
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.83 (dd, J = 5.6, 3.2 Hz, 2H), 7.49 (d, J = 8.4 Hz, 1H), 7.20 (d, J = 8.4 Hz, 1H), 6.71 (dd, J = 17.6, 11.6 Hz, 1H), 5.84 – 5.75 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.6, 137.1, 135.5, 134.6, 133.6, 131.8, 130.8, 129.3, 129.0, 128.9, 124.1, 123.8.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_9\text{Cl}_2\text{NO}_2$ $[\text{M}+\text{H}]^+$: 318.0083, found: 318.0079.

Melting point 198–199 °C.

2-(5,6,7,8-Tetrahydronaphthalen-2-yl)isoindoline-1,3-dione (43a), 2-(5,6,7,8-Tetrahydronaphthalen-1-yl)isoindoline-1,3-dione (43b)



A43 (132.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 7.9:1) to afford **43a** and **43b** as a white solid (35.5 mg, 64%); **43a/43b** = 7.9:1 (the isomer ratio was determined by $^1\text{H NMR}$); the isolated product was an inseparable mixture of isomers.

R_f = 0.47 (hexane : ethyl acetate = 4:1).

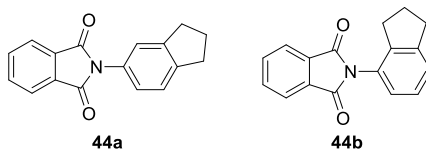
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.94 (qd, J = 5.2, 2.0 Hz, 2H), 7.81 – 7.74 (m, 2H), 7.23 – 7.01 (m, 3H), 2.86 – 2.52 (m, 4H), 1.85 – 1.73 (m, 4H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.6, 139.1, 138.2, 137.7, 135.6, 134.3, 132.1, 131.9, 130.7, 129.9, 128.7, 127.3, 126.1, 126.1, 123.9, 123.7, 123.7, 29.6, 29.4, 29.2, 24.9, 23.0, 22.9, 22.6, 22.5.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{15}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 278.1176, found: 278.1182.

Melting point 162–164 °C.

2-(2,3-Dihydro-1H-inden-5-yl)isoindoline-1,3-dione (44a), 2-(2,3-Dihydro-1H-inden-4-yl)isoindoline-1,3-dione (44b)



A44 (118.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6.5:1) to afford **44a** and **44b** as a white solid (34.7 mg, 66%); **44a/44b** = 6.5:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.45 (hexane : ethyl acetate = 4:1).

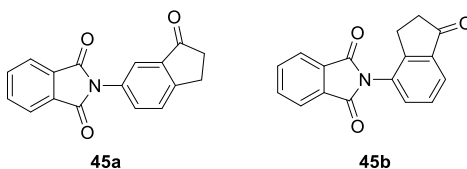
^1H NMR (400 MHz, CDCl_3) δ 7.94 (dt, J = 6.8, 3.6 Hz, 2H), 7.78 (dt, J = 5.6, 2.8 Hz, 2H), 7.35 – 7.07 (m, 3H), 3.03 – 2.79 (m, 4H), 2.16 – 2.06 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.7, 167.1, 146.5, 145.5, 144.8, 142.3, 134.3, 132.1, 131.9, 129.5, 127.2, 125.4, 125.2, 124.9, 124.8, 123.8, 123.7, 122.9, 33.3, 33.0, 32.7, 31.2, 25.6, 24.9.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 264.1019, found: 264.1019.

Melting point 154–155 °C.

2-(3-Oxo-2,3-dihydro-1H-inden-5-yl)isoindoline-1,3-dione (45a), 2-(1-Oxo-2,3-dihydro-1H-inden-4-yl)isoindoline-1,3-dione (45b)



A45 (132.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 9:1) to afford **45a** and **45b** as a white solid (28.8 mg, 52%); **45a/45b** = 9:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

R_f = 0.38 (hexane : ethyl acetate = 4:1).

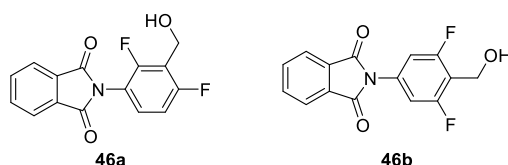
^1H NMR (400 MHz, CDCl_3) δ 8.03 – 7.93 (m, 2H), 7.90 – 7.76 (m, 3H), 7.69 – 7.55 (m, 2H), 3.23 – 3.05 (m, 2H), 2.79 – 2.71 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 205.8, 167.0, 166.7, 154.5, 138.0, 134.7, 134.6, 134.1, 132.7, 131.7, 131.1, 128.6, 127.4, 124.1, 123.9, 122.0, 36.7, 25.7.

Melting point 192–193 °C.

Analytic data match the literature⁶.

2-(2,4-Difluoro-3-(hydroxymethyl)phenyl)isoindoline-1,3-dione (46a), 2-(3,5-Difluoro-4-(hydroxymethyl)phenyl)isoindoline-1,3-dione (46b)



A46 (144.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **46** as a white solid (31.8 mg, 55%).

R_f = 0.33 (hexane : ethyl acetate = 4:1).

¹H NMR (400 MHz, CDCl₃) δ 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.35 – 7.29 (m, 1H), 7.07 (td, J = 8.8, 1.6 Hz, 1H), 4.84 (s, 2H).

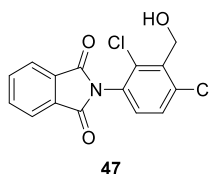
¹³C NMR (100 MHz, CDCl₃) δ 166.5, 134.7, 131.8, 130.1, 130.0, 124.1, 117.9, 112.1, 112.0, 111.9, 111.8, 60.4, 53.2, 53.1, 53.1, 21.1, 14.2.

¹⁹F NMR (376 MHz, CDCl₃) δ -71.3, -113.3, -120.0 (t, J = 8.4 Hz).

HRMS (ESI-TOF) m/z calcd for C₁₅H₉F₂NO₃ [M+H]⁺: 290.0623, found: 290.0622.

Melting point 174–176 °C.

2-(2,4-Dichloro-3-(hydroxymethyl)phenyl)isoindoline-1,3-dione (47)



A47 (177.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 3:1) to afford **47** as a white solid (32.7 mg, 51%).

R_f = 0.26 (hexane : ethyl acetate = 2:1).

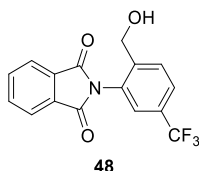
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.03 (dt, J = 7.2, 3.6 Hz, 2H), 7.96 (dd, J = 5.2, 3.2 Hz, 2H), 7.71 – 7.62 (m, 2H), 5.43 (t, J = 5.2 Hz, 1H), 4.76 (d, J = 5.2 Hz, 2H).

¹³C NMR (100 MHz, DMSO-*d*₆) δ 166.7, 138.1, 136.8, 135.6, 135.4, 131.9, 129.8, 129.3, 124.3, 59.3.

HRMS (ESI-TOF) m/z calcd for $C_{15}H_9Cl_2NO_3$ $[M+H]^+$: 322.0032, found: 322.0030.

Melting point 170–172 °C.

2-(2-(Hydroxymethyl)-5-(trifluoromethyl)phenyl)isoindoline-1,3-dione (48)



A48 (176.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 3:1) to afford **48** as a white solid (30.8 mg, 48%).

R_f = 0.25 (hexane : ethyl acetate = 2:1).

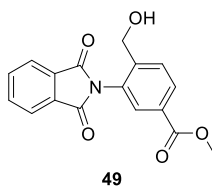
1H NMR (400 MHz, $CDCl_3$) δ 7.98 (dt, J = 7.2, 3.6 Hz, 2H), 7.85 (dd, J = 5.6, 3.2 Hz, 2H), 7.81 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 9.2 Hz, 1H), 7.54 (s, 1H), 4.59 (d, J = 4.0 Hz, 2H), 2.39 (t, J = 5.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 142.6, 134.9, 131.7, 131.2 (q, J = 125.6 Hz), 130.6, 129.9, 126.5 (q, J = 13.5 Hz), 126.1 (q, J = 13.9 Hz), 124.8, 124.2, 61.4.

HRMS (ESI-TOF) m/z calcd for $C_{16}H_{13}NO_3$ $[M+H]^+$: 268.0968, found: 268.0977.

Melting point 140–141 °C.

Methyl 3-(1,3-dioxoisoindolin-2-yl)-4-(hydroxymethyl)benzoate (49)



A49 (166.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 3:1) to afford **49** as a white solid (34.2 mg, 55%).

R_f = 0.23 (hexane : ethyl acetate = 2:1).

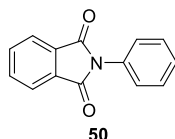
1H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.95 (d, J = 1.6 Hz, 1H), 7.84 (dd, J = 5.6, 3.2 Hz, 2H), 7.75 (d, J = 8.0 Hz, 1H), 4.59 (d, J = 6.4 Hz, 2H), 3.93 (s, 3H), 2.36 (t, J = 6.4 Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.7, 143.6, 134.8, 131.7, 130.9, 130.8, 130.3, 130.1, 124.1, 61.5, 52.4, 31.6, 22.7, 14.1.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{NO}_5$ $[\text{M}+\text{H}]^+$: 312.0866, found: 312.0871.

Melting point 174–176 °C.

2-Phenylisoindoline-1,3-dione (**50**)



A50 (78.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **50** as a white solid (31.7 mg, 71%).

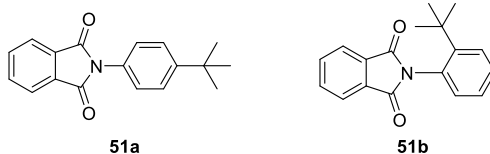
R_f = 0.53 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.80 (dd, J = 5.6, 3.2 Hz, 2H), 7.54 – 7.49 (m, 2H), 7.46 – 7.39 (m, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.3, 134.4, 131.8, 131.7, 129.2, 128.2, 126.6, 123.8.

Analytic data match the literature⁴.

2-(4-(Tert-butyl)phenyl)isoindoline-1,3-dione (**51a**), 2-(2-(Tert-butyl)phenyl)isoindoline-1,3-dione (**51b**)



A51 (134.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **51** as a white solid (30.7 mg, 55%).

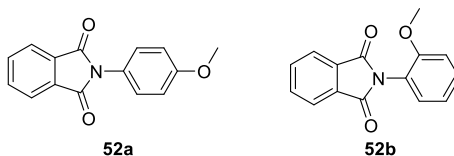
R_f = 0.52 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 7.96 (dd, J = 5.6, 3.2 Hz, 2H), 7.79 (dd, J = 5.6, 3.2 Hz, 2H), 7.53 (d, J = 2.0 Hz, 1H), 7.54 – 7.34 (m, 4H), 1.36 (s, 8H), 1.32 (s, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.5, 151.2, 134.4, 131.9, 128.9, 126.2, 126.1, 125.3, 123.9, 123.7, 34.7, 31.6, 31.3, 31.3.

Analytic data match the literature⁴.

2-(4-Methoxyphenyl)isoindoline-1,3-dione (52a), 2-(2-Methoxyphenyl)isoindoline-1,3-dione (52b)



A52 (108.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **52a** and **52b** as a white solid (26.8 mg, 53%); **52a/52b** = 18:1 (the isomer ratio was determined by ^1H NMR); the isolated product was an inseparable mixture of isomers.

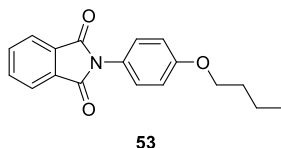
R_f = 0.37 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 7.95 (dd, J = 5.6, 3.2 Hz, 2H), 7.79 (dd, J = 5.6, 3.2 Hz, 2H), 7.35 – 7.33 (m, 2H), 7.04 – 7.01 (m, 2H), 3.85 and 3.80 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.6, 159.3, 134.4, 131.9, 128.0, 124.3, 123.7, 114.5, 55.5.

Analytic data match the literature⁴.

2-(4-Butylphenyl)isoindoline-1,3-dione (53)



A53 (150.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **53** as a white solid (27.1 mg, 46%).

R_f = 0.47 (hexane : ethyl acetate = 4:1).

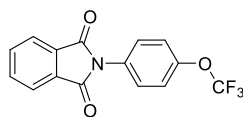
^1H NMR (400 MHz, CDCl_3) δ 7.94 (dd, J = 5.6, 3.2 Hz, 2H), 7.78 (dd, J = 5.6, 3.2 Hz, 2H), 7.36 – 7.27 (m, 2H), 7.04 – 6.97 (m, 2H), 4.00 (t, J = 6.4 Hz, 2H), 1.82 – 1.75 (m, 2H), 1.55 – 1.46 (m, 2H), 0.99 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.7, 158.9, 134.3, 131.9, 127.9, 124.0, 123.7, 115.0, 68.0, 31.2, 19.2, 13.8.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 296.1281, found: 296.1279.

Melting point 193–195 °C.

2-(4-(Trifluoromethoxy)phenyl)isoindoline-1,3-dione (54)



54

A54 (162.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **54** as a white solid (34.4 mg, 56%).

R_f = 0.44 (hexane : ethyl acetate = 4:1).

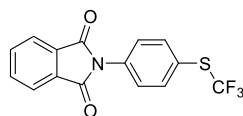
^1H NMR (400 MHz, CDCl_3) δ 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.53 – 7.51 (m, 2H), 7.36 (d, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 148.4, 134.7, 131.6, 130.2, 127.9, 124.0, 121.7, 120.4 (J = 257 Hz).

^{19}F NMR (376 MHz, CDCl_3) δ -57.85.

Analytic data match the literature⁴.

2-(4-((Trifluoromethyl)thio)phenyl)isoindoline-1,3-dione (**55**)



55

A55 (178.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **55** as a white solid (40.1 mg, 62%).

R_f = 0.45 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 7.98 (ddd, J = 5.6, 3.2, 1.2 Hz, 2H), 7.84 – 7.69 (m, 4H), 7.66 – 7.56 (m, 2H).

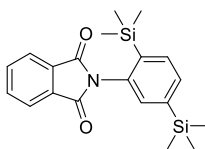
^{13}C NMR (100 MHz, CDCl_3) δ 166.8, 137.0, 134.8 (J = 173 Hz), 134.7, 131.5, 130.0, 128.7, 127.0, 124.0.

^{19}F NMR (376 MHz, CDCl_3) δ -42.36 (d, J = 12.4 Hz).

HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_8\text{F}_3\text{NO}_2\text{S}$ $[\text{M}+\text{H}]^+$: 324.0301, found: 324.0293.

Melting point 184–186 °C.

2-(2,5-Bis(trimethylsilyl)phenyl)isoindoline-1,3-dione (**56**)



56

A56 (222.5 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **56** as a white solid (40.4 mg, 55%).

R_f = 0.47 (hexane : ethyl acetate = 4:1).

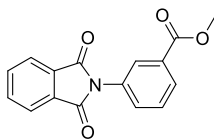
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 (dd, J = 5.6, 3.2 Hz, 2H), 7.64 (dd, J = 5.6, 3.2 Hz, 2H), 7.51 (d, J = 7.2 Hz, 1H), 7.44 (d, J = 7.2 Hz, 1H), 7.08 (s, 1H), 0.10 (s, 9H), -0.00 (s, 9H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.9, 144.0, 141.0, 136.3, 135.6, 134.8, 134.3, 134.3, 132.7, 124.3.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{20}\text{H}_{25}\text{NO}_2\text{Si}_2$ $[\text{M}+\text{H}]^+$: 368.1497, found: 368.1498.

Melting point 151–153 °C.

Methyl 3-(1,3-dioxoisindolin-2-yl)benzoate (**57**)



57

A57 (136.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **57** as a white solid (33.1 mg, 57%).

R_f = 0.31 (hexane : ethyl acetate = 4:1).

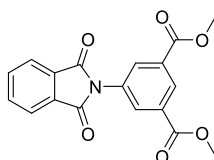
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.19 – 8.08 (m, 2H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.68 – 7.58 (m, 2H), 3.95 (s, 1H), 3.94 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.0, 166.2, 135.9, 134.7, 134.6, 132.0, 131.6, 131.6, 131.3, 130.9, 130.5, 129.3, 129.3, 129.2, 127.7, 126.0, 124.0, 123.9, 52.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 282.0761, found: 282.0759.

Melting point 193–195 °C.

Dimethyl 5-(1,3-dioxoisindolin-2-yl)isophthalate (**58**)



58

A58 (194.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **58** as a white solid (34.6 mg, 51%).

R_f = 0.27 (hexane : ethyl acetate = 4:1).

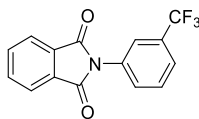
¹H NMR (400 MHz, CDCl₃) δ 8.73 (s, 1H), 8.35 (d, J = 1.6 Hz, 2H), 8.00 (dd, J = 5.6, 3.2 Hz, 2H), 7.84 (dd, J = 5.6, 3.2 Hz, 2H), 3.97 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 166.7, 165.4, 134.8, 132.4, 131.8, 131.7, 131.5, 130.1, 124.1, 52.6.

HRMS (ESI-TOF) m/z calcd for C₁₈H₁₃NO₆ [M+H]⁺: 340.0816, found: 340.0811.

Melting point 197–199 °C.

2-(3-(Trifluoromethyl)phenyl)isoindoline-1,3-dione (**59**)



59

A59 (146.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **59** as a white solid (35.0 mg, 60%).

R_f = 0.33 (hexane : ethyl acetate = 4:1).

¹H NMR (400 MHz, CDCl₃) δ 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.83 (dd, J = 5.6, 3.2 Hz, 2H), 7.78 (s, 1H), 7.67 (dt, J = 10.0, 7.2 Hz, 3H).

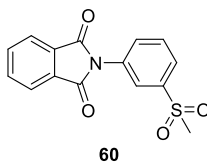
¹³C NMR (100 MHz, CDCl₃) δ 166.8, 134.8, 132.3, 131.6 (J = 32 Hz), 131.5, 129.7, 129.6, 124.0, 123.6 (J = 271 Hz), 124.7 (J = 4 Hz), 123.4 (J = 4 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -62.64 (d, J = 10.8 Hz).

HRMS (ESI-TOF) m/z calcd for C₁₅H₈F₃NO₂ [M+H]⁺: 292.0580, found: 292.0577.

Melting point 200–201 °C.

2-(3-(Methylsulfonyl)phenyl)isoindoline-1,3-dione (**60**)



A60 (156.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **60** as a white solid (36.7 mg, 61%).

R_f = 0.33 (hexane : ethyl acetate = 4:1).

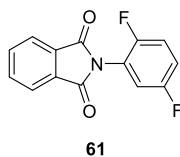
¹H NMR (400 MHz, CDCl₃) δ 8.12 – 8.08 (m, 1H), 8.01 – 7.97 (m, 3H), 7.85 – 7.71 (m, 4H), 3.13 (s, 3H), 3.10 (s, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 166.6, 141.6, 135.0, 134.9, 132.9, 131.4, 131.3, 130.2, 128.4, 126.7, 126.5, 125.4, 124.2, 124.1, 44.6.

HRMS (ESI-TOF) m/z calcd for C₁₅H₁₁NO₄S [M+H]⁺: 302.0482, found: 302.0490.

Melting point 213–215 °C.

2-(2,5-Difluorophenyl)isoindoline-1,3-dione (**61**)



A61 (114.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **61** as a white solid (30.0 mg, 58%).

R_f = 0.47 (hexane : ethyl acetate = 4:1).

¹H NMR (400 MHz, CDCl₃) δ 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.83 (dd, J = 5.6, 3.2 Hz, 2H), 7.23 (dt, J = 9.2, 4.4 Hz, 1H), 7.19 – 7.10 (m, 2H).

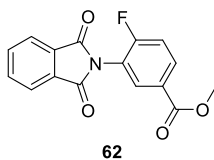
¹³C NMR (100 MHz, CDCl₃) δ 166.1, 159.5 (J = 5 Hz), 157.4 (J = 4 Hz), 155.4 (J = 4 Hz), 152.9 (J = 1 Hz), 134.7, 131.8, 124.1, 117.7, 117.6, 117.4 (J = 2 Hz), 117.2 (J = 8 Hz), 117.0, 116.7.

¹⁹F NMR (376 MHz, CDCl₃) δ -116.8, -123.7.

HRMS (ESI-TOF) m/z calcd for C₁₄H₇F₂NO₂ [M+H]⁺: 260.0518, found: 260.0515.

Melting point 194–197 °C.

Methyl 3-(1,3-dioxoisoindolin-2-yl)-4-fluorobenzoate (**62**)



A62 (154.1 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **62** as a white solid (25.2 mg, 42%).

R_f = 0.37 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 8.17 (ddd, J = 8.8, 4.8, 2.4 Hz, 1H), 8.10 (dd, J = 7.2, 2.4 Hz, 1H), 7.99 (dd, J = 5.6, 3.2 Hz, 2H), 7.83 (dd, J = 5.6, 3.2 Hz, 2H), 7.34 (t, J = 9.2 Hz, 1H), 3.93 (s, 3H).

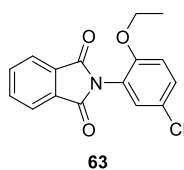
^{13}C NMR (100 MHz, CDCl_3) δ 166.2, 165.3, 160.8 (J = 259 Hz), 134.7, 134.4, 132.5, 132.4, 131.9, 131.8, 127.2 (J = 3 Hz), 124.1, 123.6, 119.7 (J = 14 Hz), 117.0 (J = 21 Hz), 52.5.

^{19}F NMR (376 MHz, CDCl_3) δ -111.2.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{10}\text{FNO}_4$ $[\text{M}+\text{H}]^+$: 300.0667, found: 300.0669.

Melting point 198–200 °C.

2-(5-Chloro-2-ethoxyphenyl)isoindoline-1,3-dione (**63**)



A63 (156.6 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **63** as a white solid (27.7 mg, 46%).

R_f = 0.41 (hexane : ethyl acetate = 4:1).

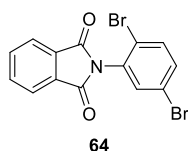
^1H NMR (400 MHz, CDCl_3) δ 7.95 (dd, J = 5.6, 3.2 Hz, 2H), 7.79 (dd, J = 5.6, 3.2 Hz, 2H), 7.37 (dd, J = 8.8, 2.8 Hz, 1H), 7.26 (s, 1H), 6.96 (d, J = 8.8 Hz, 1H), 4.04 (q, J = 7.2 Hz, 2H), 1.26 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 153.6, 134.3, 132.1, 130.4, 130.1, 125.3, 123.8, 121.5, 114.1, 64.7, 14.5.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{12}\text{ClNO}_3$ $[\text{M}+\text{H}]^+$: 302.0578, found: 302.0571.

Melting point 190–193 °C.

2-(2,5-Dibromophenyl)isoindoline-1,3-dione (**64**)



A64 (235.9 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **64** as a white solid (31.8 mg, 42%).

R_f = 0.45 (hexane : ethyl acetate = 4:1).

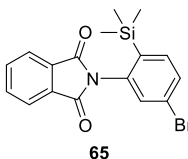
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.99 (dd, J = 5.6, 3.2 Hz, 2H), 7.83 (dd, J = 5.6, 3.2 Hz, 2H), 7.61 (dd, J = 8.0, 1.2 Hz, 1H), 7.51 – 7.48 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.2, 134.7, 134.6, 134.0, 133.9, 132.7, 131.7, 124.2, 122.3, 121.5.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{14}\text{H}_7\text{Br}_2\text{NO}_2$ $[\text{M}+\text{H}]^+$: 379.8916, found: 379.8912.

Melting point 185–187 °C.

2-(5-Bromo-2-(trimethylsilyl)phenyl)isoindoline-1,3-dione (**65**)



A65 (229.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **65** as a white solid (36.6 mg, 49%).

R_f = 0.39 (hexane : ethyl acetate = 4:1).

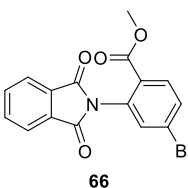
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.72 (d, J = 8.0 Hz, 1H), 7.47 (dd, J = 8.0, 1.6 Hz, 1H), 7.42 (d, J = 1.6 Hz, 1H), 0.28 (s, 9H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.1, 143.1, 137.1, 136.6, 135.7, 134.2, 133.2, 132.1, 125.3, 125.2.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{16}\text{BrNO}_2\text{Si}$ $[\text{M}+\text{H}]^+$: 374.0206, found: 374.0205.

Melting point 171–172 °C.

Methyl 4-bromo-2-(1,3-dioxoisindolin-2-yl)benzoate (**66**)



A66 (215.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **66** as a white solid (28.7 mg, 40%).

R_f = 0.38 (hexane : ethyl acetate = 4:1).

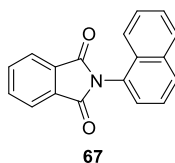
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.01 (ddd, J = 8.8, 4.8, 2.4 Hz, 4H), 7.85 – 7.83 (m, 3H), 3.93 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.4, 165.4, 134.7, 134.4, 133.8, 132.0, 131.8, 131.7, 130.8, 129.0, 124.1, 123.6, 52.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{10}\text{BrNO}_4$ $[\text{M}+\text{H}]^+$: 359.9866, found: 359.9873.

Melting point 187–188 °C.

2-(Naphthalen-1-yl)isoindoline-1,3-dione (**67**)



A67 (128.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **67** as a white solid (30.1 mg, 55%).

R_f = 0.40 (hexane : ethyl acetate = 4:1).

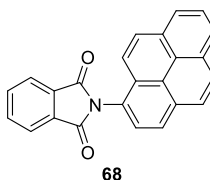
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.02 (dt, J = 6.0, 3.2 Hz, 2H), 7.98 – 7.94 (m, 2H), 7.85 (dd, J = 5.6, 3.2 Hz, 2H), 7.62 – 7.58 (m, 2H), 7.56 – 7.46 (m, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.8, 134.5, 134.5, 132.1, 130.3, 130.0, 128.6, 128.2, 127.2, 127.0, 126.6, 125.4, 124.0, 122.5.

Melting point 178–181 °C.

Analytic data match the literature⁴.

2-(Pyren-1-yl)isoindoline-1,3-dione (**68**)



A68 (202.3 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **68** as a white solid (32.0 mg, 46%).

R_f = 0.41 (hexane : ethyl acetate = 4:1).

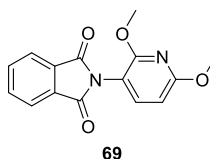
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.31 (d, J = 8.0 Hz, 1H), 8.24 (dd, J = 14.2, 7.6 Hz, 2H), 8.18 – 8.10 (m, 3H), 8.08 – 8.03 (m, 3H), 7.95 (d, J = 8.0 Hz, 1H), 7.89 – 7.84 (m, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.1, 134.6, 132.2, 132.1, 131.1, 130.8, 128.9, 128.5, 128.4, 127.2, 126.4, 126.4, 126.1, 125.9, 125.4, 125.1, 125.1, 124.5, 124.1, 121.7.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{24}\text{H}_{13}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 348.1019, found: 348.1018.

Melting point 191–192 °C.

2-(2,6-Dimethoxypyridin-3-yl)isoindoline-1,3-dione (**69**)



A69 (139.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **69** as a white solid (25.0 mg, 44%).

R_f = 0.30 (hexane : ethyl acetate = 4:1).

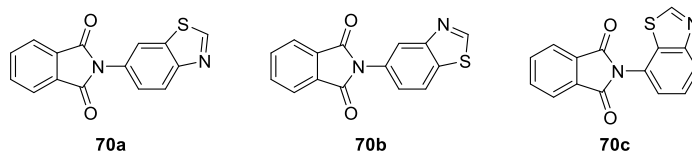
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.93 (dd, J = 5.6, 3.2 Hz, 2H), 7.77 (dd, J = 5.6, 3.2 Hz, 2H), 7.45 (d, J = 8.4 Hz, 1H), 6.43 (d, J = 8.4 Hz, 1H), 3.96 (s, 3H), 3.92 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.4, 163.3, 158.5, 140.9, 134.2, 132.2, 123.7, 106.5, 101.7, 53.9, 53.8.

Melting point 171–172 °C.

Analytic data match the literature⁴.

2-(Benzo[d]thiazol-6-yl)isoindoline-1,3-dione (**70a**), 2-(Benzo[d]thiazol-5-yl)isoindoline-1,3-dione (**70b**), 2-(Benzo[d]thiazol-7-yl)isoindoline-1,3-dione (**70c**)



A70 (135.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **70a**, **70b** and **70c** as a white solid (34.2 mg, 61%); **70a/70b/70c** = 2:1:1 (the isomer ratio was determined by $^1\text{H NMR}$); the isolated product was an inseparable mixture of isomers.

$R_f = 0.33$ (hexane : ethyl acetate = 4:1).

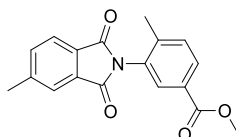
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.10 – 9.05 (m, 1H), 8.28 – 8.24 (m, 1H), 8.11 – 8.09 (m, 1H), 8.03 – 7.99 (m, 2H), 7.87 – 7.82 (m, 2H), 7.71 – 7.49 (m, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.3, 166.2, 155.5, 155.3, 155.0, 154.3, 153.7, 152.6, 134.8, 134.6, 134.6, 134.3, 133.6, 132.3, 131.7, 131.7, 131.6, 130.1, 129.2, 126.7, 126.3, 125.3, 125.0, 124.2, 124.1, 124.0, 123.9, 122.3, 122.0, 120.2.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_9\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 281.0379, found: 281.0382.

Melting point 188–189 °C.

Methyl 4-methyl-3-(5-methyl-1,3-dioxisoindolin-2-yl)benzoate (**71**)



71

B2 (35.4 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **71** as a white solid (41.4 mg, 67%).

$R_f = 0.37$ (hexane : ethyl acetate = 4:1).

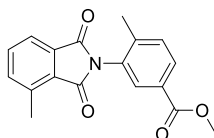
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.90 (d, $J = 1.6$ Hz, 1H), 7.84 (d, $J = 7.6$ Hz, 1H), 7.77 (s, 1H), 7.60 (d, $J = 7.6$ Hz, 1H), 7.44 (d, $J = 8.0$ Hz, 1H), 3.90 (s, 3H), 2.56 (s, 3H), 2.26 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.3, 167.2, 166.1, 145.9, 142.3, 135.1, 132.3, 131.3, 131.0, 130.4, 130.3, 129.3, 129.2, 124.4, 123.8, 52.2, 22.1, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 310.1074, found: 310.1075.

Melting point 131–132 °C.

Methyl 4-methyl-3-(4-methyl-1,3-dioxisoindolin-2-yl)benzoate (**72**)



72

B3 (35.4 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **72** as a white solid (29.1 mg, 47%).

R_f = 0.36 (hexane : ethyl acetate = 4:1).

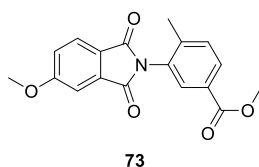
^1H NMR (400 MHz, CDCl_3) δ 8.07 – 8.02 (m, 1H), 7.90 (d, J = 1.6 Hz, 1H), 7.79 (d, J = 7.2 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.75 (s, 3H), 2.28 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.9, 167.1, 166.1, 142.3, 138.7, 136.9, 134.0, 132.3, 131.3, 131.0, 130.4, 130.3, 129.2, 128.6, 121.6, 52.2, 18.4, 17.8.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 310.1074, found: 310.1075.

Melting point 123–124 °C.

Methyl 3-(5-methoxy-1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**73**)



B4 (38.6 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **73** as a white solid (40.3 mg, 62%).

R_f = 0.31 (hexane : ethyl acetate = 4:1).

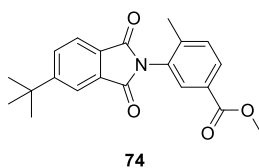
^1H NMR (400 MHz, CDCl_3) δ 8.07 – 8.01 (m, 1H), 7.90 (d, J = 1.6 Hz, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.28 – 7.24 (m, 1H), 3.96 (d, J = 1.2 Hz, 3H), 3.90 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 166.9, 166.1, 165.1, 142.3, 134.6, 131.3, 131.0, 130.4, 130.3, 129.2, 125.6, 123.8, 120.5, 108.4, 56.2, 52.2, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_5$ $[\text{M}+\text{H}]^+$: 326.1023, found: 326.1029.

Melting point 157–159 °C.

Methyl 3-(5-(tert-butyl)-1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**74**)



B5 (43.8 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **74** as a yellow solid (39.3 mg, 56%).

R_f = 0.40 (hexane : ethyl acetate = 4:1).

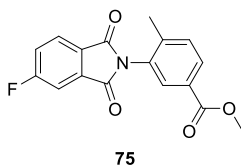
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (dd, J = 8.0, 1.6 Hz, 1H), 8.01 – 7.98 (m, 1H), 7.89 (d, J = 7.6 Hz, 2H), 7.83 (dd, J = 8.0, 1.6 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.27 (s, 3H), 1.42 (s, 9H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.6, 167.2, 166.1, 159.3, 142.3, 132.1, 131.6, 131.3, 131.0, 130.4, 130.3, 129.2, 123.8, 121.1, 52.2, 35.9, 31.2, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{21}\text{H}_{22}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 352.1543, found: 352.1540.

Melting point 140–142 °C.

Methyl 3-(5-(tert-butyl)-1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**75**)



B6 (36.2 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **75** as a white solid (30.2 mg, 43%).

R_f = 0.43 (hexane : ethyl acetate = 4:1).

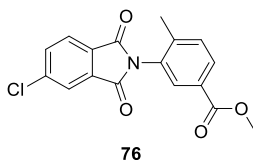
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (dd, J = 8.0, 1.6 Hz, 1H), 8.01 – 7.98 (m, 1H), 7.89 (d, J = 7.6 Hz, 2H), 7.83 (dd, J = 8.0, 1.6 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.27 (s, 3H), 1.42 (s, 9H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.0, 166.0, 165.7, 165.5 (d, J = 124.1 Hz), 142.1, 134.7 (d, J = 37.6 Hz), 131.4, 130.6, 130.6, 130.2, 127.7 (d, J = 11.3 Hz), 126.4 (d, J = 33.8 Hz), 121.6 (d, J = 90.2 Hz), 111.7 (d, J = 94.0 Hz), 52.3, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{FNO}_4$ $[\text{M}+\text{H}]^+$: 314.0823, found: 314.0828.

Melting point 147–148 °C.

Methyl 3-(5-chloro-1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**76**)



B7 (39.6 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **76** as a white solid (38.2 mg, 58%).

R_f = 0.32 (hexane : ethyl acetate = 4:1).

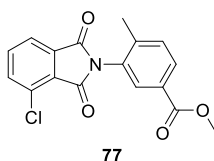
^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.2 Hz, 1H), 7.94 (d, J = 1.2 Hz, 1H), 7.90 (d, J = 8.0 Hz, 2H), 7.78 (dd, J = 8.0, 1.2 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 166.1, 166.0, 165.8, 142.1, 141.3, 134.6, 133.5, 131.4, 130.6, 130.6, 130.1, 129.9, 129.3, 125.2, 124.4, 52.3, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{ClNO}_4$ $[\text{M}+\text{H}]^+$: 330.0528, found: 330.0531.

Melting point 145–146 °C.

Methyl 3-(4-chloro-1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**77**)



B8 (39.6 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **77** as a white solid (33.6 mg, 51%).

R_f = 0.42 (hexane : ethyl acetate = 4:1).

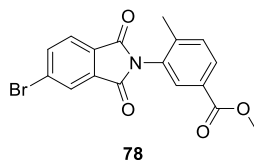
^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.89 (dt, J = 8.4, 3.2 Hz, 2H), 7.76 – 7.71 (m, 2H), 7.45 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H), 2.28 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 166.0, 165.6, 164.6, 142.2, 136.3, 135.4, 133.9, 132.1, 131.4, 130.6, 130.5, 130.2, 129.3, 127.6, 122.4, 52.2, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{ClNO}_4$ $[\text{M}+\text{H}]^+$: 330.0528, found: 330.0531.

Melting point 144–146 °C.

Methyl 3-(5-bromo-1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**78**)



B9 (48.4 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **78** as a yellow solid (47.7 mg, 64%).

R_f = 0.40 (hexane : ethyl acetate = 4:1).

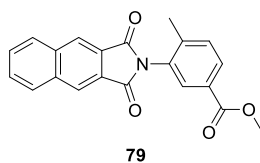
^1H NMR (400 MHz, CDCl_3) δ 8.10 (t, J = 1.6 Hz, 1H), 8.05 (dt, J = 8.0, 1.6 Hz, 1H), 7.95 (dt, J = 8.0, 1.6 Hz, 1H), 7.89 (d, J = 1.2 Hz, 1H), 7.83 (dd, J = 8.0, 1.2 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 3.90 (d, J = 1.2 Hz, 3H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 166.3, 166.0, 165.7, 142.1, 137.6, 133.5, 131.4, 130.6, 130.6, 130.4, 130.1, 129.5, 129.3, 127.3, 125.3, 52.3, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{BrNO}_4$ $[\text{M}+\text{H}]^+$: 374.0022, found: 374.0027.

Melting point 165–167 °C.

Methyl 3-(1,3-dioxo-1,3-dihydro-2H-benzo[f]isoindol-2-yl)-4-methylbenzoate (**79**)



B10 (42.6 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **79** as a white solid (33.1 mg, 48%).

R_f = 0.45 (hexane : ethyl acetate = 4:1).

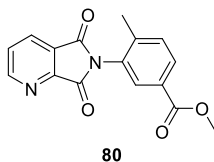
^1H NMR (400 MHz, CDCl_3) δ 8.47 (s, 2H), 8.12 (dt, J = 6.4, 3.2 Hz, 2H), 8.06 (dd, J = 8.0, 1.6 Hz, 1H), 7.96 (d, J = 1.6 Hz, 1H), 7.75 (dt, J = 6.4, 3.2 Hz, 2H), 7.47 (d, J = 8.0 Hz, 1H), 3.91 (s, 3H), 2.30 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 166.9, 166.1, 142.1, 135.7, 131.4, 131.2, 130.5, 130.4, 130.2, 129.5, 129.2, 127.5, 125.6, 52.2, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{21}\text{H}_{16}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 346.1074, found: 346.1068.

Melting point 173–175 °C.

Methyl 3-(5,7-dioxo-5,7-dihydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-methylbenzoate (**80**)



80

B11 (42.6 mg, 0.2 mmol, 1 equiv.) and **A12** (150.2 mg, 1 mmol, 5 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 6:1) to afford **80** as a white solid (19.0 mg, 32%).

R_f = 0.40 (hexane : ethyl acetate = 4:1).

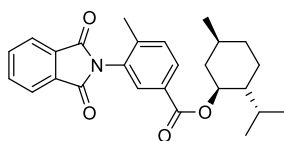
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.29 (d, J = 1.2 Hz, 1H), 9.18 (d, J = 4.8 Hz, 1H), 8.09 (dd, J = 8.0, 1.6 Hz, 1H), 7.95 – 7.84 (m, 2H), 7.48 (d, J = 8.0 Hz, 1H), 3.92 (s, 3H), 2.28 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.9, 165.9, 165.6, 156.1, 145.5, 142.0, 139.2, 131.5, 130.8, 130.2, 130.1, 129.4, 125.7, 117.3, 52.3, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{21}\text{H}_{16}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 297.0870, found: 297.0877.

Melting point 193–195 °C.

(1S,2S,5S)-2-Isopropyl-5-methylcyclohexyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (81)



81

A71 (274.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **81** as a white solid (45.3 mg, 54%).

R_f = 0.47 (hexane : ethyl acetate = 8:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dt, J = 6.8, 3.6 Hz, 2H), 7.89 (d, J = 1.6 Hz, 1H), 7.82 (dt, J = 6.8, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 4.93 (td, J = 10.8, 4.4 Hz, 1H), 2.27 (s, 3H), 2.10 (d, J = 11.6 Hz, 1H), 1.93 (td, J = 7.2, 2.8 Hz, 1H), 1.71 (d, J = 11.6 Hz, 2H), 1.54 (dd, J = 9.2, 6.0 Hz, 2H), 1.10 (p, J = 12.4 Hz, 3H), 0.91 (dd, J = 8.8, 6.8 Hz, 6H), 0.78 (d, J = 6.8 Hz, 3H).

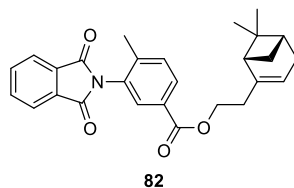
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.2, 166.1, 164.0, 140.9, 133.5, 130.9, 130.9, 130.2, 129.8, 129.5, 129.1, 129.0, 122.9, 122.9, 74.0, 46.2, 39.9, 33.3, 30.4, 25.4, 22.5, 21.0, 19.8, 17.3, 15.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{26}\text{H}_{30}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 420.2169, found: 420.2166.

Melting point 194–196 °C.

2-((1*S*,5*R*)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (82)

3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate



A72 (284.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **82** as a white solid (38.6 mg, 45%).

R_f = 0.40 (hexane : ethyl acetate = 8:1).

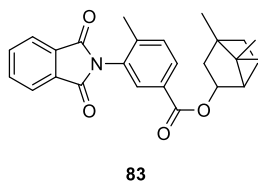
¹H NMR (400 MHz, CDCl₃) δ 8.03 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.89 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.37 – 5.31 (m, 1H), 4.31 (td, J = 7.2, 4.2 Hz, 2H), 2.44 – 2.34 (m, 3H), 2.27 (s, 3H), 2.22 (d, J = 11.2 Hz, 2H), 2.12 – 2.04 (m, 2H), 1.26 (s, 3H), 1.16 (d, J = 8.4 Hz, 1H), 0.83 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 167.1, 165.5, 144.1, 142.1, 134.5, 131.9, 131.3, 130.8, 130.4, 130.24, 129.6, 123.9, 119.0, 63.5, 45.8, 40.7, 38.0, 36.0, 31.7, 31.4, 26.3, 21.2, 18.4.

HRMS (ESI) Calculated for C₂₇H₂₈NO₄ [M+H]⁺: 430.2013, found: 430.2010.

Melting point 188–190 °C.

4,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (83)



A73 (272.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **83** as a white solid (52.7 mg, 63%).

R_f = 0.36 (hexane : ethyl acetate = 8:1).

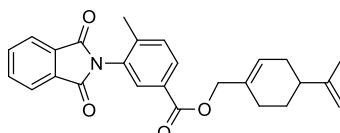
¹H NMR (400 MHz, CDCl₃) δ 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 7.99 (dd, J = 5.6, 3.2 Hz, 2H), 7.88 (d, J = 1.6 Hz, 1H), 7.83 (dd, J = 5.6, 3.2 Hz, 2H), 7.46 (d, J = 8.0 Hz, 1H), 5.11 (dt, J = 10.0, 3.2 Hz, 1H), 2.50 – 2.41 (m, 1H), 2.27 (s, 3H), 2.07 (td, J = 8.8, 4.4 Hz, 1H), 1.75 (dt, J = 21.2, 4.0 Hz, 2H), 1.39 (d, J = 12.4 Hz, 1H), 1.29 (dd, J = 8.4, 3.2 Hz, 1H), 1.11 (dd, J = 13.6, 3.2 Hz, 1H), 0.96 (s, 3H), 0.90 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.2, 167.2, 165.8, 142.0, 134.5, 132.0, 131.2, 130.8, 130.5, 130.1, 124.0, 49.1, 47.9, 45.0, 36.8, 28.1, 27.4, 19.7, 18.9, 18.4, 13.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{26}\text{H}_{28}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 418.2013, found: 418.2019.

Melting point 198–199 °C.

(4-(Prop-1-en-2-yl)cyclohex-1-en-1-yl)methyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (84)



84

A74 (270.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **84** as a white solid (34.9 mg, 42%).

R_f = 0.35 (hexane : ethyl acetate = 8:1).

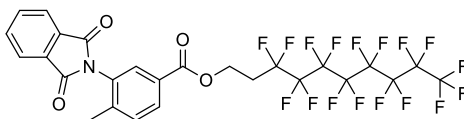
^1H NMR (400 MHz, CDCl_3) δ 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.90 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.45 (d, J = 8.0 Hz, 1H), 5.82 (td, J = 3.2, 1.6 Hz, 1H), 4.78 – 4.67 (m, 4H), 2.27 (s, 3H), 2.21 – 2.11 (m, 4H), 2.04 – 1.93 (m, 1H), 1.86 (dt, J = 12.8, 4.4, 2.4 Hz, 1H), 1.73 (t, J = 1.2 Hz, 3H), 1.51 (ddt, J = 12.8, 11.6, 8.8 Hz, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.1, 165.5, 149.7, 142.2, 134.5, 132.6, 132.0, 131.3, 130.9, 130.6, 130.2, 129.5, 126.0, 123.9, 108.8, 69.1, 40.8, 30.5, 27.3, 26.5, 20.8, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{26}\text{H}_{26}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 416.1856, found: 416.1856.

Melting point 182–184 °C.

3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Heptafluorodecyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (85)



85

A75 (582.0 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **85** as a white solid (72.7 mg, 50%).

R_f = 0.47 (hexane : ethyl acetate = 8:1).

¹H NMR (400 MHz, CDCl₃) δ 8.05 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.98 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.90 (d, *J* = 1.6 Hz, 1H), 7.82 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 1H), 4.62 (t, *J* = 6.4 Hz, 2H), 2.70 – 2.48 (m, 2H), 2.28 (s, 3H).

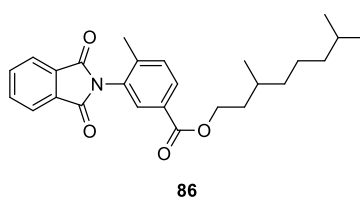
¹³C NMR (100 MHz, CDCl₃) δ 167.1, 165.1, 142.8, 134.6, 131.9, 131.5, 131.0, 130.6, 130.4, 128.6, 124.0, 57.0 (2), 30.6, 18.5.

¹⁹F NMR (376 MHz, CDCl₃) δ -80.77, -113.51, -121.63, -121.92, -122.72, -123.49, -126.12.

HRMS (ESI-TOF) *m/z* calcd for C₂₆H₁₅F₁₇NO₄ [M+H]⁺: 728.0724, found: 728.0728.

Melting point 192–194 °C.

3,7-Dimethyloctyl 3-(1,3-dioxisoindolin-2-yl)-4-methylbenzoate (**86**)



A76 (276.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **86** as a colorless oil (57.3 mg, 68%).

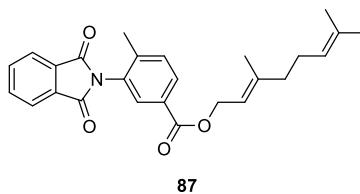
R_f = 0.63 (hexane : ethyl acetate = 8:1).

¹H NMR (400 MHz, CDCl₃) δ 8.05 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.97 (dd, *J* = 5.2, 3.2 Hz, 2H), 7.90 (d, *J* = 1.6 Hz, 1H), 7.82 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 4.40 – 4.29 (m, 2H), 2.27 (s, 3H), 1.83 – 1.73 (m, 1H), 1.55 (ddd, *J* = 20.0, 12.0, 5.6 Hz, 3H), 1.36 – 1.24 (m, 3H), 1.20 – 1.09 (m, 3H), 0.94 (d, *J* = 6.4 Hz, 3H), 0.85 (d, *J* = 6.4 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 167.1, 165.7, 142.1, 134.5, 131.9, 131.3, 130.9, 130.5, 130.2, 129.7, 123.9, 63.8, 39.2, 37.1, 35.6, 29.9, 28.0, 24.6, 22.7, 22.6, 19.6, 18.4.

HRMS (ESI-TOF) *m/z* calcd for C₂₆H₃₂NO₄ [M+H]⁺: 422.2326, found: 422.2328.

(*E*)-3,7-Dimethylocta-2,6-dien-1-yl 3-(1,3-dioxisoindolin-2-yl)-4-methylbenzoate (**87**)



A77 (272.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 8:1) to afford **87** as a colorless oil (51.7 mg, 62%).

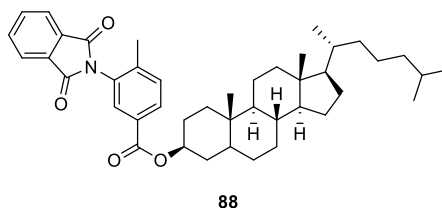
R_f = 0.52 (hexane : ethyl acetate = 4:1).

^1H NMR (400 MHz, CDCl_3) δ 8.06 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dd, J = 5.6, 3.2 Hz, 2H), 7.90 (d, J = 1.6 Hz, 1H), 7.81 (dd, J = 5.6, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.50 – 5.40 (m, 1H), 5.08 (dd, J = 9.6, 4.0 Hz, 1H), 4.83 (d, J = 7.2 Hz, 2H), 2.27 (s, 3H), 2.13 – 2.03 (m, 4H), 1.75 (s, 3H), 1.66 (s, 3H), 1.59 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.1, 165.6, 142.5, 142.1, 134.5, 131.9, 131.8, 131.2, 130.8, 130.6, 130.2, 129.7, 123.9, 123.8, 118.3, 62.0, 39.5, 26.3, 25.7, 18.4, 17.7, 16.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{26}\text{H}_{28}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 418.2013, found: 418.2021.

(3*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (88**)**



A78 (506.4 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **88** as a white solid (67.7 mg, 52%).

R_f = 0.57 (hexane : ethyl acetate = 8:1).

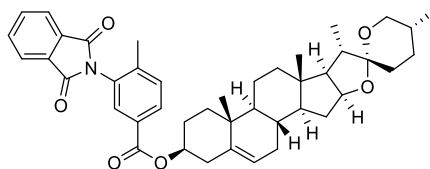
^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.97 (dt, J = 7.2, 3.6 Hz, 2H), 7.88 (d, J = 1.3 Hz, 1H), 7.82 (dq, J = 6.8, 3.6 Hz, 2H), 7.43 (d, J = 8.0 Hz, 1H), 4.93 (tt, J = 10.8, 4.8 Hz, 1H), 2.26 (s, 3H), 1.99 – 1.90 (m, 2H), 1.82 – 1.68 (m, 3H), 1.53 (ddd, J = 20.0, 10.4, 5.2 Hz, 4H), 1.38 – 1.18 (m, 10H), 1.18 – 0.96 (m, 10H), 0.90 (d, J = 6.4 Hz, 4H), 0.88 – 0.82 (m, 9H), 0.65 (s, 4H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.2, 165.1, 141.9, 134.5, 131.9, 131.2, 130.7, 130.5, 130.1, 130.1, 123.9, 56.4, 56.3, 54.2, 44.7, 42.6, 40.0, 39.5, 36.8, 36.2, 35.8, 35.5, 34.1, 32.0, 28.6, 28.3, 28.0, 27.6, 24.2, 23.9, 22.8, 22.6, 21.2, 18.7, 18.3, 12.3, 12.1.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{43}\text{H}_{58}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 652.4360, found: 652.4356.

Melting point 203–204 °C.

(4*S*,5'*R*,6*aR*,6*bS*,8*aS*,8*bR*,9*S*,10*R*,11*aS*,12*aS*,12*bS*)-5',6*a*,8*a*,9-Tetramethyl-1,3,3',4,4',5,5',6,6*a*,6*b*,6',7,8,8*a*,8*b*,9,11*a*,12,12*a*,12*b*-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-*b*]furan-10,2'-pyran]-4-yl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**89**)



89

A79 (532.4 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **89** as a white solid (66.4 mg, 49%).

R_f = 0.44 (hexane : ethyl acetate = 8:1).

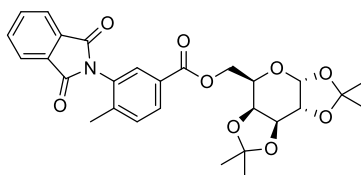
¹H NMR (400 MHz, CDCl₃) δ 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.89 (d, J = 1.6 Hz, 1H), 7.82 (dd, J = 5.6, 3.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 5.46 – 5.36 (m, 1H), 4.90 – 4.75 (m, 1H), 4.42 (q, J = 7.6 Hz, 1H), 3.54 – 3.23 (m, 2H), 2.44 (d, J = 8.0 Hz, 2H), 2.27 (s, 3H), 2.00 (td, J = 12.0, 5.6 Hz, 3H), 1.94 – 1.82 (m, 2H), 1.79 – 1.69 (m, 3H), 1.57 (s, 4H), 1.36 – 1.10 (m, 6H), 1.06 (s, 6H), 0.98 (d, J = 6.8 Hz, 3H), 0.79 (t, J = 3.2 Hz, 5H).

¹³C NMR (100 MHz, CDCl₃) δ 167.2, 164.9, 142.0, 139.7, 134.5, 132.0, 131.2, 130.8, 130.6, 130.2, 130.0, 123.9, 122.5, 109.3, 80.8, 66.9, 62.1, 56.4, 49.9, 41.6, 40.3, 39.7, 38.2, 37.0, 36.8, 32.1, 31.9, 31.4, 30.3, 28.8, 27.8, 20.8, 19.4, 18.4, 17.2, 16.3, 14.5, 14.2.

HRMS (ESI-TOF) m/z calcd for C₄₃H₅₂NO₆ [M+H]⁺: 678.3789, found: 678.3792.

Melting point 211–212 °C.

((3*aR*,5*R*,5*aS*,8*aS*,8*bR*)-2,2,7,7-Tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-5-yl)methyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (**90**)



90

A80 (378.2 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **90** as a white solid (63.8 mg, 61%).

$R_f = 0.34$ (hexane : ethyl acetate = 8:1).

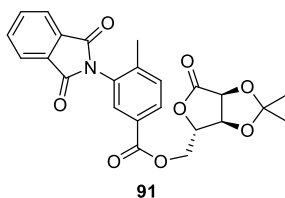
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.06 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.97 (dt, $J = 7.2, 3.6$ Hz, 2H), 7.91 (d, $J = 1.6$ Hz, 1H), 7.82 (dd, $J = 5.6, 3.2$ Hz, 2H), 7.45 (d, $J = 8.0$ Hz, 1H), 5.55 (d, $J = 4.8$ Hz, 1H), 4.64 (dd, $J = 8.0, 2.4$ Hz, 1H), 4.55 (dd, $J = 11.6, 5.2$ Hz, 1H), 4.40 (dd, $J = 11.6, 7.2$ Hz, 1H), 4.35 – 4.30 (m, 2H), 4.17 (ddd, $J = 7.2, 5.2, 2.0$ Hz, 1H), 2.27 (s, 3H), 1.48 (d, $J = 14.4$ Hz, 6H), 1.33 (d, $J = 11.2$ Hz, 6H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.1, 167.1, 165.4, 142.4, 134.5, 131.9, 131.3, 130.9, 130.6, 130.4, 129.1, 123.9, 109.7, 108.8, 96.3, 71.0, 70.7, 70.5, 66.0, 63.9, 26.1, 26.0, 25.0, 24.5, 18.4.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{28}\text{H}_{30}\text{NO}_9$ $[\text{M}+\text{H}]^+$: 524.1915, found: 524.1924.

Melting point 217–219 °C.

((3a*S*,4*S*,6a*S*)-2,2-Dimethyl-6-oxotetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)methyl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (91)



A81 (306.3 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **91** as a white solid (38.8 mg, 43%).

$R_f = 0.41$ (hexane : ethyl acetate = 8:1).

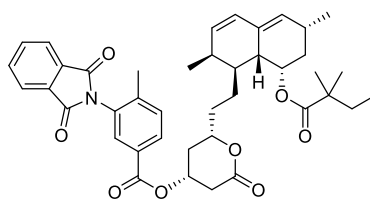
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.02 – 7.94 (m, 2H), 7.92 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.87 – 7.79 (m, 3H), 7.48 (d, $J = 8.2$ Hz, 1H), 4.88 (t, $J = 2.8$ Hz, 1H), 4.82 (d, $J = 5.6$ Hz, 1H), 4.75 (d, $J = 5.6$ Hz, 1H), 4.68 (dd, $J = 12.4, 2.4$ Hz, 1H), 4.47 (dd, $J = 12.4, 3.2$ Hz, 1H), 2.29 (s, 3H), 1.50 (s, 3H), 1.39 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 173.4, 167.0, 164.7, 143.4, 134.6, 131.9, 131.8, 131.3, 130.4, 130.2, 127.8, 124.1, 124.0, 113.9, 79.9, 77.7, 75.2, 64.0, 26.7, 25.6, 18.6.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{24}\text{H}_{22}\text{NO}_8$ $[\text{M}+\text{H}]^+$: 452.1340, found: 452.1335.

Melting point 199–201 °C.

(2*S*,4*R*)-2-(2-(((1*S*,2*S*,6*R*,8*S*,8a*R*)-8-((2,2-dimethylbutanoyl)oxy)-2,6-dimethyl-1,2,6,7,8,8a-hexahydronaphthalen-1-yl)ethyl)-6-oxotetrahydro-2H-pyran-4-yl 3-(1,3-dioxoisindolin-2-yl)-4-methylbenzoate (92)



92

A82 (536.7 mg, 1 mmol, 5 equiv.) and **B1** (32.6 mg, 0.2 mmol, 1 equiv.) were subjected to the general procedure and the product was purified by column chromatography (silica gel, hexane : ethyl acetate = 12:1) to afford **92** as a white solid (66.7 mg, 49%).

R_f = 0.32 (hexane : ethyl acetate = 8:1).

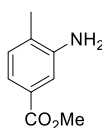
^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (dd, J = 5.6, 3.2 Hz, 2H), 7.87 (d, J = 1.6 Hz, 1H), 7.83 (dd, J = 5.6, 3.1 Hz, 2H), 7.48 (d, J = 8.2 Hz, 1H), 5.98 (d, J = 9.6 Hz, 1H), 5.81 – 5.73 (m, 1H), 5.51 (d, J = 8.4 Hz, 2H), 5.33 (d, J = 3.2 Hz, 1H), 4.61 – 4.51 (m, 1H), 2.95 – 2.80 (m, 2H), 2.46 – 2.31 (m, 2H), 2.29 (s, 3H), 2.22 (d, J = 13.6 Hz, 2H), 1.97 – 1.80 (m, 4H), 1.67 (t, J = 11.6 Hz, 1H), 1.60 – 1.40 (m, 5H), 1.07 (t, J = 5.6 Hz, 9H), 0.88 (d, J = 7.2 Hz, 3H), 0.77 (t, J = 7.6 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 177.6, 168.7, 167.1, 164.5, 143.1, 134.6, 132.8, 131.9, 131.5, 131.1, 130.5, 130.4, 129.8, 128.5, 128.4, 124.0, 67.9, 66.3, 43.0, 37.4, 36.7, 35.4, 33.4, 33.1, 33.0, 32.8, 30.6, 27.3, 24.8, 24.7, 24.1, 23.0, 18.5, 14.0, 9.3.

HRMS (ESI-TOF) m/z calcd for $\text{C}_{41}\text{H}_{48}\text{NO}_8$ $[\text{M}+\text{H}]^+$: 682.3374, found: 682.3375.

Melting point 208–209 °C.

Methyl 3-Amino-4-Methylbenzoate (93)



93

R_f = 0.23 (hexane : ethyl acetate = 3:1).

^1H NMR (400 MHz, CDCl_3) δ 7.37 (dd, J = 7.6, 1.6 Hz, 1H), 7.34 (d, J = 1.6 Hz, 1H), 7.10 (d, J = 7.6 Hz, 1H), 3.88 (s, 3H), 2.20 (s, 3H).

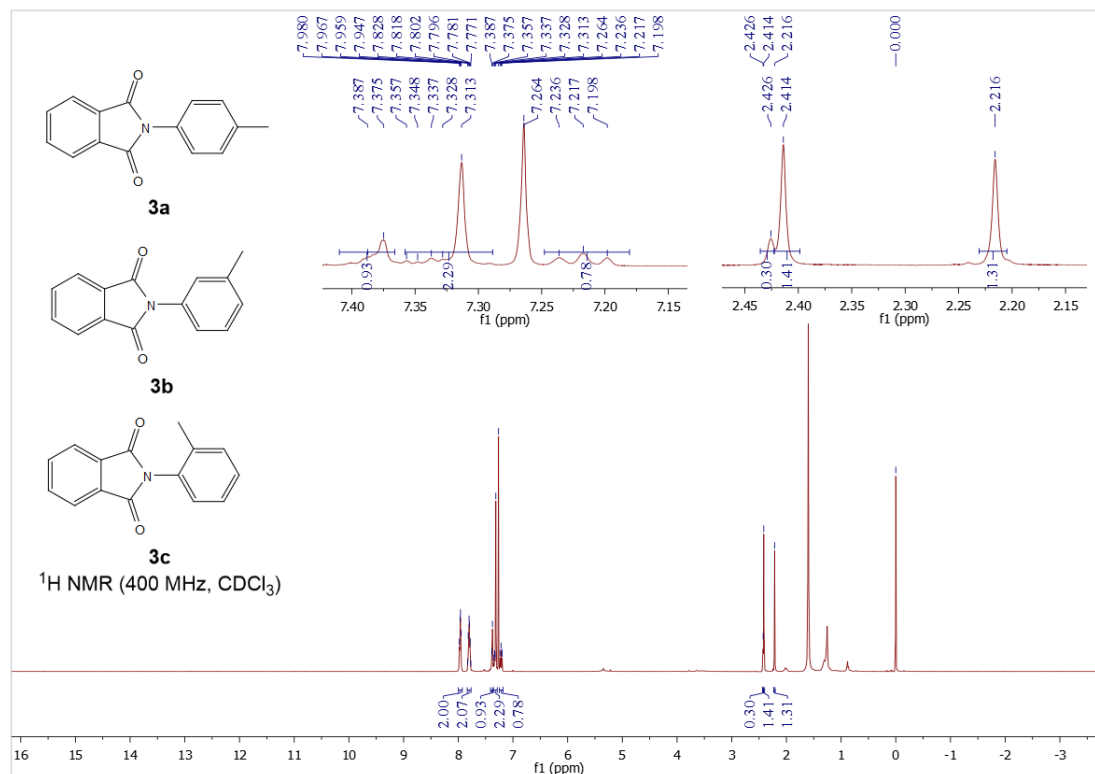
^{13}C NMR (100 MHz, CDCl_3) δ 167.4, 144.6, 130.4, 128.9, 127.7, 119.9, 115.6, 51.9, 17.6.

Melting point 165–166 °C.

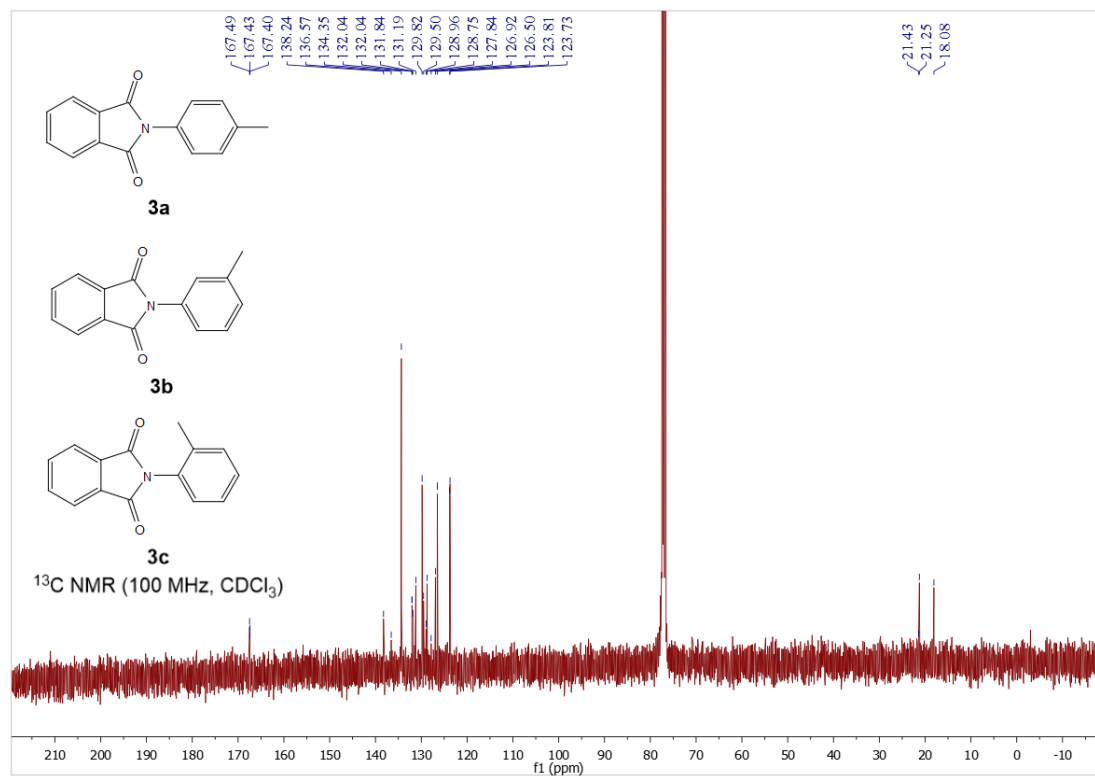
Analytic data match the literature⁷.

9 NMR Spectra of Products

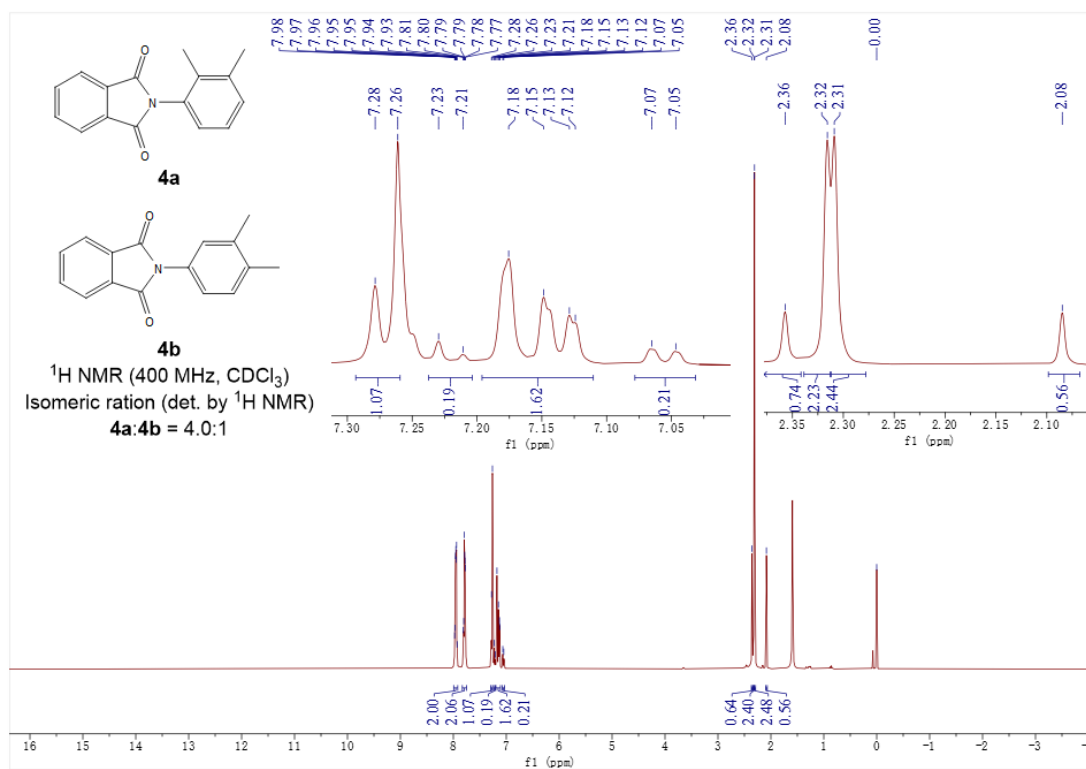
^1H NMR (400 MHz, CDCl_3) spectrum of **3**



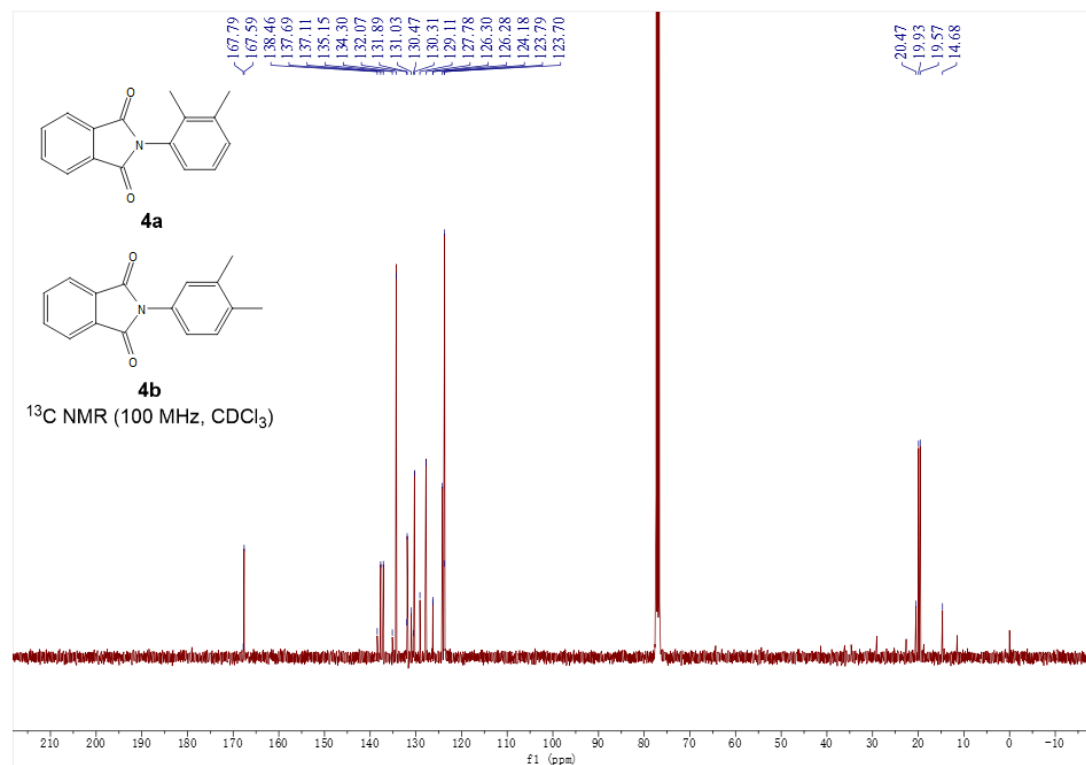
^{13}C NMR (100 MHz, CDCl_3) spectrum of **3**



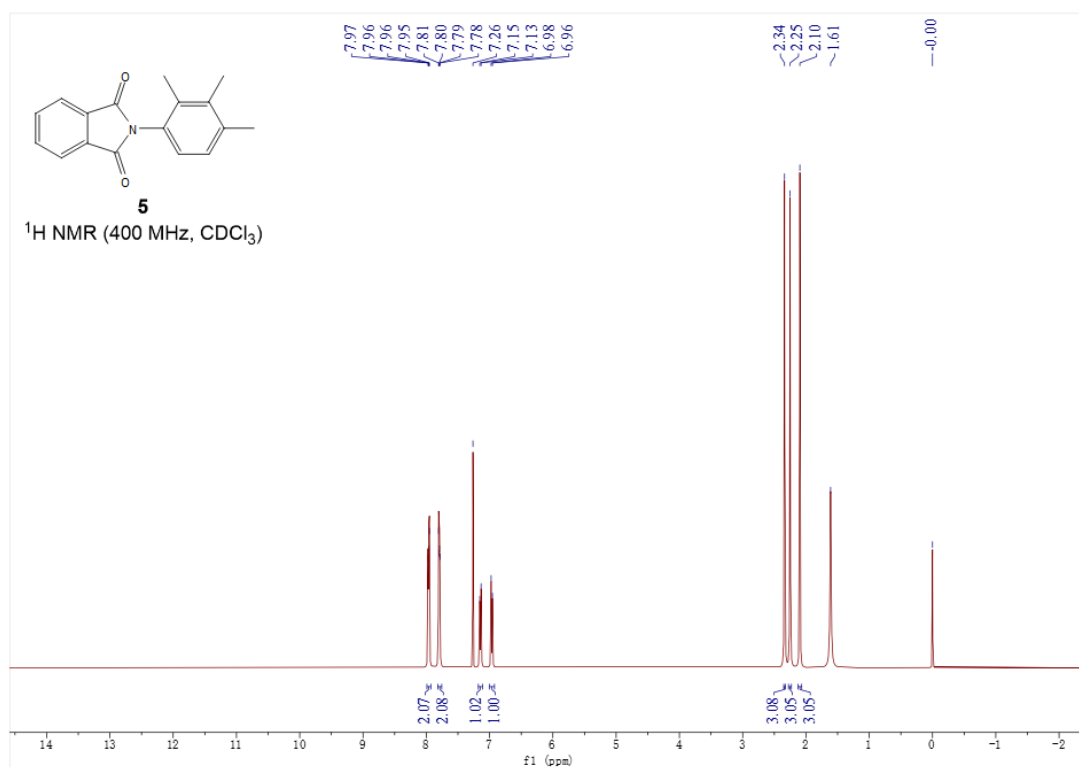
^1H NMR (400 MHz, CDCl_3) spectrum of **4**



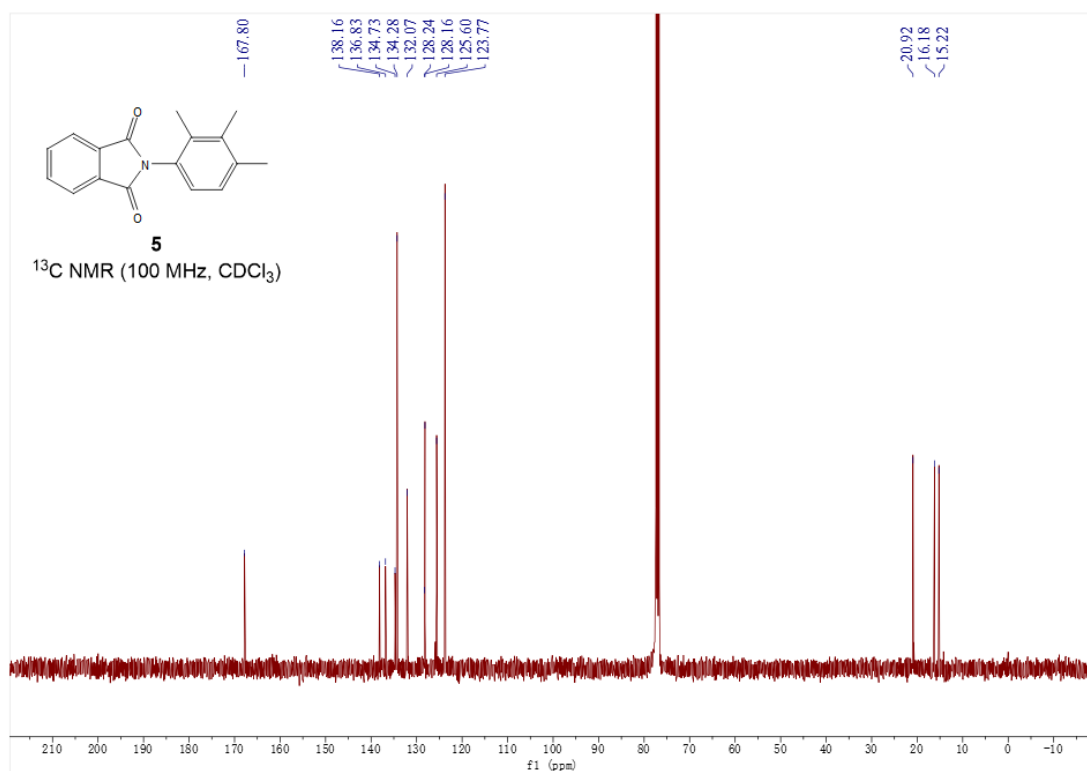
^{13}C NMR (100 MHz, CDCl_3) spectrum of **4**



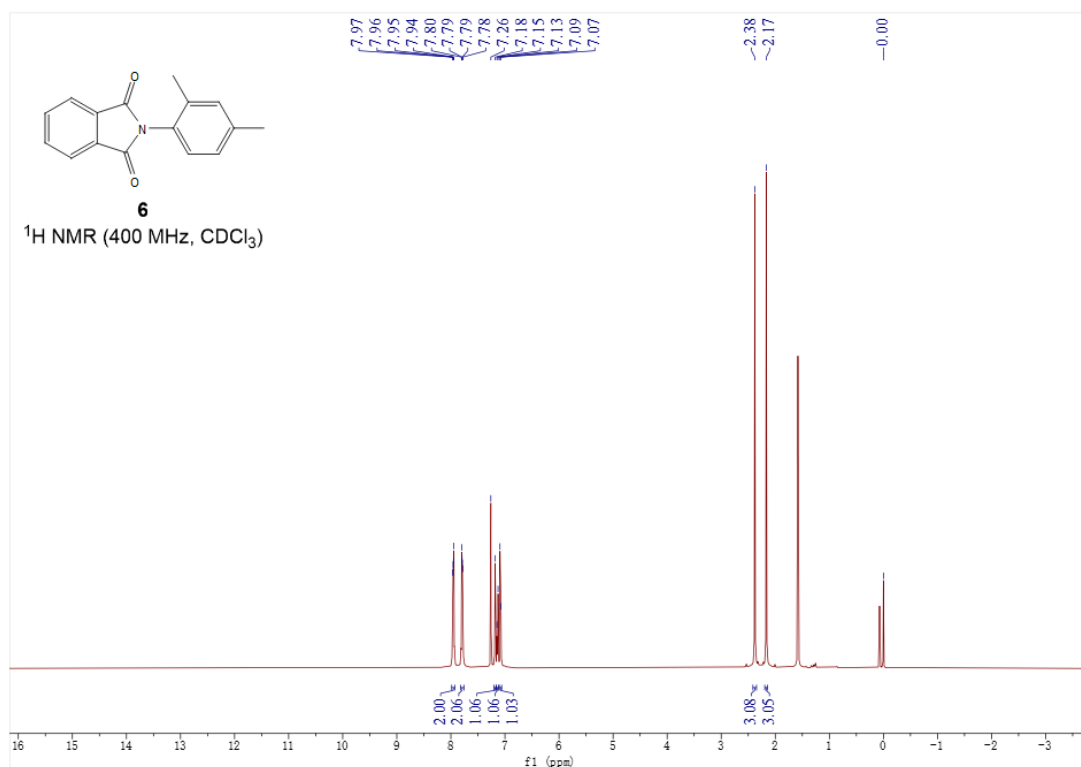
¹H NMR (400 MHz, CDCl₃) spectrum of **5**



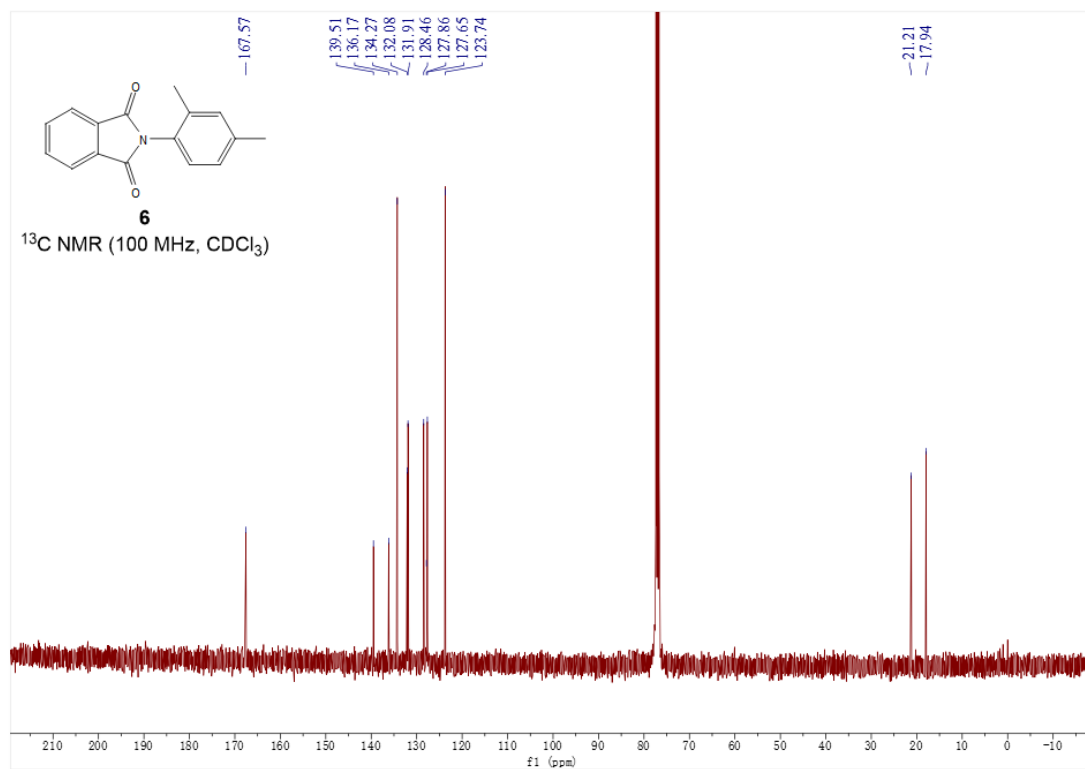
¹³C NMR (100 MHz, CDCl₃) spectrum of **5**



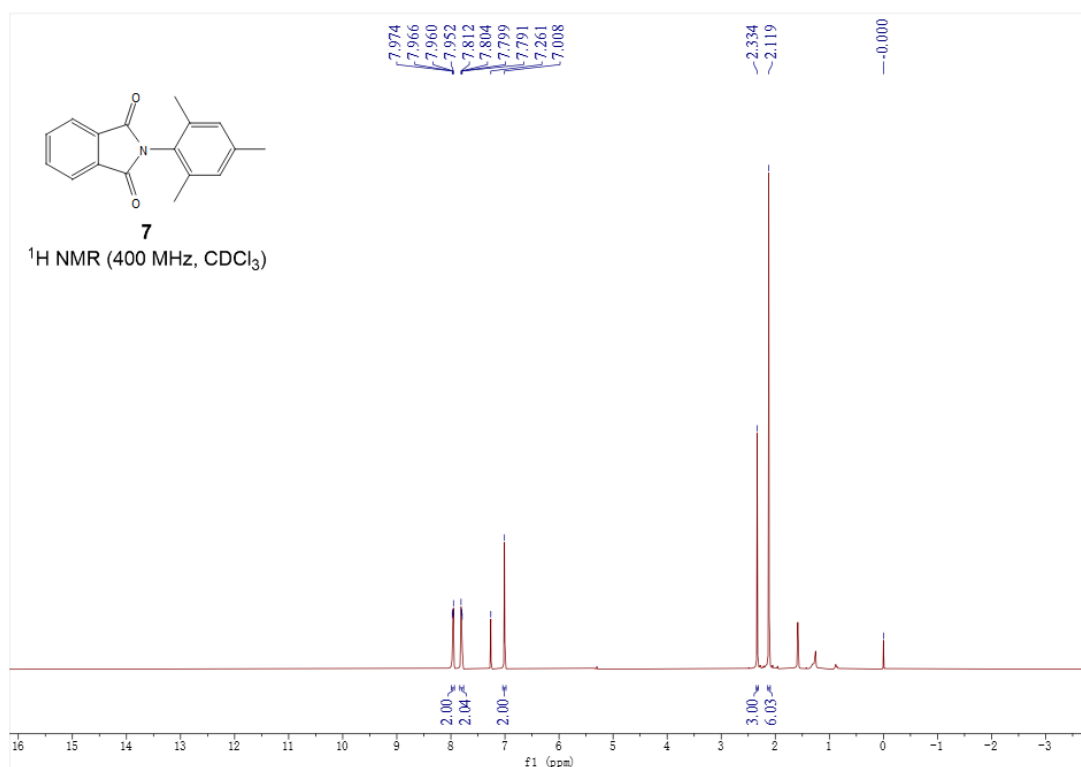
^1H NMR (400 MHz, CDCl_3) spectrum of **6**



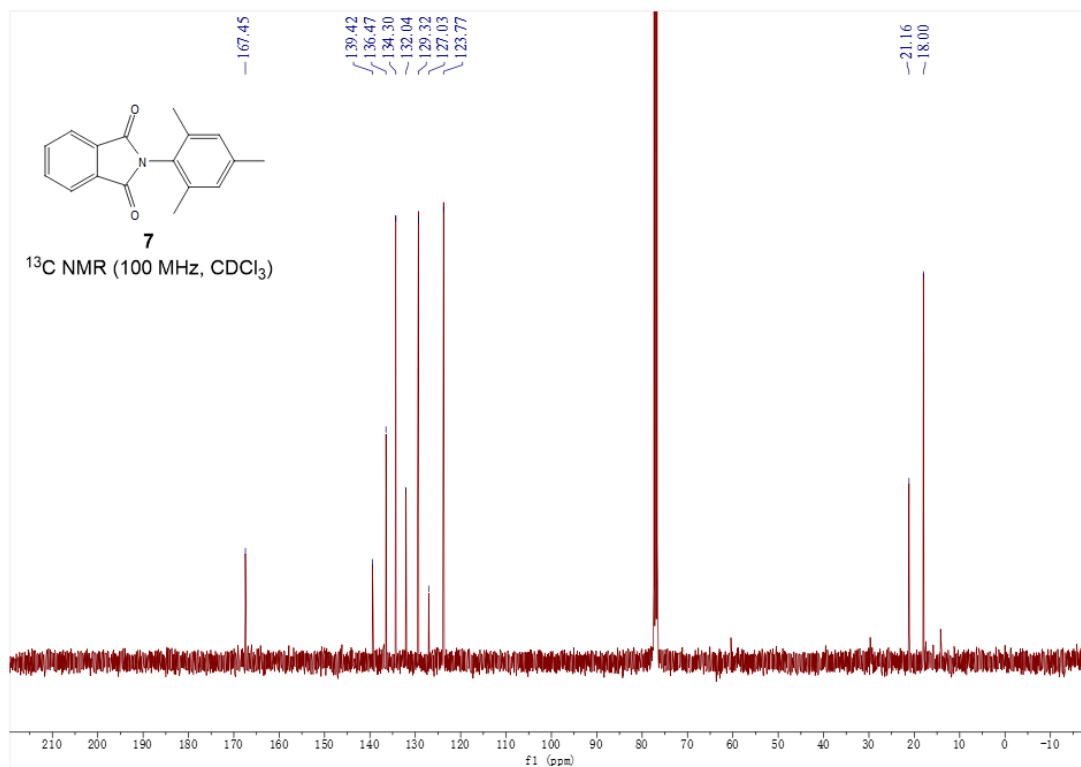
^{13}C NMR (100 MHz, CDCl_3) spectrum of **6**



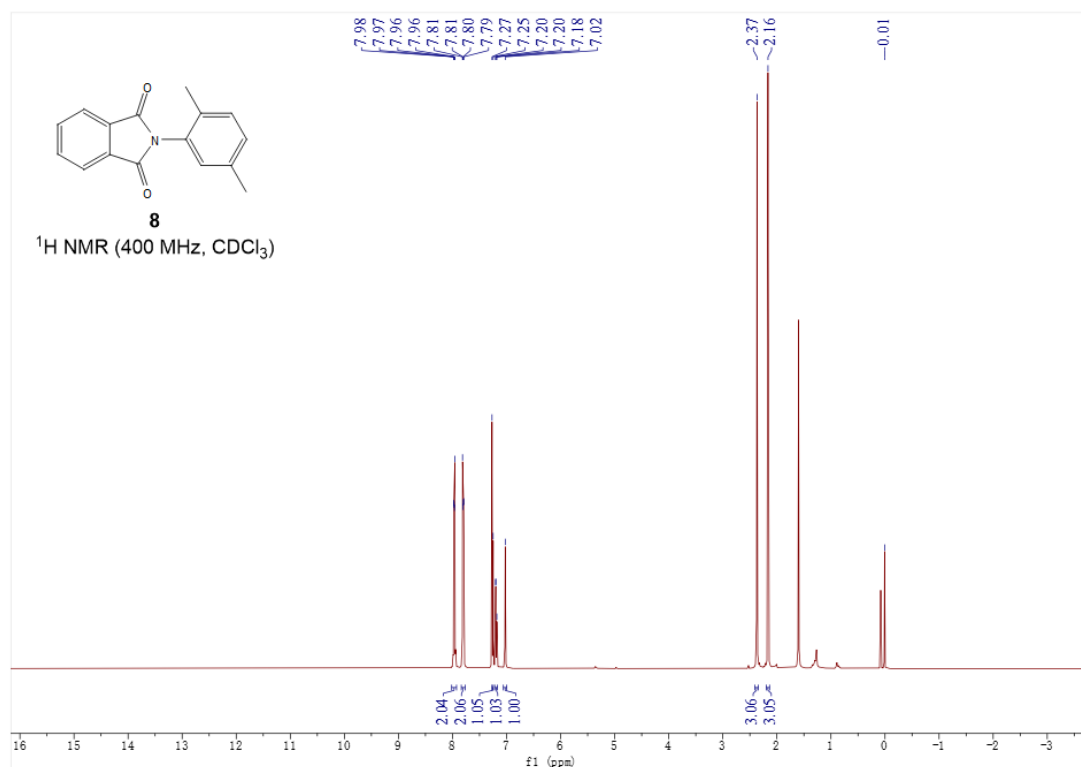
^1H NMR (400 MHz, CDCl_3) spectrum of **7**



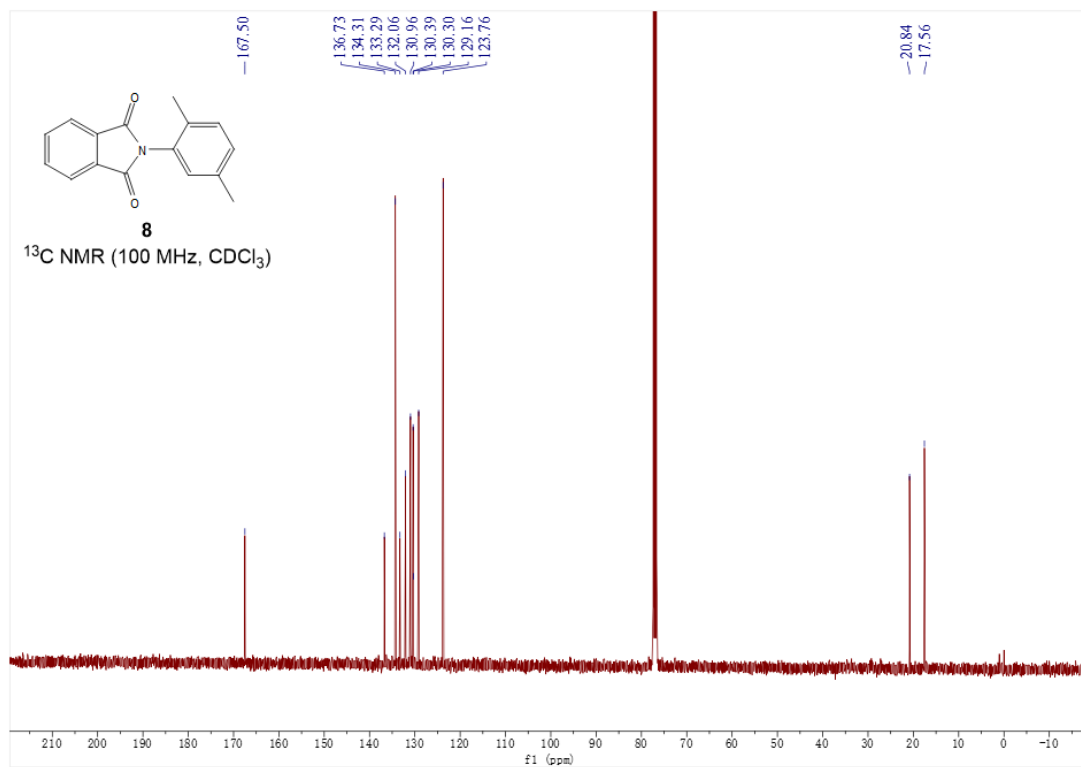
^{13}C NMR (100 MHz, CDCl_3) spectrum of **7**



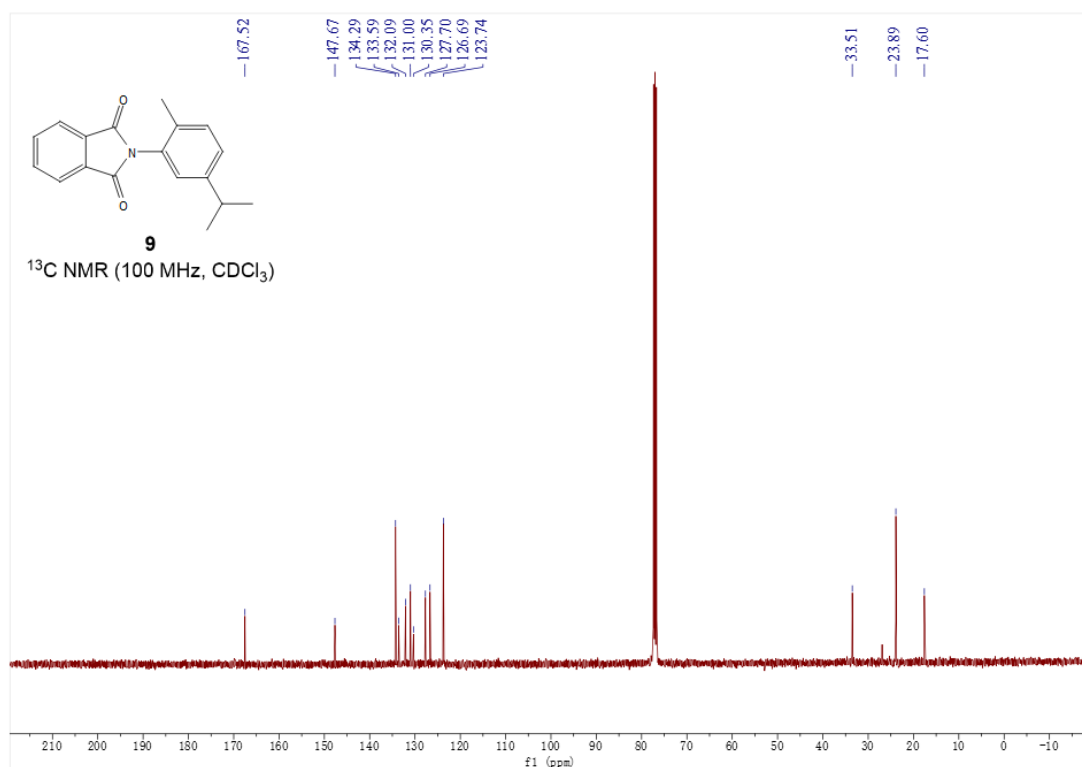
^1H NMR (400 MHz, CDCl_3) spectrum of **8**



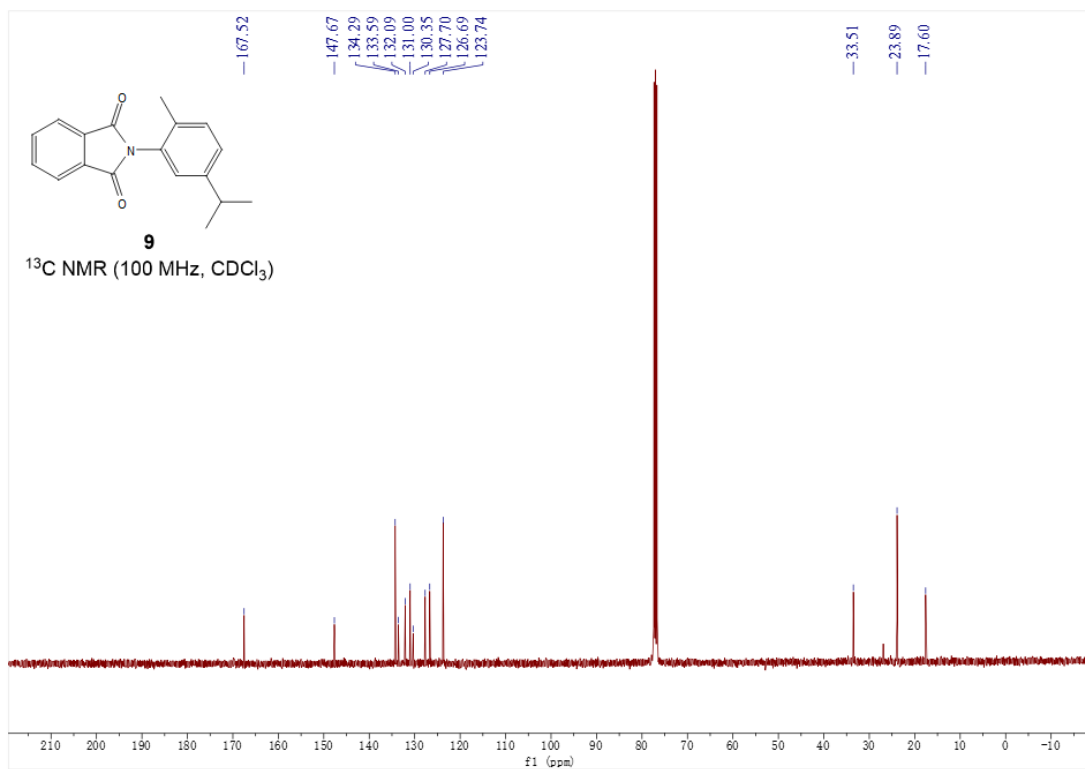
^{13}C NMR (100 MHz, CDCl_3) spectrum of **8**



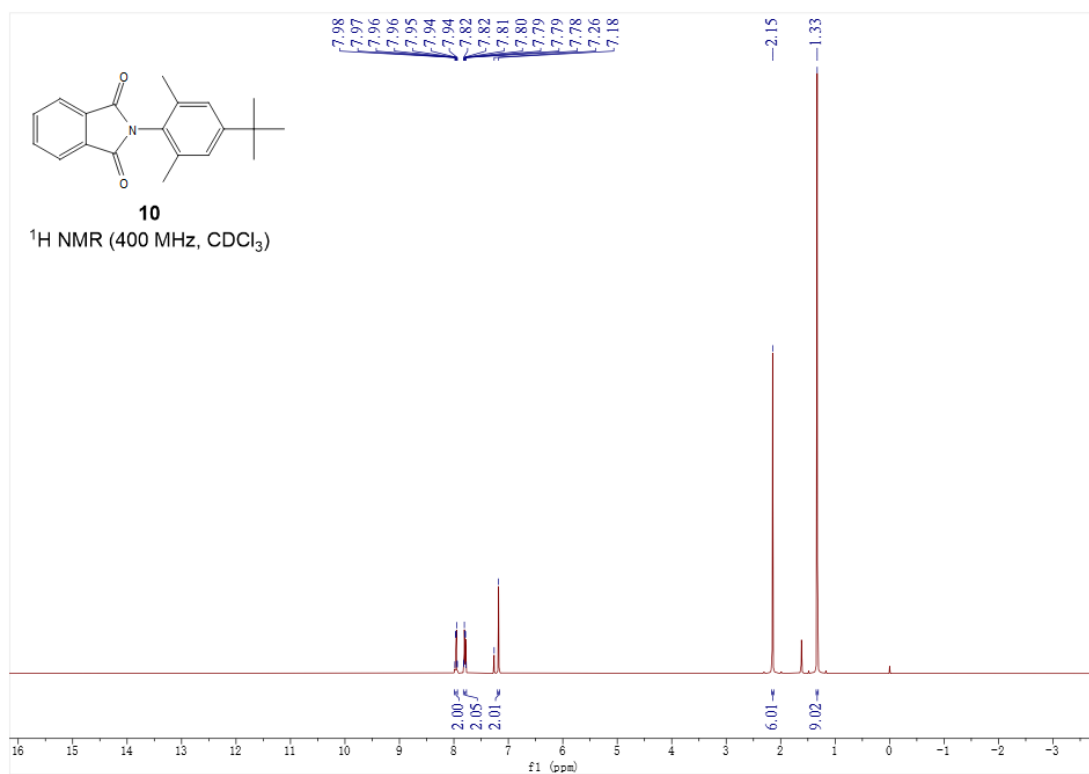
^1H NMR (400 MHz, CDCl_3) spectrum of **9**



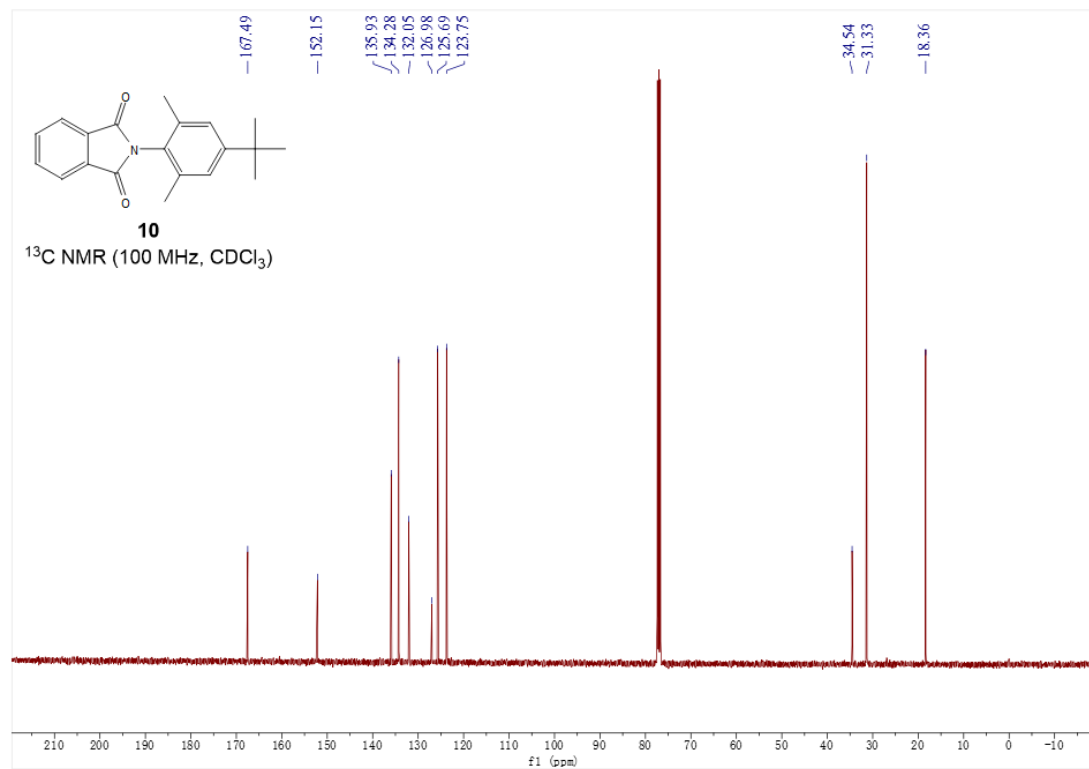
^{13}C NMR (100 MHz, CDCl_3) spectrum of **9**



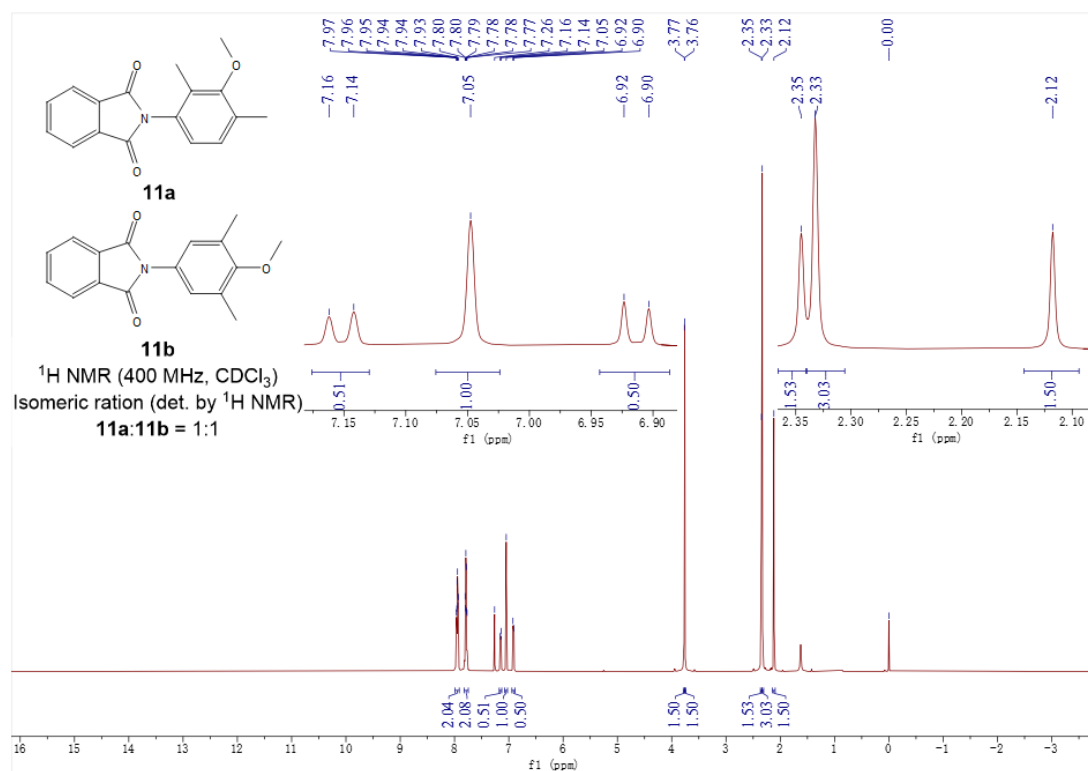
^1H NMR (400 MHz, CDCl_3) spectrum of **10**



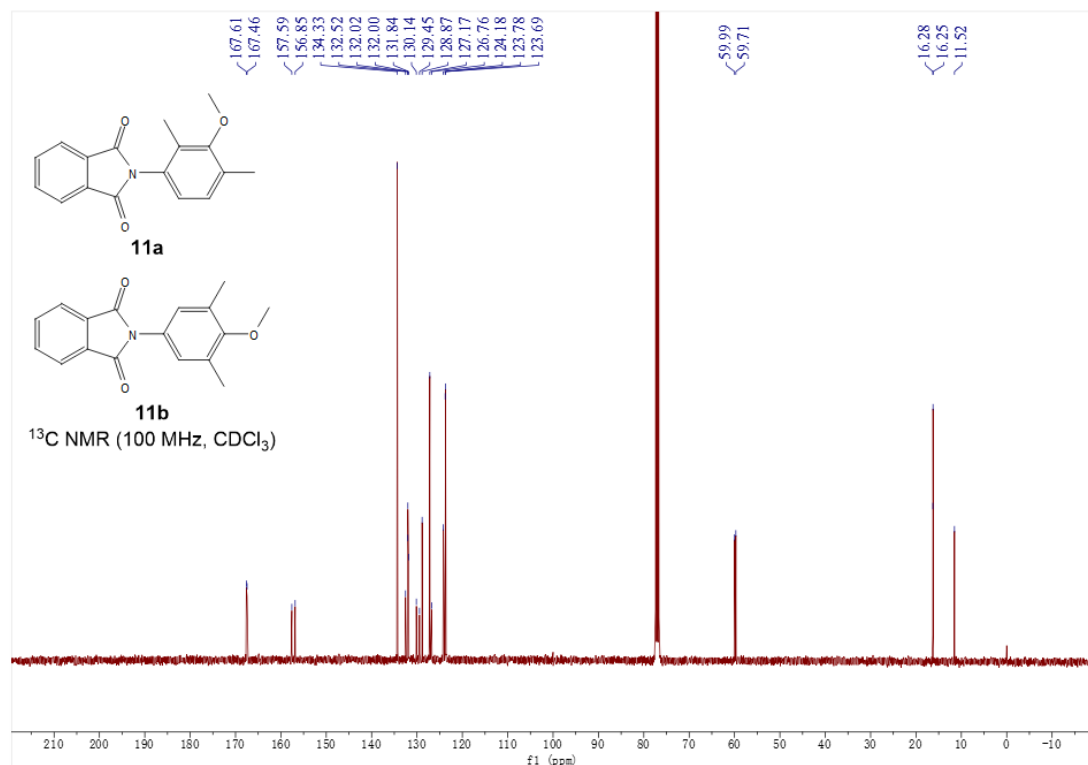
^{13}C NMR (100 MHz, CDCl_3) spectrum of **10**



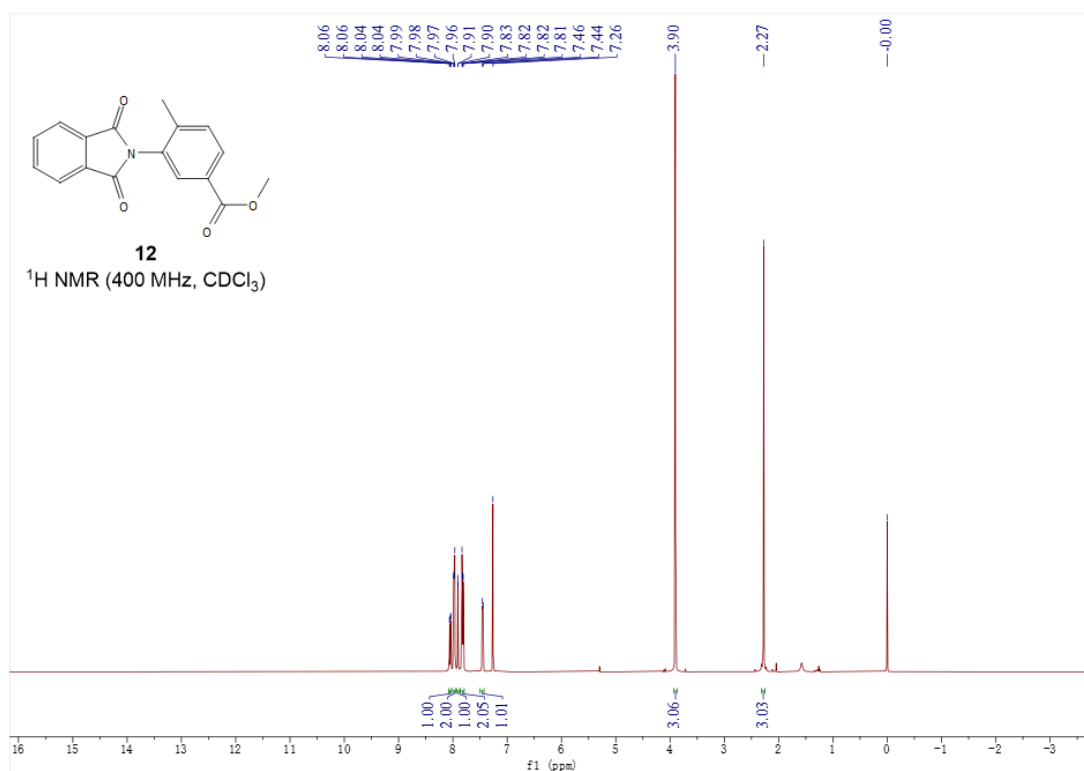
¹H NMR (400 MHz, CDCl₃) spectrum of **11**



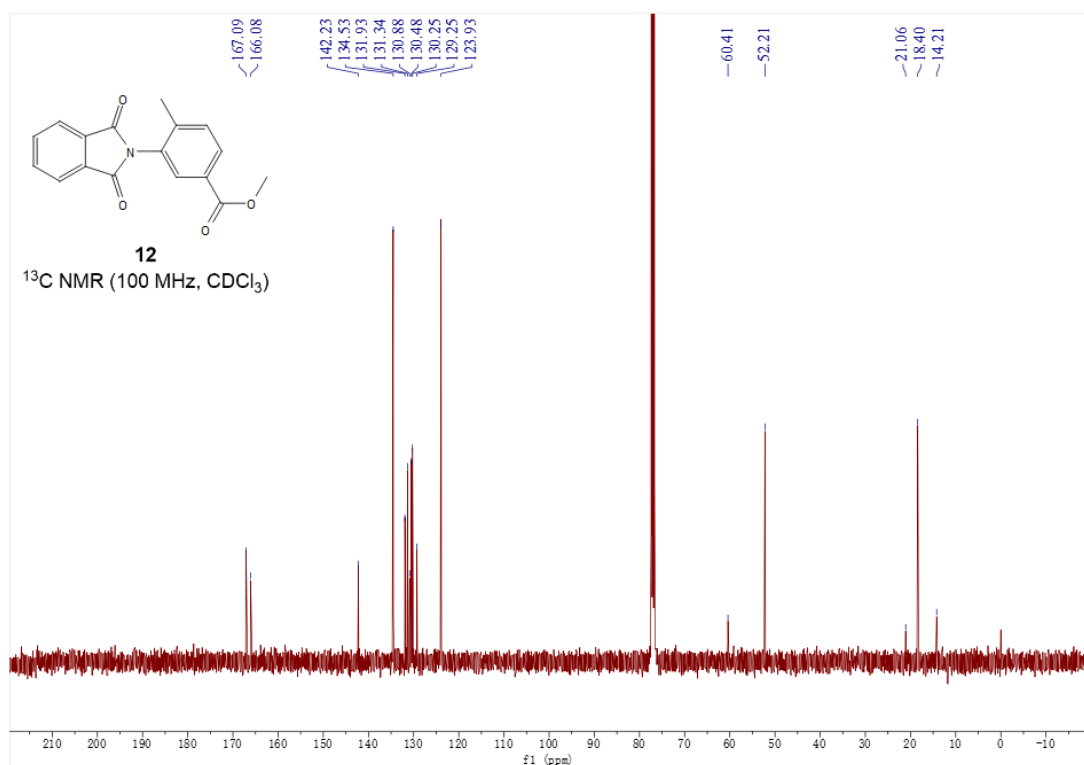
¹³C NMR (100 MHz, CDCl₃) spectrum of **11**



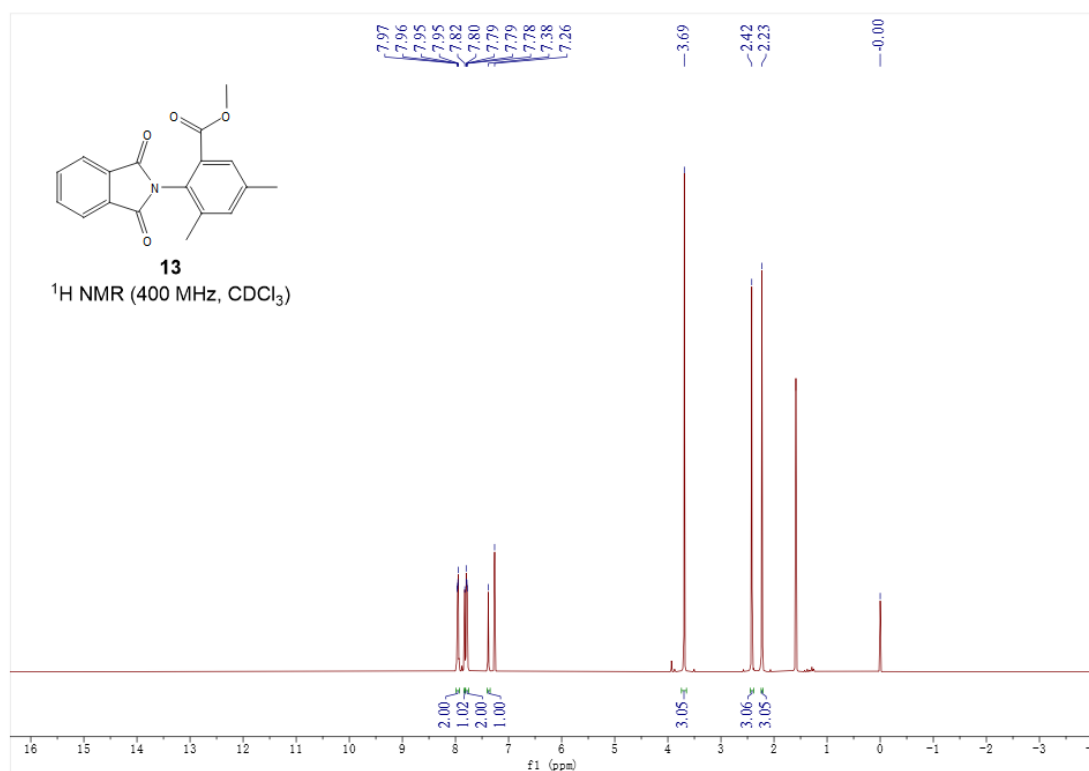
¹H NMR (400 MHz, CDCl₃) spectrum of **12**



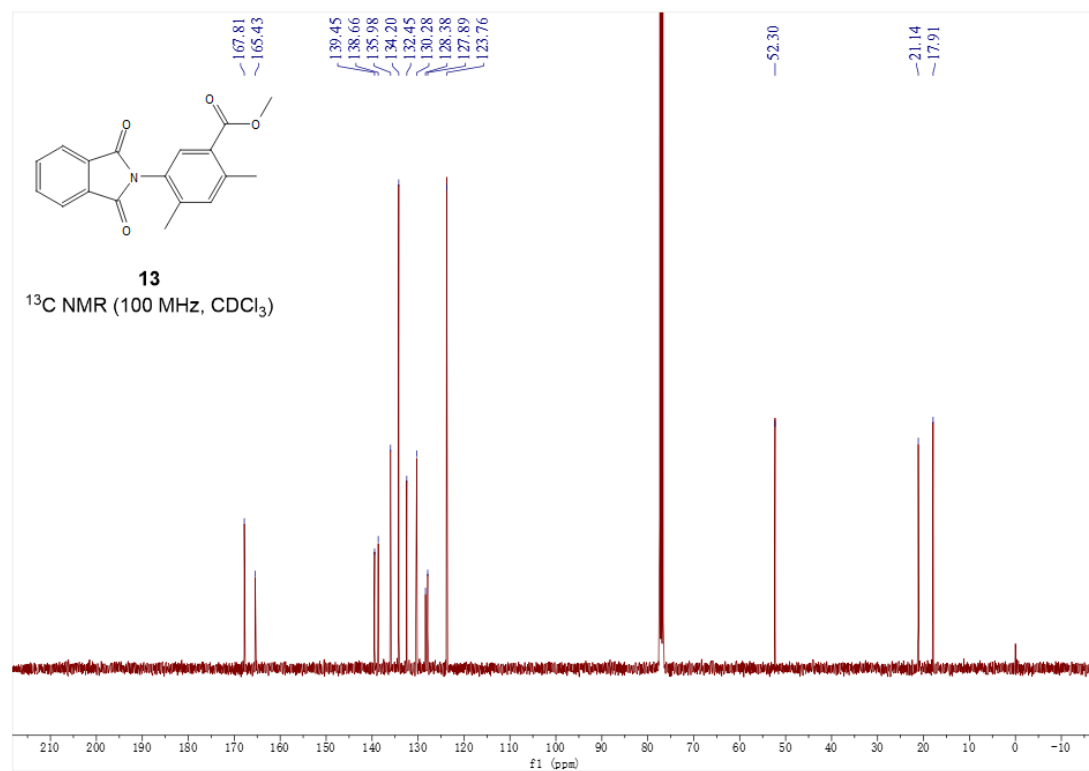
¹³C NMR (100 MHz, CDCl₃) spectrum of **12**



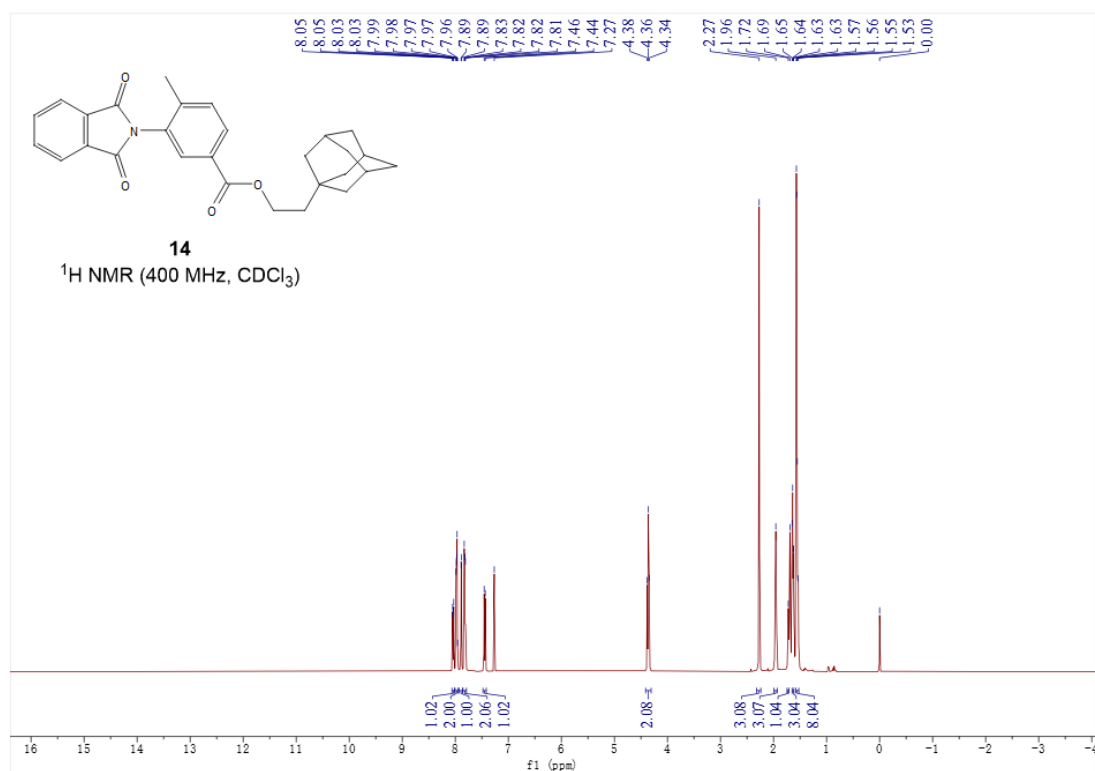
^1H NMR (400 MHz, CDCl_3) spectrum of **13**



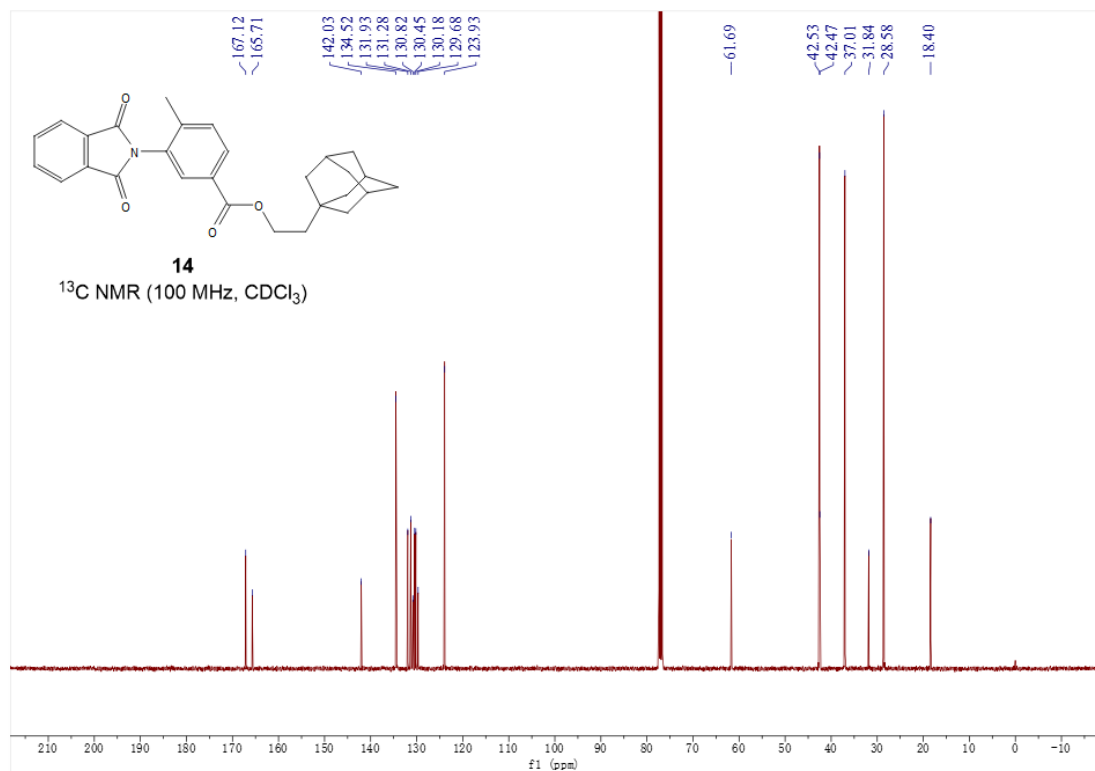
^{13}C NMR (100 MHz, CDCl_3) spectrum of **13**



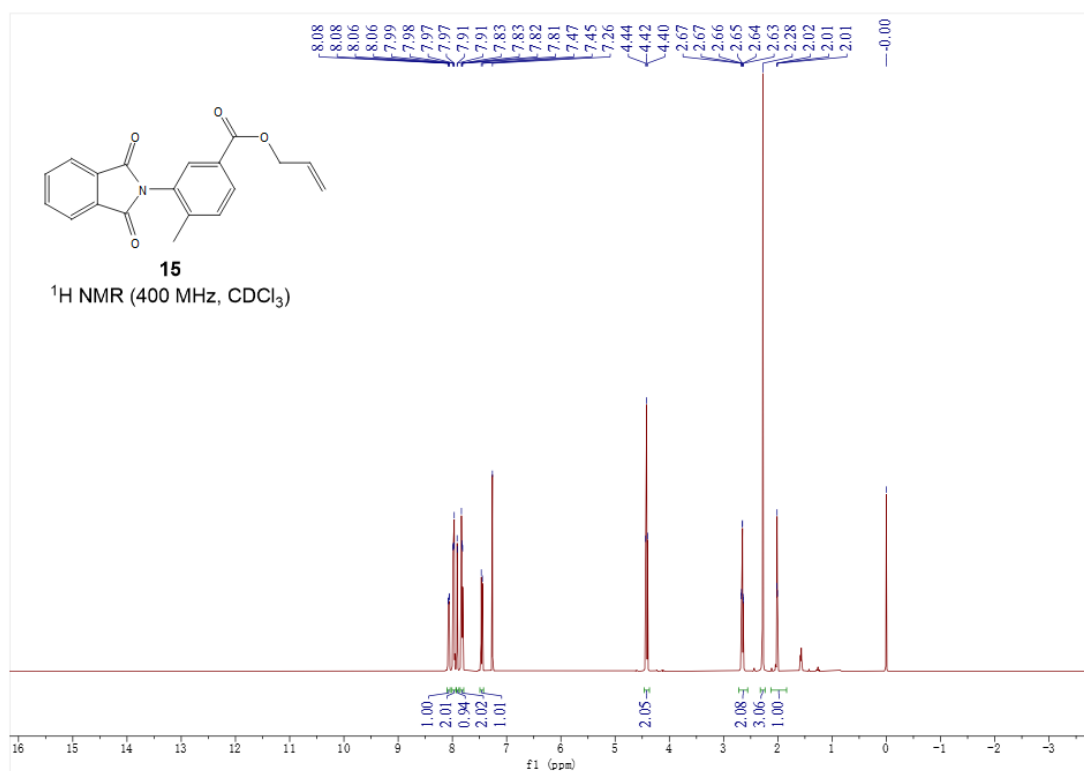
¹H NMR (400 MHz, CDCl₃) spectrum of **14**



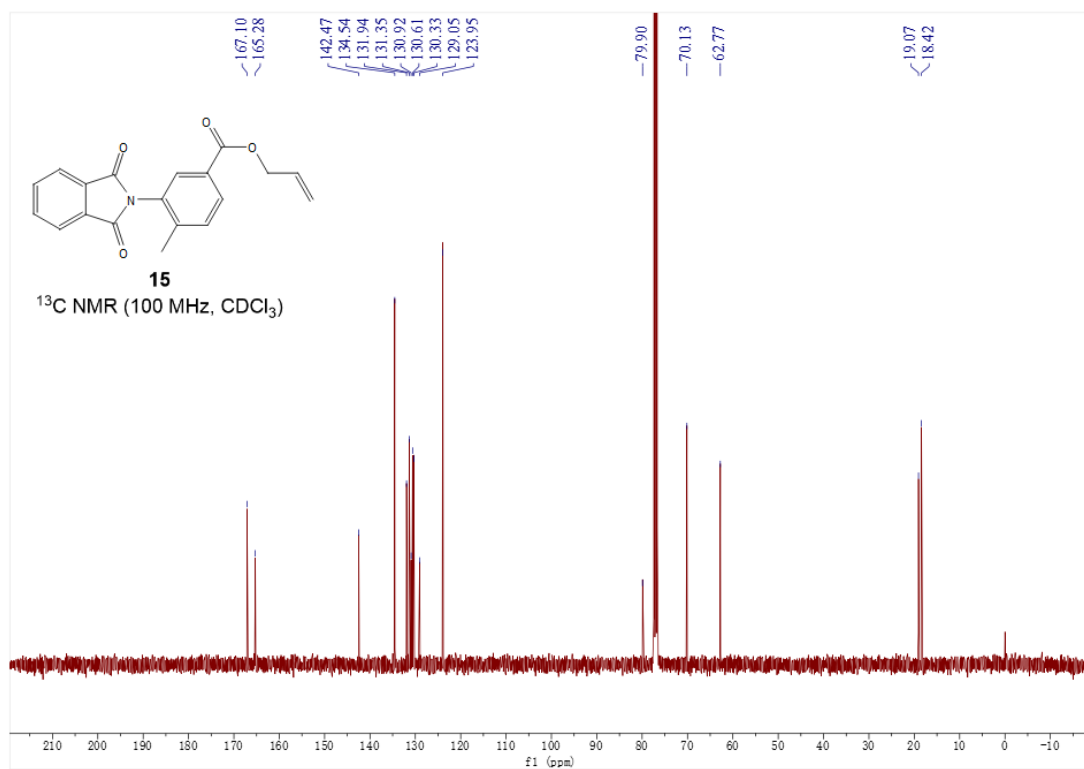
¹³C NMR (100 MHz, CDCl₃) spectrum of **14**



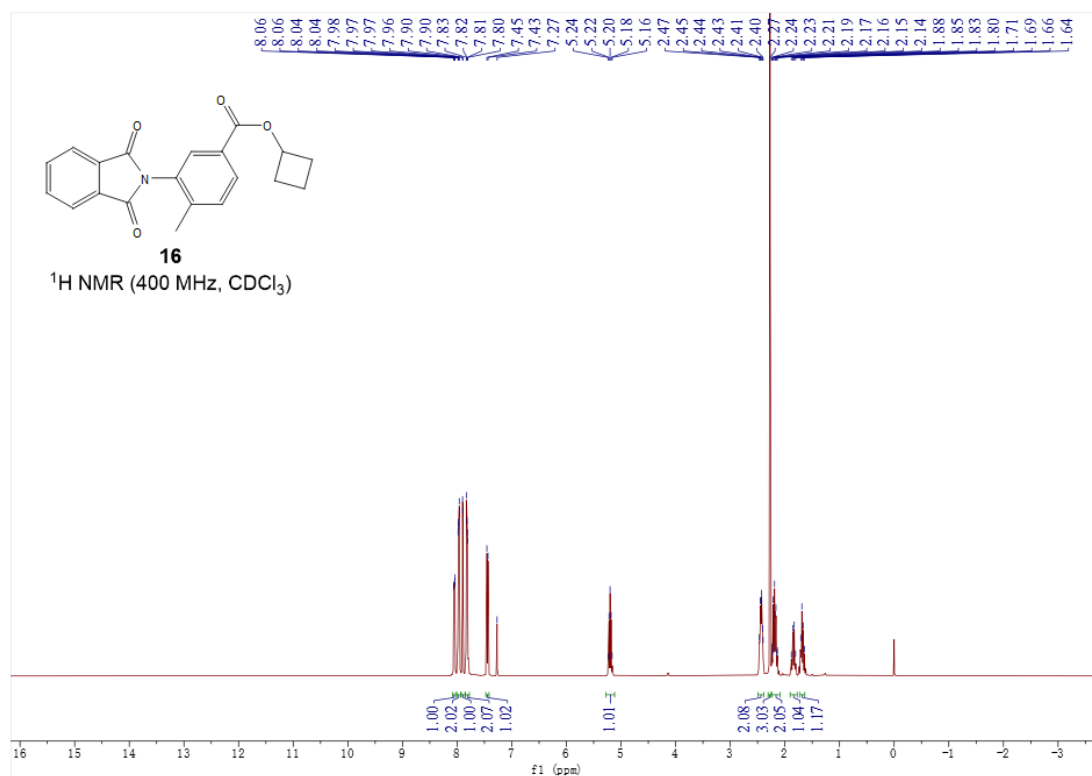
^1H NMR (400 MHz, CDCl_3) spectrum of **15**



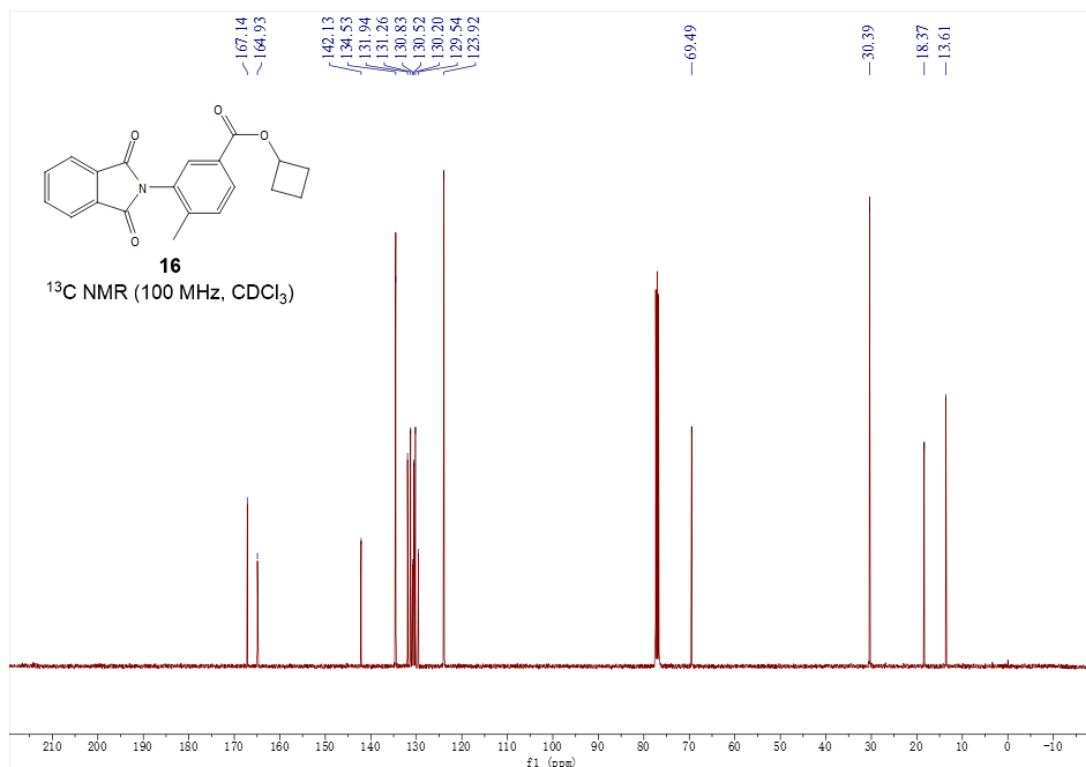
^{13}C NMR (100 MHz, CDCl_3) spectrum of **15**



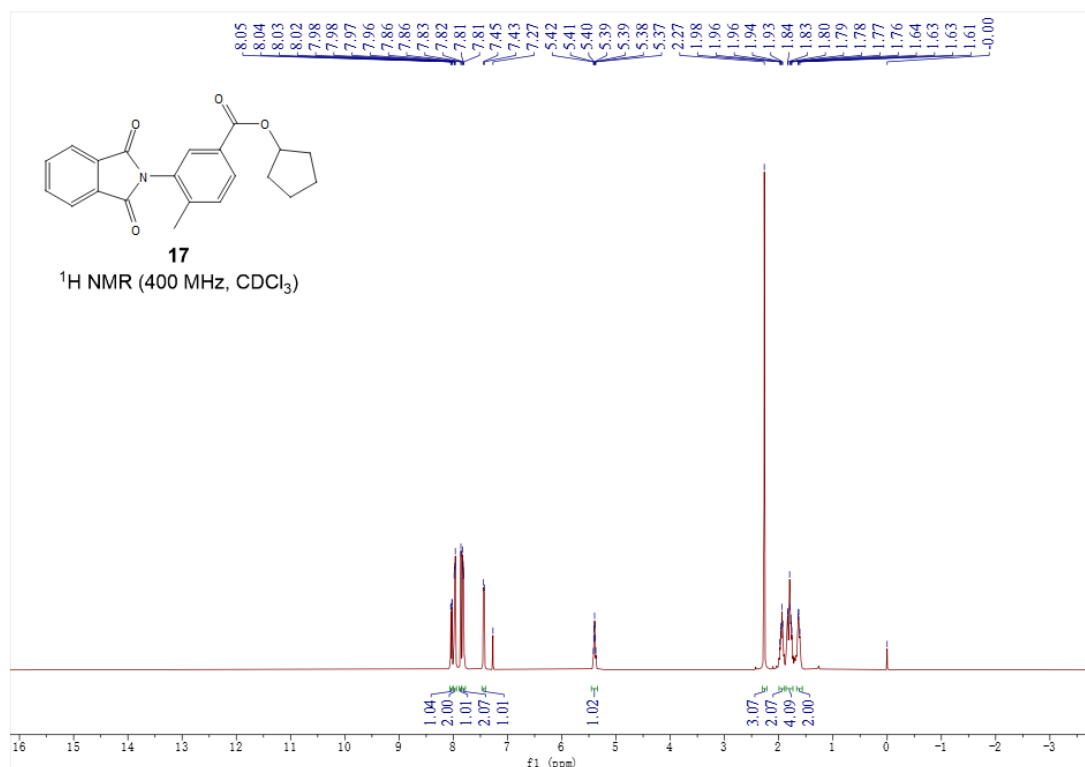
¹H NMR (400 MHz, CDCl₃) spectrum of **16**



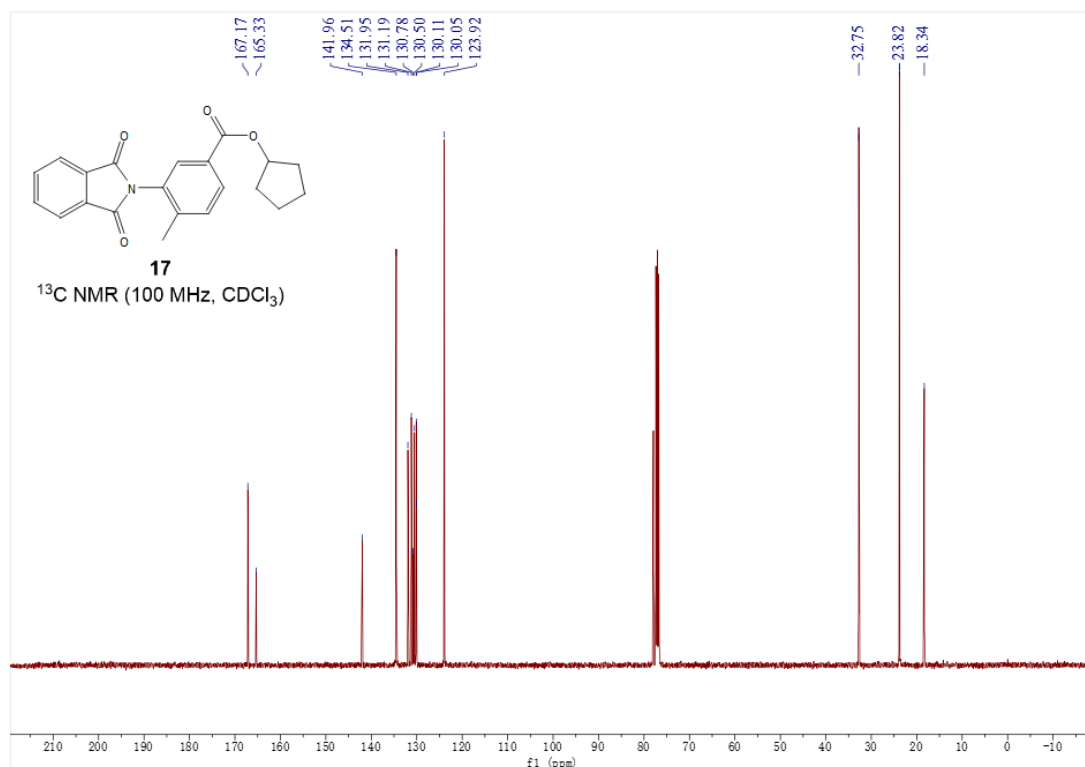
¹³C NMR (100 MHz, CDCl₃) spectrum of **16**



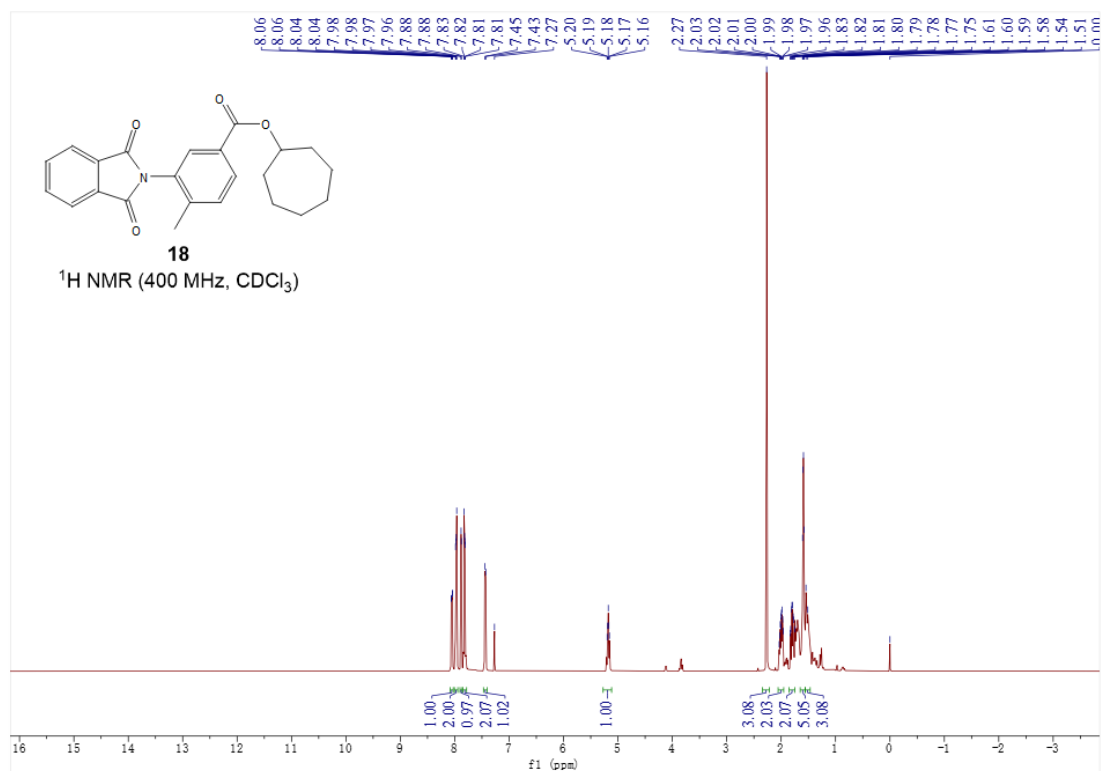
^1H NMR (400 MHz, CDCl_3) spectrum of **17**



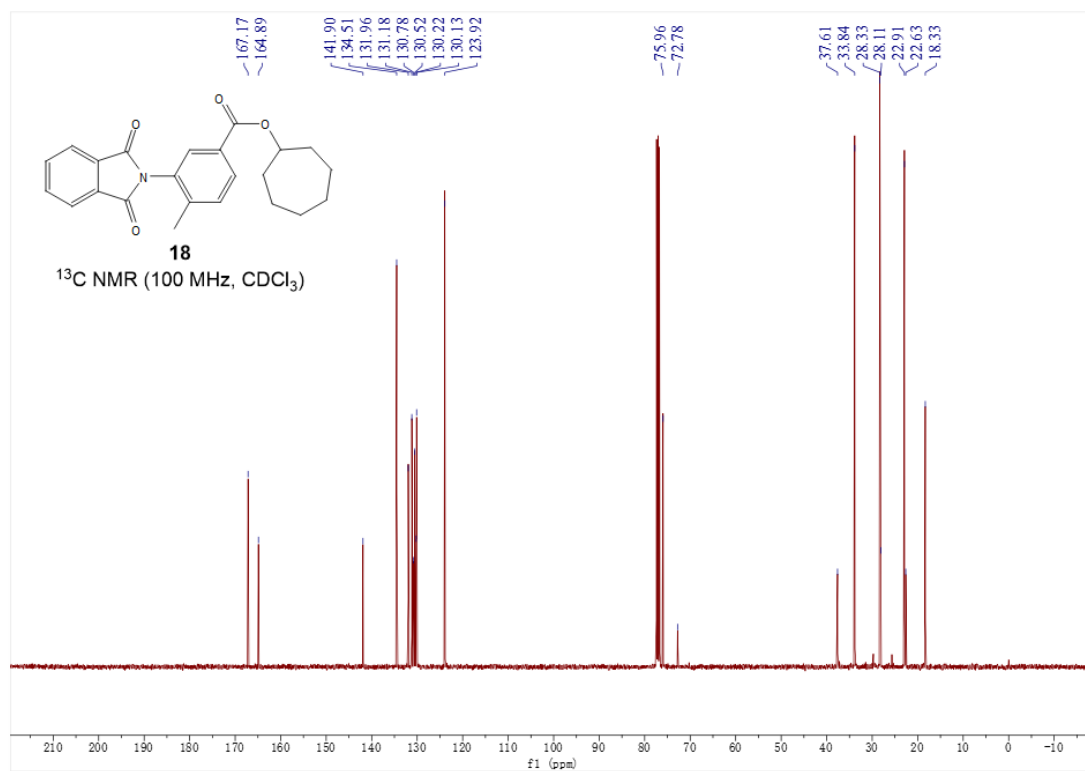
^{13}C NMR (100 MHz, CDCl_3) spectrum of **17**



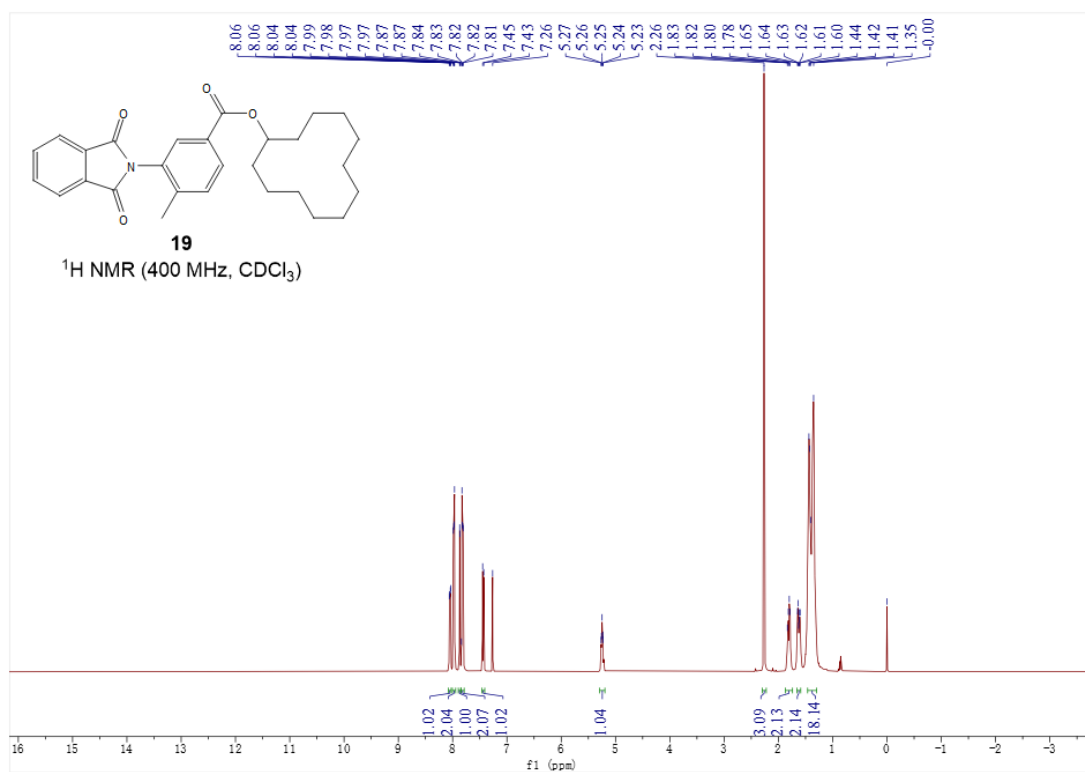
^1H NMR (400 MHz, CDCl_3) spectrum of **18**



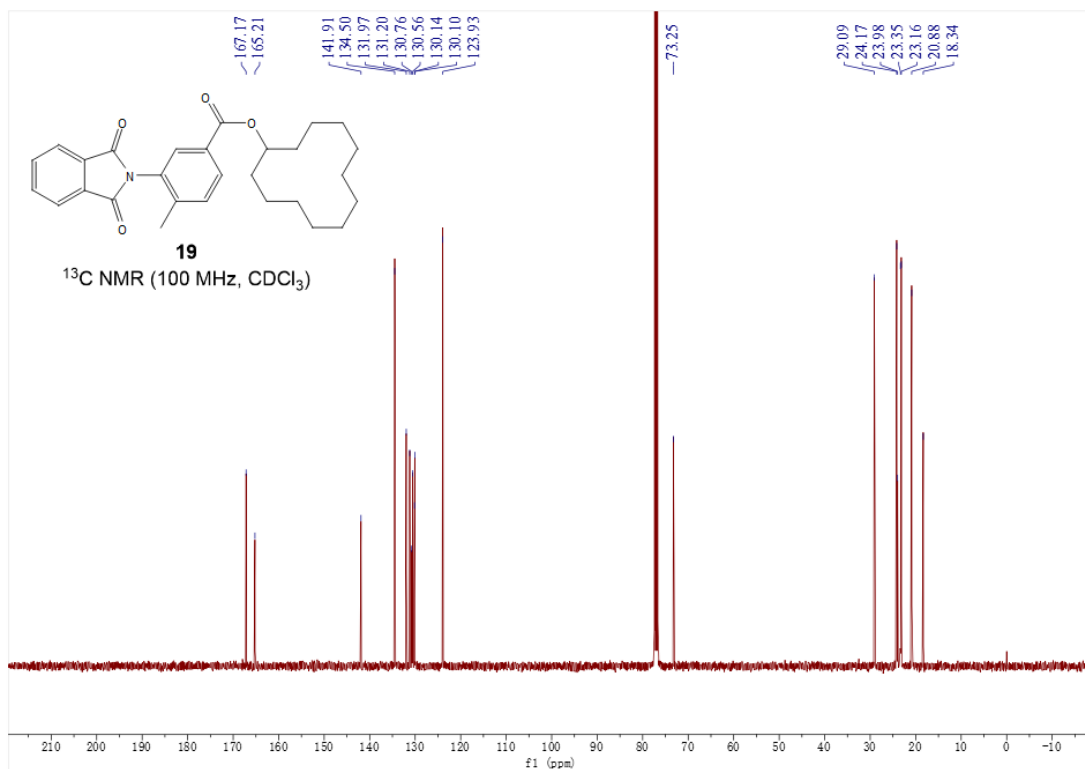
^{13}C NMR (100 MHz, CDCl_3) spectrum of **18**



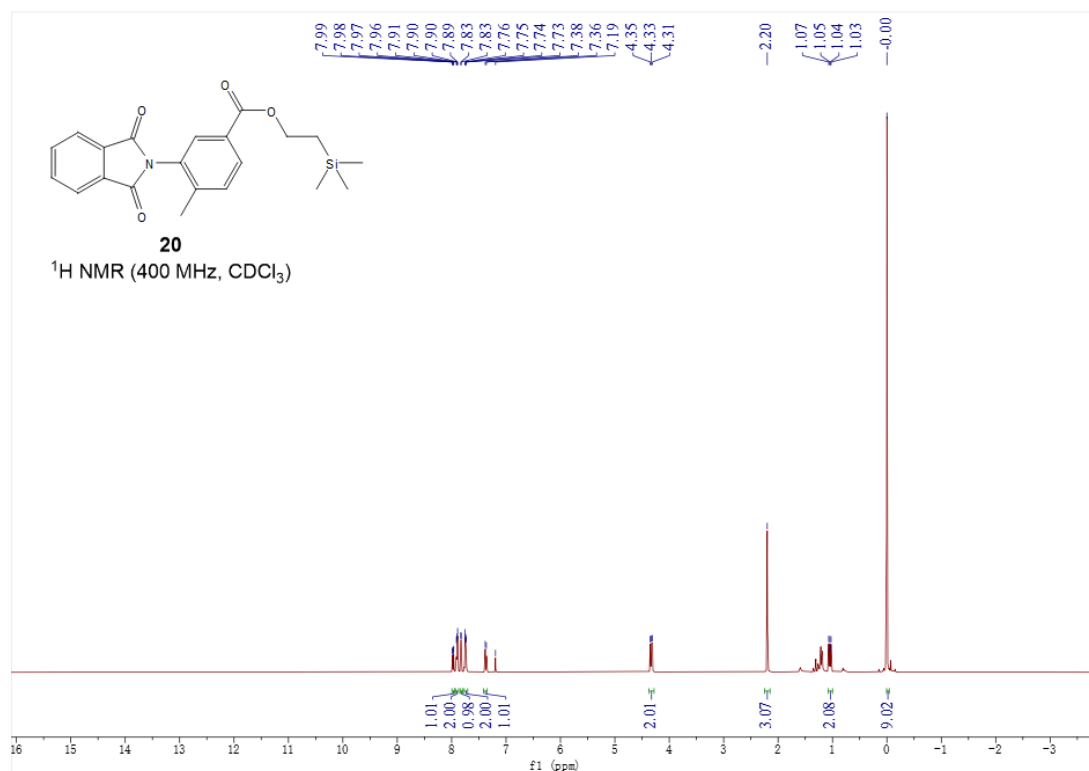
¹H NMR (400 MHz, CDCl₃) spectrum of **19**



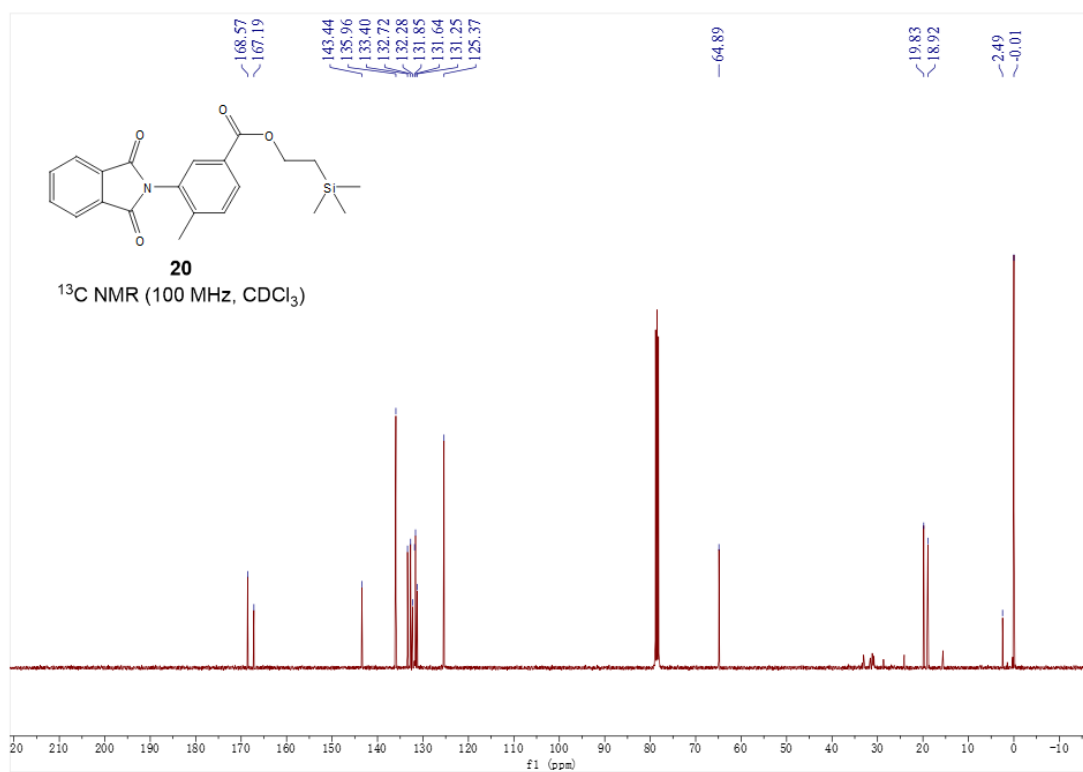
¹³C NMR (100 MHz, CDCl₃) spectrum of **19**



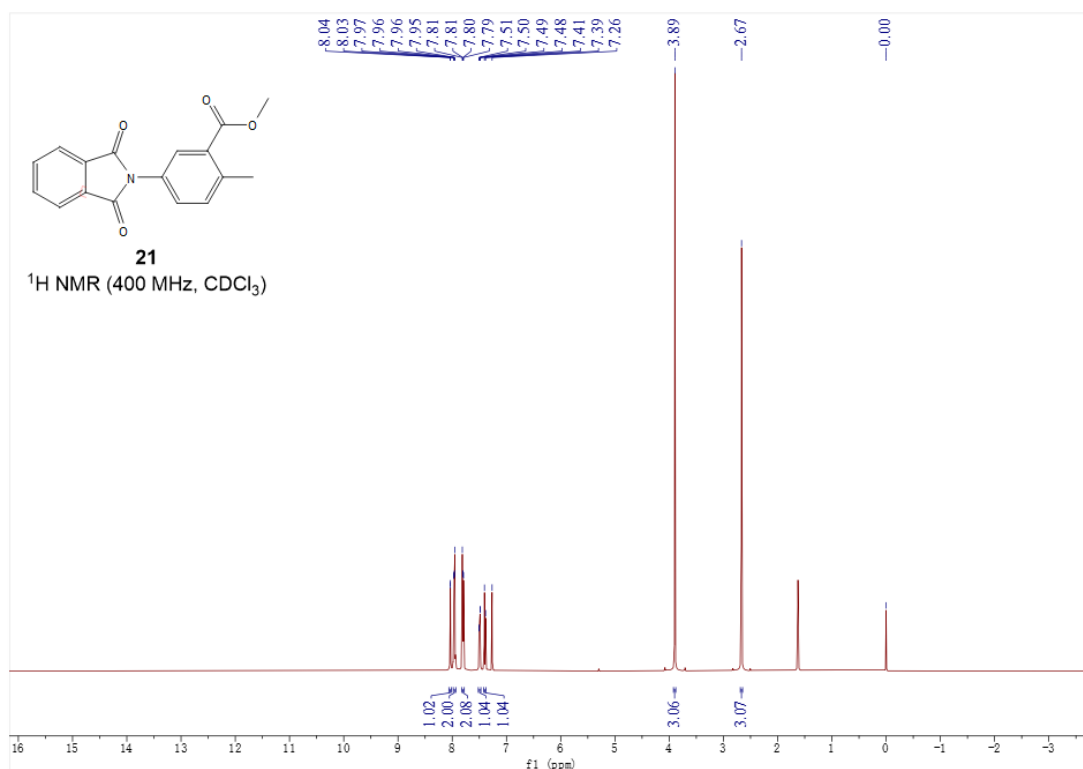
¹H NMR (400 MHz, CDCl₃) spectrum of **20**



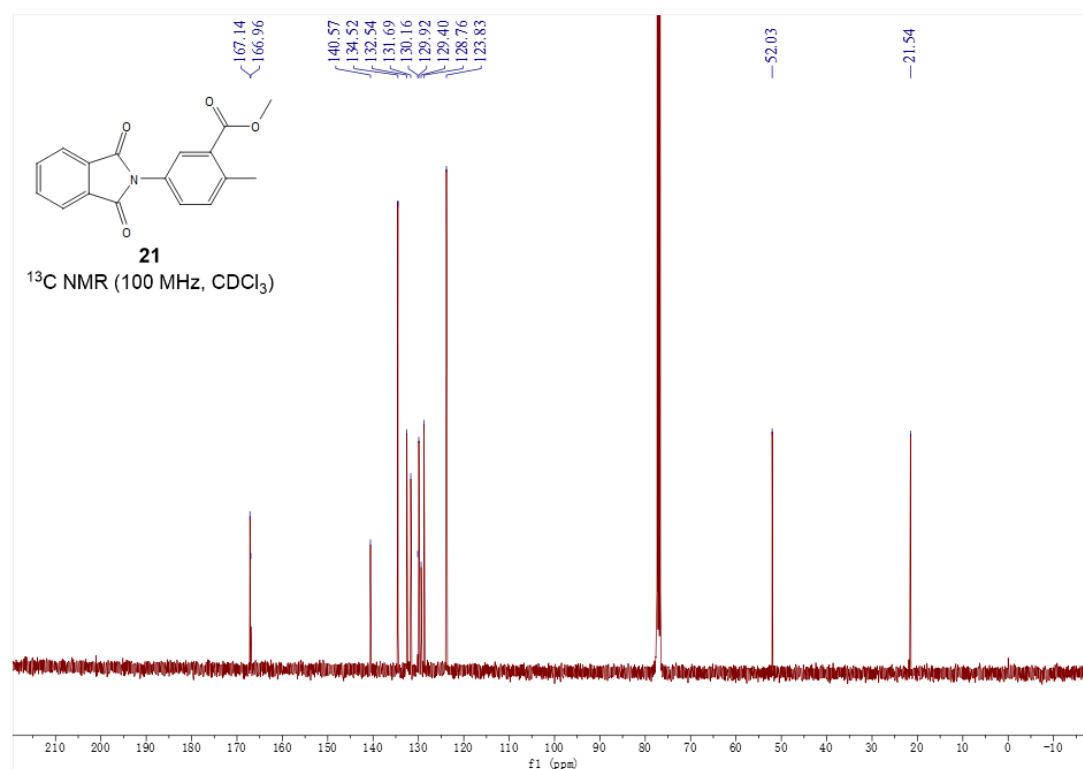
¹³C NMR (100 MHz, CDCl₃) spectrum of **20**



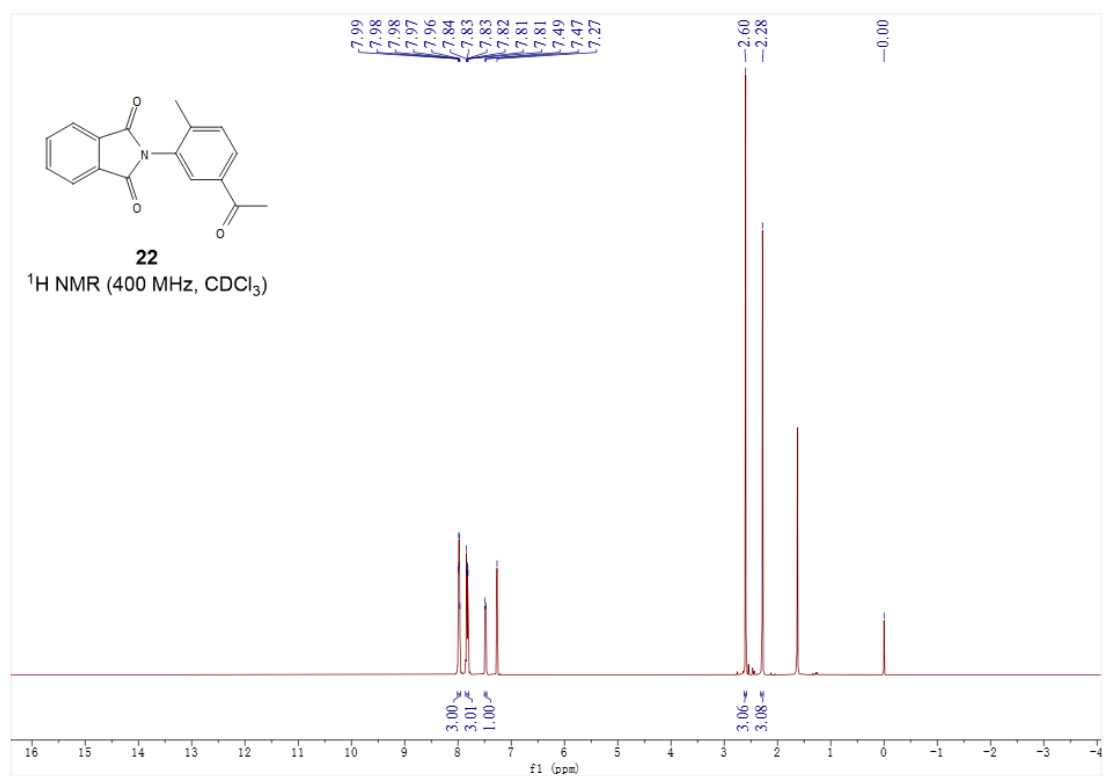
¹H NMR (400 MHz, CDCl₃) spectrum of **21**



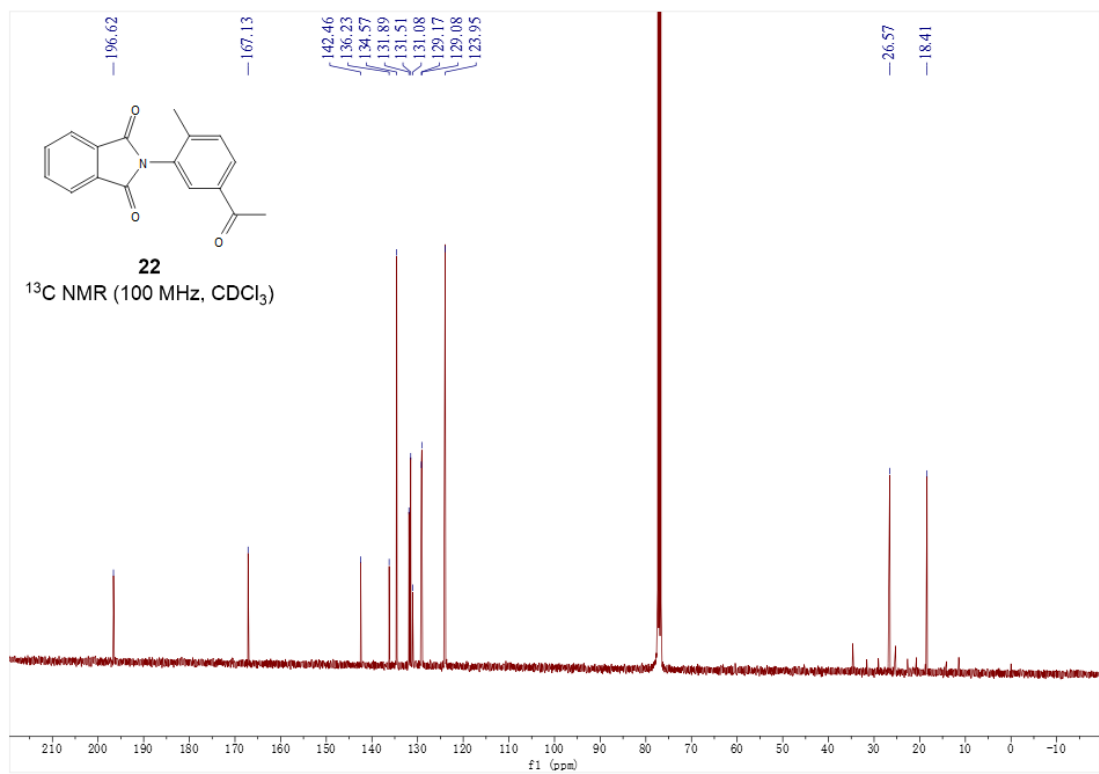
¹³C NMR (100 MHz, CDCl₃) spectrum of **21**



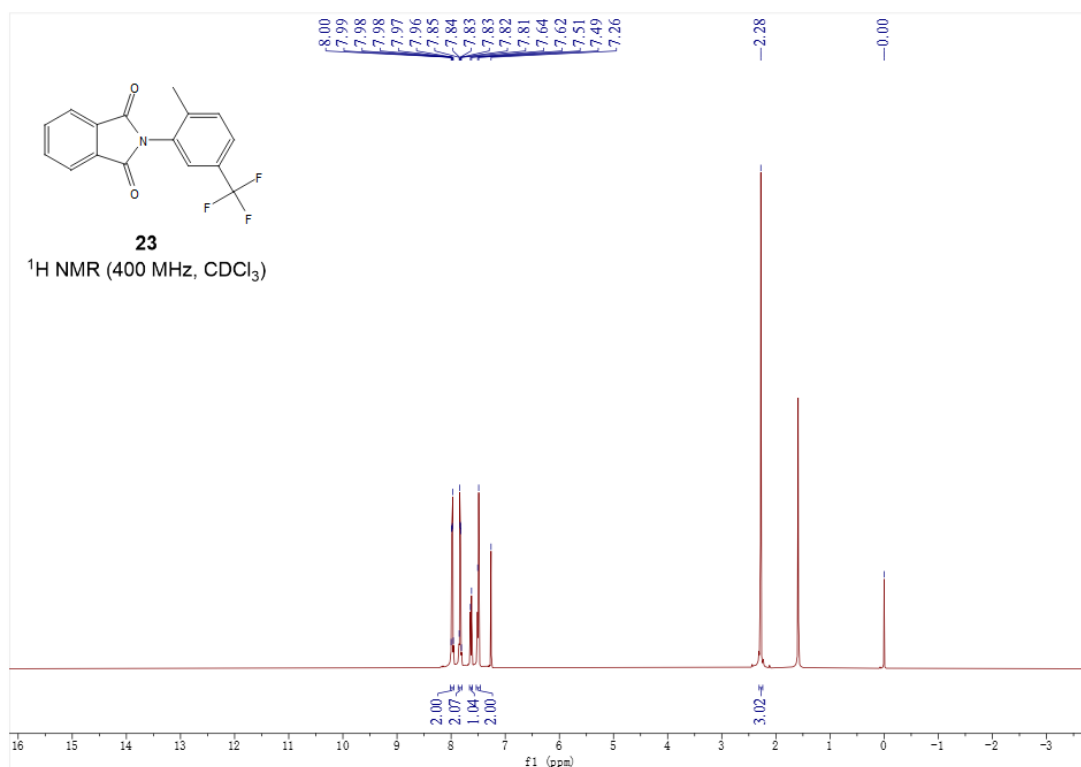
¹H NMR (400 MHz, CDCl₃) spectrum of **22**



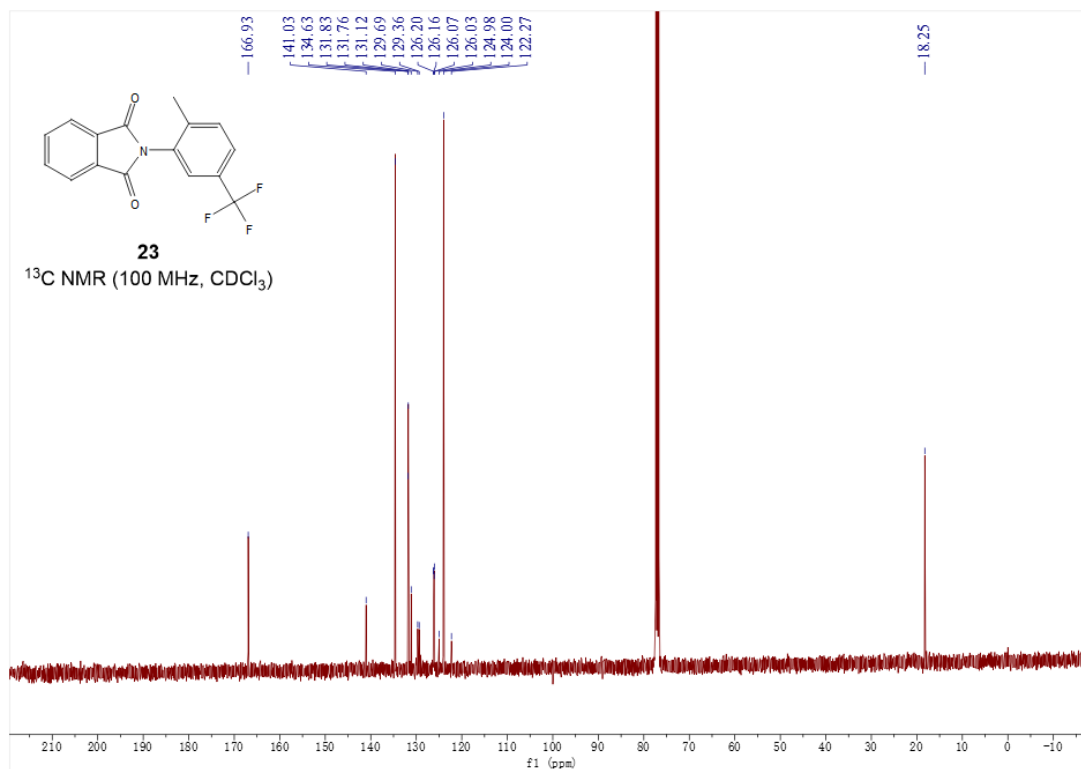
¹³C NMR (100 MHz, CDCl₃) spectrum of **22**



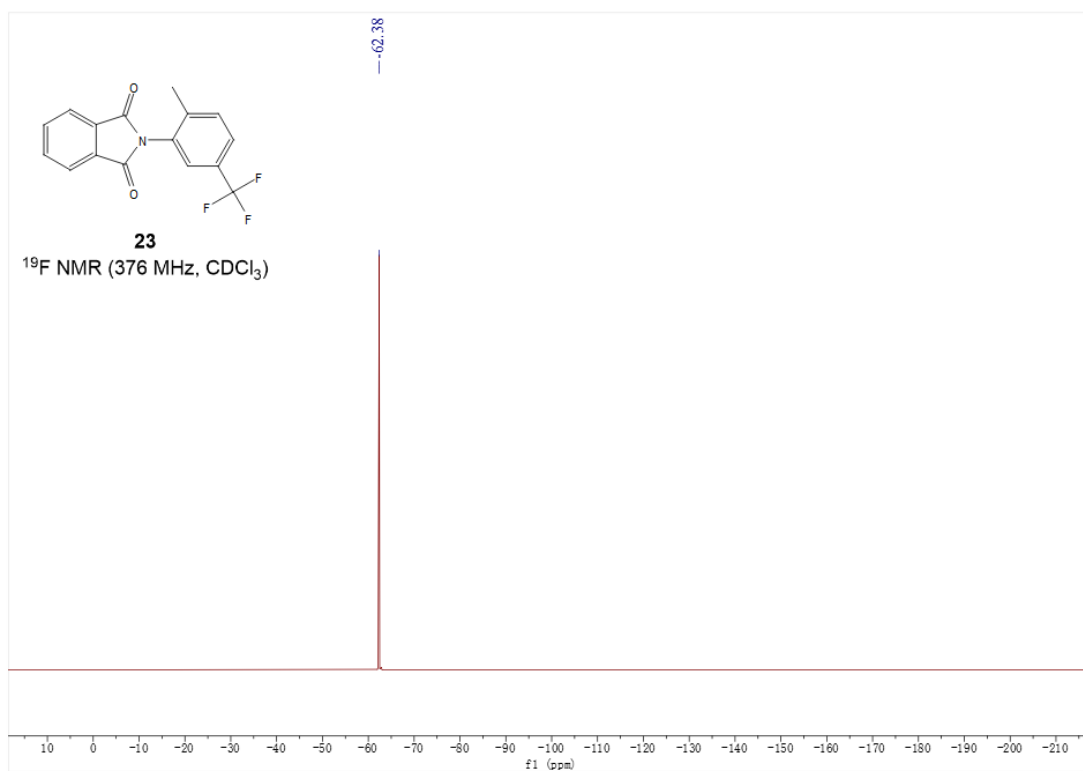
¹H NMR (400 MHz, CDCl₃) spectrum of **23**



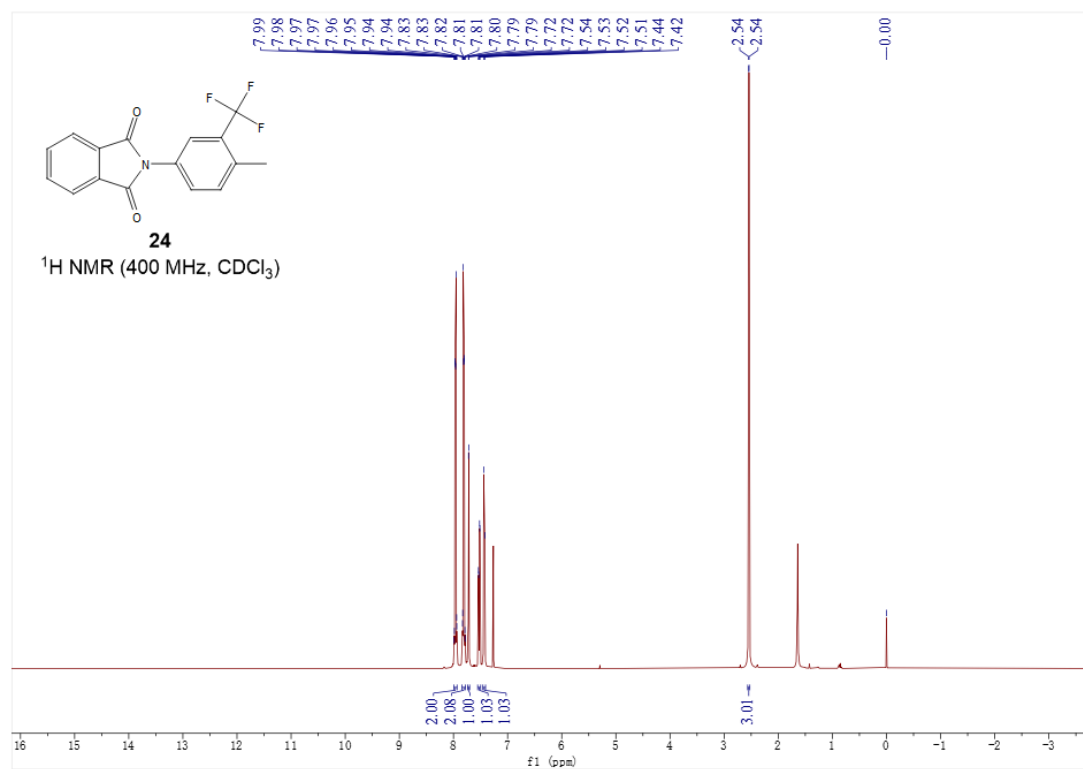
¹³C NMR (100 MHz, CDCl₃) spectrum of **23**



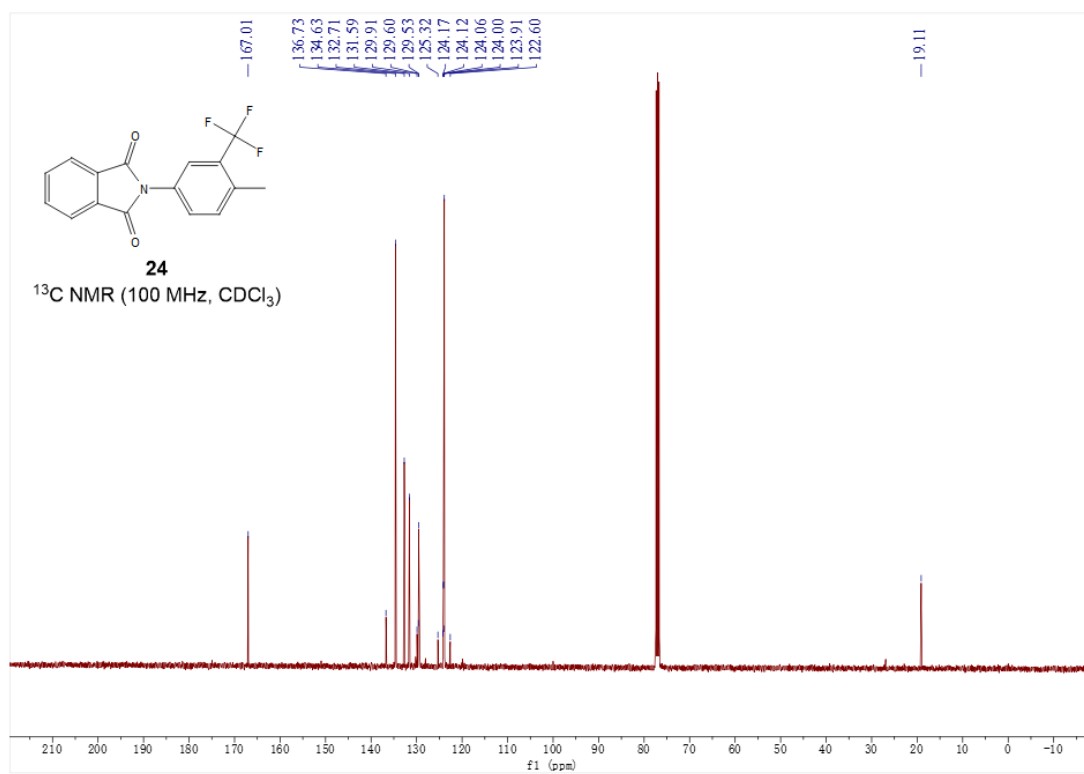
^{19}F NMR (376 MHz, CDCl_3) spectrum of **23**



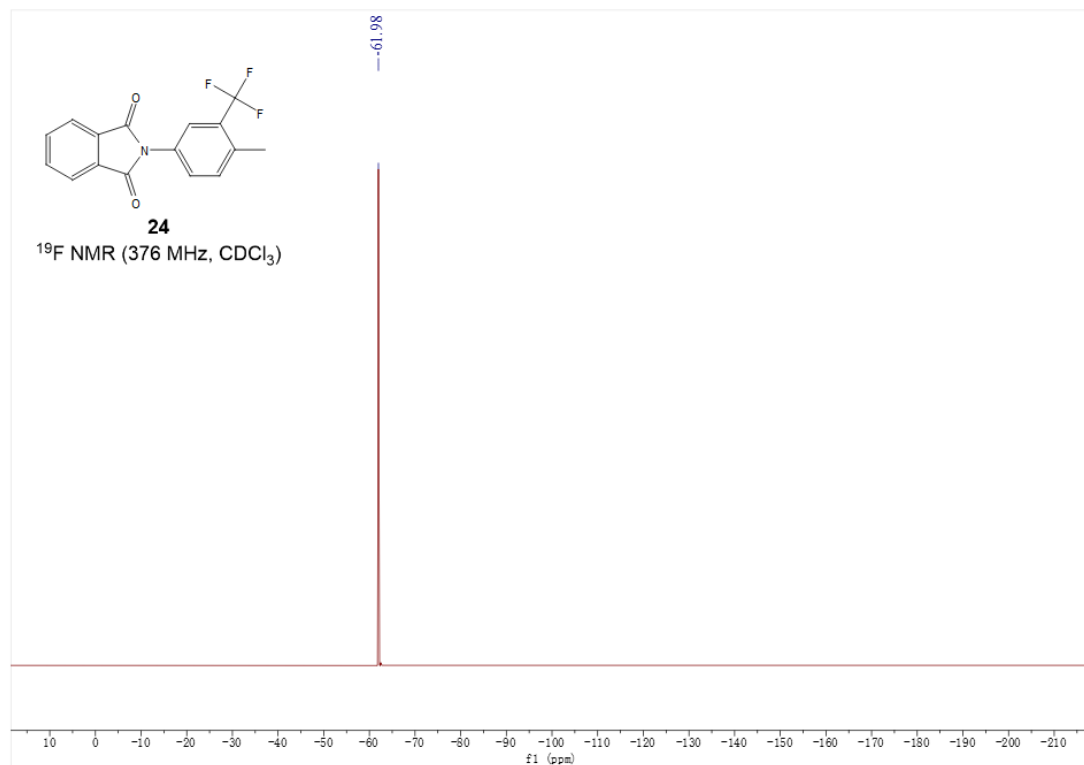
^1H NMR (400 MHz, CDCl_3) spectrum of **24**



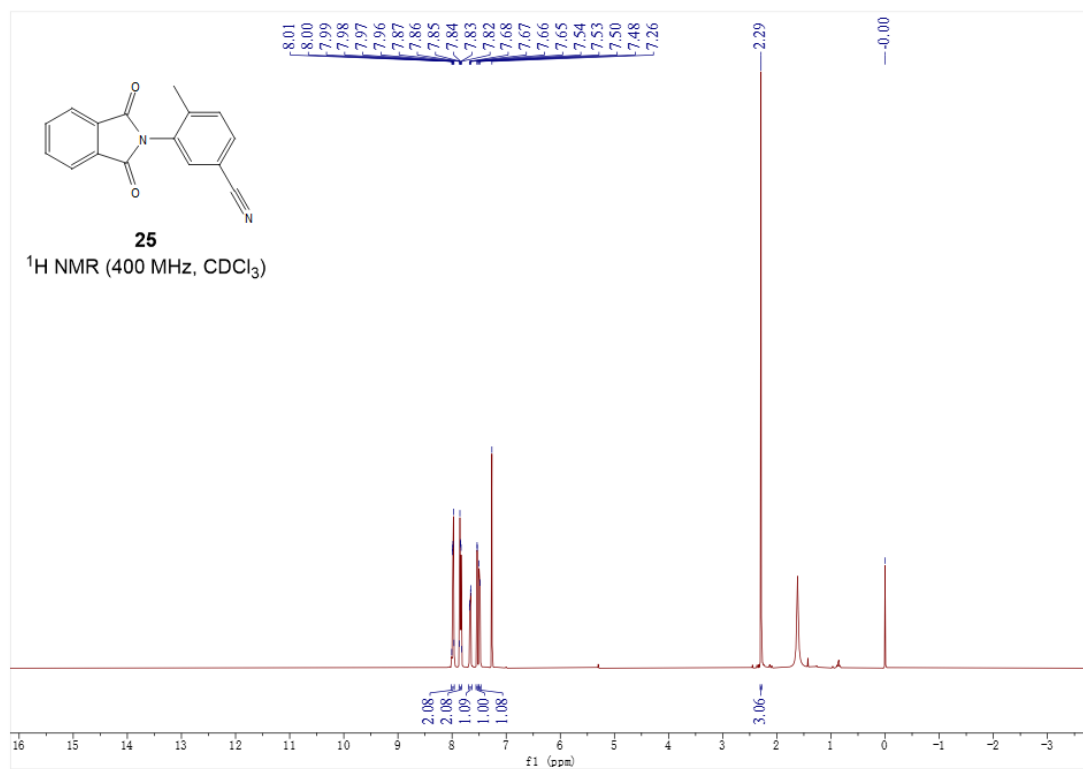
^{13}C NMR (100 MHz, CDCl_3) spectrum of **24**



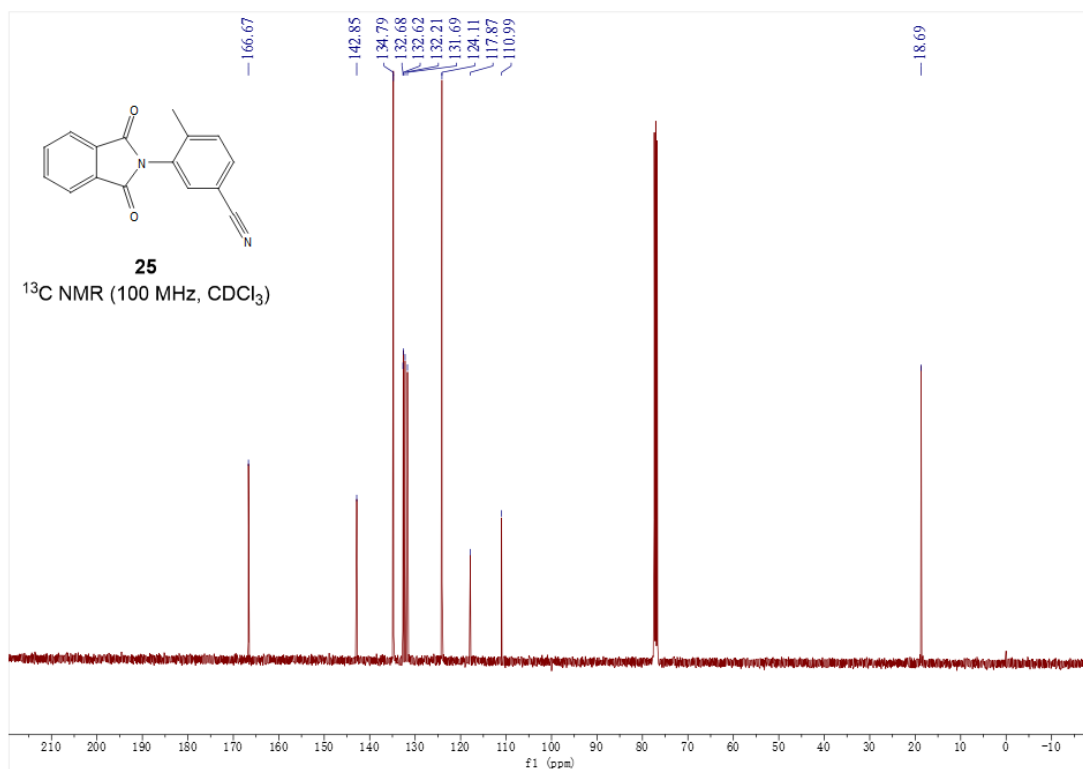
^{19}F NMR (376 MHz, CDCl_3) spectrum of **24**



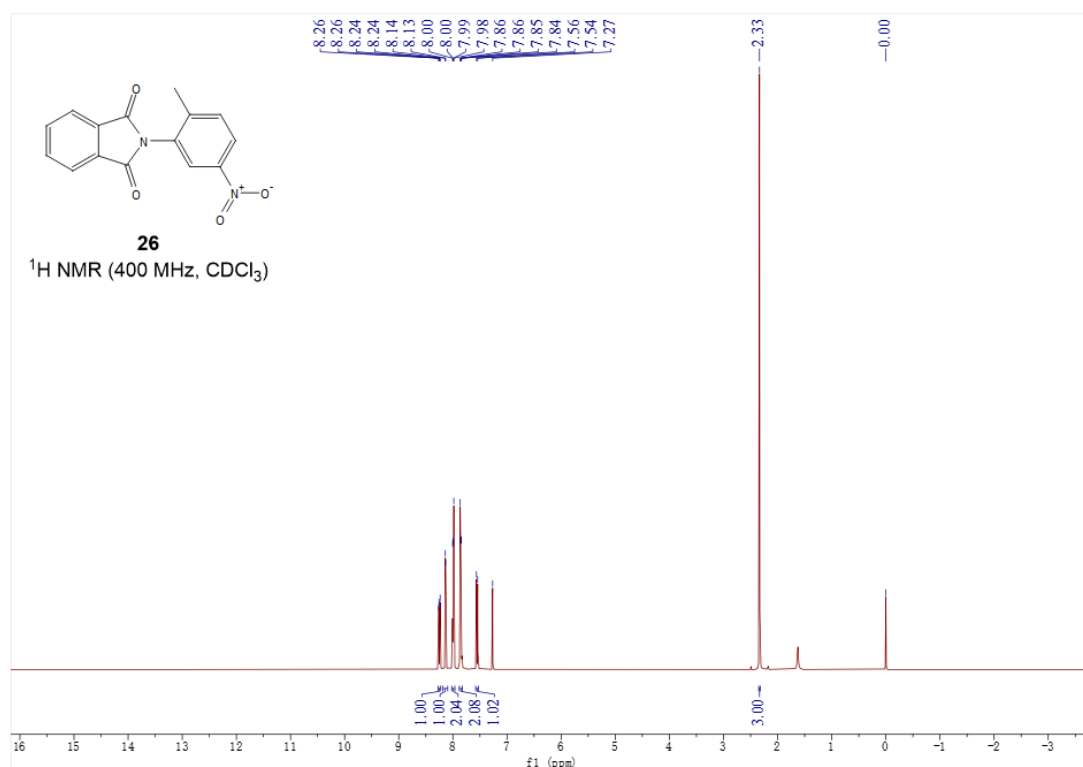
^1H NMR (400 MHz, CDCl_3) spectrum of **25**



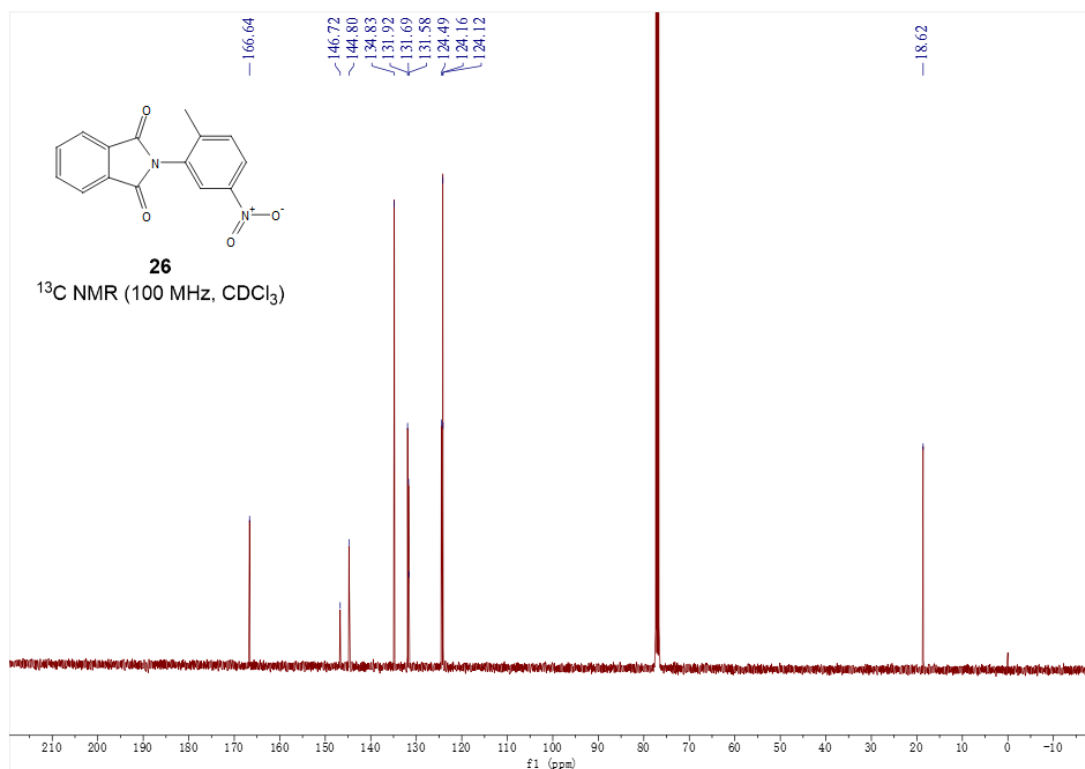
^{13}C NMR (100 MHz, CDCl_3) spectrum of **25**



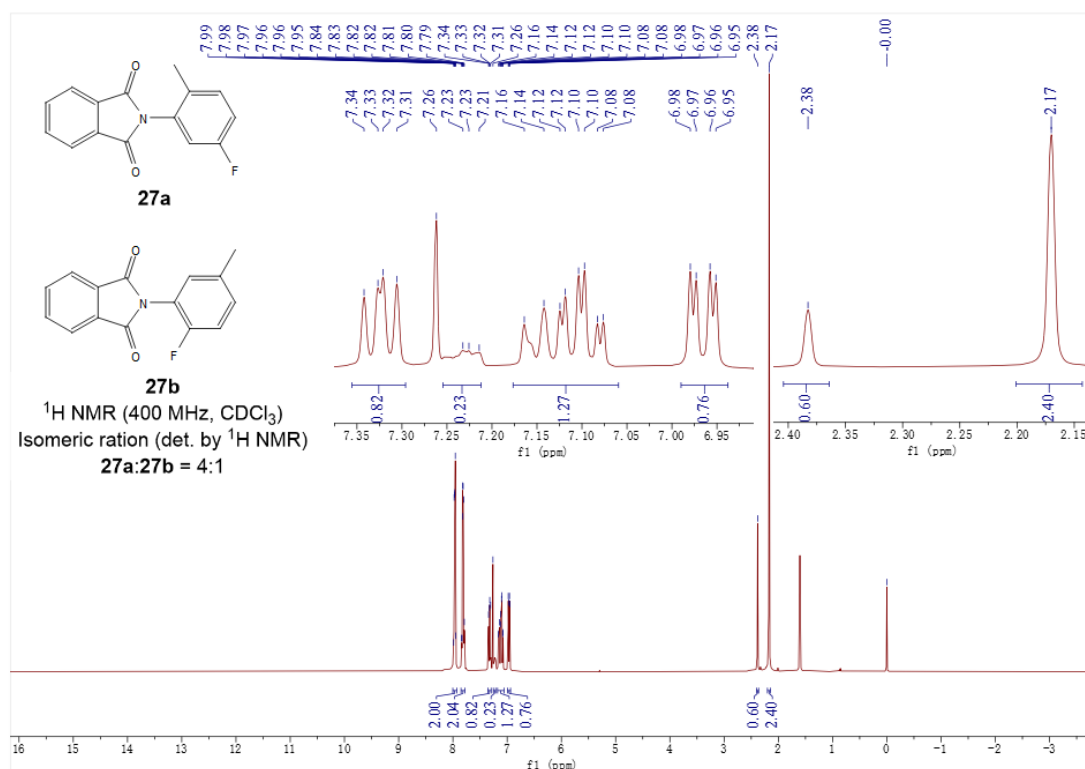
¹H NMR (400 MHz, CDCl₃) spectrum of **26**



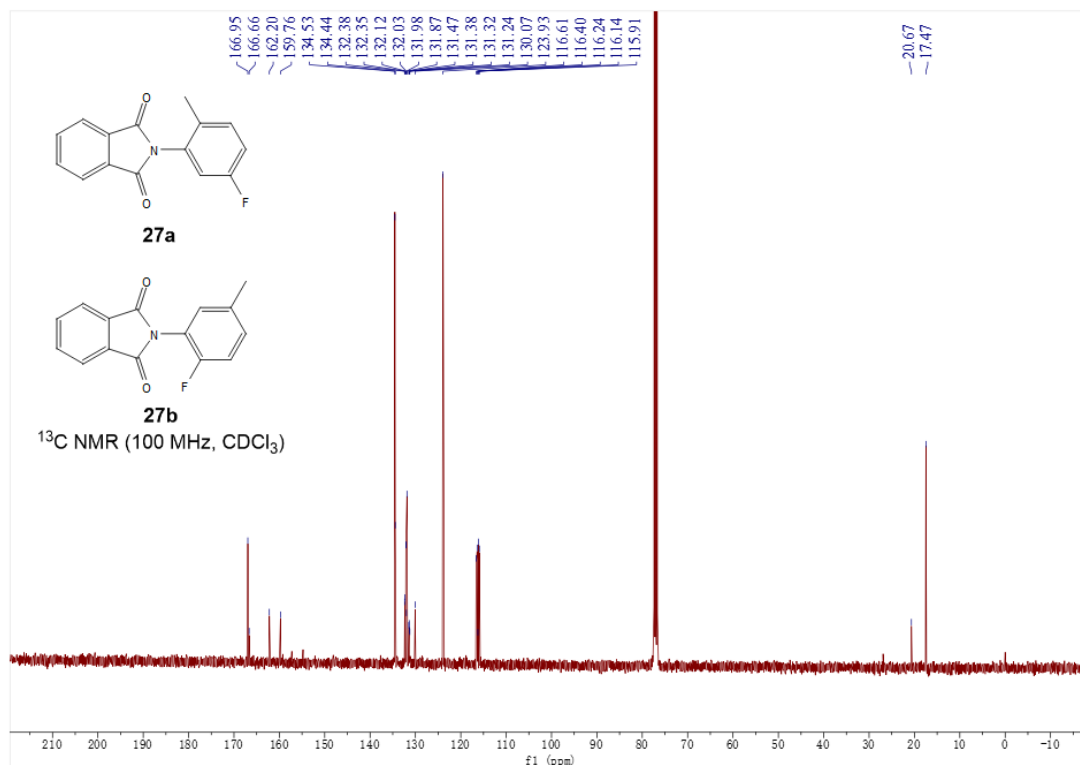
¹³C NMR (100 MHz, CDCl₃) spectrum of **26**



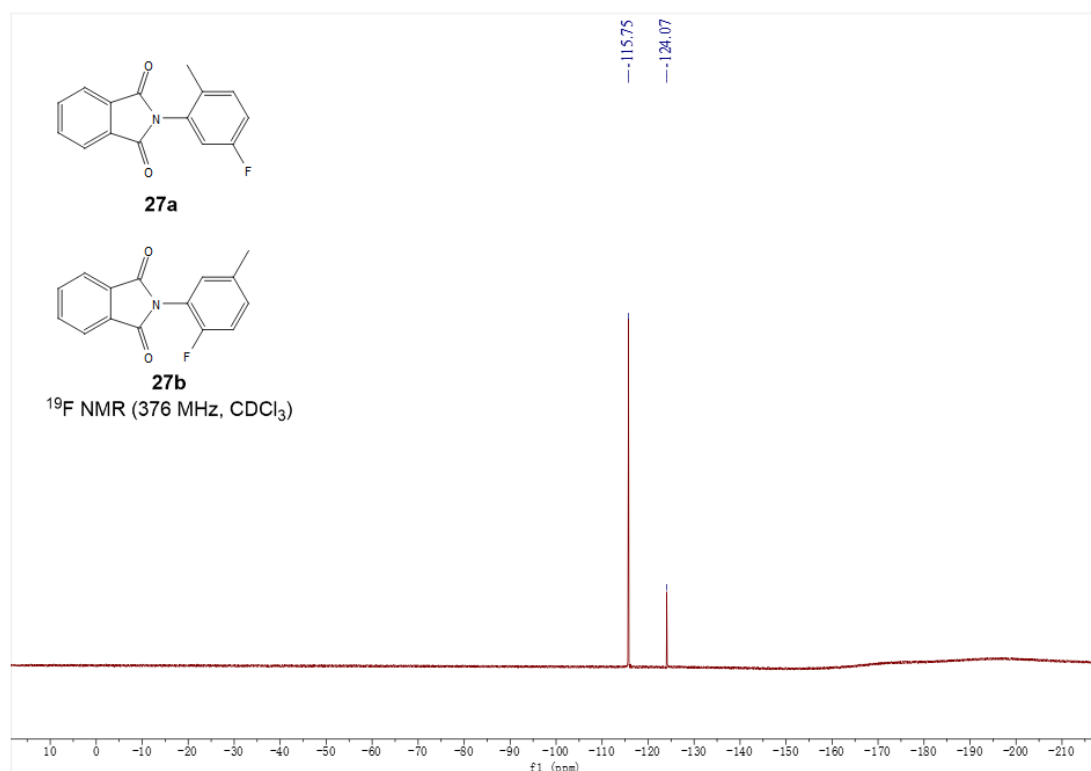
^1H NMR (400 MHz, CDCl_3) spectrum of **27**



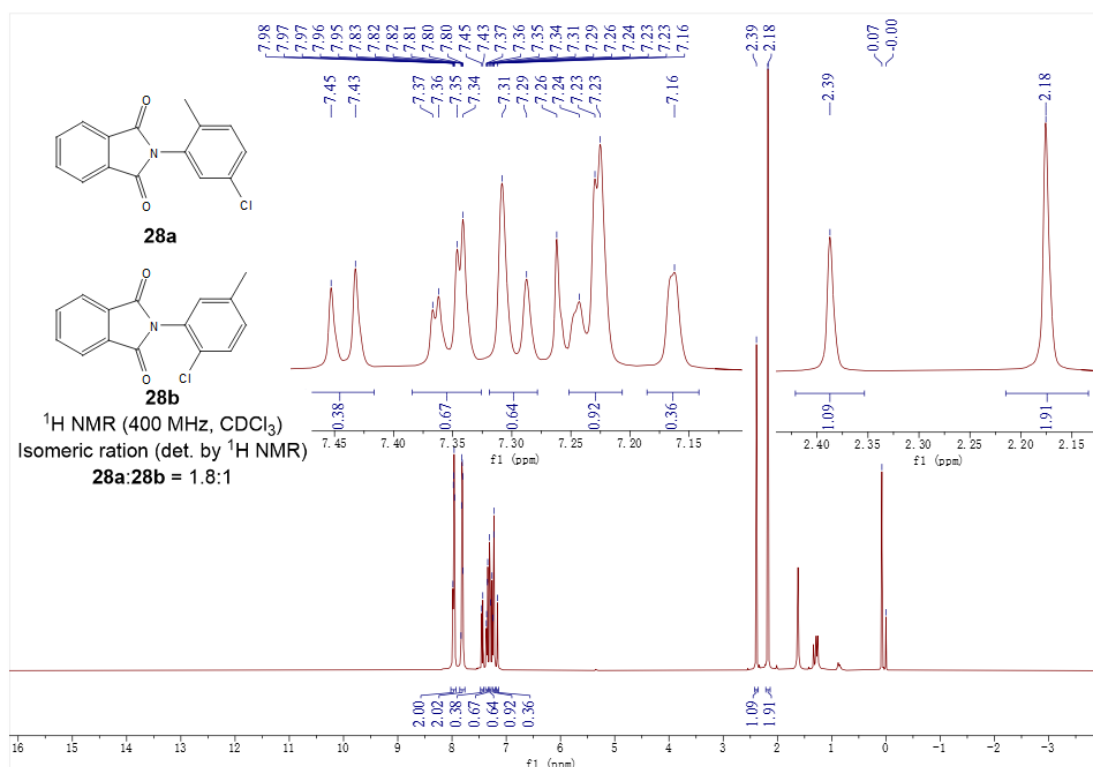
^{13}C NMR (100 MHz, CDCl_3) spectrum of **27**



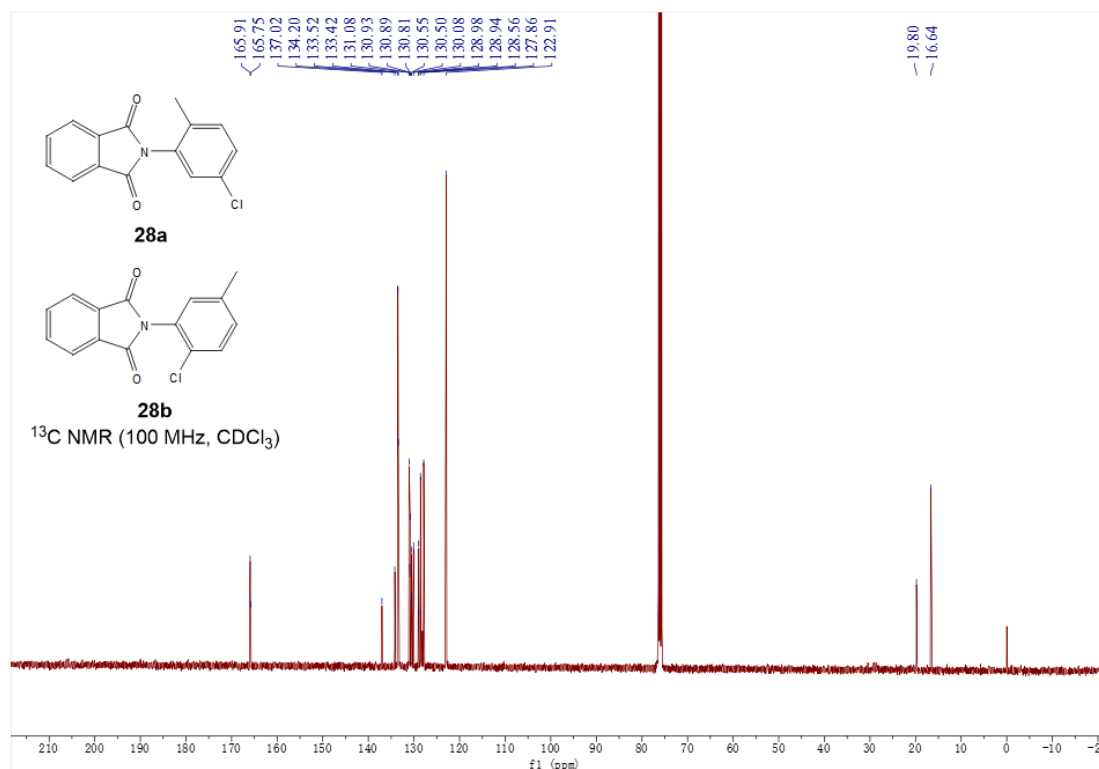
^{19}F NMR (376 MHz, CDCl_3) spectrum of **27**



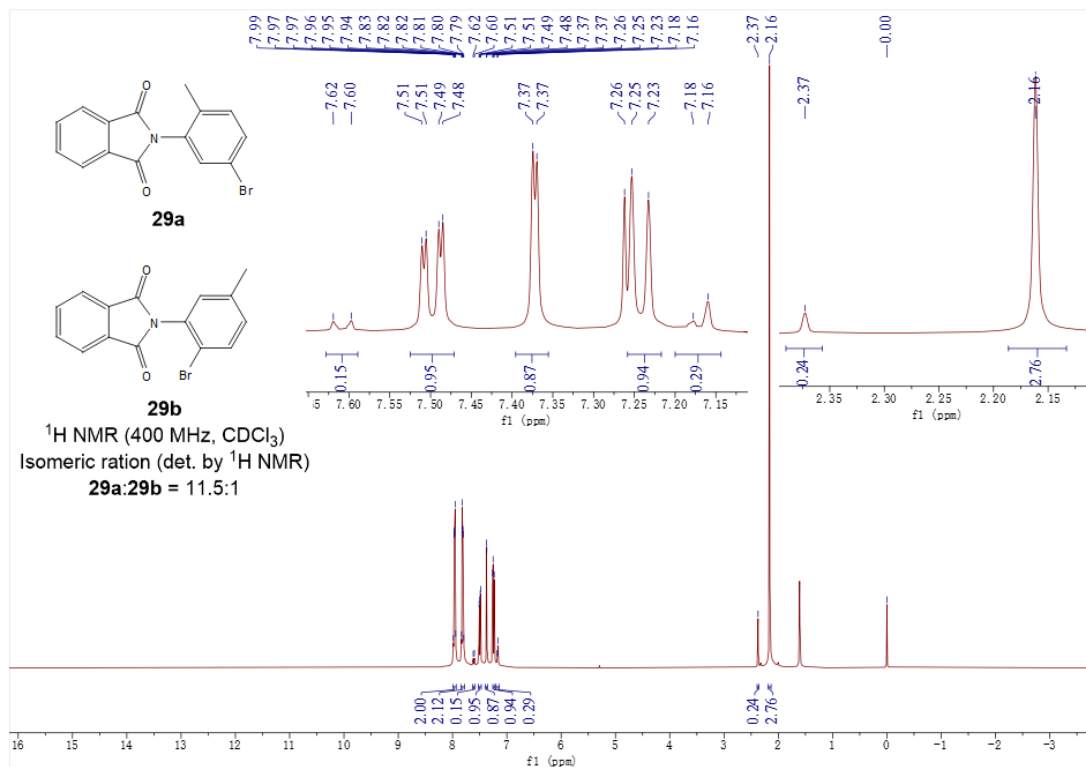
^1H NMR (400 MHz, CDCl_3) spectrum of **28**



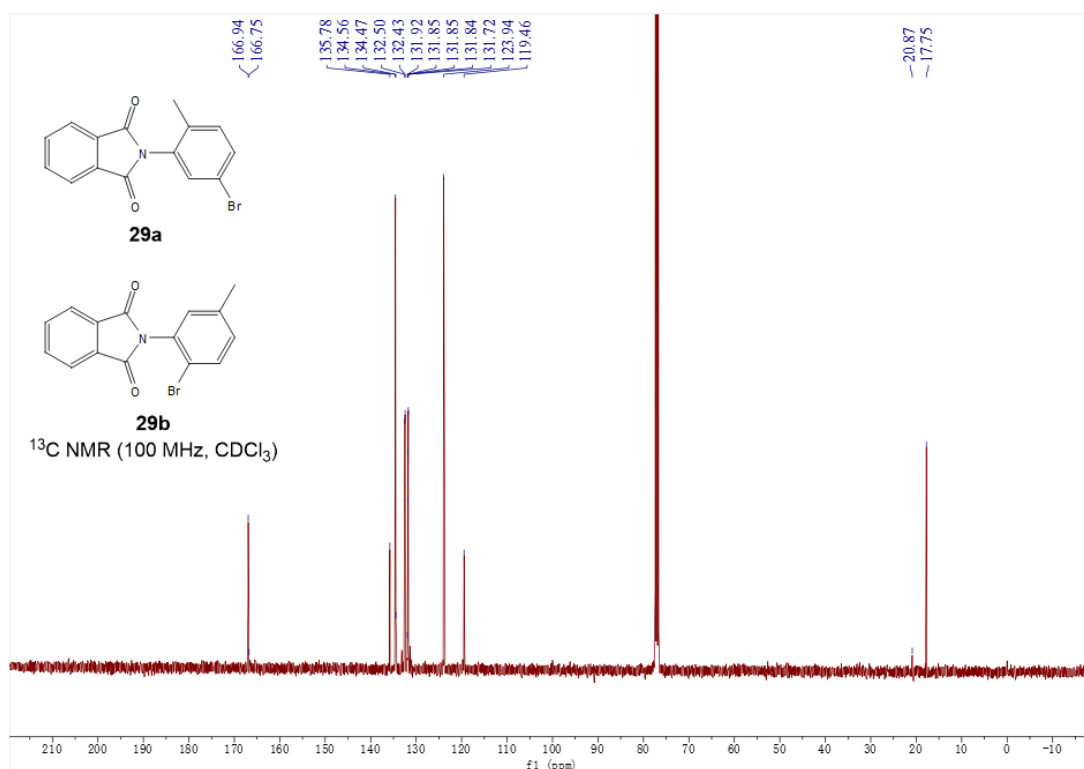
^{13}C NMR (100 MHz, CDCl_3) spectrum of **28**



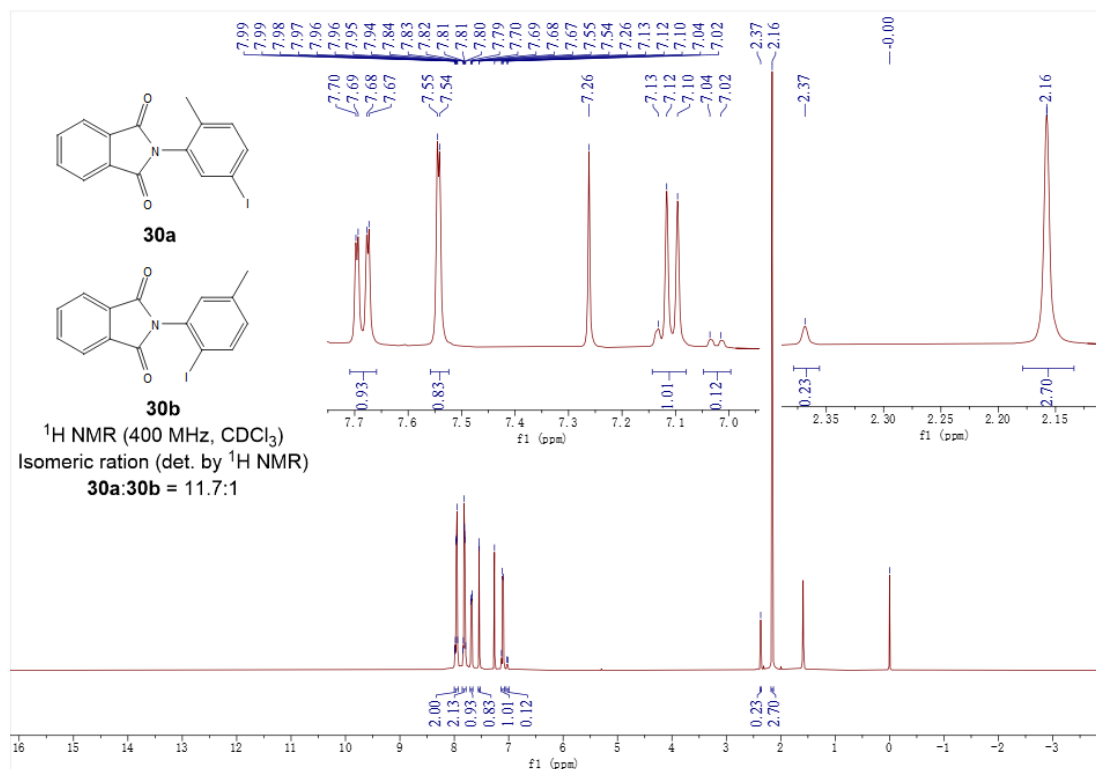
^1H NMR (400 MHz, CDCl_3) spectrum of **29**



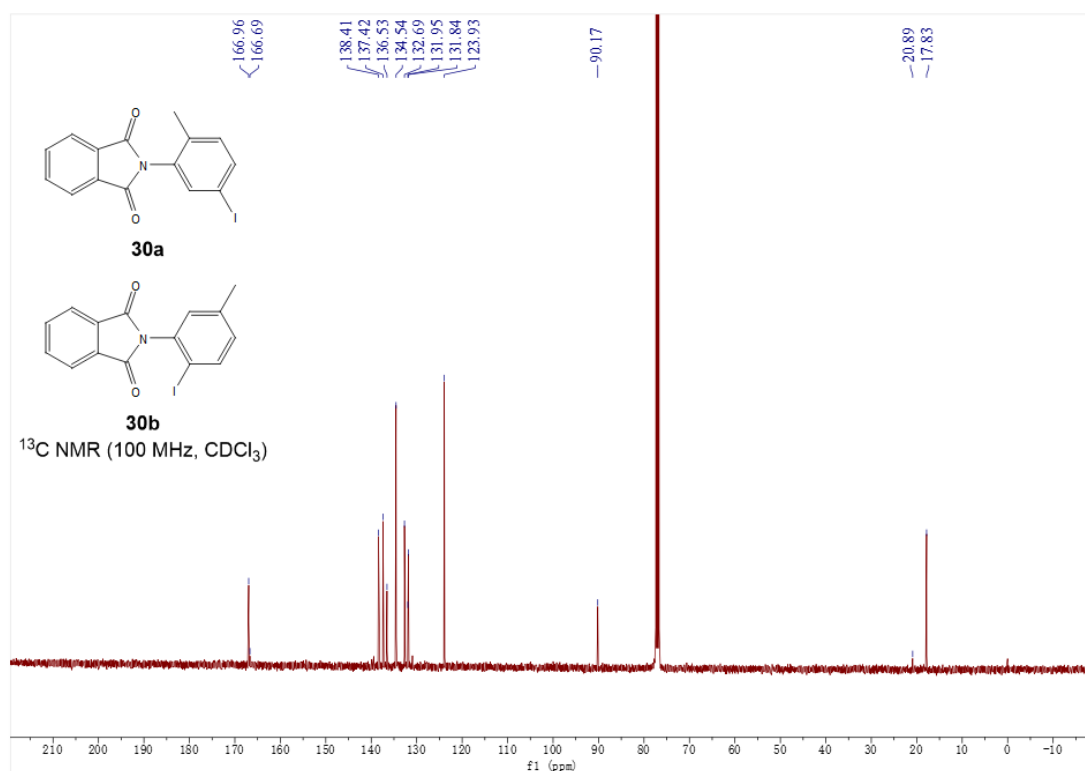
^{13}C NMR (100 MHz, CDCl_3) spectrum of **29**



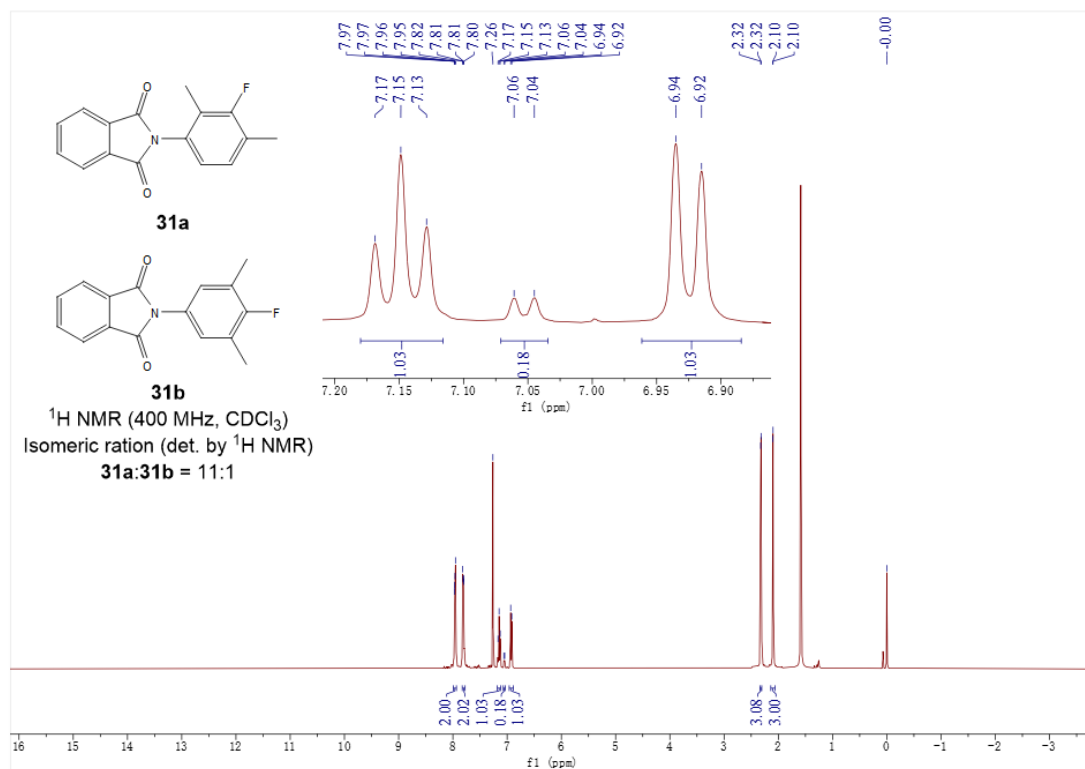
^1H NMR (400 MHz, CDCl_3) spectrum of **30**



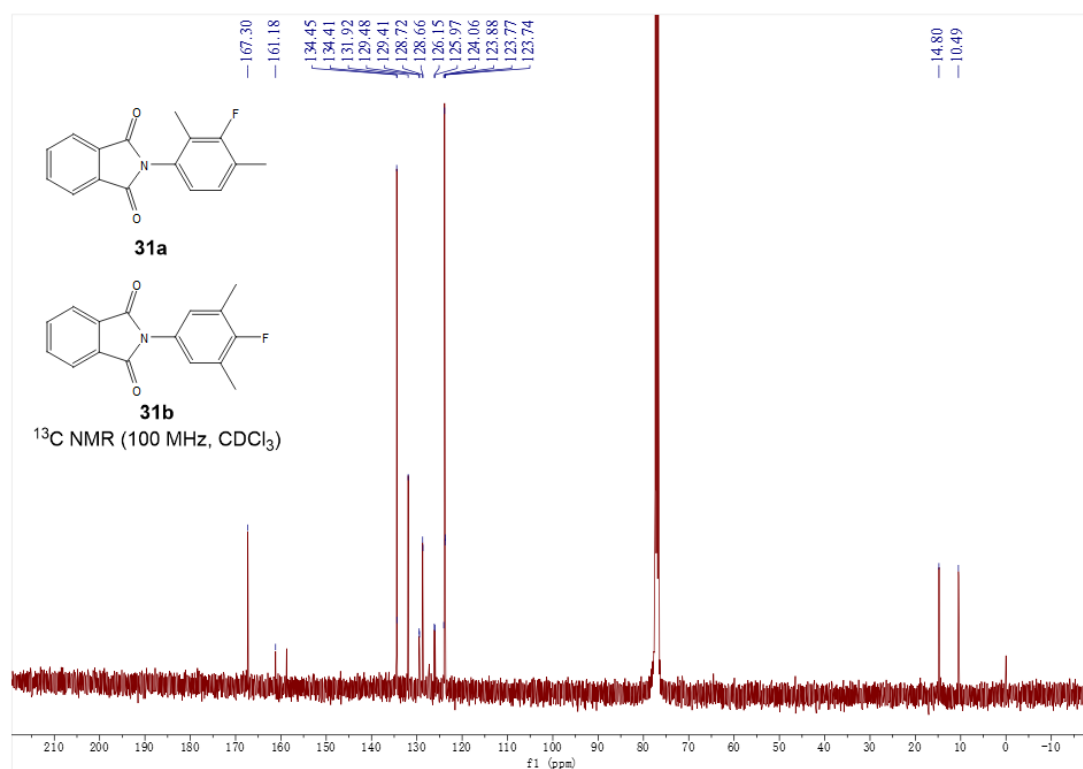
^{13}C NMR (100 MHz, CDCl_3) spectrum of **30**



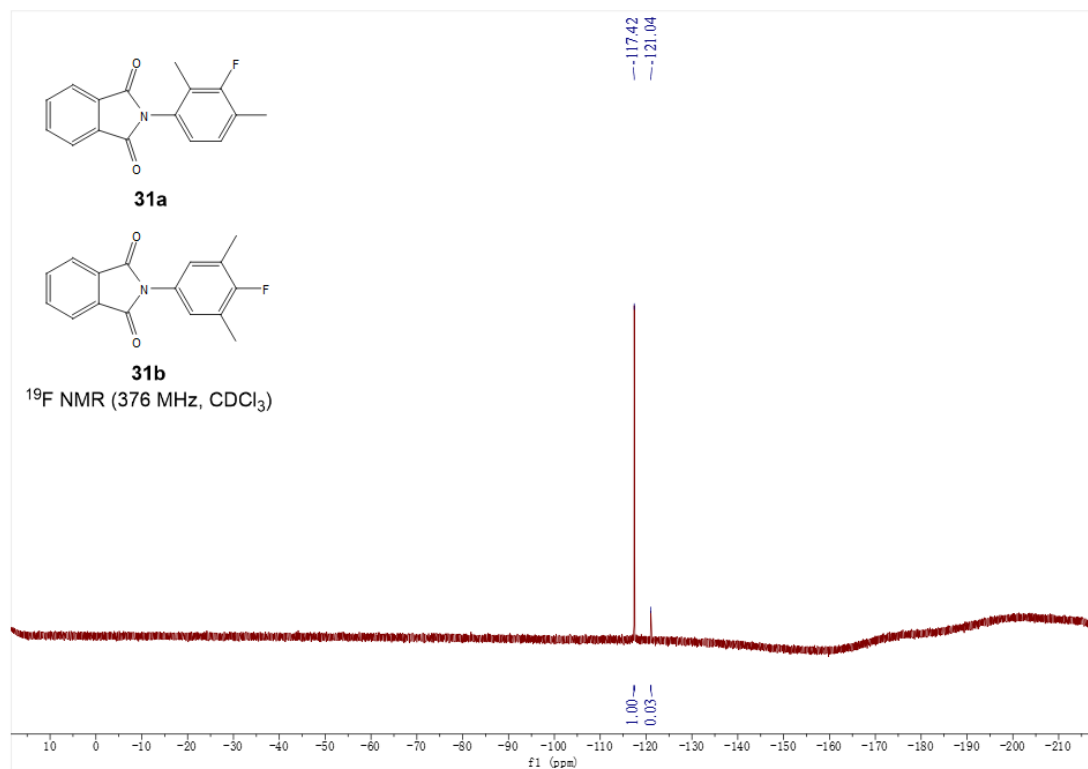
^1H NMR (400 MHz, CDCl_3) spectrum of **31**



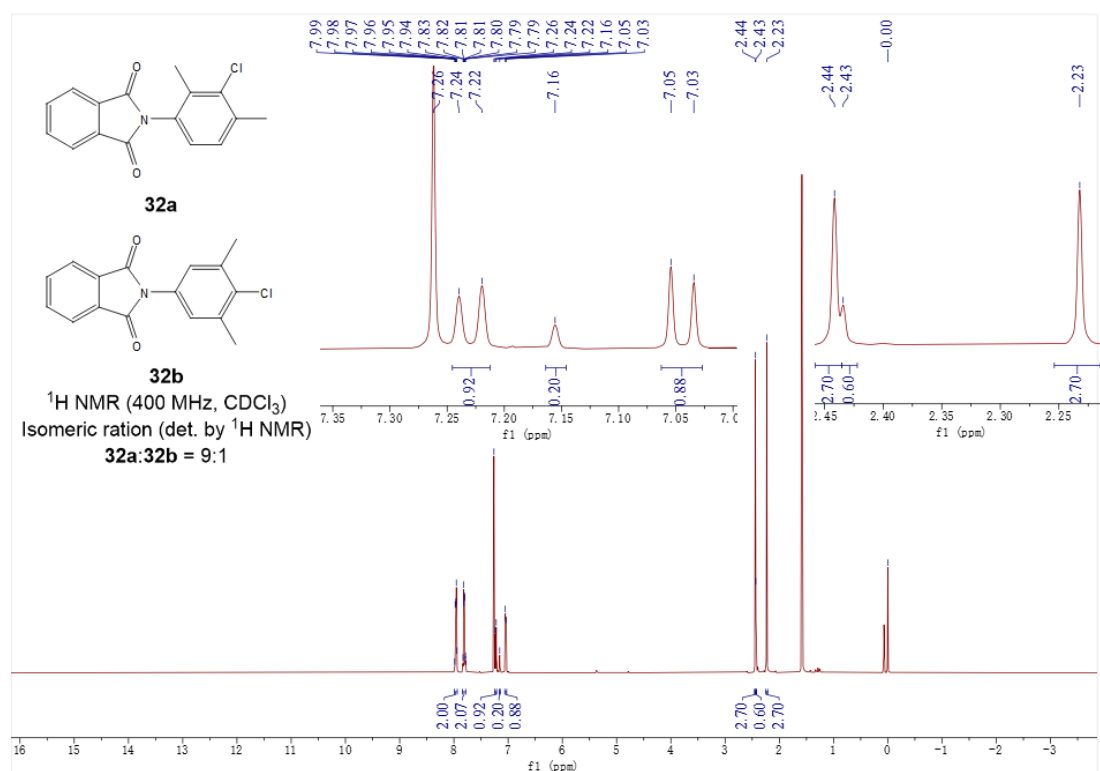
^{13}C NMR (100 MHz, CDCl_3) spectrum of **31**



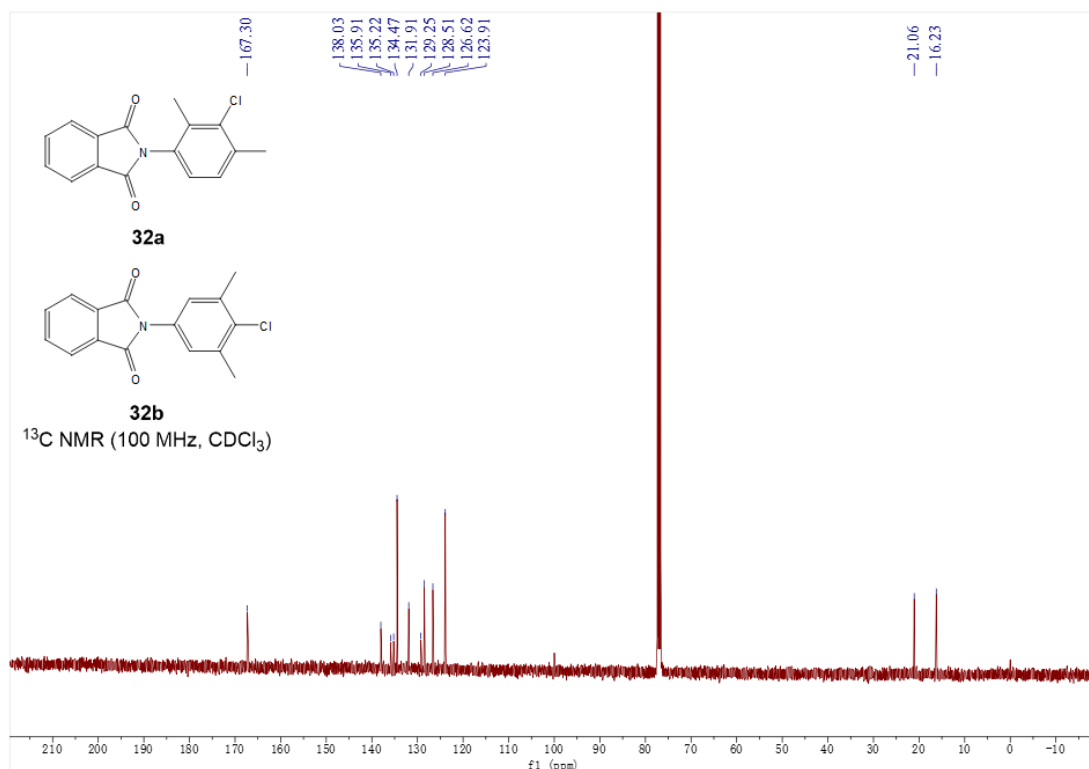
^{19}F NMR (376 MHz, CDCl_3) spectrum of **27**



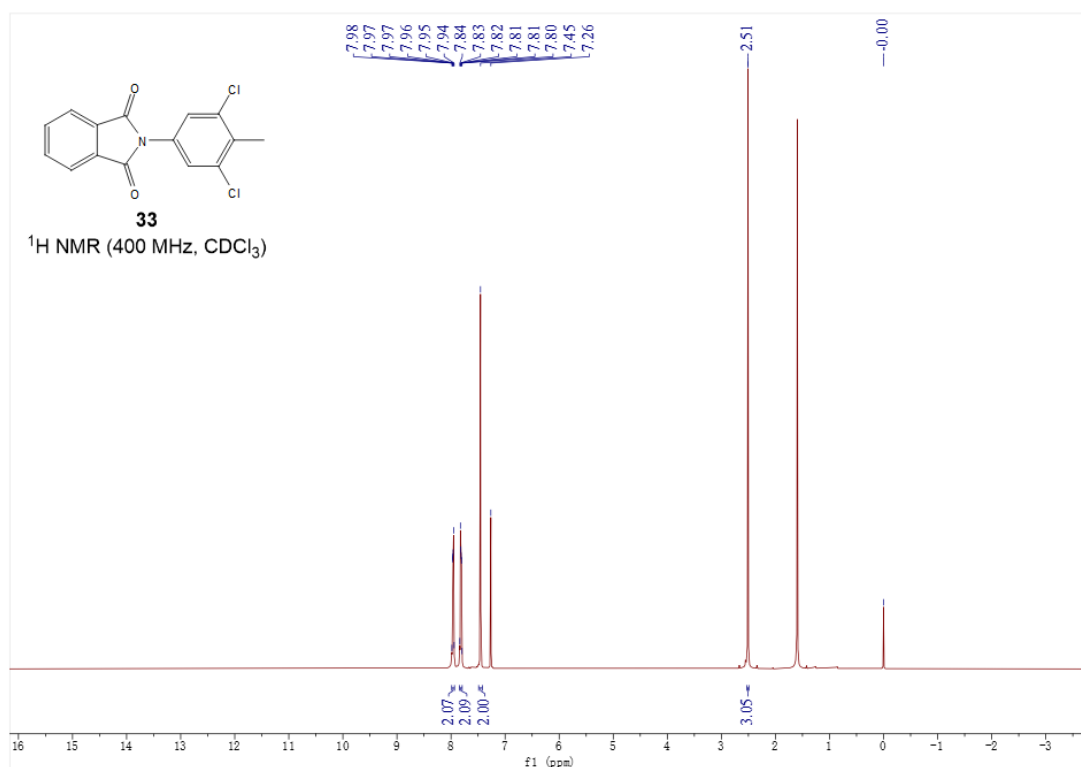
¹H NMR (400 MHz, CDCl₃) spectrum of **32**



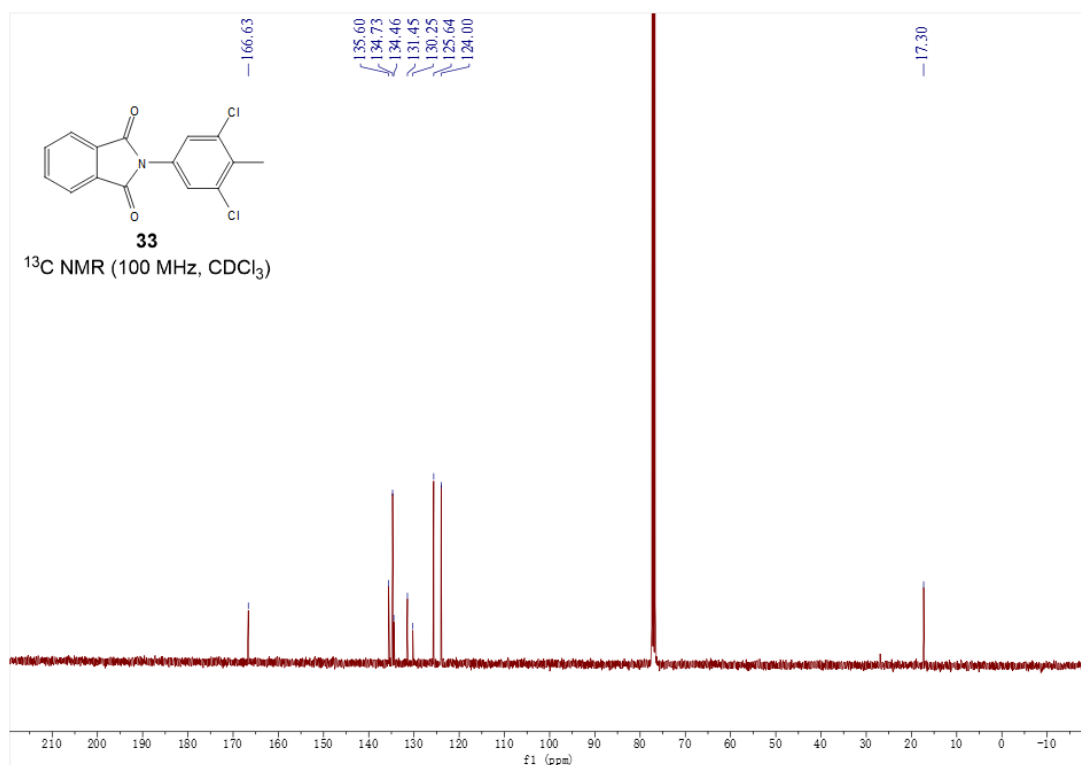
¹³C NMR (100 MHz, CDCl₃) spectrum of **32**



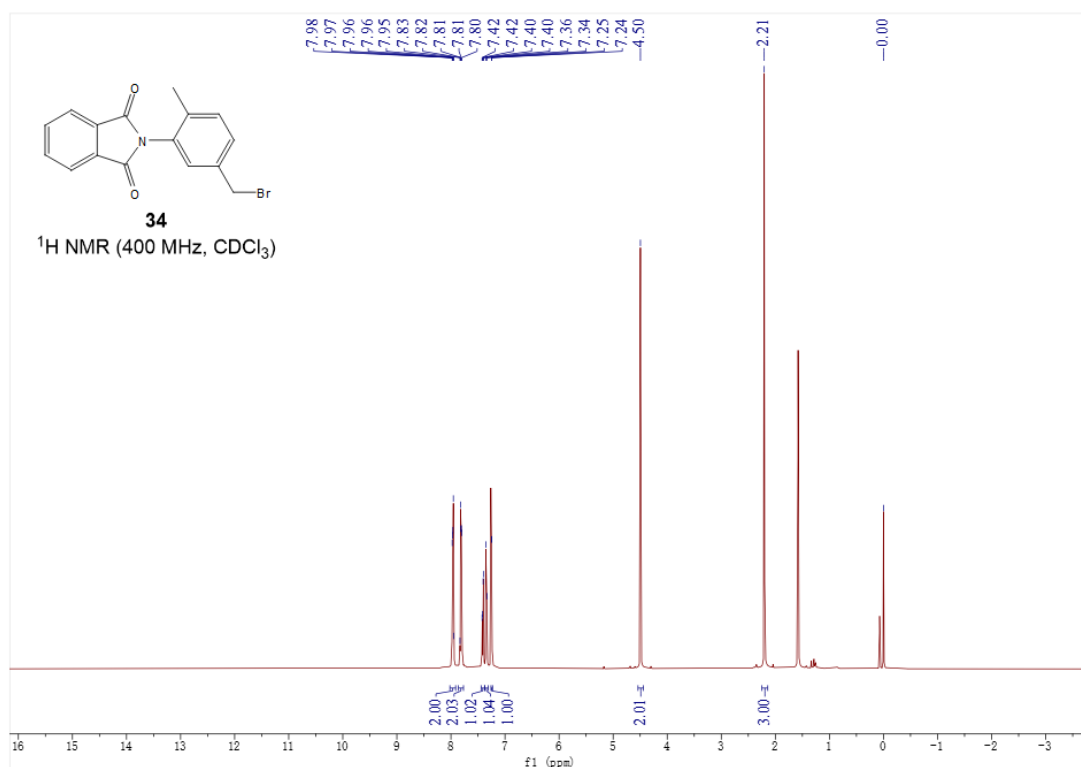
^1H NMR (400 MHz, CDCl_3) spectrum of **33**



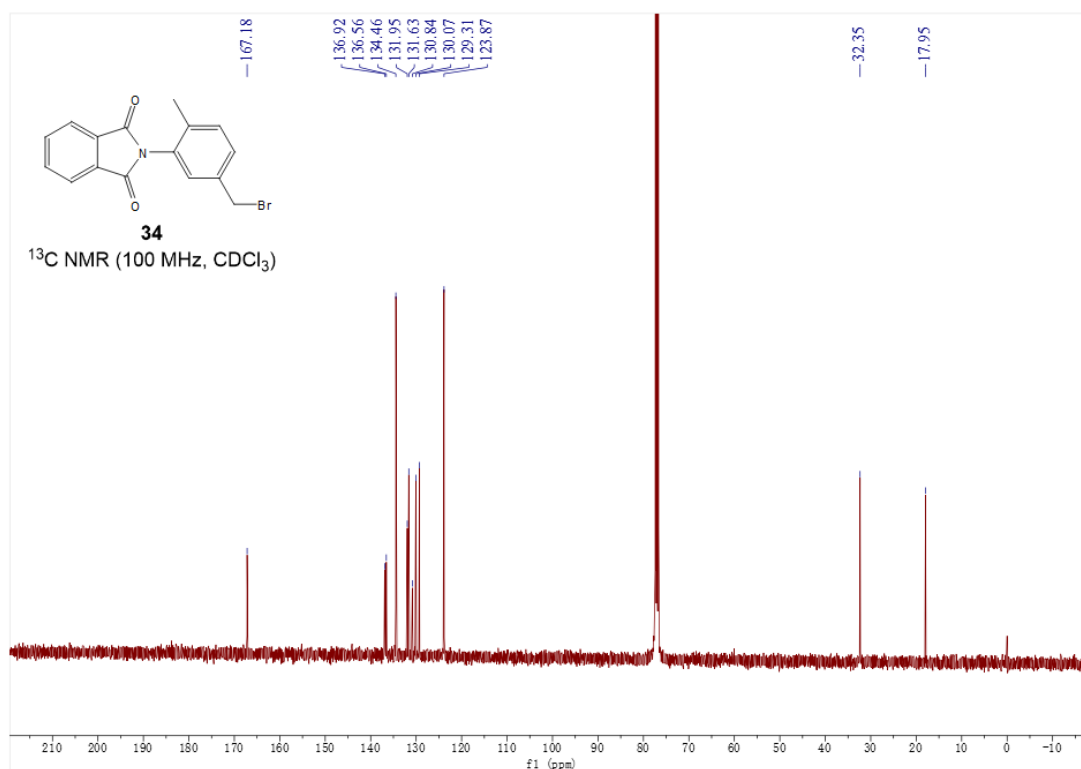
^{13}C NMR (100 MHz, CDCl_3) spectrum of **33**



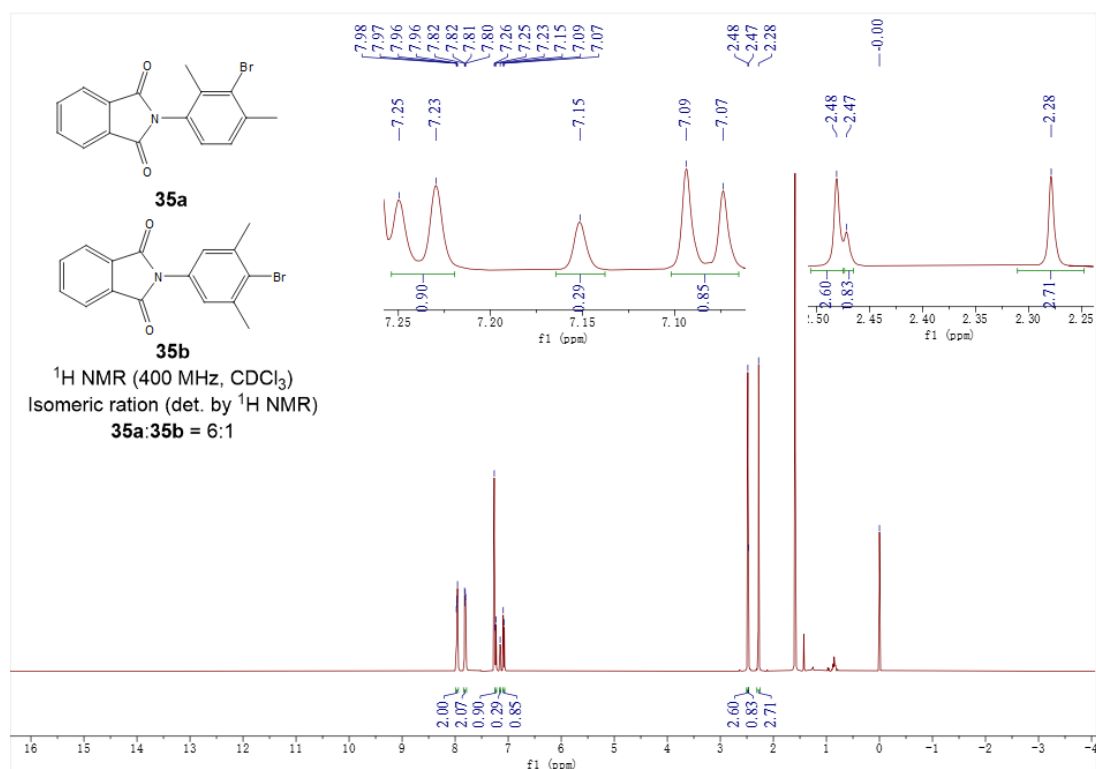
^1H NMR (400 MHz, CDCl_3) spectrum of **34**



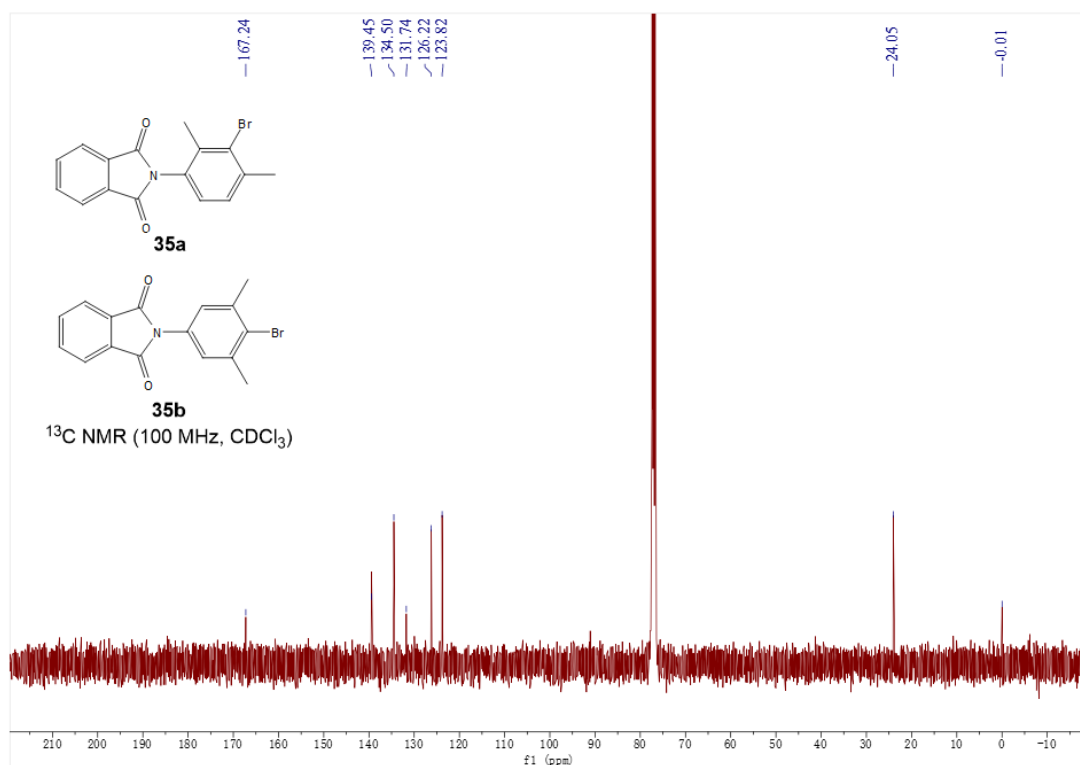
^{13}C NMR (100 MHz, CDCl_3) spectrum of **34**



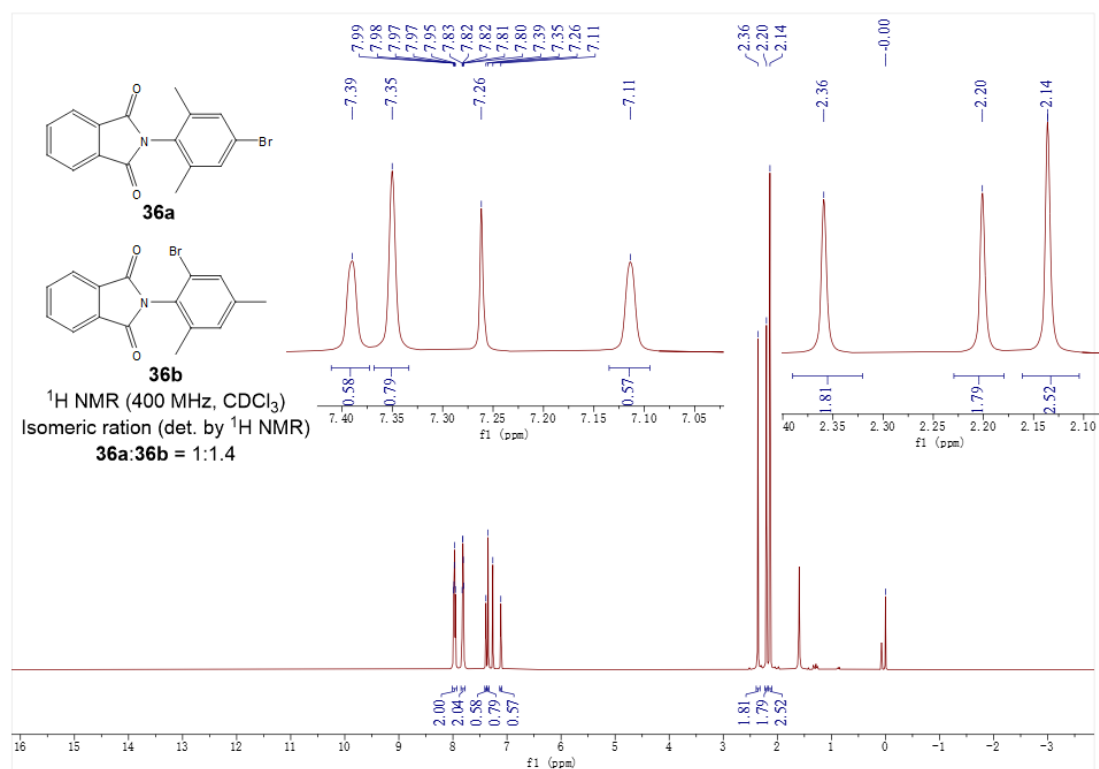
¹H NMR (400 MHz, CDCl₃) spectrum of **35**



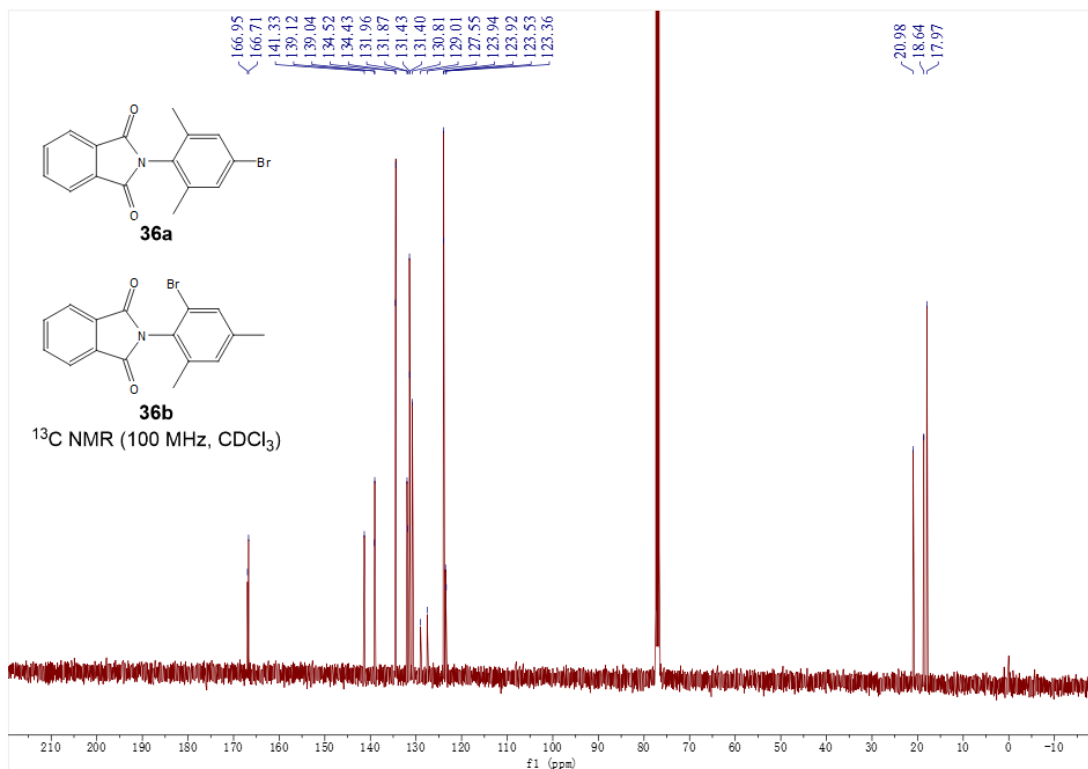
¹³C NMR (100 MHz, CDCl₃) spectrum of **35**



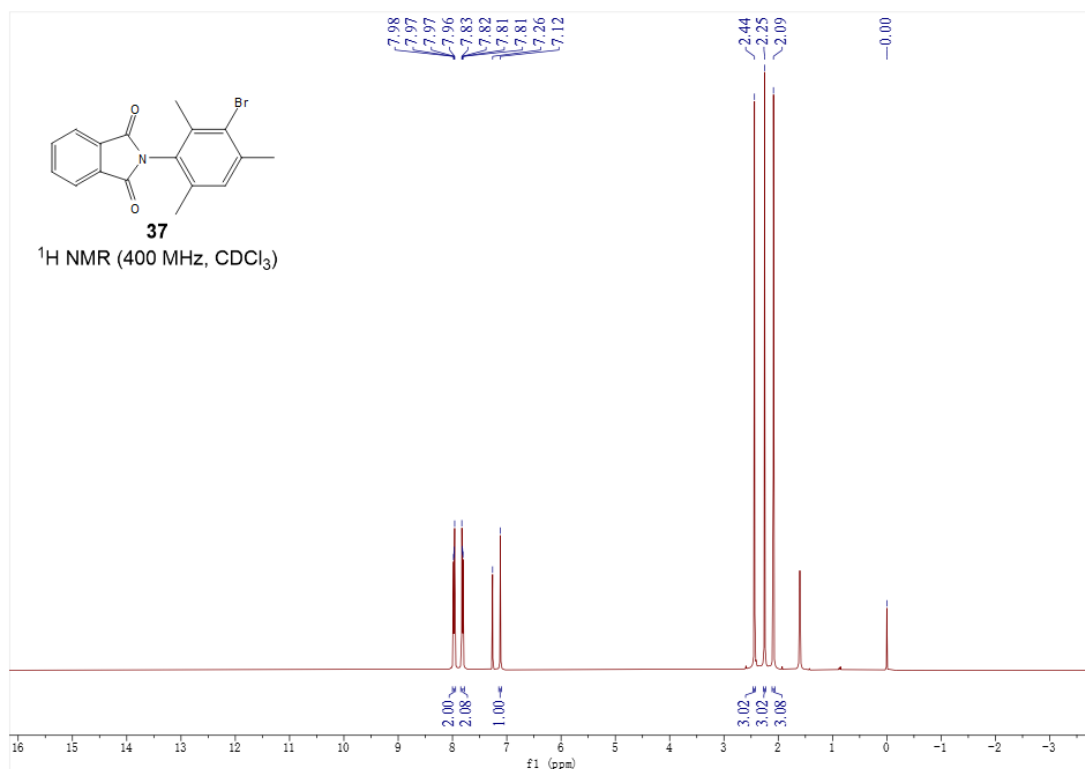
^1H NMR (400 MHz, CDCl_3) spectrum of **36**



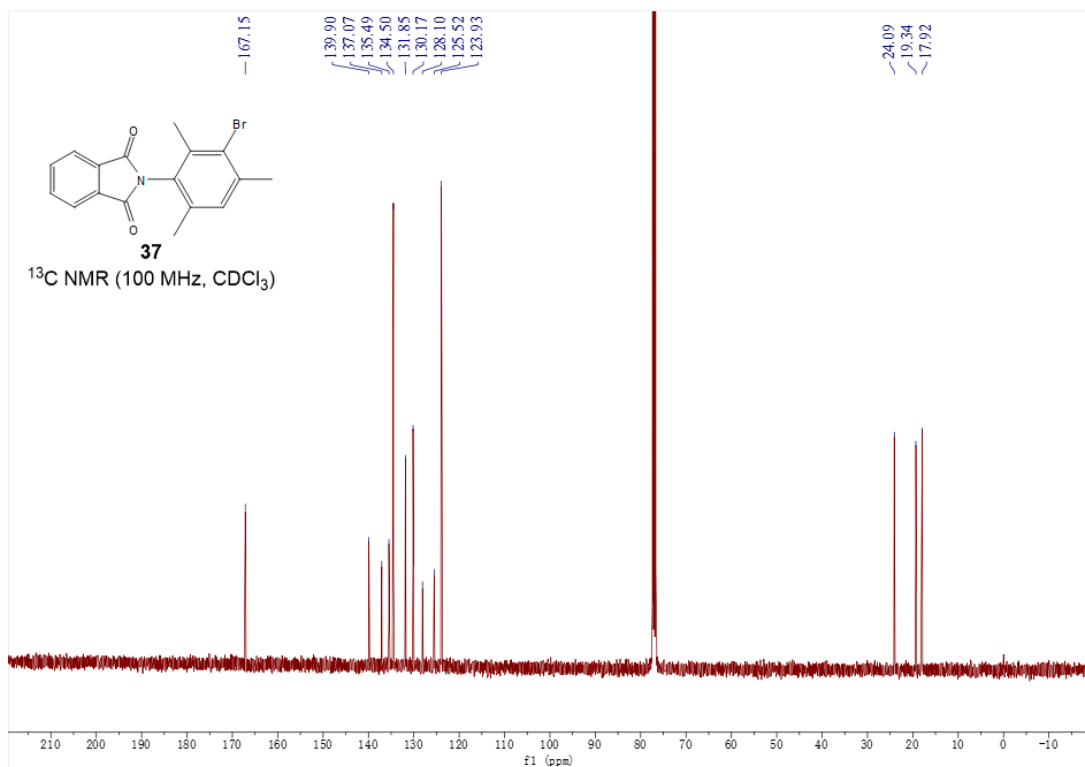
^{13}C NMR (100 MHz, CDCl_3) spectrum of **36**



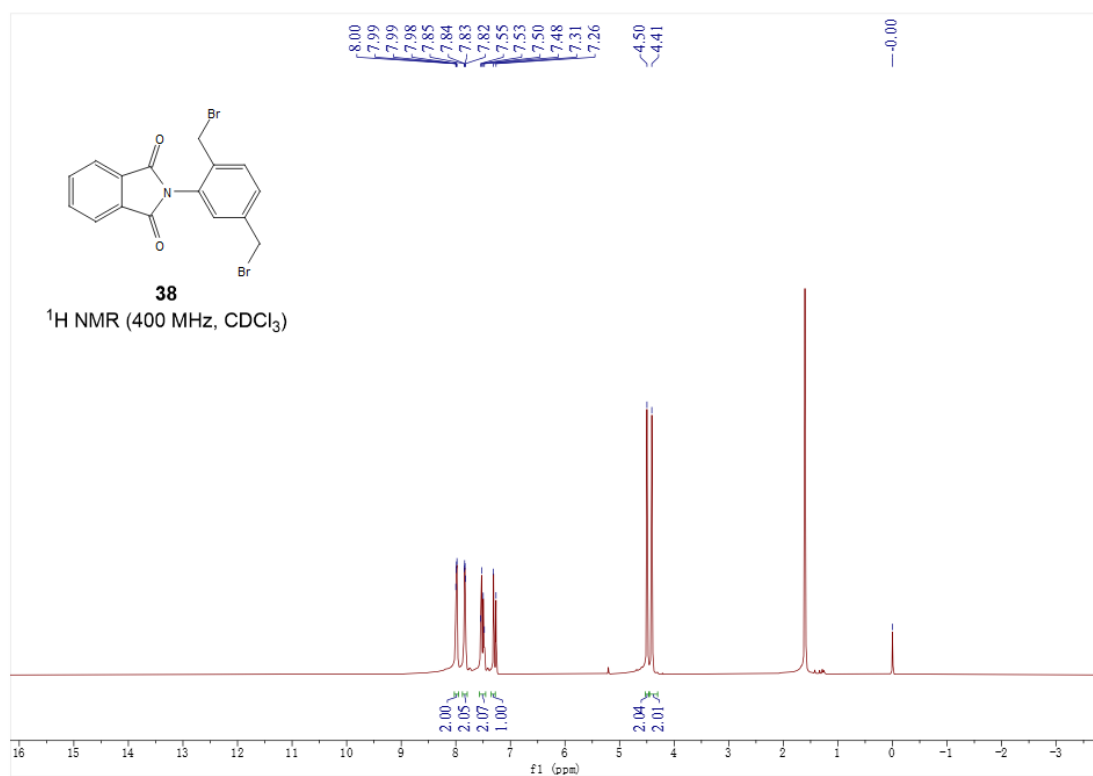
^1H NMR (400 MHz, CDCl_3) spectrum of **37**



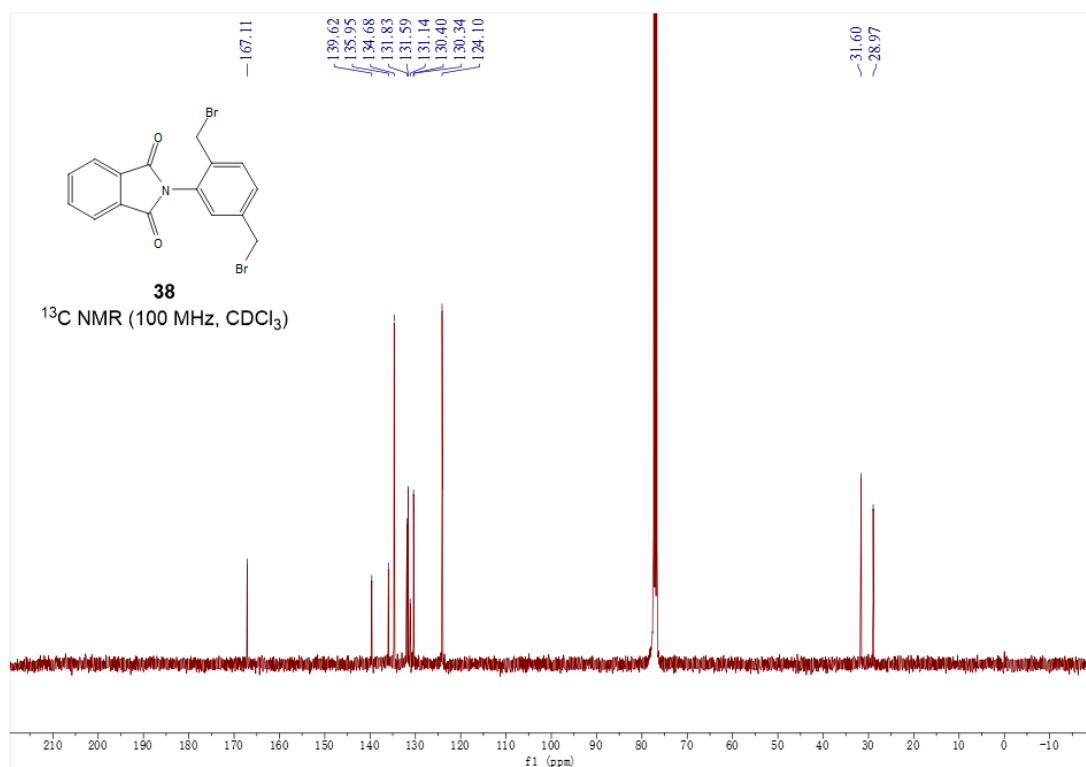
^{13}C NMR (100 MHz, CDCl_3) spectrum of **37**



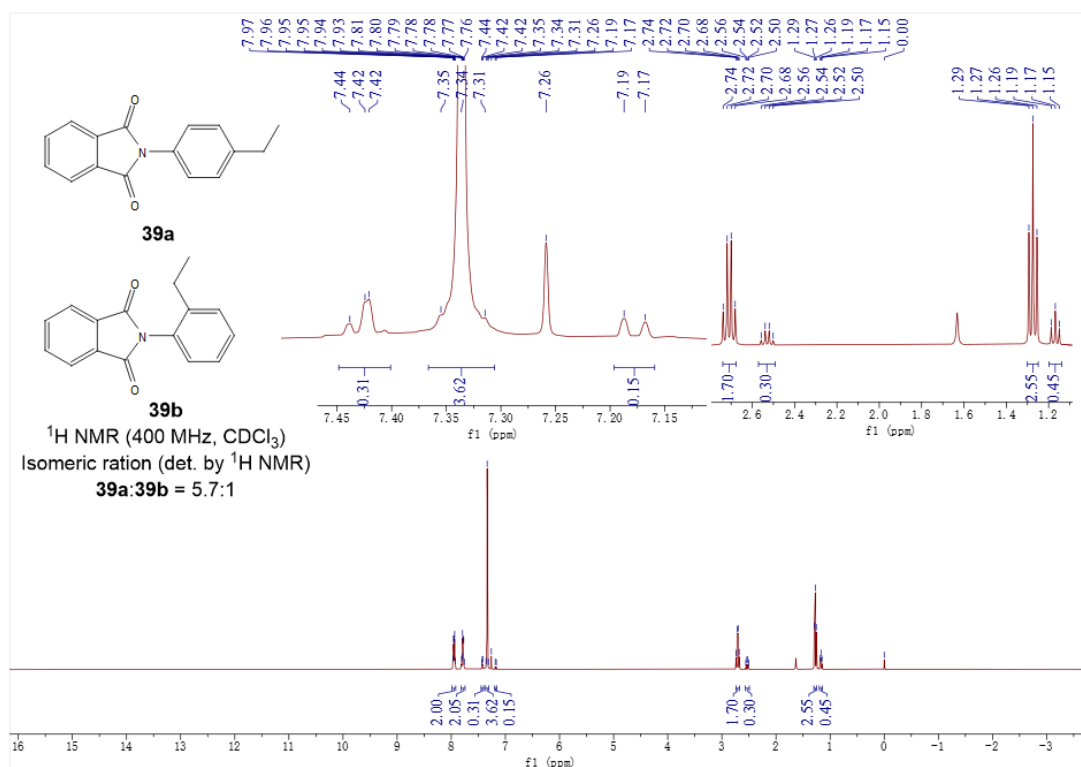
¹H NMR (400 MHz, CDCl₃) spectrum of **38**



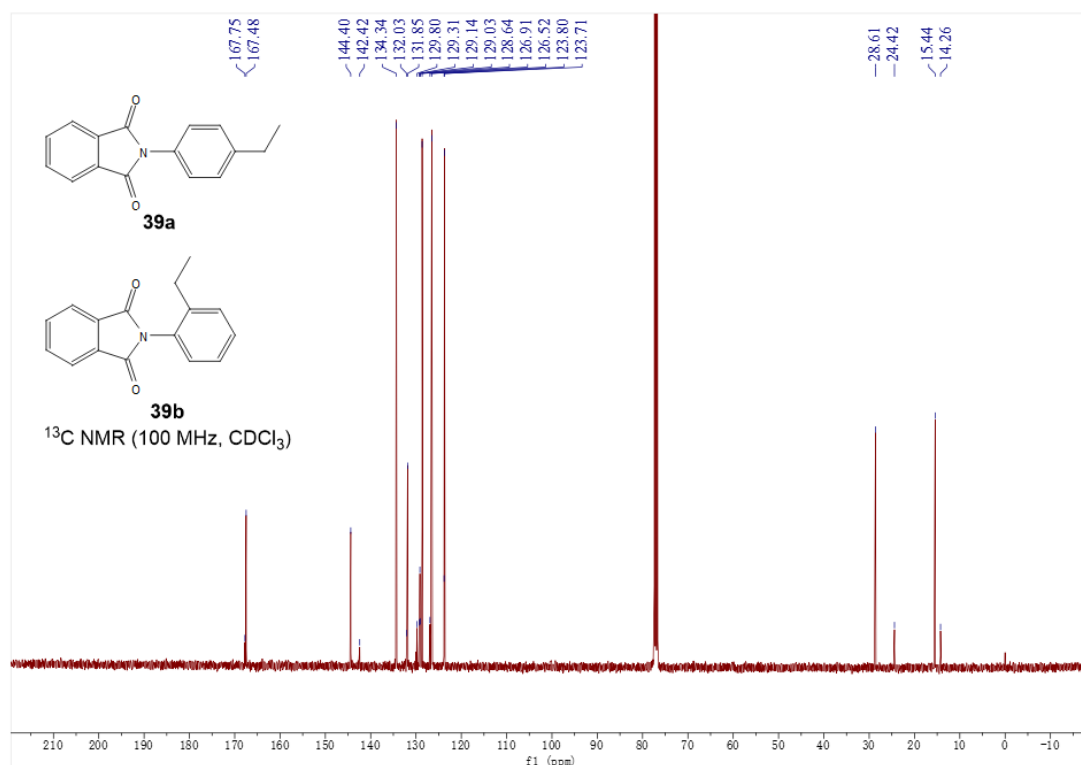
¹³C NMR (100 MHz, CDCl₃) spectrum of **38**



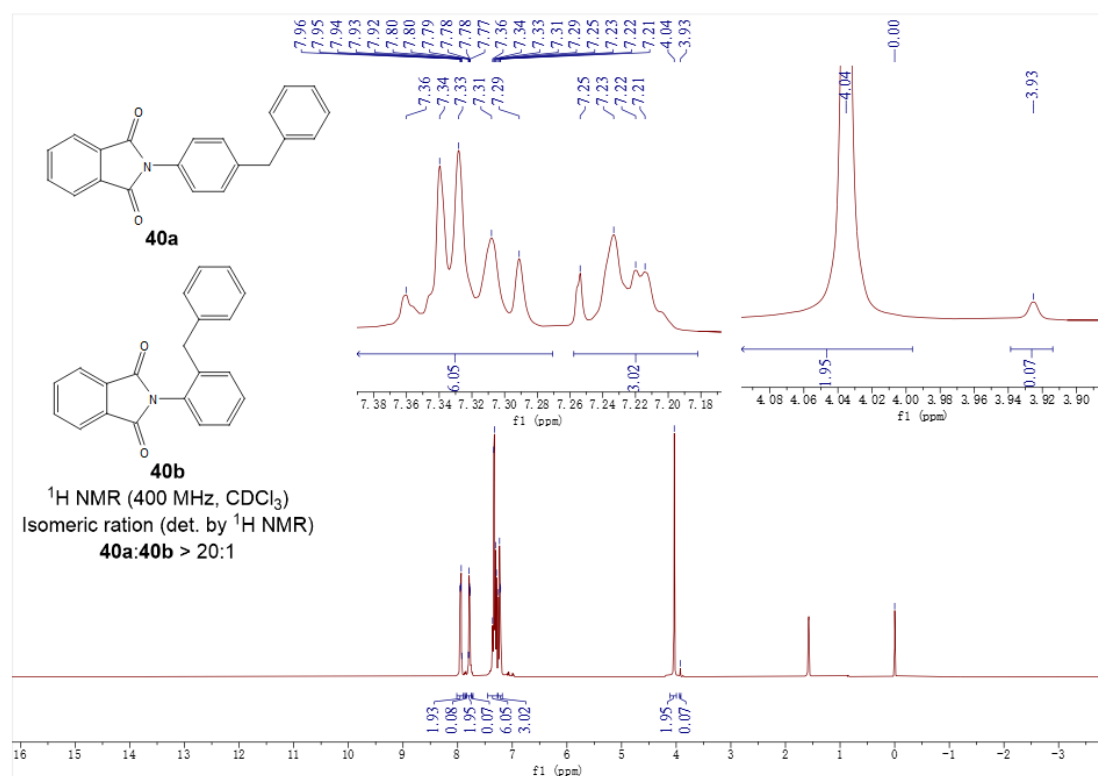
^1H NMR (400 MHz, CDCl_3) spectrum of **39**



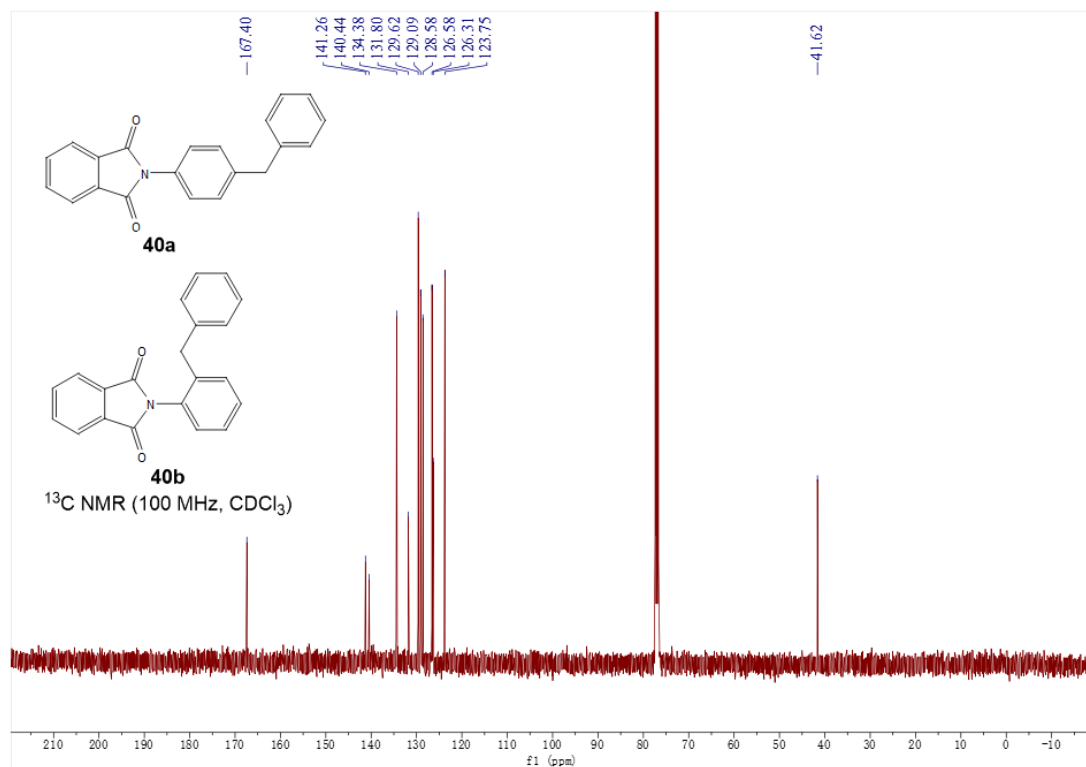
^{13}C NMR (100 MHz, CDCl_3) spectrum of **39**



¹H NMR (400 MHz, CDCl₃) spectrum of **40**



¹³C NMR (100 MHz, CDCl₃) spectrum of **40**



41a

41b

^1H NMR (400 MHz, CDCl_3)

Isomeric ration (det. by ^1H NMR)

41a:41b = 18:1

41a

C=Cc1ccc(cc1)N2C(=O)c3ccccc3C2=O

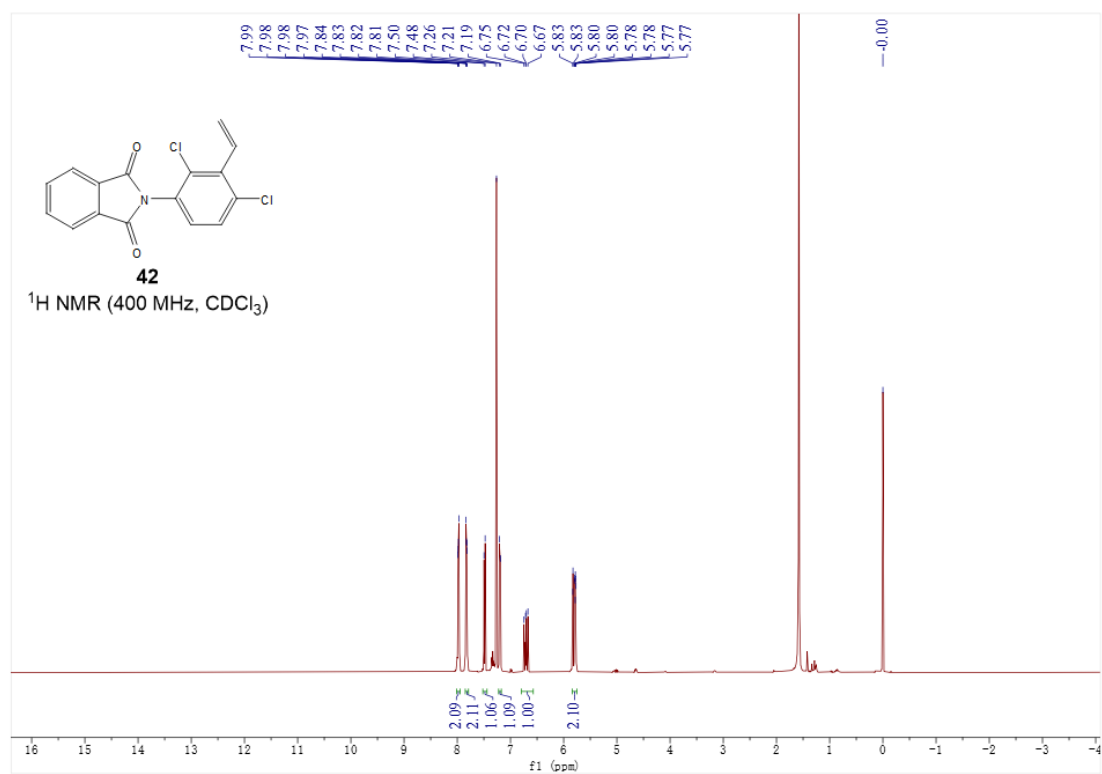
41b

C=Cc1ccccc1N2C(=O)c3ccccc3C2=O

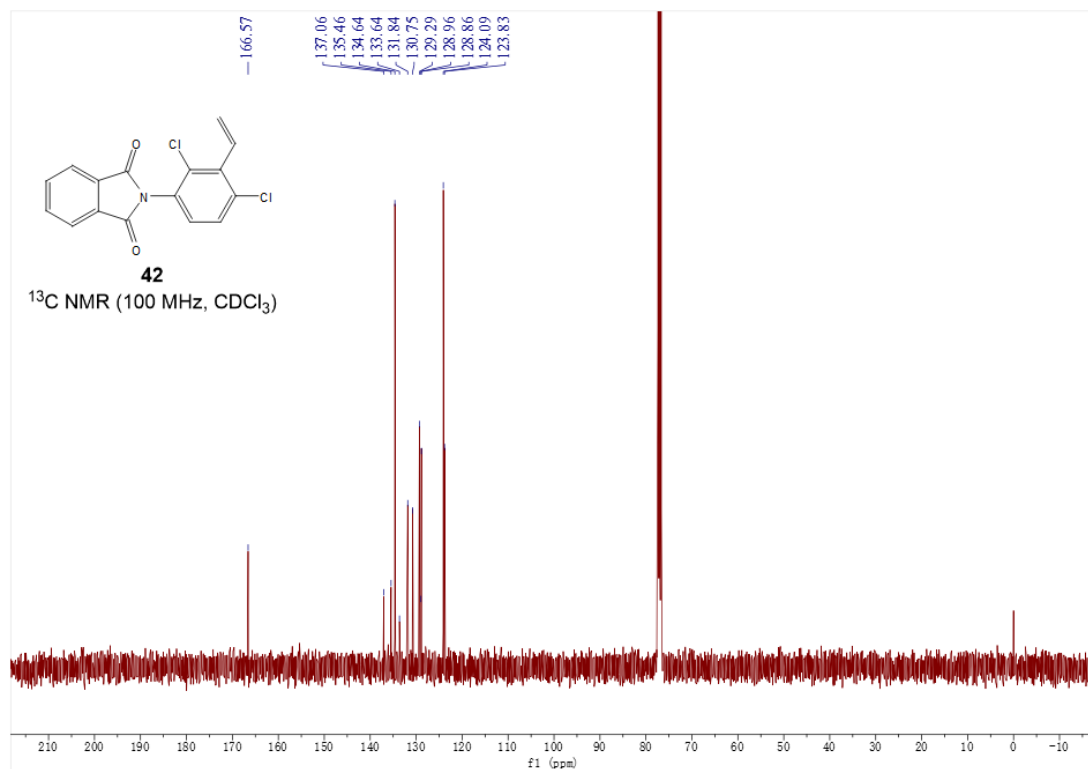
¹³C NMR (100 MHz, CDCl₃)

Chemical shift values (ppm): 167.27, 137.42, 135.98, 134.45, 131.77, 130.99, 126.86, 126.55, 123.79, 115.03.

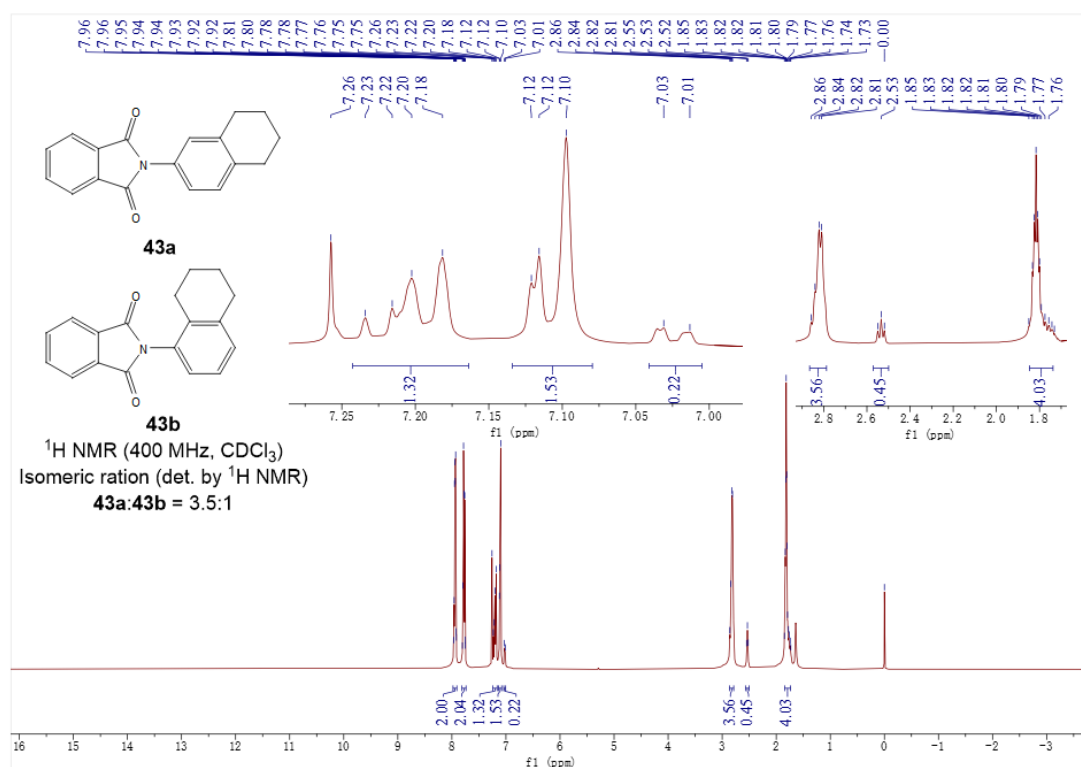
^1H NMR (400 MHz, CDCl_3) spectrum of **42**



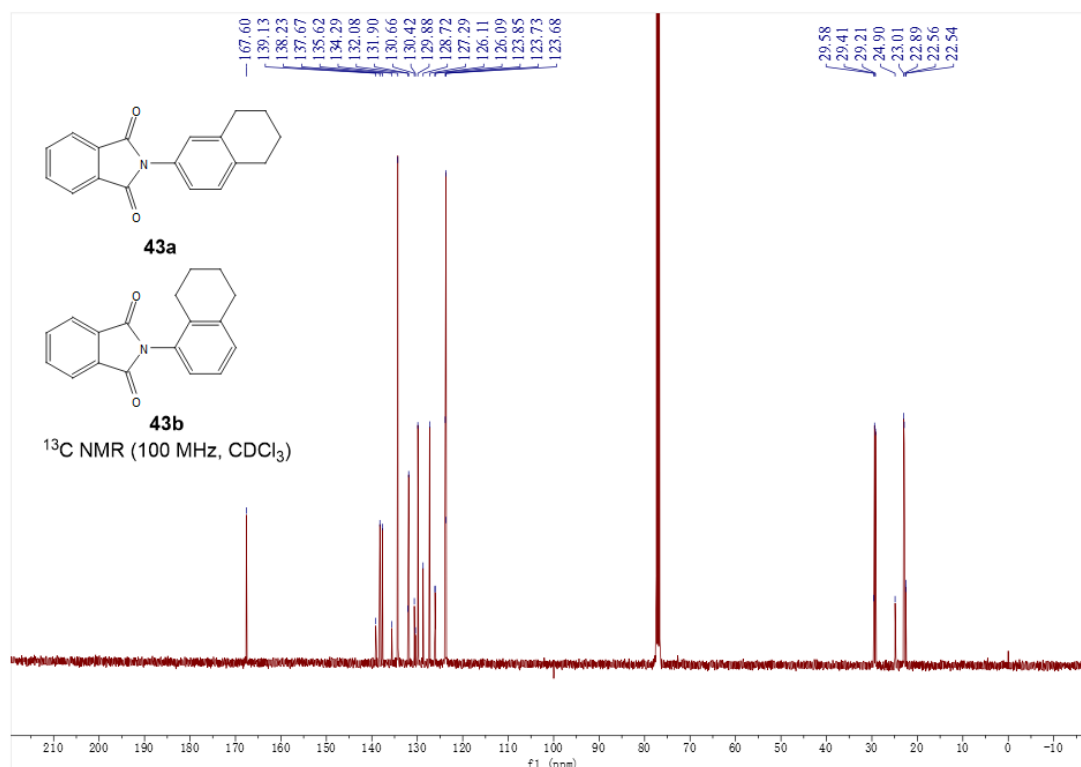
^{13}C NMR (100 MHz, CDCl_3) spectrum of **42**



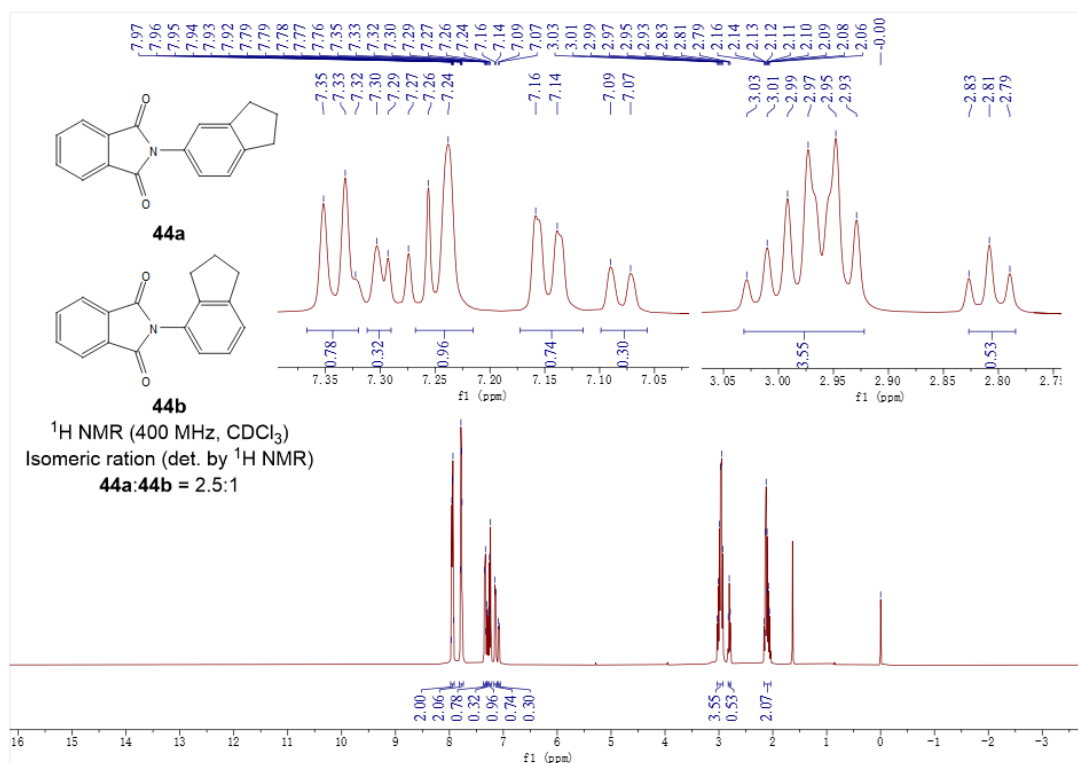
¹H NMR (400 MHz, CDCl₃) spectrum of **43**



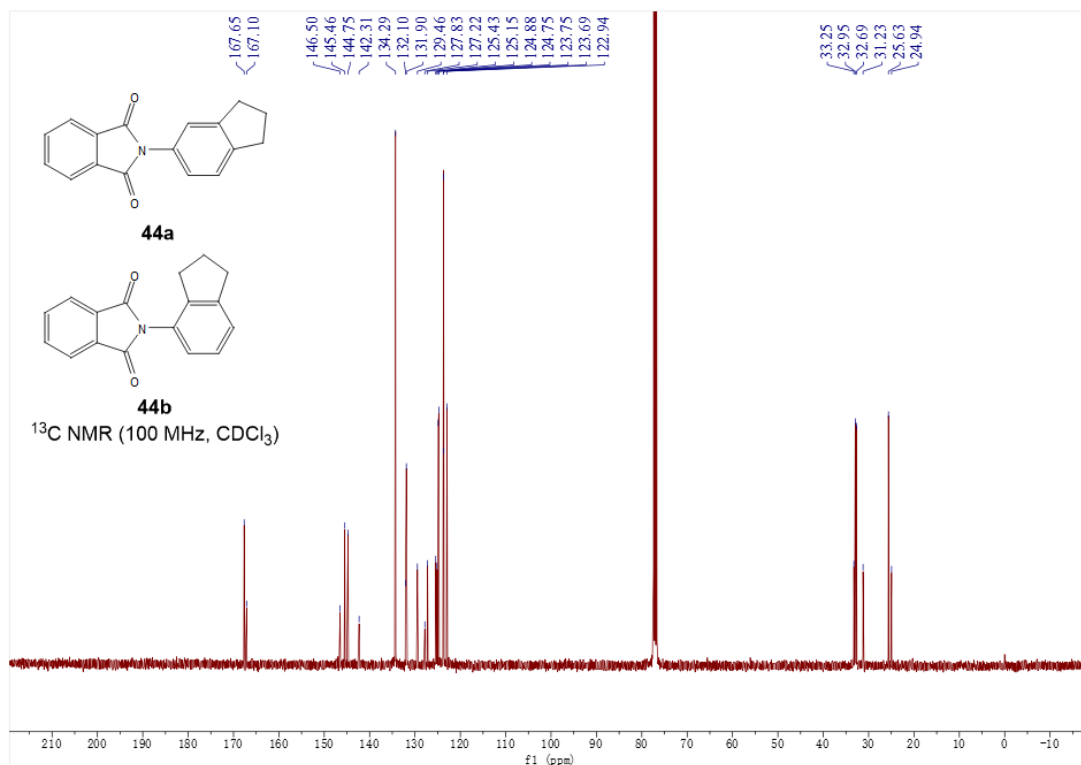
¹³C NMR (100 MHz, CDCl₃) spectrum of **43**



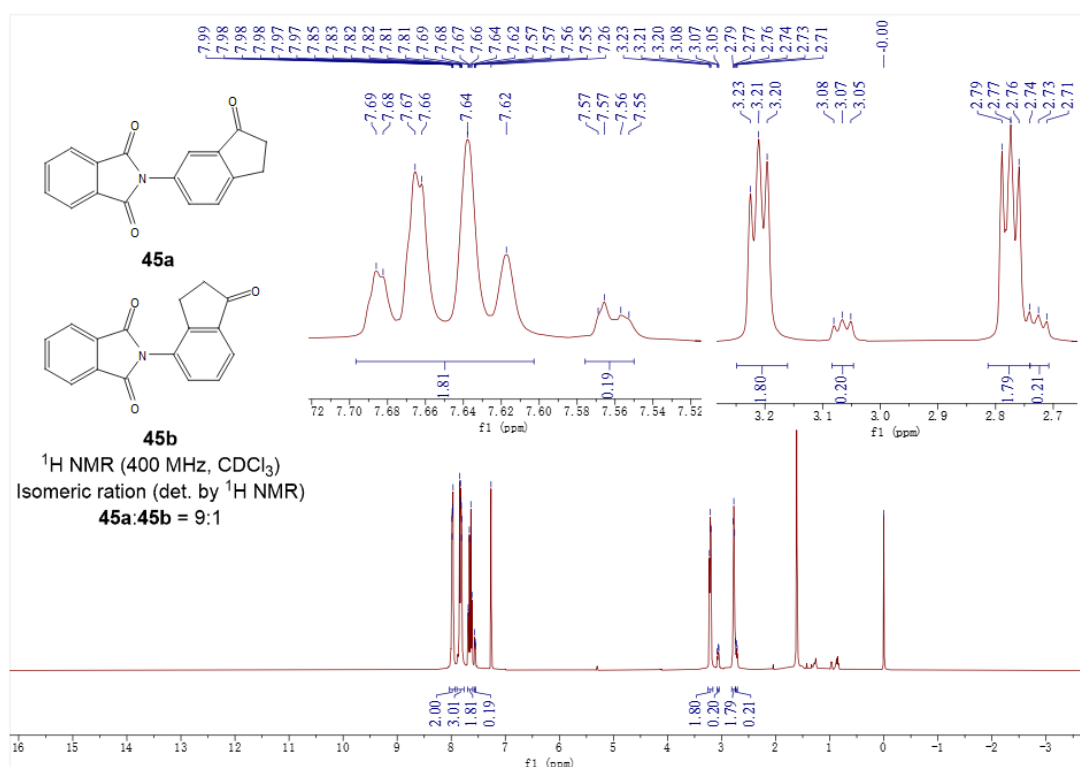
^1H NMR (400 MHz, CDCl_3) spectrum of **44**



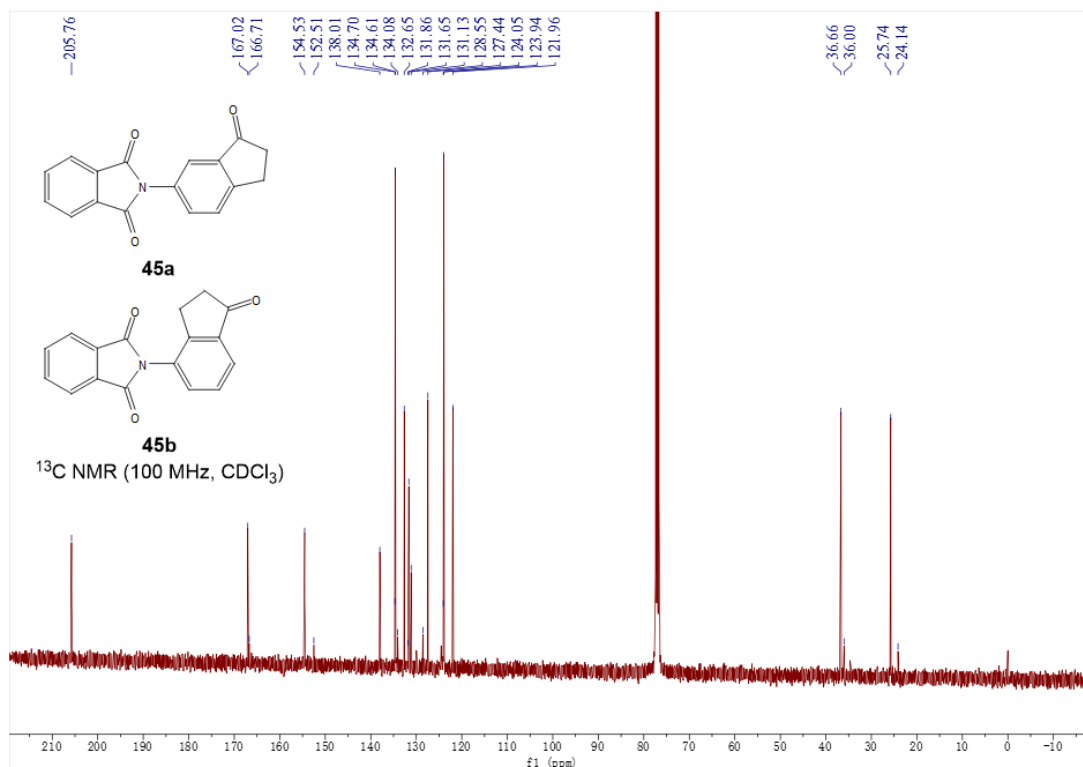
^{13}C NMR (100 MHz, CDCl_3) spectrum of **44**



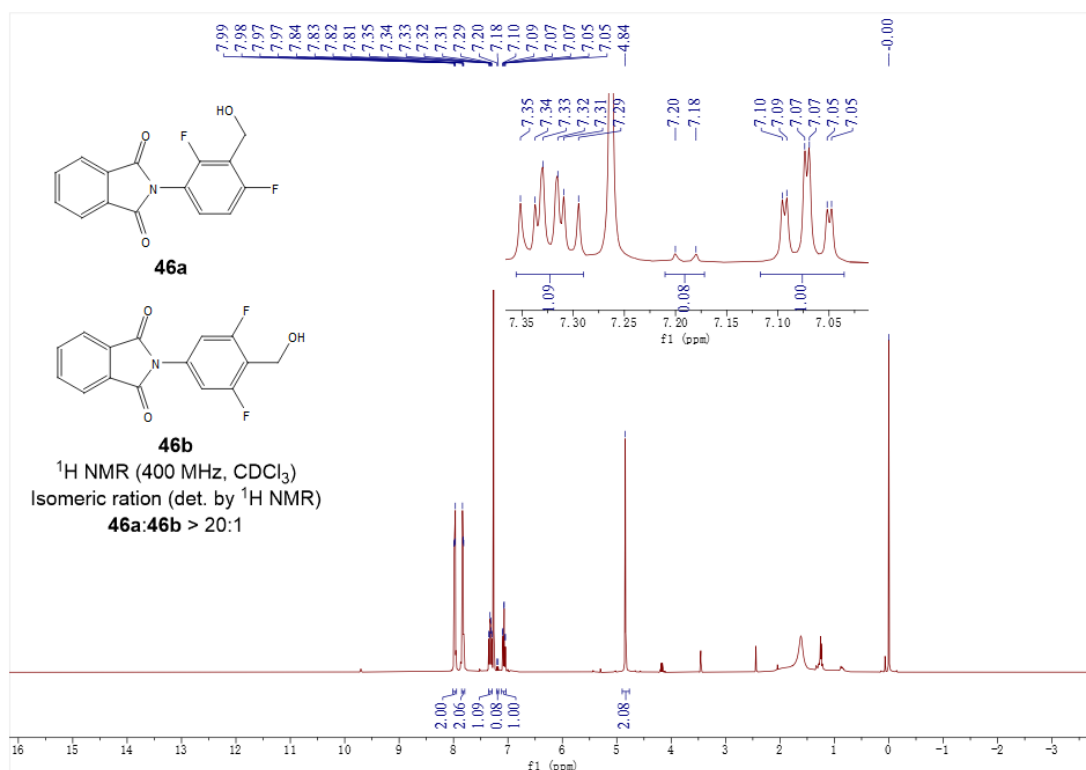
^1H NMR (400 MHz, CDCl_3) spectrum of **45**



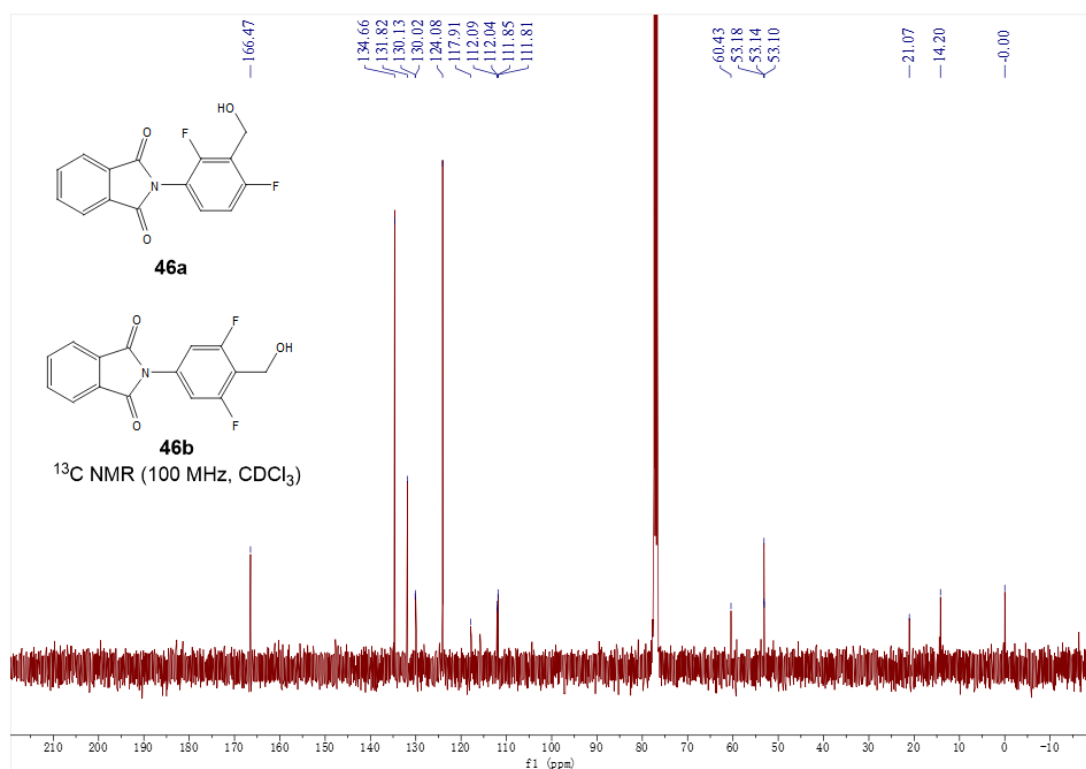
^{13}C NMR (100 MHz, CDCl_3) spectrum of **45**



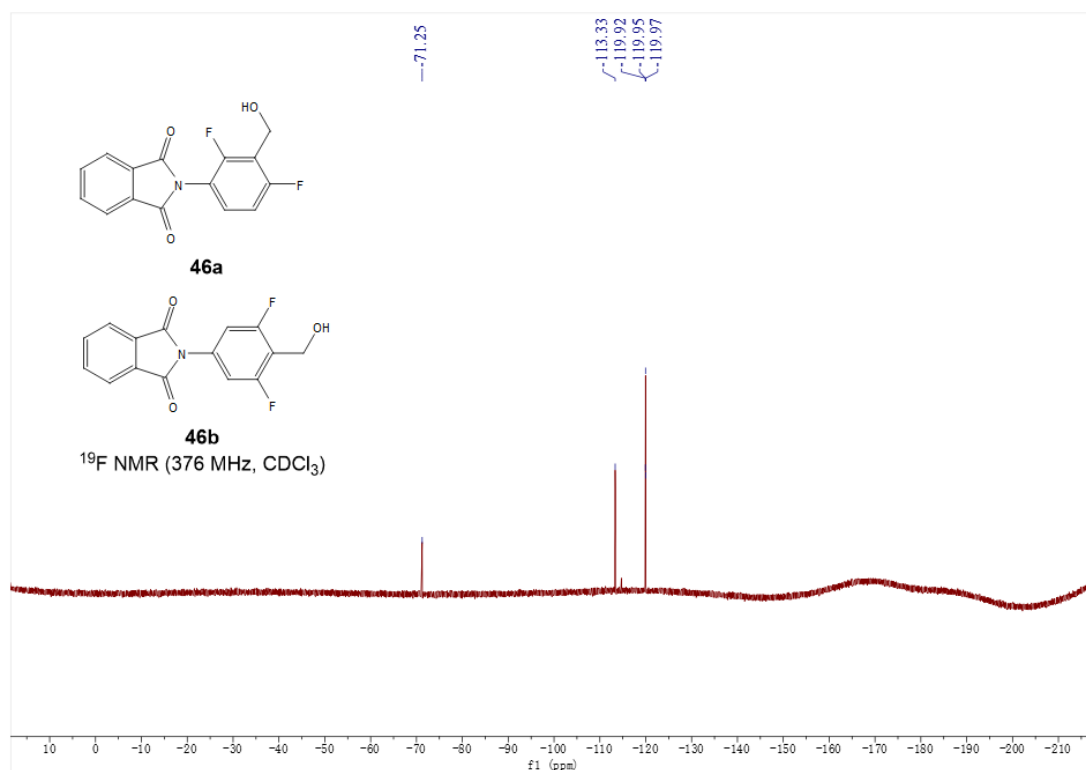
^1H NMR (400 MHz, CDCl_3) spectrum of **46**



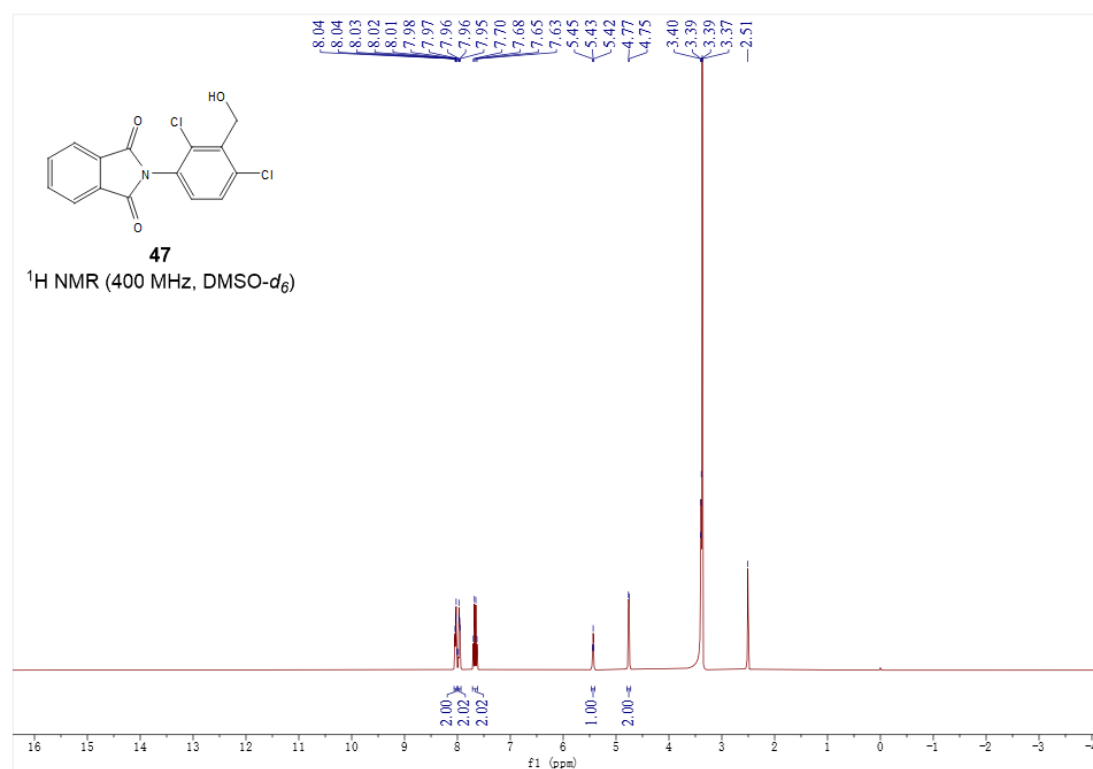
^{13}C NMR (100 MHz, CDCl_3) spectrum of **46**



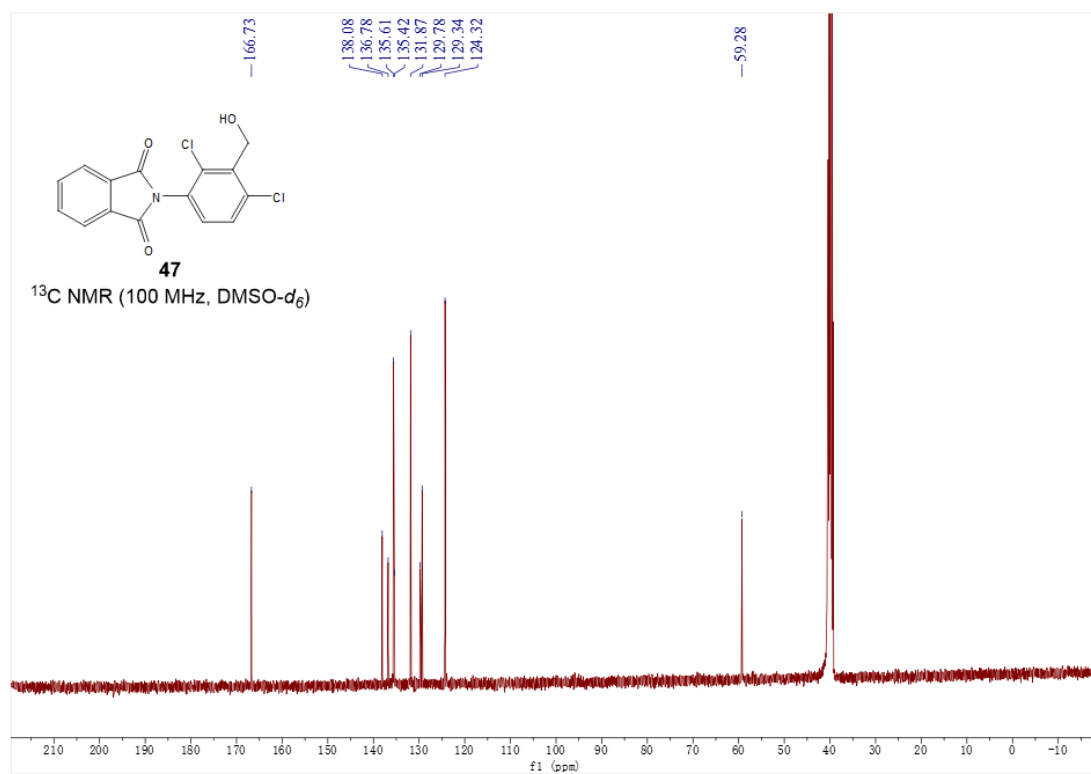
^{19}F NMR (376 MHz, CDCl_3) spectrum of **46**



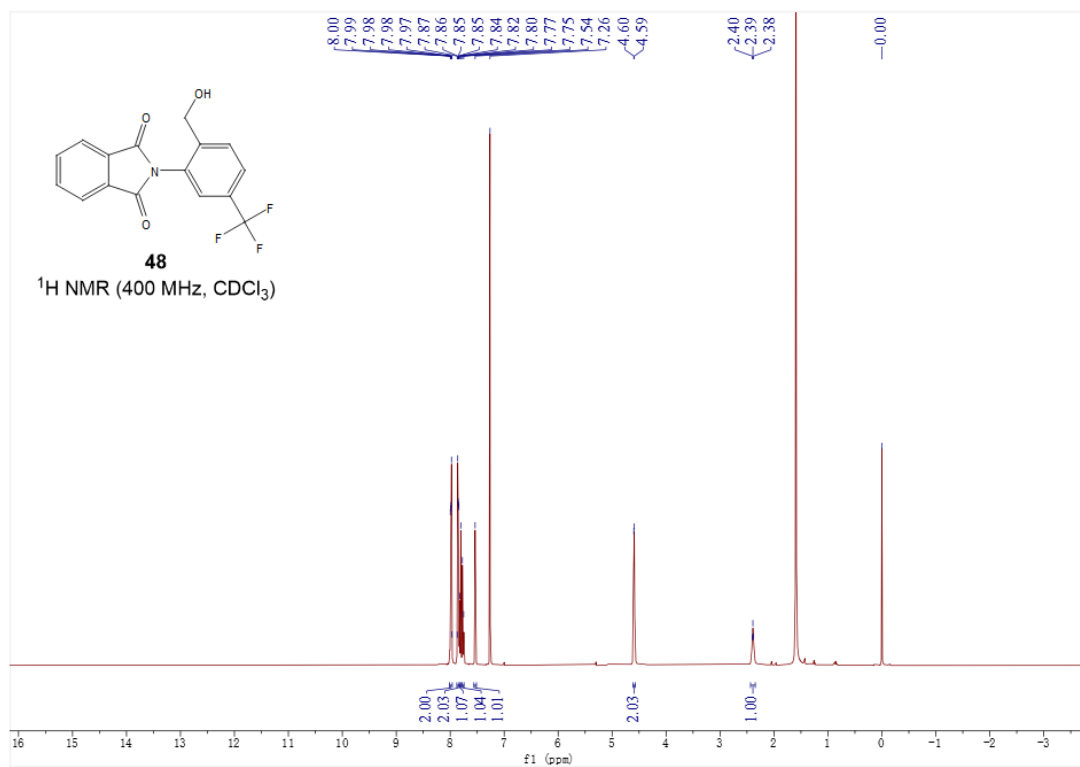
^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of **47**



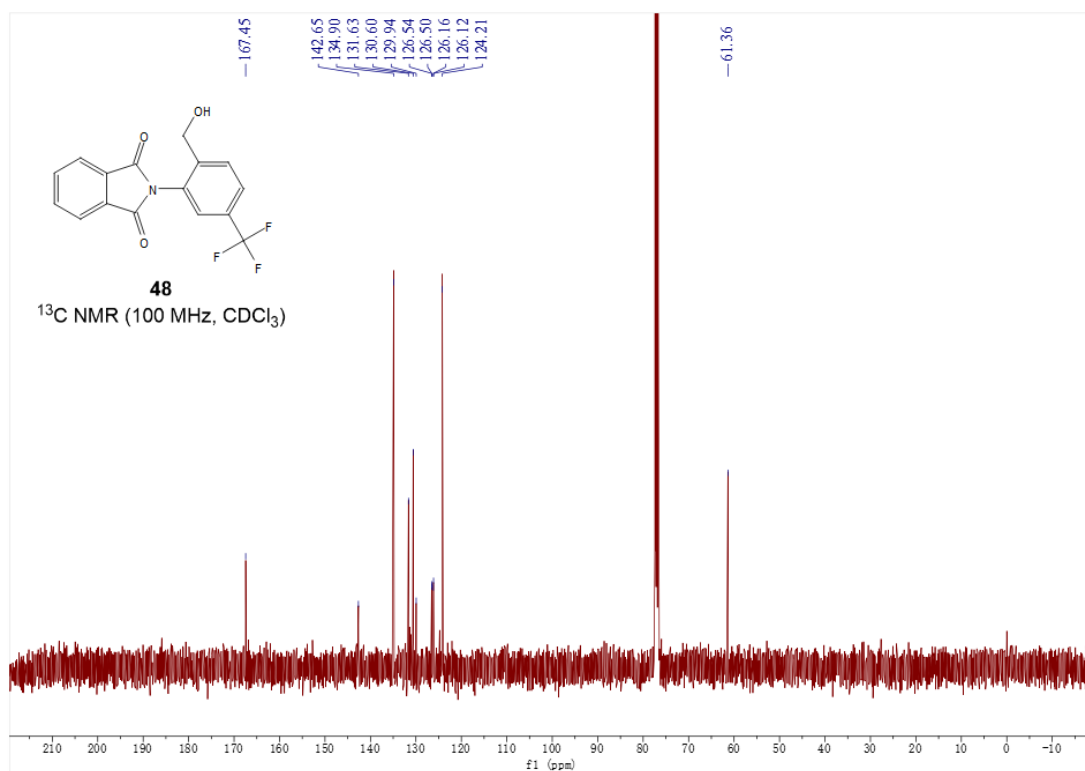
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **47**



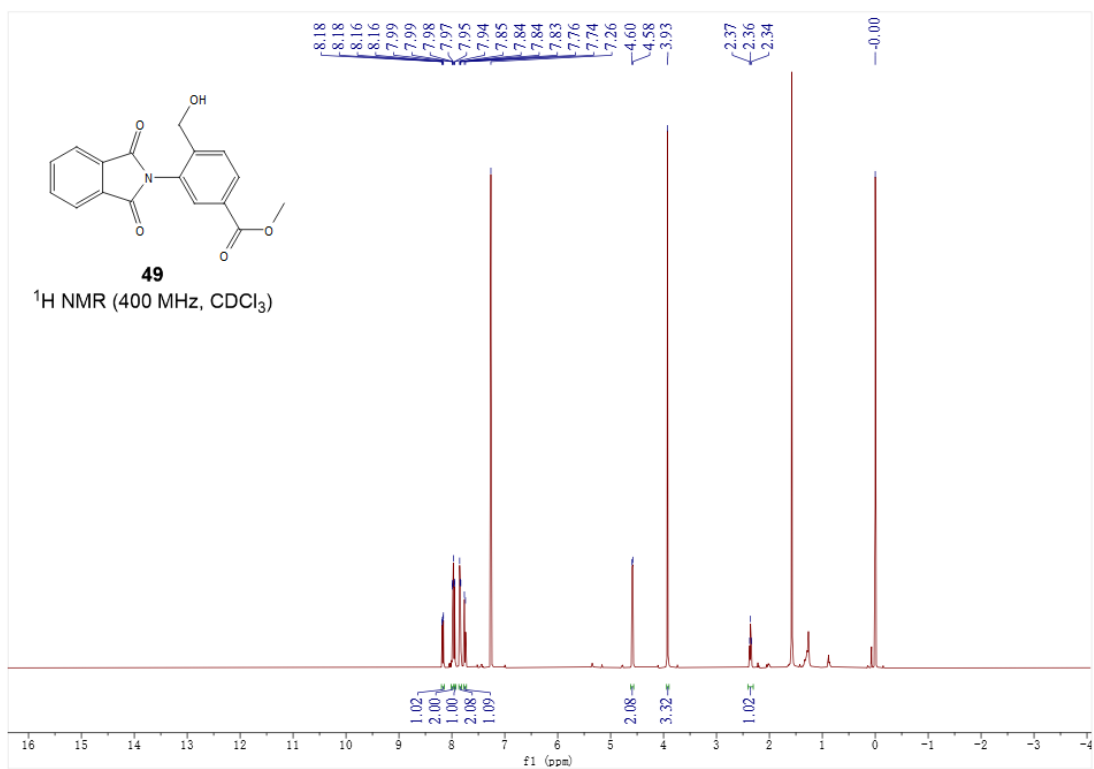
^1H NMR (400 MHz, CDCl_3) spectrum of **48**



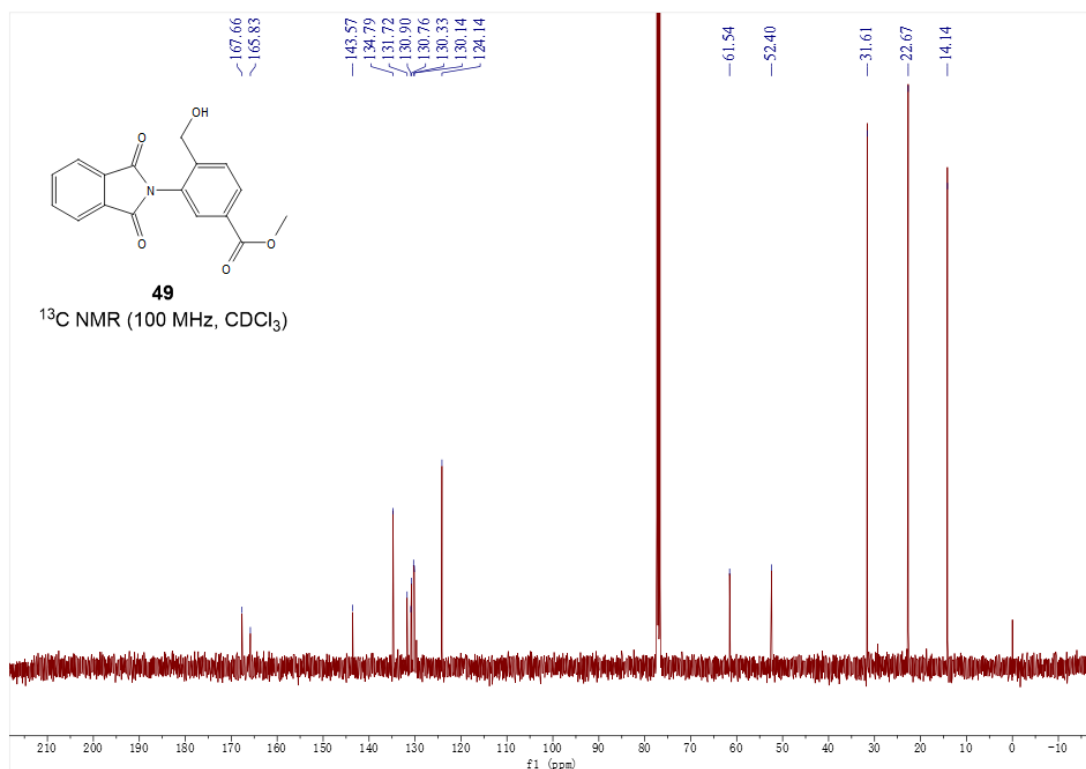
^{13}C NMR (100 MHz, CDCl_3) spectrum of **48**



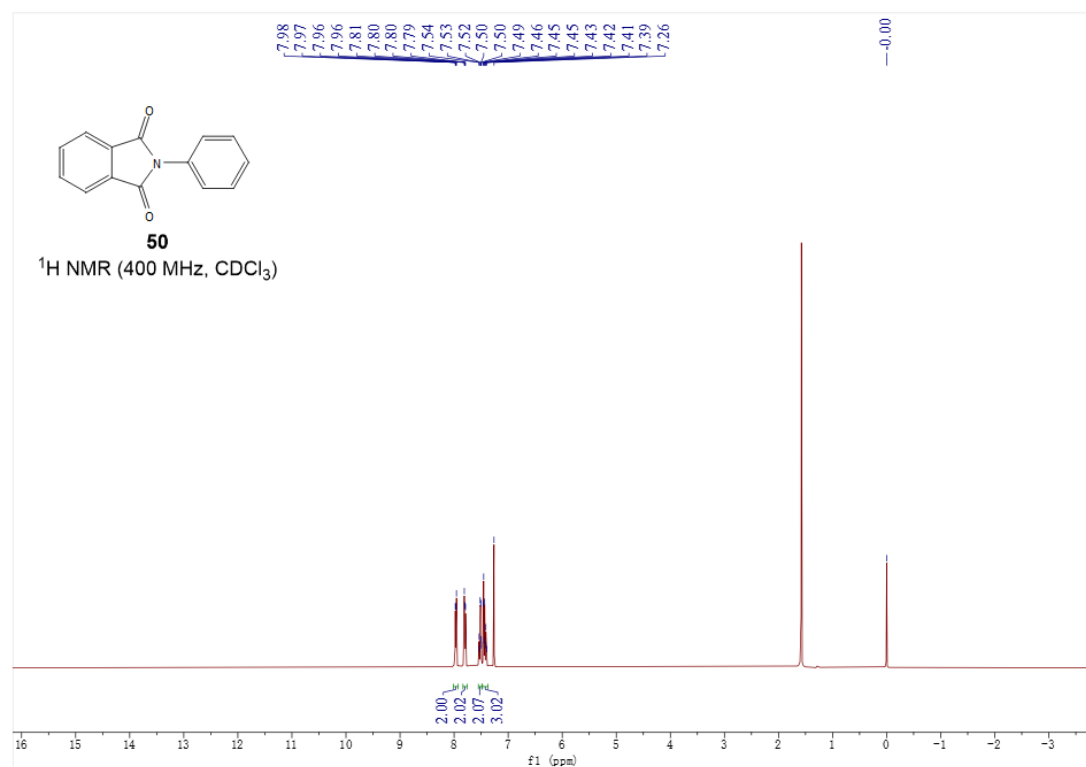
^1H NMR (400 MHz, CDCl_3) spectrum of **49**



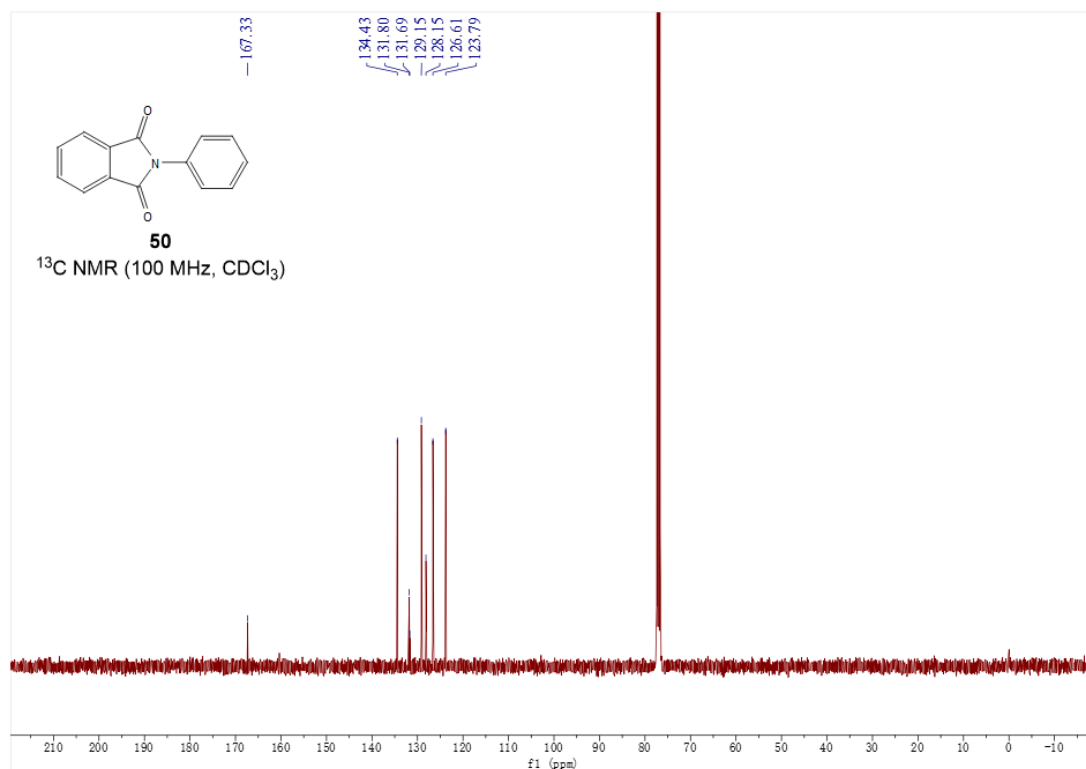
^{13}C NMR (100 MHz, CDCl_3) spectrum of **49**



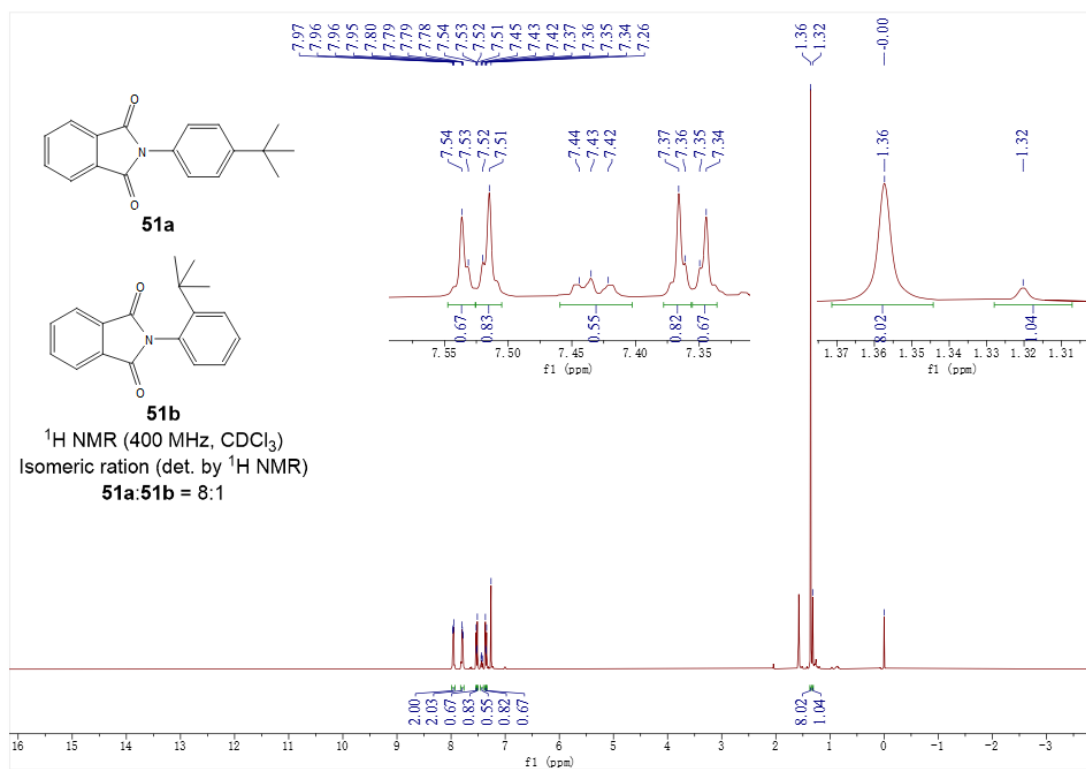
^1H NMR (400 MHz, CDCl_3) spectrum of **50**



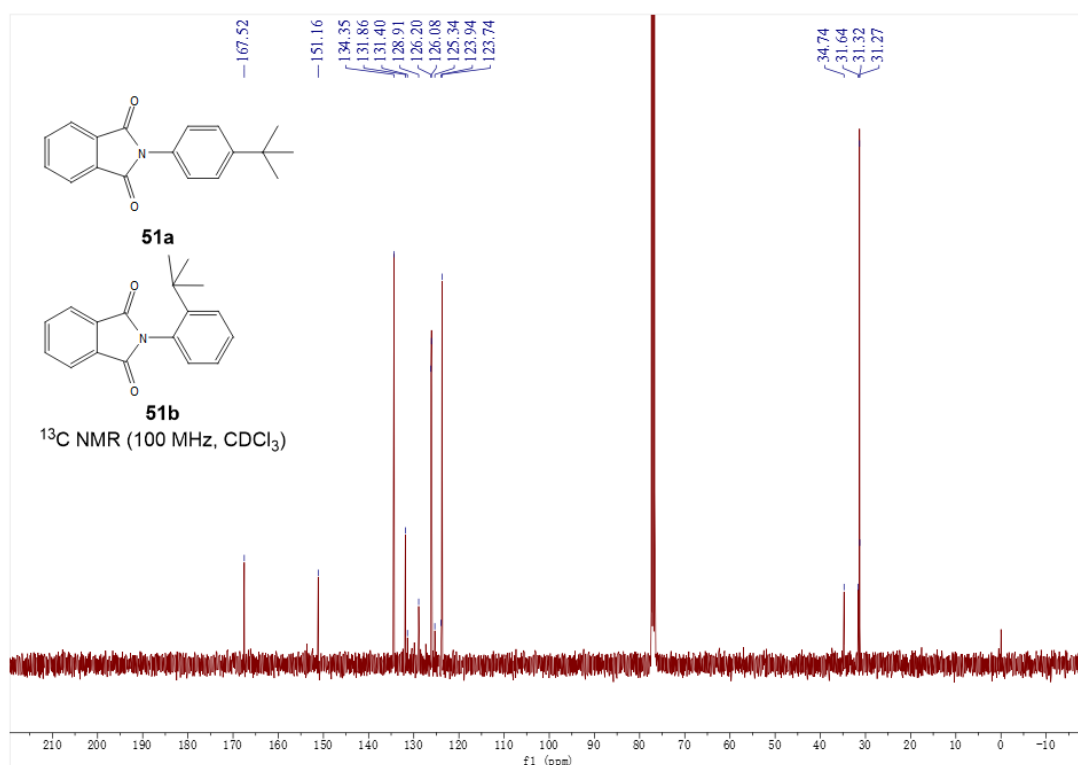
^{13}C NMR (100 MHz, CDCl_3) spectrum of **50**



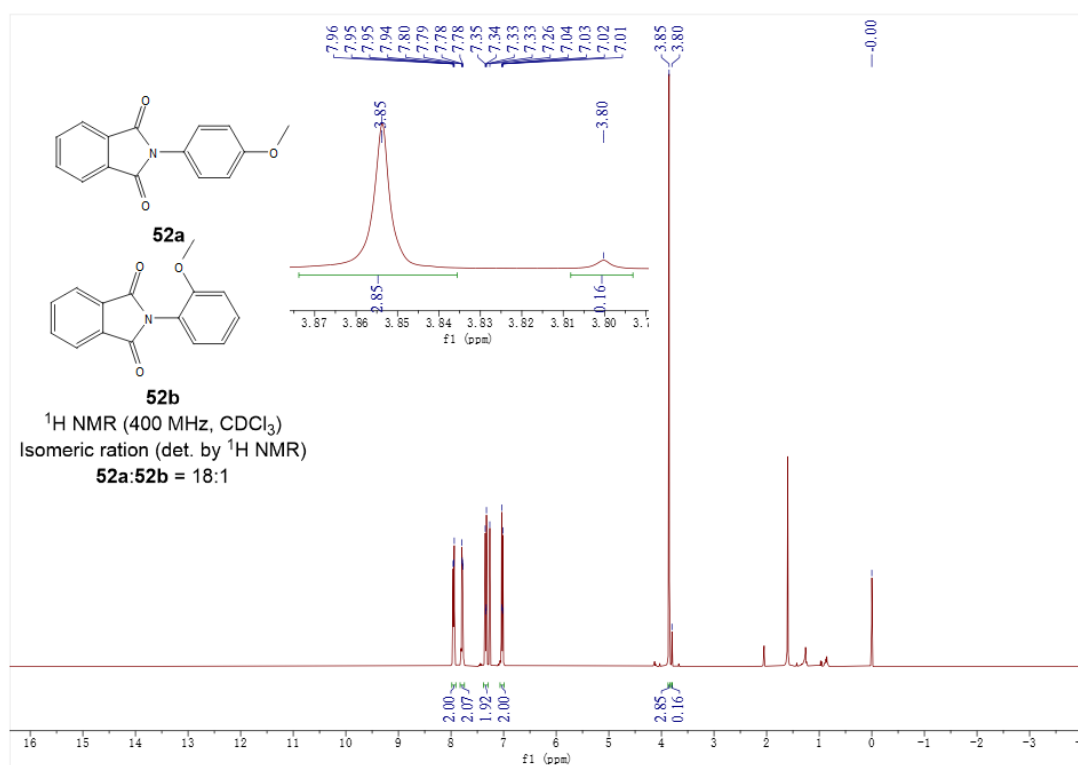
^1H NMR (400 MHz, CDCl_3) spectrum of **51**



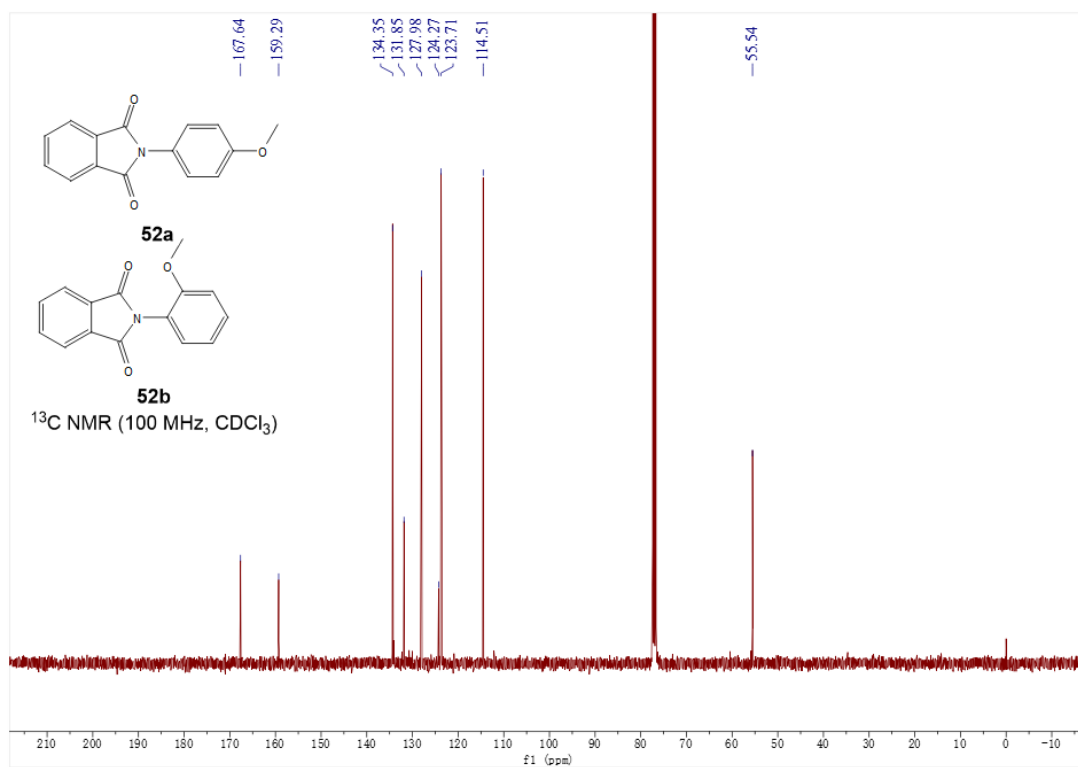
^{13}C NMR (100 MHz, CDCl_3) spectrum of **51**



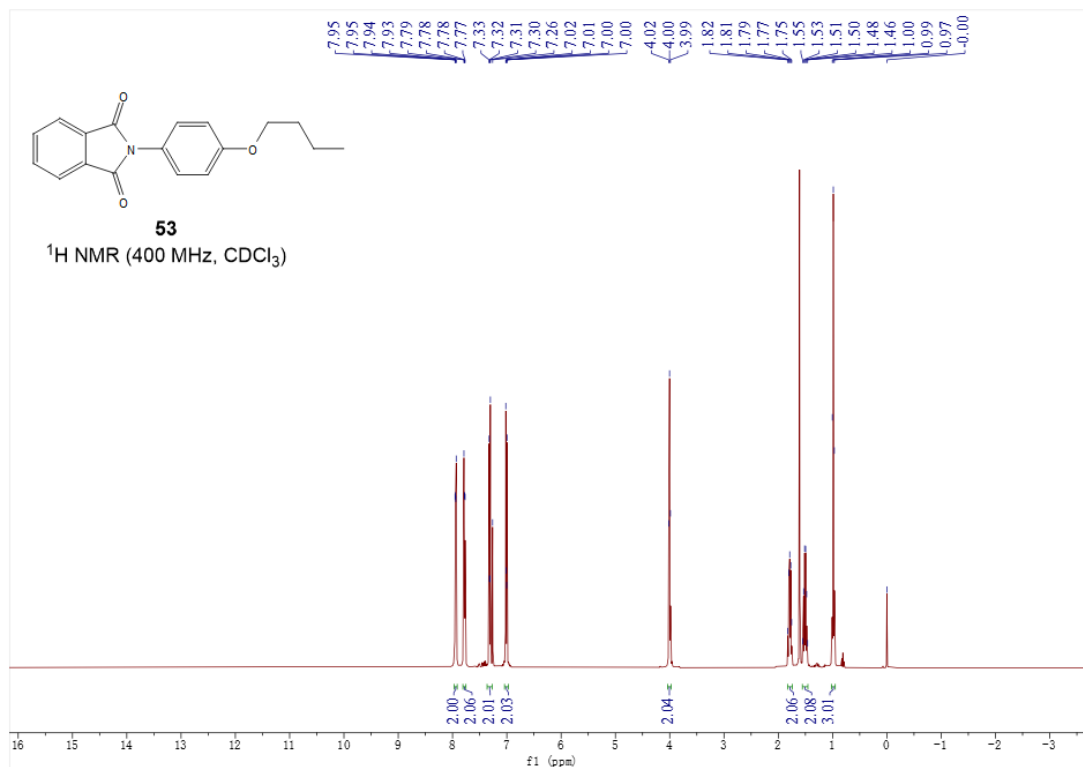
^1H NMR (400 MHz, CDCl_3) spectrum of **52**



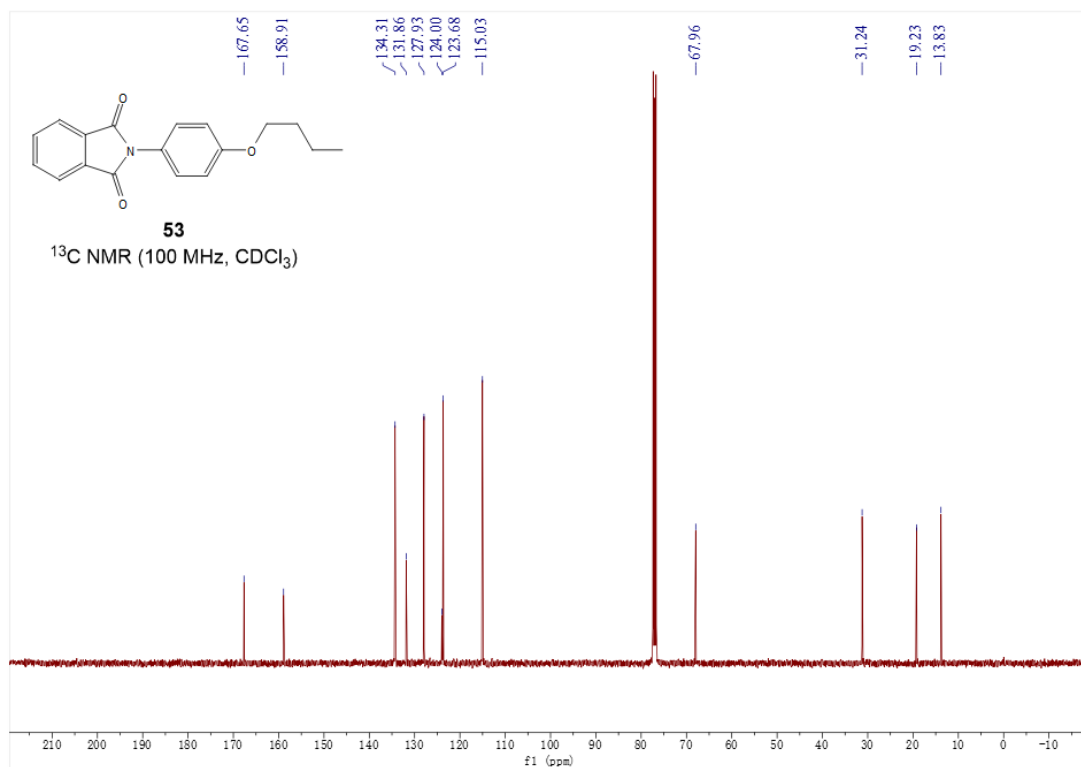
^{13}C NMR (100 MHz, CDCl_3) spectrum of **52**



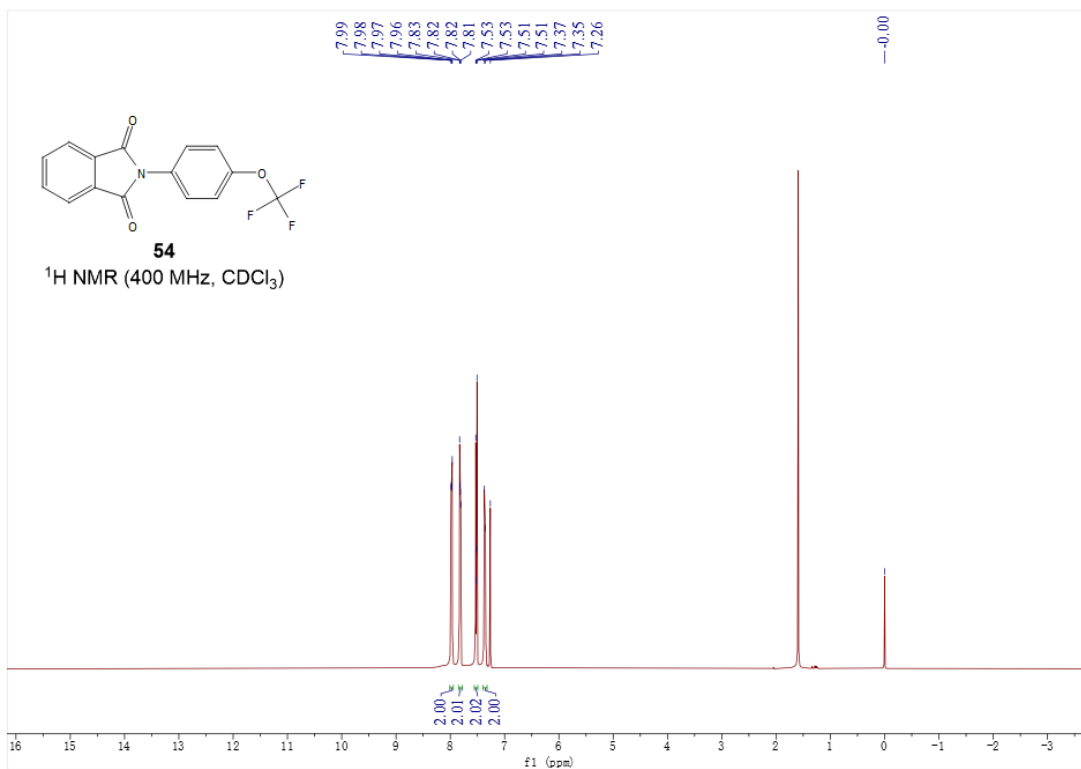
^1H NMR (400 MHz, CDCl_3) spectrum of **53**



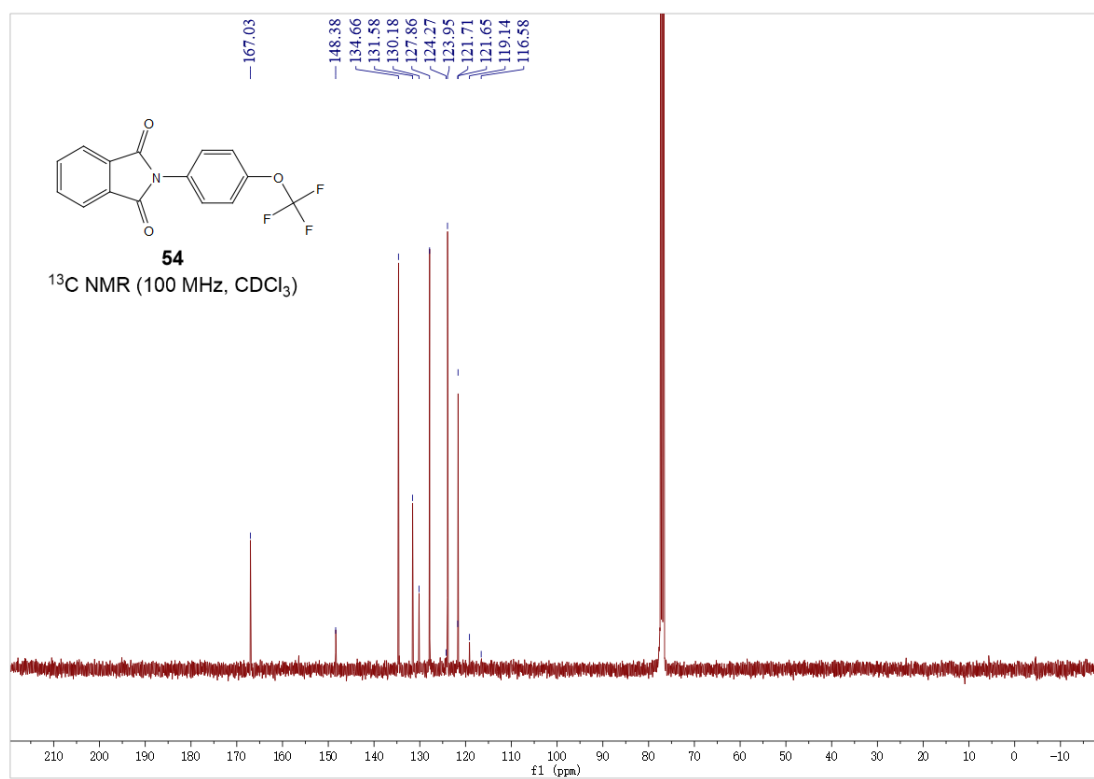
^{13}C NMR (100 MHz, CDCl_3) spectrum of **53**



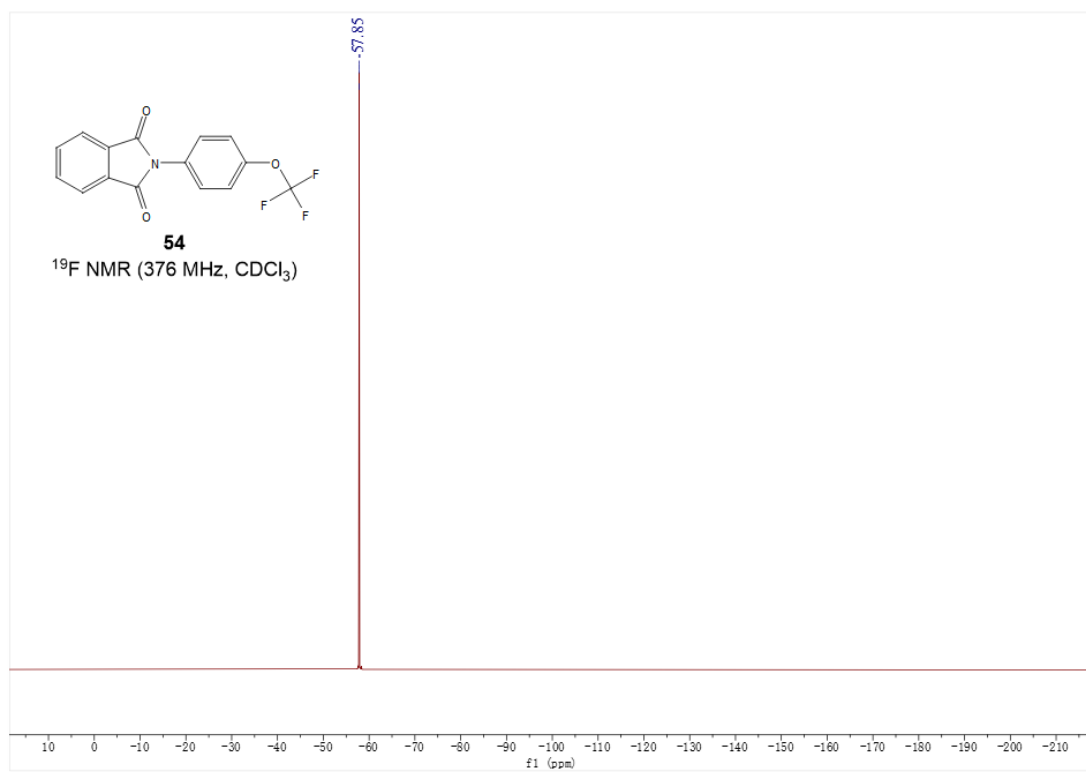
^1H NMR (400 MHz, CDCl_3) spectrum of **54**



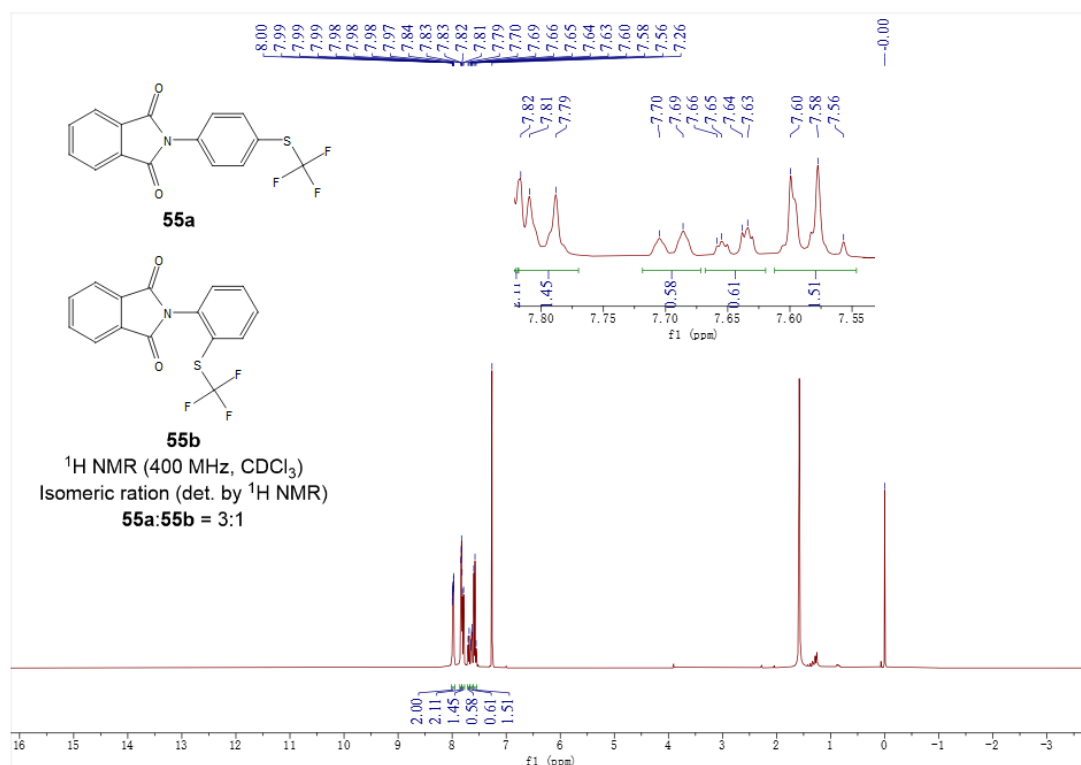
^{13}C NMR (100 MHz, CDCl_3) spectrum of **54**



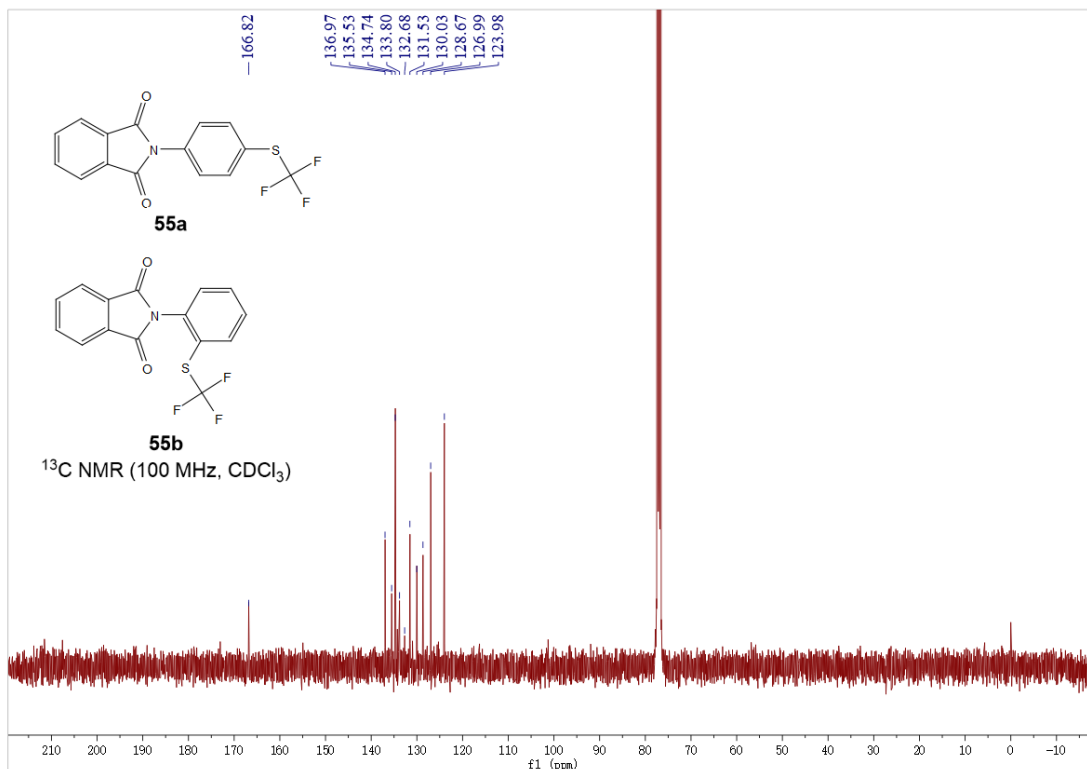
^{19}F NMR (376 MHz, CDCl_3) spectrum of **54**



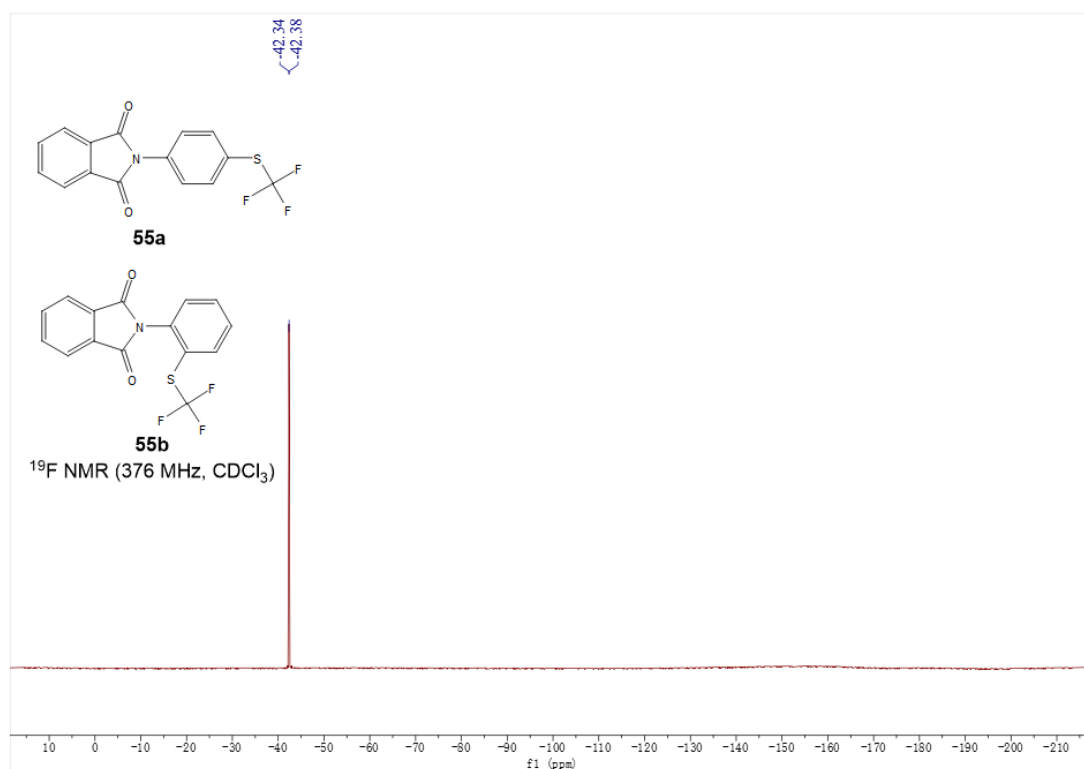
¹H NMR (400 MHz, CDCl₃) spectrum of **55**



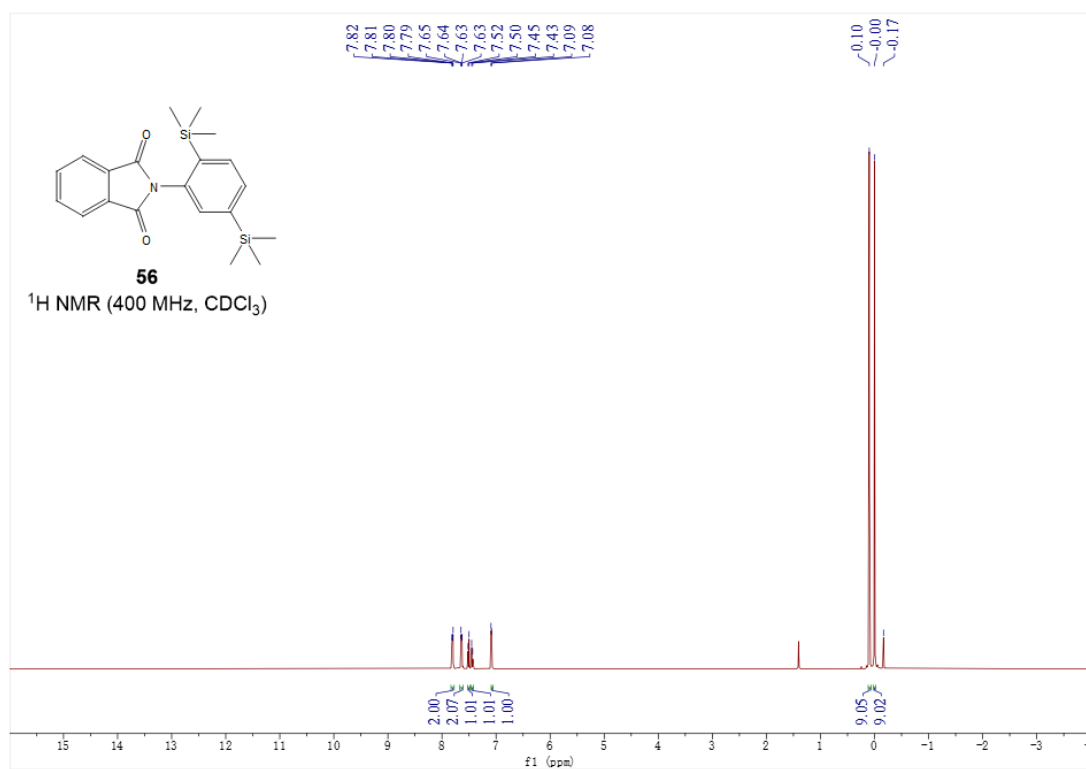
¹³C NMR (100 MHz, CDCl₃) spectrum of **55**



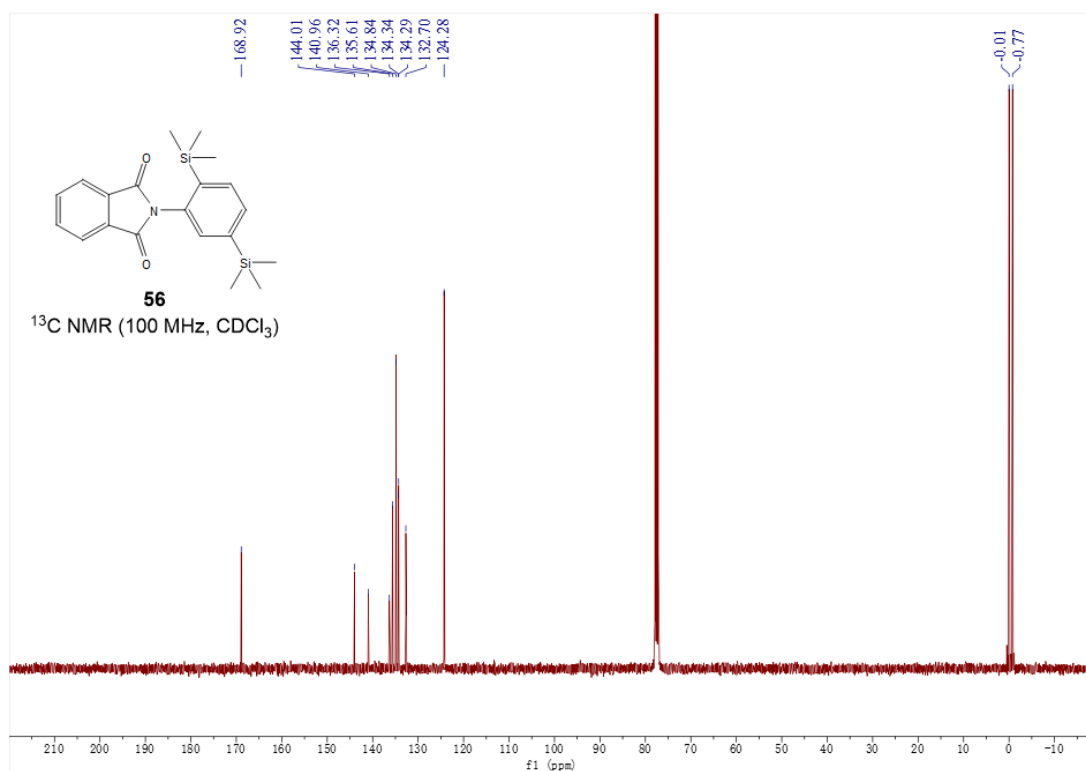
^{19}F NMR (376 MHz, CDCl_3) spectrum of **55**



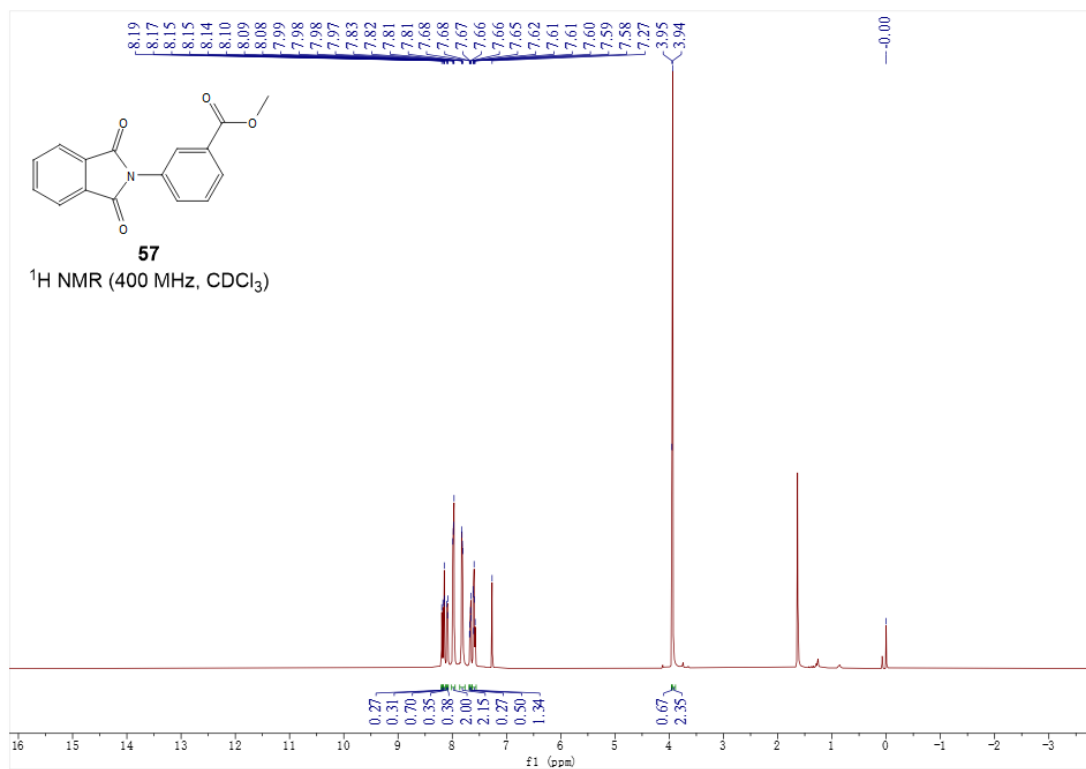
^1H NMR (400 MHz, CDCl_3) spectrum of **56**



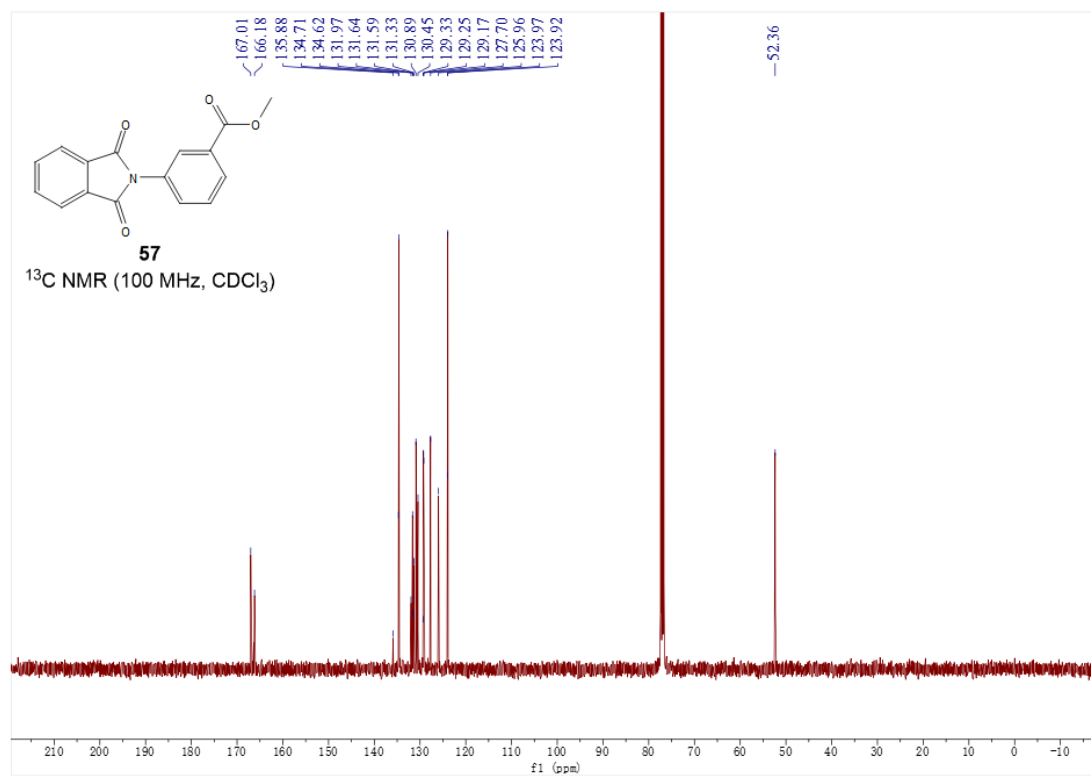
^{13}C NMR (100 MHz, CDCl_3) spectrum of **56**



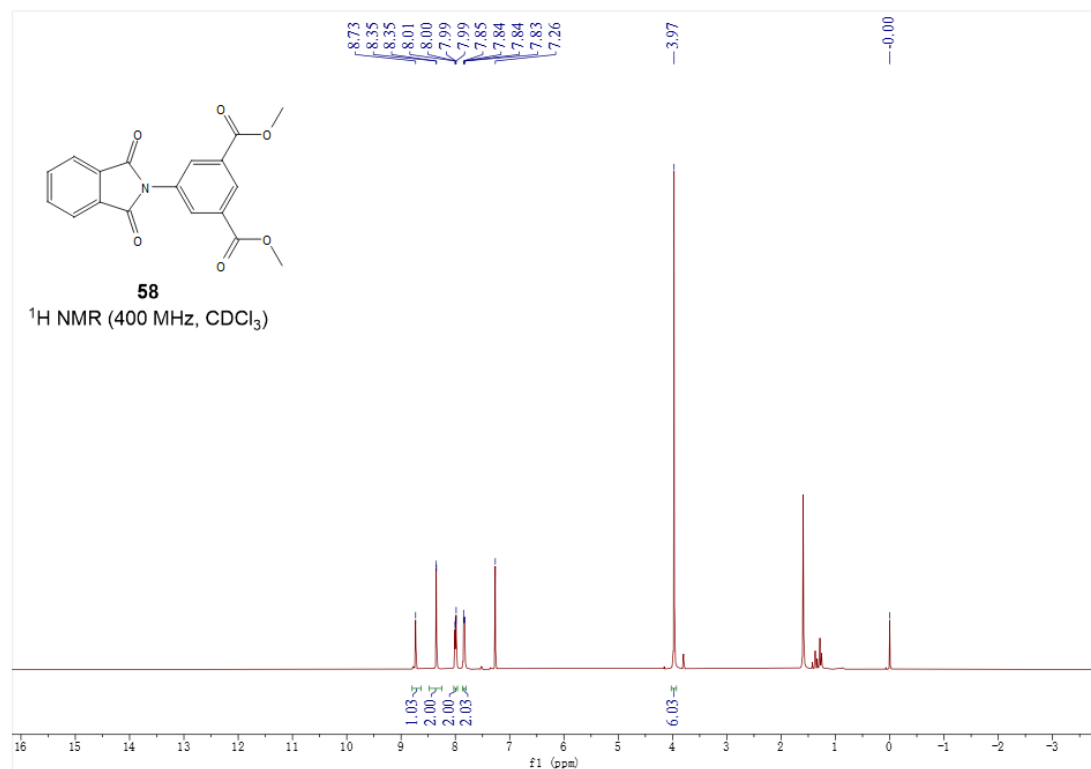
^1H NMR (400 MHz, CDCl_3) spectrum of **57**



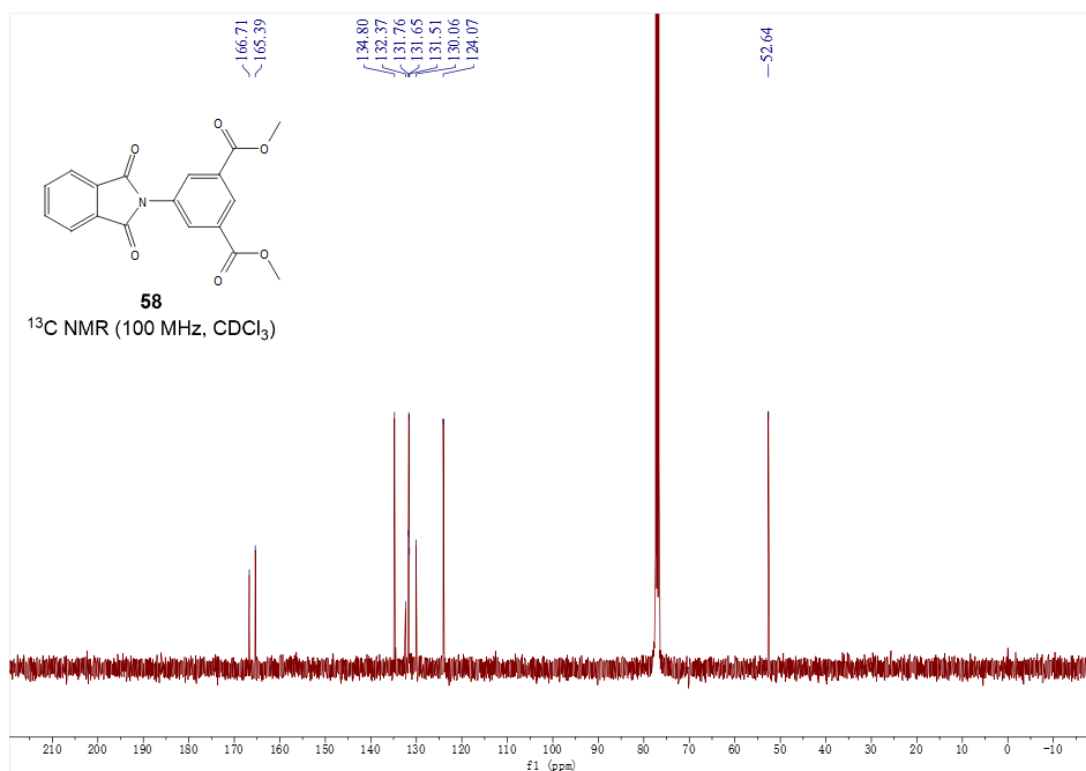
^{13}C NMR (100 MHz, CDCl_3) spectrum of **57**



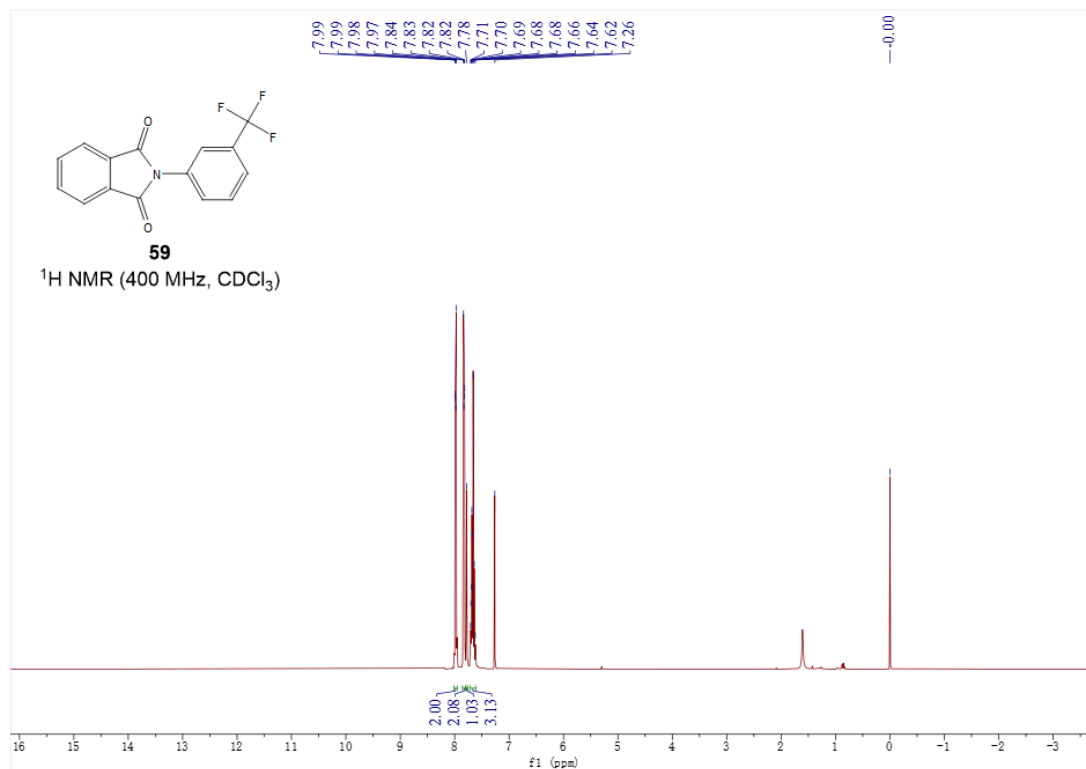
^1H NMR (400 MHz, CDCl_3) spectrum of **58**



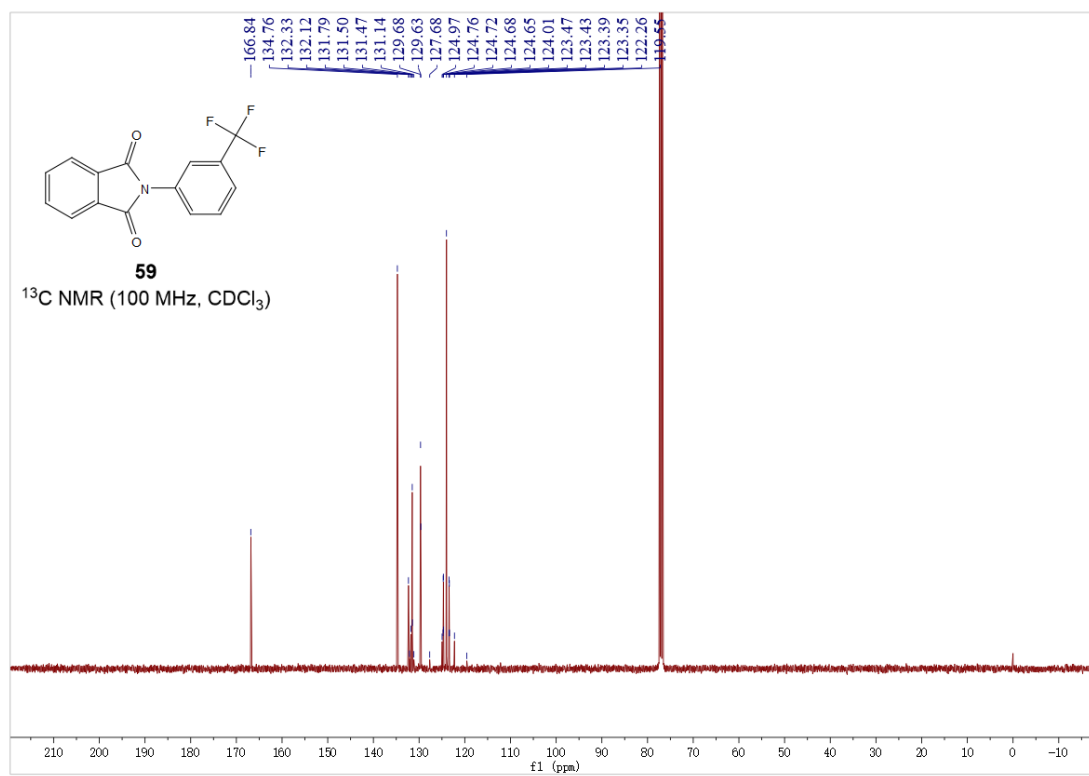
^{13}C NMR (100 MHz, CDCl_3) spectrum of **58**



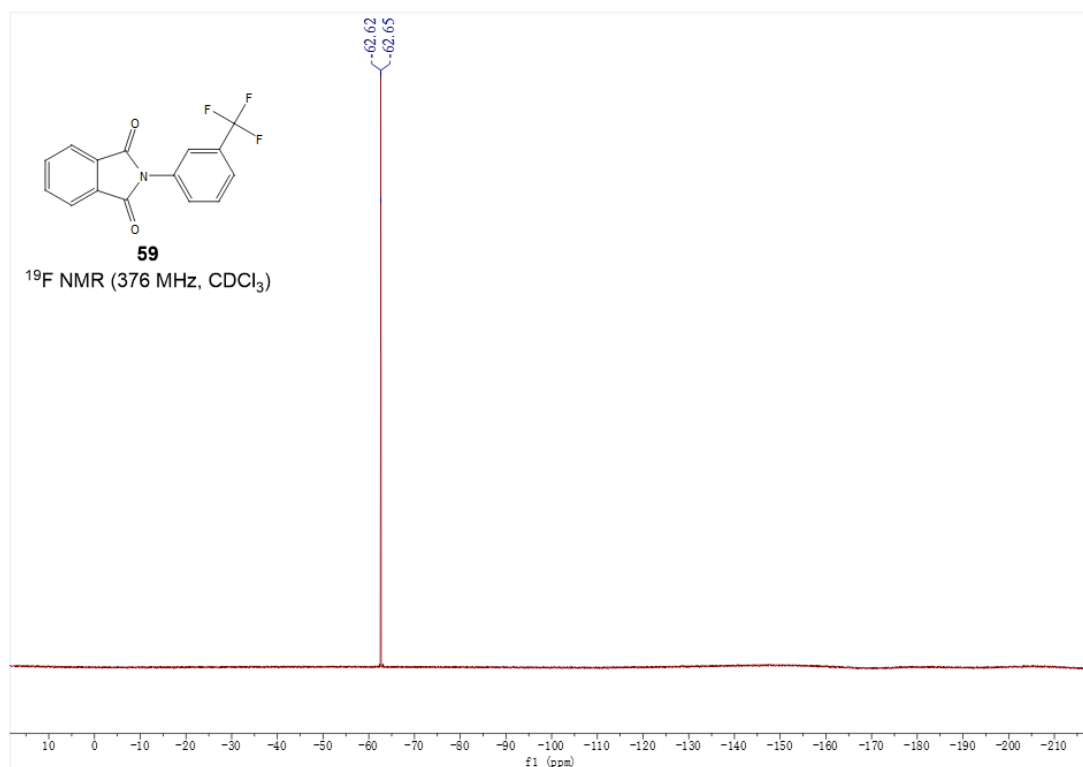
^1H NMR (400 MHz, CDCl_3) spectrum of **59**



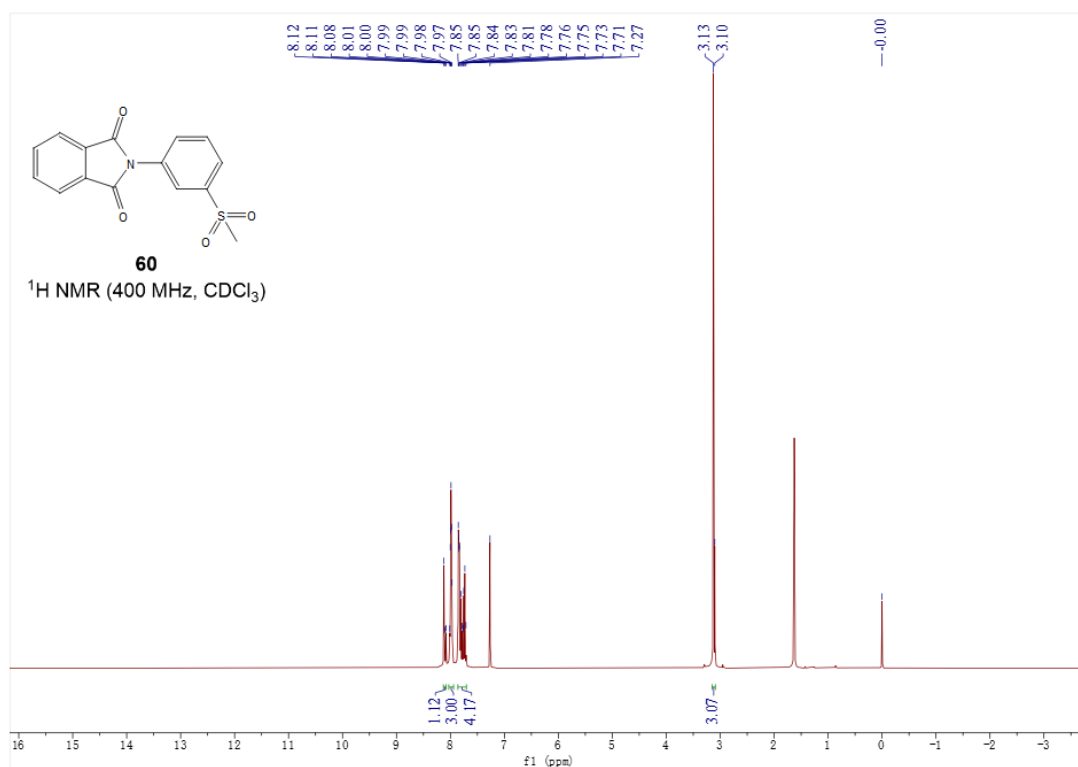
^{13}C NMR (100 MHz, CDCl_3) spectrum of **59**



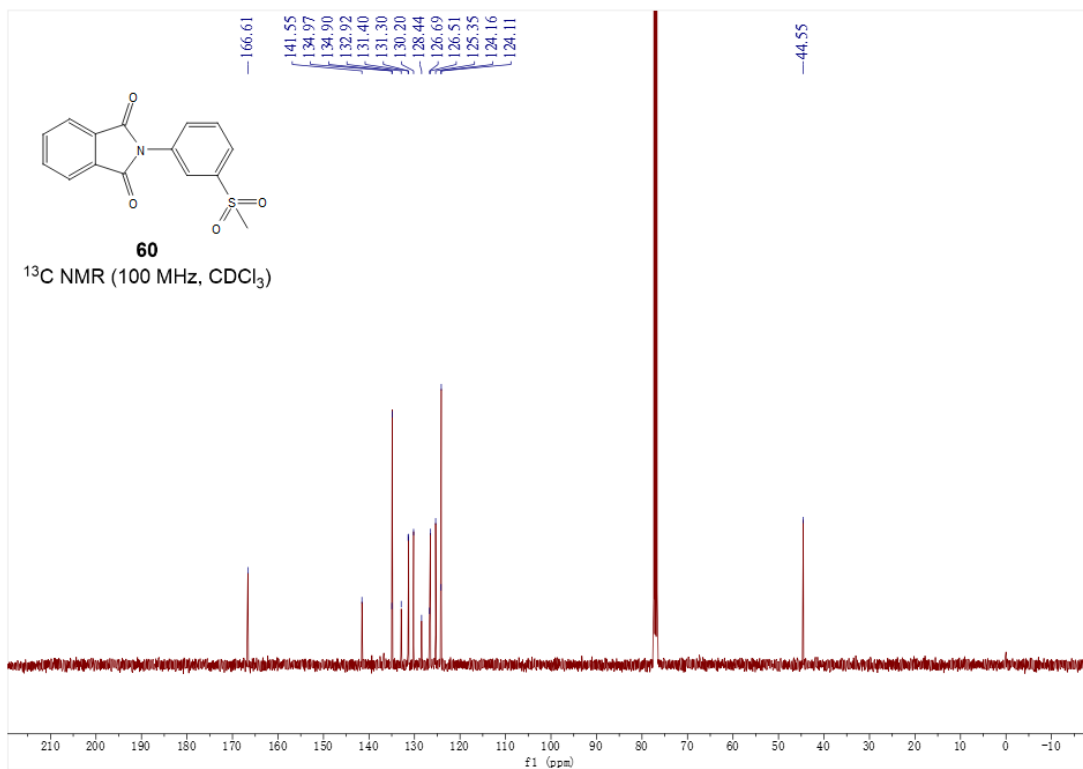
^{19}F NMR (376 MHz, CDCl_3) spectrum of **59**



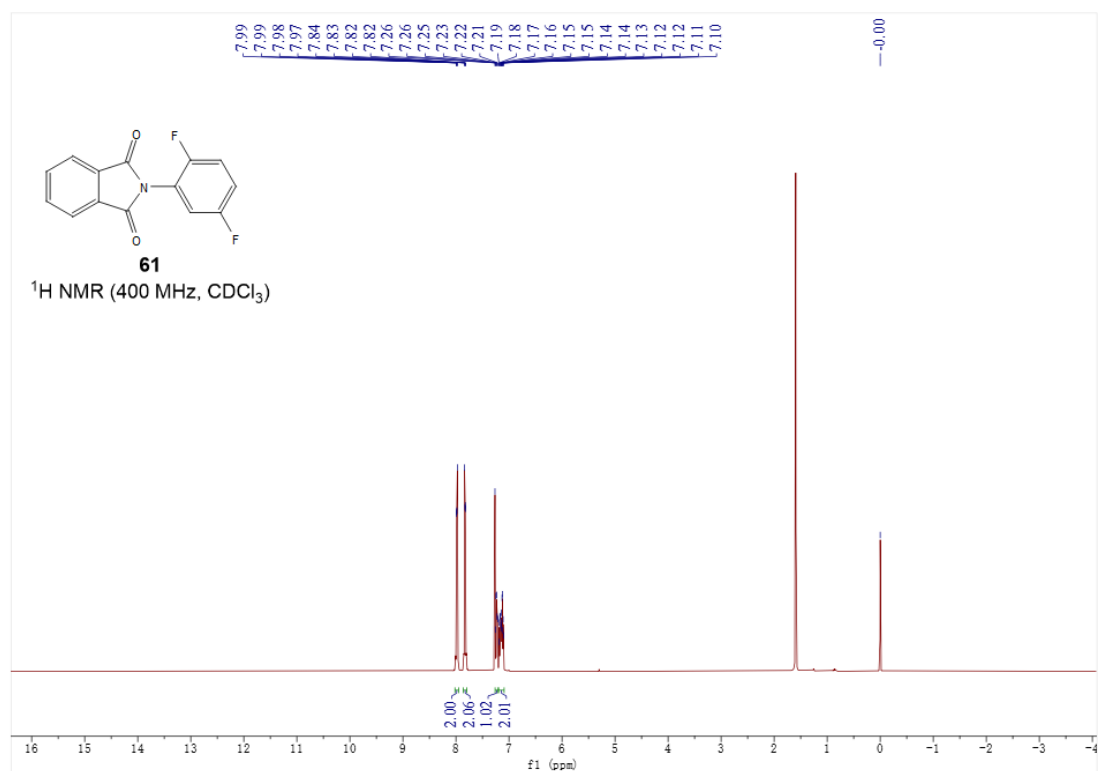
^1H NMR (400 MHz, CDCl_3) spectrum of **60**



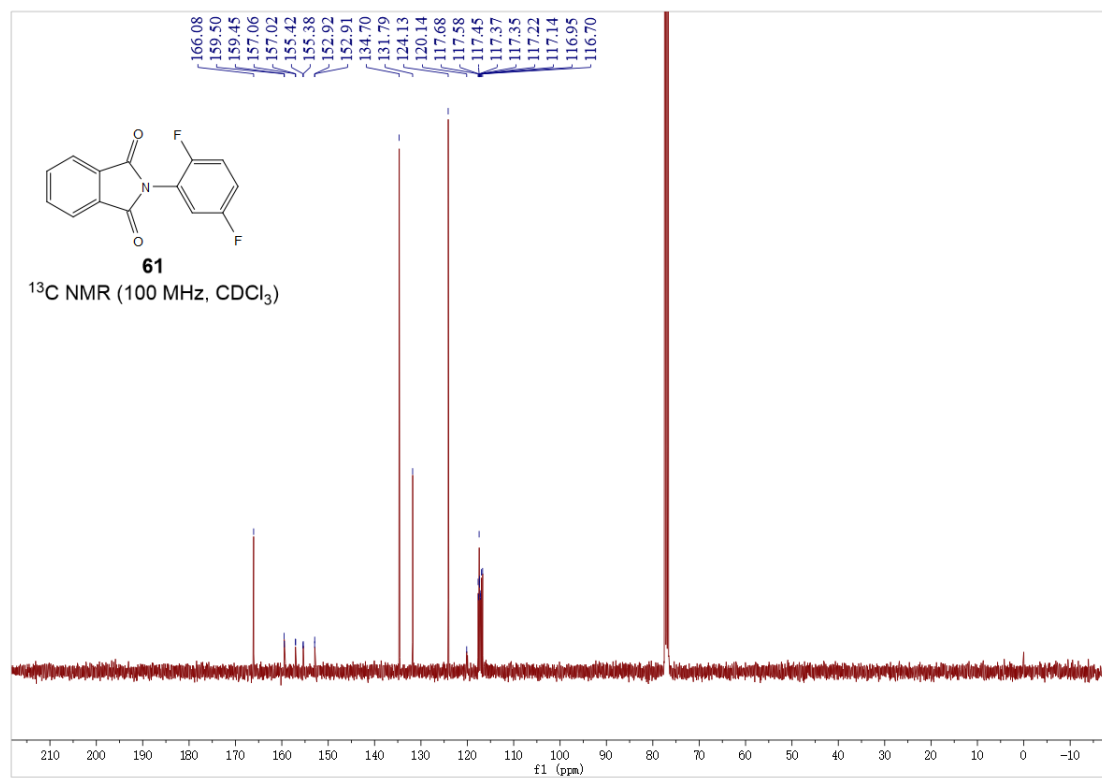
^{13}C NMR (100 MHz, CDCl_3) spectrum of **60**



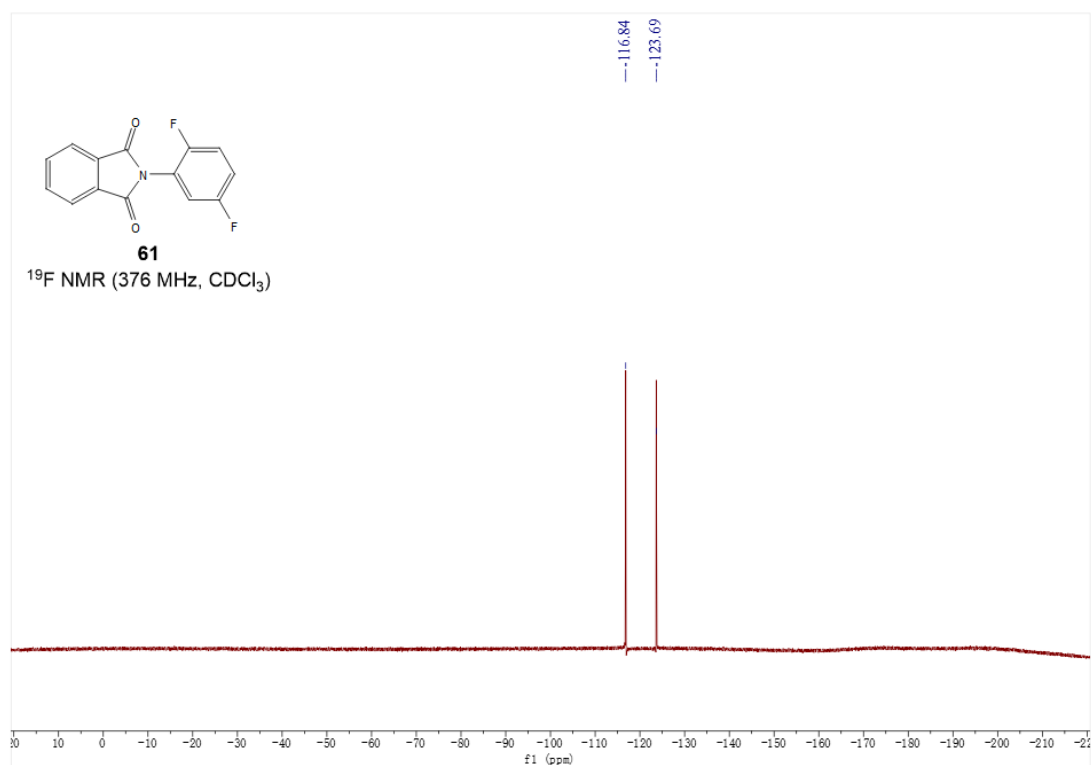
^1H NMR (400 MHz, CDCl_3) spectrum of **61**



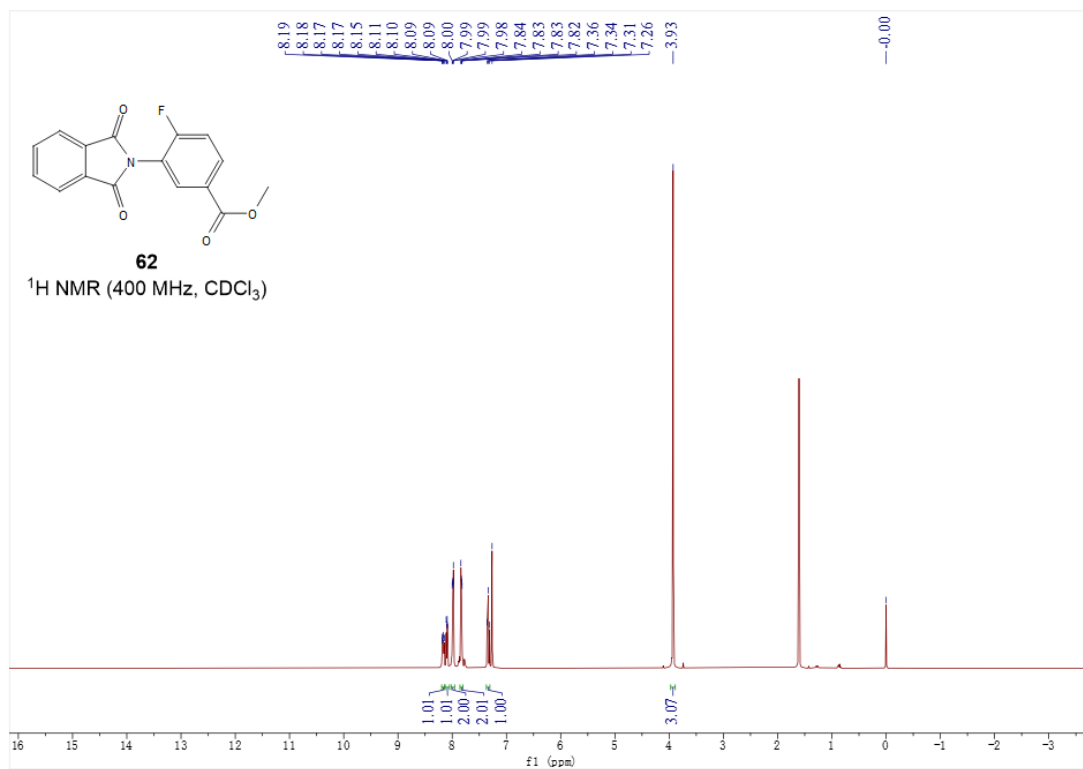
^{13}C NMR (100 MHz, CDCl_3) spectrum of **61**



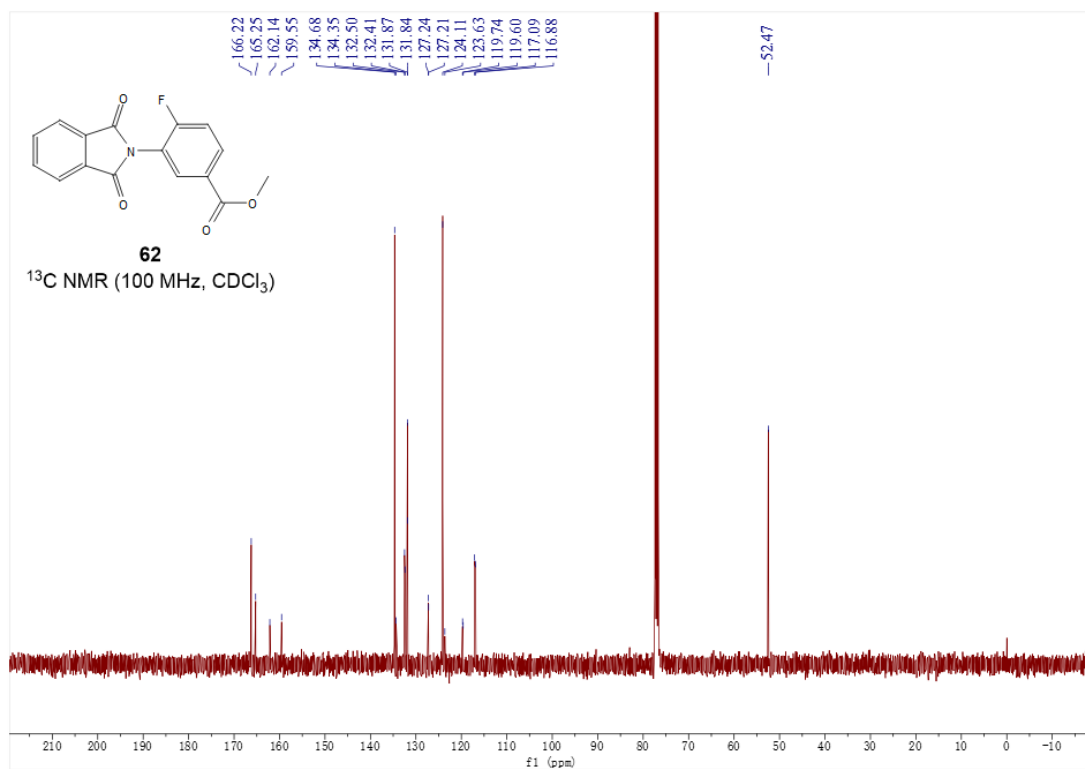
^{19}F NMR (376 MHz, CDCl_3) spectrum of **61**



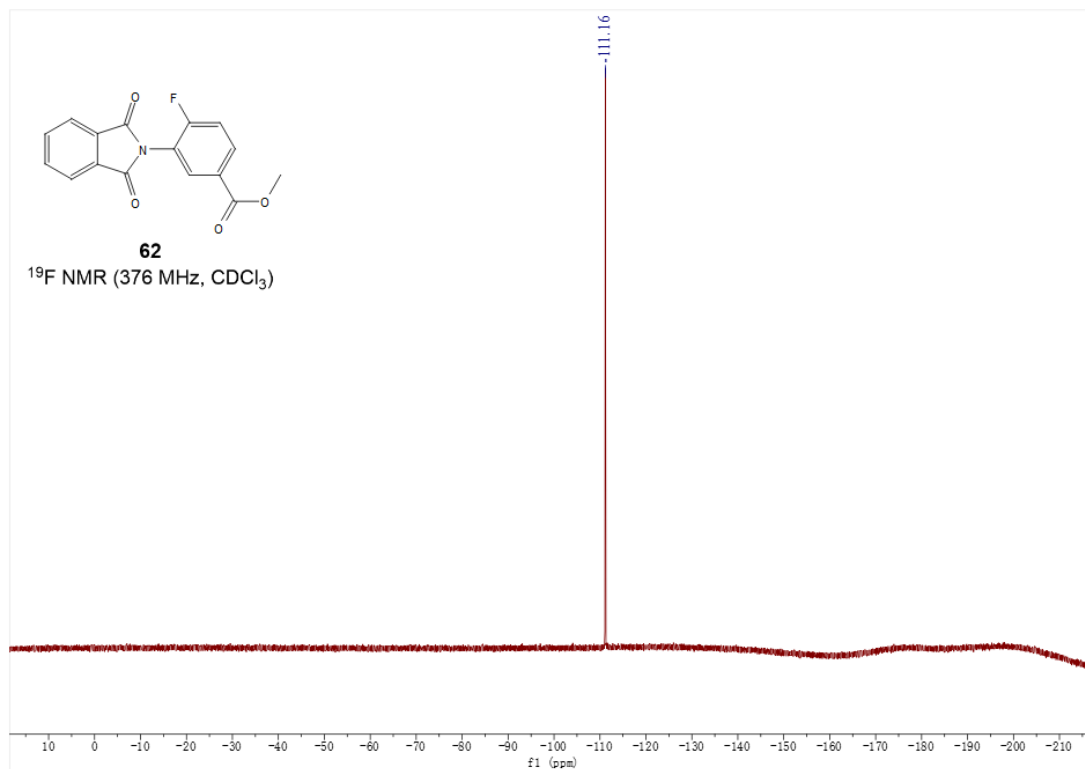
^1H NMR (400 MHz, CDCl_3) spectrum of **62**



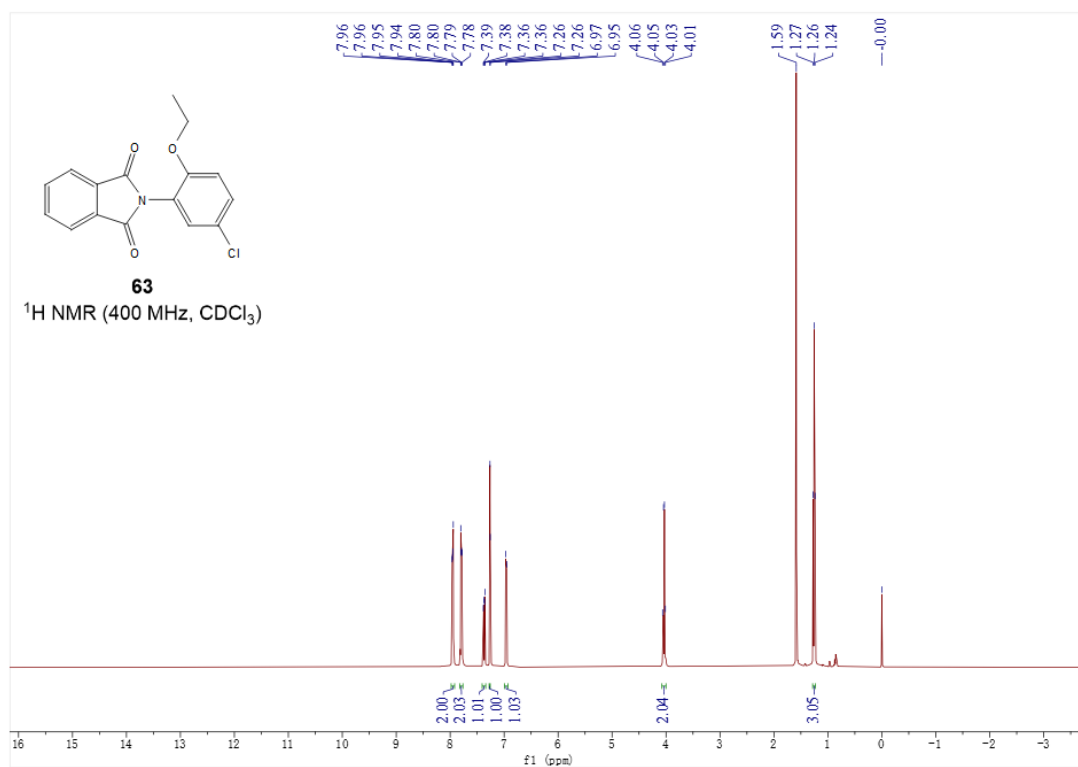
^{13}C NMR (100 MHz, CDCl_3) spectrum of **62**



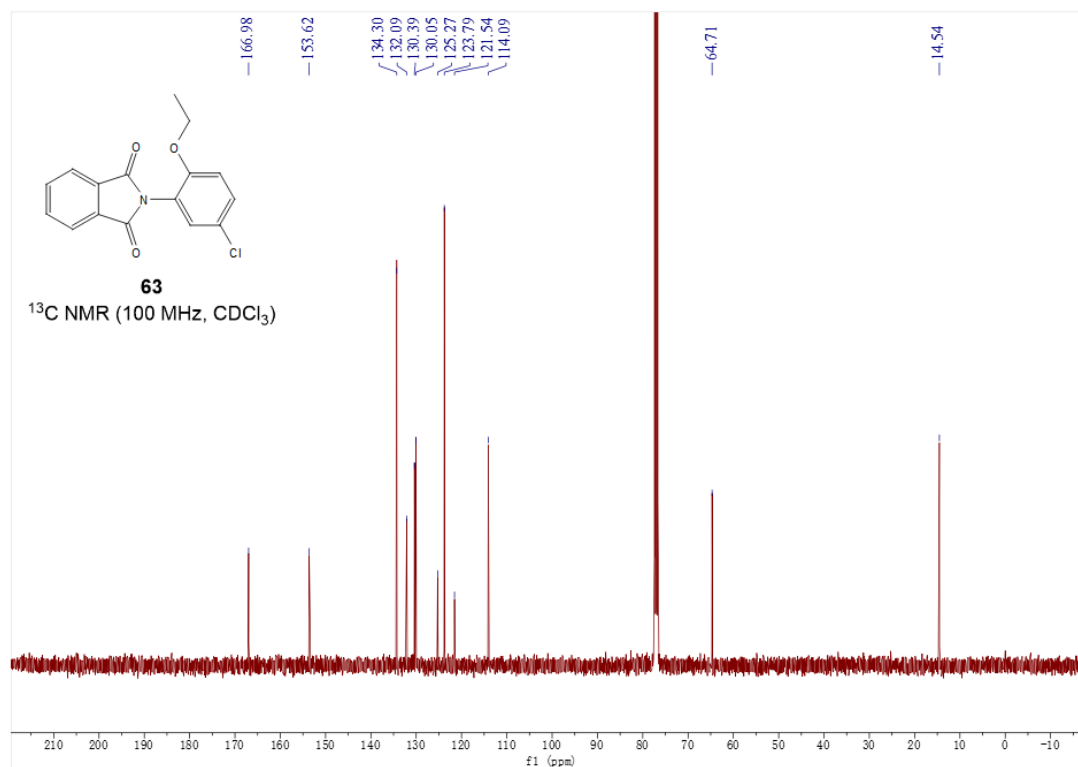
^{19}F NMR (376 MHz, CDCl_3) spectrum of **62**



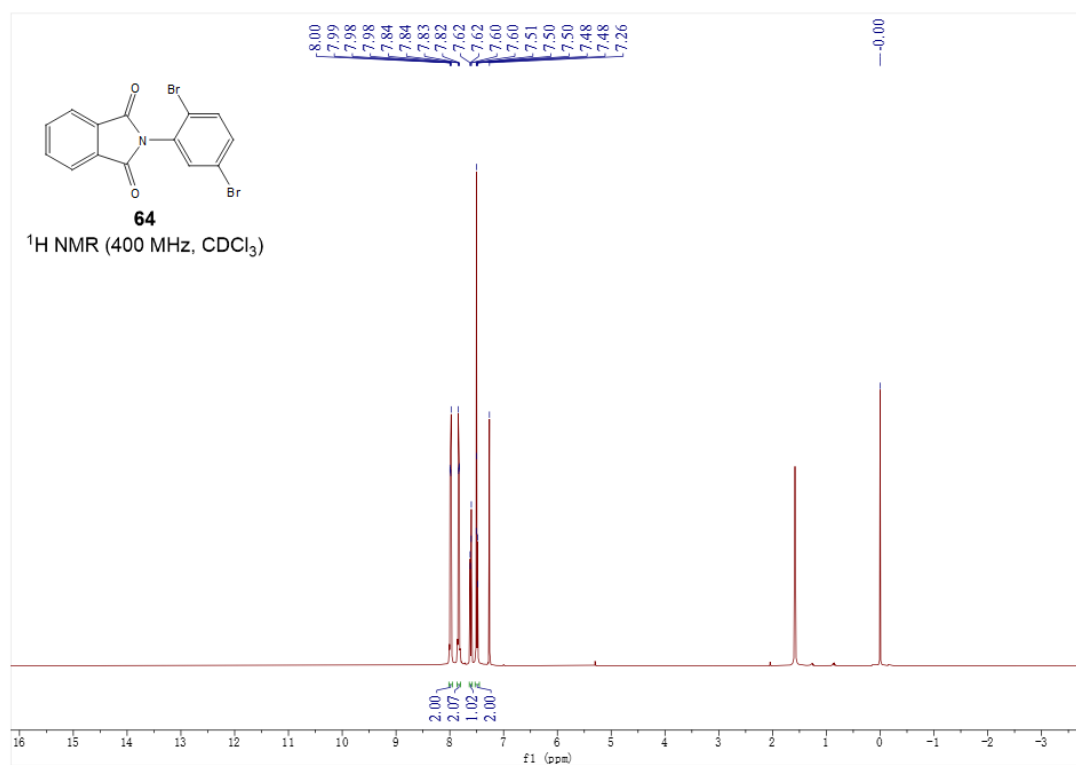
^1H NMR (400 MHz, CDCl_3) spectrum of **63**



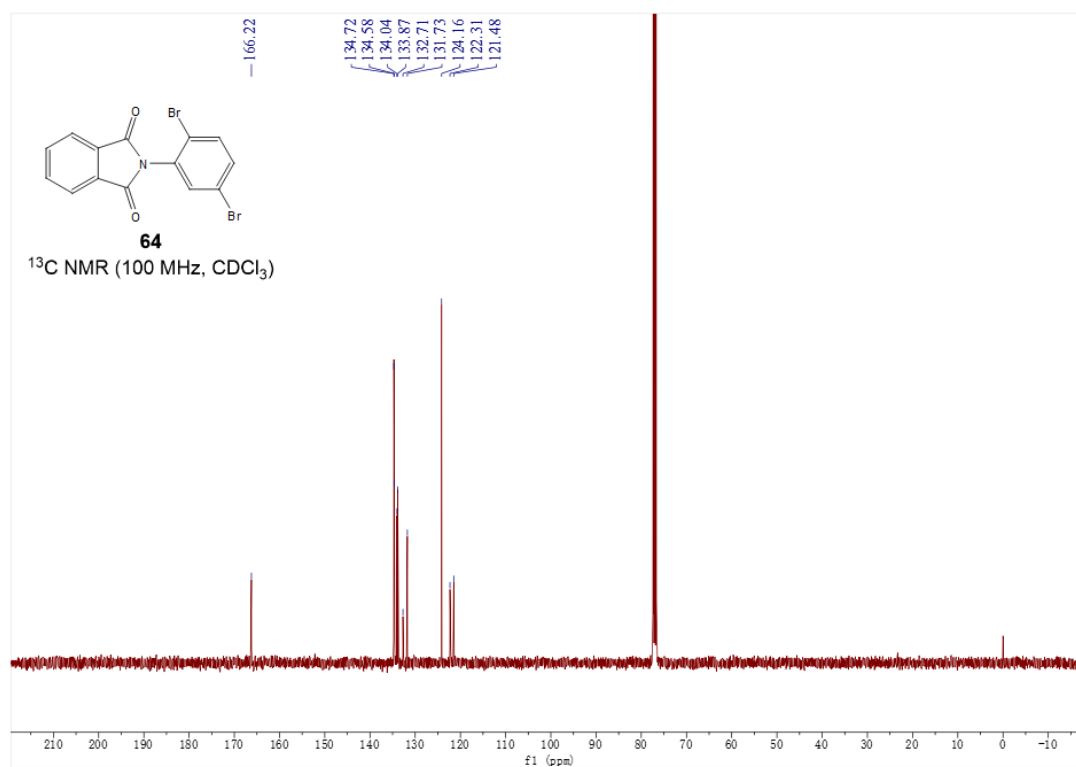
^{13}C NMR (100 MHz, CDCl_3) spectrum of **63**



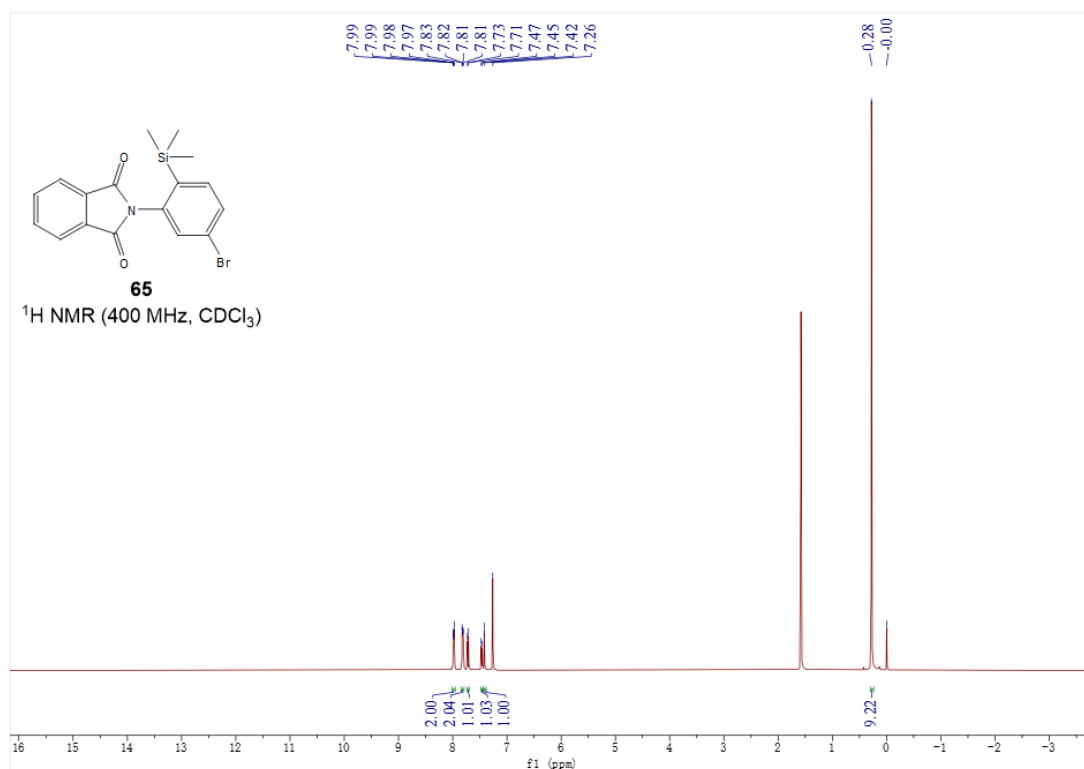
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **64**



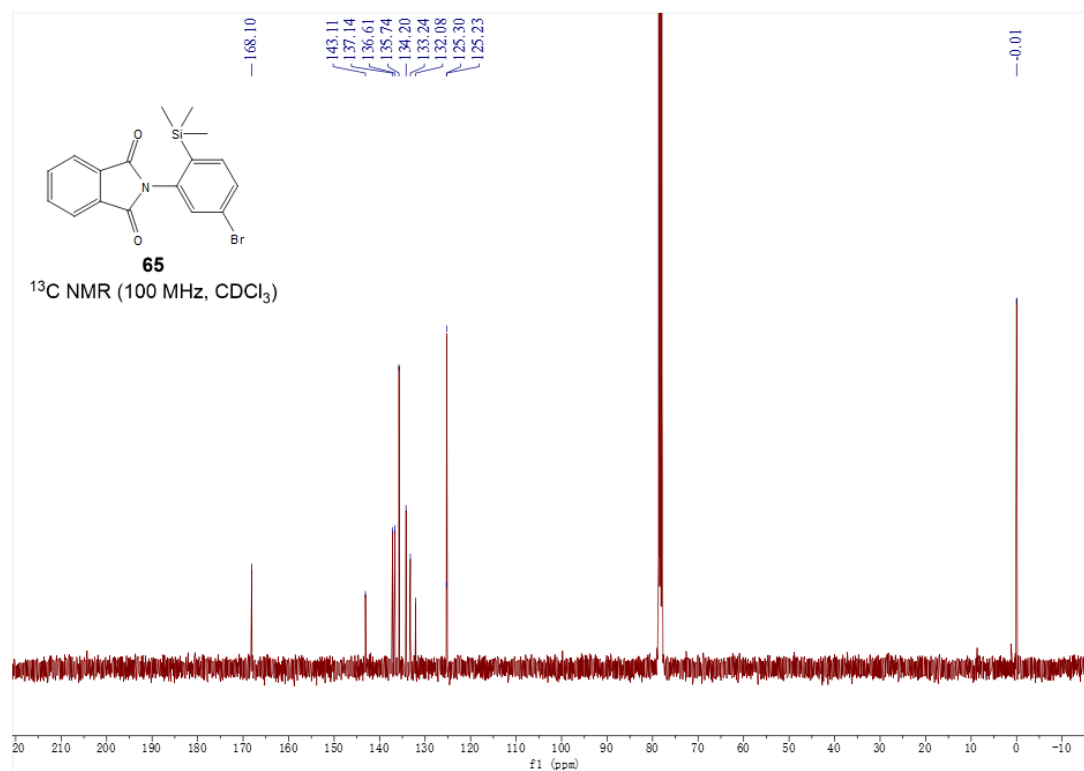
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **64**



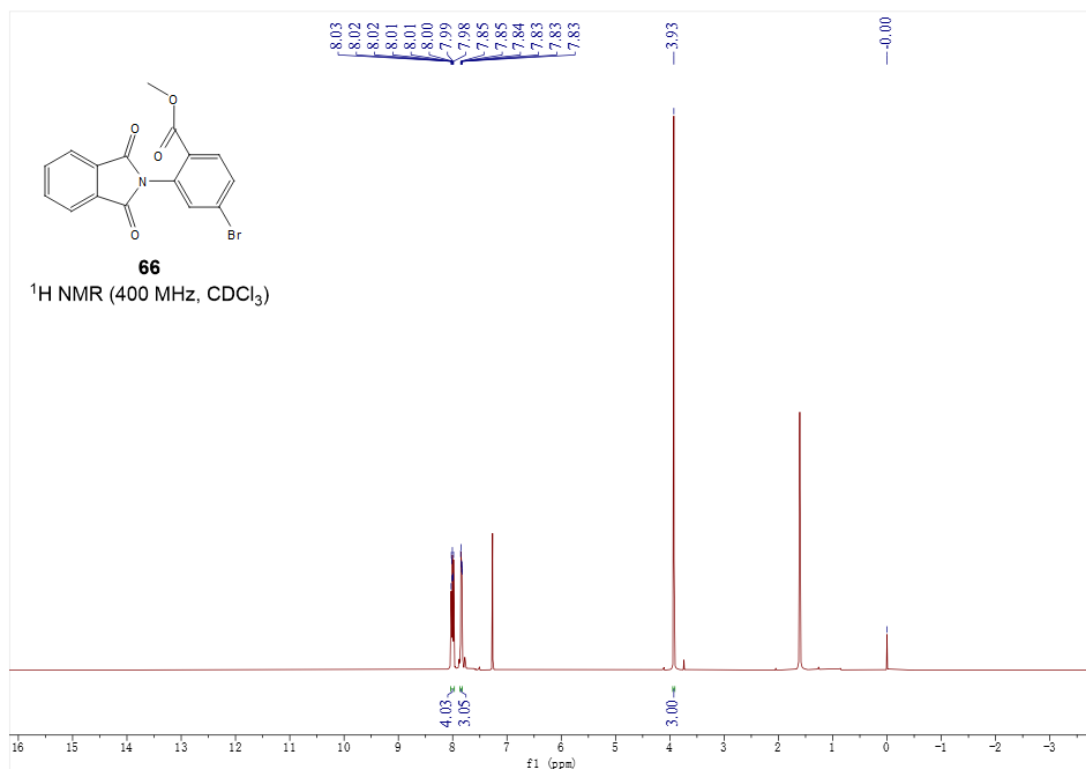
^1H NMR (400 MHz, CDCl_3) spectrum of **65**



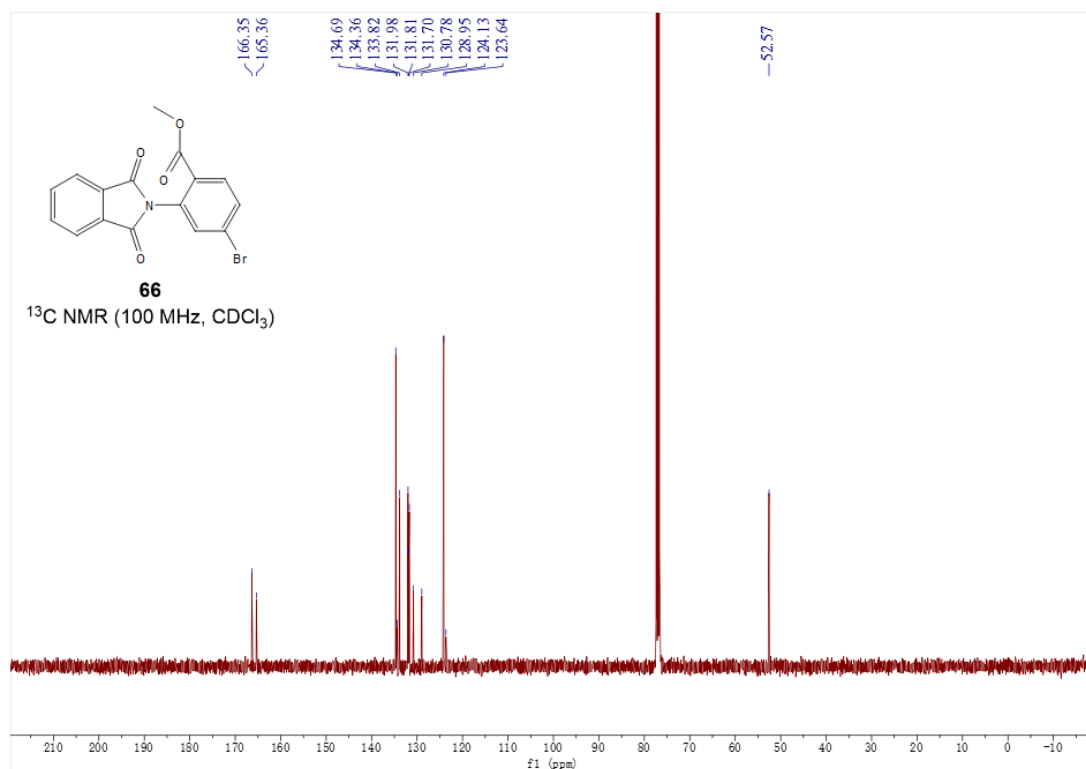
^{13}C NMR (100 MHz, CDCl_3) spectrum of **65**



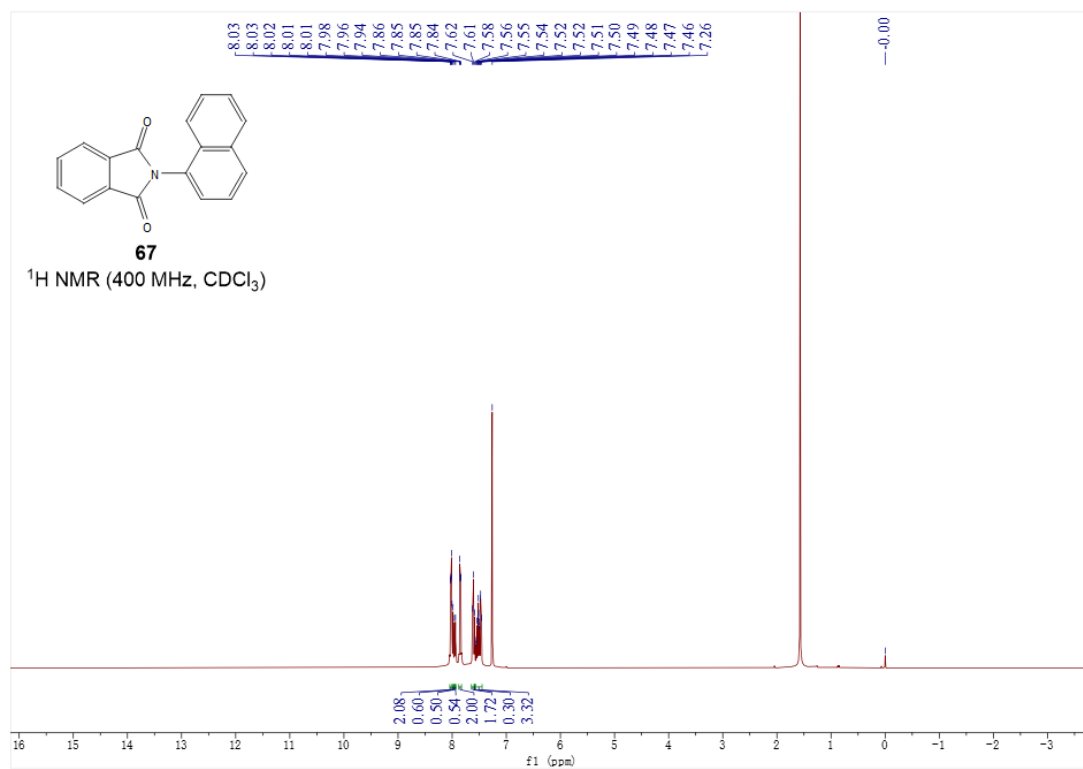
^1H NMR (400 MHz, CDCl_3) spectrum of **66**



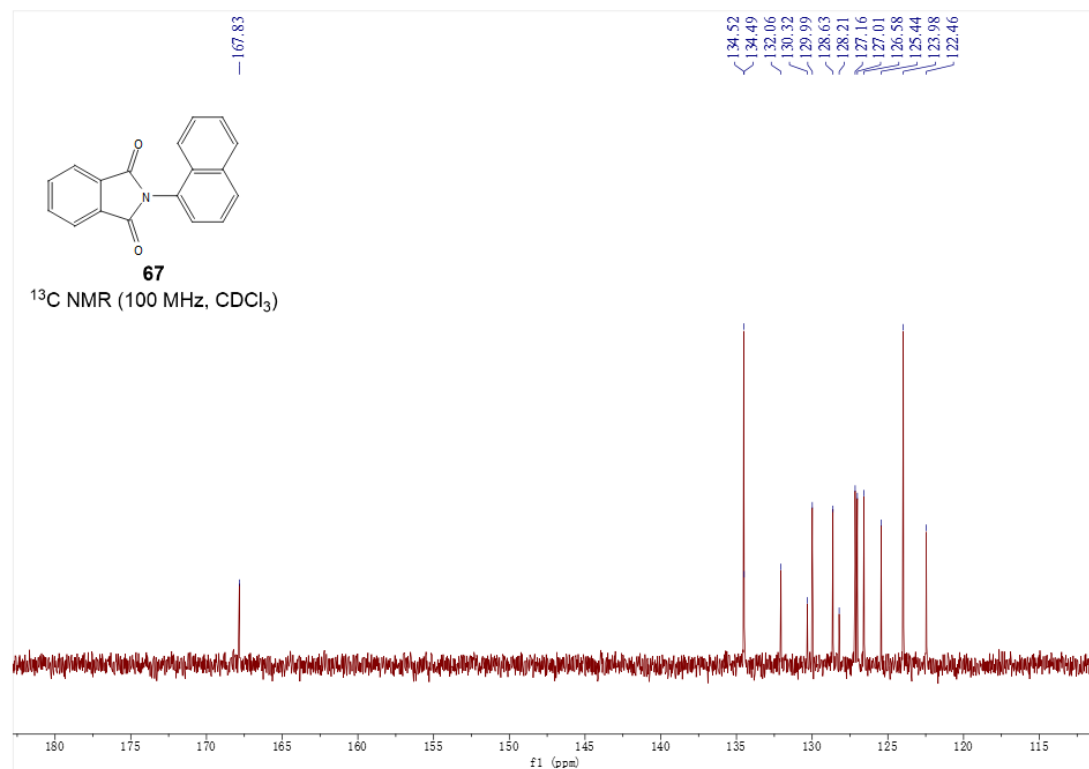
^{13}C NMR (100 MHz, CDCl_3) spectrum of **66**



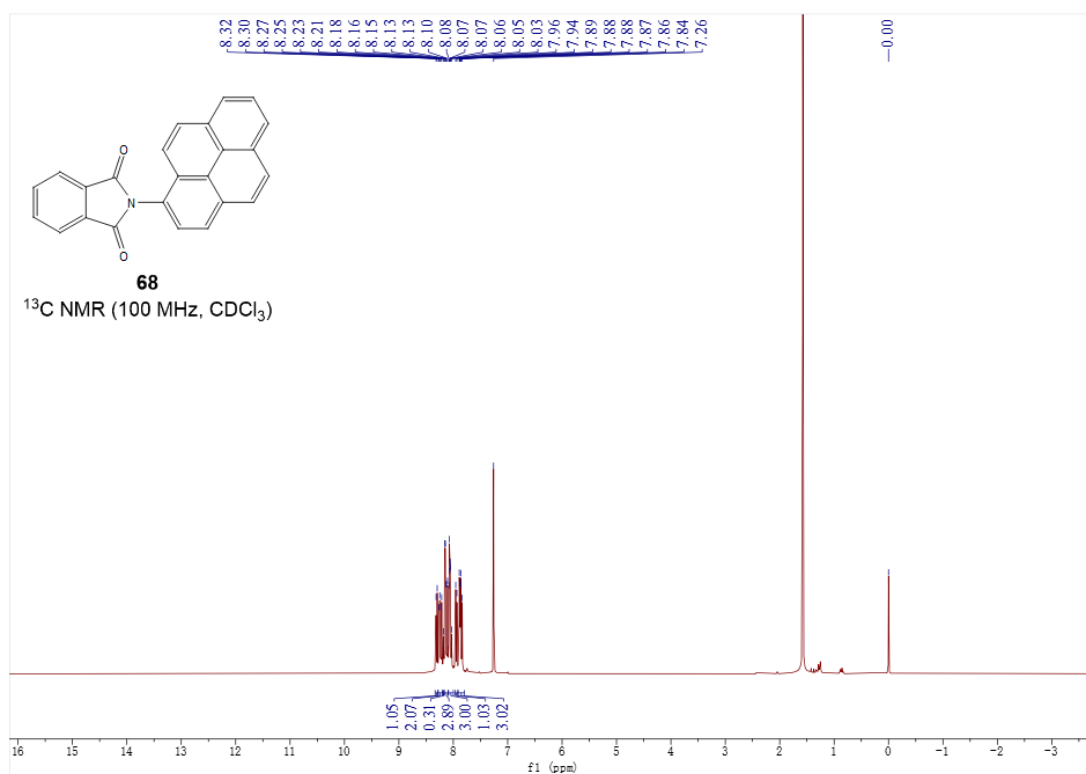
^1H NMR (400 MHz, CDCl_3) spectrum of **67**



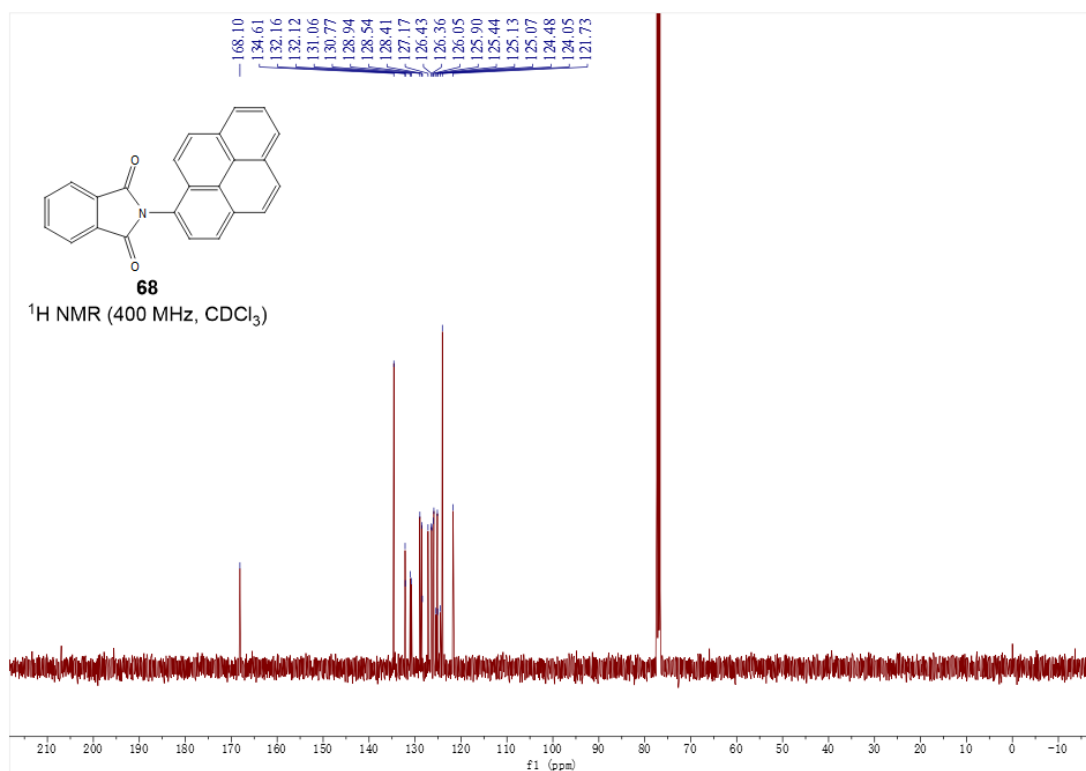
^{13}C NMR (100 MHz, CDCl_3) spectrum of **67**



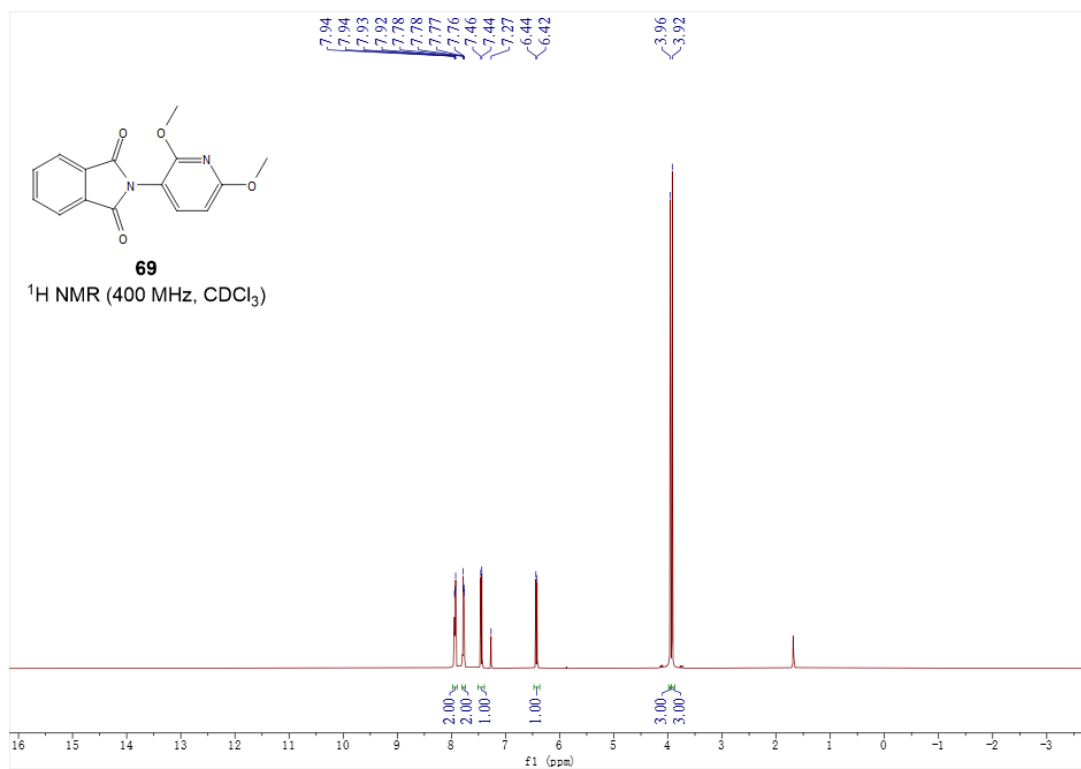
^1H NMR (400 MHz, CDCl_3) spectrum of **68**



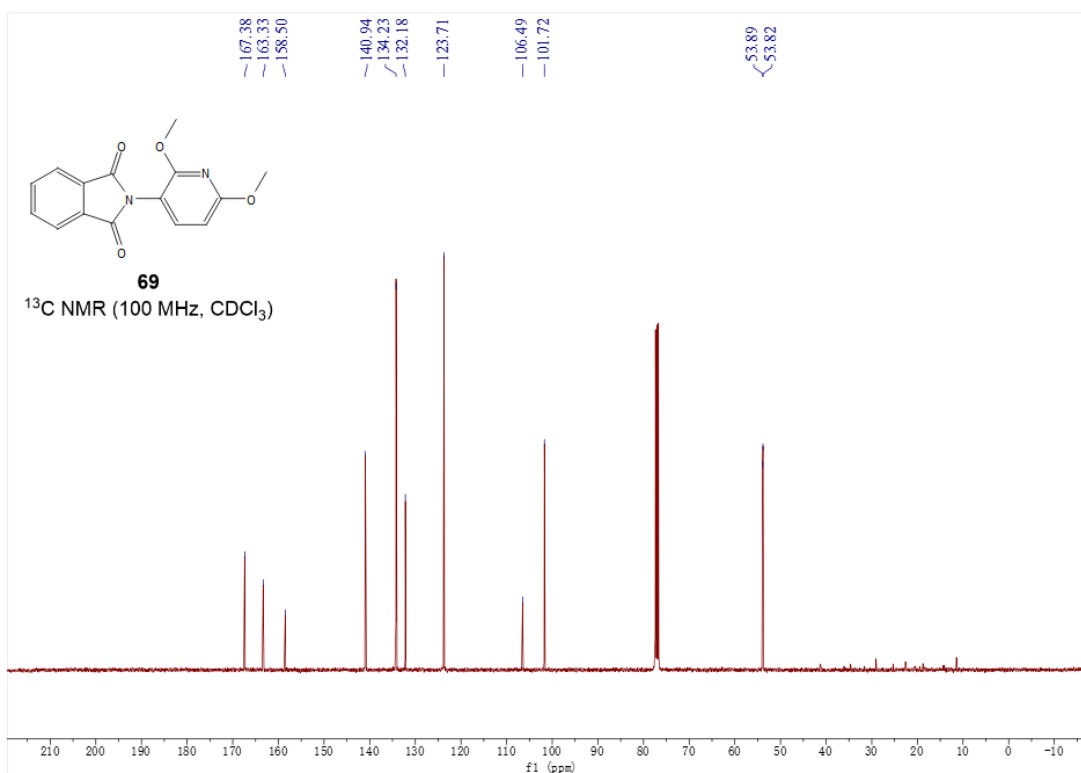
^{13}C NMR (100 MHz, CDCl_3) spectrum of **68**



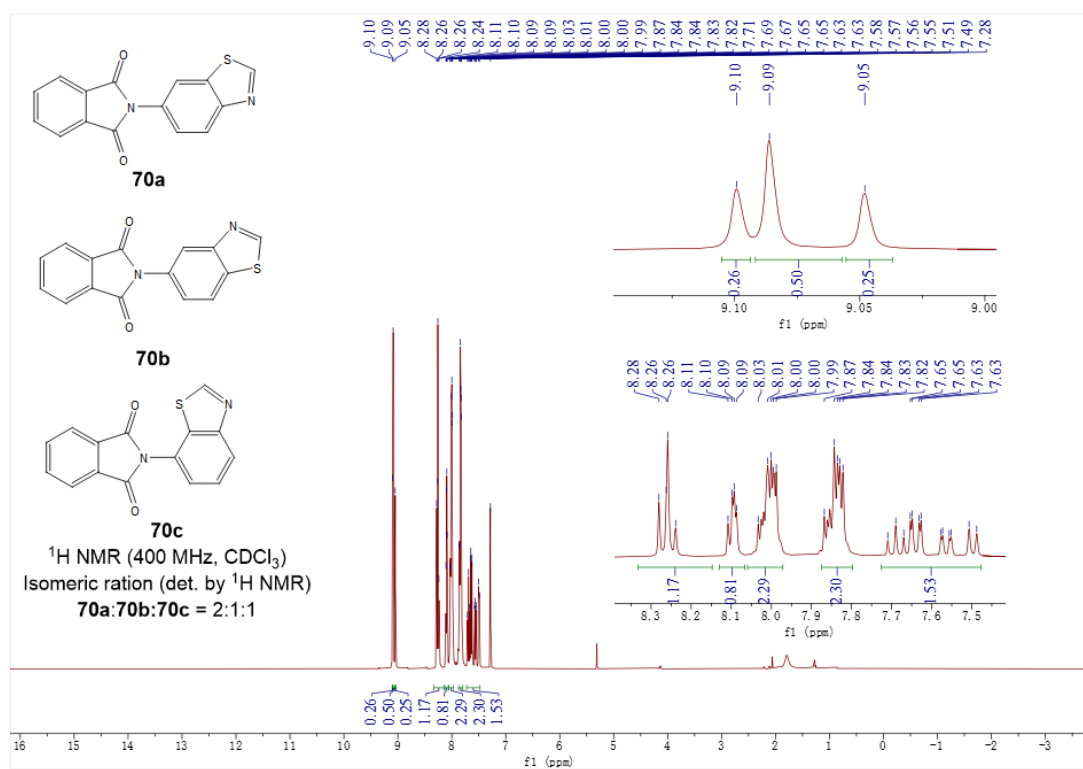
^1H NMR (400 MHz, CDCl_3) spectrum of **69**



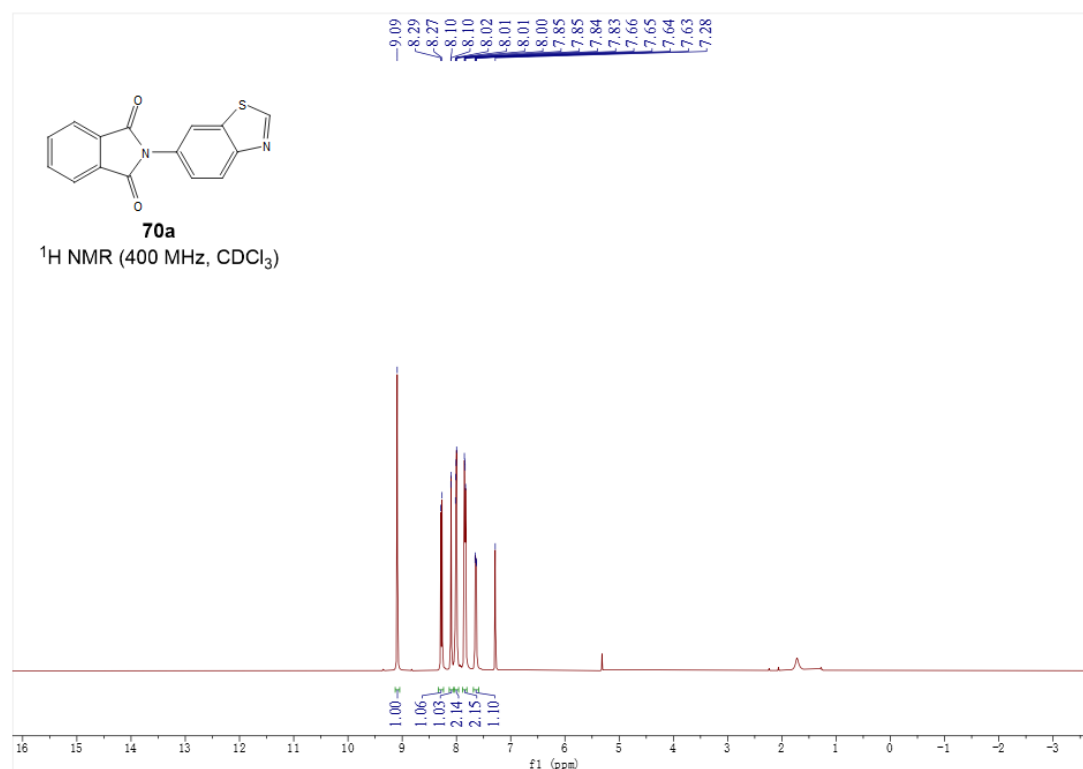
^{13}C NMR (100 MHz, CDCl_3) spectrum of **69**



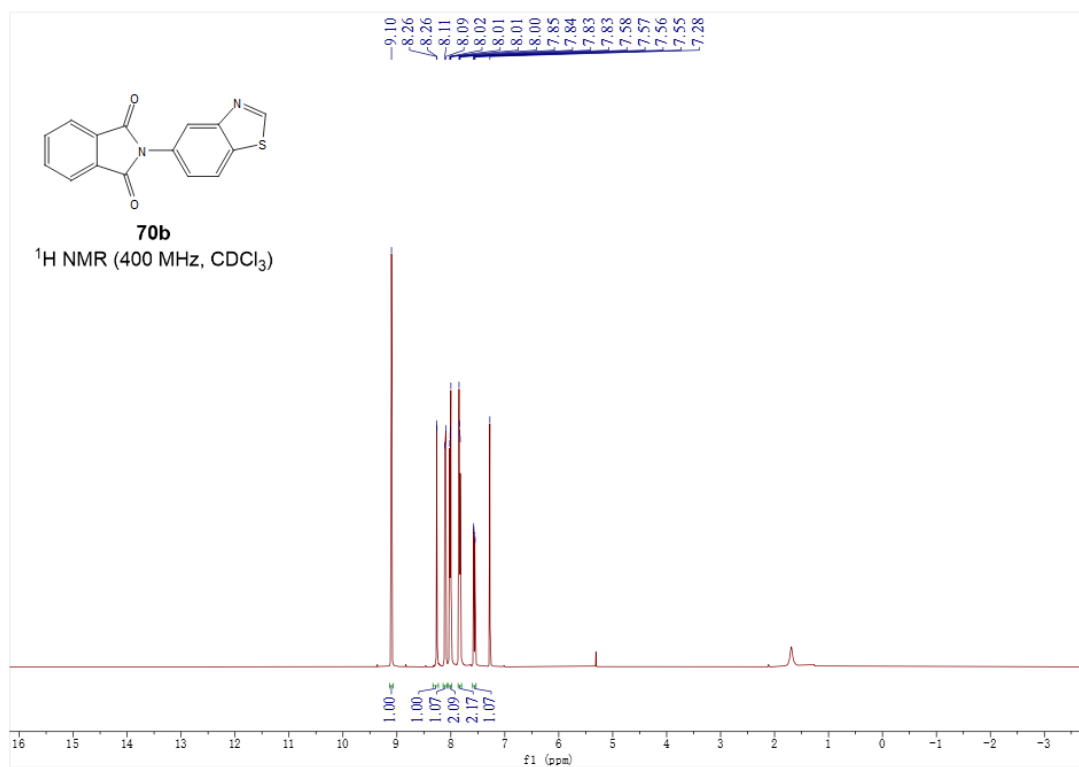
^1H NMR (400 MHz, CDCl_3) spectrum of **70**



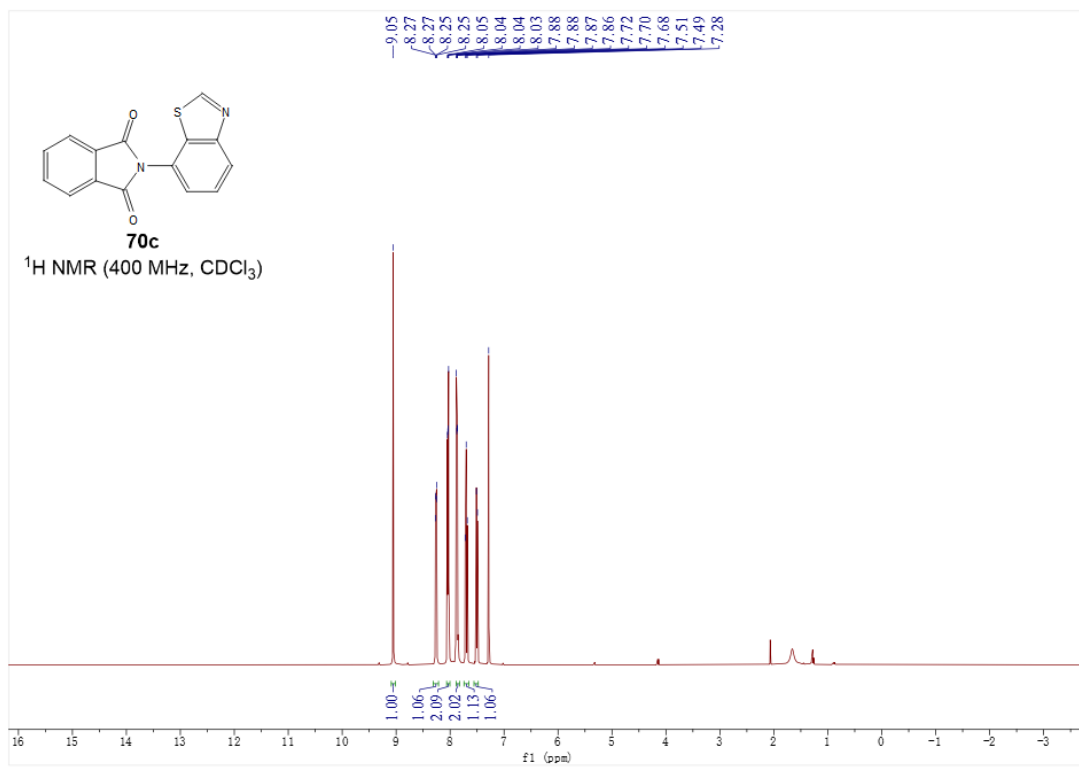
^1H NMR (400 MHz, CDCl_3) spectrum of **70a**



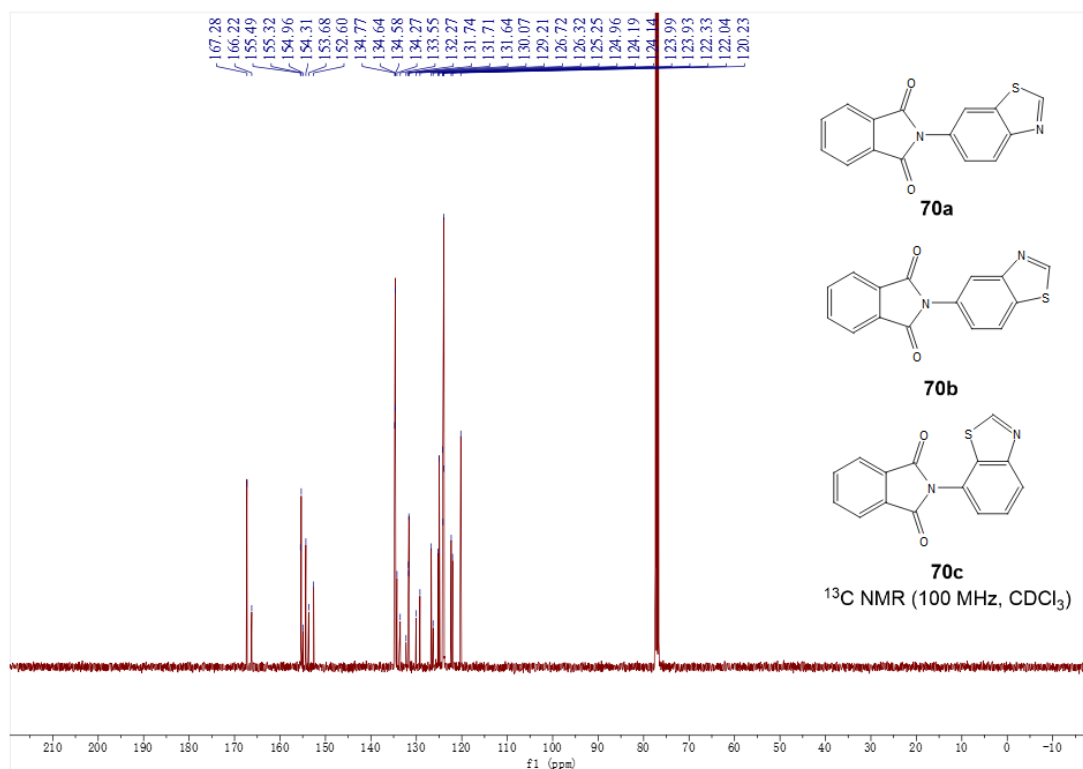
^1H NMR (400 MHz, CDCl_3) spectrum of **70b**



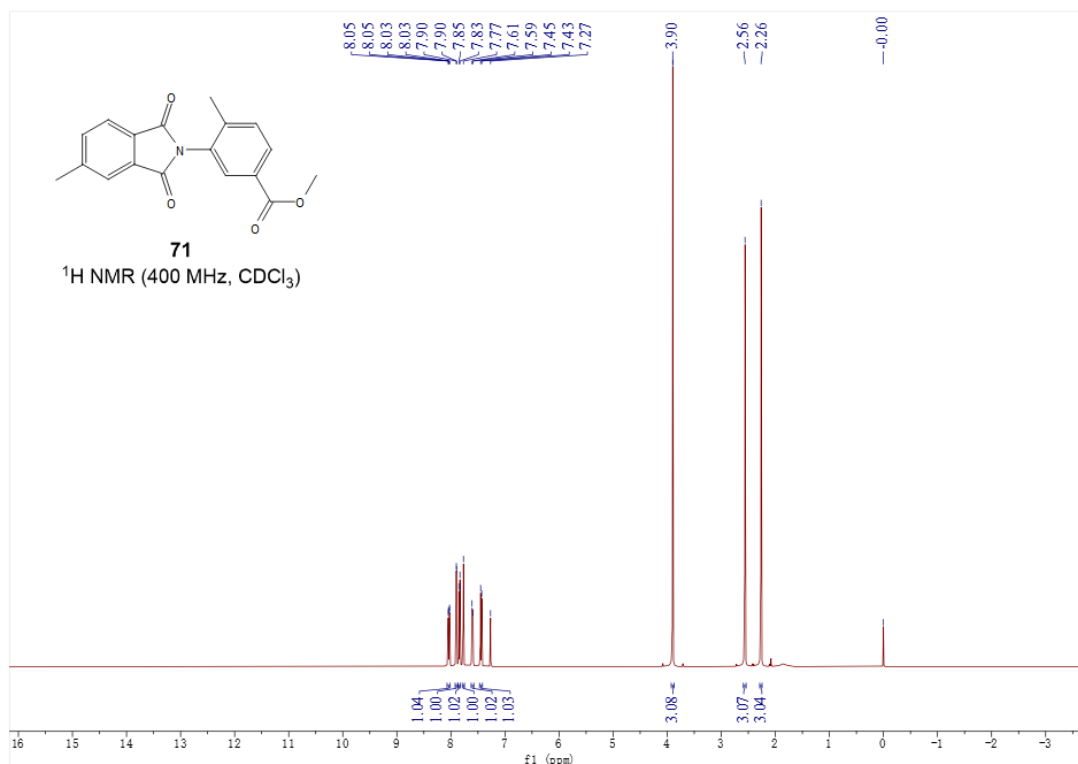
^1H NMR (400 MHz, CDCl_3) spectrum of **70c**



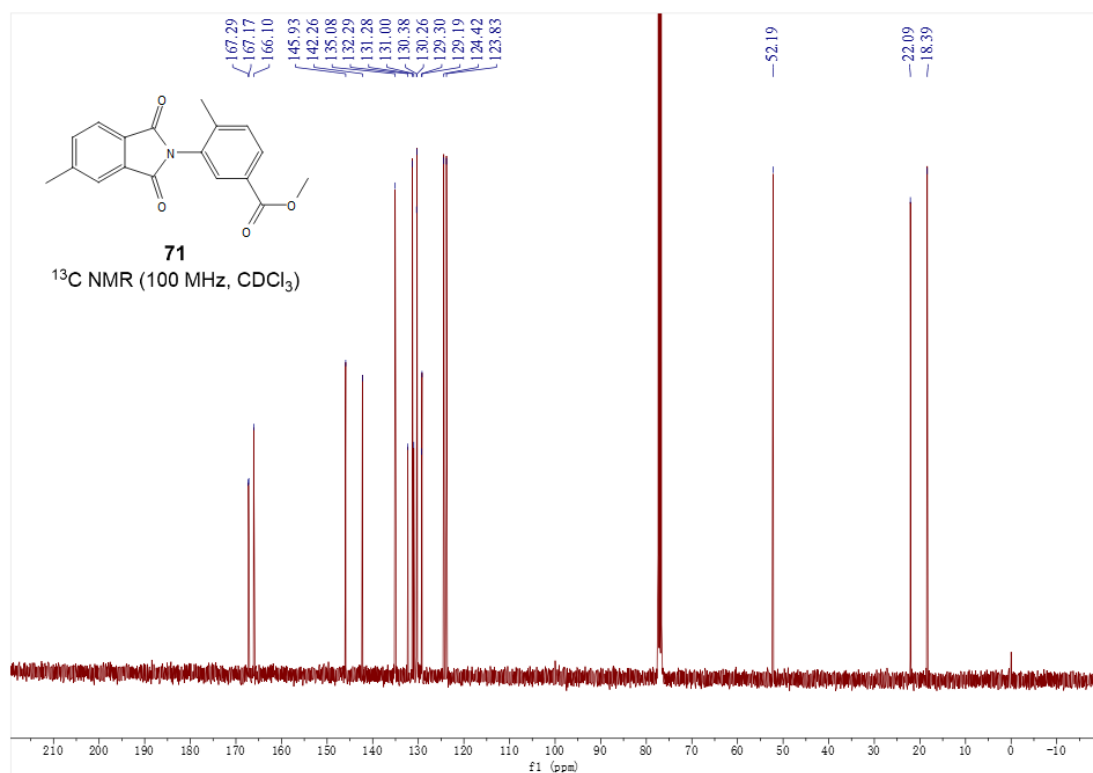
^{13}C NMR (100 MHz, CDCl_3) spectrum of **70**



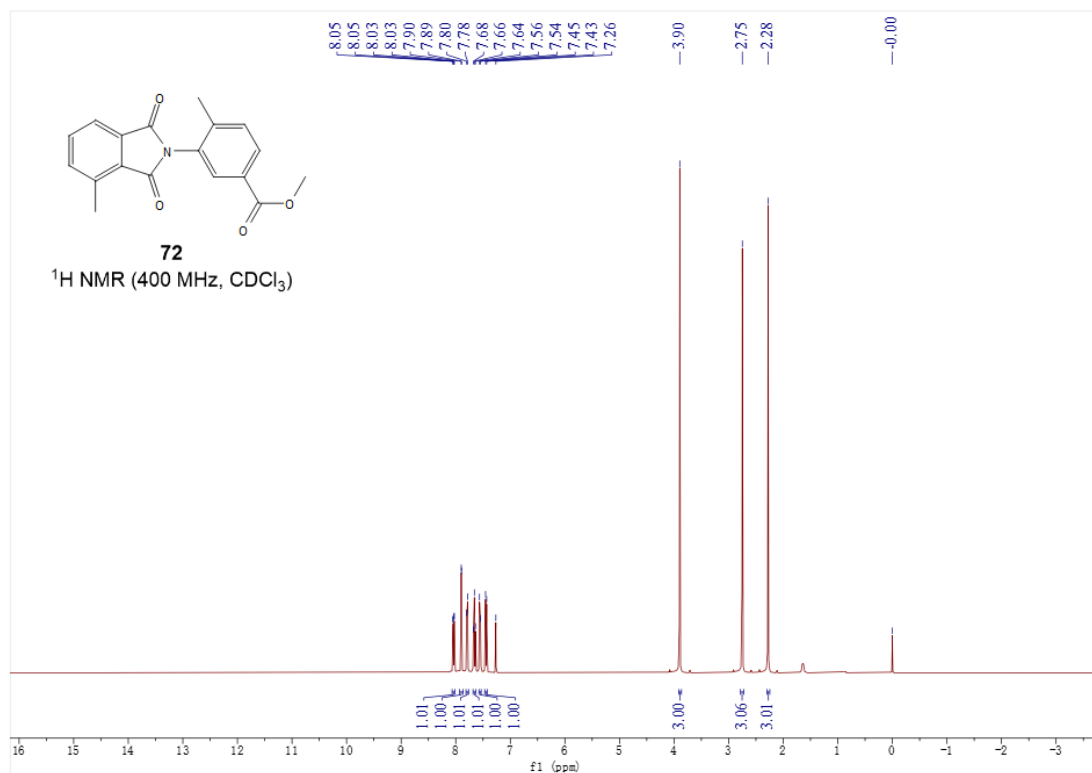
^1H NMR (400 MHz, CDCl_3) spectrum of **71**



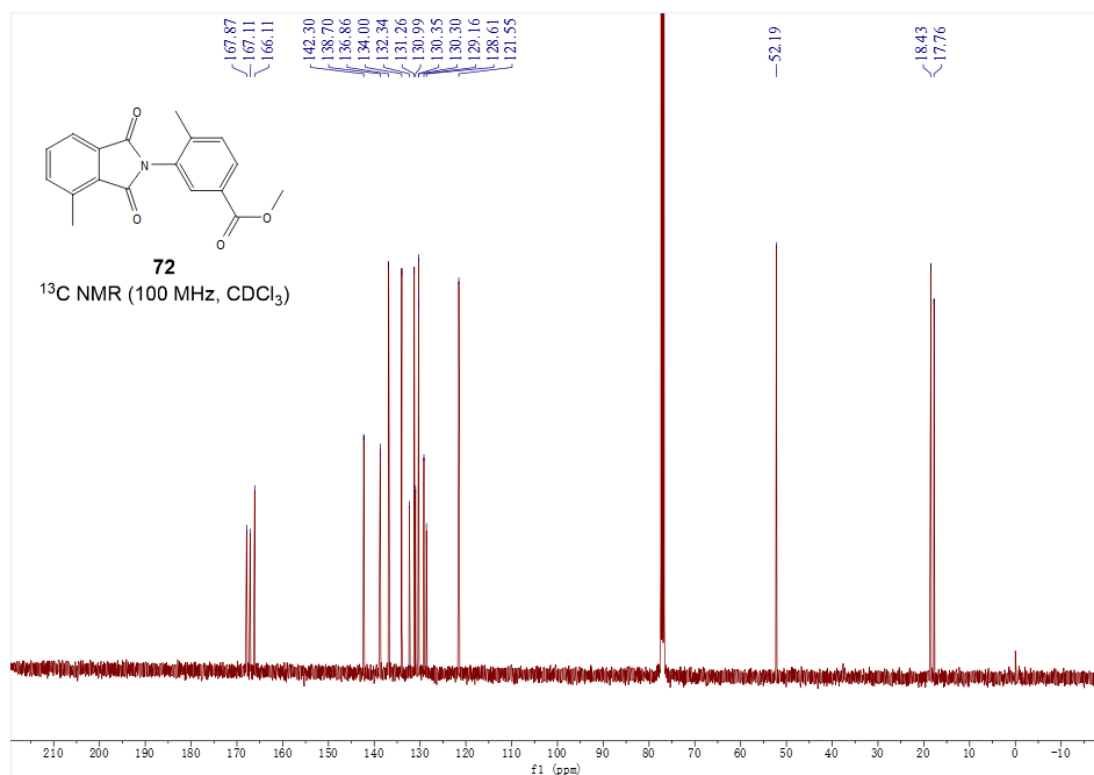
^{13}C NMR (100 MHz, CDCl_3) spectrum of **71**



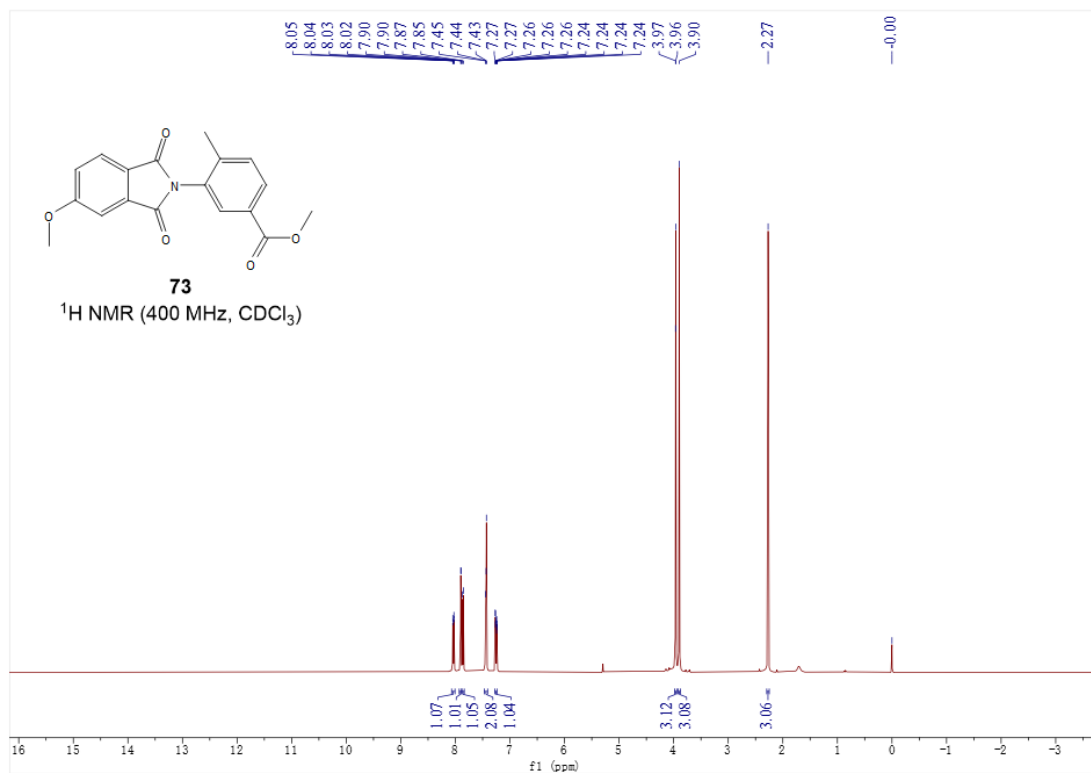
^1H NMR (400 MHz, CDCl_3) spectrum of **72**



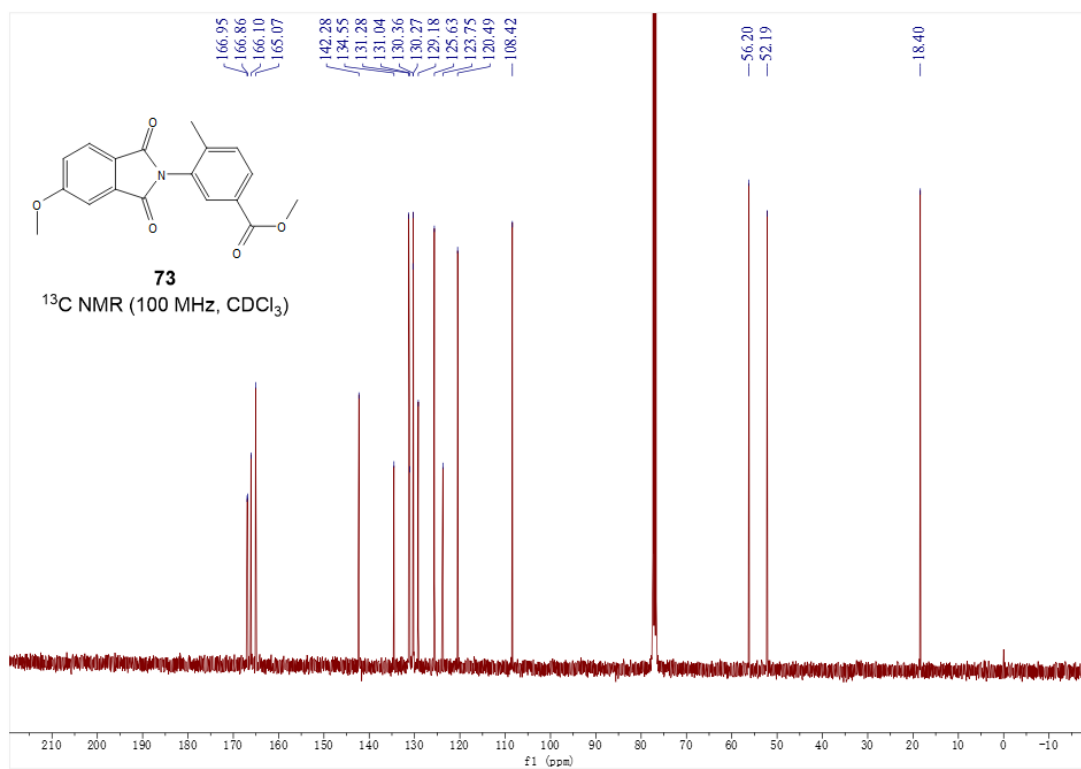
^{13}C NMR (100 MHz, CDCl_3) spectrum of **72**



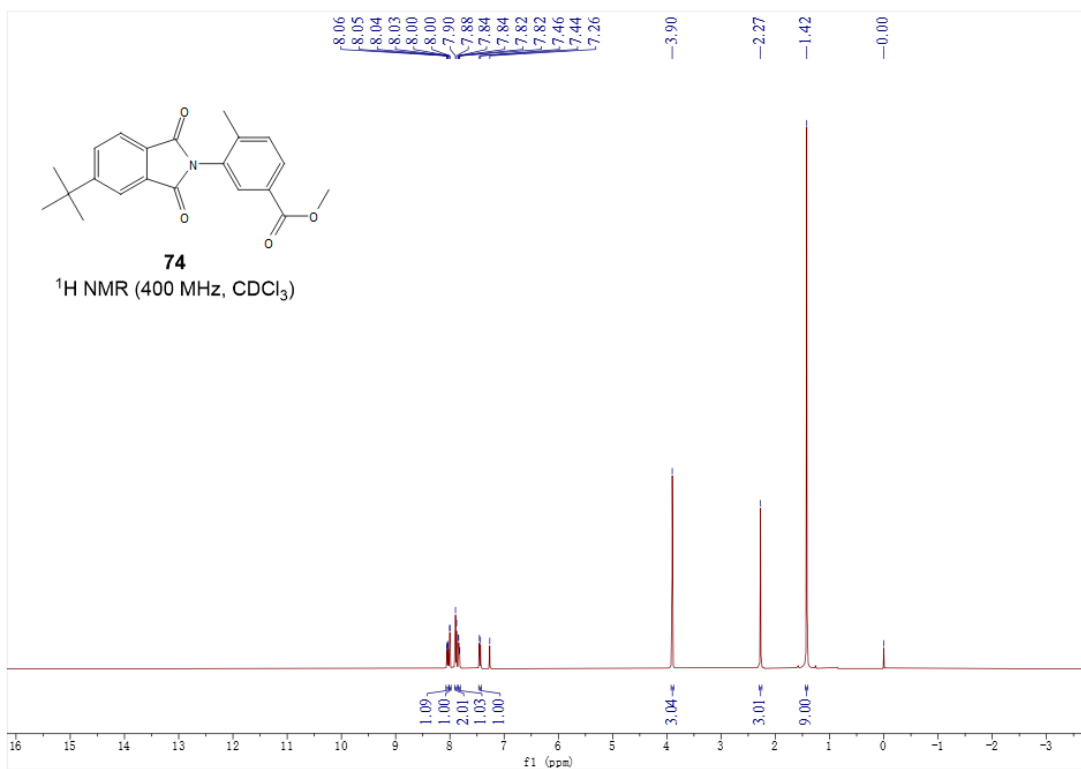
^1H NMR (400 MHz, CDCl_3) spectrum of **73**



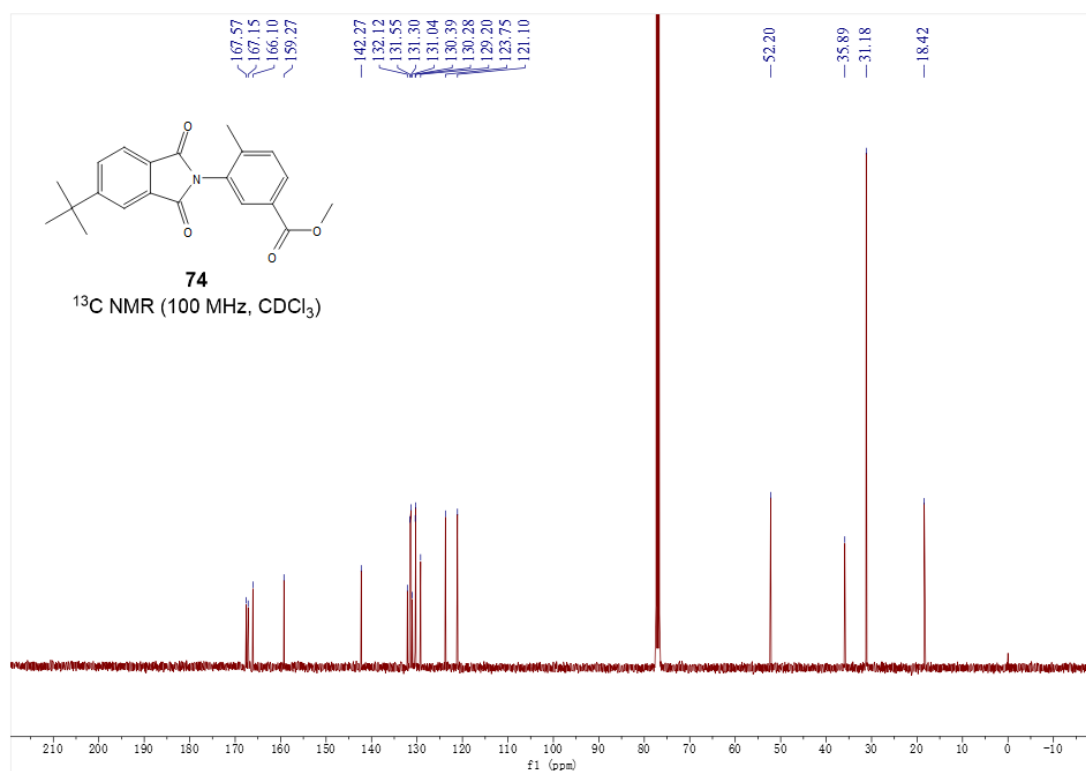
^{13}C NMR (100 MHz, CDCl_3) spectrum of **73**



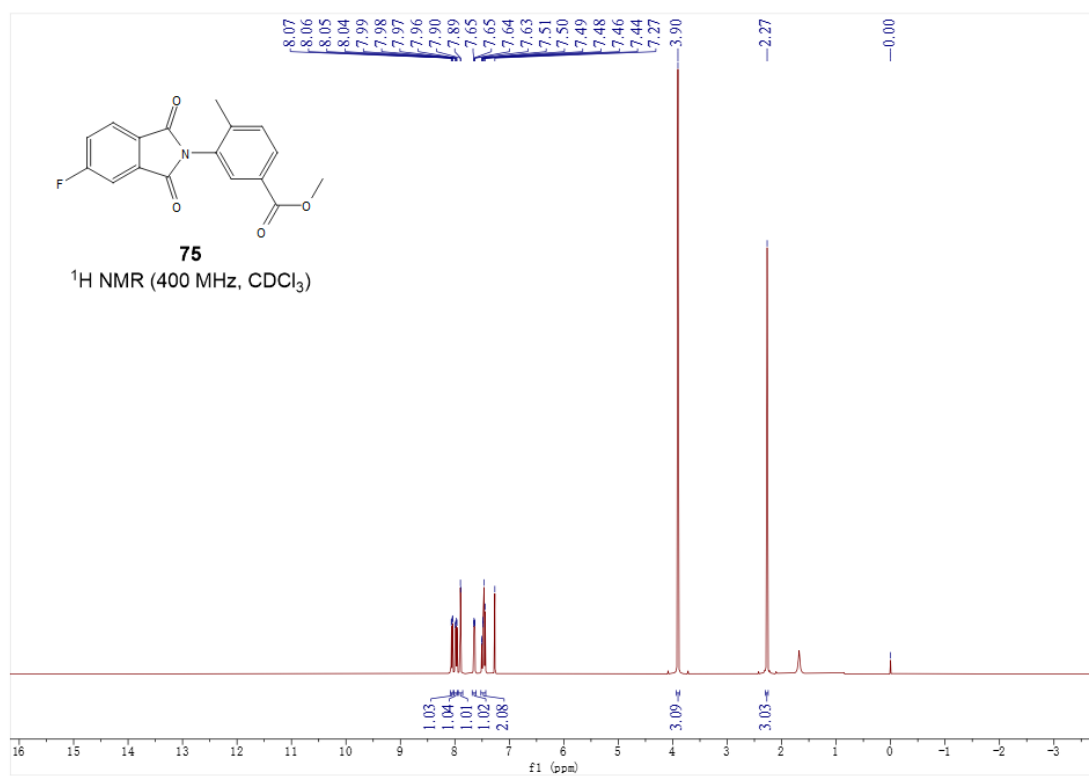
^1H NMR (400 MHz, CDCl_3) spectrum of **74**



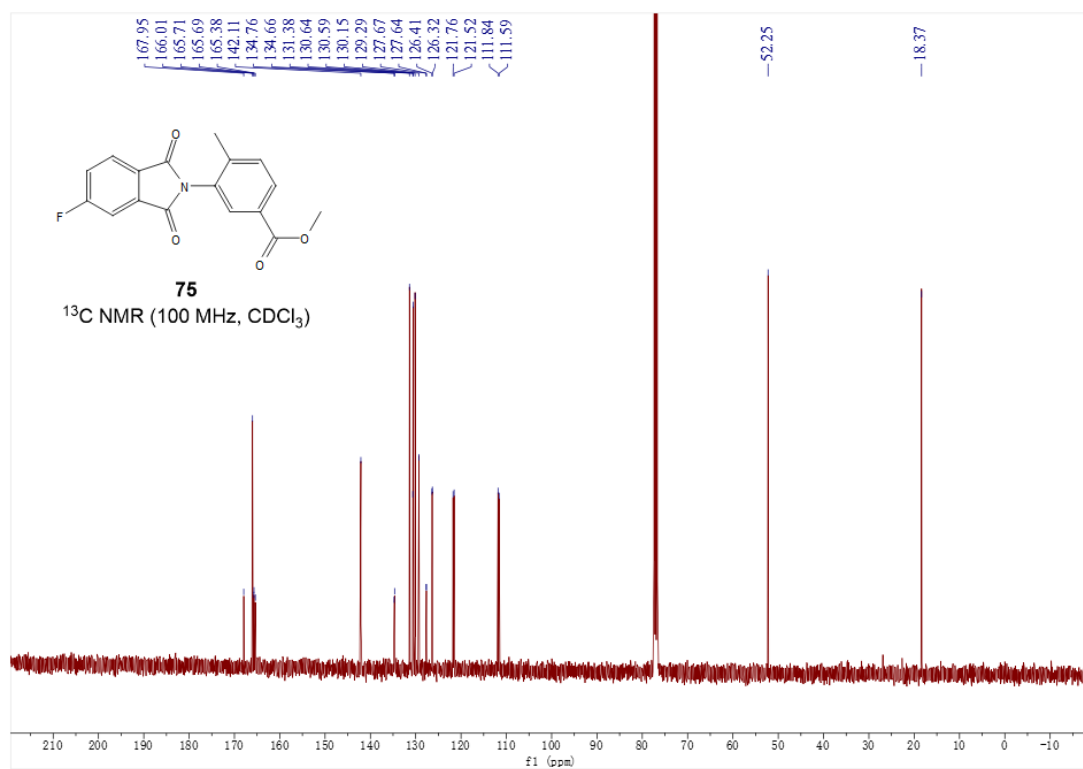
^{13}C NMR (100 MHz, CDCl_3) spectrum of **74**



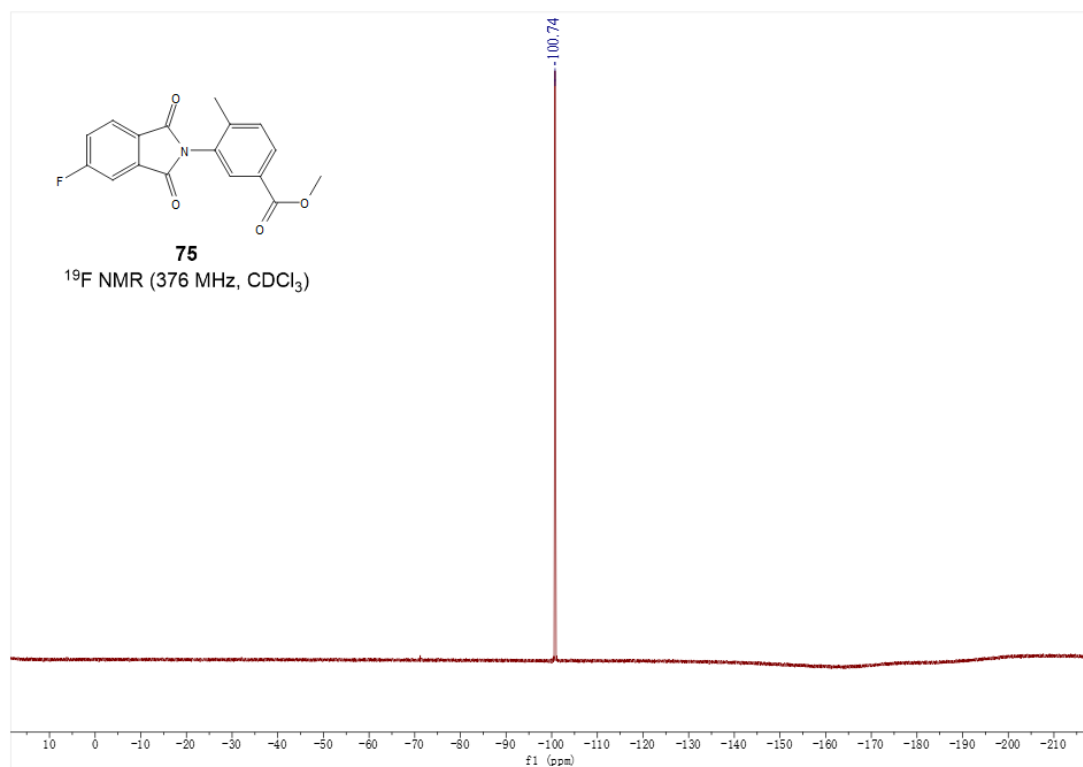
^1H NMR (400 MHz, CDCl_3) spectrum of **75**



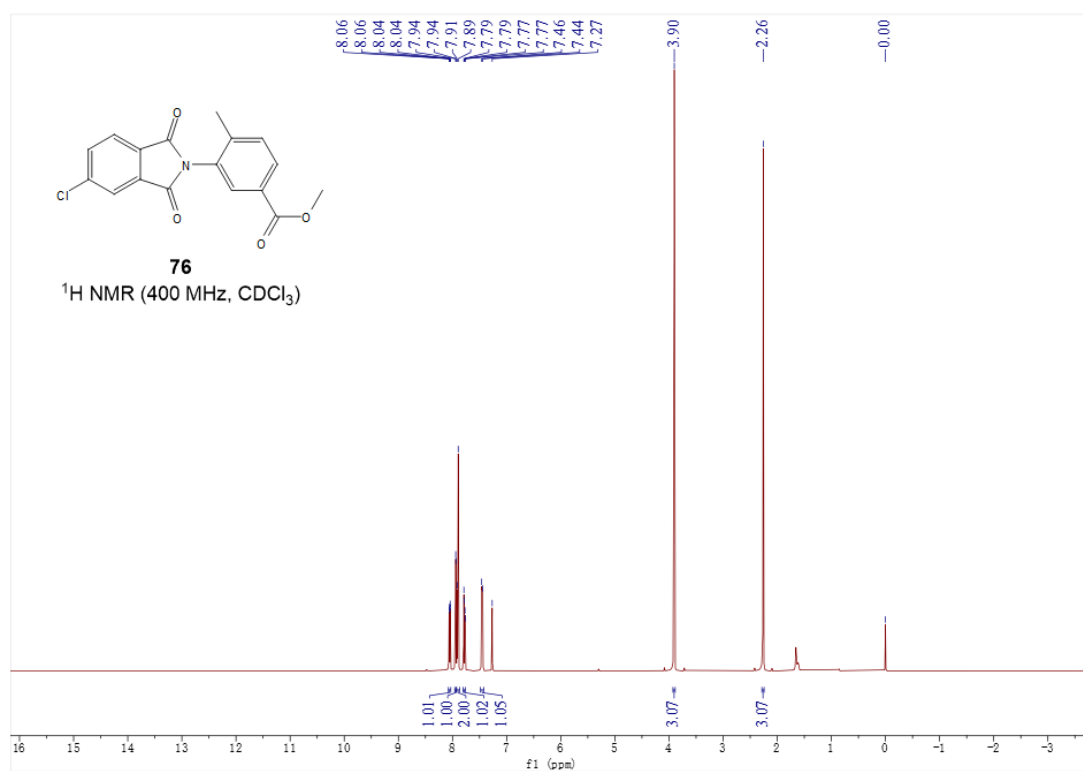
^{13}C NMR (100 MHz, CDCl_3) spectrum of **75**



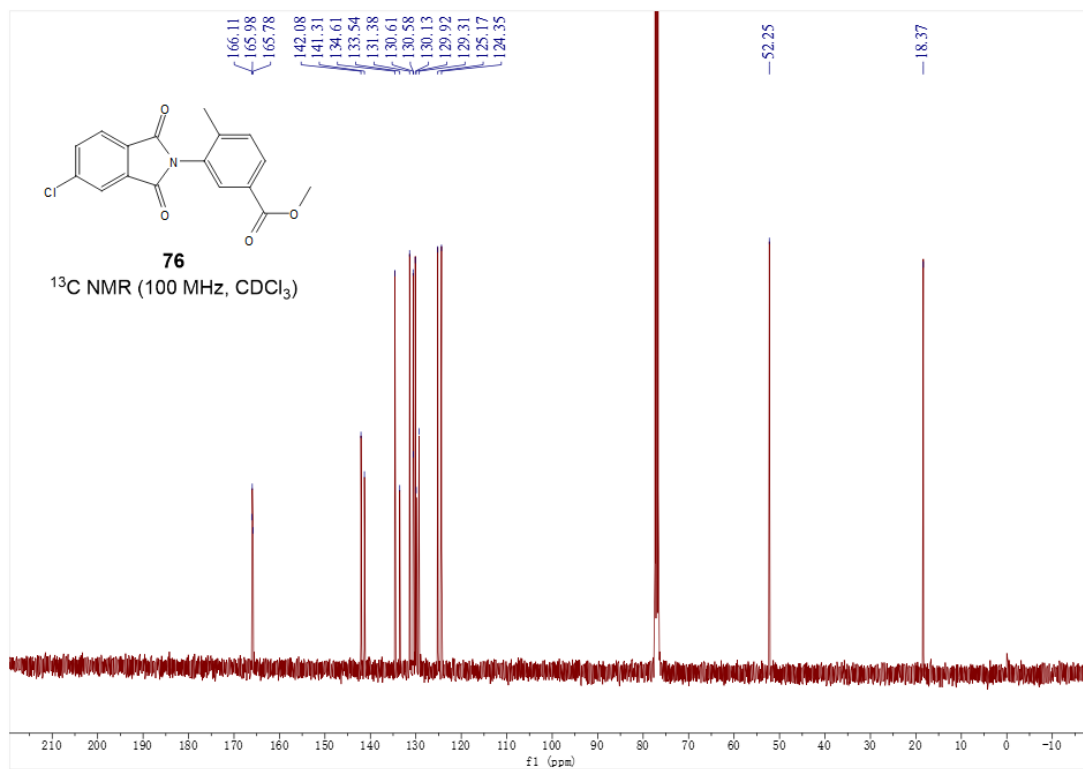
^{19}F NMR (376 MHz, CDCl_3) spectrum of **75**



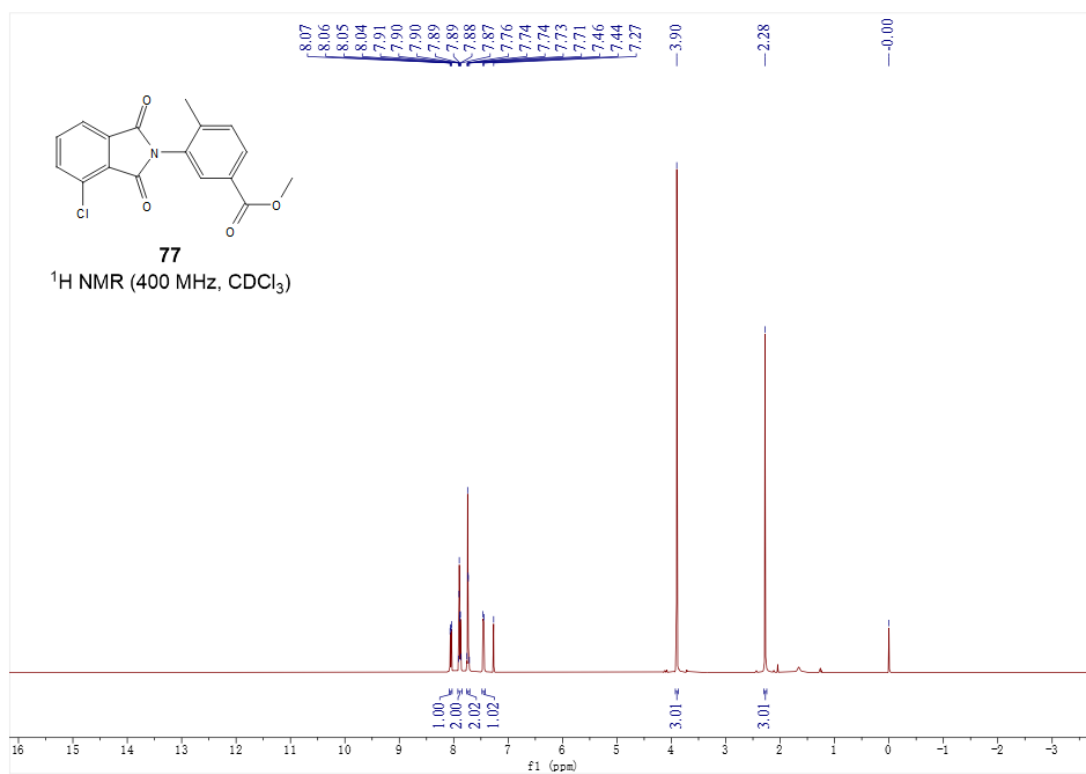
^1H NMR (400 MHz, CDCl_3) spectrum of **76**



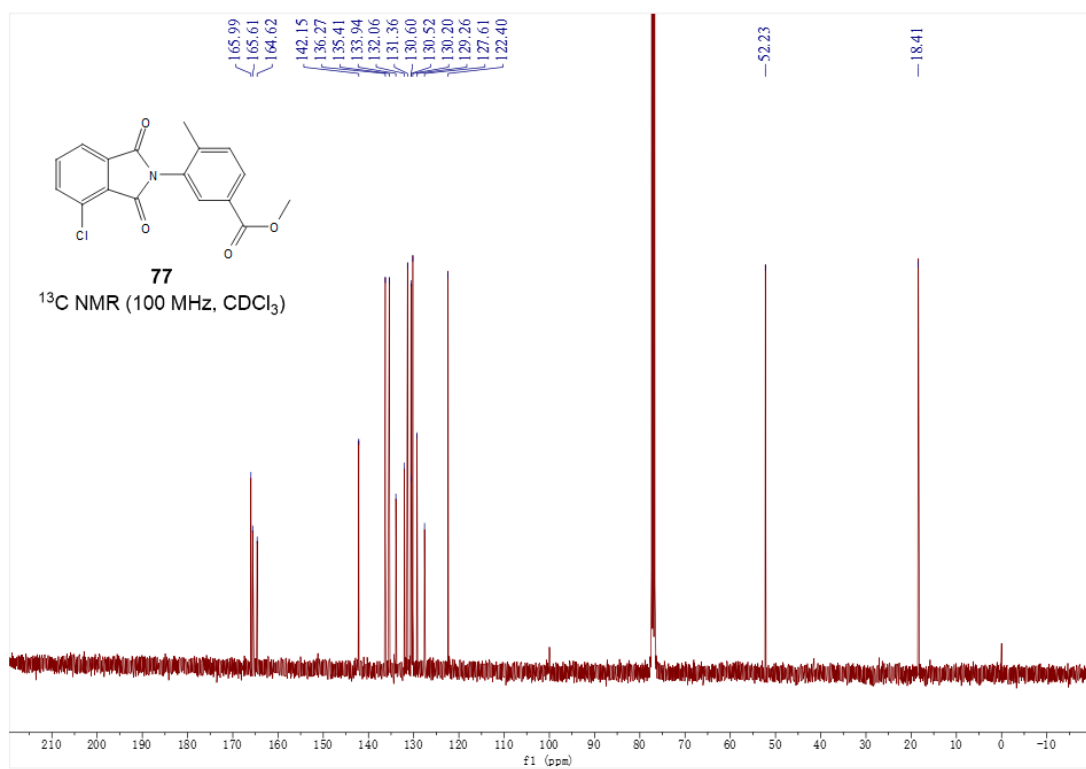
^{13}C NMR (100 MHz, CDCl_3) spectrum of **76**



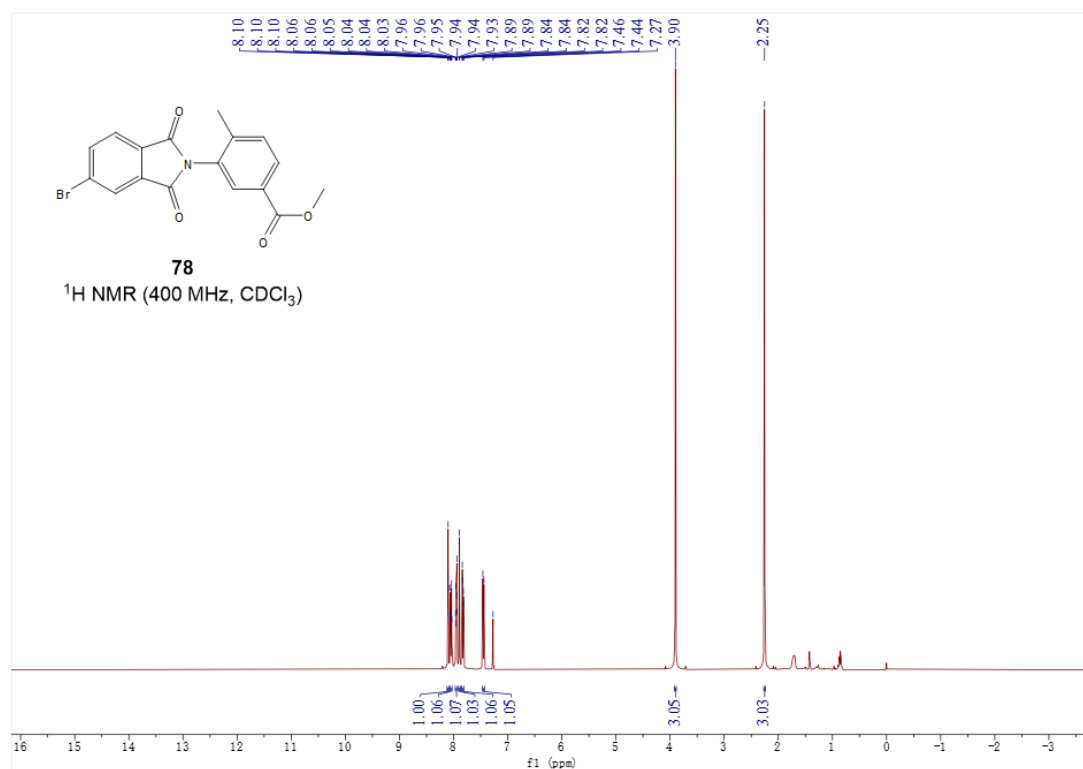
^1H NMR (400 MHz, CDCl_3) spectrum of **77**



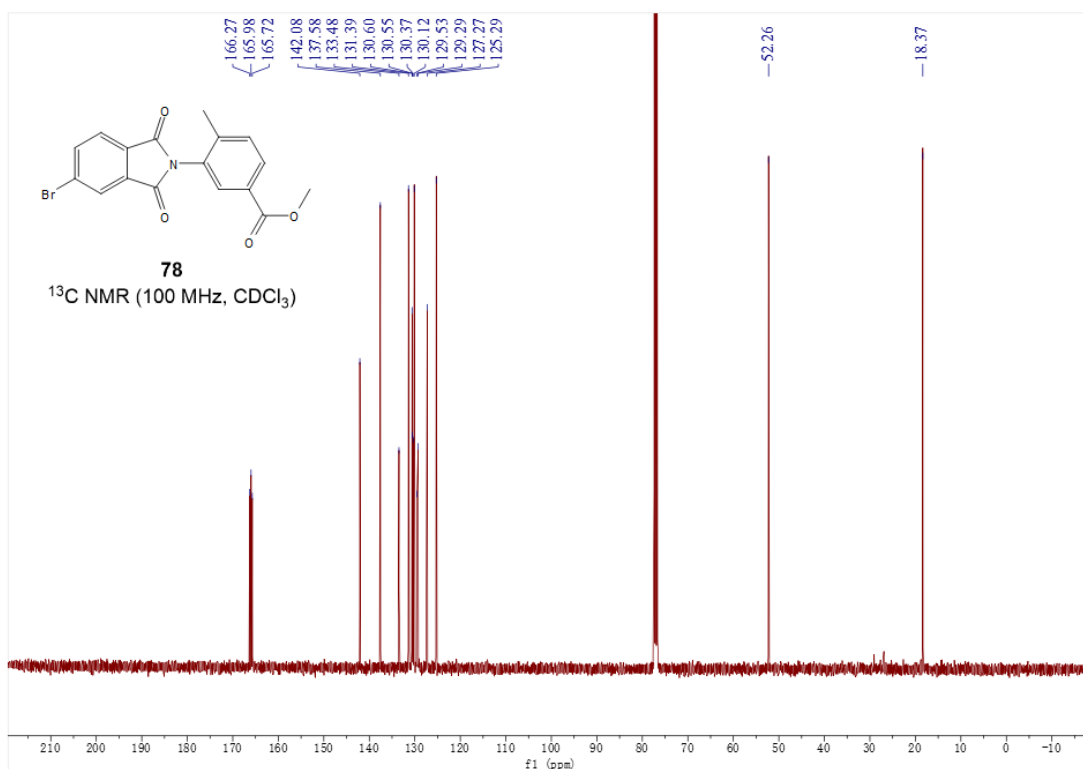
^{13}C NMR (100 MHz, CDCl_3) spectrum of **77**



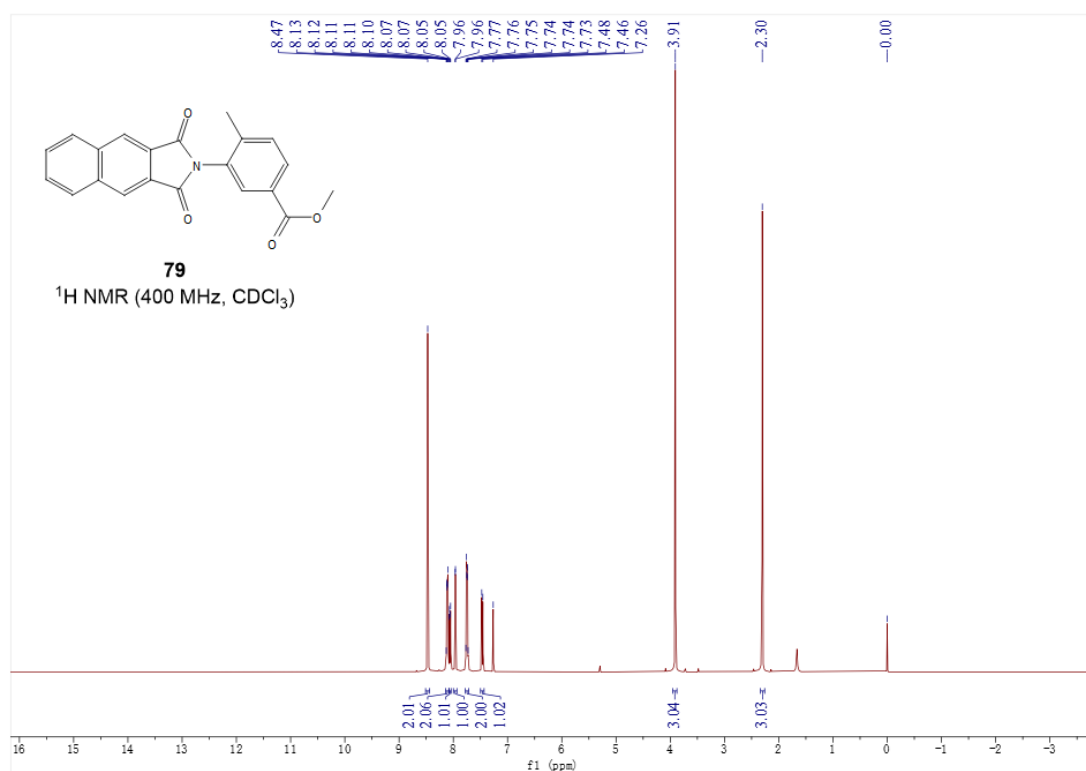
^1H NMR (400 MHz, CDCl_3) spectrum of **78**



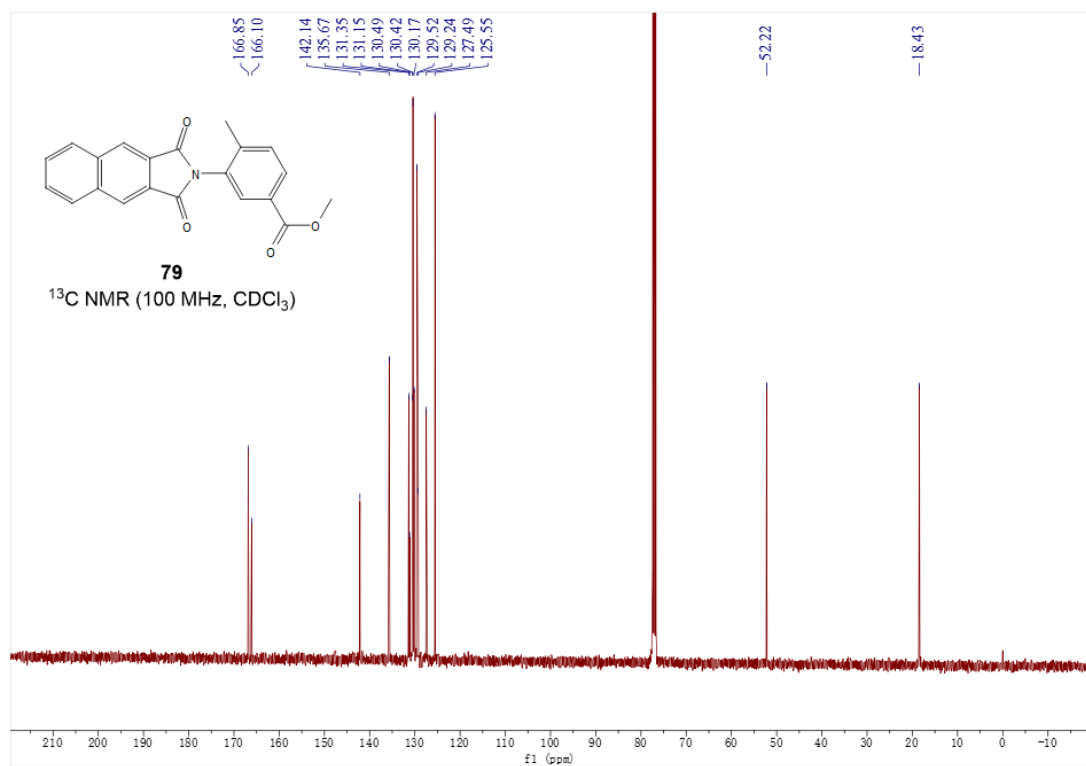
^{13}C NMR (100 MHz, CDCl_3) spectrum of **78**



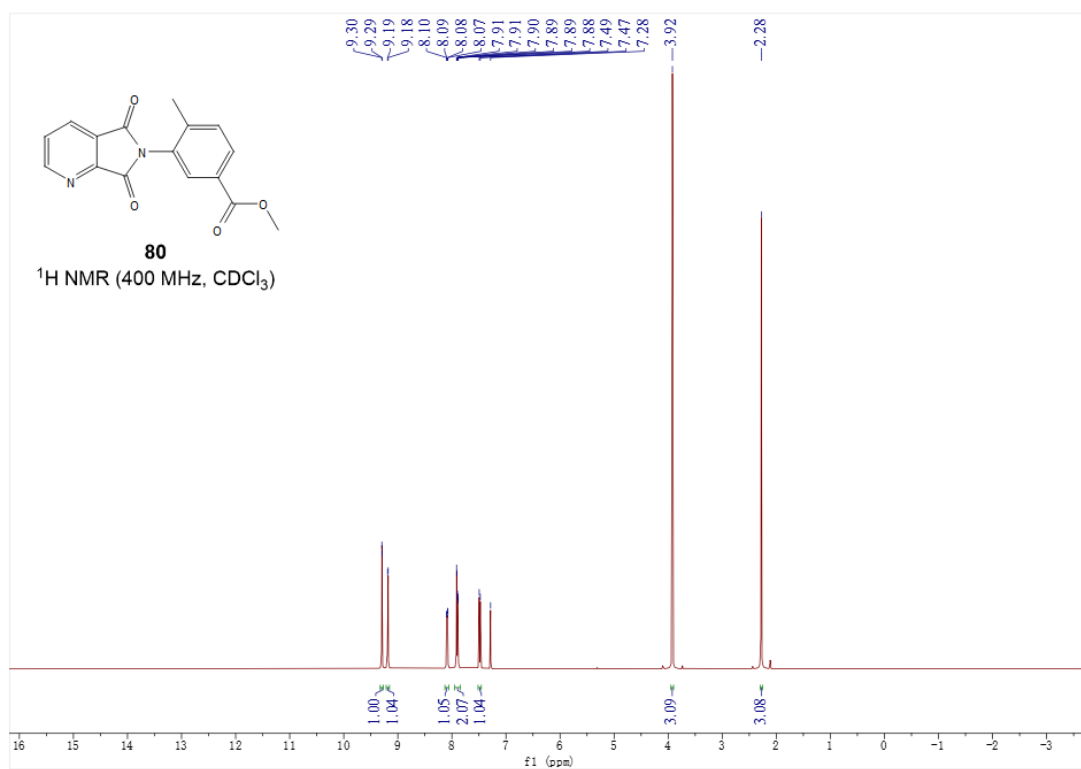
^1H NMR (400 MHz, CDCl_3) spectrum of **79**



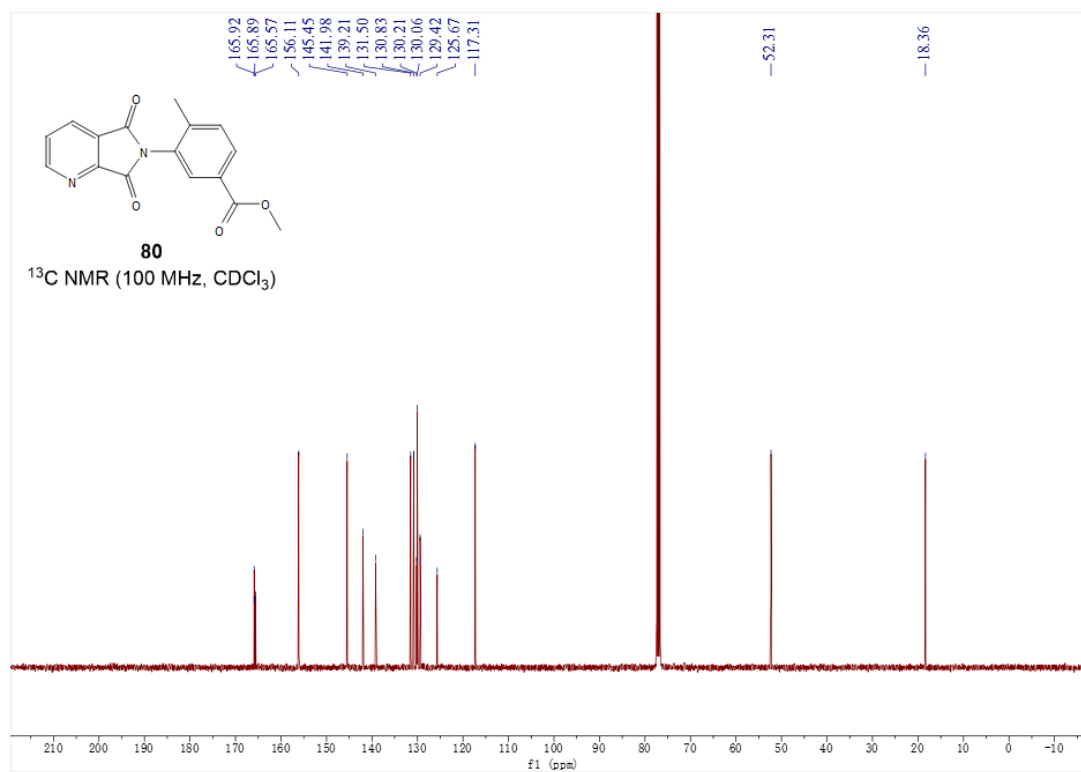
^{13}C NMR (100 MHz, CDCl_3) spectrum of **79**



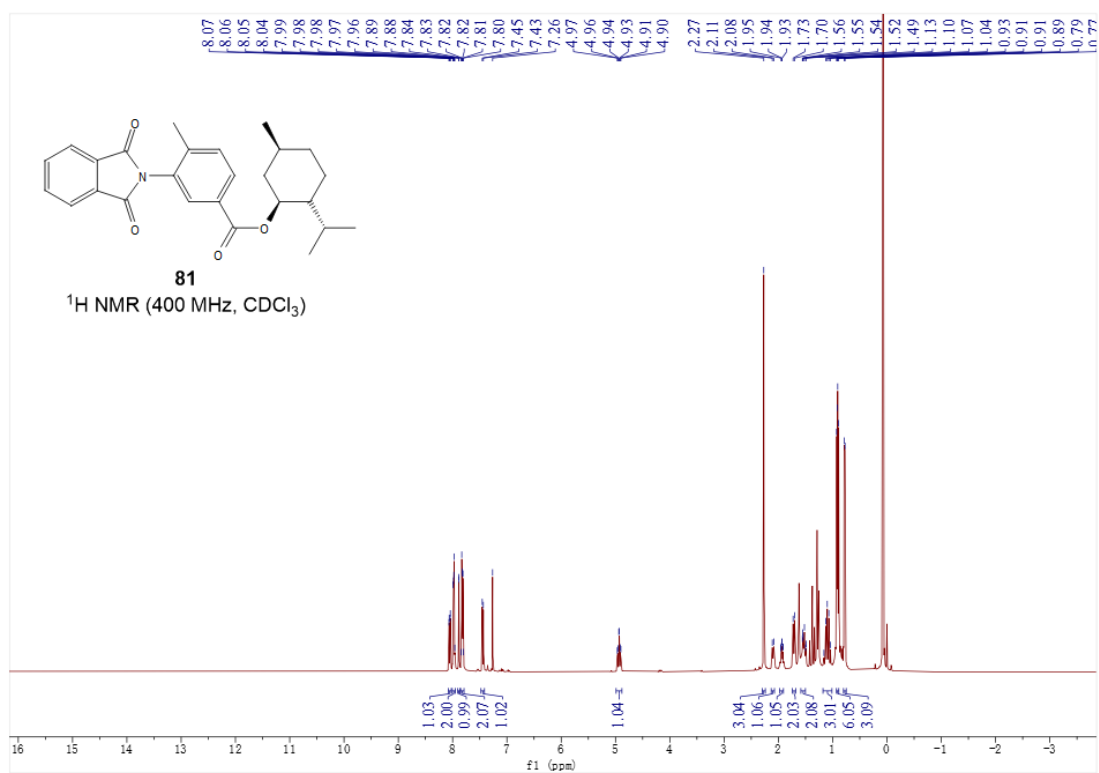
^1H NMR (400 MHz, CDCl_3) spectrum of **80**



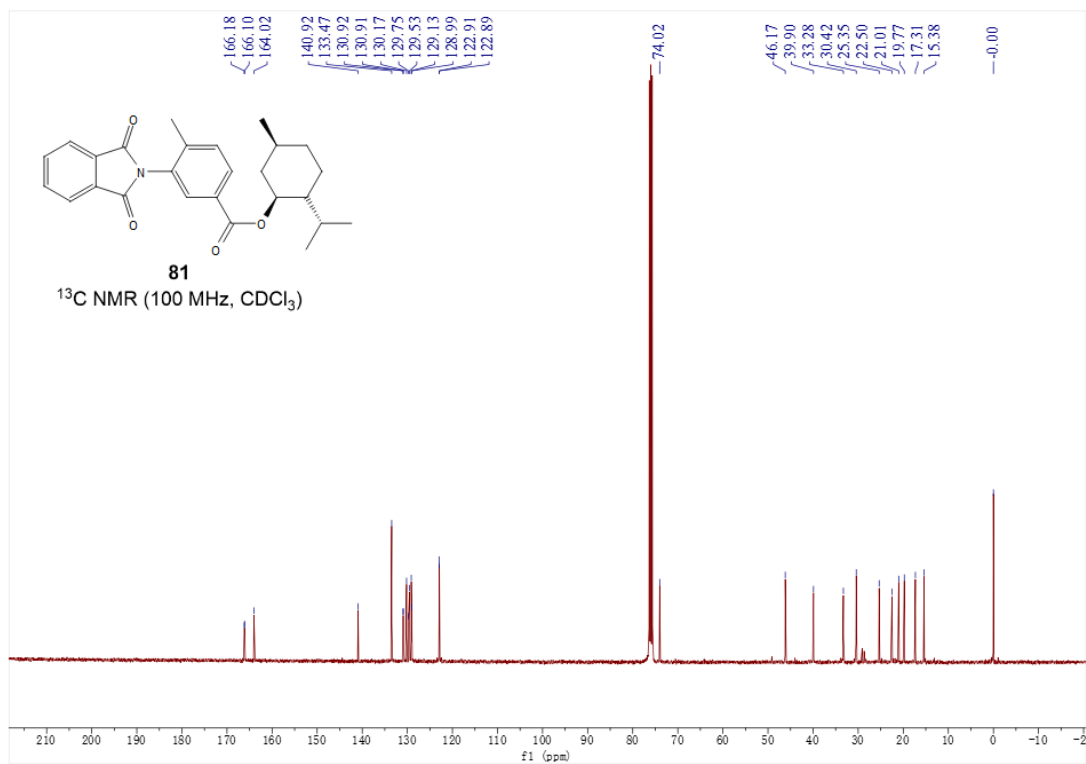
^{13}C NMR (100 MHz, CDCl_3) spectrum of **80**



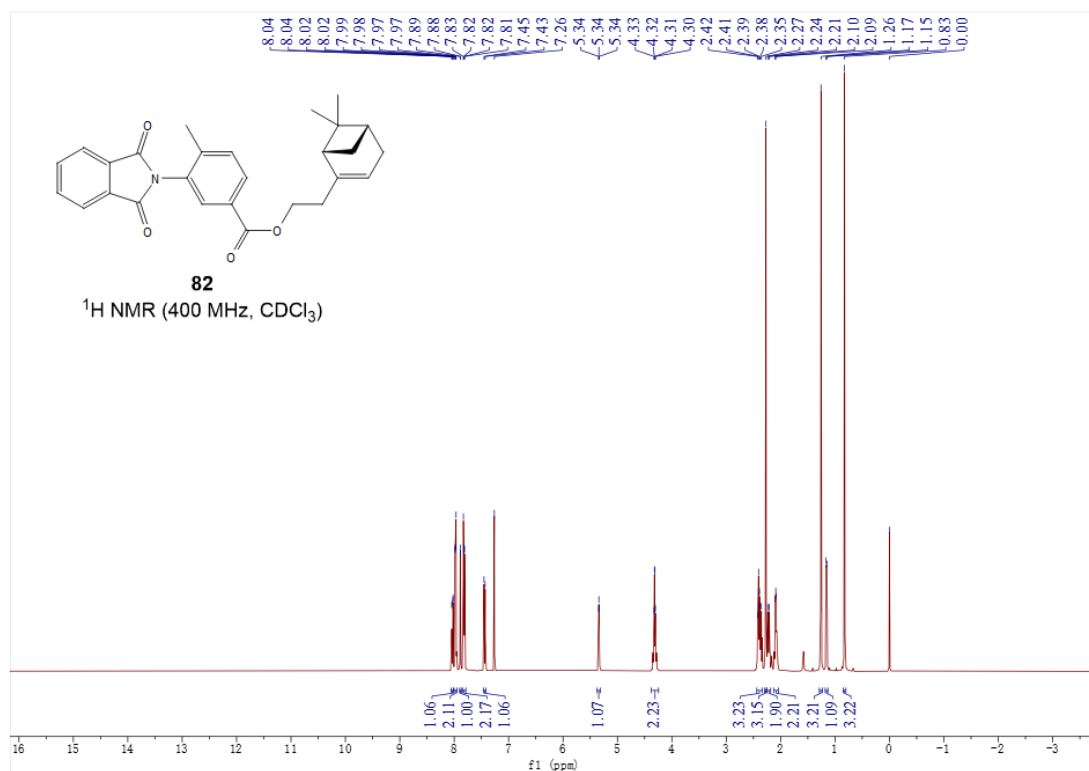
^1H NMR (400 MHz, CDCl_3) spectrum of **81**



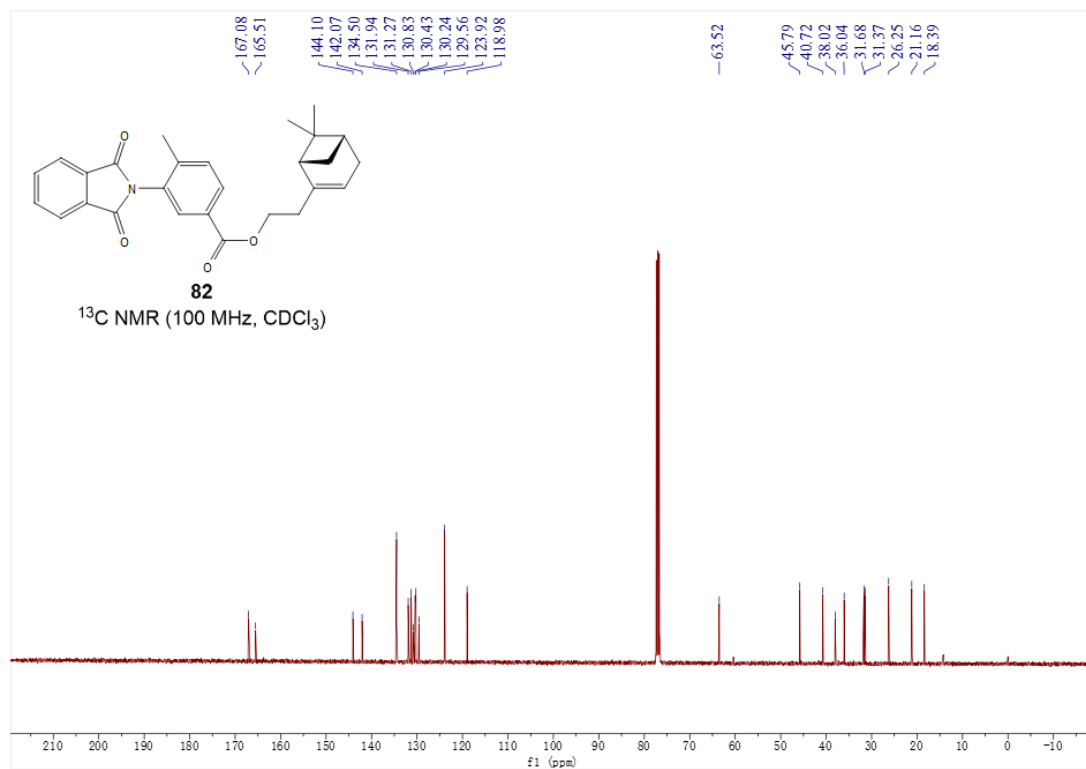
^{13}C NMR (100 MHz, CDCl_3) spectrum of **81**



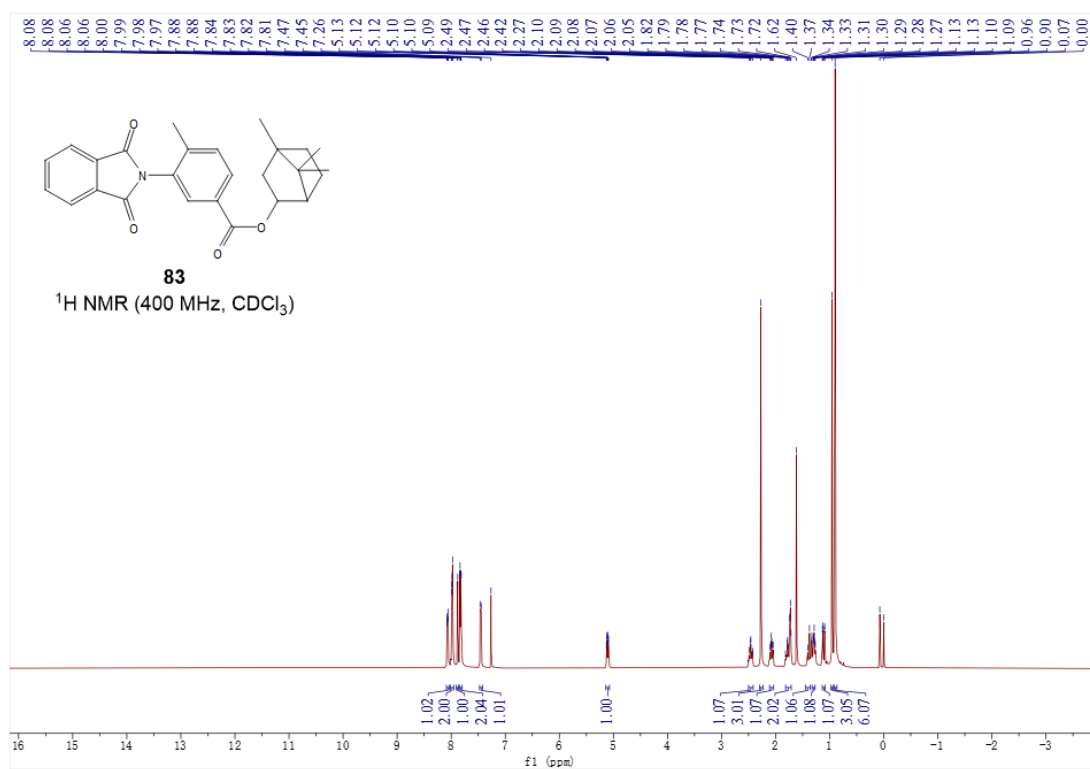
^1H NMR (400 MHz, CDCl_3) spectrum of **82**



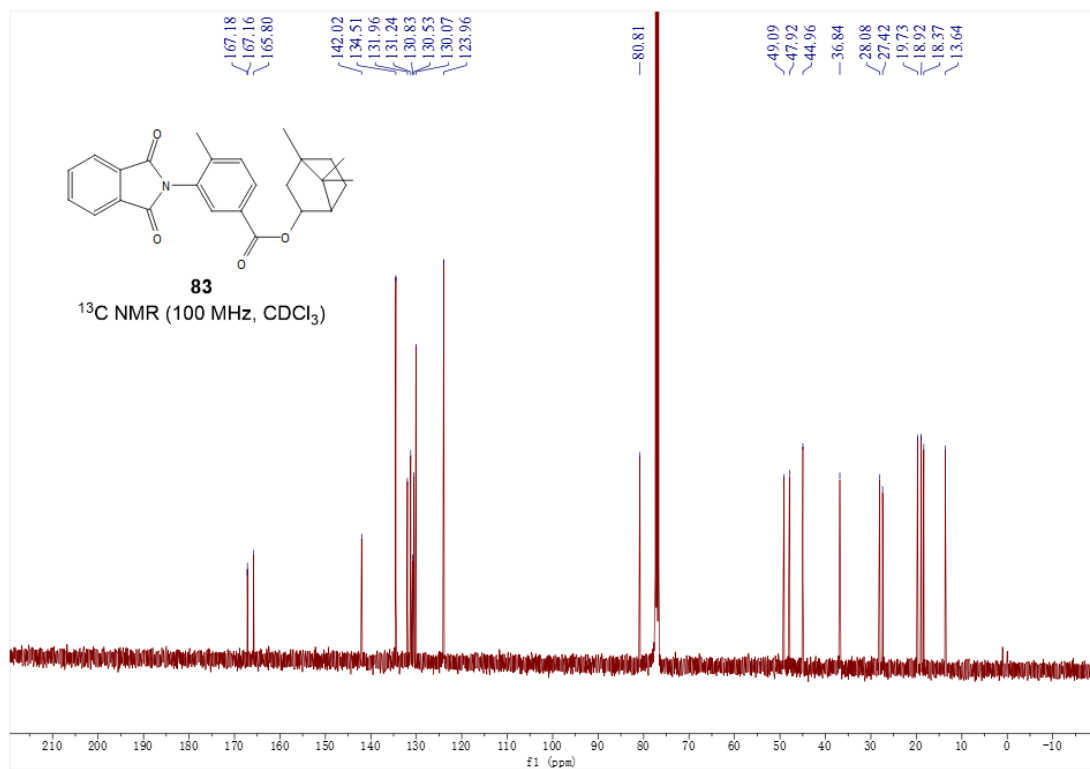
^{13}C NMR (100 MHz, CDCl_3) spectrum of **82**



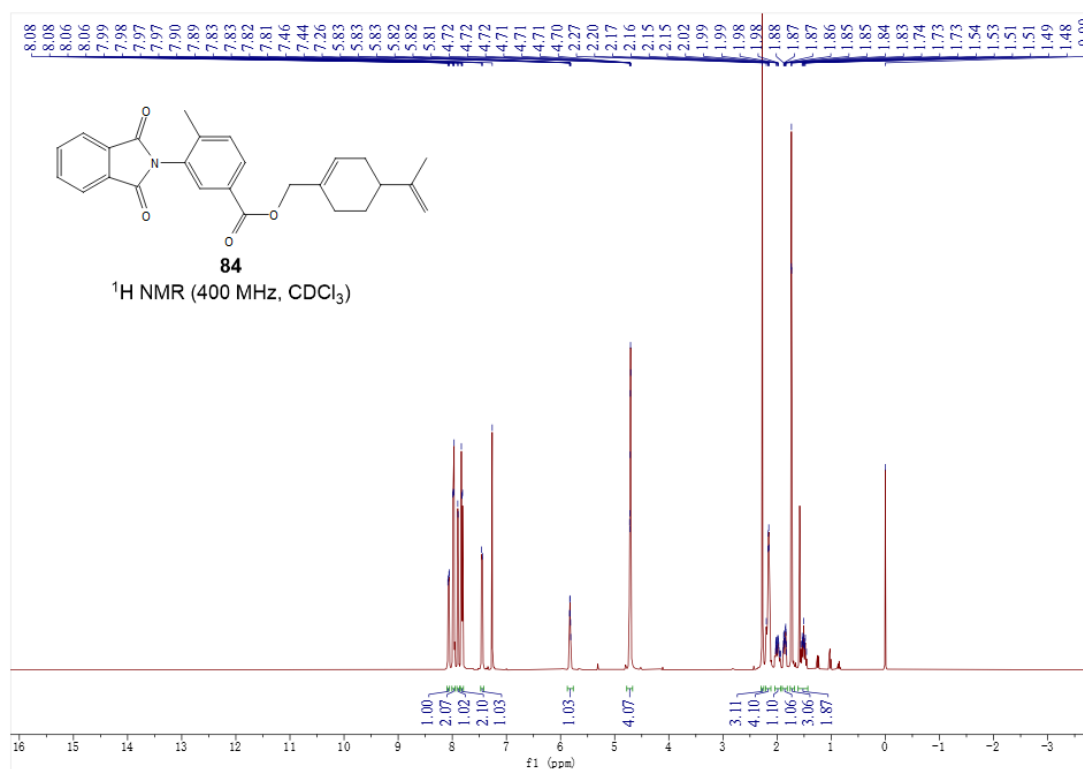
^1H NMR (400 MHz, CDCl_3) spectrum of **83**



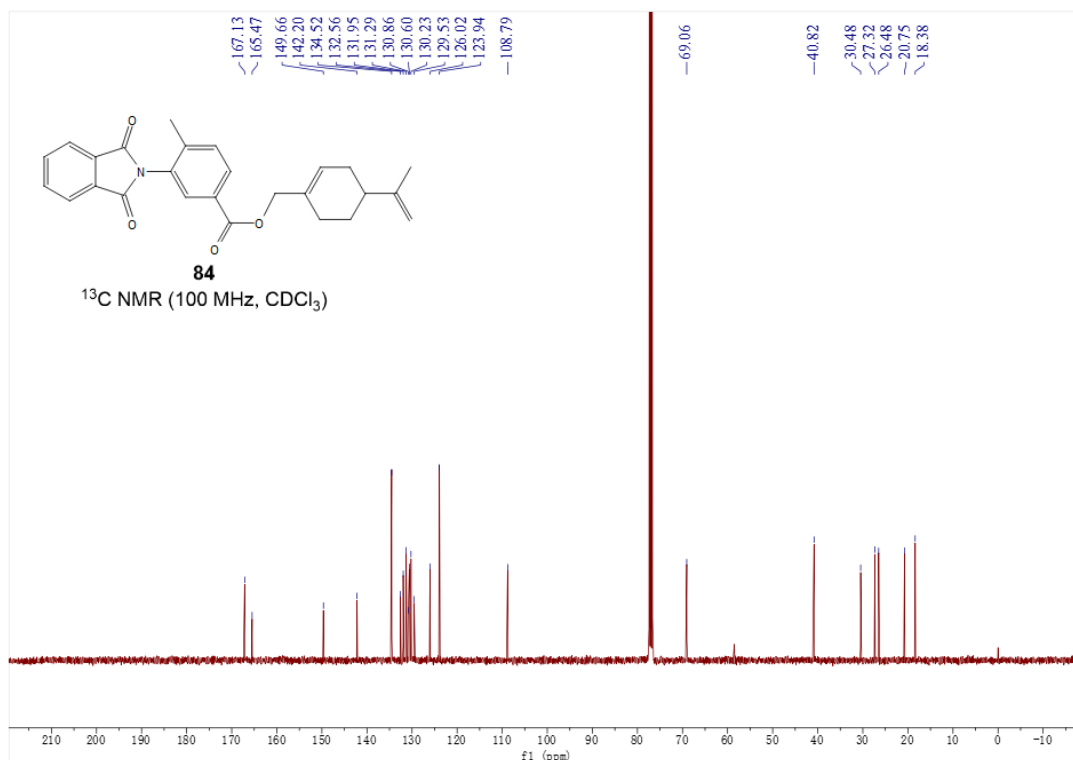
^{13}C NMR (100 MHz, CDCl_3) spectrum of **83**



^1H NMR (400 MHz, CDCl_3) spectrum of **84**



^{13}C NMR (100 MHz, CDCl_3) spectrum of **84**



85

^1H NMR (400 MHz, CDCl_3)

Chemical structure of compound 85: CC1=CC=C(C(=O)N1C2=CC=C(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C2)C3=CC=CC=C3

^1H NMR (400 MHz, CDCl_3) spectrum showing chemical shifts (ppm) and integration values:

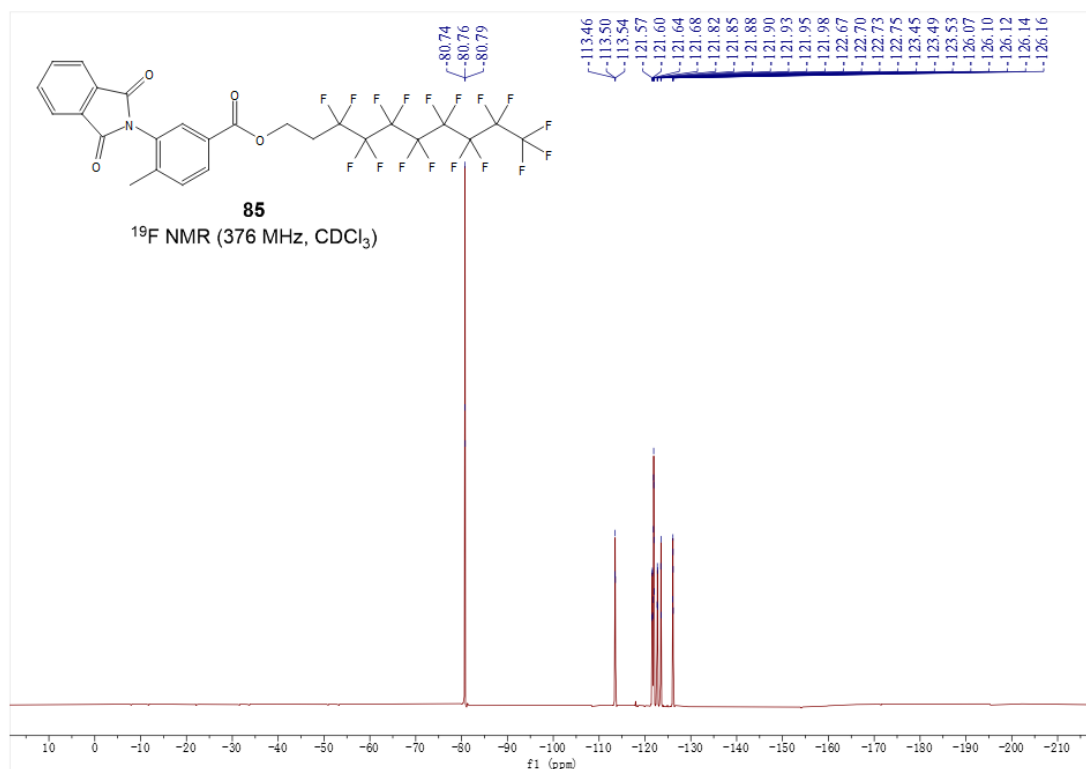
Chemical Shift (ppm)	Integration
8.06, 8.05, 8.04, 8.03, 7.99, 7.98, 7.97, 7.90, 7.89, 7.84, 7.83, 7.82, 7.81, 7.48, 7.46, 7.26, 4.64, 4.62, 4.60	1.07, 2.00, 1.05, 2.02, 1.00
2.65, 2.62, 2.60, 2.58, 2.56, 2.28	2.01, 2.08, 3.08
-0.00	

85

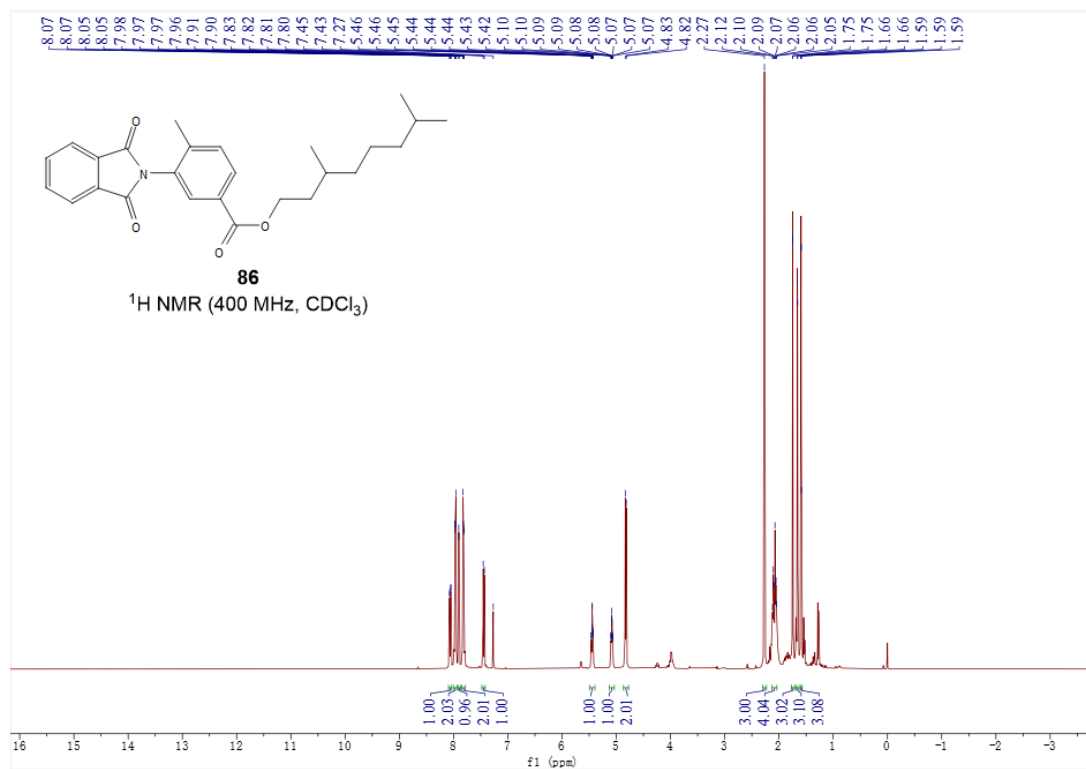
^{13}C NMR (100 MHz, CDCl_3)

167.06
165.12
142.80
134.55
131.91
131.46
131.03
130.55
130.35
128.57
123.96
57.03
56.98
30.64
18.45

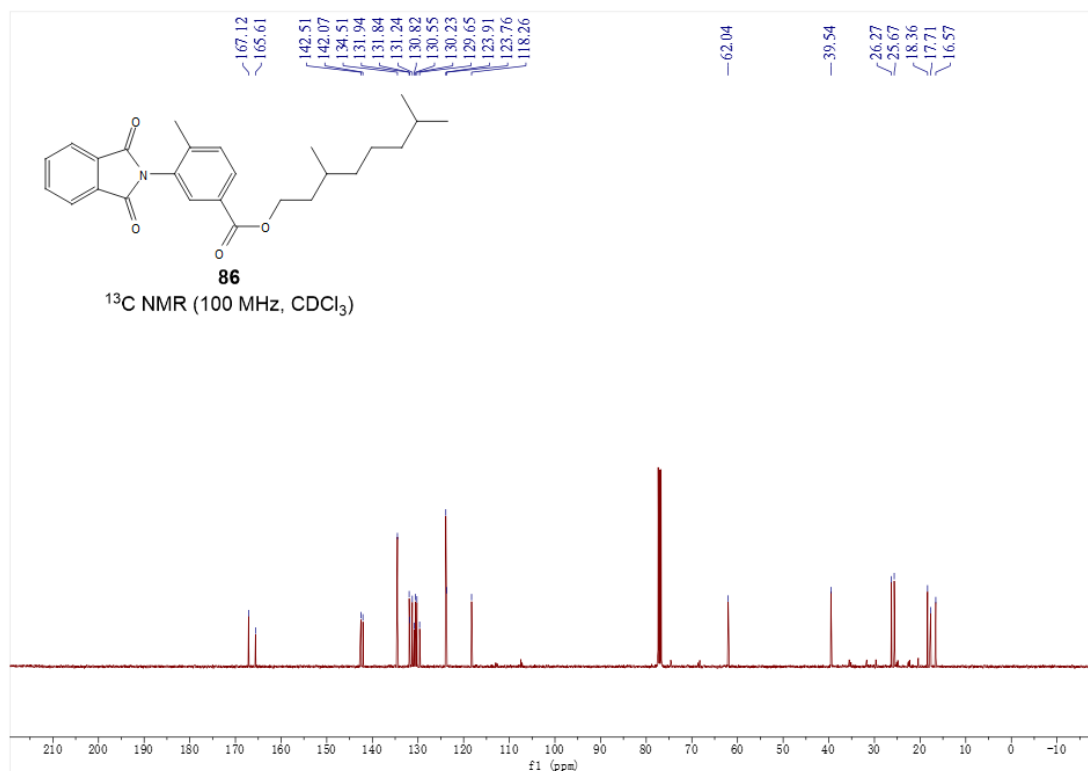
^{19}F NMR (376 MHz, CDCl_3) spectrum of **85**



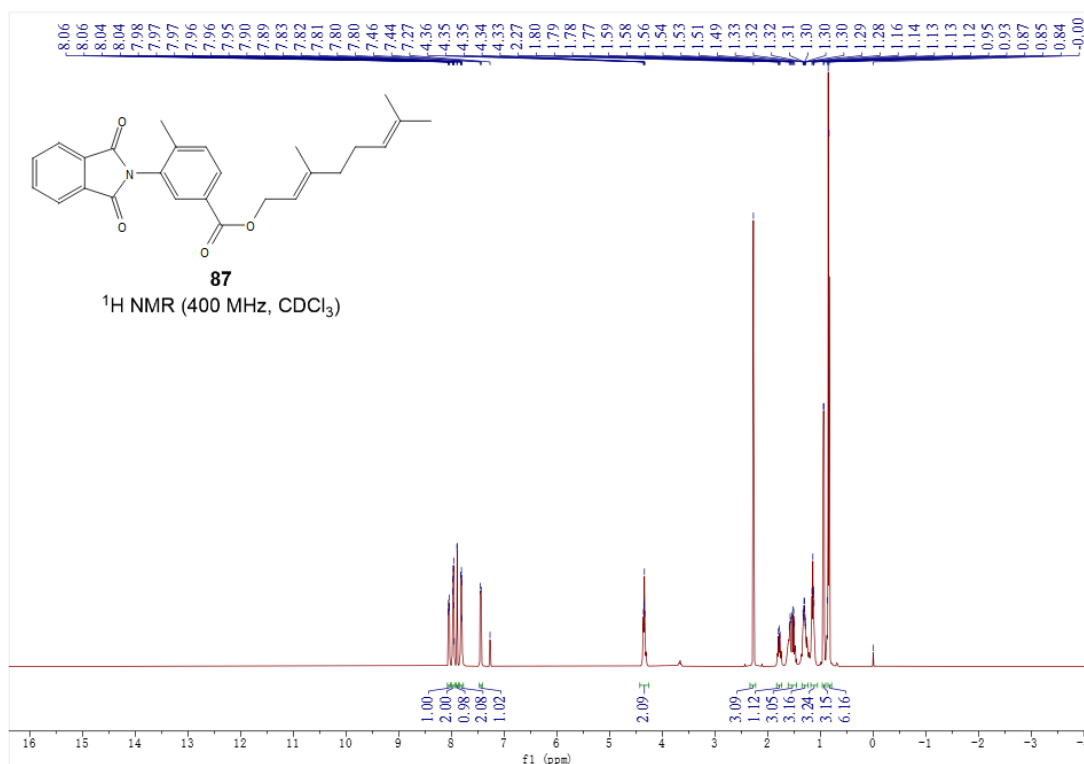
^1H NMR (400 MHz, CDCl_3) spectrum of **86**



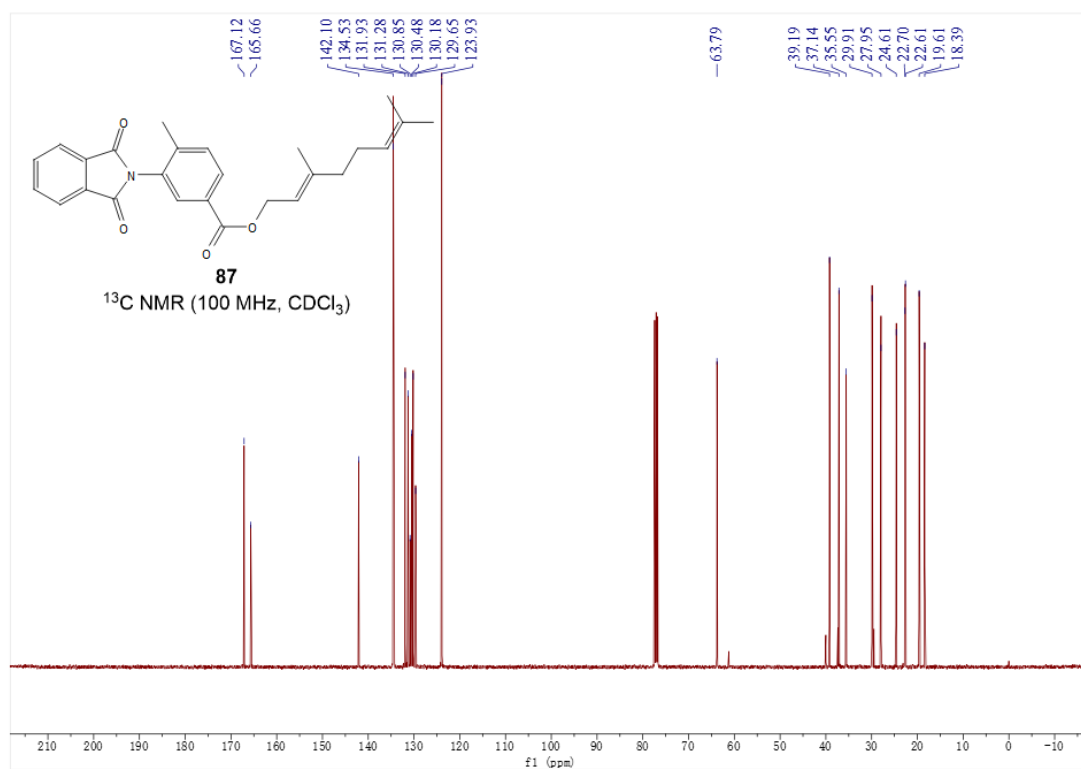
^{13}C NMR (100 MHz, CDCl_3) spectrum of **86**



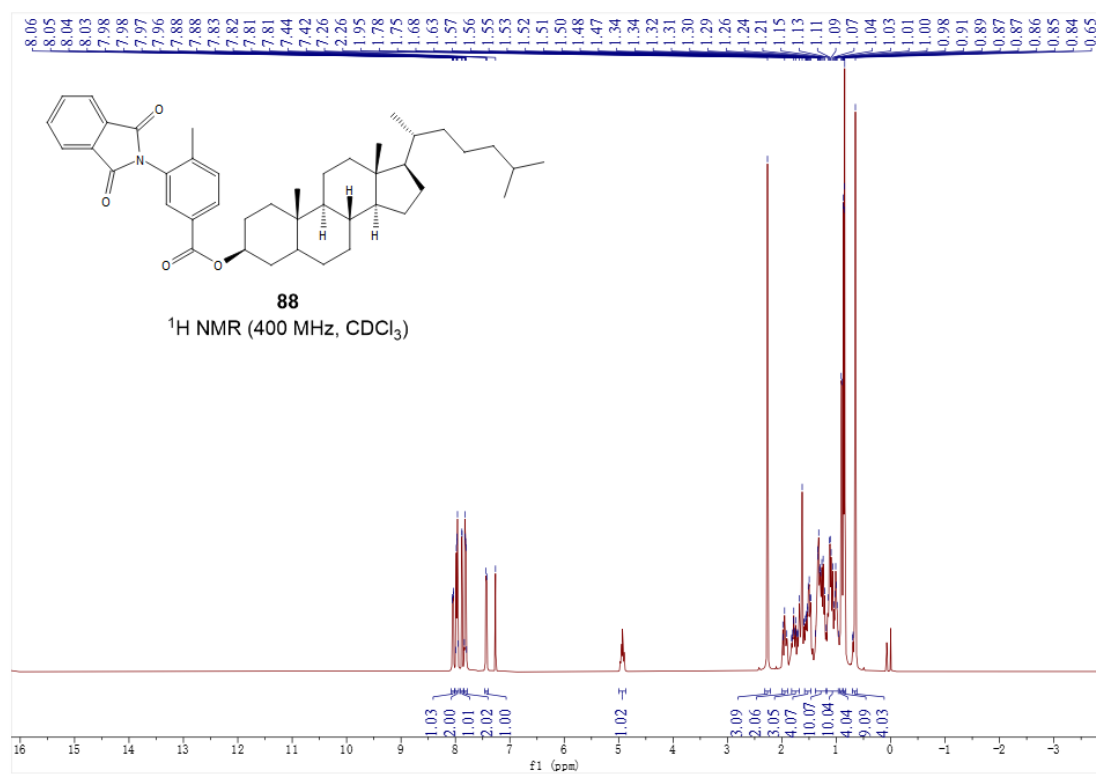
^1H NMR (400 MHz, CDCl_3) spectrum of **87**



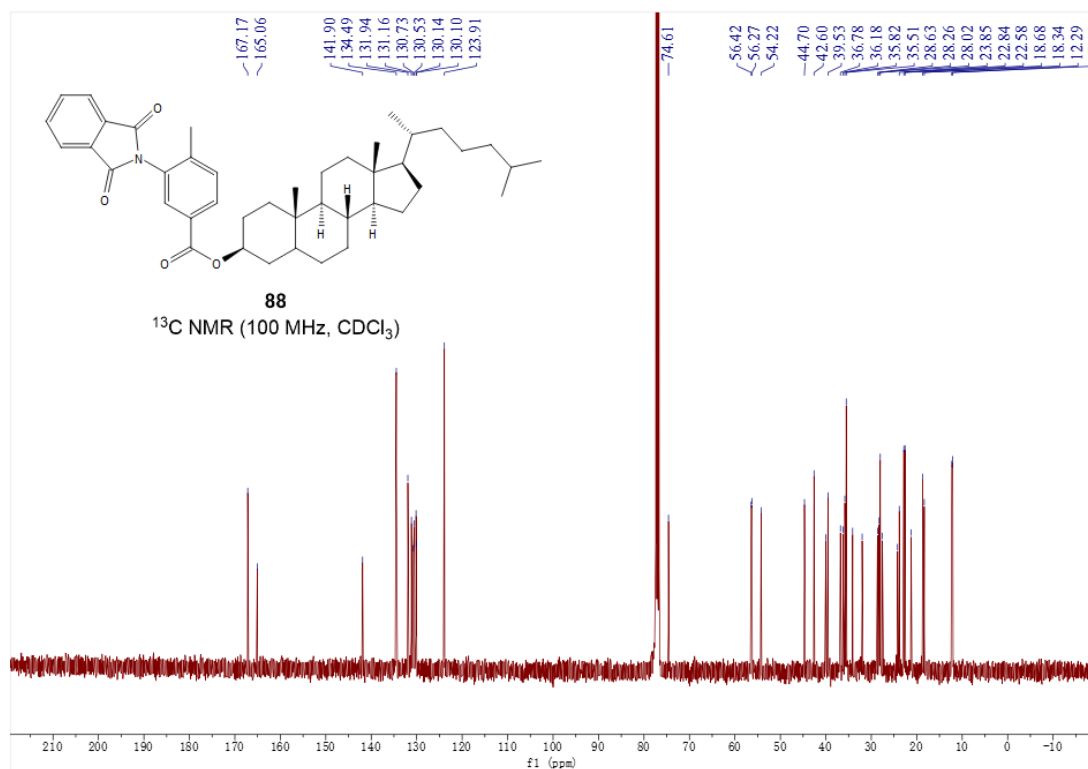
^{13}C NMR (100 MHz, CDCl_3) spectrum of **87**



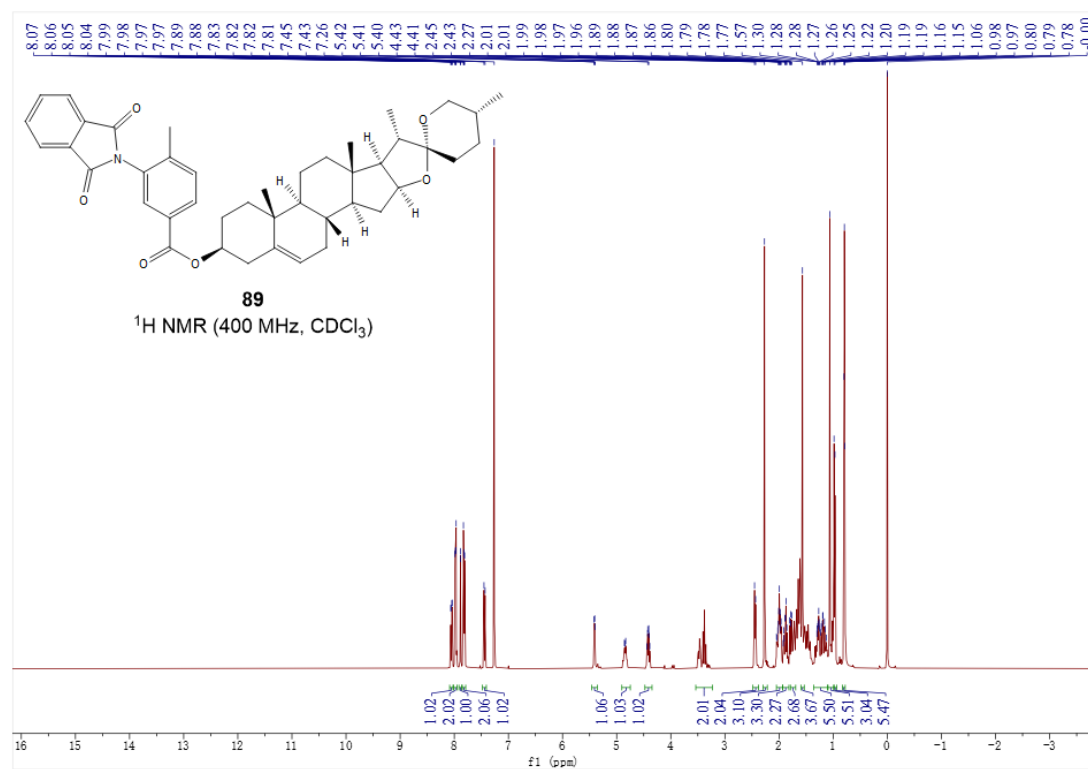
^1H NMR (400 MHz, CDCl_3) spectrum of **88**



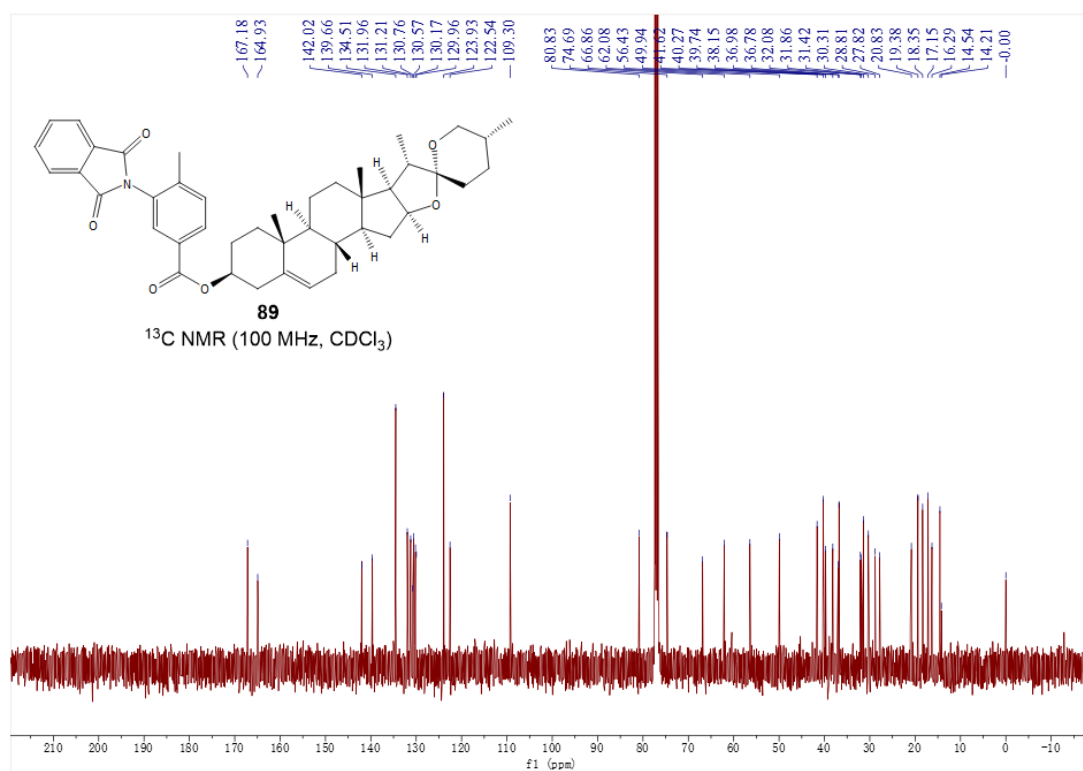
^{13}C NMR (100 MHz, CDCl_3) spectrum of **88**



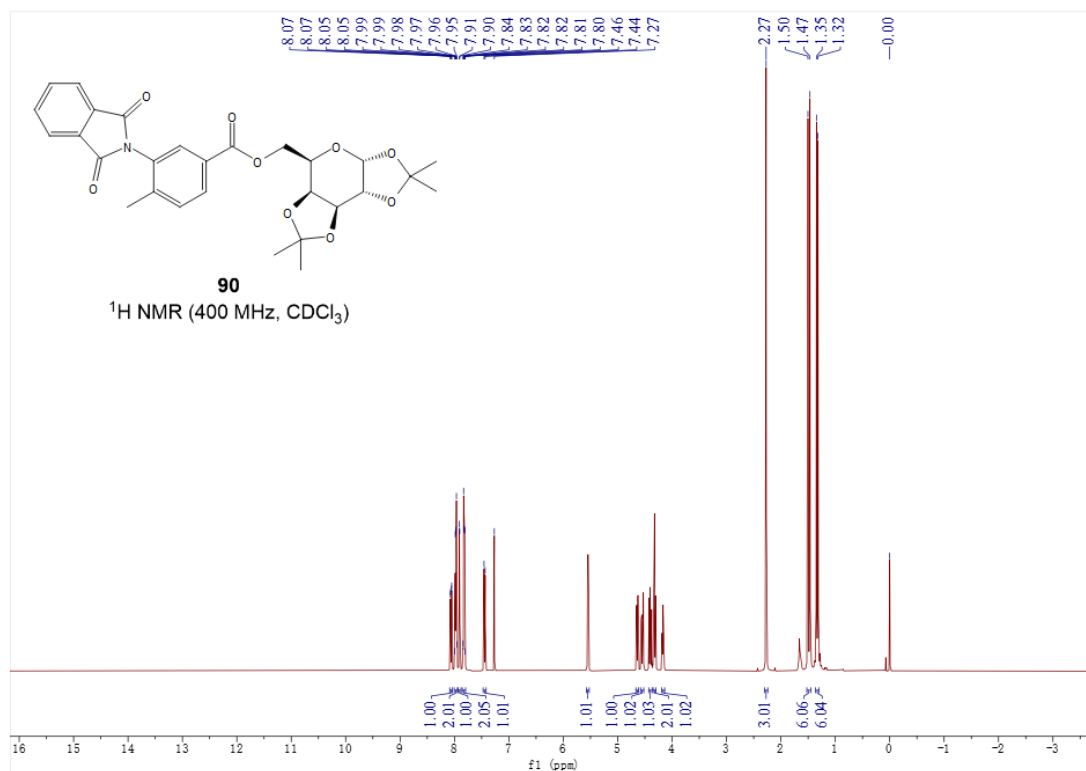
^1H NMR (400 MHz, CDCl_3) spectrum of **89**



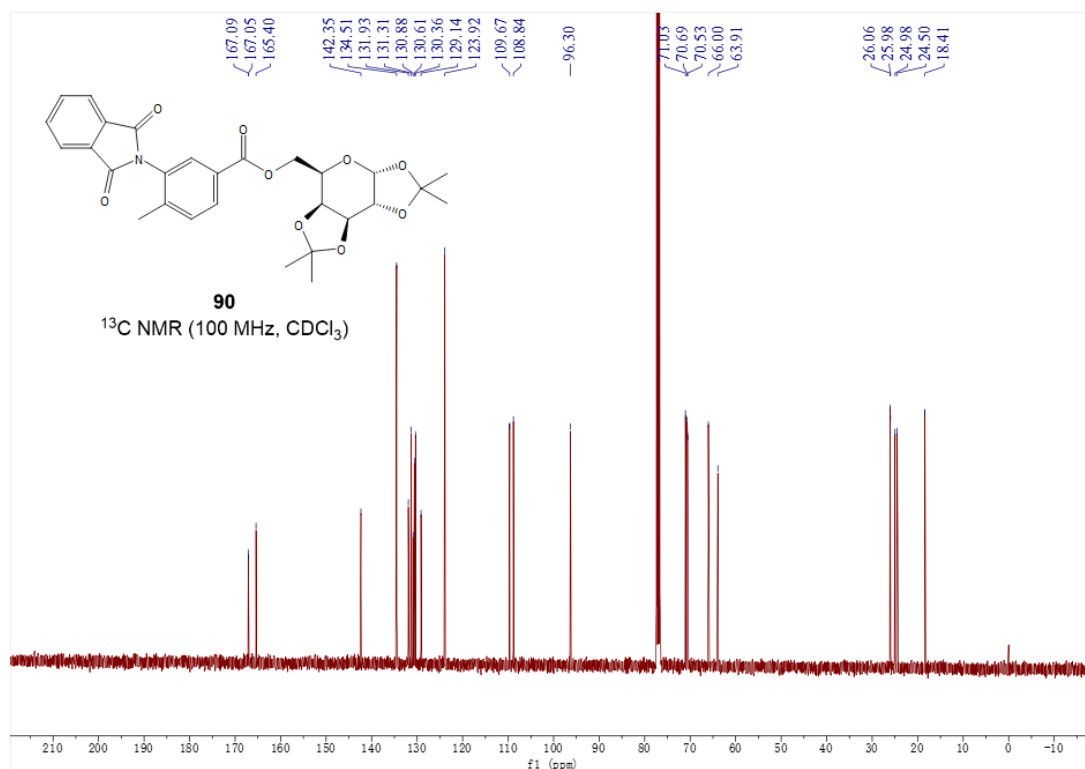
^{13}C NMR (100 MHz, CDCl_3) spectrum of **89**



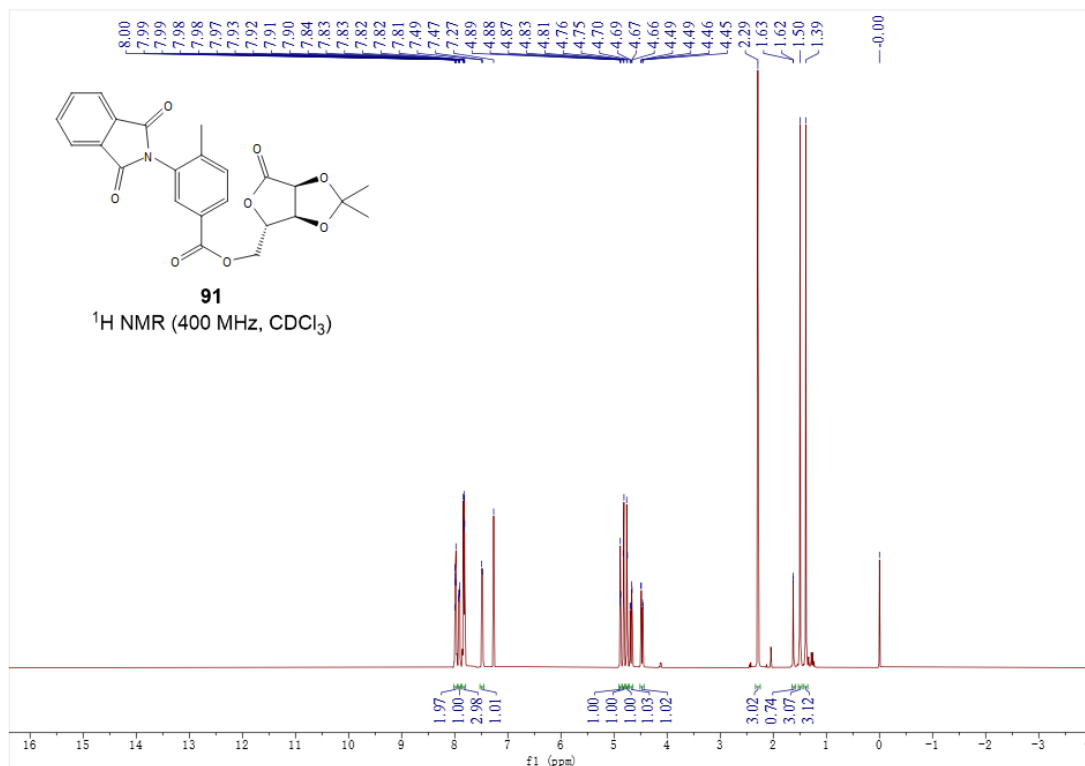
^1H NMR (400 MHz, CDCl_3) spectrum of **90**



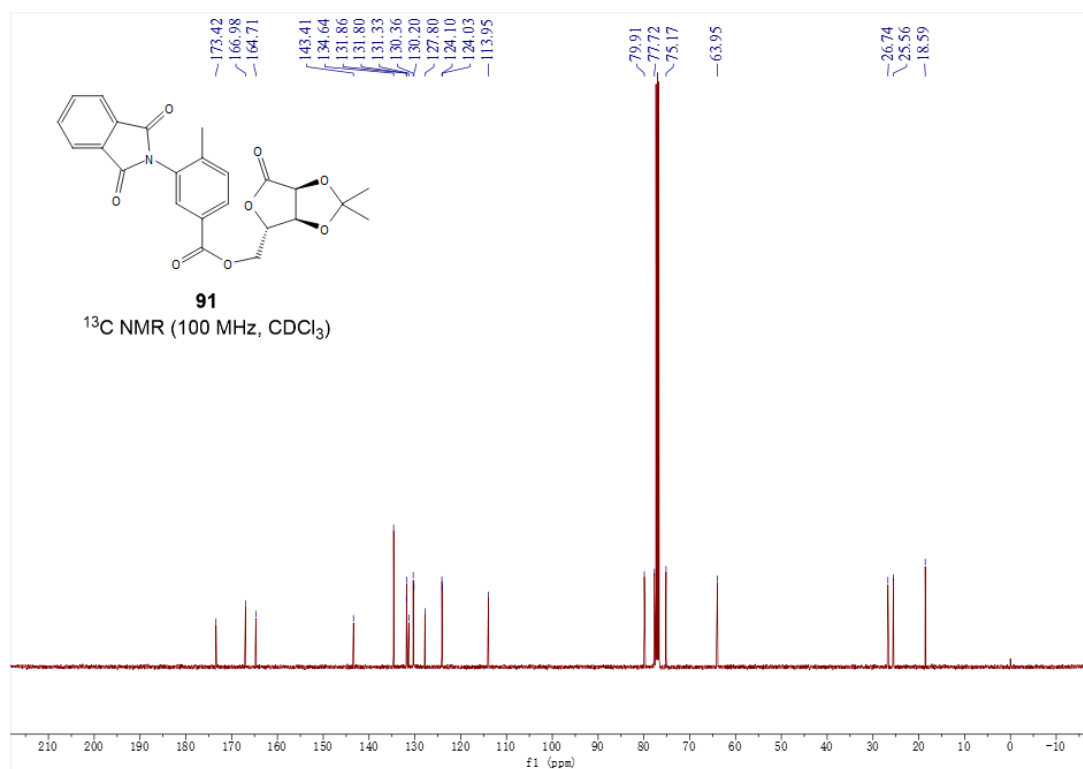
^{13}C NMR (100 MHz, CDCl_3) spectrum of **90**



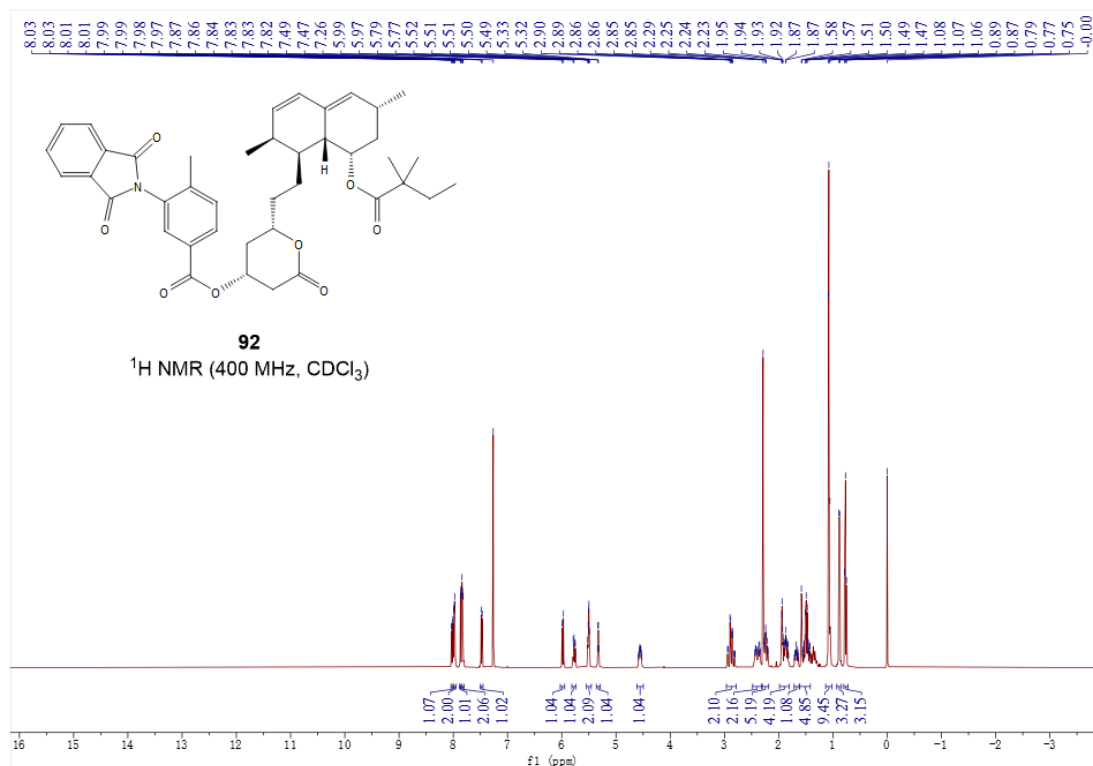
^1H NMR (400 MHz, CDCl_3) spectrum of **91**



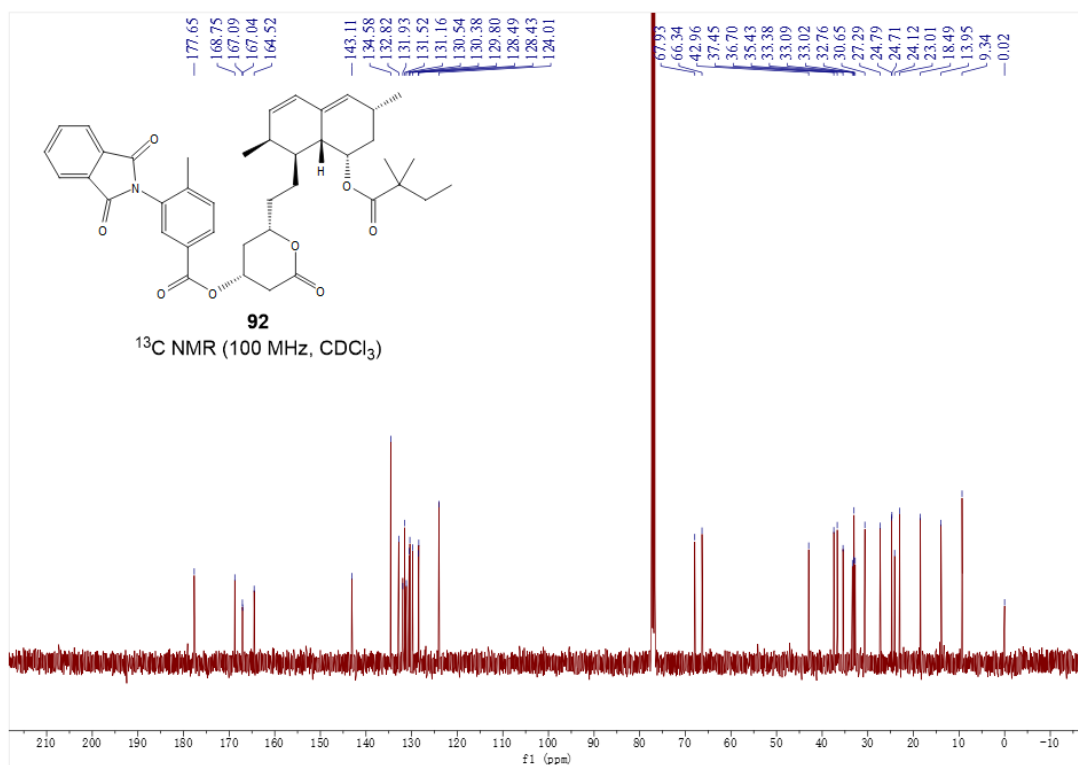
^{13}C NMR (100 MHz, CDCl_3) spectrum of **91**



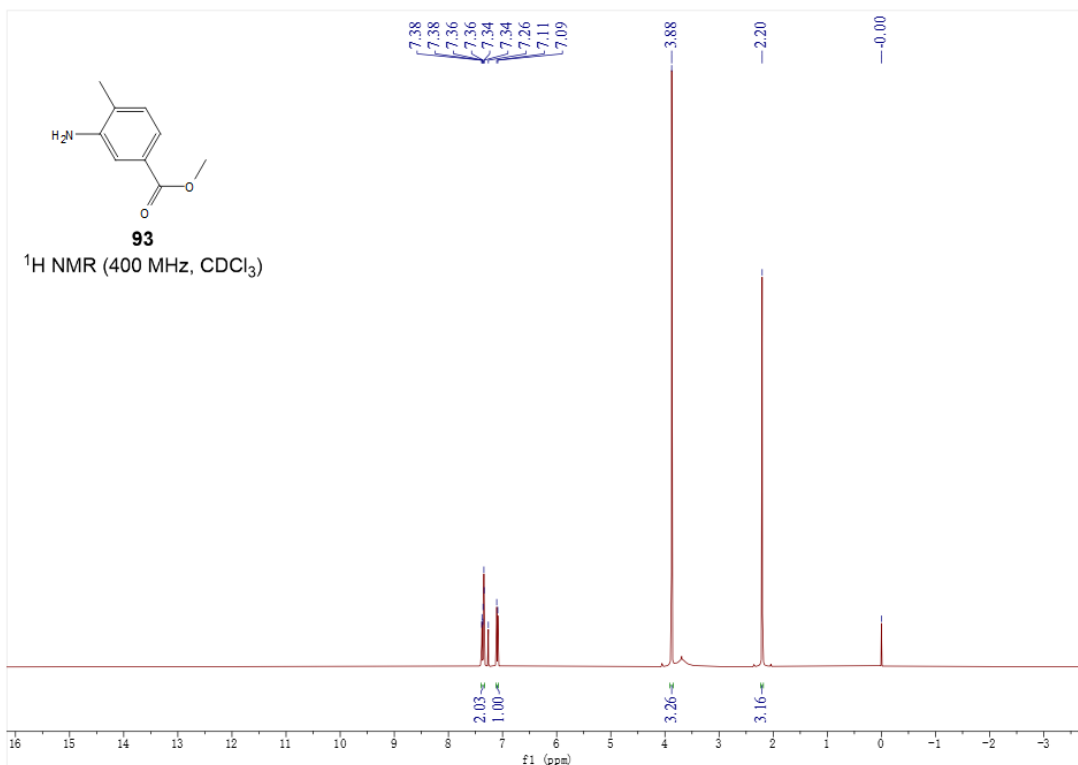
^1H NMR (400 MHz, CDCl_3) spectrum of **92**



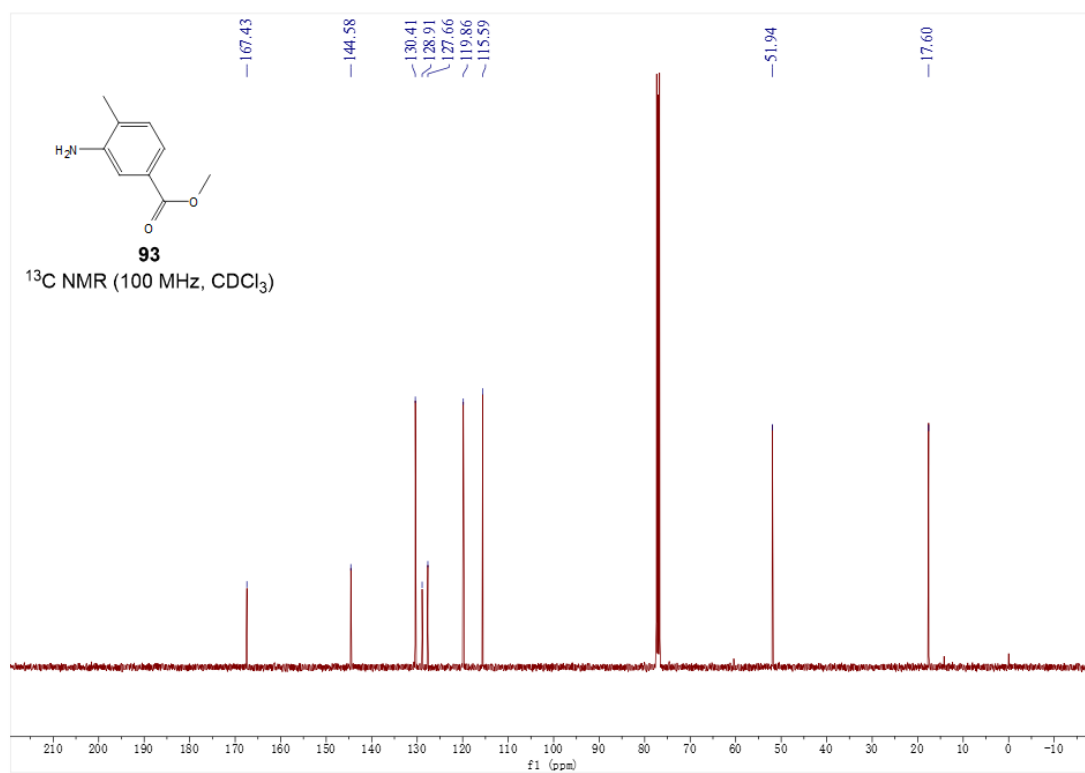
^{13}C NMR (100 MHz, CDCl_3) spectrum of **92**



^1H NMR (400 MHz, CDCl_3) spectrum of **93**



^{13}C NMR (100 MHz, CDCl_3) spectrum of **93**



10 References

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