Supporting information

Visible Light-Promoted Aerobic Oxidative Cleavage and Cyclization of Olefins to Access 3-hydroxy-isoindolinones

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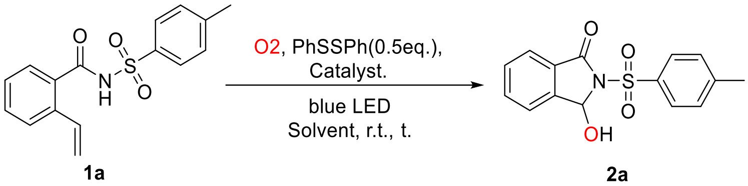
1. General information

Unless otherwise indicated, all the regents and solvents were purchased from commercial suppliers and used without any further purification. ^{1}H spectra were recorded in $CDCl_3$ or (Methyl sulfoxide)-d6 on 400MHz NMR spectrometers and resonances (•) are given in parts per million relatives to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q =quartet, p = penta, dd = doublet of doublets, dt = doublet of triplets, ddt = doublet of doublet of triplets, dtd = doublet of triplet of doublets, m = multiplet, br = broad), coupling constant (*J*) in Hertz (Hz), and integration. ^{13}C NMR were recorded at 100 MHz and chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent. Column chromatography was generally performed on Silicycle silica gel (200-300 mesh). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm coated silica gel plates (HSGF 254) and visualized the course of the reactions using a UV light (254 nm or 365 nm). High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrosprayionization-time of flight).

2. Optimization of reaction conditions of 1a

Table S1. Screening of reaction conditions for the synthesis of product **2a**[a]

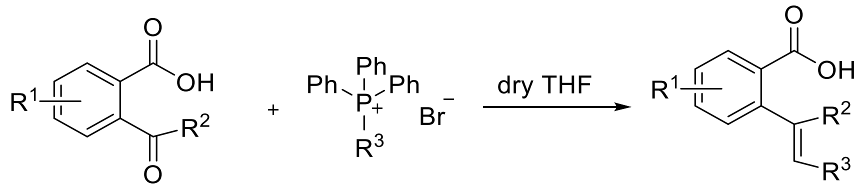


Entry	Catalyst	Solvent	T (h)	Yield (%)[b]
1	$FeCl_3$	DCE	10	43
2	$FeCl_3$	DMF	10	trace
3	$FeCl_3$	THF	10	30
4	$FeCl_3$	DMSO	10	trace
5	$FeCl_3$	MeCN/H_2O (5/1)	10	25
6	$FeCl_3$	MeCN/HFIP (5/1)	10	45
7	$ZnCl_2$	MeCN/MeOH (5/1)	10	52
8	$NiCl_2$	MeCN/MeOH (5/1)	10	21
9	$CuCl_2$	MeCN/MeOH (5/1)	10	21
10	CuCl	MeCN/MeOH (5/1)	10	33
11	$CoCl_2$	MeCN/MeOH (5/1)	10	trace
12	$Fe(acac)_3$	MeCN/MeOH (5/1)	10	trace
13	$FeSO_4 \cdot 7H_2O$	MeCN/MeOH (5/1)	10	31
14	$FeCl_3$	MeCN/MeOH (5/1)	2	12
15	$FeCl_3$	MeCN/MeOH (5/1)	4	38
16	$FeCl_3$	MeCN/MeOH (5/1)	6	52
17	$FeCl_3$	MeCN/MeOH (5/1)	8	68
18	$FeCl_3$	MeCN/MeOH (5/1)	12	75

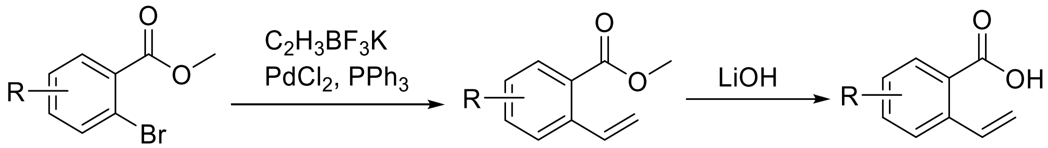
[a] Reaction conditions： O_2, blue LED (426 nm, 30 W), **1a** (0.3 mmol, 1.0 eq.), PhSSPh (0.15 mmol, 0.5eq.), catalyst, MeCN/MeOH (3 mL, v/v = 5/1), room temperature, 10 h, pressure cylindrical. [b] Isolated yield.

3. Experimental section

General procedure for the synthesis of 2-olefin benzoic acid[1]



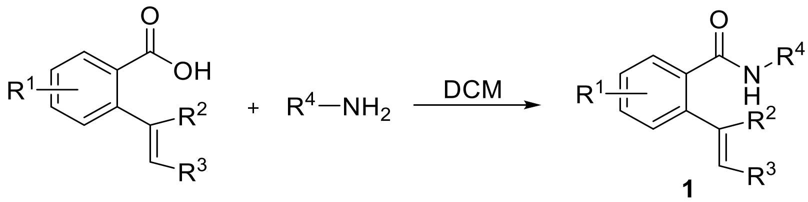
Under nitrogen, to a solution of *t*-BuOK (2.6 equiv.) in dry THF (0.5 M) was added bromo-(alkyl/aryl)-triphenylphosphorane (1.3 equiv.) in portions at 0 °C. The mixture was stirred at 0° C for 30 min and a solution of ketone (1.0 equiv.) in dry THF (1 M) was added dropwise and the reaction was stirred at 0 °C for 1 h and at rt overnight. The solvent was removed in vacuo and the residue diluted with DCM and aqueous NaOH (1 M). The aqueous layer was separated, washed with dichloromethane, and acidified to pH 1 with concentrated HCl. DCM was added and the organic compound was extracted twice with DCM. The organic layer was washed with water, dried over $MgSO_4$ and concentrated. The crude product was purified by SiO_2 column chromatography (DCM/MeOH: 100/0 to 95/5 to 9/1) to give pure enoic acid.



A 50 mL sealable Schlenk tube was charged with methyl 2-bromobenzoate (4.1 mmol), potassium vinyltrifluoroborate (4.4 mmol), cesium carbonate (4.1 g), palladium (II) chloride (29 mg), triphenylphosphine (130 mg), THF (9 mL) and degassed water (1 mL). The reaction mixture was stirred at 85°C for 40 h. After cooling down, the reaction mixture was diluted with DCM (50 mL) and water (30 mL). After the solution was filtered over Celite, the organic layer was separated. The aqueous layer was extracted with DCM (50 mL × 2). The combined organic layers were dried over MgSO4, filtered and concentrated in vacuo. The residue was purified by flash chromatography on silica gel (petroleum/EtOAc) to give the compound methyl 2-vinyl benzoate (86%).

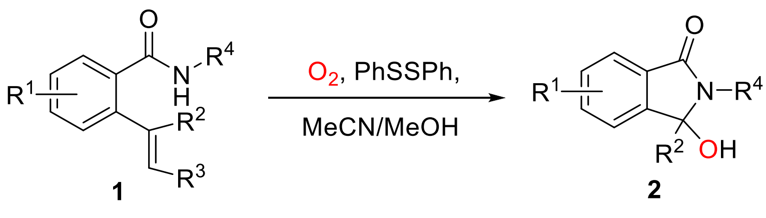
To a solution of methyl 2-vinyl benzoate (7.26 mmol) in a mixed solvent (30 mL, volume ratio of THF: MeOH: H2O = 4: 1: 1) was added lithium hydroxide (21.8 mmol). The reaction mixture was stirred at 70 °C for 12 h. After cooling down to room temperature, the reaction mixture was adjusted to pH = 1 using 1 M HCl. The mixture was extracted with ethyl acetate (20 mL × 2). The combined organic layers were dried over MgSO4, filtered and concentrated in vacuo. The residue was recrystallized from ethanol to give the 2-vinyl benzoic acid (99%).

General procedure for the synthesis of 2-olefin benzimide[2]



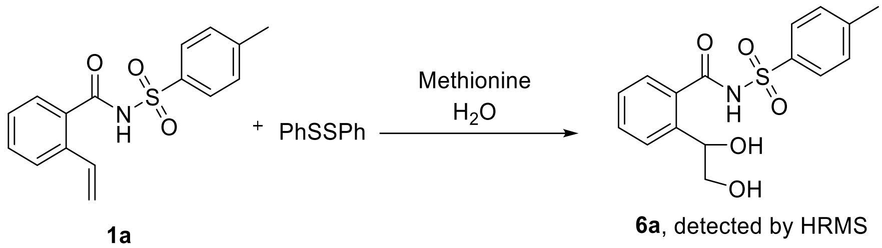
A dichloromethane solution (100 mL) containing 2-vinylbenzoic acid (0.98 g, 6.6 mmol), tosylamine (0.90 g, 5.3 mmol), DMAP (1.61 g, 13.2 mmol), and 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC·HCl) (2.53 g, 13.2 mmol) was stirred overnight at rt. The reaction mixture was quenched with HCl aq. and extracted with dichloromethane. The organic phase was dried with $MgSO_4$ and concentrated in vacuo. The crude mixture was purified by column chromatography (SiO_2, eluent: dichloromethane) to give raw material **1**.

General procedure for the synthesis of product 2



A 35 mL glass tube was charged with 2 (0.3 mmol), PhSSPh (0.15 mmol, 0.5 equiv.), $FeCl_3$ (0.03 mmol, 0.1 equiv.), MeCN/MeOH (3mL, v/v = 5/1), O_2 and a magnetic stir bar. The reaction mixture was stirred and irradiated by blue LED (426 nm, 30W) at room temperature for 10 hours. After completing reaction, it was monitored with TLC. Then the reaction mixture was washed with saturated NH_4Cl solution and extracted with ethyl DCM. The organic layer was dried with anhydrous sodium sulfate and the solvent was removed under vacuum. The pure product **2** was obtained by flash chromatography on silica gel using DCM and MeOH as the eluent.

General procedure for the synthesis of product 6a[3]



A 35 mL glass tube was charged with 2 (0.3 mmol), PhSSPh (0.15 mmol, 0.5 equiv.), $FeCl_3$ (0.03 mmol, 0.1 equiv.), methionine (0.3 mmol, 1 equiv.), H_2O (1mL), MeCN/MeOH (3Ml, v/v = 5/1), O_2 and a magnetic stir bar. The reaction mixture was stirred and irradiated by blue LED (426 nm, 30W) at room temperature for 10 hours. After completing reaction, it was monitored with TLC. The product **6a** was detected *via* high-resolution mass spectroscopy.

4. X-ray crystallography structure of compound 2n

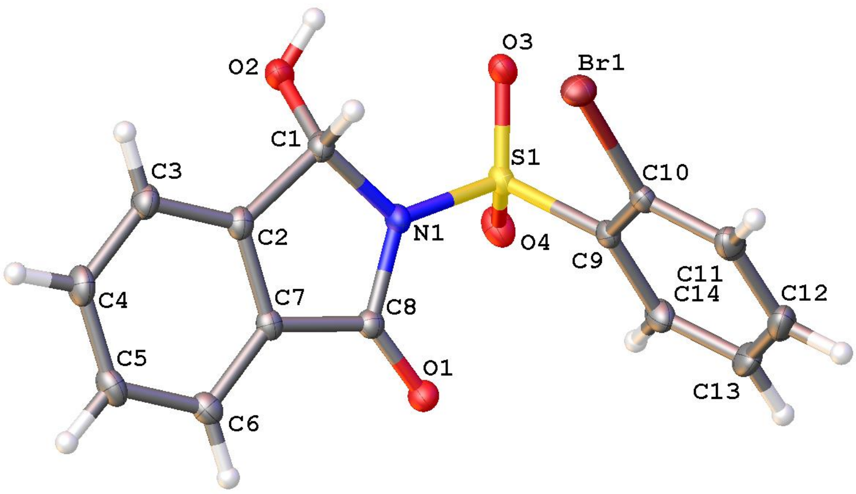


Fig. S1. X-ray structure of **2n**

5. HRMS Spectra for compound 3a, 4a, 6a and 7ai

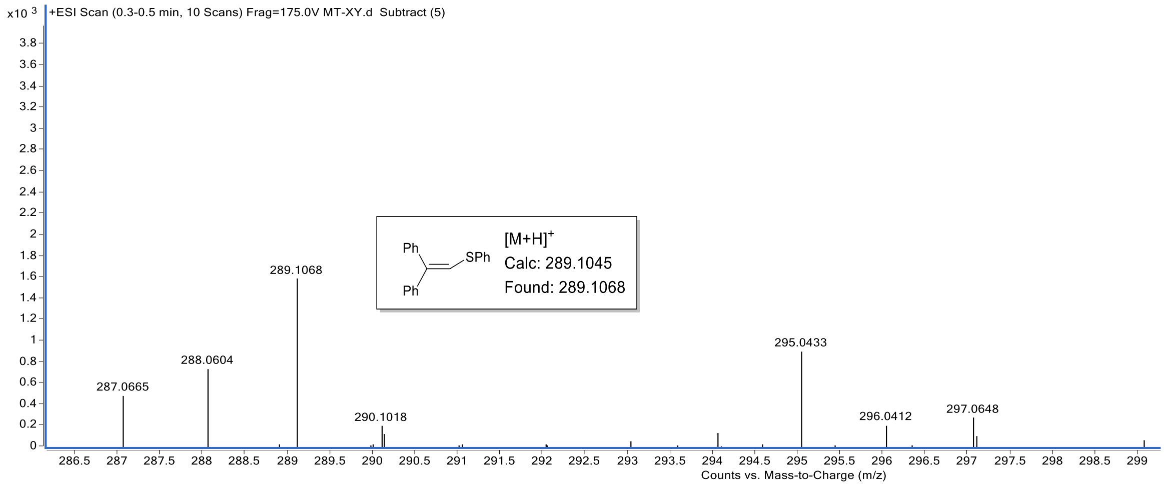


Fig. S2. HRMS Spectra for compound **3a**

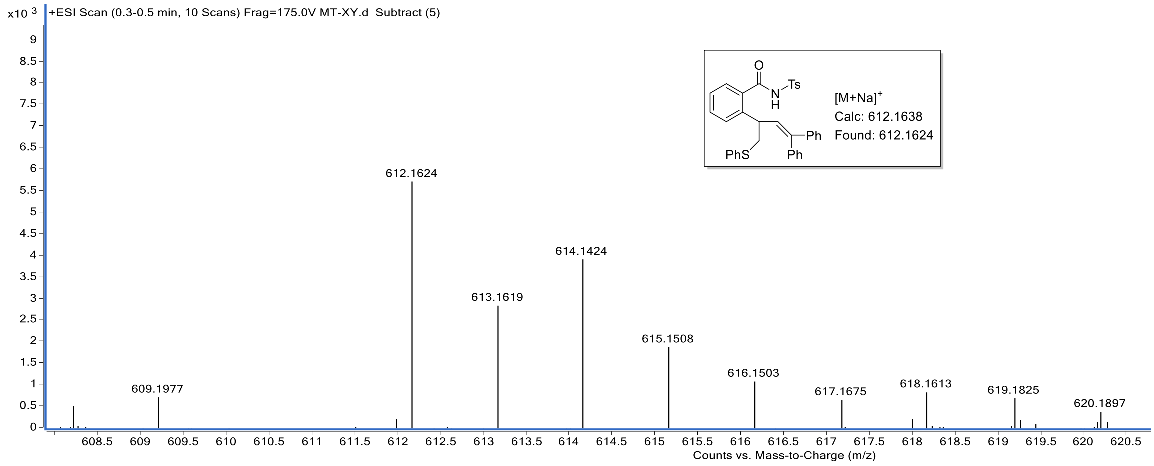


Fig. S2. HRMS Spectra for compound **4a**

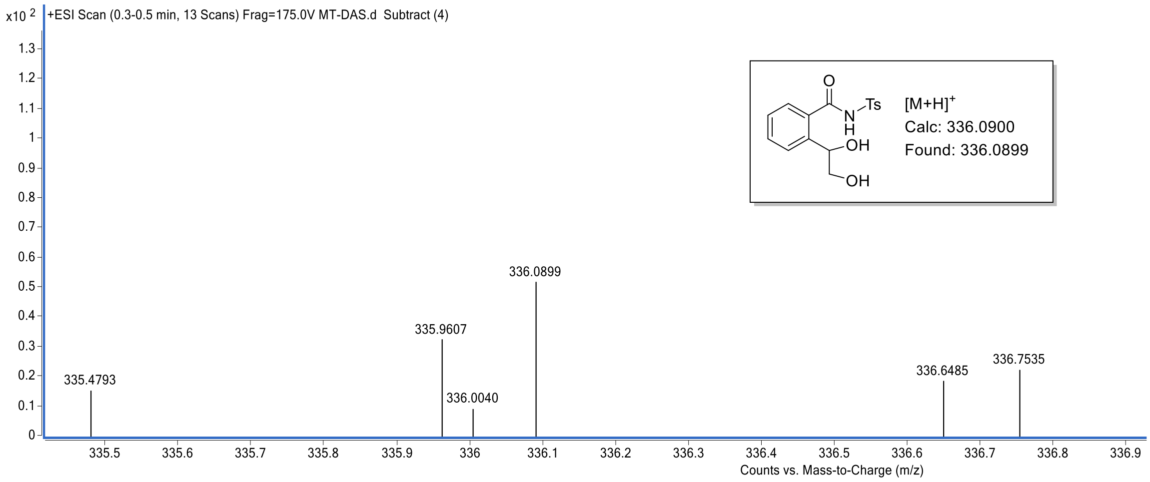


Fig. S4. HRMS Spectra for compound **6a**

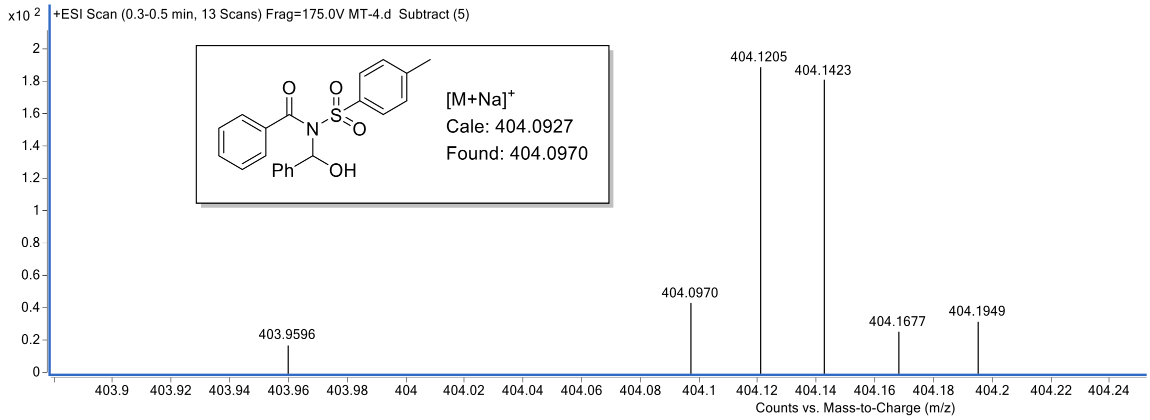
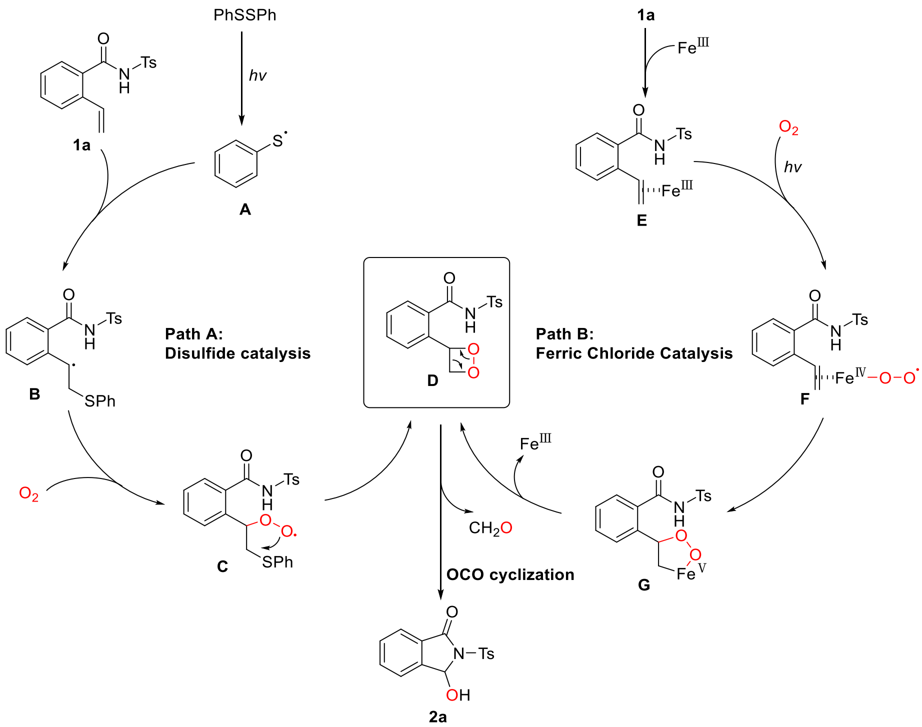


Fig. S5. HRMS Spectra for compound **7ai**

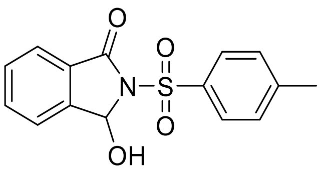
6. Plausible reaction mechanism *via* diphenyl disulfide or ferric chloride

Based on the experimental results and previous reports[4], another plausible mechanism was speculated *via* diphenyl disulfide or ferric chloride in scheme S1. Similarly, diphenyl disulfide was split into two molecules of phenyl sulfide radical **A** and free radical intermediate **B** is formed through radicals **A** attacks unsaturated double bond of substrate **1a** in high regioselectivity. Then, intermediate **C** is gotten when molecular oxygen capture radical **B**, and afterwards, the key intermediate **D** would be formed *via* C-S bond cleavage. Next, unstable intermediate **D** could give desired product **2a** through the fracture of dioxetane immediately (Scheme S1, Path A). On the other hand, iron salt could combine with C=C bond and generate intermediate **G** with the participation of oxygen. Subsequently, unstable intermediate **D** proceeds through removal of iron salt, which gives goal product isoindolinone 2a at same way as path A (Scheme S1, Path B).

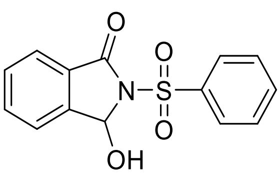


Scheme S1. Plausible reaction mechanism *via* diphenyl disulfide or ferric chloride

7. Analytical data of products 2

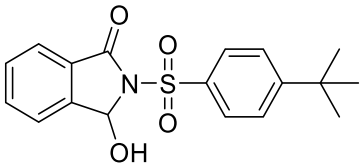


3-hydroxy-2-tosylisoindolin-1-one **(2a)**. White solid (75%, 0.068g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (s, 2H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.61 (td, *J* = 7.5, 1.0 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 1H), 7.49 - 7.42 (m, 1H), 7.26 (d, *J* = 8.3 Hz, 2H), 6.58 (d, *J* = 4.9 Hz, 1H), 4.47 (d, *J* = 5.0 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.79, 145.44, 142.51, 135.50, 134.56, 130.63, 129.76, 129.21, 128.35, 124.66, 124.24, 82.48, 21.71. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{15}H_{14}NO_4S^+$ 304.0638 found 304.0635.

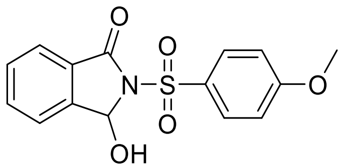


3-hydroxy-2-(phenylsulfonyl)isoindolin-1-one **(2b)**. White solid (78%, 0.068g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (dt, *J* = 8.6, 1.7 Hz, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.63 (td, *J* = 7.5, 1.1

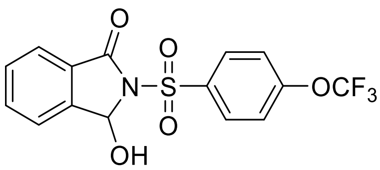
Hz, 1H), 7.60 – 7.54 (m, 2H), 7.52 - 7.44 (m, 3H), 6.60 (d, *J* = 4.9 Hz, 1H), 4.31 (d, *J* = 5.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.66, 141.37, 137.40, 133.60, 133.21, 129.68, 128.11, 127.24, 123.69, 123.23, 81.44. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{14}H_{12}NO_4S^+$ 290.0482 found 290.0479.



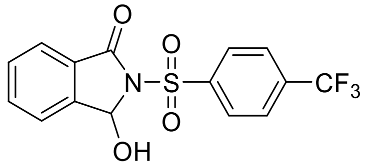
2-((4-(tert-butyl)phenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2c)**. White solid (80%, 0.083g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 - 8.02 (m, 2H), 7.78 (td, *J* = 7.5, 1.1 Hz, 1H), 7.73 - 7.66 (m, 4H), 7.65 (d, *J* = 2.3 Hz, 1H), 7.62 - 7.57 (m, 1H), 6.73 (s, 1H), 1.29 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.18, 157.66, 145.33, 136.81, 135.20, 130.71, 128.74, 128.17, 126.52, 125.00, 124.16, 83.80, 35.47, 31.16. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{18}H_{20}NO_4S^+$ 346.1108 found 346.1122.



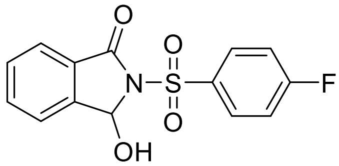
3-hydroxy-2-((4-methoxyphenyl)sulfonyl)isoindolin-1-one **(2d)**. White solid (65%, 0.062g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 (d, *J* = 8.9 Hz, 2H), 7.77 (t, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.65 (s, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 9.0 Hz, 2H), 6.68 (s, 1H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.13, 163.90, 145.32, 135.15, 131.05, 130.70, 130.66, 128.78, 124.98, 124.11, 114.77, 83.72, 56.30. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{15}H_{14}NO_5S^+$ 320.0587 found 320.0592.



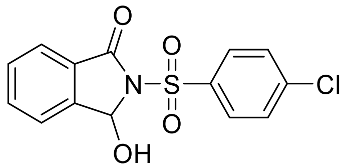
3-hydroxy-2-((4-(trifluoromethoxy)phenyl)sulfonyl)isoindolin-1-one **(2e)**. Colorless solid (72%, 0.081g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.24 – 8.10 (m, 2H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.65 (td, *J* = 7.5, 1.1 Hz, 1H), 7.58 (d, *J* = 7.4 Hz, 1H), 7.53 - 7.46 (m, 1H), 7.37 – 7.24 (m, 2H), 6.61 (d, *J* = 5.3 Hz, 1H), 4.30 (d, *J* = 5.3 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.70, 152.25, 141.38, 135.52, 133.79, 129.81, 129.68, 127.90, 123.76, 123.28, 119.71, 119.13 (q, *J* = 259 Hz), 81.53. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.63 (s, 3F). HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{15}H_{11}NO_5F_3S^+$ 374.0305 found 374.0326.



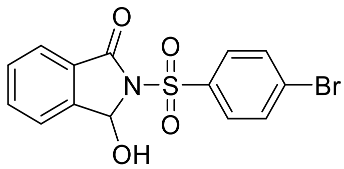
3-hydroxy-2-((4-(trifluoromethyl)phenyl)sulfonyl)isoindolin-1-one **(2f)**. White solid (85%, 0.091g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.36 (d, *J* = 8.3 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.79 - 7.67 (m, 3H), 7.64 (t, *J* = 7.5 Hz, 1H), 6.81 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.24, 145.39, 143.37, 135.42, 134.01 (q, *J* = 32 Hz), 130.79, 129.27, 128.43, 126.91, 125.02, 124.32, 123.78 (q, *J* = 271 Hz), 84.18. ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.87 (s, 3F). HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{15}H_{11}NO_4F_3S^+$ 358.0355 found 358.0381.



2-((4-fluorophenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2g)**. White solid (72%, 0.066g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 8.8, 5.0 Hz, 2H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.15 (t, *J* = 8.5 Hz, 2H), 6.60 (s, 1H), 4.31 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.30, 163.72 (d, *J* = 4 Hz), 141.34, 133.71, 133.36 (d, *J* = 3 Hz), 130.32 (d, *J* = 10 Hz), 129.77, 127.97, 123.71, 123.25, 115.44 (d, *J* = 22 Hz), 81.46. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -102.22 (s, 1F). HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{14}H_{11}NO_4FS^+$ 308.0387 found 308.0396.

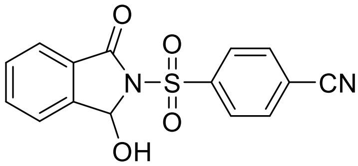


2-((4-chlorophenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2h)**. White solid (82%, 0.080g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (d, *J* = 8.7 Hz, 2H), 7.80 (t, *J* = 7.5 Hz, 1H), 7.76 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.68 (s, 1H), 7.67 (s, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 6.74 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.20, 145.37, 139.59, 138.42, 135.35, 130.78, 130.19, 129.83, 128.53, 125.01, 124.26, 84.02. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{14}H_{11}NO_4ClS^+$ 324.0092 found 324.0088.

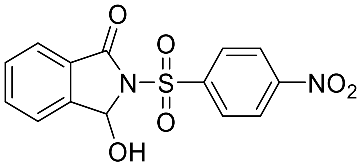


2-((4-bromophenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2i)**. White solid (88%, 0.097g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.07 (d, *J* = 8.6 Hz, 2H), 7.91 (d, *J* = 8.5 Hz, 2H), 7.83 - 7.78 (m, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.55 (s, 1H), 6.77 (s, 1H).

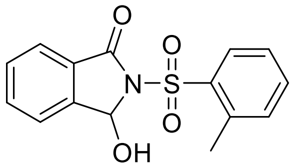
^{13}C NMR (101 MHz, DMSO-d_6) δ 165.21, 145.35, 138.85, 135.33, 132.78, 130.77, 130.24, 128.74, 128.55, 125.00, 124.27, 84.04. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{14}H_{11}NO_4BrS^+$ 367.9587 found 367.9596.



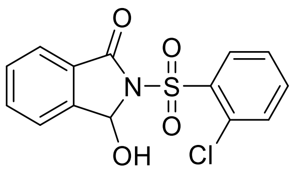
4-((1-hydroxy-3-oxoisoindolin-2-yl)sulfonyl)benzonitrile **(2j)**. White solid (80%, 0.075g). ^1H NMR (400 MHz, DMSO-d_6) δ 8.29 (d, *J* = 8.4 Hz, 2H), 8.18 (s, 2H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.73 (dd, *J* = 21.5, 7.6 Hz, 3H), 7.64 (t, *J* = 7.5 Hz, 1H), 6.80 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.26, 145.39, 143.39, 135.50, 133.85, 130.84, 128.95, 128.34, 125.03, 124.37, 118.00, 116.86, 84.22. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{15}H_{11}N_2O_4S^+$ 315.0434 found 315.0420.



3-hydroxy-2-((4-nitrophenyl)sulfonyl)isoindolin-1-one **(2k)**. White solid (71%, 0.071g). ^1H NMR (400 MHz, DMSO-d_6) δ 8.49 (d, *J* = 8.8 Hz, 2H), 8.37 (d, *J* = 8.7 Hz, 2H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.80 - 7.72 (m, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 8.5 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.25, 150.99, 145.41, 144.67, 135.53, 130.85, 129.93, 128.32, 125.04, 124.97, 124.38, 84.27. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{14}H_{11}N_2O_6S^+$ 335.0332 found 335.0350.

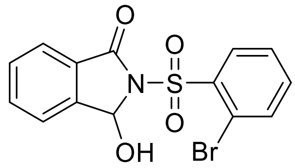


3-hydroxy-2-(o-tolylsulfonyl)isoindolin-1-one **(2l)**. White solid (71%, 0.071g). White solid (68%, 0.062g). ^1H NMR (400 MHz, DMSO-d_6) δ 8.10 (d, *J* = 7.9 Hz, 1H), 7.80 (t, *J* = 7.5 Hz, 1H), 7.74 - 7.66 (m, 3H), 7.65 - 7.56 (m, 2H), 7.51 - 7.38 (m, 2H), 6.74 (d, *J* = 9.3 Hz, 1H), 2.61 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.39, 145.27, 138.00, 137.82, 135.33, 134.38, 133.03, 130.82, 130.75, 128.52, 126.97, 125.11, 124.26, 83.98, 20.26. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{15}H_{14}NO_4S^+$ 304.0638 found 304.0630.

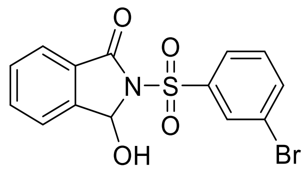


2-((2-chlorophenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2m)**. White solid (66%, 0.064g). ^1H

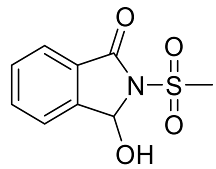
NMR (400 MHz, DMSO-d_6) δ 8.26 (d, *J* = 7.8 Hz, 1H), 7.84 (t, *J* = 7.5 Hz, 1H), 7.77 - 7.71 (m, 3H), 7.70 (s, 1H), 7.68 (s, 1H), 7.66 (s, 1H), 7.65 - 7.60 (m, 1H), 6.82 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.03, 145.24, 136.50, 136.04, 135.55, 133.07, 132.28, 131.17, 130.88, 128.36, 128.08, 125.17, 124.36, 85.06. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{14}H_{11}NO_4ClS^+$ 324.0092 found 324.0098.



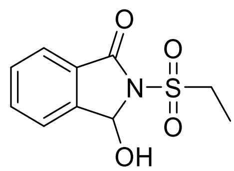
2-((2-bromophenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2n)**. Colorless solid (70%, 0.077g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 - 8.22 (m, 1H), 7.87 - 7.77 (m, 3H), 7.73 - 7.67 (m, 3H), 7.66 - 7.59 (m, 2H), 6.84 (d, *J* = 9.5 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.96, 145.18, 138.13, 135.95, 135.73, 135.56, 133.41, 130.89, 128.81, 128.10, 125.15, 124.35, 119.75, 85.45. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{14}H_{11}NO_4BrS^+$ 367.9587 found 367.9599.



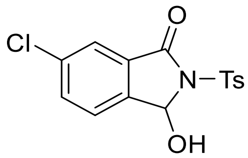
2-((3-bromophenyl)sulfonyl)-3-hydroxyisoindolin-1-one **(2o)**. White solid (74%, 0.082g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.82 (t, *J* = 7.4 Hz, 1H), 7.79 - 7.64 (m, 4H), 7.62 (d, *J* = 8.0 Hz, 1H), 6.79 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.23, 145.38, 141.44, 137.39, 135.41, 131.89, 130.80, 130.53, 128.47, 127.35, 125.02, 124.33, 122.39, 84.11. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{14}H_{11}NO_4BrS^+$ 367.9587 found 367.9600.



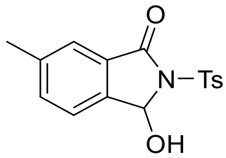
3-hydroxy-2-(methylsulfonyl)isoindolin-1-one **(2p)**. White solid (71%, 0.049g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.80 (dd, *J* = 7.0, 4.3 Hz, 2H), 7.65 (t, *J* = 8.1 Hz, 2H), 7.40 (d, *J* = 9.2 Hz, 1H), 6.49 (d, *J* = 9.1 Hz, 1H), 3.36 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.03, 145.44, 135.18, 130.70, 128.97, 124.88, 124.26, 83.60, 42.15. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_9H_{10}NO_4S^+$ 228.0325 found 228.0340.



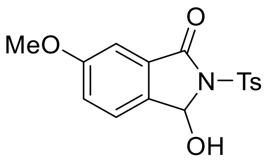
2-(ethylsulfonyl)-3-hydroxyisoindolin-1-one **(2q)**. White solid (76%, 0.055g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 6.53 (d, *J* = 4.0 Hz, 1H), 4.59 (d, *J* = 4.8 Hz, 1H), 3.58 - 3.44 (m, 2H), 1.34 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.76, 141.75, 133.74, 129.70, 127.99, 123.73, 123.37, 81.16, 47.73, 6.48. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{10}H_{12}NO_4S^+$ 242.0482 found 242.0455.



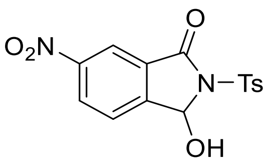
6-chloro-3-hydroxy-2-tosylisoindolin-1-one **(2r)**. White solid (78%, 0.079g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 (d, *J* = 8.3 Hz, 2H), 7.82 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.74 (d, *J* = 1.7 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.46 (d, *J* = 8.2 Hz, 2H), 6.73 (s, 1H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.85, 145.36, 143.94, 136.54, 135.46, 135.06, 130.73, 130.08, 128.33, 126.93, 123.82, 83.59, 21.56. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{16}H_{16}NO_4S^+$ 3180795 found 318.0803. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{15}H_{13}NO_4ClS^+$ 338.0248 found 338.0267.



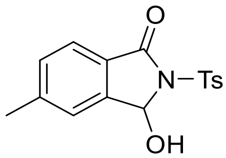
3-hydroxy-6-methyl-2-tosylisoindolin-1-one **(2s)**. White solid (67%, 0.064g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 8.7 Hz, 2H), 7.49 (s, 1H), 7.44 (d, *J* = 8.2 Hz, 2H), 6.65 (d, *J* = 8.5 Hz, 1H), 2.39 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.24, 145.12, 142.73, 140.69, 136.82, 135.99, 130.04, 128.86, 128.23, 124.73, 124.03, 83.69, 21.55, 21.21. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{16}H_{16}NO_4S^+$ 318.0795 found 318.0788.



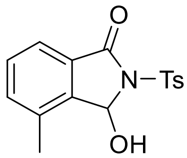
3-hydroxy-6-methoxy-2-tosylisoindolin-1-one **(2t)**. White solid (80%, 0.080g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.53 (dd, *J* = 13.1, 8.7 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.32 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.15 (d, *J* = 2.4 Hz, 1H), 6.63 (d, *J* = 8.8 Hz, 1H), 3.81 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.07, 161.33, 145.16, 137.67, 136.78, 130.21, 130.04, 128.24, 126.12, 122.73, 106.99, 83.59, 56.26, 21.55. HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{16}H_{16}NO_5S^+$ 334.0744 found 334.0787.



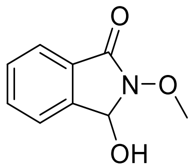
3-hydroxy-6-nitro-2-tosylisoindolin-1-one **(2u)**. Yellow solid (86%, 0.090g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.63–8.53 (m, 1H), 8.36 (s, 1H), 7.99 (d, *J* = 8.1 Hz, 2H), 7.91 (t, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 8.1 Hz, 2H), 6.85 (d, *J* = 4.8 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.27, 150.67, 149.57, 145.58, 136.34, 130.25, 130.16, 129.93, 128.39, 126.83, 119.37, 83.66, 21.58. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{15}H_{13}N_2O_6S^+$ 340.0489 found 349.0491.



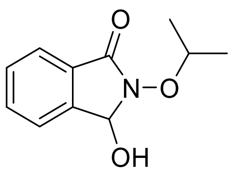
3-hydroxy-5-methyl-2-tosylisoindolin-1-one **(2v)**. White solid (73%, 0.070g). ^1H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, *J* = 8.3 Hz, 2H), 7.58 (s, 1H), 7.56 (s, 1H), 7.45 (d, *J* = 2.8 Hz, 2H), 7.42 (s, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 6.64 (s, 1H), 2.44 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.09, 146.05, 145.71, 145.09, 136.87, 131.55, 130.03, 128.22, 126.15, 125.20, 124.05, 83.60, 21.97, 21.55. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{16}H_{16}NO_4S^+$ 318.0795 found 318.0803.



3-hydroxy-4-methyl-2-tosylisoindolin-1-one **(2w)**. White solid (77%, 0.073g). ^1H NMR (400 MHz, DMSO-d_6) δ 7.98 (d, *J* = 8.3 Hz, 2H), 7.58–7.50 (m, 2H), 7.50–7.46 (m, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 6.75 (s, 1H), 2.42 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.37, 145.14, 143.25, 136.86, 136.30, 135.59, 130.73, 130.02, 128.76, 128.29, 121.54, 83.34, 21.55, 17.33. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{16}H_{16}NO_4S^+$ 318.0795 found 318.0788.

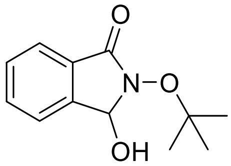


3-hydroxy-2-methoxyisoindolin-1-one **(2x)**. White solid (58%, 0.031g). ^1H NMR (400 MHz, DMSO-d_6) δ 7.69 (dt, *J* = 6.8, 3.3 Hz, 2H), 7.57 (d, *J* = 7.6 Hz, 2H), 7.10 (d, *J* = 8.6 Hz, 1H), 5.98 (d, *J* = 8.6 Hz, 1H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.48, 142.59, 133.30, 130.07, 129.53, 124.15, 122.98, 81.39, 64.55. HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_9H_{10}NO_3^+$ 180.0655 found 180.0678.

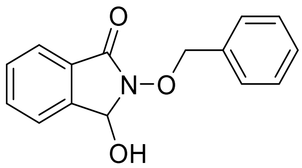


3-hydroxy-2-isopropoxyisoindolin-1-one **(2y)**. Colorless oil (65%, 0.041g). ^1H NMR (400 MHz, DMSO-d_6) δ 7.68 (d, *J* = 7.2 Hz, 2H), 7.57 (d, *J* = 6.8 Hz, 2H), 7.04 (d, *J* = 8.9 Hz, 1H), 5.88 (d, *J* = 8.9 Hz, 1H), 4.44 (p, *J* = 6.2 Hz, 1H), 1.28 (d, *J* = 2.4 Hz, 3H), 1.26 (d, *J* = 2.5 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.11, 142.87, 133.27, 130.06, 129.60, 124.14, 122.98, 82.72, 78.30, 21.53.

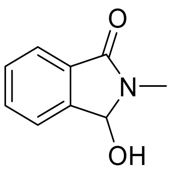
HRMS (TOF) m/z [M + H]+ Calcd for $C_{11}H_{14}NO_3^+$ 208.0968 found 208.0971.



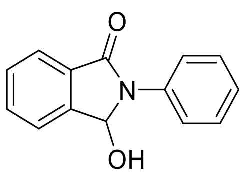
2-(*tert*-butoxy)-3-hydroxyisoindolin-1-one **(2z)**. White solid (61%, 0.040g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.72-7.66 (m, 2H), 7.59-7.54 (m, 2H), 6.94 (d, *J* = 9.0 Hz, 1H), 5.80 (d, *J* = 9.0 Hz, 1H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.78, 143.54, 133.38, 130.09, 129.52, 124.32, 123.05, 83.71, 82.72, 28.06. HRMS (TOF) m/z [M + H]+ Calcd for $C_{12}H_{16}NO_3^+$ 222.1125 found 222.1148.



2-(benzyloxy)-3-hydroxyisoindolin-1-one **(2aa)**. White solid (69%, 0.053g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 - 7.69 (m, 1H), 7.68 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.59 (d, *J* = 2.5 Hz, 1H), 7.58 - 7.53 (m, 3H), 7.45 - 7.35 (m, 3H), 7.20 (d, *J* = 8.6 Hz, 1H), 5.99 (d, *J* = 8.6 Hz, 1H), 5.17 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.74, 142.64, 135.87, 133.32, 130.12, 129.62, 129.52, 129.03, 128.81, 124.18, 123.05, 81.90, 78.54. HRMS (TOF) m/z [M + H]+ Calcd for $C_{15}H_{14}NO_3^+$ 256.0968 found 256.0951.

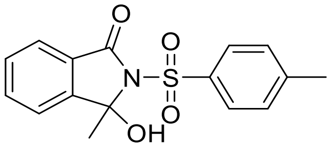


3-hydroxy-2-methylisoindolin-1-one **(2ac)**. White solid (35%, 0.017g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.64 (d, *J* = 7.4 Hz, 1H), 7.63 - 7.57 (m, 2H), 7.52 (td, *J* = 7.1, 1.9 Hz, 1H), 6.59 (d, *J* = 8.9 Hz, 1H), 5.72 (d, *J* = 8.5 Hz, 1H), 2.96 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.47, 145.34, 132.28, 132.23, 129.70, 123.91, 122.63, 82.61, 26.20. HRMS (TOF) m/z [M + H]+ Calcd for $C_9H_{10}NO_2^+$ 164.0706 found 164.0752.

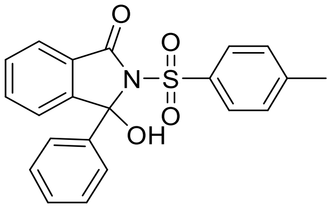


3-hydroxy-2-phenylisoindolin-1-one **(2ad)**. White solid (44%, 0.030g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 - 7.57 (m, 4H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 2H), 7.13 (t, *J* = 7.4 Hz, 1H), 6.28 (d, *J* = 10.6 Hz, 1H), 3.44 (d, *J* = 11.0 Hz, 1H). ^{13}C NMR

(101 MHz, Chloroform-*d*) δ 165.47, 141.73, 136.03, 131.86, 130.36, 129.19, 128.02, 124.29, 122.81, 122.22, 120.82, 81.88. HRMS (TOF) m/z [M + H]+ Calcd for $C_{14}H_{12}NO_2^+$ 226.0863 found 226.0856.



3-hydroxy-3-methyl-2-tosylisoindolin-1-one **(2ae)**. White solid (86%, 0.082g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.82 - 7.75 (m, 1H), 7.75 - 7.67 (m, 2H), 7.65 (s, 1H), 7.58 (td, *J* = 7.4, 1.0 Hz, 1H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.40 - 7.33 (m, 1H), 2.39 (s, 2.3H, major), 2.38 (s, 0.7H, minor), 2.12 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.21, 149.83, 144.92, 137.24, 135.39, 130.49, 129.82, 129.77, 128.48, 127.17, 126.12, 124.03, 123.12, 94.50, 27.62, 21.53. HRMS (TOF) m/z [M + H]+ Calcd for $C_{16}H_{16}NO_4S^+$ 318.0795 found 318.0825.



3-hydroxy-3-phenyl-2-tosylisoindolin-1-one **(2af)**. White solid (54%, 0.061g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 (s, 1H), 7.80 - 7.63 (m, 4H), 7.59 - 7.41 (m, 3H), 7.41 - 7.29 (m, 5H), 7.23 (d, *J* = 7.7 Hz, 1H), 2.37 (s, 2.1H, major), 2.37 (s, 1.0H, minor). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.70, 150.20, 145.05, 142.33, 141.93, 140.89, 136.92, 135.67, 130.53, 129.77, 129.66, 128.72, 128.61, 126.98, 126.11, 124.18, 123.85, 95.42, 21.55 (major), 21.38 (minor). HRMS (TOF) m/z [M + H]+ Calcd for $C_{21}H_{18}NO_4S^+$ 380.0951 found 380.0947.

8. References

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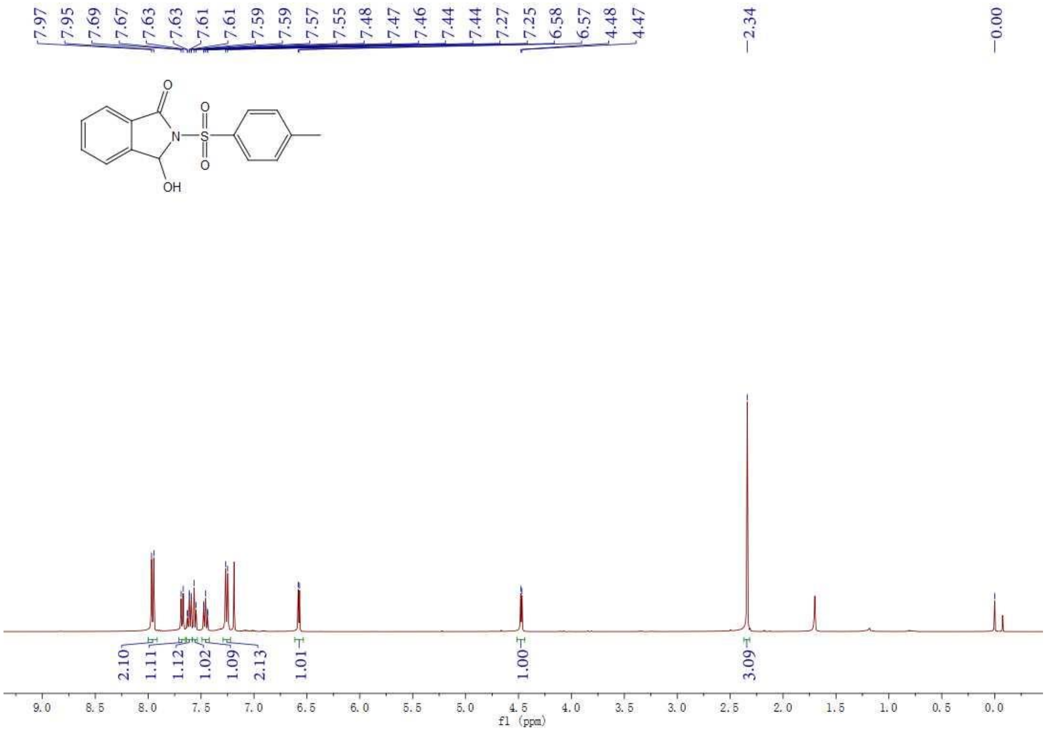
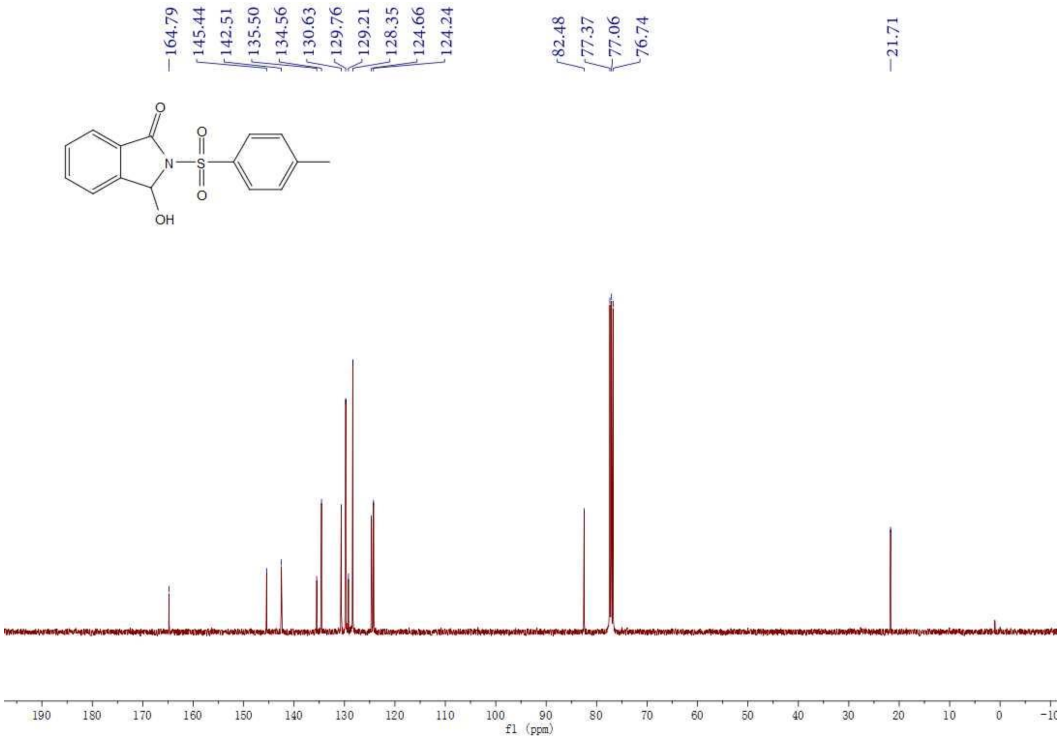
9. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra

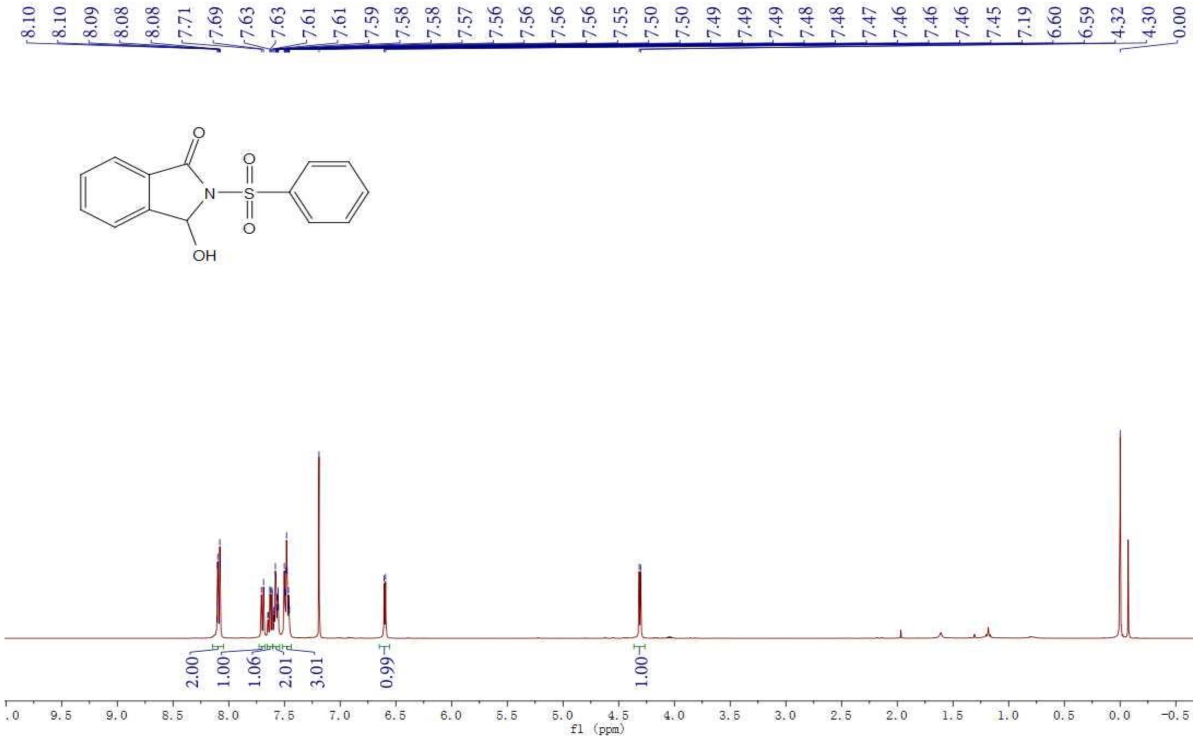
^{1}H NMR of compound **2a**



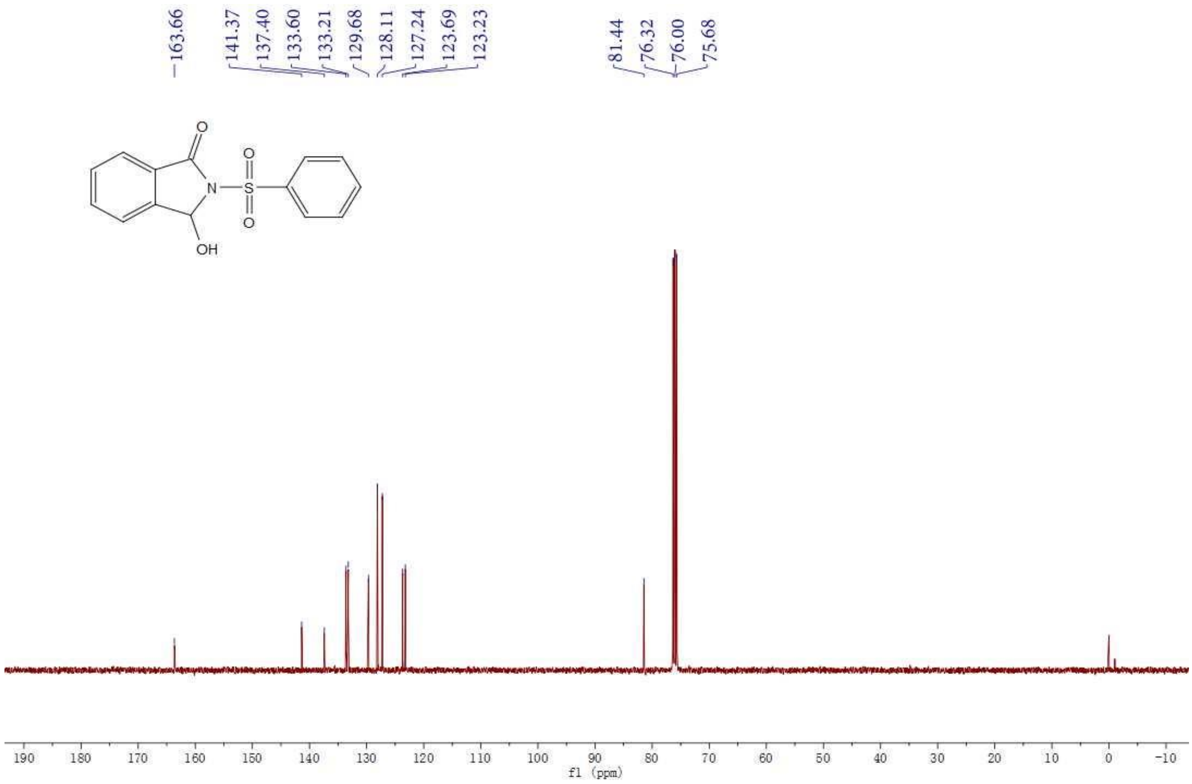
^{13}C NMR of compound **2a**



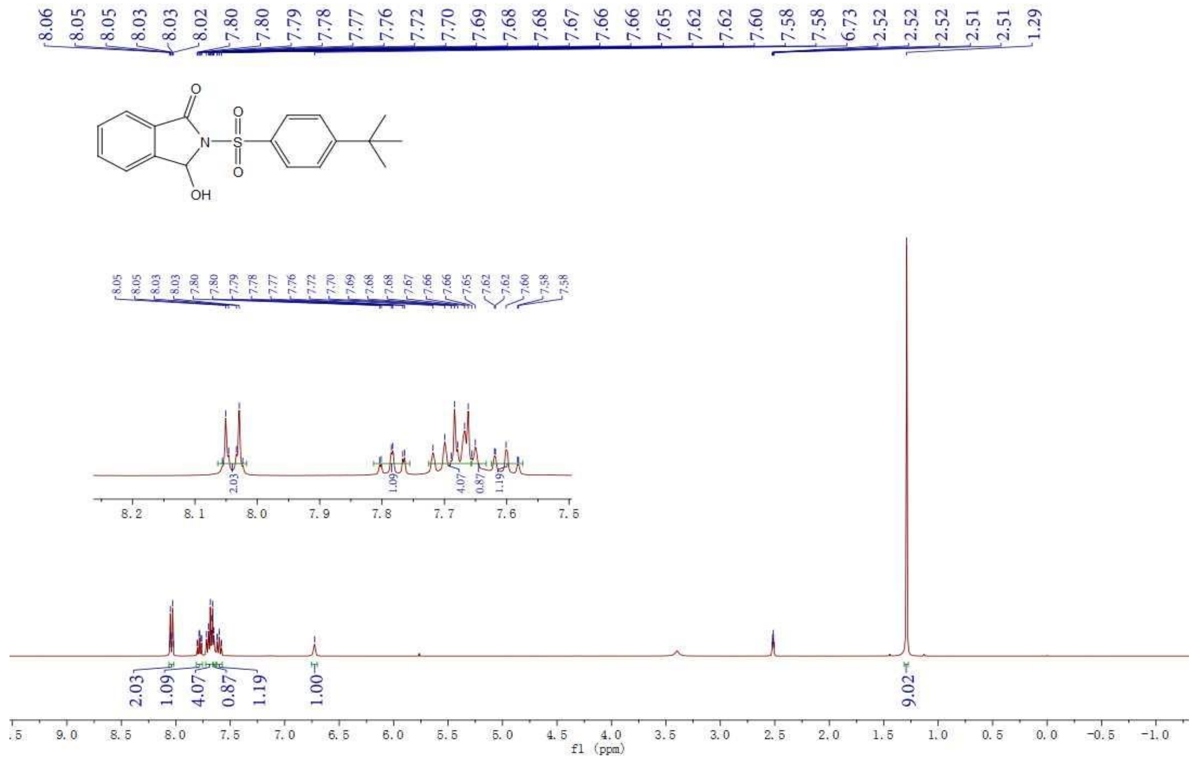
[1]H NMR of compound **2b**



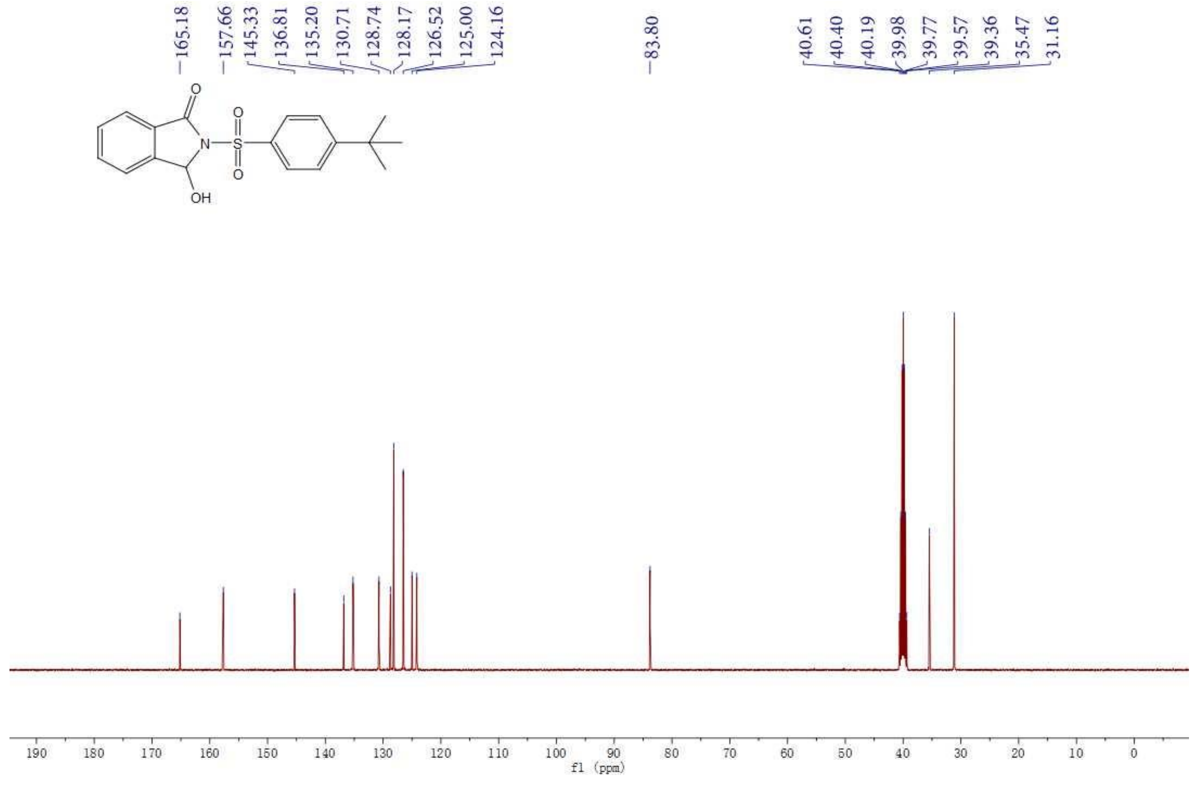
[13]C NMR of compound **2b**



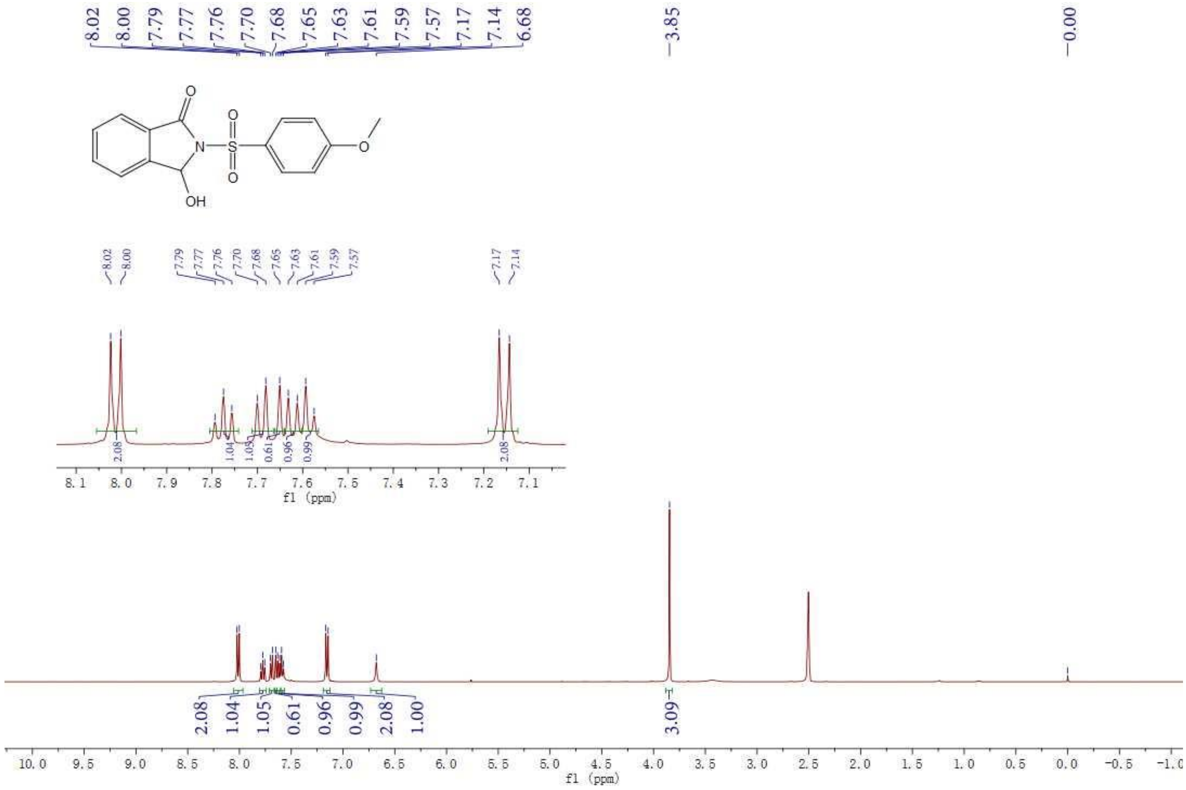
^{1}H NMR of compound **2c**



^{13}C NMR of compound **2c**



^{1}H NMR of compound **2d**



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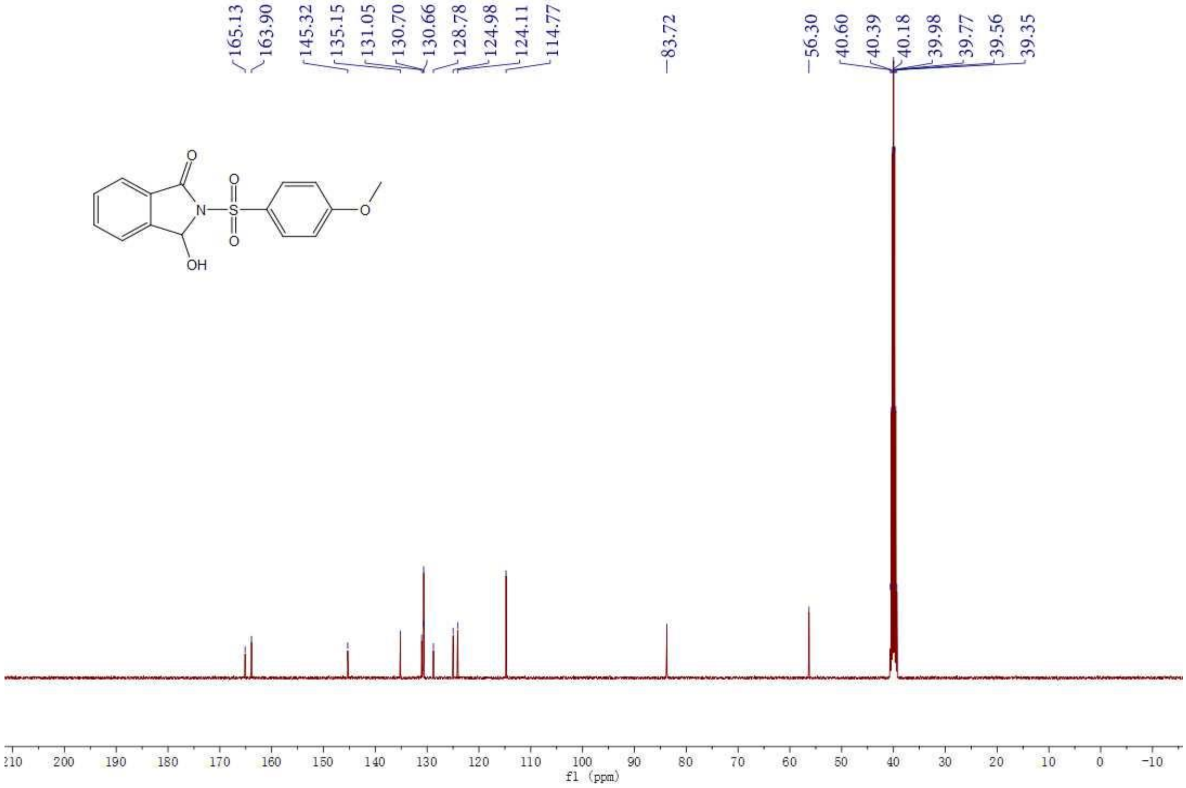

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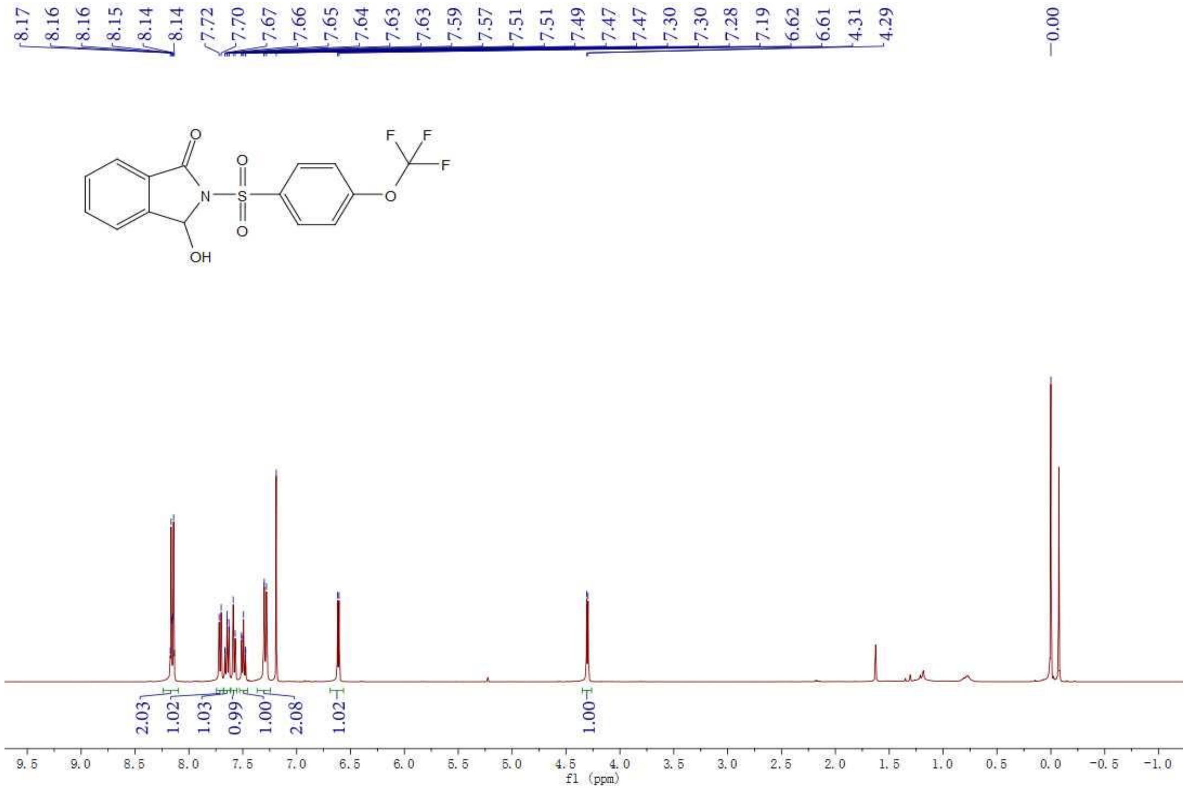
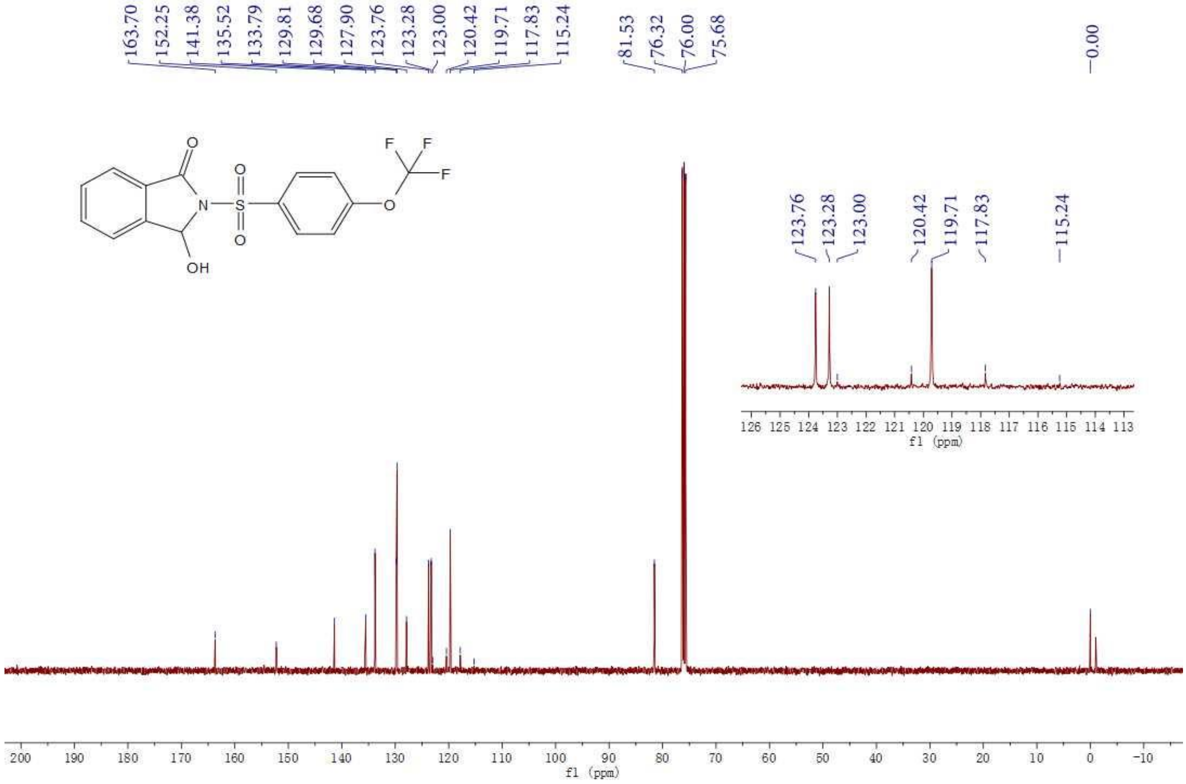


^{13}C NMR of compound **2e**



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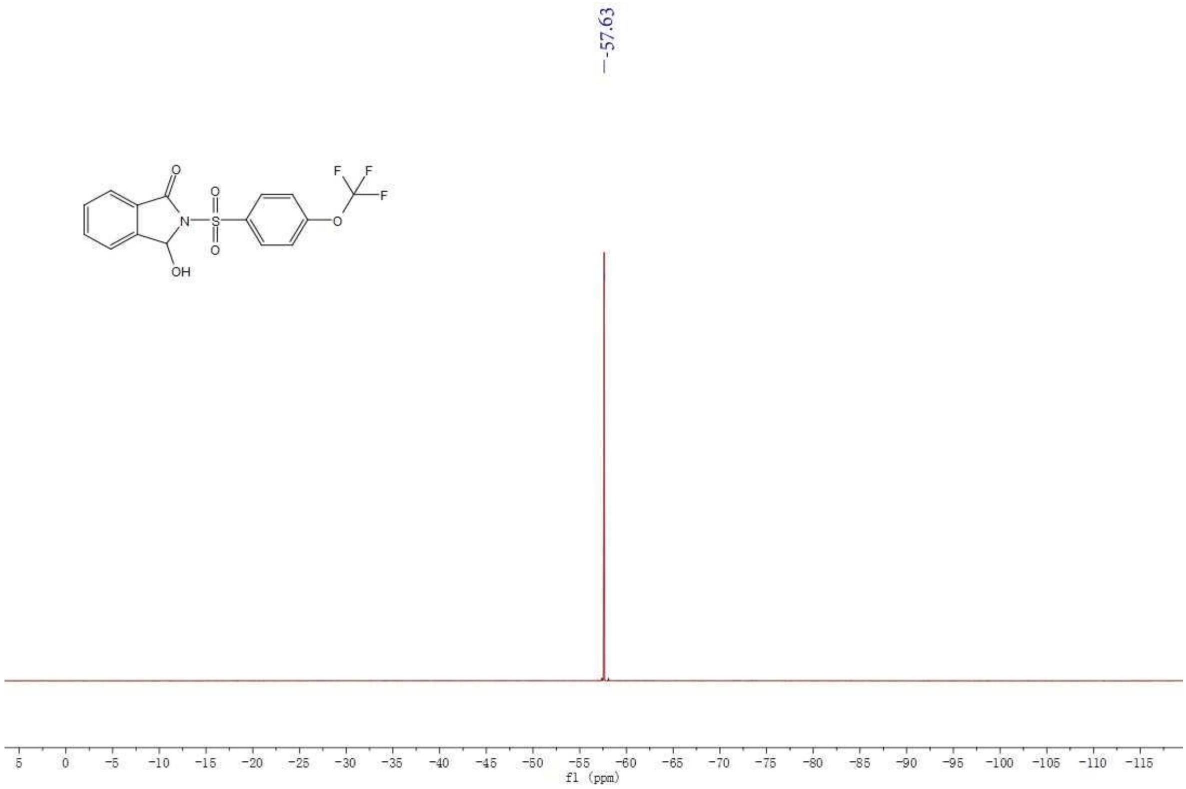

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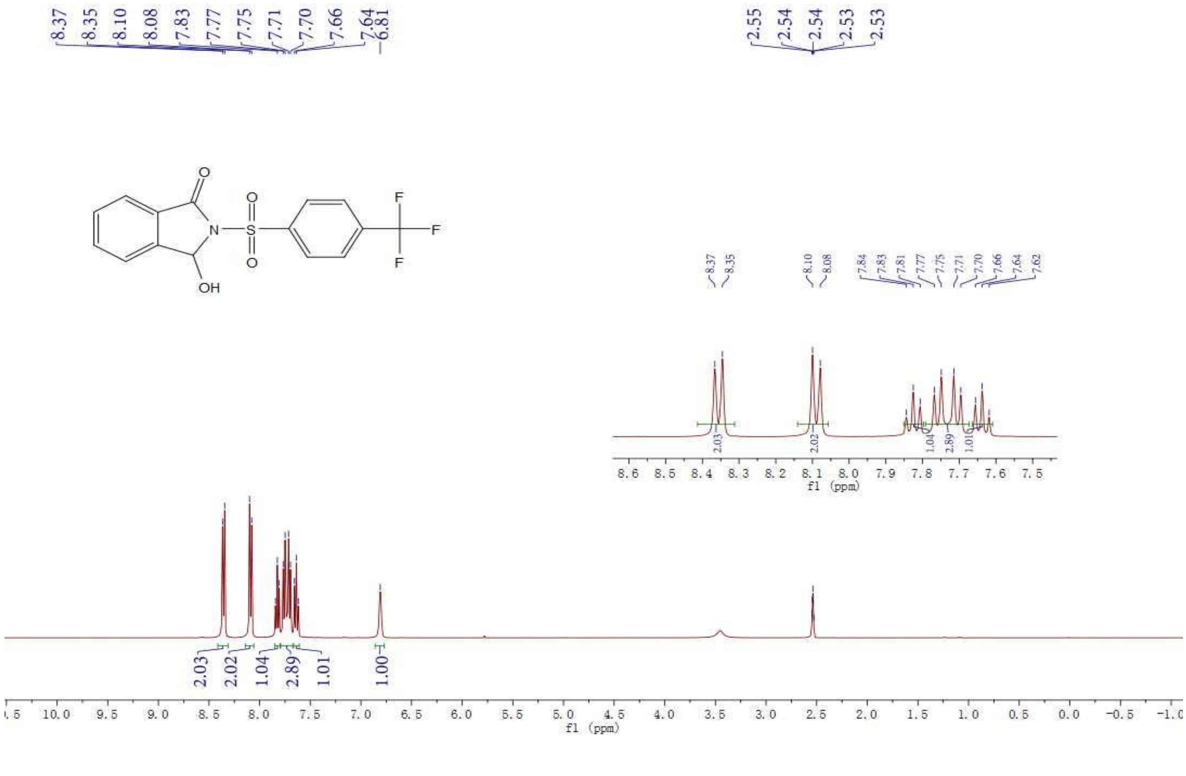

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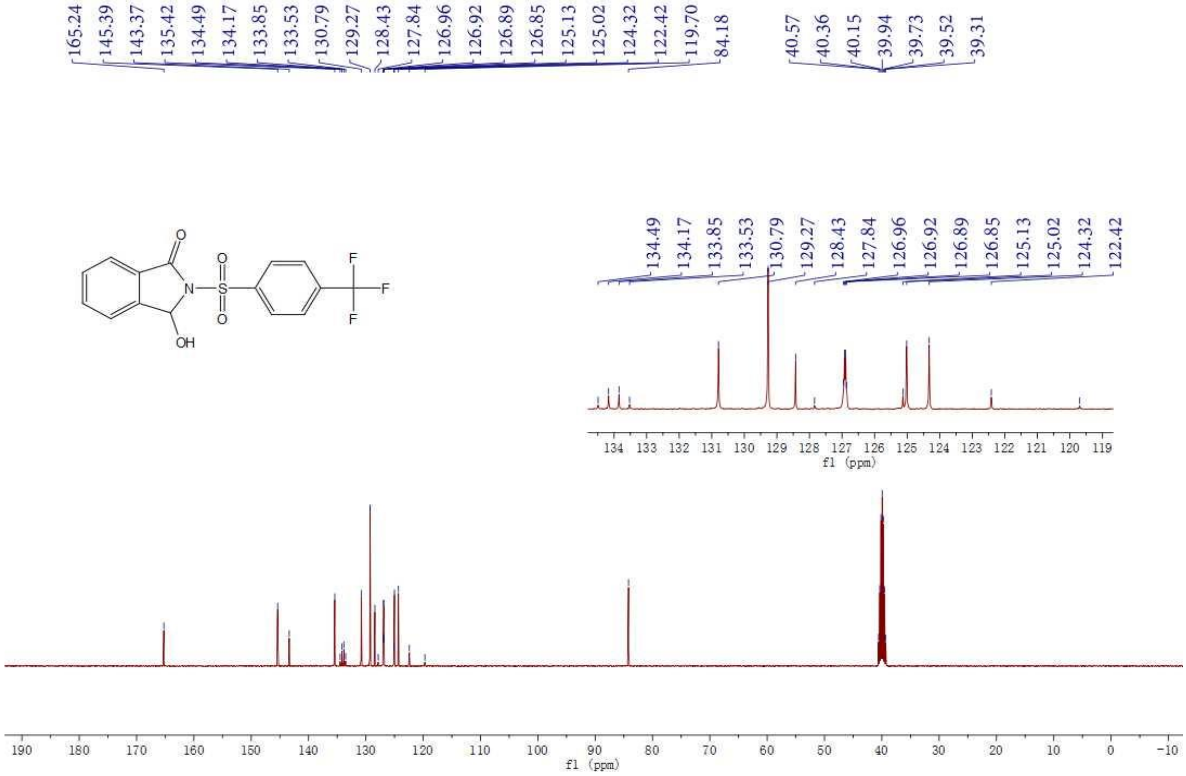

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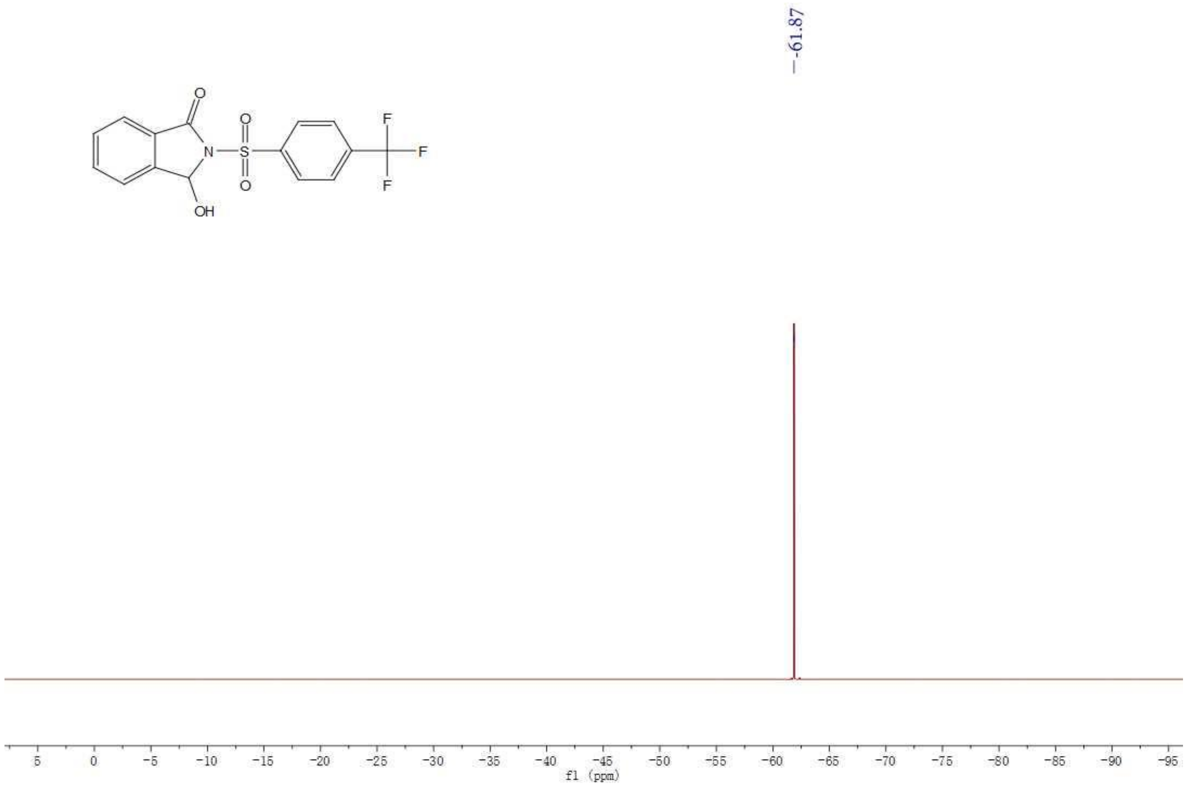
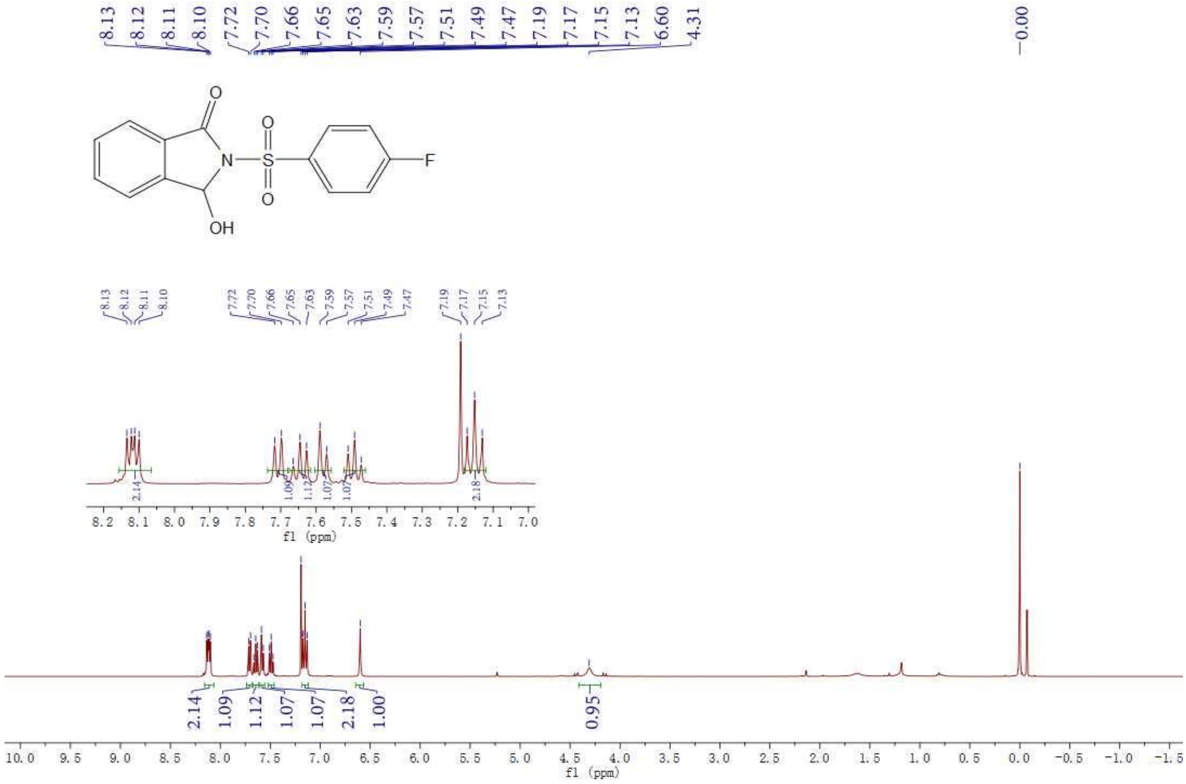
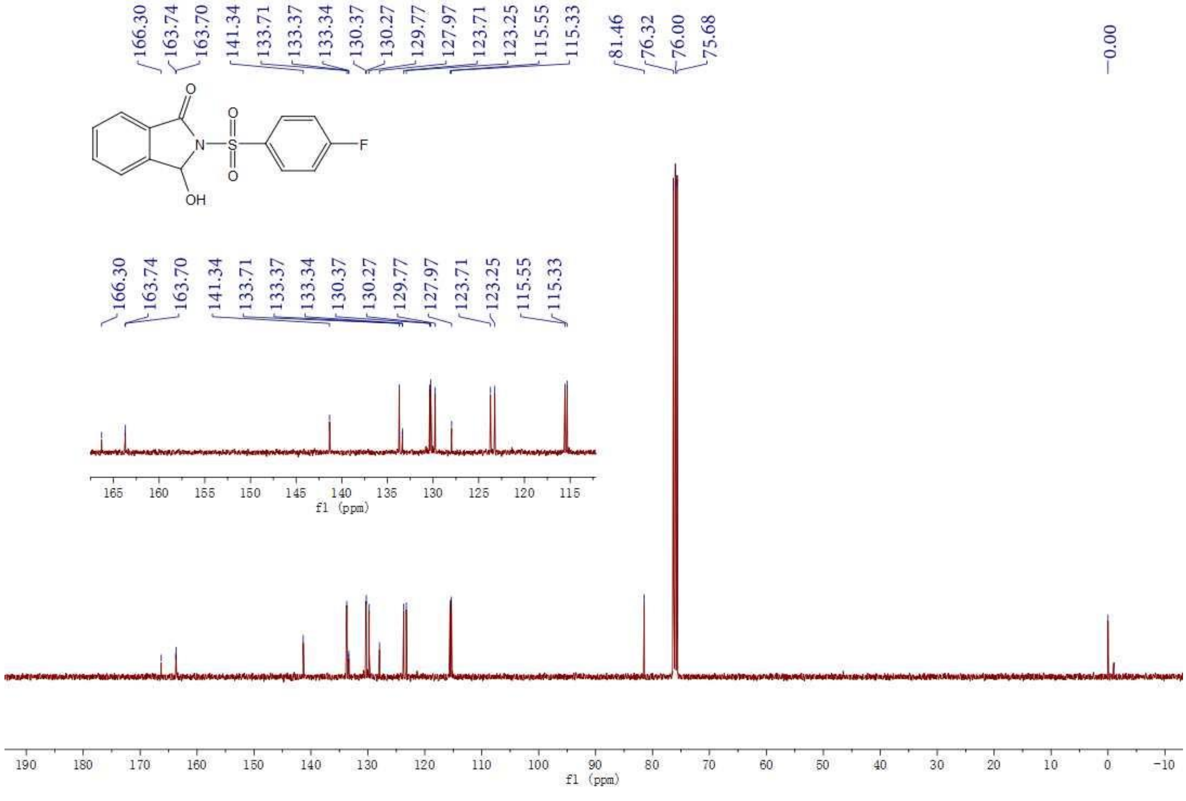


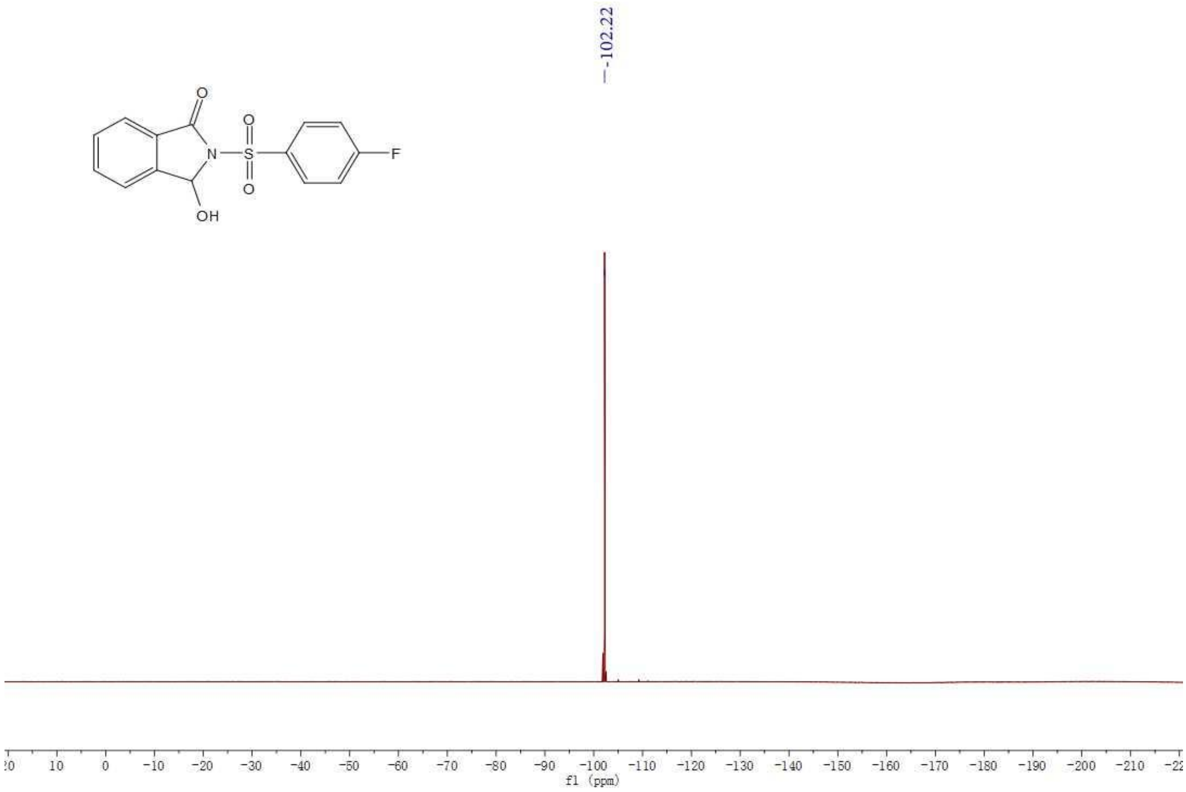
¹H NMR of compound **2g**



¹³C NMR of compound **2g**



^{19}F NMR of compound **2g**



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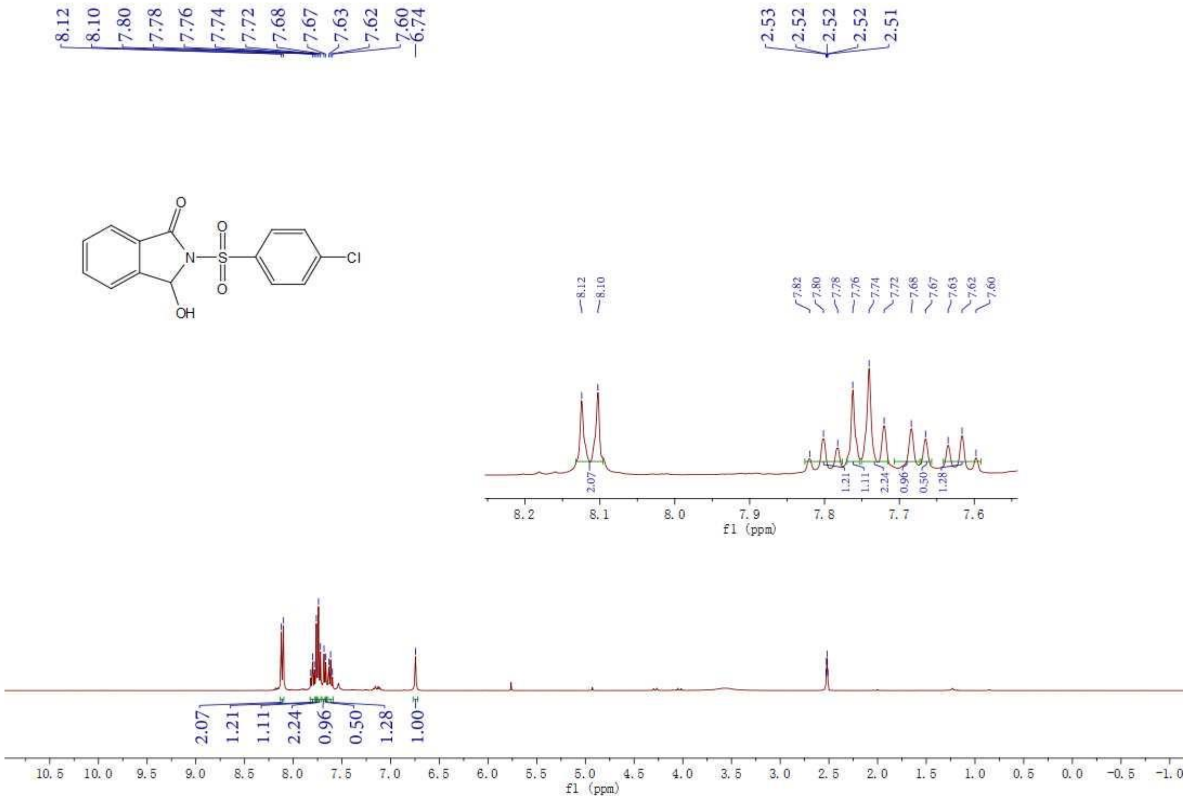

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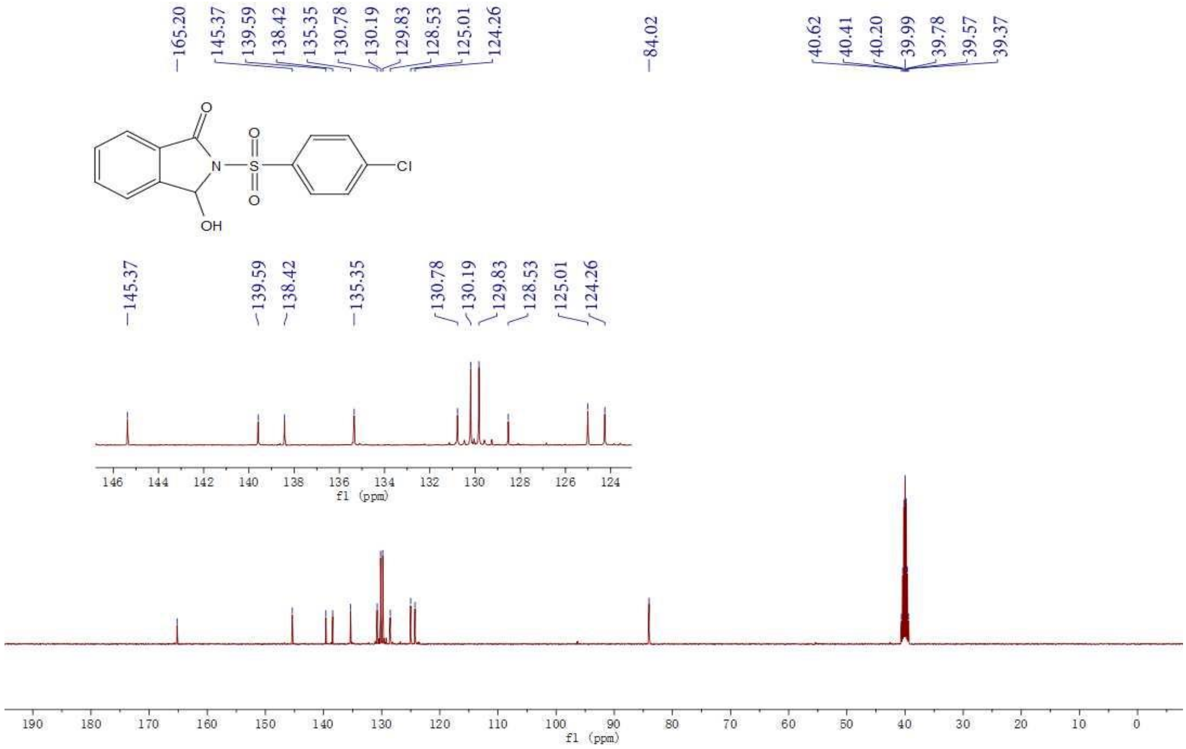
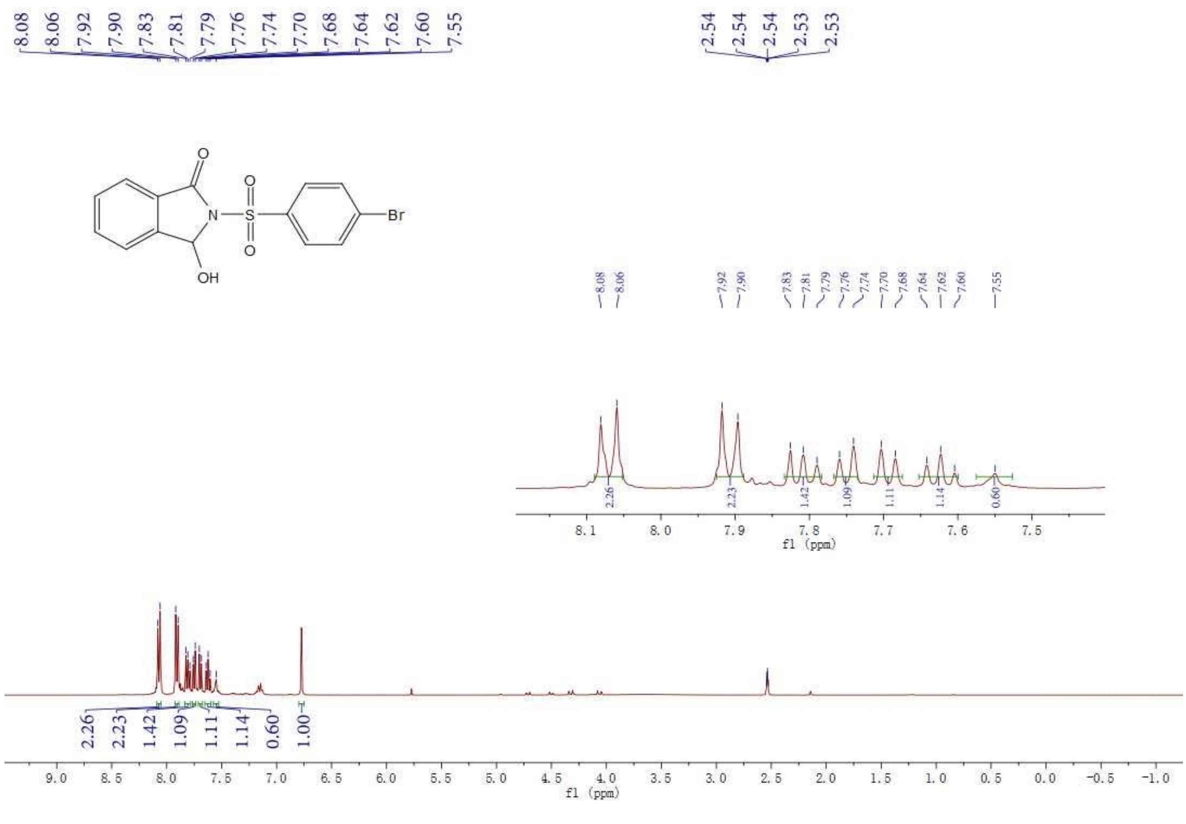


^{1}H NMR of compound **2i**



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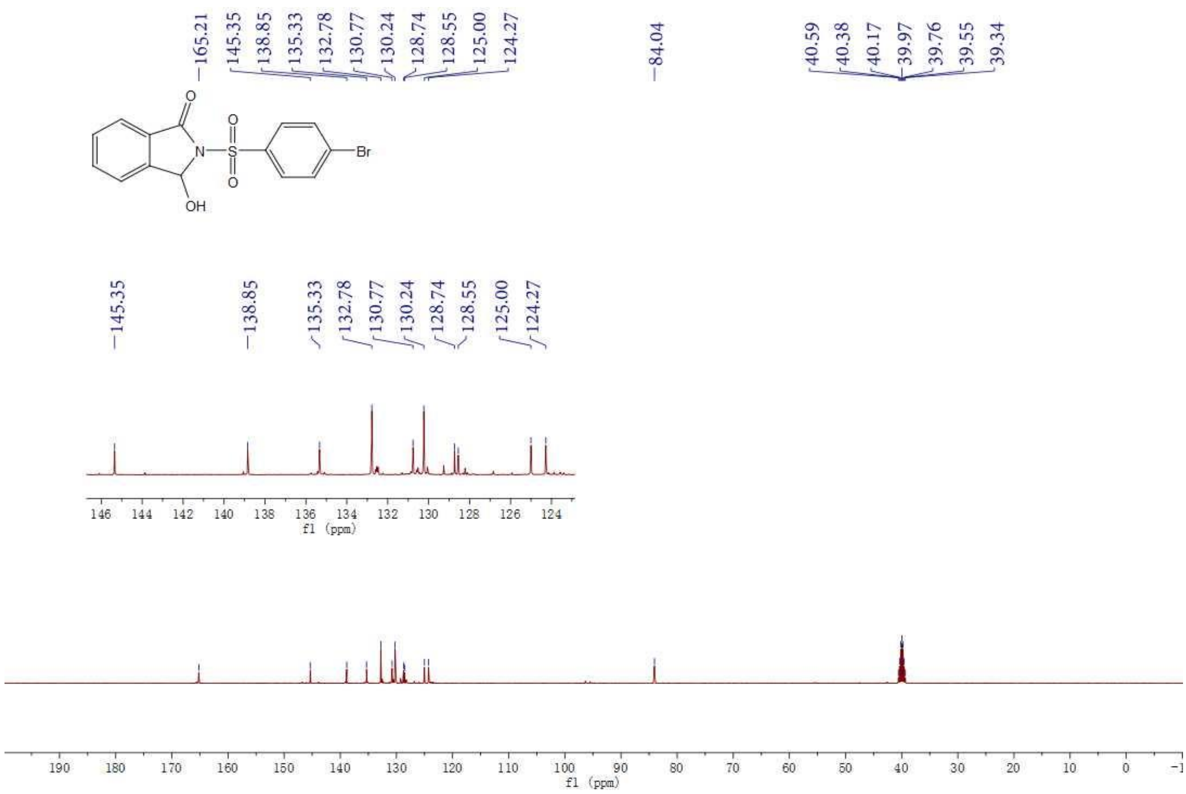

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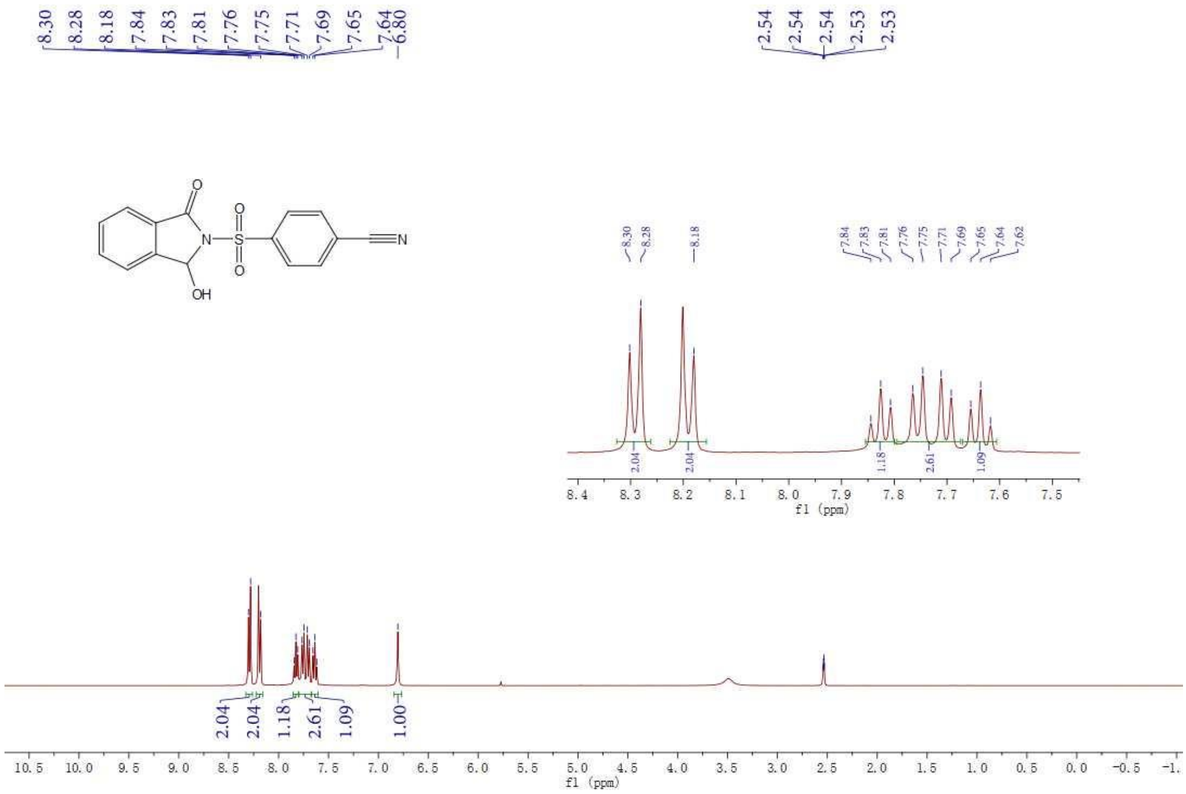

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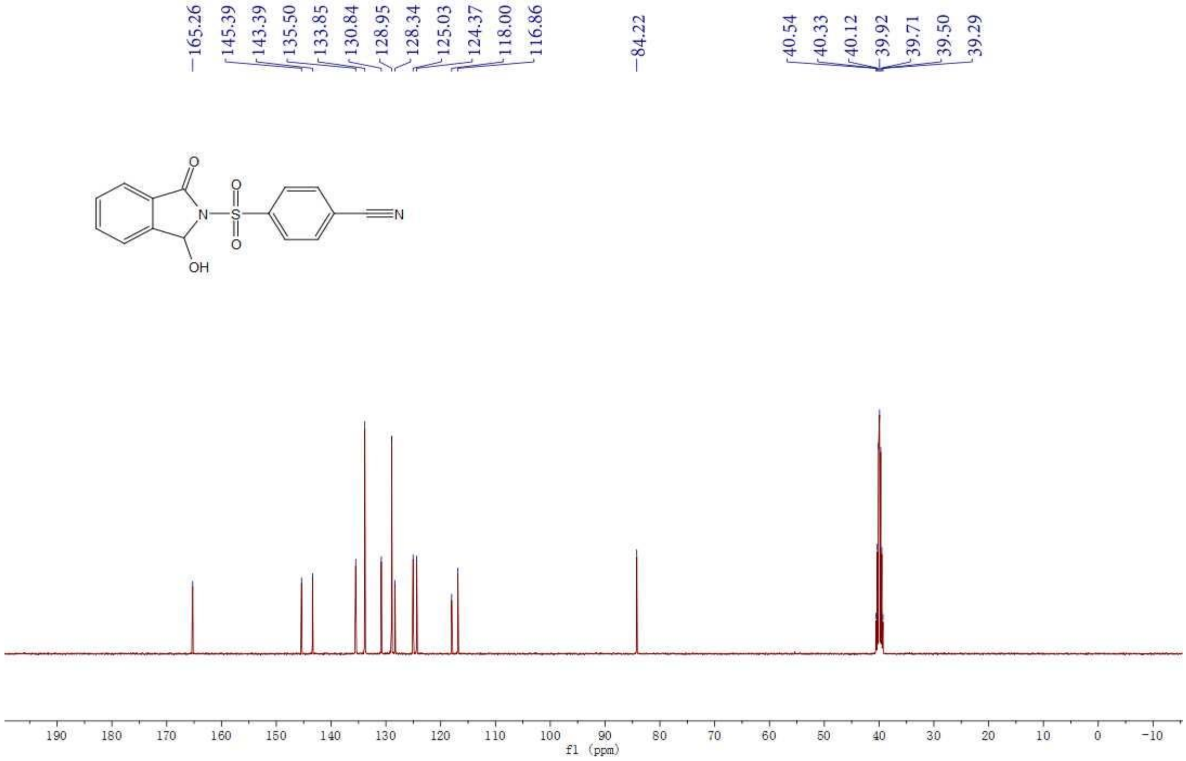

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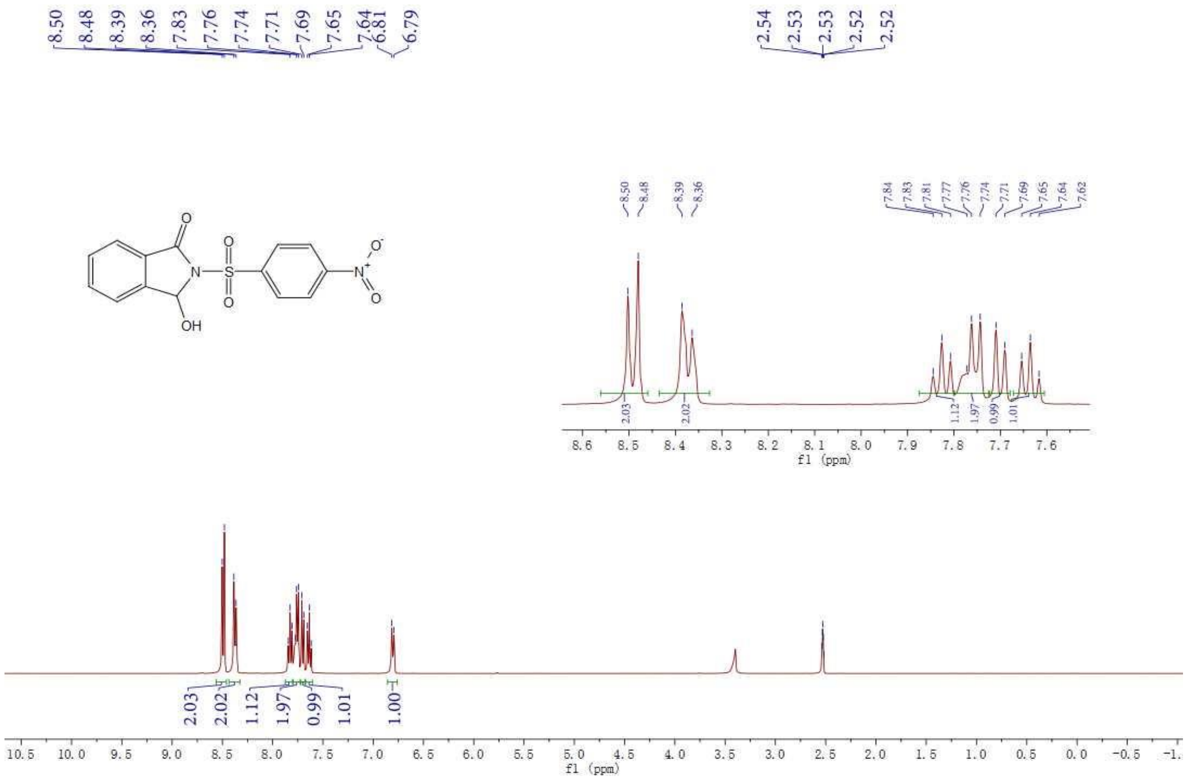

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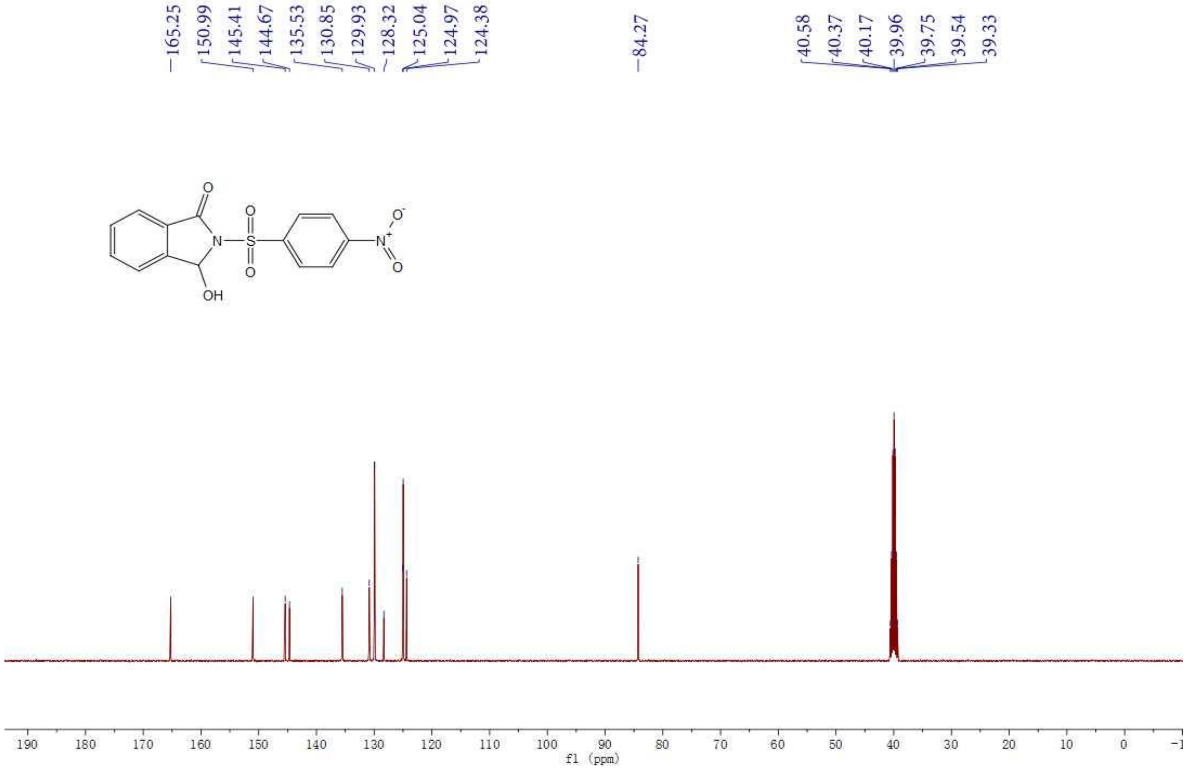

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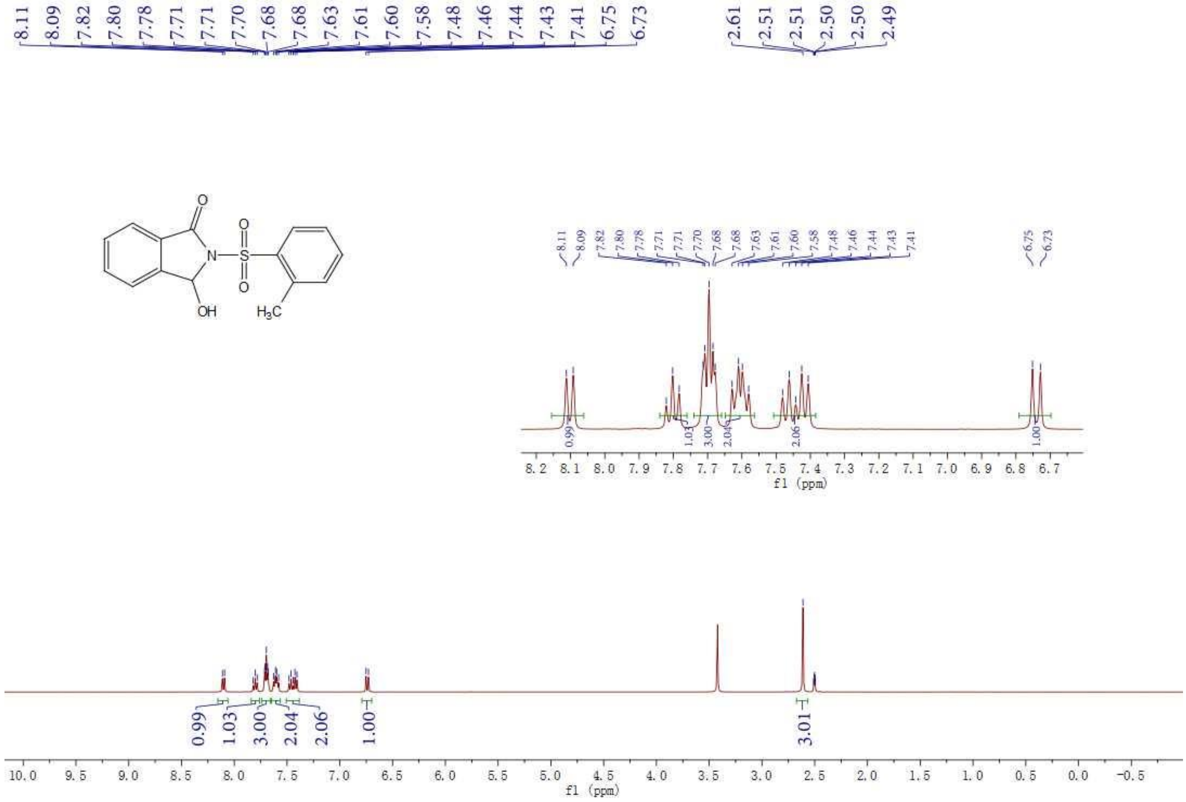

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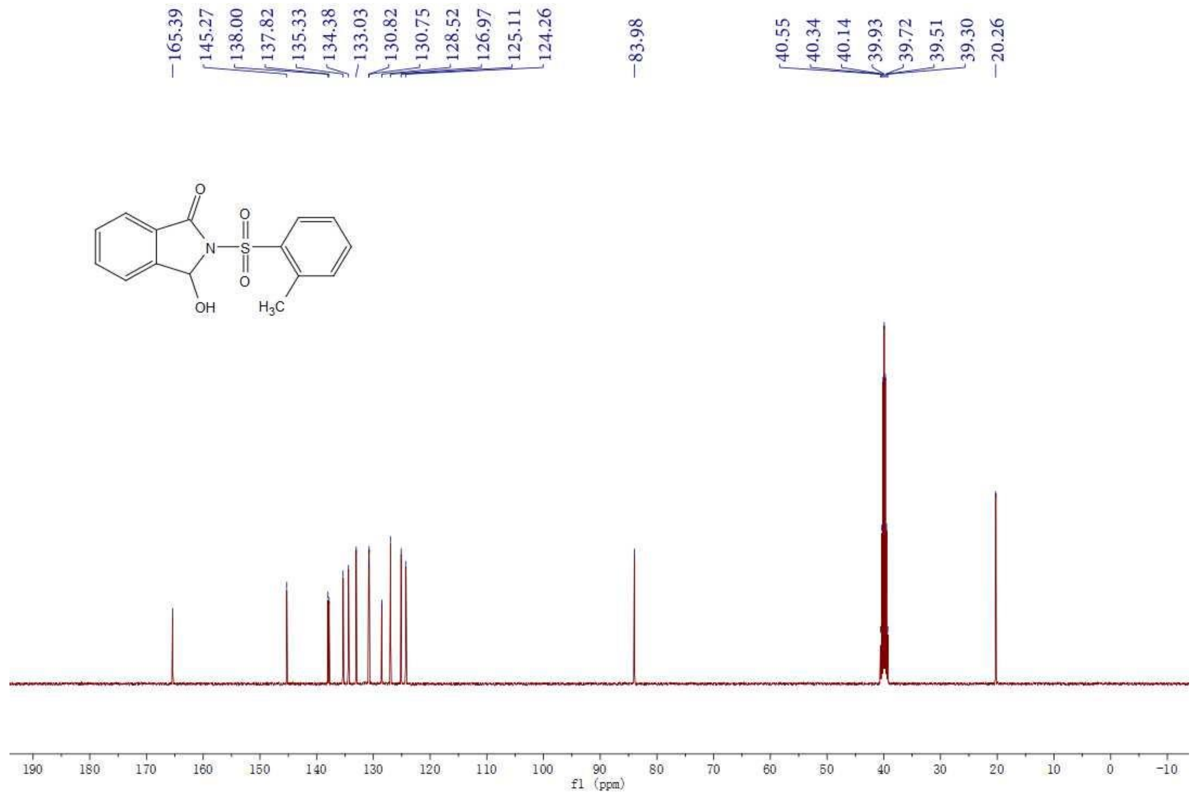
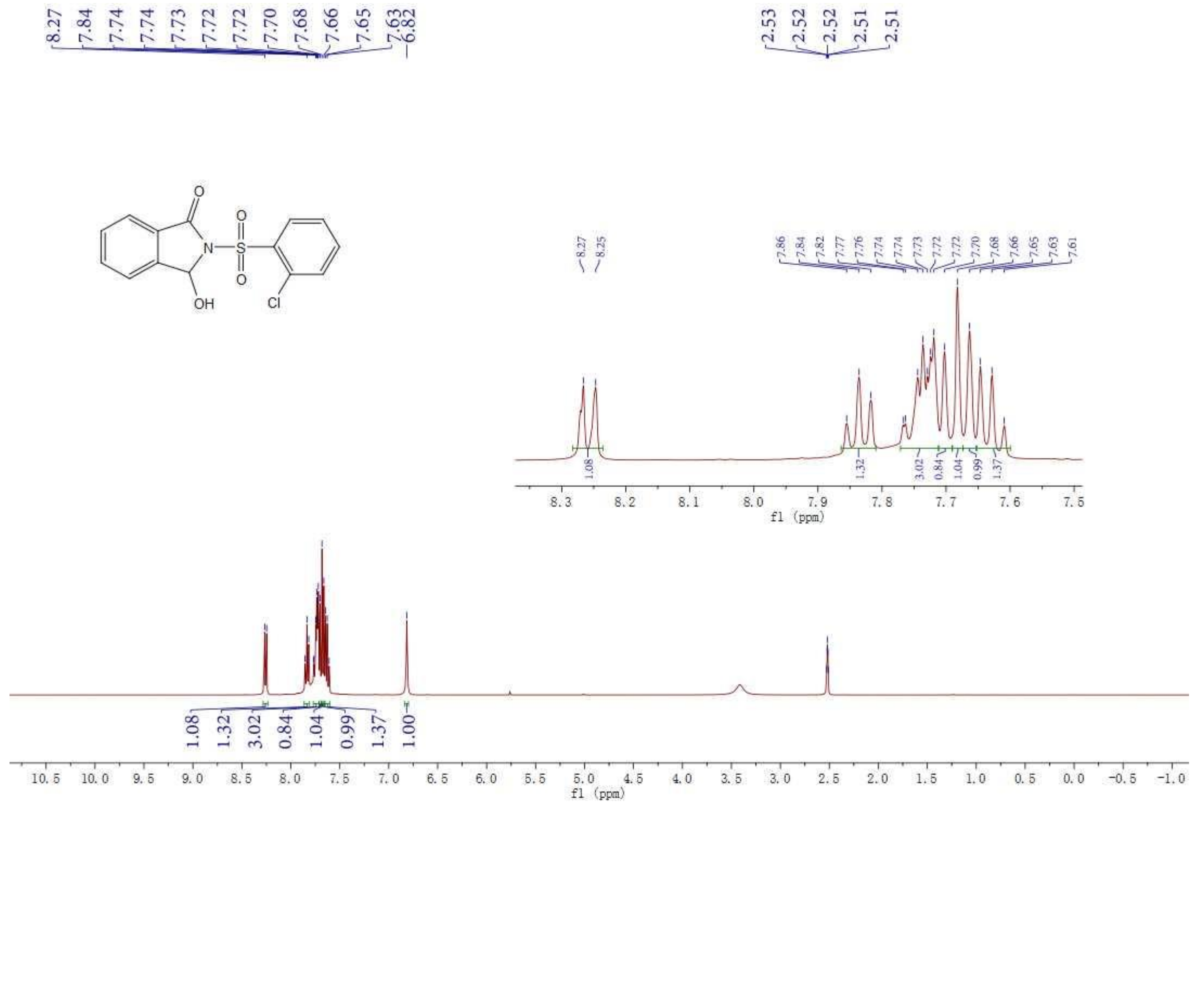
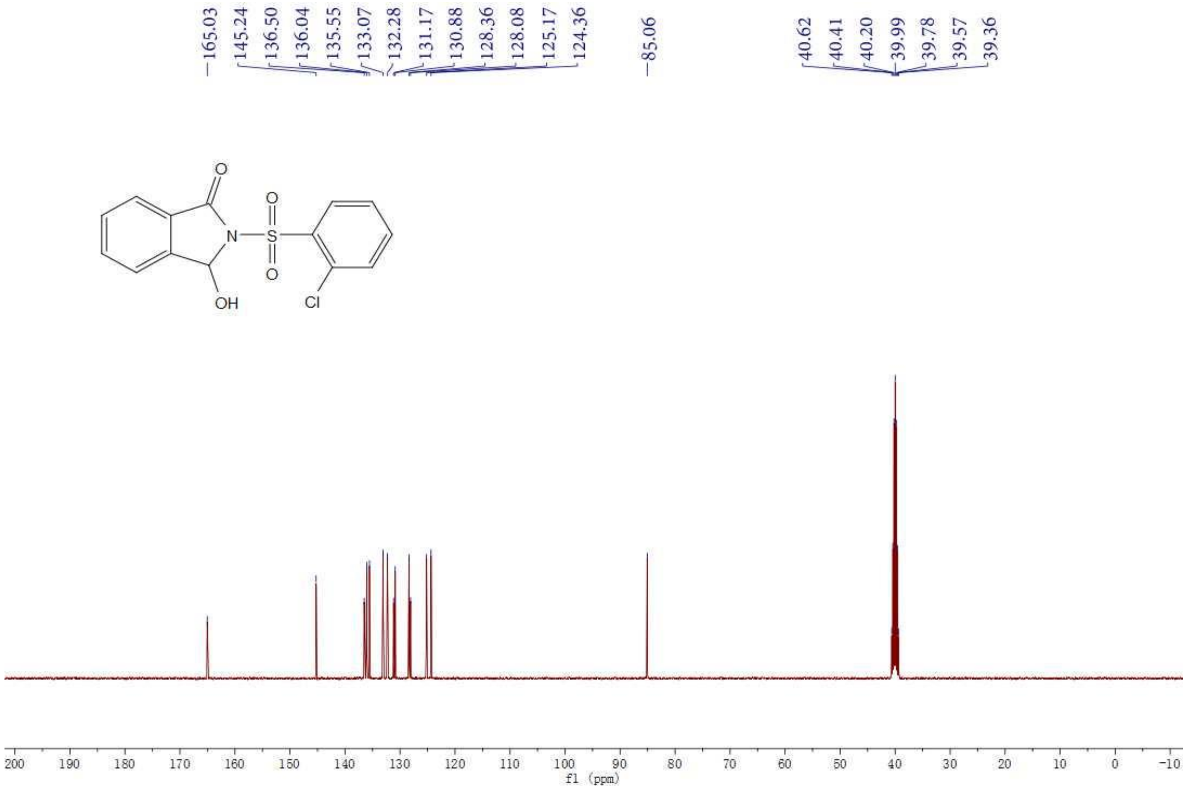


^{1}H NMR of compound **2m**



^{13}C NMR of compound **2m**



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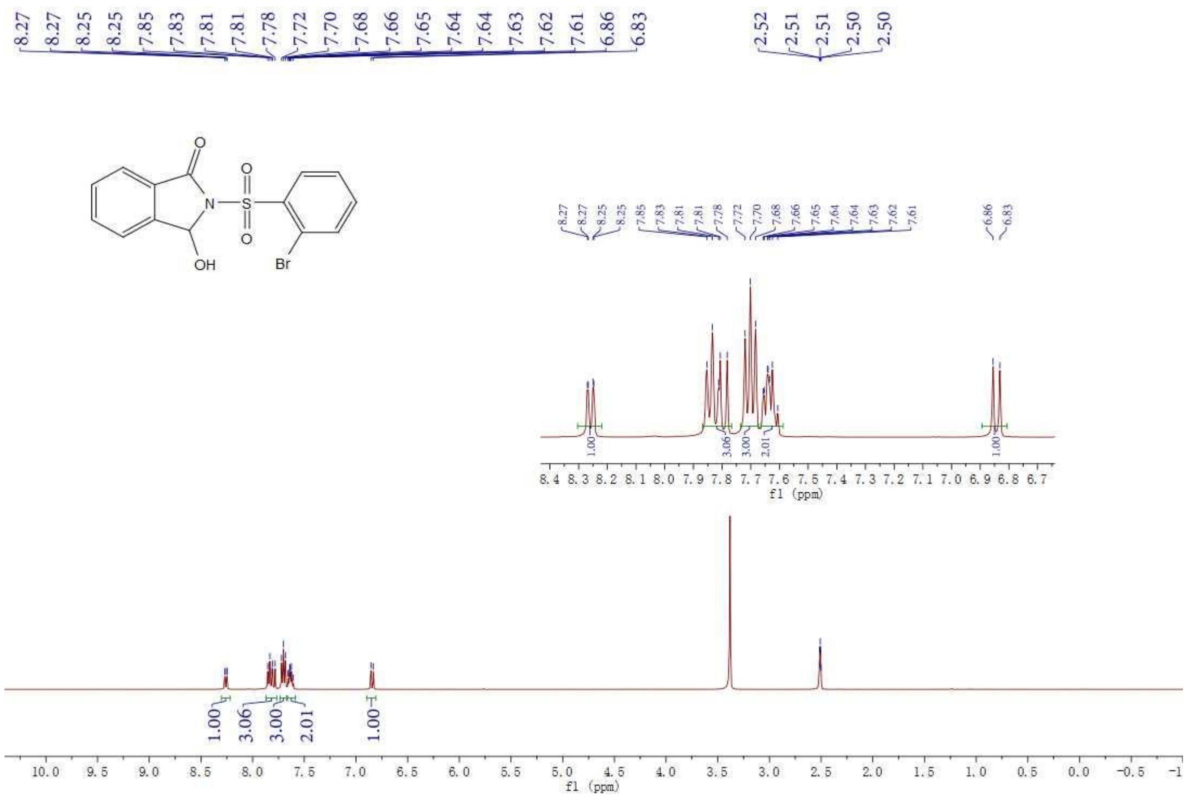
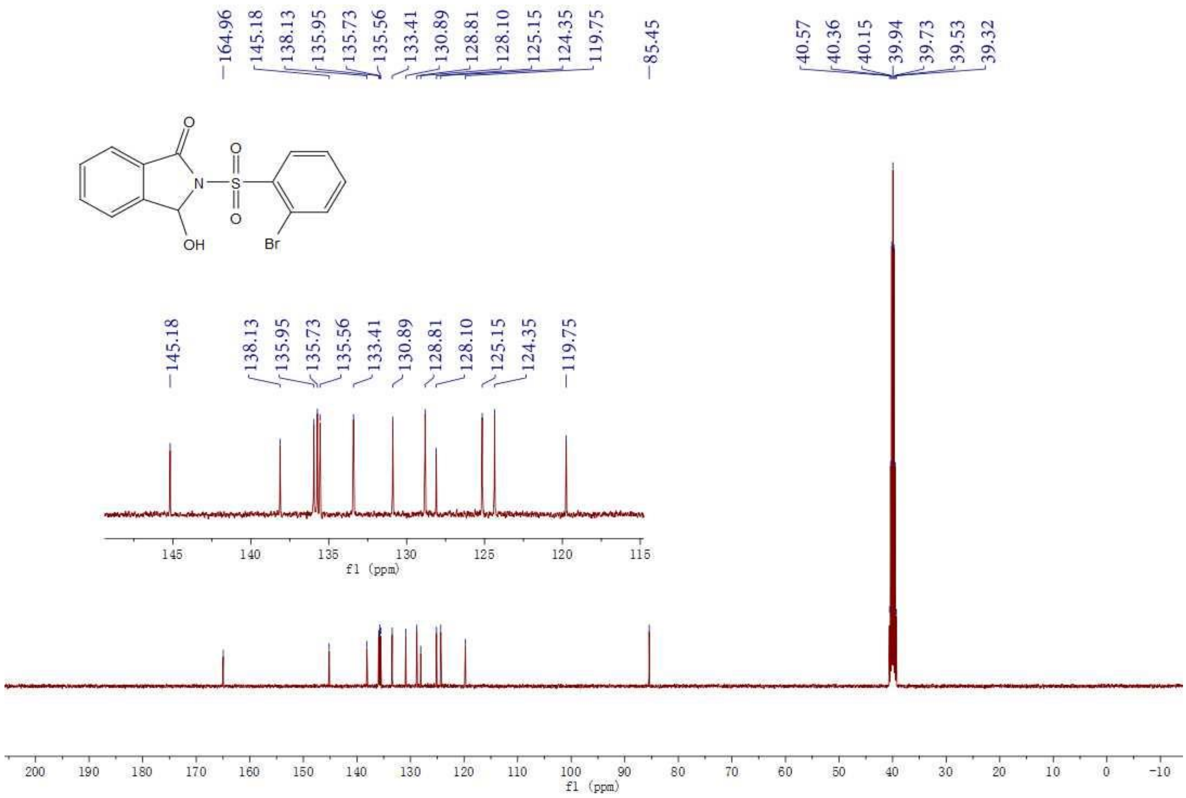
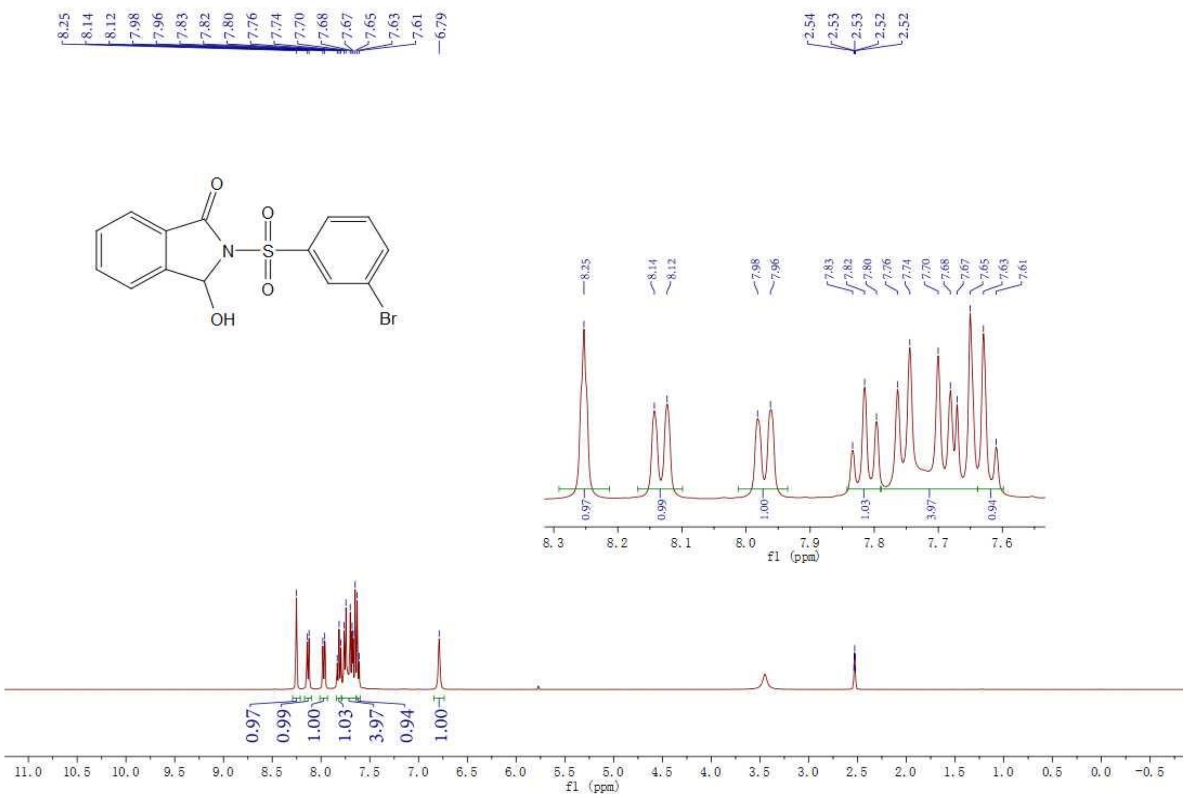


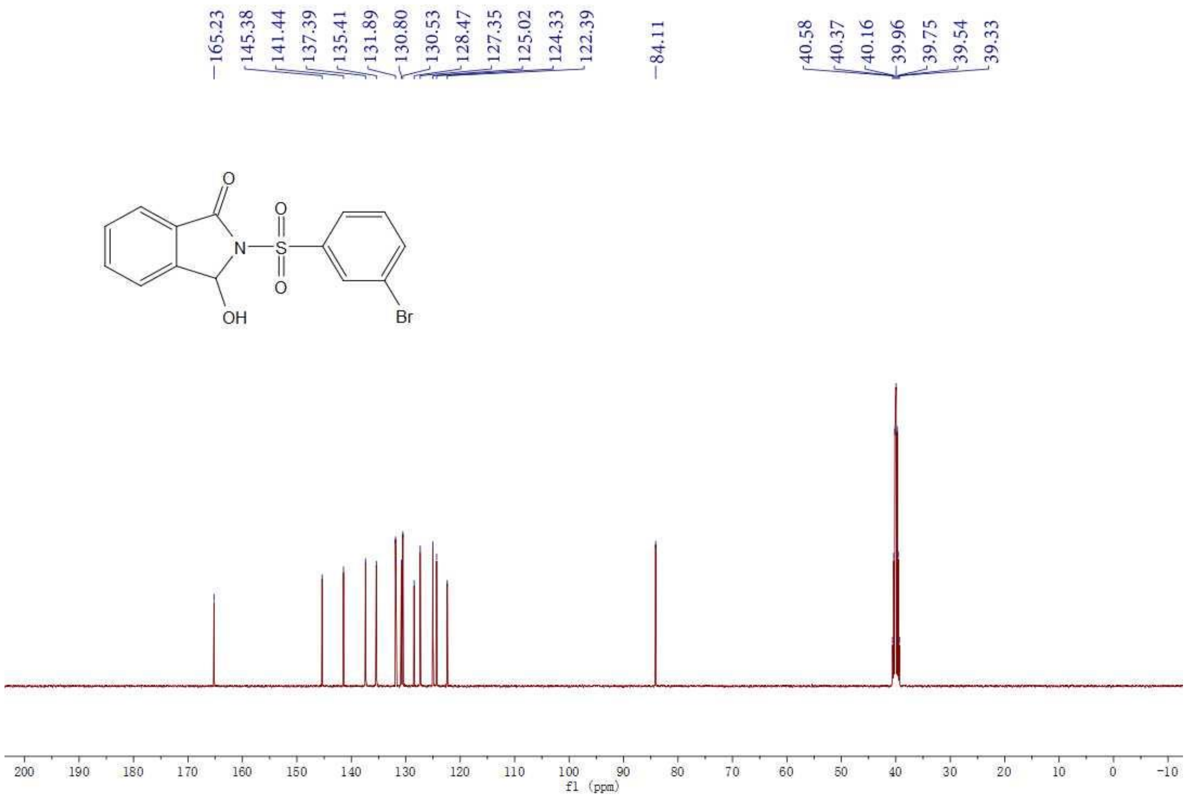
^{13}C NMR of compound **2n**



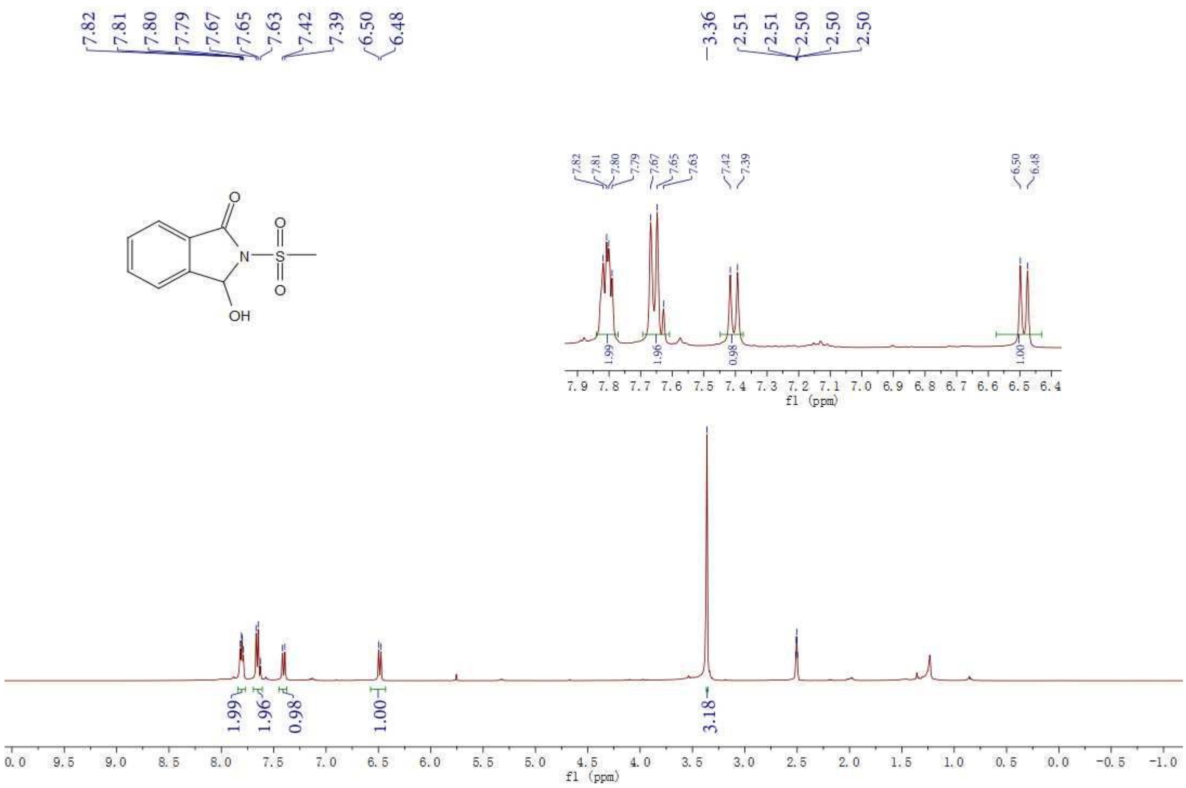
^{1}H NMR of compound **2o**



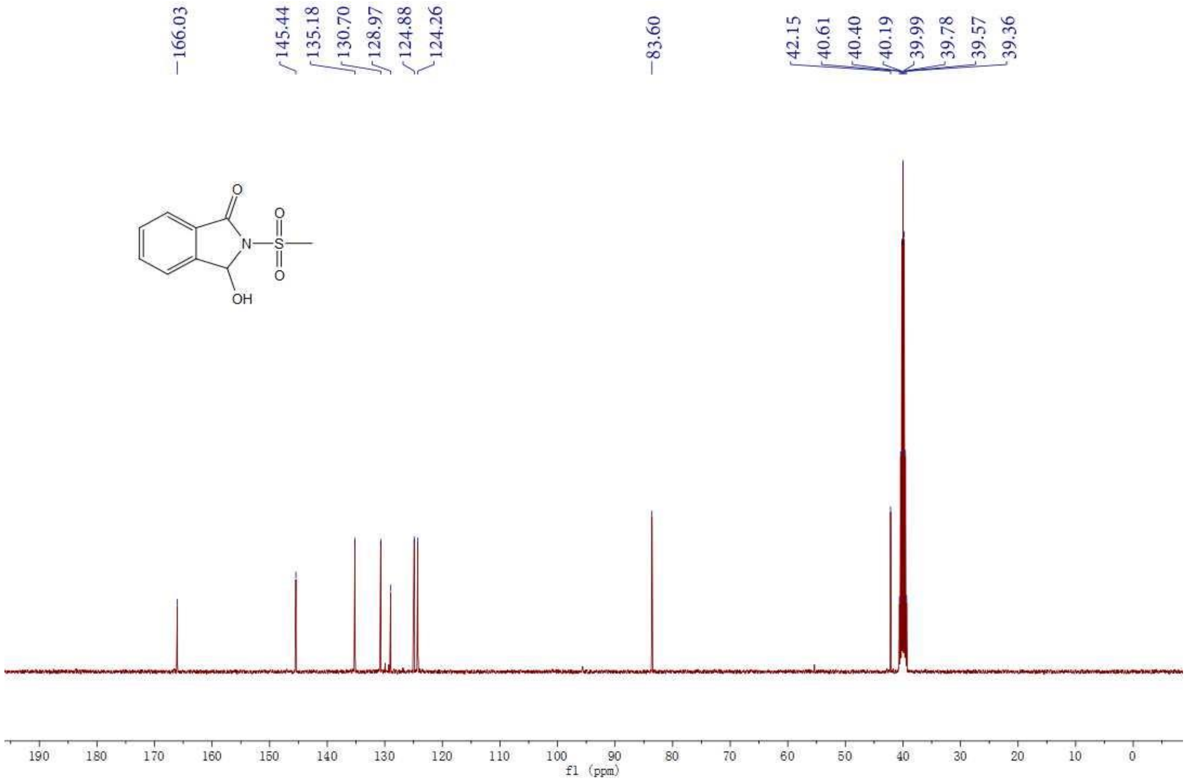
^{13}C NMR of compound **2o**



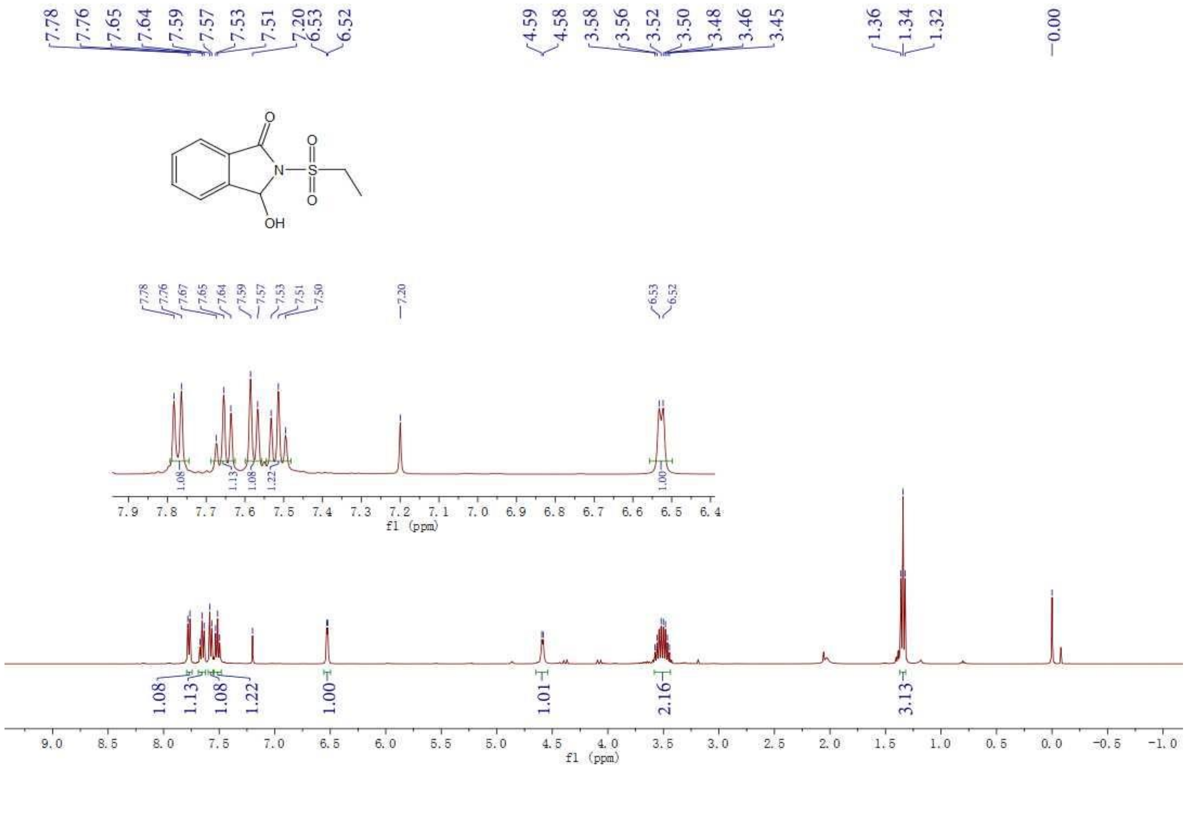
^{1}H NMR of compound **2p**



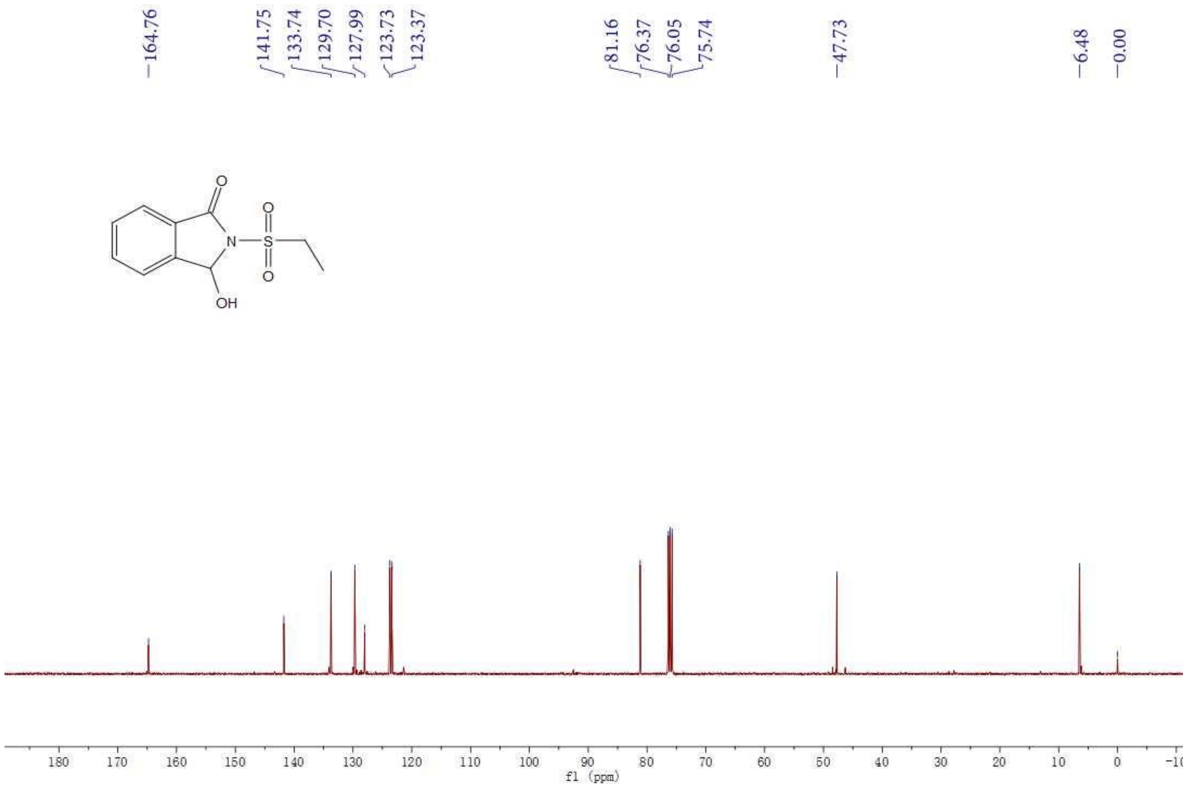
^{13}C NMR of compound **2p**



^{1}H NMR of compound **2q**



^{13}C NMR of compound **2q**



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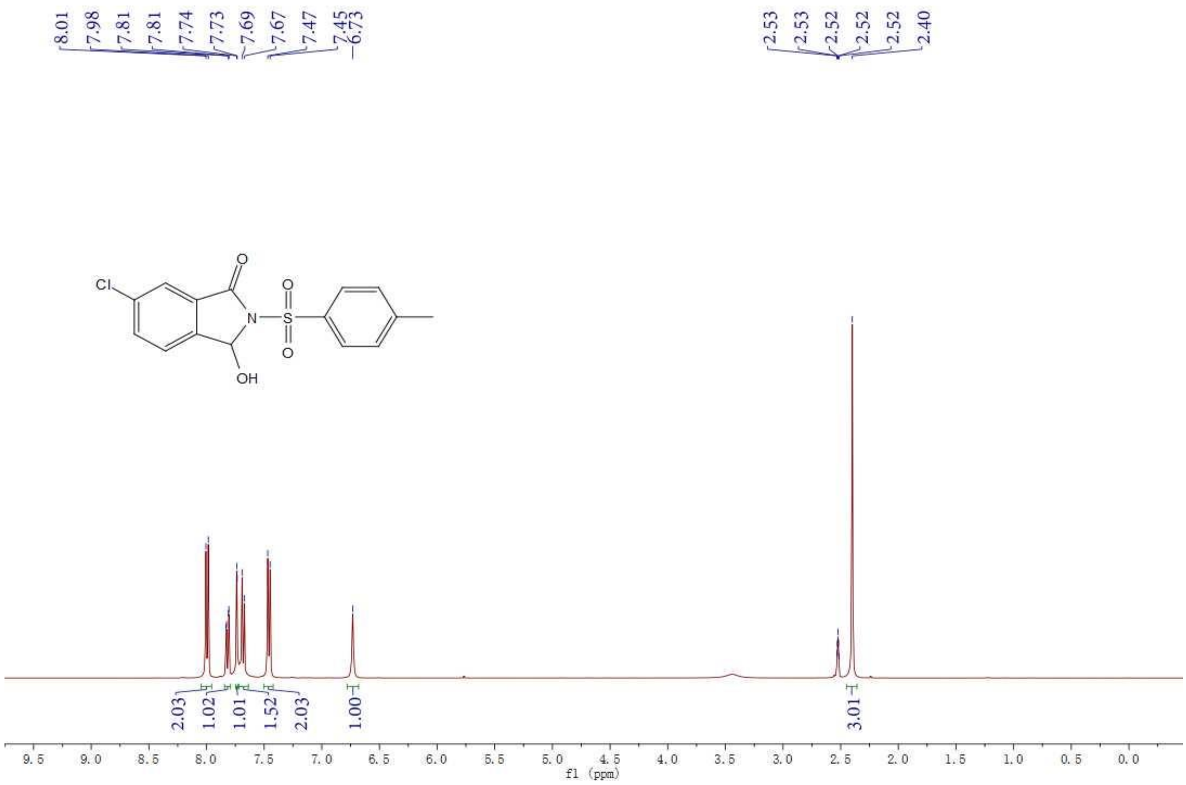
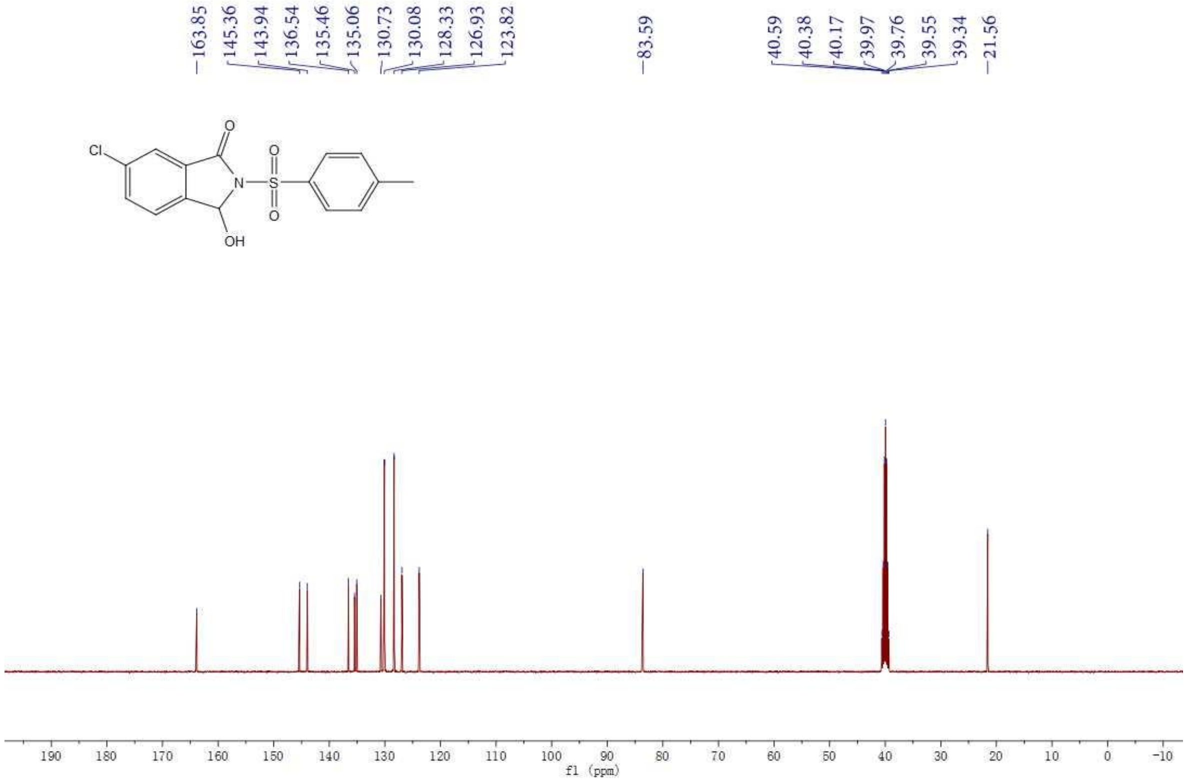
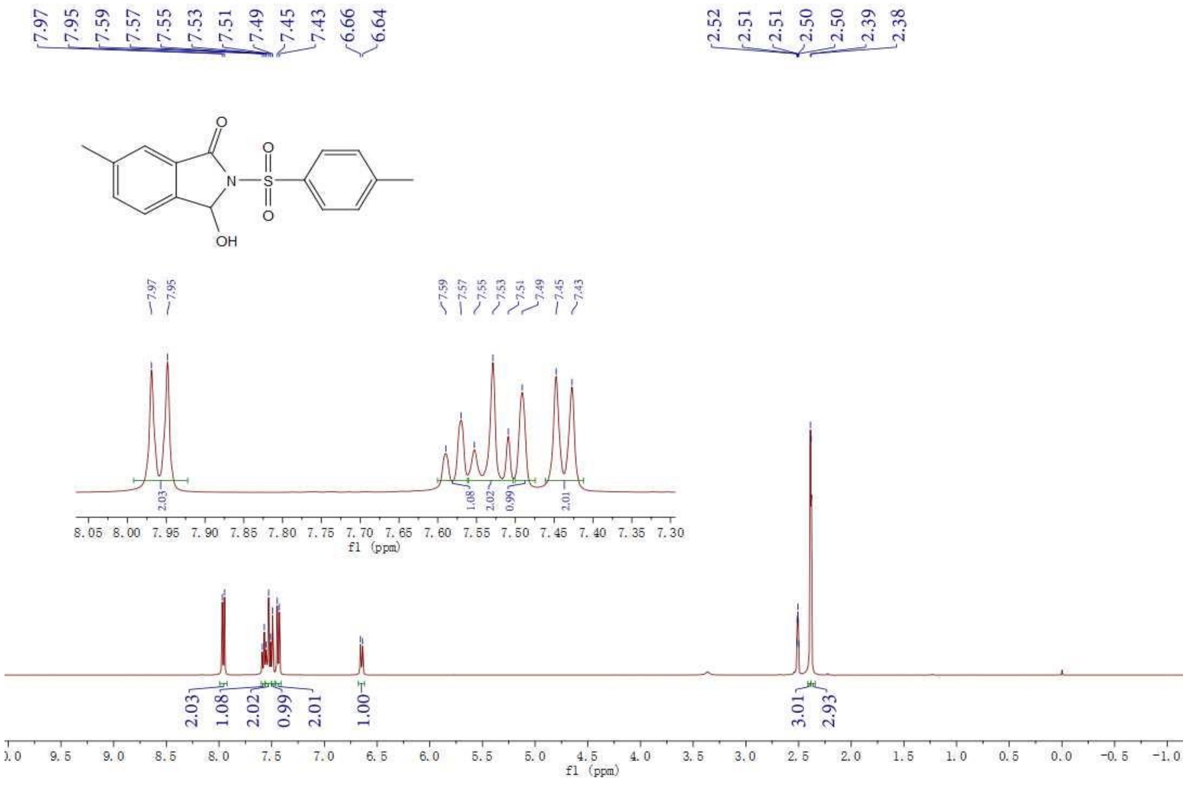


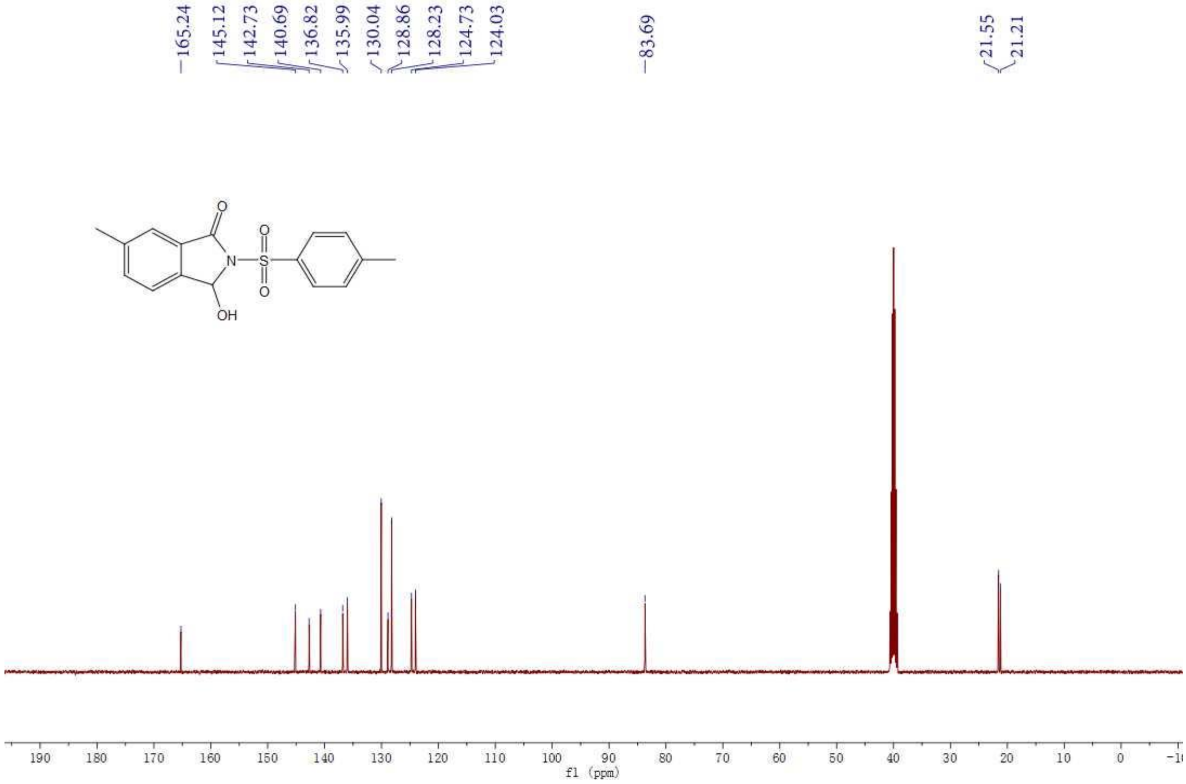
[13]C NMR of compound **2r**



[1]H NMR of compound **2s**



^{13}C NMR of compound **2s**



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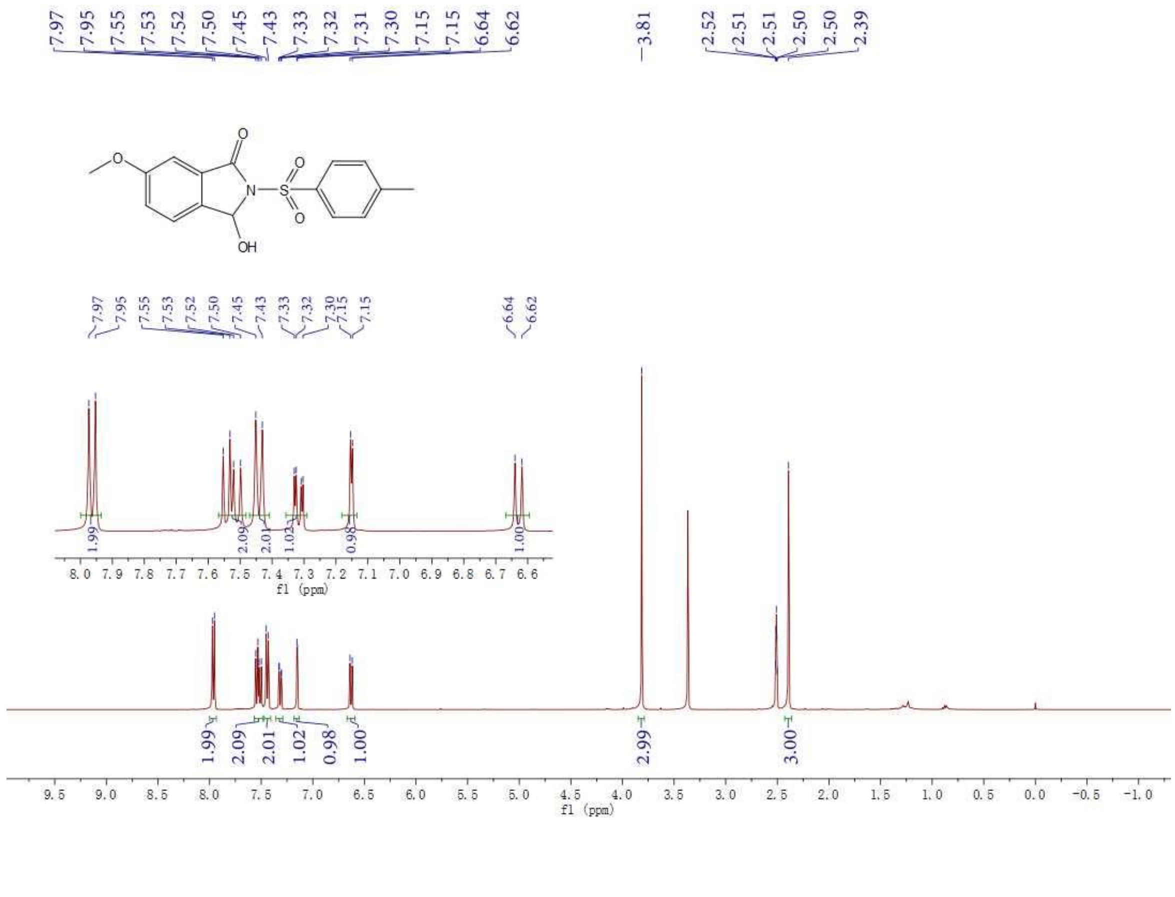

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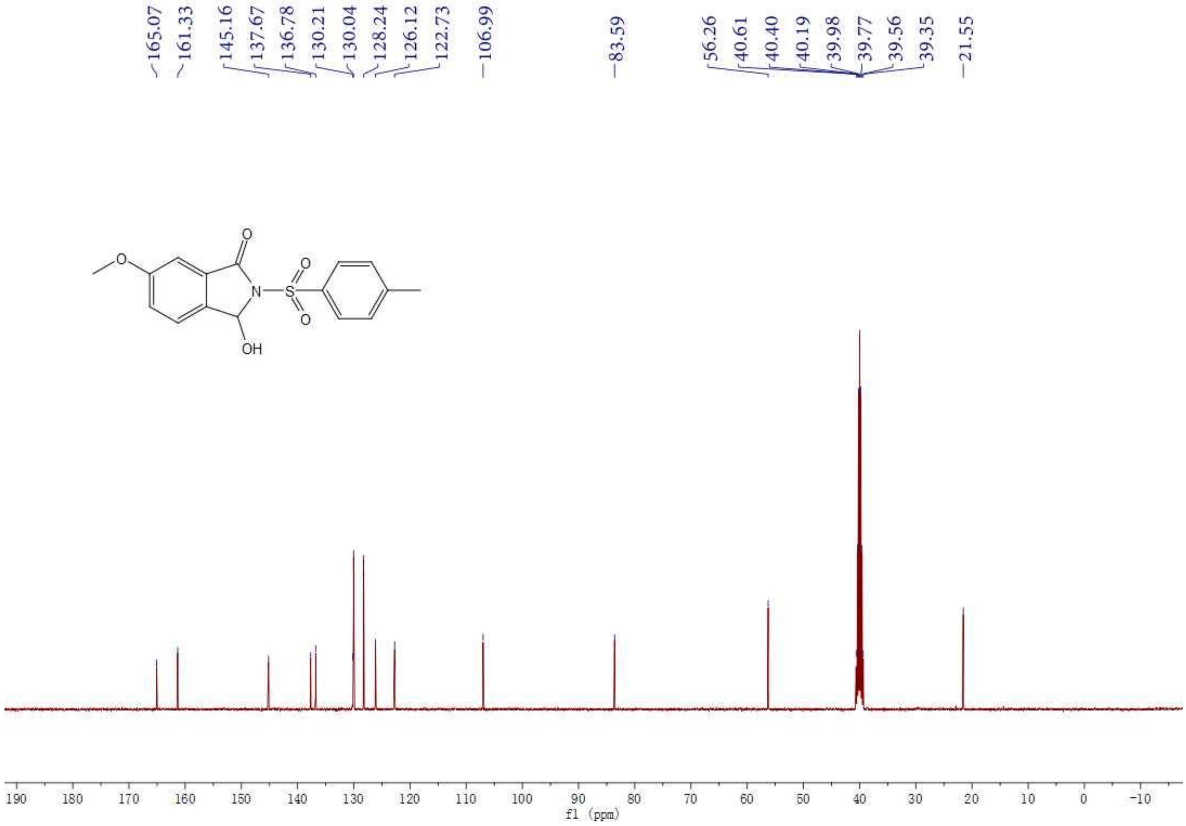

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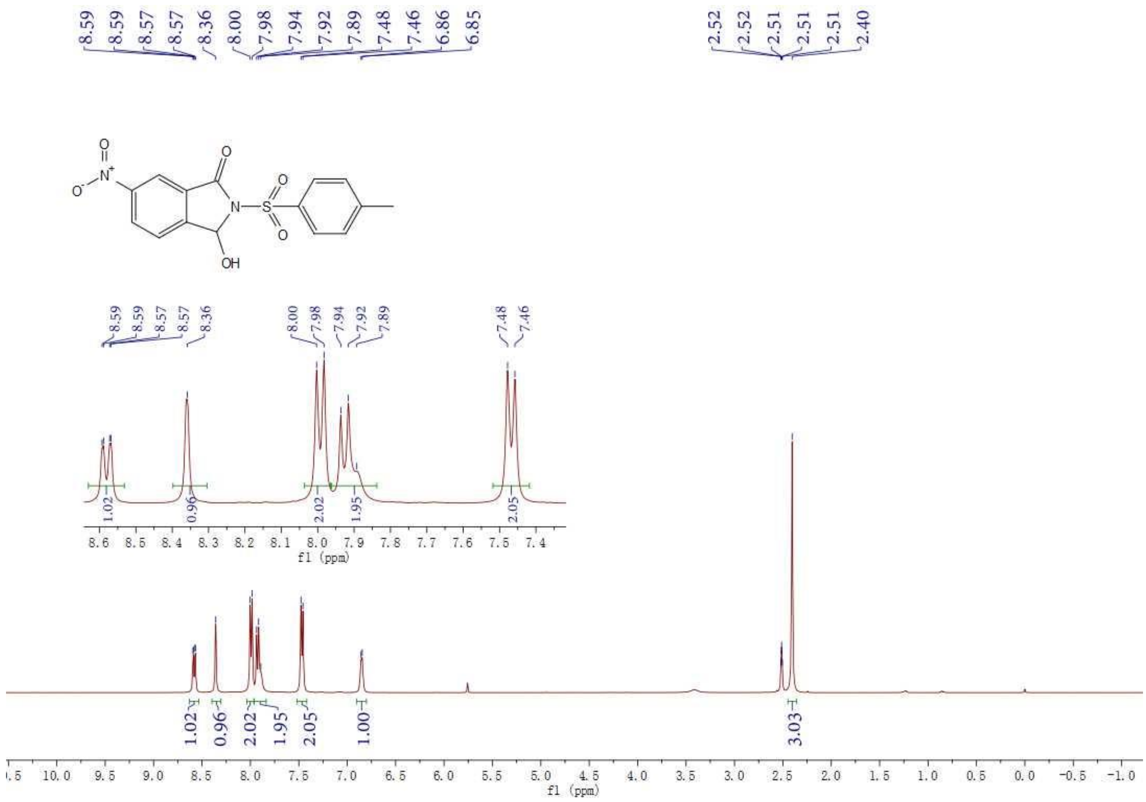

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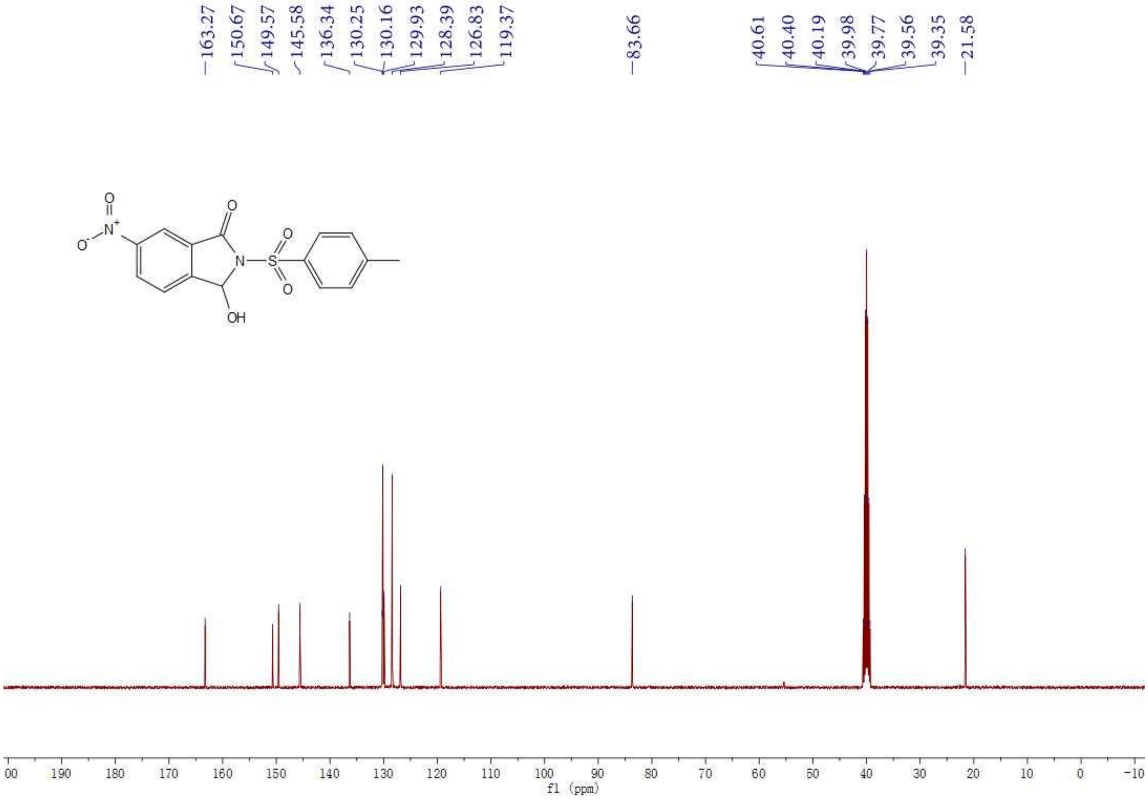
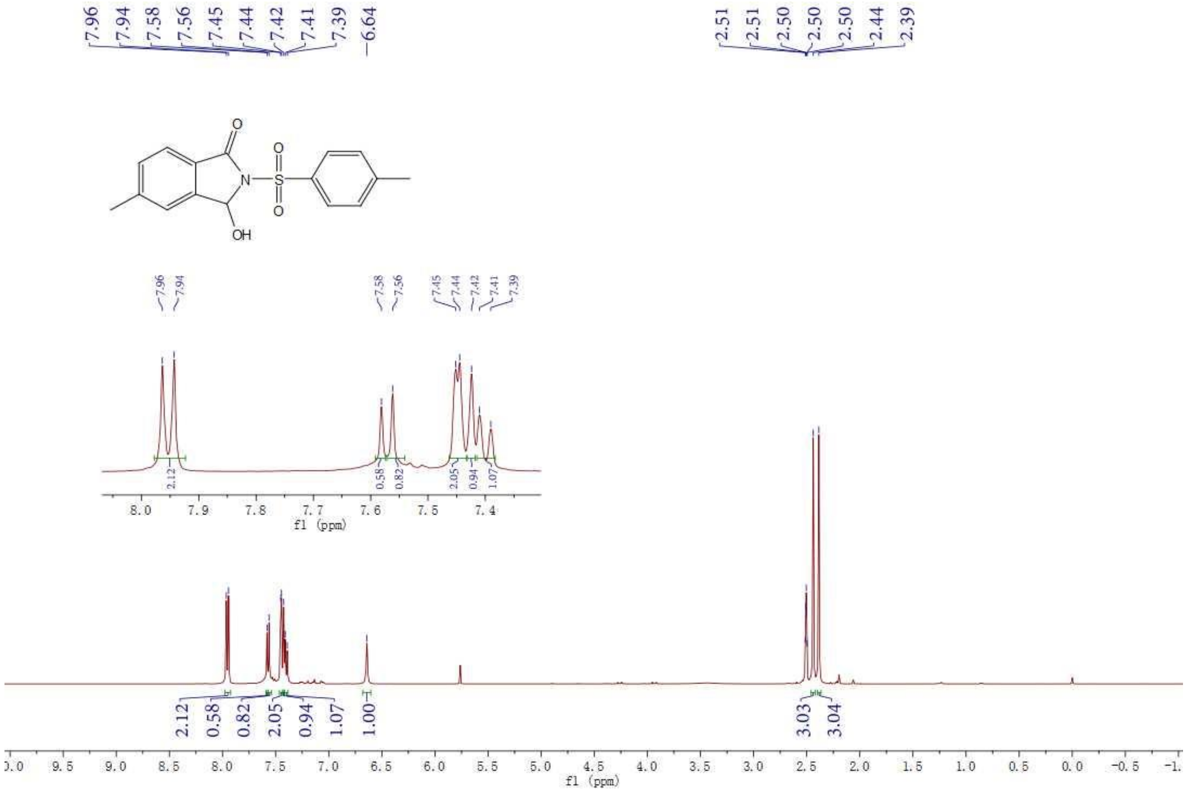
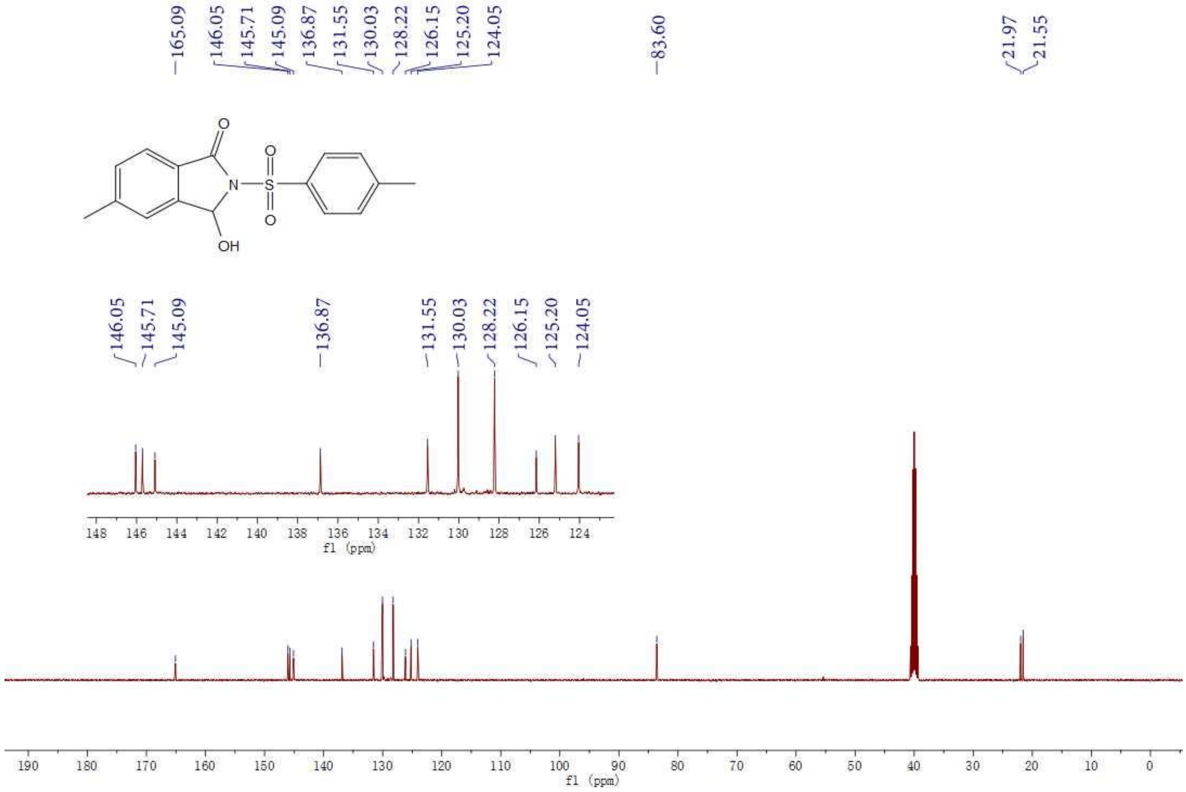


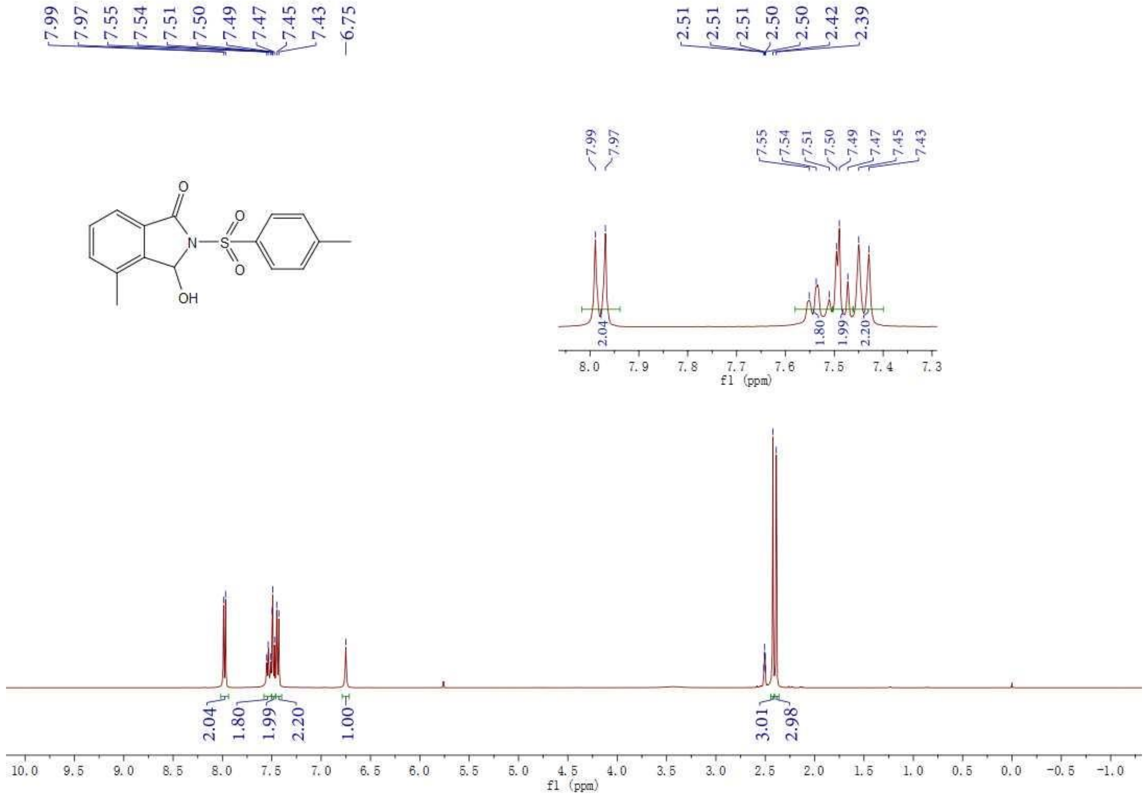
^{1}H NMR of compound **2v**



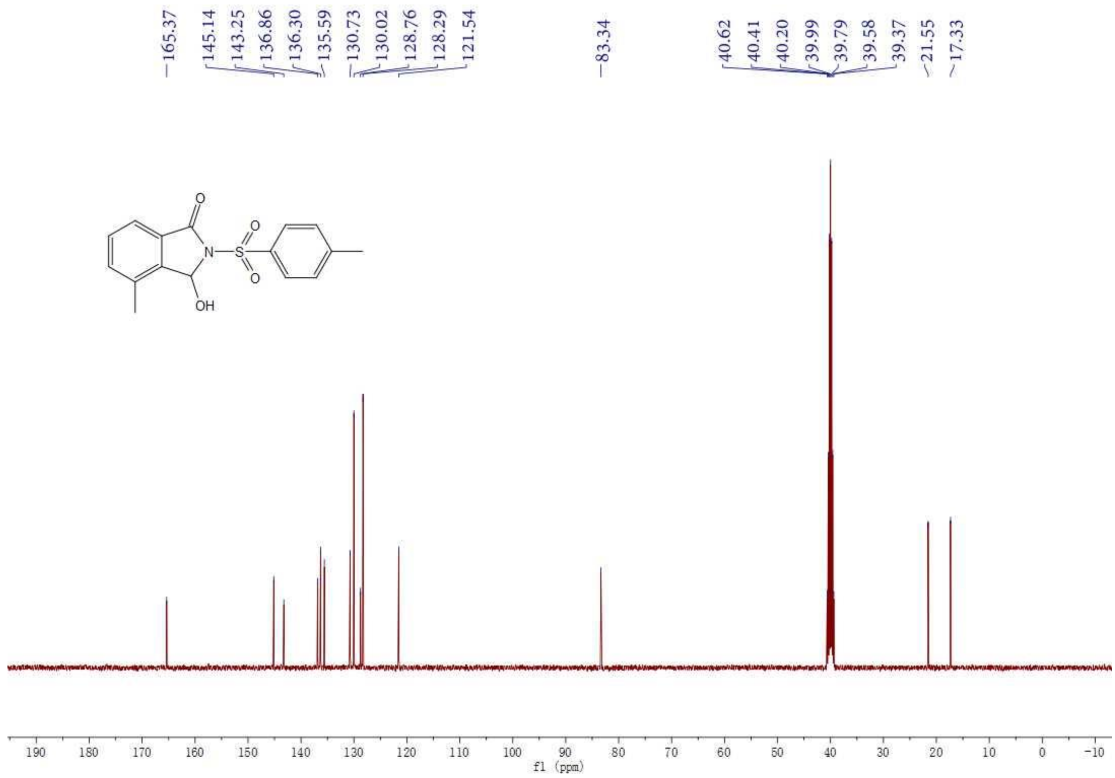
^{13}C NMR of compound **2v**



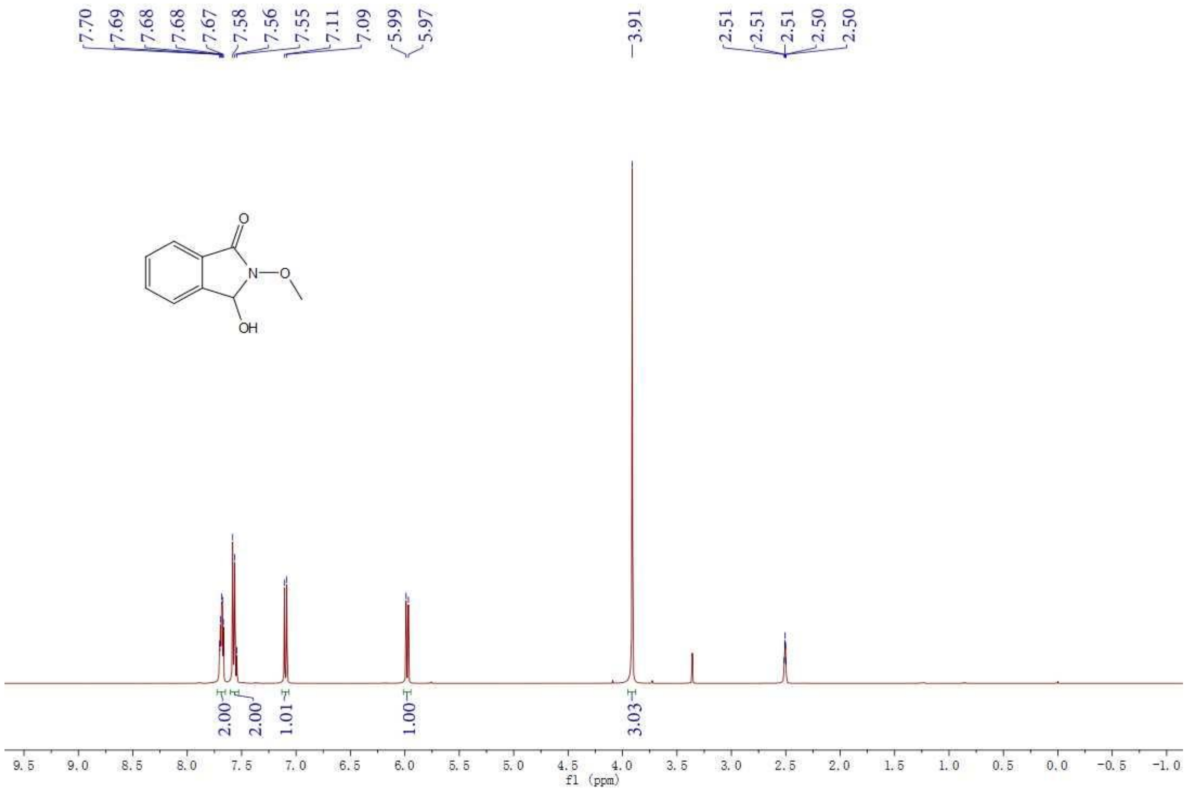
^{1}H NMR of compound **2w**



^{13}C NMR of compound **2w**



^{1}H NMR of compound **2x**



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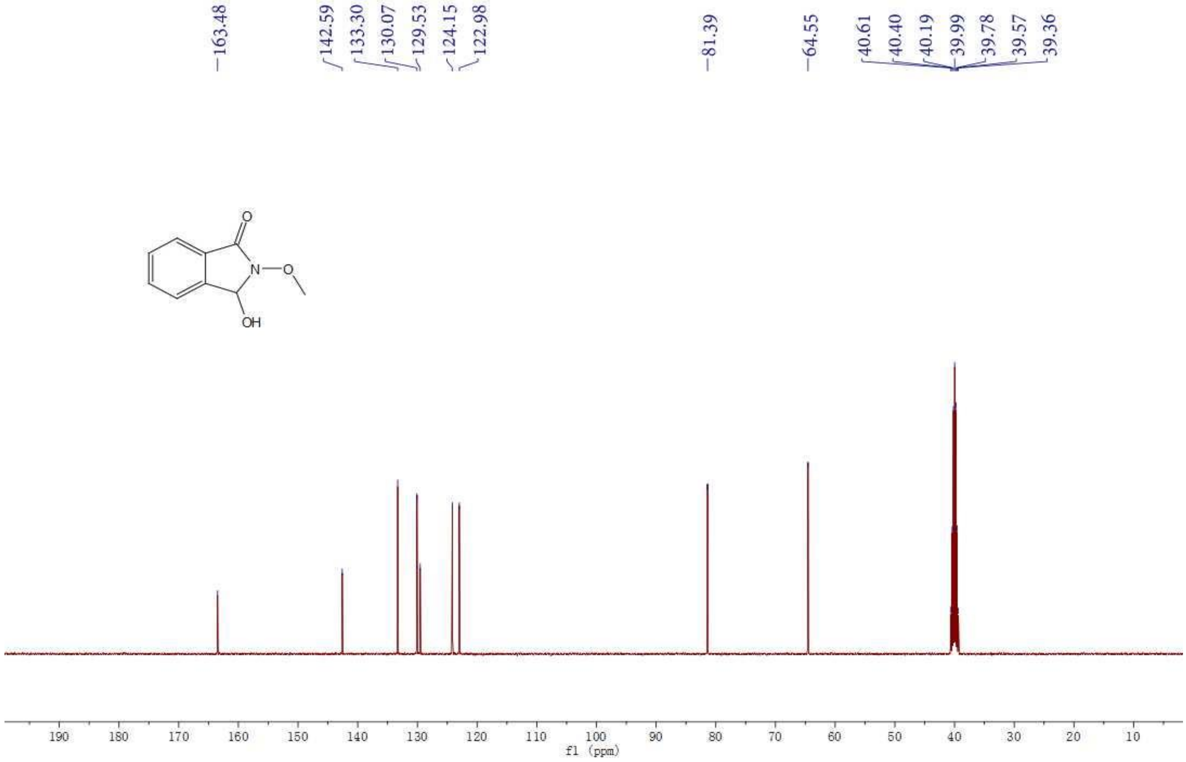
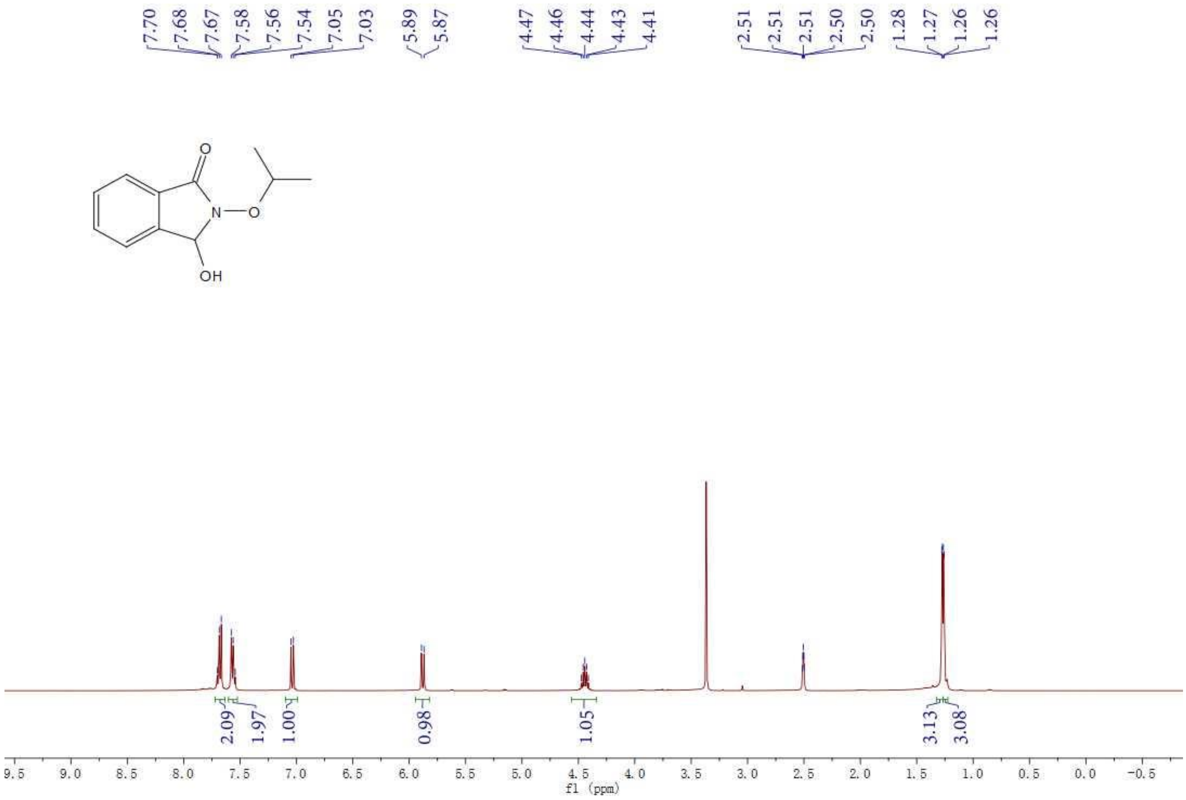
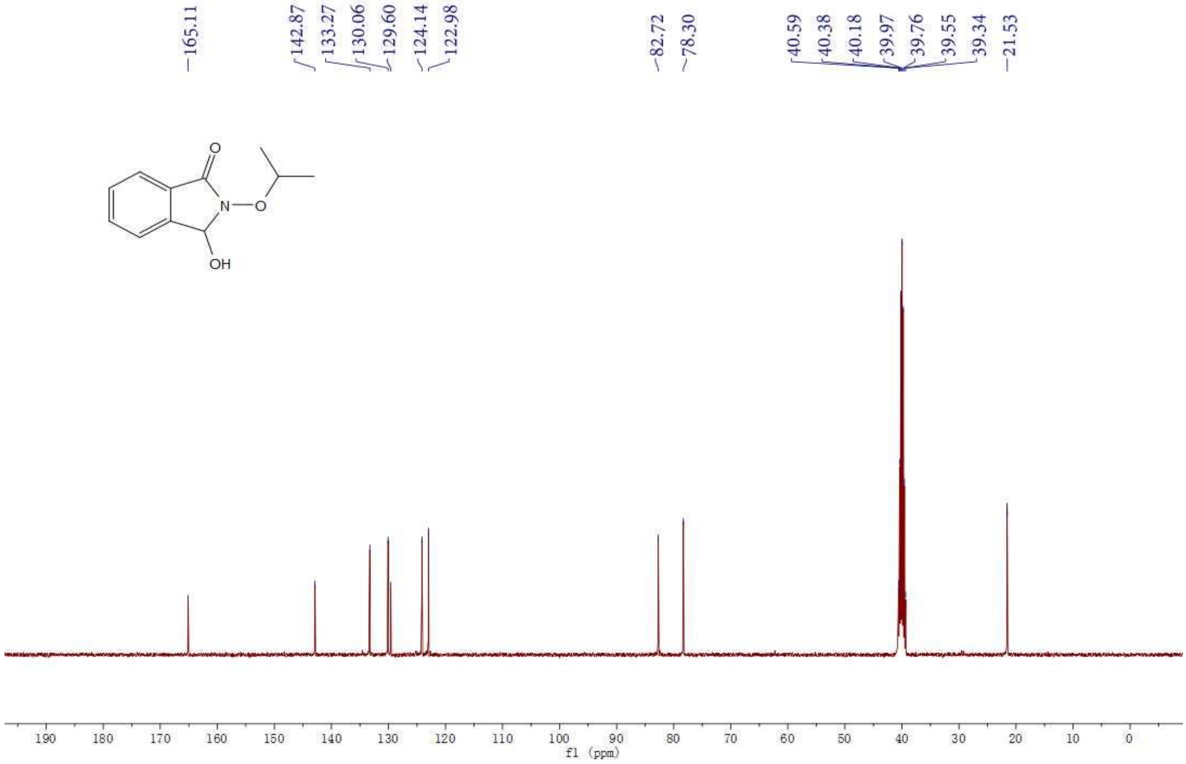


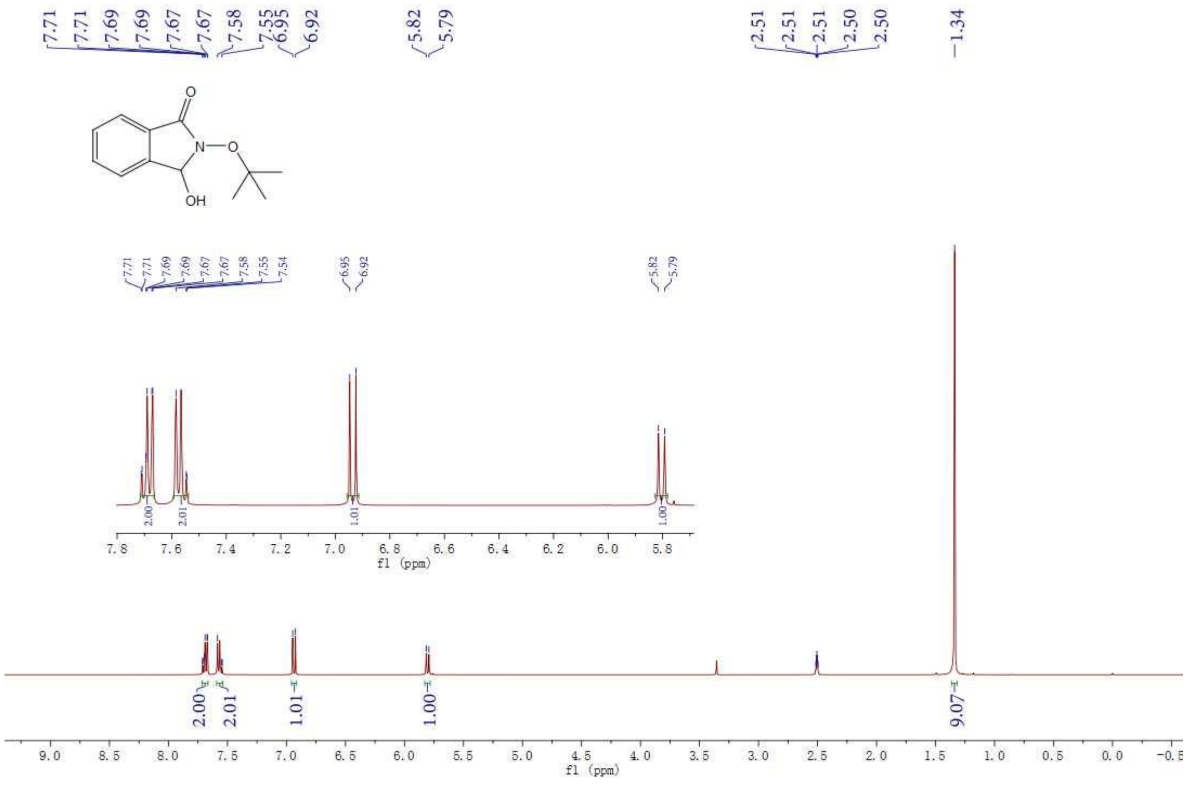
^{1}H NMR of compound **2y**



^{13}C NMR of compound **2y**



^{1}H NMR of compound **2z**



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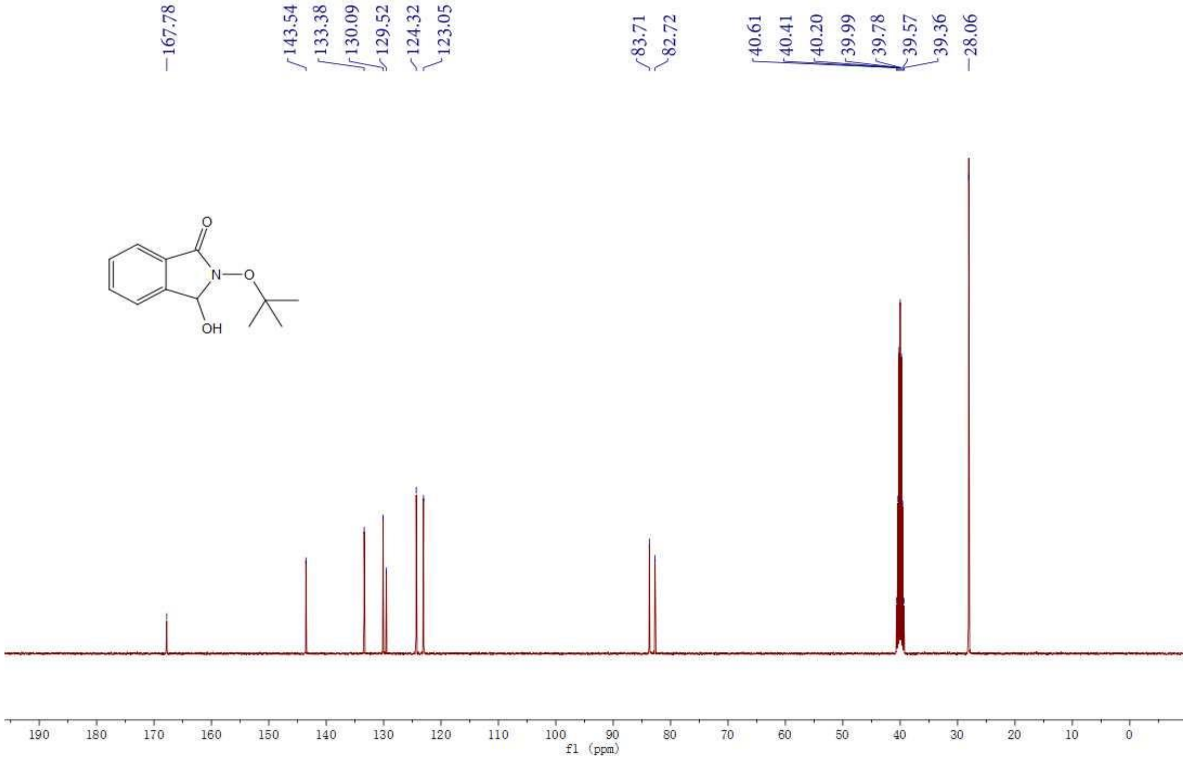
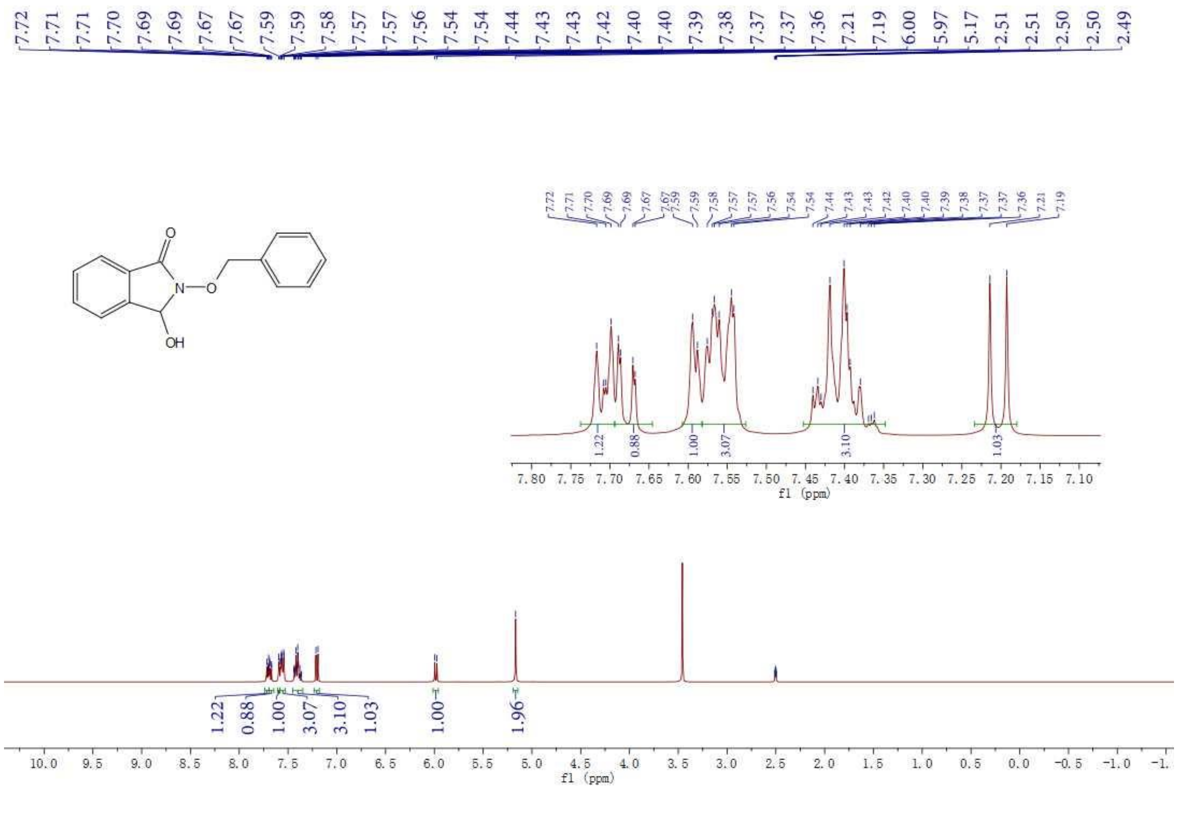
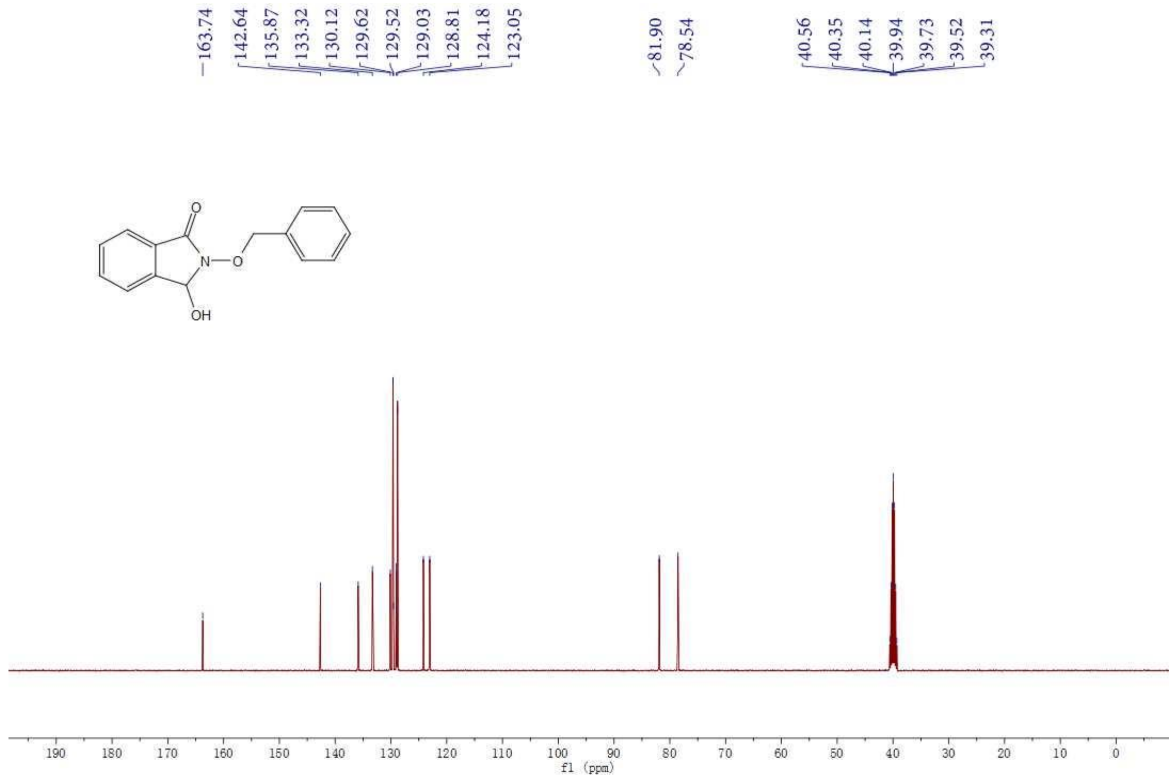


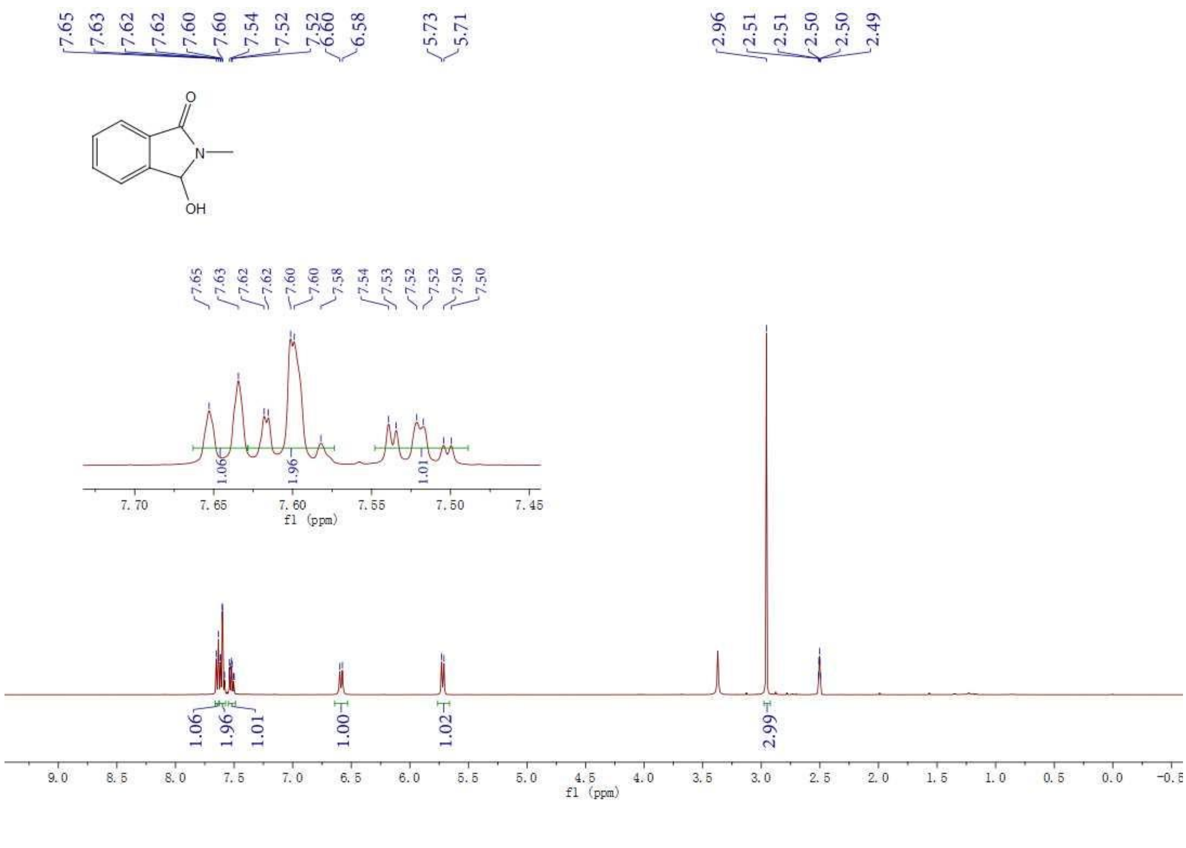
^{1}H NMR of compound **2aa**



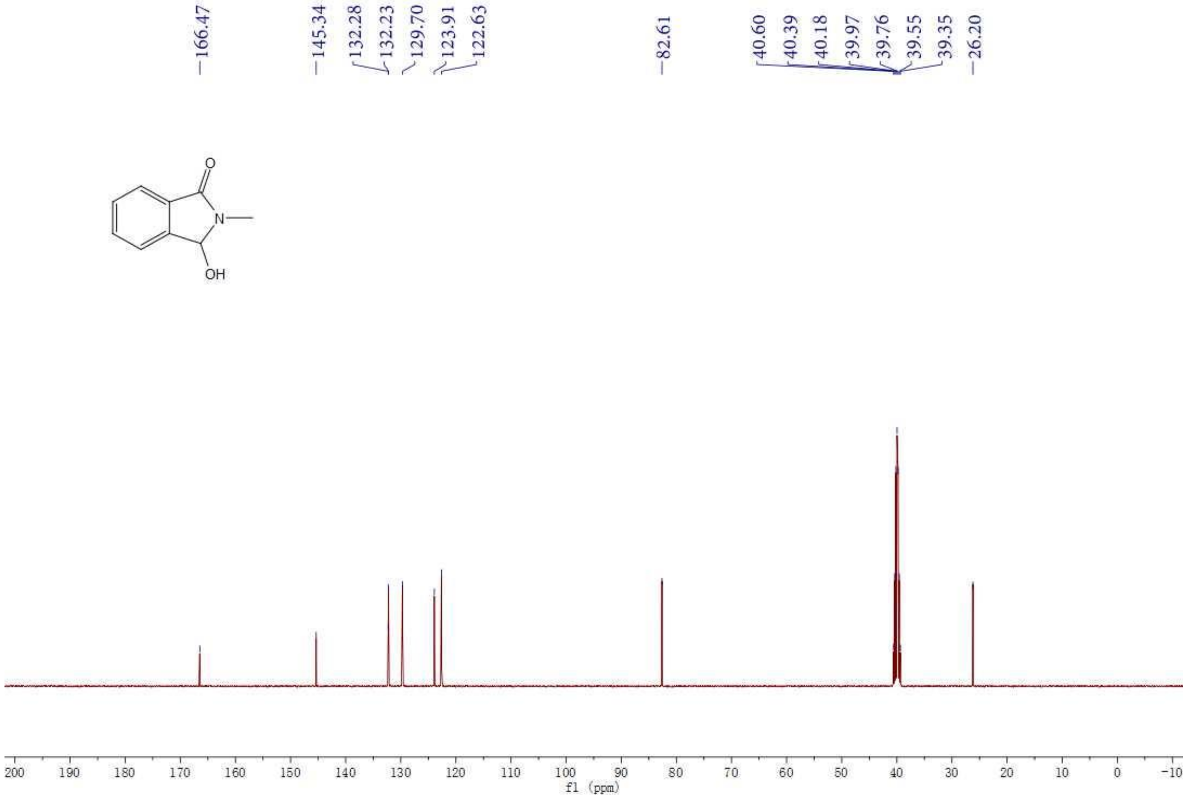
^{13}C NMR of compound **2aa**



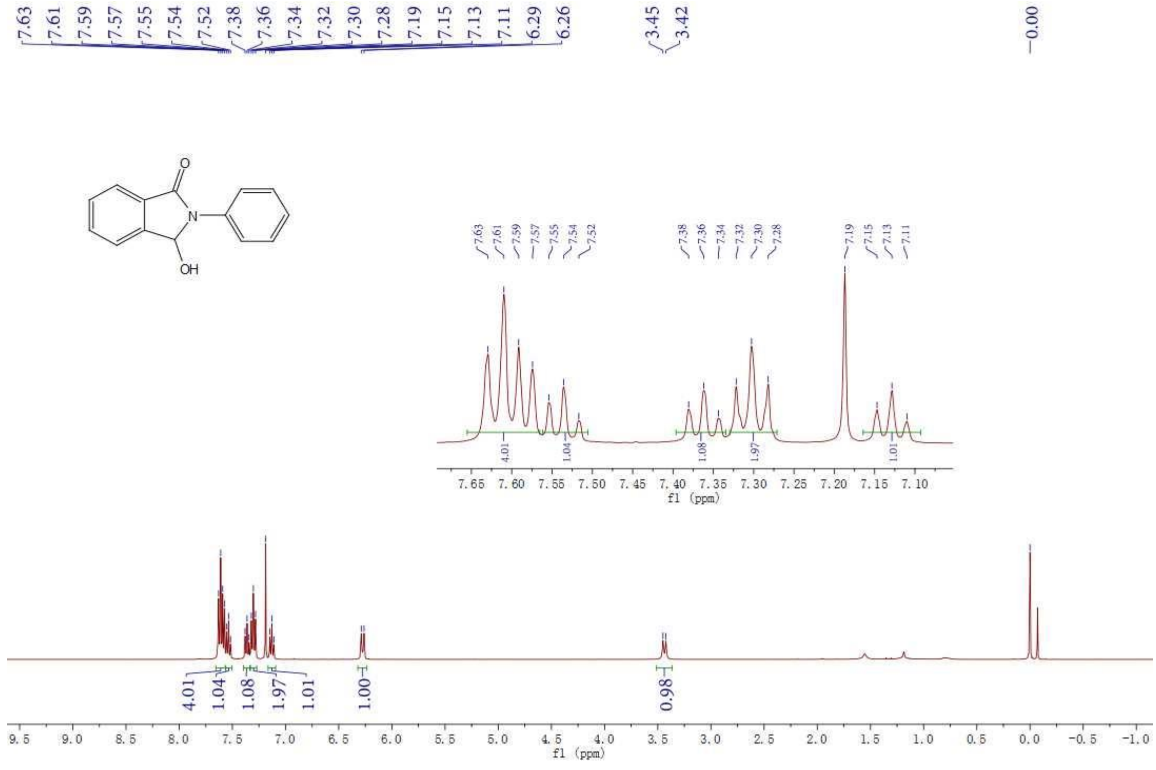
^{1}H NMR of compound **2ac**



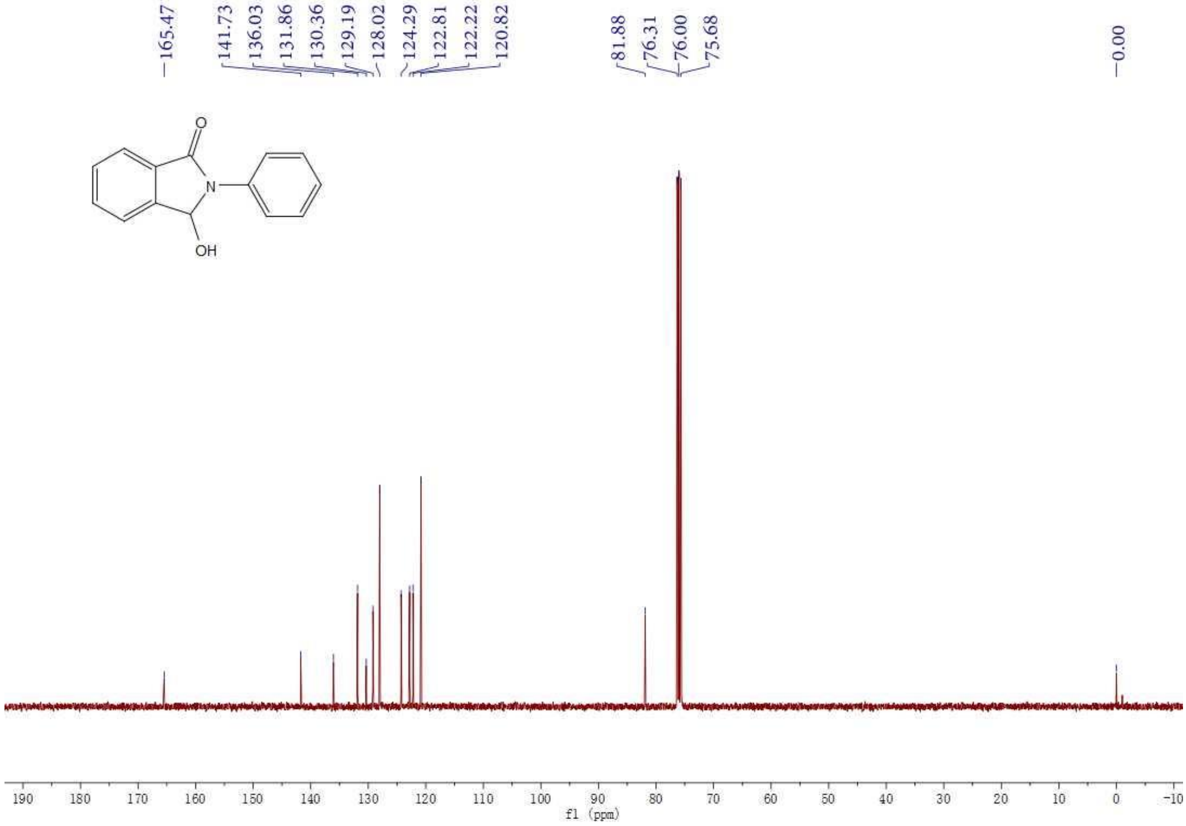
¹³C NMR of compound **2ac**



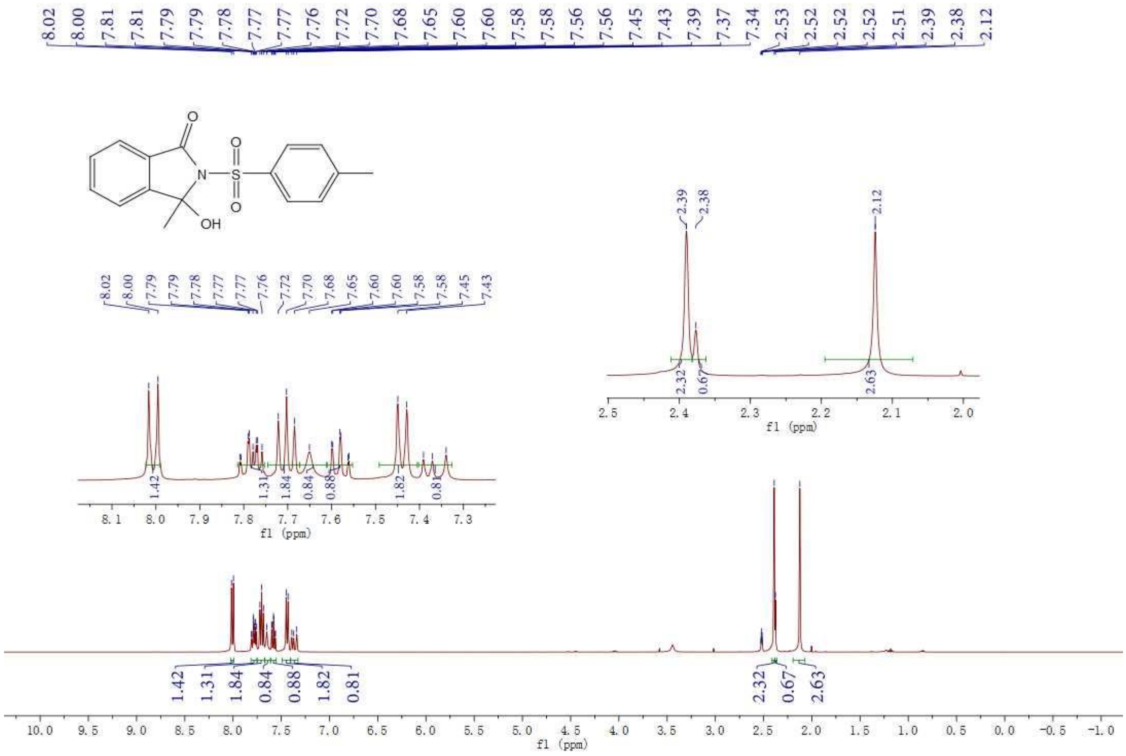
¹H NMR of compound **2ad**



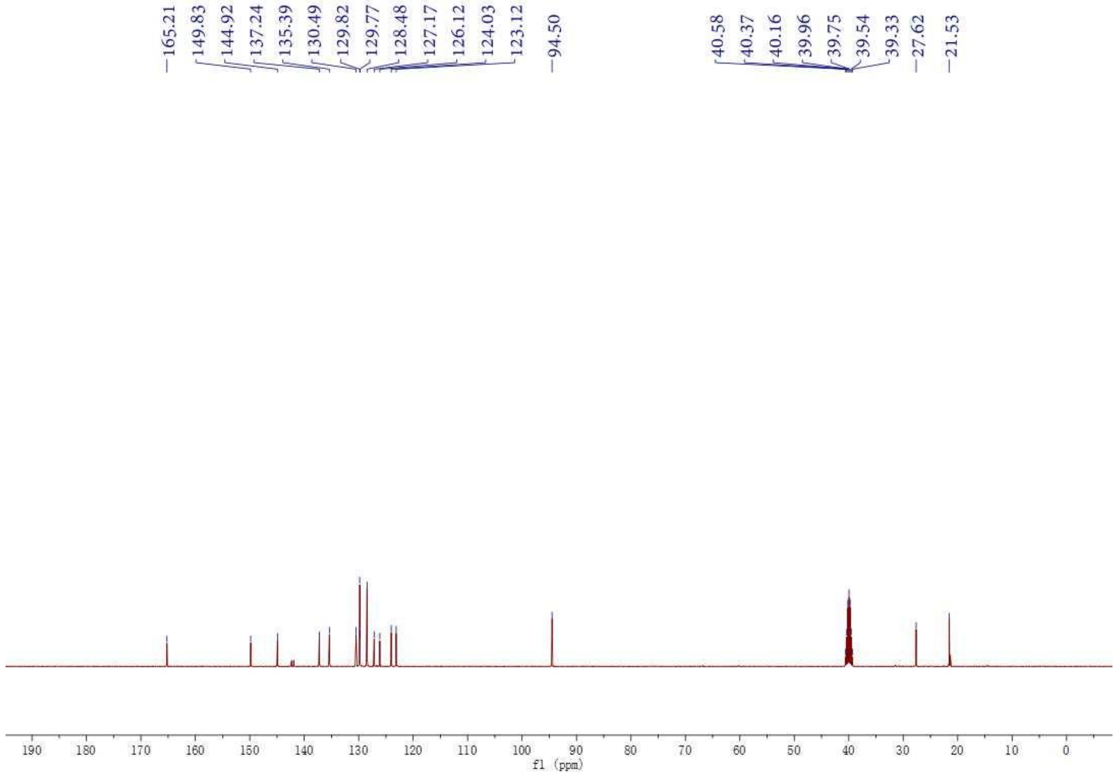
^{13}C NMR of compound **2ad**



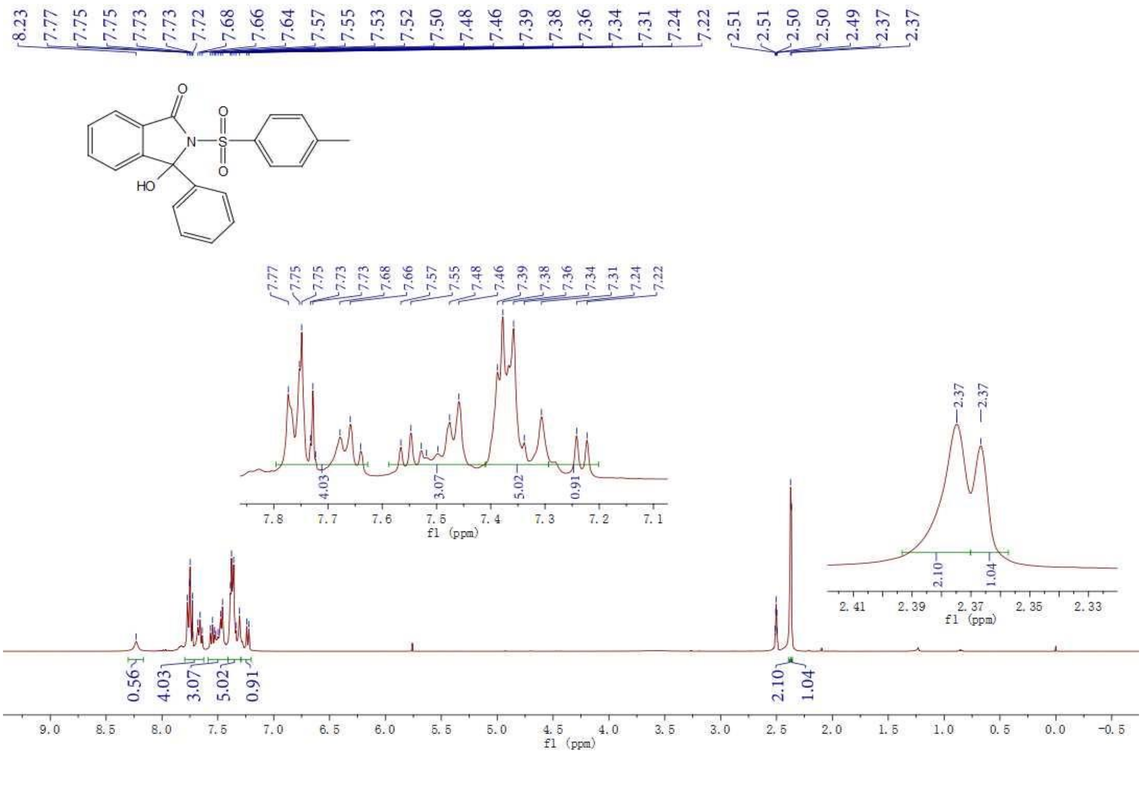
^{1}H NMR of compound **2ae**



^{13}C NMR of compound **2ae**



^{1}H NMR of compound **2af**



^{13}C NMR of compound **2af**