Supplementary Information

Comparison of optical characteristics of pseudoresonance structures with non-pseudoresonance structures

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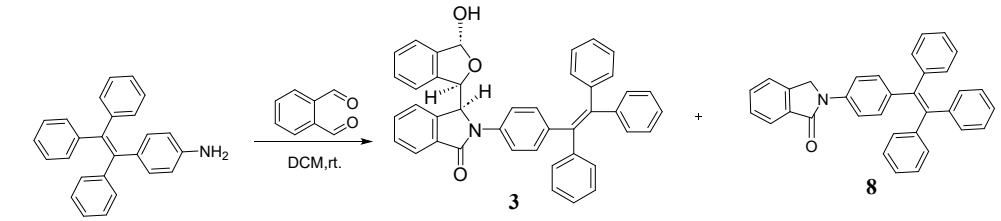
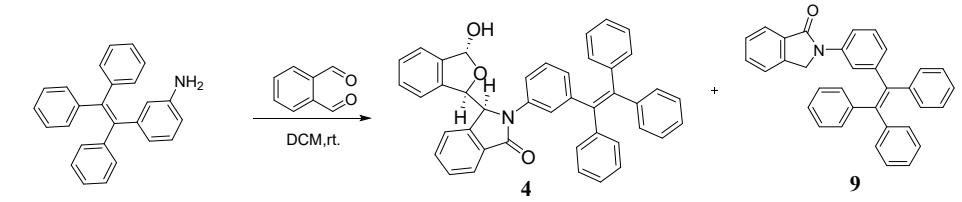
Content

1、The synthesis of compound 3 - 15.





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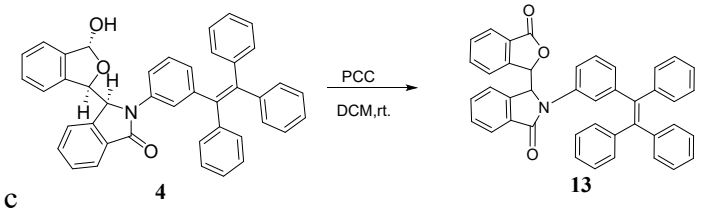
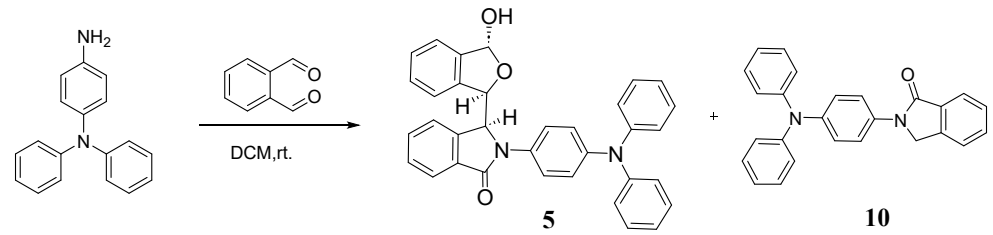
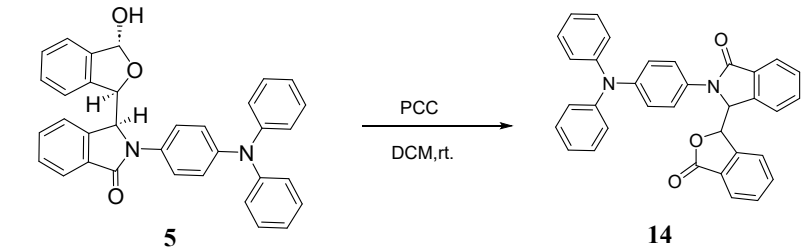
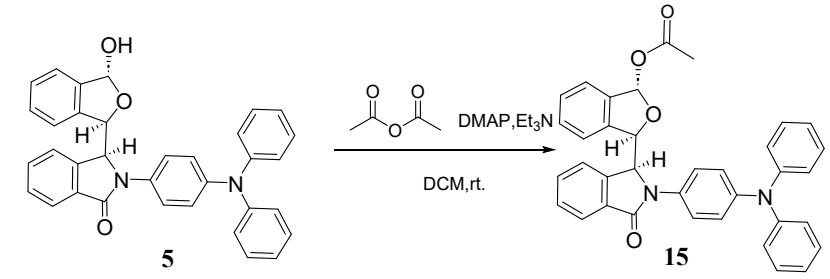
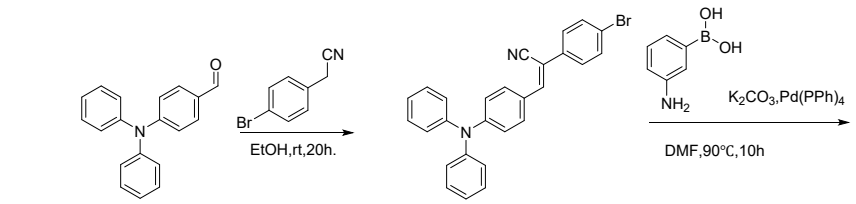


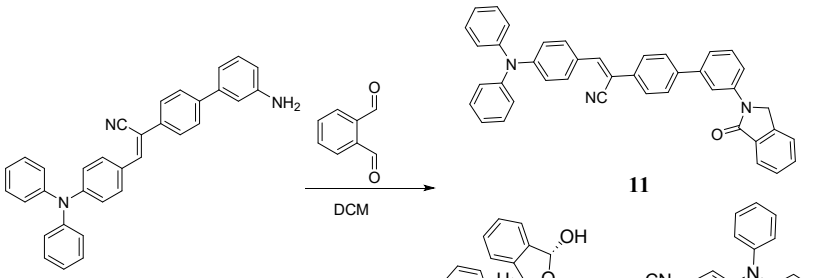








CN-1



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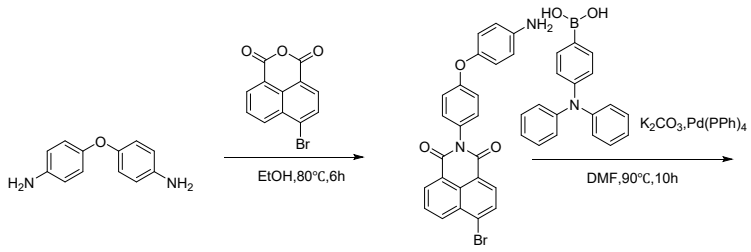
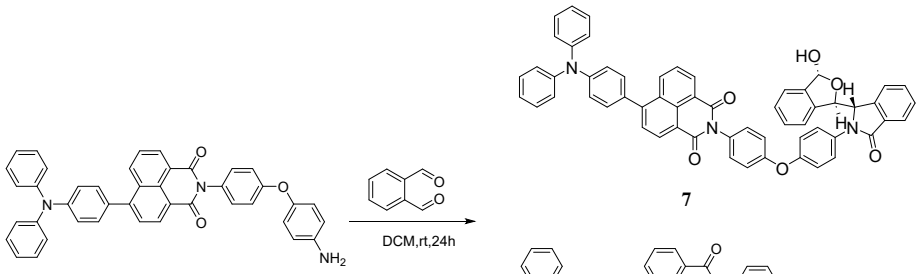
CN-2

6



NG-1



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NG-2

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Synthesis of Compound **3** and Compound **8**:Separate solutions of (2-(4-aminophenyl)ethene-1,1,2-triyl)tribenzene (600.0 mg) and phthalaldehyde (347.4 mg) in dichloromethane (DCM) were prepared. After both solutions were cooled in an ice bath for 20 minutes, the solution of (2-(4-aminophenyl)ethene-1,1,2-triyl)tribenzene

was added dropwise to the phthalaldehyde solution. The reaction was allowed to proceed at room temperature with monitoring by thin-layer chromatography (TLC). Upon completion, the mixture was concentrated under reduced pressure. The crude product was purified by column chromatography using a petroleum ether (PE) : ethyl acetate (EA) = 6 : 1 solvent system to afford 369 mg of Compound 8 with a yield of 46%. Elution with a PE : EA = 3 : 1 solvent system yielded 211 mg of Compound 3 with a yield of 21%.

Compound **3**: ^{1}H NMR (600 MHz, Chloroform-d) δ 7.95 (d, J = 7.6 Hz, 0.7H), 7.89 (d, J = 7.2 Hz, 1H), 7.52 (p, J = 7.5 Hz, 3H), 7.38 (dq, J = 22.2, 7.6 Hz, 3H), 7.30 (d, J = 7.5 Hz, 2.4H), 7.25 (s, 3.4H), 7.20 – 7.15 (m, 5.7H), 7.15 – 7.05 (m, 10H), 7.05 – 7.00 (m, 8.5H), 6.97 (d, J = 8.2 Hz, 2H), 6.78 (d, J = 7.4 Hz, 0.7H), 6.59 (d, J = 7.6 Hz, 0.7H), 6.27 (d, J = 7.6 Hz, 1H), 6.08 (s, 0.7H), 5.90 (s, 1H), 5.65 (s, 1H), 5.60 (s, 0.7H), 5.55 (s, 0.7H), 5.28 (s, 0.7H), 5.16 (d, J = 2.3 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-d) δ 166.3, 166.2, 143.9, 143.6, 142.5, 142.4, 142.3, 142.3, 140.4, 140.3, 139.4, 139.3, 139.3, 139.2, 139.2, 139.0, 136.9, 136.5, 135.5, 135.3, 133.1, 132.5, 130.4, 130.4, 130.3, 130.1, 128.4, 128.3, 128.2, 128.1, 128.0, 128.0, 127.9, 127.6, 126.8, 126.8, 126.7, 126.7, 126.7, 125.6, 125.6, 125.5, 125.5, 125.3, 123.6, 123.1, 123.1, 122.8, 122.6, 122.2, 121.3, 121.2, 120.6, 120.5, 100.3, 100.0, 64.1, 63.7. HRMS (ESI) *m*/*z*: $[M + H]^+$ calcd for $C_{42}H_{31}NO_3$, 598.2382; found, 598.2372.

Compound **8**: ^{1}H NMR (600 MHz, Chloroform-d) δ 7.89 (d, J = 7.2 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.57 (td, J = 7.4, 1.1 Hz, 1H), 7.48 (t, J = 7.4 Hz, 2H), 7.13 – 7.01 (m, 17H), 4.79 (s, 2H).^{13}C NMR (151 MHz, Chloroform-d) δ 167.4, 144.4, 143.8, 143.5, 143.2, 141.3, 140.6, 140.1, 138.8, 133.3, 131.9, 131.4, 131.3, 128.6, 128.3, 127.8, 127.7, 127.7, 127.5, 126.6, 126.5, 124.1, 50.6. HRMS (ESI) *m*/*z*: $[M + H]^+$ calcd for $C_{34}H_{25}NO$, 464.2014; found, 464.2004.

Synthesis of Compound **4** and Compound **9**:Separate solutions of (2-(3-aminophenyl)ethene-1,1,2-triyl)tribenzene (600.0 mg) and phthalaldehyde (347.4 mg)

in dichloromethane (DCM) were prepared. After both solutions were cooled in an ice bath for 20 minutes, the solution of (2-(3-aminophenyl)ethene-1,1,2-triyl)tribenzene was added dropwise to the phthalaldehyde solution. The reaction was allowed to proceed at room temperature with monitoring by TLC. Upon completion, the mixture was concentrated under reduced pressure. Purification by column chromatography using a PE : EA = 6 : 1 solvent system afforded 379 mg of Compound 9 with a yield of 47%. Subsequent elution with a PE : EA = 3 : 1 solvent system yielded 278 mg of Compound 4 with a yield of 27%.

Compound **4**: ^{1}H NMR (600 MHz, Chloroform-d) δ 7.93 (d, J = 7.6 Hz, 1H), 7.87 (d, J = 7.6 Hz, 0.8H), 7.61 (ddd, J = 8.0, 2.4, 1.1 Hz, 1H), 7.47 – 7.41 (m, 3.9H), 7.40 – 7.34 (m, 1.7H), 7.34 – 7.28 (m, 3.4H), 7.24 – 7.21 (m, 1.2H), 7.18 (t, J = 7.9 Hz, 1H), 7.11 (dq, J = 5.2, 3.2, 2.4 Hz, 15H), 7.09 – 7.05 (m, 6H), 7.05 – 6.99 (m, 8.4H), 6.97 (ddd, J = 8.3, 4.1, 2.6 Hz, 2H), 6.92 – 6.85 (m, 1H), 6.61 (d, J = 7.5 Hz, 0.8H), 6.42 (d, J = 7.6 Hz, 0.8H), 6.09 (d, J = 7.6 Hz, 1H), 5.41 (t, J = 2.3 Hz, 0.8H), 5.36 – 5.32 (m, 0.8H), 5.29 (d, J = 2.1 Hz, 1.6H), 5.15 (d, J = 2.2 Hz, 1H), 4.95 (d, J = 2.2 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-d) δ 167.3, 167.1, 144.9, 144.6, 143.5, 143.5, 143.4, 143.3, 141.5, 140.4, 140.3, 140.3, 140.3, 140.2, 140.0, 137.9, 137.6, 136.5, 136.4, 134.2, 133.6, 131.4, 131.4, 131.3, 131.3, 131.1, 129.4, 129.4, 129.4, 129.3, 129.2, 129.0, 128.9, 128.6, 127.9, 127.9, 127.8, 127.7, 127.7, 126.6, 126.6, 126.5, 126.3, 124.7, 124.1, 124.1, 123.8, 123.6, 123.2, 122.4, 122.2, 121.6, 121.5, 101.3, 101.0, 81.7, 65.1, 64.7. HRMS (ESI) m/z: [M + H]+ calcd for $C_{42}H_{31}NO_3$, 598.2382; found, 598.2371.

Compound **9**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.96 (ddd, *J* = 8.2, 2.3, 1.0 Hz, 1H), 7.87 (dt, *J* = 7.6, 1.0 Hz, 1H), 7.55 (td, *J* = 7.5, 1.2 Hz, 1H), 7.46 (td, *J* = 7.5, 0.9 Hz, 1H), 7.42 (dt, *J* = 7.5, 0.9 Hz, 1H), 7.22 – 7.01 (m, 17H), 6.84 (dt, *J* = 7.8, 1.2 Hz, 1H), 4.44 (s, 2H).^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.4, 144.4, 143.8, 143.5, 143.2, 141.3, 140.6, 140.1, 138.8, 133.3, 131.9, 131.4, 131.3, 128.6, 128.3, 127.8, 127.7, 127.6, 127.5, 126.6, 126.5, 124.1, 122.5, 122.2, 118.4, 50.6. HRMS (ESI) m/z: [M + H]+ calcd for $C_{34}H_{25}NO$, 464.2014; found,464.2006.

Synthesis of Compound **13**:At room temperature, a solution of 50 mg of Compound 4 in 10 mL of DCM was prepared. To this solution, 117.0 mg (5 equiv) of pyridinium chlorochromate (PCC) was added. Upon completion of the reaction, the mixture was filtered, and the filtrate was concentrated under reduced pressure to remove DCM. The residue was purified by column chromatography using a DCM : EA = 15 : 1 solvent system, yielding 37 mg of Compound 13 with a yield of 74%.

Compound **13**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.5 Hz, 1H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.67 – 7.62 (m, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 9.9 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.19 (dt, *J* = 32.5, 7.7 Hz, 4H), 7.11 – 6.89 (m, 14H), 6.71 (t, *J* = 7.6 Hz, 1H), 6.06 (d, *J* = 7.6 Hz, 1H), 5.31 (s, 1H), 5.07 (s, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.9, 167.0, 145.4, 145.0, 143.6, 143.5, 143.2, 141.5, 140.3, 137.8, 135.8, 133.9, 133.4, 131.7, 131.5, 131.4, 131.3, 130.1, 129.6, 129.5, 129.2, 127.9, 127.8, 127.7, 126.7, 126.5, 126.3, 126.1, 124.7, 124.1, 122.4, 121.9, 63.1.

Synthesis of Compound **5** and Compound **10**: Separate solutions of 500 mg of 4-aminotriphenylamine and 386 mg of phthalaldehyde in 15 mL of dichloromethane (DCM) were prepared. The solution of 4-aminotriphenylamine was added dropwise to the solution of phthalaldehyde in an ice bath. The reaction mixture was then stirred at room temperature for 24 hours. After completion, the solvent was removed under reduced pressure. The crude product was purified by column chromatography. Elution with a solvent system of petroleum ether (PE) and DCM (1:1) afforded 326 mg of Compound 10 with a yield of 44%. Subsequent elution with a DCM:ethyl acetate (EA) (15:1) solvent system yielded 221 mg of Compound 5 with a yield of 22%.

Compound **5**: ^{1}H NMR (600 MHz, Chloroform-d) δ 7.92 (d, J = 7.5 Hz, 1H), 7.86 (d, J = 7.5 Hz, 0.6H), 7.56 – 7.35 (m, 5H), 7.35 – 7.28 (m, 2H), 7.28 – 7.20 (m, 7.2H), 7.10 – 6.94 (m, 17.6H), 6.76 – 6.71 (m, 1.4H), 6.61 – 6.55 (m, 1.3H), 6.05 (d, J = 7.6 Hz, 0.8H), 5.88 (s, 0.7H), 5.63 (d, J = 1.9 Hz, 1H), 5.52 (s, 1.2H), 5.38 – 5.36 (m, 0.7H), 5.28 (t, J = 4.9 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.3, 167.3, 147.6, 147.4, 146.4, 140.5 (d, *J* = 8.2 Hz), 140.3, 140.2, 137.1, 131.7, 129.7, 129.6, 129.1,

129.1, 126.4, 126.0, 124.8, 124.7, 124.5, 123.8, 123.5, 123.3, 123.0, 122.4, 101.5, 101.4, 82.8, 82.2, 65.1, 65.0.

Compound **10**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.7 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.1 Hz, 2H), 7.17 (t, *J* = 7.7 Hz, 4H), 7.07 (d, *J* = 8.7 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 4H), 6.93 (t, *J* = 7.3 Hz, 2H), 4.75 (s, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.3, 147.7, 144.4, 140.1, 134.4, 133.3, 132.0, 129.3, 128.4, 124.9, 124.1, 124.0, 122.7, 122.6, 120.8, 51.0. HRMS (ESI) m/z: [M + H]+ calcd for $C_{26}H_{20}N_2O$, 377.1654; found, 377.1649.

Synthesis of Compound **14**: At room temperature, a solution of 50 mg of Compound 5 in 10 mL of DCM was prepared. To this solution, 105.0 mg (5 equiv) of pyridinium chlorochromate (PCC) was added. Upon completion of the reaction, the mixture was filtered, and the filtrate was concentrated under reduced pressure to remove DCM. The residue was purified by column chromatography using a DCM:EA (15:1) solvent system, yielding 42 mg of the product (Compound 14) with a yield of 84%.

Compound **14**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 7.4 Hz, 1H), 7.72 – 7.63 (m, 1H), 7.56 – 7.40 (m, 4H), 7.20 (t, *J* = 8.1 Hz, 4H), 7.07 (d, *J* = 8.1 Hz, 4H), 7.02 – 6.87 (m, 7H), 6.57 (d, *J* = 6.2 Hz, 1H), 5.90 (s, 1H), 5.78 (s, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.7, 166.9, 147.6, 146.5, 144.4, 138.7, 134.1, 133.3, 132.2, 130.1, 129.8, 129.3, 127.3, 126.0, 125.9, 124.8, 124.5, 124.1, 123.0, 122.4, 121.8, 80.6, 62.7.

Synthesis of Compound **15**: At room temperature, a solution of 100 mg of Compound 5 in 15 mL of chloroform was prepared. To this solution, 2.0 mg (0.1 equiv) of 4-dimethylaminopyridine (DMAP), 81 μL (3 equiv) of triethylamine, and 37 μL (2 equiv) of acetic anhydride were added. After the reaction was complete, the mixture was washed three times with saturated sodium chloride solution. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. Purification by column chromatography using a DCM:EA (20:1) solvent system afforded 52 mg of the product (Compound 15) with a yield of 49%.

Compound **15**: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.02 – 7.94 (m, 1H), 7.67 – 7.57 (m, 2H), 7.39 – 7.31 (m, 4H), 7.28 – 7.22 (m, 3H), 7.19 (d, *J* = 7.7 Hz, 4H), 7.07 (dd, *J* = 16.0, 9.3 Hz, 5H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.42 (d, *J* = 2.1 Hz, 1H), 6.30 (d, *J* = 7.7 Hz, 1H), 6.09 (s, 1H), 5.77 (s, 1H), 2.07 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.1, 167.3, 147.7, 145.9, 140.0, 138.1, 137.0, 133.4, 132.1, 131.1, 129.9, 129.4, 126.3, 124.5, 124.4, 123.9, 123.3, 123.0, 122.5, 121.0, 100.0, 85.4, 64.2, 21.3.

Synthesis of **CN-1**: A mixture of 2 g of 4-(diphenylamino)benzaldehyde and 1.548 g (1.1 equiv) of (4-bromophenyl)acetonitrile was dissolved in 50 mL of anhydrous ethanol, followed by the addition of 352 mg (1.2 equiv) of sodium hydroxide. The reaction was stirred at room temperature for 20 hours. Upon completion, the mixture was washed with an acetic acid aqueous solution three times and subsequently with brine three times. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure to afford 3.5 g of the crude product, corresponding to a 98% yield.

Compound **CN-1**: ^{1}H NMR (600 MHz, Chloroform-d) δ 7.69 (d, J = 9.0 Hz, 2H), 7.47 (d, J = 9.0 Hz, 2H), 7.43 (d, J = 9.0 Hz, 2H), 7.32 (s, 1H), 7.25 (t, J = 7.8 Hz, 4H), 7.08 (dd, J = 14.4, 8.4 Hz, 6H), 6.96 (d, J = 9.0 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-d) ^{13}C NMR (151 MHz, Chloroform-d) δ 150.2, 146.5, 142.0, 134.1, 132.1, 130.8, 129.6, 127.2, 126.0, 125.8, 122.6, 120.7, 118.4, 106.4.

Synthesis of **CN-2**: Under a nitrogen atmosphere, a mixture of 2 g of CN-1, 670 mg (1.1 equiv) of 3-aminophenylboronic acid, and 257 mg (0.05 equiv) of tetrakis(triphenylphosphine)palladium(0) in 40 mL of DMF was heated to 90 °C. A solution of 1.84 g (3 equiv) of potassium carbonate in 3 mL of water was then added dropwise to the reaction system. The reaction was allowed to proceed for 10 hours. After completion, the mixture was quenched with 200 mL of saturated sodium chloride solution and extracted three times with ethyl acetate (EA). The combined organic extracts were washed three times with brine, dried over anhydrous sodium sulfate, and

concentrated. The crude product was purified by column chromatography using dichloromethane (DCM) as the eluent, yielding 1.46 g of CN-2 with a yield of 71%.

Compound **CN-2**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 7.8 Hz, 2H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.24 (t, *J* = 7.8 Hz, 4H), 7.21 – 7.12 (m, 6H), 7.08 (s, 2H), 7.07 – 6.95 (m, 9H), 6.92 (dd, *J* = 15.0, 7.8 Hz, 2H), 6.84 (d, *J* = 13.8 Hz, 2H), 6.73 (d, *J* = 8.4 Hz, 1H), 6.61 (t, *J* = 9.0 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 150.0, 149.5, 146.9, 146.6, 143.7, 142.0, 141.6, 141.3, 133.9, 132.3, 131.2, 130.7, 129.9, 129.8, 129.6, 129.5, 129.2, 127.7, 127.6, 126.0, 125.7, 124.4, 124.4, 121.0, 120.4, 118.8, 117.5, 117.5, 114.6, 114.5, 113.7, 113.6, 107.4.

Synthesis of Compound **6** and Compound **11**: Separate solutions of 500 mg of CN-2 and 217 mg (1.5 equiv) of phthalaldehyde, each in 15 mL of DCM, were prepared. The CN-2 solution was added dropwise to the phthalaldehyde solution in an ice bath. The reaction mixture was then stirred at room temperature for 24 hours. After completion, the solvent was removed under reduced pressure. The residue was subjected to column chromatography; elution with a solvent system of petroleum ether (PE) to ethyl acetate (EA) (5:1) yielded 256 mg of Compound 11 with a yield of 41%. Further elution with PE:EA (2:1) afforded 176 mg of Compound 6 with a yield of 23%.

Compound **6**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.93 (t, *J* = 7.0 Hz, 1H), 7.87 (t, *J* = 7.1 Hz, 1H), 7.73 (d, *J* = 8.6 Hz, 2H), 7.66 – 7.60 (m, 2H), 7.58 – 7.52 (m, 3H), 7.51 – 7.27 (m, 20H), 7.25 (t, *J* = 7.7 Hz, 4H), 7.23 – 7.19 (m, 6H), 7.17 – 7.13 (m, 3H), 7.12 – 6.95 (m, 18H), 6.87 (d, *J* = 7.5 Hz, 1H), 6.76 (d, *J* = 8.7 Hz, 3H), 6.60 (d, *J* = 7.6 Hz, 1H), 6.44 (dd, *J* = 13.9, 7.6 Hz, 1H), 6.01 – 5.95 (m, 1H), 5.89 (d, *J* = 7.1 Hz, 1H), 5.67 (s, 1H), 5.61 (d, *J* = 7.4 Hz, 2H), 5.20 (d, *J* = 14.8 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-d) δ 167.4, 167.3, 150.0, 149.6, 146.6, 146.6, 143.9, 143.9, 141.6, 141.5, 140.8, 140.6, 133.6, 133.3, 132.0, 131.8, 131.3, 130.8, 130.8, 130.7, 129.8, 129.7, 129.6, 129.6, 129.6, 129.5, 129.3, 129.3, 129.2, 127.9, 127.8, 127.8, 127.6, 126.1, 126.1, 125.8, 124.8, 124.7, 124.6, 124.5, 124.4, 124.4, 124.4, 124.2, 123.5,

123.2, 123.2, 122.6, 122.5, 121.2, 121.0, 120.9, 120.4, 120.4, 101.3, 65.1, 65.1, 64.8, 64.7, 60.4. HRMS (ESI) m/z: [M + H]+ calcd for $C_{49}H_{35}N_3O_3$, 714.2757; found, 714.2743.

Compound **11**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.13 (s, 1H), 7.86 (t, *J* = 6.9 Hz, 1H), 7.74 (dd, *J* = 14.3, 9.5 Hz, 2H), 7.67 – 7.60 (m, 2H), 7.60 – 7.50 (m, 2H), 7.50 – 7.38 (m, 4H), 7.34 (dd, *J* = 13.2, 8.0 Hz, 1H), 7.26 – 7.15 (m, 5H), 7.11 – 6.96 (m, 8H), 6.78 – 6.72 (m, 1H), 4.84 (d, *J* = 4.2 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.7, 150.0, 149.6, 146.6, 146.6, 143.9, 141.5, 141.4, 141.2, 141.2, 141.0, 140.1, 134.3, 133.2, 132.7, 132.2, 131.3, 130.8, 129.7, 129.7, 129.6, 129.6, 129.3, 128.5, 127.9, 127.8, 126.5, 126.1, 125.7, 124.4, 124.4, 124.2, 123.2, 123.1, 122.7, 120.9, 120.4, 118.7, 118.6, 118.3, 118.2, 110.1, 107.2, 60.4. HRMS (ESI) m/z: [M + H]+ calcd for $C_{41}H_{29}N_3O$, 580.2389; found, 580.2386.

Synthesis of **NG-1:** A mixture of 1.358 g of 4-bromo-1,8-naphthalic anhydride and 1 g (1 equiv) of 4,4'-diaminodiphenyl ether in 20 mL of anhydrous ethanol was heated to 80 °C and stirred under reflux for 6 hours. Upon completion of the reaction, the mixture was concentrated under reduced pressure. The crude product was purified by column chromatography using a solvent system of dichloromethane (DCM) and ethyl acetate (EA) in a ratio of 80:1, yielding 2.25 g of NG-1 with a yield of 98%.

Compound **NG-1**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.61 (d, *J* = 8.4 Hz, 1H), 8.53 (d, *J* = 8.5 Hz, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.87 – 7.72 (m, 1H), 7.12 (d, *J* = 8.8 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.63 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) ^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.0, 163.9, 159.3, 147.8, 143.2, 133.6, 132.5, 131.6, 131.2, 130.8, 130.7, 129.6, 129.3, 128.6, 128.2, 123.3, 122.4, 121.8, 117.5, 116.3.

Synthesis of **NG-2**: Under a nitrogen atmosphere, a mixture of 1 g of NG-1, 630 mg (1 equiv) of 4-(diphenylamino)phenylboronic acid, and 146 mg (0.05 equiv) of tetrakis(triphenylphosphine)palladium(0) was dissolved in 20 mL of N,N-dimethylformamide (DMF). The solution was heated to 90 °C. Subsequently, 900 mg

of potassium carbonate dissolved in 3 mL of water was added to the reaction system. The reaction was allowed to proceed for 10 hours. After completion, the reaction was quenched by adding 150 mL of saturated sodium chloride solution. The mixture was extracted three times with ethyl acetate (EA). The combined organic extracts were washed three times with saturated sodium chloride solution, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. Purification by column chromatography using a solvent system of DCM:EA = 80:1 afforded 918 mg of NG-2 with a yield of 67%.

Compound **NG-2**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.61 – 8.54 (m, 2H), 8.38 (d, *J* = 8.5 Hz, 1H), 7.72 – 7.60 (m, 2H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.29 – 7.22 (m, 4H), 7.16 – 7.08 (m, 8H), 7.06 – 6.94 (m, 4H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.63 (d, *J* = 8.8 Hz, 2H).^{13}C NMR (151 MHz, Chloroform-*d*) ^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 164.5, 148.5, 148.0, 147.3, 147.1, 143.0, 133.2, 131.9, 131.6, 131.3, 130.8, 130.2, 129.7, 129.5, 129.3, 129.1, 127.8, 126.8, 125.1, 123.7, 123.1, 122.5, 121.7, 121.4, 117.5, 116.4.

Synthesis of Compound **7** and Compound **12**: Solutions of 881 mg of NG-2 and 284 mg (1.5 equiv) of phthalaldehyde, each dissolved in 15 mL of dichloromethane (DCM), were prepared. The solution of NG-2 was added dropwise to the solution of phthalaldehyde at 0 °C. The resulting mixture was then allowed to react at room temperature for 24 hours. Upon completion, the crude mixture was subjected to column chromatography. Elution with a solvent system of DCM:EA = 100:1 yielded 480 mg of Compound 12 with a yield of 43%. Further elution with a solvent system of DCM:EA = 10:1 yielded 246 mg of Compound 7 with a yield of 21%.

Compound **7**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.62 – 8.57 (m, 4H), 8.40 (d, *J* = 8.5 Hz, 2H), 7.92 (d, *J* = 7.3 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.67 (dd, *J* = 7.7, 3.9 Hz, 4H), 7.47 (td, *J* = 7.5, 2.8 Hz, 3H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.38 – 7.29 (m, 12H), 7.28 – 7.19 (m, 19H), 7.17 – 7.09 (m, 20H), 7.07 – 7.00 (m, 7H), 6.83 (d, *J* = 7.4 Hz, 1H), 6.81 (d, *J* = 7.5 Hz, 1H), 6.51 (d, *J* = 7.6 Hz, 1H), 6.48 (d, *J* = 7.6 Hz, 1H), 6.02

(d, *J* = 12.2 Hz, 1H), 5.86 (s, 1H), 5.57 (d, *J* = 11.9 Hz, 2H), 5.49 (s, 1H), 5.29 (d, *J* = 8.3 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-d) δ 167.4, 164.7, 164.5, 157.3, 155.2, 154.5, 148.5, 147.3, 147.2, 140.6, 140.4, 140.3, 133.8, 133.3, 132.6, 132.4, 131.8, 131.8, 131.6, 131.6, 131.4, 130.8, 130.5, 130.3, 130.2, 130.2, 130.1, 129.8, 129.6, 129.5, 129.4, 129.4, 129.3, 129.3, 129.1, 127.8, 127.1, 126.9, 126.8, 125.1, 124.7, 124.3, 123.7, 123.6, 123.3, 123.0, 122.5, 122.5, 122.4, 121.3, 121.2, 121.1, 120.0, 119.8, 119.5, 119.2, 101.3, 101.3, 82.9, 65.4, 65.0. HRMS (ESI) m/z: [M + Na]+ calcd for $C_{58}H_{39}N_3O_6$, 896.2737; found, 896.2735.

Compound **12**: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.60 (dd, *J* = 7.4, 3.9 Hz, 2H), 8.40 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.82 – 7.78 (m, 2H), 7.70 – 7.66 (m, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.32 (d, *J* = 8.6 Hz, 2H), 7.25 (t, *J* = 7.9 Hz, 4H), 7.22 (d, *J* = 8.8 Hz, 2H), 7.16 – 7.12 (m, 8H), 7.10 (d, *J* = 8.8 Hz, 2H), 7.03 (t, *J* = 7.3 Hz, 2H), 4.80 (s, 2H) ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.41, 164.69, 164.47, 157.80, 153.02, 147.33, 140.09, 135.58, 133.27, 133.17, 132.08, 131.82, 131.64, 131.39, 131.13, 130.84, 130.21, 130.02, 129.52, 129.27, 128.45, 127.79, 126.78, 125.10, 124.20, 123.70, 123.00, 122.65, 122.48, 121.31, 121.28, 120.50, 118.73, 51.03. HRMS (ESI) m/z: [M + H]+ calcd for $C_{50}H_{33}N_3O_4$, 740.2549; found, 740.2546.

2、NMR and partial MS spectra of compound 3-15.

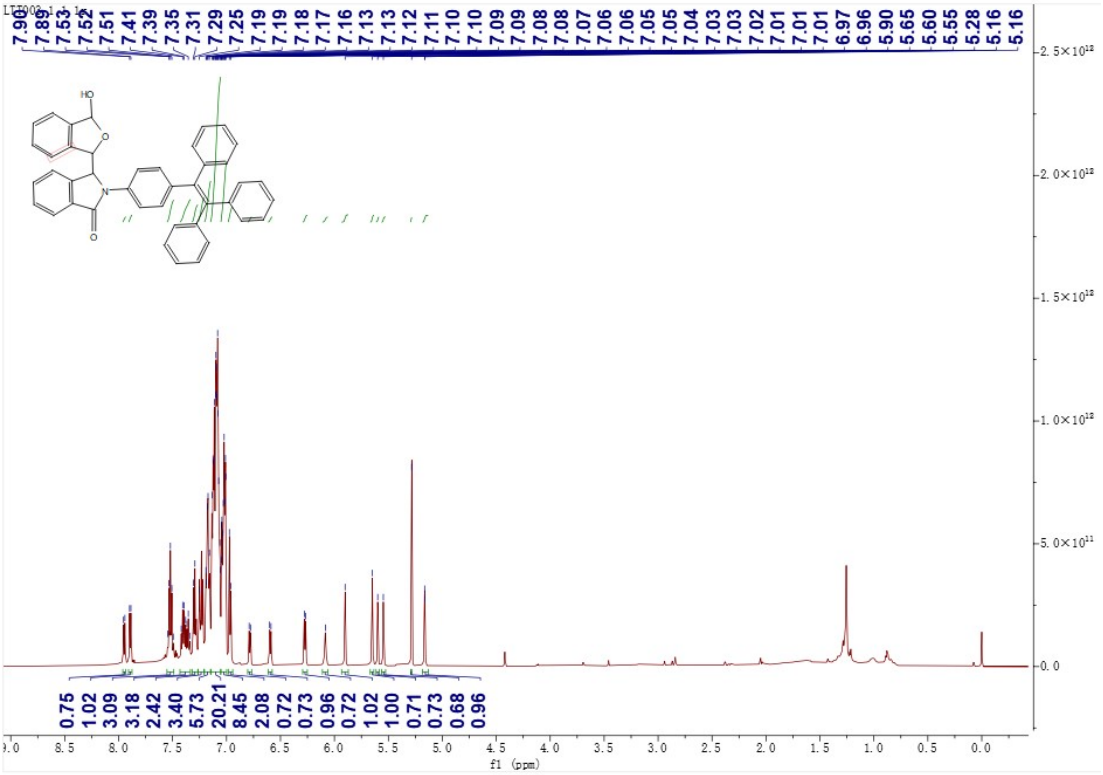

Figure S1. The ^{1}H NMR spectrum of Compound **3**.

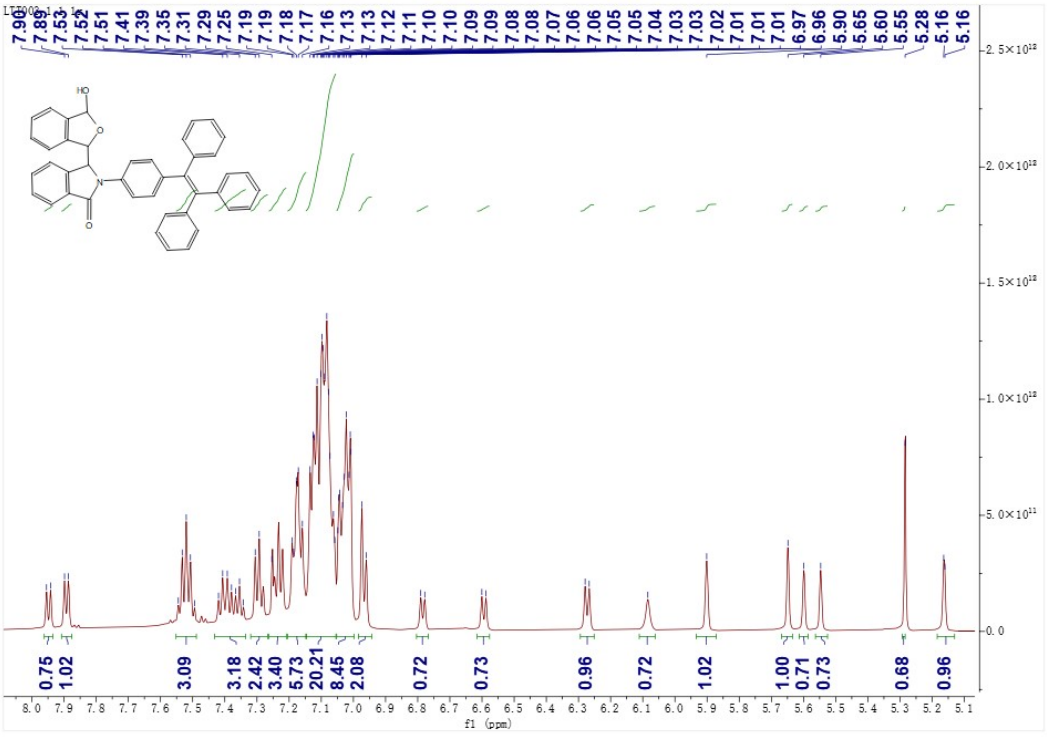

Figure S2. The expanded view of the ^{1}H NMR spectrum for Compound **3**.

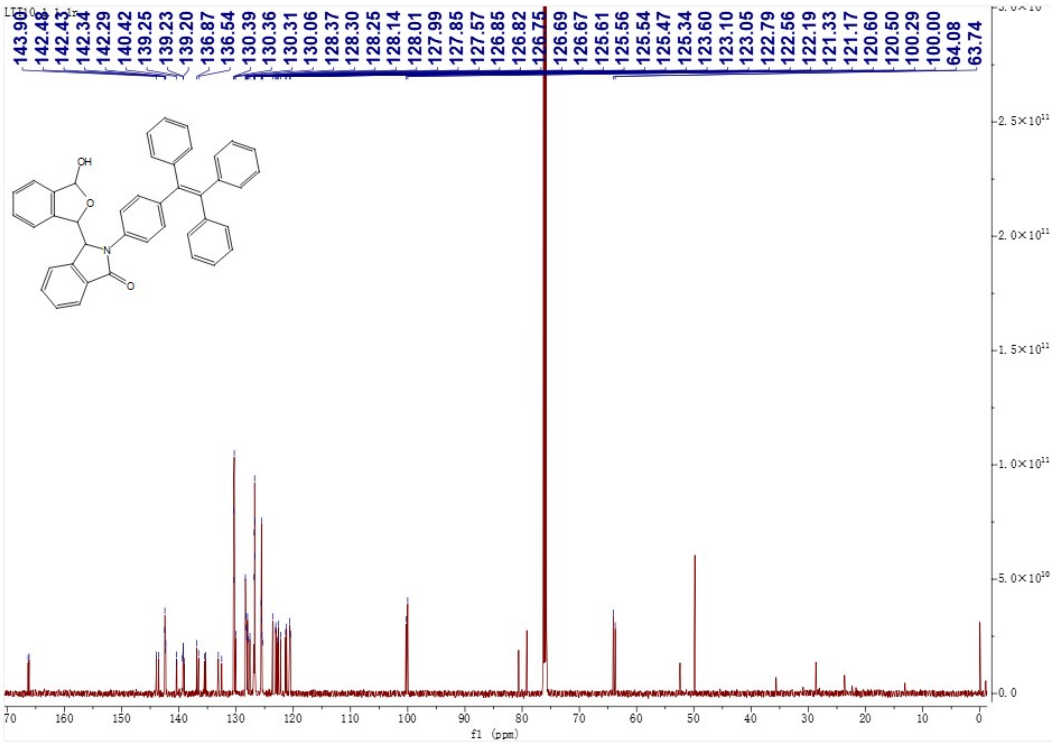

Figure S3. The ^{13}C NMR spectrum of Compound **3.**

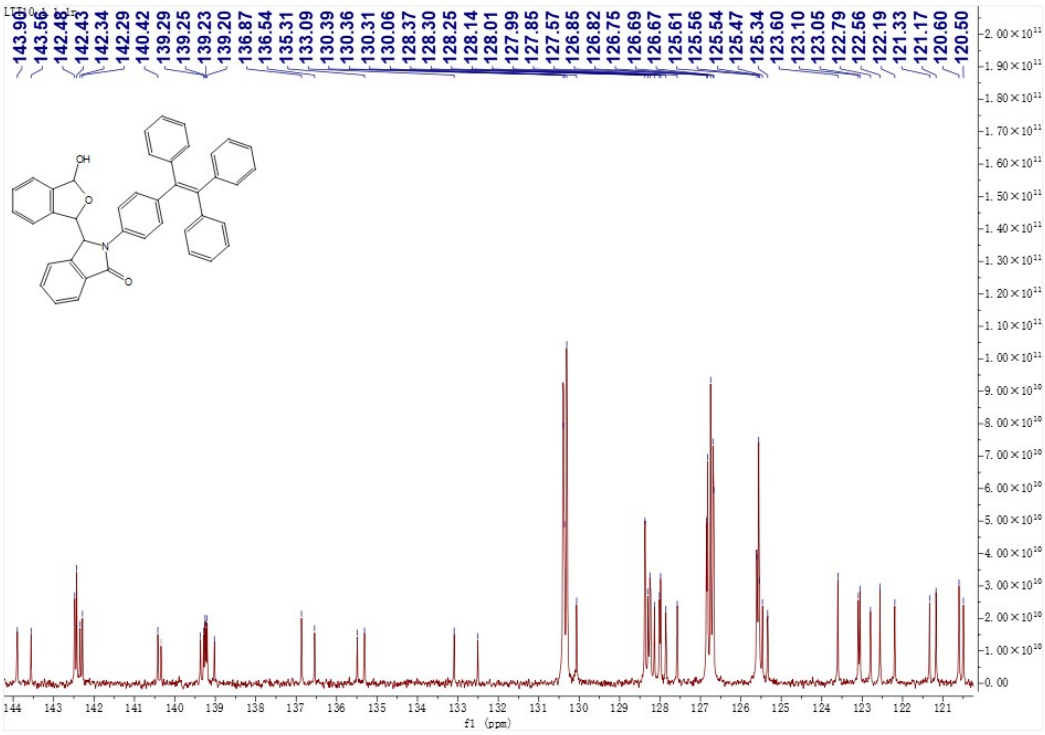

Figure S4. The expanded view of the ^{13}C NMR spectrum for Compound **3**.

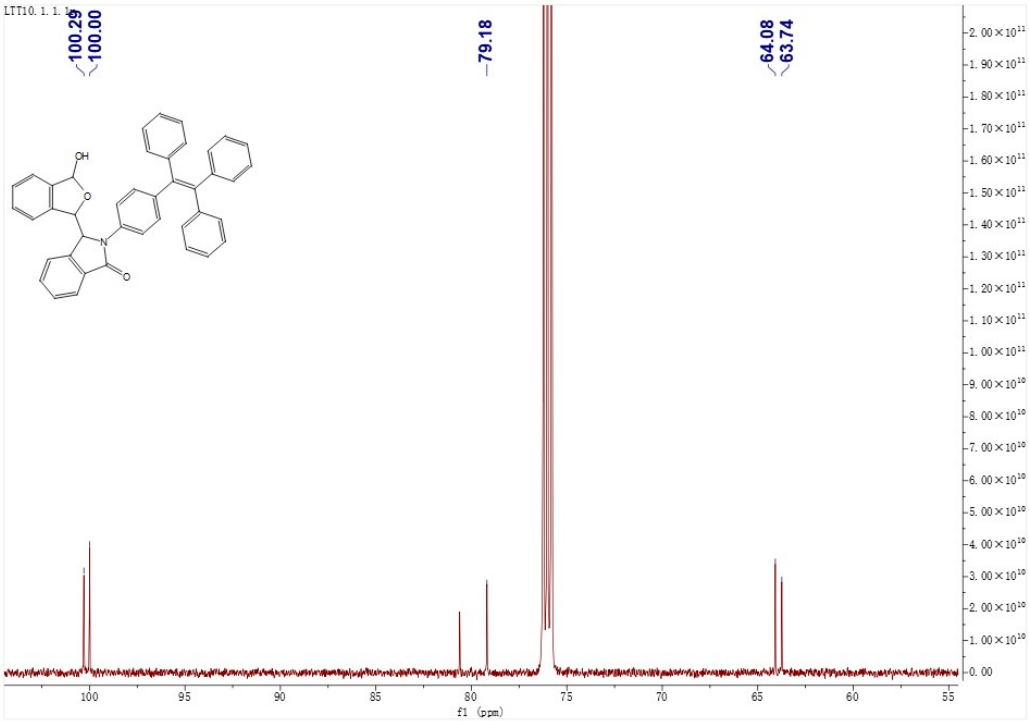

Figure S5. The expanded view of the ^{13}C NMR spectrum for Compound **3**.

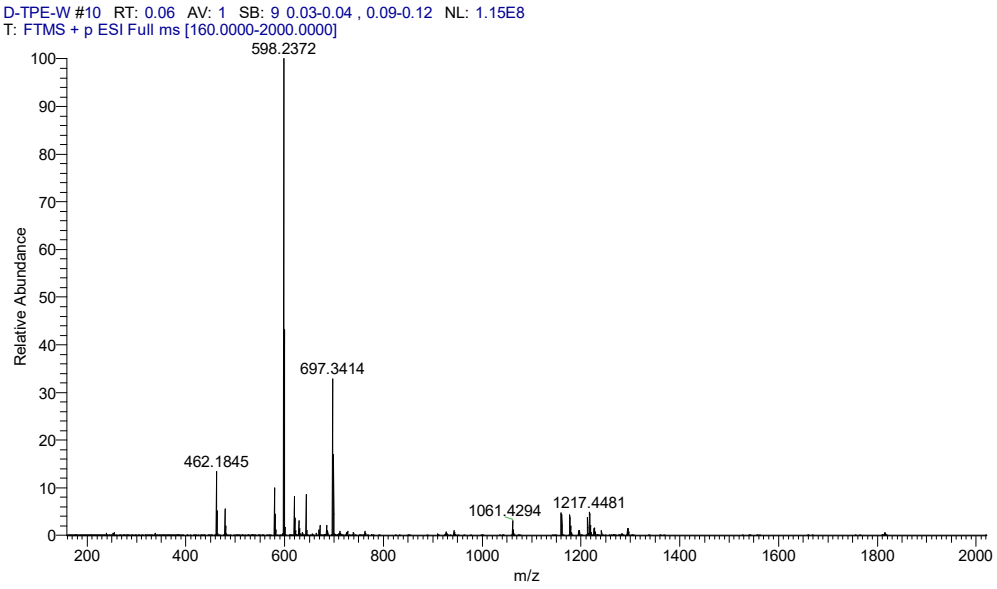

Figure S6. The MS spectrum of Compound **3**.

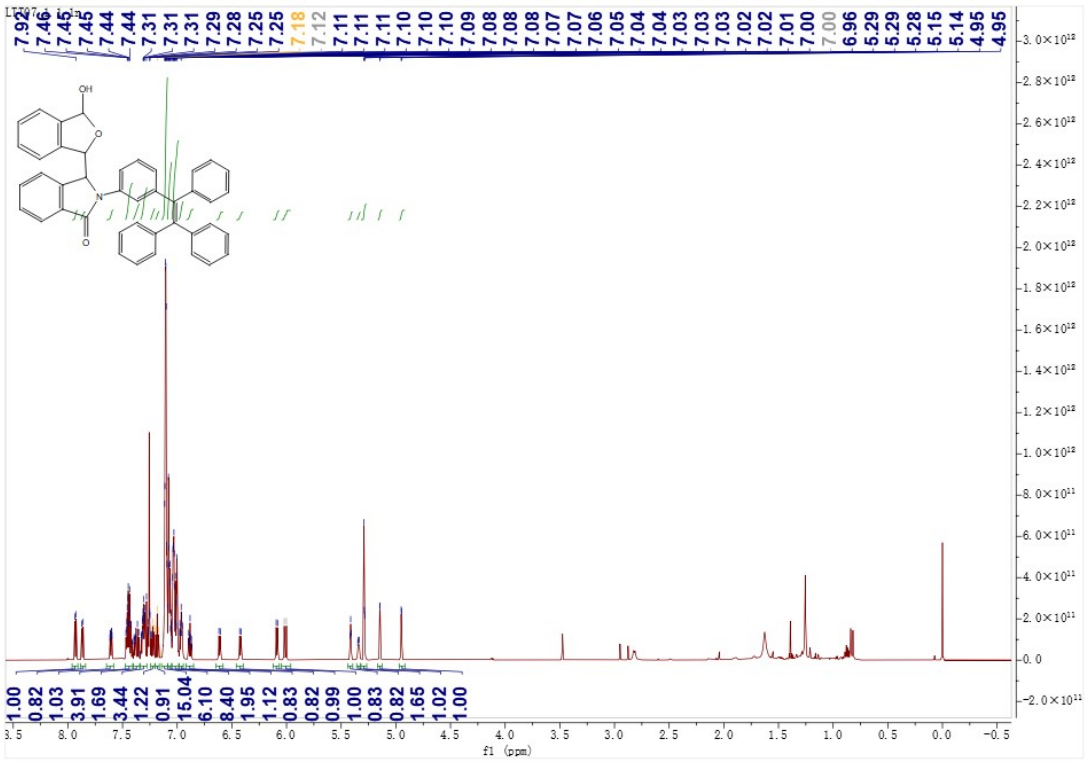

Figure S7. The ^{1}H NMR spectrum of Compound **4**.

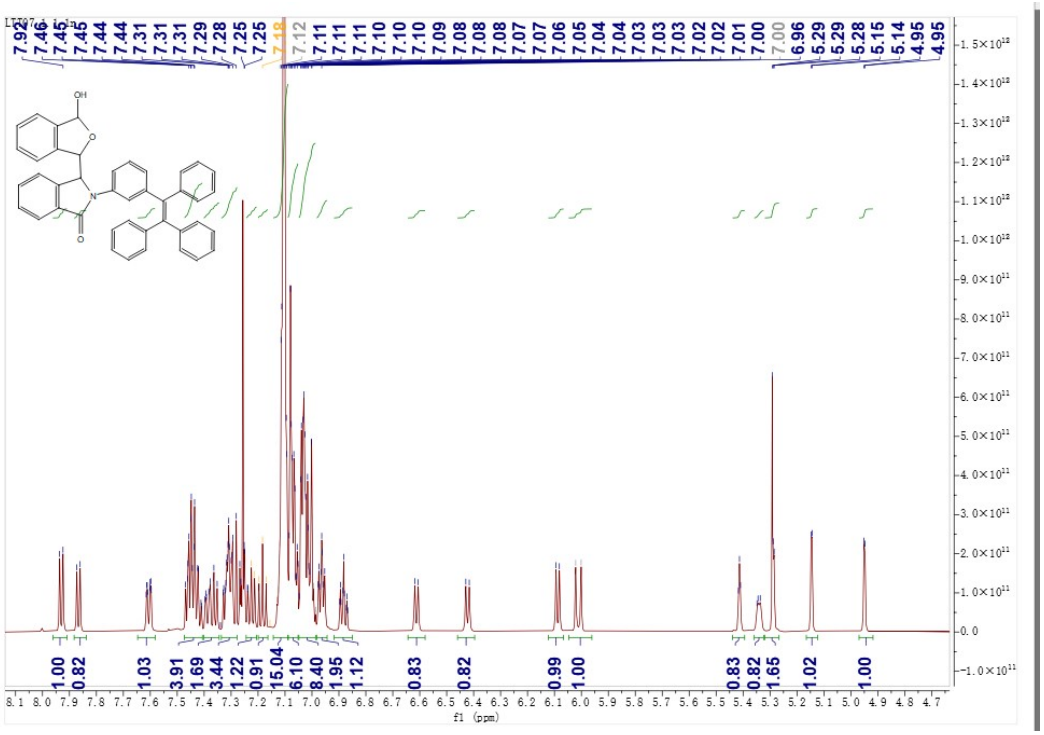

Figure S8. The expanded view of the ^{1}H NMR spectrum for Compound **4**.

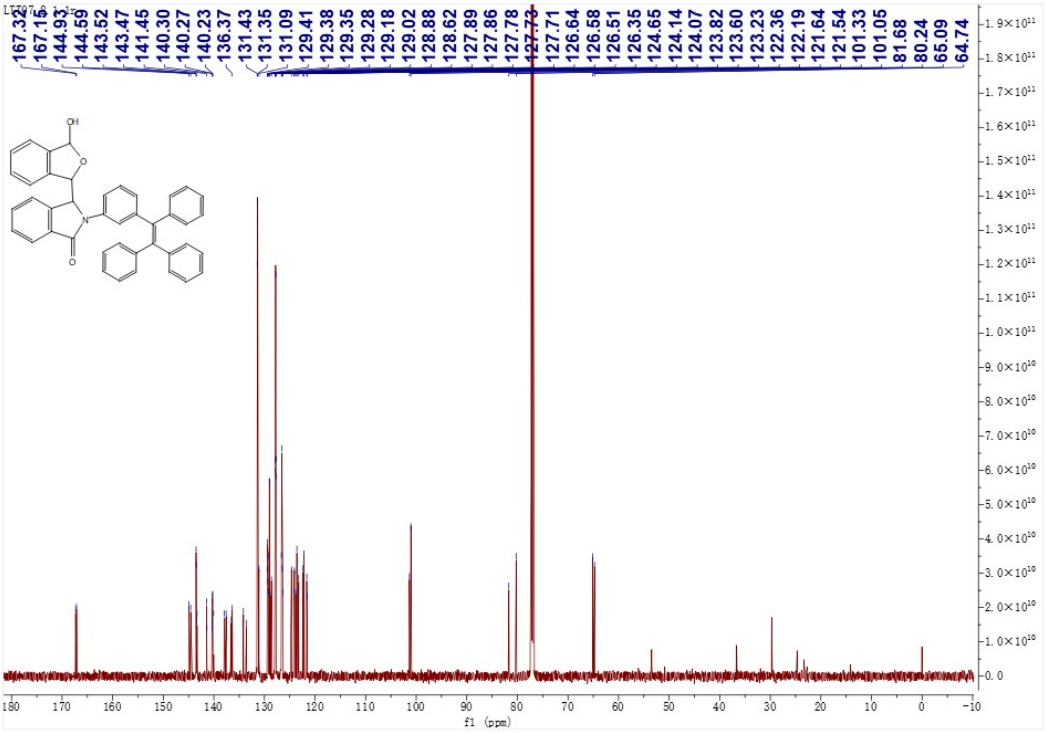

Figure S9. The ^{13}C NMR spectrum of Compound **4**.

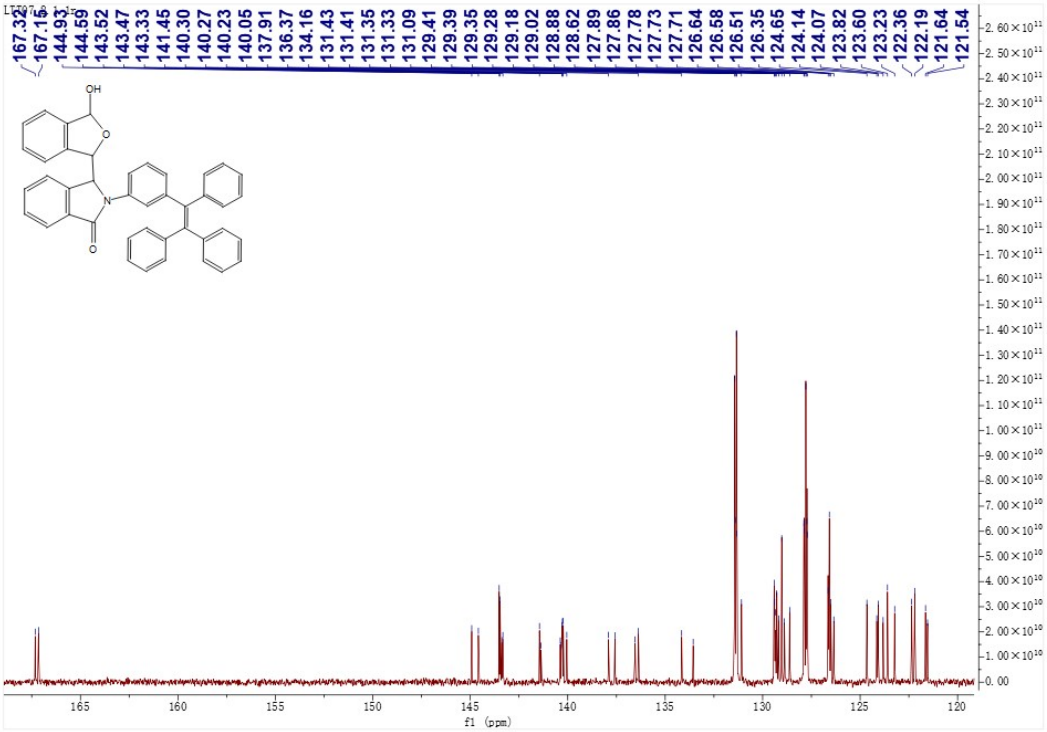

Figure S10. The expanded view of the ^{13}C NMR spectrum for Compound **4**.

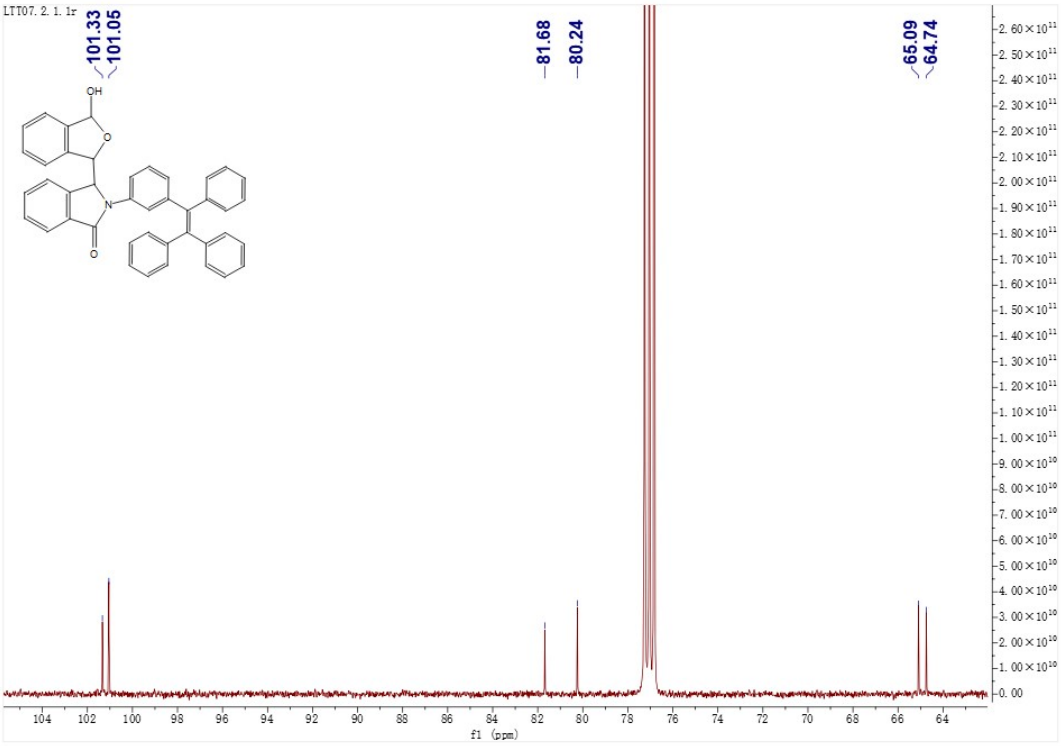

Figure S11. The expanded view of the ^{13}C NMR spectrum for Compound **4**.

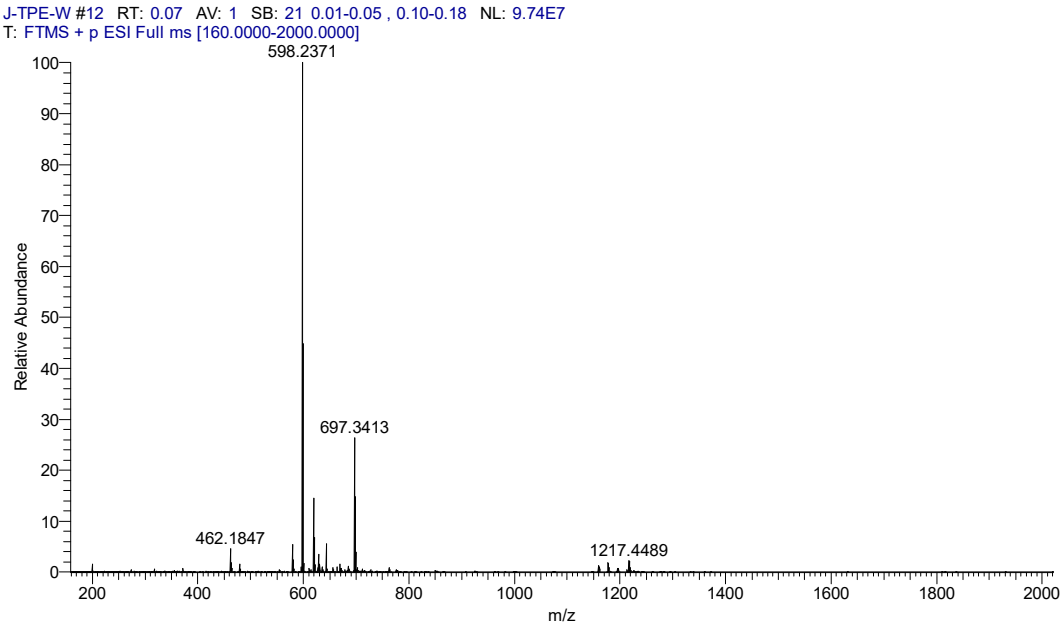

Figure S12. The MS spectrum of Compound **4**

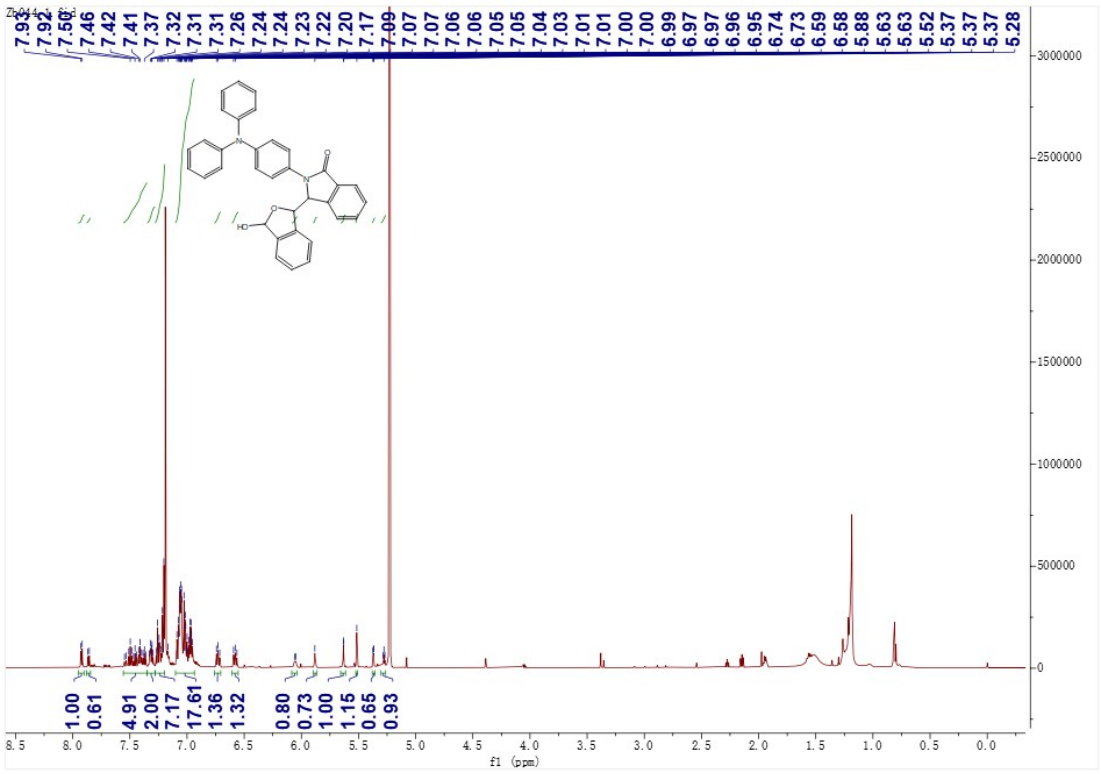

Figure S13. The ^{1}H NMR spectrum of Compound **5**.

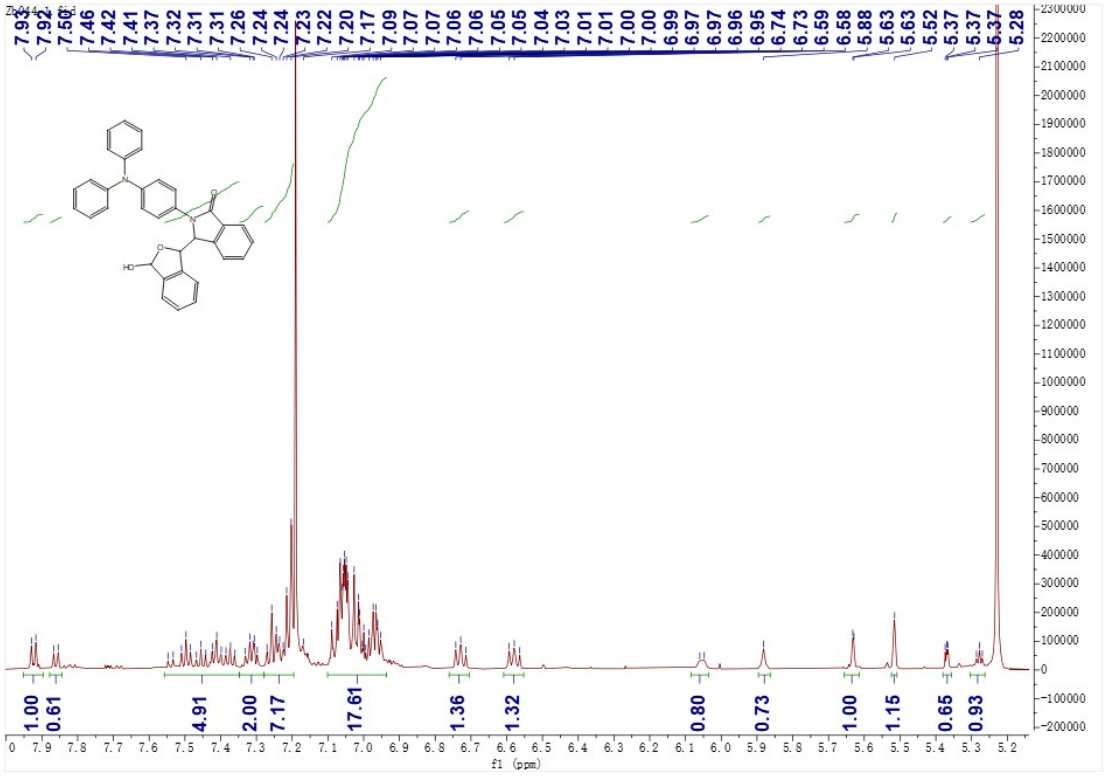

Figure S14. The expanded view of the ^{1}H NMR spectrum for Compound **5**.

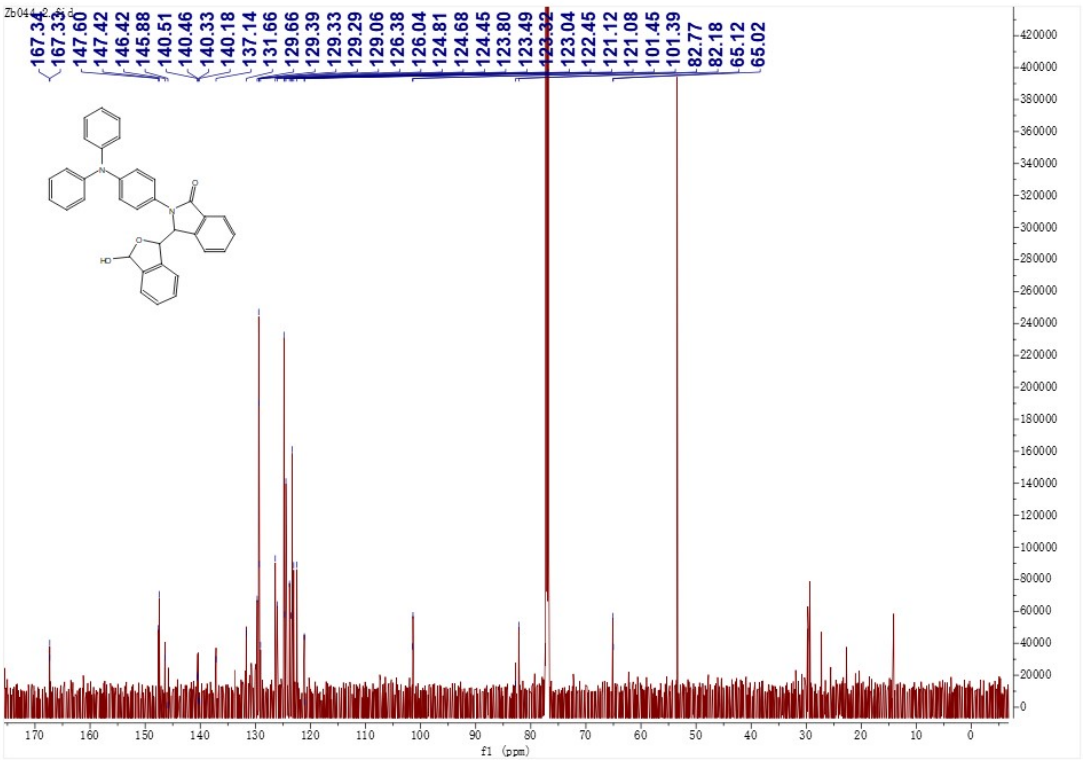

Figure S15. The ^{13}C NMR spectrum of Compound **5**.

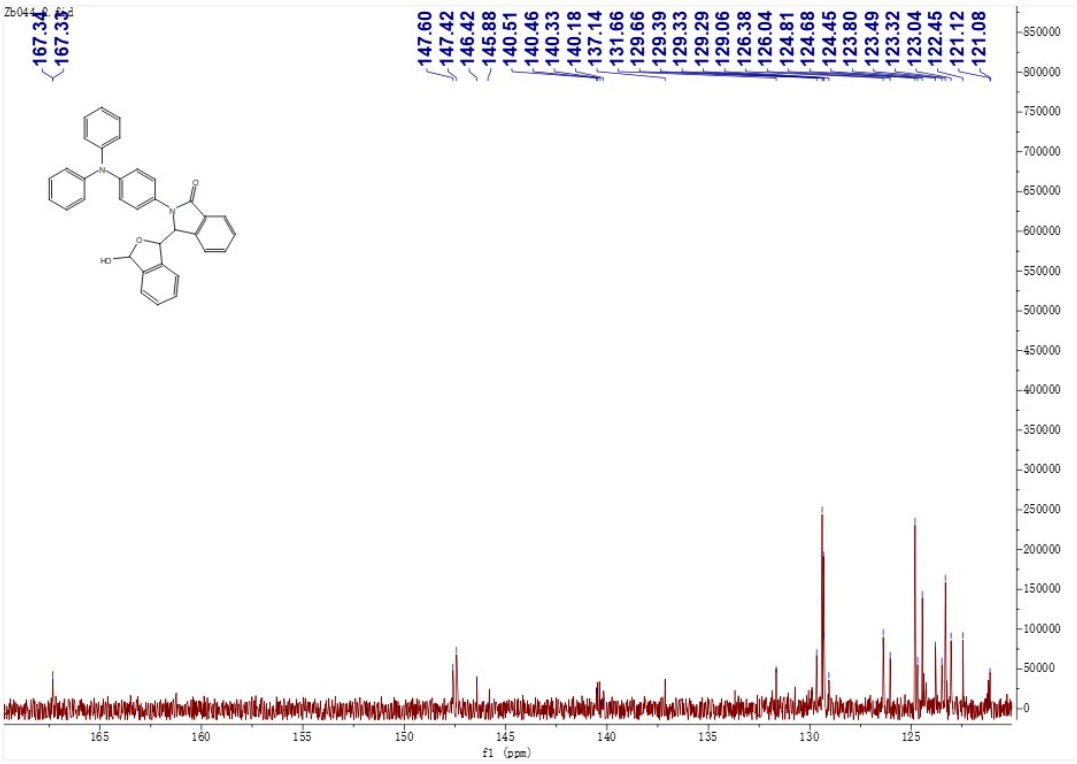

Figure S16. The expanded view of the ^{13}C NMR spectrum for Compound **5**.

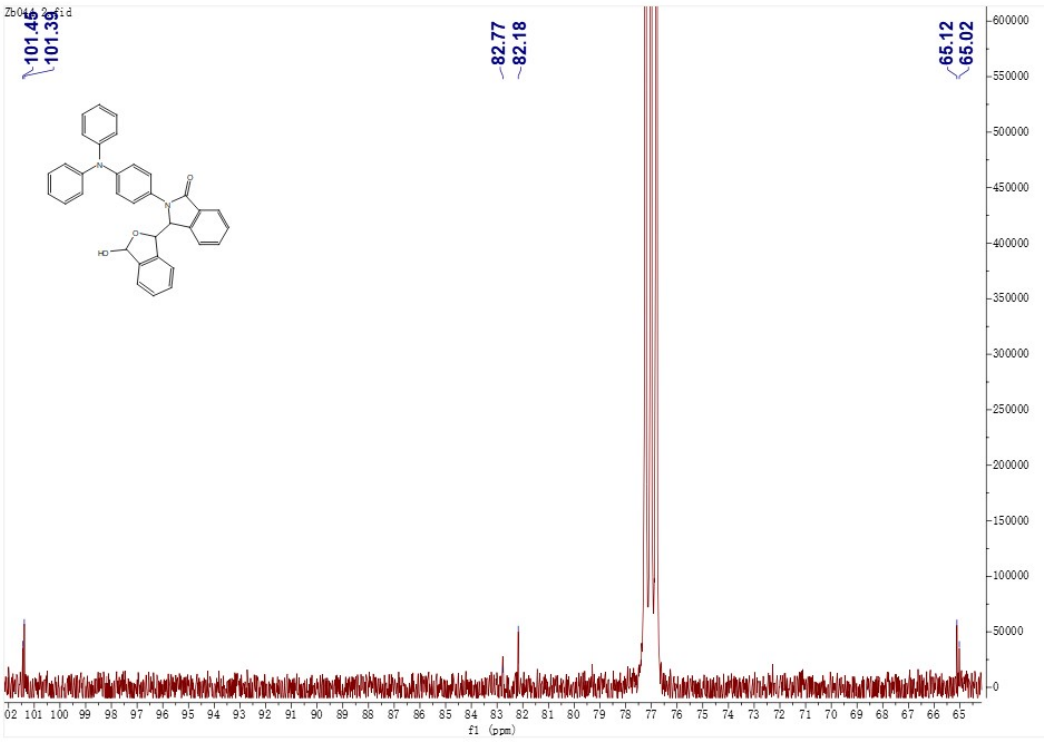

Figure S17. The expanded view of the ^{13}C NMR spectrum for Compound **5**.

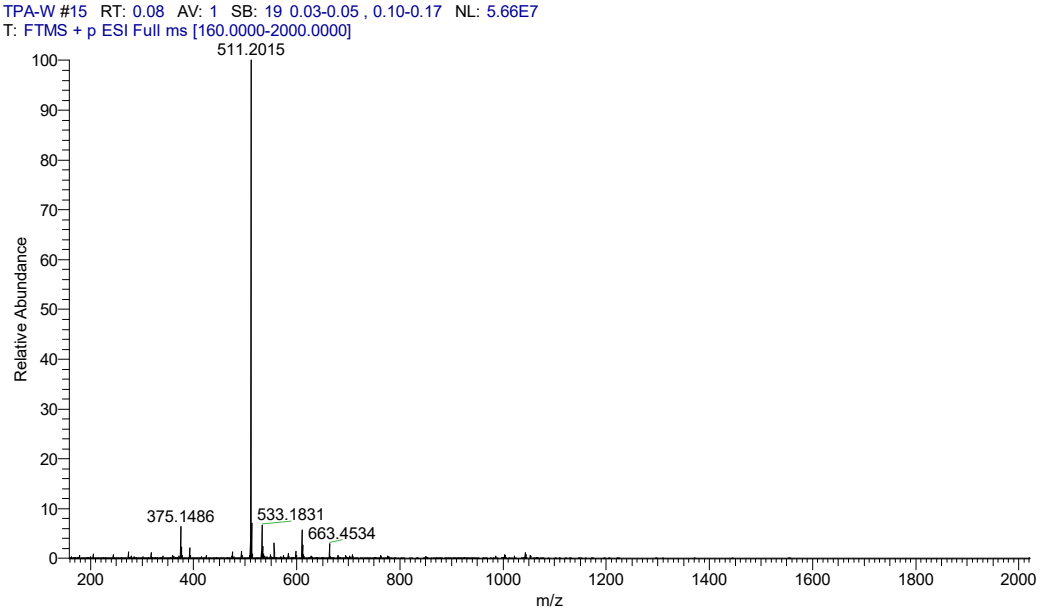

Figure S18. The MS spectrum of Compound **5.**

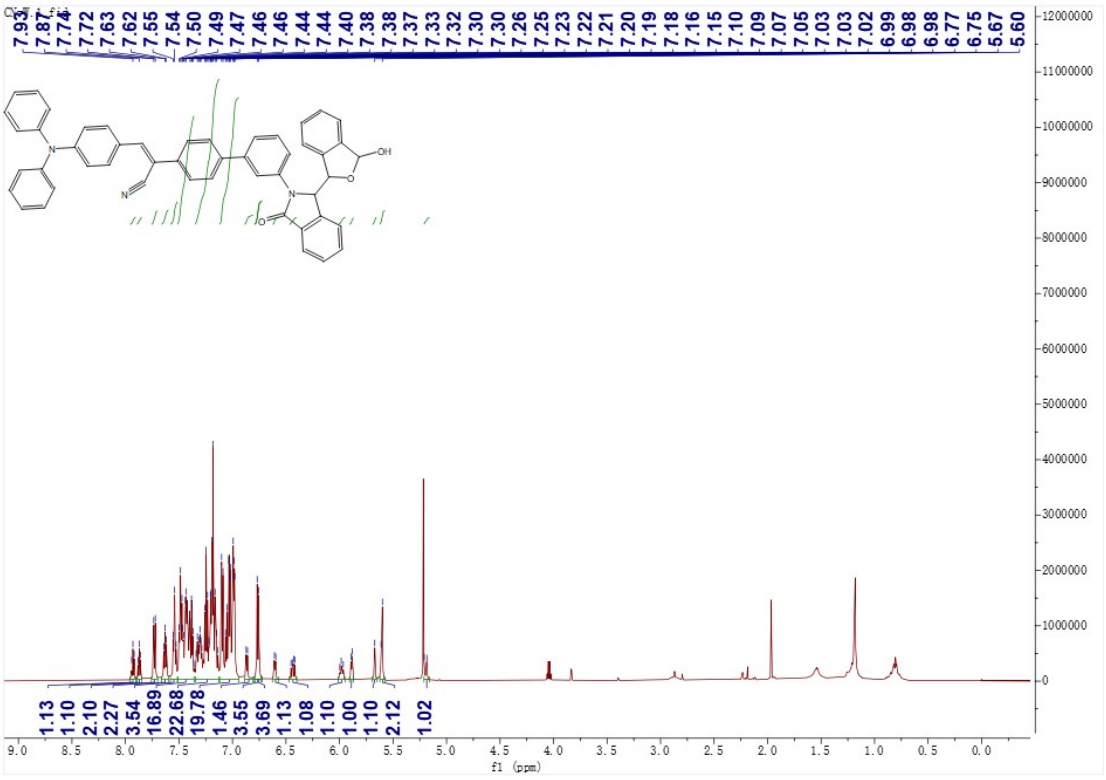

Figure S19. The ^{1}H NMR spectrum of Compound **6**.

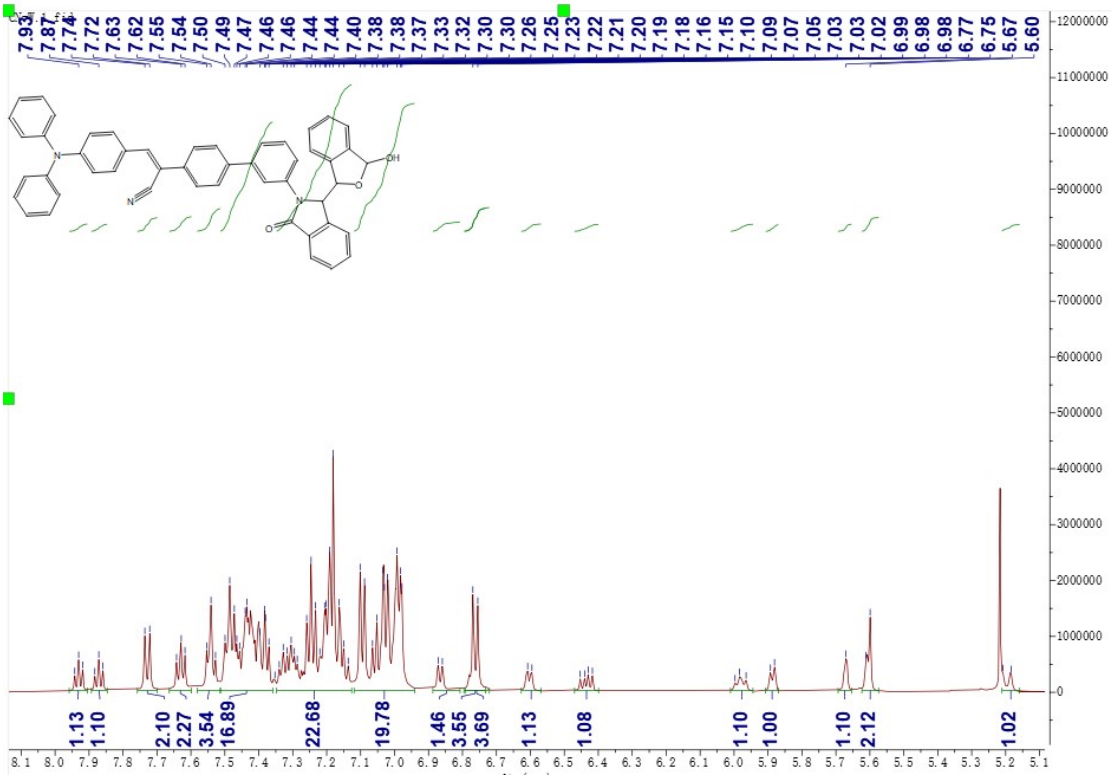

Figure S20. The expanded view of the ^{1}H NMR spectrum for Compound **6**.

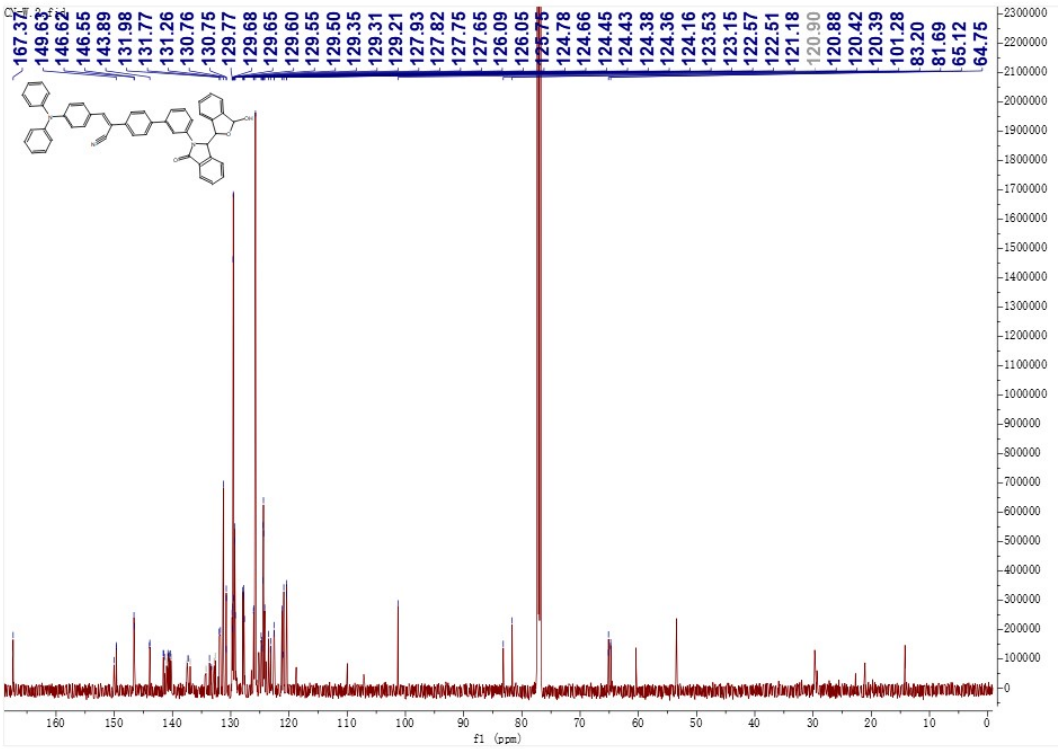

Figure S21. The ^{13}C NMR spectrum of Compound **6**.

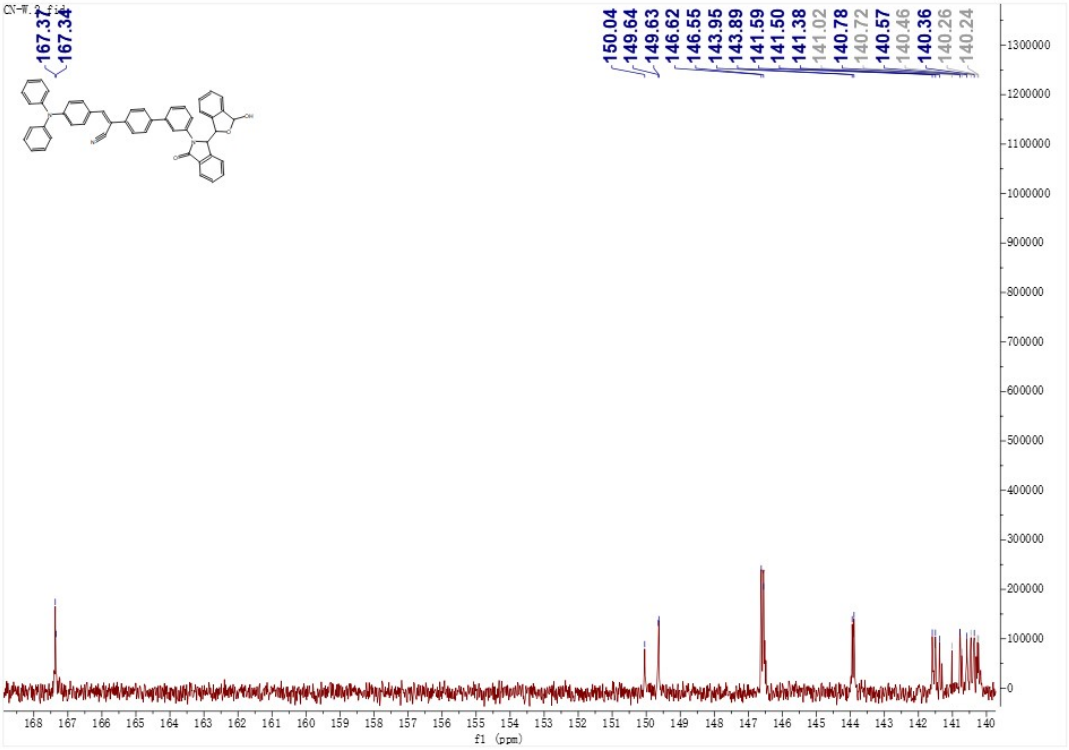

Figure S22. The expanded view of the ^{13}C NMR spectrum for Compound **6**.

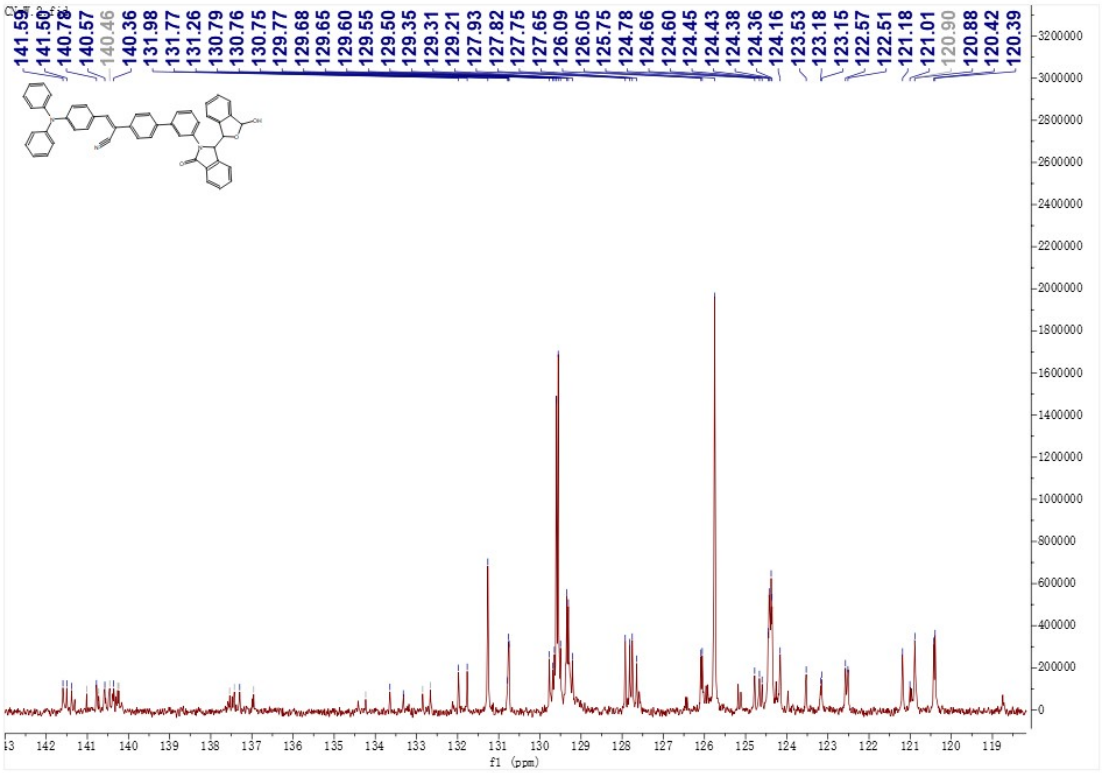

Figure S23. The expanded view of the ^{13}C NMR spectrum for Compound **6**.

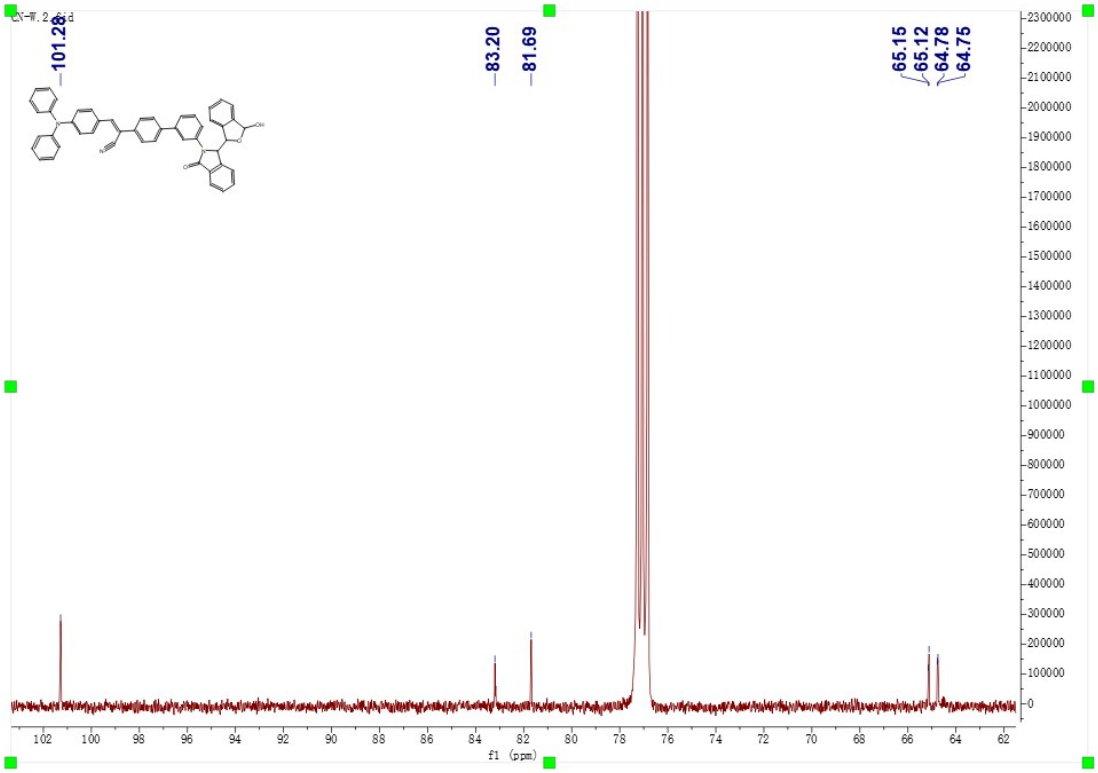

Figure S24. The expanded view of the ^{13}C NMR spectrum for Compound **6**.

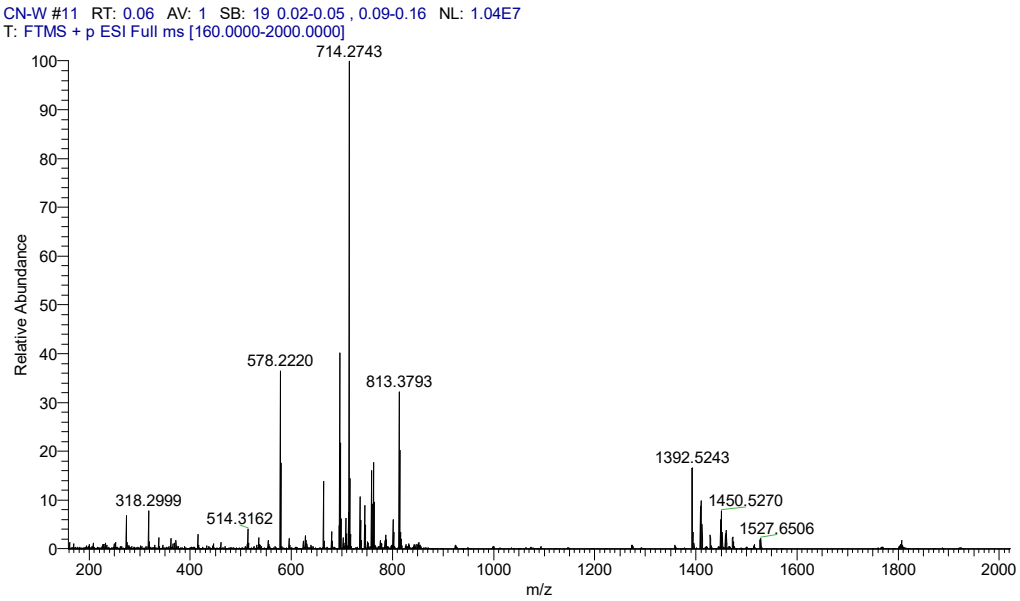

Figure S25. The MS spectrum of Compound **6.**

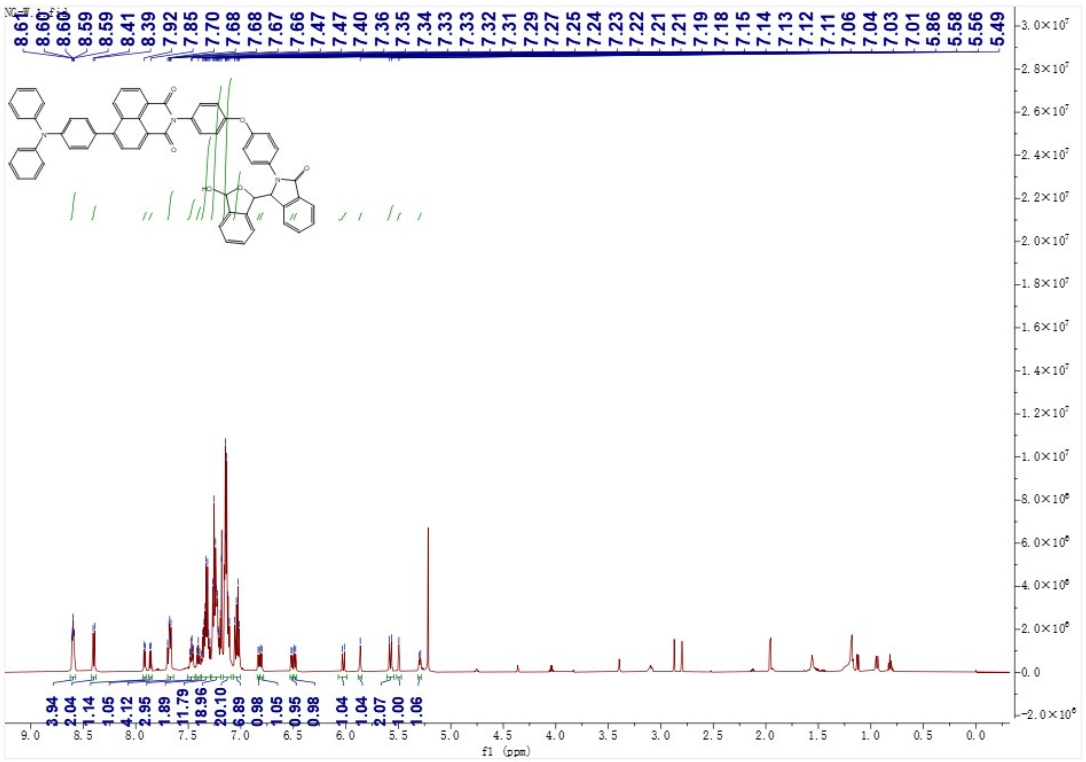

Figure S26. The ^{1}H NMR spectrum of Compound **7**.

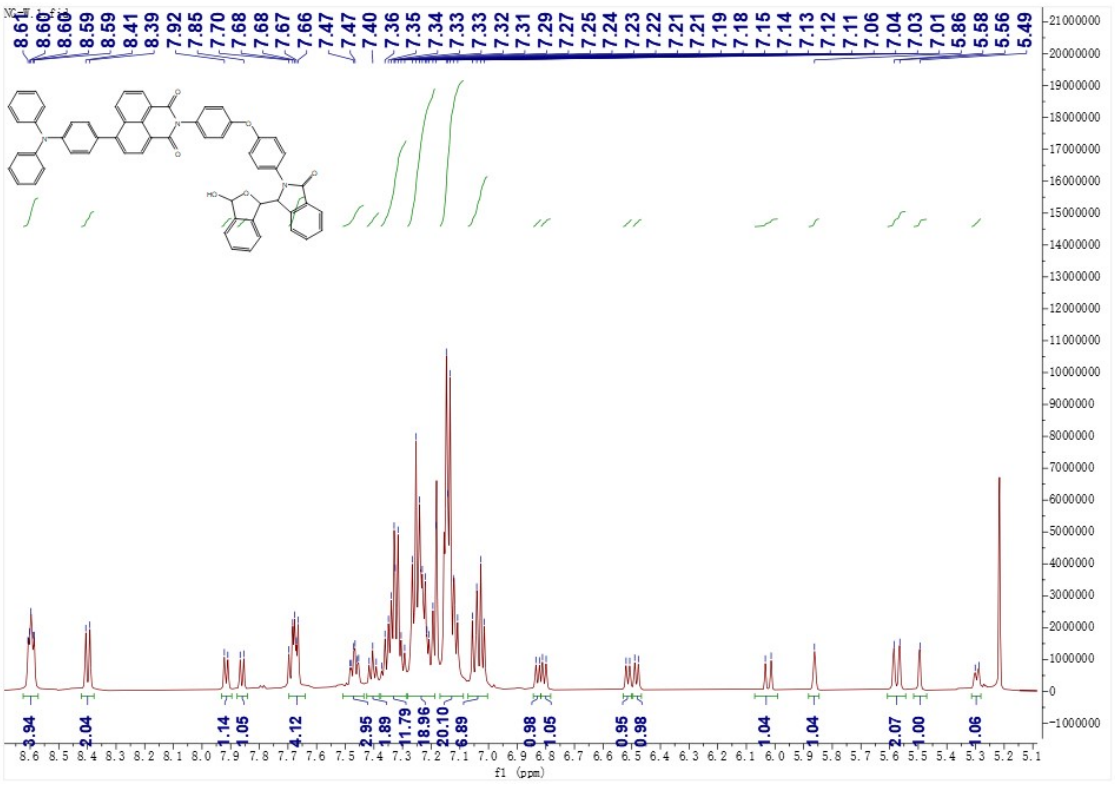

Figure S27. The expanded view of the ^{1}H NMR spectrum for Compound **7**.

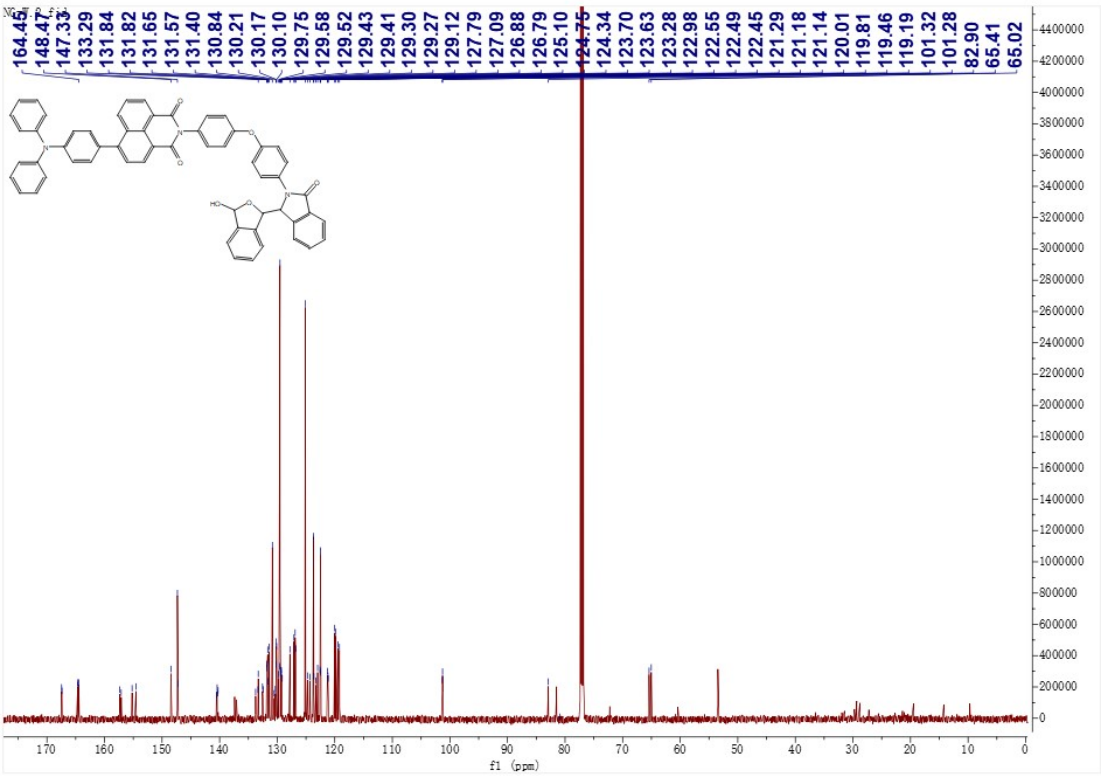

Figure S28. The ^{13}C NMR spectrum of Compound **7**.

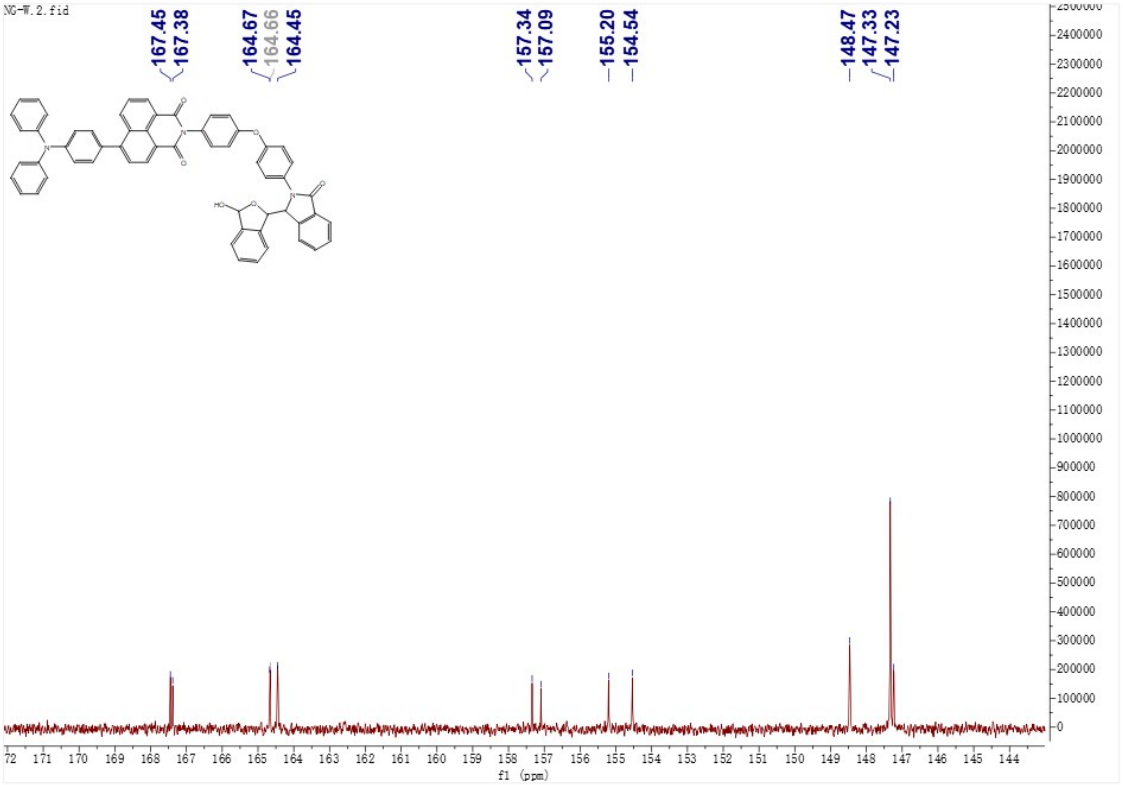

Figure S29. The expanded view of the ^{13}C NMR spectrum for Compound **7**.

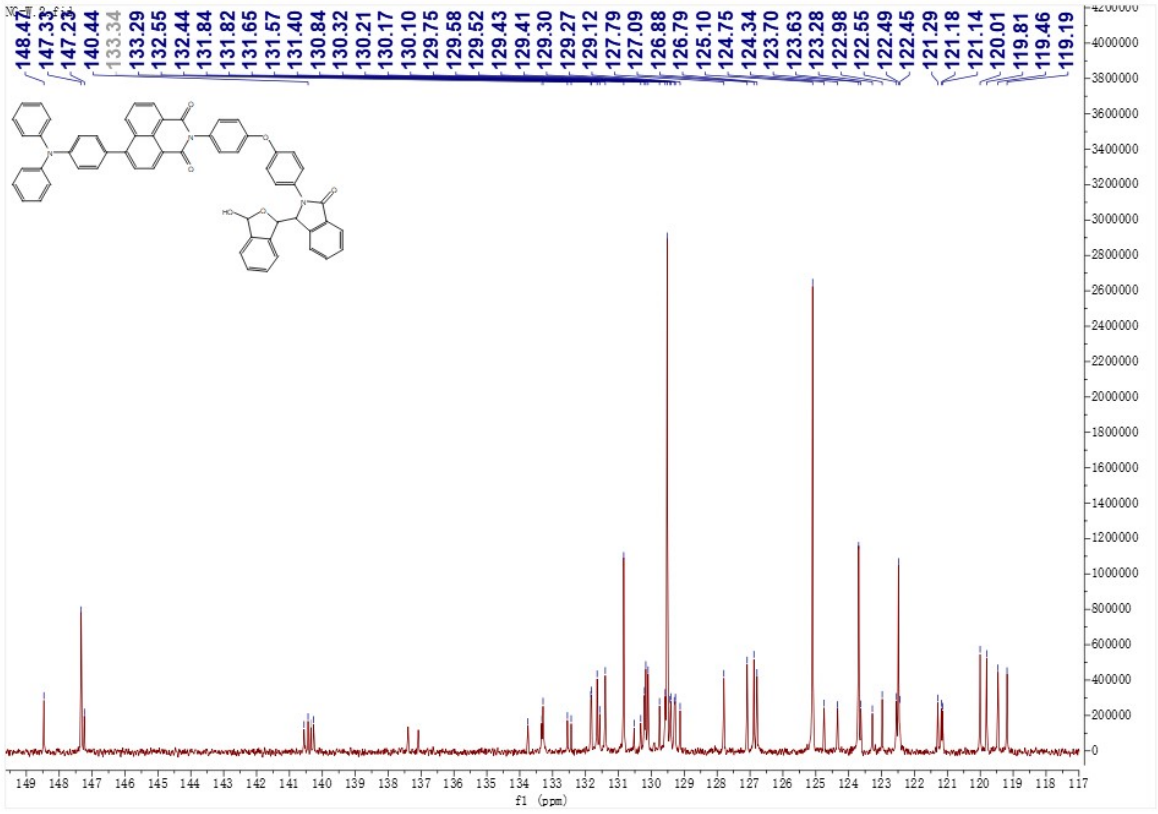

Figure S30. The expanded view of the ^{13}C NMR spectrum for Compound **7**.

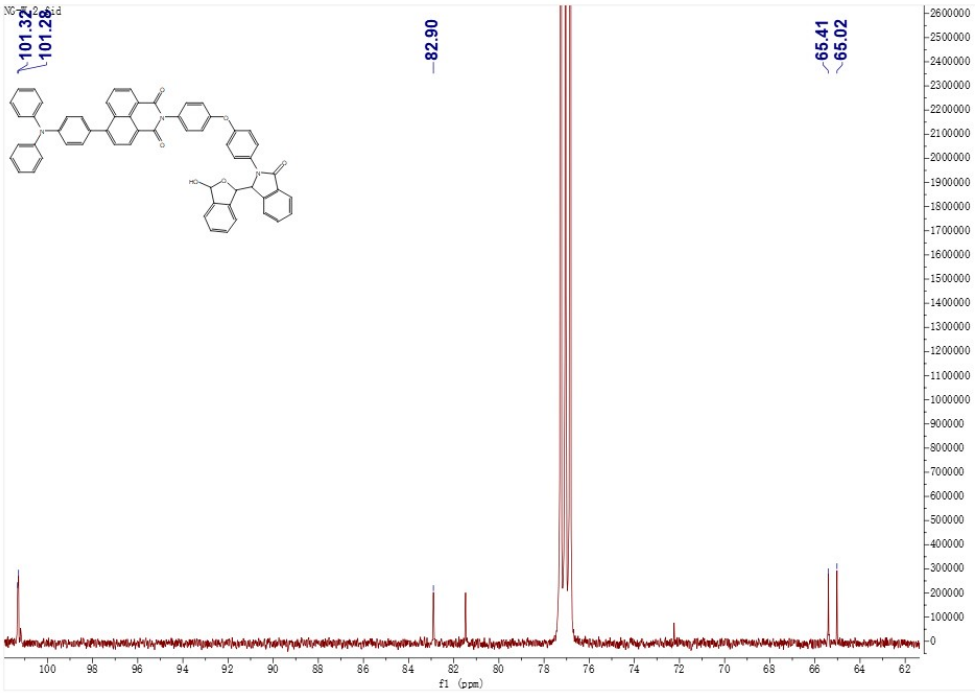

Figure S31. The expanded view of the ^{13}C NMR spectrum for Compound **7**.

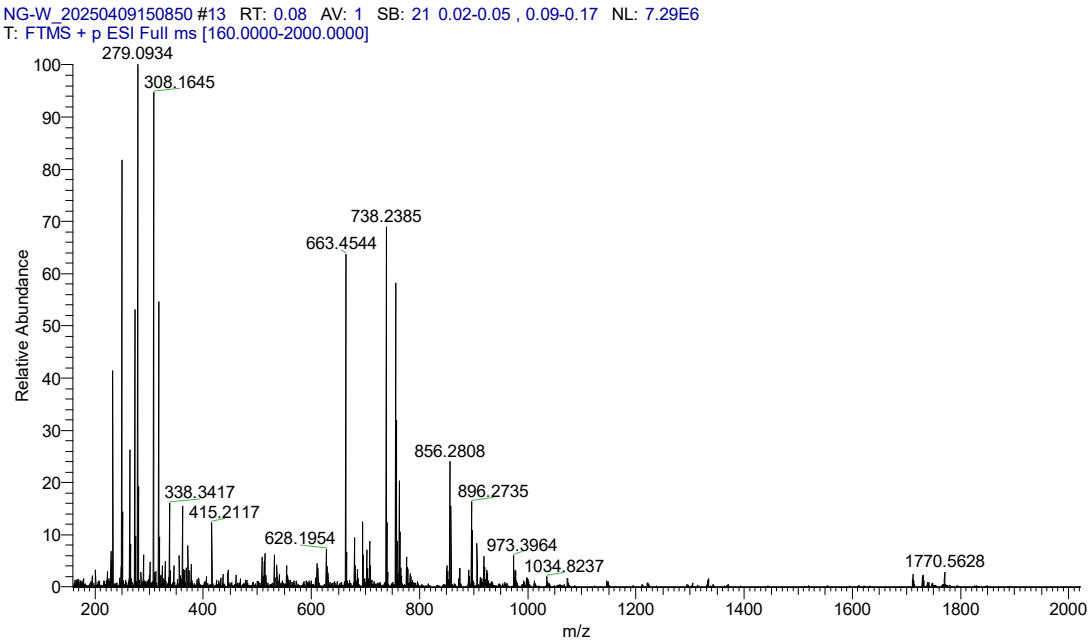

Figure S32. The MS spectrum of Compound **7.**

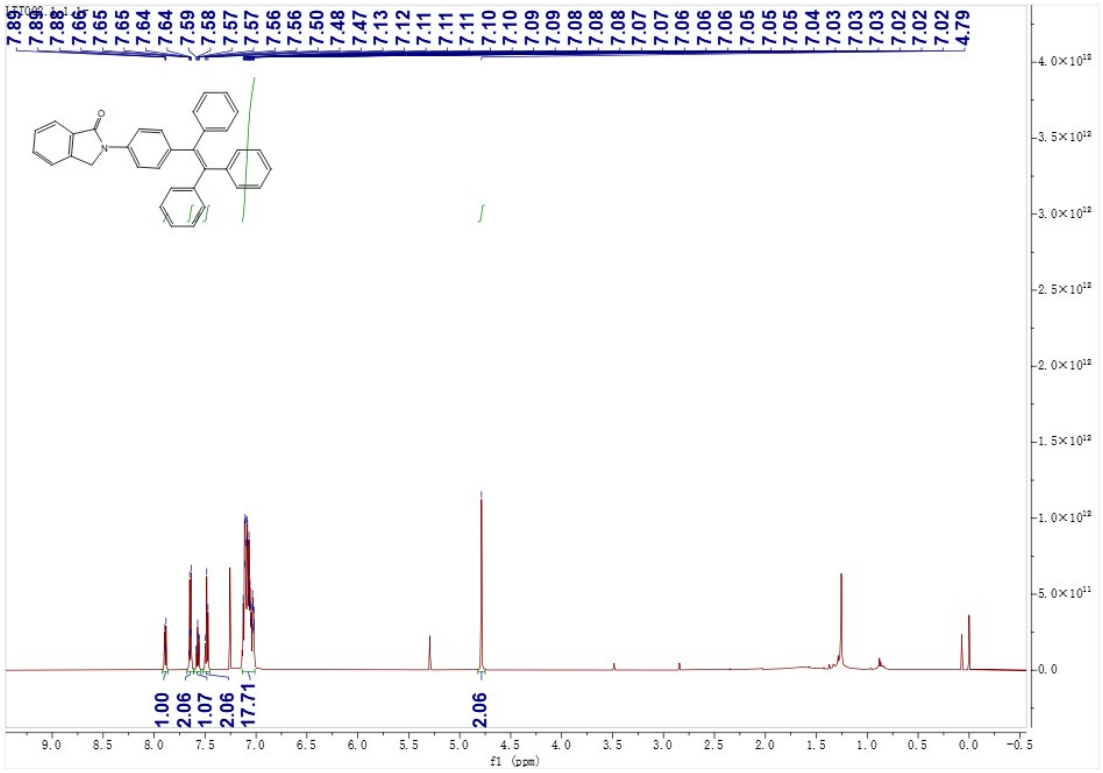

Figure S33. The ^{1}H NMR spectrum of Compound **8**.

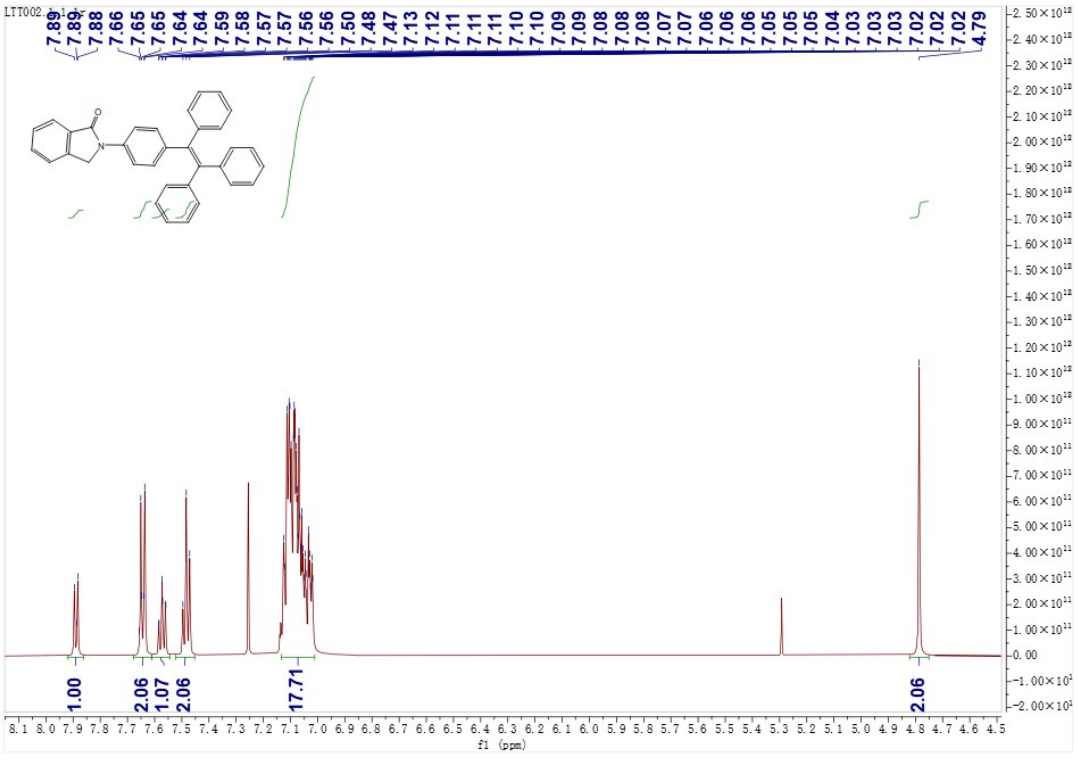

Figure S34. The expanded view of the ^{1}H NMR spectrum for Compound **8**.

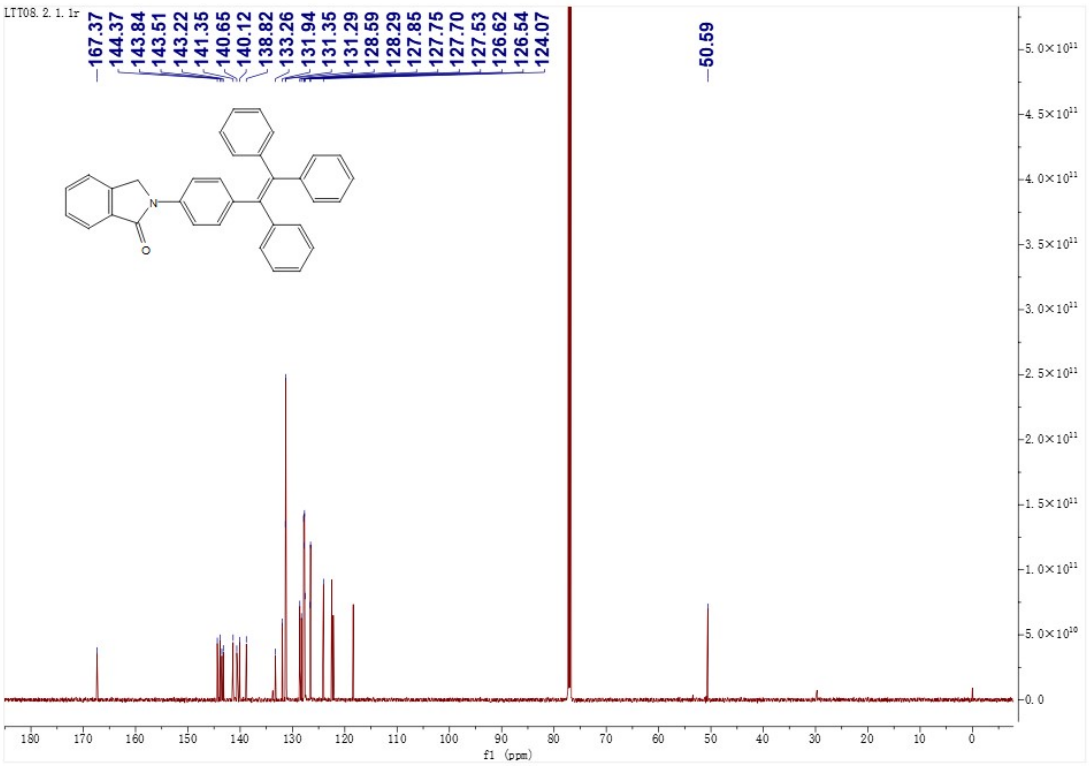

Figure S35. The ^{13}C NMR spectrum of Compound **8**.

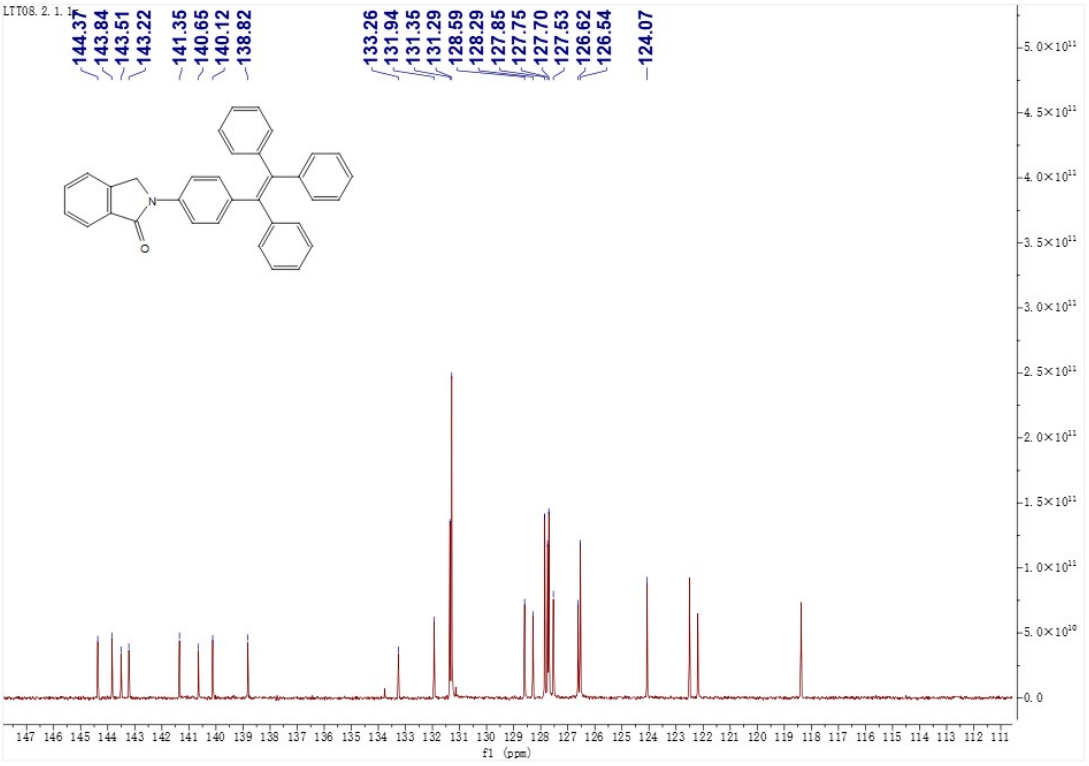

Figure S36. The expanded view of the ^{13}C NMR spectrum for Compound **8**.

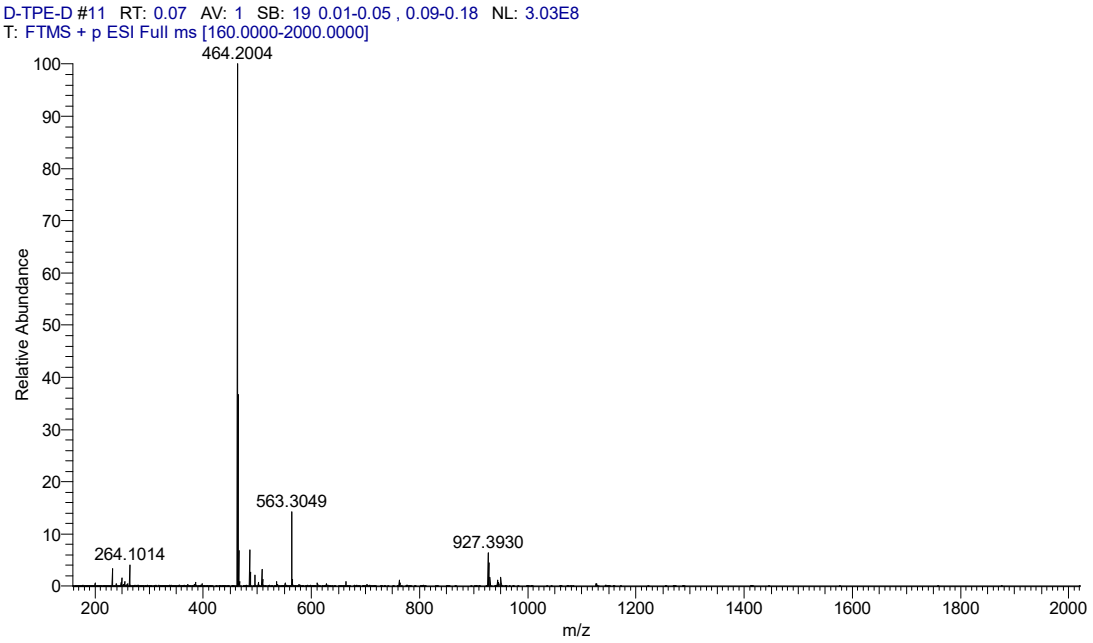

Figure S37. The MS spectrum of Compound **8.**

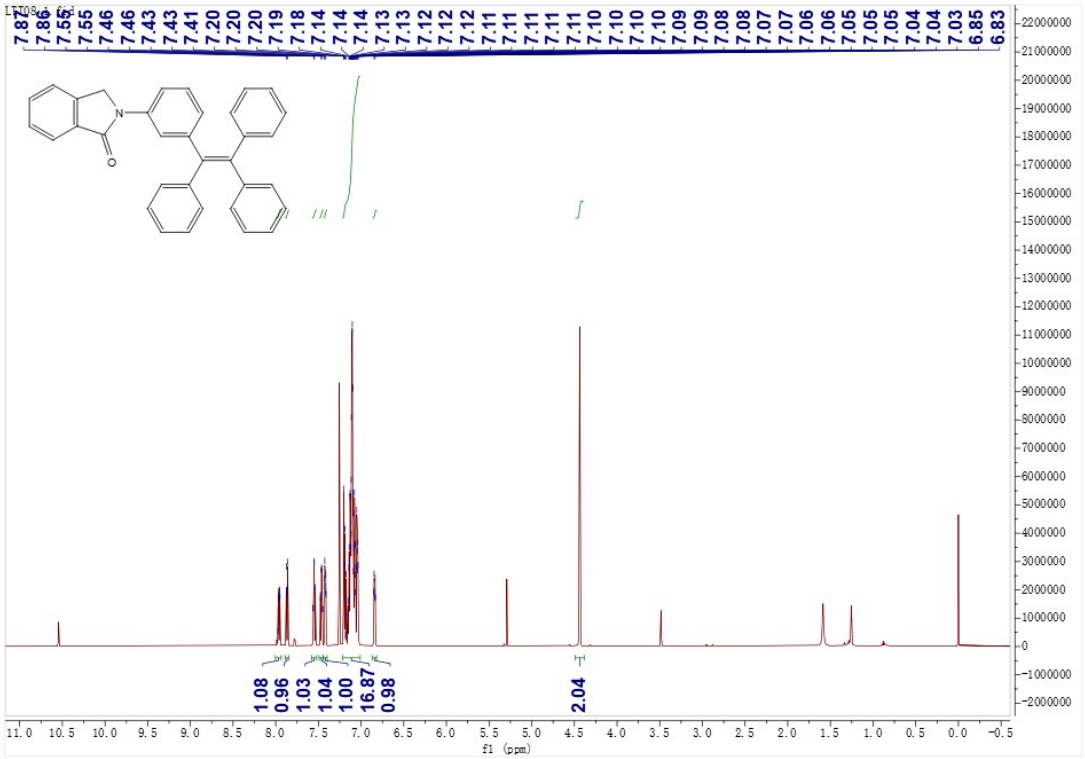

Figure S38. The ^{1}H NMR spectrum of Compound **9**.

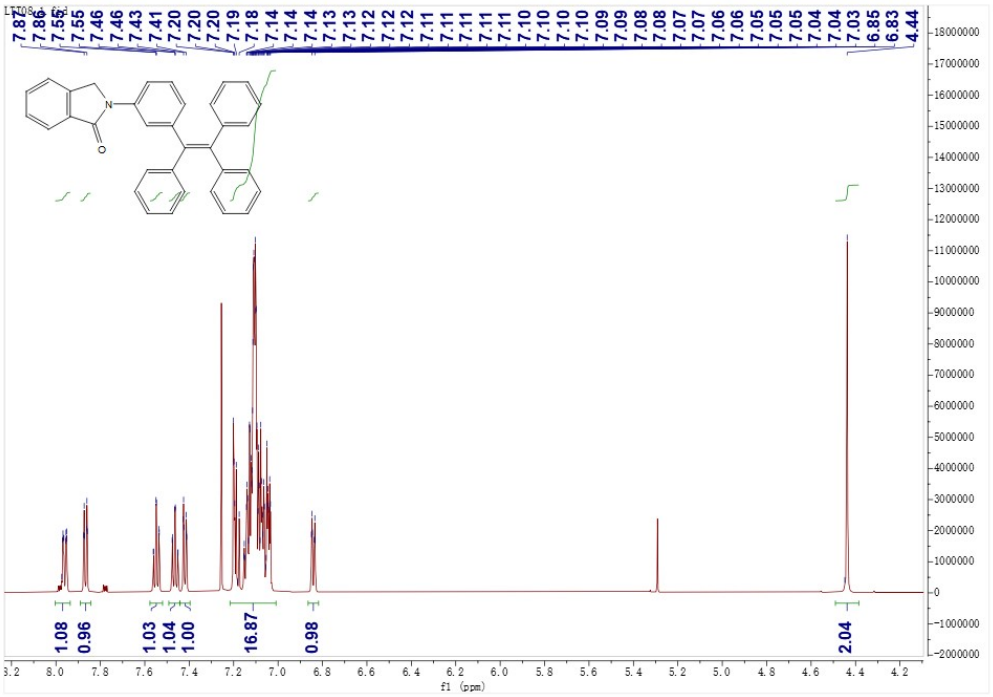

Figure S39. The expanded view of the ^{1}H NMR spectrum for Compound **9**.

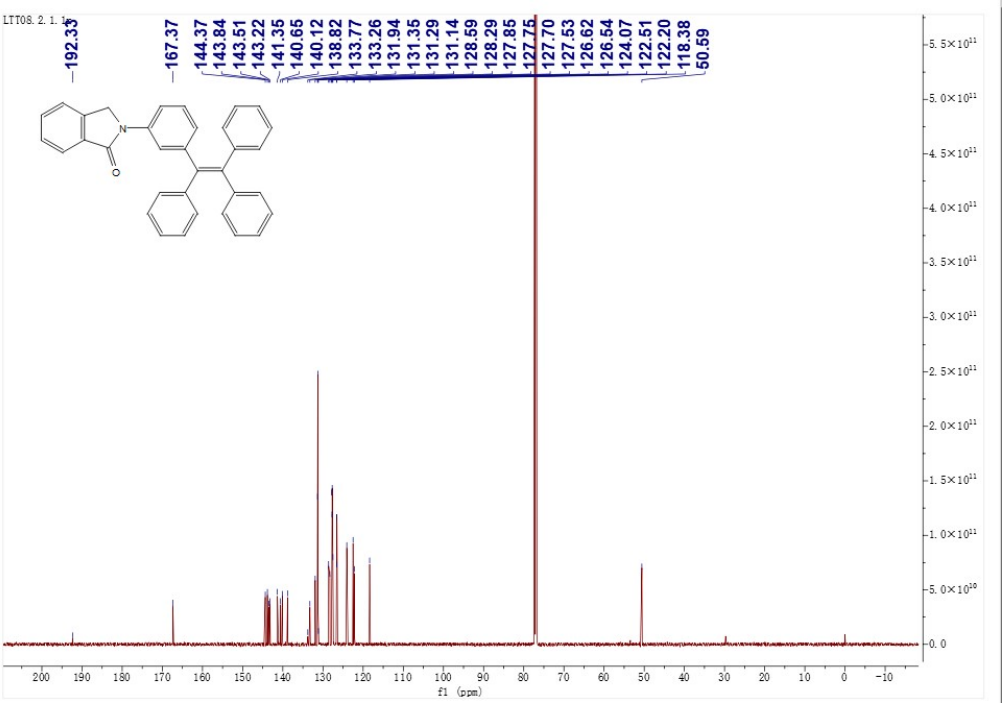

Figure S40. The ^{13}C NMR spectrum of Compound **9**.

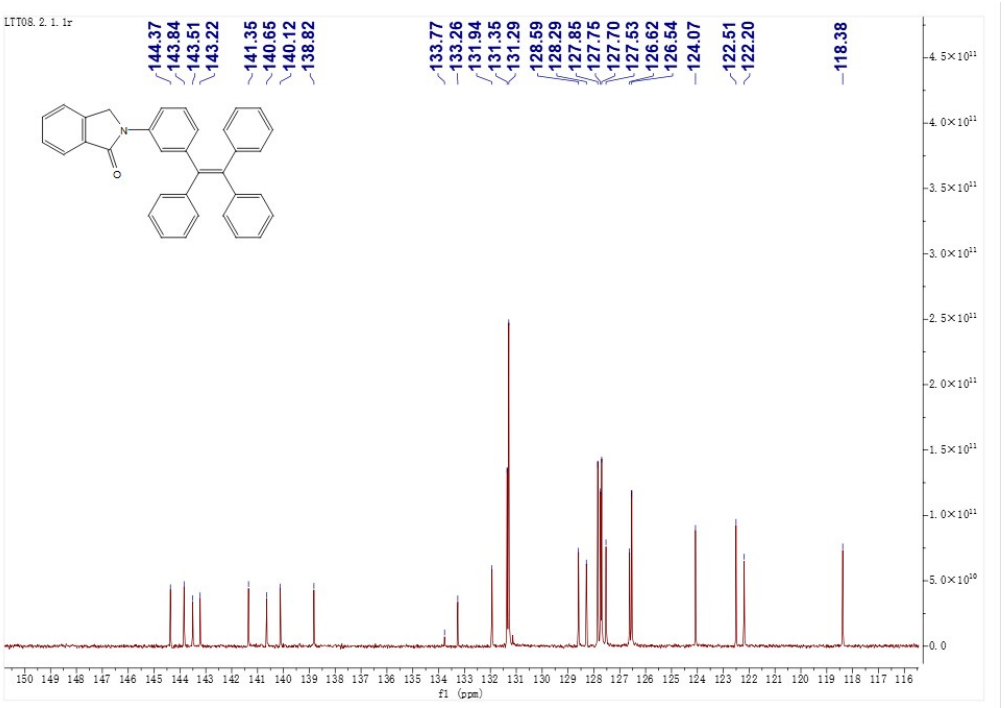

Figure S41. The expanded view of the ^{13}C NMR spectrum for Compound **9**.

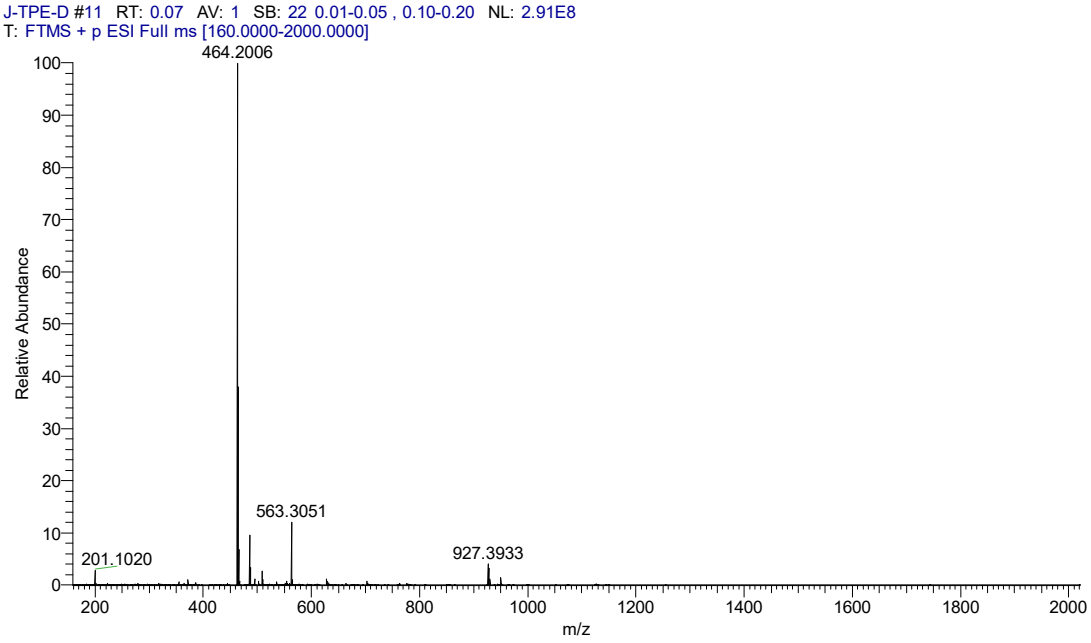

Figure S42. The MS spectrum of Compound **9.**

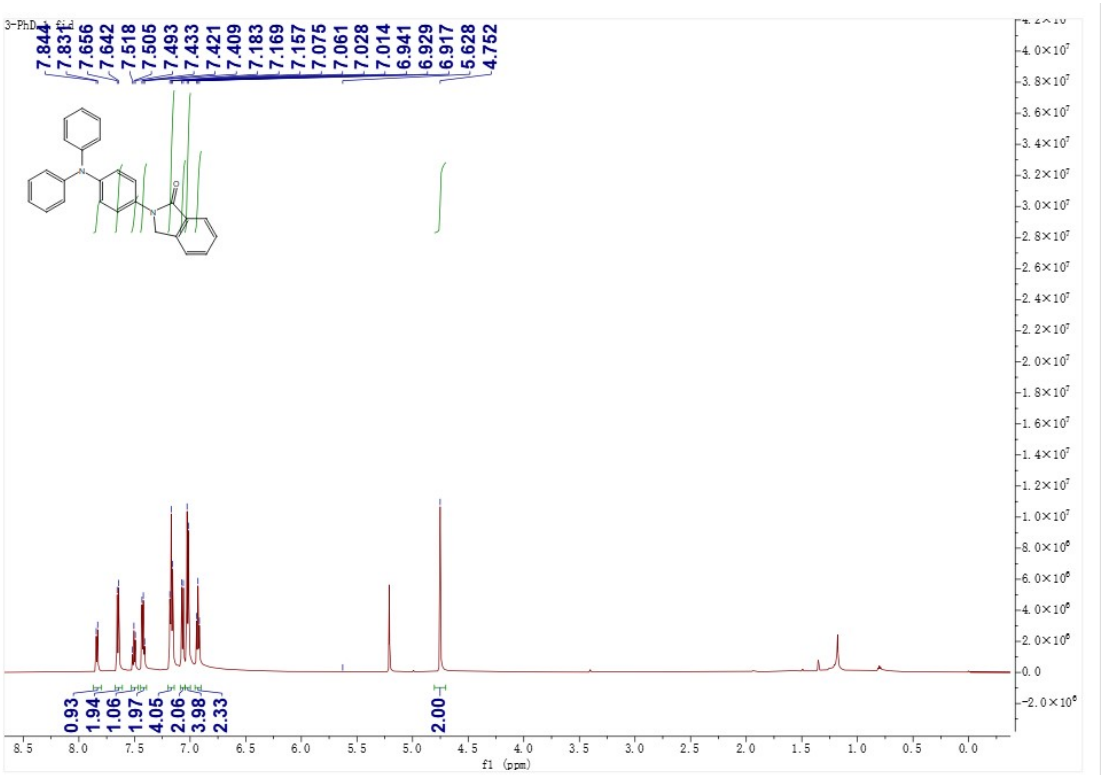

Figure S43. The ^{1}H NMR spectrum of Compound **10**.

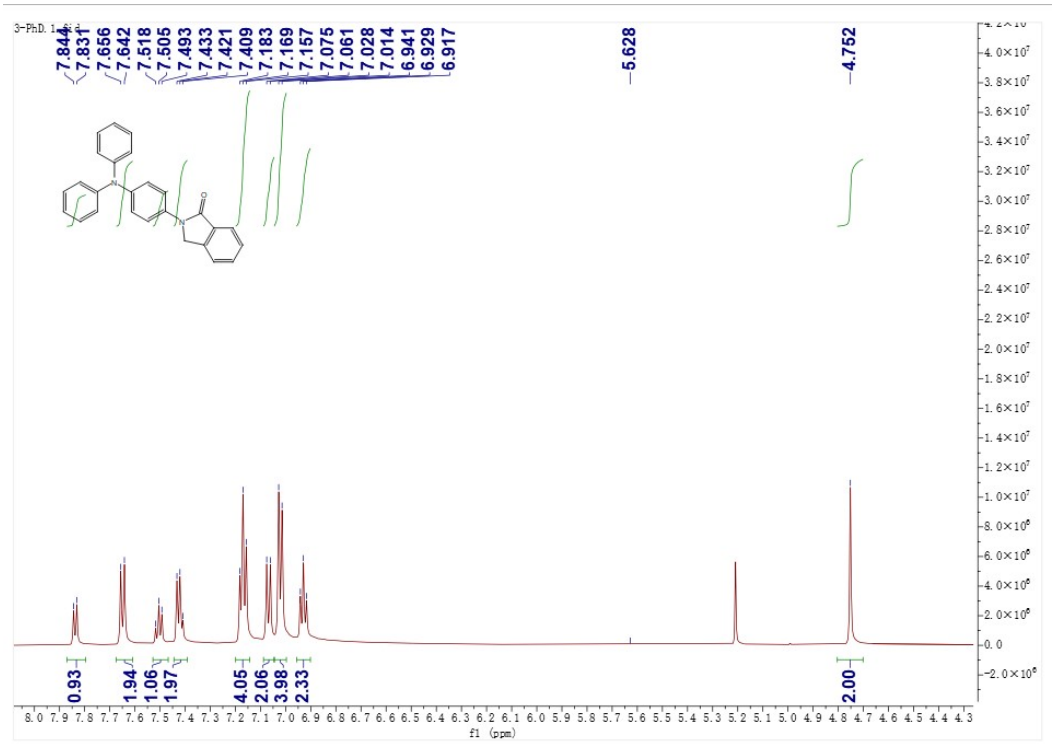

Figure S44. The expanded view of the ^{1}H NMR spectrum for Compound **10**.

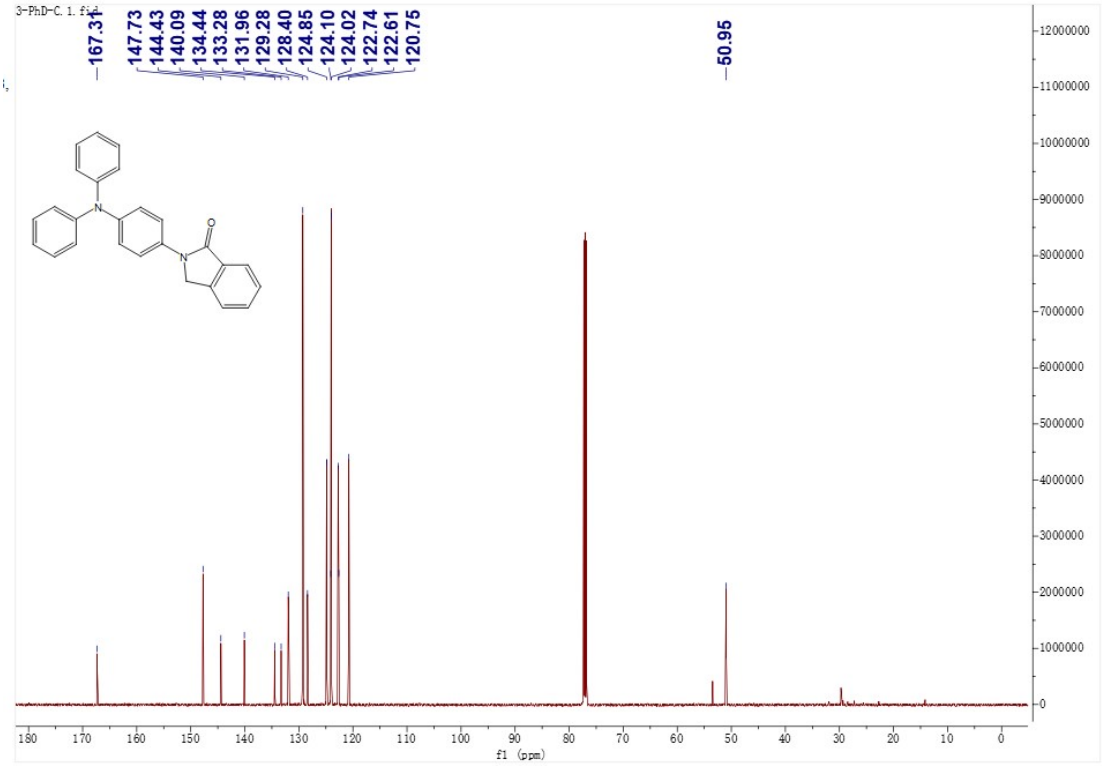

Figure S45. The ^{13}C NMR spectrum of Compound **10**.

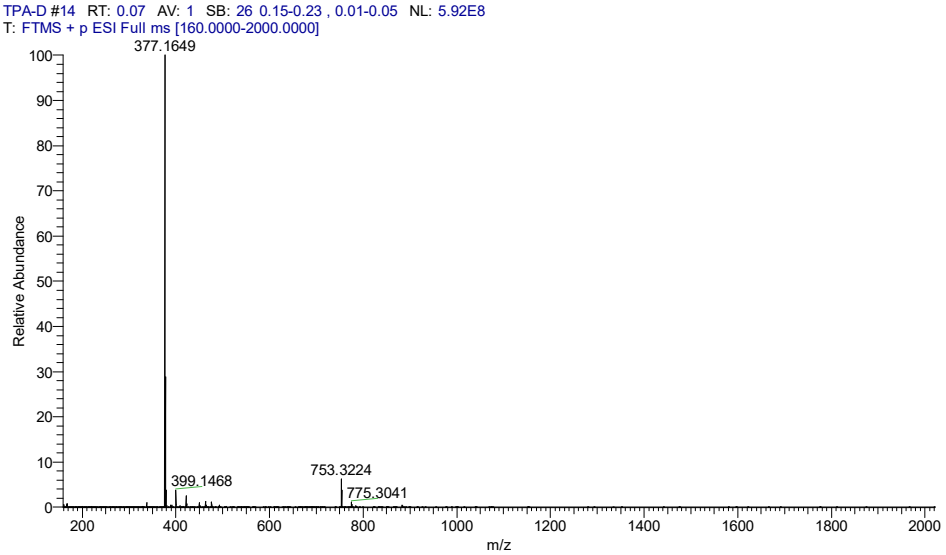

Figure S46. The MS spectrum of Compound **10.**

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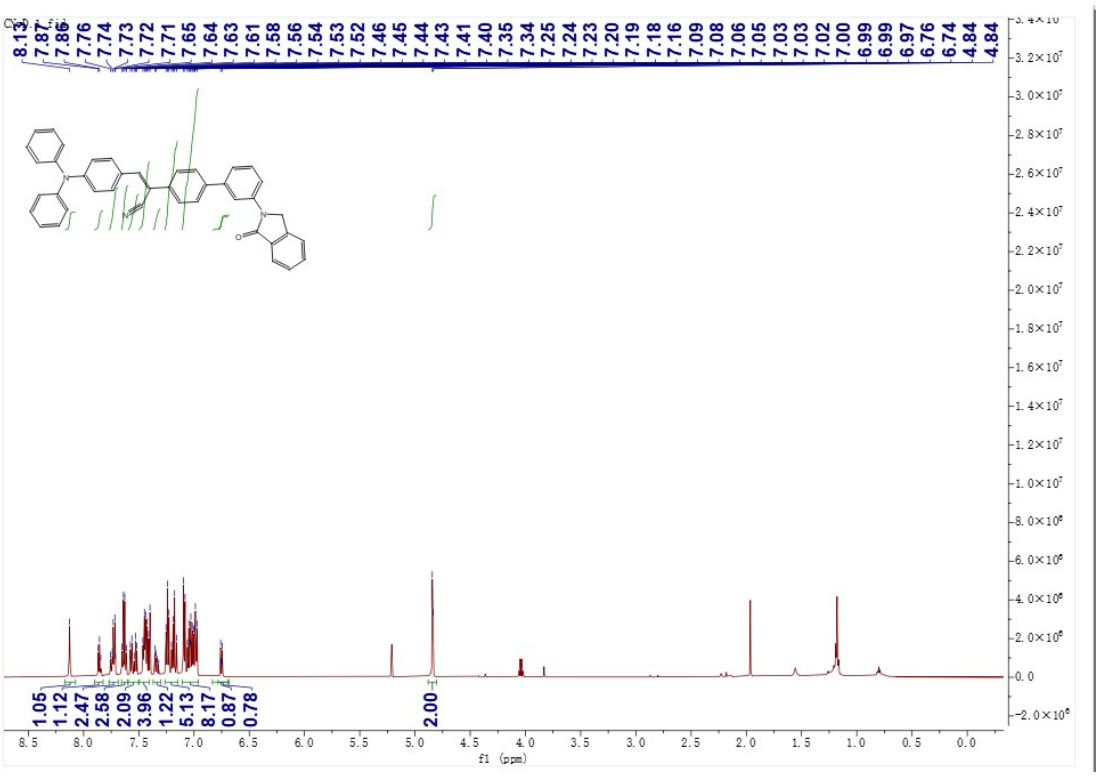


Figure S47. The ^{1}H NMR spectrum of Compound **11**.

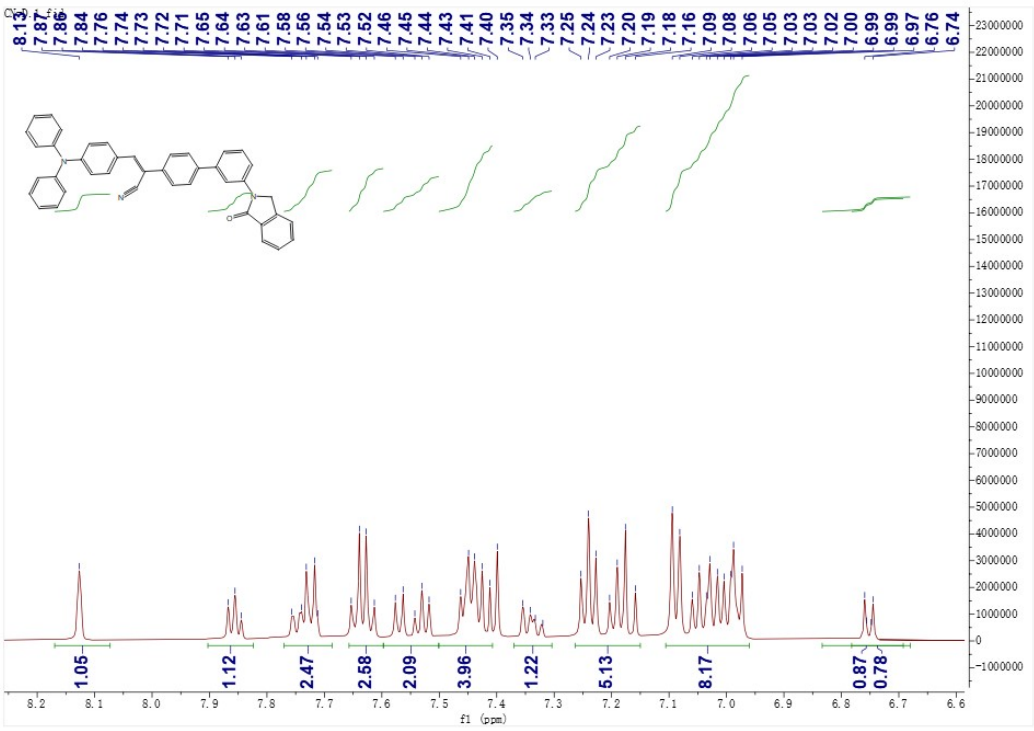


Figure S48. The expanded view of the ^{1}H NMR spectrum for Compound **11**.

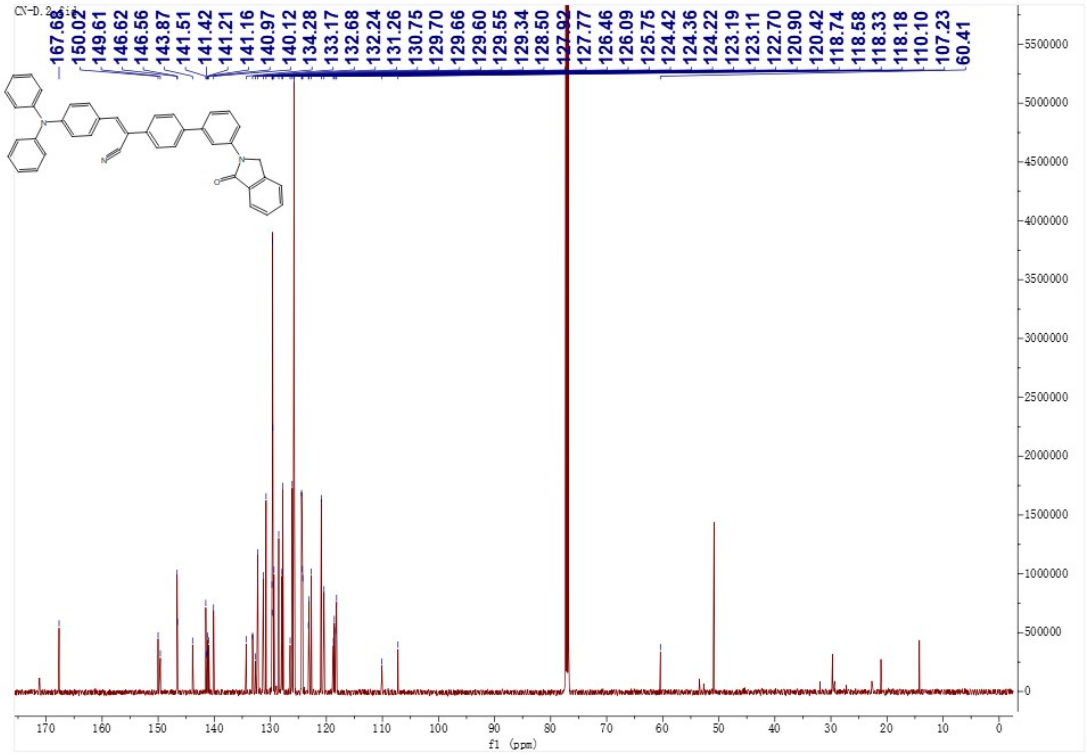


Figure S49. The ^{13}C NMR spectrum of Compound **11**.

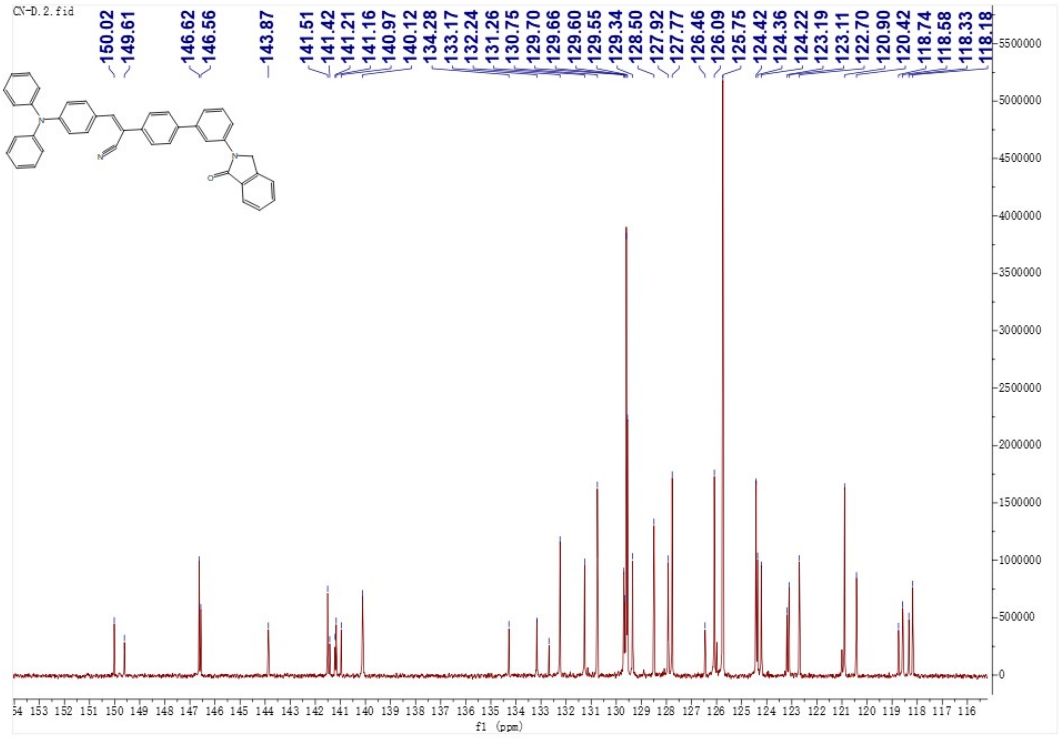


Figure S50. The expanded view of the ^{13}C NMR spectrum for Compound **11**.

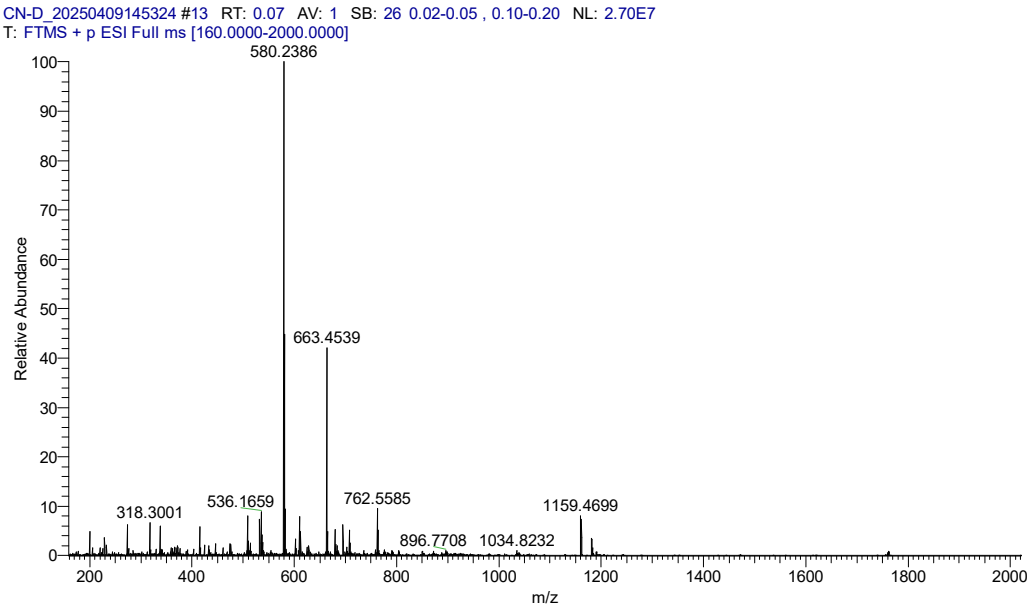


Figure S51. The MS spectrum of Compound **11.**

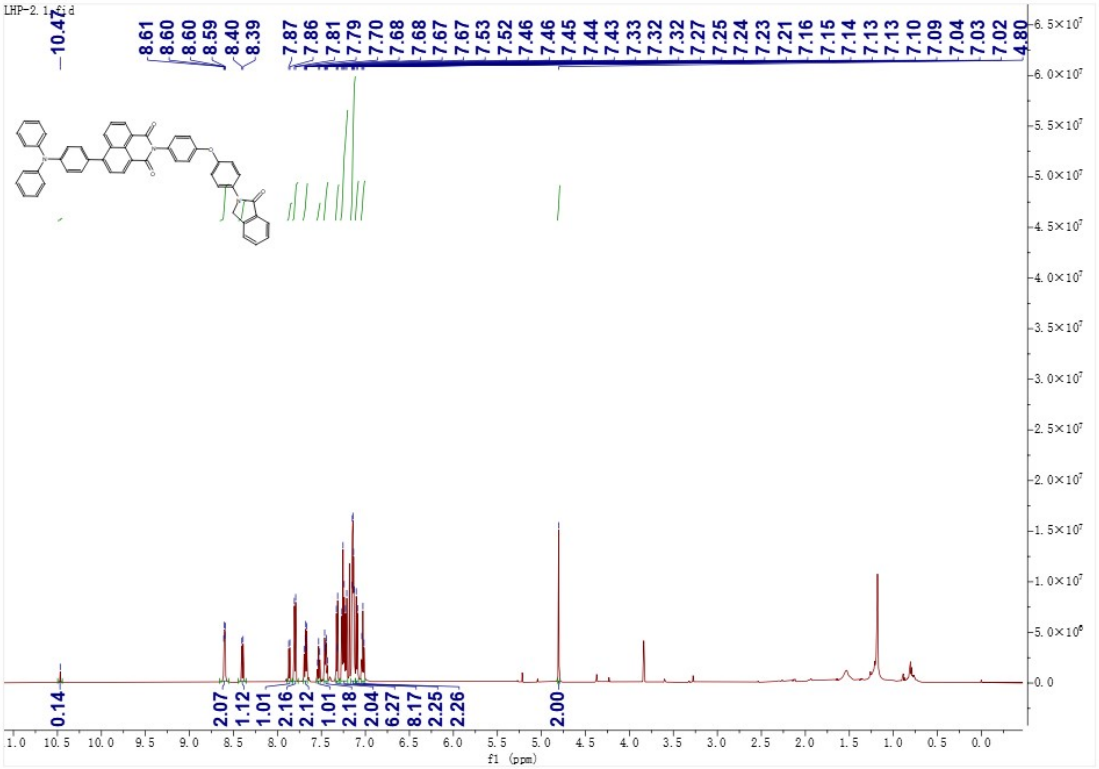


Figure S52. The 1H NMR spectrum of Compound **12**.

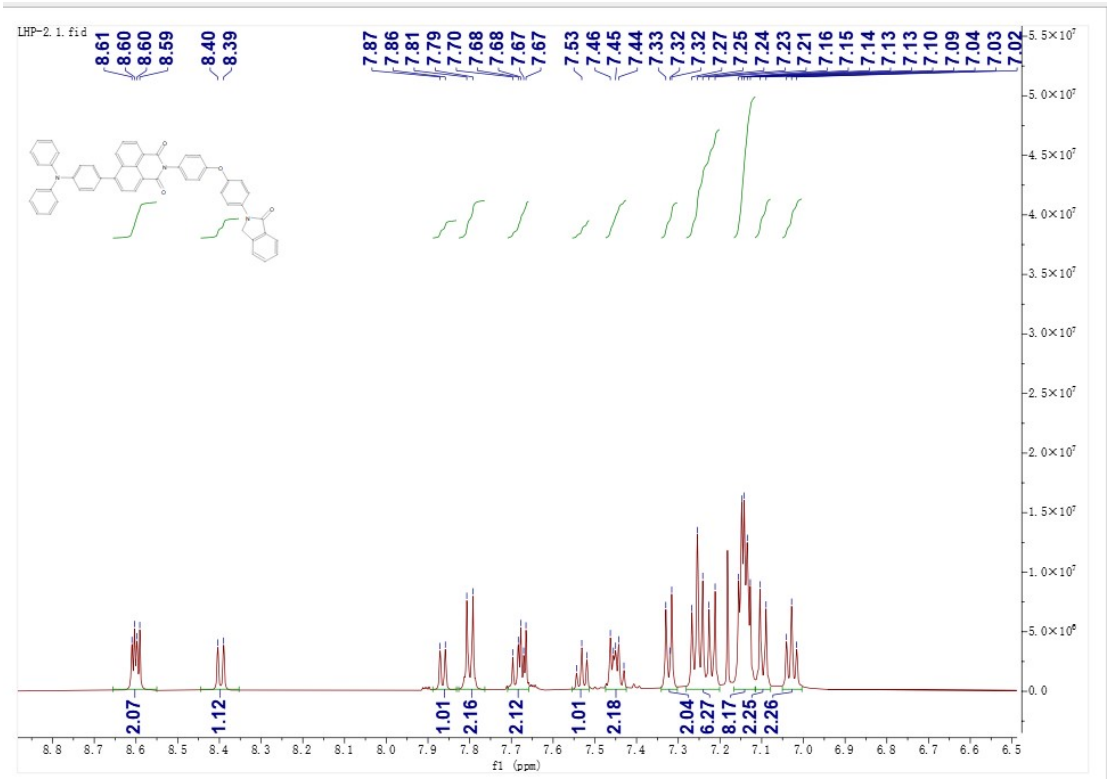


Figure S53. The expanded view of the ^{1}H NMR spectrum for Compound **12**.

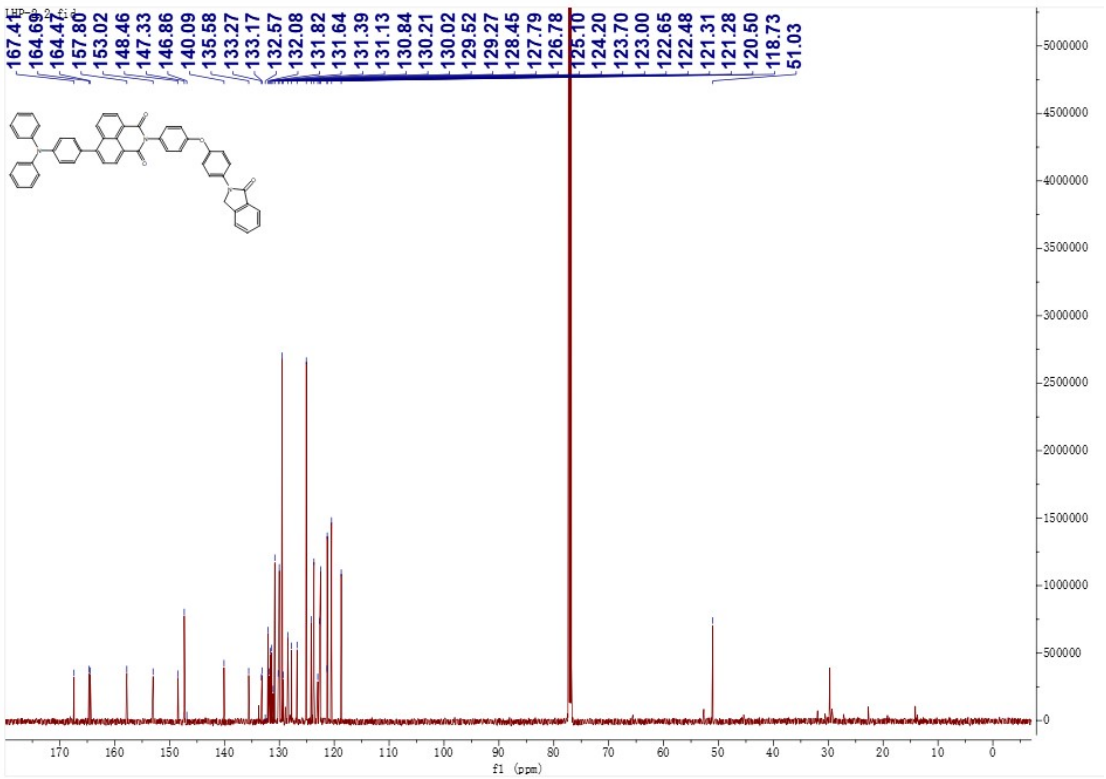


Figure S54. The ^{13}C NMR spectrum of Compound **12**.

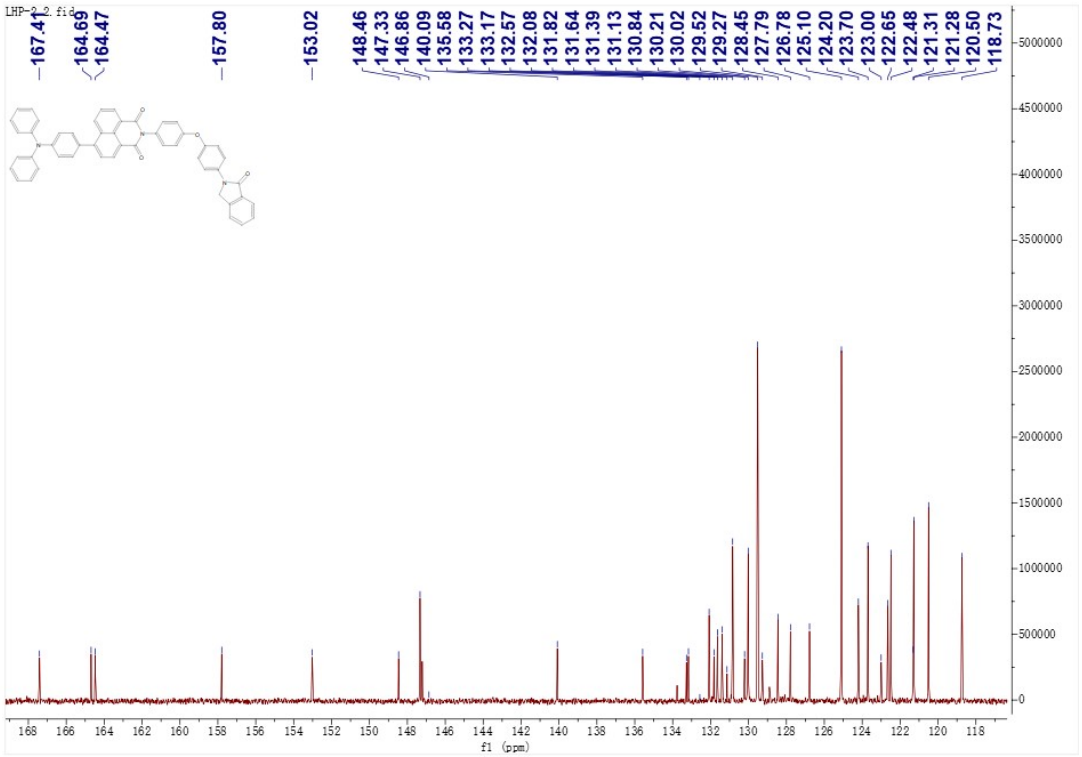


Figure S55. The expanded view of the ^{13}C NMR spectrum for Compound **12**.

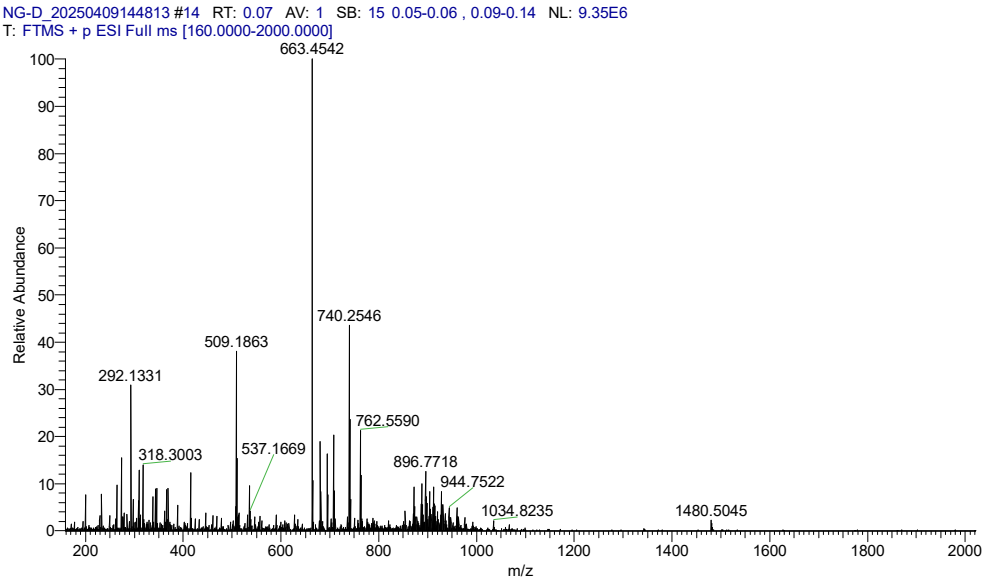


Figure S56. The MS spectrum of Compound **12.**

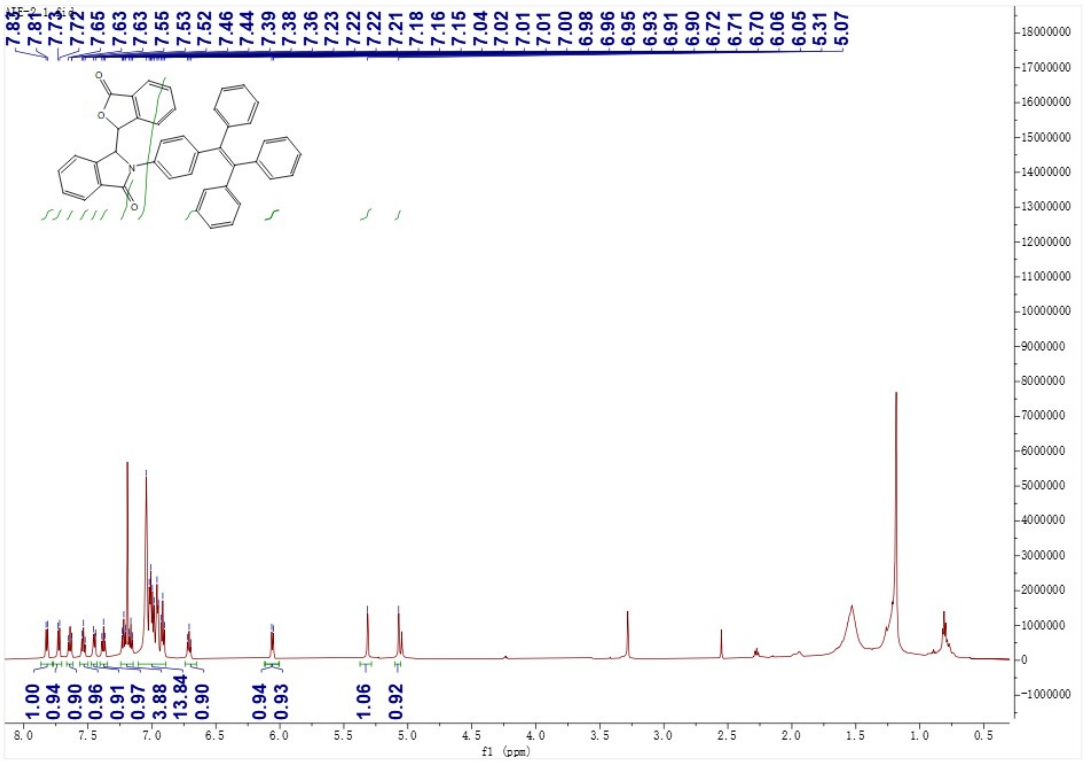


Figure S57. The 1H NMR spectrum of Compound **13**.

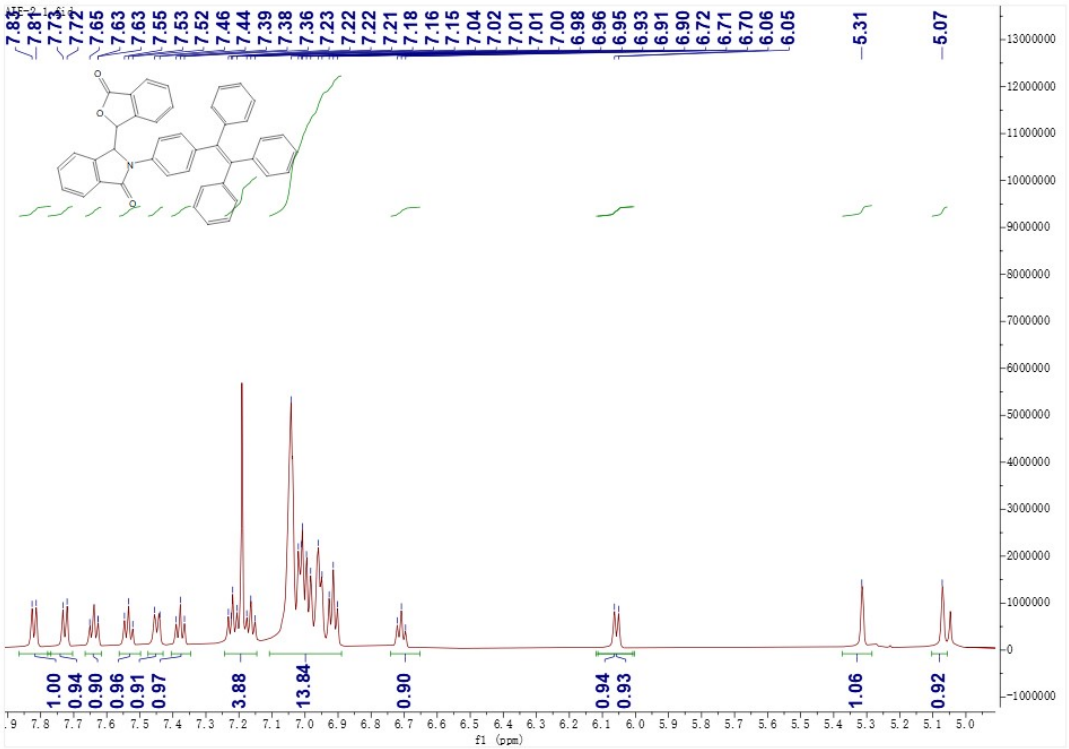


Figure S58. The expanded view of the ^{1}H NMR spectrum for Compound **13**.

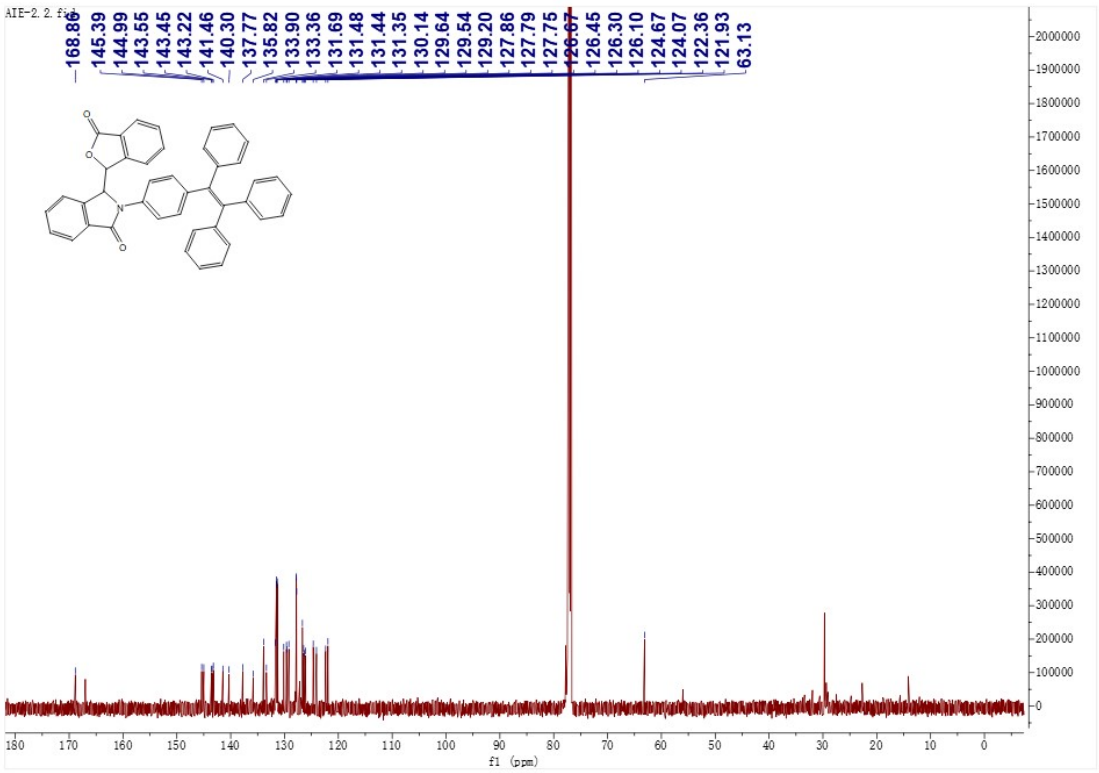


Figure S59. The ^{13}C NMR spectrum of Compound **13**.

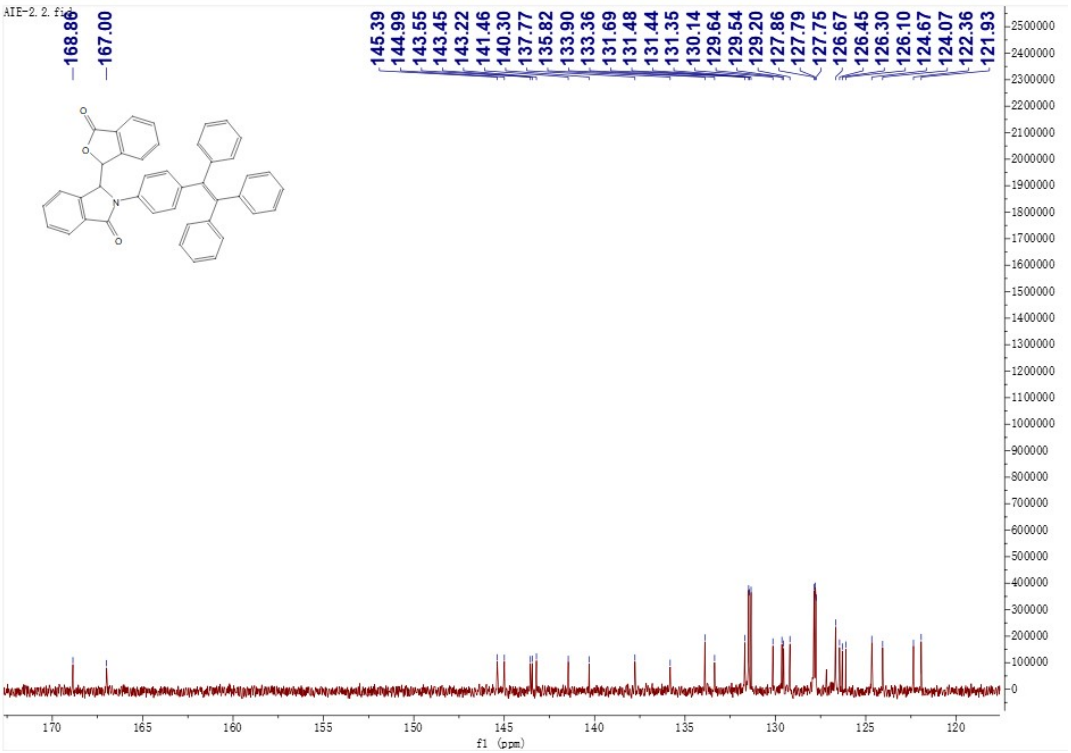


Figure S60. The expanded view of the ^{13}C NMR spectrum for Compound **13**.

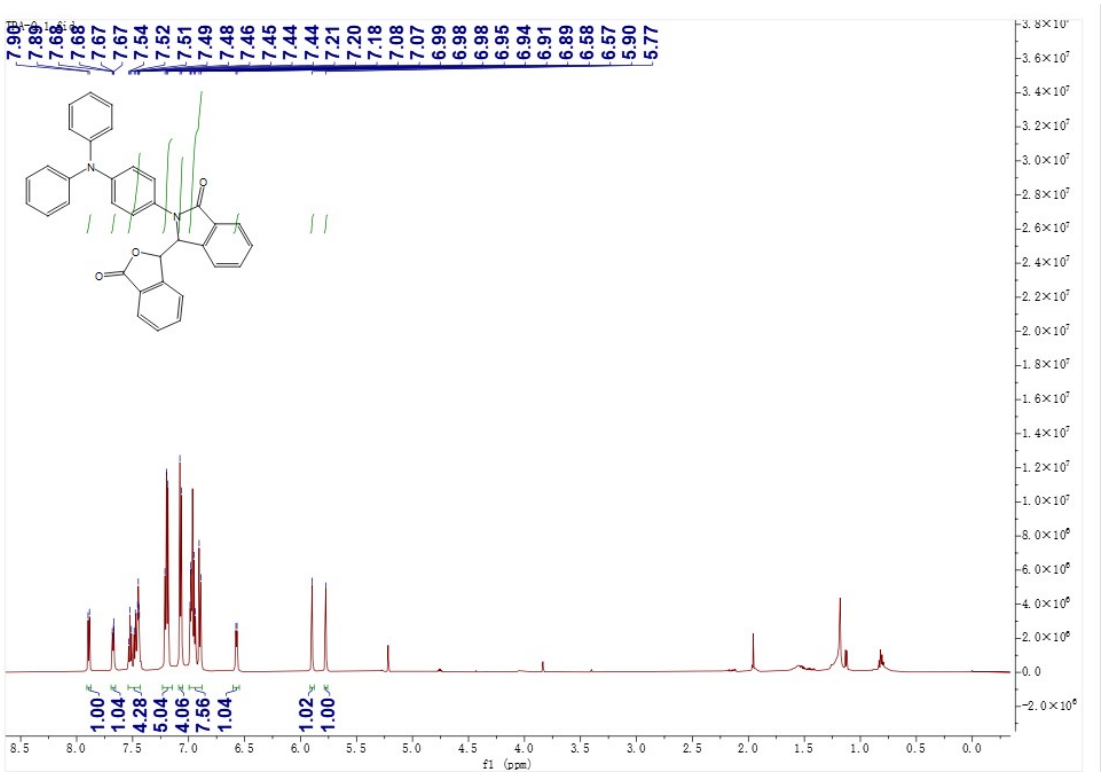


Figure S61. The 1H NMR spectrum of Compound **14**.

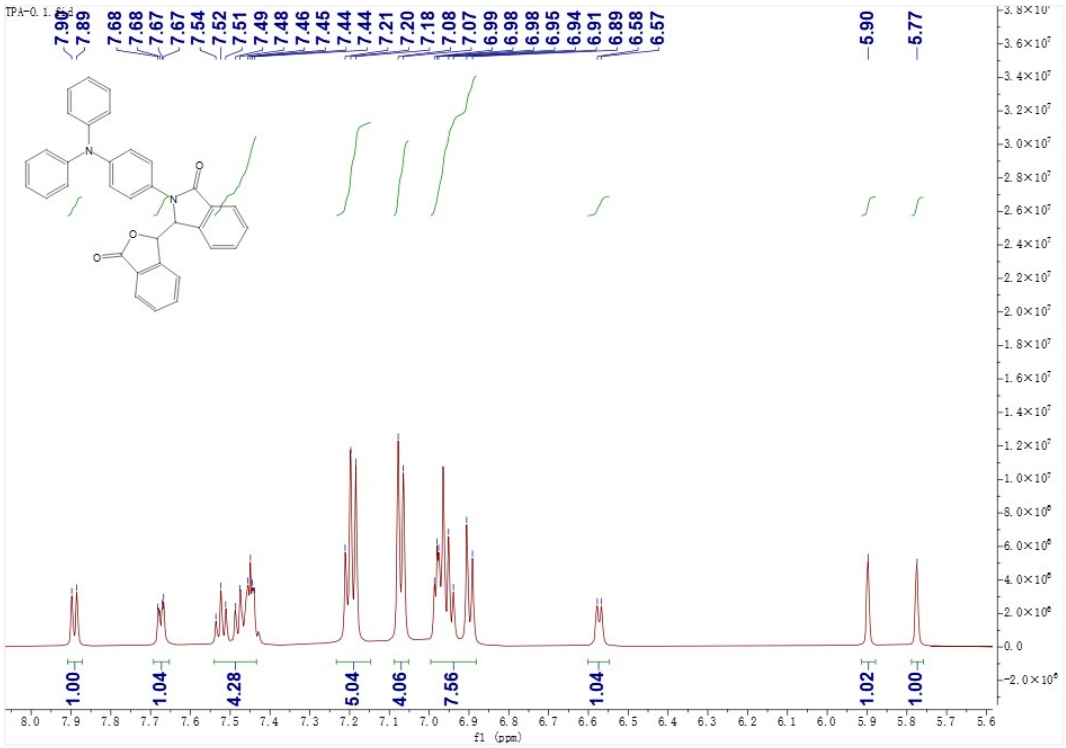


Figure S62. The expanded view of the ^{1}H NMR spectrum for Compound **14**.

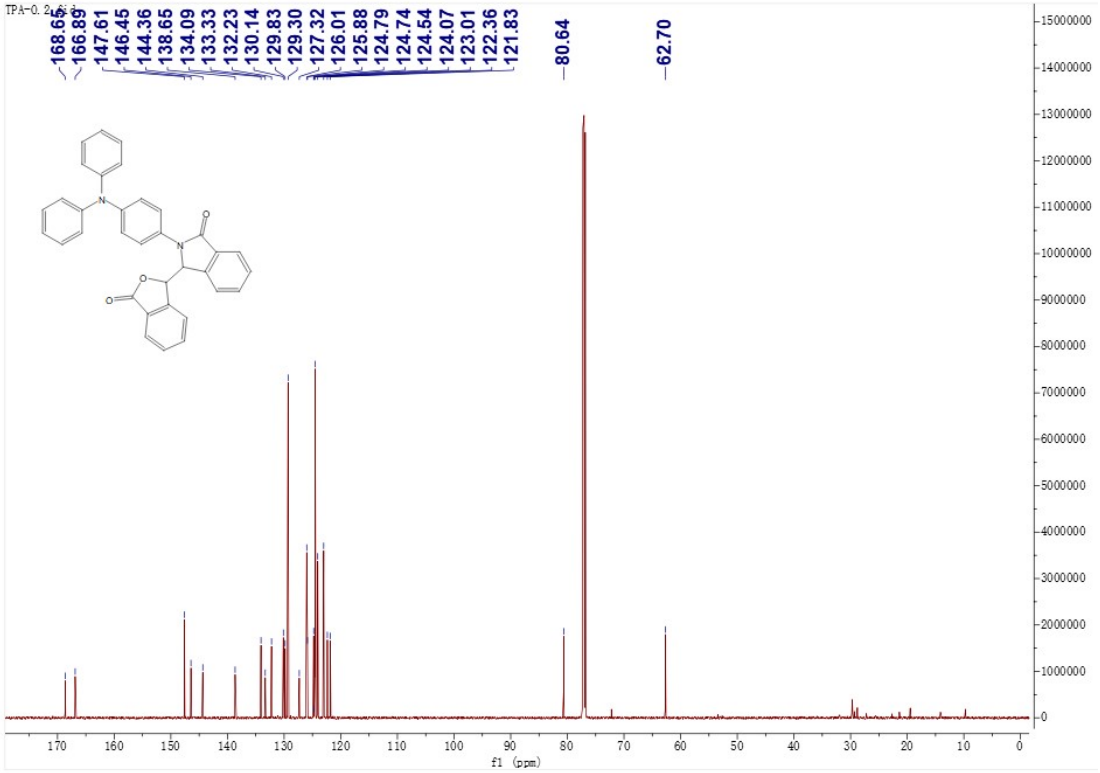


Figure S63. The ^{13}C NMR spectrum of Compound **14**.

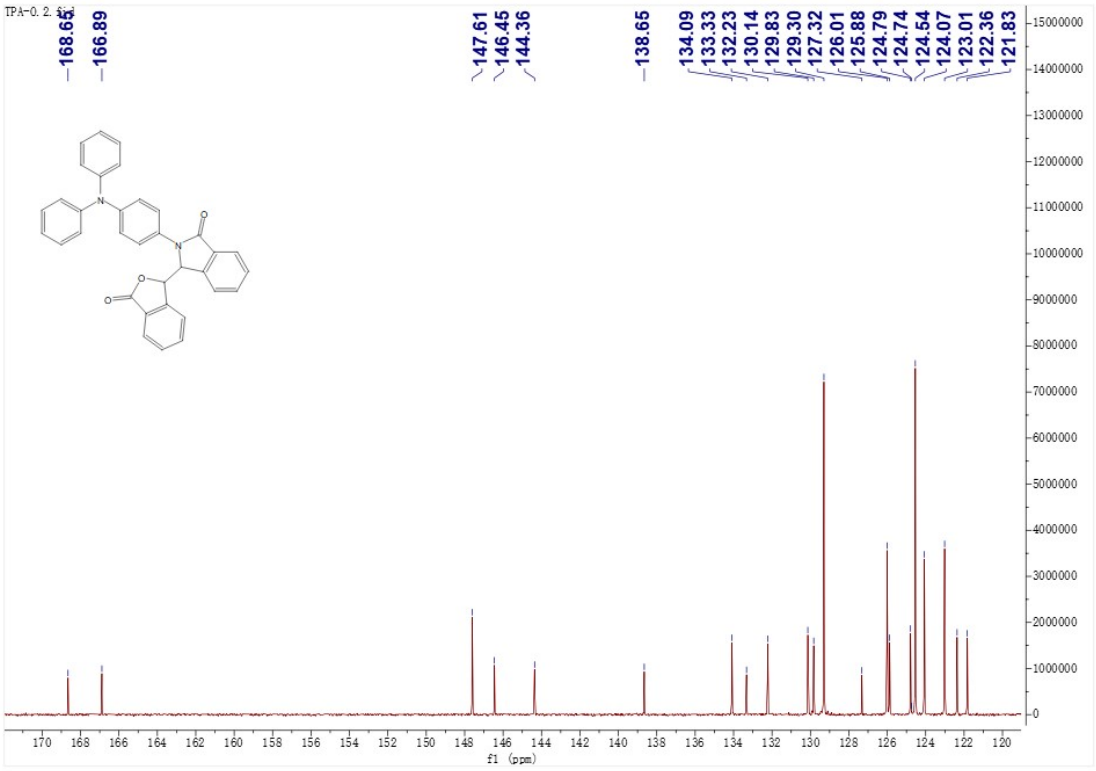


Figure S64. The expanded view of the ^{13}C NMR spectrum for Compound **14**.

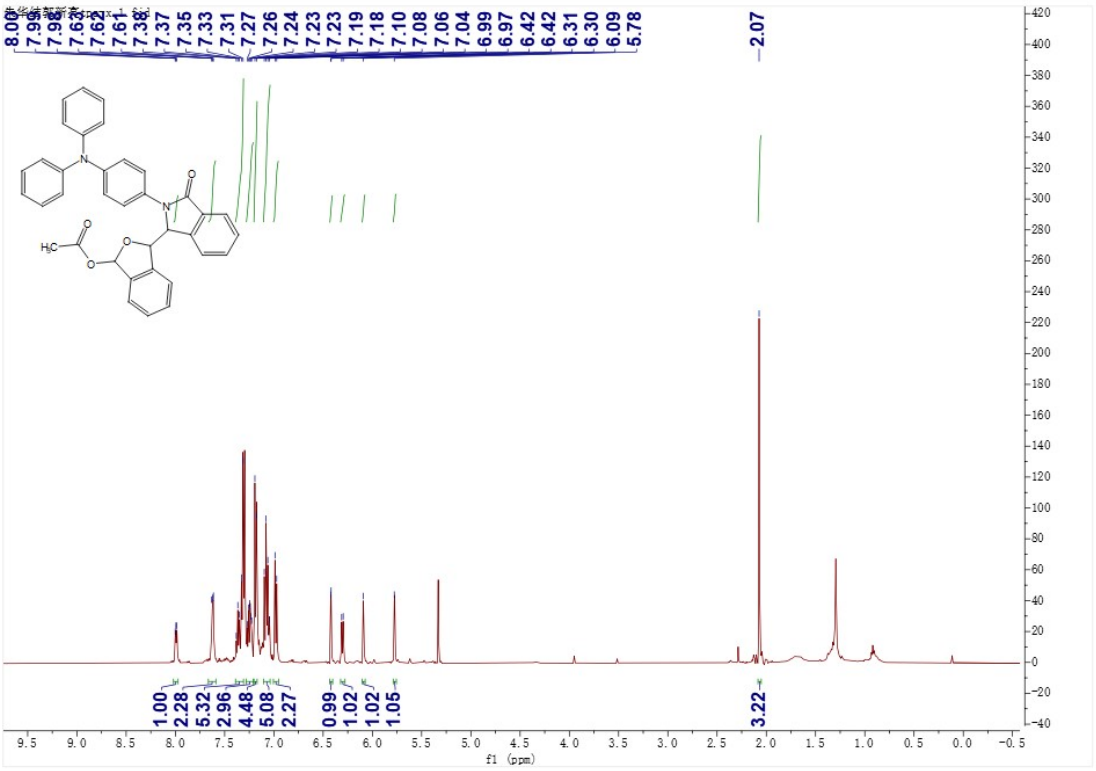


Figure S65. The 1H NMR spectrum of Compound **15**.

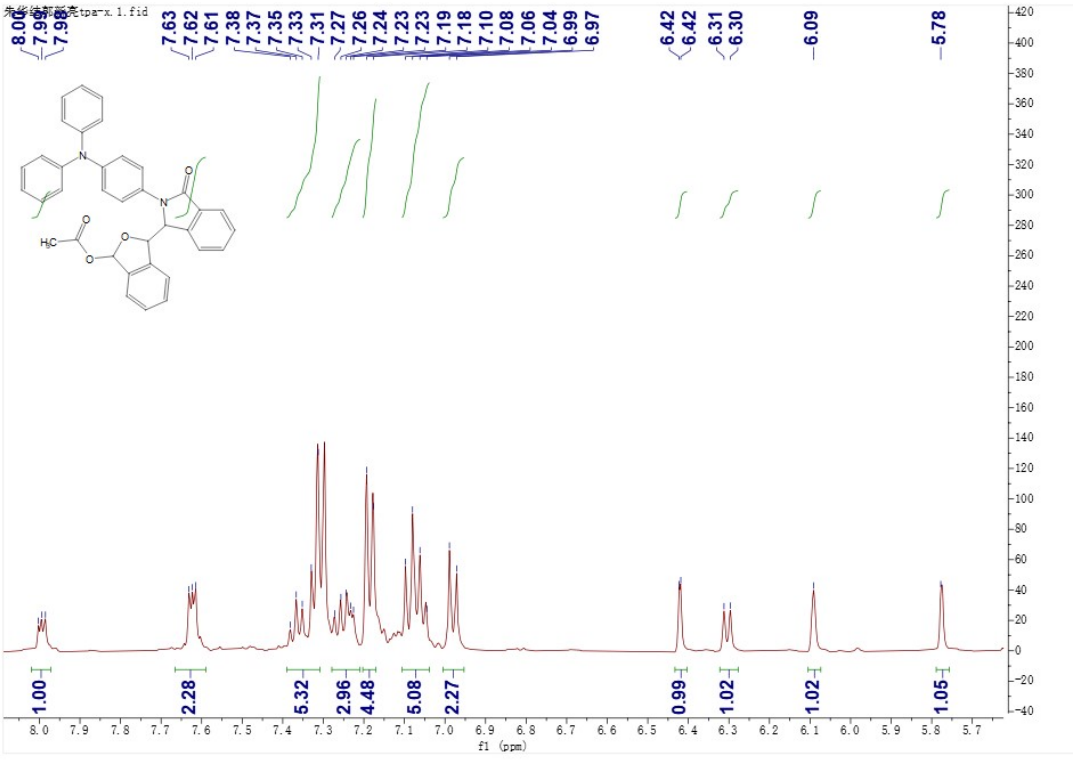


Figure S66. The expanded view of the ^{1}H NMR spectrum for Compound **15**.

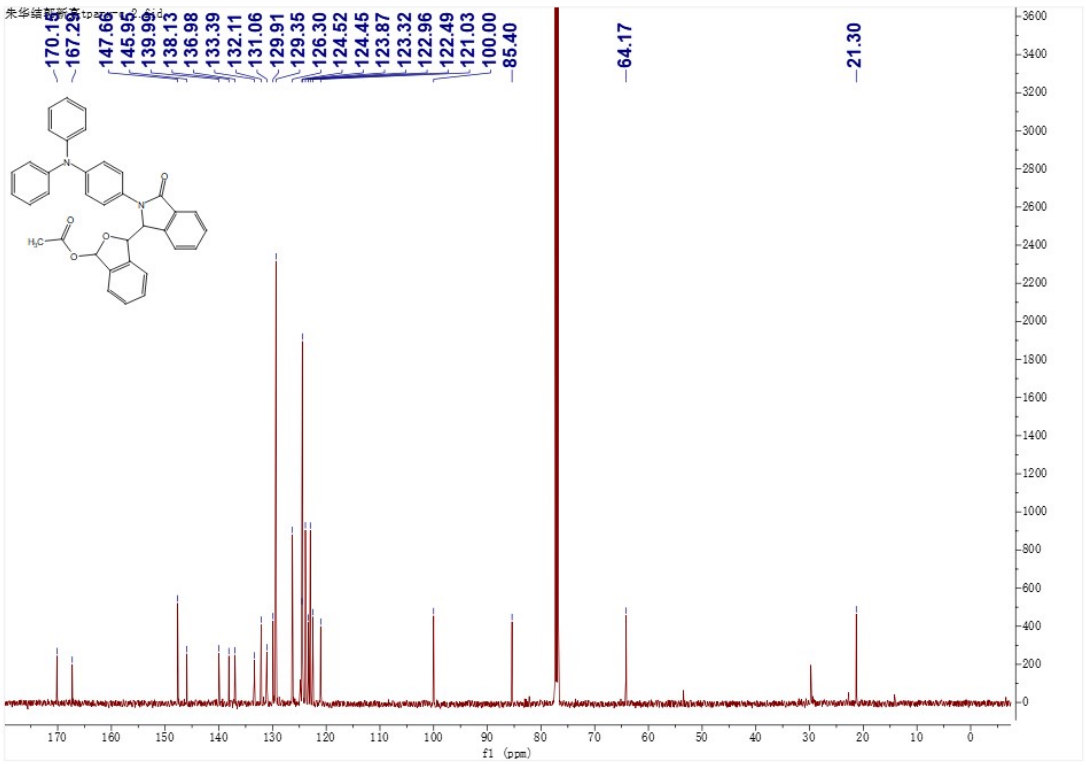


Figure S67. The ^{13}C NMR spectrum of Compound **15**.

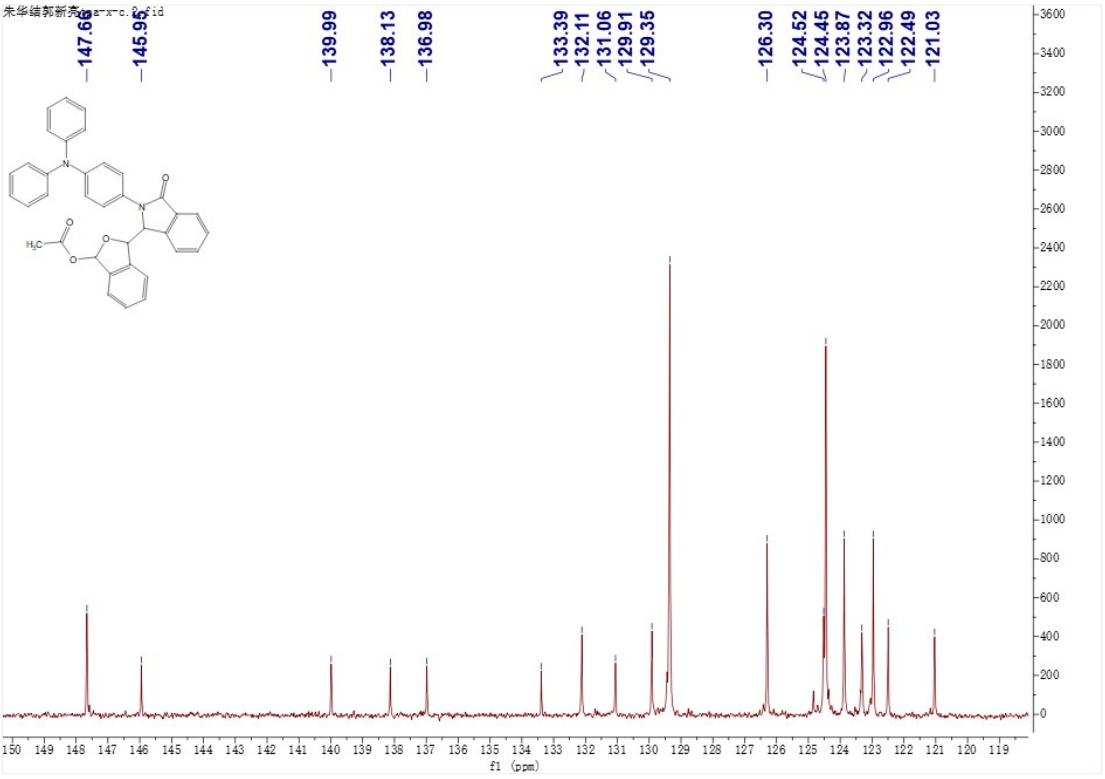


Figure S68. The expanded view of the ^{13}C NMR spectrum for Compound **15**.

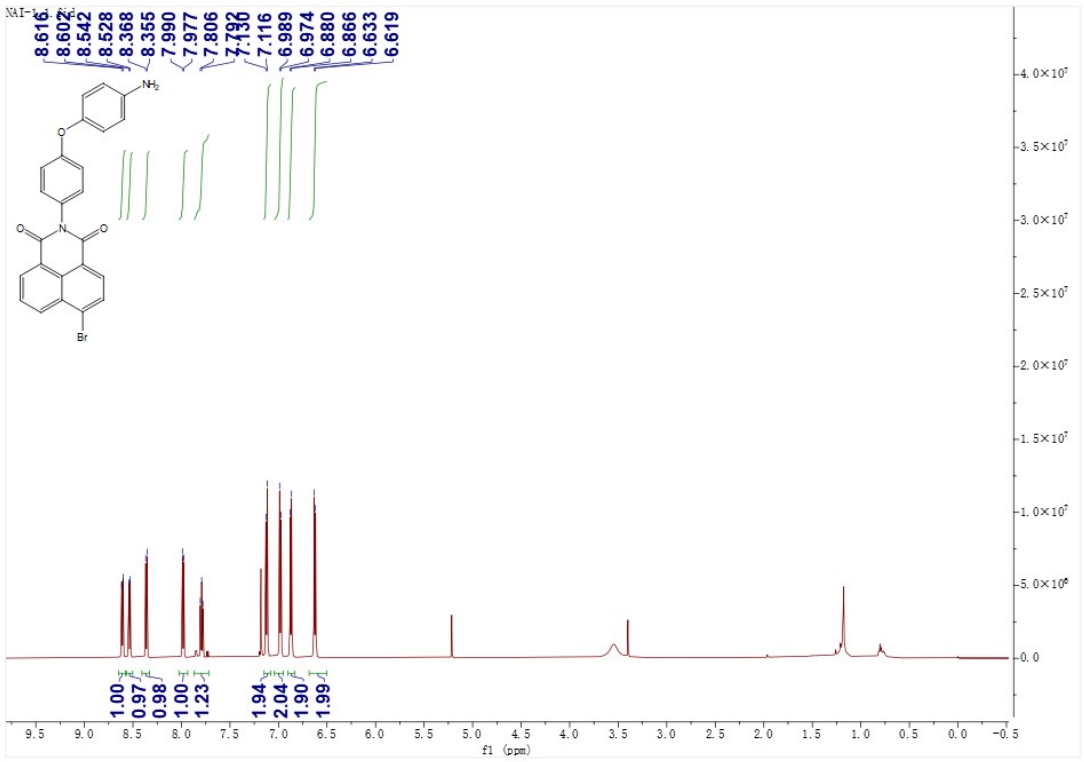


Figure S69. The 1H NMR spectrum of Compound **NG-1**.

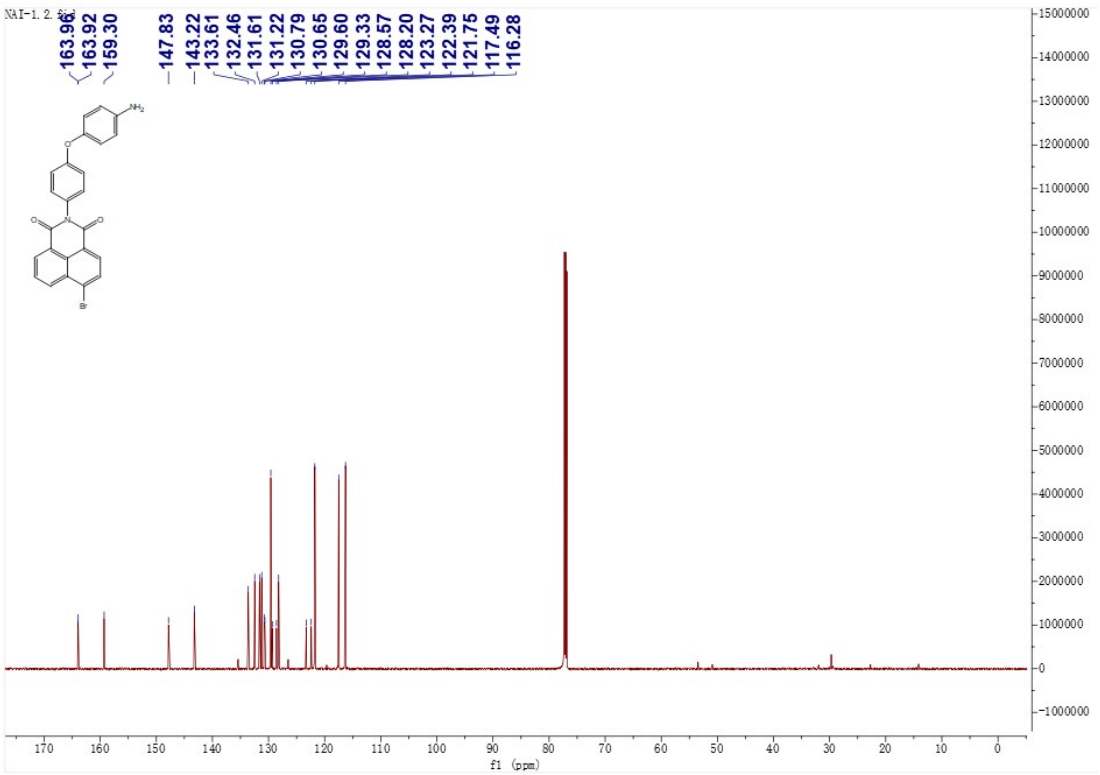


Figure S70. The ^{13}C NMR spectrum of Compound **NG-1**.

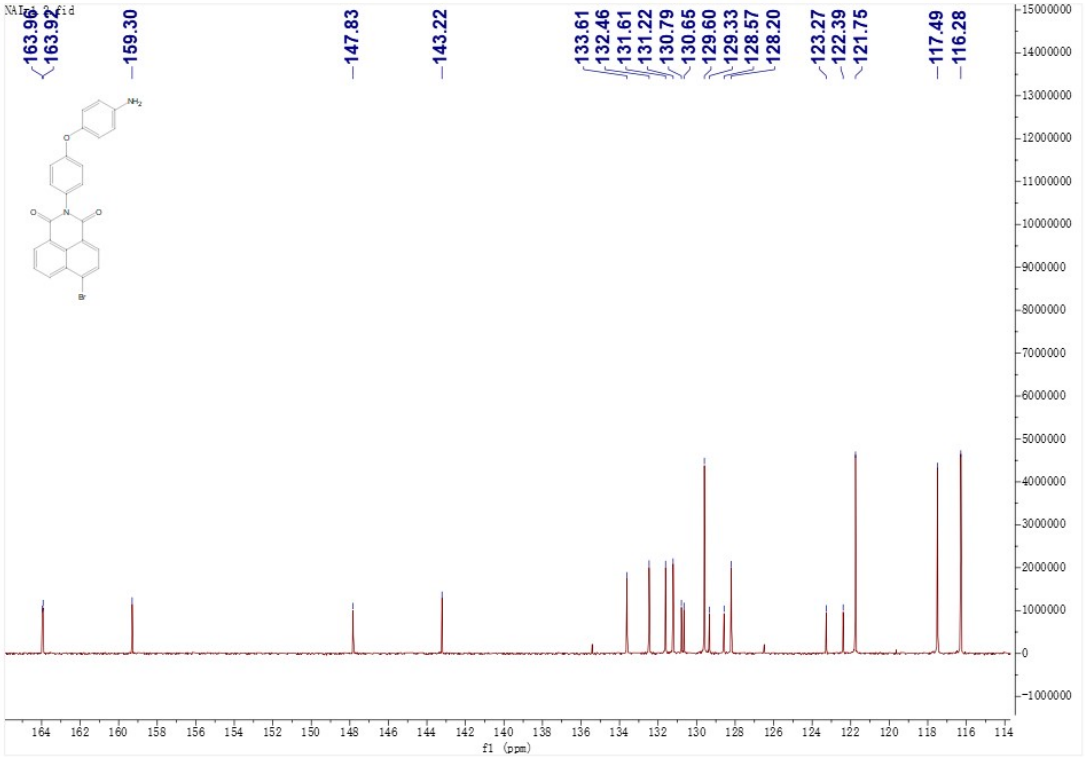


Figure S71. The expanded view of the ^{13}C NMR spectrum for Compound **NG-1**.

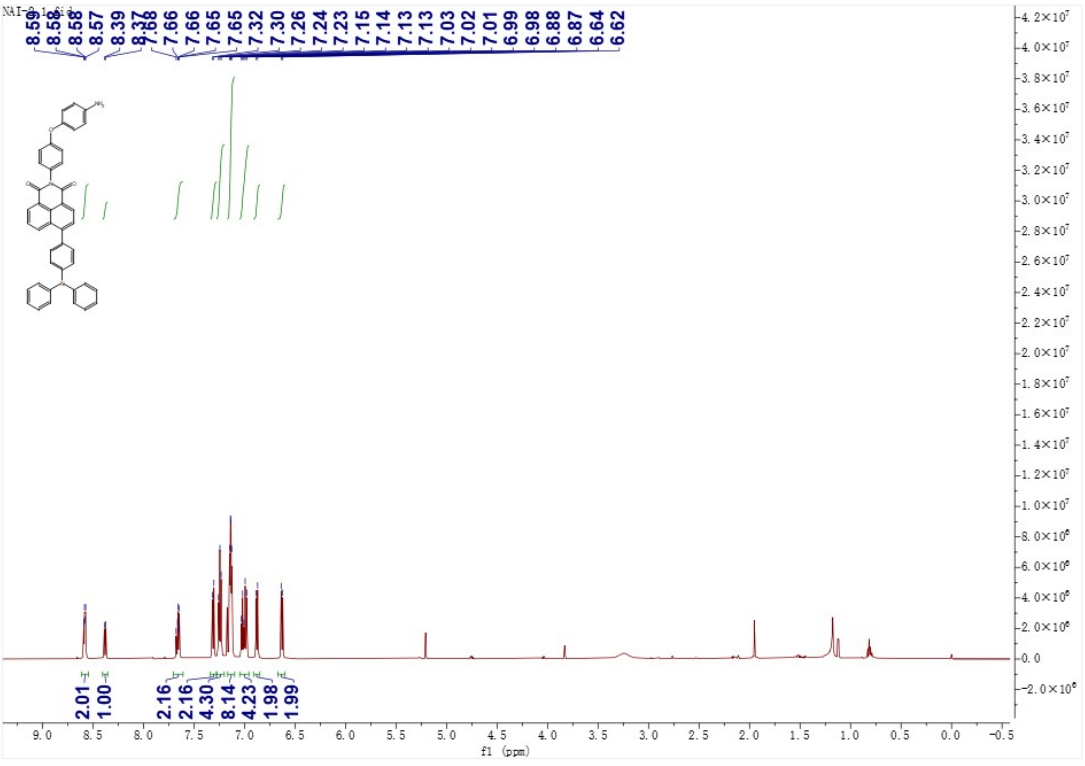


Figure S72. The 1H NMR spectrum of Compound **NG-2**.

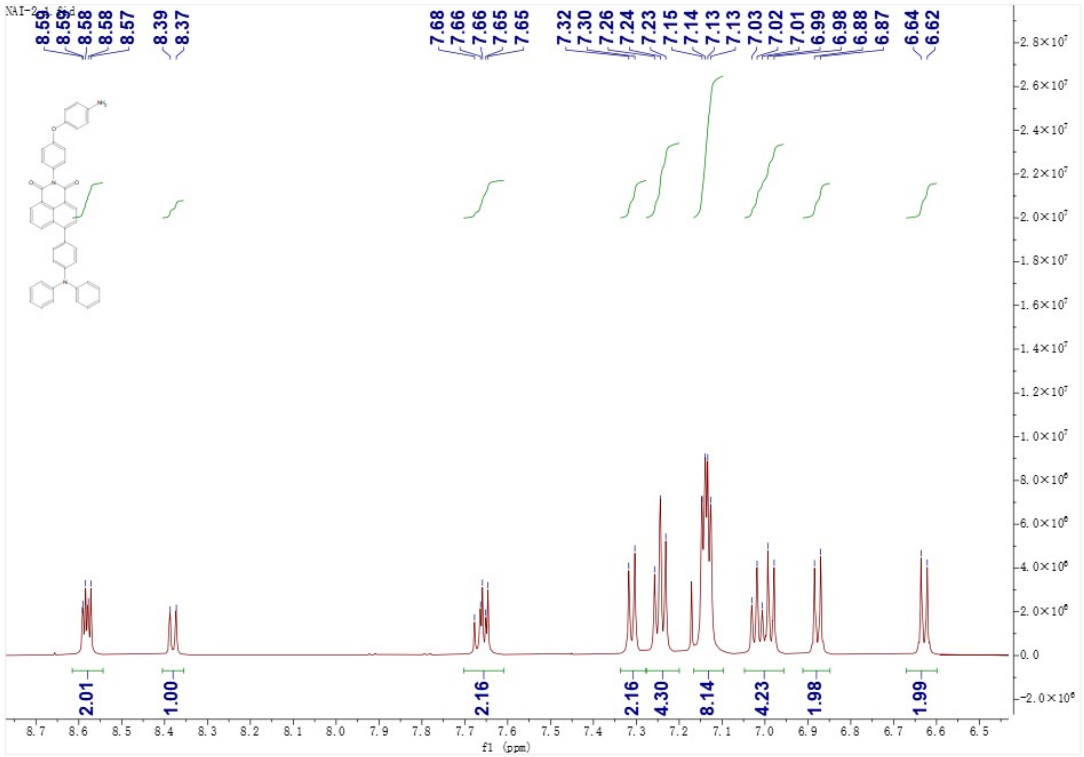


Figure S73. The expanded view of the ^{1}H NMR spectrum for Compound **NG-2**.

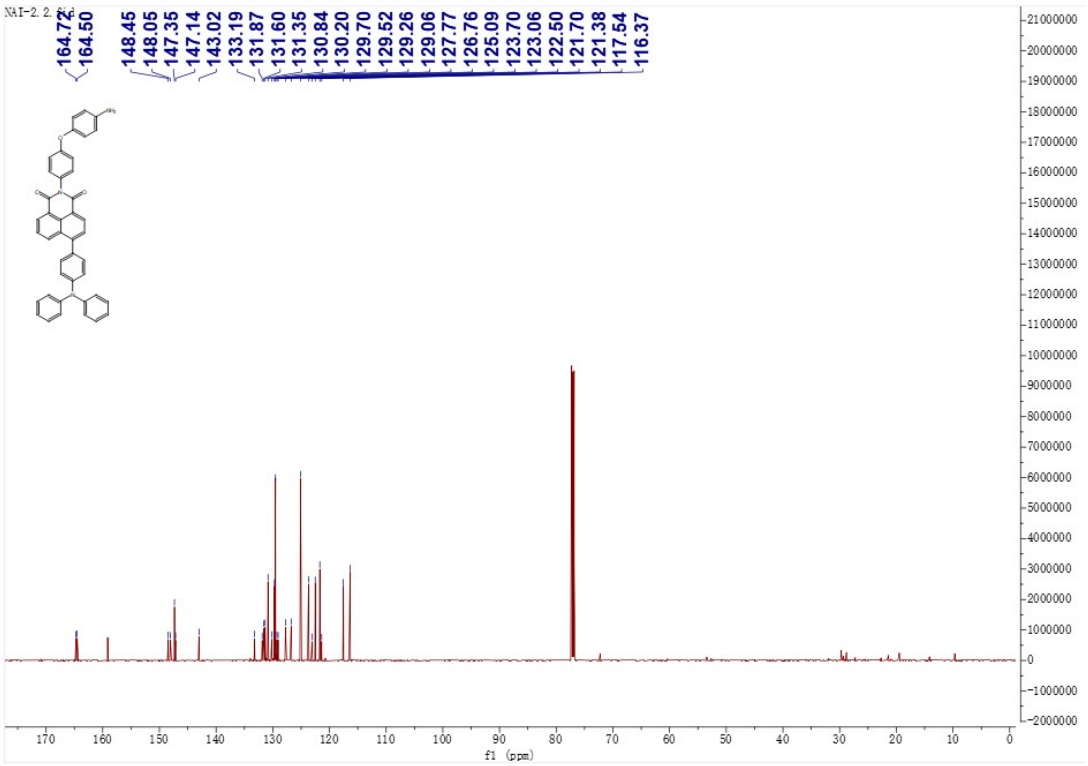


Figure S74. The ^{13}C NMR spectrum of Compound **NG-2**.

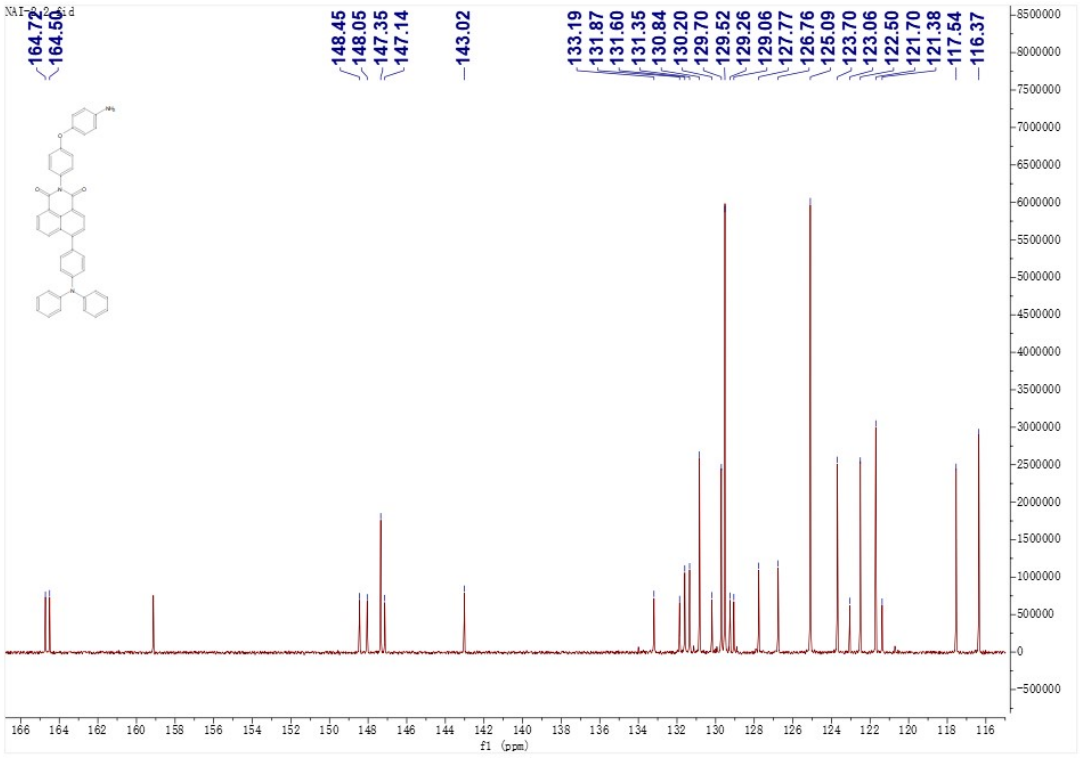


Figure S75. The expanded view of the ^{13}C NMR spectrum for Compound **NG-2**.

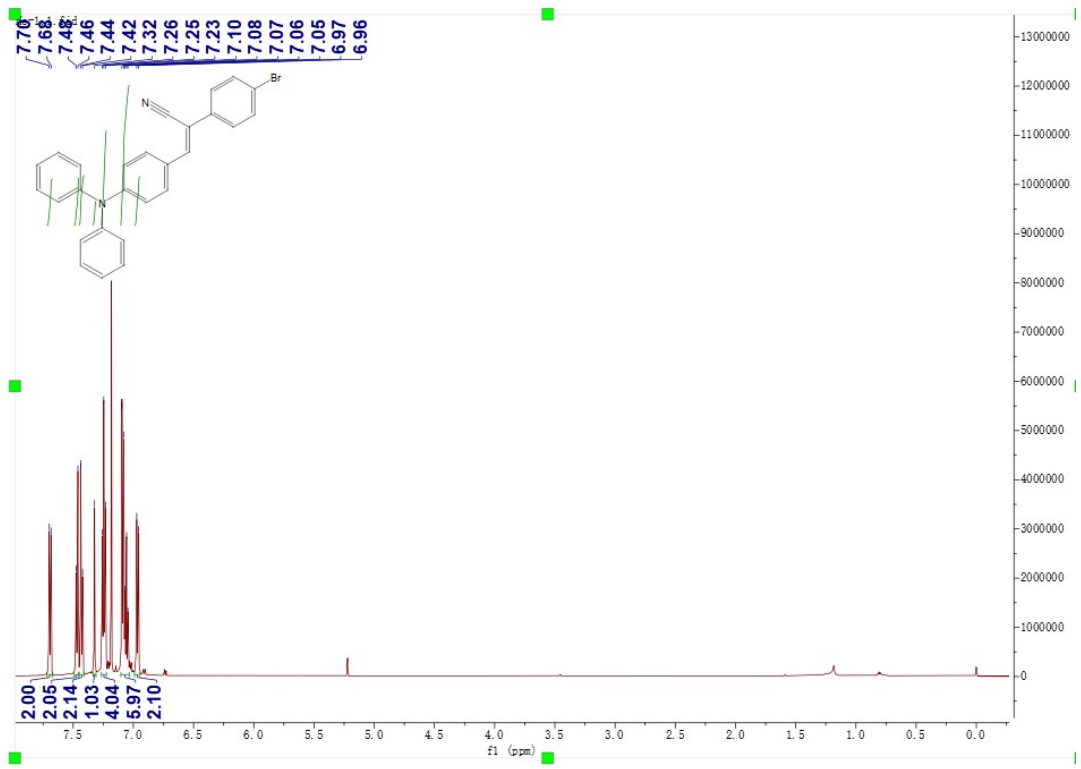


Figure S76. The 1H NMR spectrum of Compound **CN-1**.

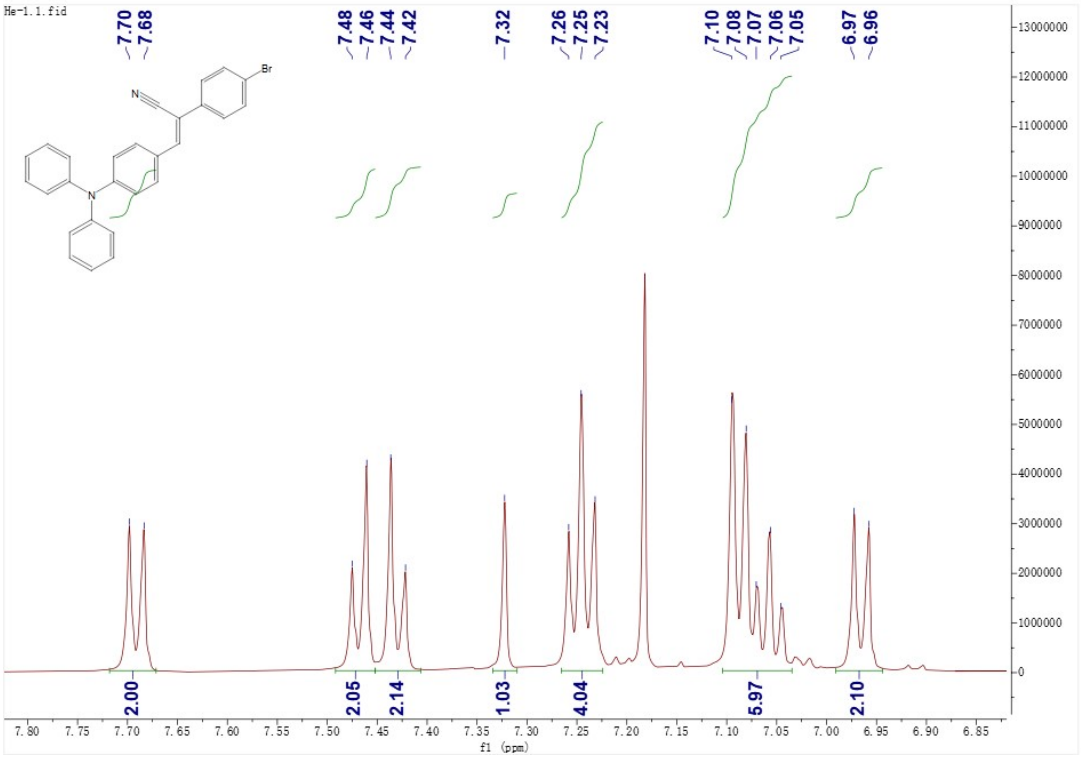


Figure S77. The expanded view of the ^{1}H NMR spectrum for Compound **CN-1**.

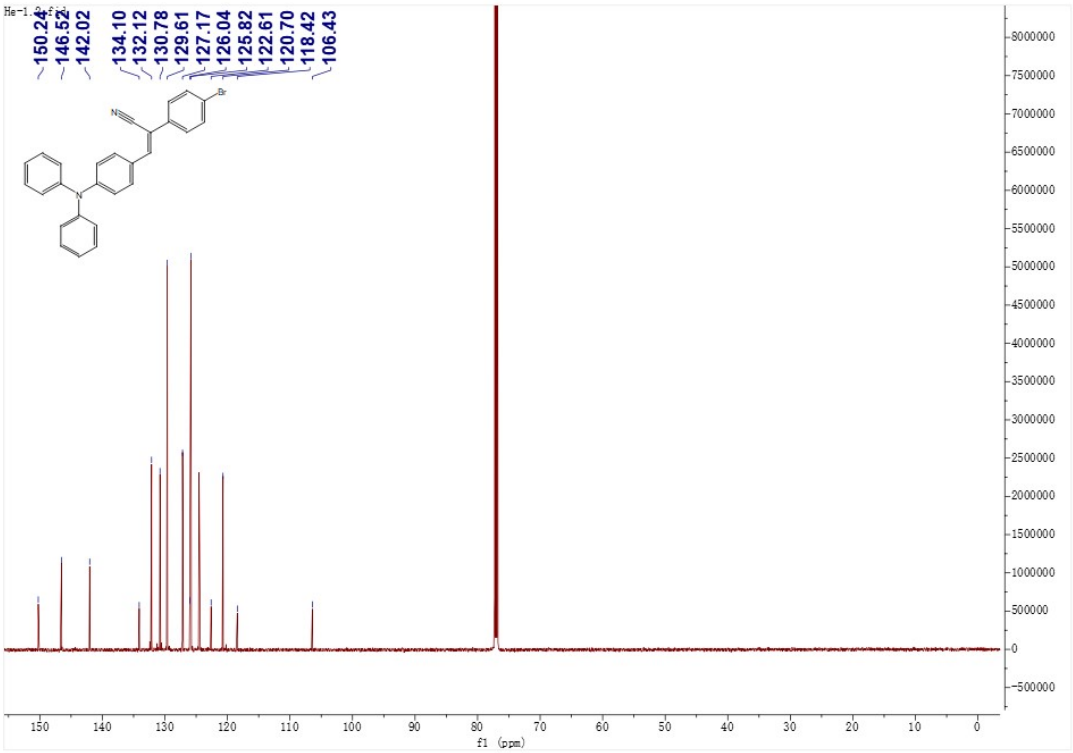


Figure S78. The ^{13}C NMR spectrum of Compound **CN-1**.

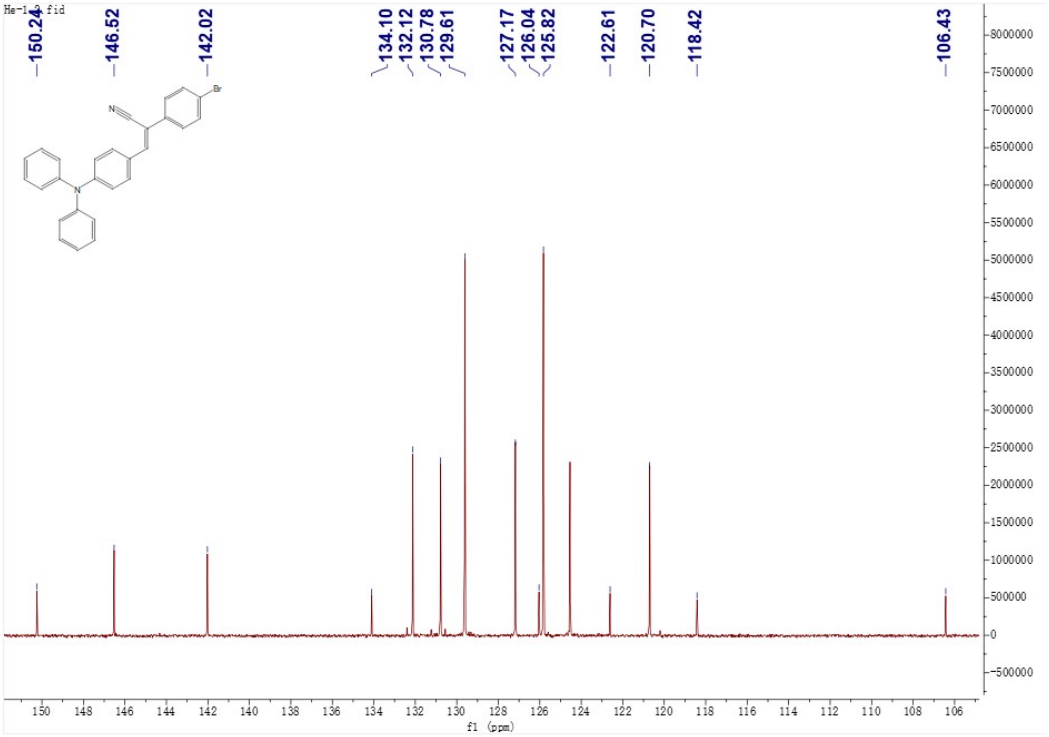


Figure S79. The expanded view of the ^{13}C NMR spectrum for Compound **CN-1**.

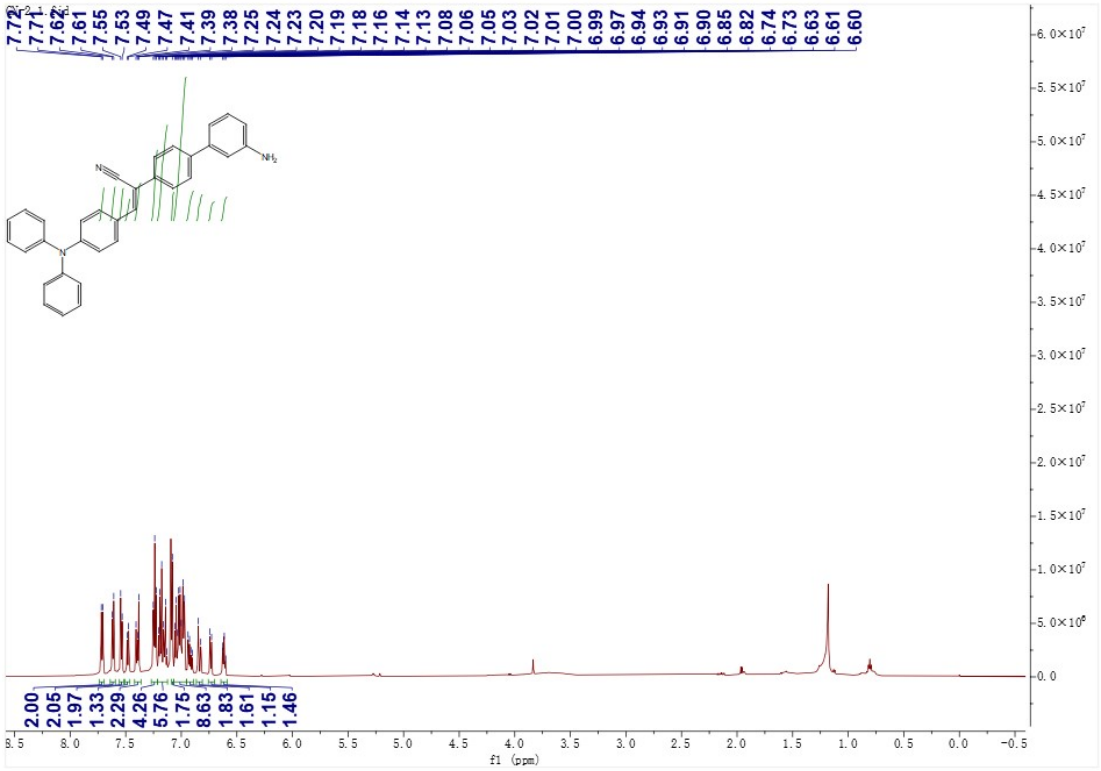


Figure S80. The 1H NMR spectrum of Compound **CN-2**.

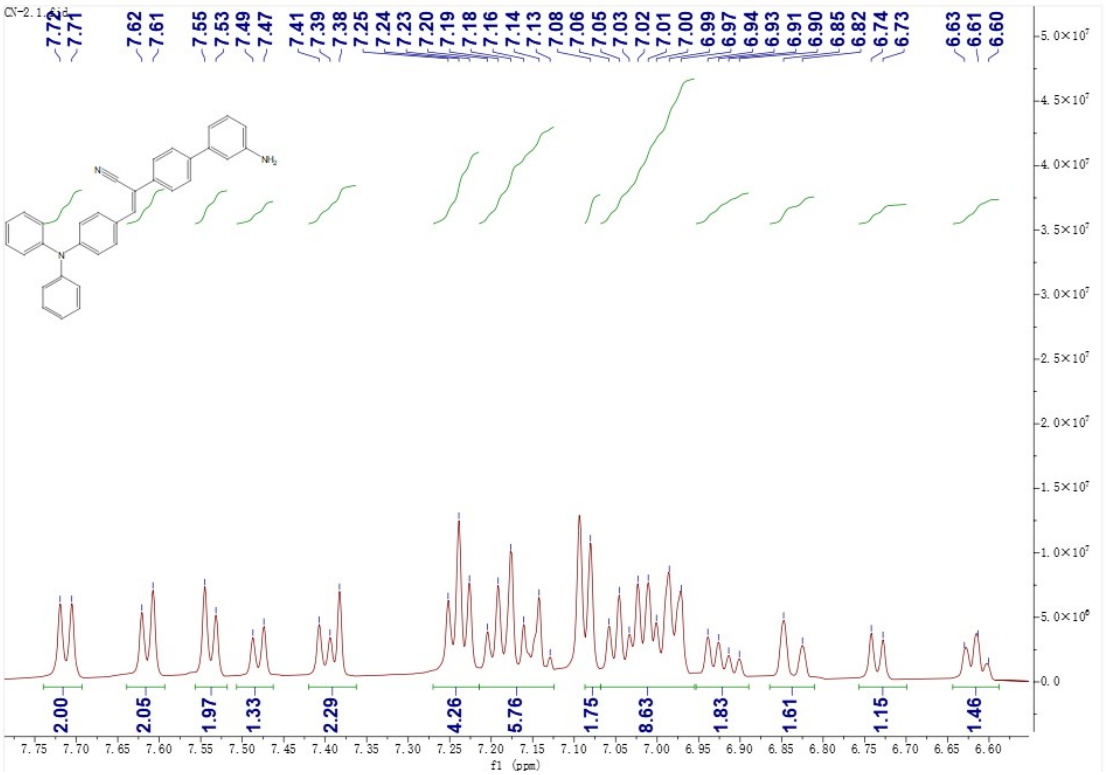


Figure S81. The expanded view of the ^{1}H NMR spectrum for Compound **CN-2**.

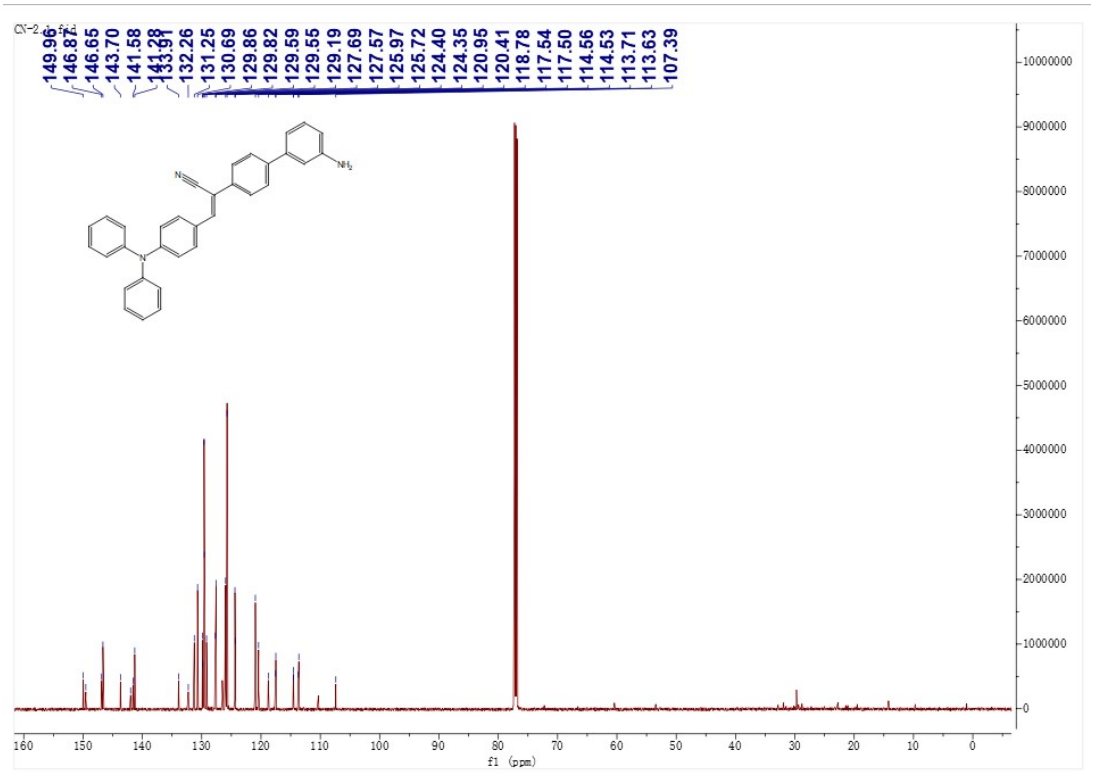


Figure S82. The ^{13}C NMR spectrum of Compound **CN-2**.

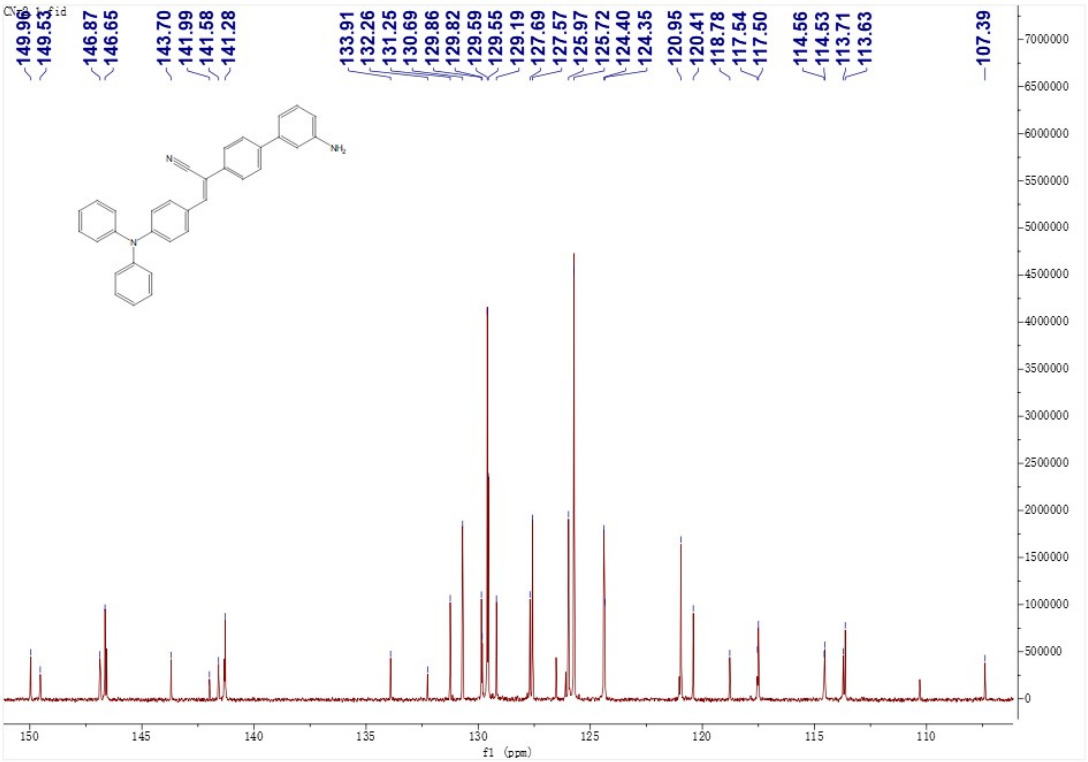


Figure S83. The expanded view of the ^{13}C NMR spectrum for Compound **CN-2**.

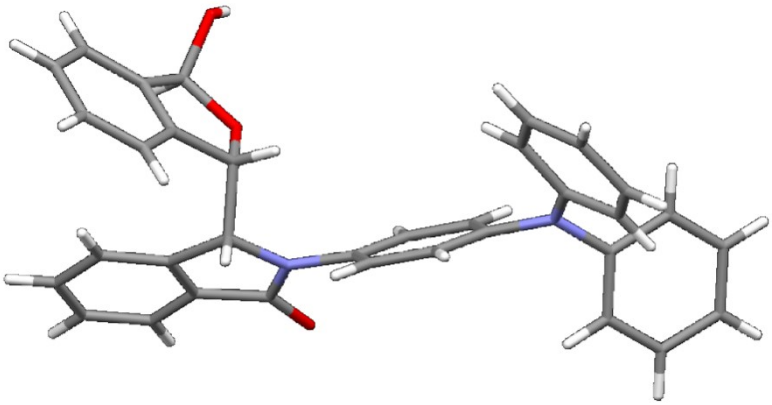
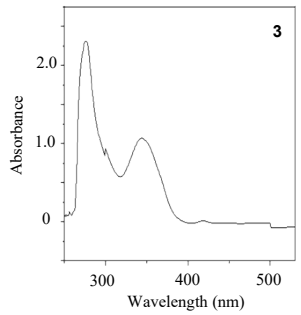
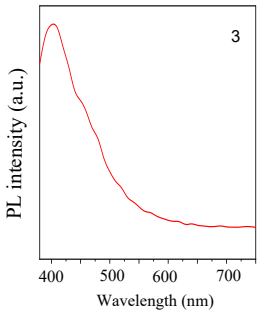
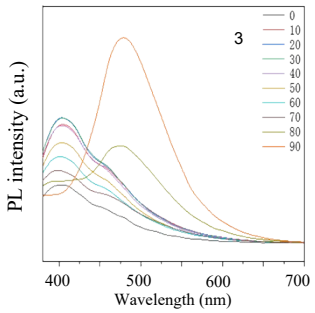


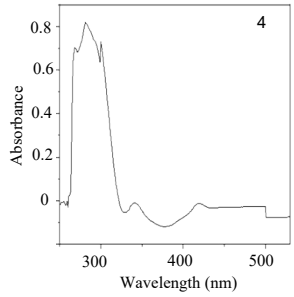
Figure S84. X-Ray structure of compound **5.**

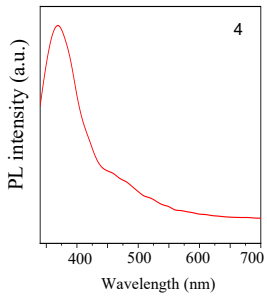
3、UV and PL tests of compounds 3 - 12.

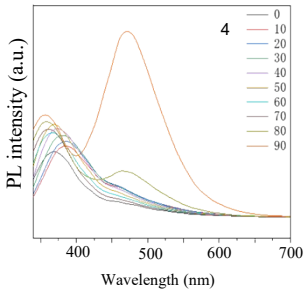


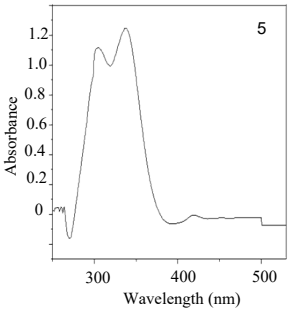


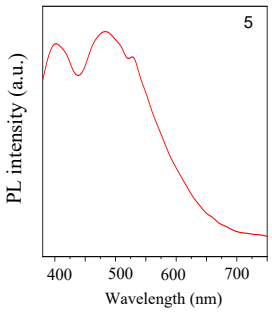


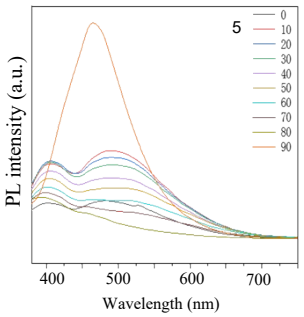


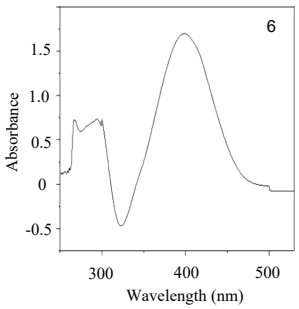


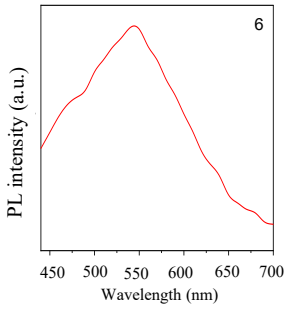


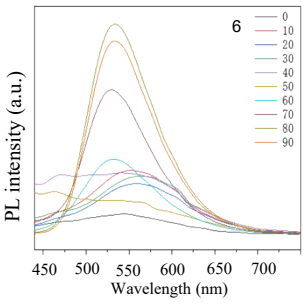


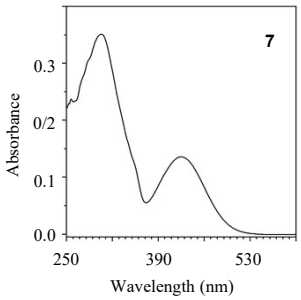


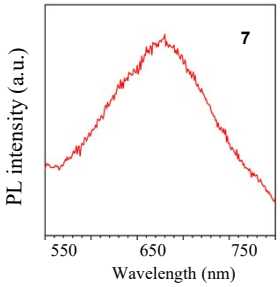


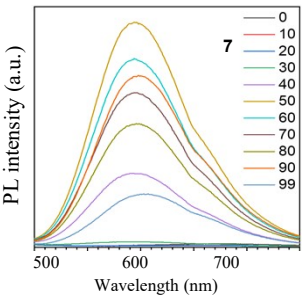












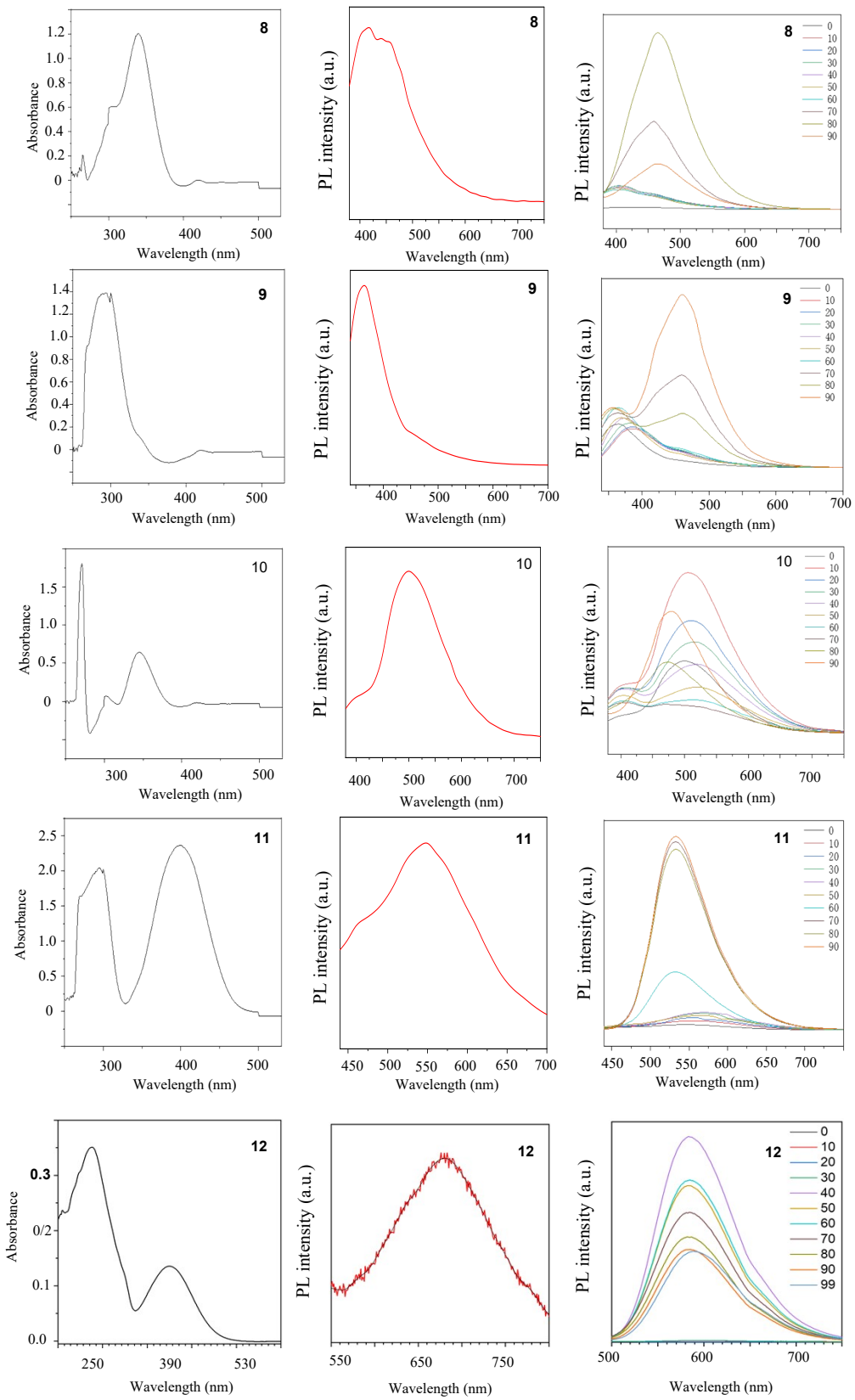


Figure S85. The UV and PL of the compounds **3** - **12**, including the UV and PL of different AIE samples from 0% to 90%.

4、Concentration gradient NMR of compound 3

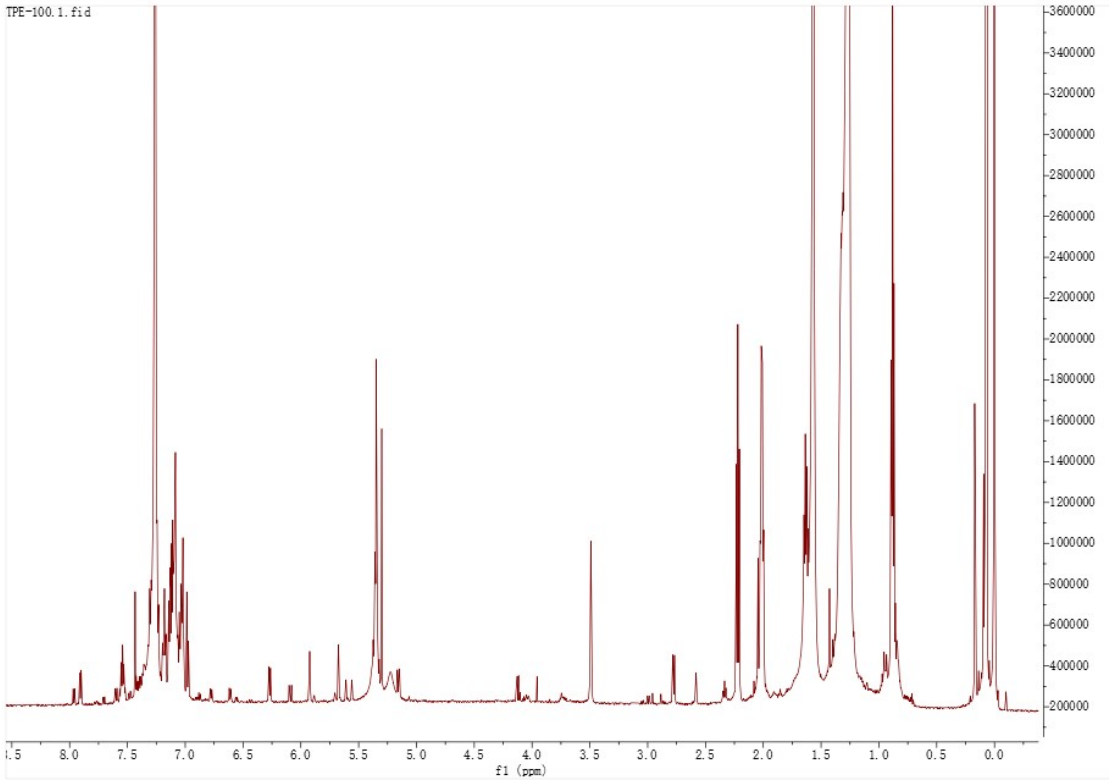


Figure S86. ^{1}H NMR of compound **3** at 0.1 mg/mL

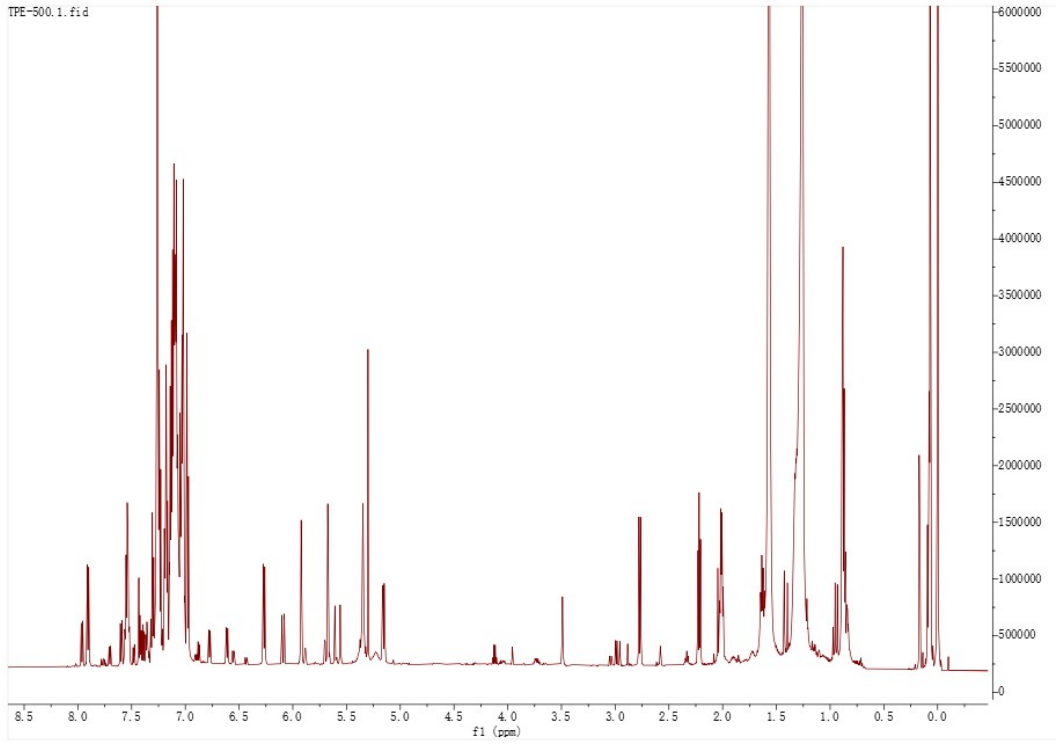


Figure S87. ^{1}H NMR of compound **3** at 0.5 mg/mL

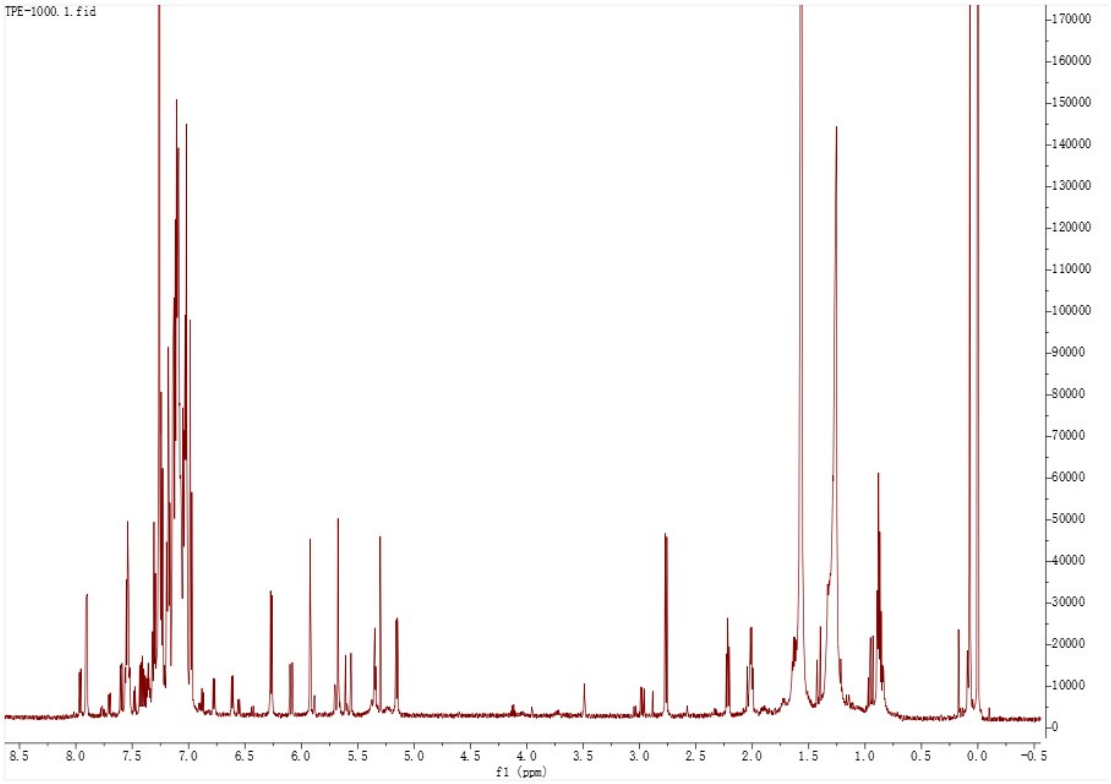


Figure S88. ^{1}H NMR of compound **3** at 1.0 mg/mL

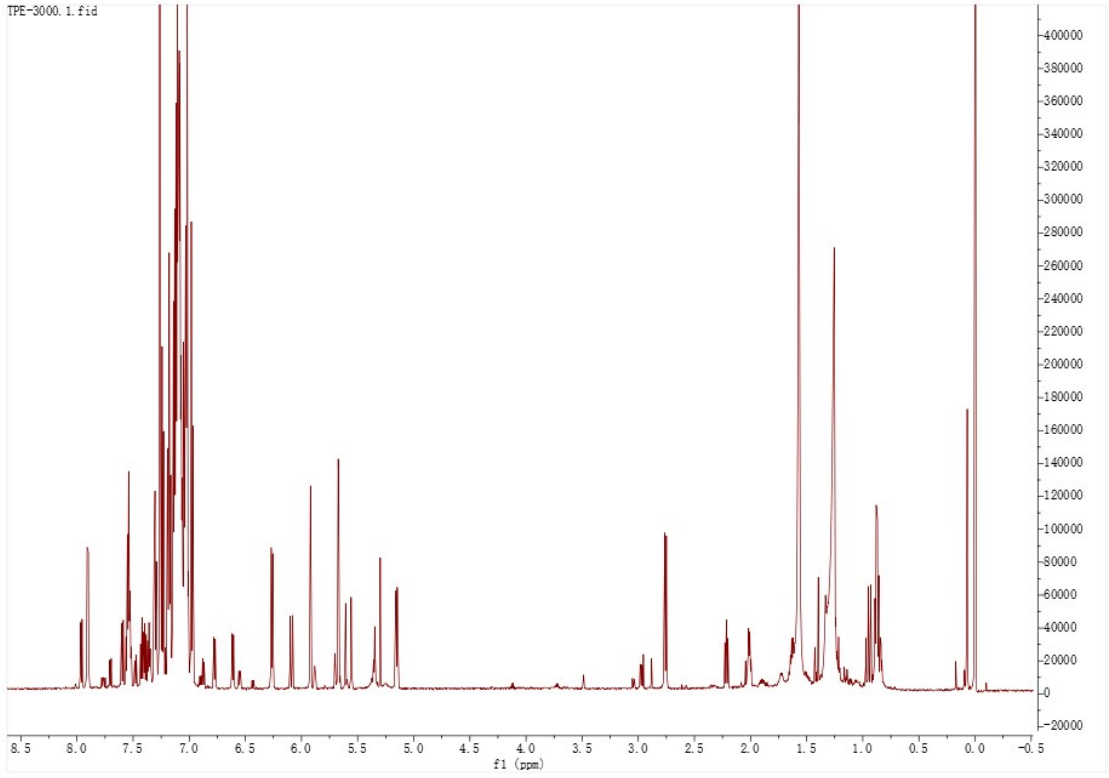


Figure S89. ^{1}H NMR of compound **3** at 3.0 mg/mL

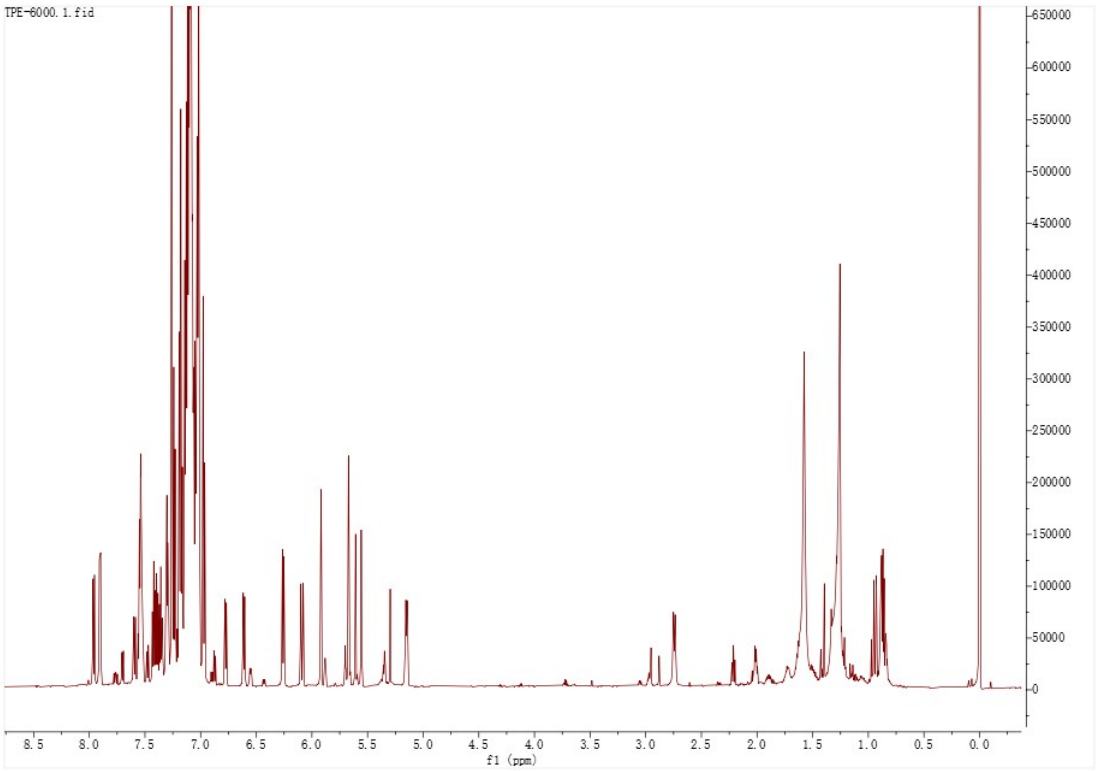


Figure S90. ^{1}H NMR of compound **3** at 6.0 mg/mL

5、Variable-temperature NMR of compound 3

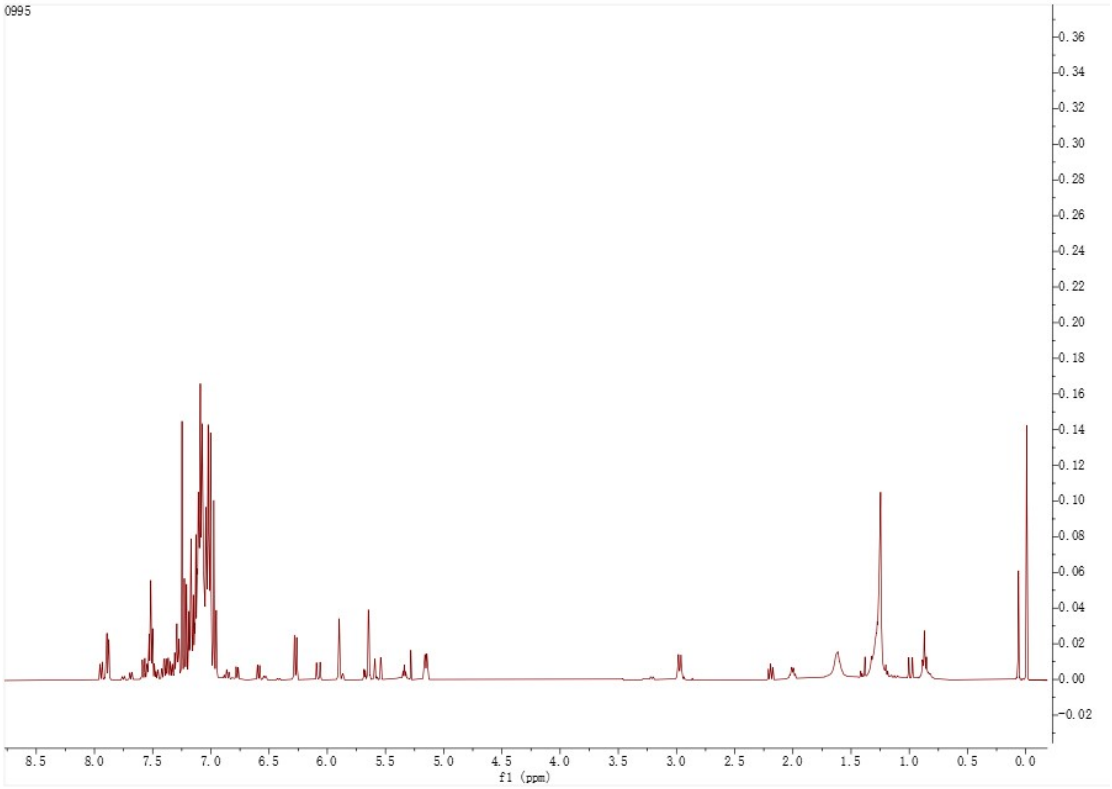


Figure S91. ^{1}H NMR of compound **3** at 298K.

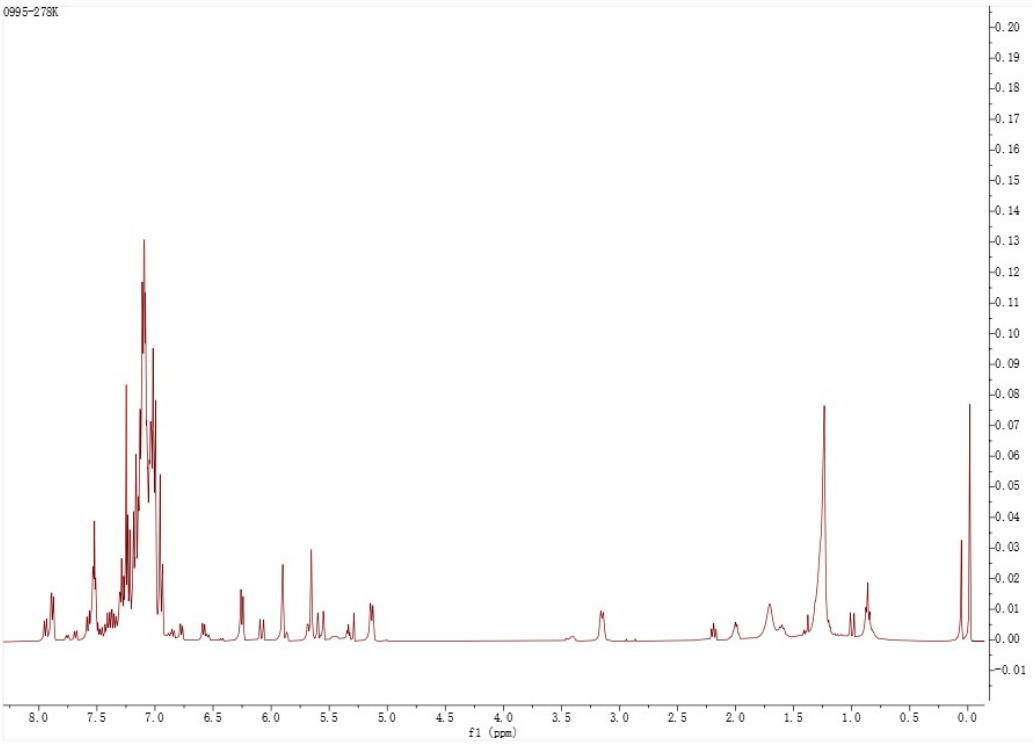


Figure S92. ^{1}H NMR of compound **3** at 278K.

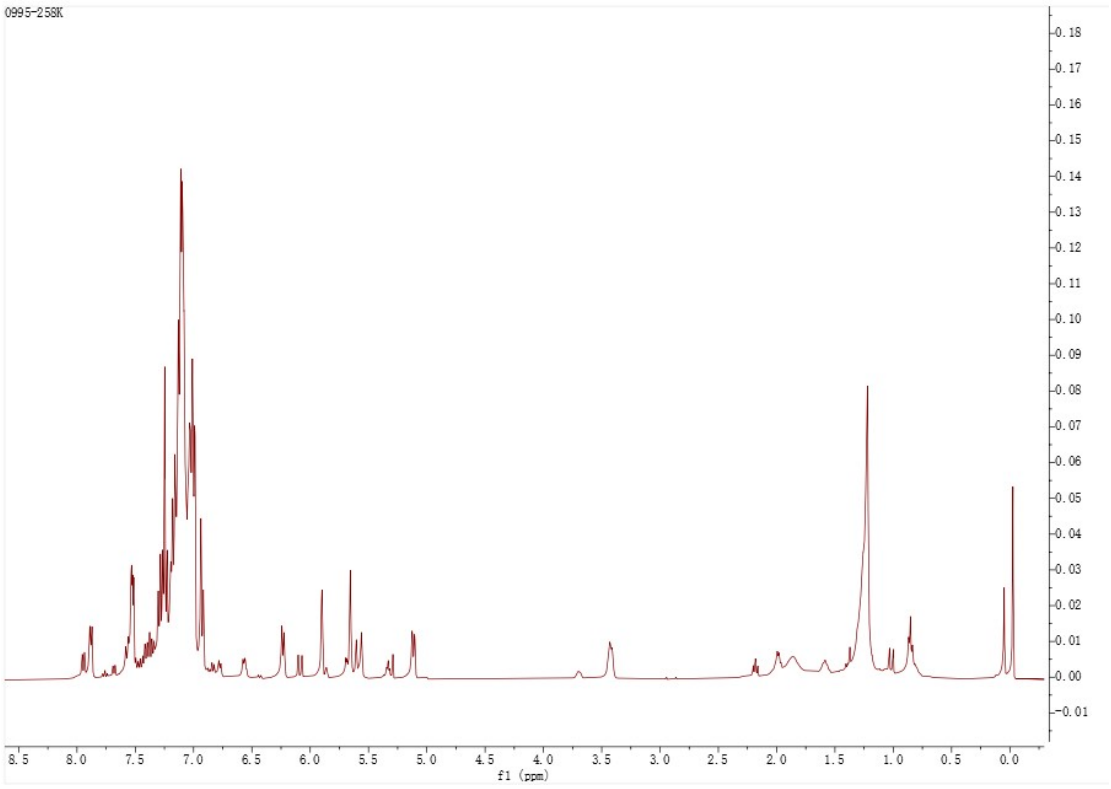


Figure S93. ^{1}H NMR of compound **3** at 258K.

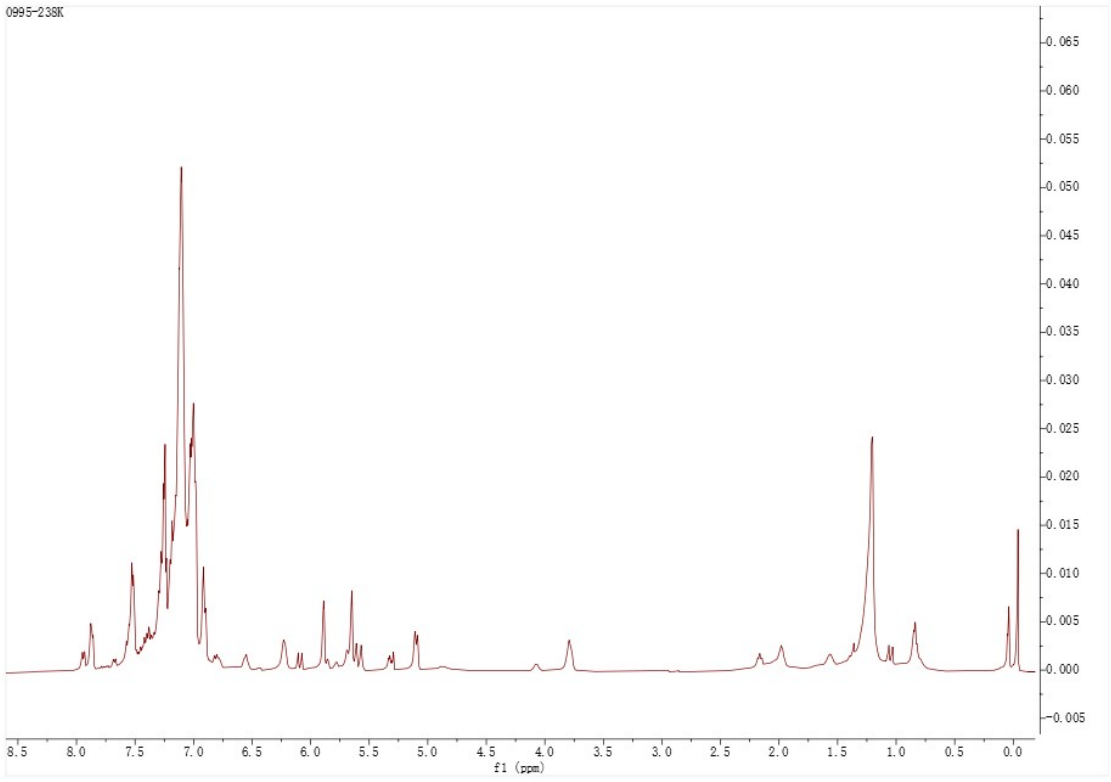


Figure S94. ^{1}H NMR of compound **3** at 238K.

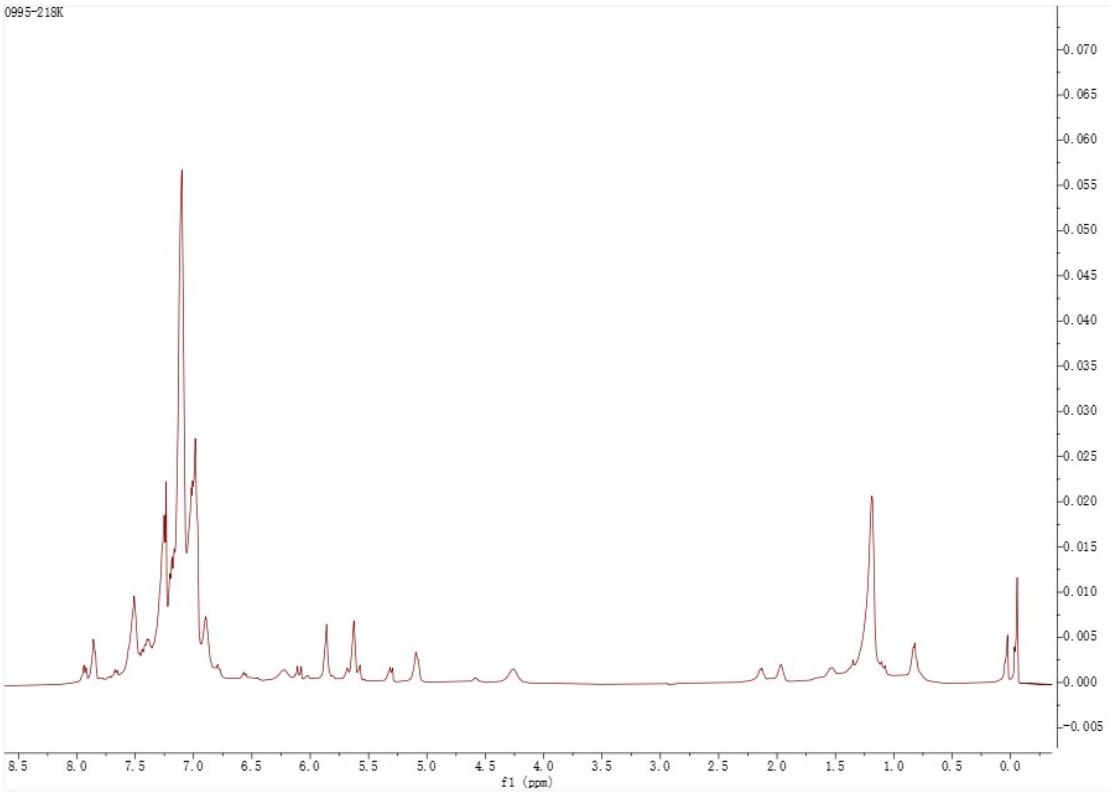
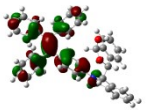
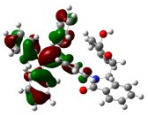
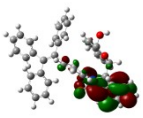
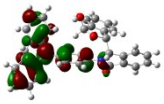
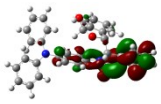
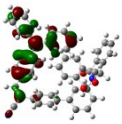
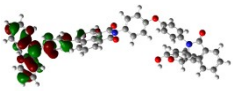
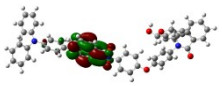
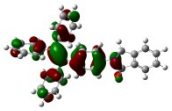
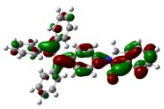
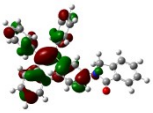
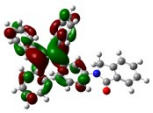
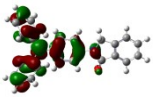
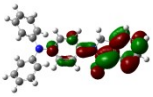
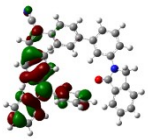
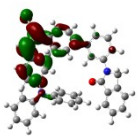
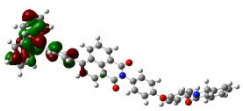
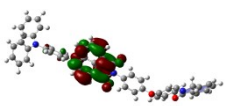
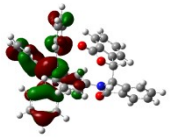
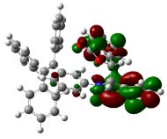


Figure S95. ^{1}H NMR of compound **3** at 218K.

6、Calculation of Compound 3-15 Homo-Lumo.

Table S1. The electronic orbitals and their energy data for the compounds **3-13** [a]

Cpd	HOMO	LUMO	Energy (Hartree) [b]
3			-0.2687_{Homo} → 0.010_{Lumo} ΔE= 0.2697
4			-0.2764_{Homo} → 0.0174_{Lumo} ΔE=0.2938
5			-0.2574_{Homo} → 0.0171_{Lumo} ΔE= 0.2935
6			-0.2640_{Homo} → 0.0096_{Lumo} ΔE= 0.2736
7			-0.2651_{Homo} → 0.069_{Lumo} ΔE=0.2720
8			-0.2651_{Homo} → 0.0082_{Lumo} ΔE=0.2733
9			-0.2727_{Homo} → 0.0269_{Lumo} ΔE=0.2920
10			-0.2528_{Homo} → 0.0132_{Lumo} ΔE= 0.2660
11			-0.2591_{Homo} → -0.0059_{Lumo} ΔE= 0.2708
12			-0.2649_{Homo} → 0.0103_{Lumo} ΔE= 0.2752
13			-0.2743_{Homo} → -0.0276_{Lumo} ΔE= 0.2373

[a)] The isovalue was 0.03 used in the calculations. [b)] 1 Hartree=27.211 eV.

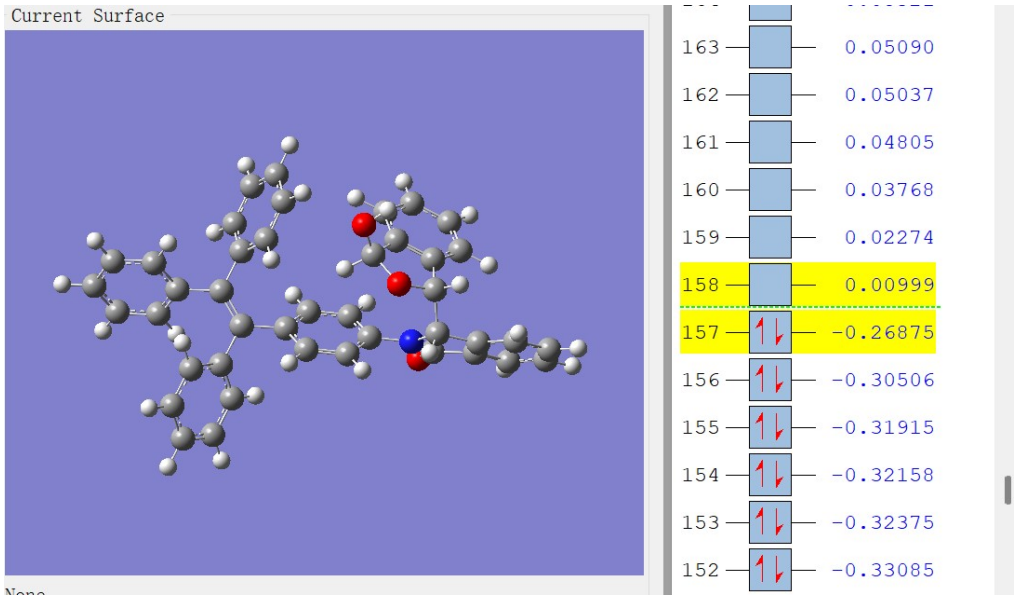


Figure S96. Original HOMO-LUMO difference diagram of compound **3** in GaussView.

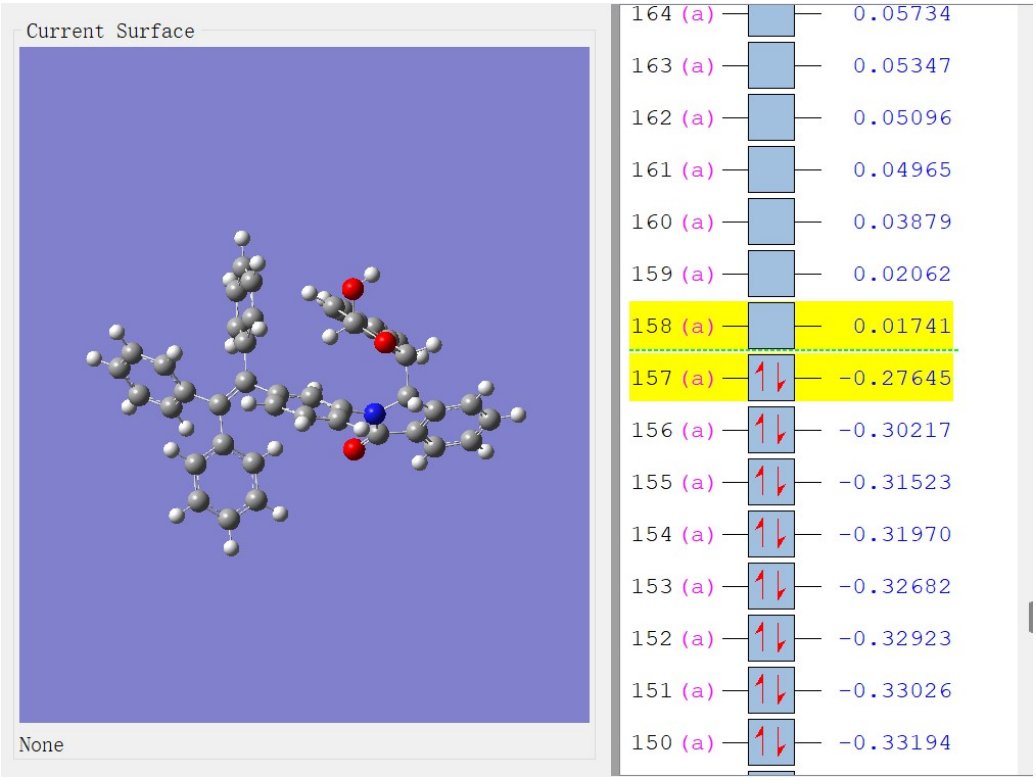


Figure S97. Original HOMO-LUMO difference diagram of compound **4** in GaussView.

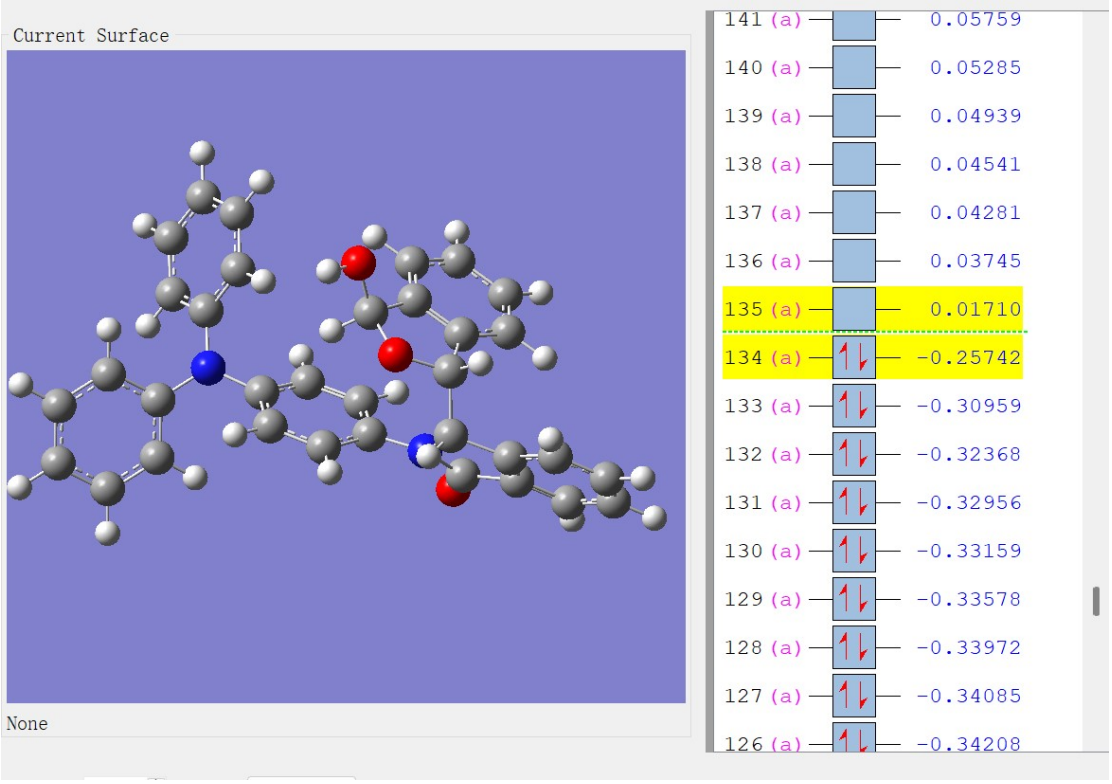


Figure S98. Original HOMO-LUMO difference diagram of compound **5** in GaussView.

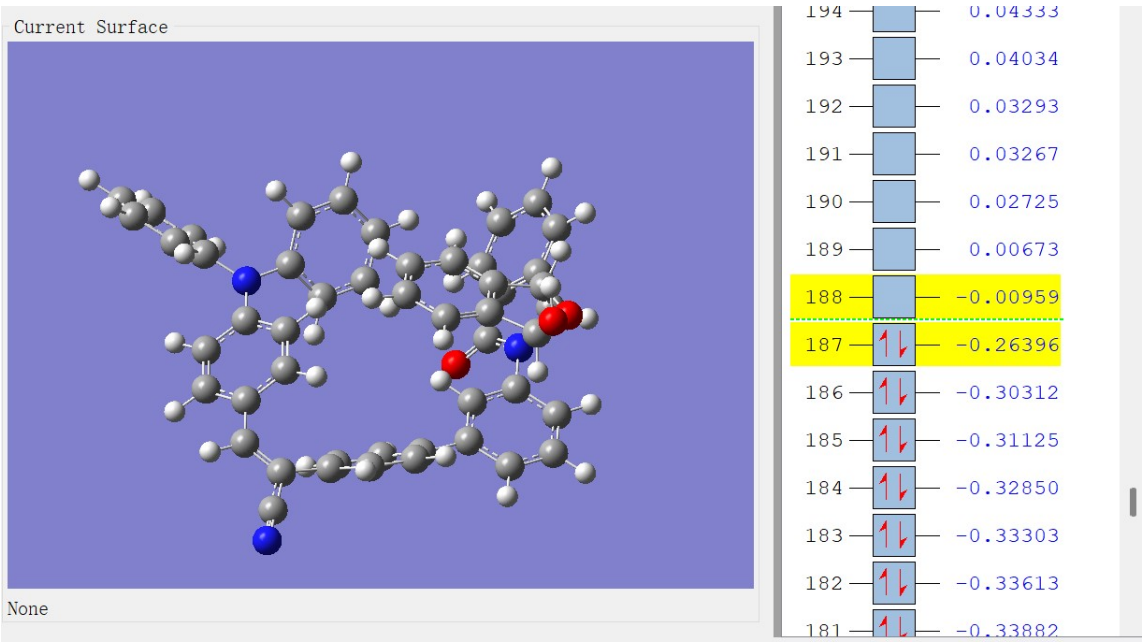


Figure S99. Original HOMO-LUMO difference diagram of compound **6** in GaussView.

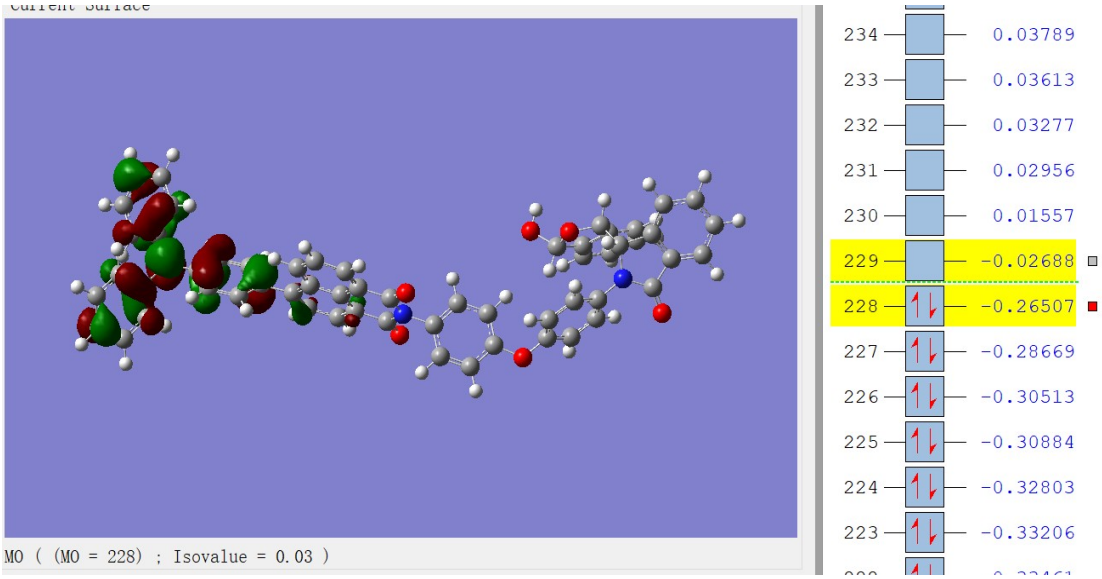


Figure S100. Original HOMO-LUMO difference diagram of compound **7** in GaussView.

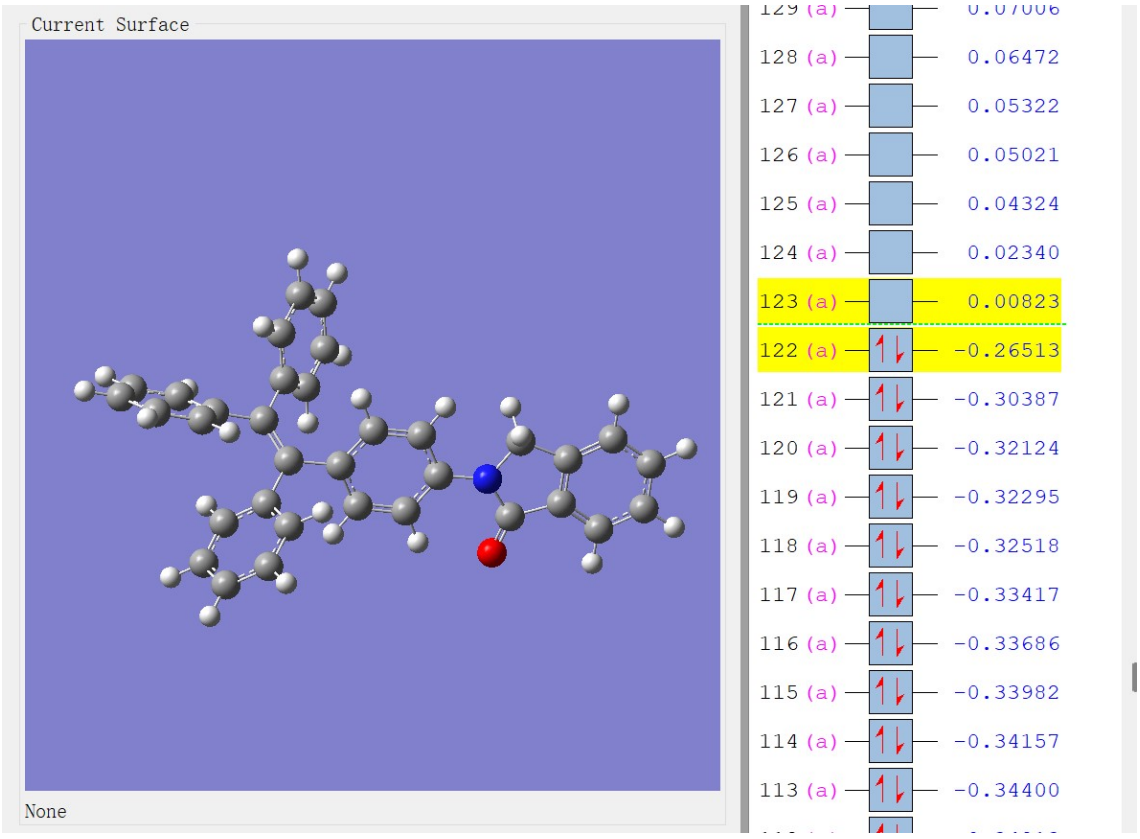


Figure 101. Original HOMO-LUMO difference diagram of compound **8** in GaussView.

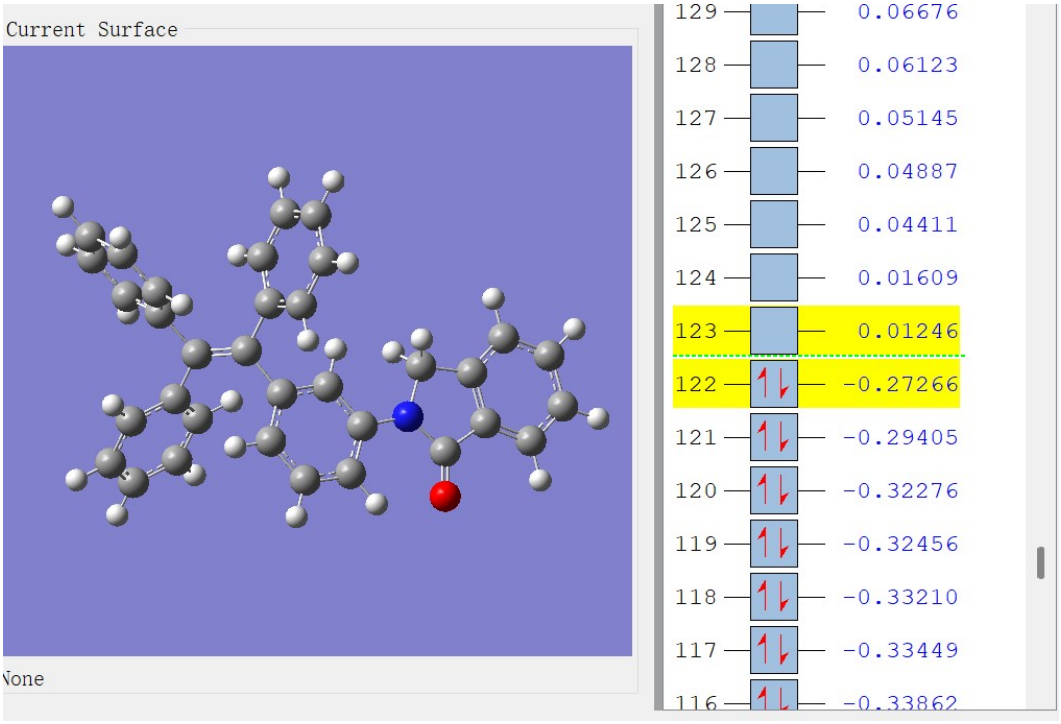


Figure S102. Original HOMO-LUMO difference diagram of compound **9** in GaussView.

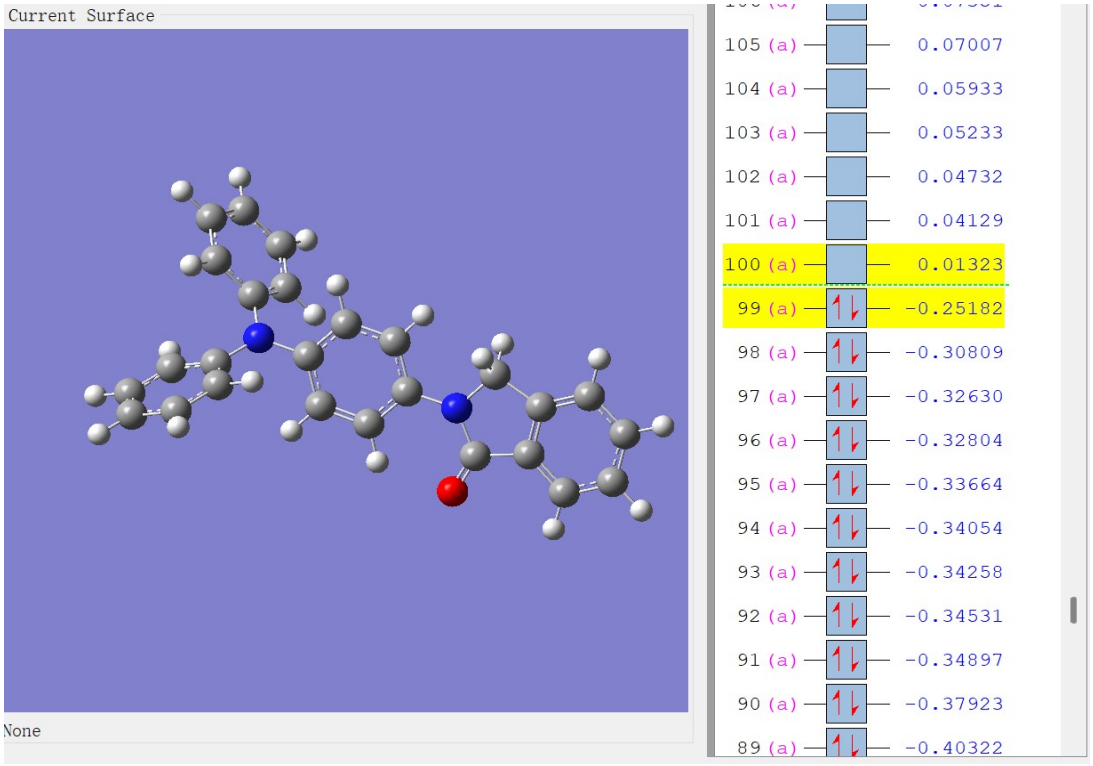


Figure 103. Original HOMO-LUMO difference diagram of compound **10** in

GaussView.

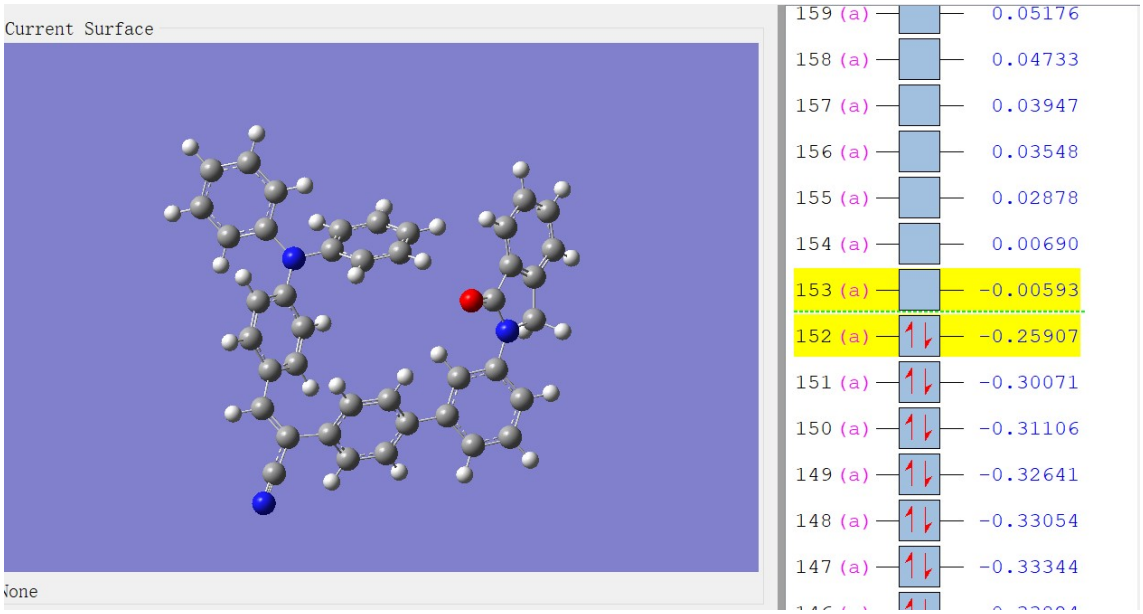


Figure S104. Original HOMO-LUMO difference diagram of compound **11** in GaussView.

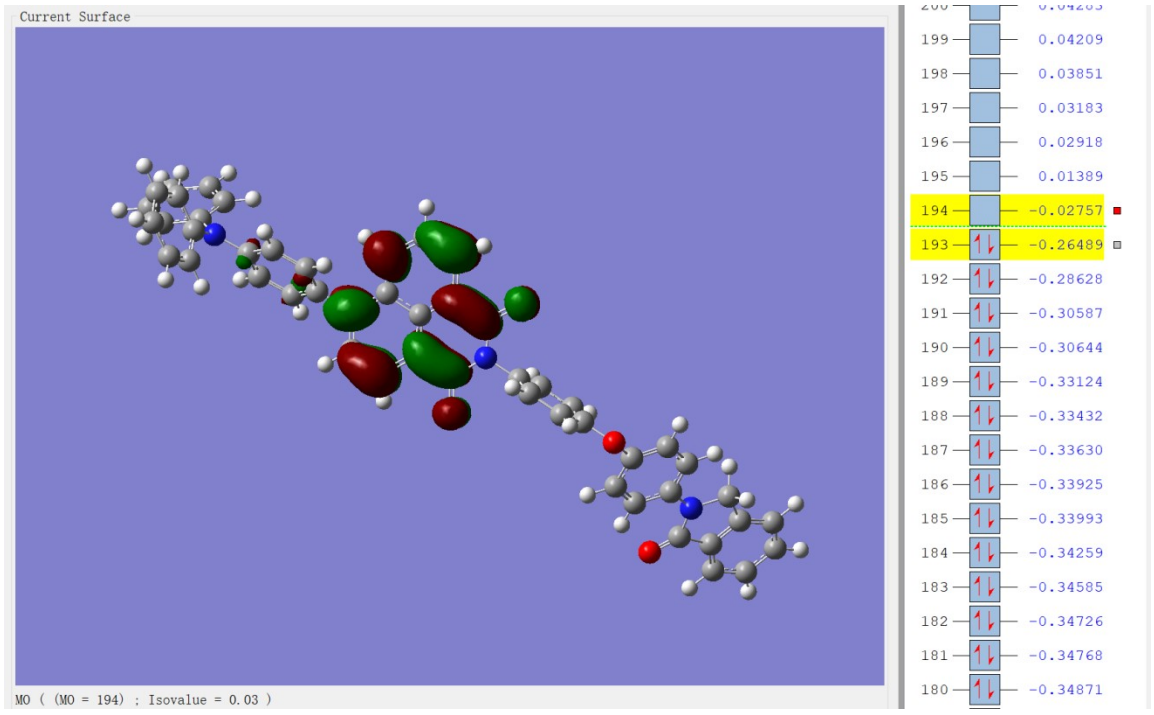


Figure S105. Original HOMO-LUMO difference diagram of compound **12** in GaussView.

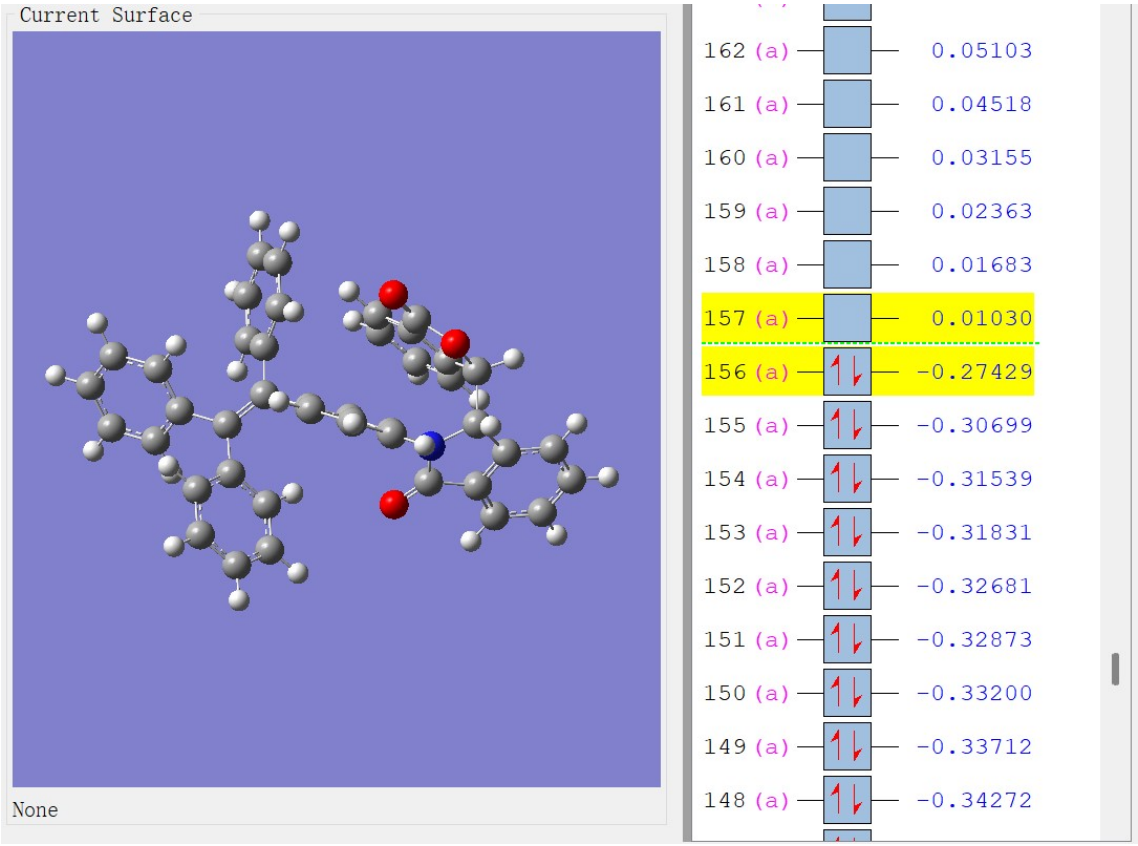


Figure S106. Original HOMO-LUMO difference diagram of compound **13** in GaussView.

7. The atom force microscopy (AFM) study for the compound 7.

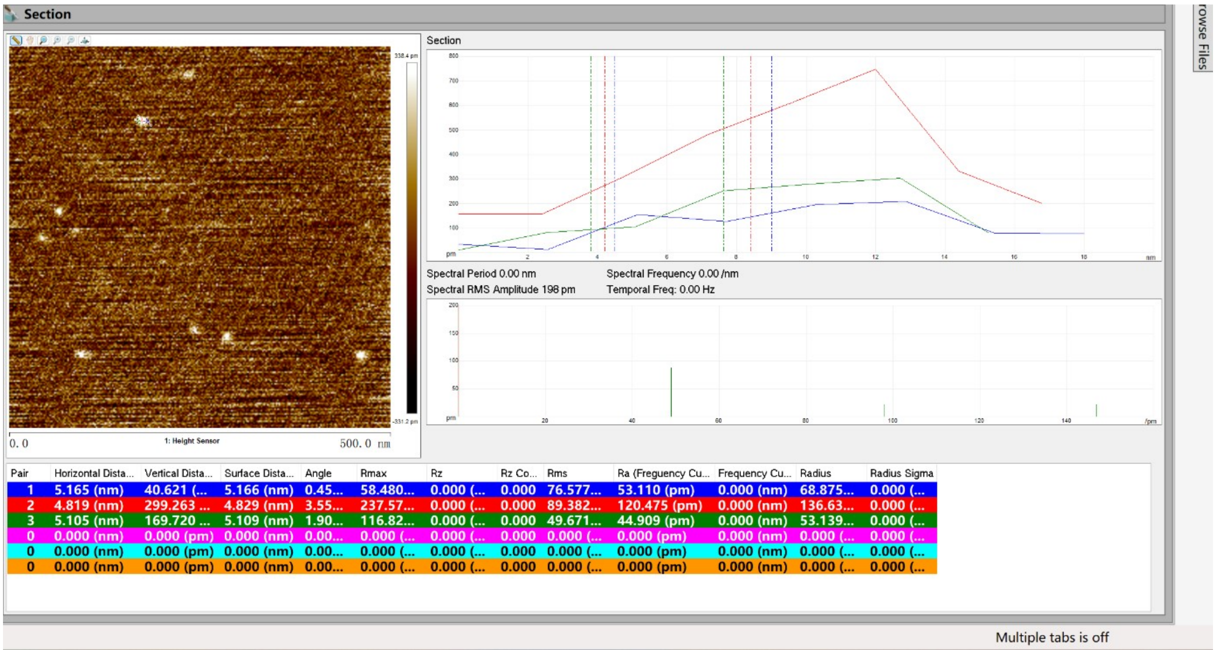


Figure S107. The atom force microscopy (AFM) study for the compound **7**.

8. Cell Staining Experiment.

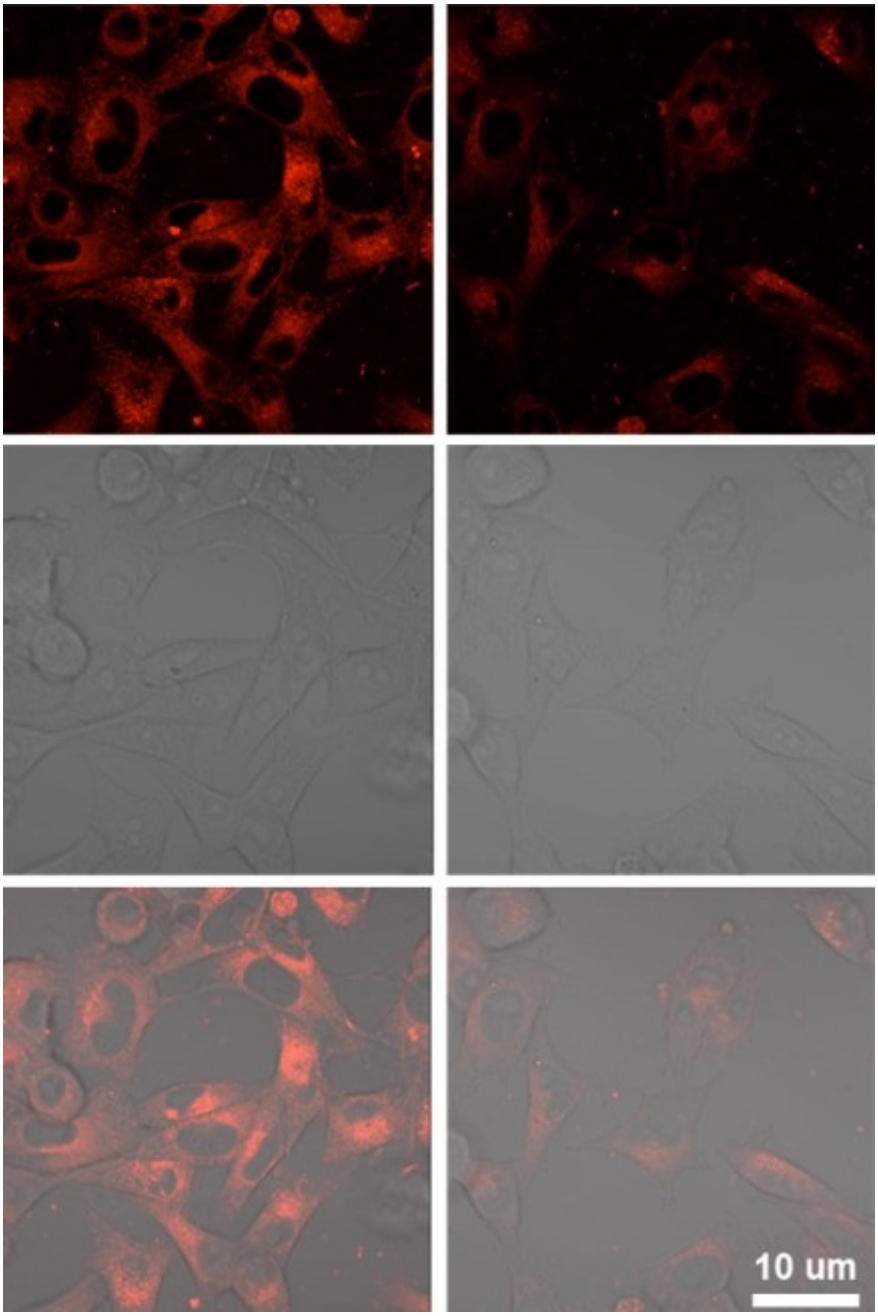


Figure S108. Confocal microscopic images of compounds **6** and **7** after staining for five hours, with a molecular concentration of 10 mM and an excitation wavelength of 405 nm.

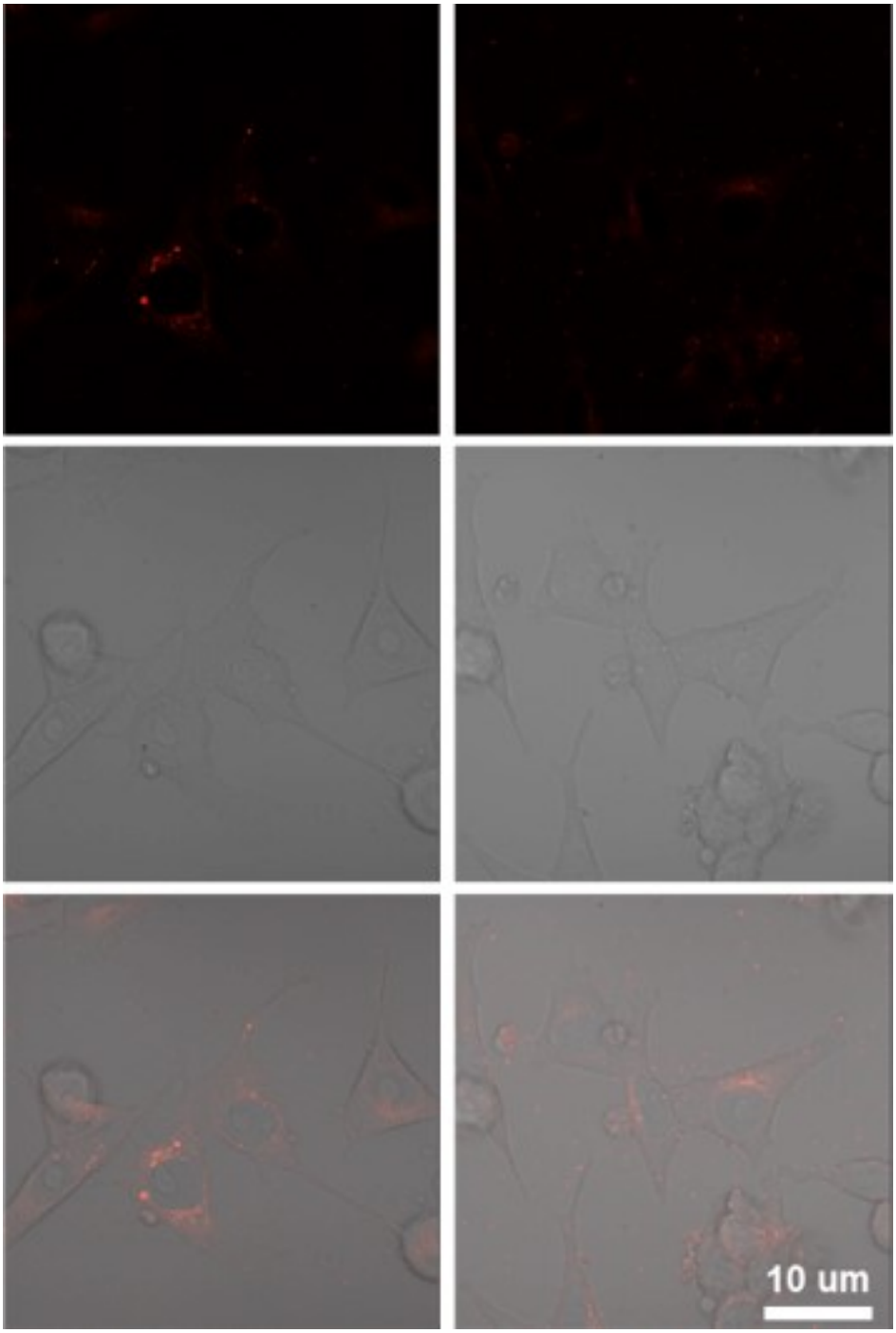


Figure S109. Confocal microscopic images of compounds **11** and **12** after staining for five hours, with a molecular concentration of 10 mM and an excitation wavelength of 405 nm.

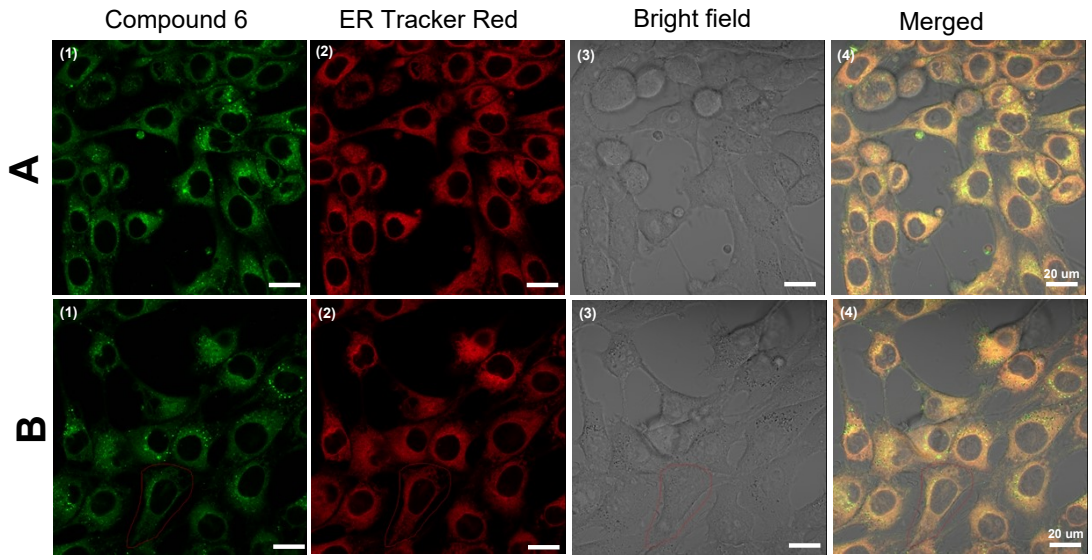


Figure S110. Confocal imaging of compound 6 in the endoplasmic reticulum. A(1) and B(1) are confocal images of endoplasmic reticulum staining of compound **6** in 4T1 cells; A(2) and B(2) are confocal images of endoplasmic reticulum staining of ER Track Red in 4T1 cells; A(3) and B(3) are bright-field microscopy images of 4T1 cells; A(4) and B(4) are merged images of 1, 2, and 3. Compound concentration: 10 μM, staining time: 1 hour.， scale bar = 20 μm。

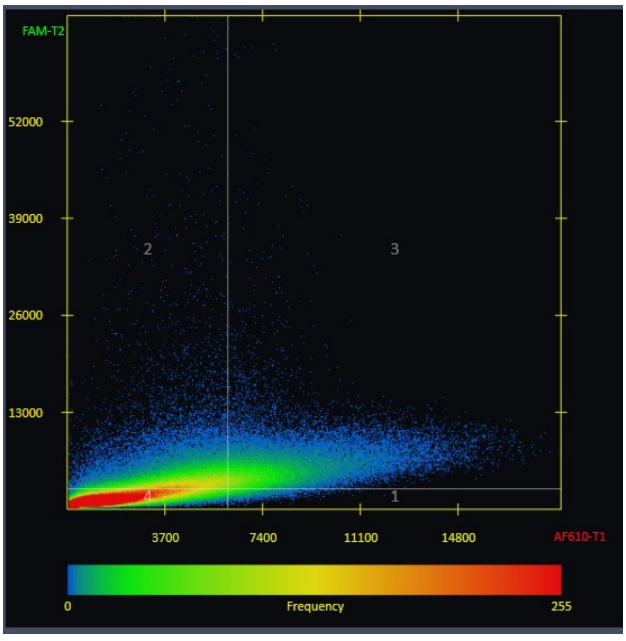


Figure S111. Heatmap of Pearson Correlation Coefficients for Co-localization Experiment of Compound **6** in the Endoplasmic Reticulum， Pearson ecoefficiency: 76 %.

9. Cell phototoxicity and dark toxicity experiments of compounds 6-7 and 11-12.

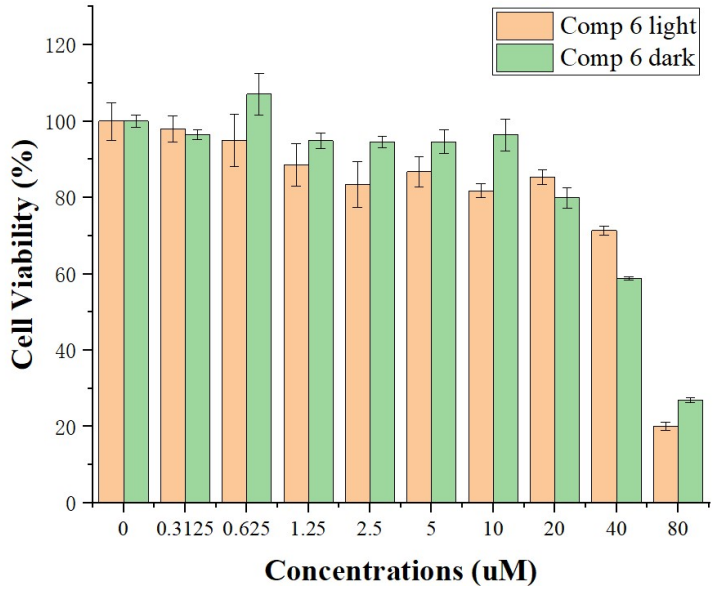


Figure S112. Phototoxicity and Dark Toxicity Data Chart of Compound **6.**

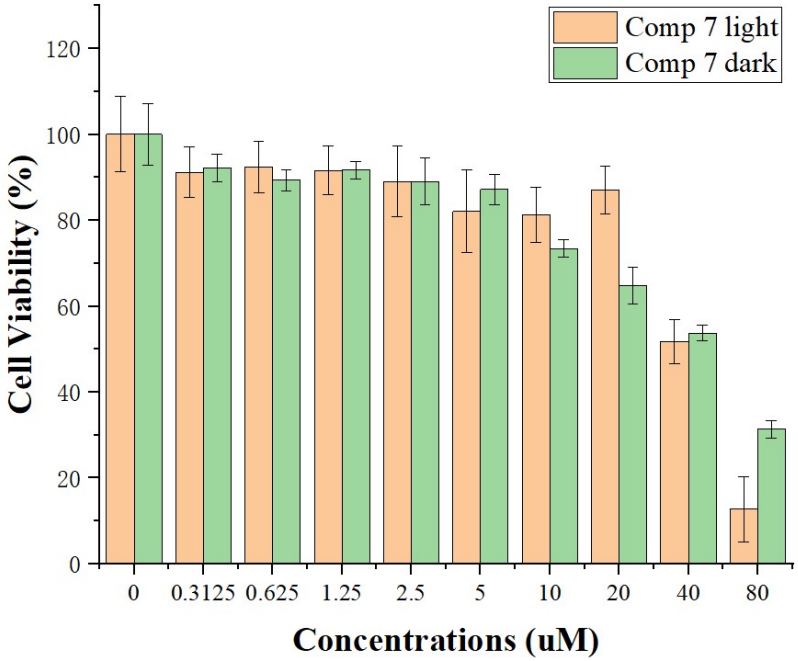


Figure S113. Phototoxicity and Dark Toxicity Data Chart of Compound **7.**

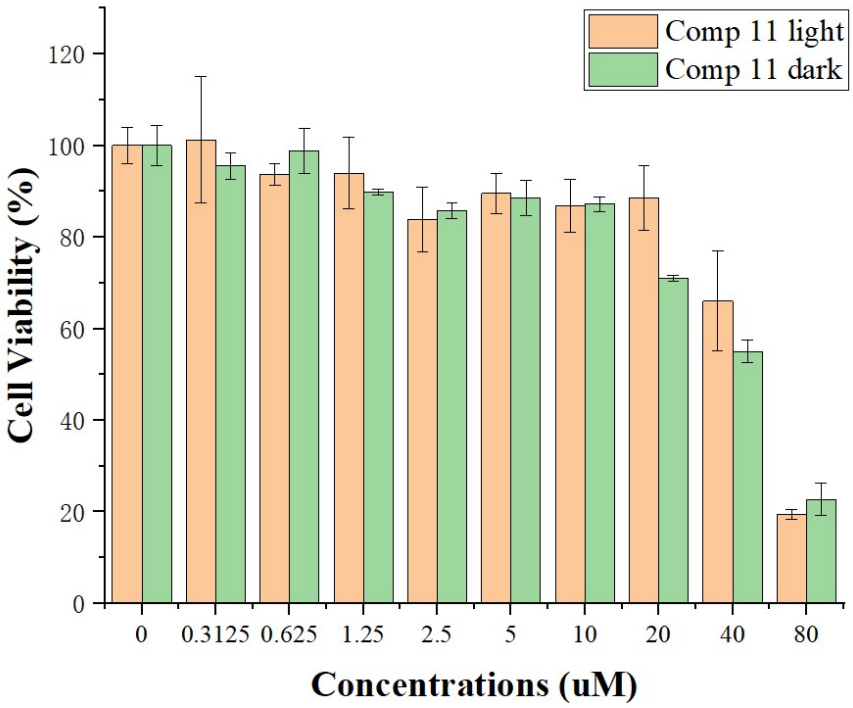


Figure S114. Phototoxicity and Dark Toxicity Data Chart of Compound **11.**

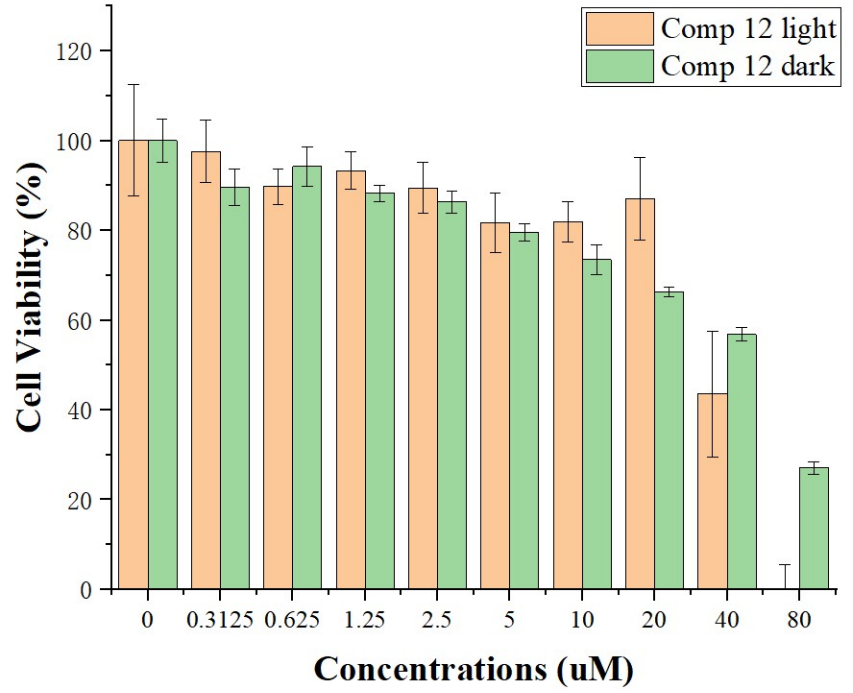


Figure S115. Phototoxicity and Dark Toxicity Data Chart of Compound **12.**