

Supplementary Information

An Approach to Unsymmetrical 3,3'-Diindolylmethanes through Pd-Catalyzed Cascade Heck Cyclization of Allenamides and *o*-Ethynylanilines

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1. General Information

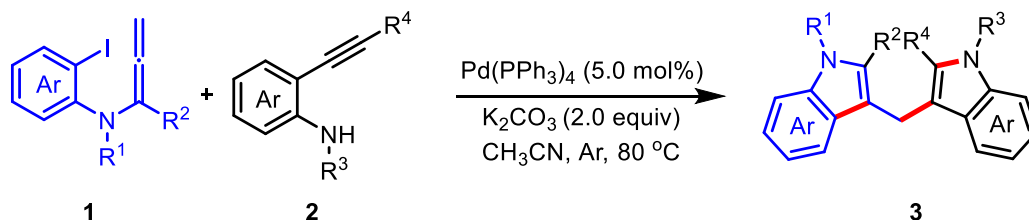
Unless otherwise noted, all chemicals were purchased from commercial suppliers (Adamas, Energy and Aladdin, etc.) and used without further purification. ^1H and ^{13}C NMR spectra were collected on BRUKER AV-300 (300 and 400 MHz) spectrometer using CDCl_3 as solvent. Chemical shifts of ^1H NMR were recorded in parts per million (ppm, δ) relative to tetramethylsilane ($\delta = 0.00$ ppm) with the solvent resonance as the internal standard (CDCl_3 : $\delta = 7.26$ ppm). Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (Hz) and integration. Chemical shifts of ^{13}C NMR were reported in ppm with the solvent as the internal standard (CDCl_3 : $\delta = 77.0$ ppm). High Resolution Mass measurement was performed on Agilent QTOF 6520 mass spectrometer with electron spray ionization (ESI) as the ion source. Melting point (m. p.) was measured on a microscopic melting point apparatus. Flash column chromatography was carried out using commercially available 200-300 mesh under pressure unless otherwise indicated. Gradient flash chromatography was conducted eluting with PE/EA, they are listed as volume/volume ratios.

2. General Procedure for the Preparation of Starting Materials

Substituted allenamides **1** were synthesized from the corresponding *o*-haloanilines and propargyl bromide.¹ *o*-Alkynylanilines **2** were prepared following the reported procedure (Sonogashira coupling of the corresponding 2-iodoanilines and alkynes followed by *N*-tosylation).² All of the NMR spectroscopy were in full accordance with the data in the literatures.

3. General Experimental Procedures

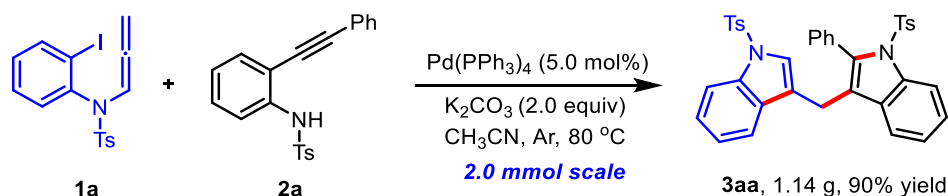
Scheme S1. General Experimental Procedures



A sealed tube was charged with substituted allenamides **1** (0.1 mmol, 1.0 equiv), *o*-ethynylanilines **2** (0.11 mmol, 1.1 equiv), Pd(PPh₃)₄ (5.8 mg, 5.0 mol%), K₂CO₃ (27.6 mg, 2.0 equiv) in CH₃CN (2.0 mL). Under an argon atmosphere, the reaction mixture was stirred at 80 °C for 24 h. Then the mixture was cooled to room temperature. Saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na₂SO₄. The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate) to afford the corresponding products **3**.

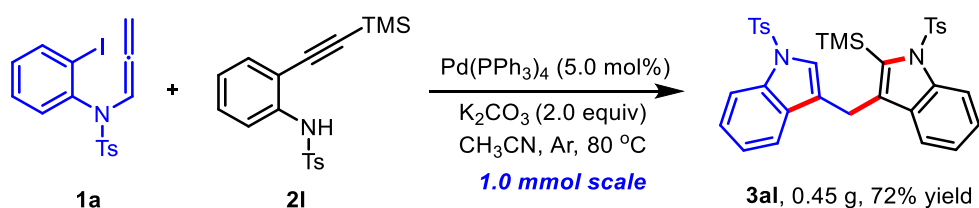
4. Scale-up Experiments and Synthetic Transformations of 3aa and 3al

Scheme S2. Scale-up (2.0 mmol) Experiment of 3aa



A sealed tube was charged with *N*-(2-iodophenyl)-4-methyl-*N*-(propa-1,2-dien-1-yl)benzenesulfonamide **1a** (2.0 mmol, 1.0 equiv), 4-methyl-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide **2a** (2.2 mmol, 1.1 equiv), Pd(PPh₃)₄ (115.6 mg, 5.0 mol%), K₂CO₃ (552.0 mg, 2.0 equiv) and CH₃CN (40.0 mL). Under an argon atmosphere, the reaction mixture was stirred at 80 °C for 48 h. Then the mixture was cooled to room temperature. Saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na₂SO₄. The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **3aa** (1.14 g, 90% yield). When the reaction was carried out in the round-bottomed flask, the product **3aa** was obtained in 96% yield (1.21 g).

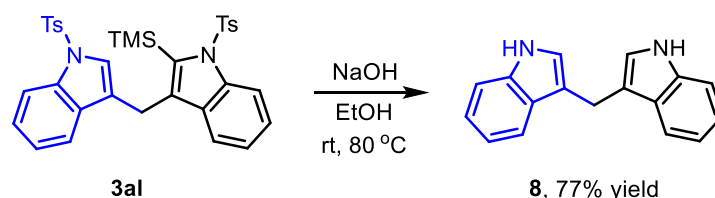
Scheme S3. Scale-up (1.0 mmol) Experiment of 3al



A sealed tube was charged with *N*-(2-iodophenyl)-4-methyl-*N*-(propa-1,2-dien-1-yl)benzenesulfonamide **1a** (1.0 mmol, 1.0 equiv), 4-methyl-*N*-(2-((trimethylsilyl)ethynyl)phenyl)benzenesulfonamide **2l** (1.1 mmol, 1.1 equiv), Pd(PPh₃)₄ (57.8 mg, 5.0 mol%), K₂CO₃ (276.0 mg, 2.0 equiv) in CH₃CN (20.0 mL). Under an argon atmosphere, the reaction mixture was stirred at 80 °C for 24 h. Then the mixture was cooled to room temperature. Saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic

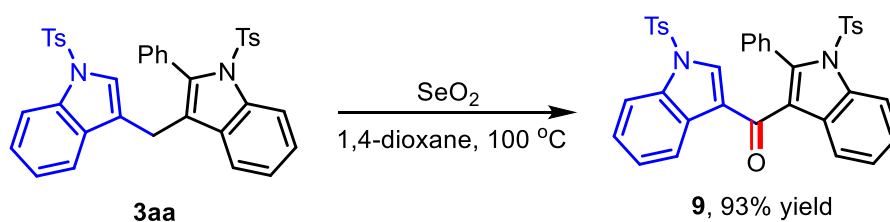
phase was washed with saturated brine and dried over Na_2SO_4 . The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **3al** (0.45 g, 72% yield).

Scheme S4. Synthetic Transformation (**3al** to **8**³)



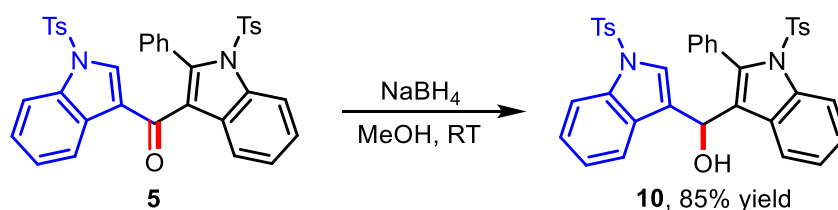
A sealed tube was charged with **3al** (0.1 mmol, 1.0 equiv), NaOH (0.6 mmol, 6.0 equiv) and EtOH (1.0 mL). The reaction mixture was stirred at 80 °C for 18 h. Then the saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na_2SO_4 . The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 50:1 to 5:1) to afford the corresponding product **8** (18.9 mg, 77% yield). When the reaction was carried out in the round-bottomed flask, the product **8** was obtained in 84% yield.

Scheme S5. Synthetic Transformation (**3aa** to **9**⁴)



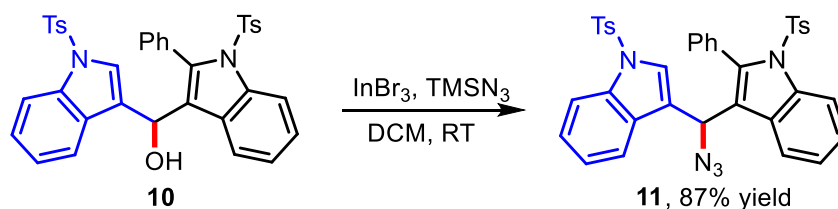
A sealed tube was charged with **3aa** (0.05 mmol, 1.0 equiv), SeO_2 (1.0 mmol, 20.0 equiv) and 1,4-dioxane (3.0 mL). The reaction mixture was stirred at 100 °C for 72 h. Then the mixture was cooled to room temperature. Saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na_2SO_4 . The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **9** (30.0 mg, 93% yield). When the reaction was carried out in the round-bottomed flask, the product **9** was obtained in 78% yield.

Scheme S6. Synthetic Transformation (3aa to 10⁵)



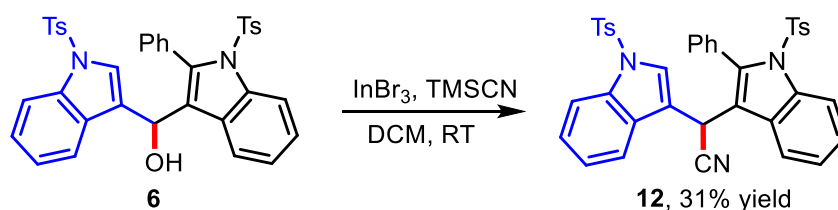
A sealed tube was charged with **5** (0.05 mmol, 1.0 equiv) and MeOH (1.0 mL). The reaction mixture was cooled to -0 °C and NaBH₄ (0.1 mmol, 2.0 equiv) was added. The reaction mixture was allowed to warm to room temperature and stirred for 16 h. Then the saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na₂SO₄. The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 20:1 to 2:1) to afford the corresponding product **10** (27.5 mg, 85% yield). When the reaction was carried out in the round-bottomed flask, the product **10** was obtained in 77% yield.

Scheme S7. Synthetic Transformation (10 to 11⁶)



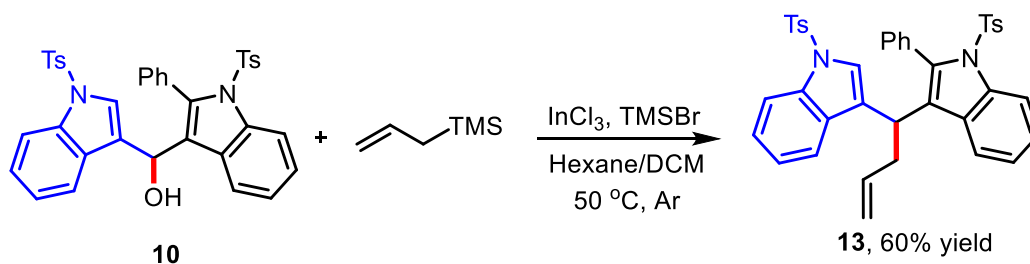
A sealed tube was charged with **10** (0.05 mmol, 1.0 equiv), InBr₃ (0.01 mmol, 0.2 equiv), TMSN₃ (0.15 mmol, 3.0 equiv) and DCM (0.4 mL). The reaction mixture was stirred at room temperature for 11 h. Then the saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na₂SO₄. The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **11** (29.3 mg, 87% yield). When the reaction was carried out in the round-bottomed flask, the product **11** was obtained in 77% yield.

Scheme S8. Synthetic Transformation (10 to 12⁷)



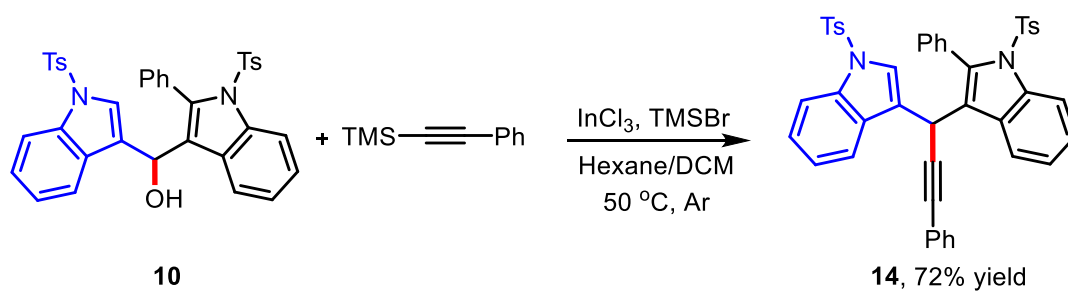
A sealed tube was charged with **10** (0.05 mmol, 1.0 equiv), InBr_3 (0.01 mmol, 0.2 equiv), TMSCN (0.15 mmol, 3.0 equiv) and DCM (0.4 mL). The reaction mixture was stirred at room temperature for 5 h. Then the saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na_2SO_4 . The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **12** (10.1 mg, 31% yield). When the reaction was carried out in the round-bottomed flask, the product **12** was obtained in 40% yield.

Scheme S9. Synthetic Transformation (10 to 13⁸)



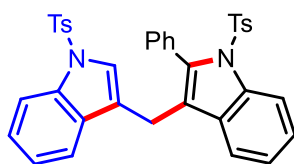
A sealed tube was charged with **10** (0.05 mmol, 1.0 equiv), InCl_3 (0.01 mmol, 0.2 equiv), TMSBr (0.01 mmol, 0.2 equiv) and allyltrimethylsilane (0.2 mmol, 4.0 equiv) in Hexane/DCM (3:2, 1.0 mL). Under an argon atmosphere, the reaction mixture was stirred at 50 °C for 2 h. Then the mixture was cooled to room temperature. Saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na_2SO_4 . The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **13** (20.1 mg, 60% yield).

Scheme S10. Synthetic Transformation (**10** to **14**⁸)



A sealed tube was charged with **10** (0.05 mmol, 1.0 equiv), InCl₃ (0.01 mmol, 0.2 equiv), TMSBr (0.03 mmol, 0.6 equiv) and trimethyl(phenylethynyl)silane (0.2 mmol, 4.0 equiv) in Hexane/DCM (3:2, 1.0 mL). Under an argon atmosphere, the reaction mixture was stirred at 50 °C for 4 h. Then the mixture was cooled to room temperature. Saturated ammonium chloride solution was added to the reaction mixture and extracted with EtOAc. The combined organic phase was washed with saturated brine and dried over Na₂SO₄. The solvent was evaporated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1 to 5:1) to afford the corresponding product **14** (26.2 mg, 72% yield).

5. Characterization of the Products



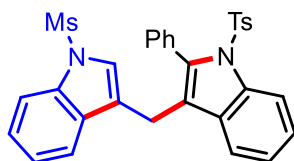
2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3aa):

61.2 mg, 97% yield; light yellow solid, **m. p.** 192–193 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.39 – 7.27 (m, 12H), 7.18 – 7.03 (m, 7H), 6.55 (s, 1H), 3.77 (s, 2H), 2.34 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 144.6, 138.3, 137.9, 135.5, 134.7, 134.3, 130.8, 130.8, 130.6, 129.6, 129.4, 128.8, 127.5, 126.5, 125.1, 124.9, 124.1, 123.6, 123.3, 122.1, 120.8, 119.4, 119.2, 116.9, 114.0, 21.6, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{30}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 648.1985, found 648.1981.



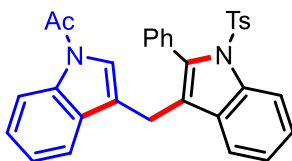
3-((1-(methylsulfonyl)-1H-indol-3-yl)methyl)-2-phenyl-1-tosyl-1H-indole (3ba):

43.2 mg, 78% yield; light yellow solid, **m. p.** 162–163 °C (PE/EA = 5:1, R_f = 0.4).

^1H NMR (300 MHz, CDCl_3) δ 8.37 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.2 Hz, 1H), 7.44 – 7.32 (m, 8H), 7.30 – 7.18 (m, 5H), 7.12 – 7.09 (m, 2H), 6.50 (s, 1H), 3.86 (s, 2H), 2.90 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.0, 138.2, 137.8, 135.4, 134.5, 130.9, 130.9, 130.8, 130.4, 129.4, 128.8, 127.6, 126.5, 125.2, 125.1, 124.2, 123.4, 123.0, 121.3, 120.6, 119.6, 119.2, 116.8, 113.2, 40.2, 21.5, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{31}\text{H}_{26}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 572.1672, found 572.1674.



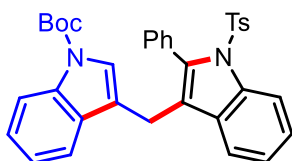
1-(3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1H-indol-1-yl)ethan-1-one (3ca):

19.0 mg, 37% yield; light yellow solid, **m. p.** 185–186 °C (PE/EA = 10:1, R_f = 0.5).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.40 – 8.34 (m, 2H), 7.43 – 7.30 (m, 11H), 7.25 – 7.17 (m, 2H), 7.09 (d, J = 8.1 Hz, 2H), 6.46 (s, 1H), 3.85 (s, 2H), 2.31 (s, 3H), 2.30 (s, 3H) ppm.

$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 168.0, 144.5, 137.9, 137.5, 135.9, 135.1, 131.0, 130.8, 130.1, 129.2, 128.8, 127.6, 126.9, 125.4, 125.2, 124.2, 123.4, 122.2, 121.1, 120.8, 119.4, 118.7, 116.5, 23.8, 21.5, 20.5 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{32}\text{H}_{26}\text{N}_2\text{O}_3\text{S} + \text{NH}_4]^+$ 536.2002, found 536.2011.



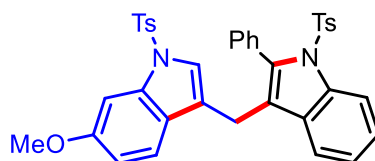
tert-butyl 3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1H-indole-1-carboxylate (3da):

51.0 mg, 88% yield; light yellow solid, **m. p.** 129–130 °C (PE/EA = 20:1, R_f = 0.3).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.35 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 8.1 Hz, 1H), 7.41 – 7.25 (m, 11H), 7.19 – 7.09 (m, 4H), 6.77 (s, 1H), 3.83 (s, 2H), 2.33 (s, 3H), 1.63 (s, 9H) ppm.

$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 149.7, 144.7, 137.9, 137.7, 135.1, 134.6, 131.1, 130.9, 130.3, 129.4, 128.6, 127.5, 126.5, 125.0, 124.3, 124.2, 123.1, 122.3, 121.4, 119.6, 119.1, 118.8, 116.6, 115.1, 83.5, 28.2, 21.5, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{35}\text{H}_{32}\text{N}_2\text{O}_4\text{S} + \text{NH}_4]^+$ 594.2421, found 594.2424.



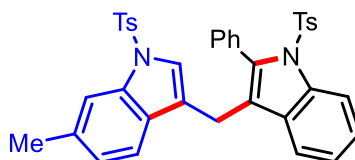
6-methoxy-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ea):

53.0 mg, 80% yield; light yellow solid, **m. p.** 109–110 °C (PE/EA = 10:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, $J = 8.4$ Hz, 1H), 7.49 (d, $J = 2.2$ Hz, 1H), 7.42 – 7.1 (m, 10H), 7.17 – 7.02 (m, 7H), 6.78 (dd, $J = 8.6, 2.3$ Hz, 1H), 6.45 (s, 1H), 3.85 (s, 3H), 3.72 (s, 2H), 2.35 (s, 3H), 2.32 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 158.2, 145.3, 144.6, 138.2, 137.9, 136.6, 134.7, 134.3, 130.9, 130.9, 130.8, 129.6, 129.4, 128.7, 127.5, 126.5, 126.4, 125.1, 124.4, 124.1, 122.3, 122.2, 121.0, 119.7, 119.4, 116.9, 112.3, 98.3, 55.7, 21.6, 21.5, 20.8 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_5\text{S}_2 + \text{H}]^+$ 661.1825, found 661.1832.



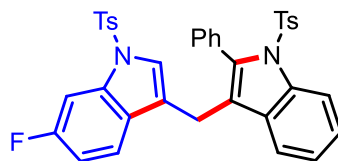
6-methyl-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3fa):

55.0 mg, 85% yield; light yellow solid, **m. p.** 143–144 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, $J = 8.4$ Hz, 1H), 7.76 (s, 1H), 7.45 – 7.31 (m, 10H), 7.19 – 6.97 (m, 8H), 6.49 (s, 1H), 3.74 (s, 2H), 2.44 (s, 3H), 2.34 (s, 3H), 2.32 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.2, 144.5, 138.2, 137.9, 135.9, 135.1, 134.8, 134.3, 130.9, 130.9, 130.8, 129.6, 129.4, 128.7, 128.3, 127.5, 126.5, 126.4, 125.1, 124.8, 124.1, 122.9, 122.0, 121.0, 119.4, 118.8, 116.8, 114.0, 21.8, 21.5, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 662.2142, found 662.2147.



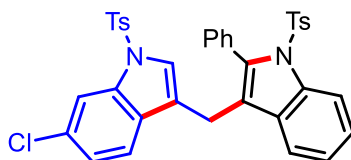
6-fluoro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ga):

60.0 mg, 92% yield; light yellow solid, **m. p.** 184–185 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, $J = 8.4$ Hz, 1H), 7.67 (dd, $J = 9.7, 2.3$ Hz, 1H), 7.44 – 7.31 (m, 10H), 7.21 – 7.11 (m, 6H), 7.05 – 7.02 (m, 1H), 6.90 (td, $J = 9.0, 2.3$ Hz, 1H), 6.56 (s, 1H), 3.74 (s, 2H), 2.36 (s, 3H), 2.32 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 161.0 (d, $J_{\text{C-F}} = 241.0$ Hz), 145.3, 144.9, 138.3, 137.8, 135.8, 135.6, 134.5, 134.4, 130.8, 130.7, 129.7, 129.4, 128.8, 127.6, 126.8, 126.5, 125.2, 124.1, 123.8 (d, $J_{\text{C-F}} = 3.8$ Hz), 121.8, 120.6, 120.1, 120.0 (d, $J_{\text{C-F}} = 9.7$ Hz), 116.8, 111.7 (d, $J_{\text{C-F}} = 23.9$ Hz), 101.5, 101.1, 21.55, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{FN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 666.1891, found 666.1893.



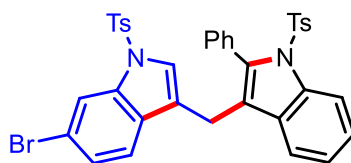
6-chloro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ha):

53.0 mg, 80% yield; light yellow solid, **m. p.** 173–174 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, $J = 8.4$ Hz, 1H), 7.96 (s, 1H), 7.42 – 7.31 (m, 10H), 7.18 – 7.09 (m, 7H), 7.02 (d, $J = 7.7$ Hz, 1H), 6.58 (s, 1H), 3.74 (s, 2H), 2.36 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 145.0, 138.3, 137.9, 135.8, 134.6, 134.5, 131.0, 130.8, 130.7, 129.8, 129.4, 129.0, 128.8, 127.6, 126.5, 125.2, 124.1, 123.9, 121.8, 120.5, 120.0, 119.2, 116.9, 114.1, 21.6, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{ClN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 682.1596, found 682.1603.



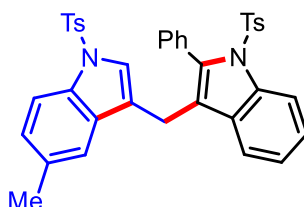
6-bromo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ia):

50.0 mg, 70% yield; light yellow solid, **m. p.** 136–137 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, $J = 8.4$ Hz, 1H), 8.12 (s, 1H), 7.42 – 7.31 (m, 10H), 7.27 – 7.24 (m, 1H), 7.17 – 7.10 (m, 6H), 7.02 (d, $J = 7.7$ Hz, 1H), 6.57 (s, 1H), 3.74 (s, 2H), 2.37 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 145.0, 138.3, 137.9, 136.1, 134.6, 134.5, 130.8, 130.7, 129.8, 129.4, 129.4, 128.9, 127.6, 126.6, 126.6, 126.5, 125.2, 124.1, 124.1, 121.8, 120.5, 120.4, 119.2, 118.6, 117.0, 116.9, 21.6, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{BrN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 726.1090, found 726.1094.



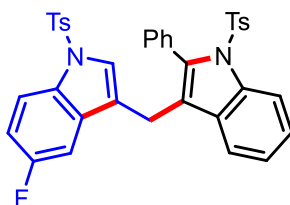
5-methyl-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ja):

47.3 mg, 73% yield; light yellow solid, **m. p.** 198–199 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, $J = 8.4$ Hz, 1H), 7.82 (d, $J = 9.1$ Hz, 1H), 7.42 – 7.31 (m, 10H), 7.18 – 7.04 (m, 8H), 6.50 (s, 1H), 3.73 (s, 2H), 2.35 (s, 3H), 2.34 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 144.5, 138.3, 138.0, 134.8, 134.4, 133.8, 133.0, 130.9, 130.8, 129.6, 129.4, 128.8, 127.6, 126.5, 126.3, 125.1, 124.1, 123.7, 122.1, 120.9, 119.4, 119.2, 116.9, 113.7, 21.6, 21.5, 21.2, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 662.2142, found 662.2140.



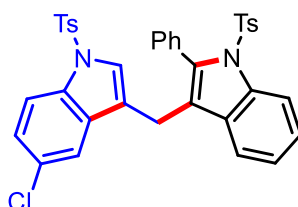
5-fluoro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ka):

57.0 mg, 88% yield; light yellow solid, **m. p.** 177–178 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 9.0, 4.4 Hz, 1H), 7.45 – 7.31 (m, 10H), 7.19 – 6.89 (m, 8H), 6.63 (s, 1H), 3.72 (s, 2H), 2.35 (s, 3H), 2.32 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 159.6 (d, $J_{\text{C-F}}$ = 239.6 Hz), 145.3, 144.9, 138.3, 137.9, 134.5, 131.8, 131.7, 131.6, 130.8, 130.8, 130.6, 129.7, 129.4, 128.9, 127.6, 126.5, 126.5, 125.3, 125.2, 124.1, 122.0 (d, $J_{\text{C-F}}$ = 4.0 Hz), 120.4, 119.3, 116.9, 115.2, 115.0, 112.9 (d, $J_{\text{C-F}}$ = 25.2 Hz), 105.0 (d, $J_{\text{C-F}}$ = 24.1 Hz), 21.6, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{FN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 666.1891, found 666.1895.



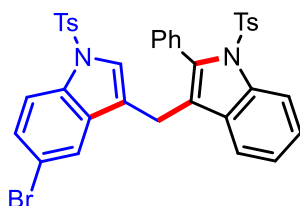
5-chloro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3la):

55.3 mg, 83% yield; light yellow solid, **m. p.** 184–185 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.46 – 7.32 (m, 10H), 7.24 – 7.04 (m, 8H), 6.61 (s, 1H), 3.72 (s, 2H), 2.35 (s, 3H), 2.32 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 145.0, 138.3, 137.8, 134.5, 134.5, 133.9, 131.8, 130.8, 130.7, 130.6, 129.7, 129.4, 129.2, 128.9, 127.6, 126.5, 126.5, 125.2, 125.2, 125.0, 124.1, 121.6, 120.3, 119.2, 119.1, 116.8, 115.0, 21.6, 20.5 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{ClN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 682.1596, found 682.1595.



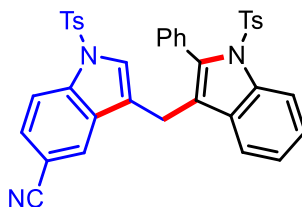
5-bromo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ma):

59.3 mg, 84% yield; light yellow solid, **m. p.** 194–195 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.7 Hz, 1H), 7.45 – 7.32 (m, 12H), 7.19 – 7.04 (m, 6H), 6.59 (s, 1H), 3.72 (s, 2H), 2.35 (s, 3H), 2.32 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.2, 145.0, 138.3, 137.8, 134.5, 134.4, 134.2, 132.3, 130.8, 130.7, 130.5, 129.7, 129.4, 128.9, 127.8, 127.6, 126.5, 126.5, 125.2, 124.8, 124.1, 122.1, 121.4, 120.2, 119.2, 116.9, 116.8, 115.4, 21.6, 20.5 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{BrN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 726.1090, found 726.1090.



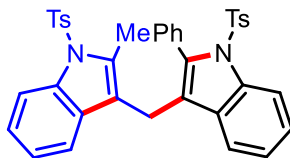
3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole-5-carbonitrile (3na):

64.1 mg, 98% yield; light yellow solid, **m. p.** 184–185 °C (PE/EA = 5:1, R_f = 0.4).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, J = 8.4 Hz, 1H), 8.02 – 7.99 (m, 1H), 7.52 – 7.30 (m, 12H), 7.22 – 7.09 (m, 6H), 6.79 (s, 1H), 3.80 (s, 2H), 2.37 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.5, 145.2, 138.3, 137.7, 137.0, 134.6, 134.3, 130.8, 130.6, 130.4, 130.2, 129.9, 129.4, 129.0, 127.8, 127.7, 126.5, 126.5, 125.6, 125.3, 124.3, 124.1, 121.4, 119.8, 119.0, 116.7, 114.6, 106.8, 21.6, 20.3 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{29}\text{N}_3\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 673.1938, found 673.1938.



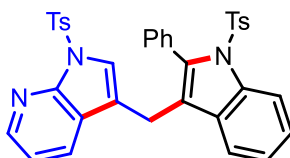
2-methyl-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (30a):

50.0 mg, 78% yield; white solid, **m. p.** 103–104 °C (PE/EA = 10:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.30 (d, J = 8.4 Hz, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.49 (d, J = 8.3 Hz, 2H), 7.41 – 7.34 (m, 3H), 7.29 – 7.27 (m, 5H), 7.19 – 7.13 (m, 1H), 7.11 (d, J = 8.2 Hz, 2H), 7.05 (d, J = 8.1 Hz, 2H), 6.97 – 6.87 (m, 4H), 3.77 (s, 2H), 2.33 (s, 3H), 2.31 (s, 3H), 2.27 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 144.5, 144.5, 137.2, 137.1, 136.3, 136.2, 135.2, 133.1, 131.3, 131.0, 130.5, 130.2, 129.7, 129.3, 128.7, 127.5, 126.7, 126.1, 124.8, 123.8, 123.7, 123.2, 120.9, 119.3, 118.5, 117.7, 116.1, 114.6, 21.5, 20.5, 12.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_4\text{S}_2 + \text{Na}]^+$ 667.1696, found 667.1691.



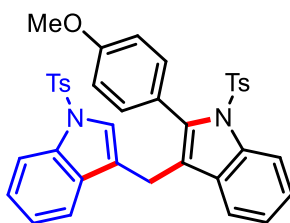
3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-pyrrolo[2,3-b]pyridine (3pa):

58.0 mg, 92% yield; light yellow solid, **m. p.** 159–160 °C (PE/EA = 5:1, R_f = 0.3).

^1H NMR (300 MHz, CDCl_3) δ 8.40 – 8.36 (m, 2H), 7.82 (d, J = 8.4 Hz, 2H), 7.50 (dd, J = 7.9, 1.5 Hz, 1H), 7.43 – 7.30 (m, 8H), 7.24 – 7.13 (m, 6H), 7.07 – 7.02 (m, 1H), 6.84 (s, 1H), 3.80 (s, 2H), 2.36 (s, 3H), 2.34 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 147.6, 145.2, 145.0, 144.9, 138.2, 137.7, 135.2, 134.5, 130.9, 130.8, 130.6, 129.5, 129.4, 128.8, 127.7, 127.6, 127.6, 126.5, 125.3, 124.2, 123.3, 122.7, 120.2, 119.2, 118.6, 118.00, 116.7, 21.6, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{36}\text{H}_{29}\text{N}_3\text{O}_4\text{S}_2 + \text{H}]^+$ 632.1672, found 632.1674.



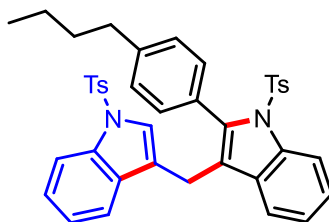
2-(4-methoxyphenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ab):

64.8 mg, 98% yield; light yellow solid, **m. p.** 201–202 °C (PE/EA = 10:1, R_f = 0.2).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.39 (d, J = 8.3 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.42 – 7.25 (m, 9H), 7.19 – 7.01 (m, 7H), 6.91 – 6.86 (m, 2H), 6.54 (s, 1H), 3.84 (s, 3H), 3.76 (s, 2H), 2.34 (s, 3H), 2.33 (s, 3H) ppm.

$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 159.9, 145.2, 144.6, 138.2, 137.8, 135.5, 134.7, 134.5, 132.1, 130.9, 130.6, 129.6, 129.4, 126.5, 126.5, 124.9, 124.0, 123.6, 123.2, 122.9, 122.2, 120.2, 119.2, 114.0, 113.0, 55.2, 21.6, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_5\text{S}_2 + \text{NH}_4]^+$ 678.2091, found 678.2084.



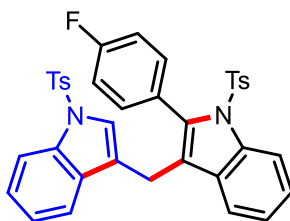
2-(4-butylphenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ac):

65.0 mg, 95% yield; light yellow solid, **m. p.** 158–159 °C (PE/EA = 20:1, R_f = 0.2).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.38 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.41 – 7.25 (m, 9H), 7.18 – 7.01 (m, 9H), 6.56 (s, 1H), 3.77 (s, 2H), 2.67 (t, J = 7.8 Hz, 2H), 2.35 (s, 3H), 2.33 (s, 3H), 1.70 – 1.60 (m, 2H), 1.46 – 1.34 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H) ppm.

$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 145.2, 144.6, 143.6, 138.6, 137.9, 135.6, 134.8, 134.5, 130.9, 130.7, 129.6, 129.4, 128.0, 127.6, 126.6, 126.5, 125.0, 124.9, 124.0, 123.7, 123.2, 122.3, 120.5, 119.3, 119.2, 116.9, 114.0, 35.5, 33.3, 22.5, 21.5, 20.8, 14.0 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{41}\text{H}_{38}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 704.2611, found 704.2617.



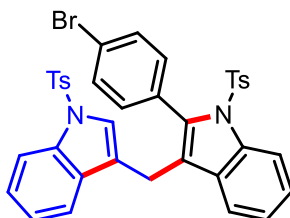
2-(4-fluorophenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ad):

54.0 mg, 83% yield; light yellow solid, **m. p.** 188–189 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.34 (dd, J = 9.1, 4.5 Hz, 1H), 7.98 (d, J = 8.3 Hz, 1H), 7.42 – 7.29 (m, 8H), 7.22 – 7.08 (m, 9H), 6.66 (dd, J = 8.5, 2.5 Hz, 1H), 6.52 (s, 1H), 3.77 (s, 2H), 2.35 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 160.0 (d, $J_{\text{C-F}}$ = 240.3 Hz), 145.5, 144.9, 135.7, 135.2, 134.5, 134.3, 133.9, 133.9, 131.9, 131.8, 130.5, 130.4, 130.4, 129.7, 129.5, 126.4, 126.4, 126.3, 125.1, 124.6, 123.4, 123.4, 121.7, 120.6 (d, $J_{\text{C-F}}$ = 3.9 Hz), 119.2, 118.0, 117.9, 114.1, 113.0 (d, $J_{\text{C-F}}$ = 24.8 Hz), 105.1, 104.8, 21.6, 21.5, 20.9 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{FN}_2\text{O}_4\text{S}_2 + \text{Na}]^+$ 671.1445, found 671.1453.



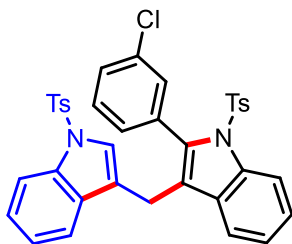
2-(4-bromophenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ae):

50.4 mg, 71% yield; light yellow solid, **m. p.** 215–216 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.1 Hz, 1H), 7.49 – 7.39 (m, 5H), 7.33 – 7.28 (m, 4H), 7.24 – 7.05 (m, 9H), 6.50 (s, 1H), 3.75 (s, 2H), 2.35 (s, 3H), 2.34 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.5, 144.7, 138.0, 137.0, 135.5, 134.8, 134.2, 132.2, 130.8, 130.8, 130.4, 129.8, 129.6, 129.5, 126.5, 126.4, 125.5, 125.1, 124.3, 123.5, 123.3, 123.2, 121.9, 121.4, 119.5, 119.1, 116.9, 114.0, 21.6, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{BrN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 726.1090, found 726.1085.



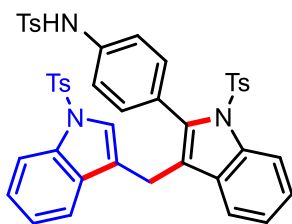
2-(3-chlorophenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3af):

37.6 mg, 57% yield; light yellow solid, **m. p.** 177–178 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.44 – 7.24 (m, 11H), 7.20 – 7.06 (m, 7H), 6.57 (s, 1H), 3.77 (s, 2H), 2.34 (s, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.5, 144.7, 137.9, 136.5, 135.5, 134.7, 134.4, 133.5, 132.6, 130.7, 130.5, 130.5, 129.7, 129.5, 129.0, 128.9, 128.9, 126.5, 125.5, 125.0, 124.2, 123.5, 123.3, 121.6, 121.5, 119.6, 119.2, 116.8, 114.0, 21.6, 21.5, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{ClN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 682.1596, found 682.1596.



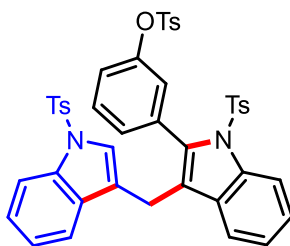
4-methyl-N-(4-(1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indol-2-yl)phenyl)benzenesulfonamide (3ag):

62.0 mg, 78% yield; white solid, **m. p.** 175–176 °C (PE/EA = 2:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.37 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.70 (d, J = 8.3 Hz, 2H), 7.41 – 7.37 (m, 3H), 7.33 – 7.27 (m, 3H), 7.22 – 7.16 (m, 7H), 7.15 – 7.03 (m, 8H), 6.51 (s, 1H), 3.70 (s, 2H), 2.34 (s, 3H), 2.32 (s, 3H), 2.31 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.4, 144.8, 144.1, 137.9, 137.3, 137.2, 135.9, 135.5, 134.6, 134.4, 131.8, 130.7, 130.5, 129.7, 129.6, 129.4, 127.4, 127.2, 126.5, 126.4, 125.3, 125.0, 124.2, 123.5, 123.3, 121.9, 120.8, 120.1, 119.4, 119.1, 116.8, 114.0, 21.6, 21.5, 21.5, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{44}\text{H}_{37}\text{N}_3\text{O}_6\text{S}_3 + \text{H}]^+$ 800.1917, found 800.1921.



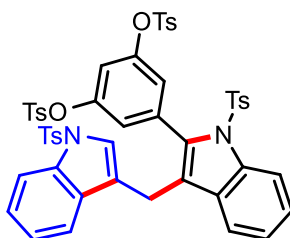
3-(1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indol-2-yl)phenyl 4-methylbenzenesulfonate (3ah):

70.0 mg, 88% yield; light yellow solid, **m. p.** 192–193 °C (PE/EA = 5:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.34 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 8.5 Hz, 1H), 7.66 (d, J = 8.2 Hz, 2H), 7.47 – 7.36 (m, 5H), 7.33 – 7.26 (m, 4H), 7.23 – 7.11 (m, 9H), 7.05 (d, J = 7.7 Hz, 1H), 6.95 (d, J = 7.9 Hz, 1H), 6.56 (s, 1H), 3.74 (s, 2H), 2.36 (s, 3H), 2.32 (s, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 148.9, 145.5, 144.8, 137.8, 136.3, 135.4, 134.7, 133.9, 132.9, 132.0, 130.7, 130.4, 130.0, 129.8, 129.7, 129.6, 128.7, 128.4, 126.6, 126.5, 125.5, 124.9, 124.3, 123.5, 123.3, 122.5, 121.9, 121.2, 119.6, 119.2, 116.8, 113.9, 21.6, 21.6, 21.5, 20.5 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{44}\text{H}_{36}\text{N}_2\text{O}_7\text{S}_3 + \text{Na}]^+$ 823.1577, found 823.1590.



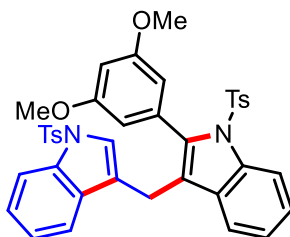
5-(1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indol-2-yl)-1,3-phenylene bis(4-methylbenzenesulfonate) (3ai):

84.0 mg, 87% yield; light yellow solid, **m. p.** 192–193 °C (PE/EA = 5:1, R_f = 0.1).

^1H NMR (300 MHz, CDCl_3) δ 8.28 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 8.1 Hz, 1H), 7.64 (d, J = 8.2 Hz, 4H), 7.48 (d, J = 8.2 Hz, 2H), 7.42 – 7.36 (m, 3H), 7.32 – 7.16 (m, 11H), 7.12 – 7.02 (m, 4H), 6.69 (t, J = 2.0 Hz, 1H), 6.54 (s, 1H), 3.70 (s, 2H), 2.39 (s, 6H), 2.33 (s, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 149.0, 145.9, 145.7, 144.9, 137.8, 135.3, 134.8, 134.7, 134.0, 133.5, 131.4, 130.5, 130.3, 130.1, 129.8, 129.7, 128.4, 126.6, 126.5, 125.8, 125.0, 124.5, 123.3, 122.7, 120.7, 119.9, 119.1, 117.4, 116.7, 113.8, 21.7, 21.6, 21.5, 20.4 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{51}\text{H}_{42}\text{N}_2\text{O}_{10}\text{S}_4 + \text{Na}]^+$ 993.1614, found 993.1606.



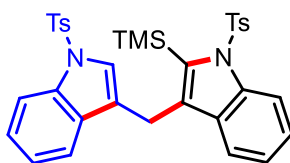
2-(3,5-dimethoxyphenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3aj):

66.4 mg, 96% yield; light yellow solid, **m. p.** 197–198 °C (PE/EA = 10:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.38 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.43 – 7.24 (m, 7H), 7.18 – 7.05 (m, 7H), 6.61 (s, 1H), 6.51 (s, 3H), 3.82 (s, 2H), 3.70 (s, 6H), 2.32 (s, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 159.8, 145.2, 144.6, 138.0, 137.9, 135.4, 134.8, 134.4, 132.6, 130.7, 130.6, 129.6, 129.4, 126.6, 126.5, 125.2, 124.9, 124.1, 123.6, 123.2, 121.9, 120.9, 119.4, 119.2, 116.8, 113.9, 109.1, 101.0, 55.2, 21.5, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{39}\text{H}_{34}\text{N}_2\text{O}_6\text{S}_2 + \text{H}]^+$ 691.1931, found 691.1936.



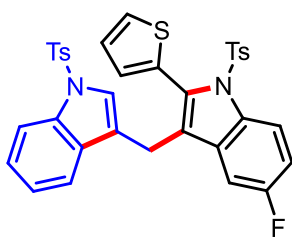
1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-2-(trimethylsilyl)-1H-indole (3al):

46.0 mg, 73% yield; light yellow solid, **m. p.** 196–197 °C (PE/EA = 40:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.05 – 7.97 (m, 2H), 7.54 – 7.52 (m, 3H), 7.43 (d, J = 8.3 Hz, 2H), 7.34 (t, J = 7.7 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.16 (d, J = 8.2 Hz, 2H), 7.07 – 6.98 (m, 4H), 6.72 (s, 1H), 4.14 (s, 2H), 2.31 (s, 3H), 2.26 (s, 3H), 0.48 (s, 9H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 144.6, 144.5, 139.6, 139.4, 135.5, 134.9, 134.7, 133.8, 132.3, 130.5, 129.6, 129.5, 126.5, 126.3, 125.4, 125.0, 123.8, 123.5, 123.3, 122.5, 119.4, 119.1, 115.6, 114.0, 22.0, 21.5, 21.5, 2.3 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{34}\text{H}_{34}\text{N}_2\text{O}_4\text{S}_2\text{Si} + \text{Na}]^+$ 649.1621, found 649.1628.



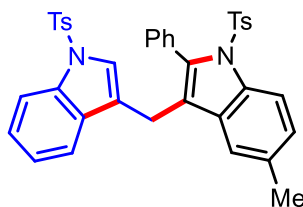
5-fluoro-2-(thiophen-2-yl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3am):

54.5 mg, 83% yield; light yellow solid, **m. p.** 209–210 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.40 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.42 – 7.38 (m, 3H), 7.32 – 7.27 (m, 6H), 7.19 – 7.01 (m, 9H), 6.54 (s, 1H), 3.75 (s, 2H), 2.34 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 162.9 (d, $J_{\text{C-F}}$ = 225.2 Hz), 145.4, 144.7, 137.9, 137.1, 135.5, 134.7, 134.4, 132.6 (d, $J_{\text{C-F}}$ = 8.3 Hz), 130.7, 130.5, 129.6, 129.5, 126.8 (d, $J_{\text{C-F}}$ = 3.4 Hz), 126.5, 126.4, 125.3, 125.0, 124.2, 123.5, 123.3, 121.9, 121.0, 119.3 (d, $J_{\text{C-F}}$ = 19.3 Hz), 116.8, 114.9, 114.6, 114.0, 21.6, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{35}\text{H}_{27}\text{FN}_2\text{O}_4\text{S}_3 + \text{Na}]^+$ 677.1009, found 677.1014.



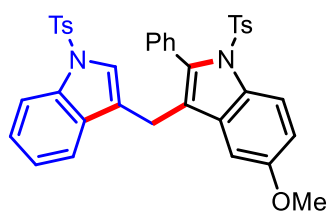
5-methyl-2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3an):

49.4 mg, 77% yield; yellow solid, **m. p.** 143–144 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.26 (d, J = 8.5 Hz, 1H), 7.96 (d, J = 8.3 Hz, 1H), 7.44 – 7.28 (m, 11H), 7.23 – 7.09 (m, 6H), 6.87 (s, 1H), 6.53 (s, 1H), 3.74 (s, 2H), 2.34 (s, 3H), 2.32 (s, 3H), 2.31 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.2, 144.6, 138.4, 136.1, 135.5, 134.8, 134.3, 133.9, 131.2, 131.0, 130.7, 130.6, 129.6, 129.4, 128.7, 127.5, 126.6, 126.5, 124.9, 123.5, 123.2, 122.1, 120.7, 119.2, 119.2, 116.6, 113.9, 21.6, 21.5, 21.3, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 662.2142, found 662.2145.



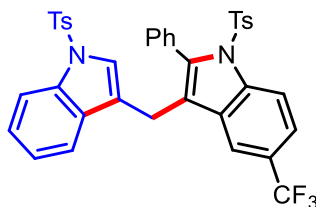
5-methoxy-2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ao):

35.2 mg, 53% yield; light yellow solid, **m. p.** 187–188 °C (PE/EA = 10:1, R_f = 0.2).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.28 (d, J = 9.1 Hz, 1H), 7.96 (d, J = 8.3 Hz, 1H), 7.44 – 7.28 (m, 11H), 7.21 – 7.17 (m, 3H), 7.07 (d, J = 8.1 Hz, 2H), 6.99 (dd, J = 9.1, 2.4 Hz, 1H), 6.53 (s, 1H), 6.41 (d, J = 2.3 Hz, 1H), 3.74 (s, 2H), 3.55 (s, 3H), 2.33 (s, 6H) ppm

$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 157.0, 145.3, 144.7, 139.2, 135.5, 134.7, 132.1, 132.3, 132.1, 130.9, 130.7, 130.6, 129.6, 129.4, 128.7, 127.6, 126.5, 126.5, 125.0, 123.6, 123.3, 122.0, 121.1, 119.1, 118.0, 114.0, 113.5, 101.9, 54.3, 21.6, 21.5, 20.7 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_5\text{S}_2 + \text{Na}]^+$ 683.1645, found 683.1654.



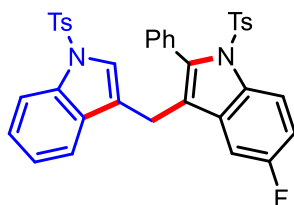
2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-5-(trifluoromethyl)-1H-indole (3ap):

54.2 mg, 78% yield; light yellow solid, **m. p.** 197–198 °C (PE/EA = 20:1, R_f = 0.2).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.53 (d, J = 8.8 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.66 (dd, J = 8.9, 1.4 Hz, 1H), 7.46 – 7.29 (m, 12H), 7.21 – 7.11 (m, 5H), 6.55 (s, 1H), 3.80 (s, 2H), 2.36 (s, 3H), 2.33 (s, 3H) ppm.

$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 145.8, 145.0, 140.0, 139.4, 135.4, 134.6, 134.4, 130.9, 130.5, 130.3, 130.0, 129.7, 129.7, 129.2, 127.7, 126.5, 126.4, 125.1, 123.2, 123.2, 121.9 (q, $J_{\text{C-F}}$ = 3.4 Hz), 121.4, 120.1, 119.2, 117.1, 116.5 (q, $J_{\text{C-F}}$ = 4.1 Hz), 113.9, 21.6, 21.4, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{29}\text{F}_3\text{N}_2\text{O}_4\text{S}_2 + \text{Na}]^+$ 721.1413, found 721.1411.



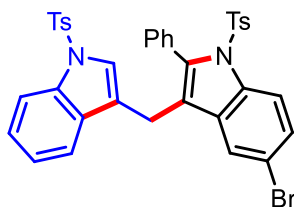
5-fluoro-2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3aq):

46.5 mg, 72% yield; white solid, **m. p.** 177–178 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.35 (dd, J = 9.1, 4.5 Hz, 1H), 7.98 (d, J = 8.9 Hz, 1H), 7.45 – 7.35 (m, 7H), 7.32 – 7.28 (m, 4H), 7.21 – 7.08 (m, 6H), 6.62 (dd, J = 8.5, 2.5 Hz, 1H), 6.52 (s, 1H), 3.73 (s, 2H), 2.36 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 160.0 (d, $J_{\text{C-F}}$ = 240.2 Hz), 145.6, 144.9, 140.2, 135.6, 134.5, 134.1, 134.1, 134.1, 132.1 (d, $J_{\text{C-F}}$ = 9.5 Hz), 130.7, 130.5, 130.4, 129.7, 129.5, 129.0, 127.6, 126.5, 126.4, 125.1, 123.6, 123.3, 121.7, 120.5 (d, $J_{\text{C-F}}$ = 3.8 Hz), 119.1, 118.2 (d, $J_{\text{C-F}}$ = 9.1 Hz), 114.1, 112.9 (d, $J_{\text{C-F}}$ = 24.9 Hz), 105.1 (d, $J_{\text{C-F}}$ = 23.8 Hz), 21.6, 21.5, 20.8 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{FN}_2\text{O}_4\text{S}_2 + \text{Na}]^+$ 671.1445, found 671.1450.



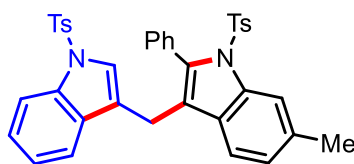
5-bromo-2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ar):

64.3 mg, 91% yield; light yellow solid, **m. p.** 164–165 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.29 (d, J = 8.9 Hz, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.50 (dd, J = 8.9, 1.9 Hz, 1H), 7.44 – 7.29 (m, 11H), 7.21 – 7.15 (m, 6H), 6.52 (s, 1H), 3.73 (s, 2H), 2.36 (s, 3H), 2.34 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.7, 144.8, 139.7, 136.7, 135.5, 134.6, 134.2, 132.7, 130.8, 130.4, 130.2, 129.8, 129.6, 129.1, 128.0, 127.6, 126.5, 126.5, 125.1, 123.4, 123.3, 121.9, 121.6, 119.8, 119.2, 118.4, 117.7, 114.0, 21.6, 21.6, 20.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{BrN}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 726.1090, found 726.1105.



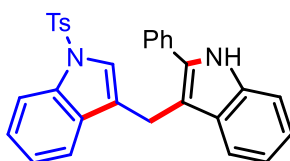
6-methyl-2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3as):

32.0 mg, 50% yield; white solid, **m. p.** 193–194 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.22 (s, 1H), 7.94 (d, J = 8.2 Hz, 1H), 7.44 – 7.26 (m, 11H), 7.18 – 7.09 (m, 5H), 6.99 – 6.92 (m, 2H), 6.56 (s, 1H), 3.73 (s, 2H), 2.56 (s, 3H), 2.35 (s, 3H), 2.34 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.2, 144.6, 138.4, 137.6, 135.5, 135.3, 134.8, 134.5, 131.0, 130.8, 130.6, 129.6, 129.4, 128.6, 128.6, 127.5, 126.5, 126.5, 125.5, 124.9, 123.6, 123.2, 122.2, 120.8, 119.2, 119.0, 117.0, 114.0, 22.1, 21.6, 21.5, 20.8 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{32}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 662.2142, found 662.2144.



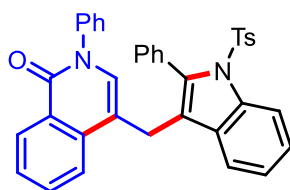
2-phenyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3au):

24.0 mg, 50% yield; light yellow solid, **m. p.** 188–189 °C (PE/EA = 10:1, R_f = 0.3).

^1H NMR (300 MHz, CDCl_3) δ 8.22 (s, 1H), 8.00 (d, J = 8.2 Hz, 1H), 7.56 (d, J = 8.4 Hz, 2H), 7.51 – 7.29 (m, 9H), 7.26 – 7.20 (m, 2H), 7.13 (d, J = 8.0 Hz, 2H), 7.08 – 7.02 (m, 2H), 4.19 (s, 2H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 144.5, 136.1, 135.8, 135.3, 134.9, 132.7, 131.0, 129.6, 129.1, 128.9, 127.8, 127.7, 126.7, 124.7, 124.3, 123.4, 123.2, 122.5, 119.7, 119.5, 119.3, 114.0, 111.0, 109.1, 21.5, 20.8 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_2\text{S} + \text{Na}]^+$ 499.1451, found 499.1454.



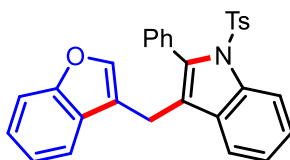
2-phenyl-4-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)isoquinolin-1(2H)-one (5):

52.2 mg, 90% yield; light yellow solid, **m. p.** 200–201 °C (PE/EA = 5:1, R_f = 0.1).

^1H NMR (300 MHz, CDCl_3) δ 8.48 (d, J = 7.2 Hz, 1H), 8.34 (d, J = 8.4 Hz, 1H), 7.66 – 7.48 (m, 3H), 7.43 – 7.29 (m, 9H), 7.23 – 7.13 (m, 6H), 6.75 (d, J = 8.2 Hz, 2H), 6.42 (s, 1H), 3.90 (s, 2H), 2.17 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 161.4, 144.5, 141.2, 138.7, 137.5, 136.5, 135.2, 132.5, 130.9, 130.5, 130.4, 130.0, 129.1, 128.9, 128.7, 127.8, 127.5, 127.1, 126.5, 126.3, 126.2, 125.3, 124.1, 122.4, 119.4, 119.2, 116.4, 113.4, 24.5, 21.5 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{28}\text{N}_2\text{O}_3\text{S} + \text{H}]^+$ 581.1893, found 581.1898.



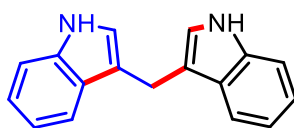
3-(benzofuran-3-ylmethyl)-2-phenyl-1-tosyl-1H-indole (7):

20.6 mg, 43% yield; white solid, **m. p.** 180–181 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.37 (d, J = 8.4 Hz, 1H), 7.43 – 7.34 (m, 7H), 7.31 – 7.24 (m, 5H), 7.22 – 7.07 (m, 4H), 6.46 (s, 1H), 3.81 (s, 2H), 2.36 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 155.4, 144.7, 141.9, 138.0, 137.9, 134.5, 131.2, 131.0, 130.8, 129.2, 128.7, 127.6, 126.8, 125.2, 124.4, 124.3, 122.4, 121.4, 119.5, 119.4, 118.9, 117.0, 111.4, 21.5, 19.4 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{30}\text{H}_{23}\text{NO}_3\text{S} + \text{Na}]^+$ 500.1291, found 500.1288.

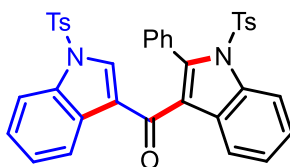


di(1H-indol-3-yl)methane (8):⁹

18.9 mg, 77% yield; reddish-brown solid (PE/EA = 10:1, R_f = 0.2).

¹H NMR (300 MHz, DMSO) δ 10.74 (s, 2H), 7.52 (d, J = 7.9 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 2.2 Hz, 2H), 7.06 – 7.00 (m, 2H), 6.94 – 6.89 (m, 2H), 4.13 (s, 2H) ppm.

¹³C NMR (75 MHz, DMSO) δ 136.8, 127.6, 123.2, 121.2, 119.1, 118.5, 114.6, 111.8, 21.4 ppm.



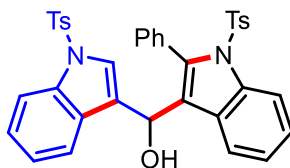
(2-phenyl-1-tosyl-1H-indol-3-yl)(1-tosyl-1H-indol-3-yl)methanone (9):

30.0 mg, 93% yield; yellow solid, **m. p.** 143–144 °C (PE/EA = 20:1, R_f = 0.2).

¹H NMR (300 MHz, CDCl₃) δ 8.45 (d, J = 8.5 Hz, 1H), 8.20 – 8.14 (m, 1H), 7.77 – 7.72 (m, 1H), 7.62 – 7.56 (m, 4H), 7.50 – 7.44 (m, 1H), 7.40 – 7.37 (m, 2H), 7.35 – 7.29 (m, 2H), 7.28 – 7.18 (m, 8H), 7.06 (d, J = 8.1 Hz, 2H), 2.36 (s, 3H), 2.31 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 186.7, 145.8, 145.3, 141.1, 137.0, 134.7, 134.5, 134.5, 134.3, 131.8, 130.1, 129.9, 129.5, 129.3, 128.9, 127.4, 127.4, 127.1, 126.9, 125.8, 125.6, 124.8, 124.6, 124.3, 122.6, 120.8, 120.5, 116.3, 112.8, 21.6, 21.5 ppm.

HRMS (ESI) m/z Calcd for [C₃₇H₂₈N₂O₅S₂ + H]⁺ 645.1512, found 645.1514.



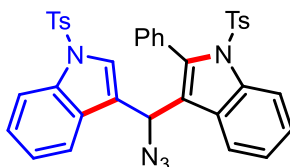
(2-phenyl-1-tosyl-1*H*-indol-3-yl)(1-tosyl-1*H*-indol-3-yl)methanol (10):

27.5 mg, 85% yield; white solid, **m. p.** 193–194 °C (PE/EA = 5:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.39 (d, $J = 8.7$ Hz, 1H), 7.94 (d, $J = 8.3$ Hz, 1H), 7.54 (d, $J = 8.2$ Hz, 2H), 7.45 – 7.04 (m, 17H), 6.99 (s, 1H), 5.86 (s, 1H), 2.35 (s, 3H), 2.34 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 144.9, 138.2, 137.9, 135.7, 134.9, 134.8, 130.1, 129.8, 129.5, 129.3, 129.1, 128.5, 127.6, 126.7, 126.6, 125.2, 124.9, 124.4, 123.9, 123.3, 123.3, 121.3, 120.6, 116.5, 113.8, 63.7, 21.6, 21.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{30}\text{N}_2\text{O}_5\text{S}_2 + \text{Na}]^+$ 669.1488, found 669.1467.



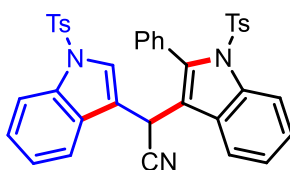
3-(azido(1-tosyl-1*H*-indol-3-yl)methyl)-2-phenyl-1-tosyl-1*H*-indole (11):

29.3 mg, 87% yield; white solid, **m. p.** 216–217 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.38 (d, $J = 8.5$ Hz, 1H), 7.93 (d, $J = 8.4$ Hz, 1H), 7.61 (d, $J = 8.3$ Hz, 2H), 7.49 – 7.00 (m, 18H), 5.76 (d, $J = 1.5$ Hz, 1H), 2.35 (s, 3H), 2.34 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.3, 145.1, 139.8, 137.6, 135.5, 134.9, 134.8, 129.8, 129.5, 128.5, 127.9, 127.8, 126.7, 126.6, 125.5, 125.0, 124.5, 124.0, 123.3, 120.7, 120.4, 120.0, 118.8, 116.3, 113.8, 54.8, 21.6, 21.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{37}\text{H}_{29}\text{N}_5\text{O}_4\text{S}_2 + \text{Na}]^+$ 694.1553, found 694.1562.



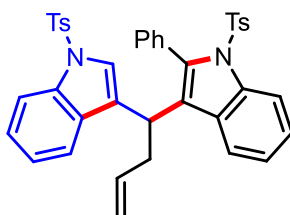
2-(2-phenyl-1-tosyl-1H-indol-3-yl)-2-(1-tosyl-1H-indol-3-yl)acetonitrile (12):

10.1 mg, 31% yield; light yellow solid, **m. p.** 205–206 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.41 (d, J = 8.6 Hz, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.3 Hz, 2H), 7.53 – 7.27 (m, 10H), 7.22 – 7.09 (m, 8H), 5.09 (d, J = 1.4 Hz, 1H), 2.37 (s, 3H), 2.36 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.5, 145.3, 139.0, 137.3, 135.4, 134.9, 134.7, 130.0, 129.9, 129.7, 129.2, 128.1, 128.0, 127.5, 126.8, 126.6, 125.8, 125.5, 124.8, 124.3, 123.7, 119.6, 119.4, 117.5, 116.4, 115.9, 114.5, 113.9, 25.8, 21.6, 21.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{38}\text{H}_{29}\text{N}_3\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 673.1938, found 673.1933.



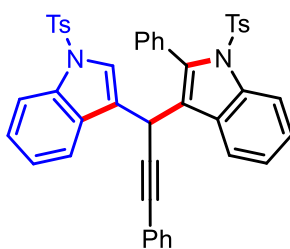
2-phenyl-1-tosyl-3-(1-(1-tosyl-1H-indol-3-yl)but-3-en-1-yl)-1H-indole (13):

20.1 mg, 60% yield; white solid, **m. p.** 220–221 °C (PE/EA = 20:1, R_f = 0.2).

^1H NMR (300 MHz, CDCl_3) δ 8.32 (d, J = 8.4 Hz, 1H), 7.88 (d, J = 8.3 Hz, 1H), 7.65 (d, J = 8.2 Hz, 2H), 7.42 (s, 4H), 7.32 – 7.27 (m, 5H), 7.22 – 7.01 (m, 7H), 6.87 (t, J = 7.5 Hz, 1H), 6.77 (d, J = 7.8 Hz, 1H), 5.45 – 5.29 (m, 1H), 4.87 – 4.79 (m, 2H), 4.17 – 4.11 (m, 1H), 2.95 – 2.74 (m, 2H), 2.34 (s, 3H), 2.33 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 144.8, 144.6, 137.8, 137.5, 135.7, 135.3, 135.1, 135.1, 131.1, 130.3, 129.8, 129.4, 129.2, 128.9, 127.5, 126.7, 126.6, 124.8, 124.6, 124.5, 123.6, 123.6, 123.0, 122.9, 120.3, 120.0, 116.8, 116.5, 113.6, 37.3, 33.5, 21.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{40}\text{H}_{34}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 688.2298, found 688.2300.



2-phenyl-3-(3-phenyl-1-(1-tosyl-1H-indol-3-yl)prop-2-yn-1-yl)-1-tosyl-1H-indole (14):

26.2 mg, 72% yield; light yellow solid, **m. p.** 105–106 °C (PE/EA = 20:1, $R_f = 0.2$).

^1H NMR (300 MHz, CDCl_3) δ 8.38 (d, $J = 8.4$ Hz, 1H), 7.92 (d, $J = 8.3$ Hz, 1H), 7.57 – 7.45 (m, 6H), 7.40 – 7.22 (m, 12H), 7.18 – 7.04 (m, 7H), 5.18 (d, $J = 1.5$ Hz, 1H), 2.35 (s, 3H), 2.31 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 145.1, 144.8, 137.8, 137.5, 135.7, 135.0, 135.0, 131.6, 130.3, 129.8, 129.8, 129.4, 129.4, 129.3, 129.2, 129.0, 128.2, 127.7, 126.7, 126.6, 125.1, 124.8, 124.2, 123.8, 123.2, 122.9, 121.7, 120.8, 120.7, 120.3, 116.5, 113.8, 87.4, 83.5, 26.8, 21.6 ppm.

HRMS (ESI) m/z Calcd for $[\text{C}_{45}\text{H}_{34}\text{N}_2\text{O}_4\text{S}_2 + \text{NH}_4]^+$ 748.2298, found 748.2298.

6. X-ray Crystallography Data of 3ab

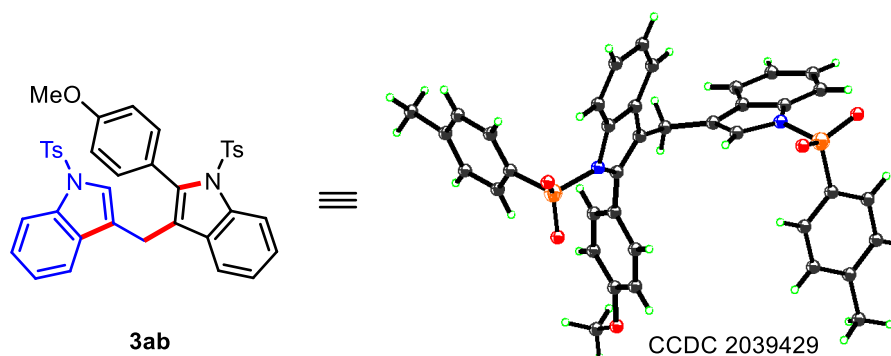


Figure S1. X-ray Crystallography of 3ab

CCDC 2039429 (**3ab**) contains the supplementary crystallographic data. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

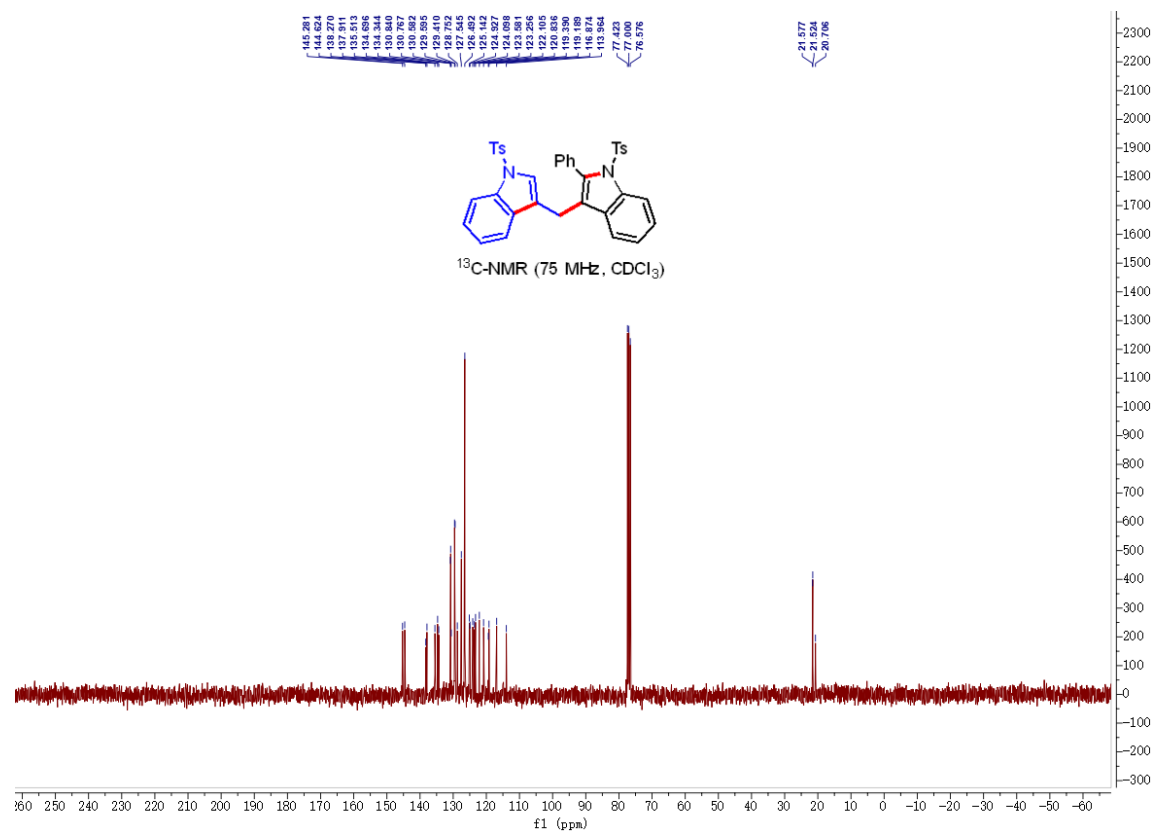
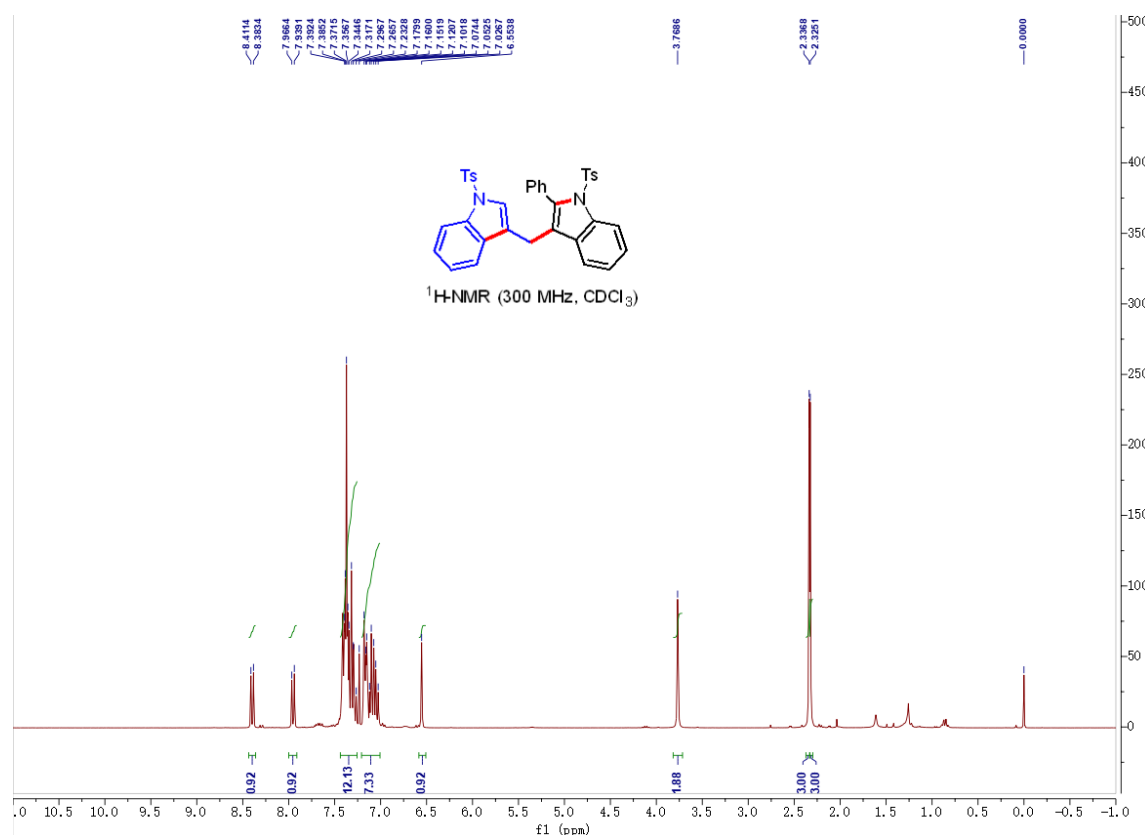
Datablock: 20200612

Bond precision:	C-C = 0.0031 Å	Wavelength=1.54178	
Cell:	a=10.9256(5)	b=12.3957(6)	c=13.8847(6)
	alpha=71.510(2)	beta=73.074(2)	gamma=72.150(2)
Temperature:	302 K		
	Calculated	Reported	
Volume	1657.87(13)	1657.87(14)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C38 H32 N2 O5 S2	C38 H32 N2 O5 S2	
Sum formula	C38 H32 N2 O5 S2	C38 H32 N2 O5 S2	
Mr	660.78	660.77	
Dx, g cm ⁻³	1.324	1.324	
Z	2	2	
Mu (mm ⁻¹)	1.839	1.839	
F000	692.0	692.0	
F000'	695.24		
h, k, lmax	13, 15, 17	13, 15, 17	
Nref	6555	6516	
Tmin, Tmax	0.754, 0.866	0.641, 0.754	
Tmin'	0.549		
Correction method=	# Reported T Limits: Tmin=0.641 Tmax=0.754		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.994	Theta(max)=	72.360
R(reflections)=	0.0370(5207)	wR2(reflections)=	0.1039(6516)
S =	1.068	Npar=	428

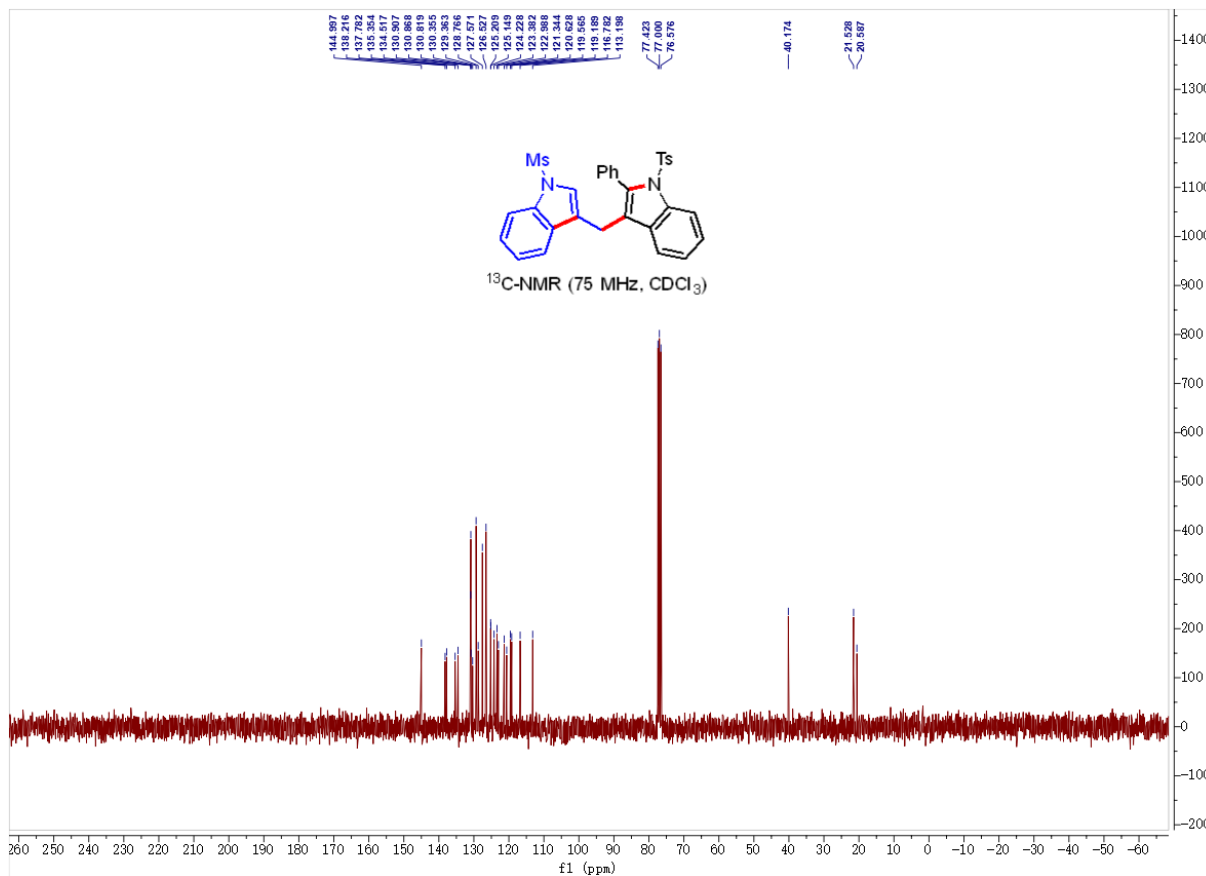
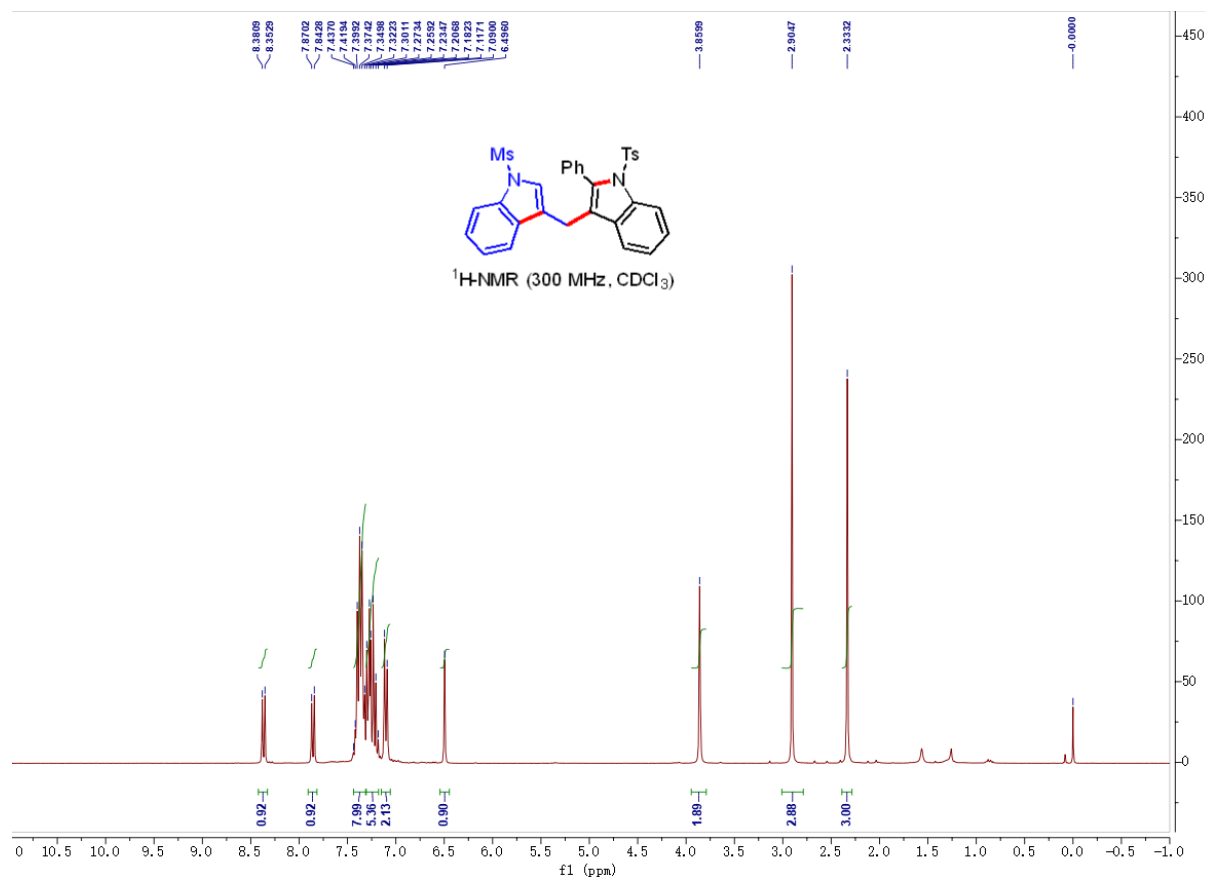
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Click on the hyperlinks for more details of the test.

7. ¹H and ¹³C NMR Spectra of Title Compounds

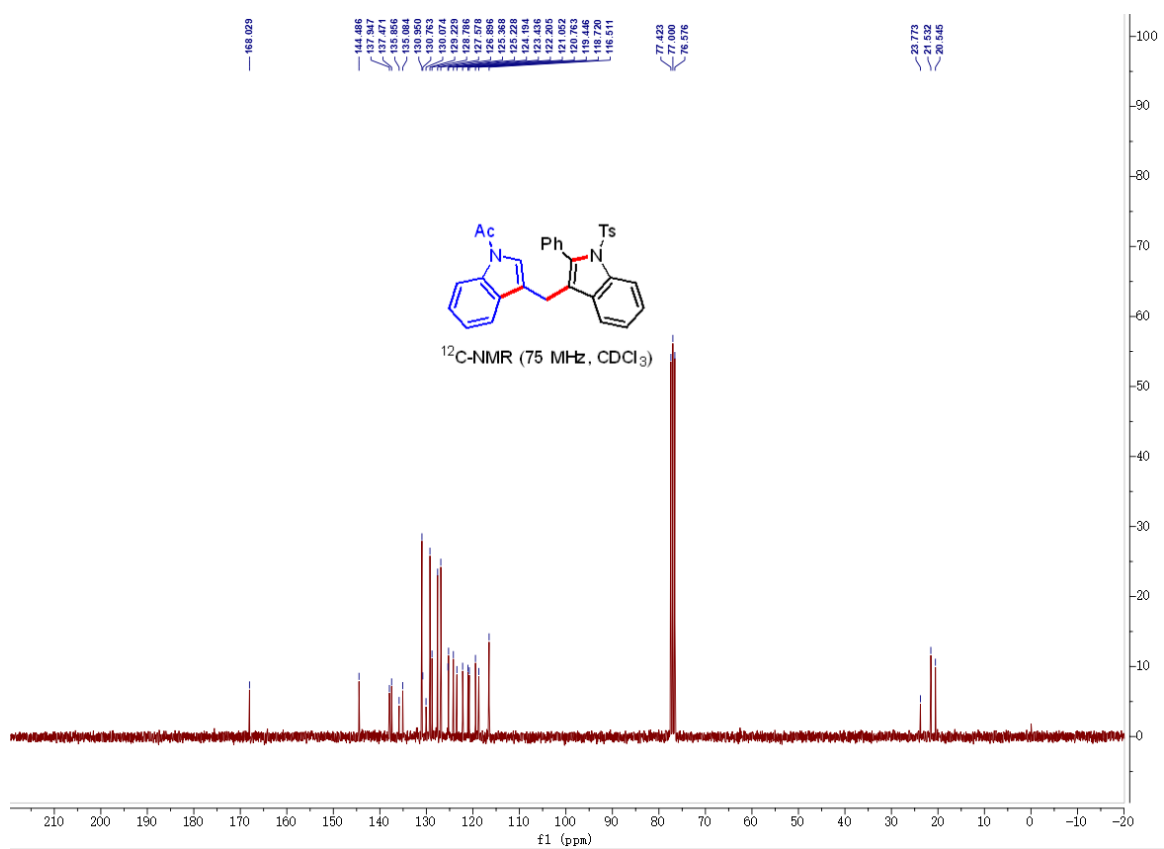
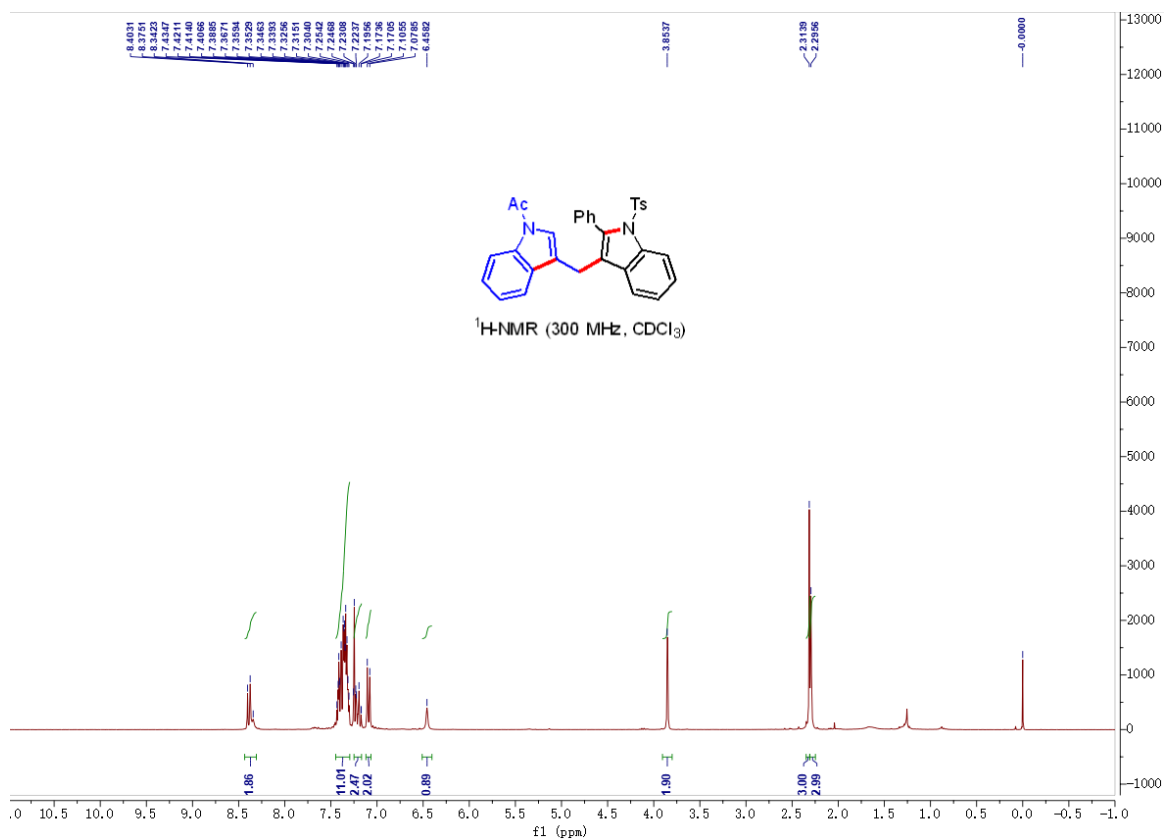
2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3aa):



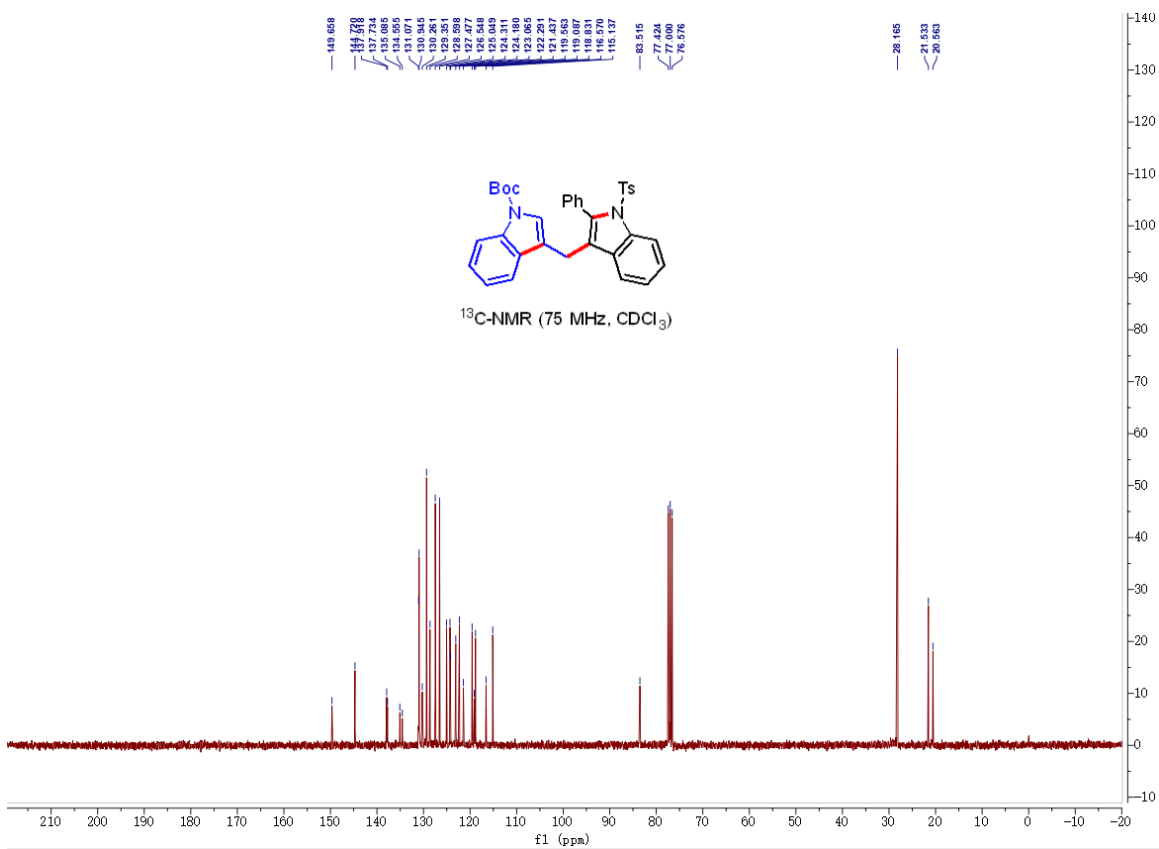
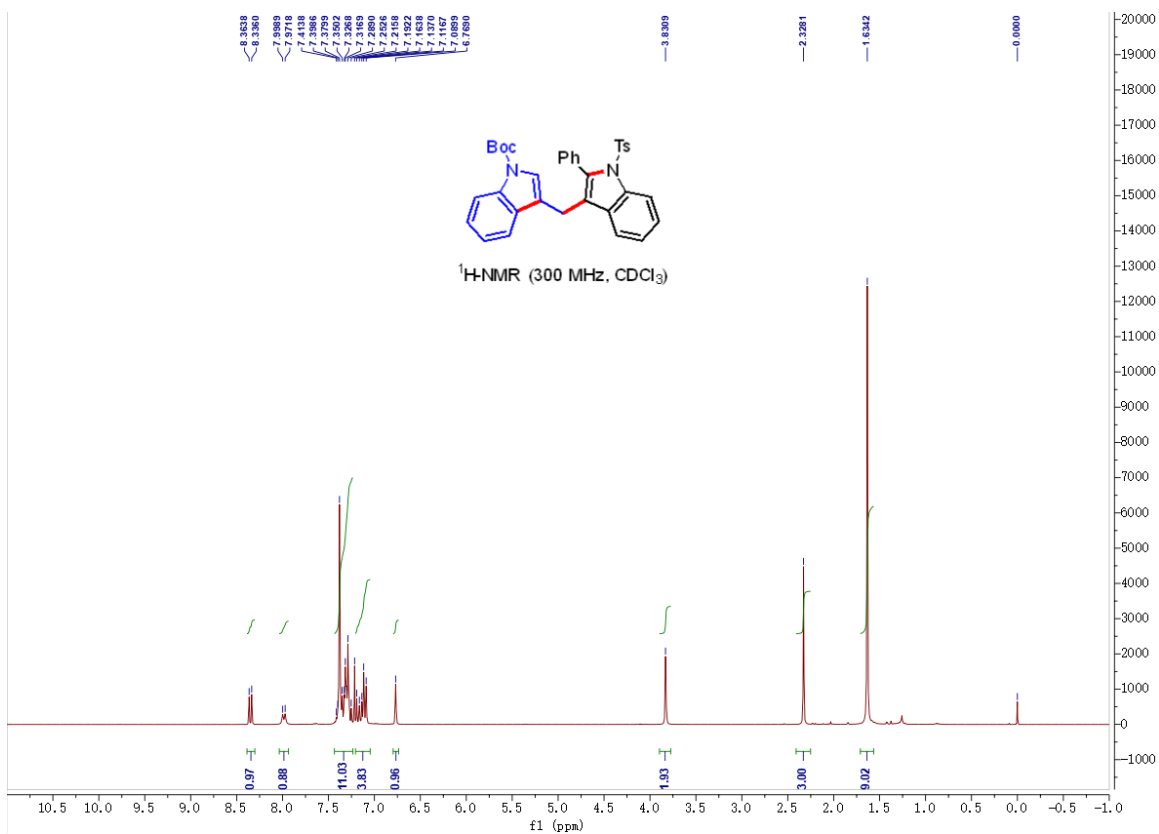
3-((1-(methylsulfonyl)-1H-indol-3-yl)methyl)-2-phenyl-1-tosyl-1H-indole (3ba):



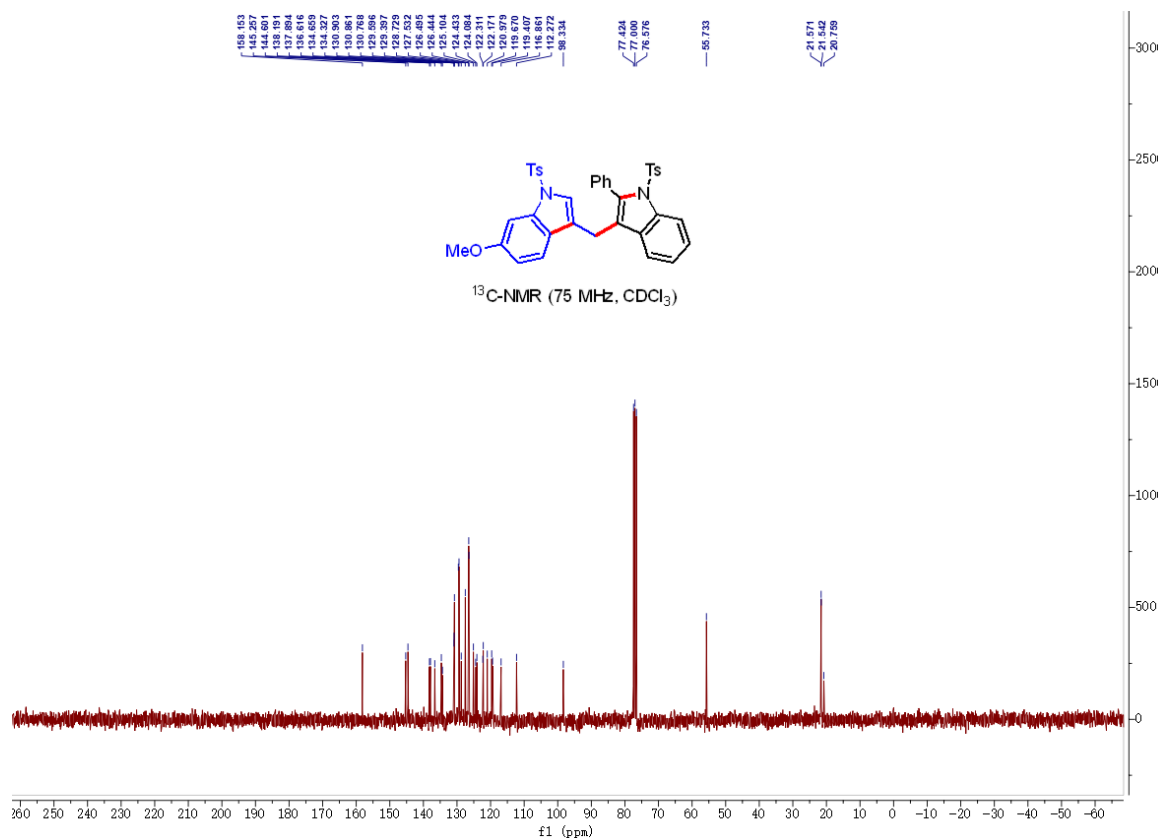
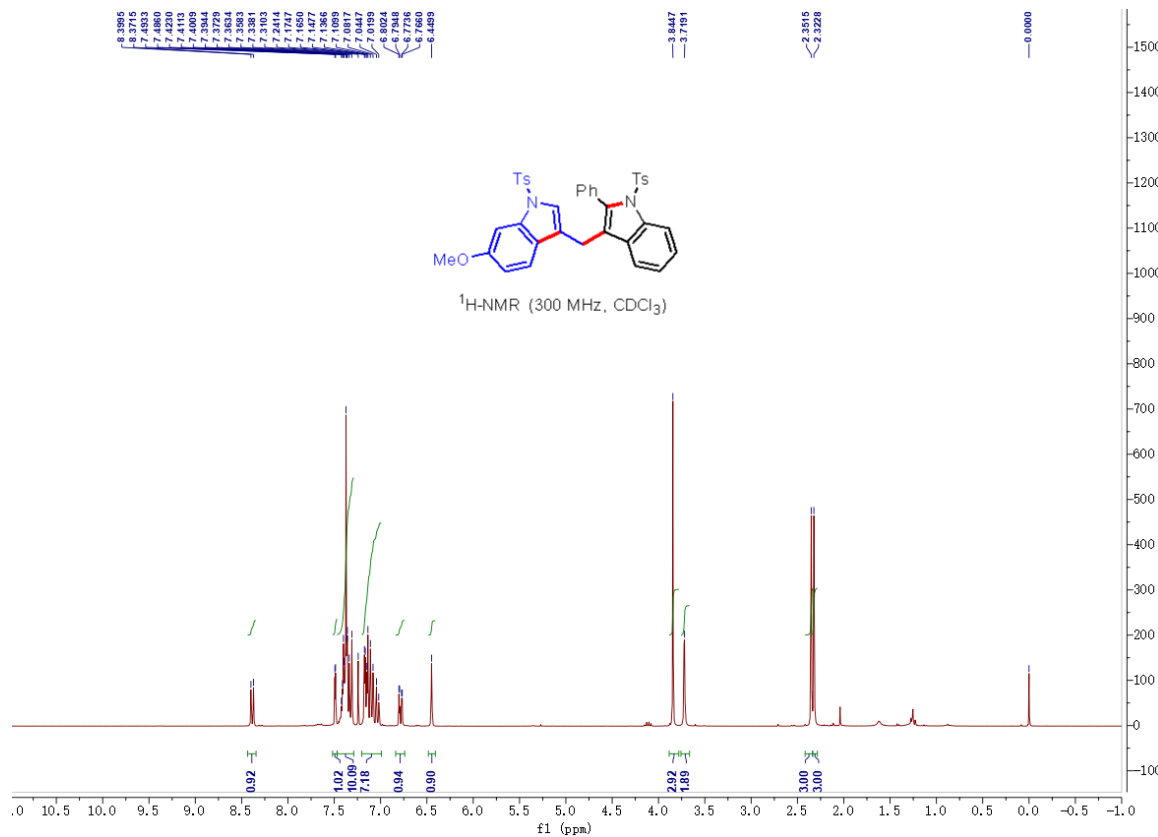
1-(3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indol-1-yl)ethan-1-one (3ca):



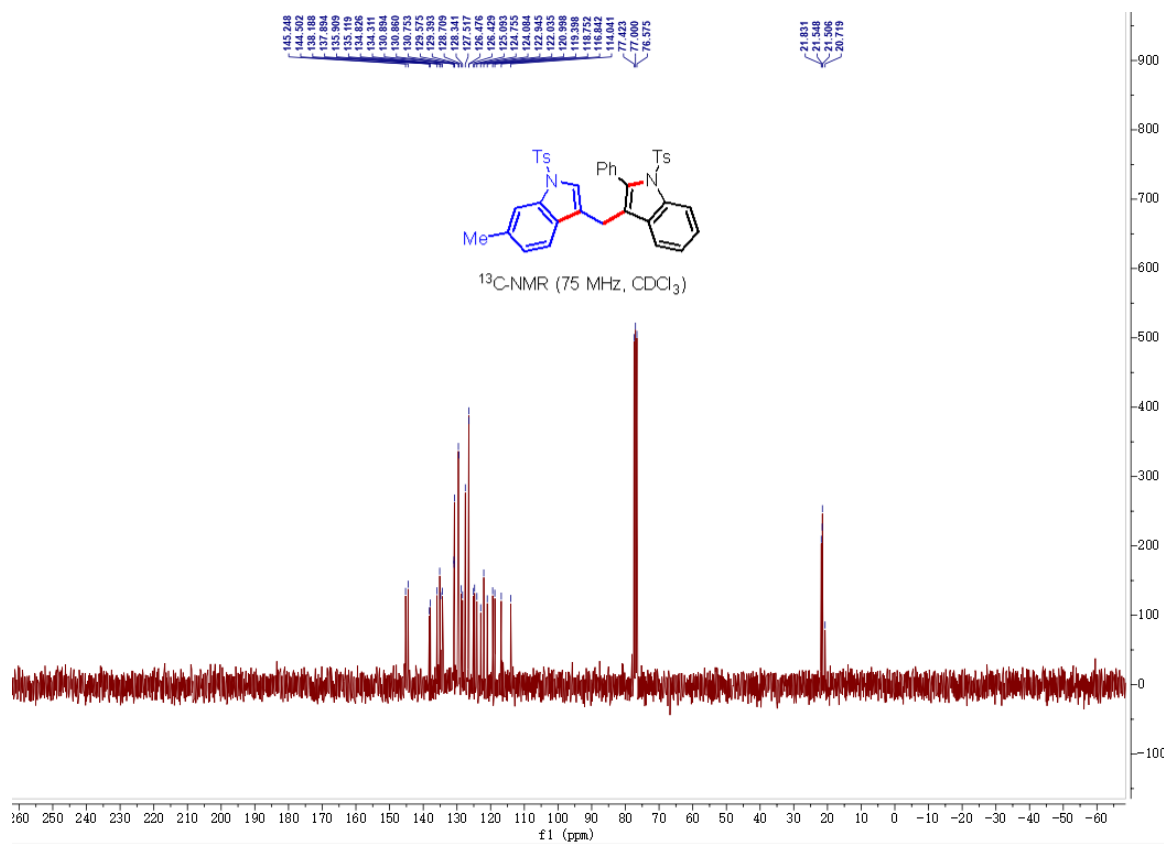
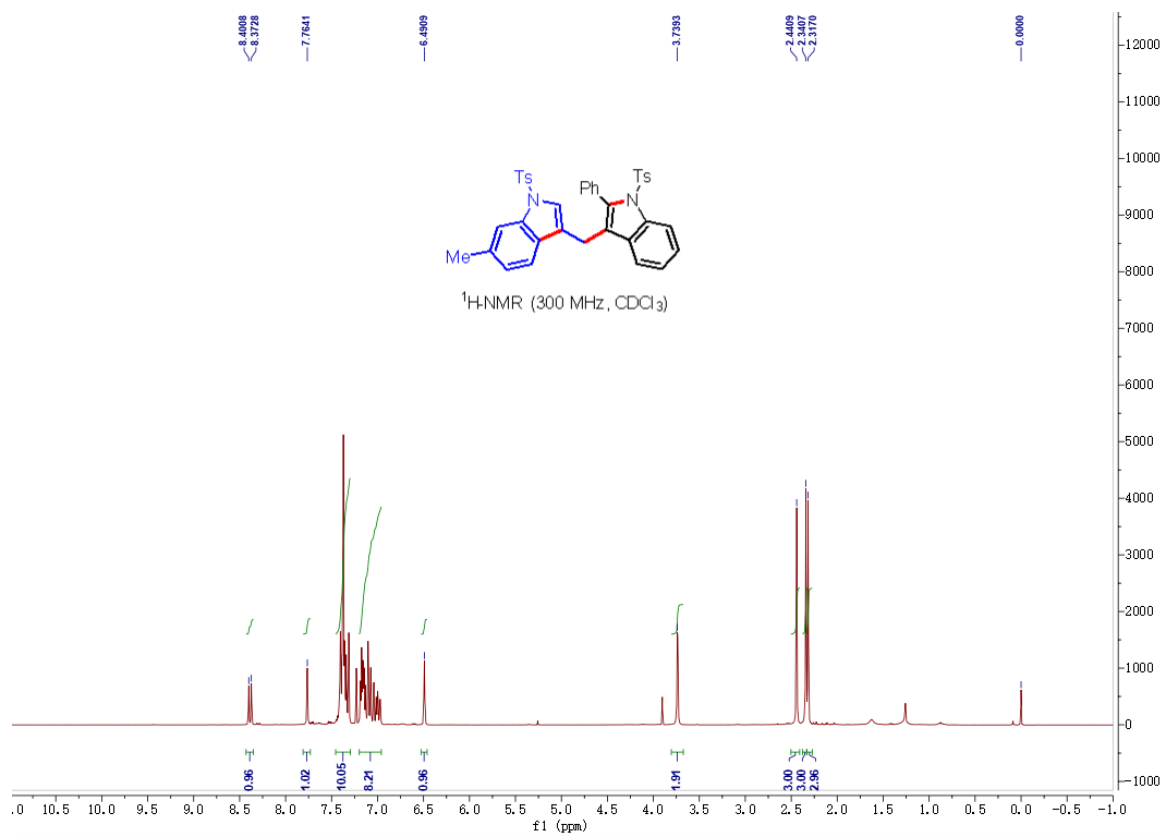
***tert*-butyl 3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole-1-carboxylate (3da):**



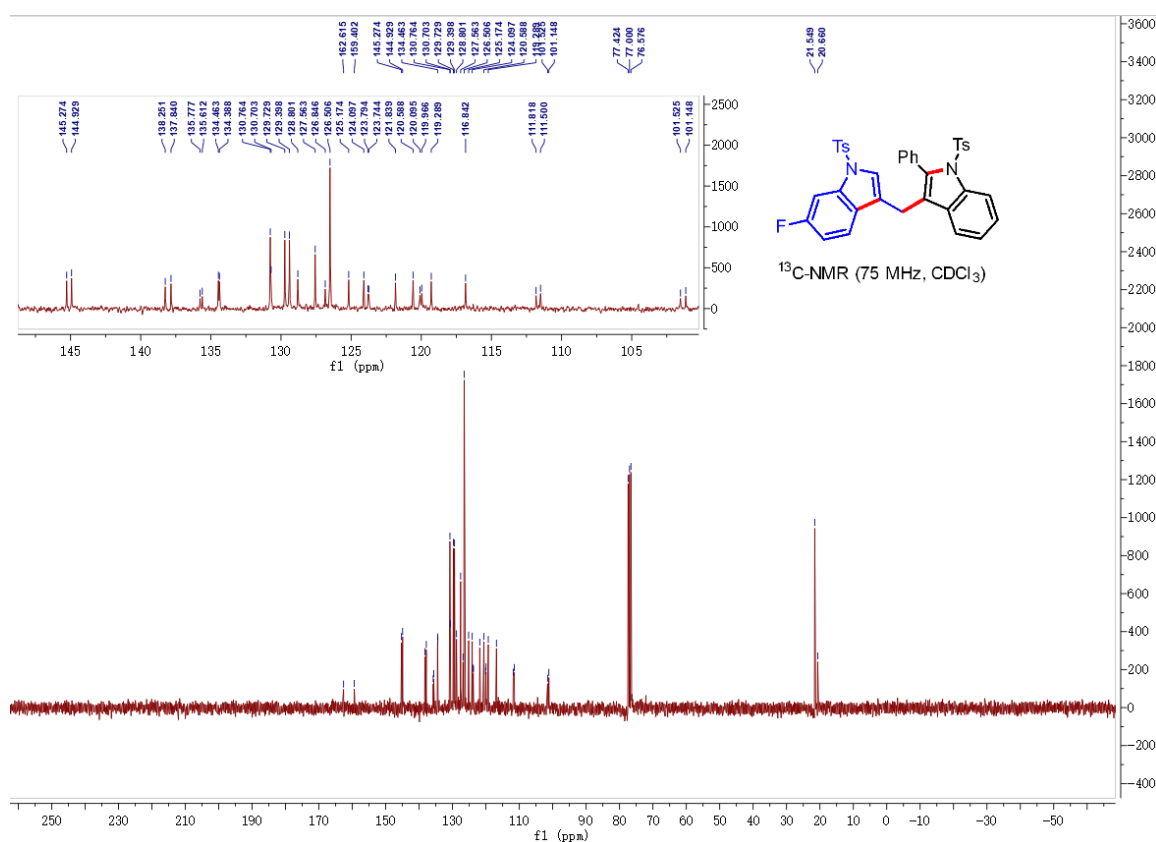
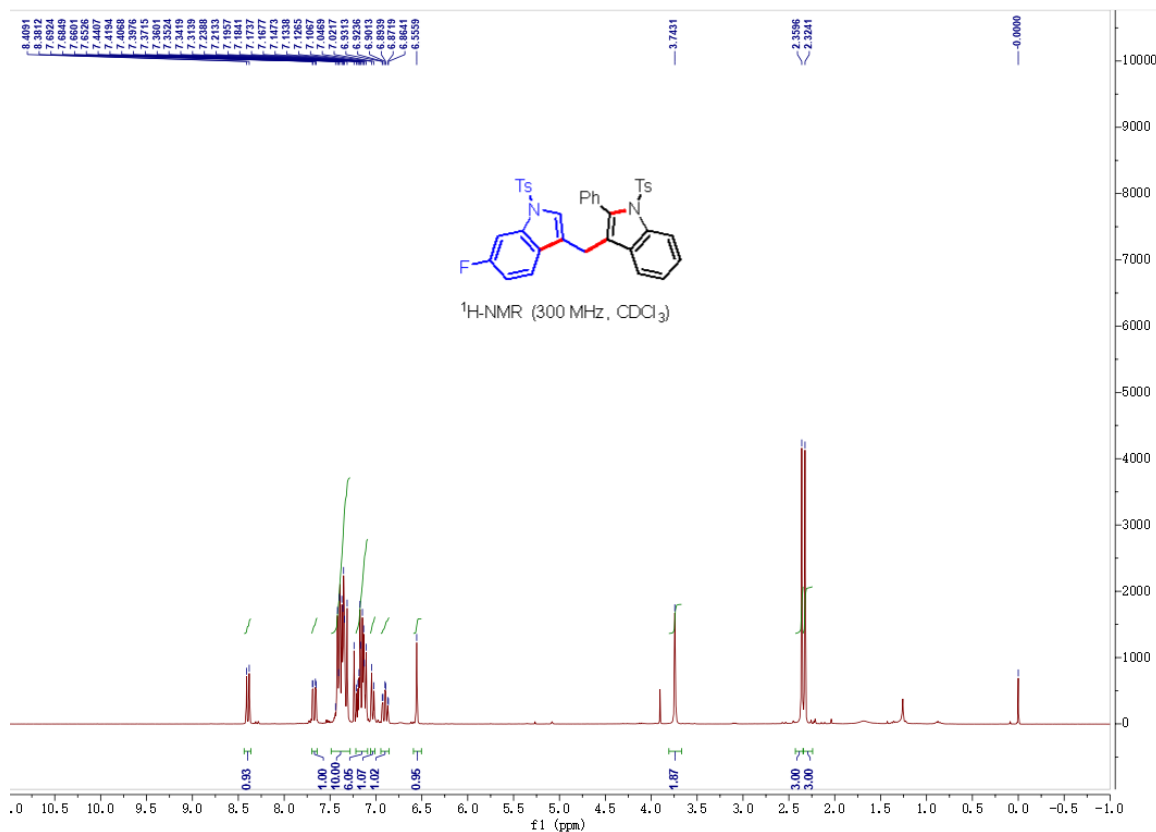
6-methoxy-3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)methyl)-1-tosyl-1*H*-indole (3ea):



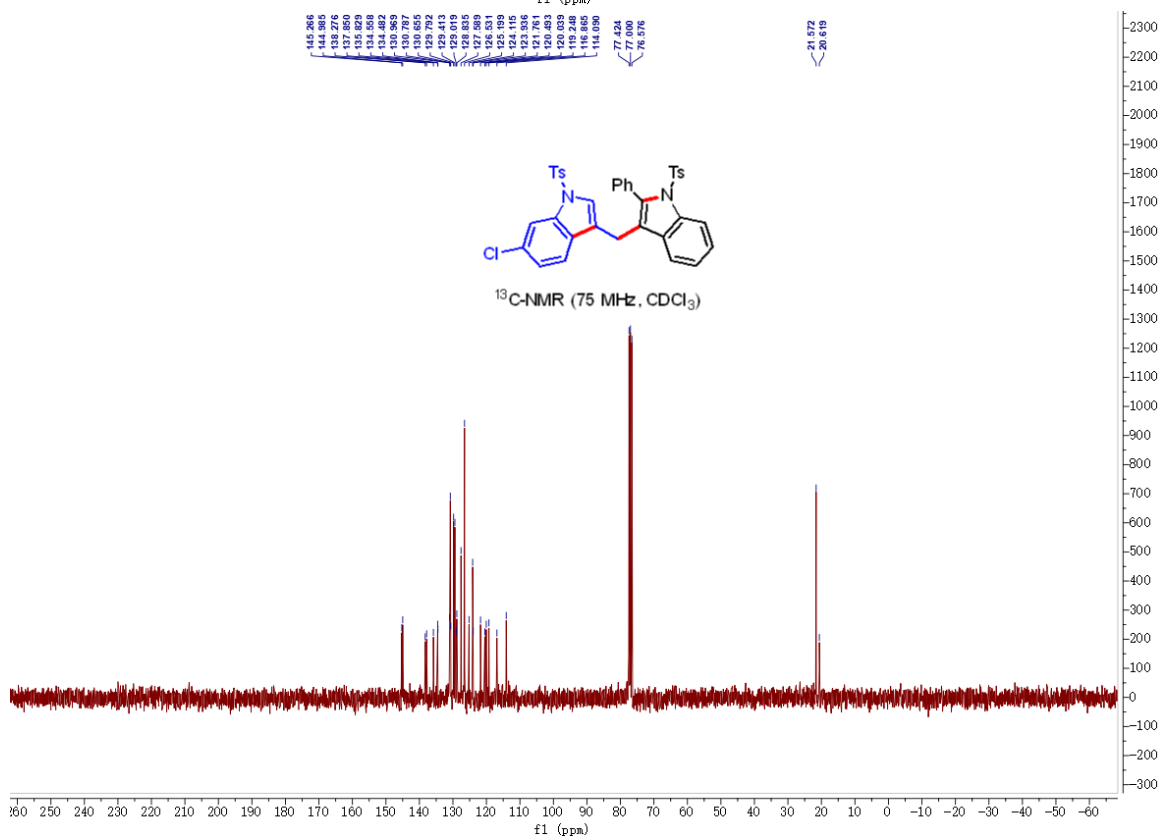
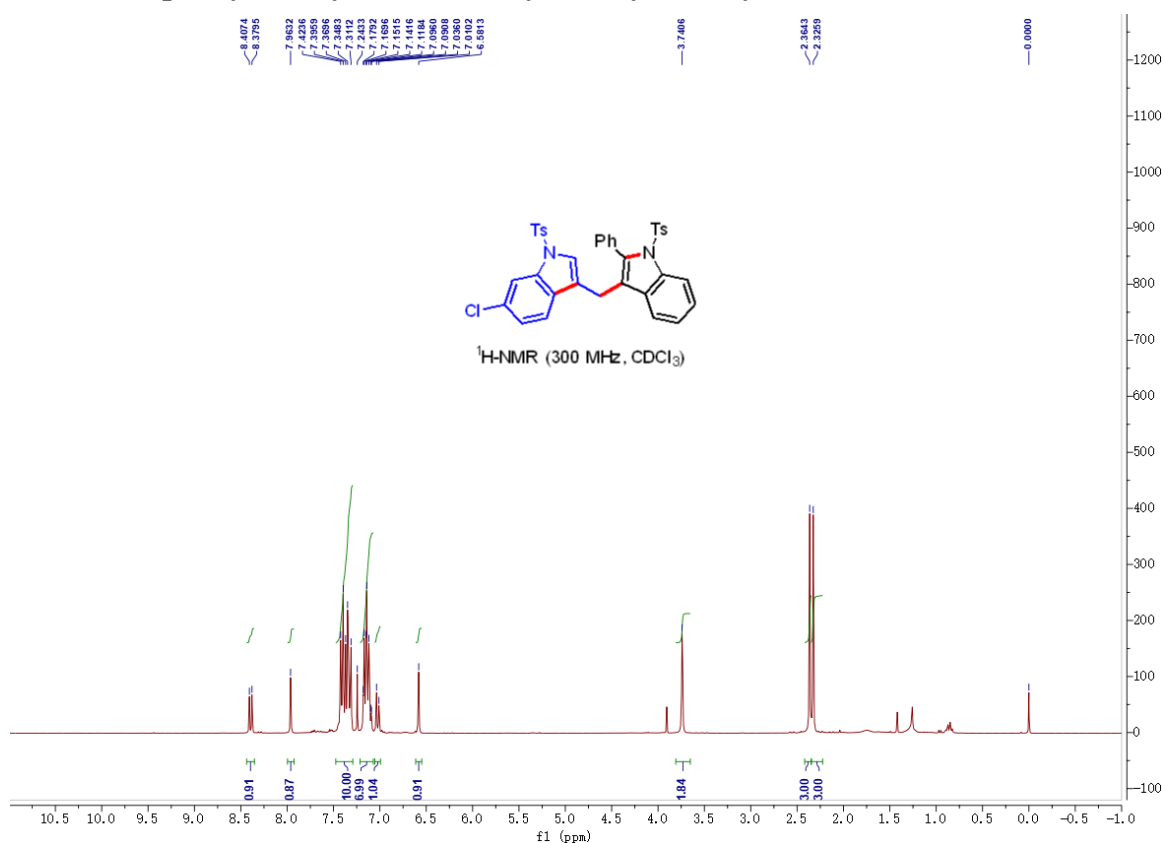
6-methyl-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3fa):



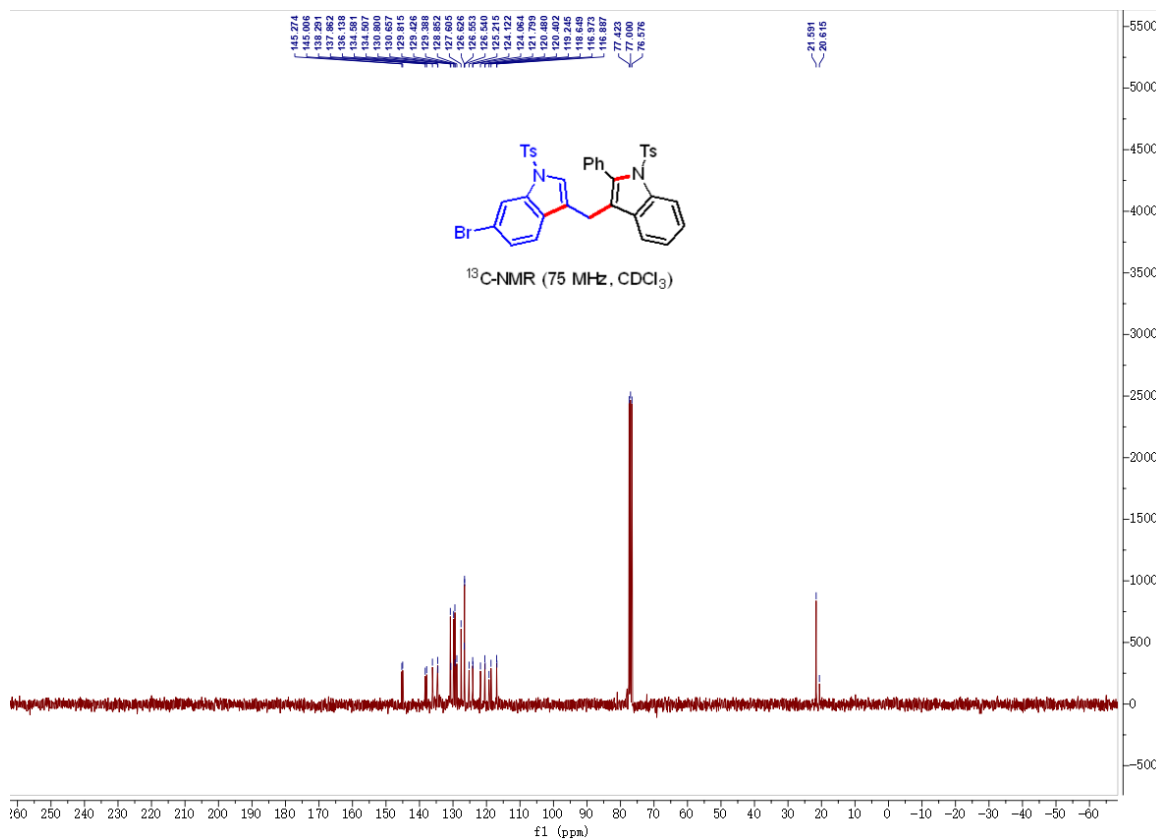
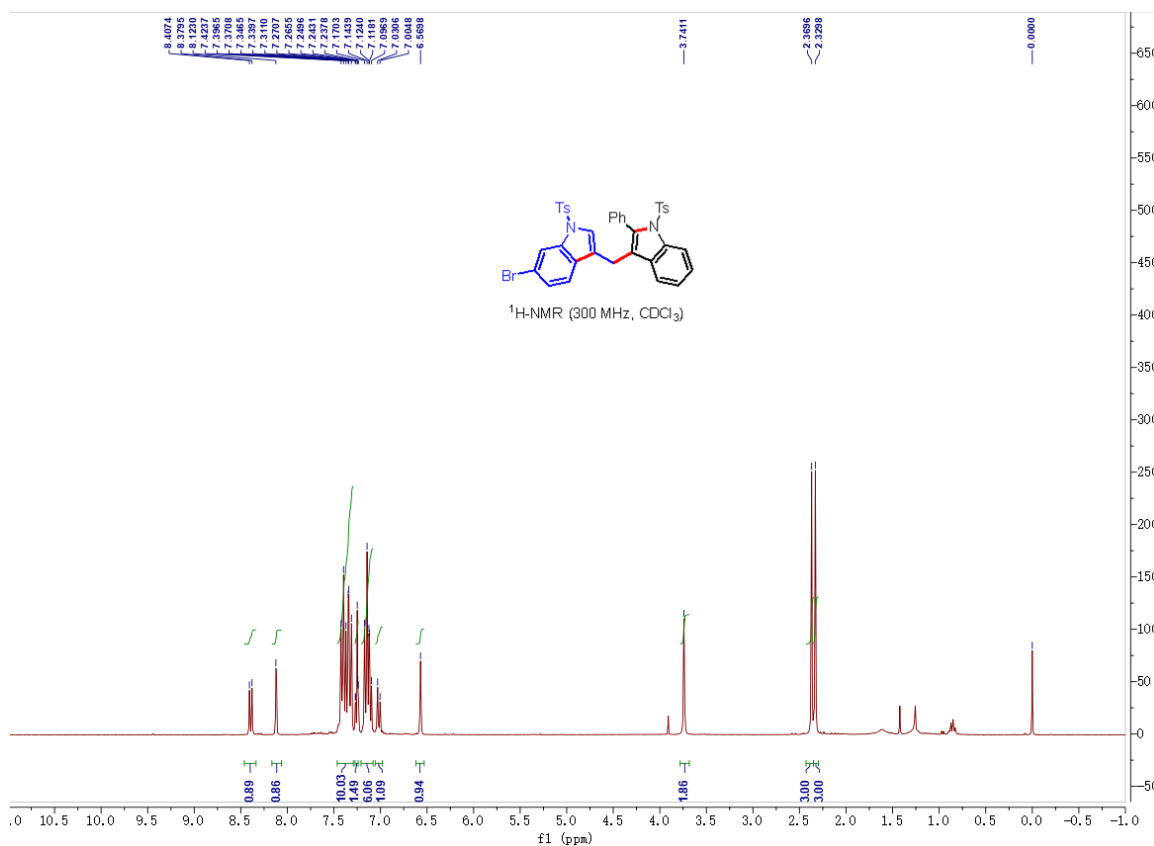
6-fluoro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ga):



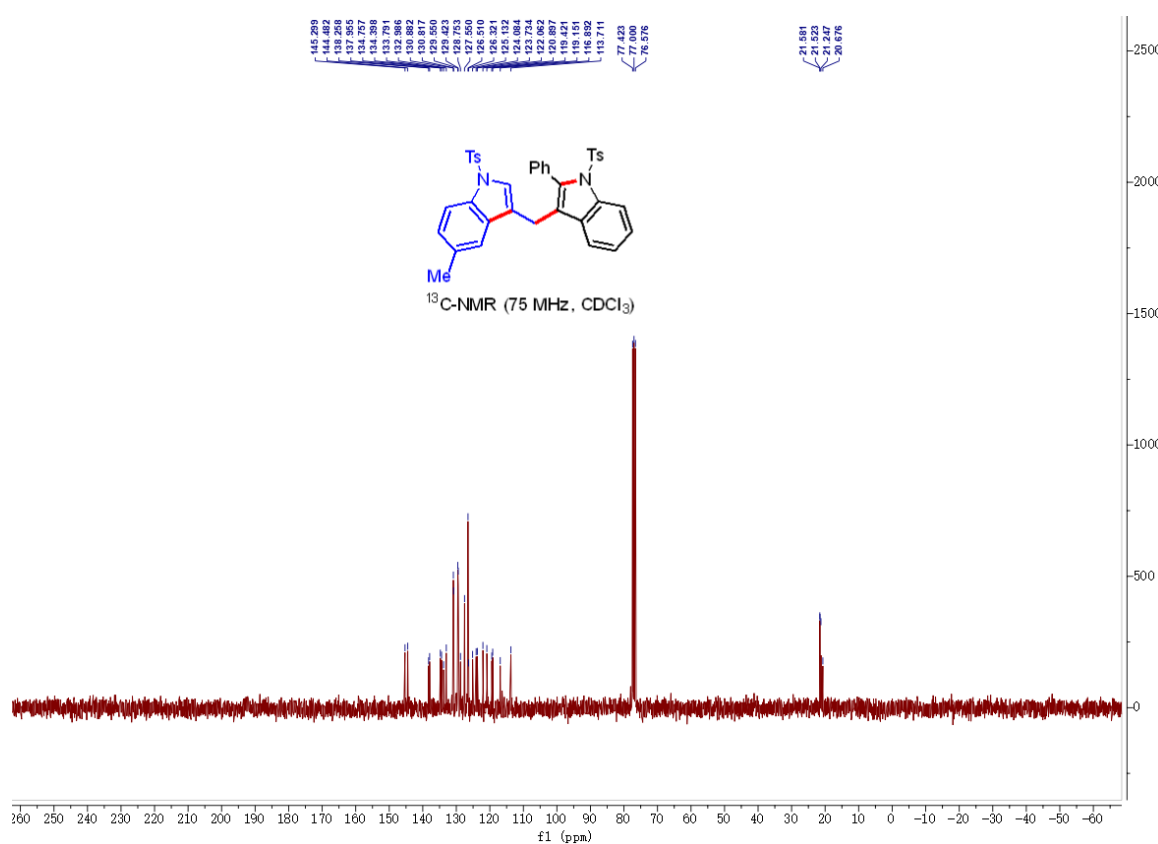
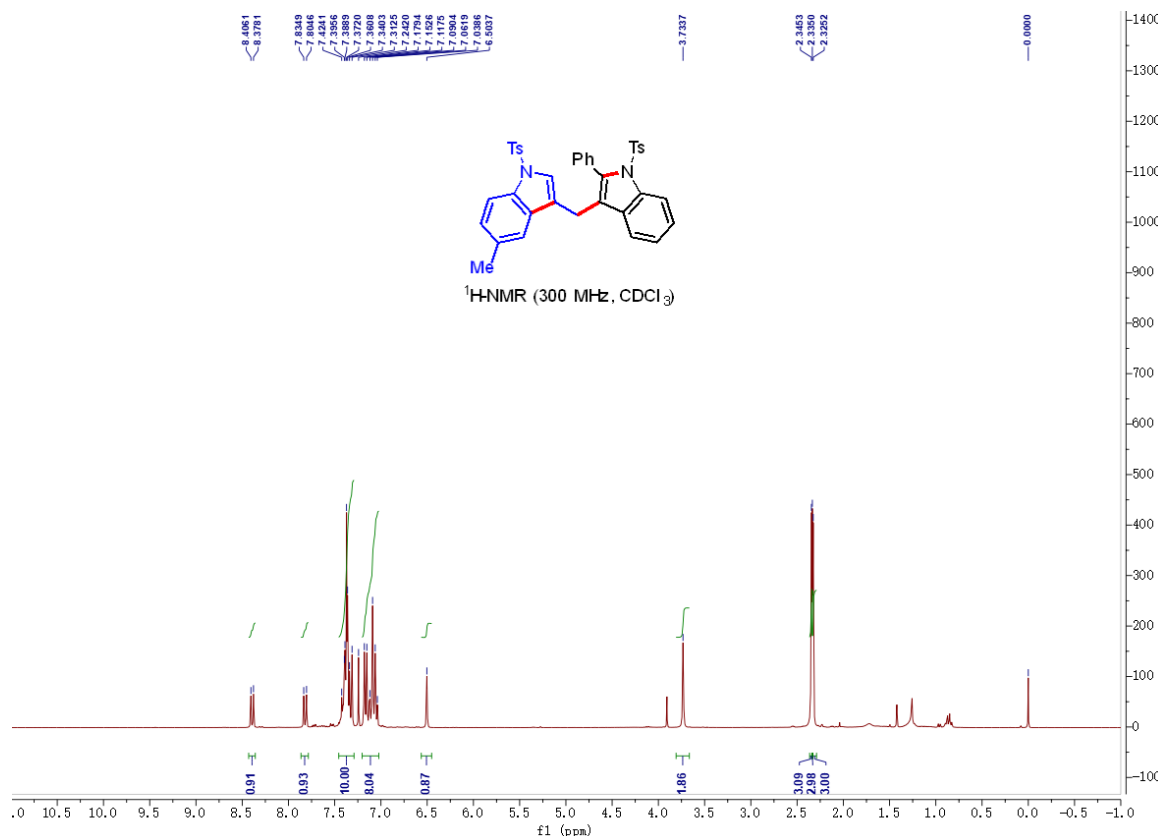
6-chloro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ha):



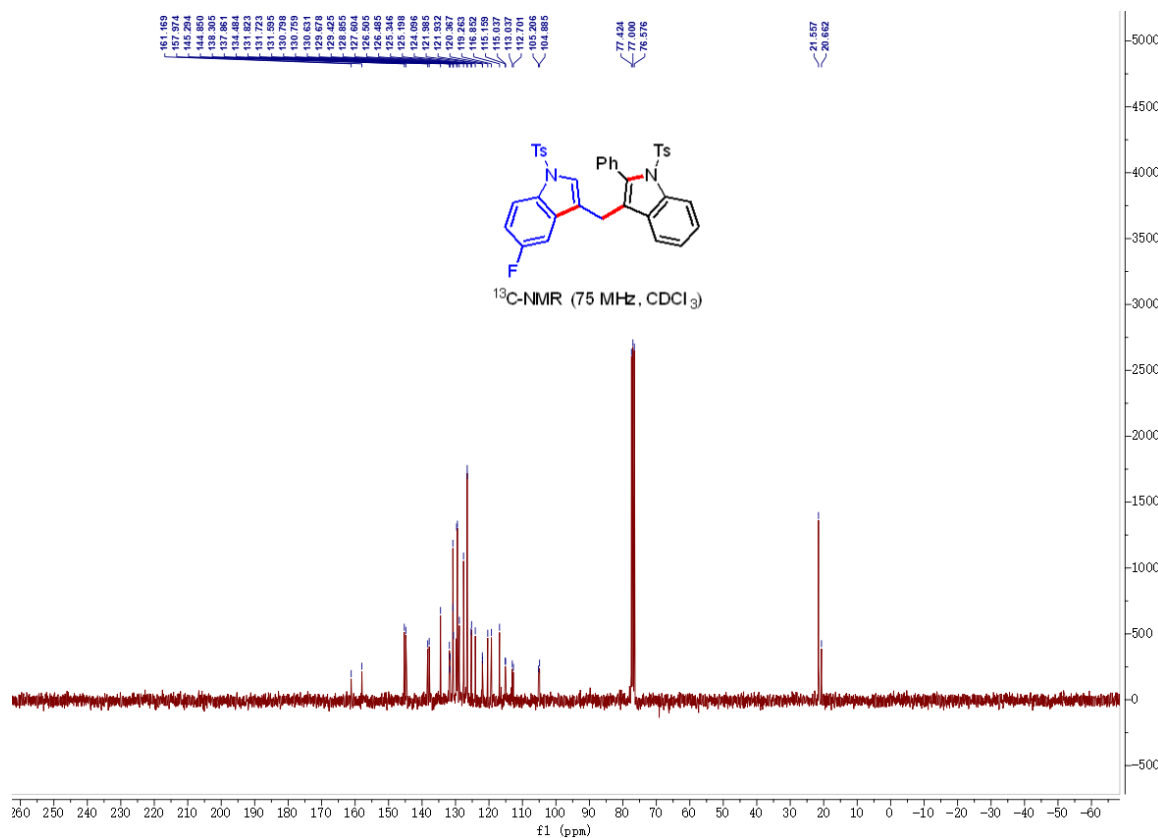
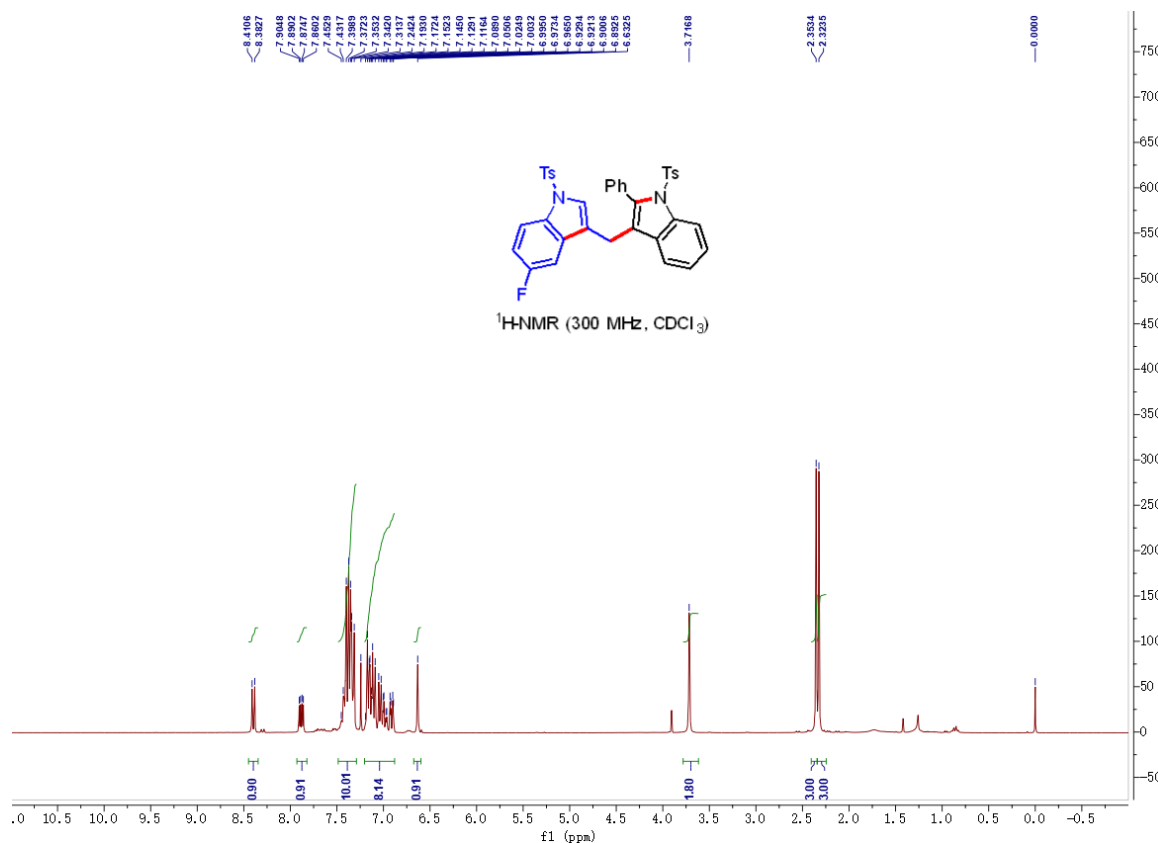
6-bromo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ia):



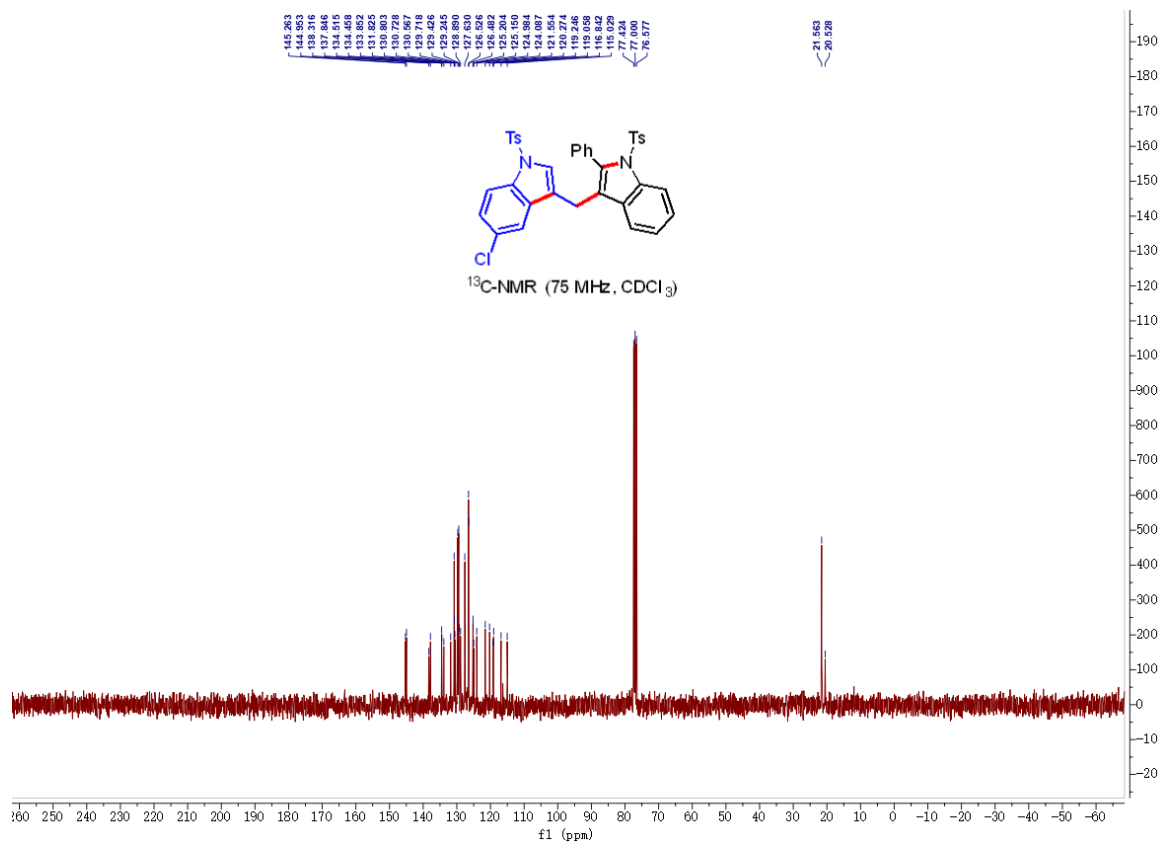
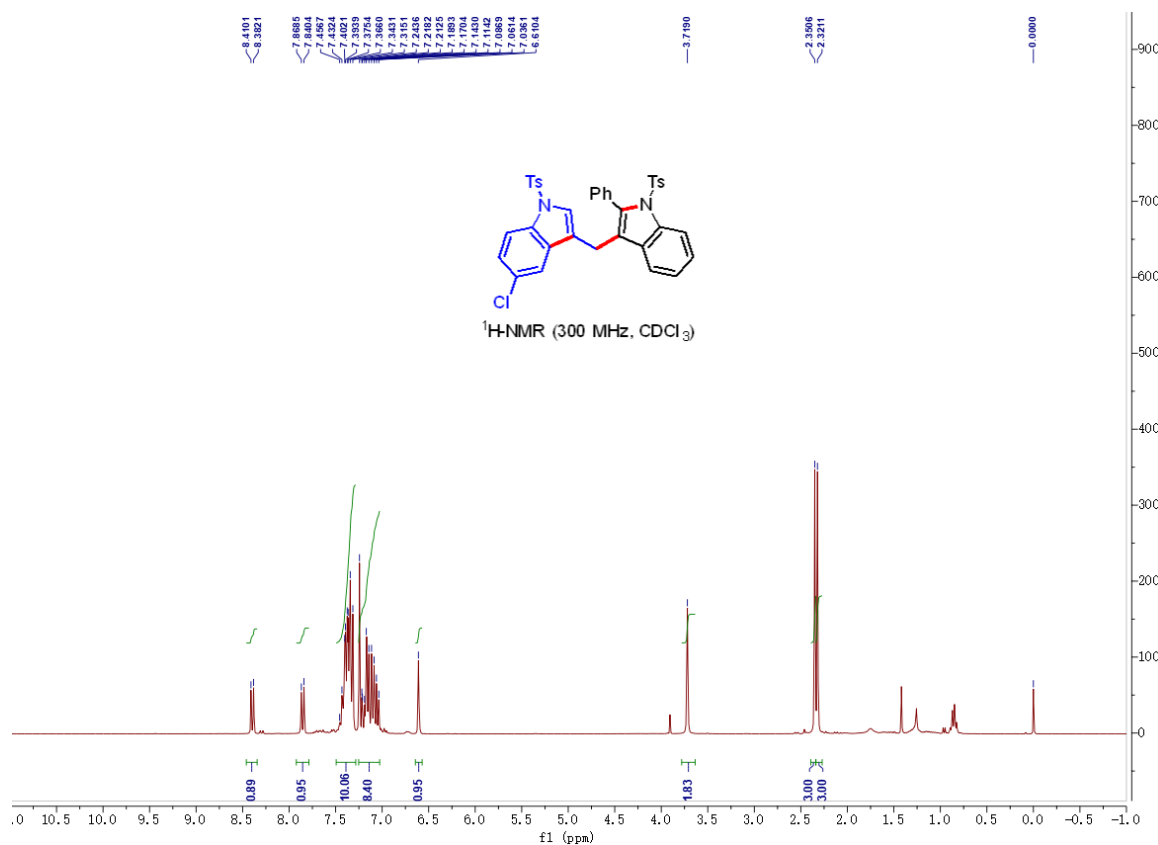
5-methyl-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ja):



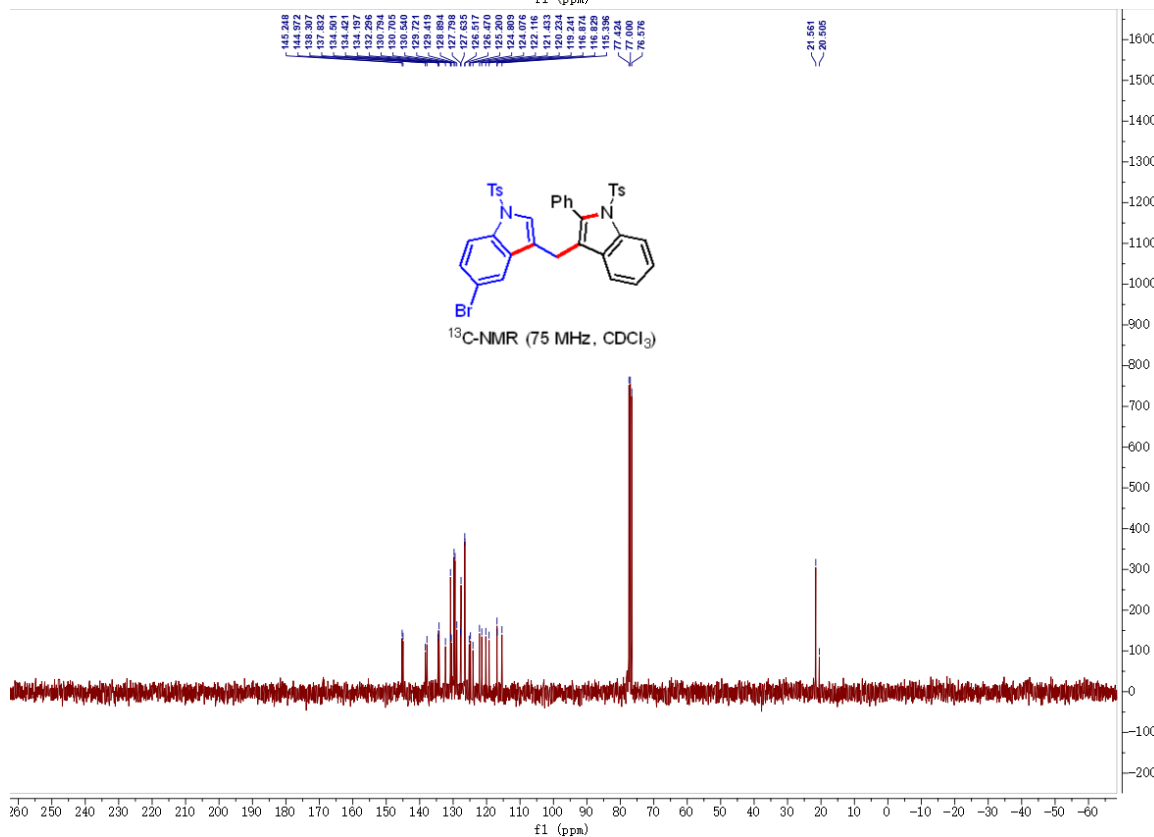
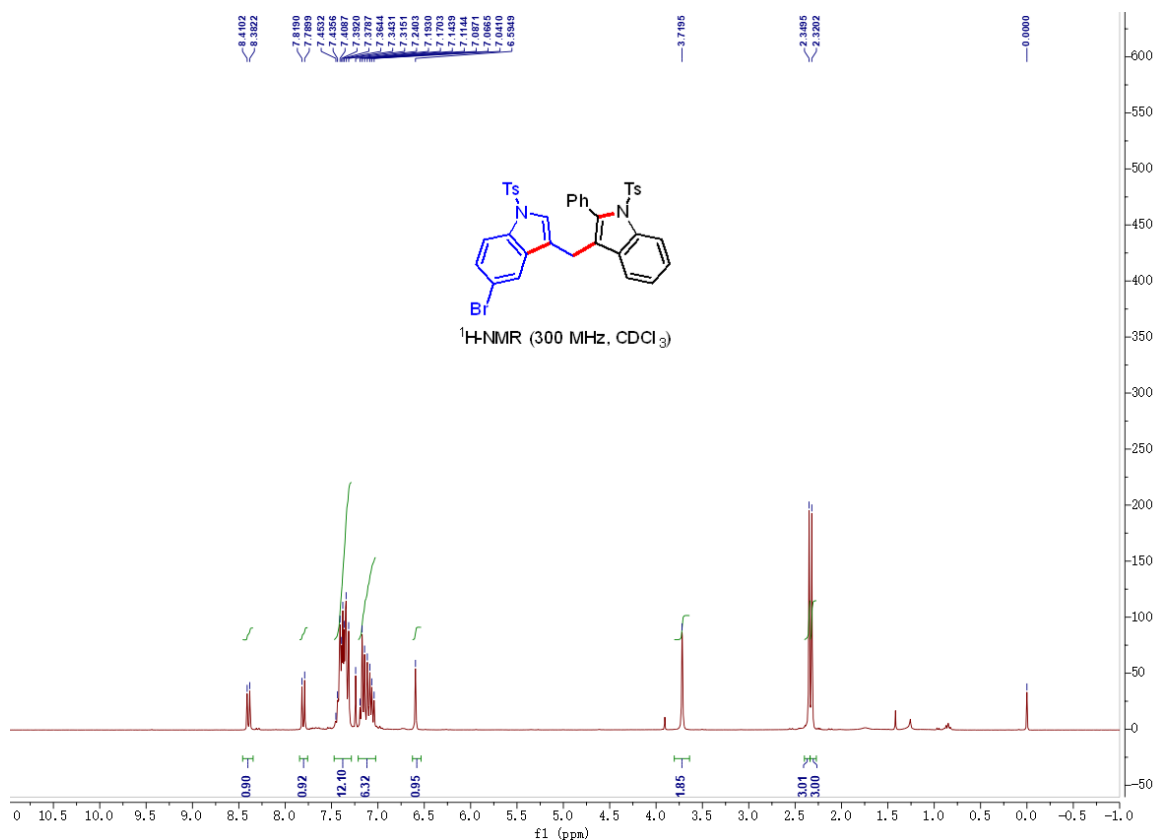
5-fluoro-3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)methyl)-1-tosyl-1*H*-indole (3ka):



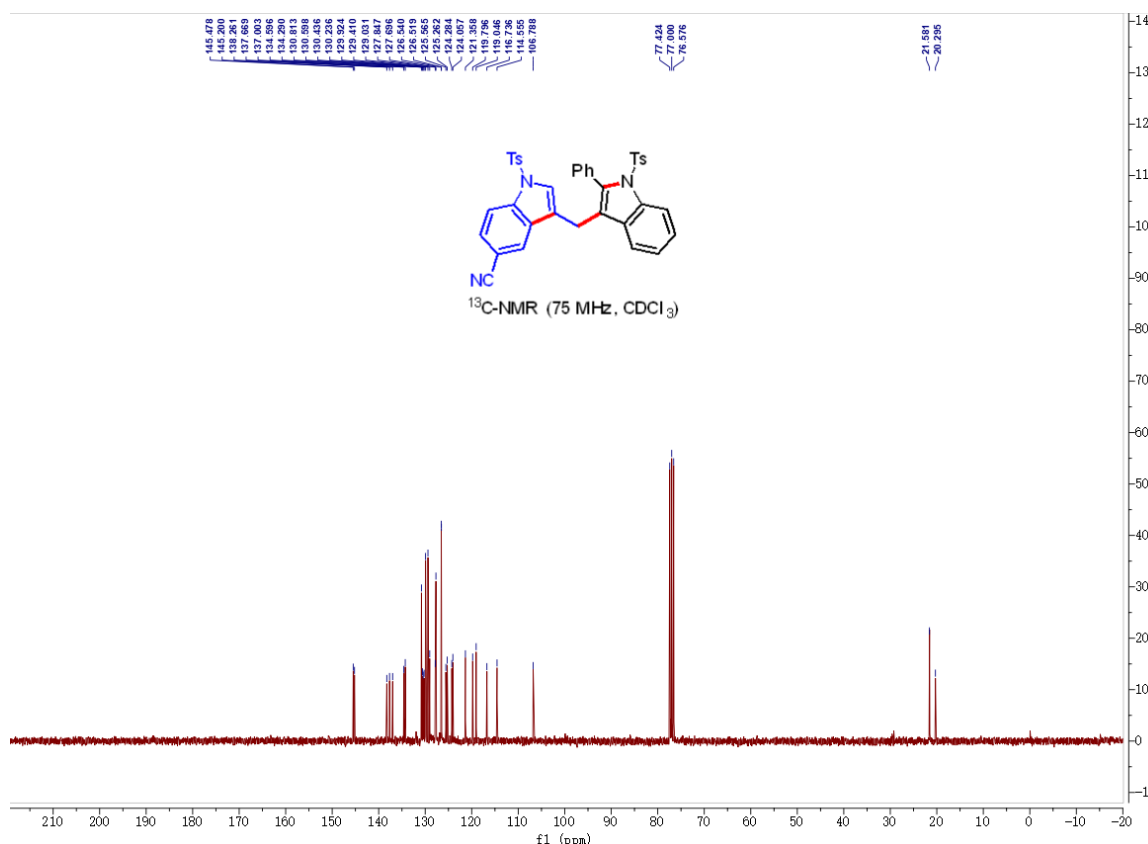
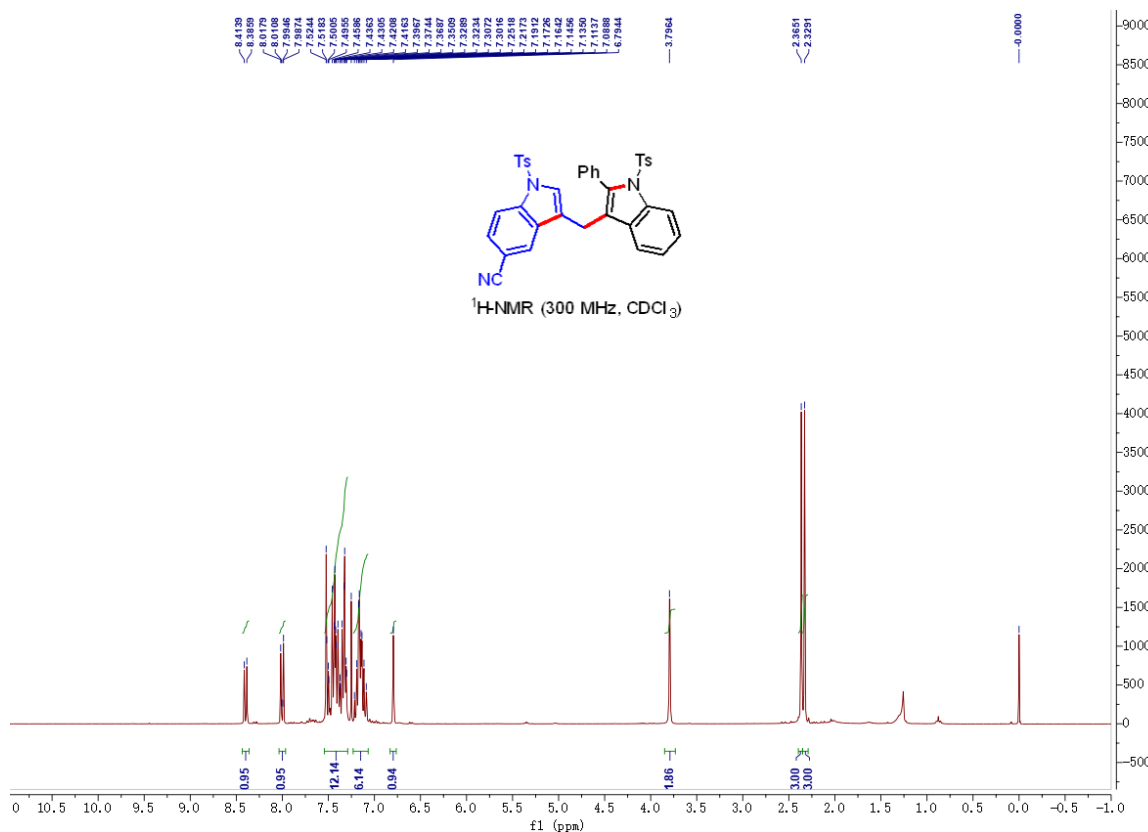
5-chloro-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (31a):



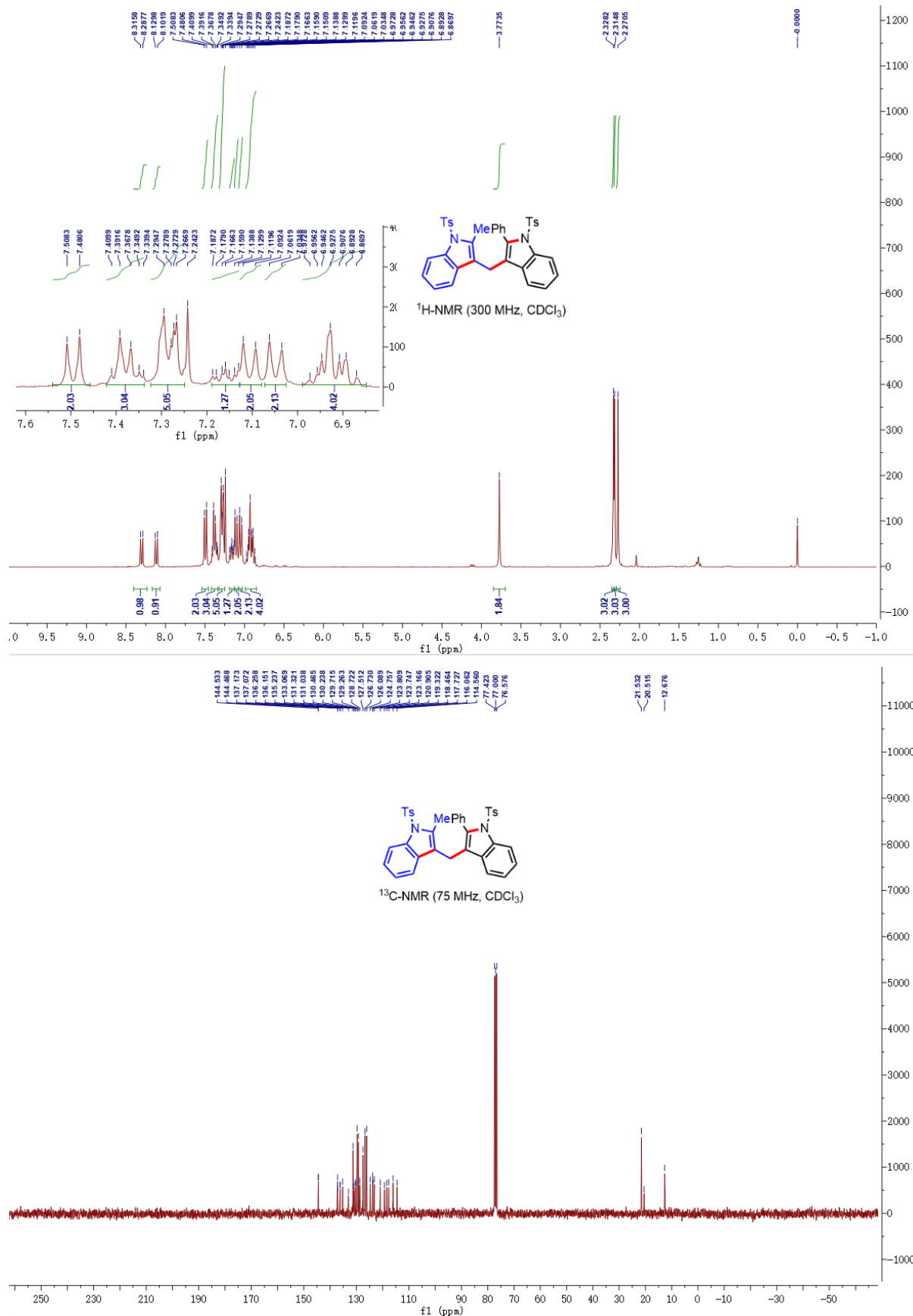
5-bromo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole (3ma):



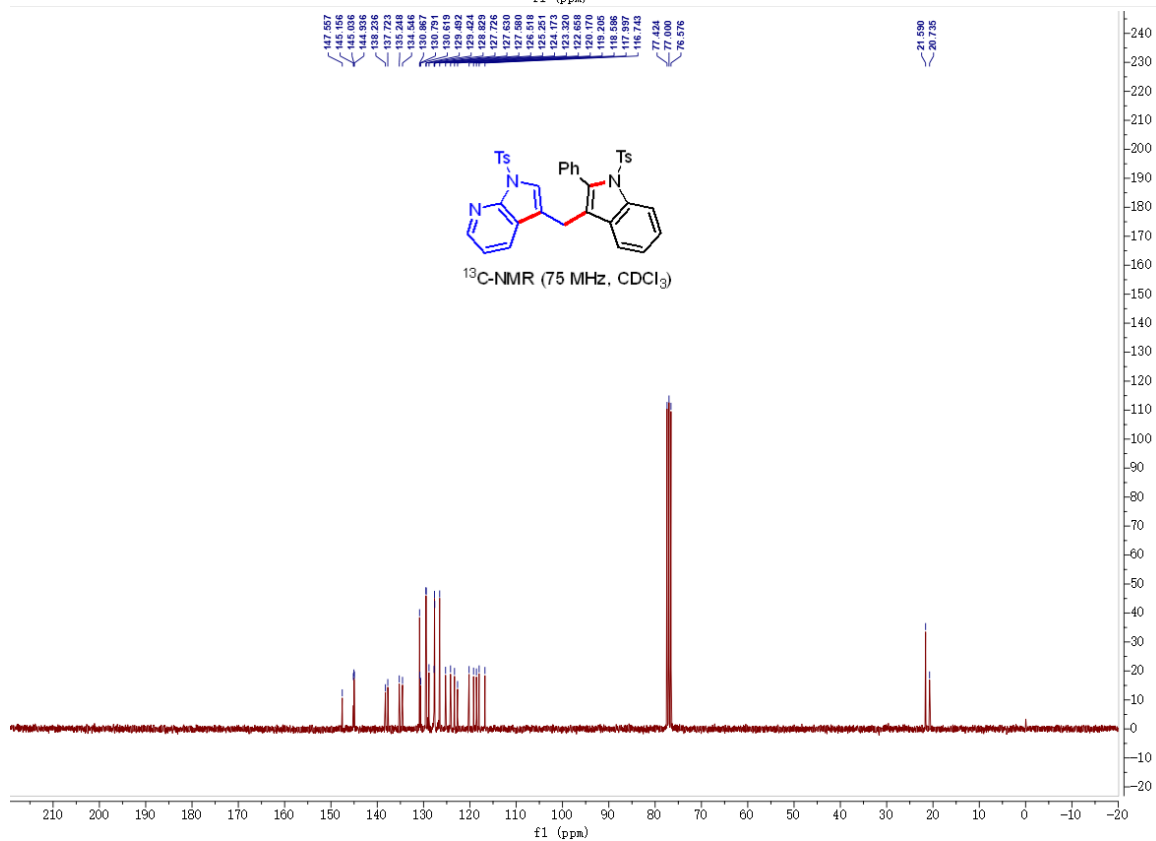
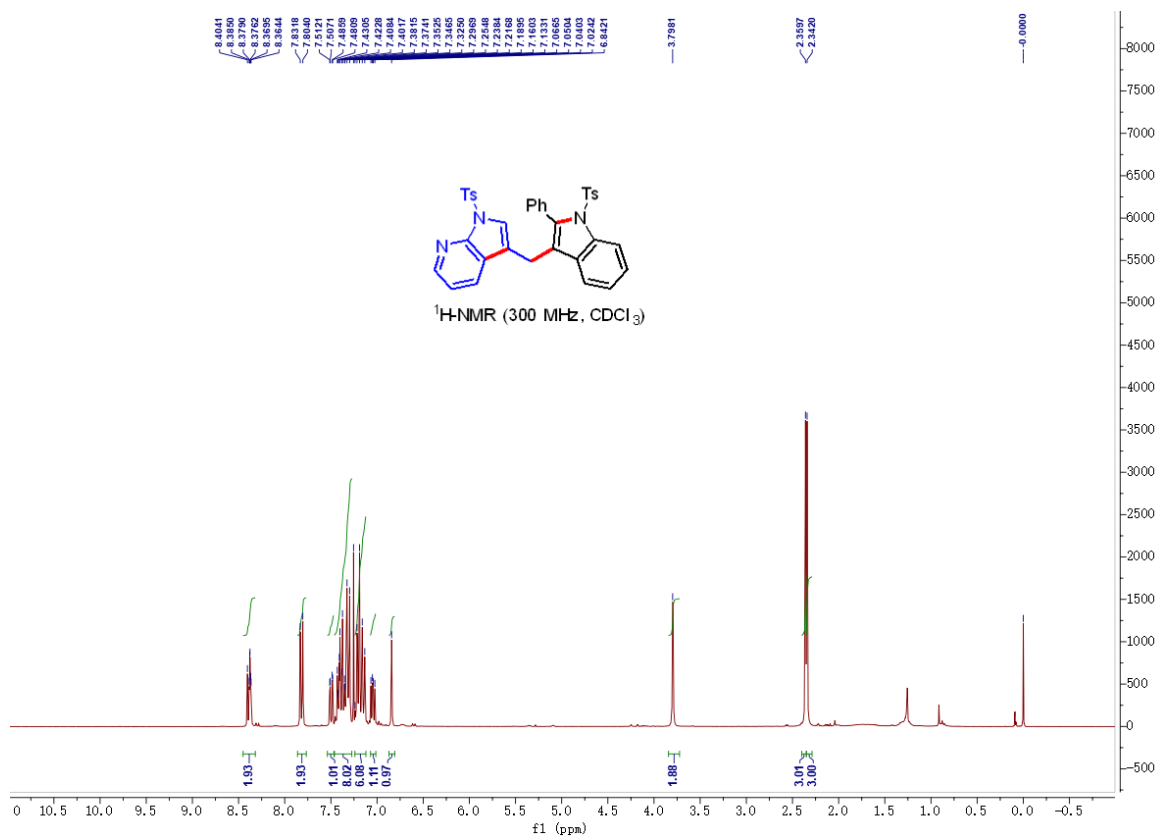
3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-indole-5-carbonitrile (3na):



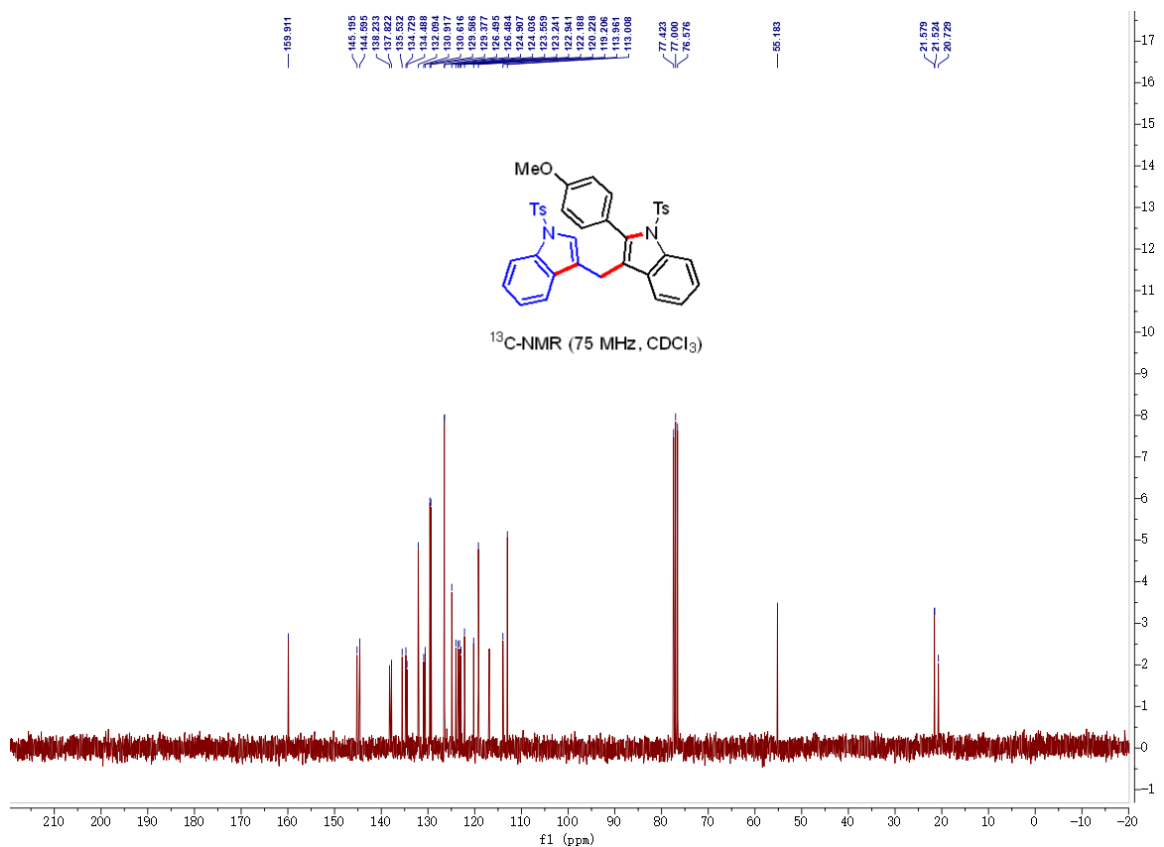
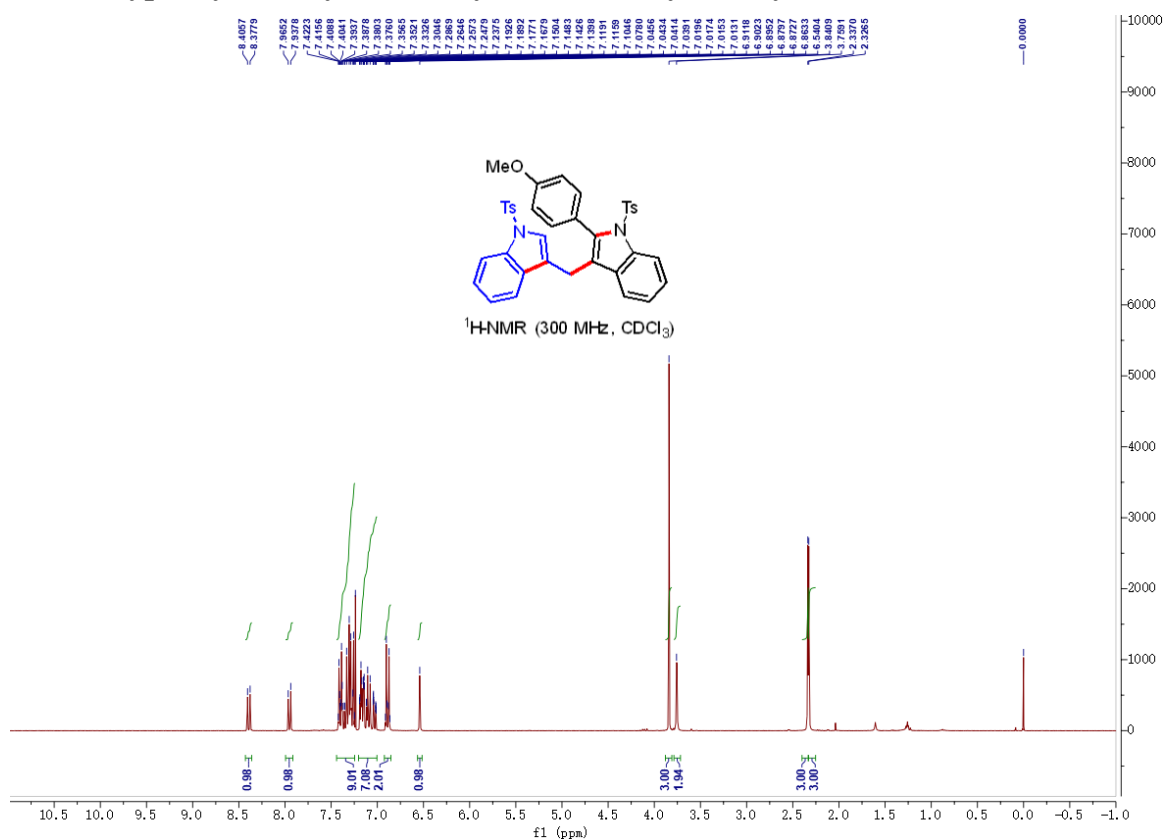
2-methyl-3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)methyl)-1-tosyl-1*H*-indole (30a):



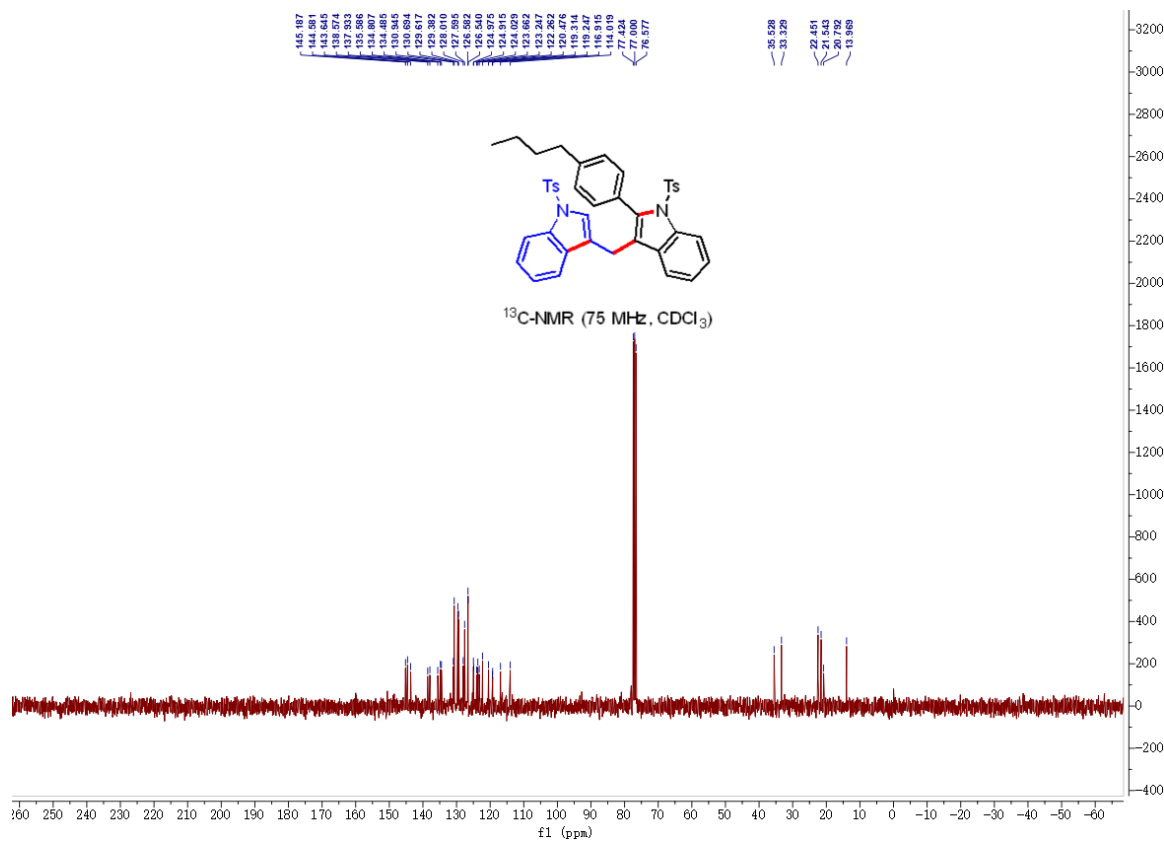
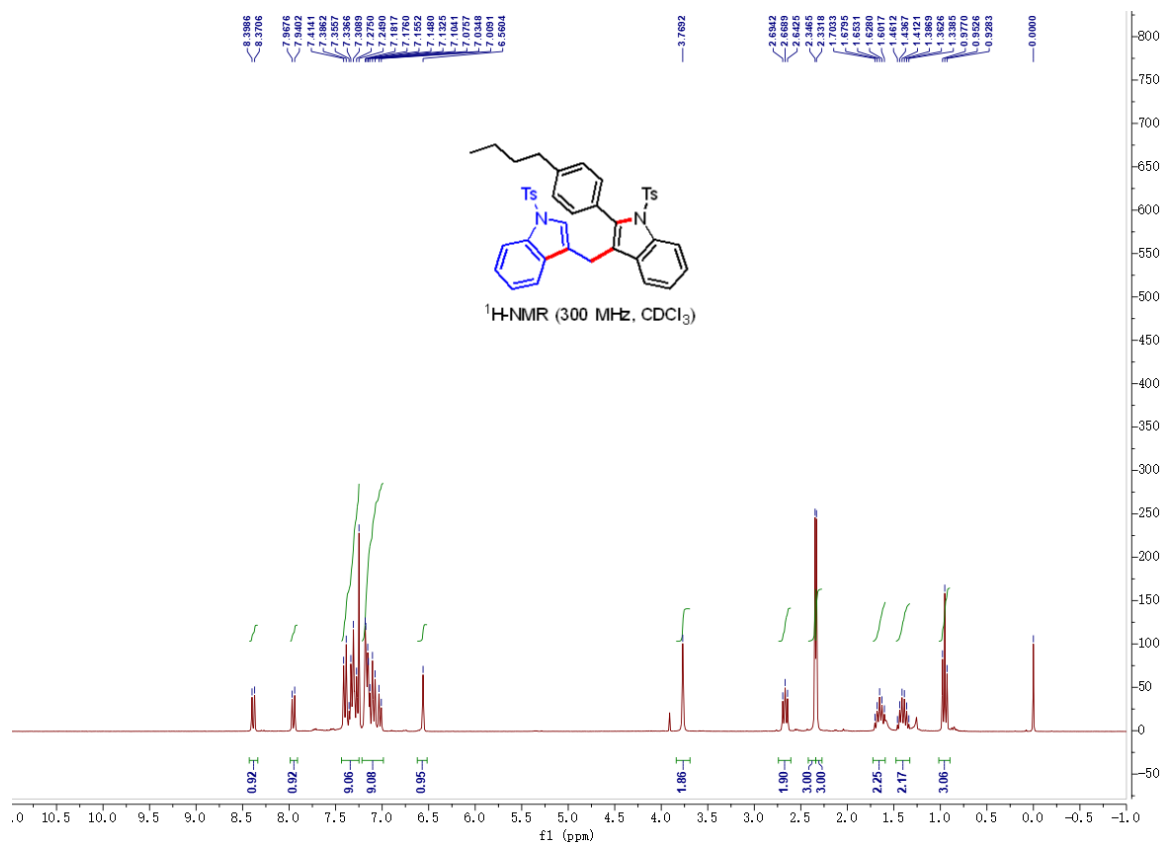
3-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)-1-tosyl-1H-pyrrolo[2,3-b]pyridine (3pa):



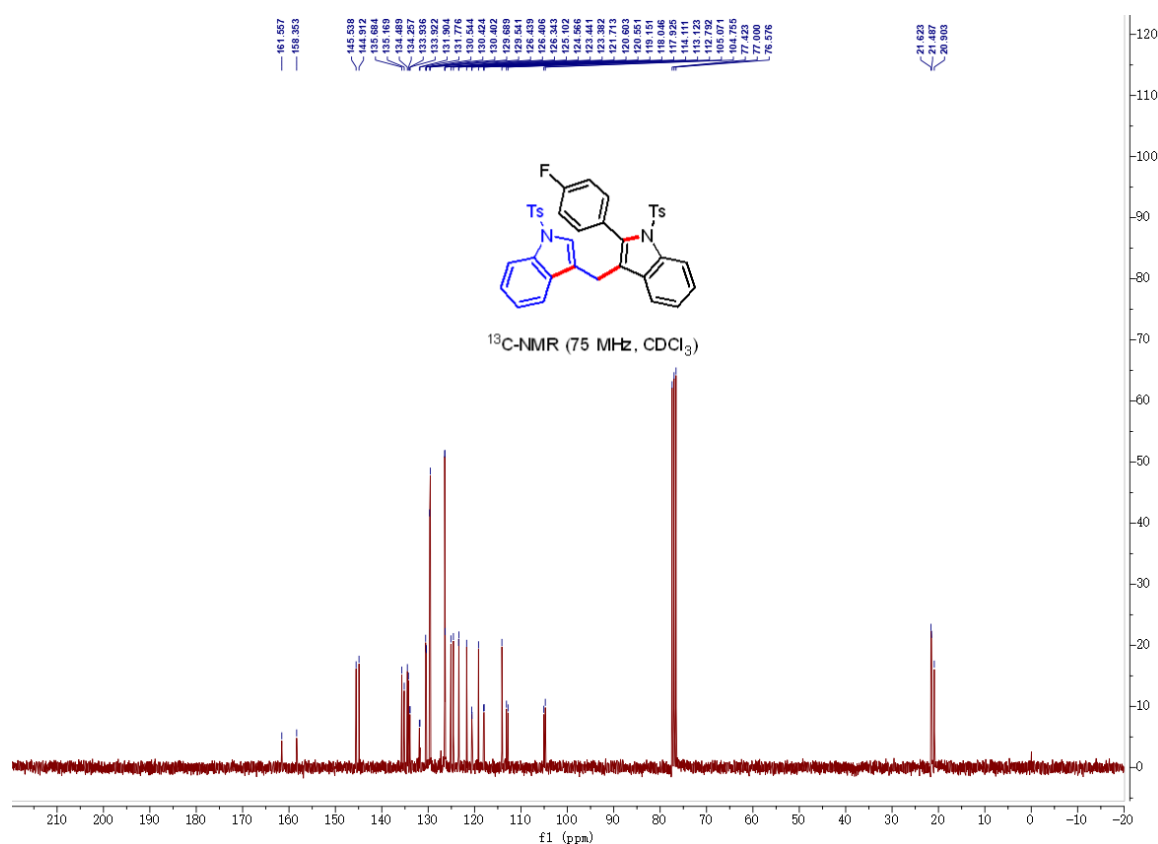
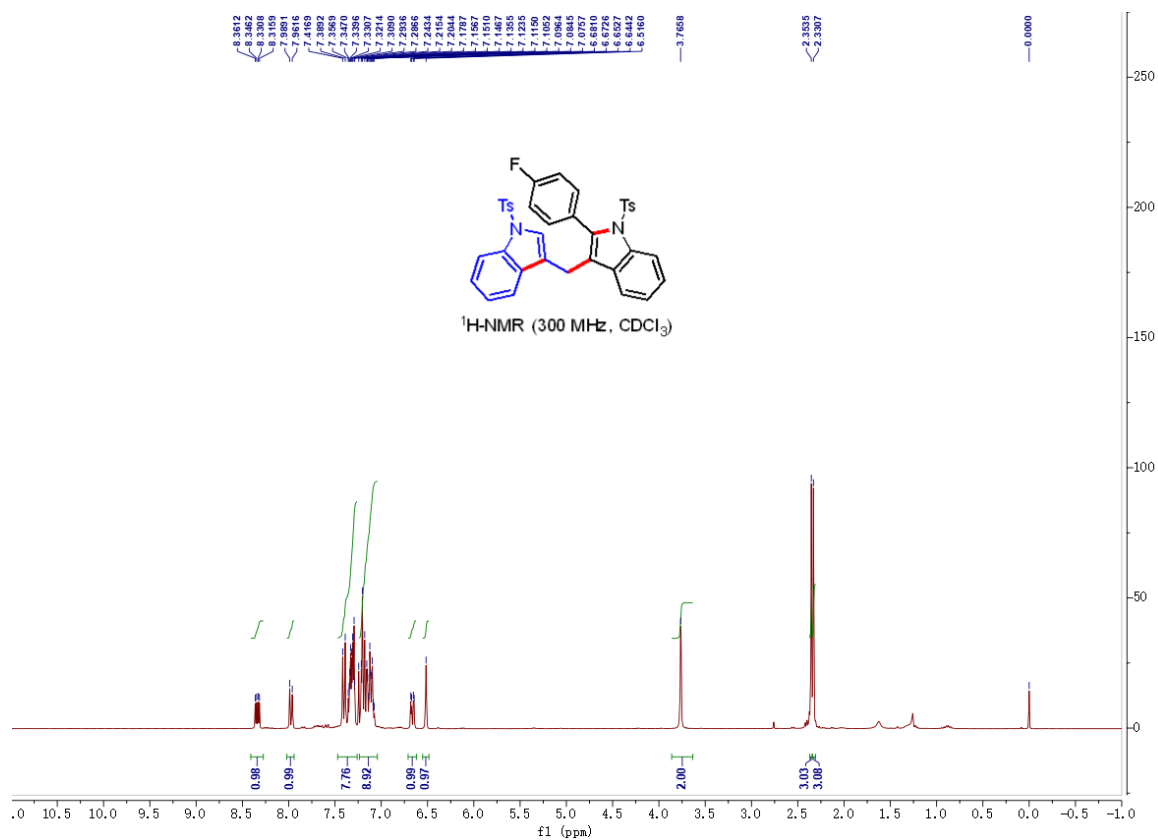
2-(4-methoxyphenyl)-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3ab):



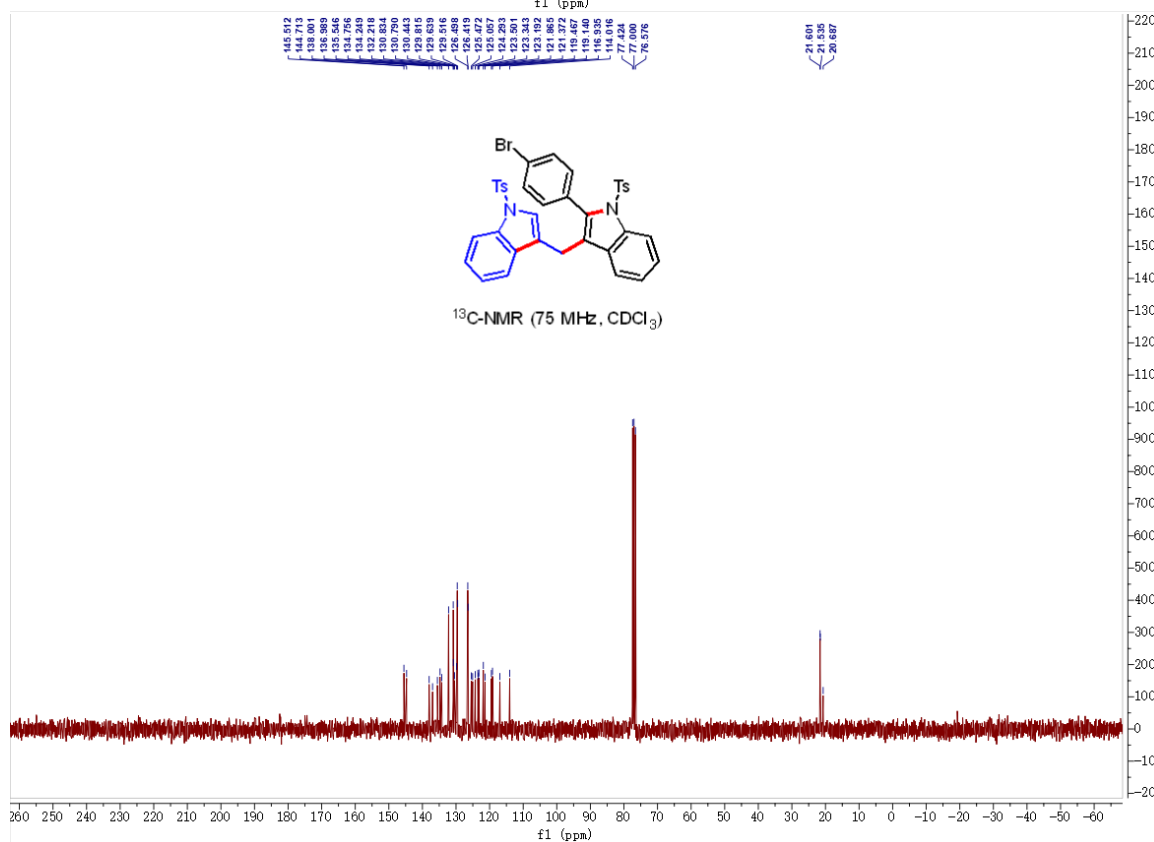
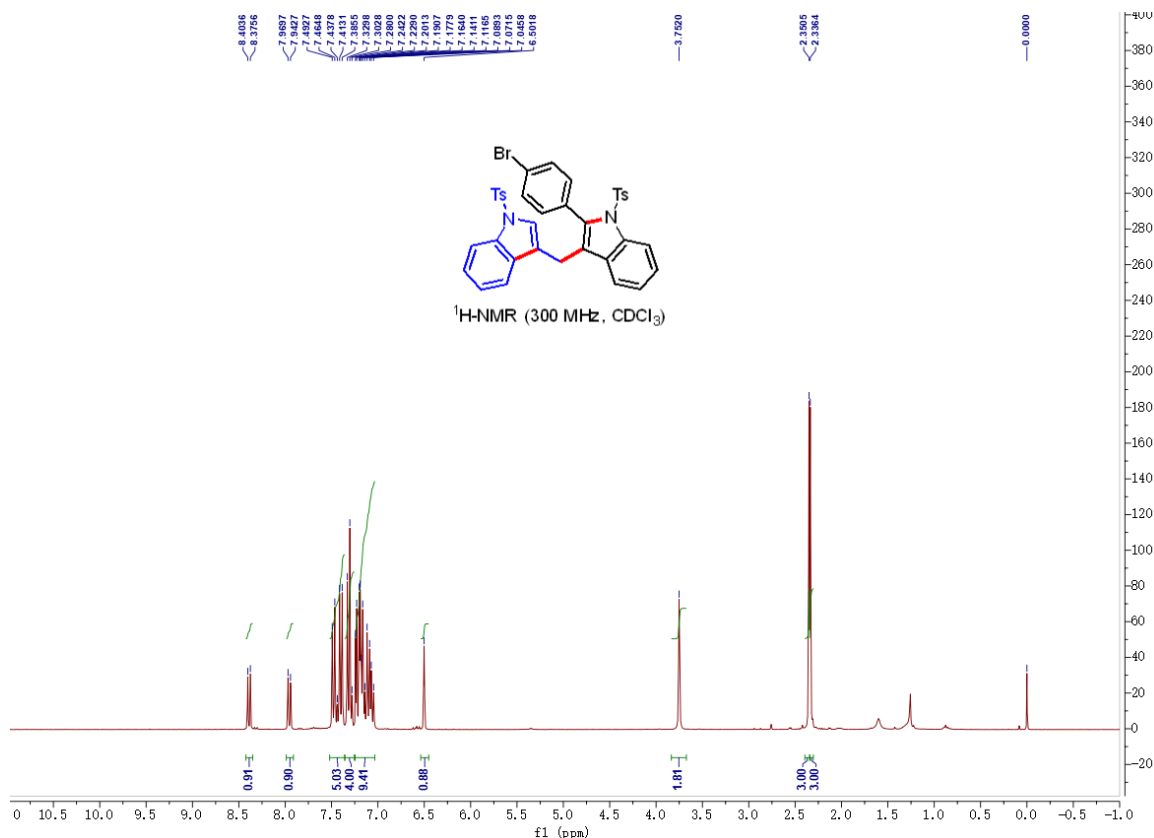
2-(4-butylphenyl)-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3ac):



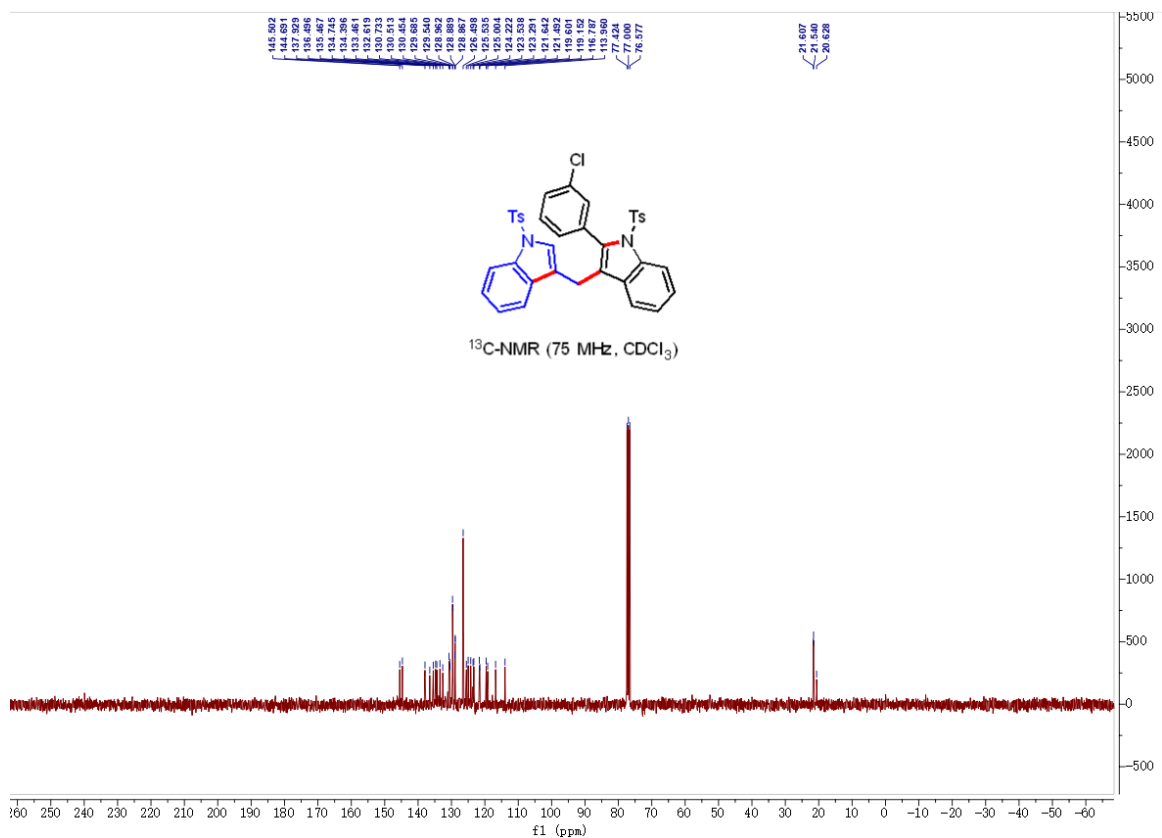
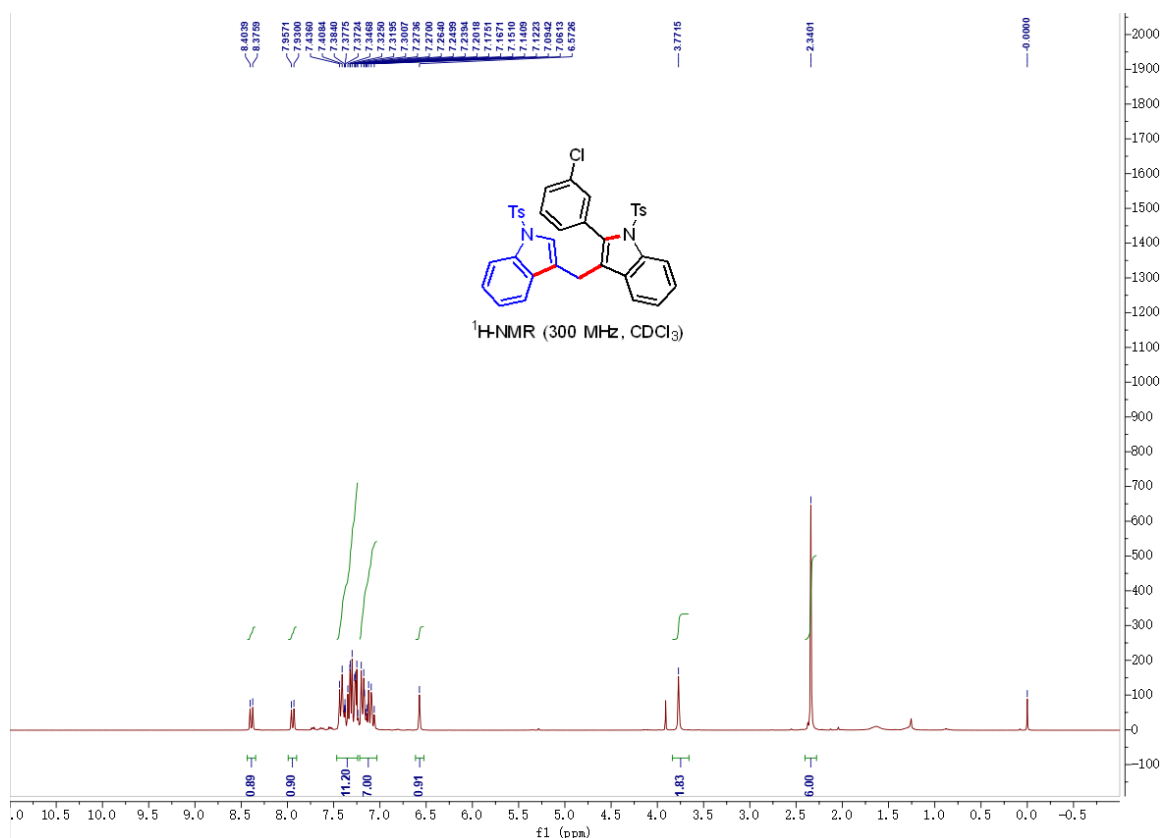
2-(4-fluorophenyl)-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3ad):



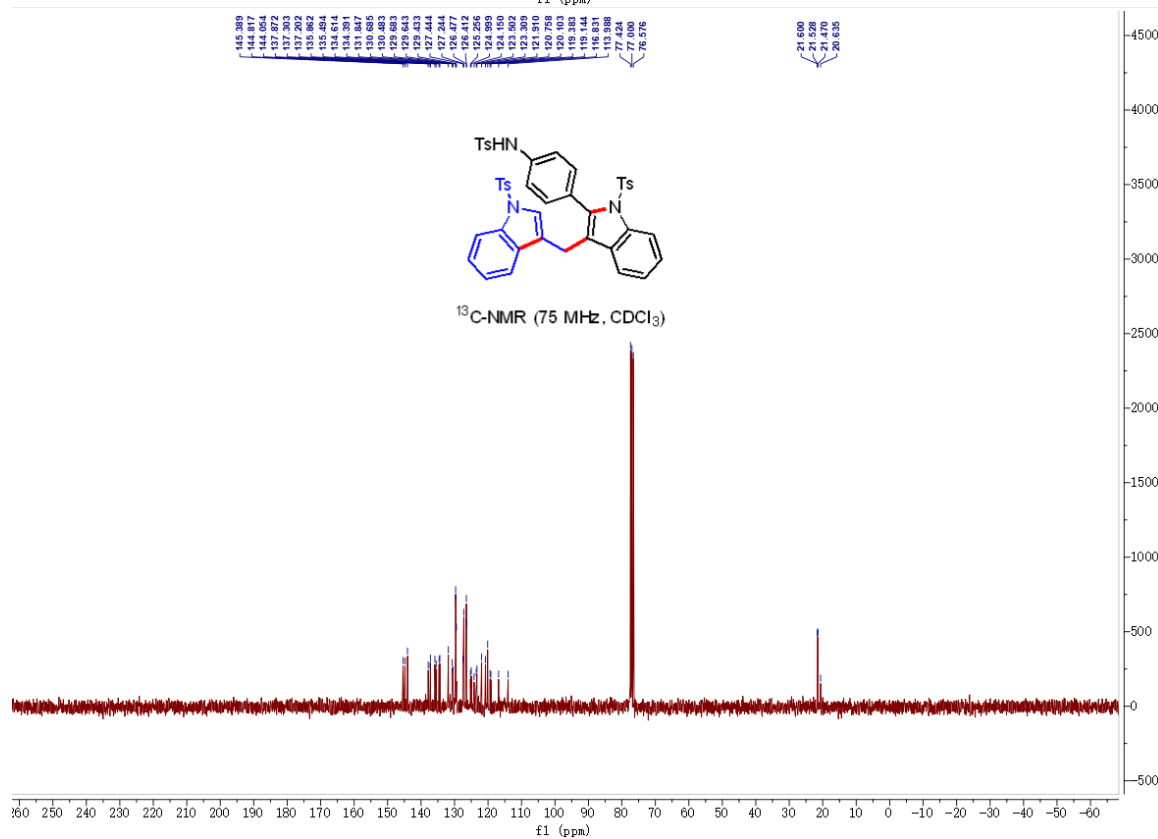
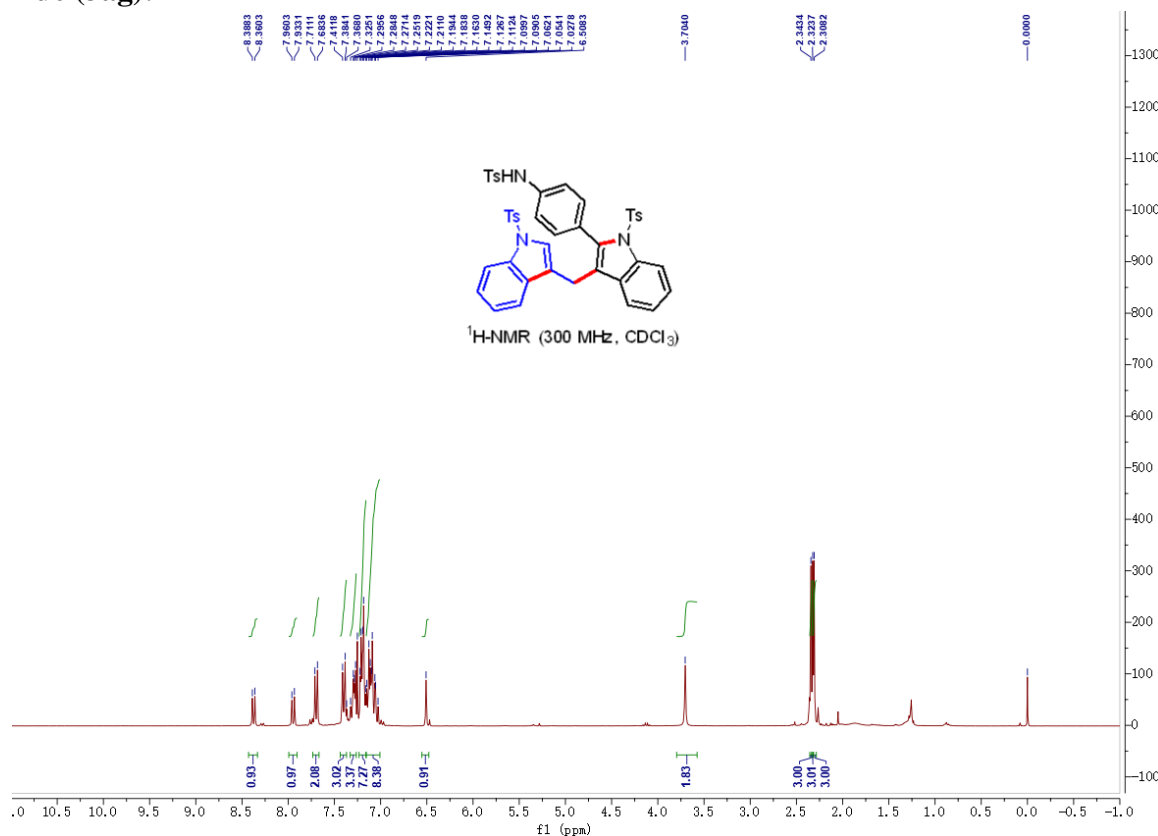
2-(4-bromophenyl)-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3ae):



2-(3-chlorophenyl)-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3af):

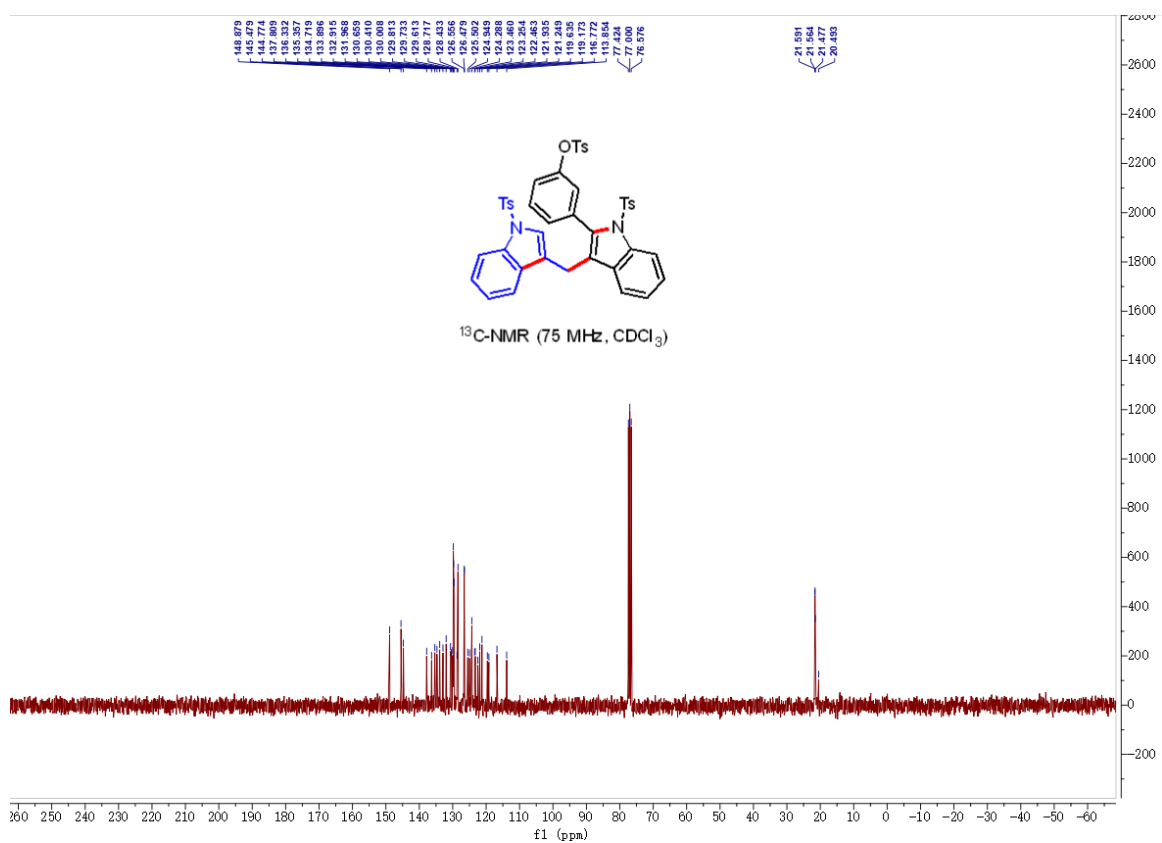
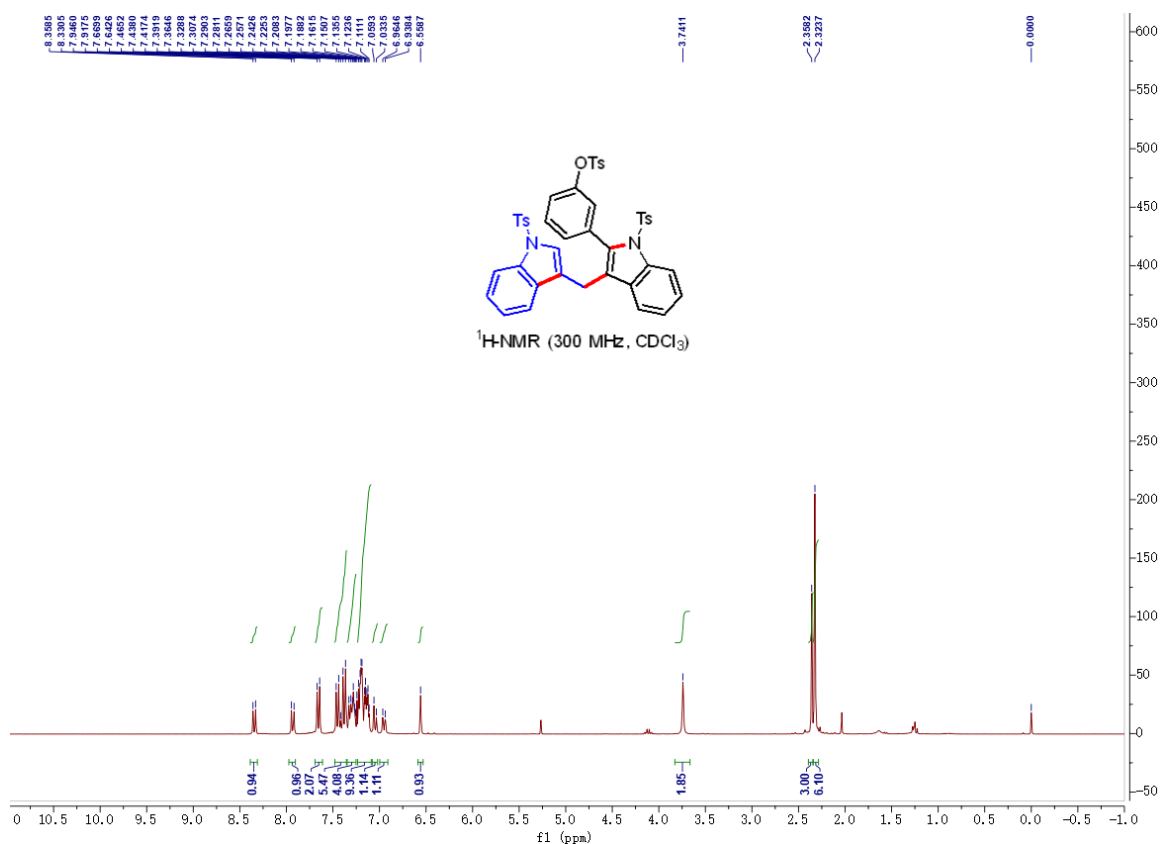


4-methyl-N-(4-(1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indol-2-yl)phenyl)benzenesulfonamide (3ag):

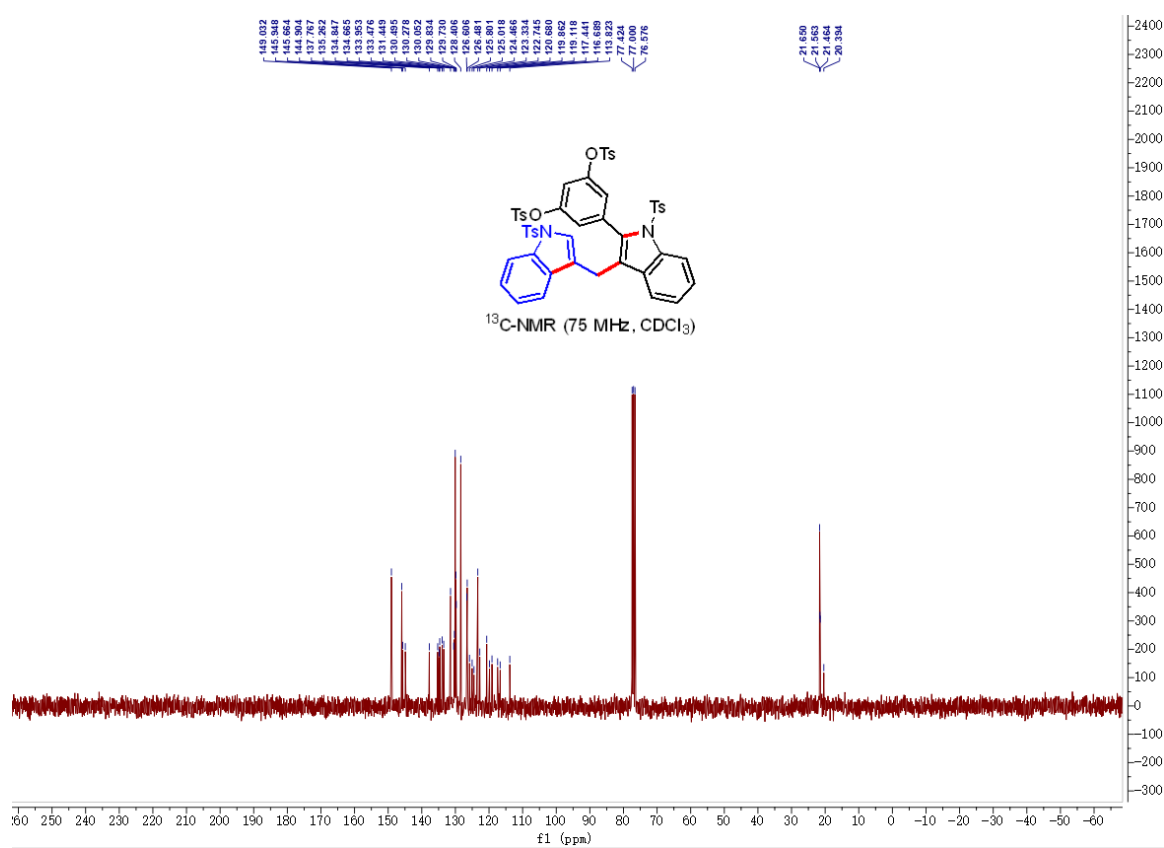
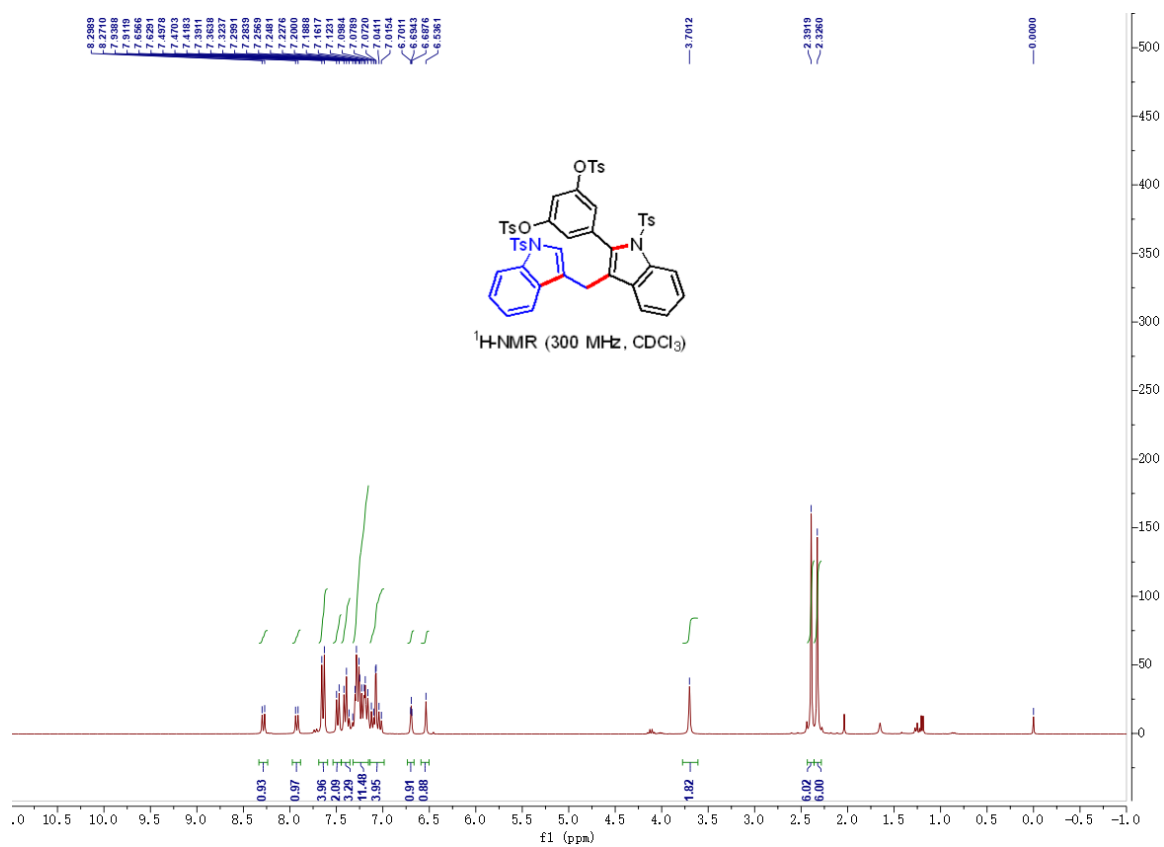


3-(1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indol-2-yl)phenyl 4-methylbenzenesulfonate

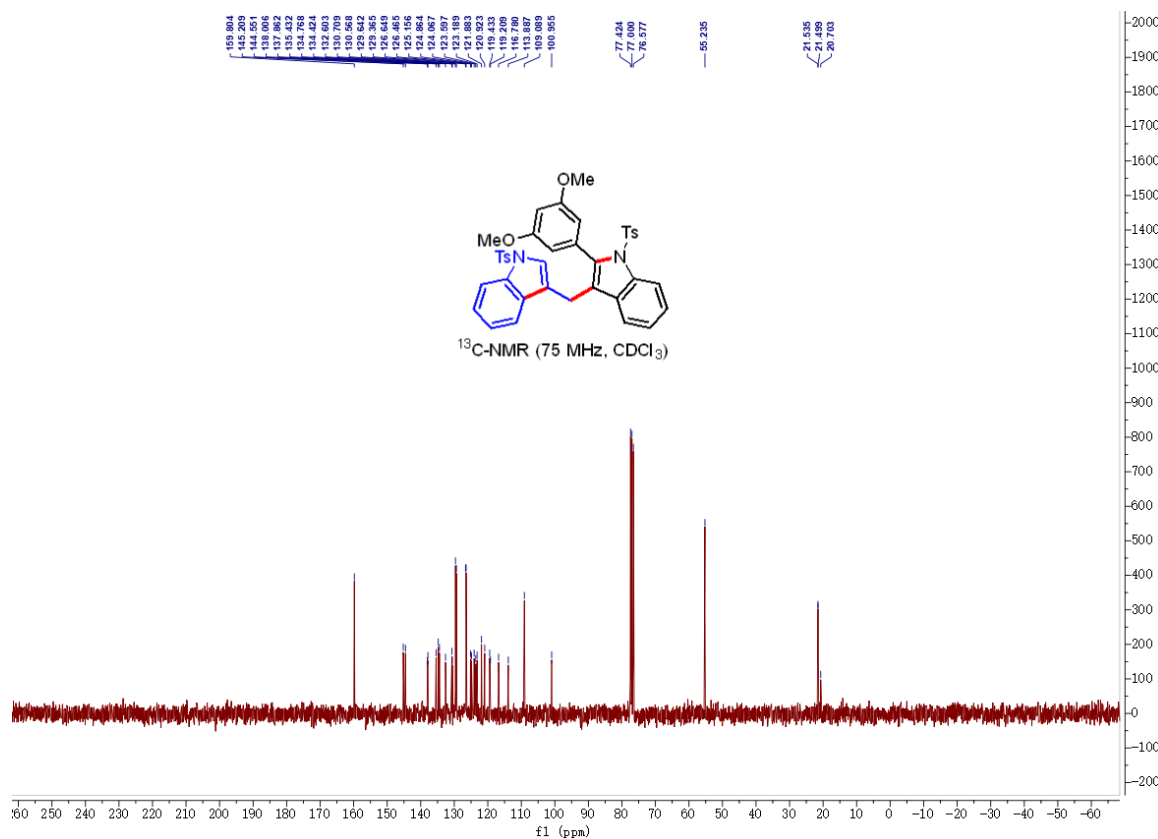
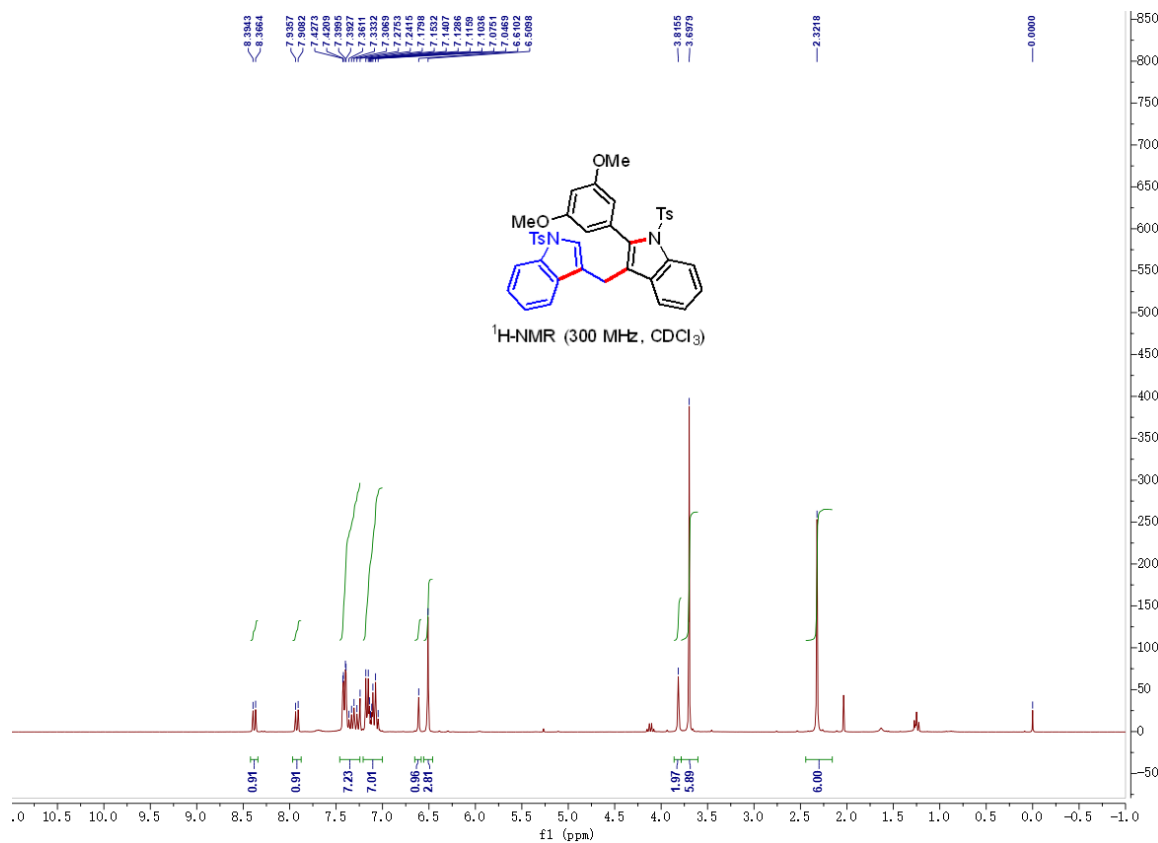
(3ah):



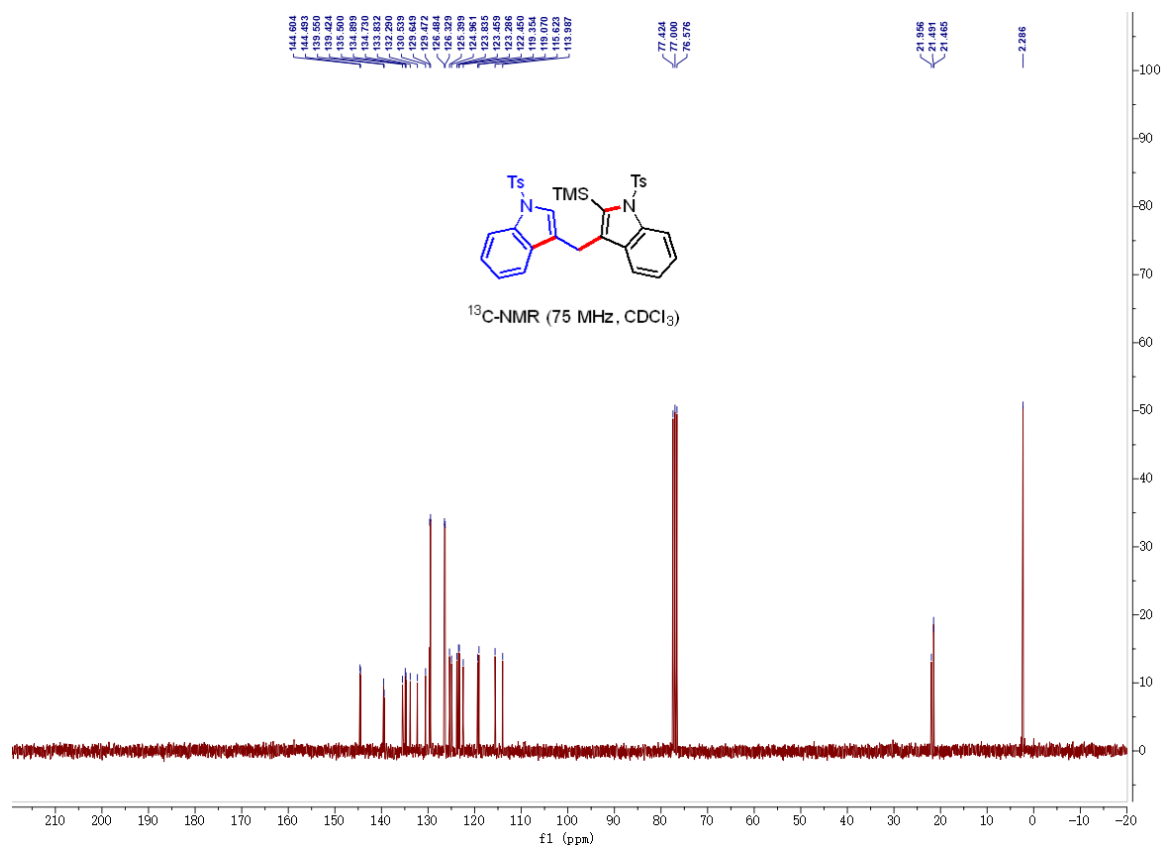
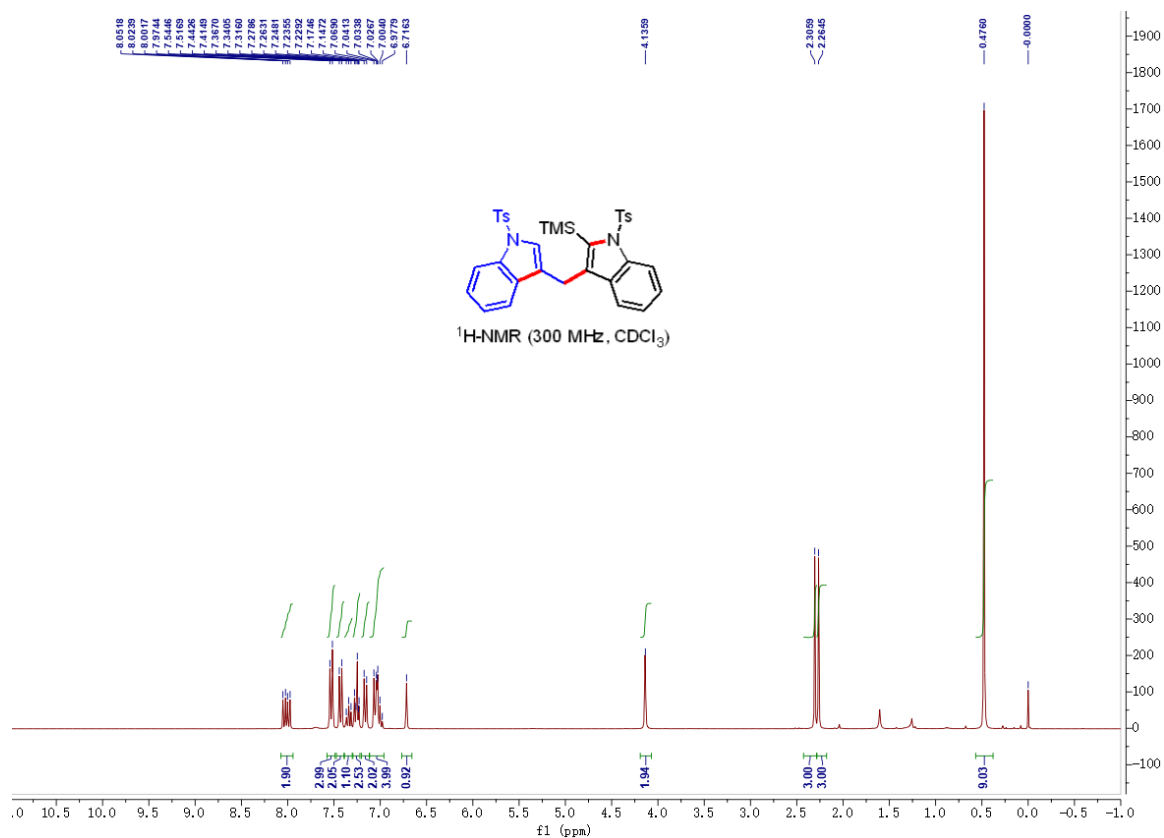
**5-(1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indol-2-yl)-1,3-phenylene
bis(4-methylbenz-enesulfonate) (3ai):**



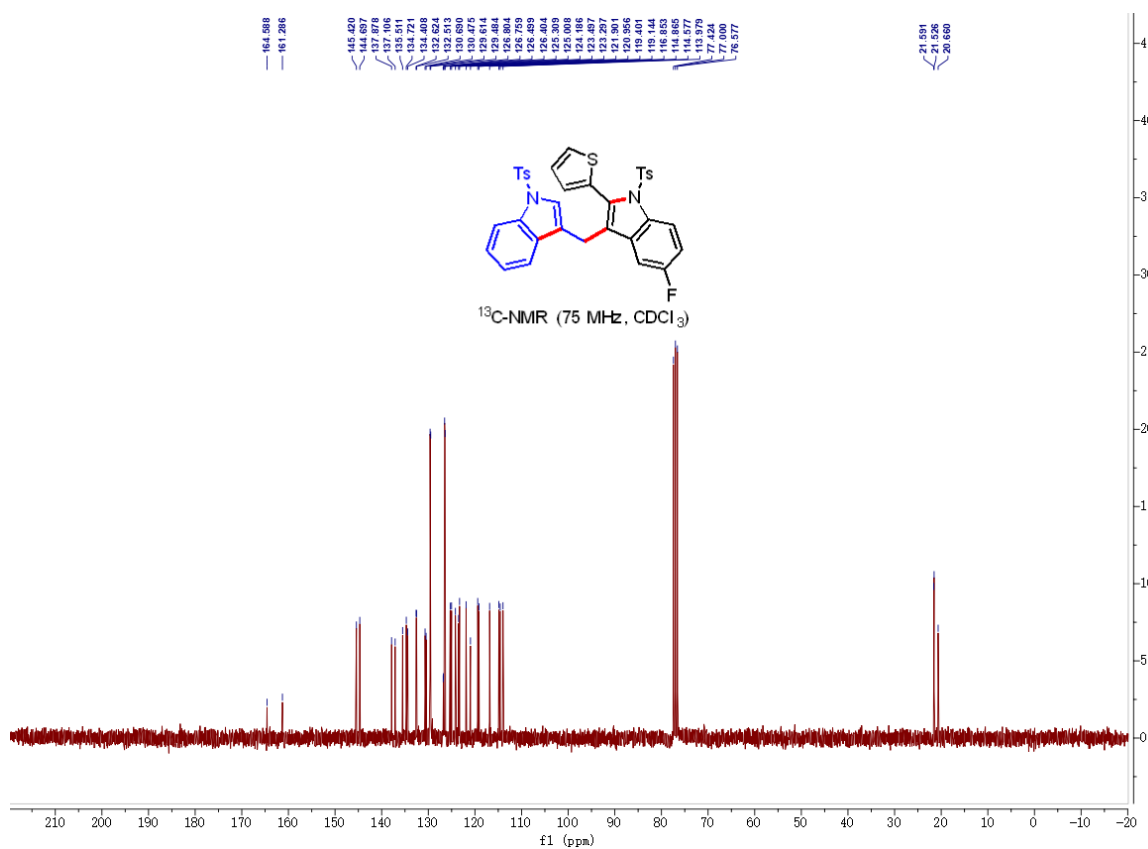
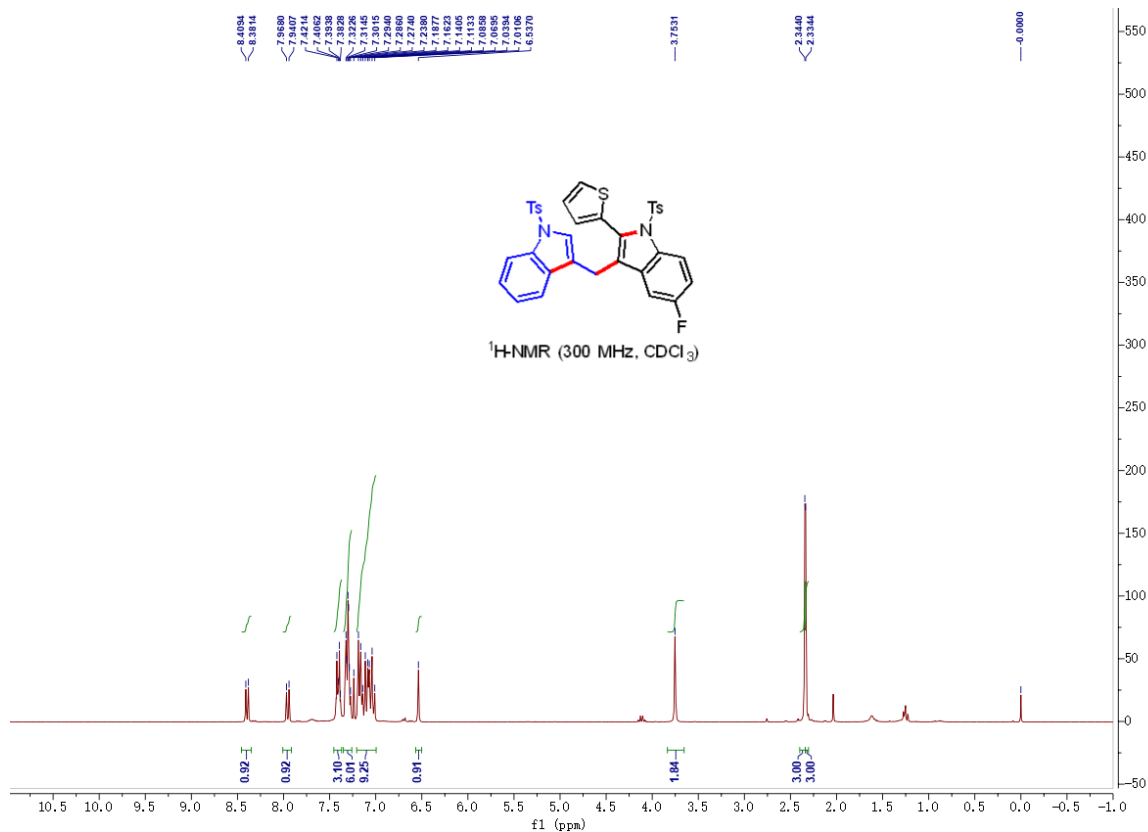
2-(3,5-dimethoxyphenyl)-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3aj):



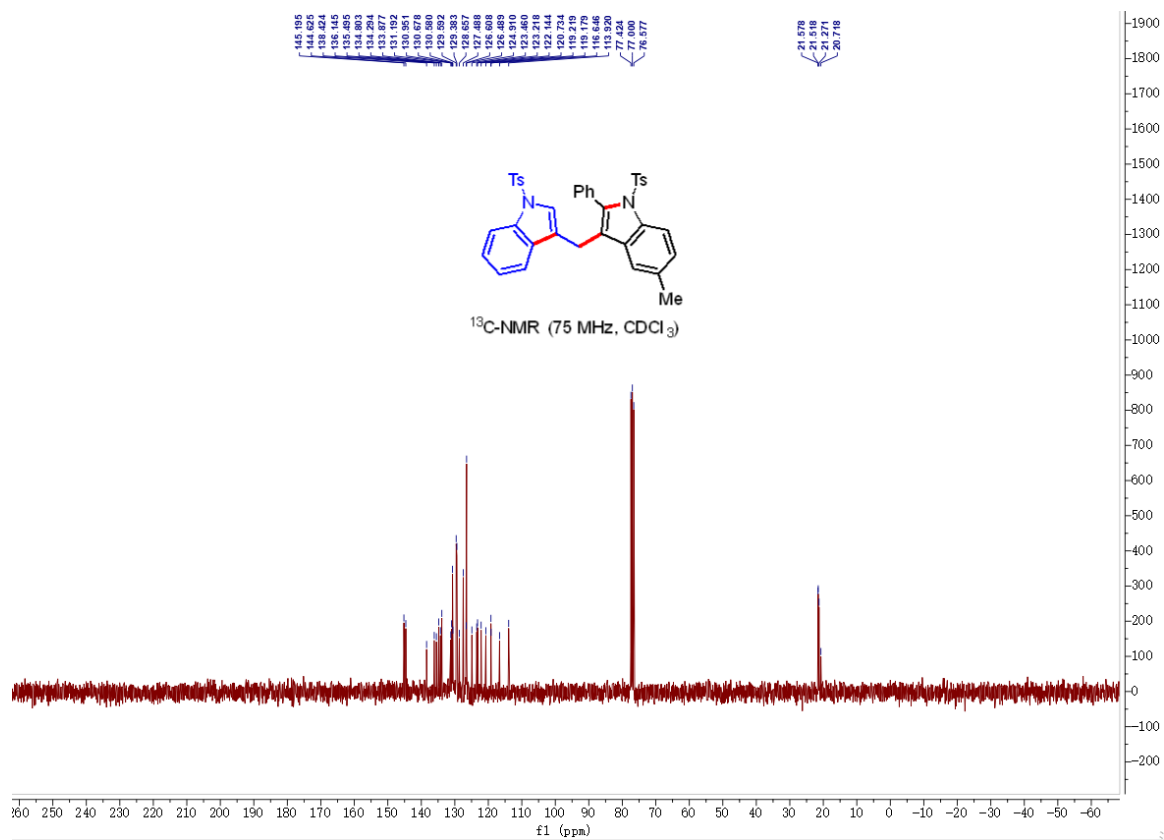
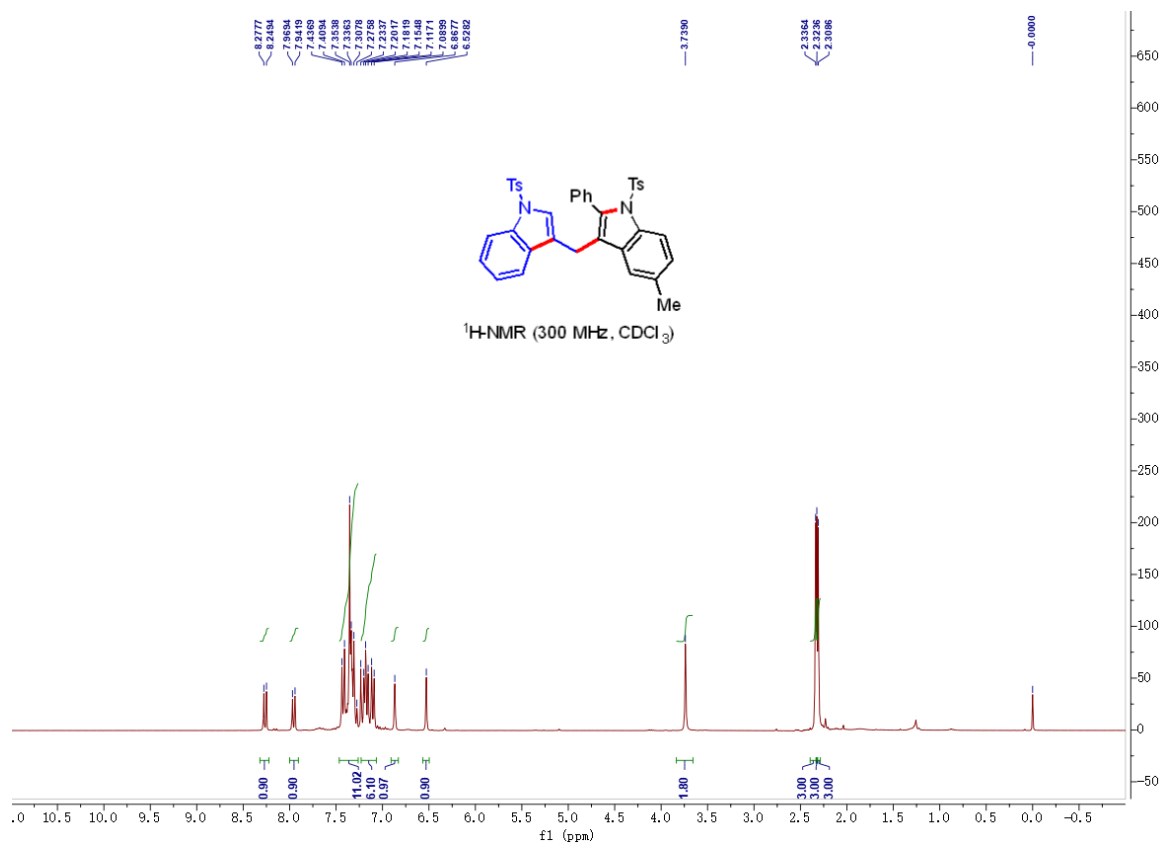
1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-2-(trimethylsilyl)-1*H*-indole (3a):



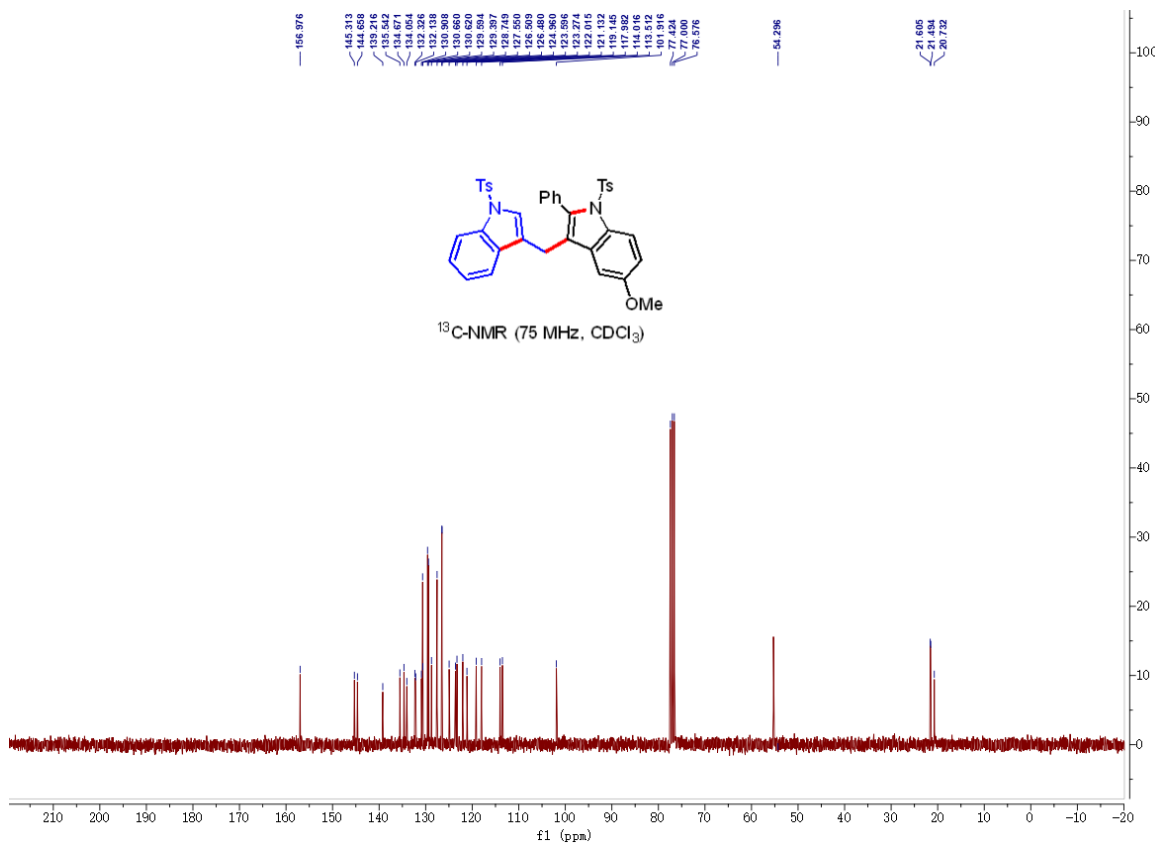
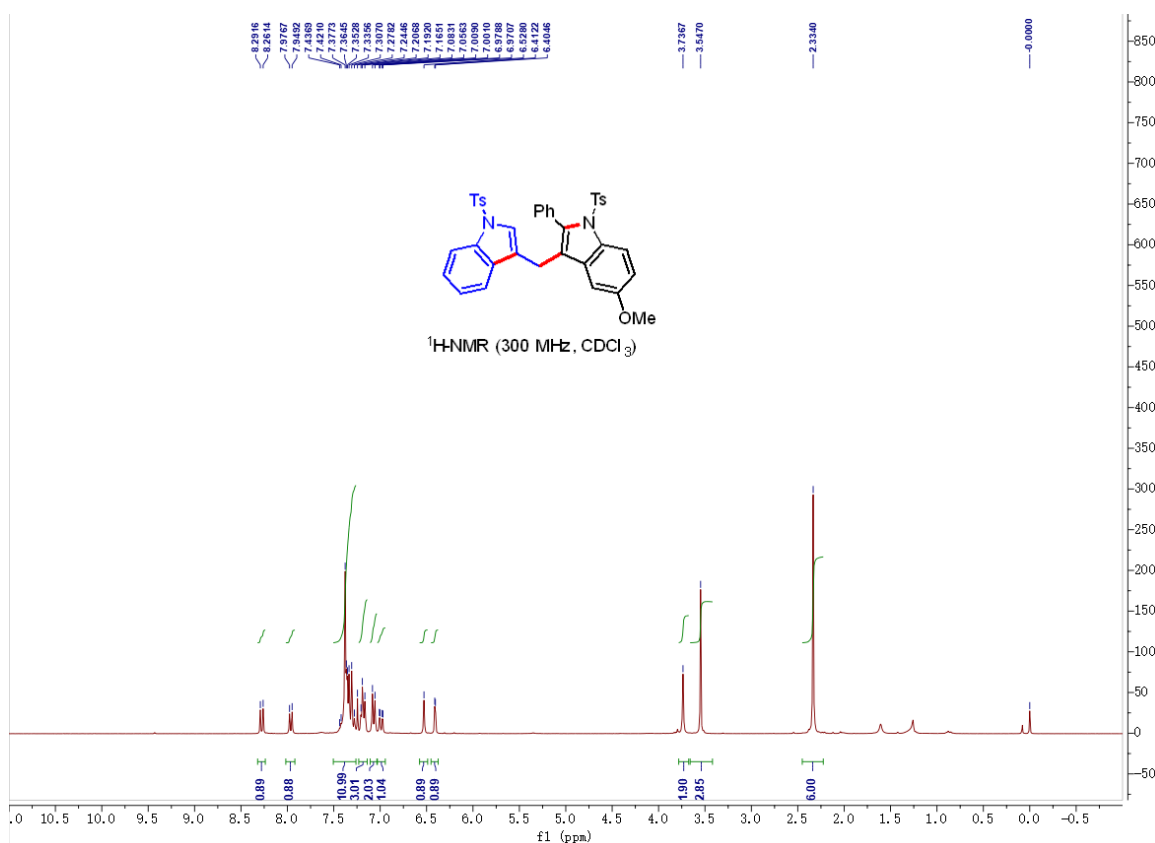
5-fluoro-2-(thiophen-2-yl)-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3am):



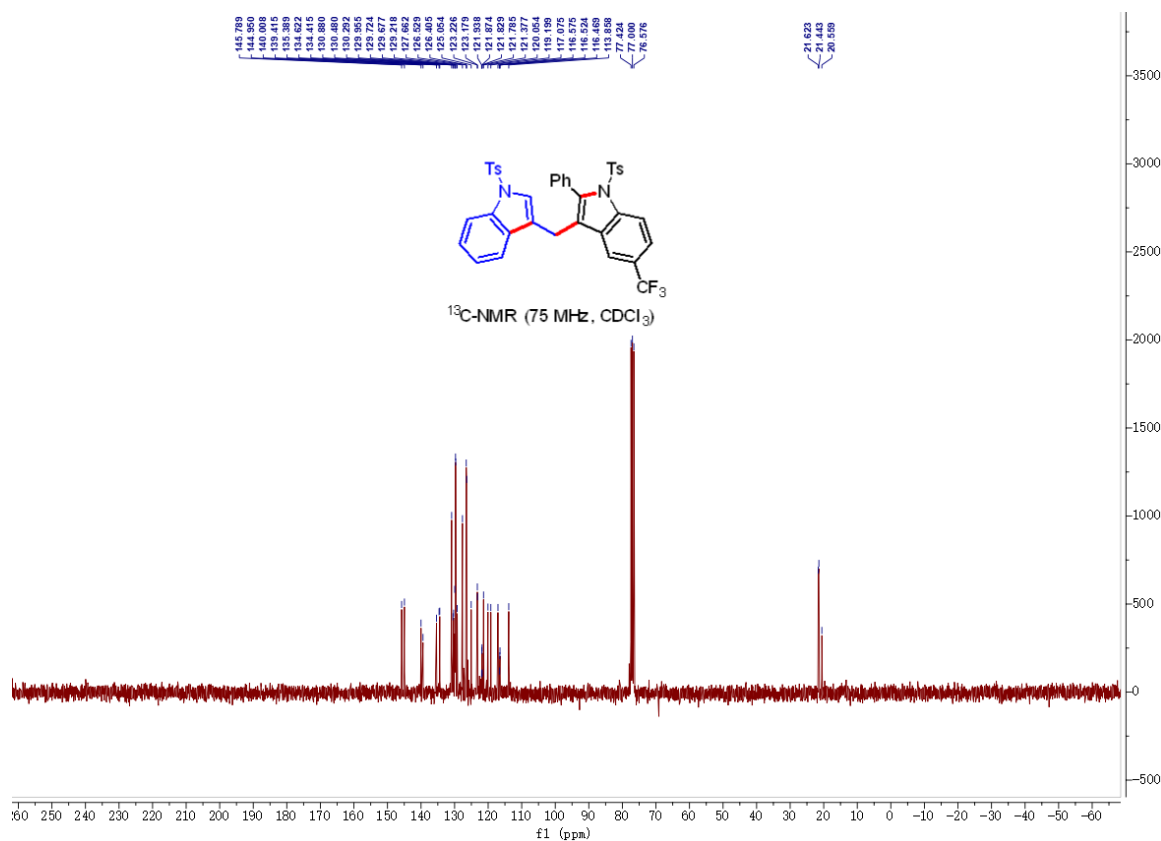
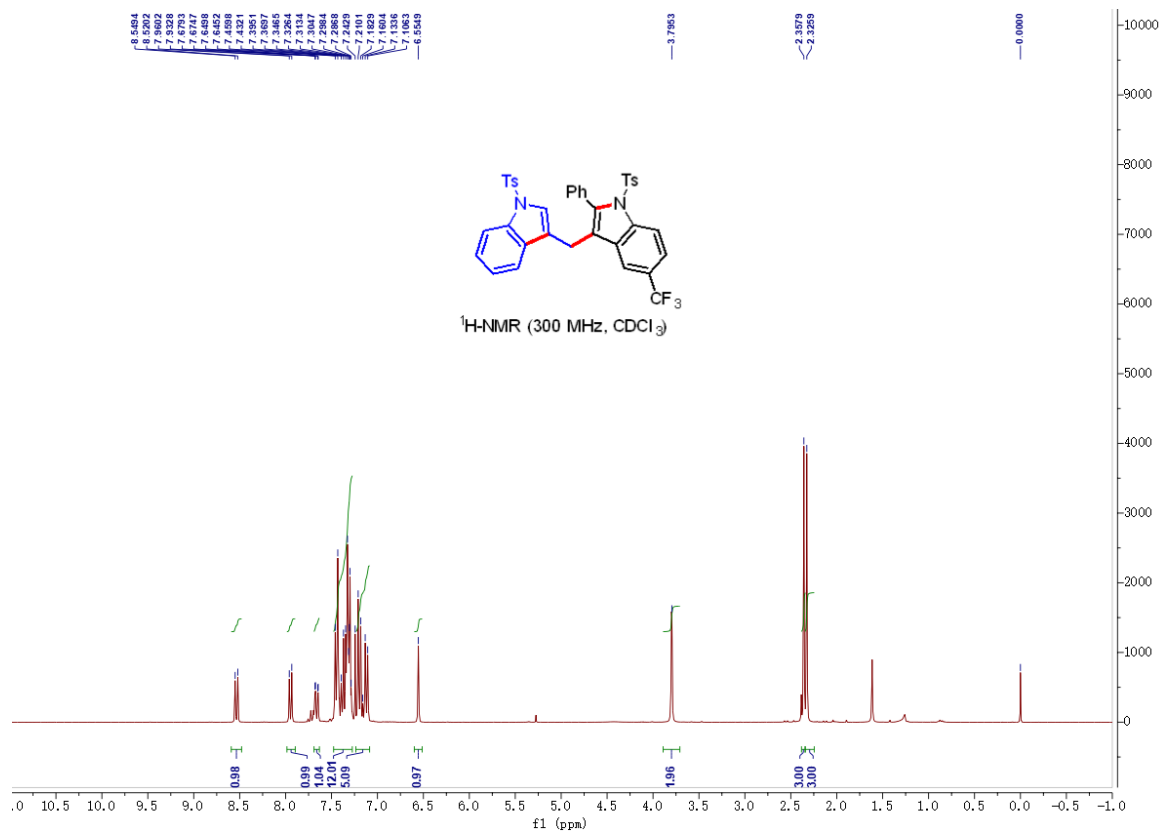
5-methyl-2-phenyl-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3an):



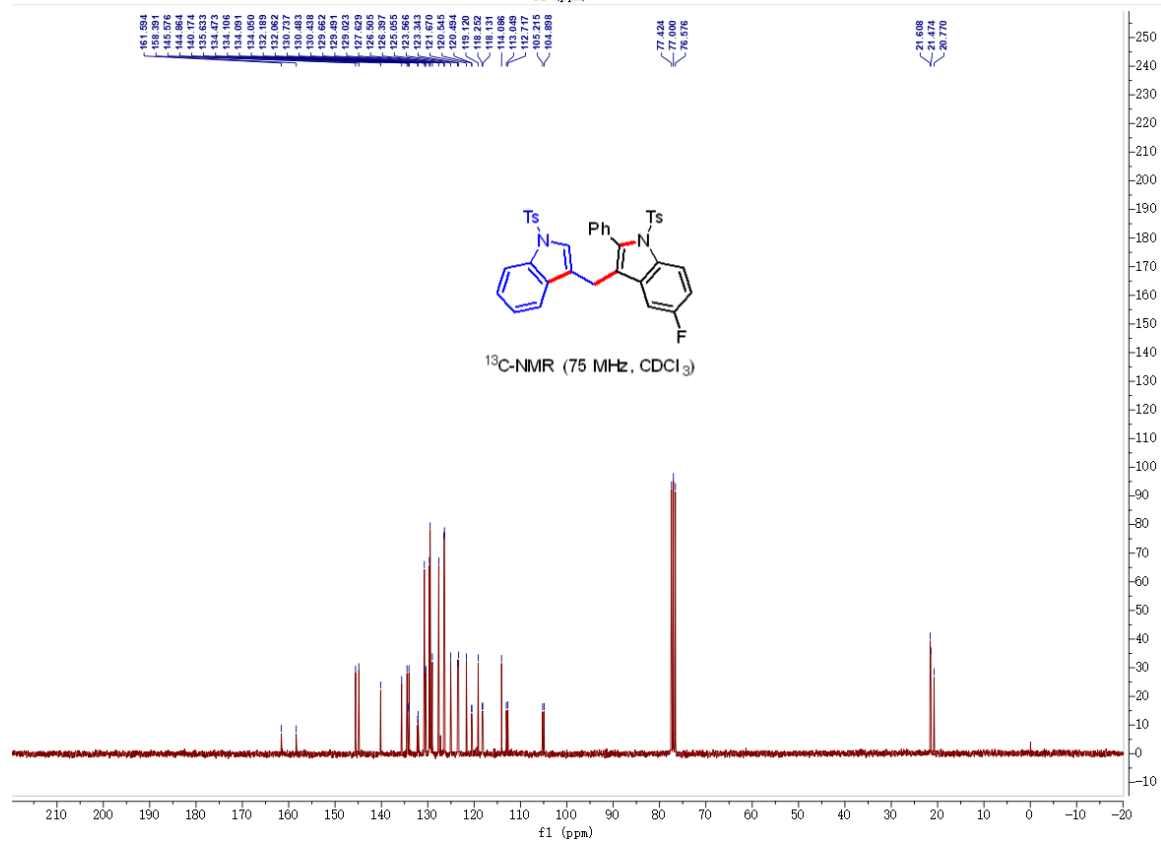
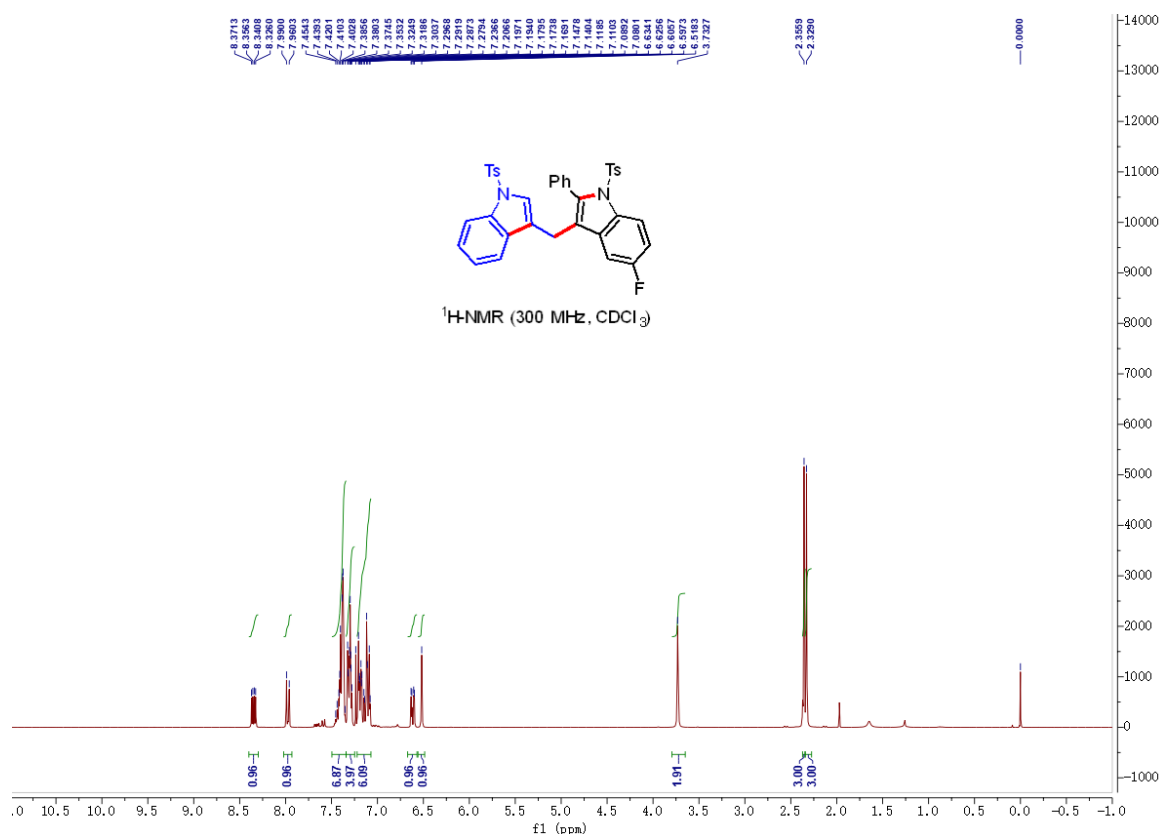
5-methoxy-2-phenyl-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3ao):



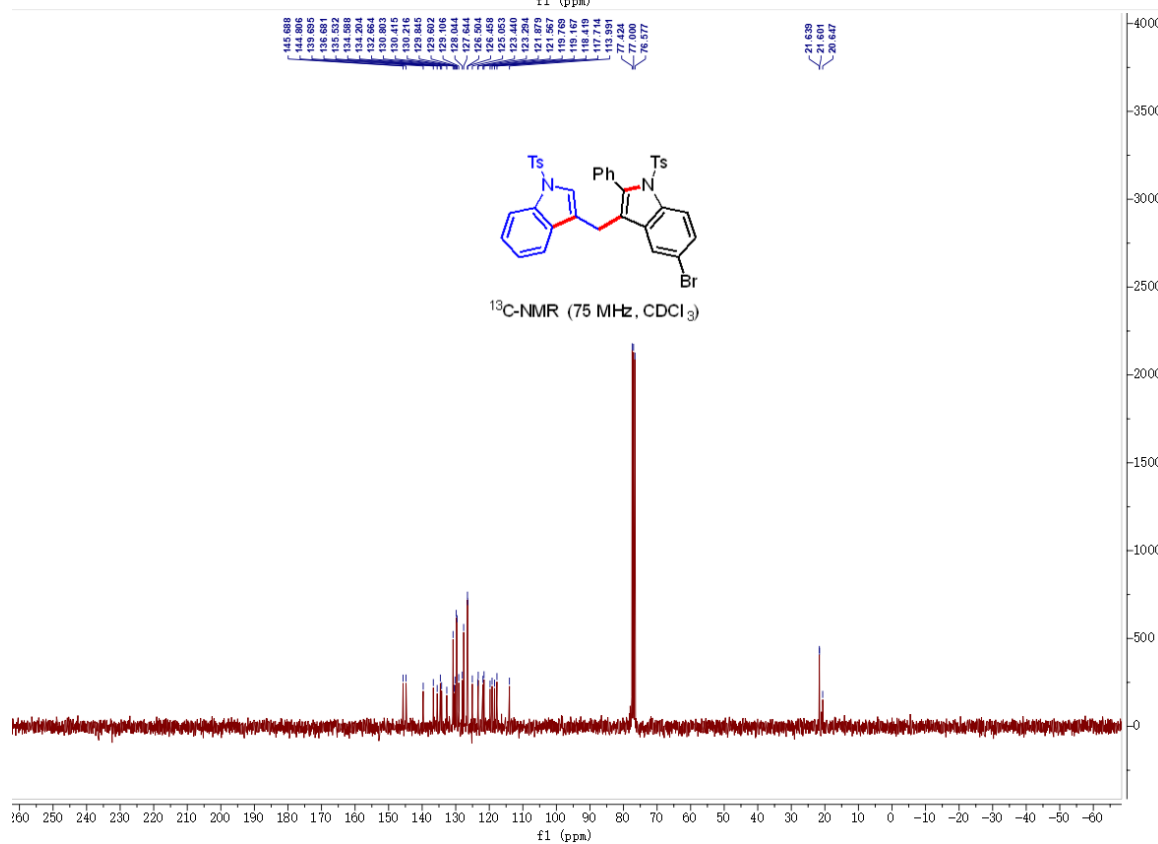
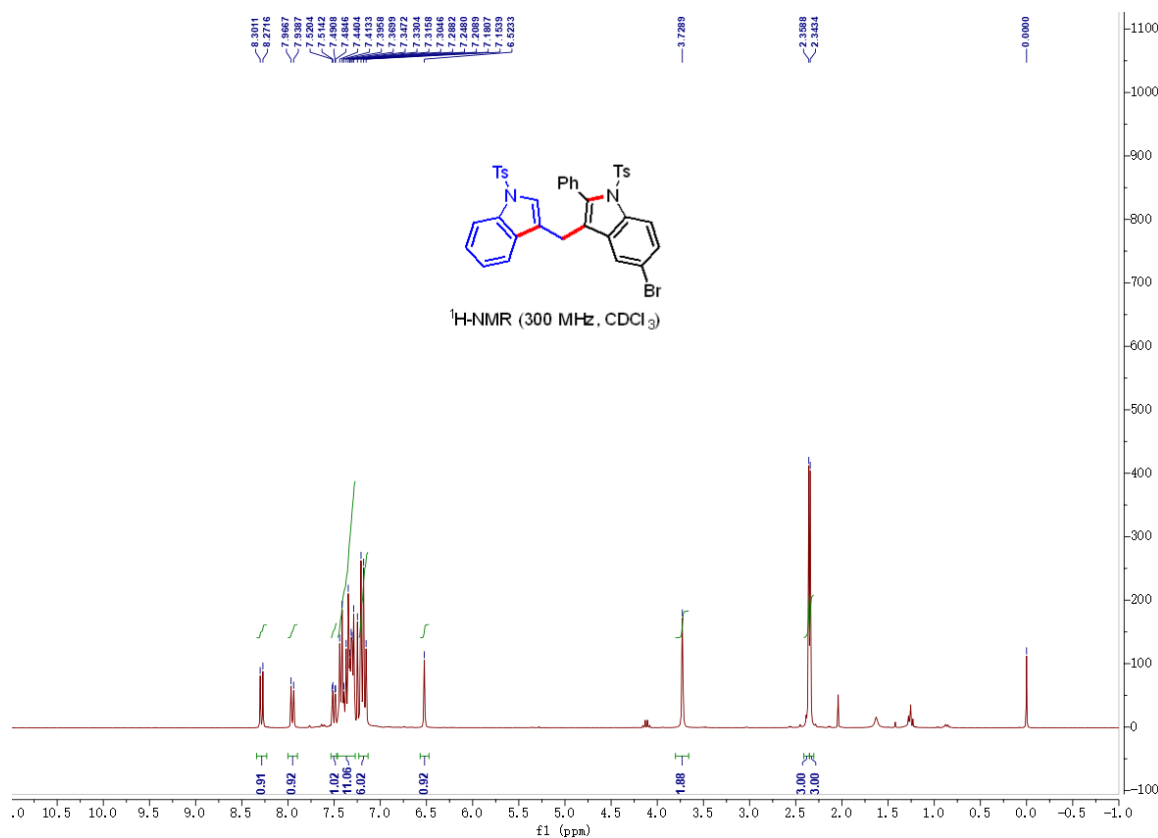
2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-5-(trifluoromethyl)-1H-indole (3ap):



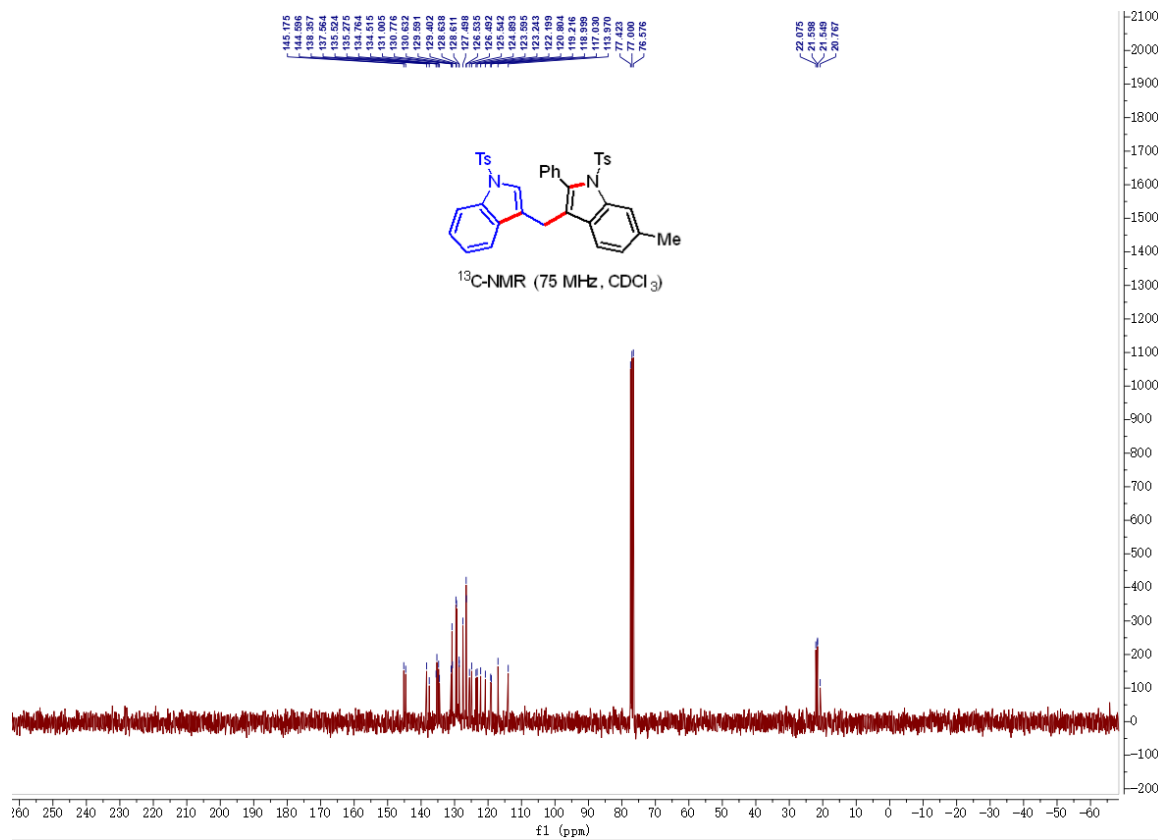
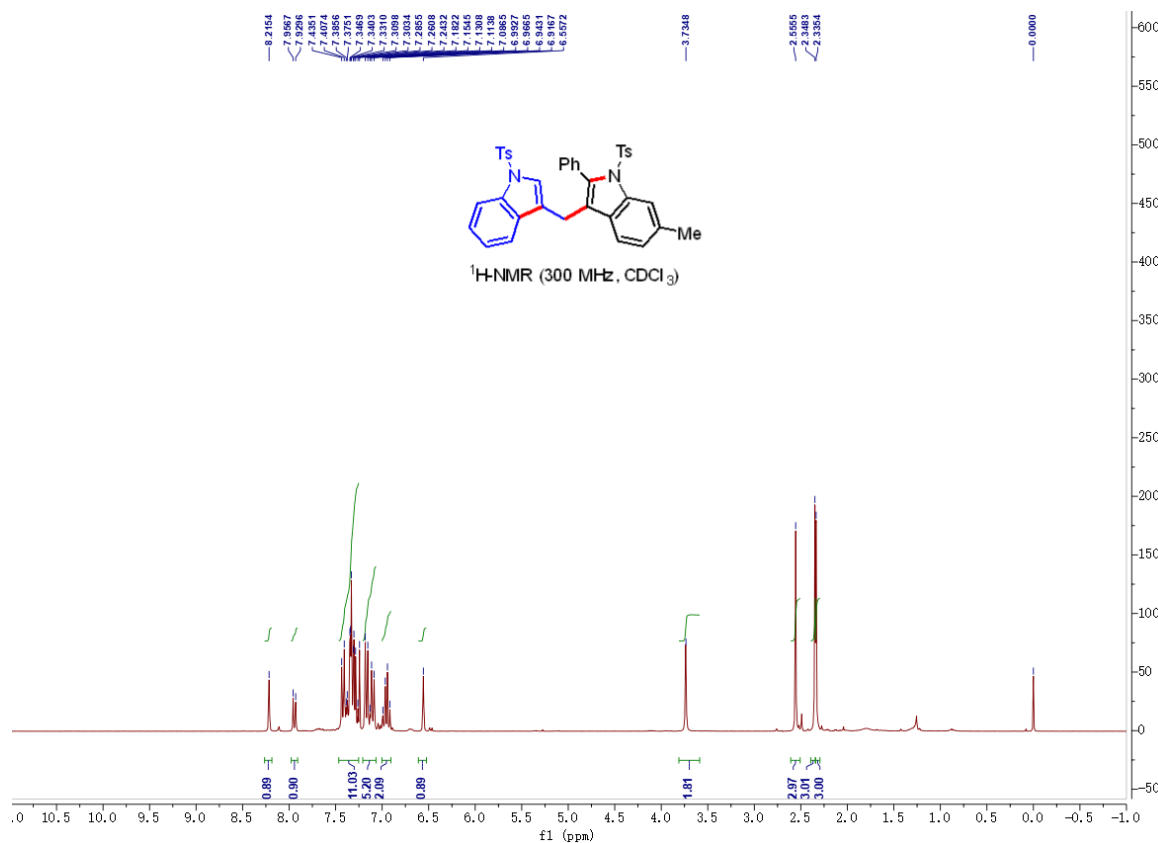
5-fluoro-2-phenyl-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3aq):



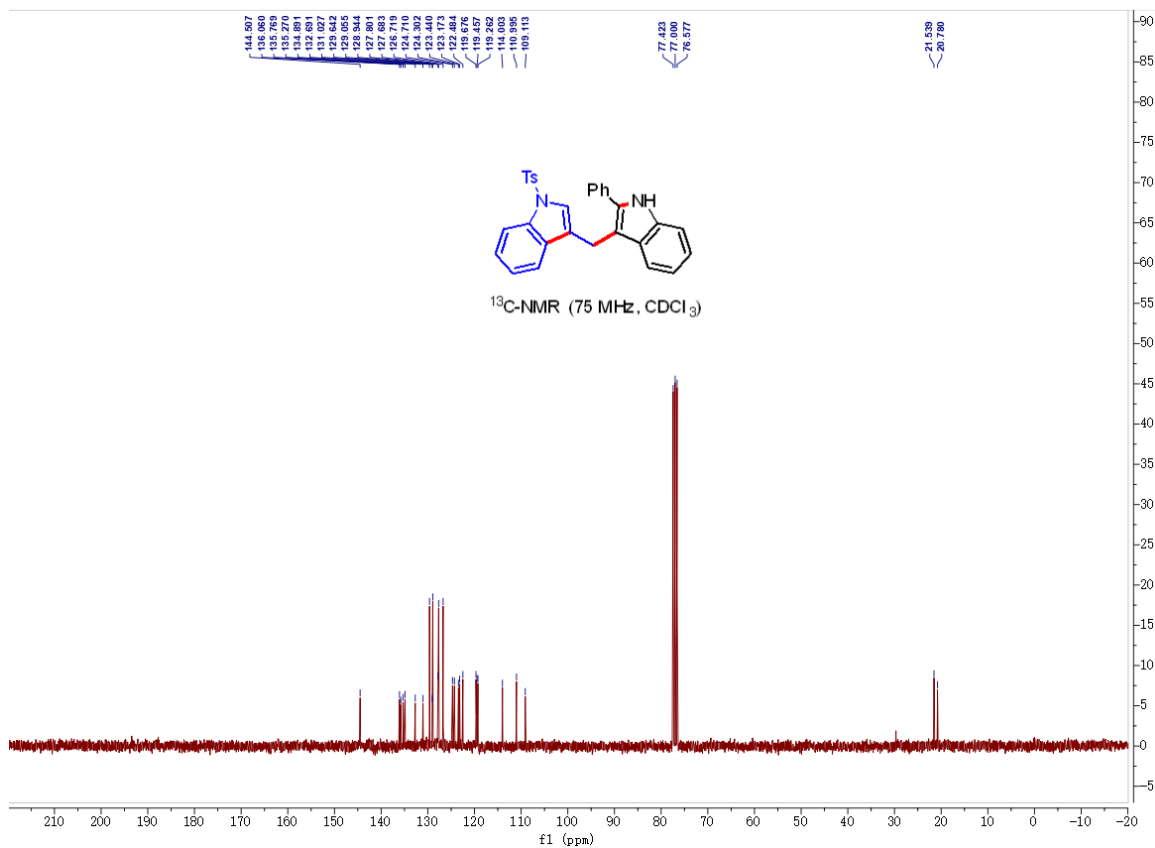
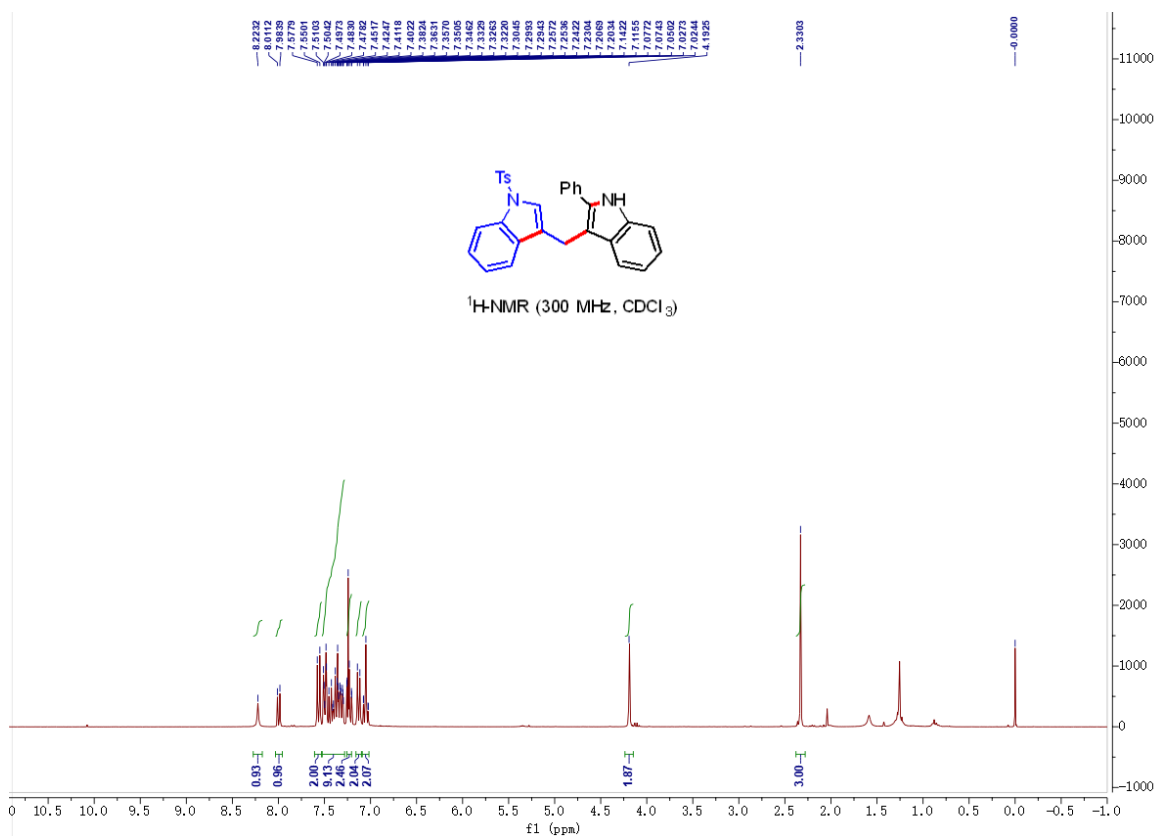
5-bromo-2-phenyl-1-tosyl-3-((1-tosyl-1*H*-indol-3-yl)methyl)-1*H*-indole (3ar):



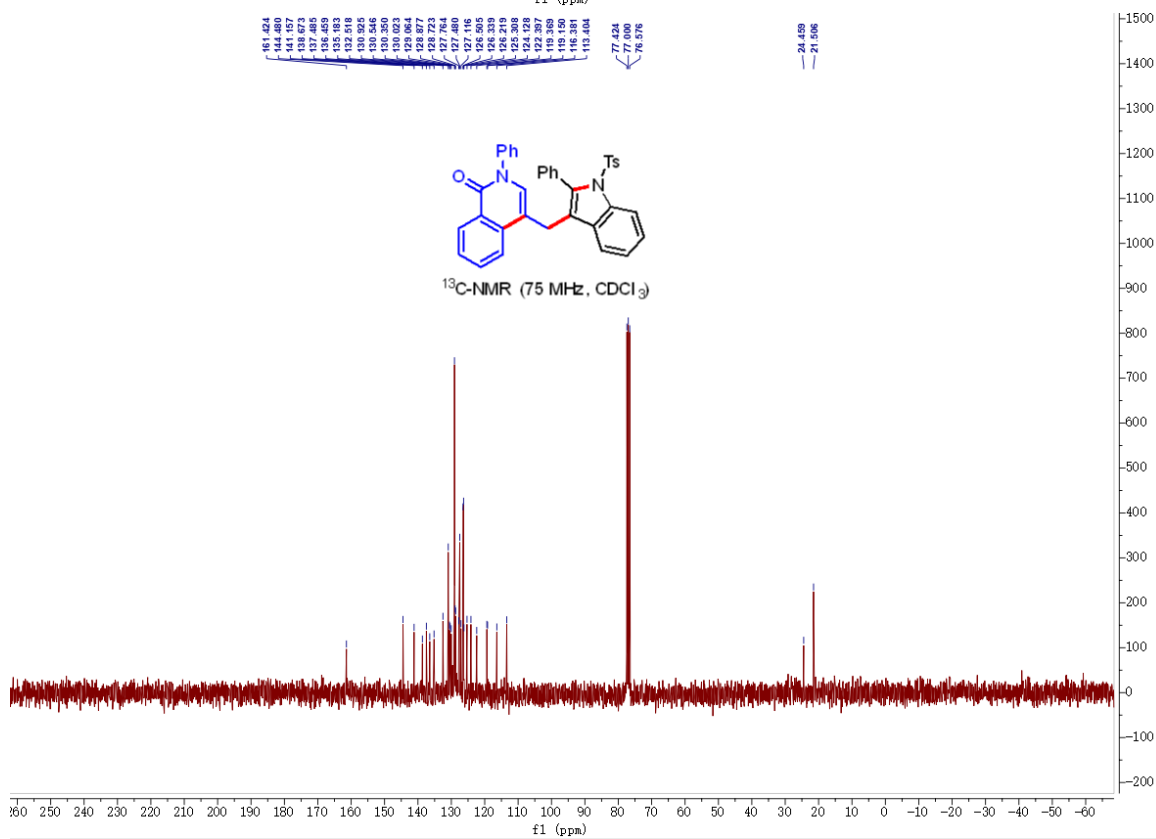
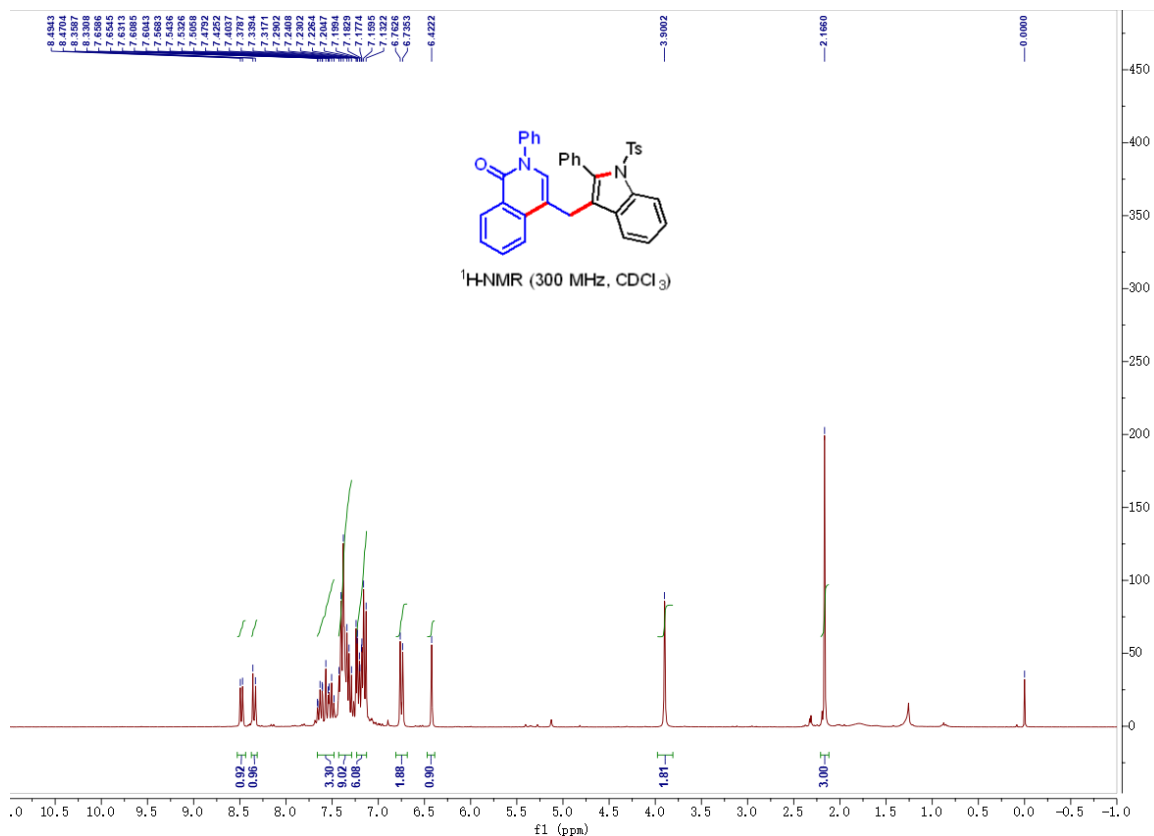
6-methyl-2-phenyl-1-tosyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3as):



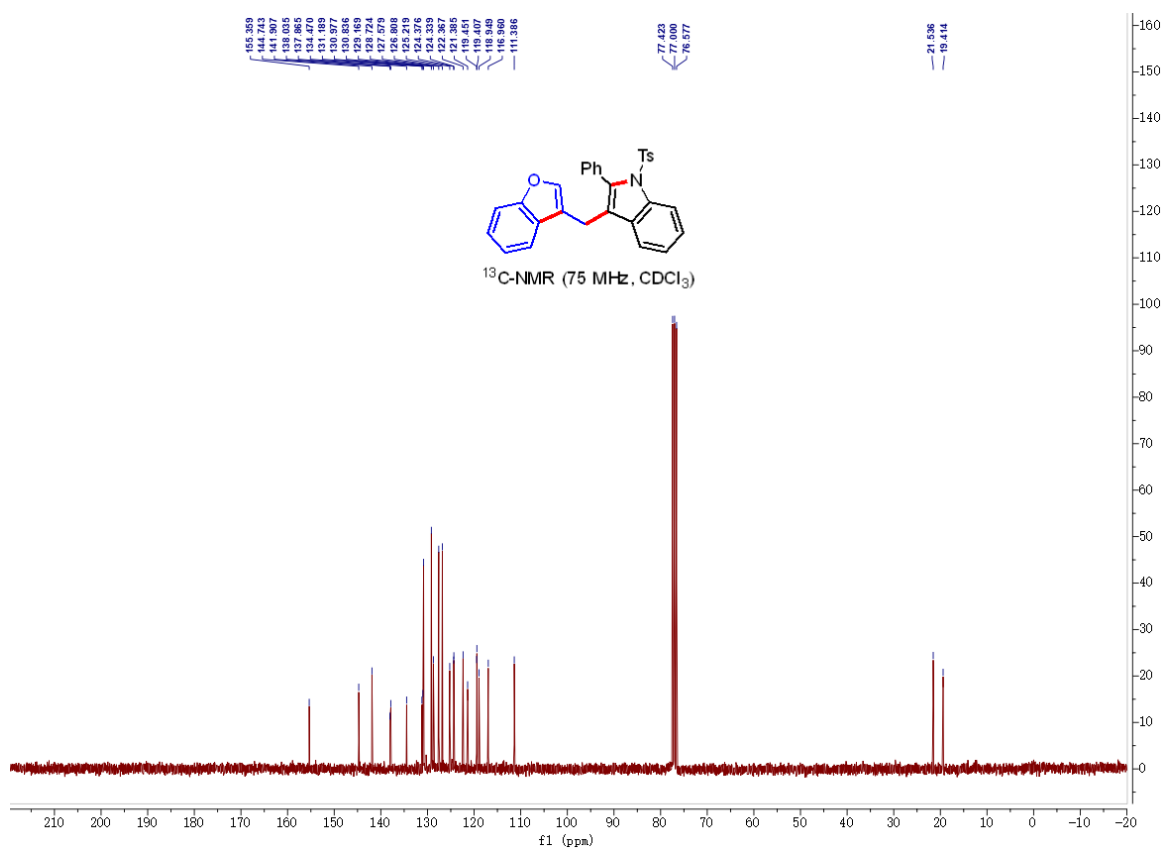
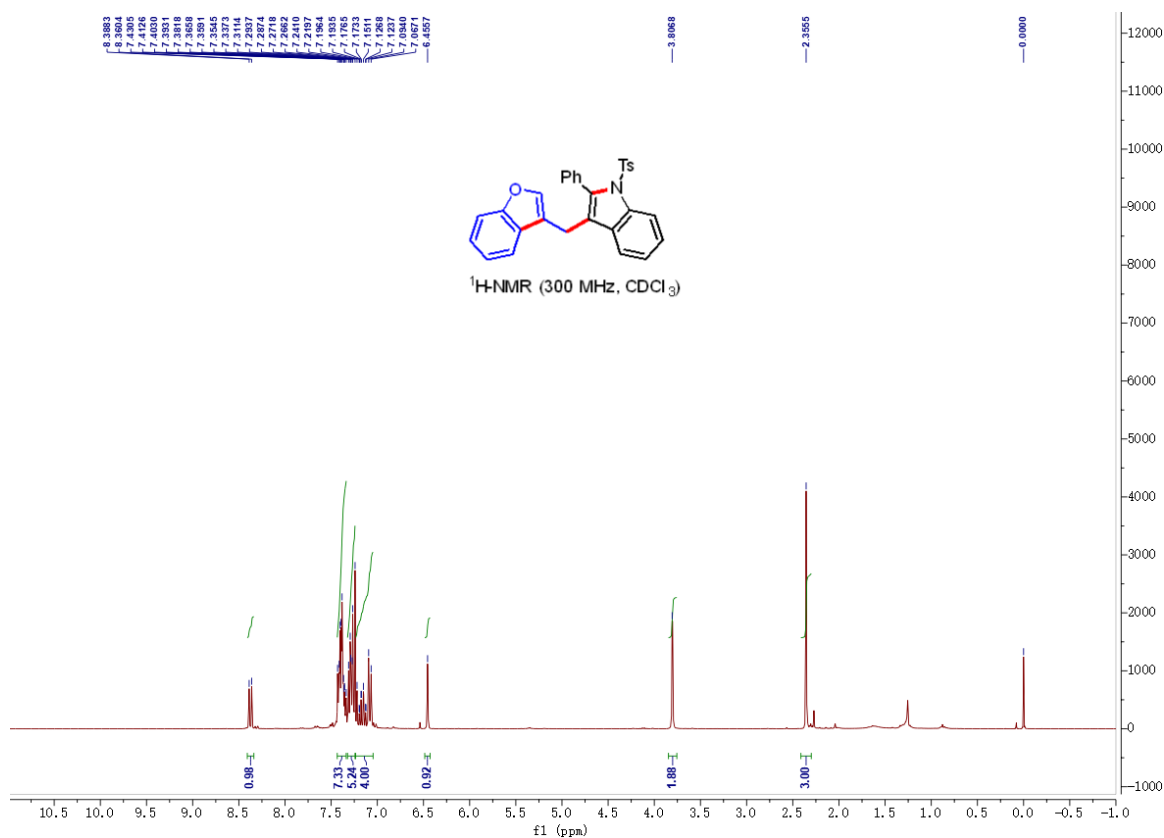
2-phenyl-3-((1-tosyl-1H-indol-3-yl)methyl)-1H-indole (3au):



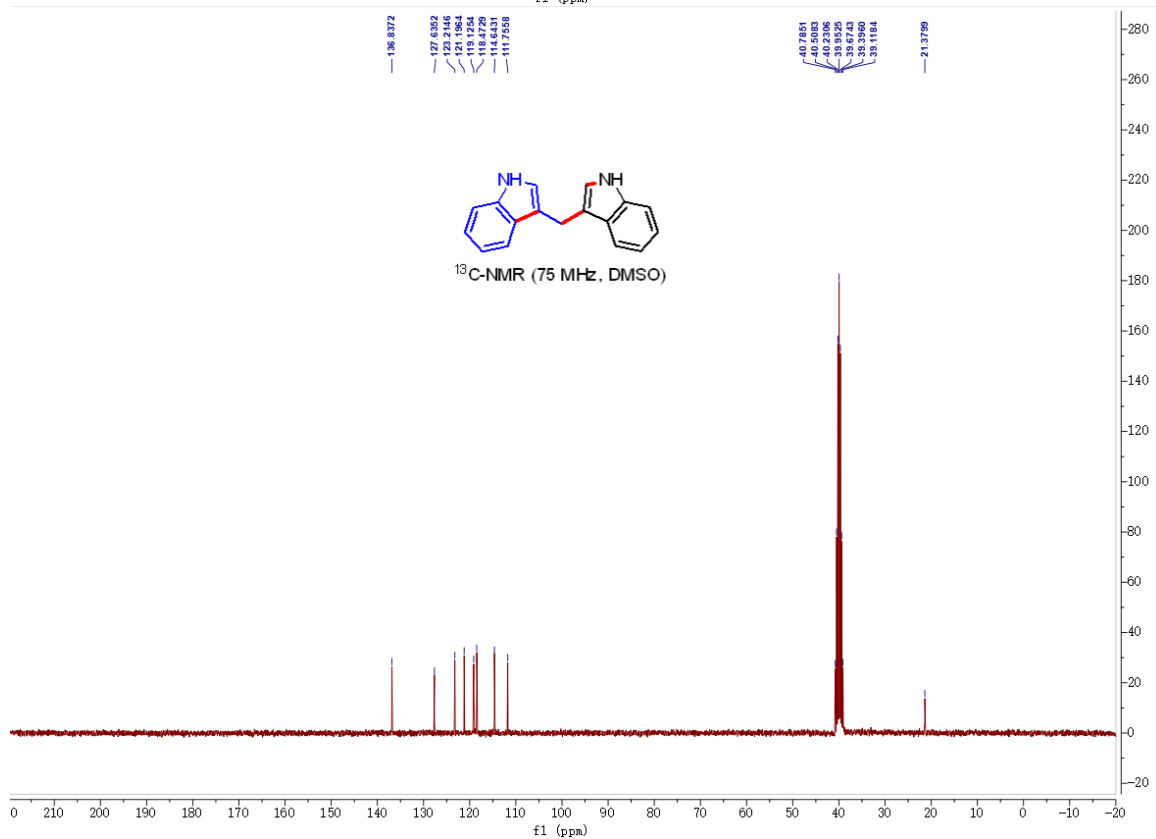
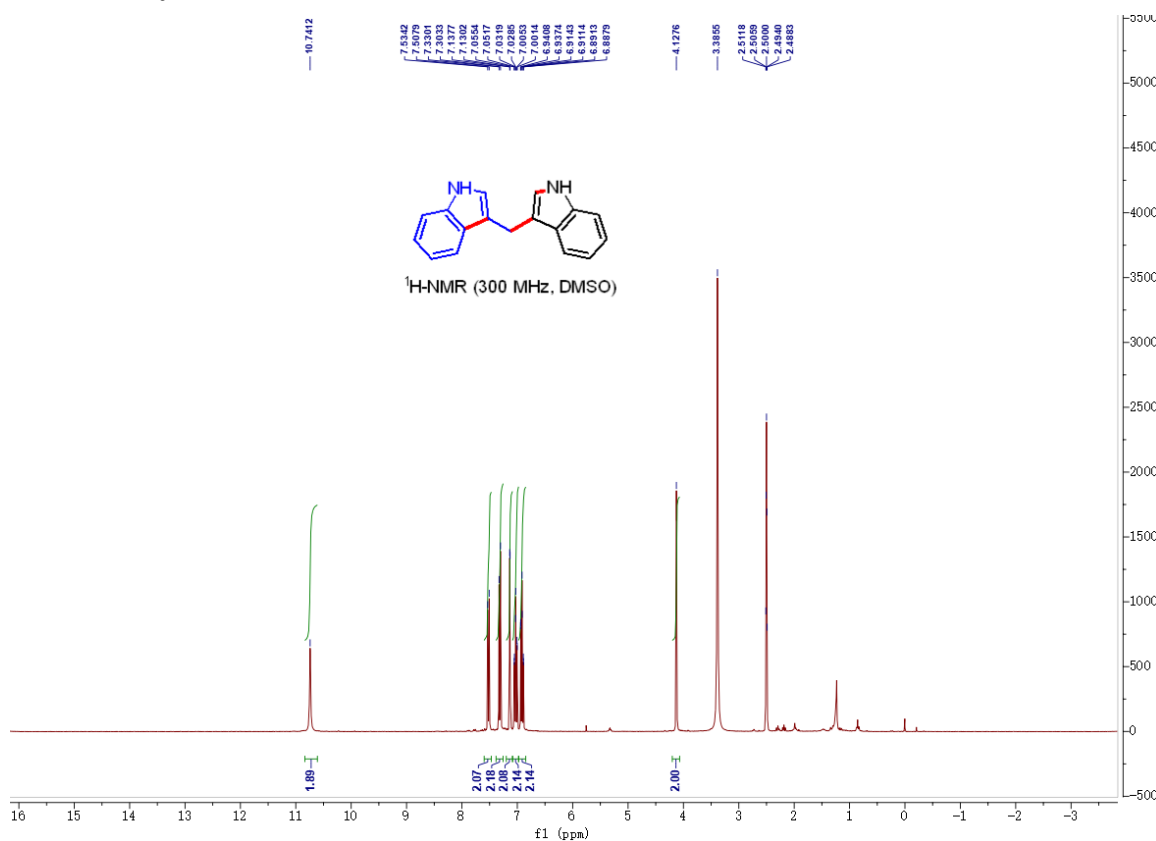
2-phenyl-4-((2-phenyl-1-tosyl-1H-indol-3-yl)methyl)isoquinolin-1(2H)-one (5):



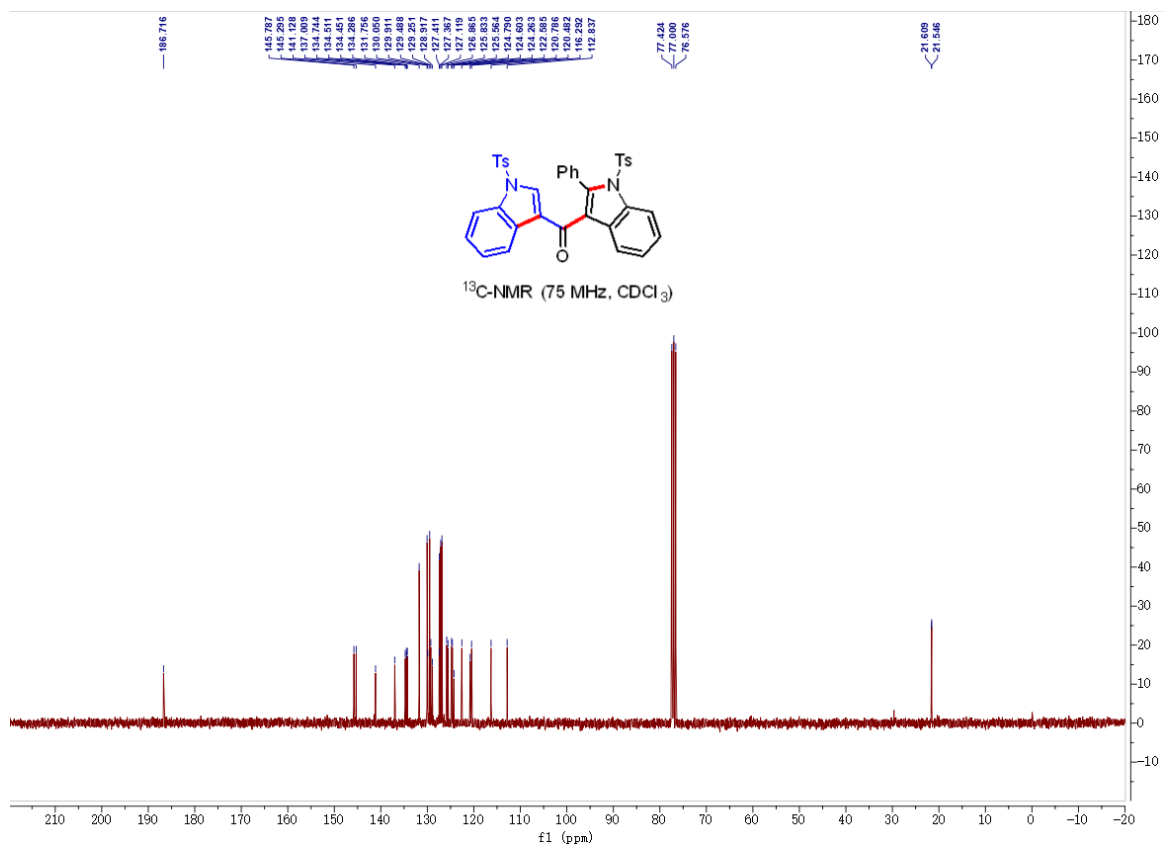
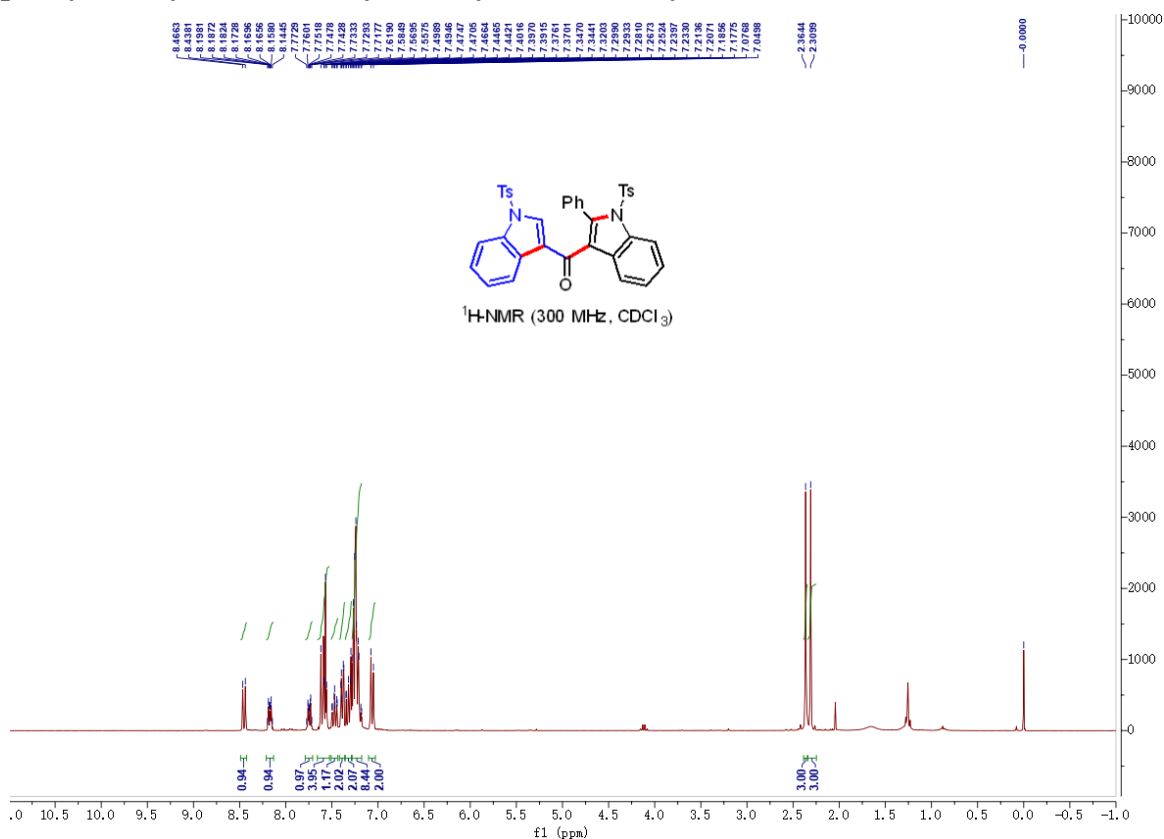
3-(benzofuran-3-ylmethyl)-2-phenyl-1-tosyl-1H-indole (7):



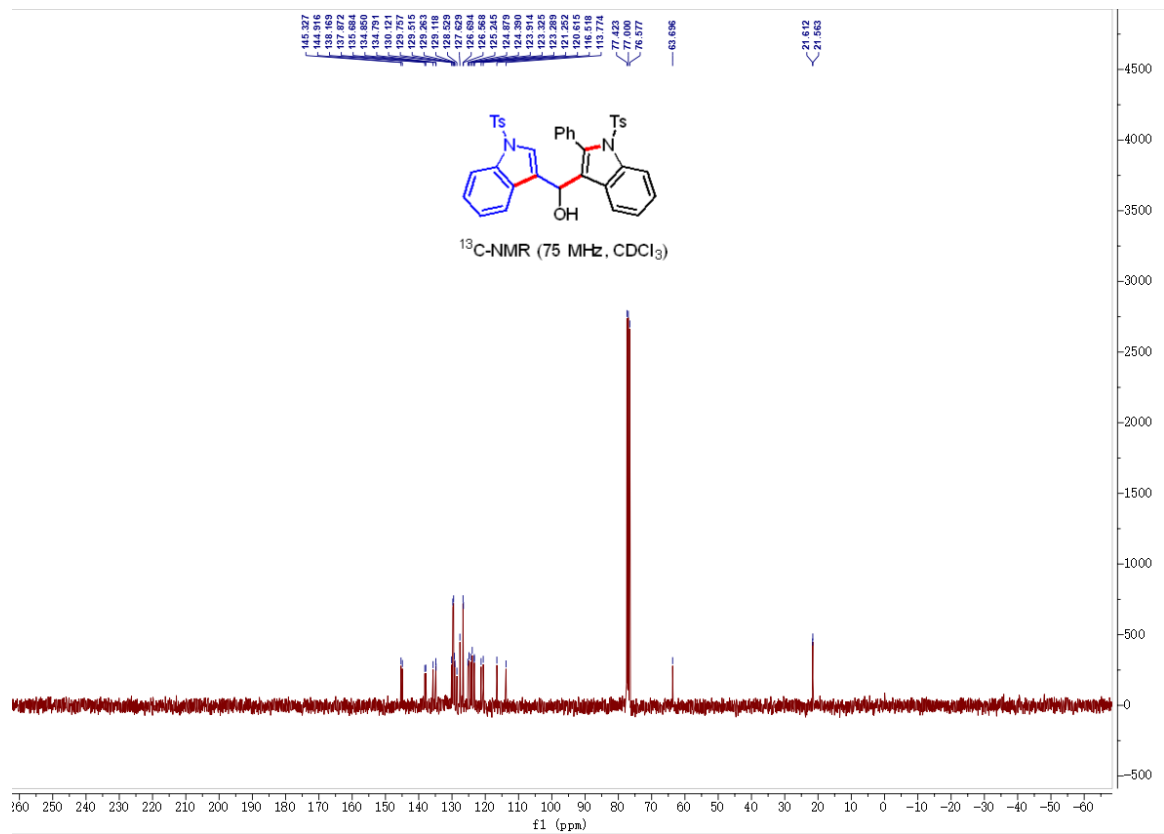
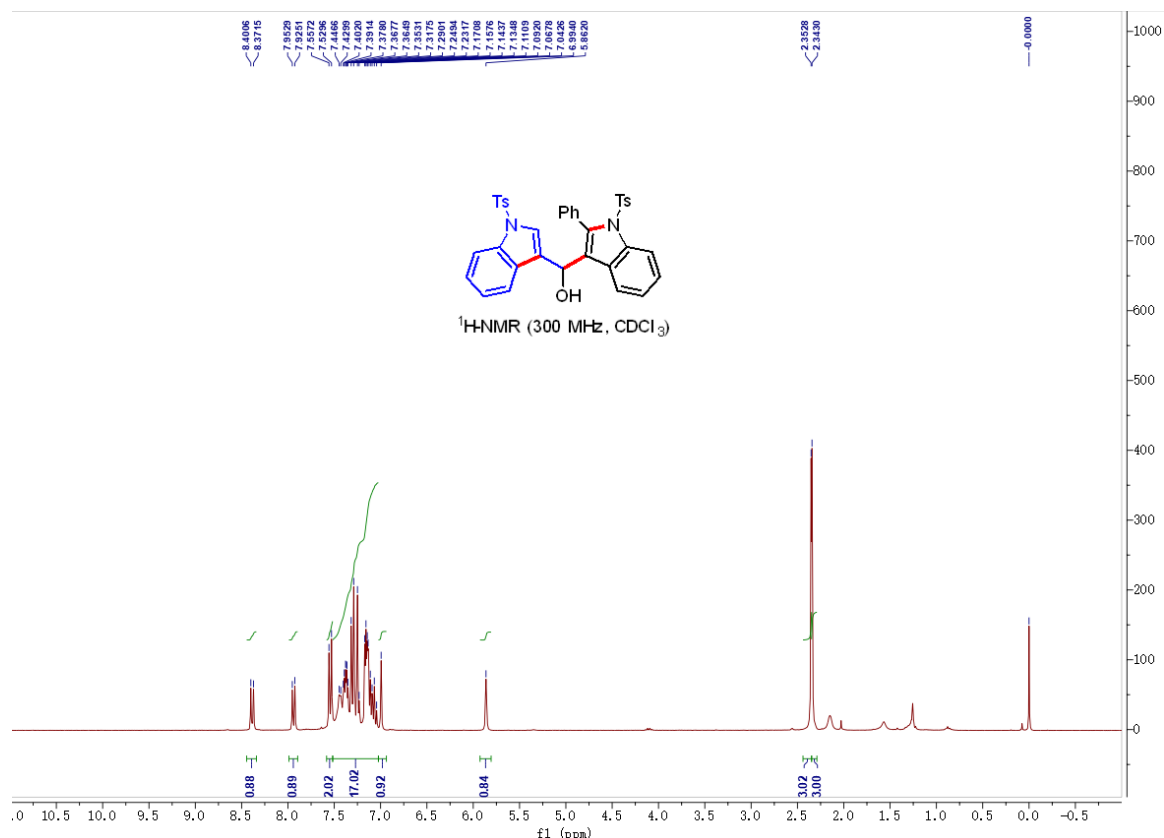
di(1H-indol-3-yl)methane (8):



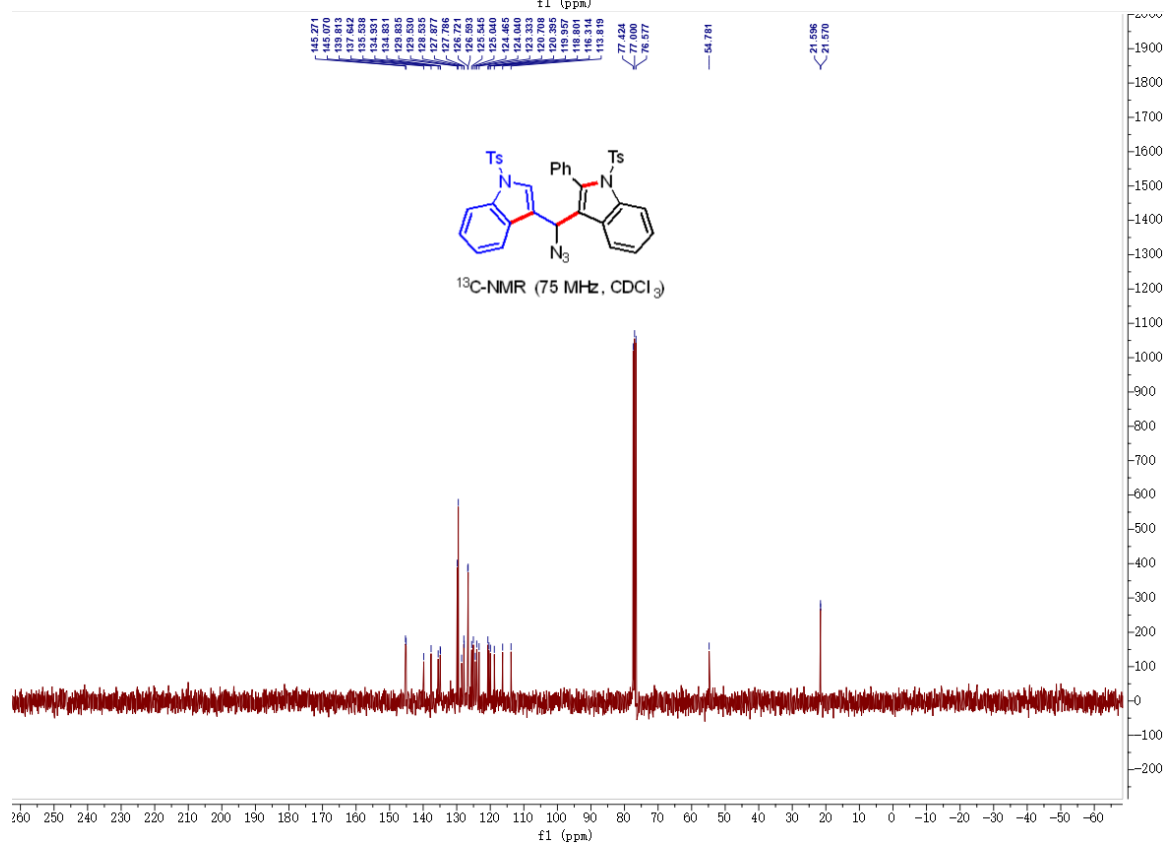
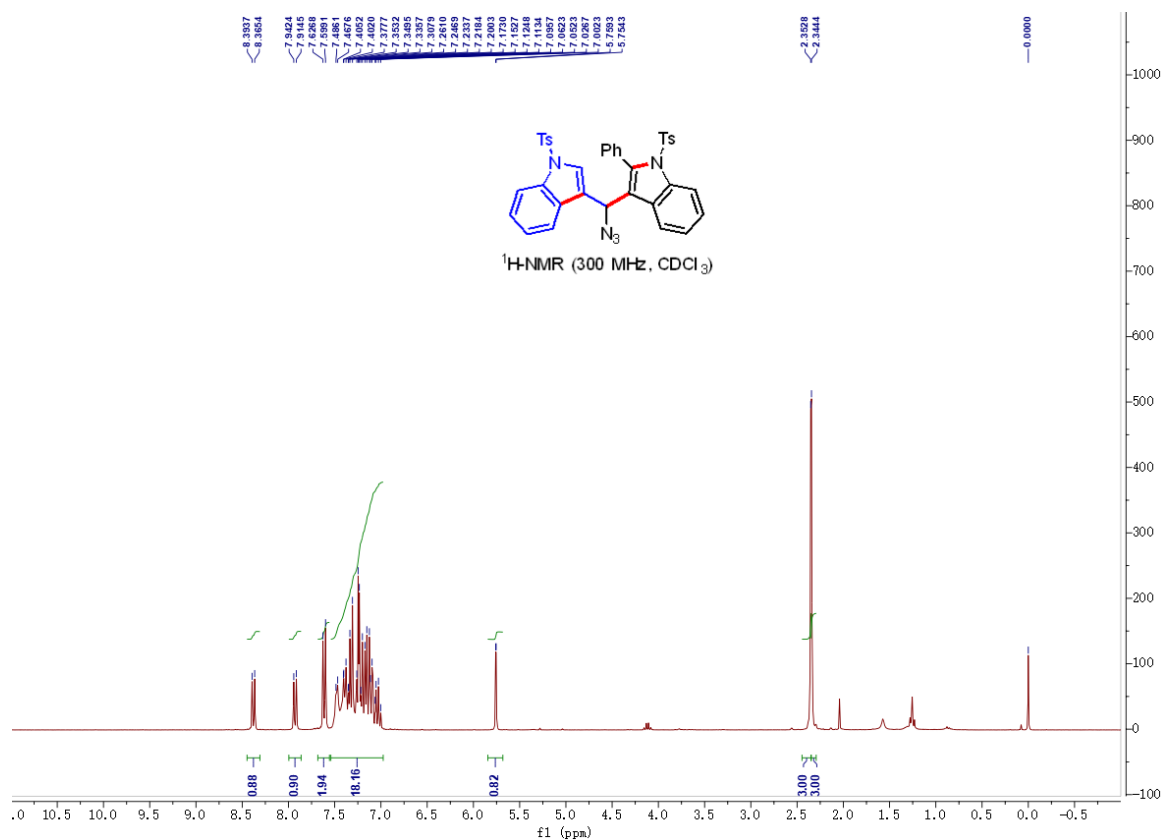
(2-phenyl-1-tosyl-1*H*-indol-3-yl)(1-tosyl-1*H*-indol-3-yl)methanone (9):



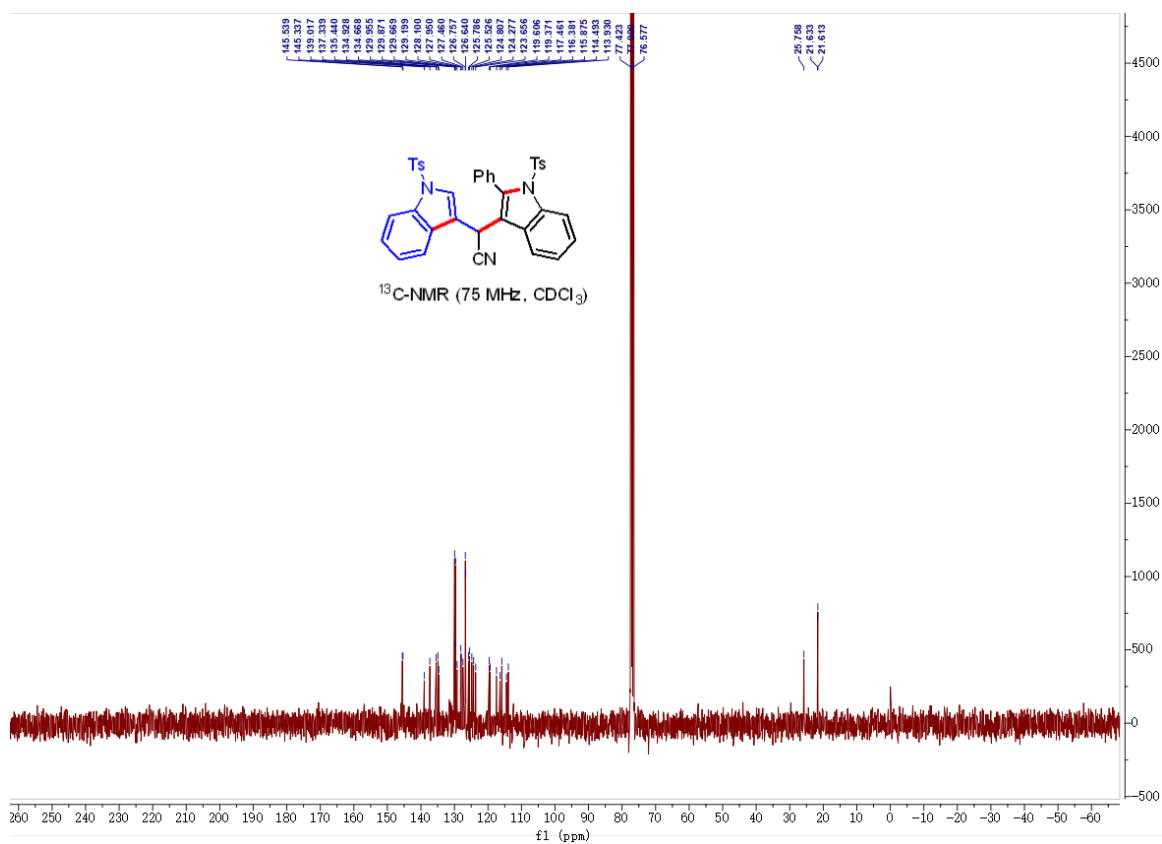
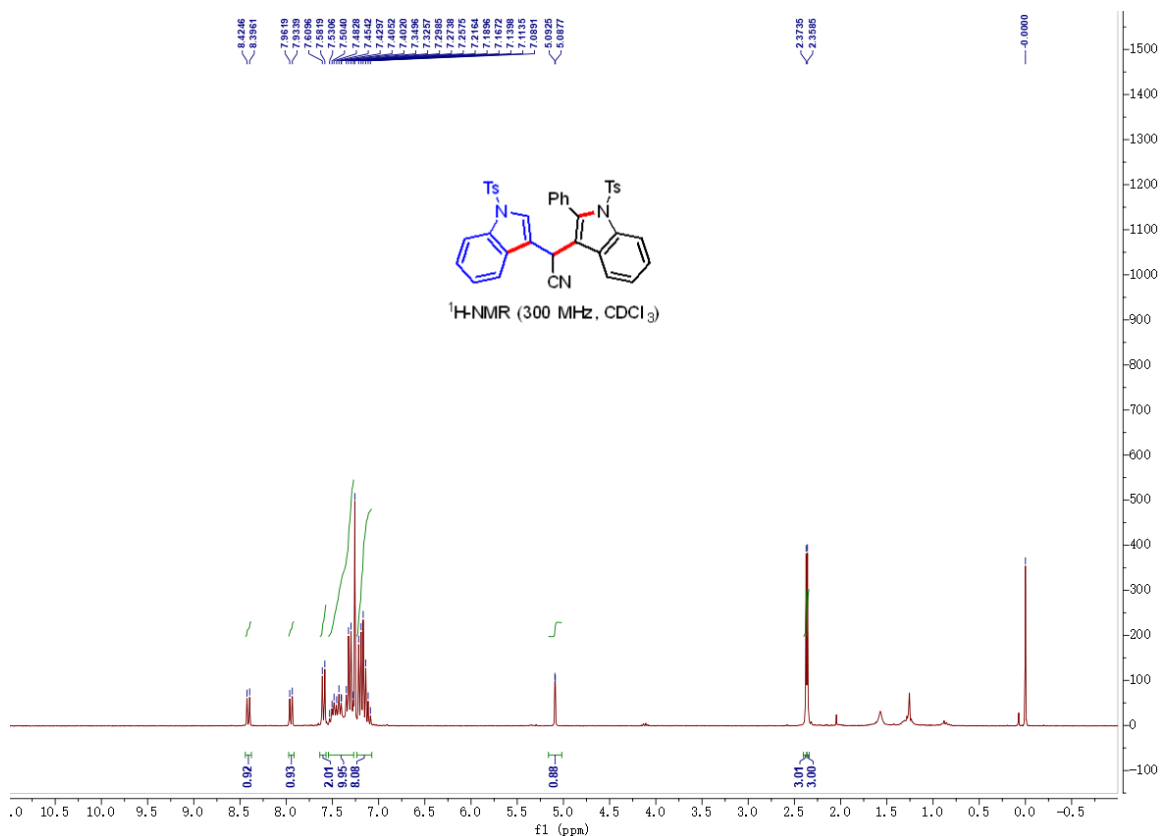
(2-phenyl-1-tosyl-1*H*-indol-3-yl)(1-tosyl-1*H*-indol-3-yl)methanol (10):



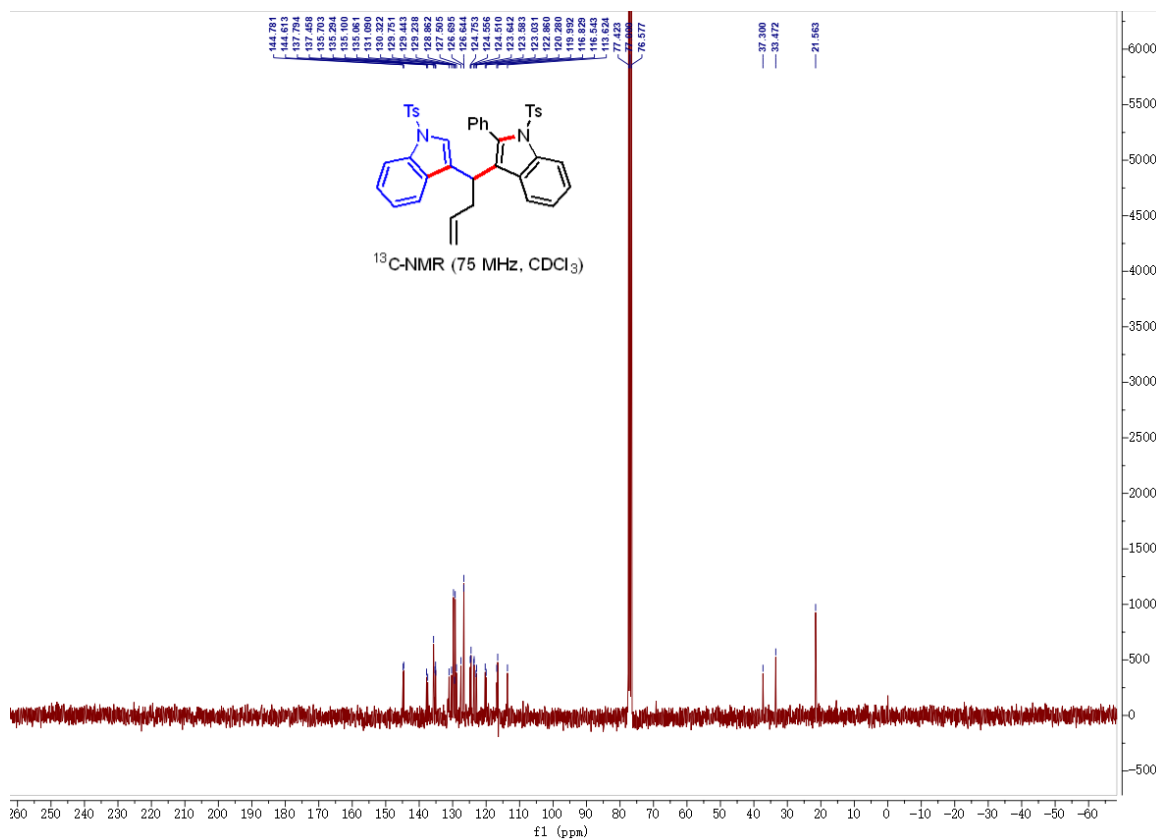
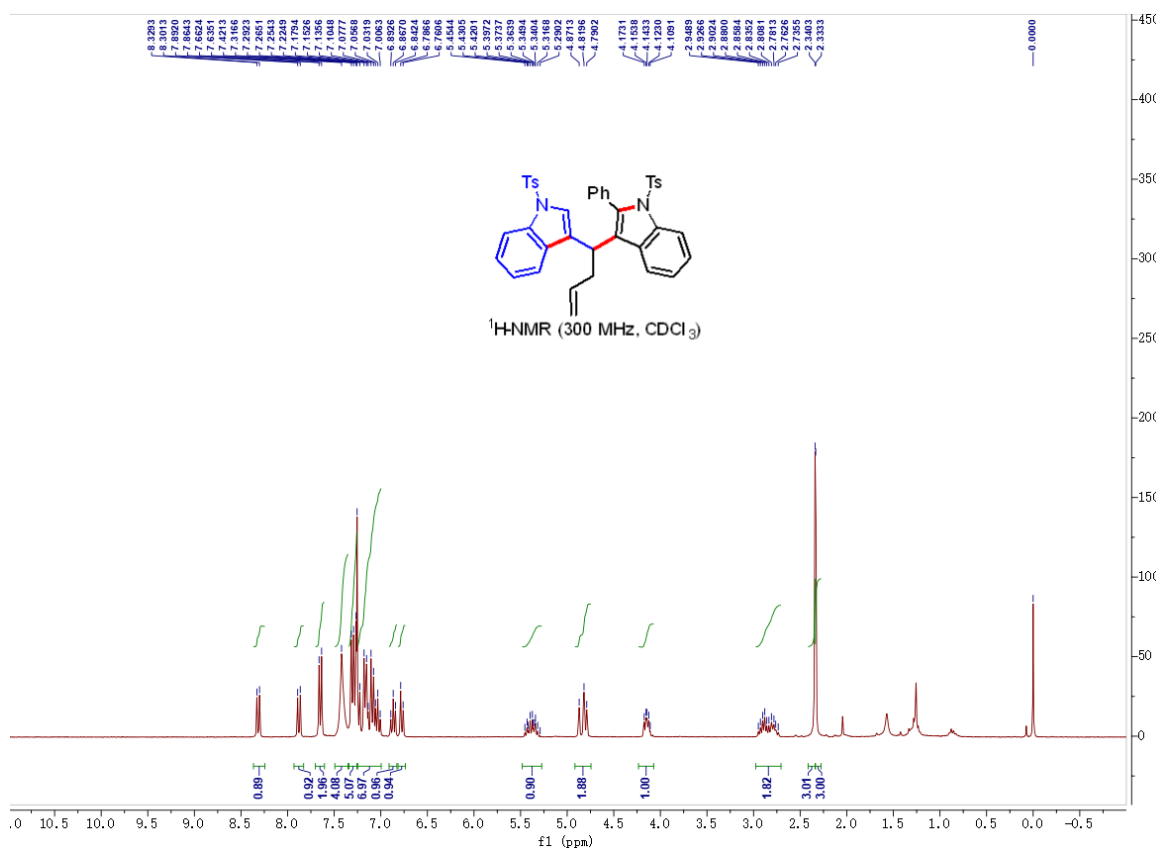
3-(azido(1-tosyl-1*H*-indol-3-yl)methyl)-2-phenyl-1-tosyl-1*H*-indole (11):



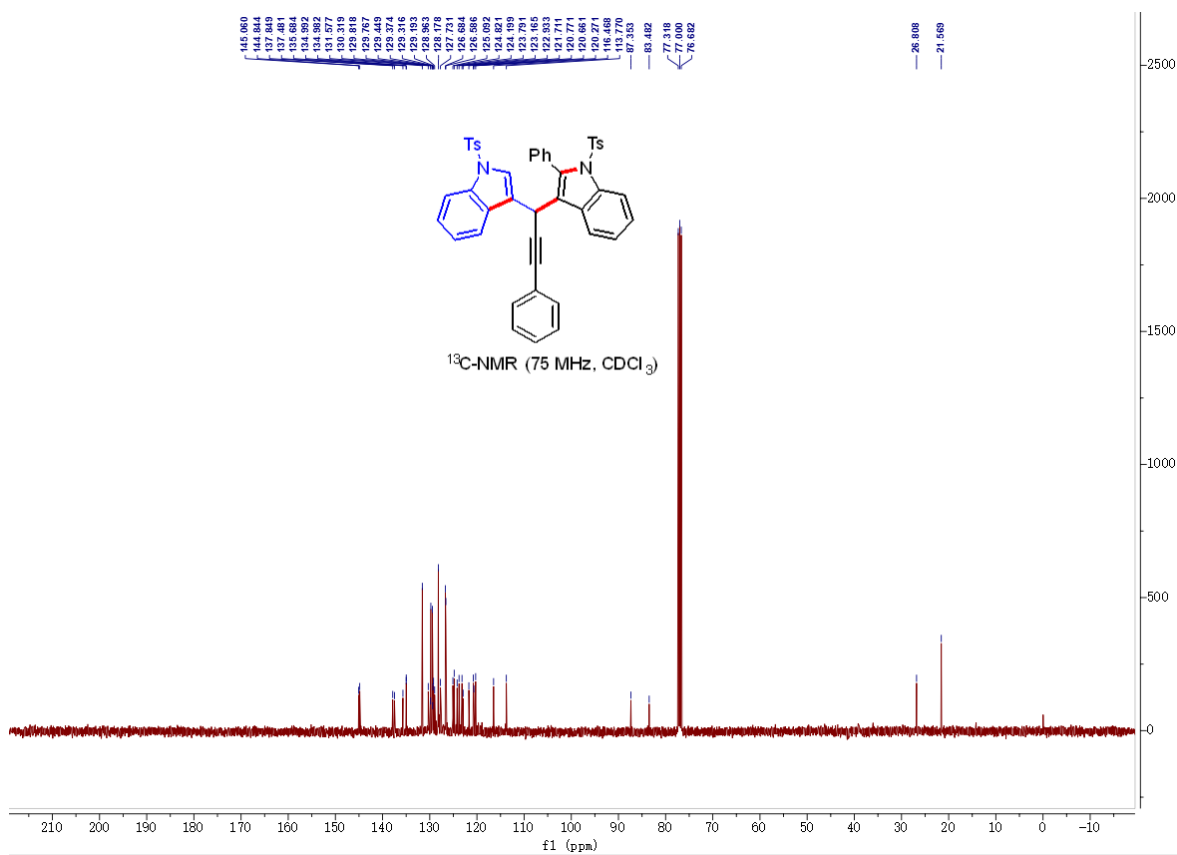
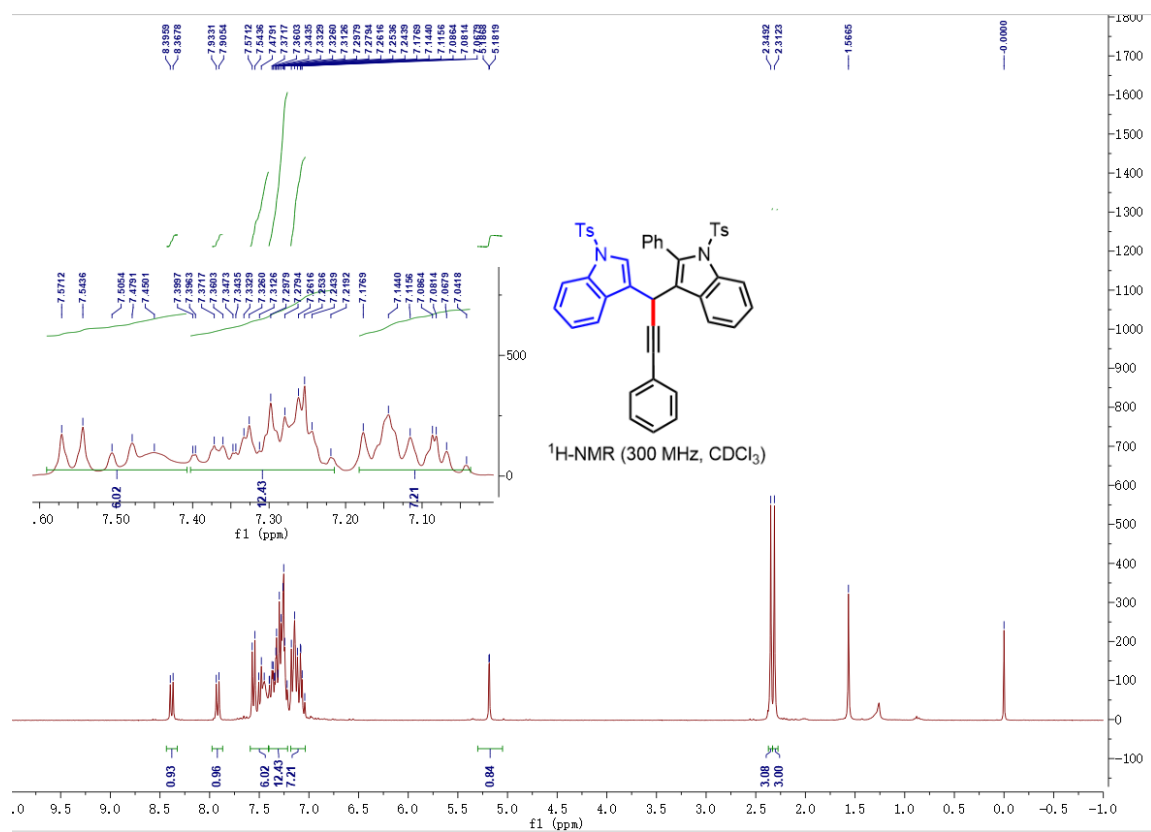
2-(2-phenyl-1-tosyl-1H-indol-3-yl)-2-(1-tosyl-1H-indol-3-yl)acetonitrile (12):



2-phenyl-1-tosyl-3-(1-(1-tosyl-1H-indol-3-yl)but-3-en-1-yl)-1H-indole (13):



2-phenyl-3-(3-phenyl-1-(1-tosyl-1*H*-indol-3-yl)prop-2-yn-1-yl)-1-tosyl-1*H*-indole (14):



8. References

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