

Supporting Information for

Direct C3 Chalcogenylation of Indolines Using a Graphene Oxide-Promoted and Visible-Light-Induced Synergistic Effect

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1. General Methods

^1H and ^{13}C NMR spectra were recorded on a Bruker spectrometers at 400 and 101 MHz, respectively. Mass spectra were recorded with Bruker Dalton Esquire 3000 plus LC-MS apparatus. Elemental analysis were carried out on a Perkin-Elmer 240B instrument. Silica gel (300-400 mesh) was used for flash column chromatography, eluting (unless otherwise stated) with an ethyl acetate/petroleum ether (PE) (60-90 °C) mixture.

Raman spectra were collected with a Horiba Jobin Y von-Labram HR UV-Visible-NIR Raman Microscope Spectrometer, using a 632 nm laser. The spectra were the average of 10 scans at a resolution of 2 cm^{-1} between $1000\text{--}2000\text{ cm}^{-1}$ Raman Shift.

2. Characterization of GO

GO was prepared by graphite oxidation using the Hummers and Offeman method and subsequent exfoliation. Further details and GO characterization have been previously reported.

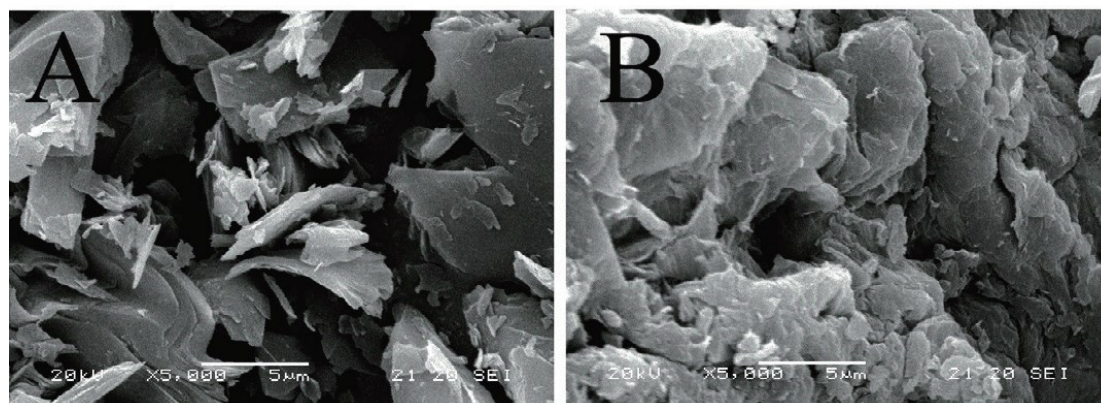


Figure S1. (A) SEM image of graphite. (B) SEM image of GO.

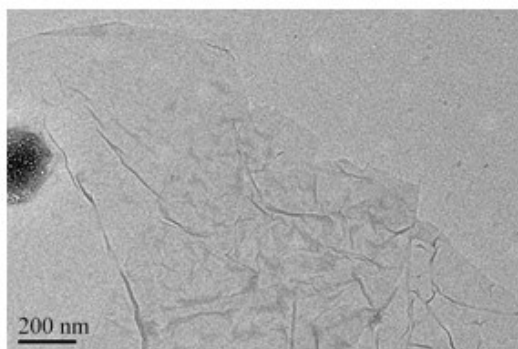


Figure S2. TEM image of graphite.

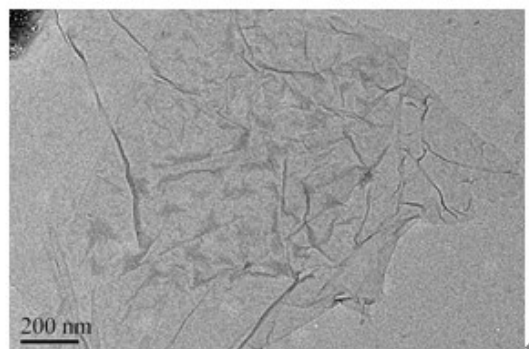


Figure S3. TEM image of GO.

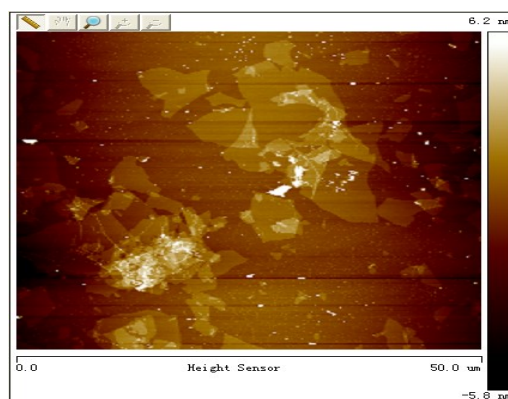


Figure S4. AFM image of GO.

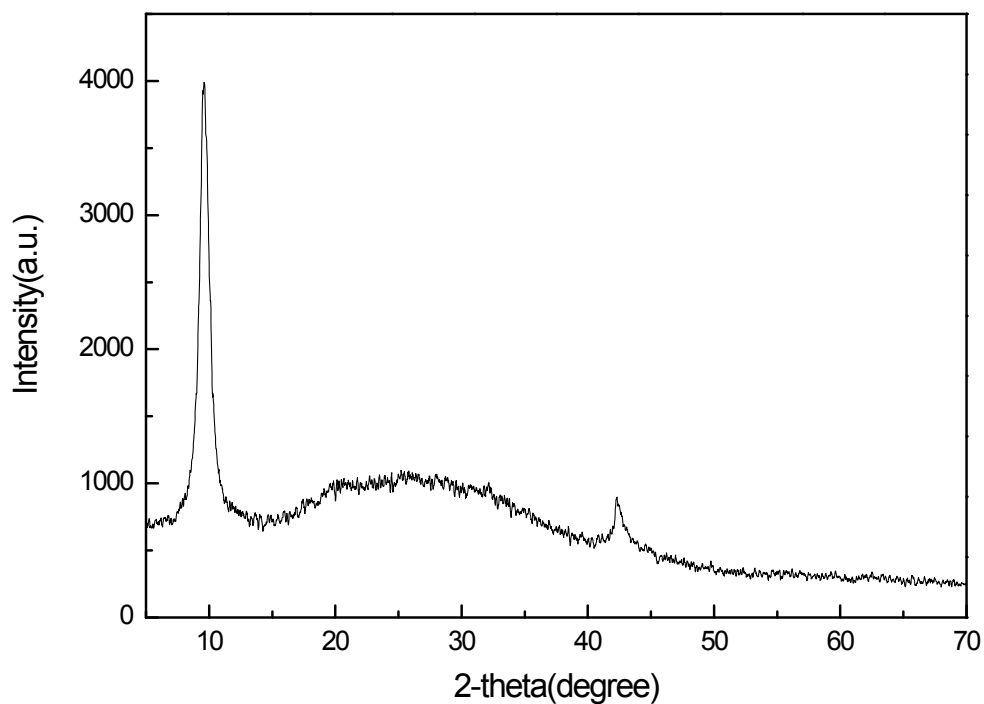


Figure S5. XRD image of GO.

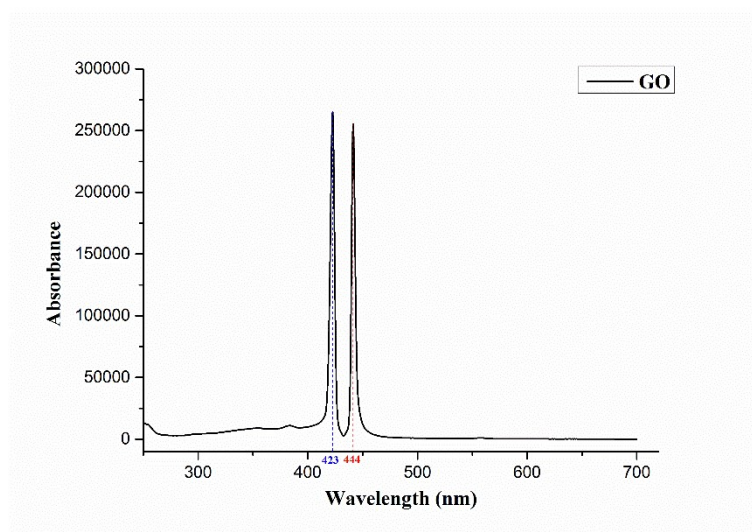
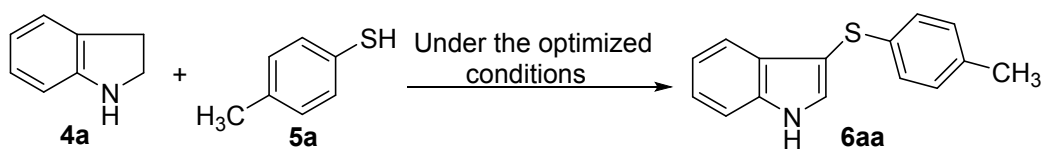


Figure S6. The fluorescence excitation spectrum of GO with the detection wavelength of 720 nm.

3. The influence of light source

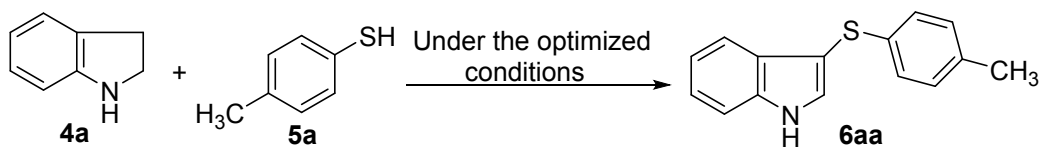
3.1 Table S1 The influence of light source



Entry	1	2	3	4	5	6
Light sources ^a	Red	Yellow	Green	Blue	Purple	White
Yield (%) ^b	0	0	0	82	23	17

^a 20W LED was used. ^b Isolated yield.

3.2 Table S2 The effect of blue LED power



Entry	1	2	3	4	5	6
Power of LED ^a	30	20	15	12	9	5
Yield (%) ^b	81	82	50	26	trace	trace

^a Blue LED was used. ^b Isolated yield.

4. Characterization of recycled GO

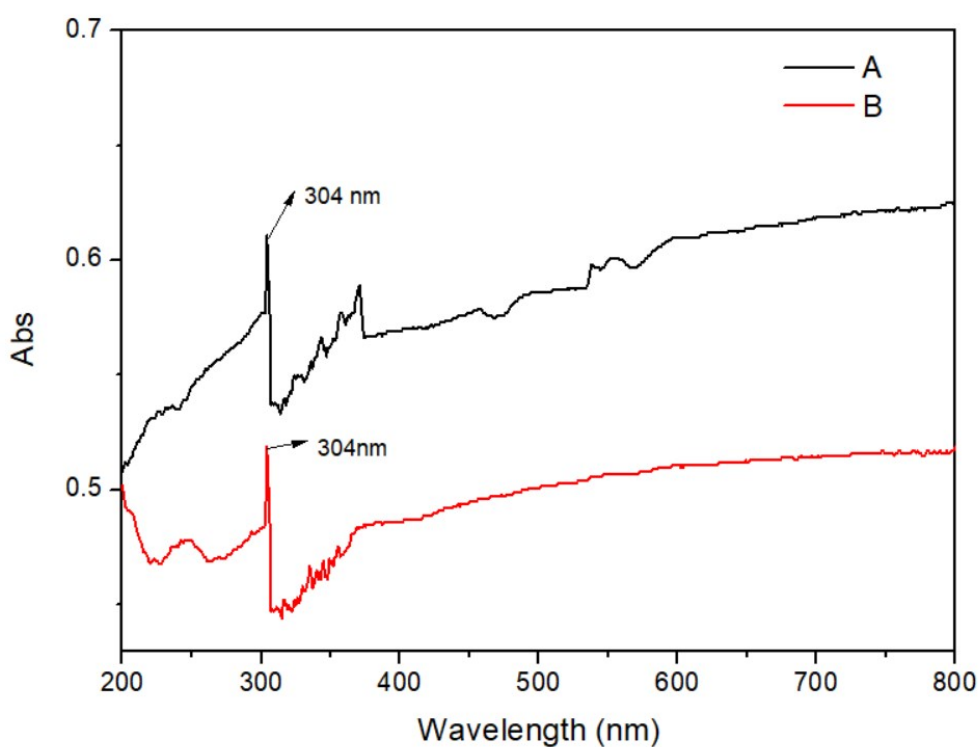


Figure S7. UV-visible spectrum of (A) freshly prepared GO and (B) recycled GO in solid state.

Table S3. Summary of elemental analysis of GO and recovered GO catalyst by EDXS measurement.

Catalyst	C%	O%	S%
GO	61	39	0.5
Recovered GO	85	13	2

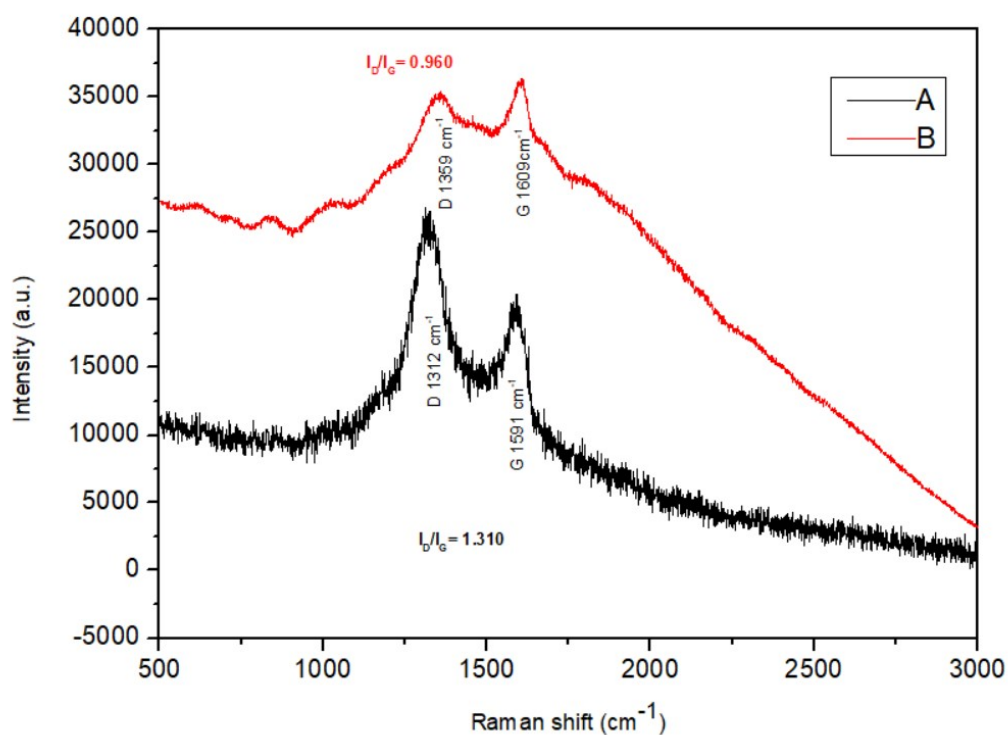


Figure S8. Raman spectra of (A) freshly prepared GO and (B) recycled GO.

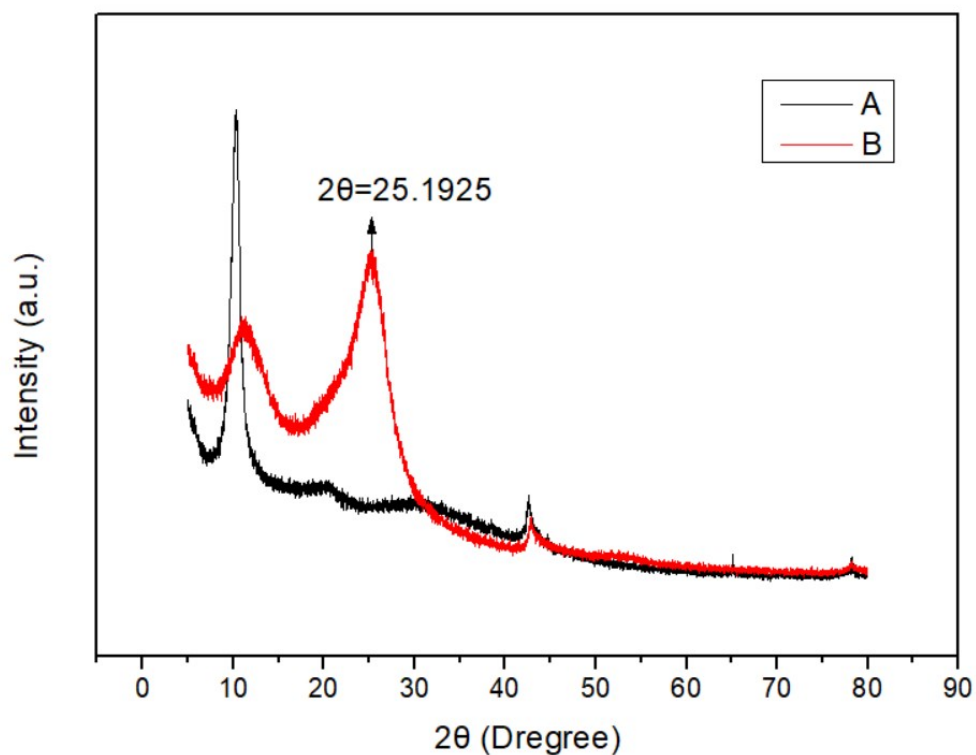
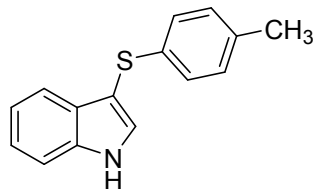


Figure S9. XRD spectra of (A) freshly prepared GO and (B) recycled GO.

5. General Procedure and Spectroscopic Data of the Products 6, 7 and 9

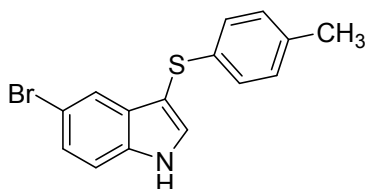
In a 10 mL Schlenk tube, indoline (0.3 mmol), GO (21.4 mg), and thiol (0.36 mmol) were stirred in DMSO (1 mL) for 15 h at room temperature under an air atmosphere irradiated by blue LEDs. The reaction mixture was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: EtOAc/PE = 1:10) to yield the corresponding product **6**.

3-(*p*-Tolylthio)-1*H*-indole (**6aa**)



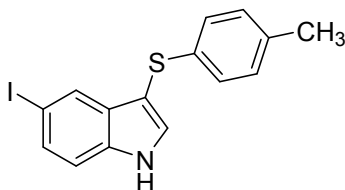
Yellow amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.37 (s, 1H, NH), 7.63 (d, *J* = 7.9 Hz, 1H, Ar-H), 7.46 (d, *J* = 2.6 Hz, 1H, Ar-H), 7.43 (d, *J* = 8.1 Hz, 1H, Ar-H), 7.26 (dt, *J* = 1.0, 8.1 Hz, 1H, Ar-H), 7.18 (t, *J* = 7.1 Hz, 1H, Ar-H), 7.05 (d, *J* = 8.3 Hz, 2H, Ar-H), 6.99 (d, *J* = 8.3 Hz, 2H, Ar-H), 2.26 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 136.5, 135.5, 134.7, 130.4, 129.5, 129.1, 126.3, 123.0, 120.8, 119.7, 111.5, 103.6, 20.8. MS (ESI): 240 (M+H⁺, 100). These assignments matched with those previously published.^{1a}

5-Bromo-3-(*p*-tolylthio)-1*H*-indole (**6ba**)



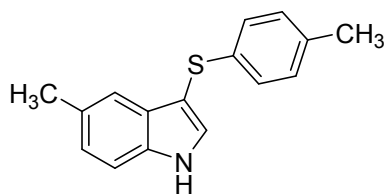
Yellow amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.42 (s, 1H, NH), 7.77 (s, 1H, Ar-H), 7.44 (s, 1H, Ar-H), 7.34 (d, *J* = 8.6 Hz, 1H, Ar-H), 7.27 (d, *J* = 8.6 Hz, 1H, Ar-H), 7.03 (d, *J* = 8.9 Hz, 2H, Ar-H), 7.01 (d, *J* = 8.9 Hz, 2H, Ar-H), 2.28 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 135.1, 135.0, 134.9, 131.7, 131.0, 129.7, 126.4, 126.0, 122.2, 114.4, 113.1, 103.4, 20.9. MS (ESI): 318 (M+H⁺, 100), 320 (M+H⁺, 100). These assignments matched with those previously published.^{1b}

5-Iodo-3-(*p*-tolylthio)-1*H*-indole (**6ca**)



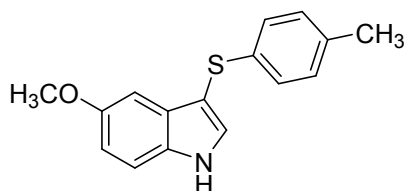
Brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.51 (s, 1H, NH), 7.99 (d, *J* = 1.5 Hz, 1H, Ar-H), 7.53 (dd, *J* = 8.5, 1.5 Hz, 1H, Ar-H), 7.43 (d, *J* = 1.5 Hz, 1H, Ar-H), 7.21 (d, *J* = 8.5 Hz, 1H, Ar-H), 7.06-7.01 (m, 4H, Ar-H), 2.29 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 135.6, 135.1, 134.9, 131.7, 131.4, 131.3, 129.6, 128.4, 126.3, 113.6, 102.8, 84.6, 20.9. MS (ESI): 366 (M+H⁺, 100). These assignments matched with those previously published.²

5-Methyl-3-(*p*-tolylthio)-1*H*-indole (**6da**)



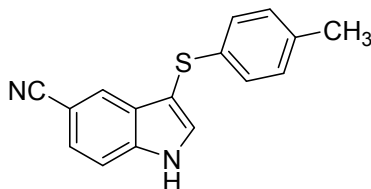
Yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.19 (s, 1H, NH), 7.55 (d, $J = 0.7$ Hz, 1H, Ar-H), 7.40 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.34 (d, $J = 8.2$ Hz, 1H, Ar-H), 7.21-7.13 (m, 3H, Ar-H), 7.08 (d, $J = 8.2$ Hz, 2H, Ar-H), 2.52 (s, 3H, CH_3), 2.36 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 135.9, 134.9, 134.7, 130.94, 130.4, 129.7, 129.5, 126.2, 124.7, 119.2, 111.5, 102.4, 21.6, 21.0. MS (ESI): 254 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{3a}

5-Methoxy-3-(*p*-tolylthio)-1*H*-indole (**6ea**)



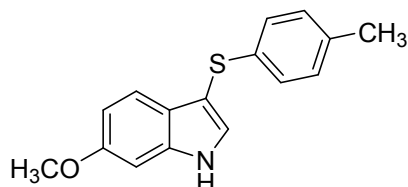
Yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.37 (s, 1H, NH), 7.40 (t, $J = 1.5$ Hz, 1H, Ar-H), 7.29 (d, $J = 8.8$ Hz, 1H, Ar-H), 7.09 (s, 1H, Ar-H), 7.06 (d, $J = 7.6$ Hz, 2H, Ar-H), 7.01 (d, $J = 7.6$ Hz, 2H, Ar-H), 6.93 (d, $J = 8.8$ Hz, 1H, Ar-H), 3.81 (s, 3H, OCH_3), 2.28 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 155.1, 135.7, 134.7, 131.4, 131.3, 130.0, 129.6, 126.1, 113.5, 112.5, 102.8, 101.0, 55.8, 20.9. MS (ESI): 270 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{3b}

3-(*p*-Tolylthio)-1*H*-indole-5-carbonitrile (**6fa**)



Yellow amorphous solid. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 12.20 (s, 1H, NH), 7.99 (d, $J = 1.6$ Hz, 1H, Ar-H), 7.81 (s, 1H, Ar-H), 7.66 (d, $J = 8.4$ Hz, 1H, Ar-H), 7.53 (d, $J = 8.4$ Hz, 1H, Ar-H), 7.04 (d, $J = 8.0$ Hz, 2H, Ar-H), 6.99 (d, $J = 8.0$ Hz, 2H, Ar-H), 2.20 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$): δ 139.1, 135.3, 135.2, 134.9, 130.1, 129.0, 126.9, 125.4, 124.1, 120.7, 114.3, 102.8, 102.5, 20.9. MS (ESI): 265 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{3a}

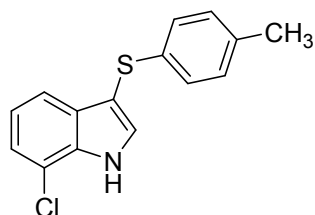
6-Methoxy-3-(*p*-tolylthio)-1*H*-indole (**6ga**)



Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.33 (s, 1H, NH), 7.51 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.34 (d, $J = 2.2$ Hz, 1H, Ar-H), 7.08 (d, $J = 8.2$ Hz, 2H, Ar-H), 7.02 (d, $J = 8.2$ Hz, 2H, Ar-H), 6.90 (d, $J = 2.2$ Hz, 1H, Ar-H), 6.86 (dd, $J = 8.6, 2.2$ Hz, 1H, Ar-H), 3.87 (s, 3H, OCH_3), 2.29 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 157.2, 137.3, 135.6, 134.7, 129.5,

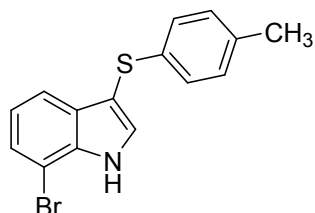
129.3, 126.3, 123.3, 120.3, 110.8, 103.4, 95.2, 55.7, 20.9. MS (ESI): 270 ($M+H^+$, 100). These assignments matched with those previously published.^{4a}

7-Chloro-3-(*p*-tolylthio)-1*H*-indole (**6ha**)



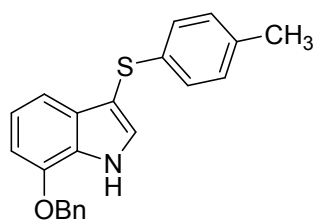
Red amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.65 (s, 1H, NH), 7.55 (dt, J = 1.0, 7.8 Hz, 1H, Ar-H), 7.54 (d, J = 2.6 Hz, 1H, Ar-H), 7.29 (dd, J = 7.8, 1.0 Hz, 1H, Ar-H), 7.12 (t, J = 7.8 Hz, 1H, Ar-H), 7.08 (d, J = 8.2 Hz, 2H, Ar-H), 7.03 (d, J = 8.2 Hz, 2H, Ar-H), 2.30 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 135.0, 134.9, 133.8, 130.9, 130.6, 129.6, 126.6, 122.4, 121.6, 118.4, 117.0, 105.2, 20.9. MS (ESI): 274 ($M+H^+$, 30), 276 ($M+H^+$, 100). Anal calcd for C₁₅H₁₂ClNS: C, 65.81; H, 4.42; N, 5.12; S, 11.71. Found C, 65.46; H, 4.81; N, 4.83; S, 11.62.

7-Bromo-3-(*p*-tolylthio)-1*H*-indole (**6ia**)



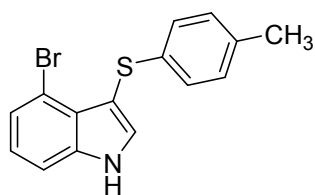
Yellow amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.59 (s, 1H, NH), 7.60 (d, J = 7.8 Hz, 1H, Ar-H), 7.54 (d, J = 2.6 Hz, 1H, Ar-H), 7.44 (dd, J = 7.8, 2.6 Hz, 1H, Ar-H), 7.08 (d, J = 8.2 Hz, 2H, Ar-H), 7.07 (t, J = 7.8 Hz, 1H, Ar-H), 7.03 (d, J = 8.2 Hz, 2H, Ar-H), 2.30 (s, 1H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 135.2, 135.0, 134.9, 130.9, 130.4, 129.6, 126.5, 125.3, 122.0, 119.0, 105.2, 105.0, 20.9. MS (ESI): 318 ($M+H^+$, 100), 320 ($M+H^+$, 100). Anal calcd for C₁₅H₁₂BrNS: C, 56.61; H, 3.80; N, 4.40; S, 10.07. Found C, 56.93; H, 4.17; N, 4.25; S, 9.81.

7-(Benzyloxy)-3-(*p*-tolylthio)-1*H*-indole (**6ja**)



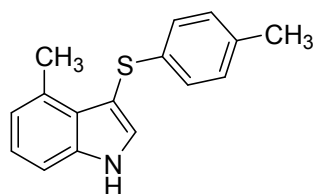
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.71 (s, 1H, NH), 7.52 (d, J = 7.1 Hz, 2H, Ar-H), 7.49-7.40 (m, 4H, Ar-H), 7.27 (d, J = 8.4 Hz, 1H, Ar-H), 7.09 (t, J = 7.8 Hz, 1H, Ar-H), 7.07 (d, J = 8.0 Hz, 2H, Ar-H), 7.01 (d, J = 8.0 Hz, 2H, Ar-H), 6.81 (d, J = 7.8 Hz, 1H, Ar-H), 5.24 (s, 2H, OCH₂), 2.28 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 145.6, 136.9, 135.7, 134.6, 130.8, 130.1, 129.5, 128.7, 128.3, 128.0, 127.2, 126.3, 121.2, 112.6, 104.0, 103.7, 70.4, 20.9. MS (ESI): 346 ($M+H^+$, 100). Anal calcd for C₂₂H₁₉NOS: C, 76.49; H, 5.54; N, 4.05; S, 9.28. Found C, 76.35; H, 5.47; N, 4.33; S, 8.95.

4-Bromo-3-(*p*-tolylthio)-1*H*-indole (**6ka**)



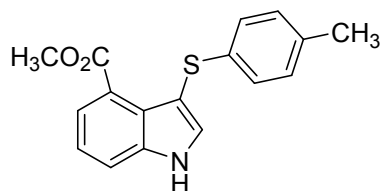
Brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.49 (s, 1H, NH), 7.79 (d, $J = 1.8$ Hz, 1H, Ar-H), 7.48 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.36 (dd, $J = 8.6, 1.8$ Hz, 1H, Ar-H), 7.31 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.04 (d, $J = 8.9$ Hz, 2H, Ar-H), 7.02 (d, $J = 8.9$ Hz, 2H, Ar-H), 2.29 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 135.1, 135.0, 134.9, 131.6, 131.0, 129.6, 126.4, 126.0, 122.3, 114.4, 113.1, 103.5, 20.9. MS (ESI): 318 ($\text{M}+\text{H}^+$, 100), 320 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{4b}

4-Methyl-3-(*p*-tolylthio)-1*H*-indole (**6la**)



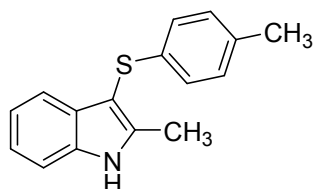
Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3) δ 8.41 (s, 1H, NH), 7.43 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.29 (d, $J = 8.1$ Hz, 1H, Ar-H), 7.17 (t, $J = 8.1$ Hz, 1H, Ar-H), 7.06-6.98 (m, 4H, Ar-H), 6.92 (d, $J = 7.1$ Hz, 1H), 2.70 (s, 3H, CH_3), 2.29 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 137.9, 137.0, 134.3, 132.2, 131.7, 129.6, 127.0, 125.5, 123.1, 122.4, 109.4, 102.9, 20.9, 18.7. MS (ESI): 254 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{3a}

Methyl 3-(*p*-tolylthio)-1*H*-indole-4-carboxylate (**6ma**)



Brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 9.19 (s, 1H, NH), 7.51 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.49 (d, $J = 1.0$ Hz, 1H, Ar-H), 7.38 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.24 (t, $J = 7.8$ Hz, 1H, Ar-H), 6.98 (s, 4H, Ar-H), 3.68 (s, 3H), 2.30 (d, $J = 37.7$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 169.6, 137.6, 136.4, 134.6, 133.4, 129.4, 126.2, 125.4, 125.3, 122.1, 122.0, 115.1, 103.1, 51.9, 20.8. MS (ESI): 298 ($\text{M}+\text{H}^+$, 100). Anal calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_2\text{S}$: C, 68.66; H, 5.08; N, 4.71; S, 10.78. Found C, 68.80; H, 5.26; N, 4.64; S, 10.57.

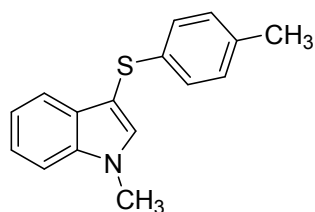
2-Methyl-3-(*p*-tolylthio)-1*H*-indole (**6na**)



Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.26 (s, 1H, NH), 7.58 (d, $J = 7.8$ Hz, 1H, Ar-H), 7.36 (dt, $J = 1.0, 7.8$ Hz, 1H, Ar-H), 7.22 (dt, $J = 1.0, 7.8$ Hz, 1H, Ar-H), 7.15 (dt, $J = 1.0, 7.8$ Hz, 1H, Ar-H), 6.99 (s, 4H, Ar-H), 2.54 (s, 3H, CH_3), 2.27 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 141.0, 135.7, 135.5, 134.4, 130.4, 129.5, 125.8, 122.1, 120.7, 119.0, 110.7,

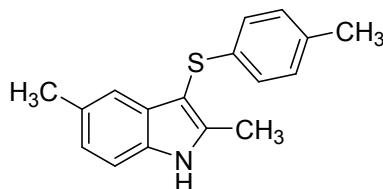
99.9, 20.9, 12.2. MS (ESI): 254 ($M+H^+$, 100). These assignments matched with those previously published.^{3a}

1-Methyl-3-(*p*-tolylthio)-1*H*-indole (**60a**)



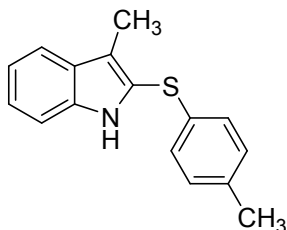
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 7.75 (d, J = 8.2 Hz, 1H, Ar-H), 7.45 (d, J = 8.2 Hz, 1H, Ar-H), 7.39 (dt, J = 1.0, 7.0 Hz, 1H, Ar-H), 7.37 (s, 1H, Ar-H), 7.28 (dt, J = 1.0, 7.0 Hz, 1H, Ar-H), 7.15 (d, J = 8.2 Hz, 2H, Ar-H), 7.07 (d, J = 8.2 Hz, 1H, Ar-H), 3.86 (s, 3H, NCH₃), 2.35 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 137.6, 136.1, 134.9, 134.6, 123.0, 129.6, 126.3, 126.2, 122.6, 120.5, 119.8, 109.8, 101.3, 33.1, 21.0. MS (ESI): 254 ($M+H^+$, 100). These assignments matched with those previously published.²

2,5-Dimethyl-3-(*p*-tolylthio)-1*H*-indole (**6pa**)



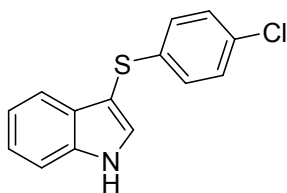
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.03 (s, 1H, NH), 7.46 (s, 1H, Ar-H), 7.25 (d, J = 8.2 Hz, 1H, Ar-H), 7.10 (dd, J = 8.2, 1.2 Hz, 1H, Ar-H), 7.46 (s, 4H, Ar-H), 2.51 (s, 3H, CH₃), 2.49 (s, 3H, CH₃), 2.34 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 141.3, 136.0, 134.3, 133.8, 130.7, 130.1, 129.6, 125.7, 123.7, 118.7, 110.5, 99.0, 21.5, 20.9, 12.1. MS (ESI): 268 ($M+H^+$, 100). These assignments matched with those previously published.^{3a}

3-Methyl-2-(*p*-tolylthio)-1*H*-indole (**6qa**)



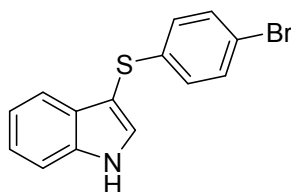
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 7.96 (s, 1H, NH), 7.71 (d, J = 7.9 Hz, 1H, Ar-H), 7.33 (d, J = 3.6 Hz, 2H, Ar-H), 7.26 (m, 1H, Ar-H), 7.12 (d, J = 8.3 Hz, 2H, Ar-H), 7.09 (d, J = 8.3 Hz, 2H, Ar-H), 2.51 (s, 3H, CH₃), 2.38 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 136.9, 135.9, 133.5, 130.0, 128.6, 127.1, 123.4, 122.3, 119.7, 119.5, 119.4, 111.0, 21.0, 9.6. MS (ESI): 254 ($M+H^+$, 100). These assignments matched with those previously published.^{3a}

3-((4-Chlorophenyl)thio)-1*H*-indole (**6ab**)



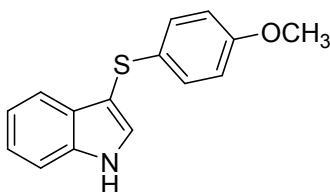
Light yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.47 (s, 1H, NH), 7.58 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.49 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.45 (d, $J = 8.2$ Hz, 1H, Ar-H), 7.29 (dt, $J = 1.0$, 8.0 Hz, 1H, Ar-H), 7.18 (dt, $J = 1.0$, 8.0 Hz, 1H, Ar-H), 7.12 (d, $J = 8.7$ Hz, 2H, Ar-H), 7.02 (d, $J = 8.7$ Hz, 2H, Ar-H). ^{13}C NMR (101 MHz, CDCl_3): δ 137.8, 136.5, 130.6, 130.5, 128.7, 128.6, 127.1, 123.1, 121.0, 119.4, 111.6, 102.4. MS (ESI): 260 ($\text{M}+\text{H}^+$, 30), 262 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.²

3-((4-Bromophenyl)thio)-1H-indole (**6ac**)



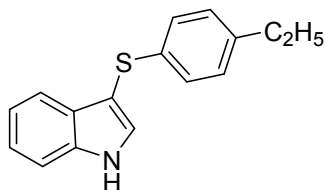
Brown amorphous solid. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 11.76 (s, 1H, NH), 7.80 (d, $J = 2.7$ Hz, 1H, Ar-H), 7.51 (d, $J = 8.1$ Hz, 1H, Ar-H), 7.41 – 7.35 (m, 3H, Ar-H), 7.20 (dt, $J = 1.1$, 8.1 Hz, 1H, Ar-H), 7.08 (dt, $J = 1.1$, 8.1 Hz, 1H, Ar-H), 6.96 (dt, $J = 2.7$, 8.6 Hz, 2H, Ar-H). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$): δ 139.5, 137.3, 133.1, 132.1, 128.9, 127.7, 122.7, 120.7, 118.6, 118.0, 112.9, 99.1. MS (ESI): 304 ($\text{M}+\text{H}^+$, 100), 306 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.²

3-((4-Methoxyphenyl)thio)-1H-indole (**6ad**)



Brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.38 (s, 1H, NH), 7.63 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.46 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.41 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.25 (dt, $J = 1.0$, 8.0 Hz, 1H, Ar-H), 7.17 (dt, $J = 1.0$, 8.0 Hz, 1H, Ar-H), 7.13 (d, $J = 8.9$ Hz, 2H, Ar-H), 6.74 (d, $J = 8.9$ Hz, 2H, Ar-H), 3.73 (s, 3H, OCH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 157.8, 136.5, 123.0, 129.5, 129.0, 128.6, 122.9, 120.8, 119.7, 114.5, 111.5, 104.7, 55.3. MS (ESI): 256 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{1a}

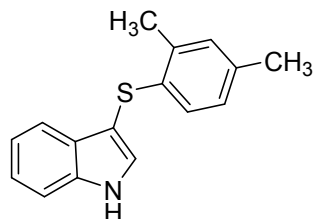
3-((4-Ethylphenyl)thio)-1H-indole (**6ae**)



Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.34 (s, 1H, NH), 7.71 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.45 (d, $J = 2.3$ Hz, 1H, Ar-H), 7.44 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.32 (dt, $J = 1.0$, 8.0 Hz, 1H, Ar-H), 7.23 (t, $J = 7.5$ Hz, 1H, Ar-H), 7.13 (d, $J = 8.2$ Hz, 2H, Ar-H), 7.06 (d, $J = 8.2$

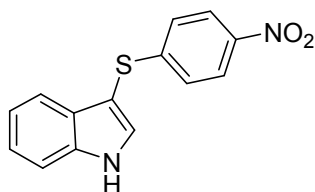
Hz, 2H, Ar-H), 2.61 (q, $J = 7.6$ Hz, 2H, CH₂), 1.23 (t, $J = 7.6$ Hz, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 141.3, 136.5, 135.9, 130.7, 129.2, 128.5, 126.3, 123.1, 120.9, 119.7, 111.8, 103.2, 28.4, 15.7. MS (ESI): 254 (M+H⁺, 100). Anal calcd for C₁₆H₁₅NS: C, 75.85; H, 5.97; N, 5.53; S, 12.65. Found C, 75.59; H, 5.63; N, 5.71; S, 12.32.

3-((2,4-Dimethylphenyl)thio)-1*H*-indole (**6af**)



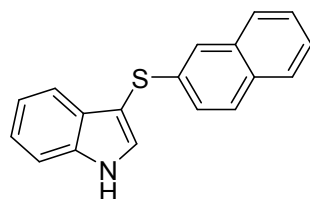
Tawny amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.28 (s, 1H, NH), 7.71 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.45 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.41 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.36 (t, $J = 7.7$ Hz, 1H, Ar-H), 7.27 (t, $J = 7.7$ Hz, 1H, Ar-H), 7.09 (s, 1H, Ar-H), 6.83 (d, $J = 8.0$ Hz, 1H, Ar-H), 6.78 (d, $J = 8.0$ Hz, 1H, Ar-H), 2.59 (s, 3H, CH₃), 2.34 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 136.6, 134.7, 134.6, 134.4, 130.9, 130.5, 129.3, 127.1, 126.1, 123.0, 120.8, 119.7, 111.6, 103.0, 20.7, 19.9. MS (ESI): 254 (M+H⁺, 100). Anal calcd for C₁₆H₁₅NS: C, 75.85; H, 5.97; N, 5.53; S, 12.65. Found C, 76.04; H, 5.83; N, 5.66; S, 12.35.

3-((4-Nitrophenyl)thio)-1*H*-indole (**6ag**)



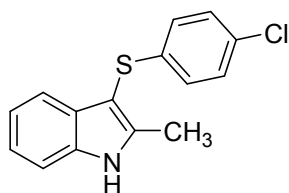
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.86 (s, 1H, NH), 8.02 (d, $J = 9.0$ Hz, 2H, Ar-H), 7.55 (t, $J = 7.7$ Hz, 1H, Ar-H), 7.54 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.53 (d, $J = 8.1$ Hz, 1H, Ar-H), 7.34 (t, $J = 8.1$ Hz, 1H, Ar-H), 7.22 (t, $J = 7.7$ Hz, 1H, Ar-H), 7.15 (d, $J = 9.0$ Hz, 2H, Ar-H). ¹³C NMR (101 MHz, CDCl₃): δ 150.0, 144.9, 136.7, 131.4, 128.5, 125.2, 123.9, 123.5, 121.4, 119.2, 112.1, 100.1. MS (ESI): 271 (M+H⁺, 100). These assignments matched with those previously published.^{5a}

3-(Naphthalen-2-ylthio)-1*H*-indole (**6ah**)



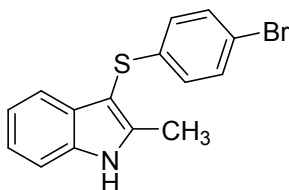
Reddish brown amorphous solid. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.74 (s, 1H, NH), 7.83 (d, $J = 2.5$ Hz, 1H, Ar-H), 7.77 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.73 (d, $J = 8.7$ Hz, 1H, Ar-H), 7.61 (d, $J = 7.5$ Hz, 1H, Ar-H), 7.50 (d, $J = 2.6$ Hz, 1H, Ar-H), 7.48 (s, 1H, Ar-H), 7.40 – 7.33 (m, 3H, Ar-H), 7.20 (dd, $J = 2.6$ Hz, 1H, Ar-H), 7.17 (t, $J = 2.6$ Hz, 1H, Ar-H), 7.03 (t, $J = 7.5$ Hz, 1H, Ar-H). ¹³C NMR (101 MHz, DMSO-*d*₆): δ 137.3, 137.2, 133.7, 133.0, 131.3, 129.1, 128.8, 128.1, 127.1, 127.0, 125.7, 124.9, 123.3, 122.6, 120.6, 118.8, 112.9, 99.8. MS (ESI): 276 (M+H⁺, 100). These assignments matched with those previously published.^{3a}

3-((4-Chlorophenyl)thio)-2-methyl-1*H*-indole (**6ai**)



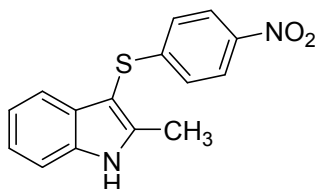
Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.28 (s, 1H, NH), 7.57 (d, $J = 7.9$ Hz, 1H, Ar-H), 7.37 (d, $J = 7.9$ Hz, 1H, Ar-H), 7.26 (dt, $J = 1.0, 8.0$ Hz, 1H, Ar-H), 7.19 (dt, $J = 1.0, 8.0$ Hz, 1H, Ar-H), 7.15 (dt, $J = 2.6, 8.6$ Hz, 2H, Ar-H), 7.00 (dt, $J = 2.6, 8.6$ Hz, 2H, Ar-H), 2.52 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 141.3, 138.0, 135.5, 130.3, 130.1, 128.8, 126.8, 122.4, 120.9, 118.8, 110.8, 99.0, 12.1. MS (ESI): 274 ($\text{M}+\text{H}^+$, 30), 276 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{5b}

3-((4-Bromophenyl)thio)-2-methyl-1H-indole (**6aj**)



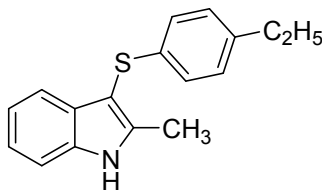
Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.27 (s, 1H, NH), 7.57 (d, $J = 7.8$ Hz, 1H, Ar-H), 7.37 (d, $J = 7.8$ Hz, 1H, Ar-H), 7.30 (dt, $J = 2.6, 8.6$ Hz, 2H, Ar-H), 7.26 (dt, $J = 1.1, 8.0$ Hz, 1H, Ar-H), 7.19 (dt, $J = 1.1, 8.0$ Hz, 1H, Ar-H), 6.94 (dt, $J = 2.6, 8.6$ Hz, 2H, Ar-H), 2.52 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 141.3, 138.7, 135.5, 131.7, 130.0, 127.1, 122.4, 120.9, 118.8, 118.0, 110.9, 98.7, 12.2. MS (ESI): 318 ($\text{M}+\text{H}^+$, 100), 320 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{5c}

2-Methyl-3-((4-nitrophenyl)thio)-1H-indole (**6ak**)



Brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.59 (s, 1H, NH), 8.02 (dt, $J = 2.6, 9.0$ Hz, 2H, Ar-H), 7.48 (d, $J = 7.8$ Hz, 1H, Ar-H), 7.42 (d, $J = 8.1$ Hz, 1H, Ar-H), 7.26 (dt, $J = 1.1, 8.1$ Hz, 1H, Ar-H), 7.18 (dt, $J = 0.8, 7.8$ Hz, 1H, Ar-H), 7.12 (dt, $J = 2.6, 9.0$ Hz, 2H, Ar-H), 2.54 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 149.9, 144.9, 141.7, 135.6, 129.6, 125.0, 123.9, 122.7, 121.2, 118.6, 111.0, 97.0, 12.1. MS (ESI): 285 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.^{5d}

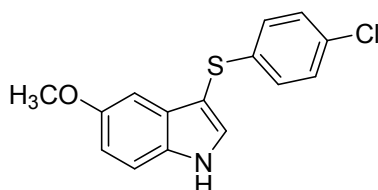
3-((4-Ethylphenyl)thio)-2-methyl-1H-indole (**6al**)



Reddish brown amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.18 (s, 1H, NH), 7.64 (d, $J = 7.7$ Hz, 1H, Ar-H), 7.36 (d, $J = 7.7$ Hz, 1H, Ar-H), 7.26 (t, $J = 7.2$ Hz, 1H, Ar-H), 7.19 (t, $J = 7.2$ Hz, 1H, Ar-H), 7.06 (s, 4H, Ar-H), 2.61 (q, $J = 7.5$ Hz, 2H, CH_2), 2.53 (s, 3H, CH_3), 1.23 (t, $J = 7.5$

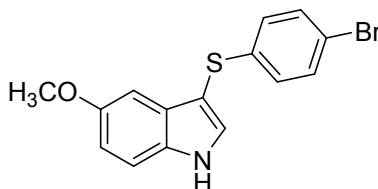
Hz, 3H, CH₃) . ¹³C NMR (101 MHz, CDCl₃): δ 141.1, 140.8, 136.0, 135.5, 130.4, 128.4, 125.8, 122.2, 120.7, 119.0, 110.7, 99.7, 28.3, 15.6, 12.2. MS (ESI): 268 (M+H⁺, 100). Anal calcd for C₁₇H₁₇NS: C, 76.36; H, 6.41; N, 5.24; S, 11.99. Found C, 76.19; H, 6.77; N, 5.30; S, 11.85.

3-((4-Chlorophenyl)thio)-5-methoxy-1*H*-indole (**6am**)



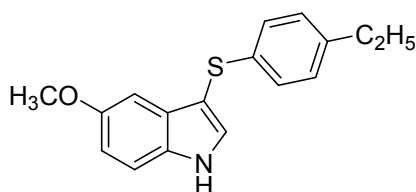
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.48 (s, 1H, NH), 7.45 (d, *J* = 2.6 Hz, 1H, Ar-H), 7.34 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.17 (t, *J* = 2.6 Hz, 1H, Ar-H), 7.15 (t, *J* = 2.6 Hz, 1H, Ar-H), 7.06 (t, *J* = 2.0 Hz, 2H, Ar-H), 7.04 (t, *J* = 2.0 Hz, 1H, Ar-H), 6.97 (dd, *J* = 8.8, 2.6 Hz, 1H, Ar-H), 3.84 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 155.2, 138.0, 131.5, 131.5, 130.5, 129.7, 128.8, 127.0, 113.7, 112.7, 101.7, 100.8, 55.9. MS (ESI): 290 (M+H⁺, 30), 292 (M+H⁺, 100). These assignments matched with those previously published.^{5b}

3-((4-Bromophenyl)thio)-5-methoxy-1*H*-indole (**6an**)



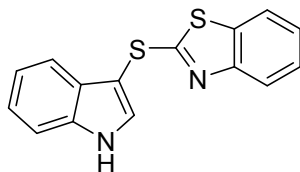
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.43 (s, 1H, NH), 7.46 (d, *J* = 2.7 Hz, 1H, Ar-H), 7.35 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.30 (dt, *J* = 2.7, 8.8 Hz, 2H, Ar-H), 7.03 (d, *J* = 2.4 Hz, 1H, Ar-H), 6.98 (dt, *J* = 2.4, 8.8 Hz, 2H, Ar-H), 6.95 (dd, *J* = 8.8, 2.7 Hz, 1H, Ar-H), 3.82 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 155.3, 138.7, 131.7, 131.5, 131.4, 129.7, 127.3, 118.3, 113.7, 112.5, 101.7, 100.8, 55.8. MS (ESI): 334 (M+H⁺, 100), 336 (M+H⁺, 100). These assignments matched with those previously published.^{5e}

3-((4-Ethylphenyl)thio)-5-methoxy-1*H*-indole (**6ao**)



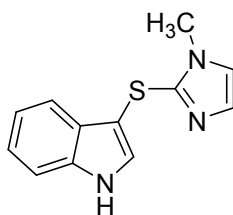
Reddish brown amorphous solid. ¹H NMR (400 MHz, CDCl₃): δ 8.38 (s, 1H, NH), 7.43 (d, *J* = 2.6 Hz, 1H, Ar-H), 7.32 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.12 (d, *J* = 2.6 Hz, 1H, Ar-H), 7.10 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.05 (d, *J* = 8.5 Hz, 2H, Ar-H), 6.95 (dd, *J* = 8.8, 2.6 Hz, 1H, Ar-H), 3.83 (s, 3H, CH₃), 2.60 (q, *J* = 7.6 Hz, 2H, CH₂), 1.22 (t, *J* = 7.6 Hz, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃): δ 155.1, 141.1, 136.0, 131.4, 131.3, 130.1, 128.4, 126.1, 113.5, 112.5, 102.7, 100.9, 55.8, 28.3, 15.6. MS (ESI): 284 (M+H⁺, 100). Anal calcd for C₁₇H₁₇NOS: C, 72.05; H, 6.05; N, 4.94; S, 11.31. Found C, 71.98; H, 5.94; N, 5.21; S, 11.06.

2-((1*H*-indol-3-yl)thio)benzo[*d*]thiazole (**6ap**)



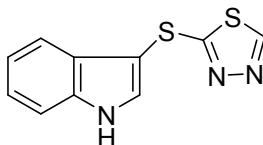
Brown amorphous solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 12.03 (s, 1H, NH), 8.04 (d, J = 2.8 Hz, 1H, Ar-H), 7.82 (dd, J = 2.8, 1.8 Hz, 1H, Ar-H), 7.80 (dd, J = 2.1, 1.0 Hz, 1H, Ar-H), 7.57 (d, J = 7.8 Hz, 1H, Ar-H), 7.56 (d, J = 7.8 Hz, 1H, Ar-H), 7.41 (dt, J = 1.2, 8.4 Hz, 1H, Ar-H), 7.30-7.23 (m, 2H, Ar-H), 7.15 (dt, J = 1.0, 7.1 Hz, 1H, Ar-H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$): δ 173.8, 154.6, 137.2, 135.4, 134.4, 128.4, 126.6, 124.4, 123.1, 122.1, 121.6, 121.3, 118.5, 113.1, 97.7. MS (ESI): 283 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.⁶

3-((1-Methyl-1H-imidazol-2-yl)thio)-1H-indole (**6aq**)



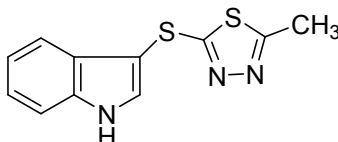
Yellow amorphous solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 11.51 (s, 1H, NH), 7.69 (s, 1H, Ar-H), 7.60 (d, J = 7.6 Hz, 1H, Ar-H), 7.39 (d, J = 7.6 Hz, 1H, Ar-H), 7.16 (s, 1H, Ar-H), 7.10 (t, J = 7.1 Hz, 1H, Ar-H), 7.04 (t, J = 7.1 Hz, 1H, Ar-H), 6.85 (s, 1H, Ar-H), 3.66 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$): δ 140.0, 136.7, 131.0, 128.9, 128.5, 124.0, 122.4, 120.3, 119.1, 112.5, 100.6, 34.0. MS (ESI): 230 ($\text{M}+\text{H}^+$, 100). Anal calcd for $\text{C}_{12}\text{H}_{11}\text{N}_3\text{S}$: C, 62.86; H, 4.84; N, 18.33; S, 13.98. Found C, 63.10; H, 5.07; N, 18.05; S, 13.61.

2-((1H-indol-3-yl)thio)-1,3,4-thiadiazole (**6ar**)



Yellow amorphous solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 11.98 (s, 1H, NH), 9.29 (s, 1H, Ar-H), 8.00 (d, J = 2.8 Hz, 1H, Ar-H), 7.56 (d, J = 8.0 Hz, 1H, Ar-H), 7.53 (d, J = 7.9 Hz, 1H, Ar-H), 7.25 (dt, J = 1.0, 8.0 Hz, 1H, Ar-H), 7.16 (d, J = 7.9 Hz, 1H, Ar-H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$): δ 173.0, 154.3, 137.2, 133.6, 127.8, 123.2, 121.3, 118.4, 113.2, 98.6. MS (ESI): 234 ($\text{M}+\text{H}^+$, 100). Anal calcd for $\text{C}_{10}\text{H}_7\text{N}_3\text{S}_2$: C, 51.48; H, 3.02; N, 18.01; S, 27.48. Found C, 51.83; H, 3.39; N, 17.85; S, 27.17.

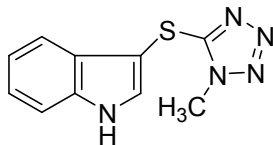
2-((1H-indol-3-yl)thio)-5-methyl-1,3,4-thiadiazole (**6as**)



Yellow amorphous solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 11.95 (s, 1H, NH), 7.96 (d, J = 2.7 Hz, 1H, Ar-H), 7.55 (d, J = 2.7 Hz, 1H, Ar-H), 7.53 (d, J = 2.7 Hz, 1H, Ar-H), 7.24 (d, J = 7.5 Hz, 1H, Ar-H), 7.16 (d, J = 7.5 Hz, 1H, Ar-H), 2.50 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 172.4, 165.7, 137.1, 133.5, 128.0, 123.1, 121.3, 118.4, 113.1, 98.8, 15.6. MS (ESI): 248 ($\text{M}+\text{H}^+$,

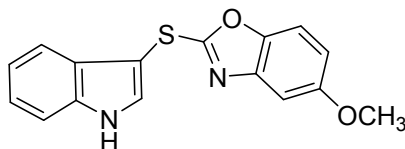
100). Anal calcd for $C_{11}H_9N_3S_2$: C, 53.42; H, 3.67; N, 16.99; S, 25.92. Found C, 53.76; H, 3.92; N, 16.84; S, 25.59.

3-((1-Methyl-1*H*-tetrazol-5-yl)thio)-1*H*-indole (**6at**)



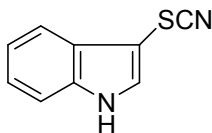
Pink amorphous solid. 1H NMR (400 MHz, $DMSO-d_6$): δ 11.85 (s, 1H, NH), 7.94 (d, $J = 2.7$ Hz, 1H, Ar-H), 7.54 (d, $J = 8.7$ Hz, 1H, Ar-H), 7.51 (d, $J = 8.7$ Hz, 1H, Ar-H), 7.22 (d, $J = 7.2$ Hz, 1H, Ar-H), 7.13 (d, $J = 7.2$ Hz, 1H, Ar-H), 4.03 (s, 3H, NCH_3). ^{13}C NMR (101 MHz, $DMSO-d_6$): δ 153.8, 136.9, 133.5, 128.8, 122.9, 121.0, 118.6, 112.9, 94.5, 34.5. MS (ESI): 232 ($M+H^+$, 100). Anal calcd for $C_{10}H_9N_5S$: C, 51.93; H, 3.92; N, 30.28; S, 13.86. Found C, 52.20; H, 4.28; N, 29.91; S, 13.93.

2-((1*H*-Indol-3-yl)thio)-5-methoxybenzo[*d*]oxazole (**6au**)



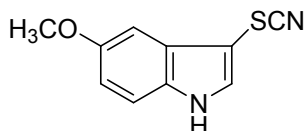
Yellow amorphous solid. 1H NMR (400 MHz, $DMSO-d_6$): δ 12.00 (s, 1H, NH), 8.00 (s, 1H, Ar-H), 7.63 (t, $J = 3.9$ Hz, 1H, Ar-H), 7.53 (d, $J = 3.9$ Hz, 2H, Ar-H), 7.35 (s, 1H, Ar-H), 7.22 (d, $J = 6.7$ Hz, 1H, Ar-H), 7.13 (t, $J = 3.9$ Hz, 1H, Ar-H), 6.88 (d, $J = 6.7$ Hz, 1H, Ar-H), 3.78 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $DMSO-d_6$): δ 174.7, 159.0, 155.8, 137.2, 134.3, 128.4, 127.1, 123.0, 122.3, 121.3, 118.5, 113.6, 113.1, 105.0, 97.7, 55.9. MS (ESI): 297 ($M+H^+$, 100). Anal calcd for $C_{16}H_{12}N_2O_2S$: C, 64.85; H, 4.08; N, 9.45; S, 10.82. Found C, 65.16; H, 4.31; N, 9.30; S, 10.55.

3-Thiocyanato-1*H*-indole (**7a**)



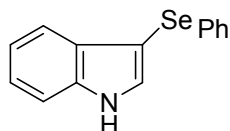
White amorphous solid. 1H NMR (400 MHz, $CDCl_3$): δ 8.76 (s, 1H, NH), 7.83 (dd, $J = 5.9, 3.1$ Hz, 1H, Ar-H), 7.52 (d, $J = 2.8$ Hz, 1H, Ar-H), 7.45 (dt, $J = 5.9, 3.1$ Hz, 1H, Ar-H), 7.35 (t, $J = 3.1$ Hz, 1H, Ar-H), 7.33 (t, $J = 3.1$ Hz, 1H, Ar-H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.0, 131.0, 127.7, 123.9, 121.9, 118.8, 112.1, 111.9, 92.3. MS (ESI): 175 ($M+H^+$, 100). These assignments matched with those previously published.⁷

6-Methoxy-3-thiocyanato-1*H*-indole (**7b**)



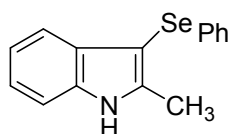
White amorphous solid. 1H NMR (400 MHz, $CDCl_3$): δ 8.55 (s, 1H, NH), 7.67 (d, $J = 8.7$ Hz, 1H, Ar-H), 7.40 (d, $J = 2.7$ Hz, 1H, Ar-H), 6.97 (dd, $J = 8.7, 2.1$ Hz, 1H, Ar-H), 6.90 (d, $J = 2.1$ Hz, 1H, Ar-H), 3.86 (s, 3H, OCH_3). ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.7, 136.9, 129.8, 121.8, 119.5, 112.1, 111.9, 95.2, 92.3, 55.7. MS (ESI): 205 ($M+H^+$, 100). These assignments matched with those previously published.⁷

3-(Phenylselanyl)-1*H*-indole (**9a**)



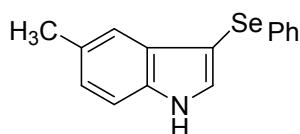
Yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.43 (s, 1H, NH), 7.69 (d, $J = 7.9$ Hz, 1H, Ar-H), 7.49 (d, $J = 2.5$ Hz, 1H, Ar-H), 7.46 (d, $J = 8.2$ Hz, 1H, Ar-H), 7.33-7.27 (m, 3H, Ar-H), 7.24-7.12 (m, 4H, Ar-H). ^{13}C NMR (101 MHz, CDCl_3): δ 136.4, 133.9, 131.3, 130.0, 129.0, 128.7, 125.6, 123.0, 120.9, 120.4, 111.4, 98.2. MS (ESI): 274 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.⁸

2-Methyl-3-(phenylselanyl)-1H-indole (**9b**)



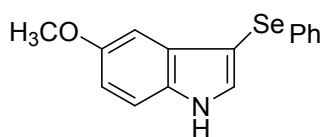
Yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.20 (s, 1H, NH), 7.64 (d, $J = 7.7$ Hz, 1H, Ar-H), 7.36 (d, $J = 7.9$ Hz, 1H, Ar-H), 7.26 (dd, $J = 3.5, 1.4$ Hz, 1H, Ar-H), 7.23 (dd, $J = 3.5, 1.4$ Hz, 2H, Ar-H), 7.20 (d, $J = 4.1$ Hz, 1H, Ar-H), 7.19-7.12 (m, 3H, Ar-H), 2.56 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 141.0, 135.8, 134.0, 131.3, 129.0, 128.4, 125.5, 122.2, 120.7, 119.8, 110.6, 96.2, 13.2. MS (ESI): 288 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.⁹

5-Methyl-3-(phenylselanyl)-1H-indole (**9c**)



Yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.30 (s, 1H, NH), 7.51 (d, $J = 0.5$ Hz, 1H, Ar-H), 7.44 (d, $J = 2.5$ Hz, 1H, Ar-H), 7.35 (d, $J = 8.3$ Hz, 1H, Ar-H), 7.31-7.28 (m, 2H, Ar-H), 7.22-7.14 (m, 4H, Ar-H), 2.49 (s, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 134.7, 134.1, 131.5, 130.4, 130.3, 129.0, 128.6, 125.6, 124.7, 119.9, 111.1, 97.4, 21.5. MS (ESI): 288 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.¹⁰

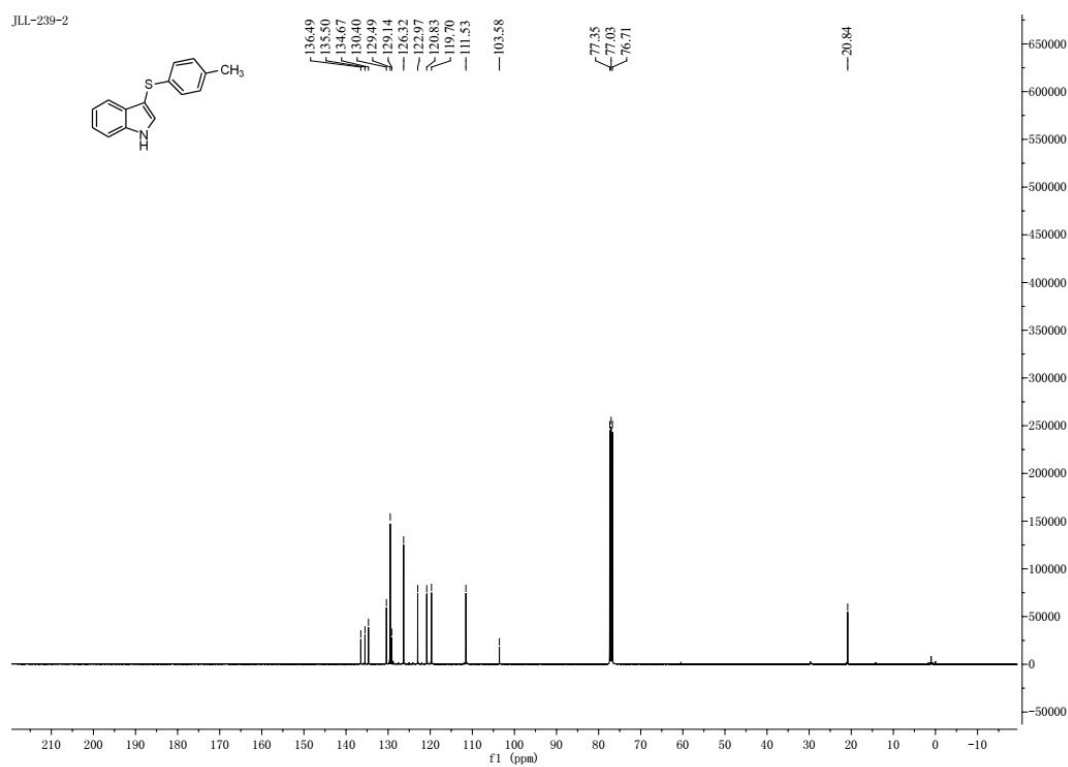
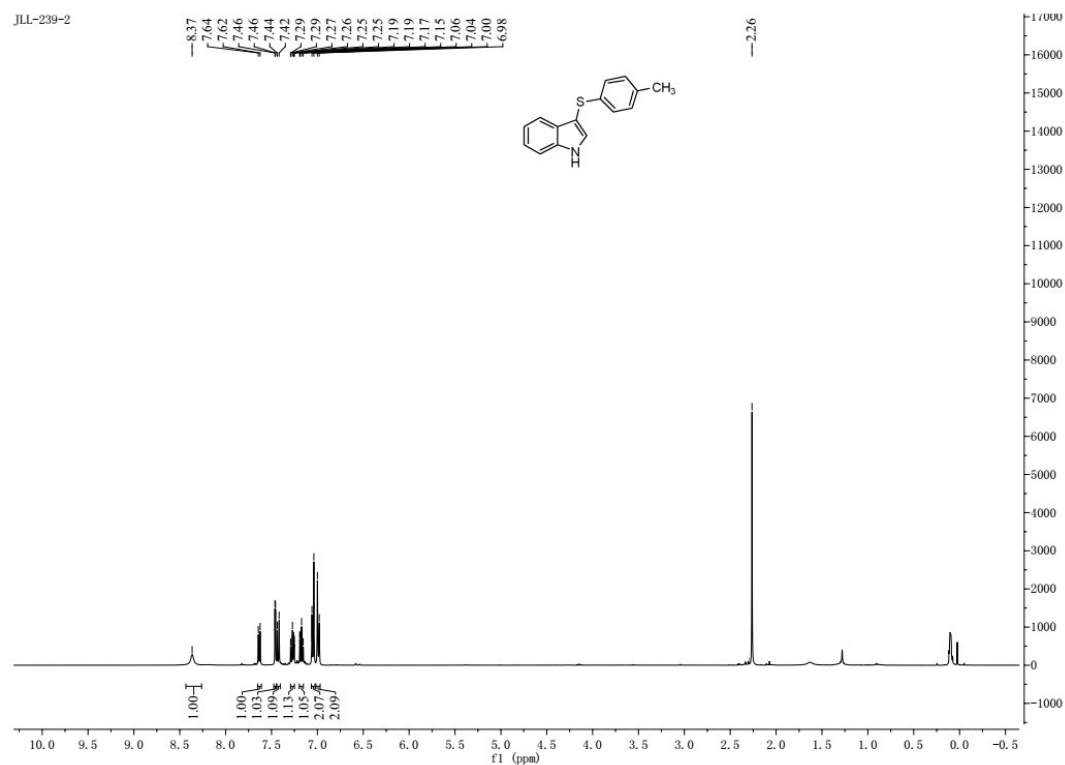
5-Methoxy-3-(phenylselanyl)-1H-indole (**9d**)



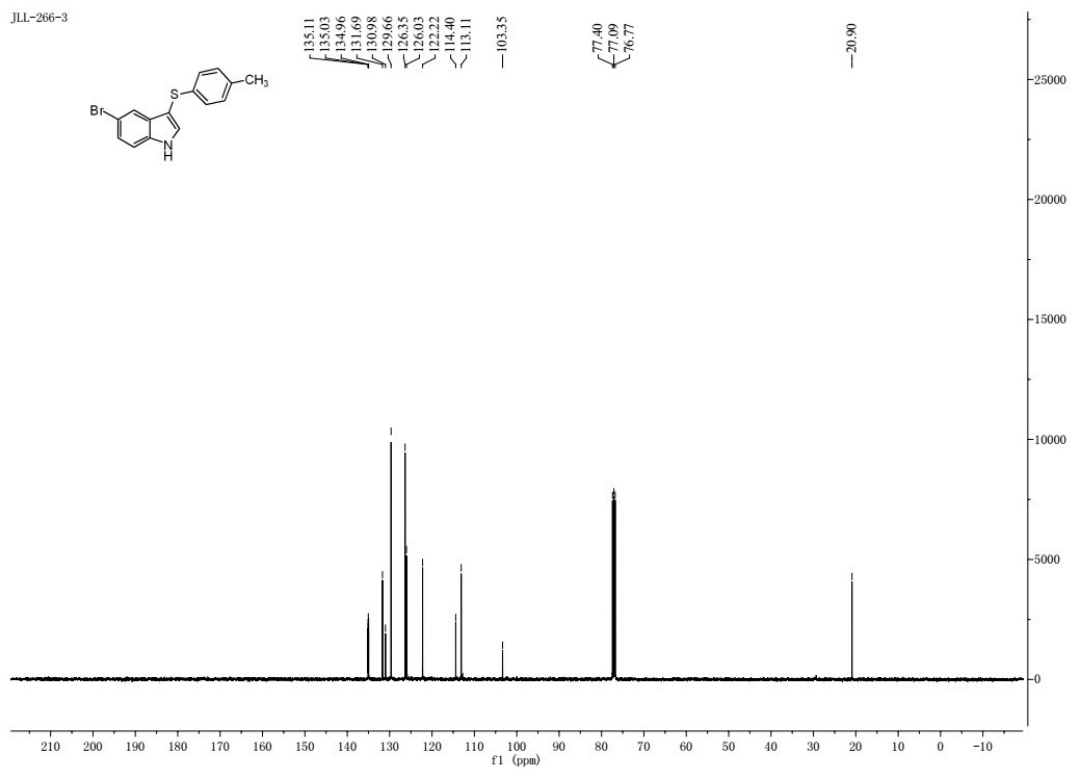
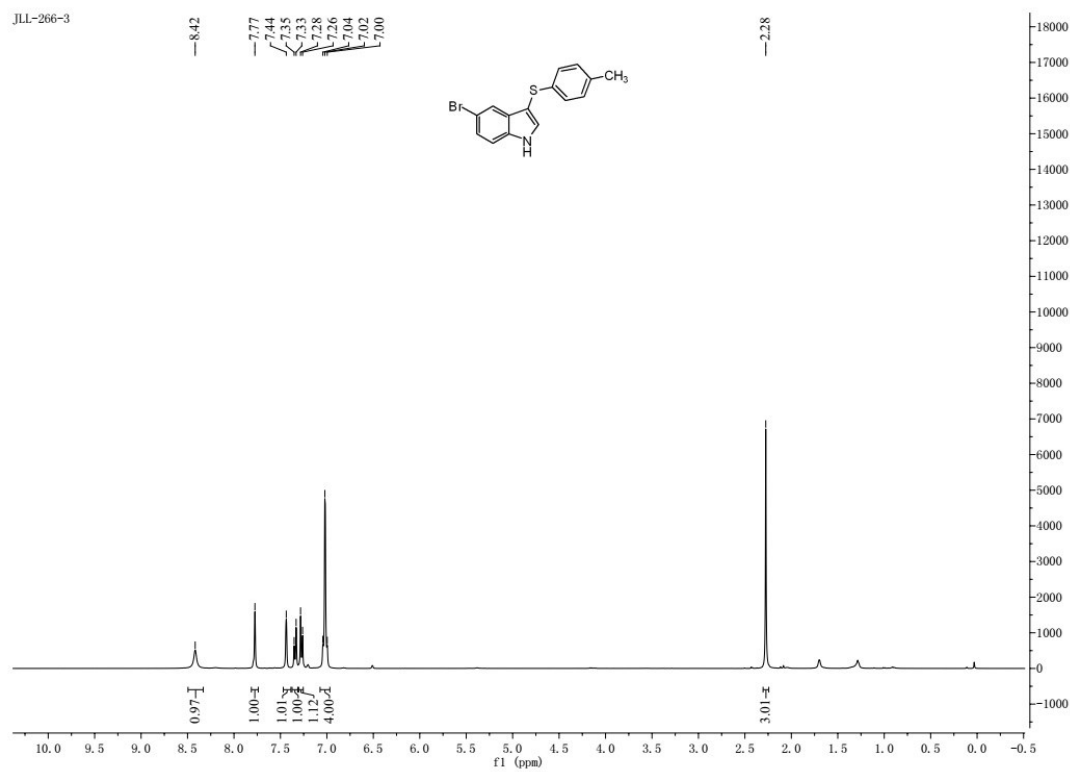
Yellow amorphous solid. ^1H NMR (400 MHz, CDCl_3): δ 8.42 (s, 1H, NH), 7.44 (d, $J = 2.5$ Hz, 1H, Ar-H), 7.33 (d, $J = 8.8$ Hz, 1H, Ar-H), 7.30 (dd, $J = 8.2, 1.5$ Hz, 1H, Ar-H), 7.29 (s, 1H, Ar-H), 7.21-7.13 (m, 4H, Ar-H), 6.97 (dd, $J = 8.8, 2.5$ Hz, 1H, Ar-H), 3.85 (s, 3H, OCH_3). ^{13}C NMR (101 MHz, CDCl_3): δ 155.1, 134.0, 132.0, 131.4, 130.8, 129.1, 128.5, 125.6, 113.5, 112.4, 101.6, 97.5, 55.9. MS (ESI): 304 ($\text{M}+\text{H}^+$, 100). These assignments matched with those previously published.¹⁰

6. Copies of ^1H and ^{13}C Spectra

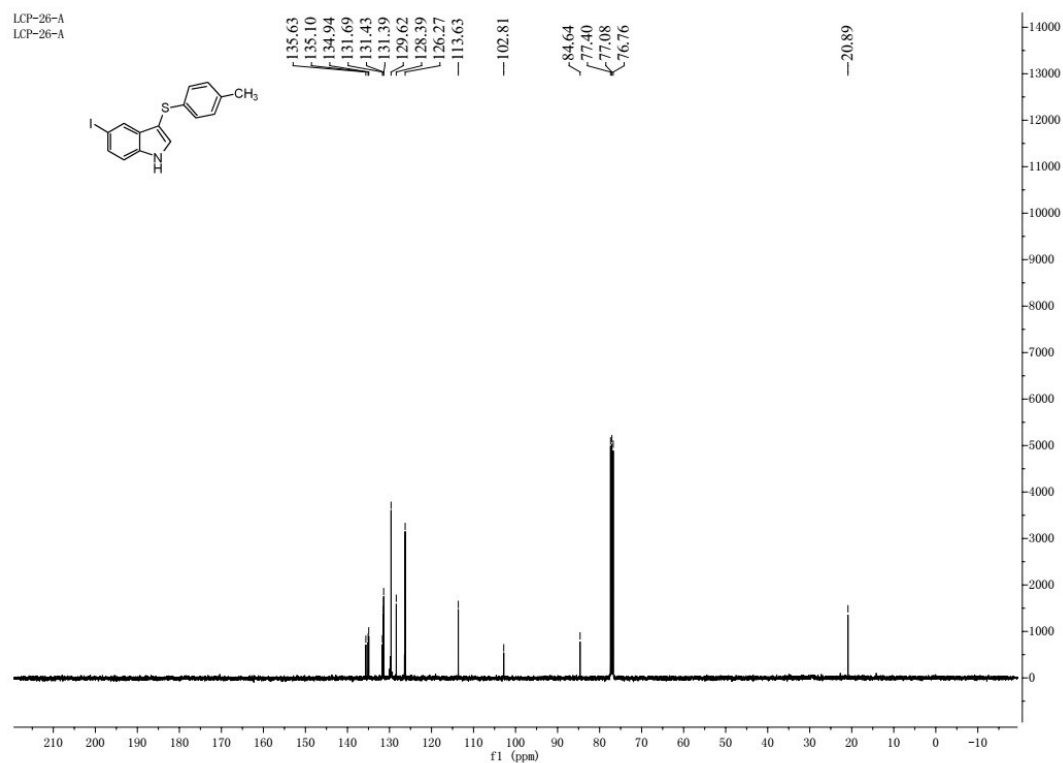
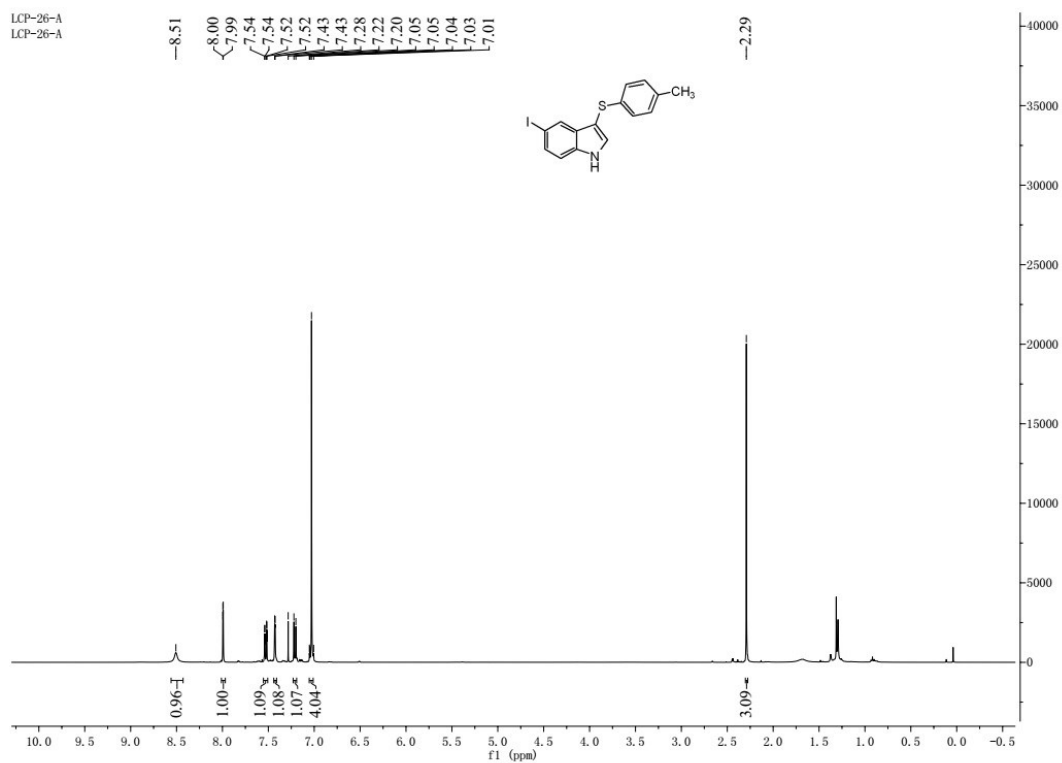
^1H and ^{13}C NMR Spectra for **6aa**



¹H and ¹³C NMR Spectra for **6ba**

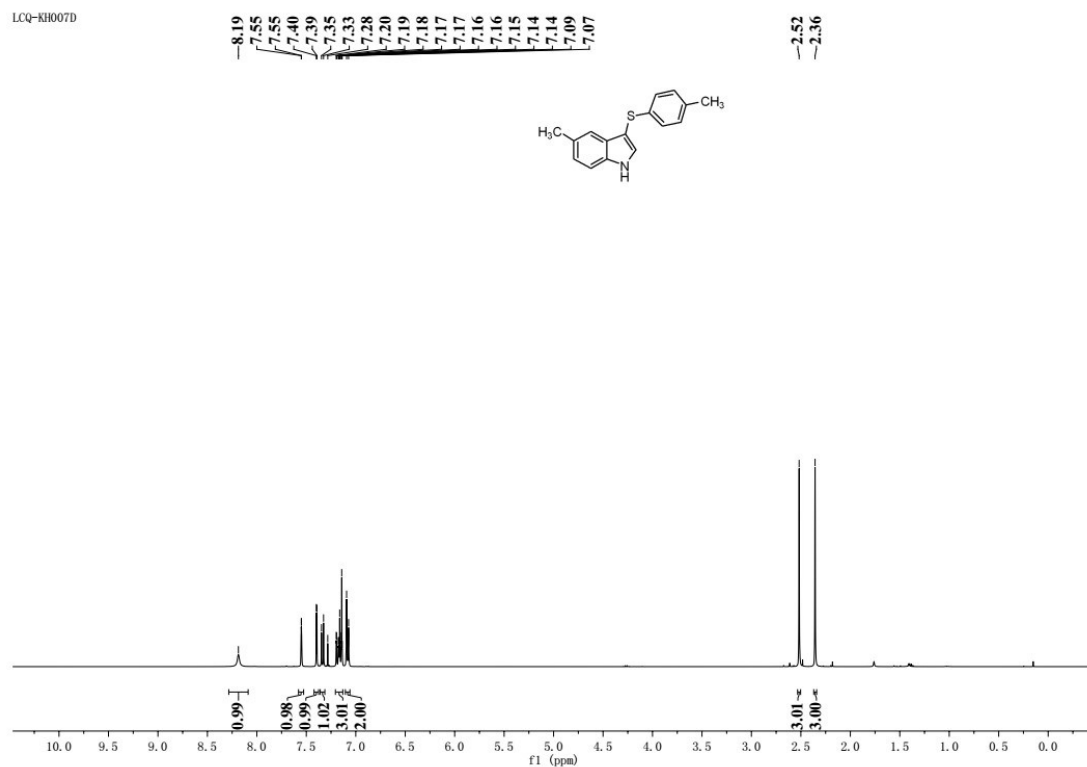


¹H and ¹³C NMR Spectra for 6ca

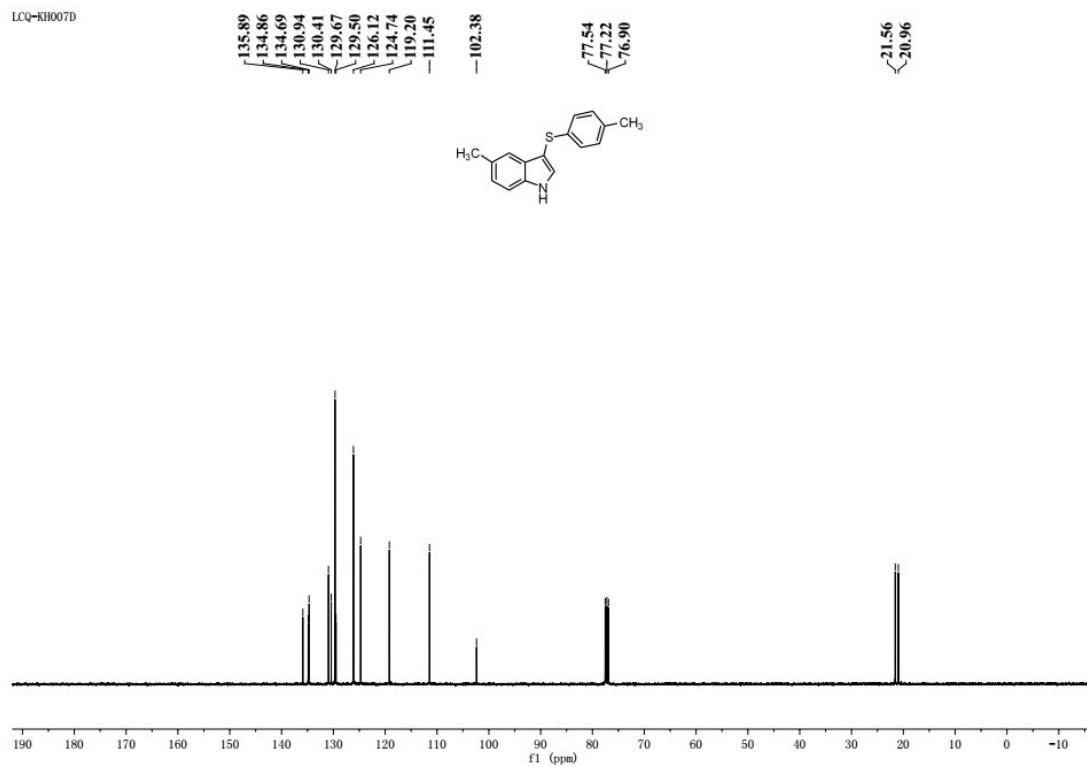


¹H and ¹³C NMR Spectra for **6da**

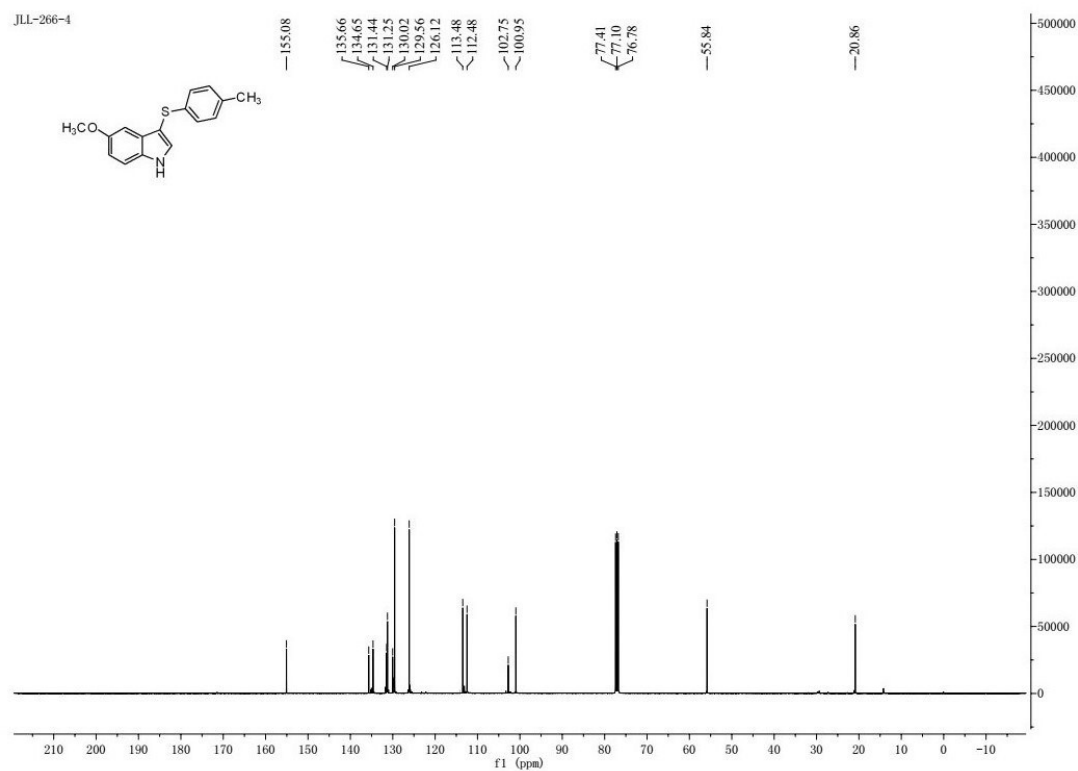
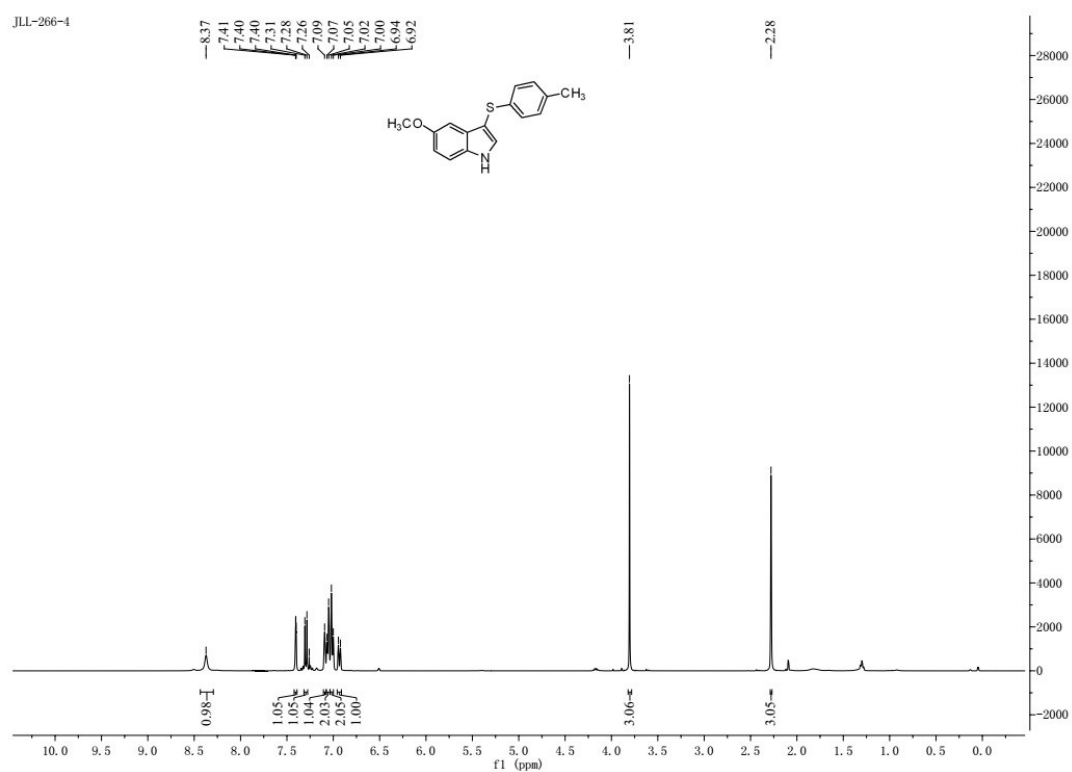
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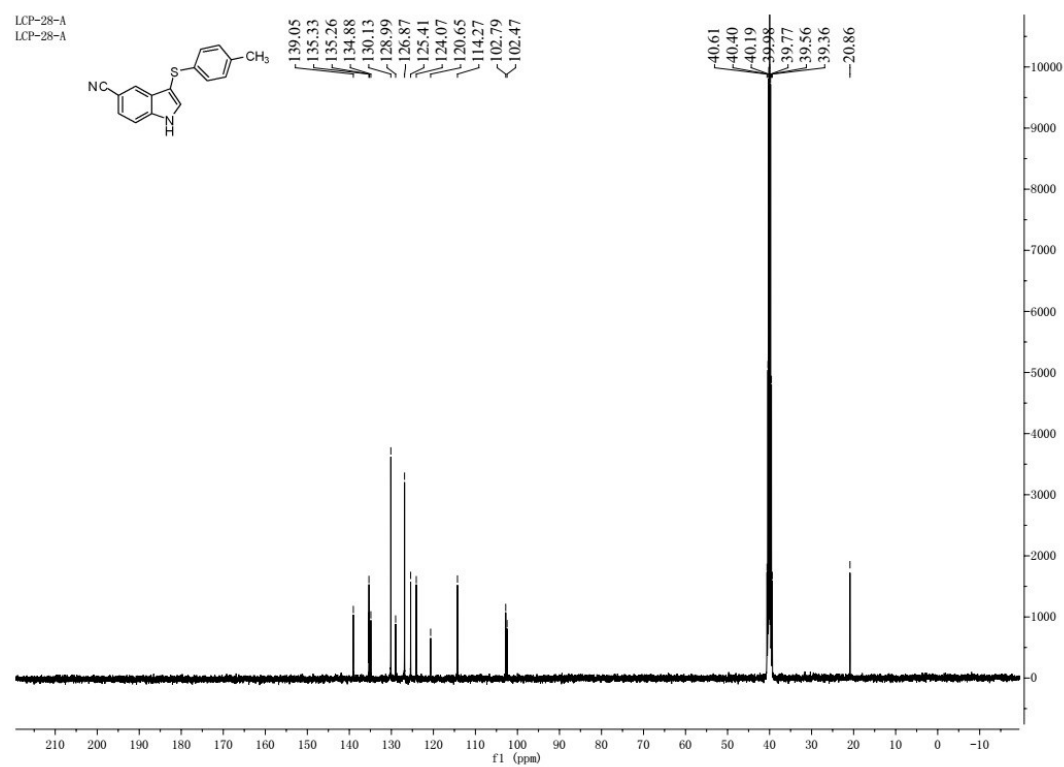
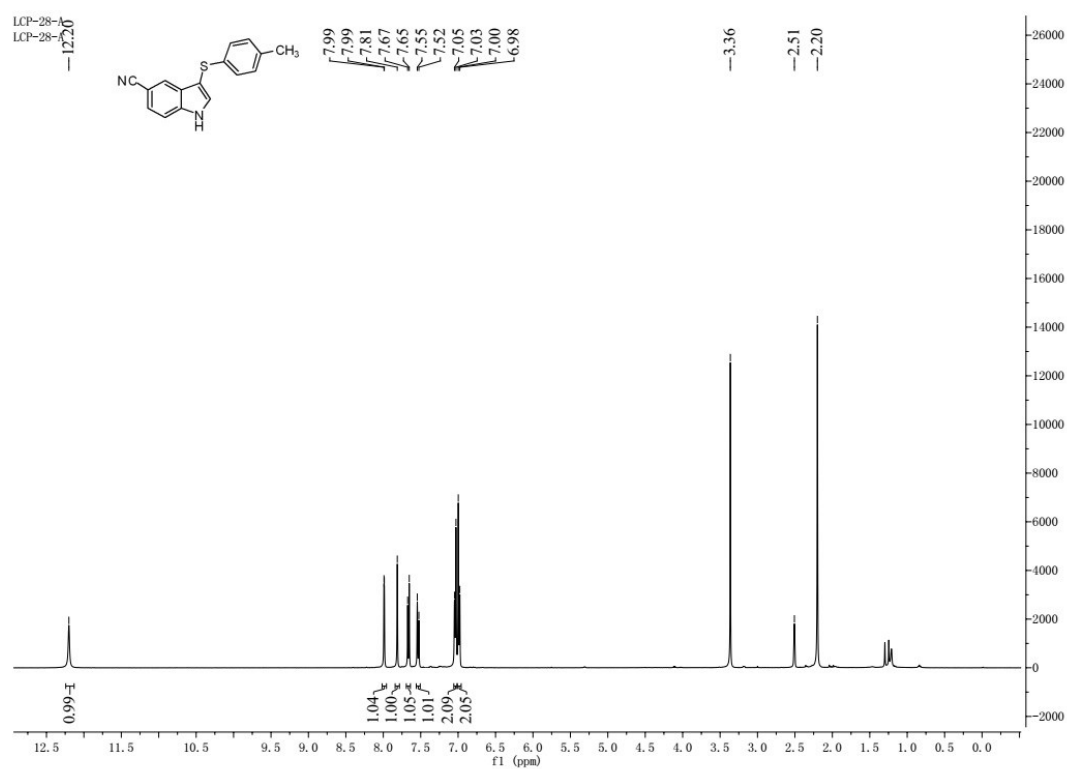
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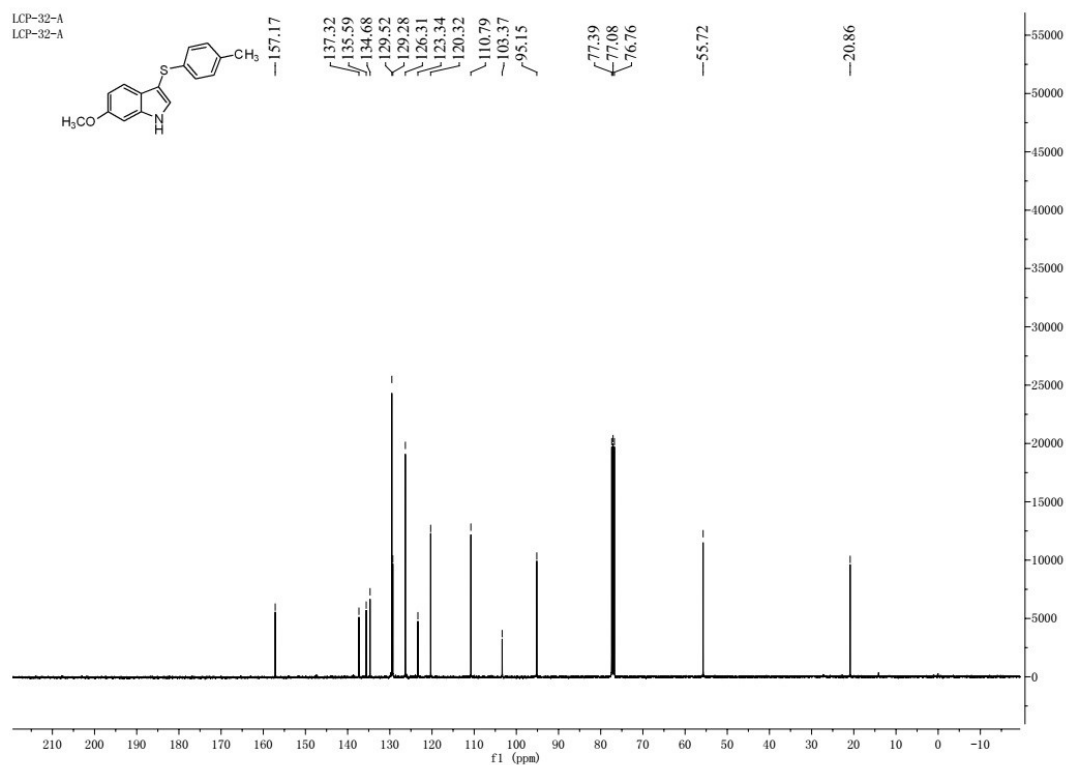
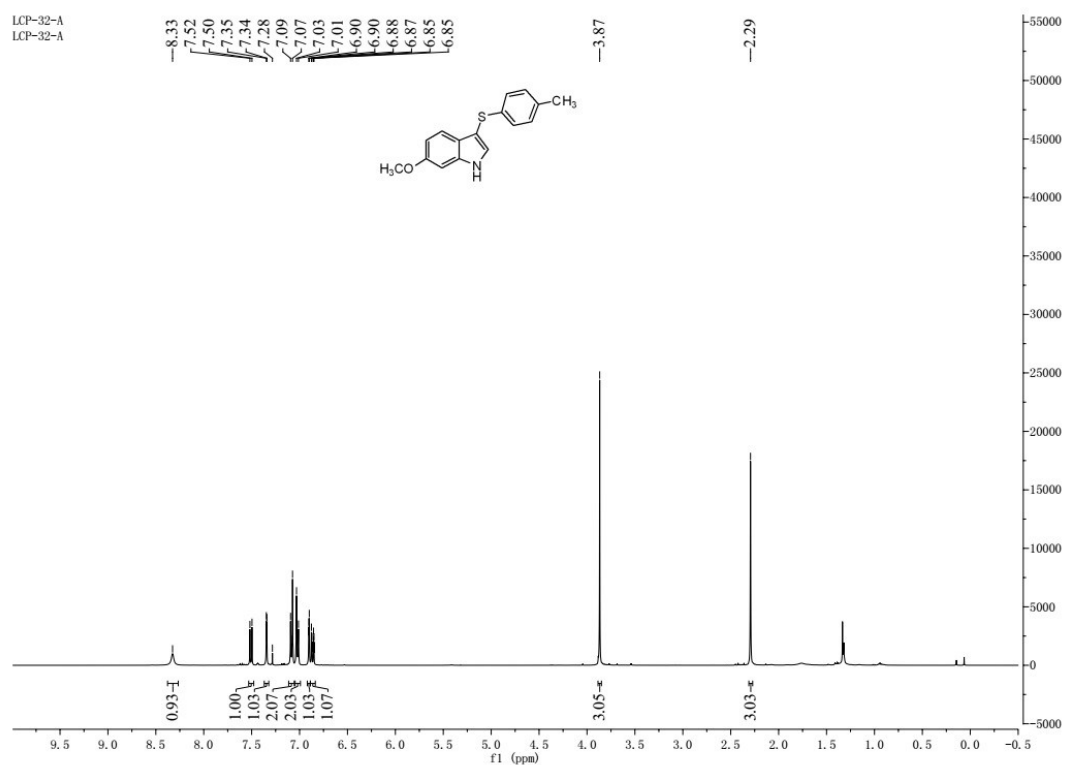
¹H and ¹³C NMR Spectra for 6ea



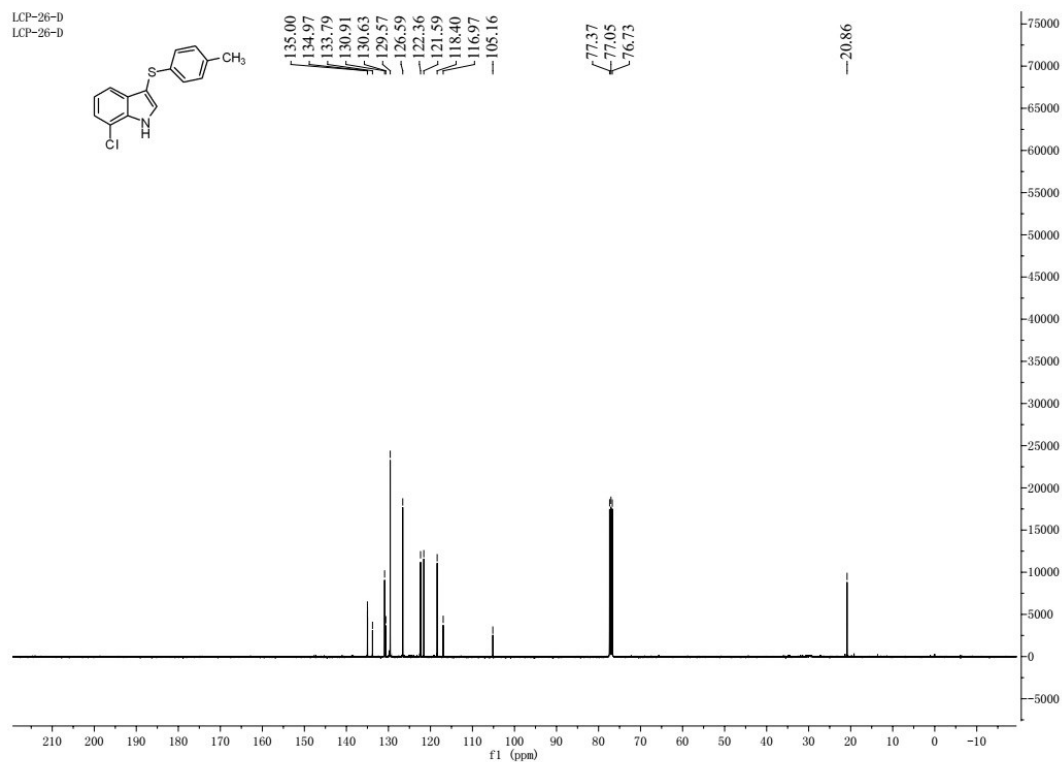
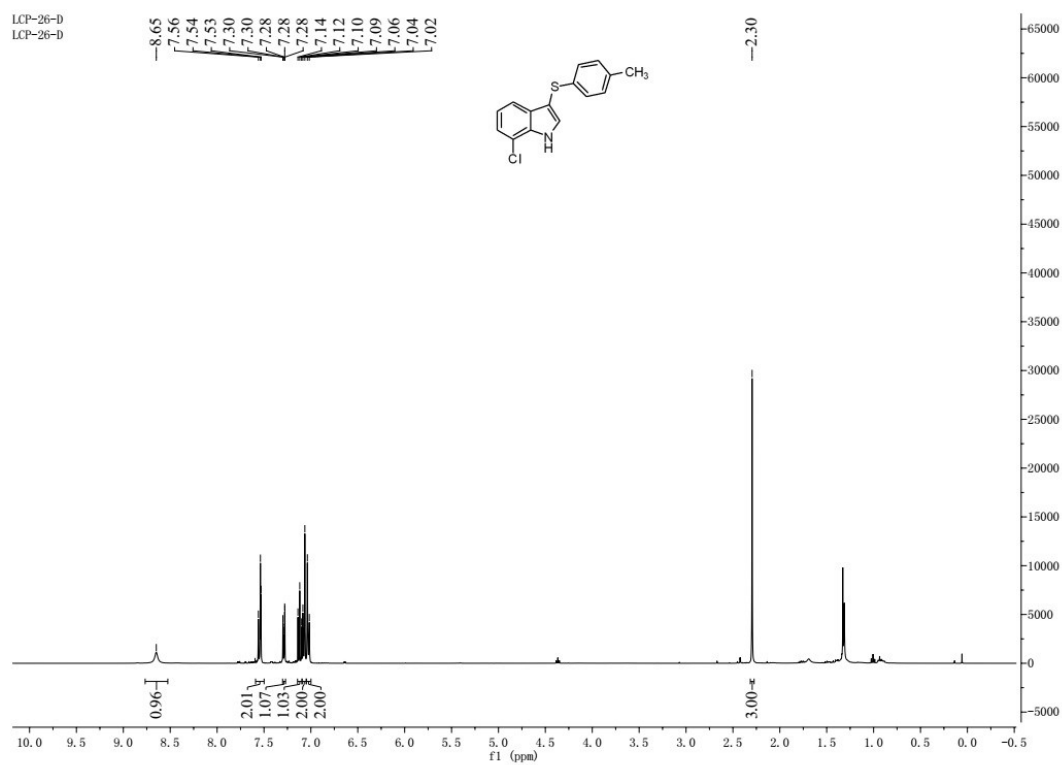
¹H and ¹³C NMR Spectra for **6fa**



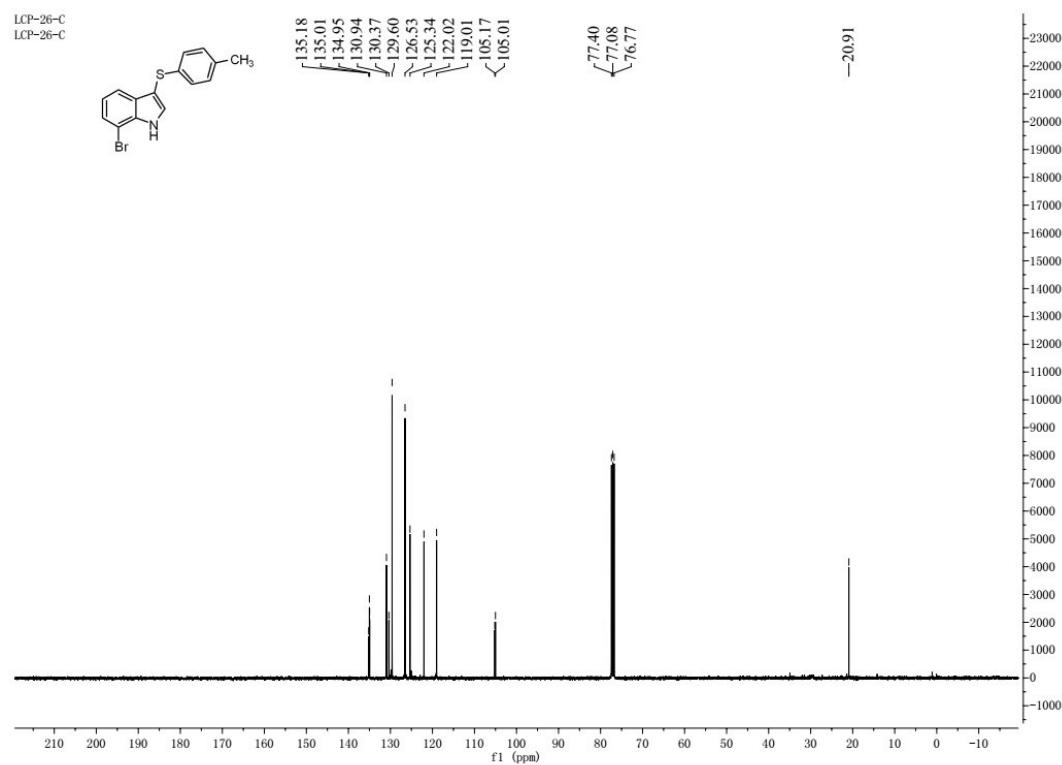
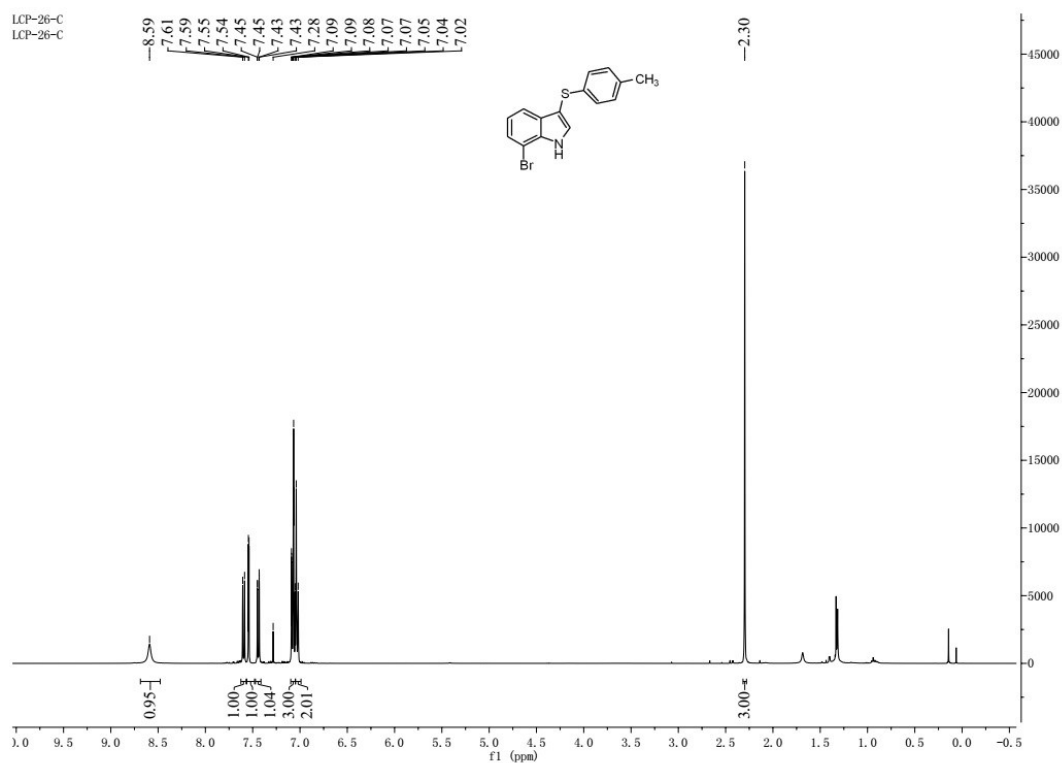
¹H and ¹³C NMR Spectra for **6ga**



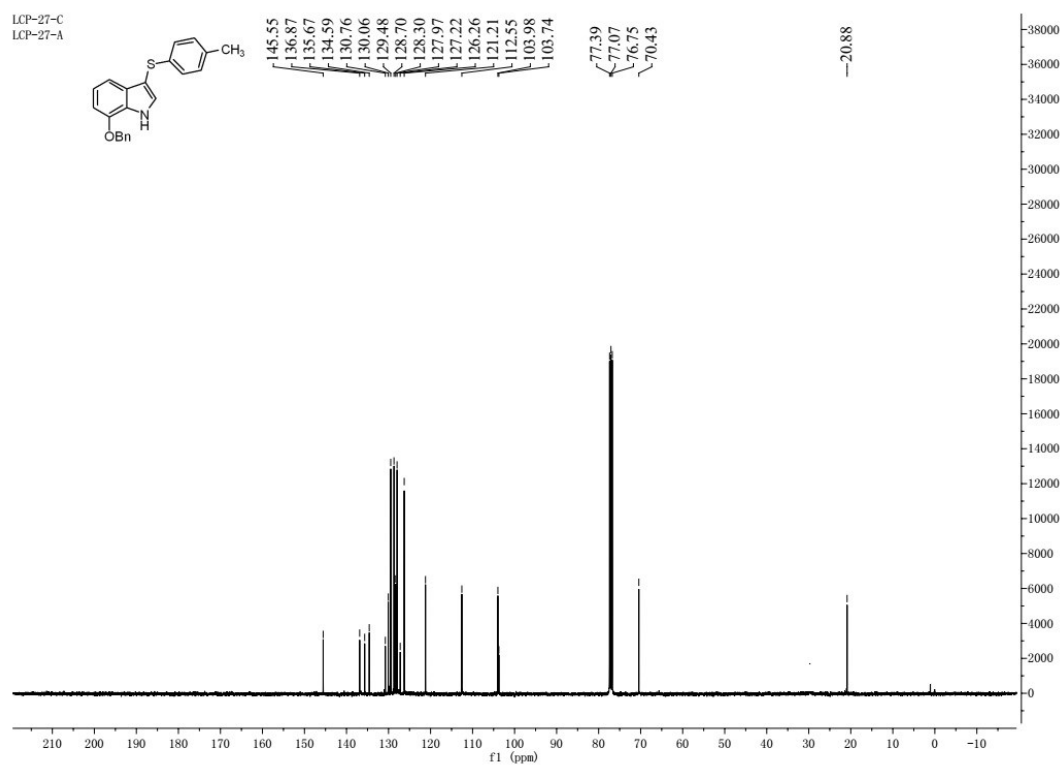
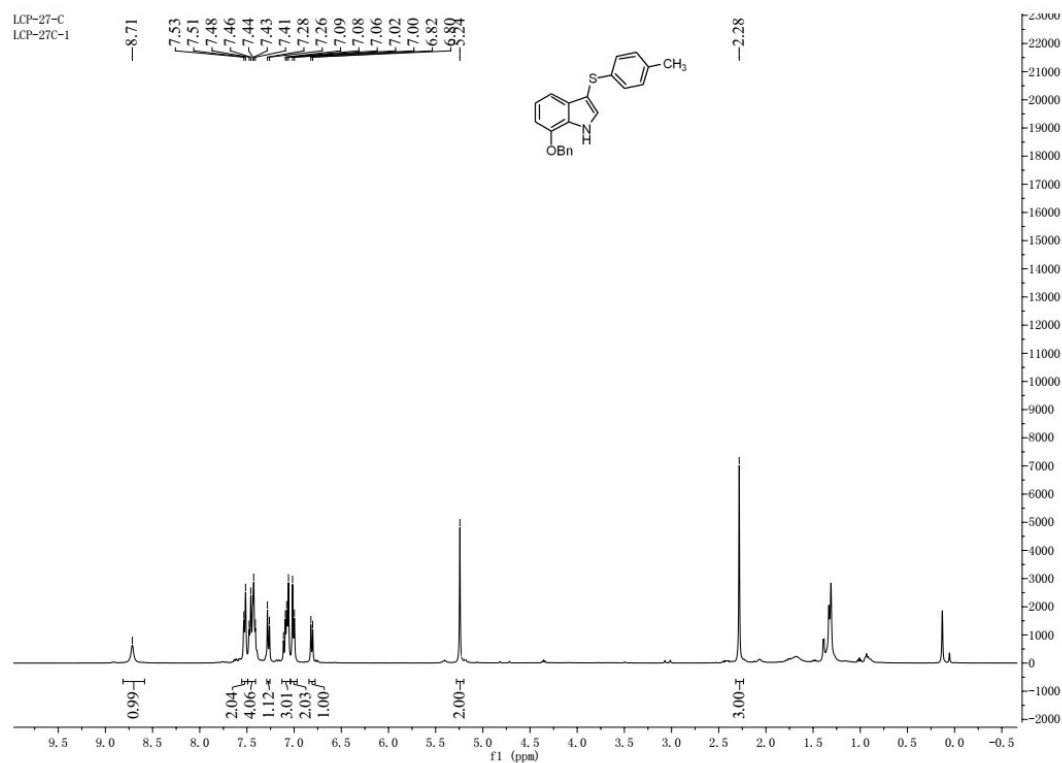
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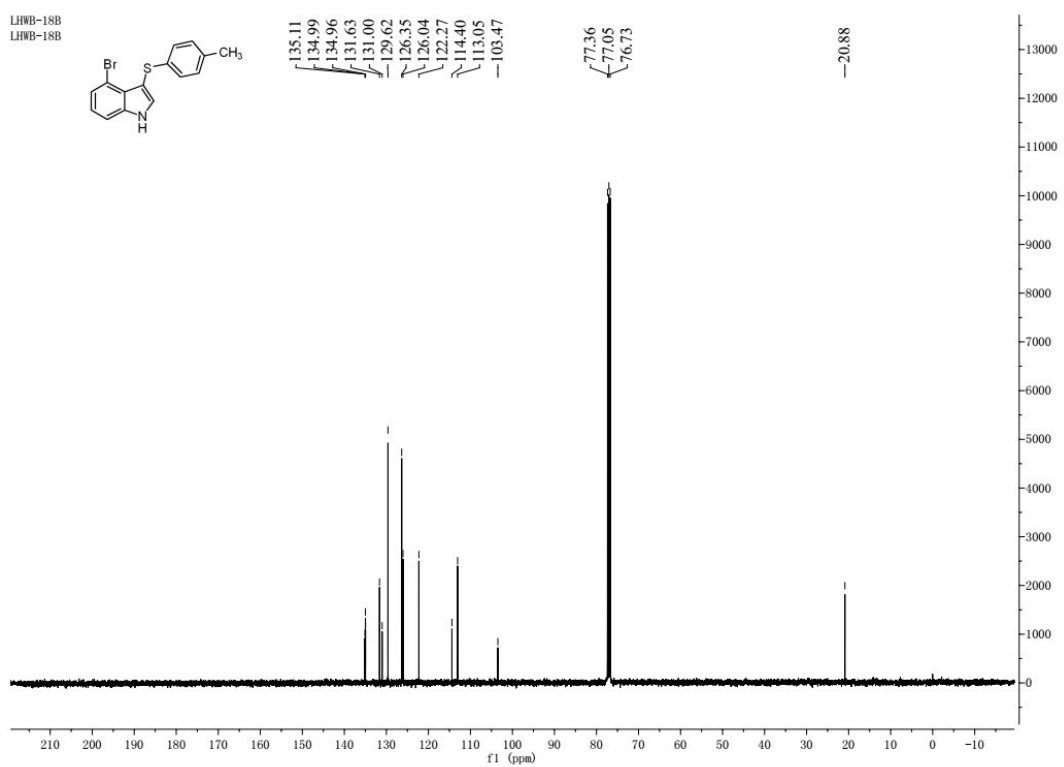
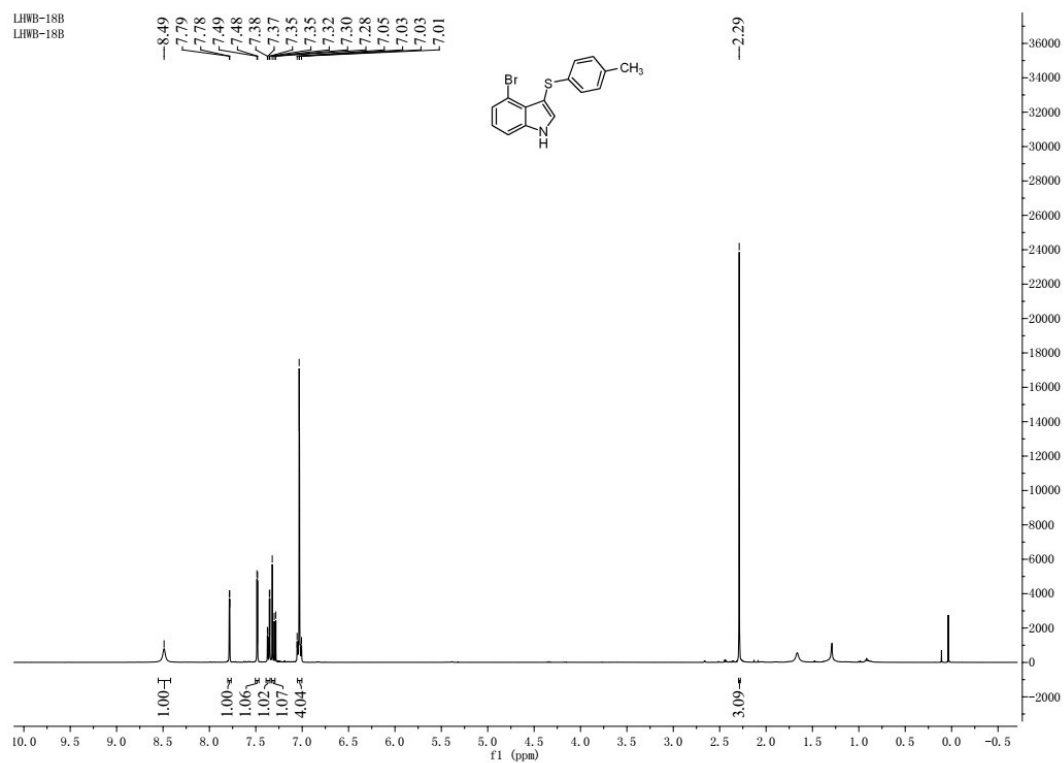
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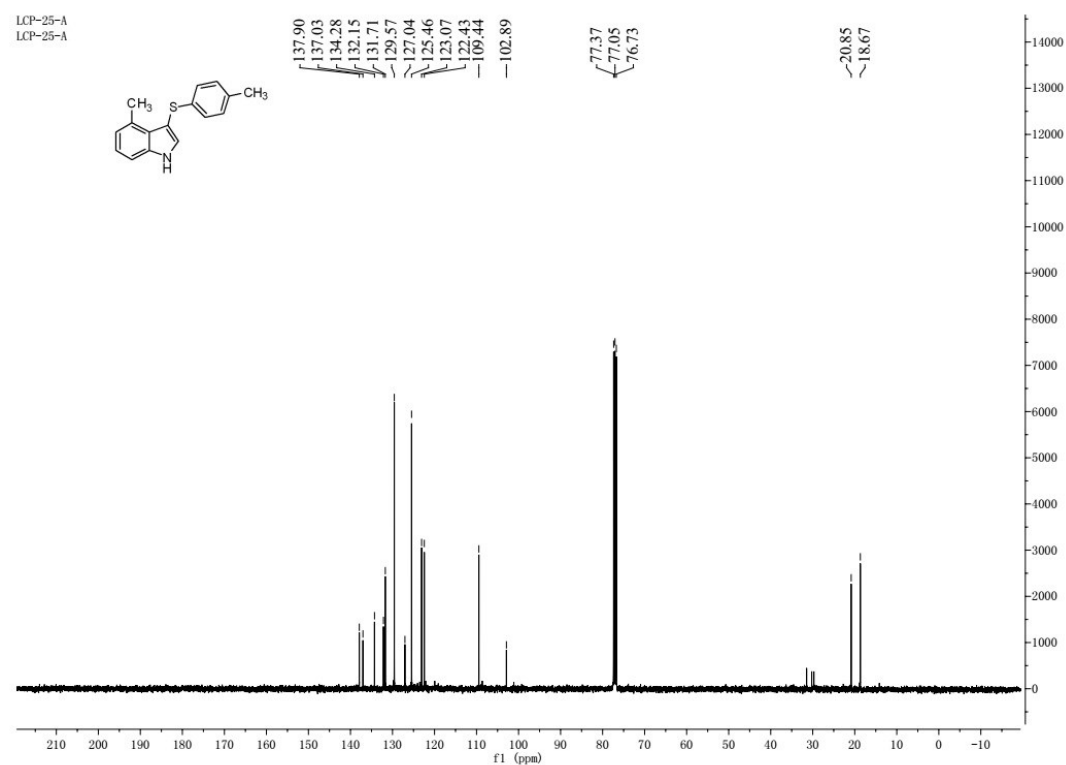
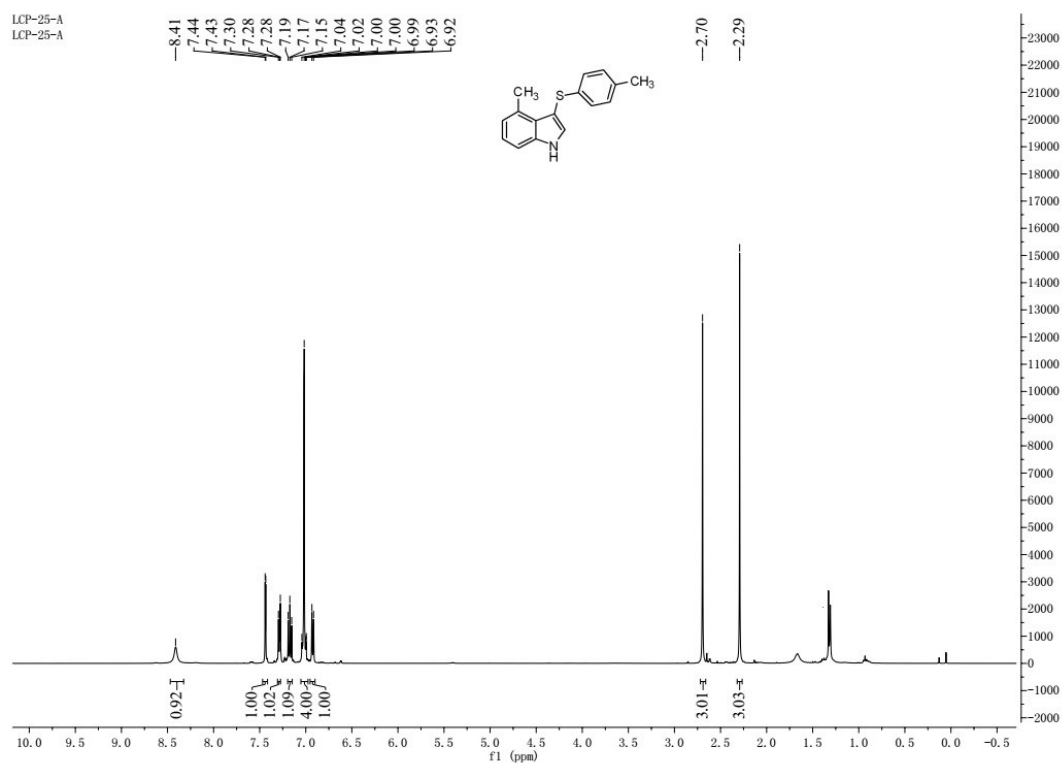
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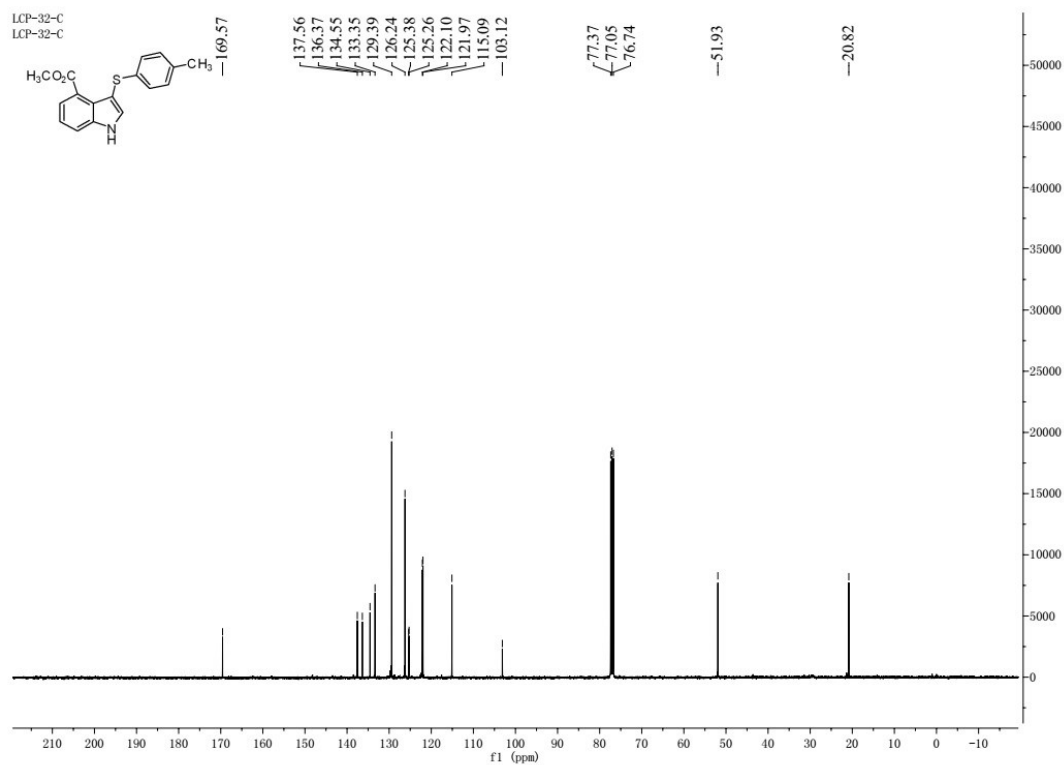
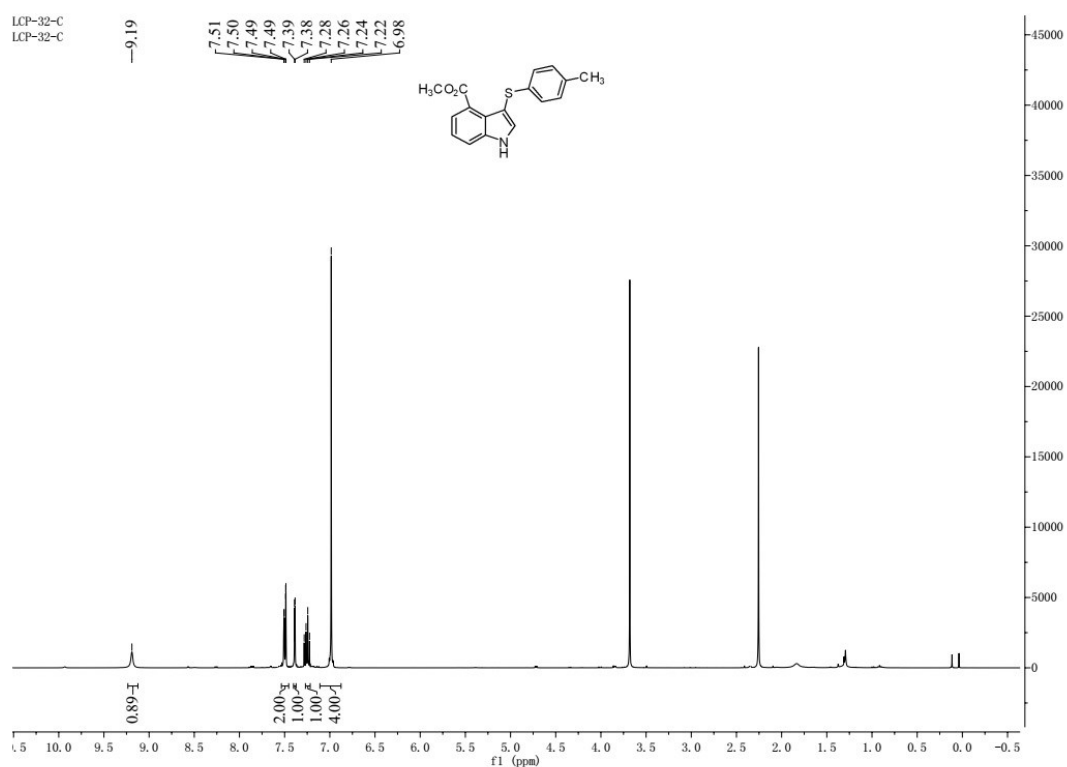
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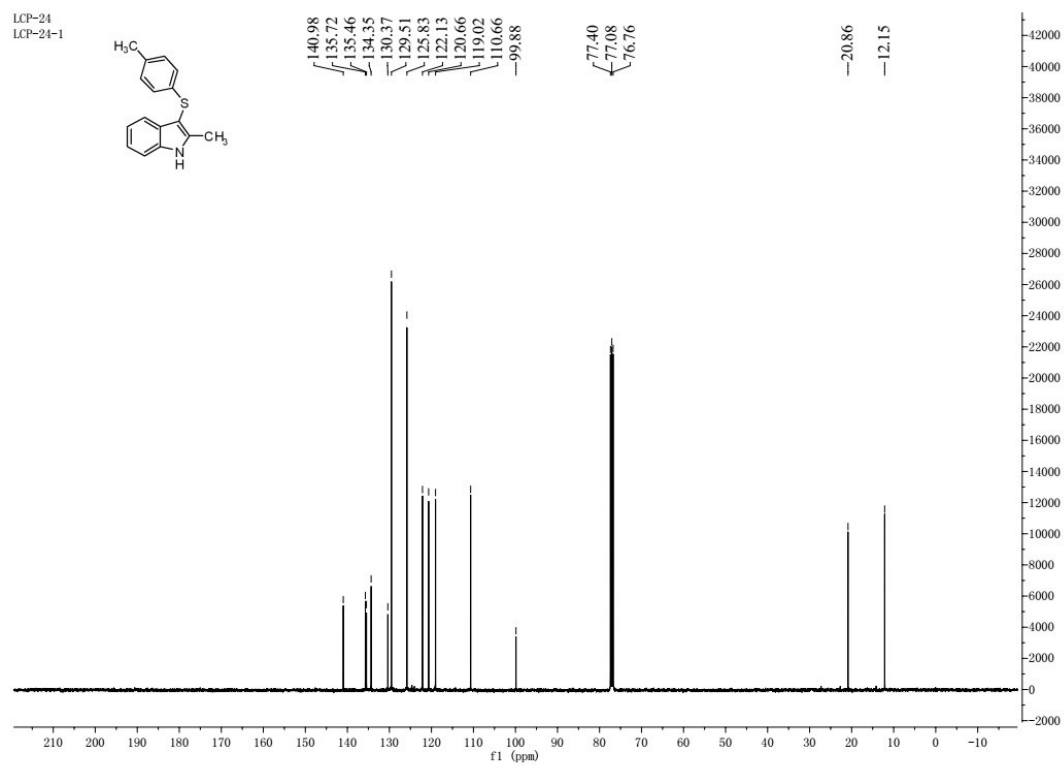
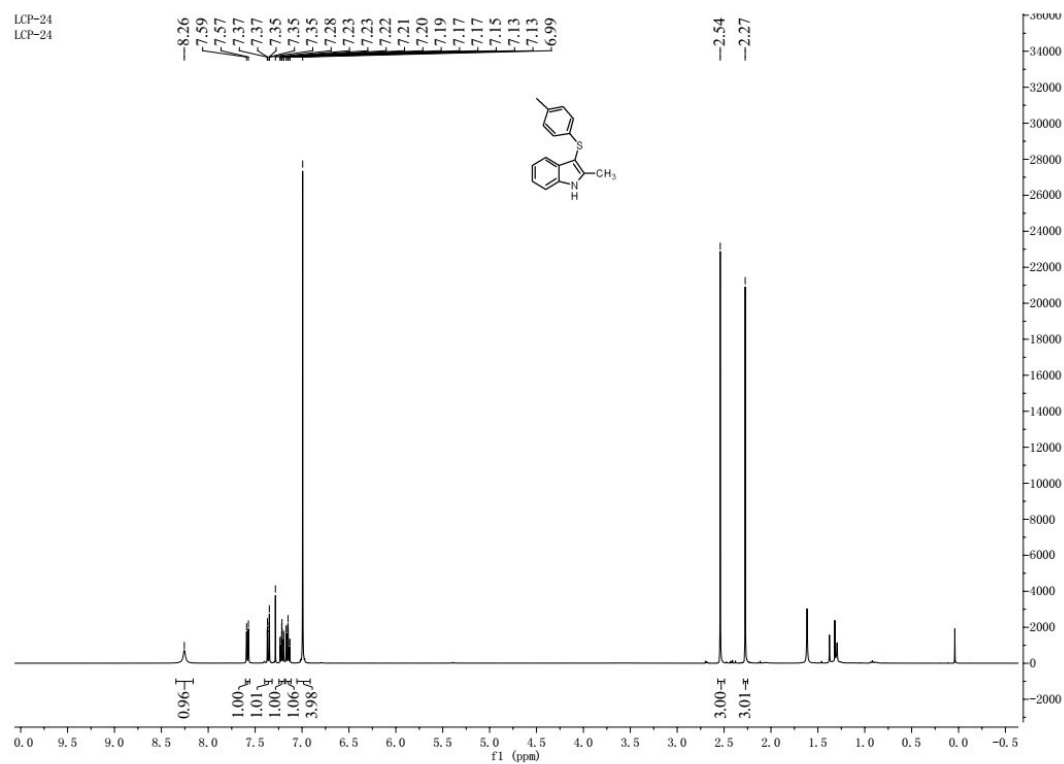
¹H and ¹³C NMR Spectra for **6la**



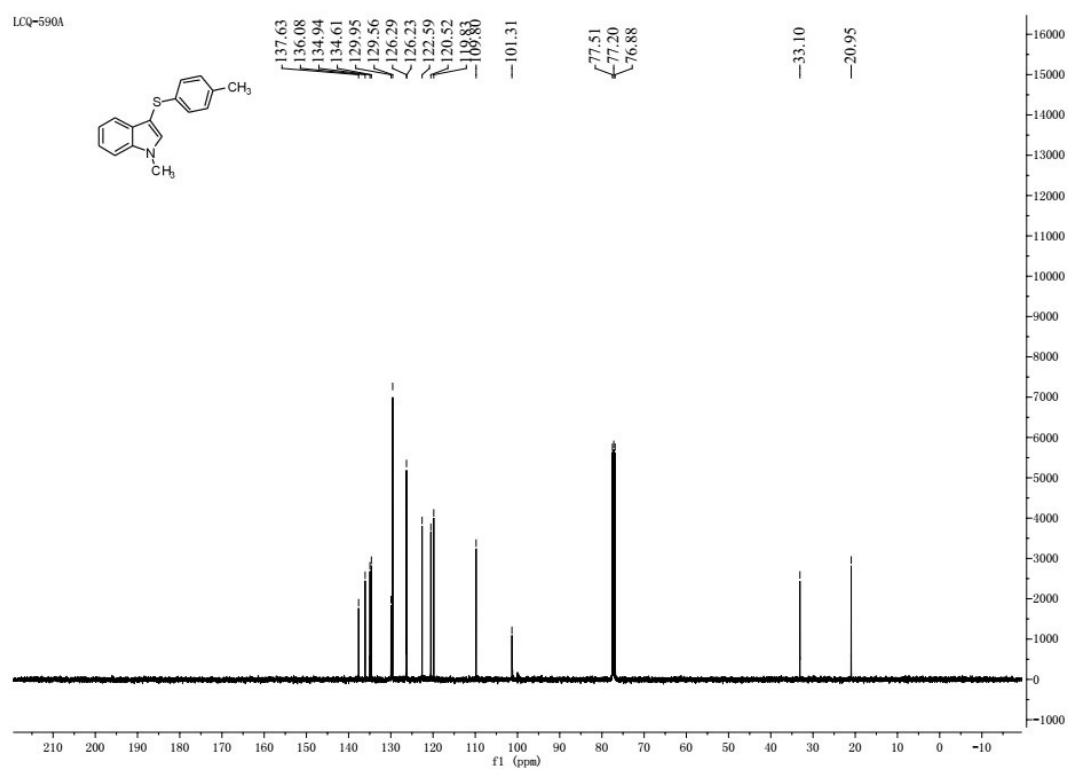
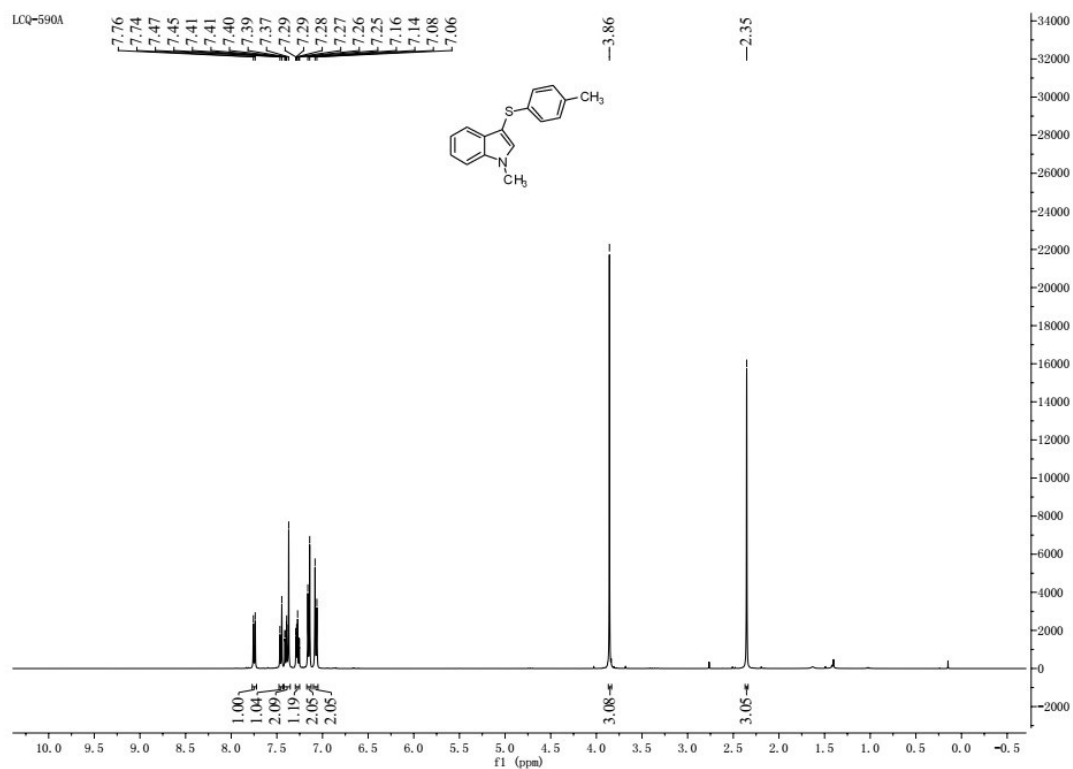
¹H and ¹³C NMR Spectra for 6ma



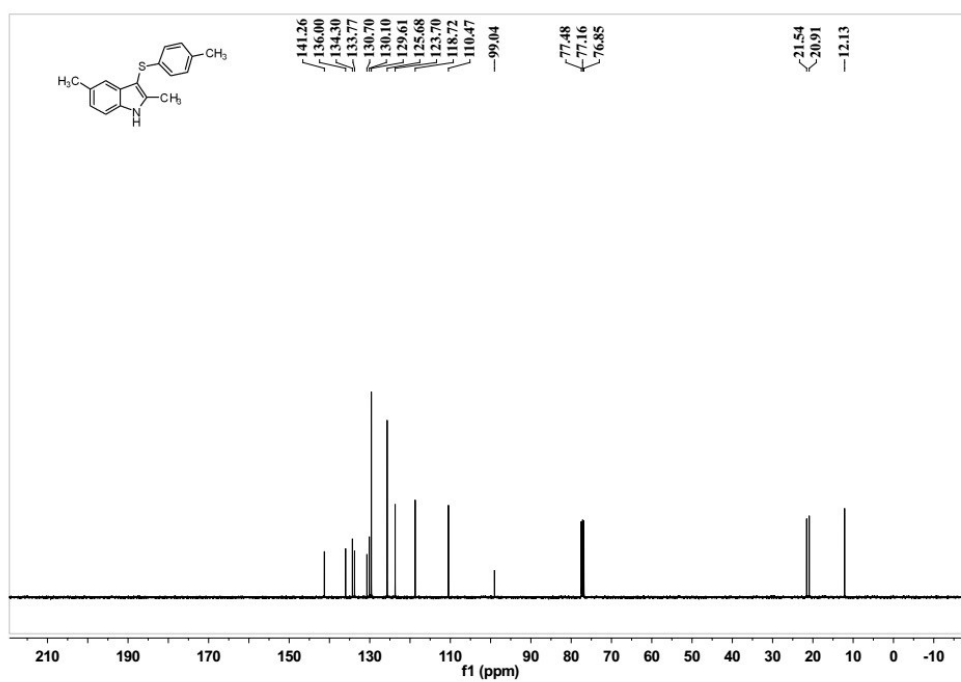
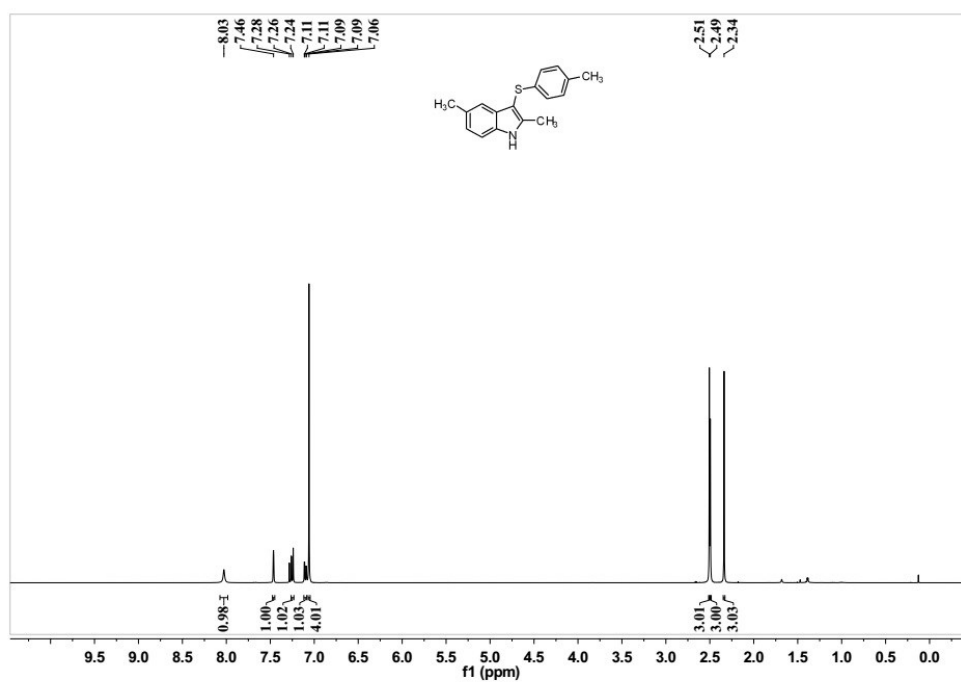
¹H and ¹³C NMR Spectra for 6na



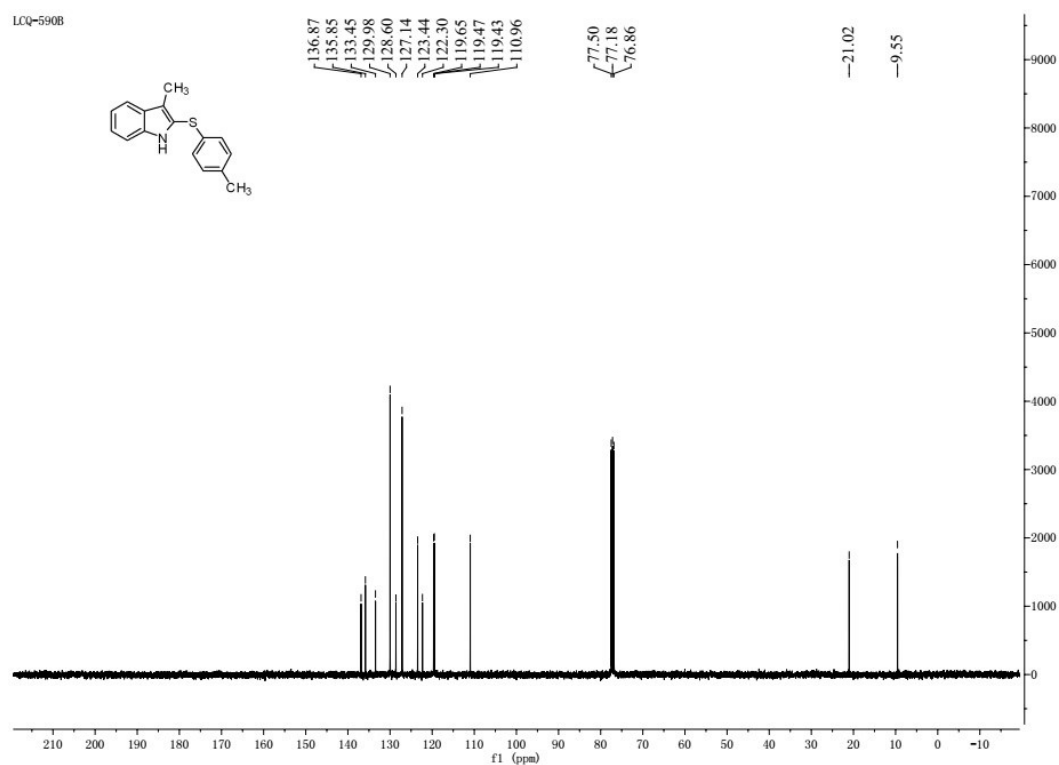
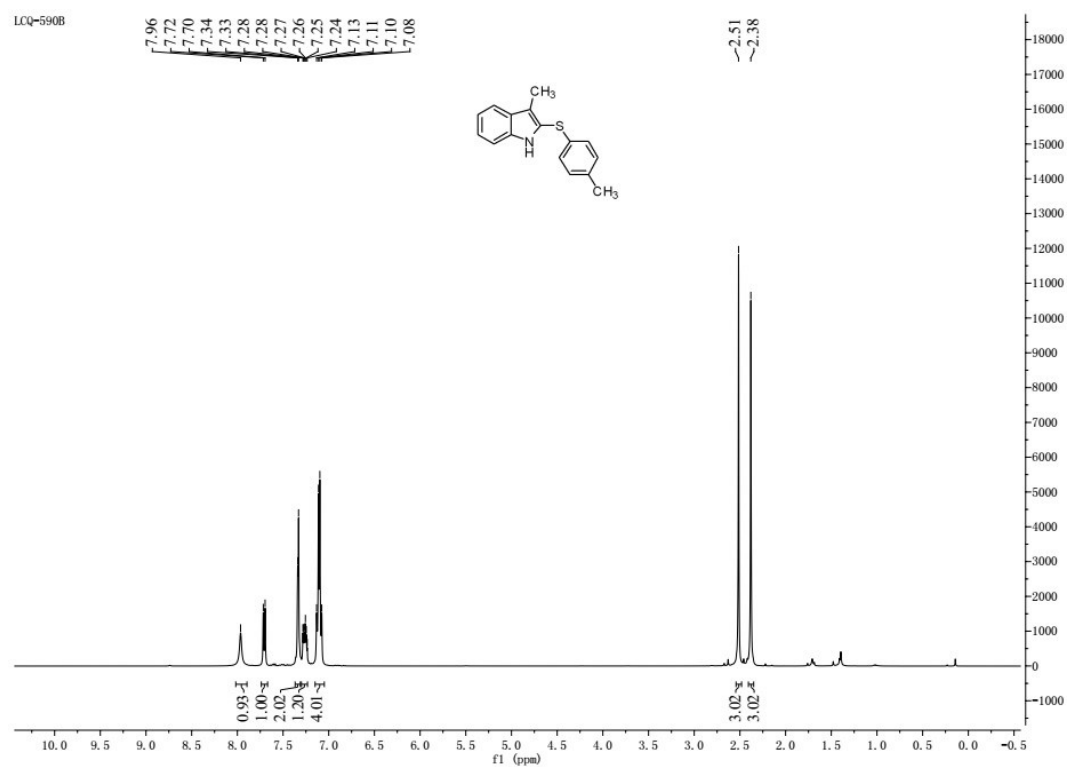
¹H and ¹³C NMR Spectra for 60a



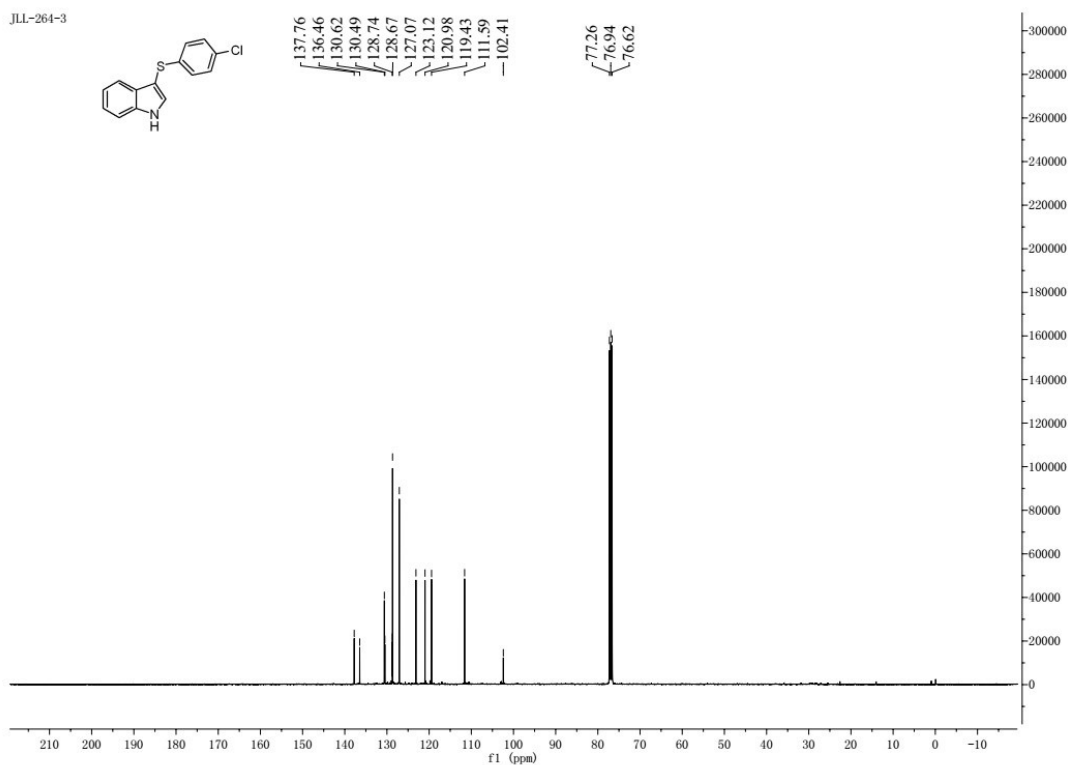
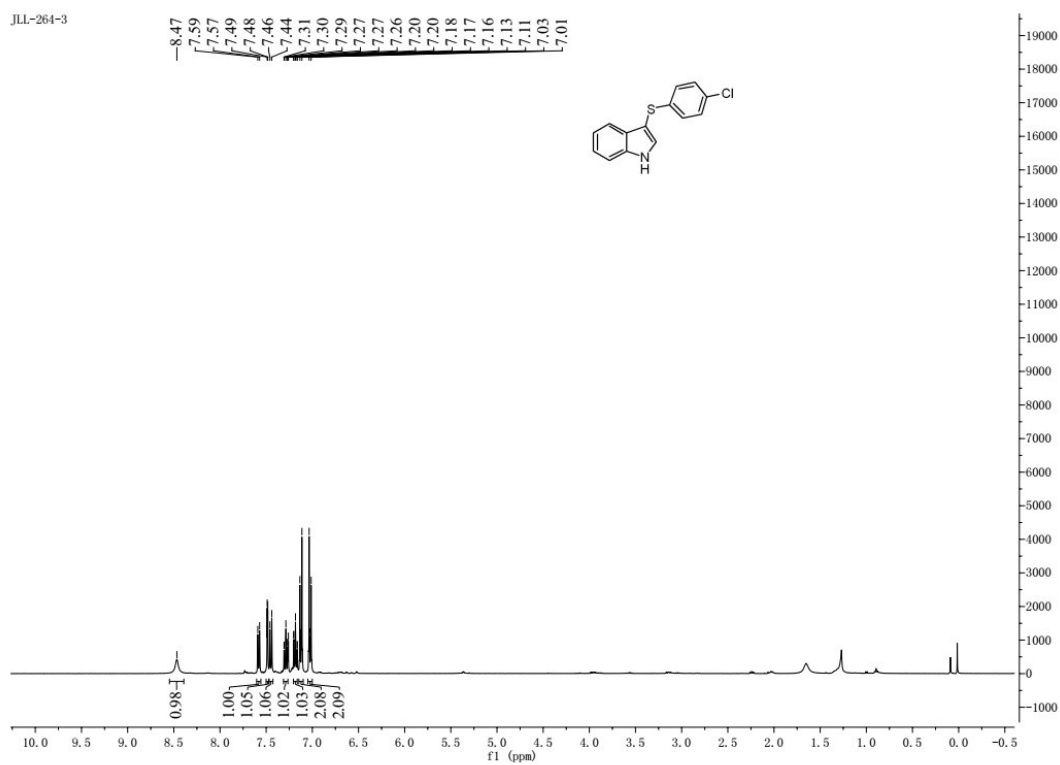
¹H and ¹³C NMR Spectra for 6pa



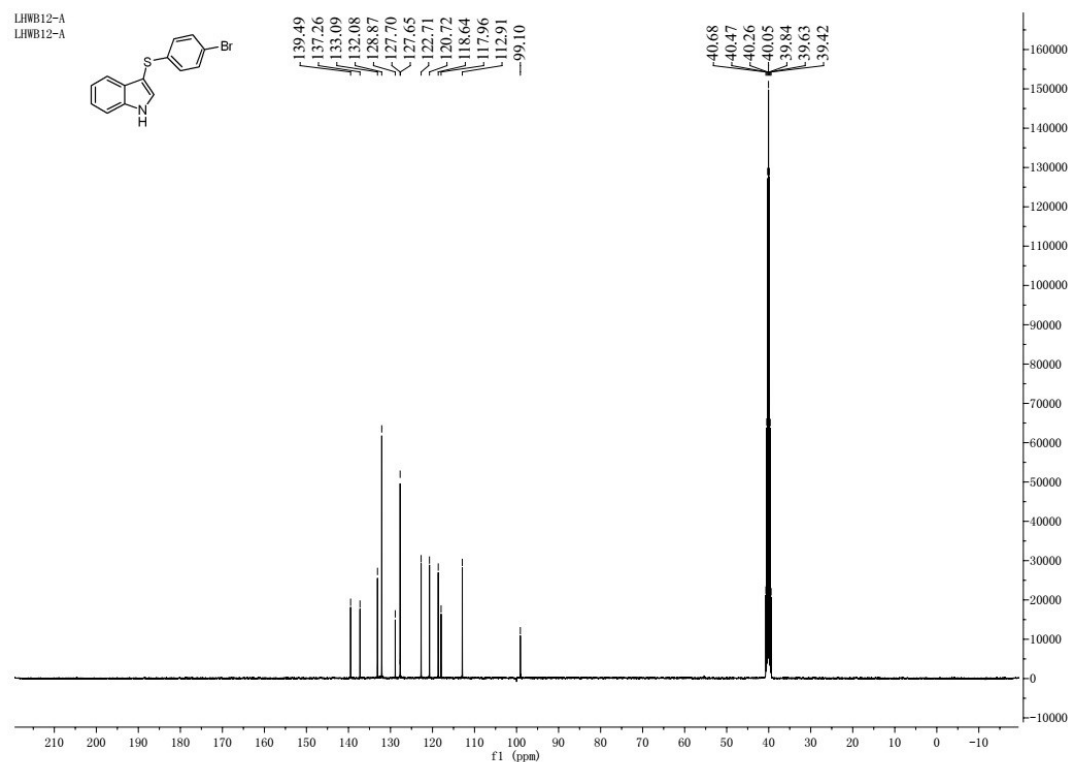
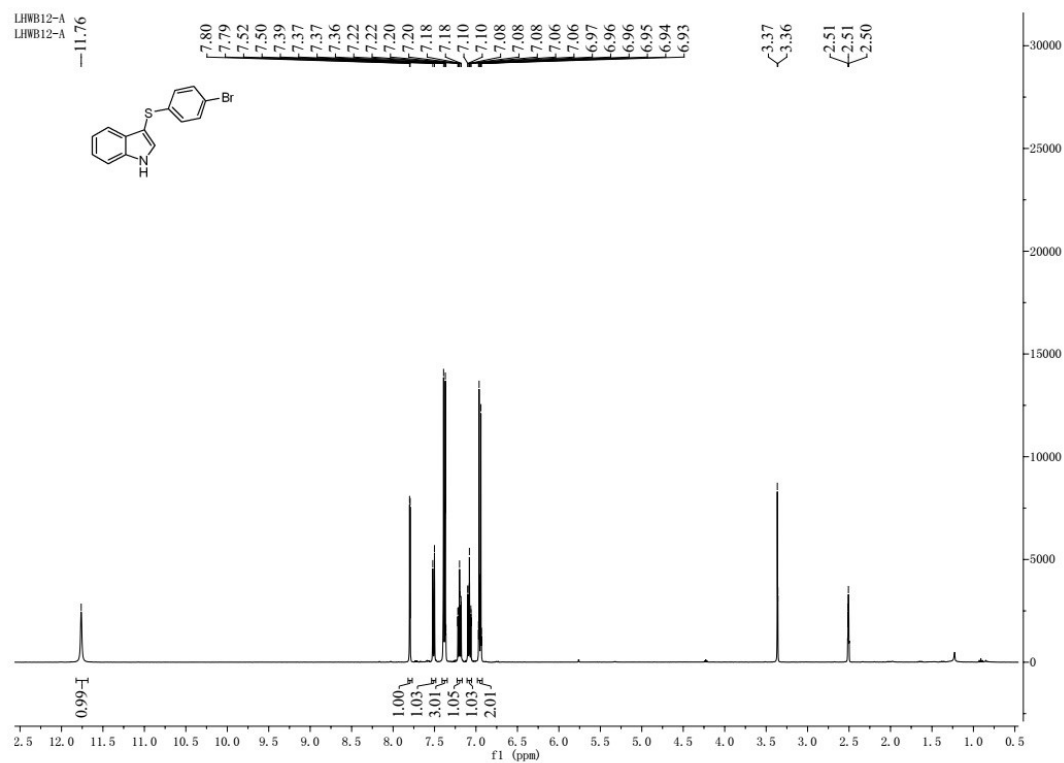
¹H and ¹³C NMR Spectra for 6qa



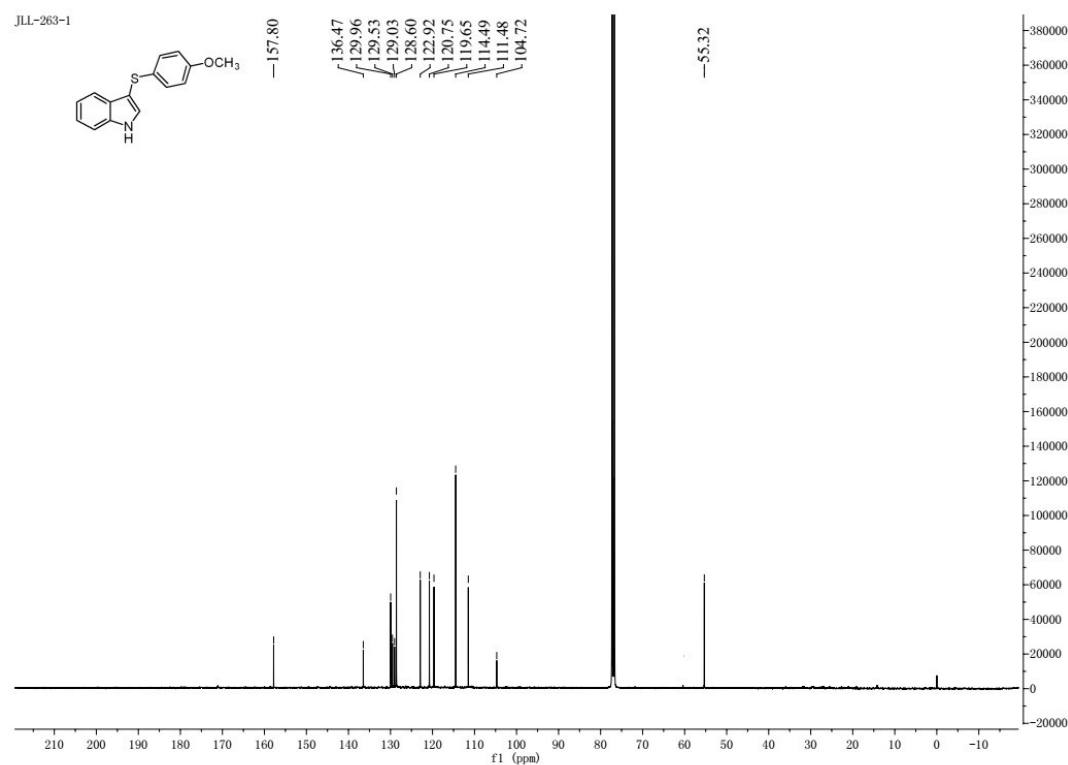
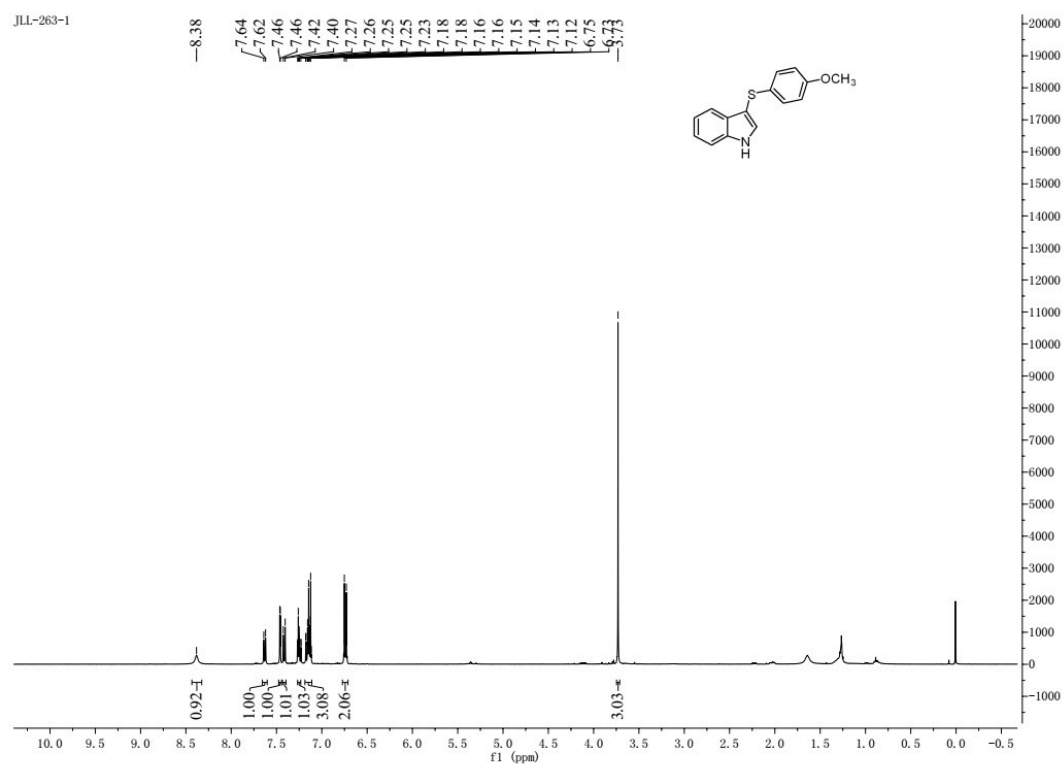
¹H and ¹³C NMR Spectra for **6ab**



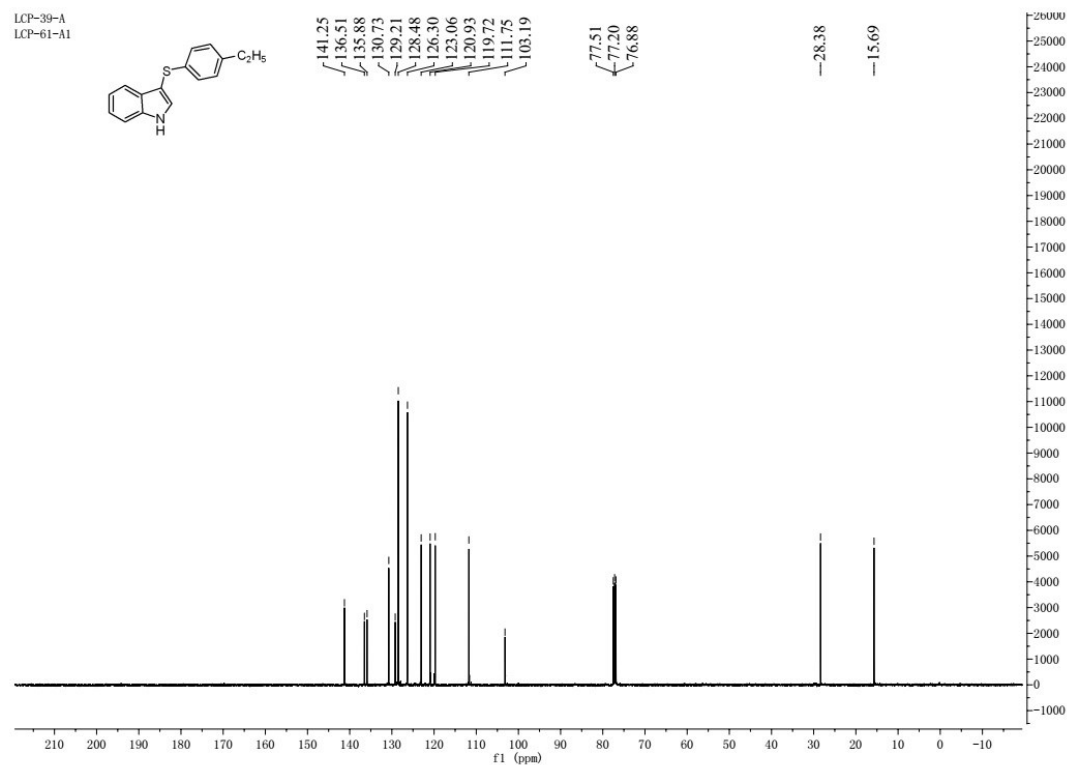
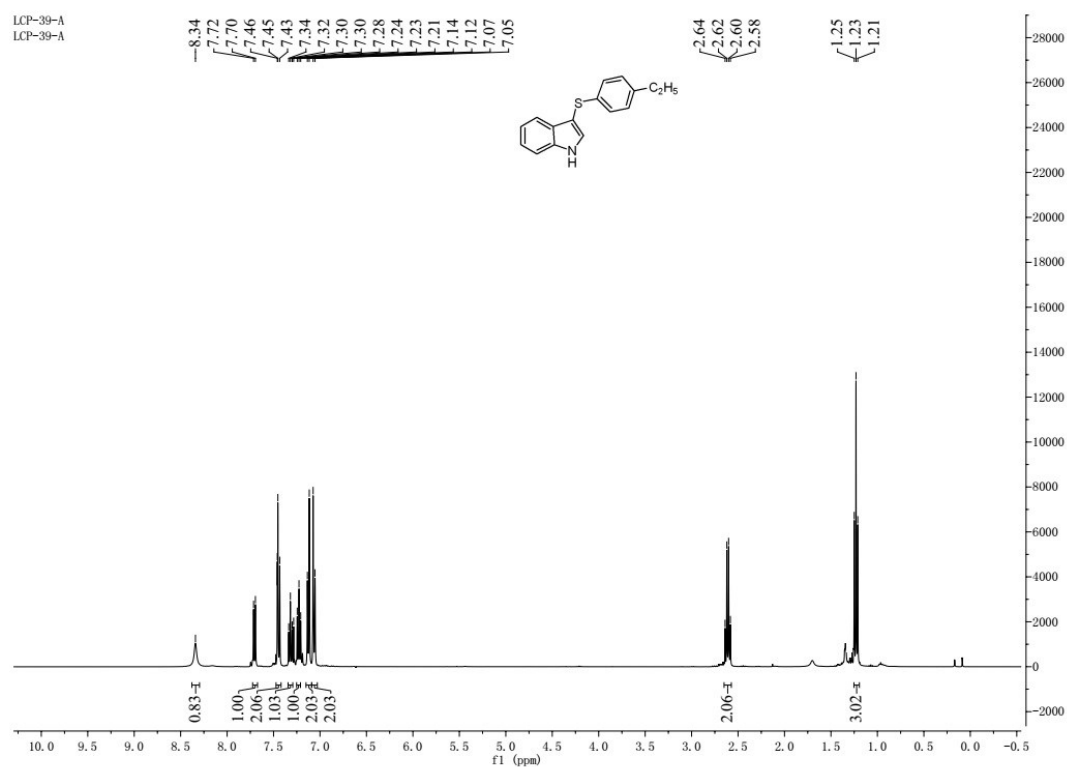
¹H and ¹³C NMR Spectra for 6ac



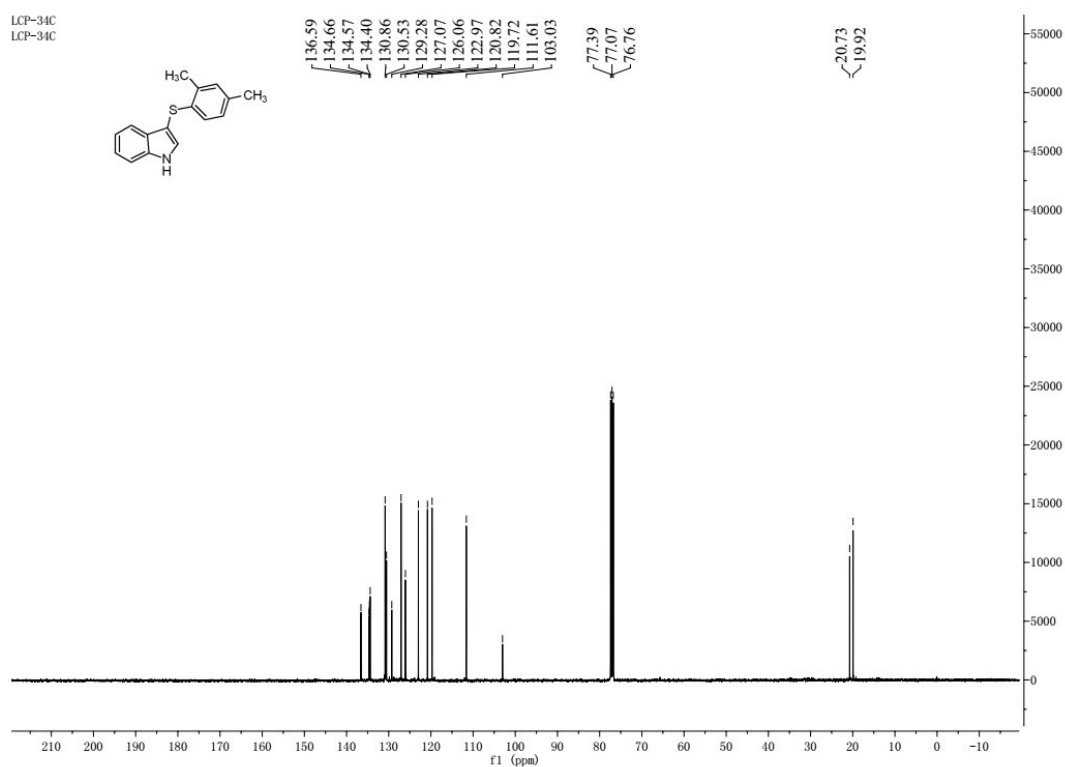
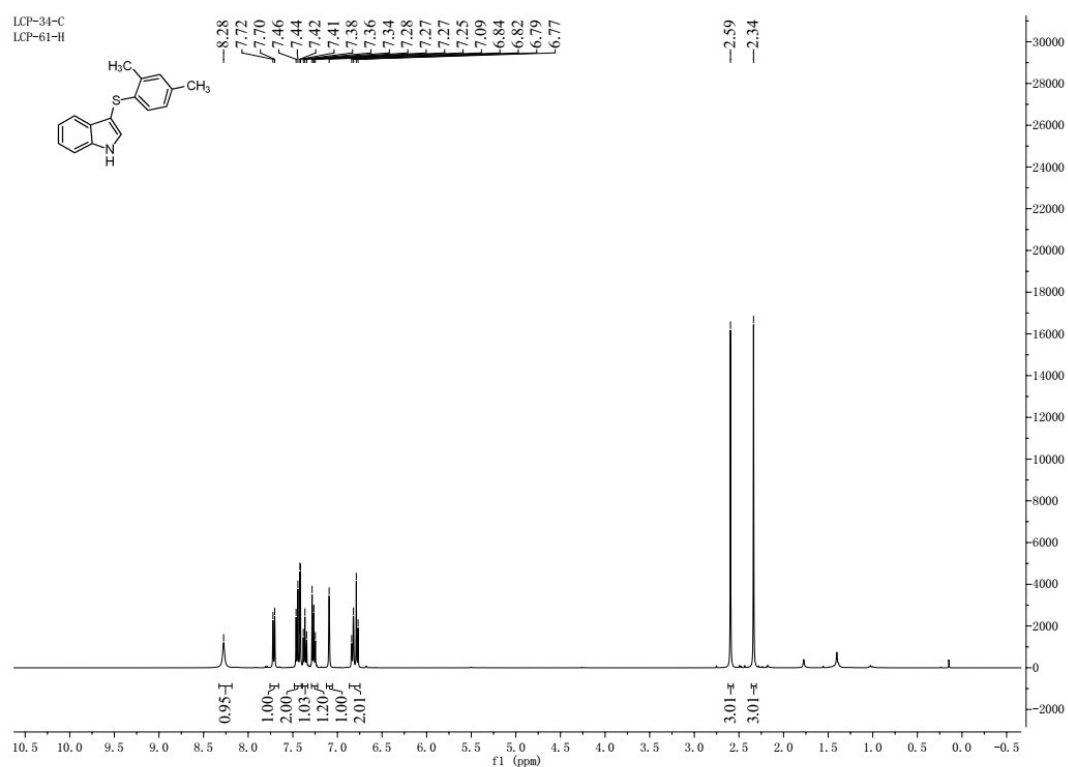
¹H and ¹³C NMR Spectra for 6ad



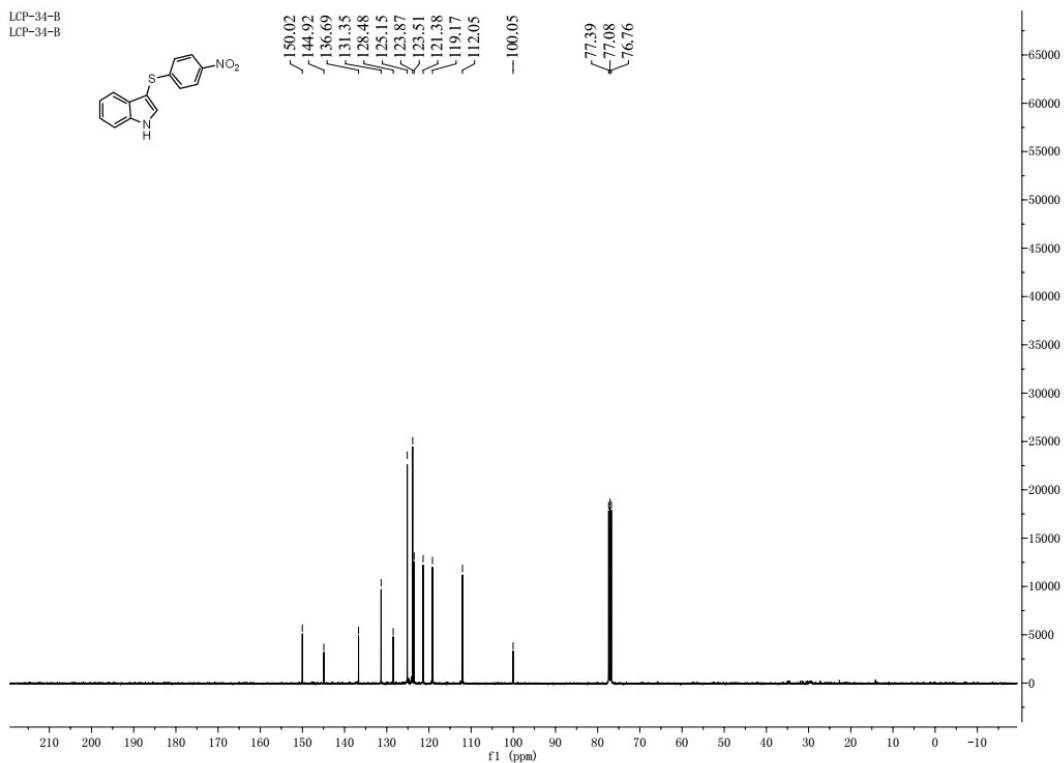
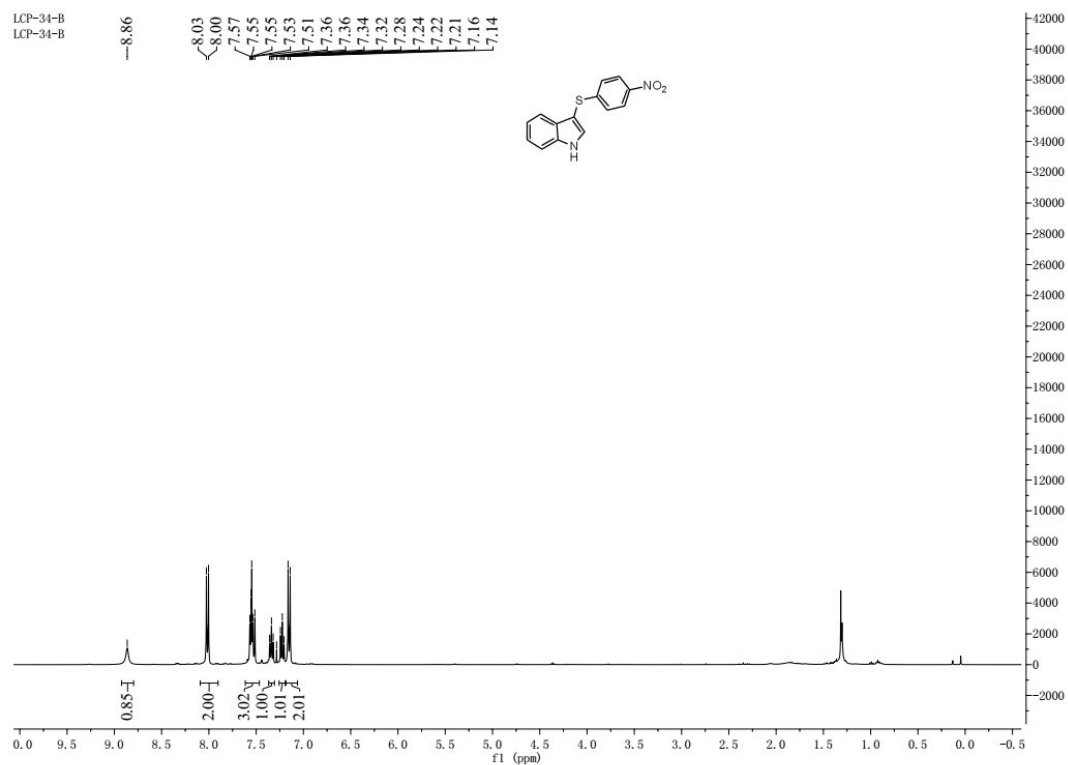
¹H and ¹³C NMR Spectra for 6ae



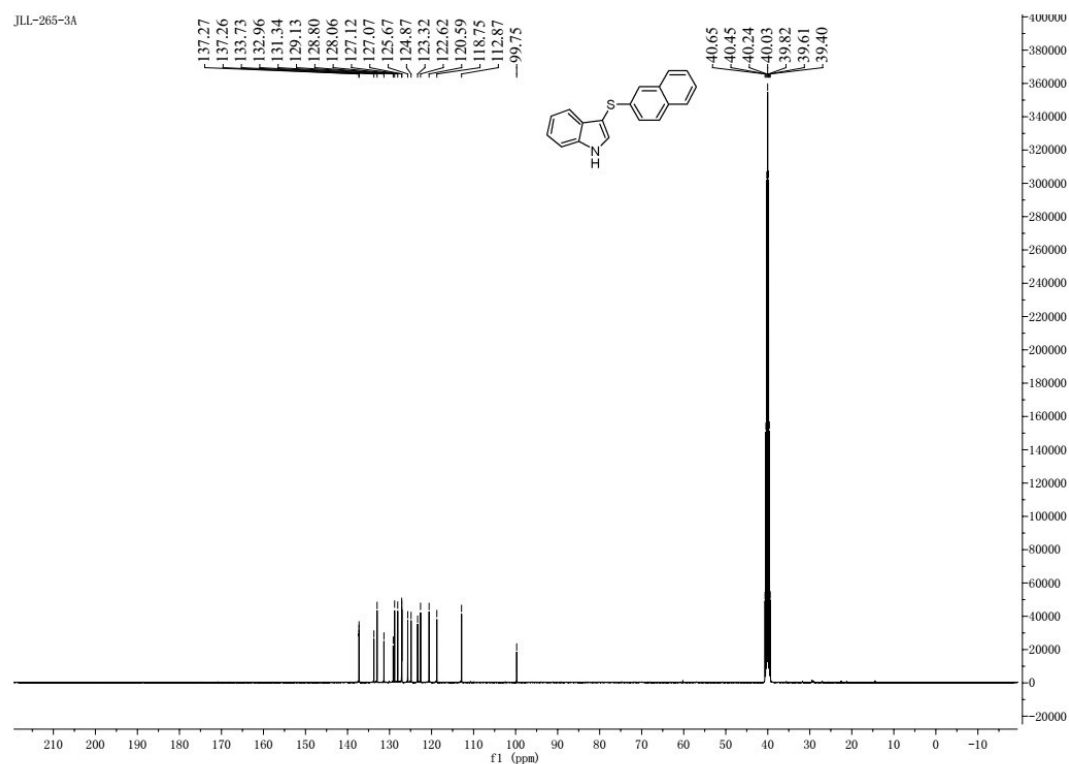
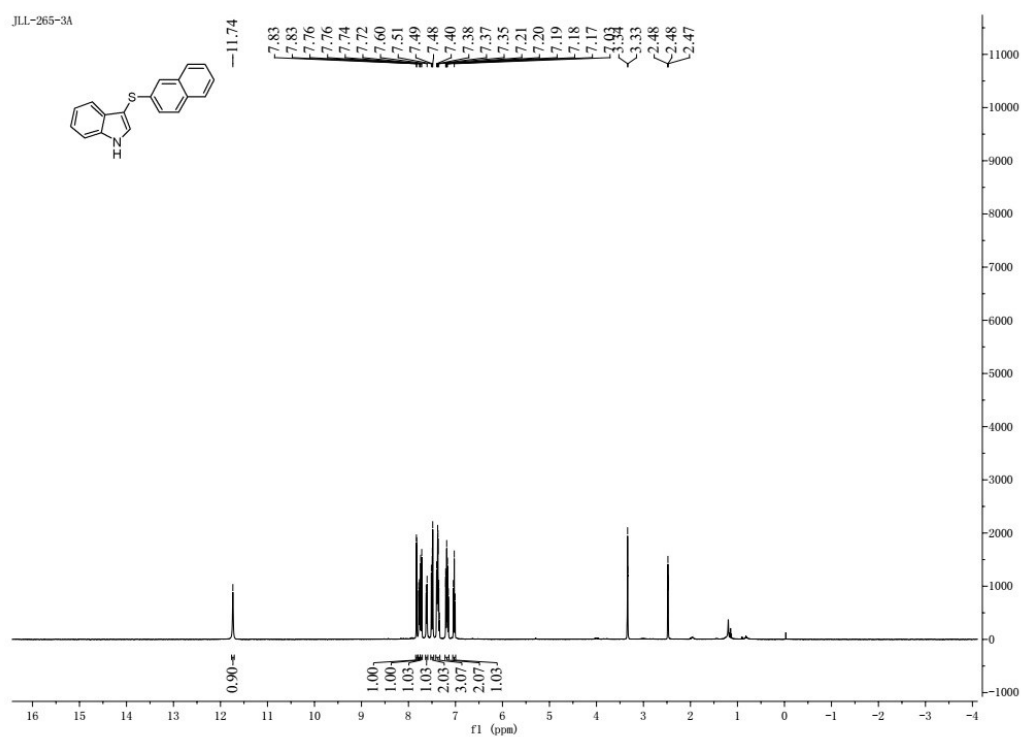
¹H and ¹³C NMR Spectra for 6af



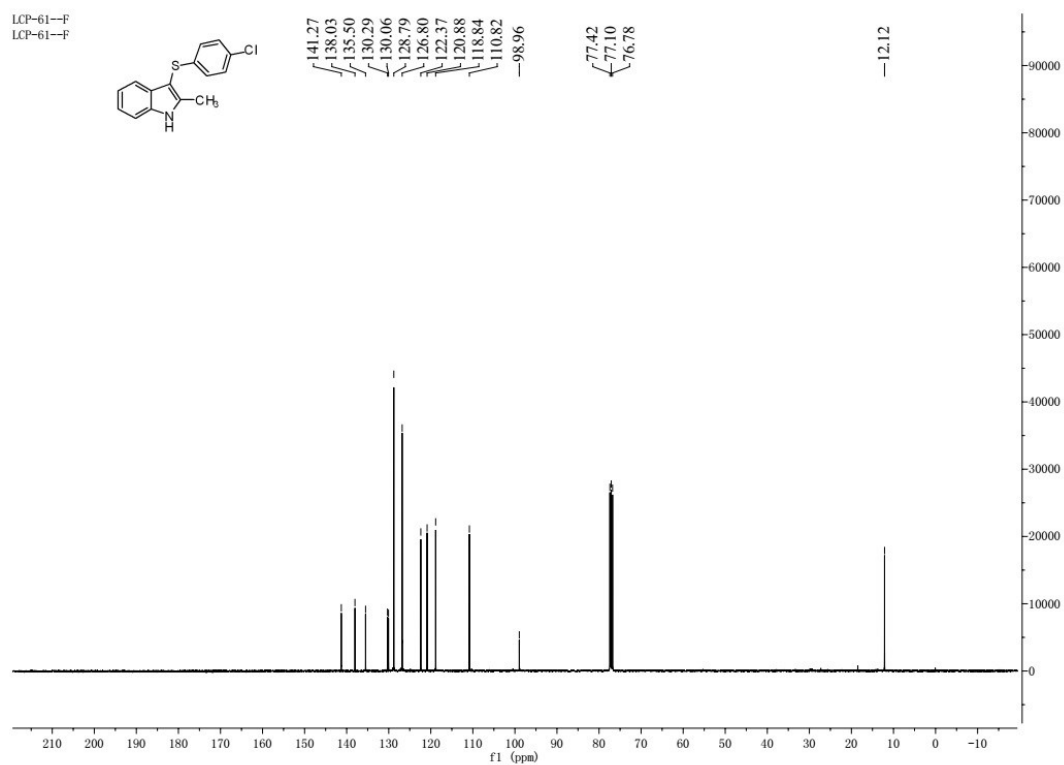
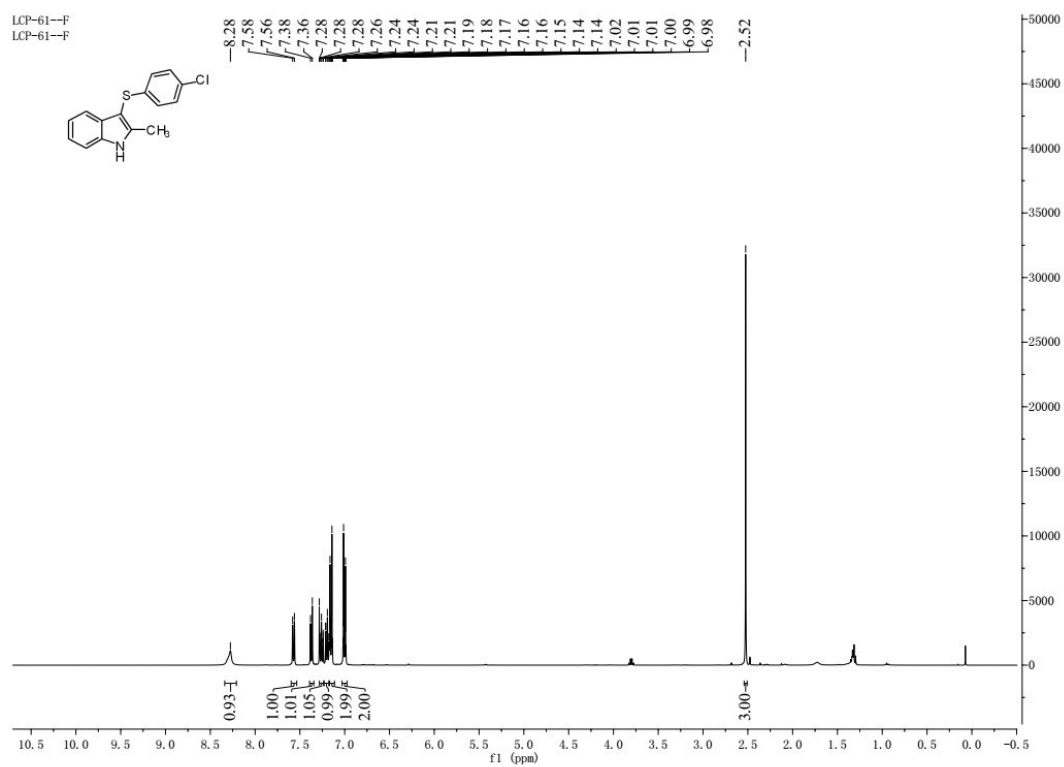
¹H and ¹³C NMR Spectra for **6ag**



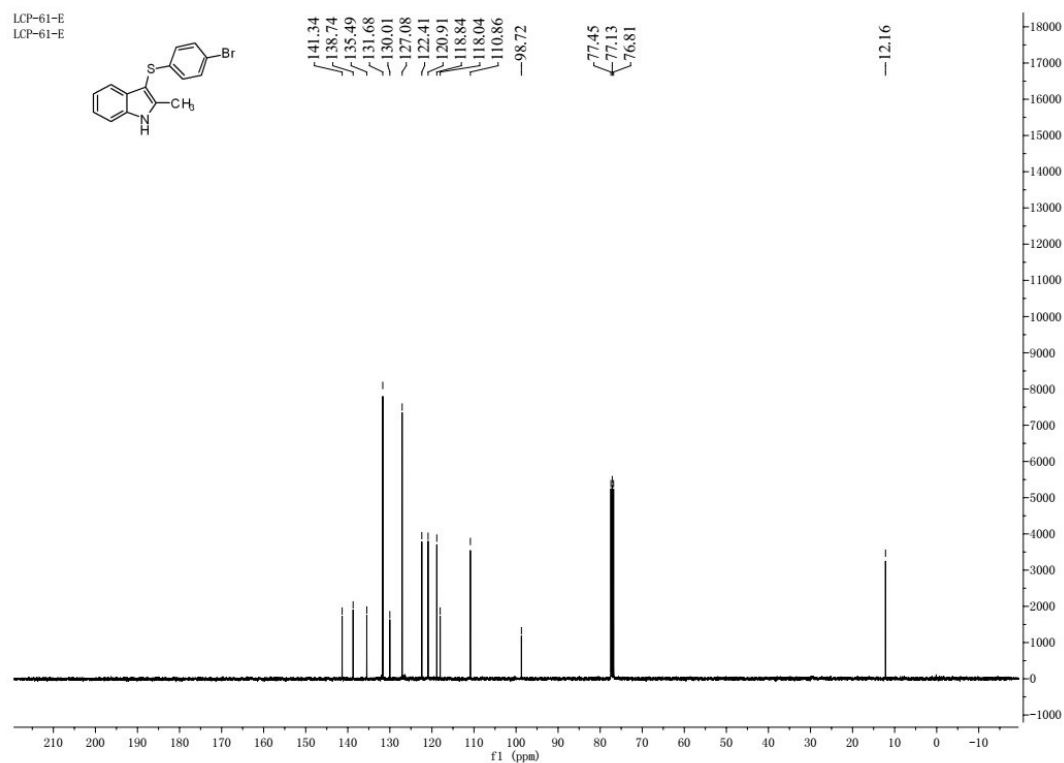
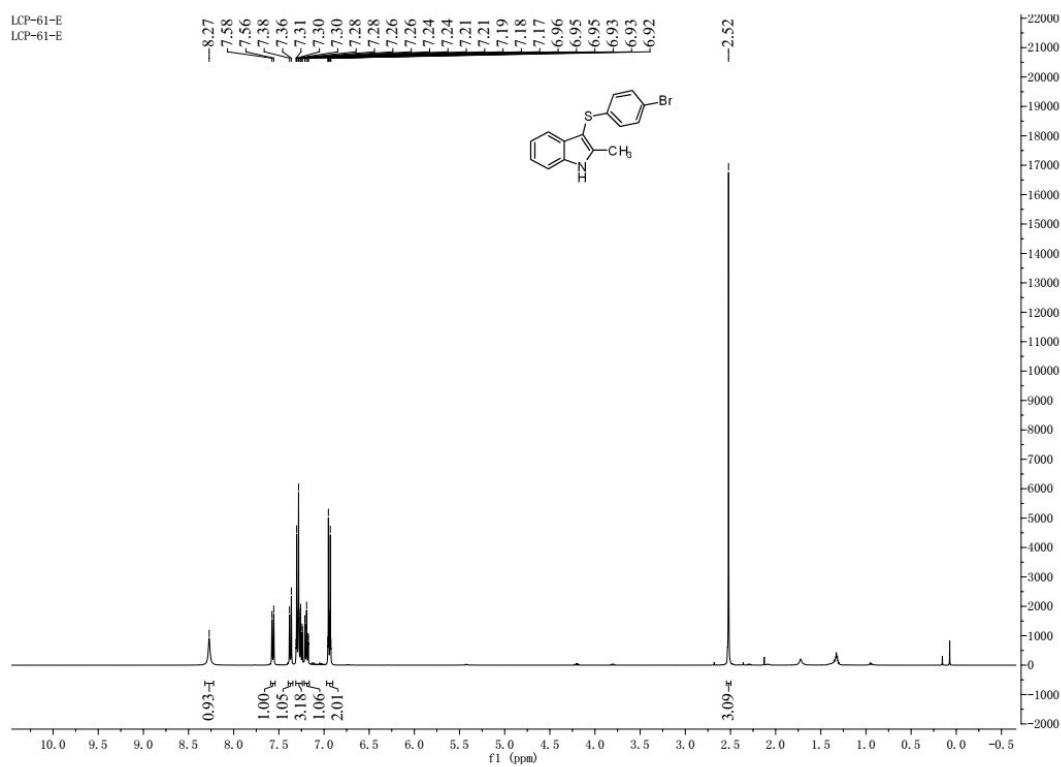
¹H and ¹³C NMR Spectra for 6ah



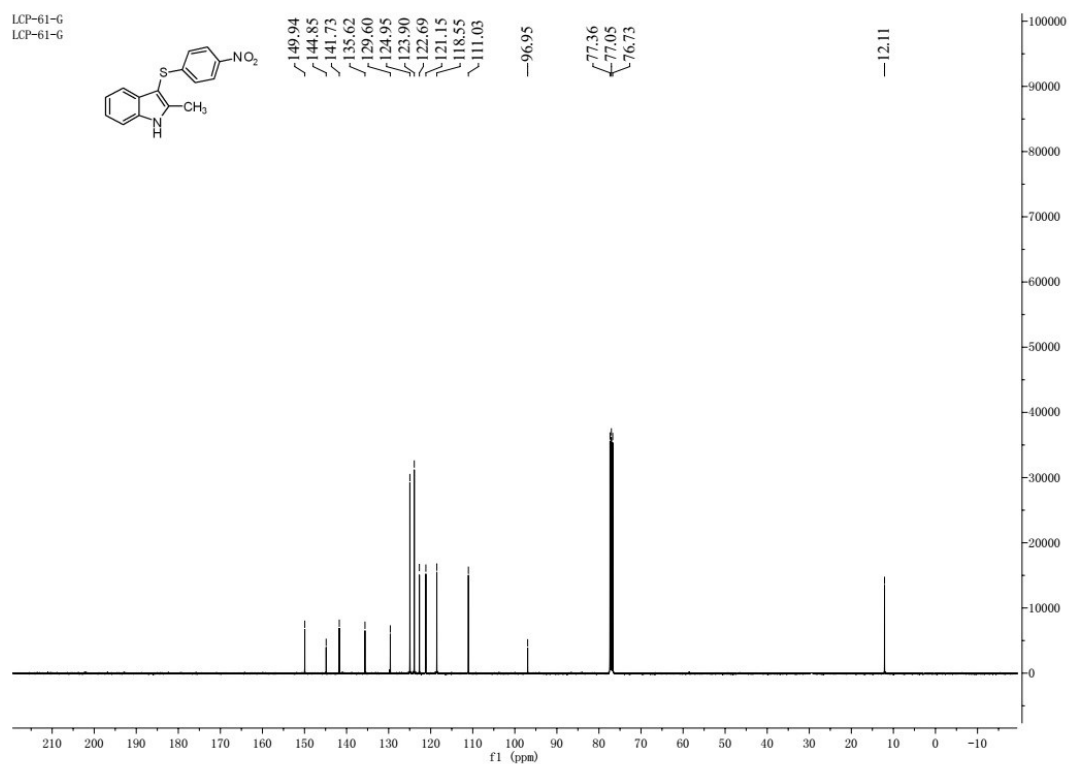
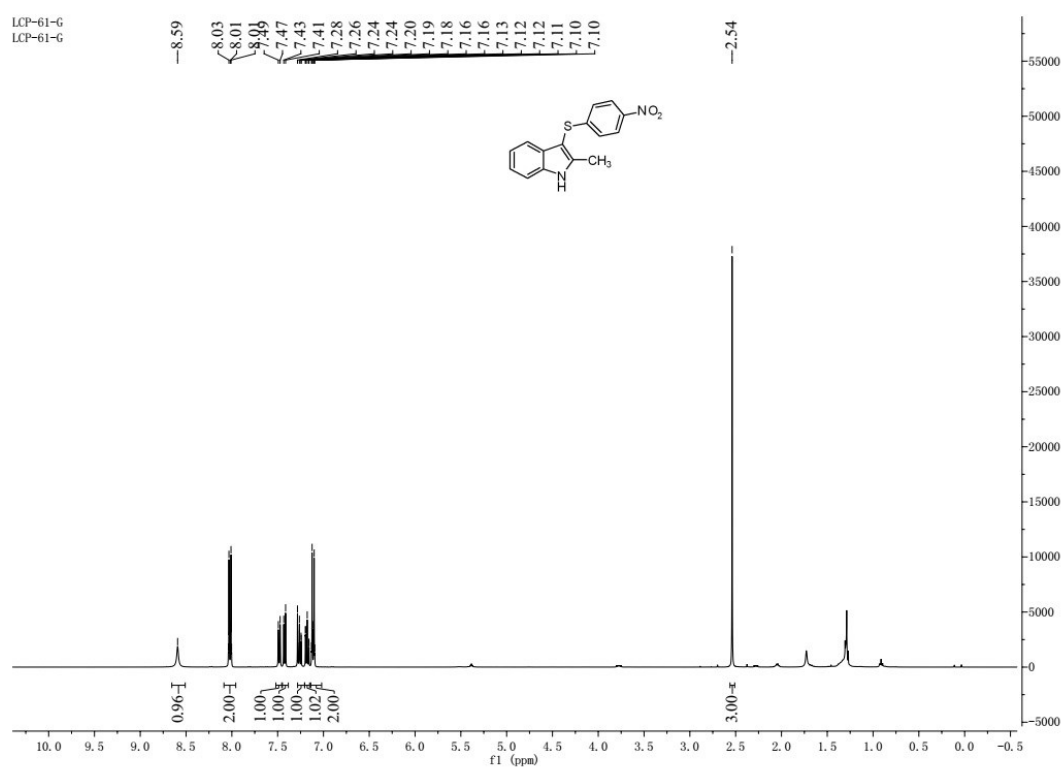
¹H and ¹³C NMR Spectra for **6ai**



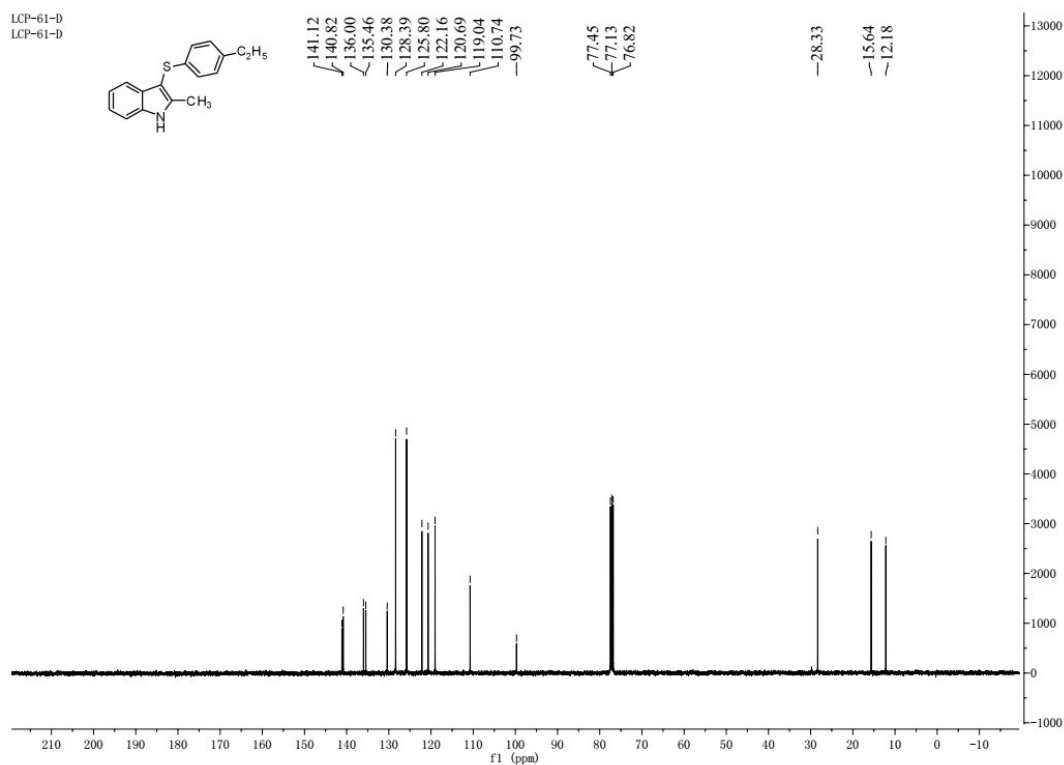
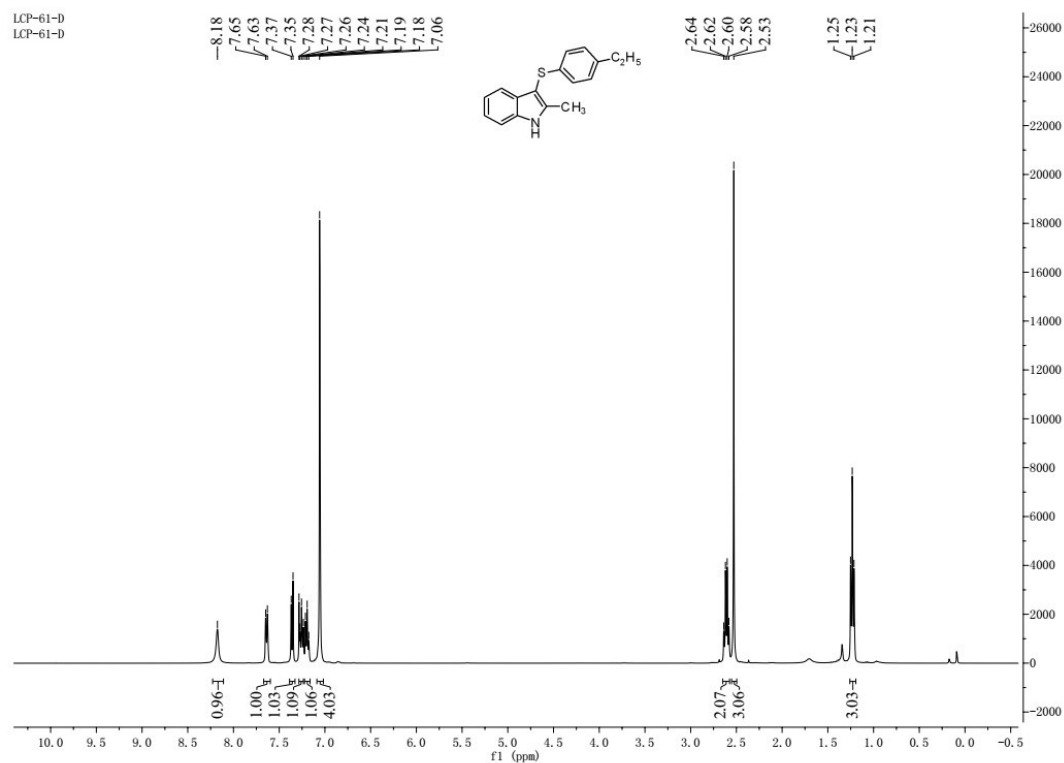
¹H and ¹³C NMR Spectra for 6aj



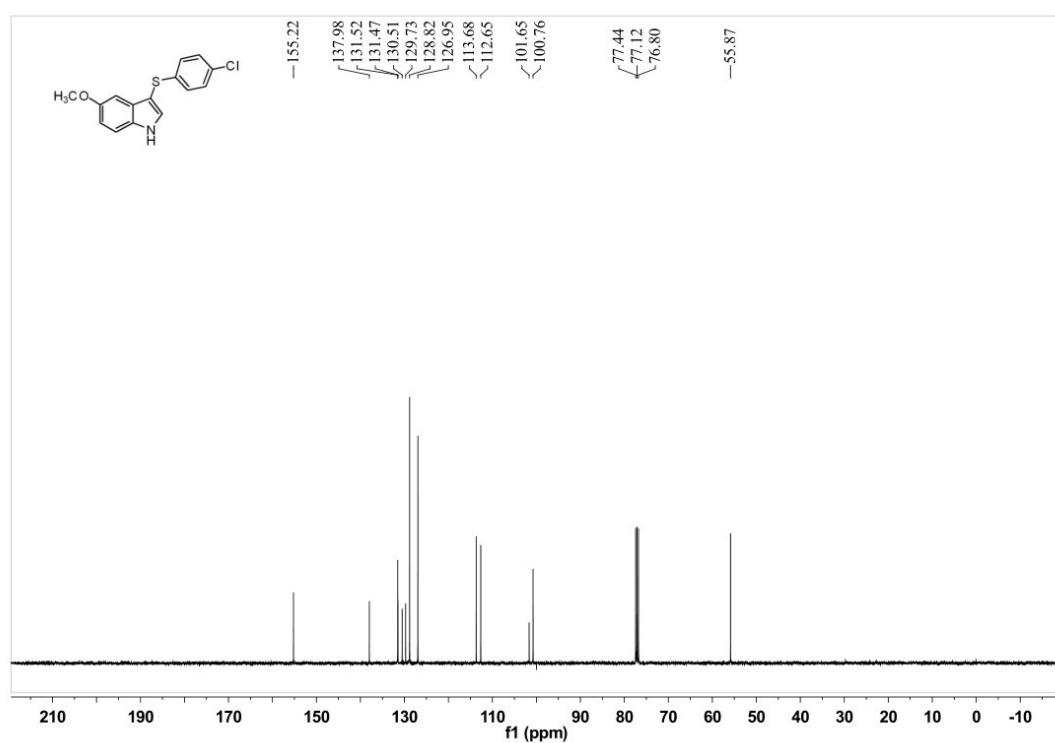
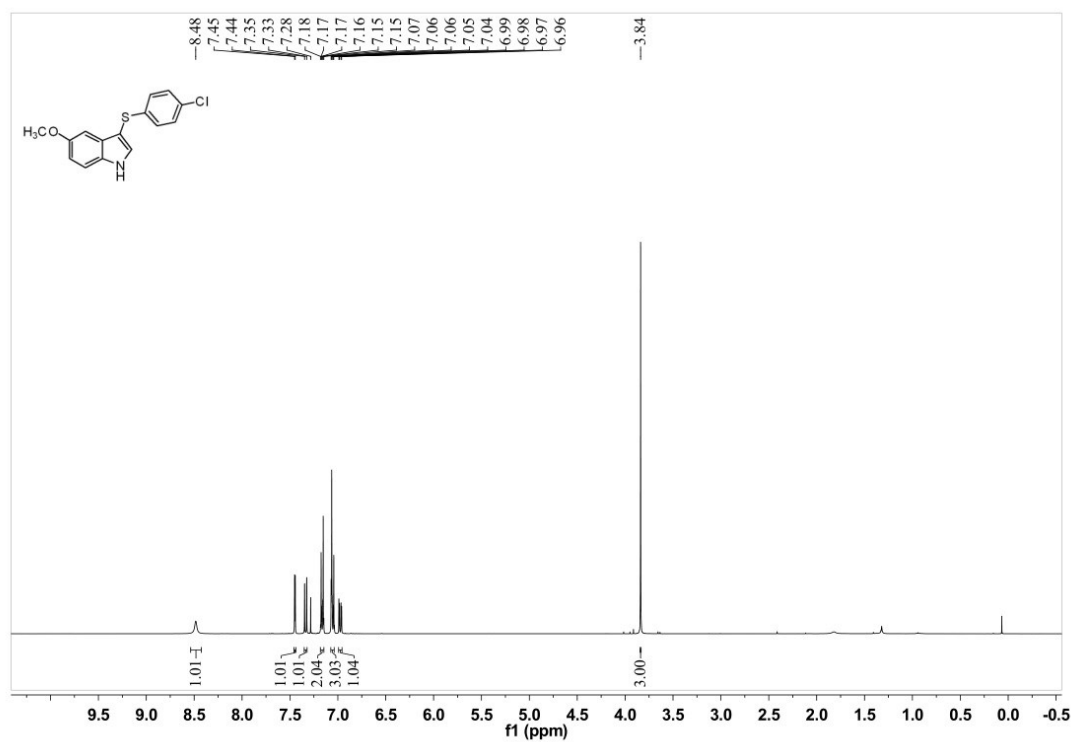
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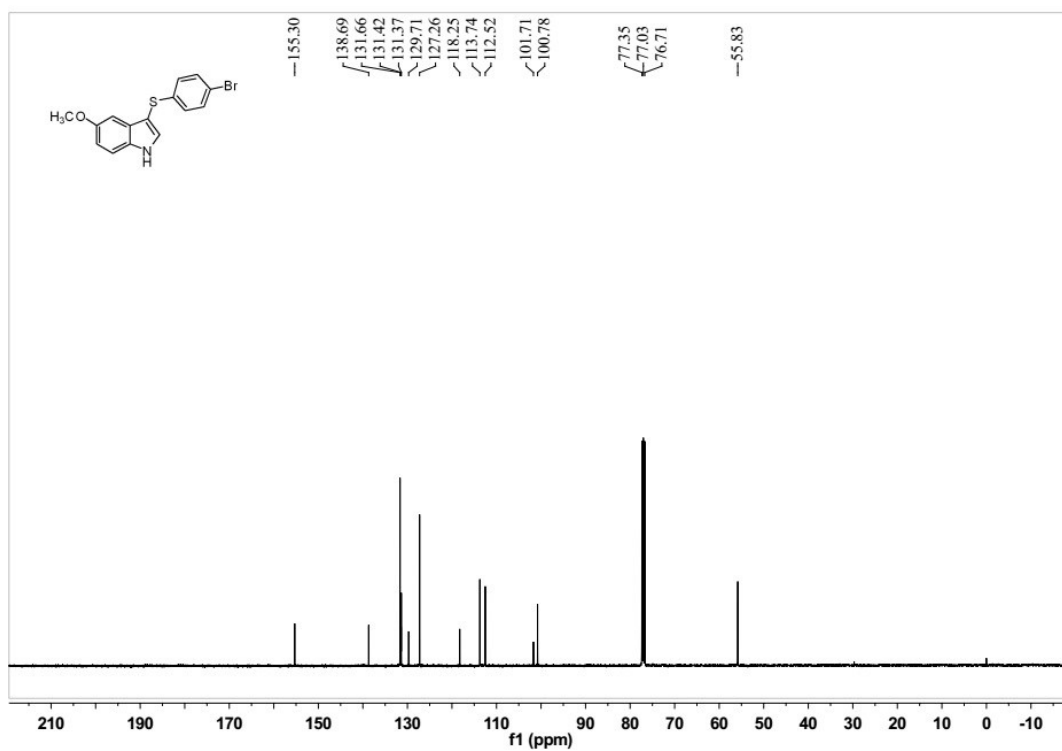
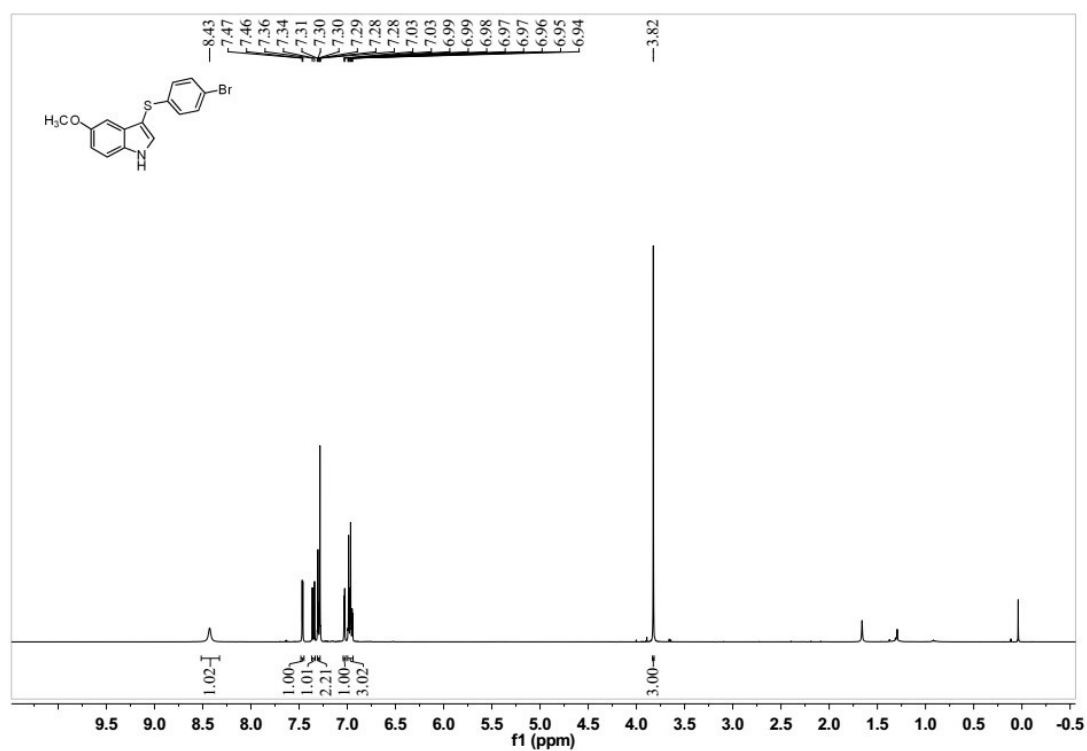
¹H and ¹³C NMR Spectra for **6al**



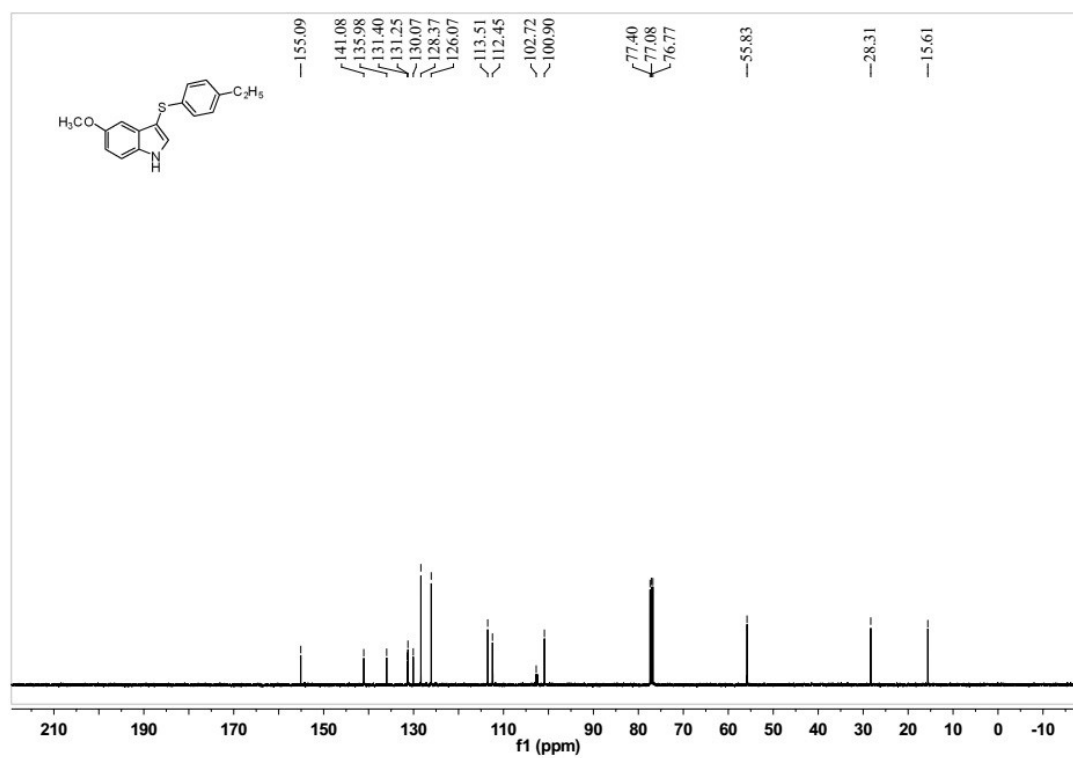
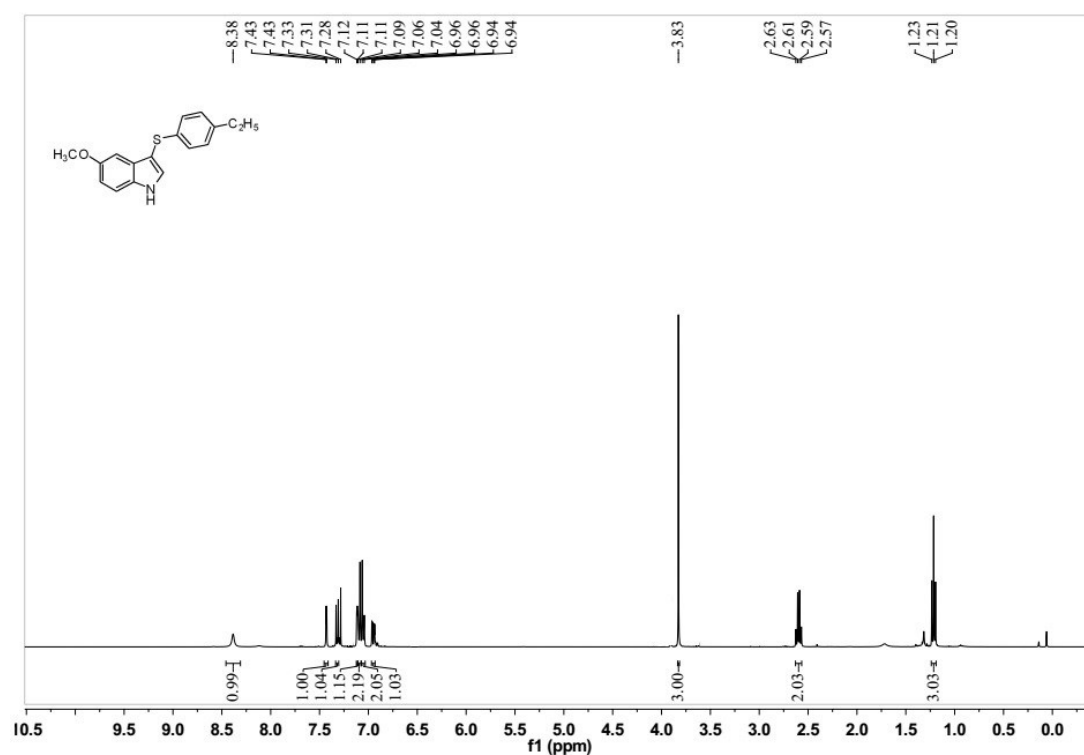
^1H and ^{13}C NMR Spectra for **6am**



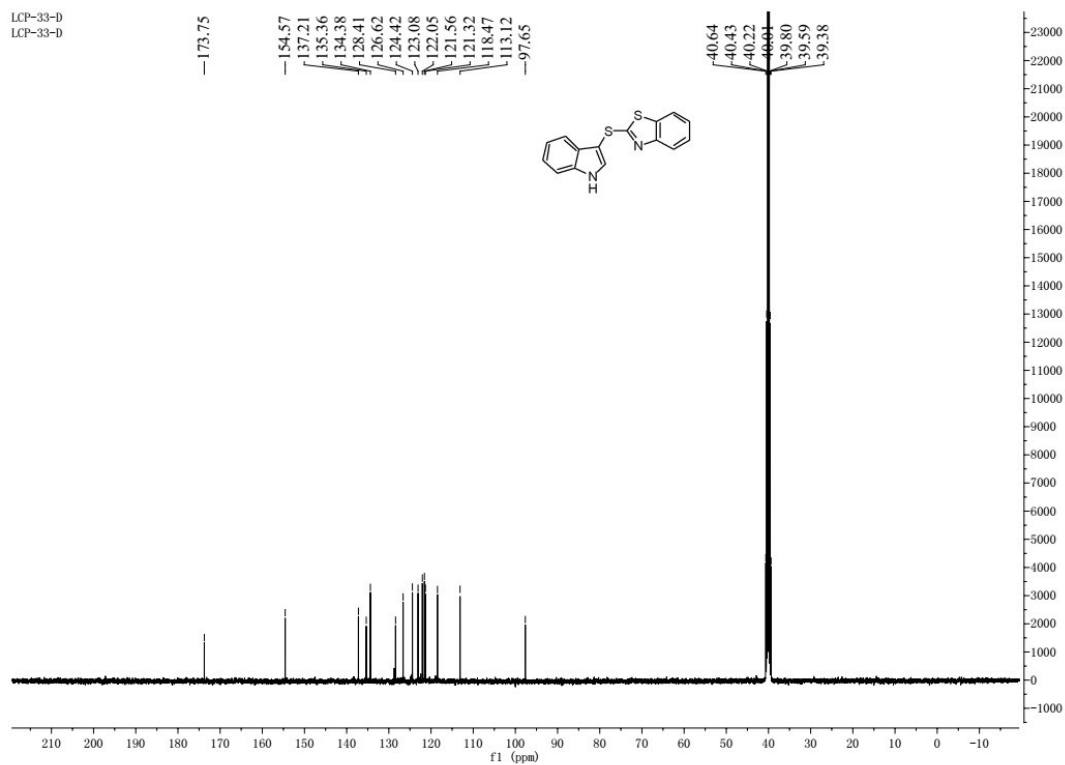
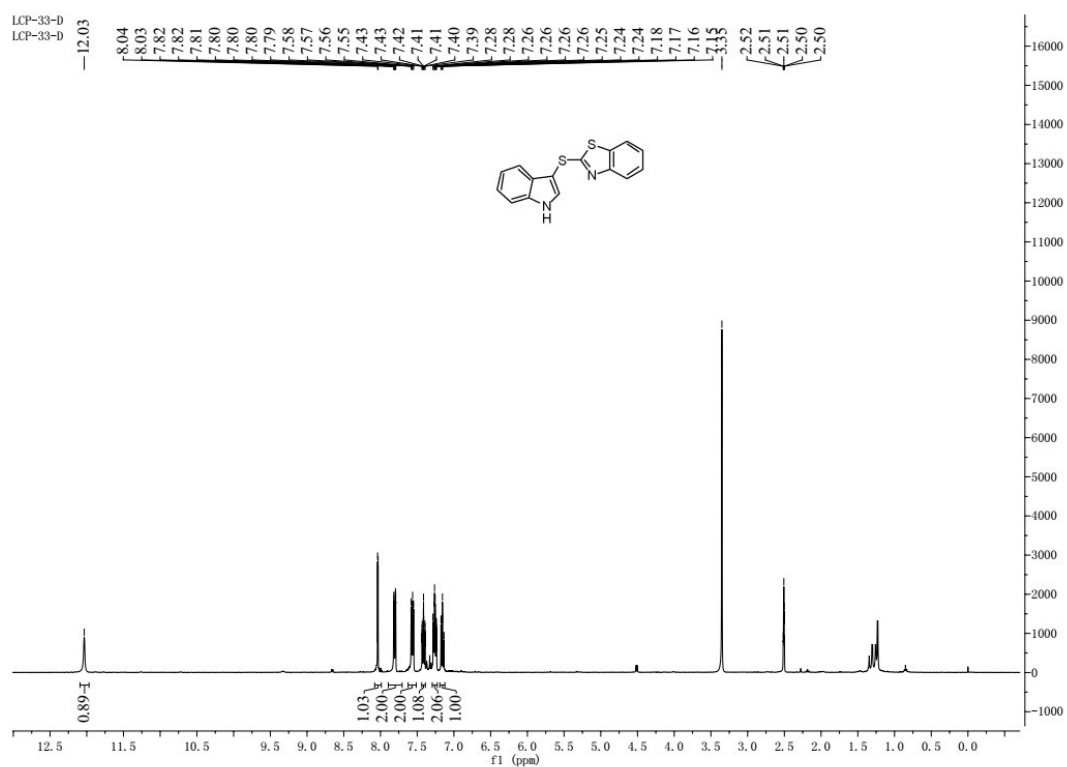
^1H and ^{13}C NMR Spectra for **6an**



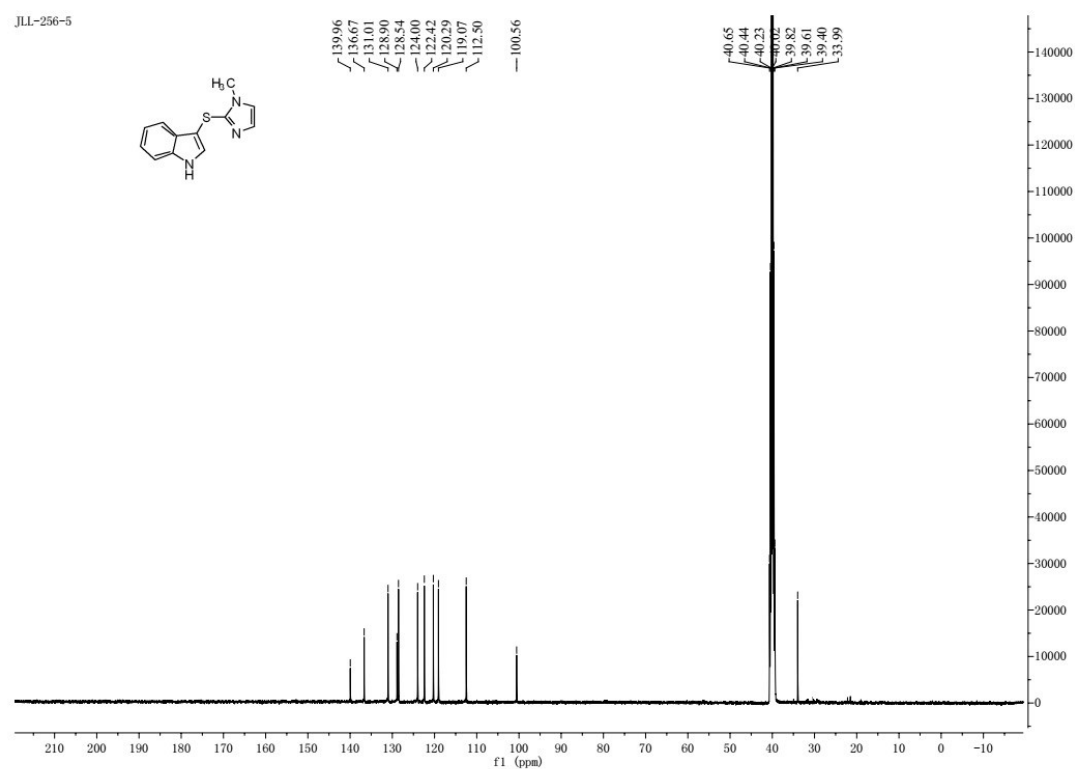
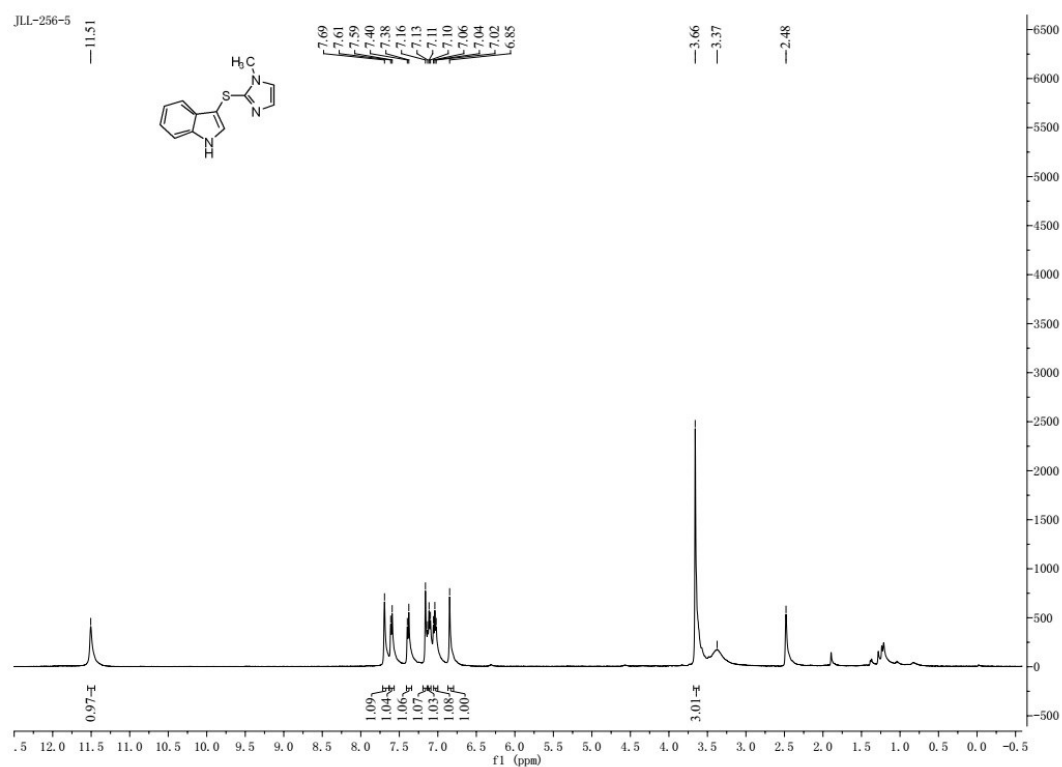
^1H and ^{13}C NMR Spectra for **6ao**



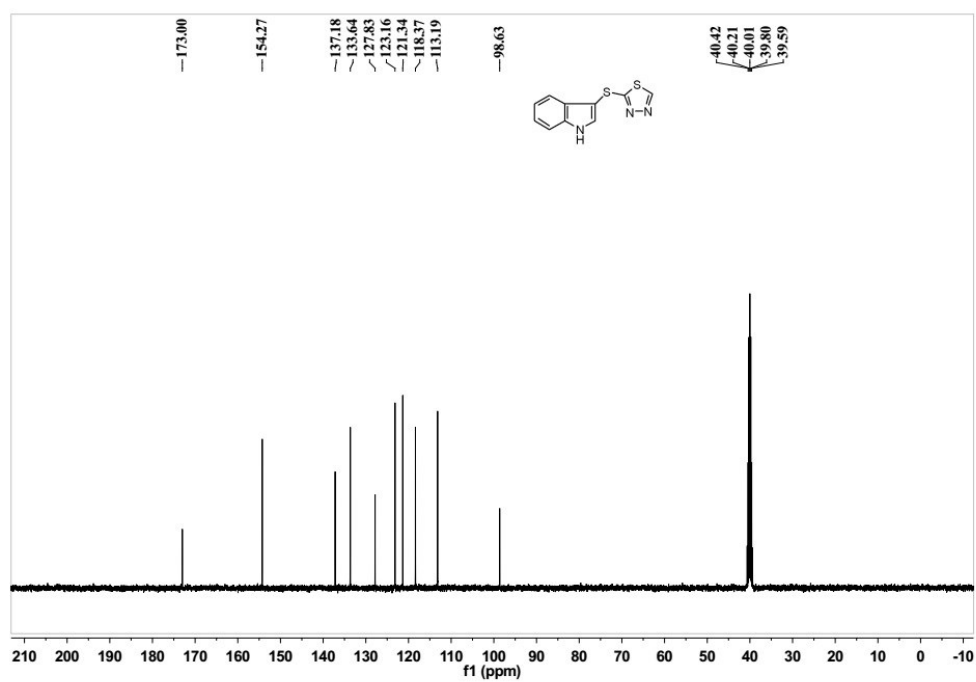
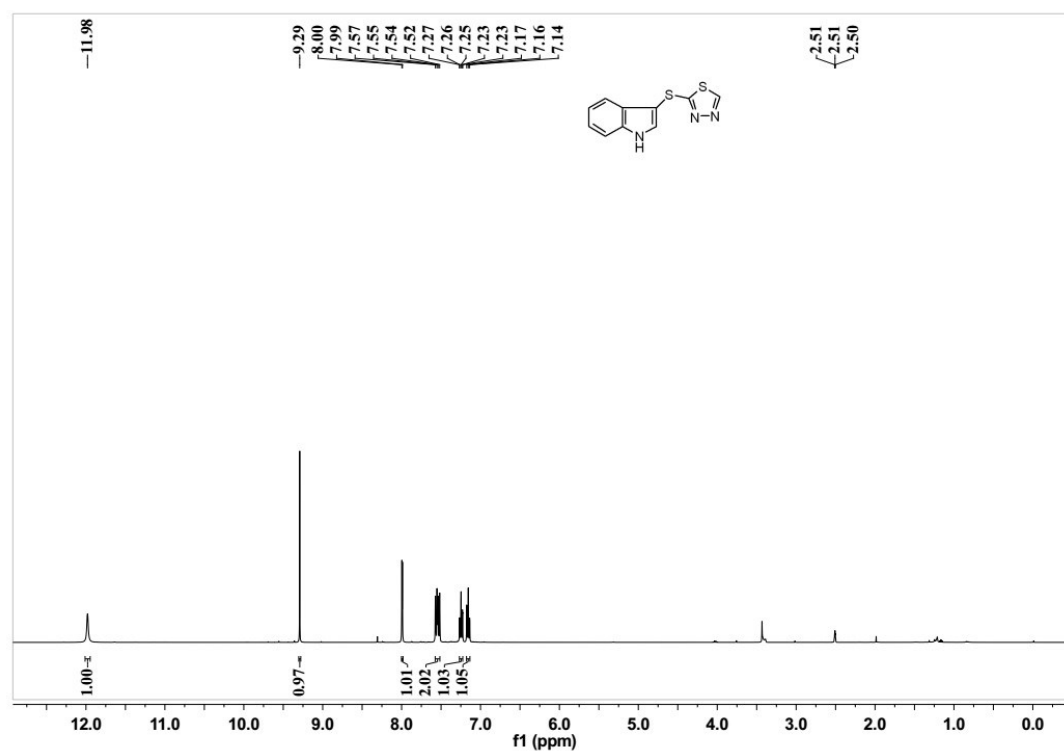
¹H and ¹³C NMR Spectra for 6ap



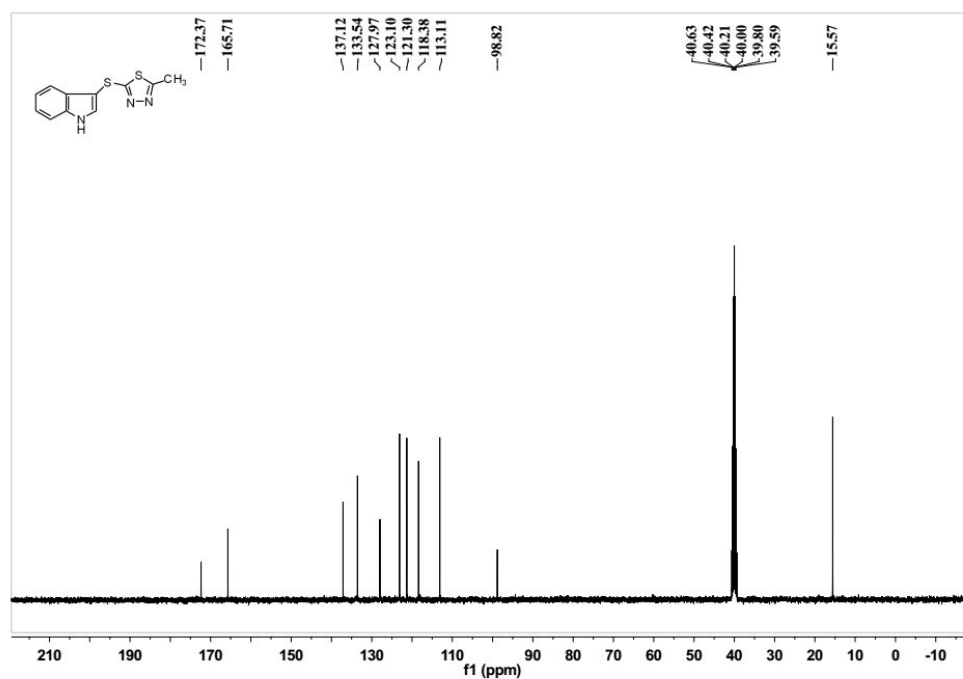
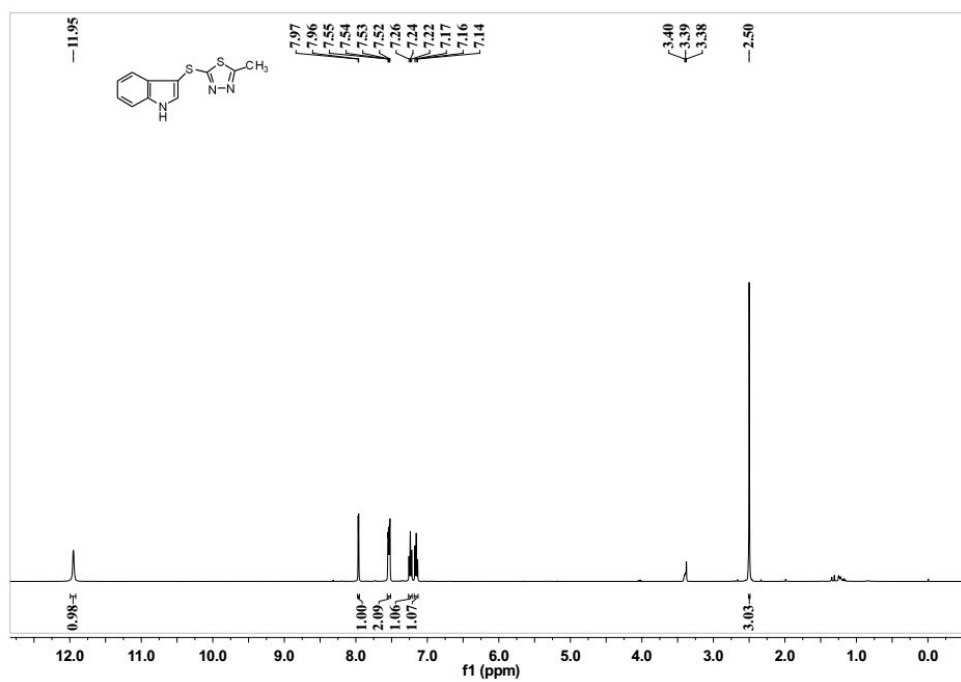
¹H and ¹³C NMR Spectra for **6aq**



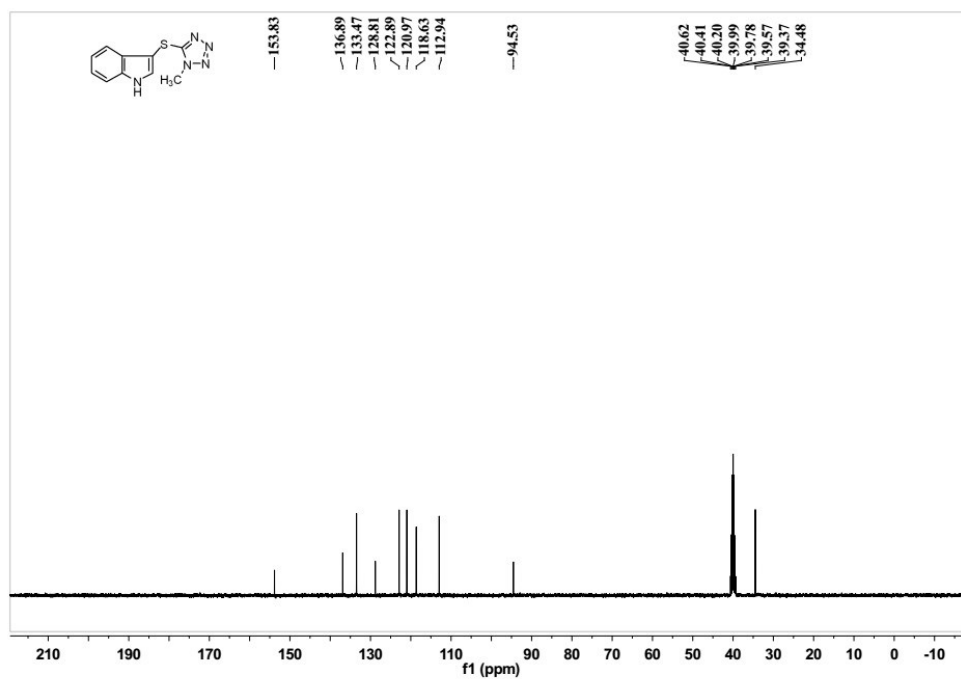
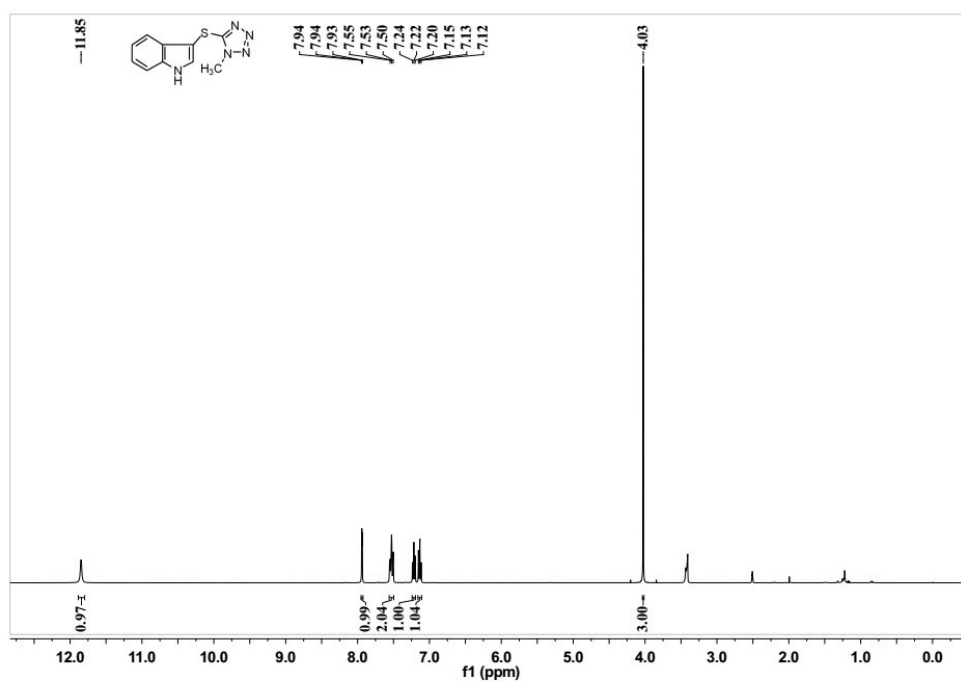
¹H and ¹³C NMR Spectra for **6ar**



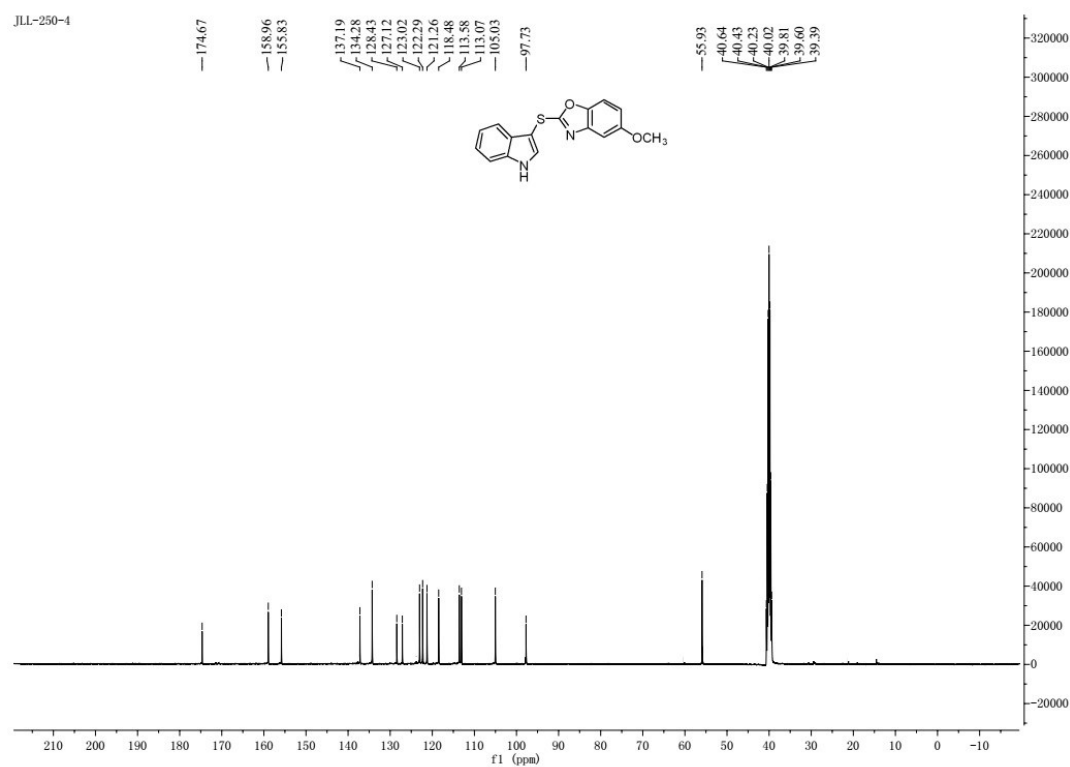
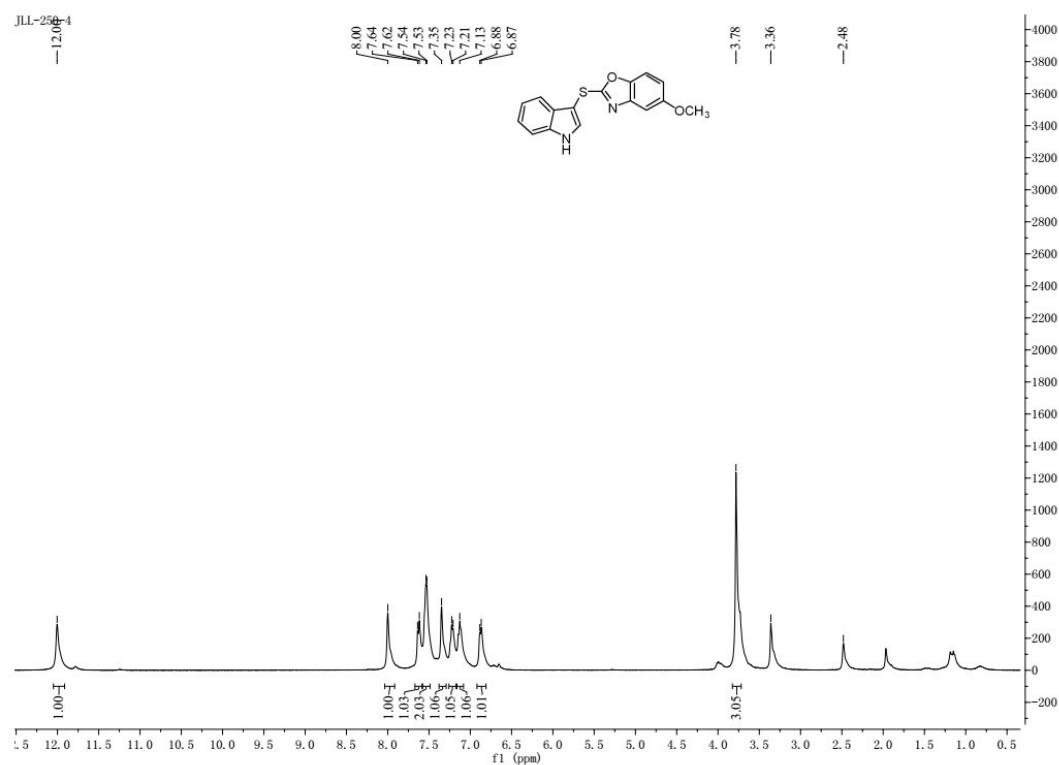
^1H and ^{13}C NMR Spectra for **6as**



^1H and ^{13}C NMR Spectra for **6at**

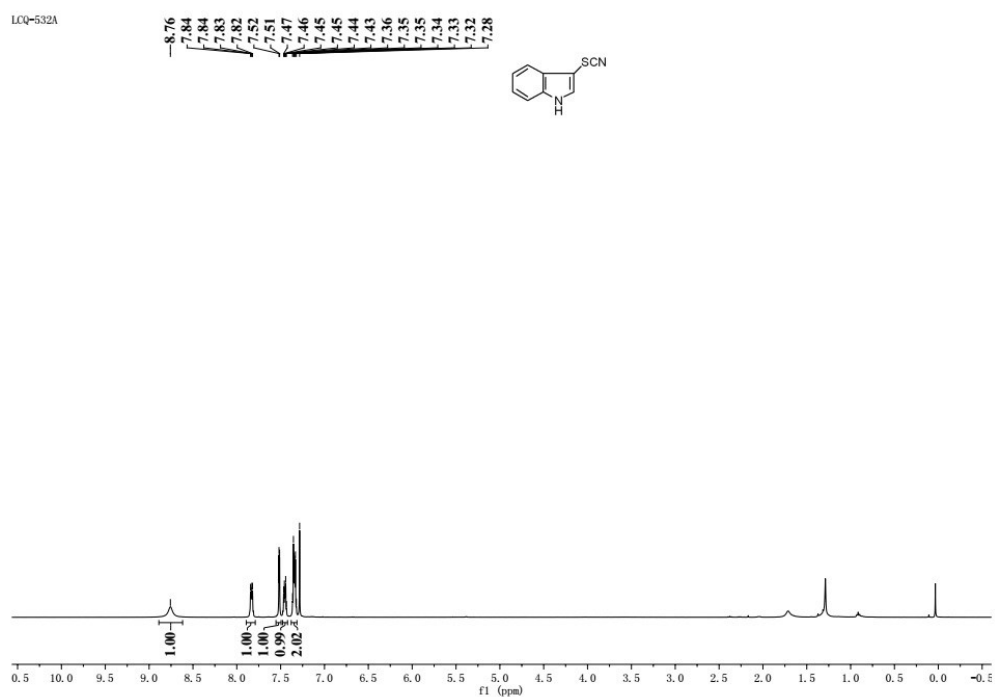


¹H and ¹³C NMR Spectra for **6au**

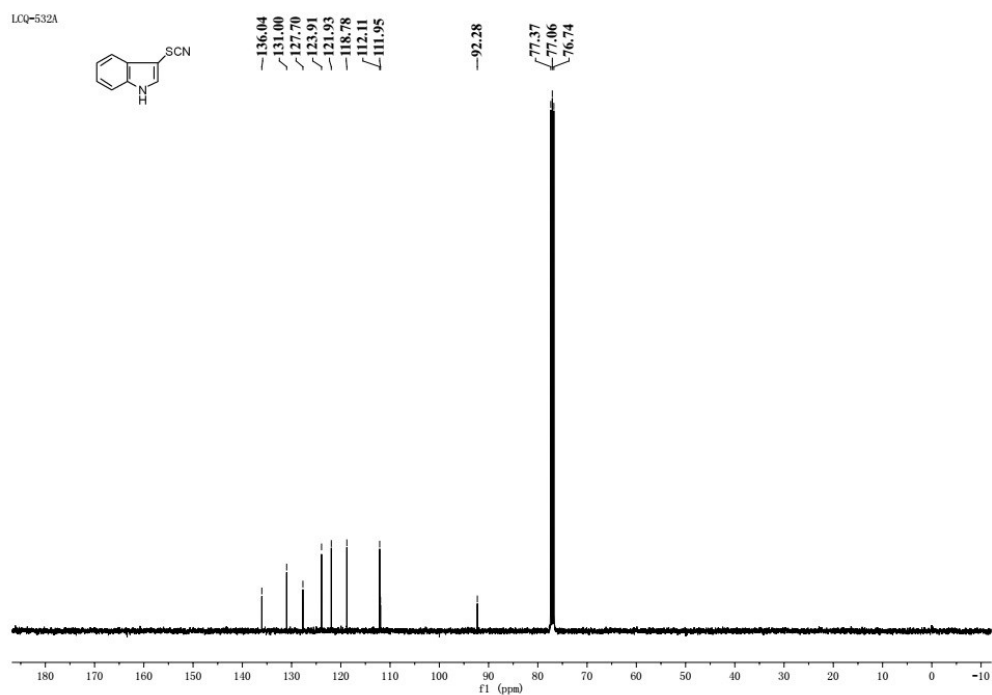


¹H and ¹³C NMR Spectra for 7a

LQ-532A

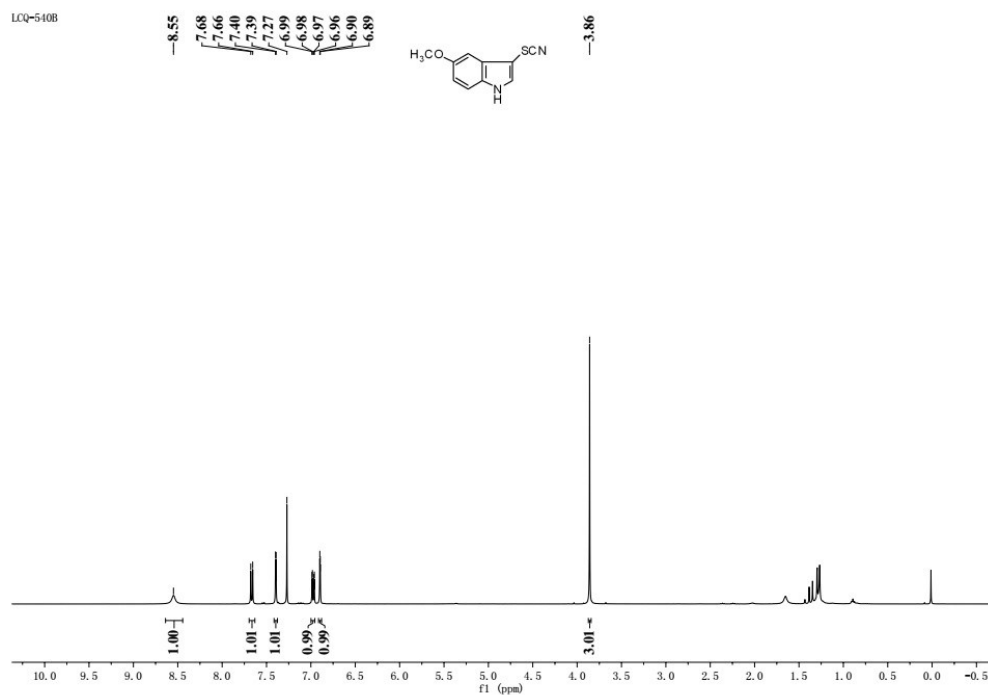


LQ-532A

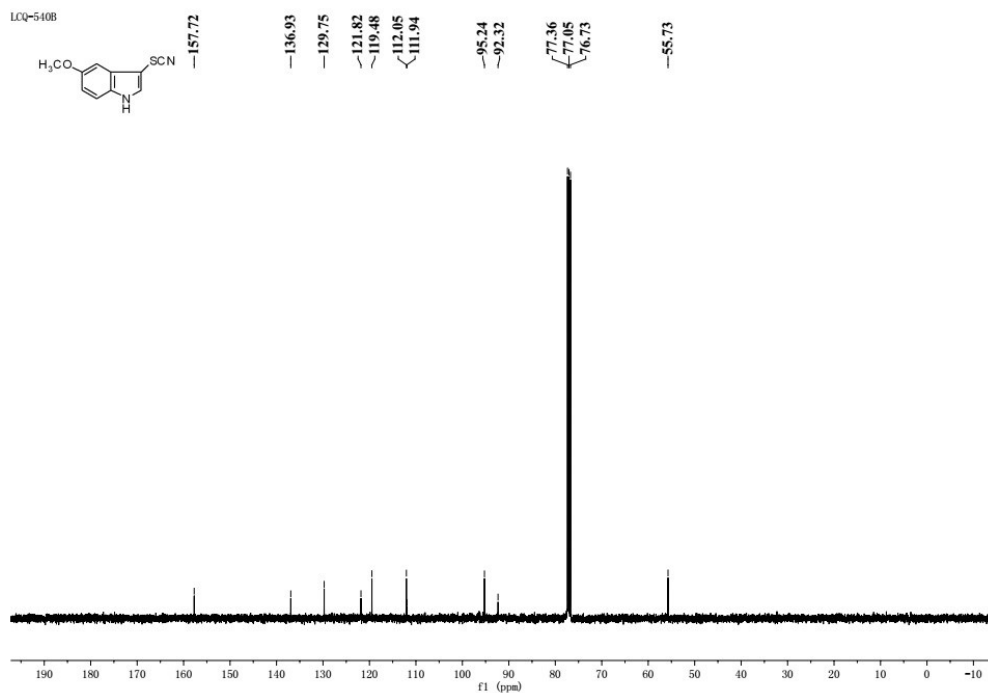


¹H and ¹³C NMR Spectra for **7b**

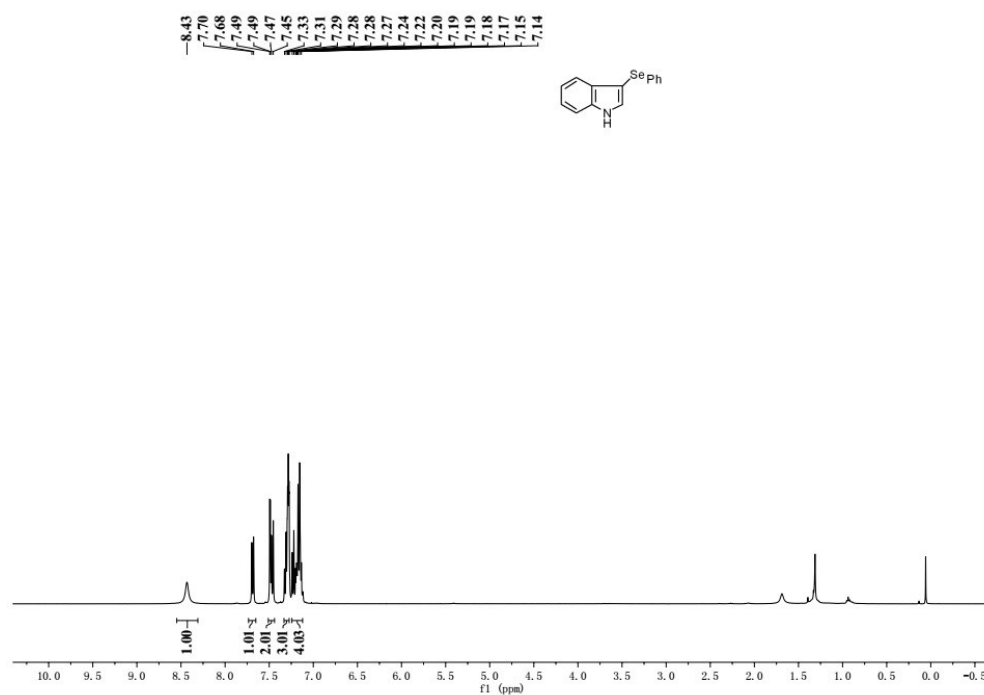
LCQ-540B



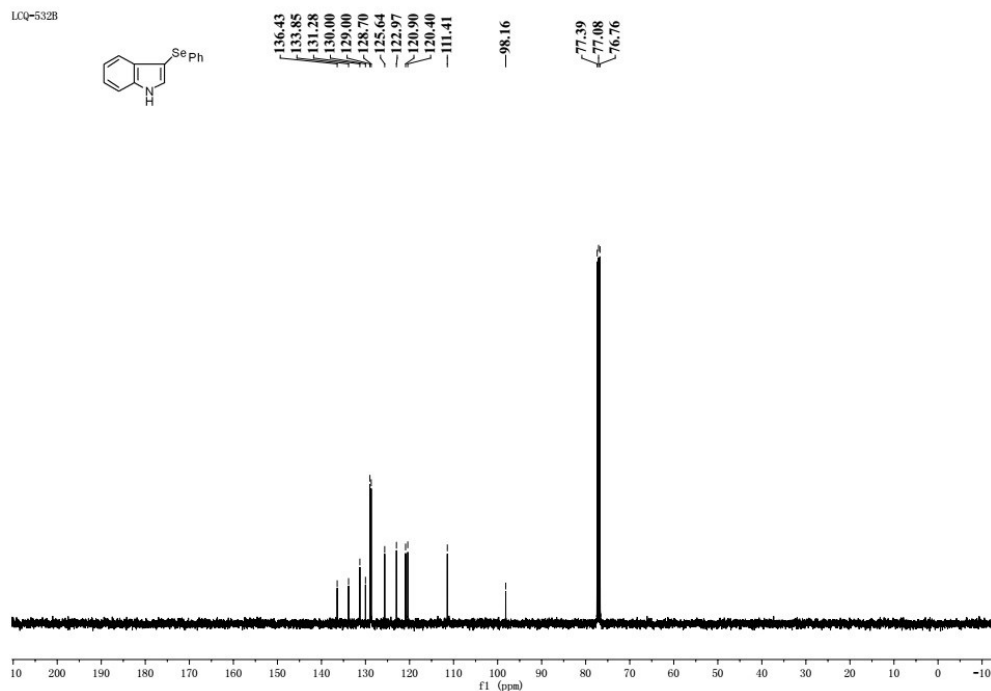
LCQ-540B



¹H and ¹³C NMR Spectra for **9a**

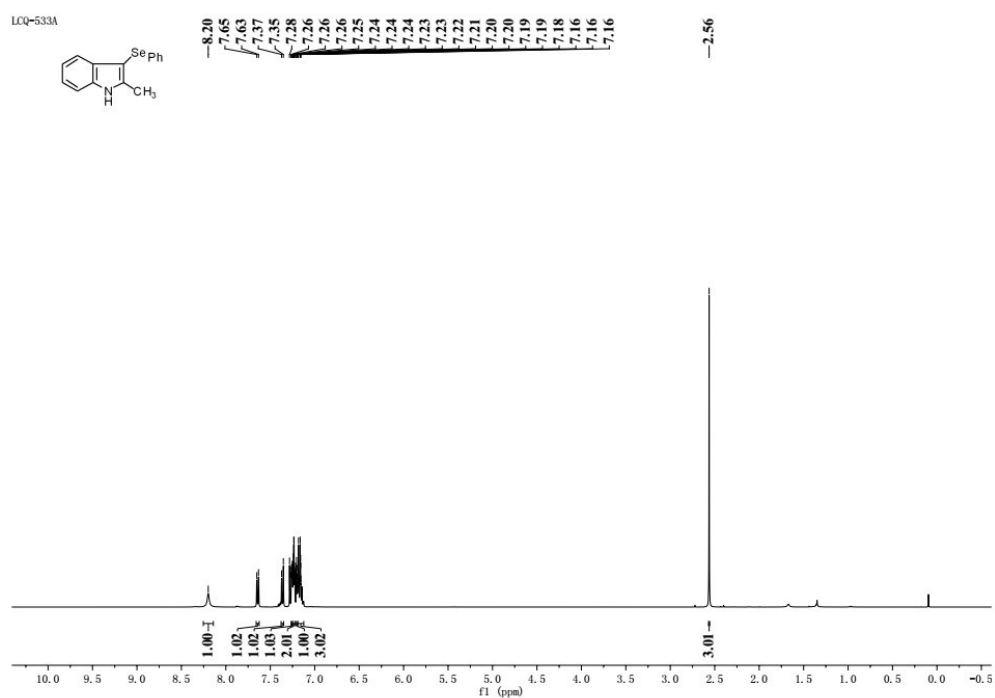
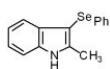


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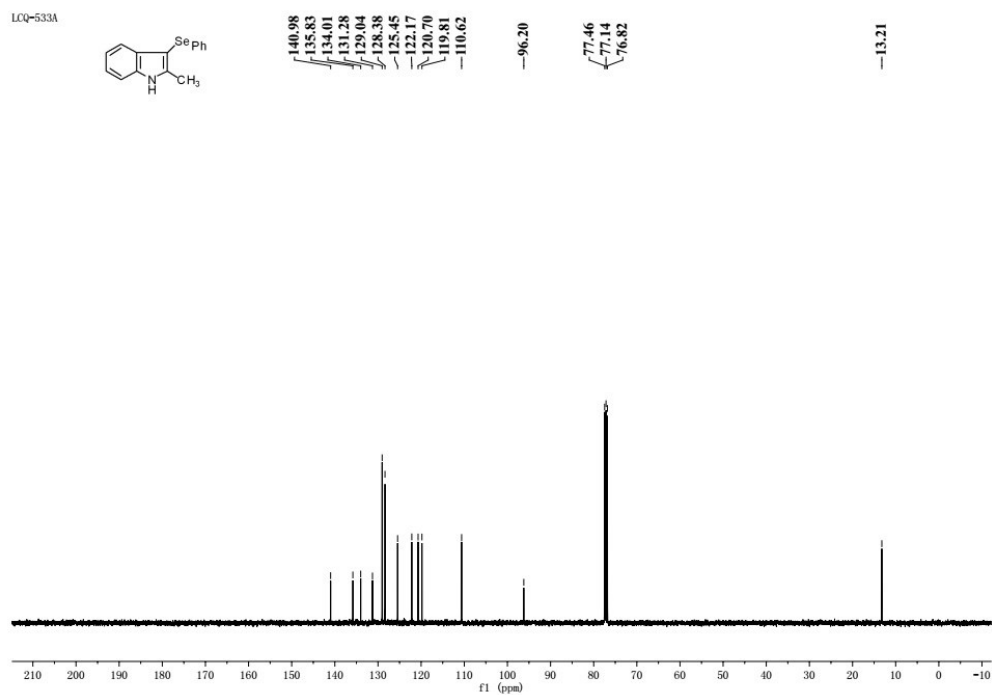
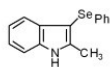


¹H and ¹³C NMR Spectra for **9b**

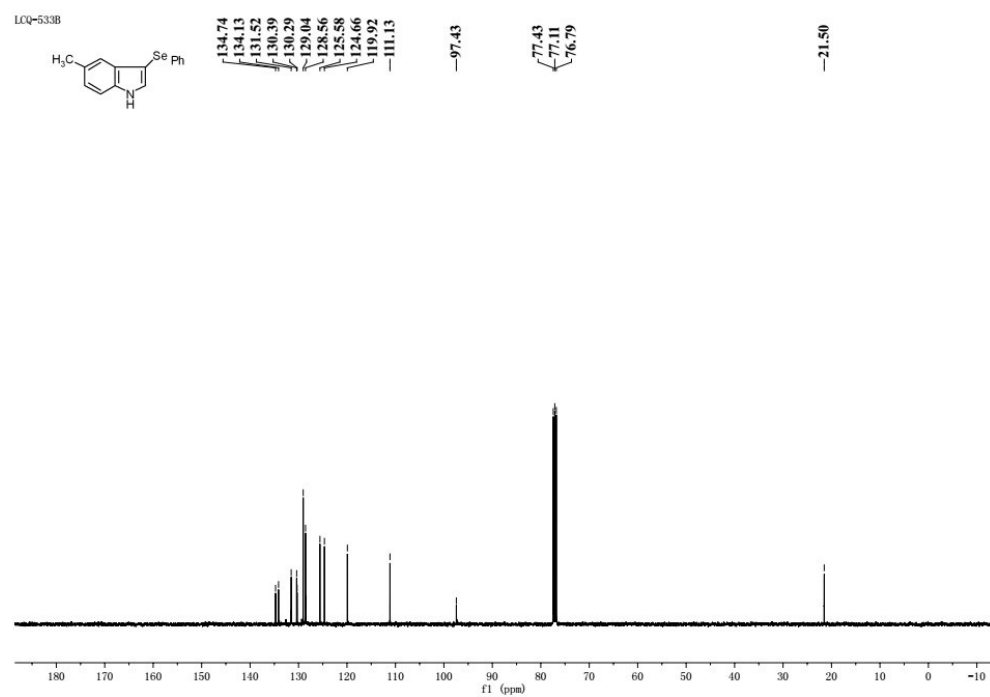
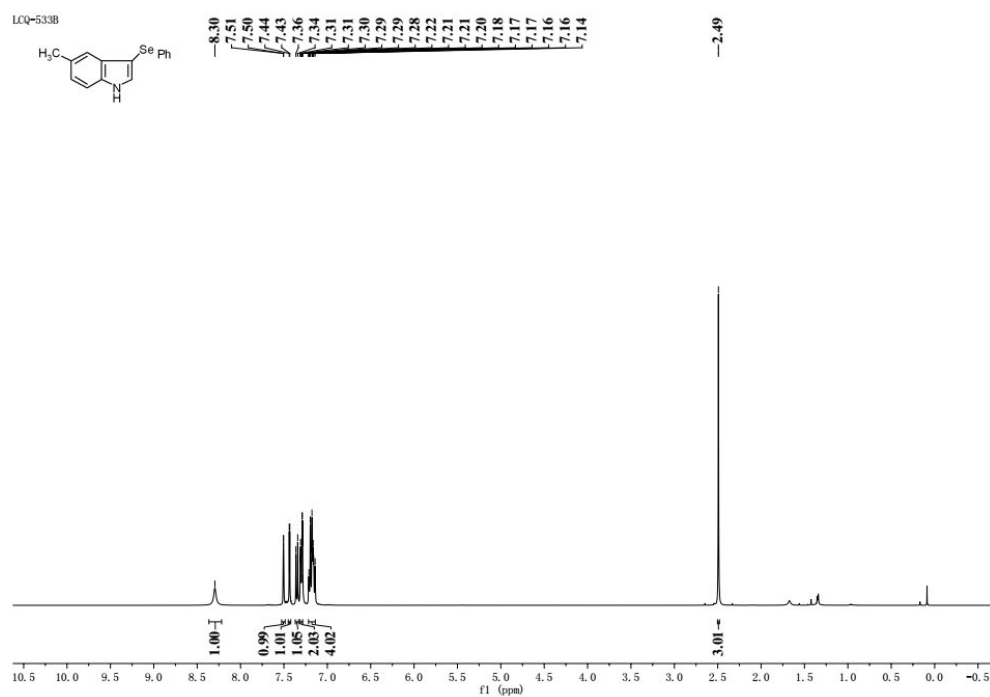
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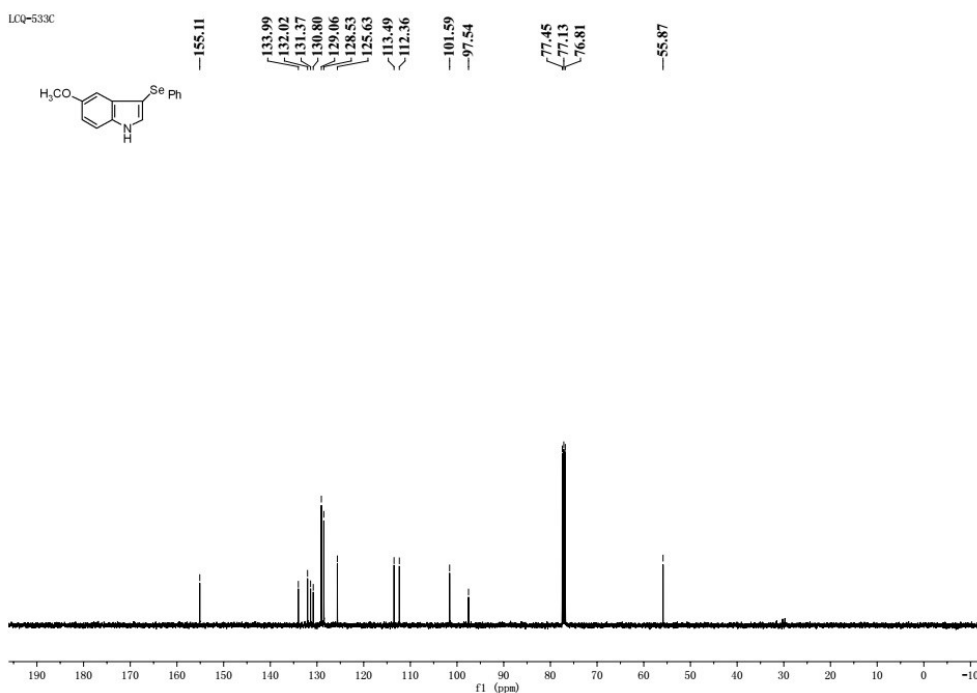
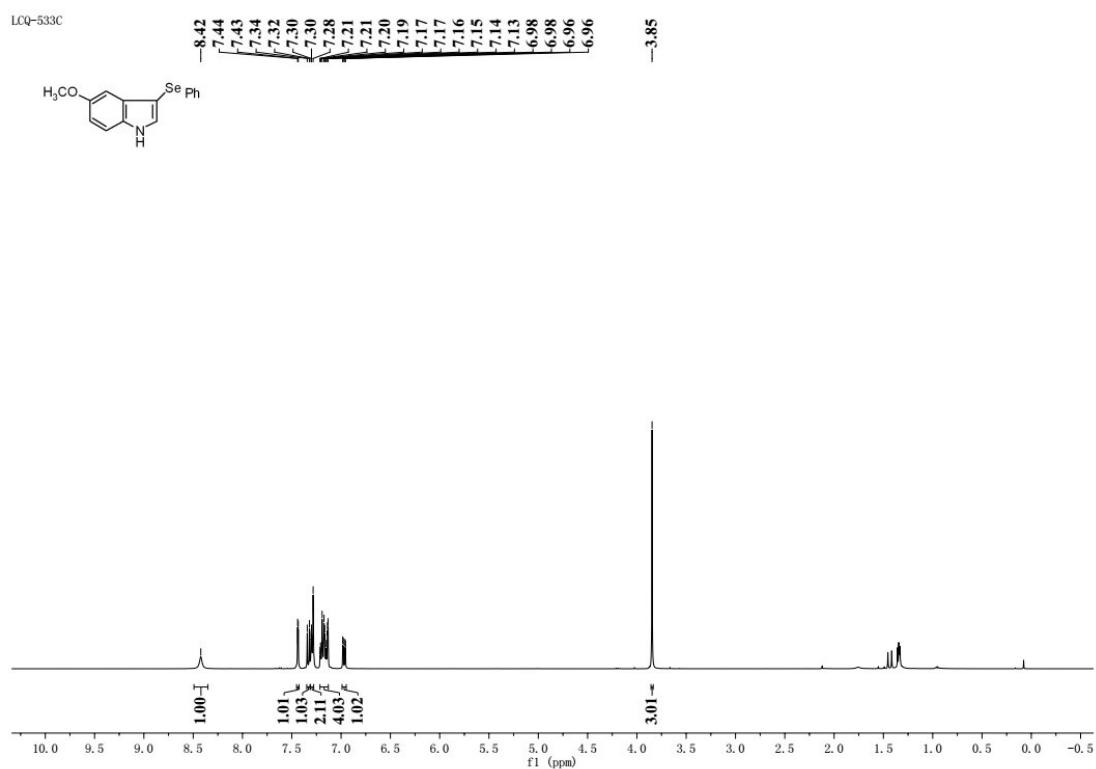
LCQ-533A



¹H and ¹³C NMR Spectra for 9c



¹H and ¹³C NMR Spectra for **9d**



7. References

- 1 (a) C. D. Prasad, S. Kumar, M. Sattar, A. Adhikary and S. Kumar, *Org. Biomol. Chem.*, 2013, **11**, 8036-8040; (b) G. S. Sorabad and M. R. Maddani, *Asian J. Org. Chem.*, 2019, **8**, 1336-1343.
- 2 (a) G. Kumaraswamy, R. Rajua and V. Narayanarao, *RSC Adv.*, 2015, **5**, 22718-22723; (b) W. Guo, W. Tan, M. Zhao, K. Tao, L. Y. Zheng, Y. Wu, D. Chen and X. L. Fan, *RSC Adv.*, 2017, **7**, 37739-37742.
- 3 (a) X. Q. Yang, Y. H. Bao, Z. H. Dai, Q. F. Zhou and F. L. Yang, *Green Chem.*, 2018, **20**, 3727-3731; (b) R. Ohkado, T. Ishikawa and H. Iida, *Green Chem.*, 2018, **20**, 984-988.
- 4 (a) J. Lin, P. N. Ibrahim, D. R. Artis, C. Zhang, W. R. Wang, S. H. Shi, WO Patent WO2006060535 A2, 2006; (b) F. X. Wang, S. D. Zhou, C. M. Wang and S. K. Tian, *Org. Biomol. Chem.*, 2017, **15**, 5284-5288.
- 5 (a) X. L. Fang, R. Y. Tang, P. Zhong and J. H. Li, *Synthesis*, 2009, 4183-4189; (b) S. Song, Y. Q. Zhang, A. Yeerlan, B. C. Zhu, J. Z. Liu and N. Jiao, *Angew. Chem. Int. Ed.*, 2017, **56**, 2487-2491; (c) S. Yi, M. Li, W. Mo, X. Hu, B. Hu, N. Sun, L. Jin and Z. Shen, *Tetrahedron Lett.*, 2016, **57**, 1912-1916; (d) D. Y. Huang, J. X. Chen, W. X. Dan, J. C. Ding, M. C. Liu and H. Y. Wu, *Adv. Synth. Catal.*, 2012, **354**, 2123-2128; (e) F. C. Bai, S. K. Zhang, L. Wei and Y. Y. Liu, *Asian J. Org. Chem.*, 2018, **7**, 371-373.
- 6 Saima, D. Equbal, A. G. Lavekar and A. K. Sinha, *Org. Biomol. Chem.*, 2016, **14**, 6111-6118.
- 7 X. Zhang, C. G. Wang, H. Jiang and L. H. Sun, *RSC Adv.*, 2018, **8**, 22042-22045.
- 8 Y. Cao, J. Liu, F. M. Liu, L. Q. Jiang and W. B. Yi, *Org. Chem. Front.*, 2019, **6**, 825-829.
- 9 Y. Z. Yu, Y. Zhou, Z. Q. Song and G. Liang, *Org. Biomol. Chem.*, 2018, **16**, 4958-4962.
- 10 X. Zhang, C. G. Wang, H. Jiang and L. H. Sun, *Chem. Commun.*, 2018, **54**, 8781-8784.