Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

for

Intermolecular Iodofunctionalization of Allenamides with indoles, pyrrole, and furan: Synthesis of iodine-substituted *Z*-enamides

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Table of contents

1. General considerations

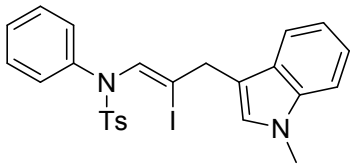
All reactions were performed using Schlenk tubes, septa, and syringes without protection of nitrogen. THF、toluene and DCM、DCE were freshly distilled over sodium/benzophenone and calcium hydride, respectively. Commercial reagents were used as supplied or were purified by standard techniques where necessary. Column chromatography was performed using Qingdao Haiyang Chemical Co., Ltd silica gel (200–300 mesh) with the appropriate solvent system, as determined by TLC analysis (Qingdao Haiyang Chemical Co., Ltd, silica gel F254) using UV light and $KMnO_4$ stain to visualize the reaction components. Melting points were determined using a WRS-1B digital melting point instrument. IR spectra were recorded on a Nicoletisso FTIR spectrometer using KBr disks. Unless otherwise noted, nuclear magnetic resonance spectra were recorded at room temperature on an Agilent 400 MHz spectrometer using $CDCl_3$ as the solvent and TMS as the internal reference. Chemical shifts for ^{13}C NMR spectra were recorded in parts per million relative to tetramethylsilane using the central peak of deuterochloroform (77.0 ppm) as the internal standard. HRMS was performed using a Bruker Daltonics Bio TOF mass spectrometer.

Allenamides **1a-1p** were prepared according to the published methods.[1, 2, 3] Indoles, pyrroles, 2-methylfuran, imidazole were obtained commercially and used without further purification.

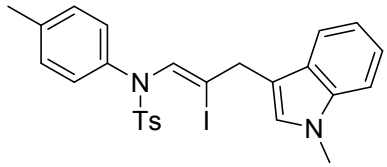
General procedure for *N*-iodosuccinimide-mediated intermolecular nucleophilic addition of allenamide 1a with indole 2a.

To a Schlenk tube were added allenamide **1a** (0.1 mmol), N-Methylindole **2a** (2.0 equiv.), *N*-iodosuccinimide (1.05 equiv.) and CH_3CN (anhydrous, 3 mL). Then the reaction mixture was stirred at r t for 1 min until complete consumption of starting material as monitored by TLC. Concentration of the reaction mixture in vacuo followed by purification through flash chromatography on silica gel column (hexane/EtOAc = 5/1 as the eluent) afforded **4a** (46.5 mg, 86% yield) as a white solid.

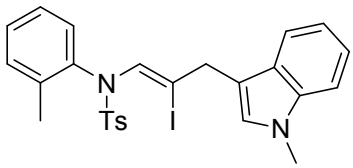
2. Analytical Data



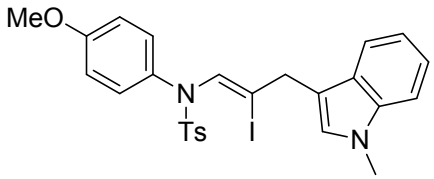
(*Z*)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**4a**) White solid; yield, 86%; m p 141.5-142.2℃; IR (neat) 3041, 2934, 2858, 1499, 1457, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.53 (d, *J* = 7.8 Hz, 1H), 7.41- 7.37 (m, 3H), 7.33 – 7.27(m, 4H), 7.24 – 7.20 (m, 1H), 7.16 – 7.07 (m, 5H), 7.01 – 6.98 (m, 1H), 3.99 (s, 2H), 3.73 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.14, 139.64, 136.69, 133.77, 131.74, 129.64, 128.72, 128.22, 127.52, 127.46, 127.12, 127.05, 121.13, 118.87, 118.45, 110.17, 109.98, 109.61, 37.80, 32.31, 21.03. HRMS (ESI) calcd for $C_{25}H_{23}IN_2NaO_2S$ $[M+Na]^+$ 565.0423; found, 565.0422.



(*Z*)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-(*p*-tolyl)benzenesulfonamide (**4b**) White solid; yield, 84%; m p 150-150.5℃; IR (neat) 3038, 2934, 2858, 1499, 1459, 756, 702 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.52 (d, *J* = 7.9 Hz, 1H), 7.39 (t, *J* = 8.4 Hz, 3H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.15 (t, *J* = 7.5 Hz, 1H), 7.12 – 7.05 (m, 4H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 8.2 Hz, 2H), 3.98 (s, 2H), 3.73 (s, 3H), 2.38 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.06, 137.01, 136.69, 136.51, 133.77, 131.84, 129.62, 129.20, 128.20, 127.55, 127.50, 127.11, 121.12, 118.87, 118.43, 110.19, 109.60, 109.32, 37.84, 32.30, 21.02, 20.52. HRMS (ESI) calcd for $C_{26}H_{25}IN_2NaO_2S$ $[M+Na]^+$ 579.0579; found, 579.0573.

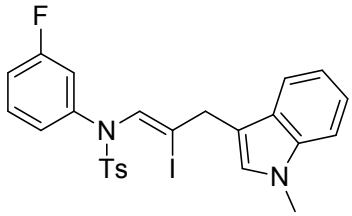


(*Z*)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-(*o*-tolyl)benzenesulfonamide (**4c**) White solid; yield, 89%; m p 99.8-100.5℃; IR (neat) 3041, 2934, 2861, 1499, 1451, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.45 – 7.42 (m, 3H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.24 – 7.22 (m, 2H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.09 (s, 1H), 7.07 (t, *J* = 7.0 Hz, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 7.9 Hz, 1H), 3.95 (s, 2H), 3.73 (s, 3H), 2.42 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.35, 138.49, 137.00, 136.72, 133.99, 131.98, 131.04, 129.83, 129.73, 128.24, 127.76, 127.09, 126.10, 121.12, 118.83, 118.42, 110.50, 109.65, 99.68, 38.87, 32.31, 21.10, 19.35. HRMS (ESI) calcd for $C_{26}H_{25}IN_2NaO_2S$ $[M+Na]^+$ 579.0579; found, 579.0584.



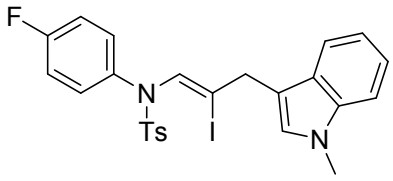
(*Z*)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-*N*-(4-methoxyphenyl)-4-methylbenzenesulfonamide (**4d**)

White solid; yield, 79%; m p 137.3-138.3℃; IR (neat) 3038, 2931, 2861, 1499, 1454, 761, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.50 (d, *J* = 7.8 Hz, 1H), 7.10 – 7.37 (m, 3H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 4.0 Hz, 2H), 7.02 – 6.93 (m, 3H), 6.86 – 6.83 (m, 2H), 3.97 (s, 2H), 3.73 (s, 3H), 3.71 (s, 2H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 158.11, 144.05, 136.70, 133.65, 131.99, 129.62, 129.43, 128.19, 127.61, 127.11, 121.12, 118.88, 118.44, 113.86, 110.26, 109.60, 109.50, 108.08, 55.23, 37.92, 32.30, 21.04. HRMS (ESI) calcd for $C_{27}H_{27}IN_2NaO_3S$ $[M+Na]^+$ 595.0528; found, 595.0523.



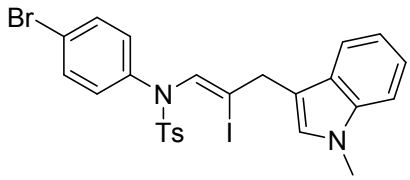
(*Z*)-*N*-(3-fluorophenyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4e**)

White solid; yield, 79%; m p 134.8-135.6℃; IR (neat) 3041, 2934, 2861, 1499, 1454, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.54 (d, *J* = 7.9 Hz, 1H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.32 (t, *J* = 8.3 Hz, 1H), 7.16 – 7.13 (m, 3H), 7.09 (t, *J* = 8.3 Hz, 1H), 7.00 (d, *J* = 7.4 Hz, 1H), 6.95 (t, *J* = 8.3 Hz, 2H), 4.01 (s, 2H), 3.73 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 161.63 (d, *J* = 242.8 Hz), 144.44, 141.22 (d, *J* = 9.9 Hz)136.71, 133.62, 131.31, 130.30 (d, *J* = 9.5 Hz), 129.79, 128.30, 127.53, 127.11, 122.89 (d, *J* = 3.1 Hz), 121.16, 118.85, 118.45, 114.07 (d, *J* = 23.7 Hz), 113.81 (d, *J* = 20.9 Hz), 111.54, 110.04, 109.65, 37.68, 32.32, 21.05. HRMS (ESI) calcd for $C_{25}H_{22}FIN_2NaO_2S$ $[M+Na]^+$ 583.0328; found, 583.0326.



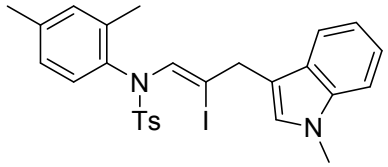
(*Z*)-*N*-(4-fluorophenyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4f**)

White solid; yield, 80%; m p 154.1-154.6℃; IR (neat) 3035, 2934, 2861, 1496, 1457, 756, 702 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.50 (d, *J* = 7.9 Hz, 1H), 7.44 – 7.32 (m, 5H), 7.20 – 7.07 (m, 7H), 6.99 (t, *J* = 7.4 Hz, 1H), 3.98 (s, 2H), 3.73 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 160.64 (d, *J* = 243.6 Hz), 159.42, 144.30, 136.70, 135.81, 133.43, 131.68, 129.95, 129.90 (d, *J* = 8.9 Hz), 128.23, 127.59, 127.11, 121.14, 118.85, 118.47, 115.62 (d, *J* = 22.7 Hz), 110.15, 109.62, 109.42, 37.81, 32.31, 21.05. HRMS (ESI) calcd for $C_{25}H_{22}FIN_2NaO_2S$ $[M+Na]^+$ 583.0328; found, 583.0322.



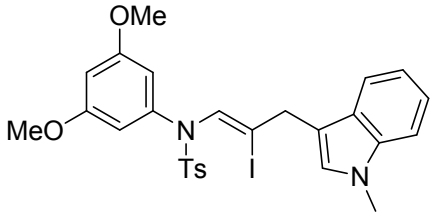
(*Z*)-*N*-(4-bromophenyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4g**)

White solid; yield, 78%; m p 149.5-150.2℃; IR (neat) 3038, 2934, 2858, 1501, 1457, 756, 702 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.51 (dd, *J* = 8.6, 2.7 Hz, 3H), 7.44 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.12 (d, *J* = 5.9 Hz, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.99 (t, *J* = 7.1 Hz, 1H), 3.99 (s, 2H), 3.73 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.39, 139.00, 136.69, 133.50, 131.74, 131.37, 129.80, 129.34, 128.25, 127.53, 127.10, 121.15, 119.86, 118.83, 118.48, 110.41, 110.09, 109.63, 37.72, 32.31, 21.05. HRMS (ESI) calcd for $C_{25}H_{22}BrIN_2NaO_2S$ $[M+Na]^+$ 642.9528; found, 642.9517.



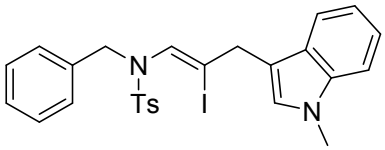
(*Z*)-*N*-(2,4-dimethylphenyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4h**)

White solid; yield, 83%; m p 54.1-54.9℃; IR (neat) 3041, 2931, 2861, 1501, 1451, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.45 – 7.34 (m, 6H), 7.22 (s, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.09 (s, 1H), 7.03 (s, 1H), 6.95 (t, *J* = 7.3 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.52 (d, *J* = 8.1 Hz, 1H), 3.94 (s, 2H), 3.73 (s, 3H), 2.42 (s, 3H), 2.22 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.31, 138.21, 137.63, 136.73, 134.39, 134.00, 132.06, 131.59, 129.74, 129.58, 128.26, 127.80, 127.10, 126.72, 121.13, 118.87, 118.42, 110.53, 109.68, 99.06, 38.98, 32.34, 21.12, 20.58, 19.27. HRMS (ESI) calcd for $C_{27}H_{27}IN_2NaO_2S$ $[M+Na]^+$ 593.0736; found, 593.0728.

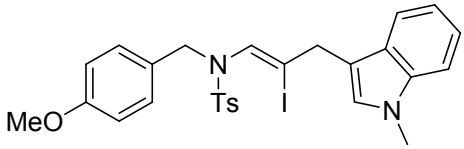


(*Z*)-*N*-(3,5-dimethoxyphenyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4i**)

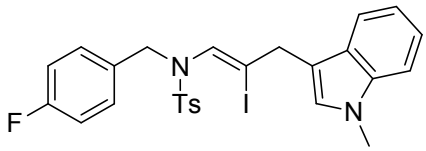
White solid; yield, 84%; m p 141.9-142.0℃; IR (neat) 3038, 2937, 2861, 1501, 1499, 761, 705 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.54 (d, *J* = 7.9 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.39 – 7.35 (m, 3H), 7.14 – 7.11 (m, 3H), 6.95 (t, *J* = 7.4 Hz, 1H), 6.34 (t, *J* = 2.0 Hz, 1H), 6.18 (d, *J* = 2.1 Hz, 2H), 4.02 (s, 2H), 3.73 (s, 3H), 3.52 (s, 6H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 159.99, 144.22, 141.08, 136.72, 133.93, 131.57, 129.63, 128.27, 127.60, 127.08, 121.10, 118.81, 118.43, 110.09, 110.02, 109.63, 105.47, 98.72, 55.10, 37.89, 32.30, 21.03. HRMS (ESI) calcd for $C_{27}H_{27}IN_2NaO_4S$ $[M+Na]^+$ 625.0634; found, 625.0629.



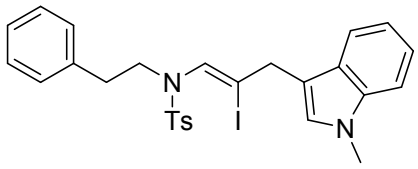
(*Z*)-*N*-benzyl-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4j**)
White solid; yield, 84%; m p 119.2-119.8℃; IR (neat) 3041, 2931, 2856, 1499, 1457, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.25 (m, 7H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.81 (s, 1H), 6.13 (s, 1H), 4.36 (s, 2H), 3.85 (s, 2H), 3.69 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 143.73, 136.57, 135.42, 135.05, 130.73, 129.78, 128.92, 128.13, 127.91, 127.65, 127.40, 127.03, 121.11, 118.68, 118.47, 114.67, 110.18, 109.54, 53.32, 38.03, 32.29, 21.04. HRMS (ESI) calcd for $C_{26}H_{25}IN_2NaO_2S$ $[M+Na]^+$ 579.0579; found, 579.0577.



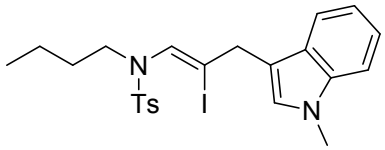
(*Z*)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-*N*-(4-methoxybenzyl)-4-methylbenzenesulfonamide (**4k**)
White solid; yield, 77%; m p 137.3-138.3℃; IR (neat) 3038, 2931, 2861, 1499, 1454, 761, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.67 (d, *J* = 7.9 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.29 (m, 2H), 7.18 - 7.14 (m, 3H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.84 (s, 1H), 6.81 (d, *J* = 4.3 Hz, 2H), 6.05 (s, 1H), 4.27 (s, 2H), 3.85 (s, 2H), 3.73 (s, 3H), 3.69 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 158.74, 143.67, 136.57, 135.06, 130.66, 130.36, 129.77, 127.93, 127.39, 127.13, 127.06, 121.11, 118.71, 118.44, 114.90, 113.48, 110.21, 109.53, 55.00, 52.76, 37.97, 32.24, 21.03. HRMS (ESI) calcd for $C_{27}H_{27}IN_2NaO_3S$ $[M+Na]^+$ 609.0685; found, 609.0683.



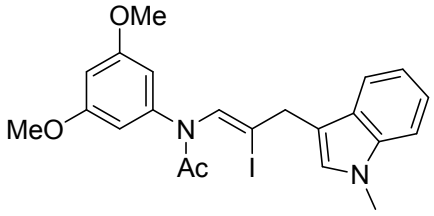
(*Z*)-*N*-(4-fluorobenzyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4l**)
White solid; yield, 81%; m p 134.7-135.7℃; IR (neat) 3035, 2934, 2864, 1501, 1459, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.43 – 7.35 (m, 3H), 7.34 – 7.26 (m, 3H), 7.17 – 7.06 (m, 3H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.88 (s, 1H), 6.08 (s, 1H), 4.31 (s, 2H), 3.86 (s, 2H), 3.71 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 161.60 (d, *J* = 242.0 Hz), 143.80, 136.59, 134.89, 131.58, 131.12 (d, *J* = 8.3 Hz), 130.56, 129.82, 127.98, 127.41, 127.03, 121.13, 118.68, 118.44, 115.49, 114.89 (d, *J* = 21.3 Hz), 110.14, 109.57, 52.57, 38.00, 32.27, 21.04. HRMS (ESI) calcd for $C_{26}H_{24}FIN_2NaO_2S$ $[M+Na]^+$ 597.0485; found, 597.0489.



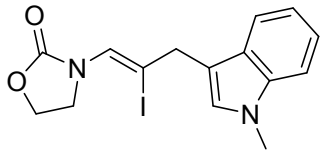
(*Z*)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-phenethylbenzenesulfonamide (**4m**)
White solid; yield, 81%; m p 118.8-119.6℃; IR (neat) 3038, 2931, 2859, 1501, 1457, 756, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.18 (s, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.19 (s, 1H), 4.00 (s, 2H), 3.76 (s, 3H), 3.33 – 3.31 (m, 2H), 2.74 – 2.64 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 143.69, 138.06, 136.73, 134.80, 130.54, 129.80, 128.58, 128.41, 128.36, 127.30, 127.09, 126.40, 121.18, 118.76, 118.51, 115.53, 110.08, 109.71, 38.87, 38.08, 34.01, 32.35, 21.00. HRMS (ESI) calcd for $C_{27}H_{27}IN_2NaO_2S$ $[M+Na]^+$ 593.0736; found, 593.0729.



(*Z*)-*N*-butyl-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methylbenzenesulfonamide (**4n**)
White solid; yield, 86%; m p 91.8-92.3℃; IR (neat) 3038, 2937, 2859, 1496, 1457, 764, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.19 – 7.13 (m, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.00 (s, 1H), 3.99 (s, 2H), 3.74 (s, 3H), 3.06 (t, *J* = 6.9 Hz, 2H), 2.38 (s, 3H), 1.36 – 1.24 (m, 7.3 Hz, 4H), 0.79 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 143.55, 136.71, 134.76, 130.78, 129.71, 128.26, 127.29, 127.09, 121.18, 118.74, 118.45, 115.54, 110.17, 109.67, 49.42, 38.14, 32.33, 29.53, 20.99, 19.57, 13.49. HRMS (ESI) calcd for $C_{23}H_{27}IN_2NaO_2S$ $[M+Na]^+$ 545.0736; found, 545.0728.

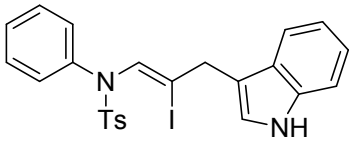


(*Z*)-*N*-(3,5-dimethoxyphenyl)-*N*-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)acetamide (**4o**)
Colorless oil liquid; yield, 82%; IR (neat) 3038, 2934, 2858, 1499, 1457, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.59 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.20 (d, *J* = 6.9 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.51 (d, *J* = 1.7 Hz, 2H), 6.39 (s, 1H), 4.02 (s, 2H), 3.74 (s, 3H), 3.65 (s, 6H), 2.03 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 160.19, 145.52, 136.75, 133.87, 133.60， 133.58, 128.40, 127.17, 121.14, 118.79, 118.51, 117.06, 109.70, 109.55, 106.59, 55.21, 41.33, 32.34, 26.45, 24.31. HRMS (ESI) calcd for $C_{22}H_{23}IN_2NaO_3S$ $[M+Na]^+$ 513.0651; found, 513.0648.



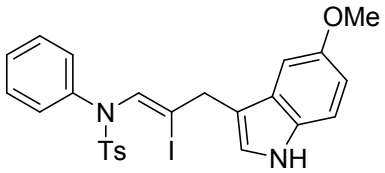
(*Z*)-3-(2-iodo-3-(1-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)oxazolidin-2-one (**4p**)

White solid; yield, 71%; m p 117.1-117.7℃; IR (neat) 3038, 2934, 2858, 1501, 1454, 761, 702 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.54 (d, *J* = 7.9 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.20 (s, 1H), 7.17 – 7.11 (m, 1H), 7.07 (s, 1H), 7.04 – 6.98 (m, 1H), 4.38 – 4.34 (m, 2H), 4.11 – 4.07 (m, 2H), 3.96 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 156.57, 136.74, 129.24, 128.29, 127.25, 121.08, 118.74, 118.53, 110.77, 109.65, 90.39, 63.11, 44.55, 39.39, 32.31. HRMS (ESI) calcd for $C_{15}H_{15}IN_2NaO_2S$ $[M+Na]^+$ 405.0076; found, 405.0070.



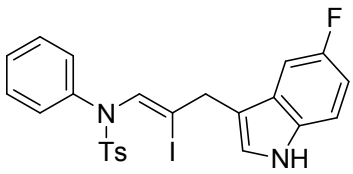
(*Z*)-*N*-(3-(1*H*-indol-3-yl)-2-iodoprop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7b**)

White solid; yield, 57%; m p 41.9-42.8℃; IR (neat) 3040, 2934, 2863, 1498, 1456, 758, 699 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 10.92 (s, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.40 – 7.26 (m, 7H), 7.26 – 7.20 (m, 1H), 7.14 (s, 1H), 7.10 – 7.06 (m, 4H), 6.96 (t, *J* = 7.4 Hz, 1H), 4.00 (s, 2H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.16, 139.69, 136.28, 133.74, 131.71, 129.67, 128.76, 127.52, 127.43, 127.09, 126.80, 124.00, 121.04, 118.64, 118.37, 111.44, 110.93, 110.39, 38.00, 21.06. HRMS (ESI) calcd for $C_{24}H_{21}IN_2NaO_2S$ $[M+Na]^+$ 551.0266; found, 551.0261.

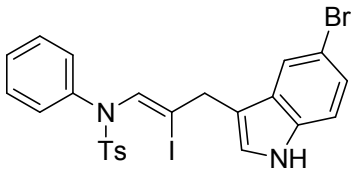


(*Z*)-*N*-(2-iodo-3-(5-methoxy-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7c**)

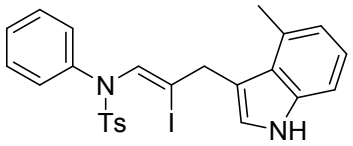
White solid; yield, 77%; m p 94.5-95.4℃; IR (neat) 3041, 2937, 2864, 1499, 1454, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 10.78 (s, 1H), 7.34 (d, *J* = 7.9 Hz, 2H), 7.31 – 7.20 (m, 6H), 7.11 (s, 1H), 7.10 – 7.03 (m, 3H), 7.01 (s, 1H), 6.73 (d, *J* = 8.8 Hz, 1H), 3.97 (s, 2H), 3.70 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 153.04, 144.16, 139.74, 133.63, 131.65, 131.41, 129.64, 128.77, 127.48, 127.38, 127.11, 124.70, 112.16, 111.39, 110.63, 110.31, 109.56, 100.22, 55.17, 38.14, 21.04. HRMS (ESI) calcd for $C_{25}H_{23}IN_2NaO_3S$ $[M+Na]^+$ 581.0372; found, 581.0372.



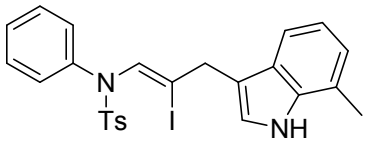
(*Z*)-*N*-(3-(5-fluoro-1*H*-indol-3-yl)-2-iodoprop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7d**) White solid; yield, 43%; m p 147.5-148.4℃; IR (neat) 3041, 2934, 2861, 1499, 1454, 756, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 11.02 (s, 1H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.34-7.27 (m, 6H), 7.24 (d, *J* = 7.1 Hz, 1H), 7.22 (s, 1H), 7.15 (s, 1H), 7.08 (d, *J* = 7.5 Hz, 2H), 6.91 (t, *J* = 9.2 Hz, 1H), 3.97 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 156.65 (d, *J* = 229.9 Hz), 144.18, 139.69, 133.79, 132.95, 131.84, 129.66, 128.73, 127.46 (d, *J* = 8.6 Hz), 127.11, 127.00, 126.14, 112.35 (d, *J* = 9.5 Hz), 111.18 (d, *J* = 4.7 Hz), 110.41, 109.54, 109.14 (d, *J* = 26.0 Hz), 103.41 (d, *J* = 23.3 Hz), 37.74, 21.04. HRMS (ESI) calcd for $C_{24}H_{20}FIN_2NaO_2S$ $[M+Na]^+$ 569.0172; found, 569.0173.



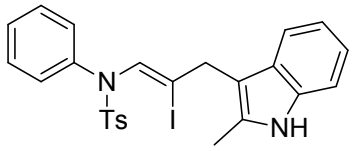
(*Z*)-*N*-(3-(5-bromo-1*H*-indol-3-yl)-2-iodoprop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7e**) White solid; yield, 50%; m p 147.2-147.8℃; IR (neat) 3041, 2931, 2864, 1496, 1454, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 11.14 (s, 1H), 7.72 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.36 – 7.26 (m, 5H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 11.3 Hz, 2H), 7.09 (d, *J* = 7.7 Hz, 2H), 3.99 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.15, 139.74, 135.00, 133.76, 131.95, 129.67, 128.75, 128.63, 127.49, 127.39, 127.09, 125.79, 123.49, 121.06, 113.44, 111.18, 110.79, 109.54, 37.62, 21.06. HRMS (ESI) calcd for $C_{24}H_{20}BrIN_2NaO_2S$ $[M+Na]^+$ 628.9371; found, 628.9368.



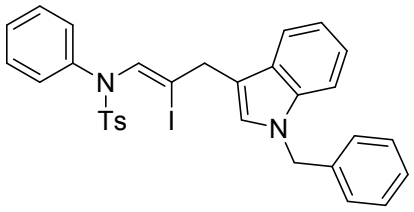
(*Z*)-*N*-(2-iodo-3-(4-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7f**) White solid; yield, 80%; m p 135-135.9℃; IR (neat) 3038, 2937, 2861, 1496, 1454, 756, 702 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 10.94 (s, 1H), 7.35 – 7.22 (m, 5H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.09 (s, 1H), 7.03-6.99 (m, 3H), 6.94 (d, *J* = 7.6 Hz, 2H), 6.77 (d, *J* = 7.1 Hz, 1H), 6.37 (s, 1H), 4.07 (s, 2H), 2.54 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.08, 139.70, 136.77, 133.15, 131.97, 129.61, 129.55, 128.83, 127.36, 127.27, 125.23, 124.39, 121.33, 120.17, 111.96, 110.97, 109.56, 109.53, 40.16, 21.02, 19.39. HRMS (ESI) calcd for $C_{25}H_{23}IN_2NaO_2S$ $[M+Na]^+$ 565.0423; found, 565.0419.



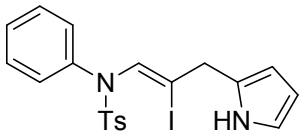
(*Z*)-*N*-(2-iodo-3-(7-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7g**)
White solid; yield, 66%; m p 145.3-146℃; IR (neat) 3040, 2934, 2863, 1495, 1453, 755, 696 cm^{-1}; ^1H NMR (400 MHz, dmso) δ 10.89 (s, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.21 (m, 5H), 7.12 (s, 1H), 7.07-7.05 (m, 3H), 6.87 (d, *J* = 4.2 Hz, 2H), 5.76 (s, 1H), 3.98 (s, 2H), 2.44 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.14, 139.72, 135.83, 133.78, 131.69, 129.64, 128.74, 127.53, 127.42, 127.08, 126.51, 123.71, 121.58, 120.49, 118.63, 116.27, 111.38, 110.52, 40.13, 21.05, 16.76. HRMS (ESI) calcd for $C_{25}H_{23}IN_2NaO_2S$ $[M+Na]^+$ 565.0423; found, 565.0417.



(*Z*)-*N*-(2-iodo-3-(2-methyl-1*H*-indol-3-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7h**)
White solid; yield, 66%; m p 68-68.9℃; IR (neat) 3042, 2937, 2860, 1496, 1454, 756, 698 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 10.83 (s, 1H), 7.42 (d, *J* = 6.5 Hz, 2H), 7.39 (s, 1H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.29 – 7.19 (m, 4H), 7.08 (s, 1H), 7.07 (d, *J* = 7.7 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.91 (t, *J* = 7.4 Hz, 1H), 3.97 (s, 2H), 2.37 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.13, 139.72, 135.11, 133.84, 133.16, 131.09, 129.65, 128.71, 128.02, 127.51, 127.42, 127.02, 120.07, 118.19, 117.79, 110.92, 110.37, 106.67, 36.58, 21.06, 11.52. HRMS (ESI) calcd for $C_{25}H_{23}IN_2NaO_2S$ $[M+Na]^+$ 565.0423; found, 565.0422.

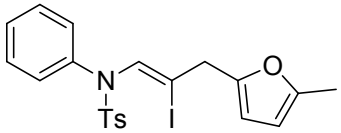


(*Z*)-*N*-(3-(1-benzyl-1*H*-indol-3-yl)-2-iodoprop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7i**)
White solid; yield, 70%; m p 133.3-133.8℃; IR (neat) 3041, 2934, 2861, 1499, 1454, 758, 700 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 9.5 Hz, 2H), 7.28 – 7.20 (m, 7H), 7.13 (d, *J* = 6.2 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 1H), 7.07 (s, 1H), 7.05 (d, J = 8.6 Hz, 2H), 6.99 (t, *J* = 7.5 Hz, 1H), 5.38 (s, 2H), 4.02 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, dmso) δ 144.12, 139.66, 138.29, 136.15, 133.66, 131.81, 129.62, 128.73, 128.43, 127.89, 127.47, 127.44, 127.22, 127.09, 126.77, 121.34, 119.05, 118.73, 111.02, 110.13, 109.81, 109.53, 48.86, 37.82, 21.03. HRMS (ESI) calcd for $C_{31}H_{27}IN_2NaO_2S$ $[M+Na]^+$ 641.0736; found, 641.0733.



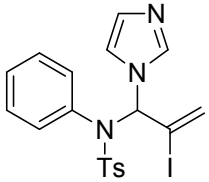
(*Z*)-*N*-(2-iodo-3-(1*H*-pyrrol-2-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7j**)

White solid; yield, 62%; m p 118.7-119.2℃; IR (neat) 3038, 2934, 2858, 1496, 1454, 758, 702 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 10.58 (s, 1H), 7.41 – 7.35 (m, 4H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 6.5 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.85 (s, 1H), 6.63 (s, 1H), 5.90 (s, 1H), 5.74 (s, 1H), 3.81 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 144.28, 139.66, 133.61, 132.10, 129.75, 128.79, 127.55, 127.49, 127.10, 117.06, 109.57, 107.50, 106.76, 106.46, 40.20, 21.07. HRMS (ESI) calcd for $C_{20}H_{19}IN_2NaO_2S$ $[M+Na]^+$ 501.0110; found, 501.0109



(*Z*)-*N*-(2-iodo-3-(5-methylfuran-2-yl)prop-1-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**7k**)

White solid; yield, 67%; m p 80.6-81.5℃; IR (neat) 3041, 2931, 2864, 1499, 1451, 756, 697 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.45 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.25 (t, *J* = 6.9 Hz, 1H), 7.09 (d, *J* = 7.1 Hz, 2H), 7.08 (s, 1H), 5.97 (d, *J* = 4.2 Hz, 2H), 3.89 (s, 2H), 2.38 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 150.68, 149.74, 144.34, 139.48, 133.68, 133.33, 129.75, 128.81, 127.52, 127.39, 127.11, 108.27, 106.51, 102.88, 40.14, 21.04, 13.28. HRMS (ESI) calcd for $C_{21}H_{20}INNaO_3S$ $[M+Na]^+$ 516.0106; found, 516.0102.

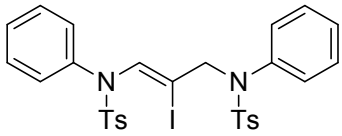


N-(1-(1*H*-imidazol-1-yl)-2-iodoallyl)-4-methyl-*N*-phenylbenzenesulfonamide (**7l**)

White solid; yield, 96%; m p 100.6-101.4 ℃; IR (neat) 3041, 2934, 2804, 1499, 1454, 758, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.0 Hz, 2H), 7.38 (s, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.25 - 7.20 (m, 4H), 6.97 (d, *J* = 8.7 Hz, 2H), 6.78 (d, *J* = 7.6 Hz, 2H), 6.75 (s, 1H), 6.68 (s, 1H), 6.25 (s, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.52, 137.25, 135.61, 134.17, 132.00, 131.93, 129.71, 129.60, 129.28, 129.11, 127.82, 119.01, 102.83, 76.33, 21.61. HRMS (ESI) calcd for $C_{19}H_{18}IN_3NaO_2S$ $[M+Na]^+$ 502.0062; found, 502.0047.

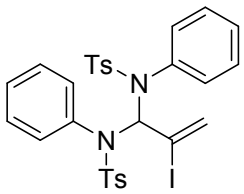
3. General procedure and spectral data of 5a and 6a

To a Schlenk tube were added allenamide **1a** (0.3 mmol) N-iodosuccinimide (1.05 equiv.) and CH_3CN (anhydrous, 5 mL). Then the reaction mixture was stirred at r t for 2 minutes until complete consumption of starting material as monitored by TLC. Concentration of the reaction mixture in vacuo followed by purification through flash chromatography on silica gel column (hexane/EtOAc = 15/1 as the eluent) afforded **6a** (6 mg, 6% yield) as a white solid, (hexane/EtOAc = 7/1 as the eluent) afforded 4-methyl-N-phenylbenzenesulfonamide (27 mg, 36% yield) as a white solid, (hexane/EtOAc = 5/1 as the eluent) afforded **5a** (30 mg, 31% yield) as a white solid.



(*Z*)-*N*,*N*'-(2-iodoprop-1-ene-1,3-diyl)bis(4-methyl-*N*-phenylbenzenesulfonamide) (**5a**)

White solid; yield, 31%; m p 140.4-141.3 ℃； IR (neat) 3041, 2934, 2861, 1499, 1457, 761, 702 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.1 Hz, 2H), 7.28 – 7.25 (m, 7H), 7.20 (t, *J* = 8.3 Hz, 3H), 7.14 (t, *J* = 7.6 Hz, 2H), 7.01 – 6.97 (m, 3H), 6.59 (d, *J* = 7.9 Hz, 2H), 4.50 (s, 2H), 2.44 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.25, 143.75, 137.98, 137.96, 135.66, 135.09, 134.23, 129.49, 129.46, 129.25, 128.90, 128.60, 128.01, 127.71, 127.57, 127.46, 109.96, 90.22, 60.64, 21.60, 21.57. HRMS (ESI) calcd for $C_{29}H_{27}IN_2NaO_4S_2$ $[M+Na]^+$ 681.0355; found, 681.0337.

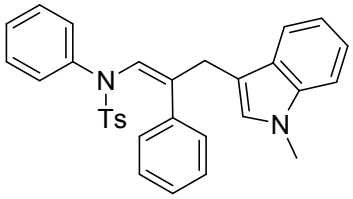


N,*N*'-(2-iodoprop-2-ene-1,1-diyl)bis(4-methyl-*N*-phenylbenzenesulfonamide) (**6a**)

White solid; yield, 6%; m p 167.1-167.9 ℃； IR (neat) 3040, 2934, 2863, 1498, 1450, 758, 699, 545 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.9 Hz, 4H), 7.29 (d, *J* = 7.3 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 4H), 7.13 (t, *J* = 7.6 Hz, 4H), 7.07 (s, 1H), 6.68 (d, *J* = 8.1 Hz, 4H), 6.52 (s, 1H), 5.93 (s, 1H), 2.42 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.01, 135.70, 134.89, 133.90, 131.49, 129.15, 128.64, 128.46, 110.01, 107.98, 81.40, 21.63. HRMS (ESI) calcd for $C_{29}H_{27}IN_2NaO_4S_2$ $[M+Na]^+$ 681.0355; found, 681.0332.

4. General procedure and spectral data of 9[4]

A mixture of **4a** (110 mg, 0.2 mmol), $Pd(PPh_3)_4$ (24 mg, 10 mmol%), Cs_2CO_3 (131 mg, 2 equiv.), and phenylboronic acid (30 mg, 1.2 equiv.) in acetonitrile–toluene (3 : 3 mL) in a flask under an argon atmosphere was stirred for 5 h at 110 °C. The reaction was monitored by TLC analysis. After the reaction was complete, the mixture was poured into ethyl acetate, filtered, evaporated under vacuum and purified through flash chromatography on silica gel column (hexane/EtOAc = 10/1 as the eluent) afforded **9** (81.8 mg, 83% yield) as a white solid.



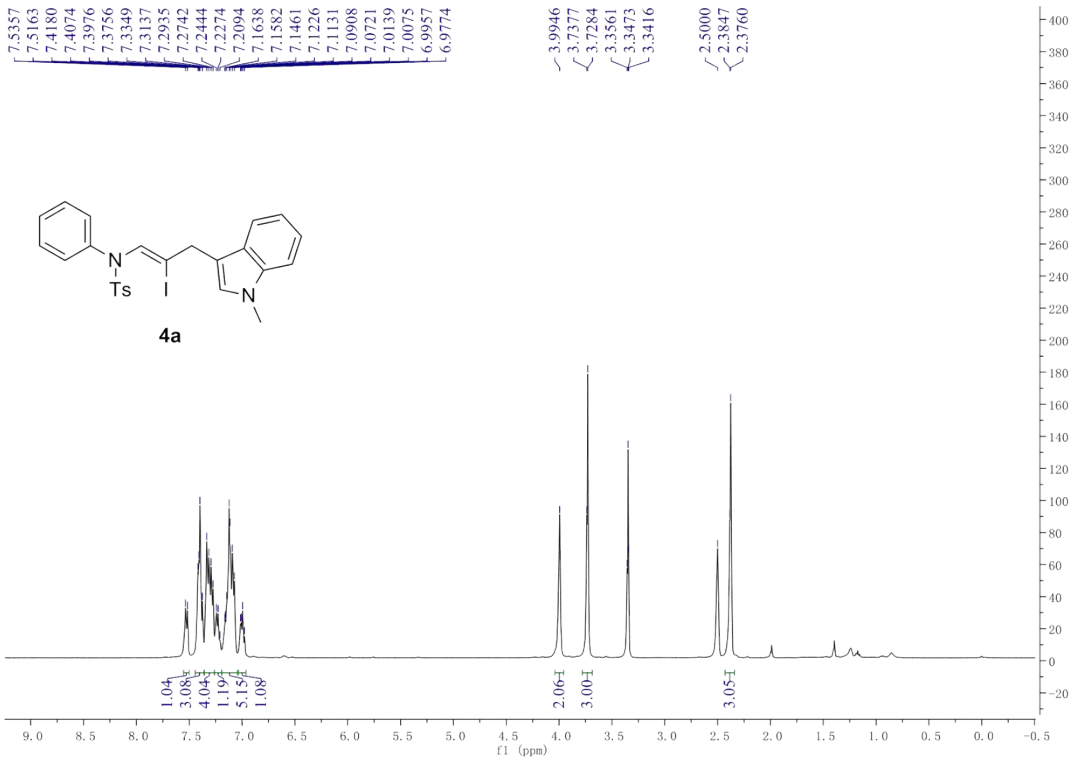
(*Z*)-4-methyl-*N*-(3-(1-methyl-1*H*-indol-3-yl)-2-phenylprop-1-en-1-yl)-*N*-phenylbenzenesulfonamide (**9**)

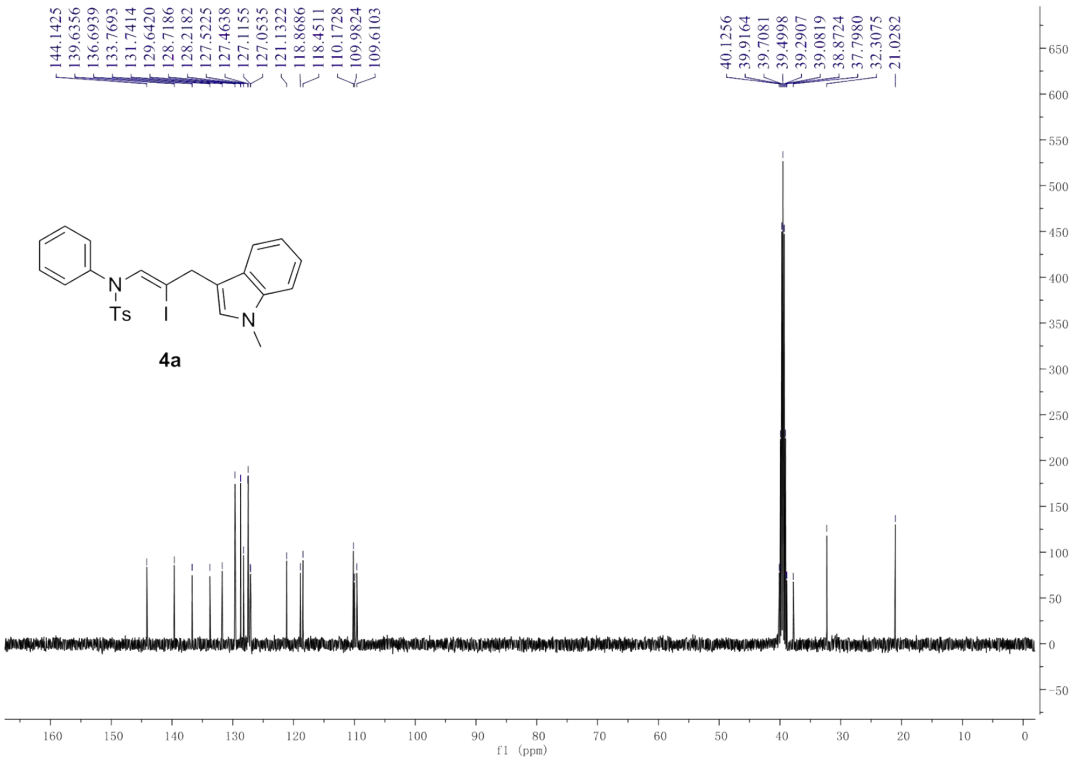
Yellow solid; yield, 83%; m p 122.5-124.0 ℃; IR (neat) 3038, 2934, 2861, 1499, 1459, 758, 705, 542 cm^{-1}; ^1H NMR (400 MHz, DMSO) δ 7.58 (d, J = 7.8 Hz, 1H), 7.37 – 7.27 (m, 5H), 7.15 (t, *J* = 7.5 Hz, 1H), 7.12 – 6.97 (m, 9H), 6.96 (s, 1H), 6.74 – 6.67 (m, 2H), 6.70 (d, *J* = 6.2 Hz, 1H), 3.78 (s, 2H), 3.67 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 143.83, 140.59, 138.13, 137.63, 136.74, 133.79, 129.58, 128.26, 127.90, 127.46, 127.40, 127.36, 126.92, 126.88, 126.55, 124.62, 121.05, 118.99, 118.37, 110.27, 109.54, 32.22, 31.56, 21.02. HRMS (ESI) calcd for $C_{31}H_{28}N_2NaO_2S$ $[M+Na]^+$ 515.1769; found, 515.1780.

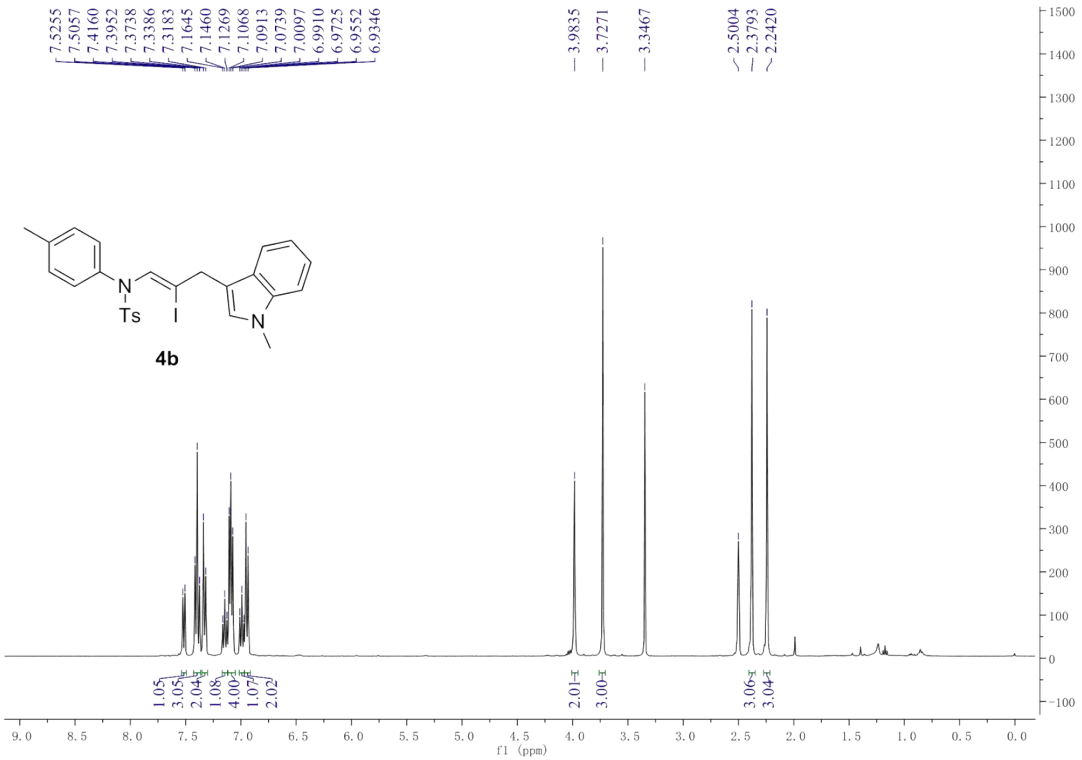
5. References

1. A. G. Gómez, L. Añorbe, A. Poblador, G. Domínguez and J. P. Castells, *Eur. J. Org. Chem*. 2008, 1370-1377.
2. L. L. Wei, J. A. Mulder, H. Xiong, C. A. Zificsak, C. J. Douglas and R. P. Hsung, *Tetrahedron*. 2001, **57**, 459-466.
3. J. M. Chapman, J. G. H. Cocolas and I. H. Hall, *J. Med. Chem*., 1983, **26**, 243-246.
4. J. K. Vandavasi, K.-K. Kuo, W.-P. Hu, H.-C. Shen, W.-S. Lo and J.-J. Wang, *Org. Biomol. Chem.*, 2013, **11**, 6520-6525.

6. NMR Spectra for 4a – 4p



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N
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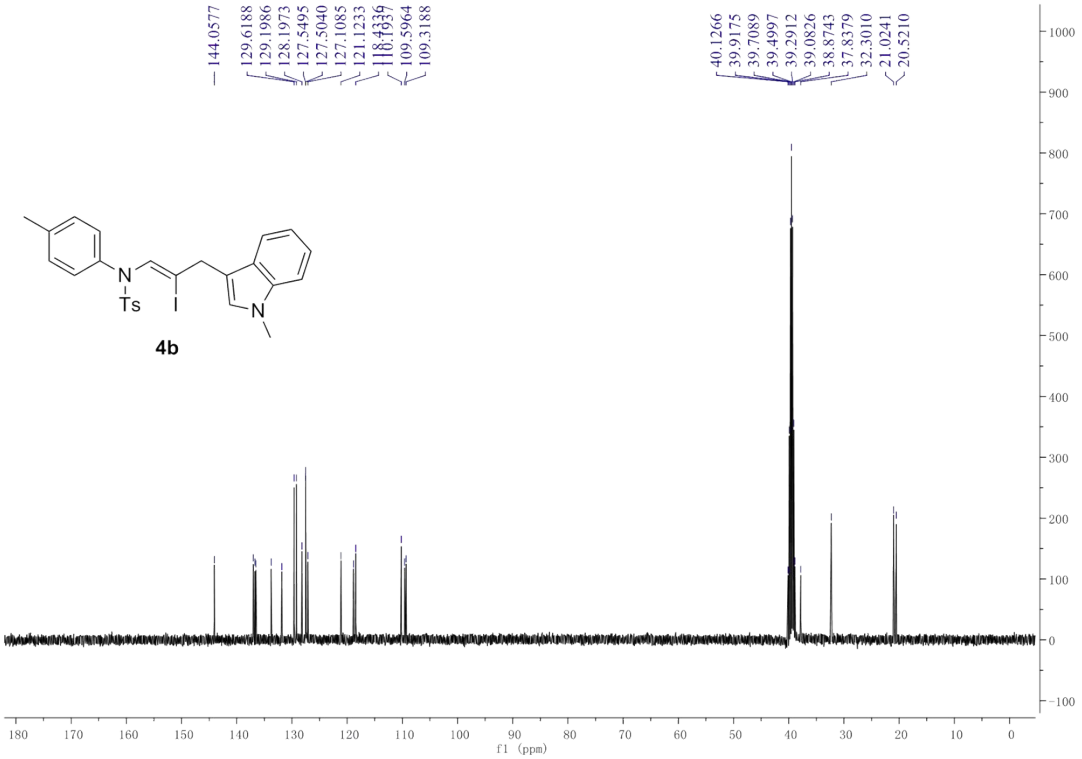
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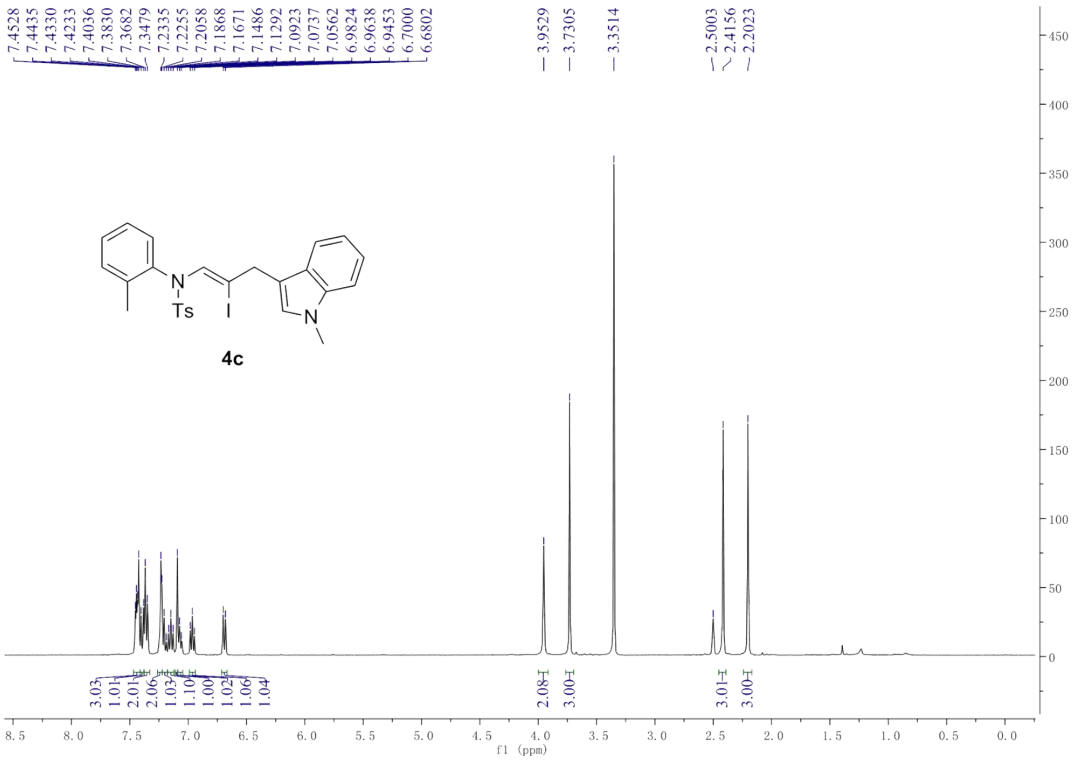
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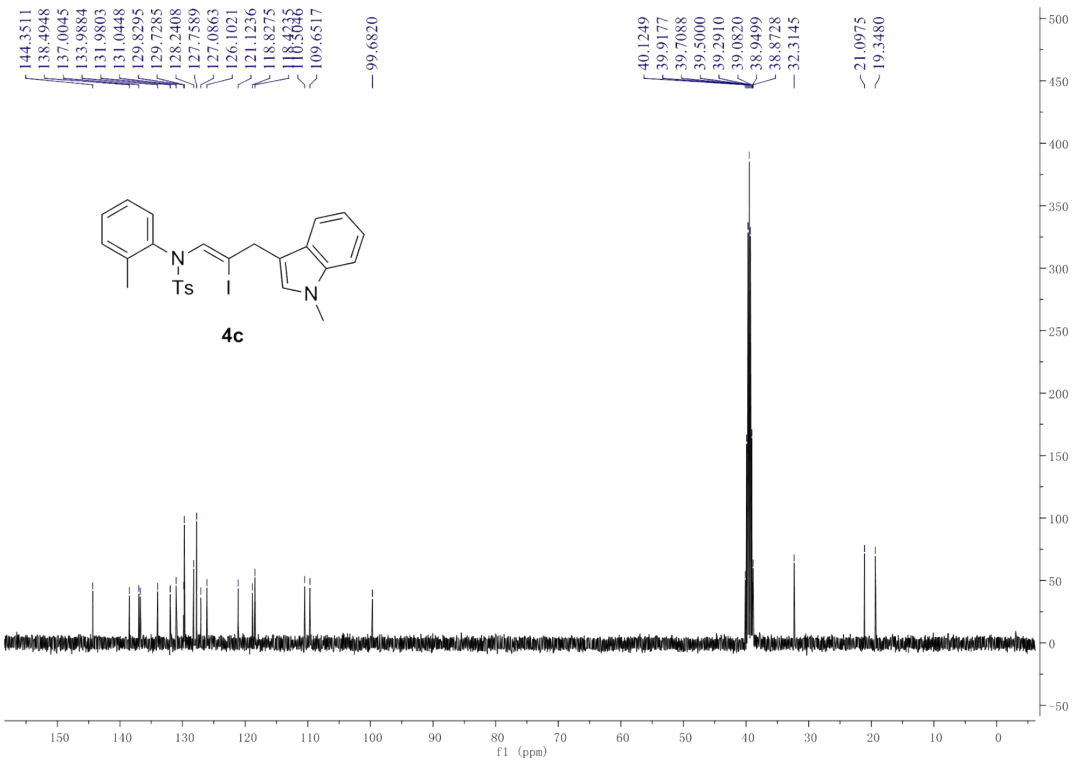
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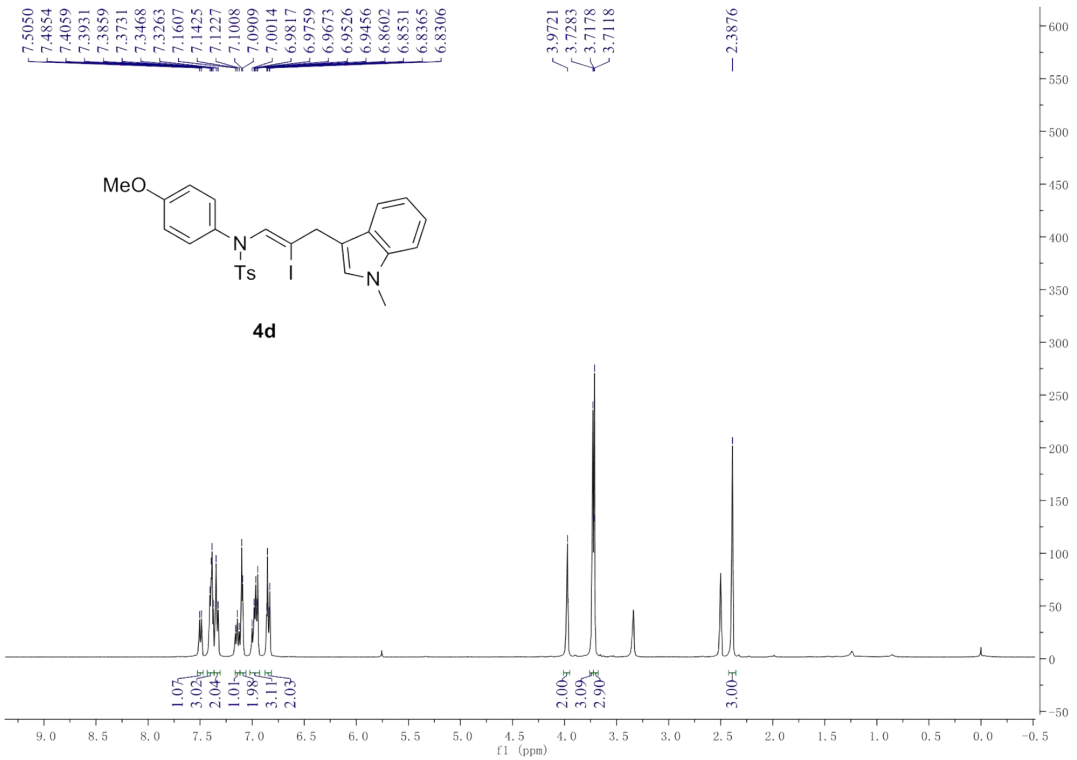
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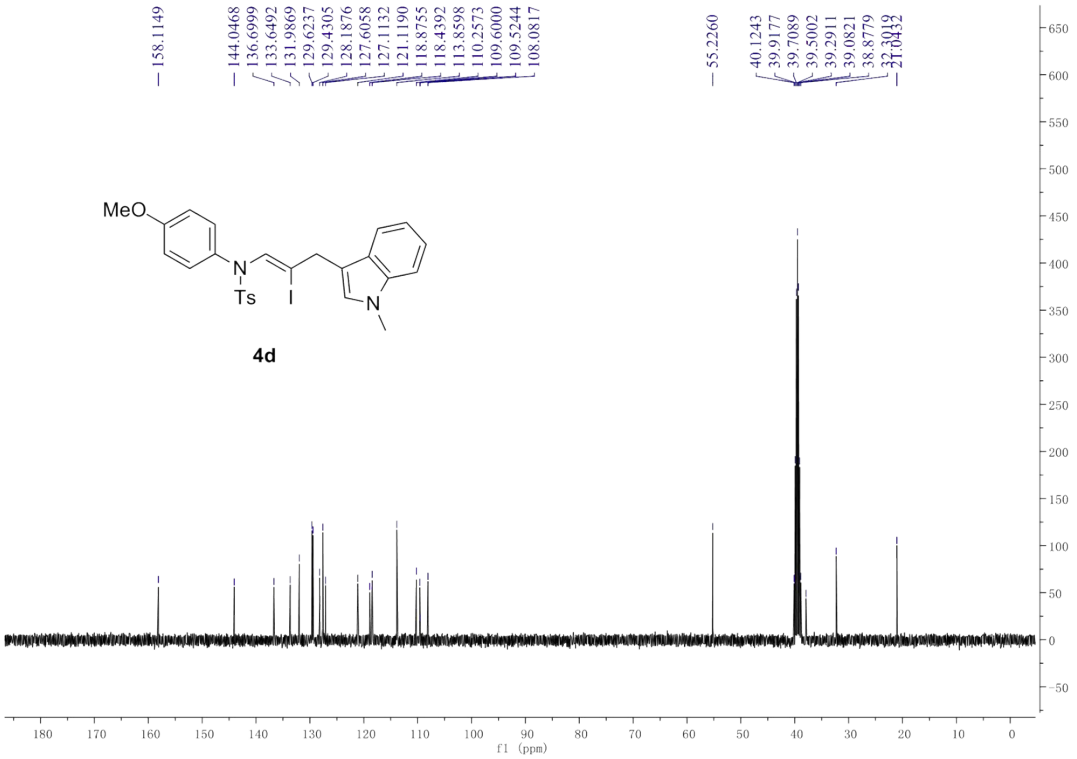
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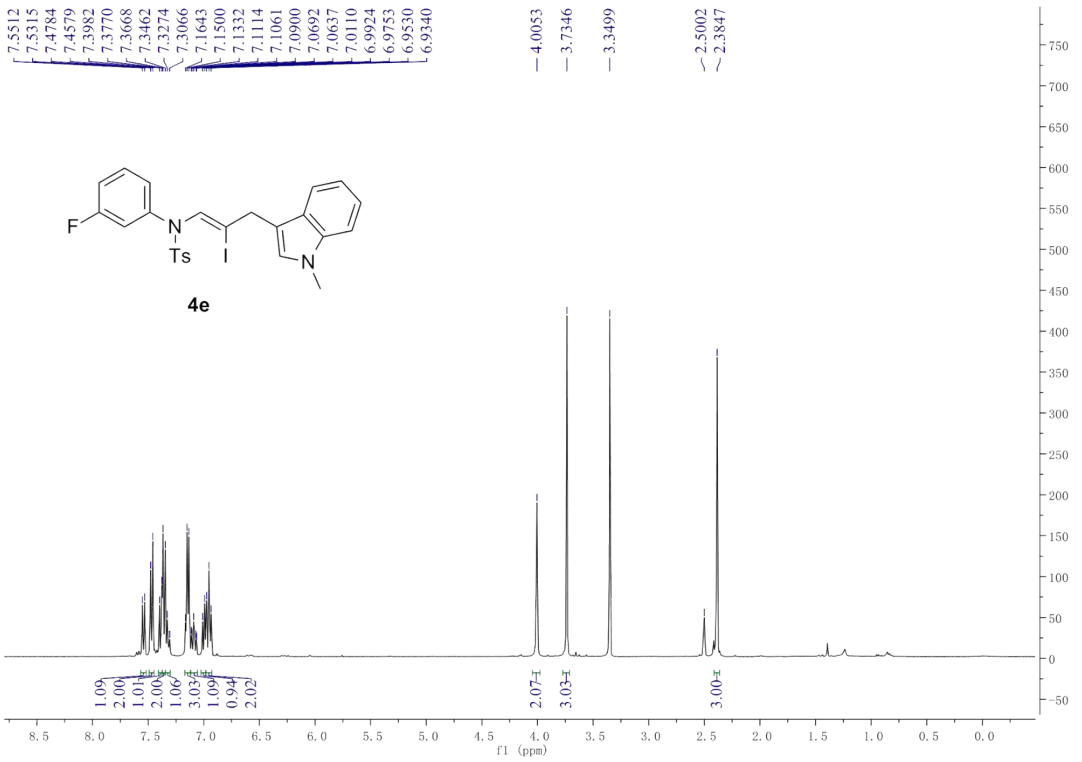
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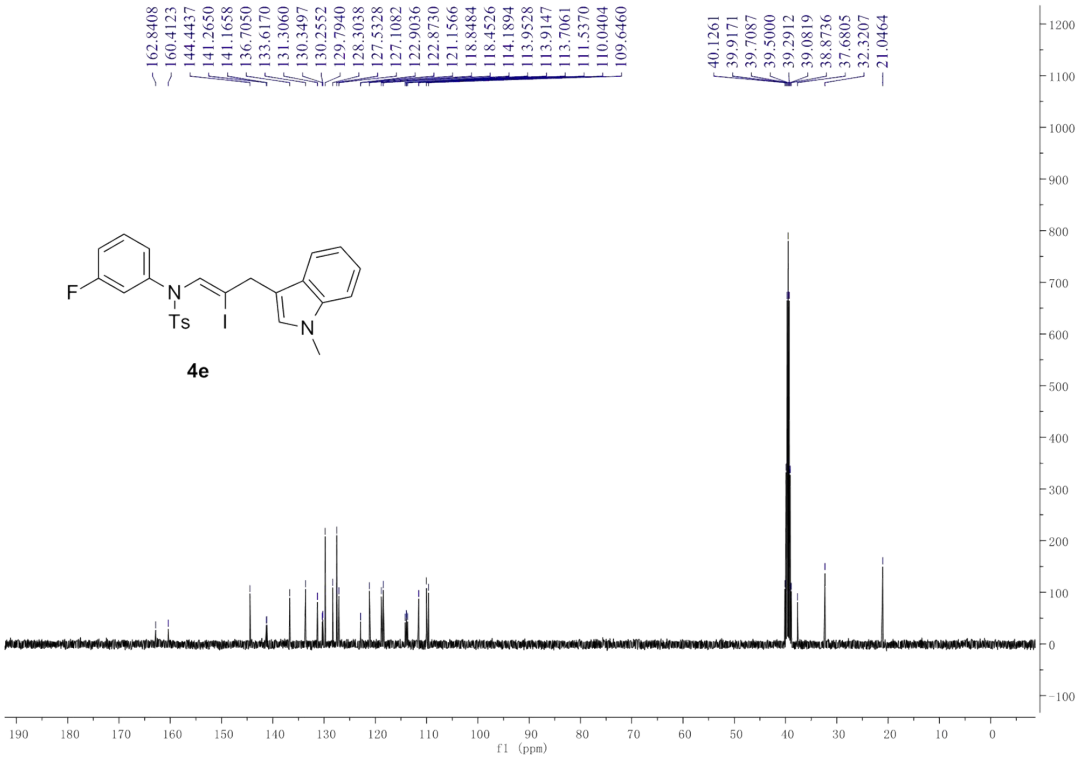
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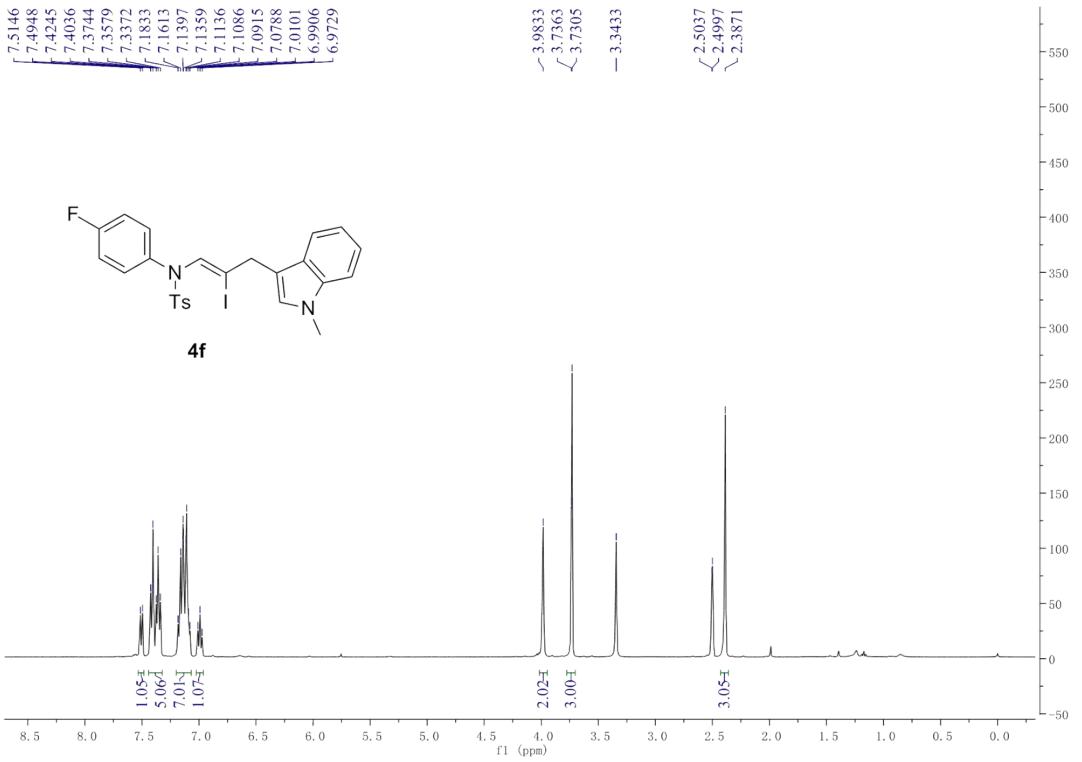
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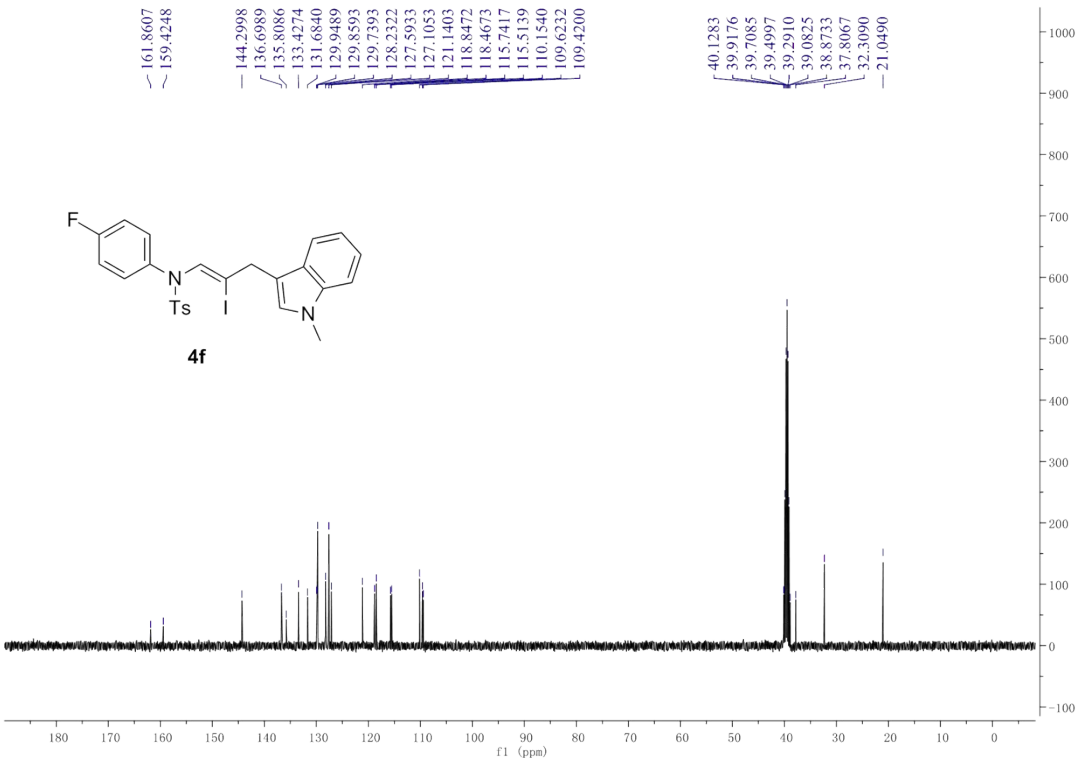
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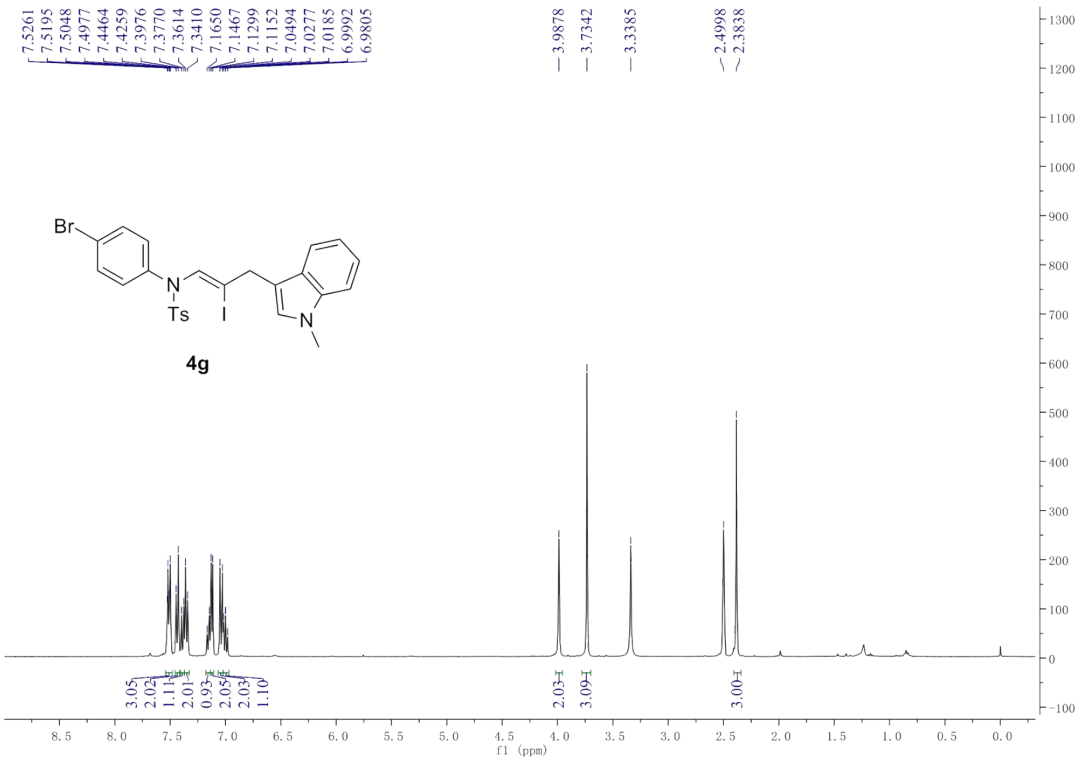
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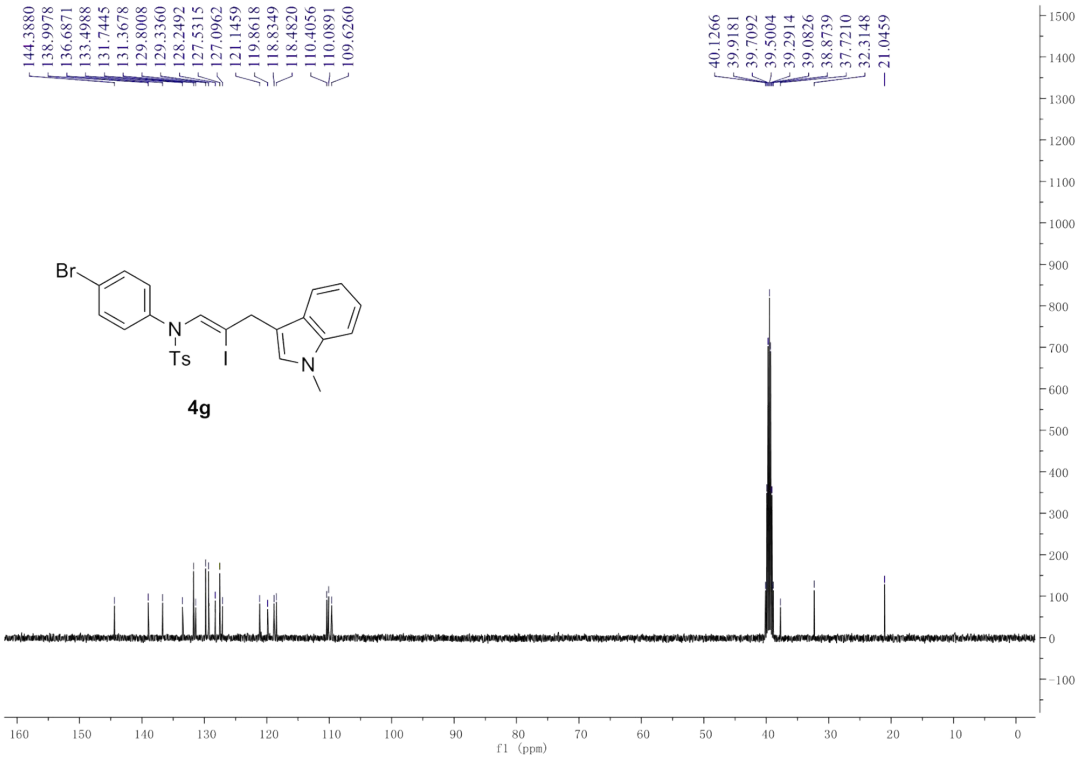
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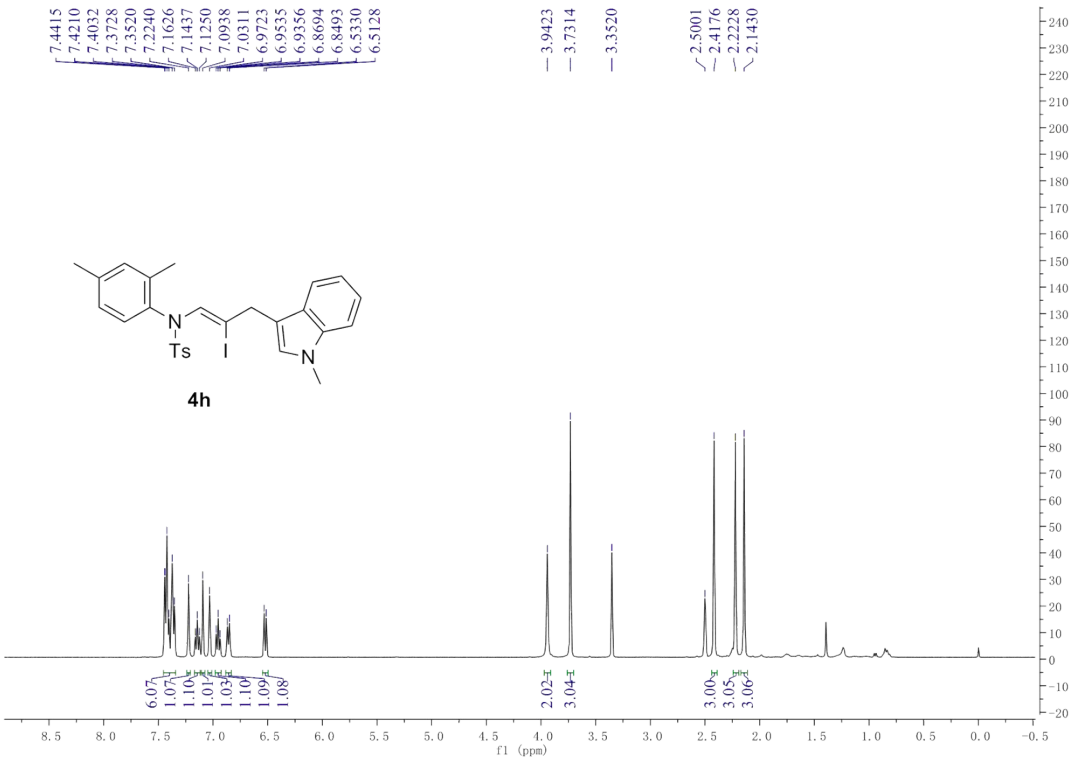
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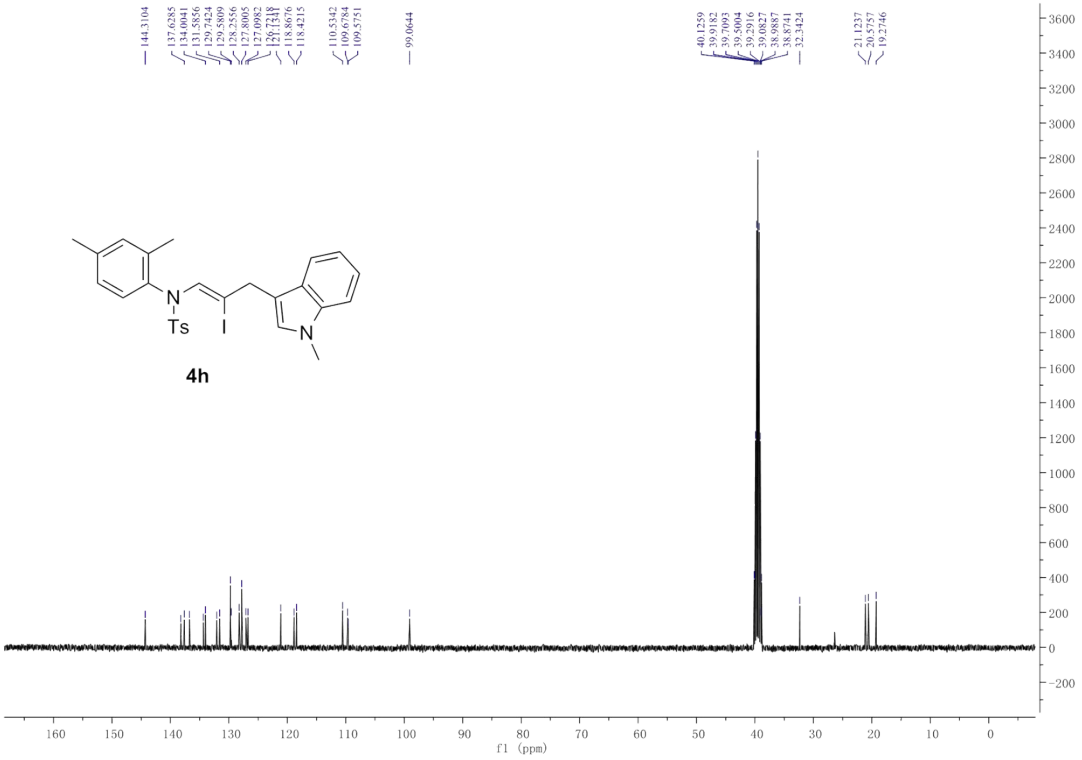
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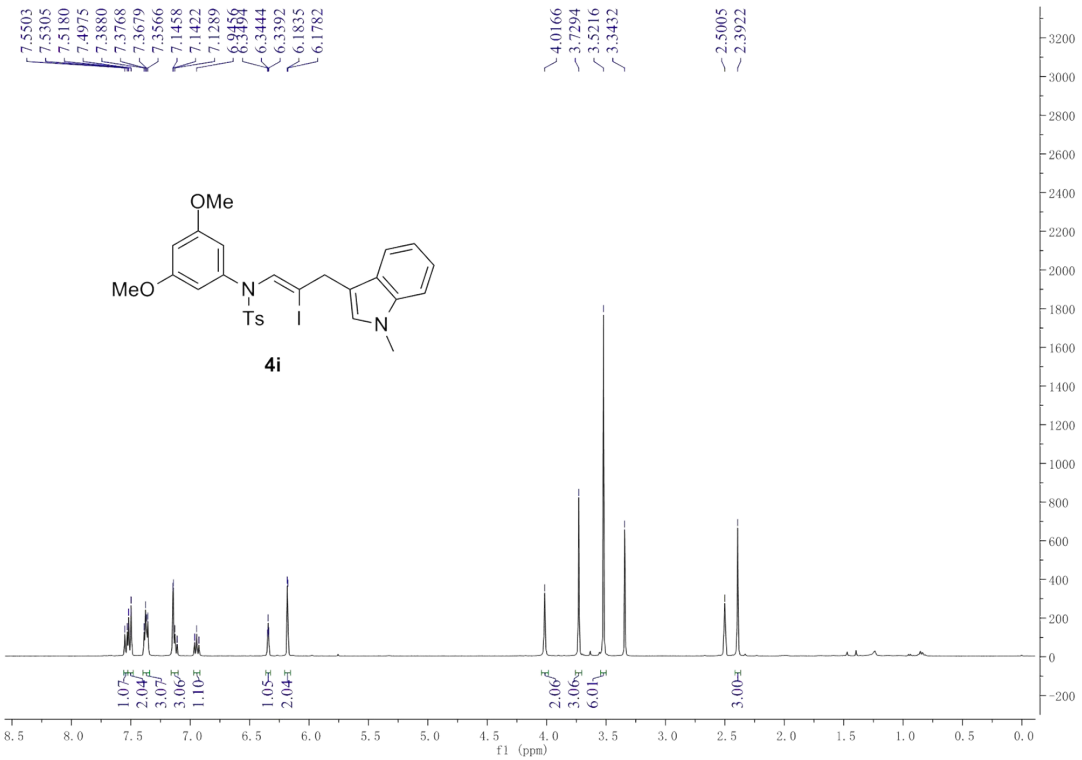
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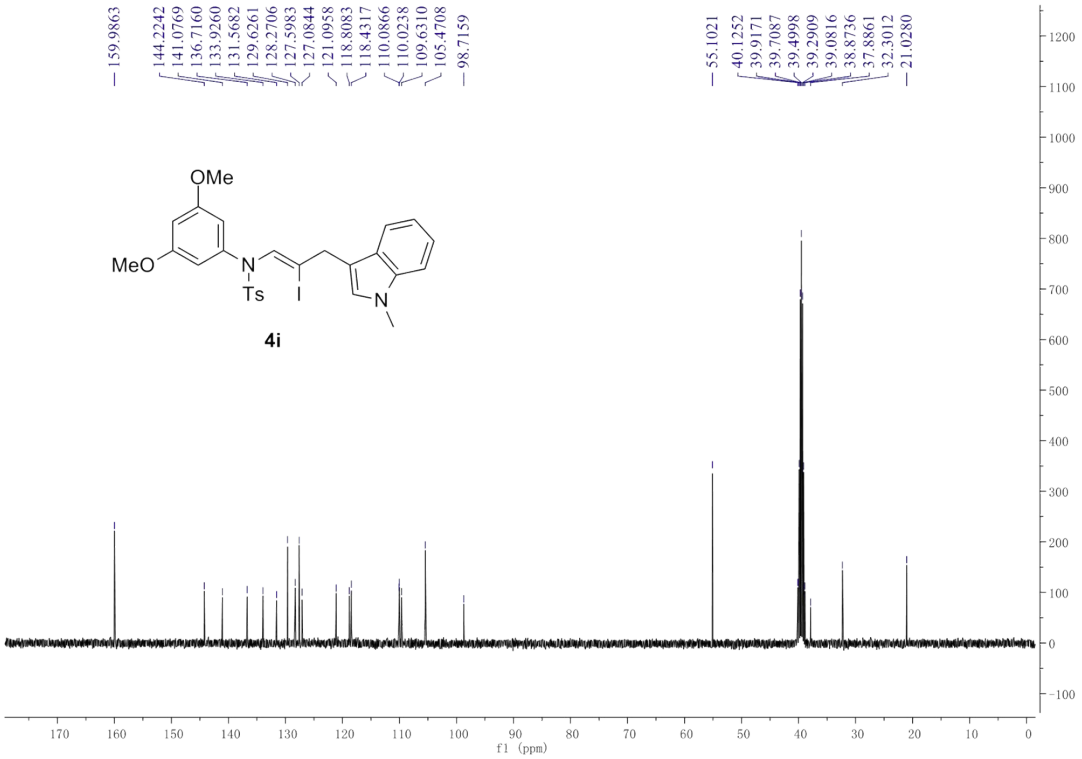
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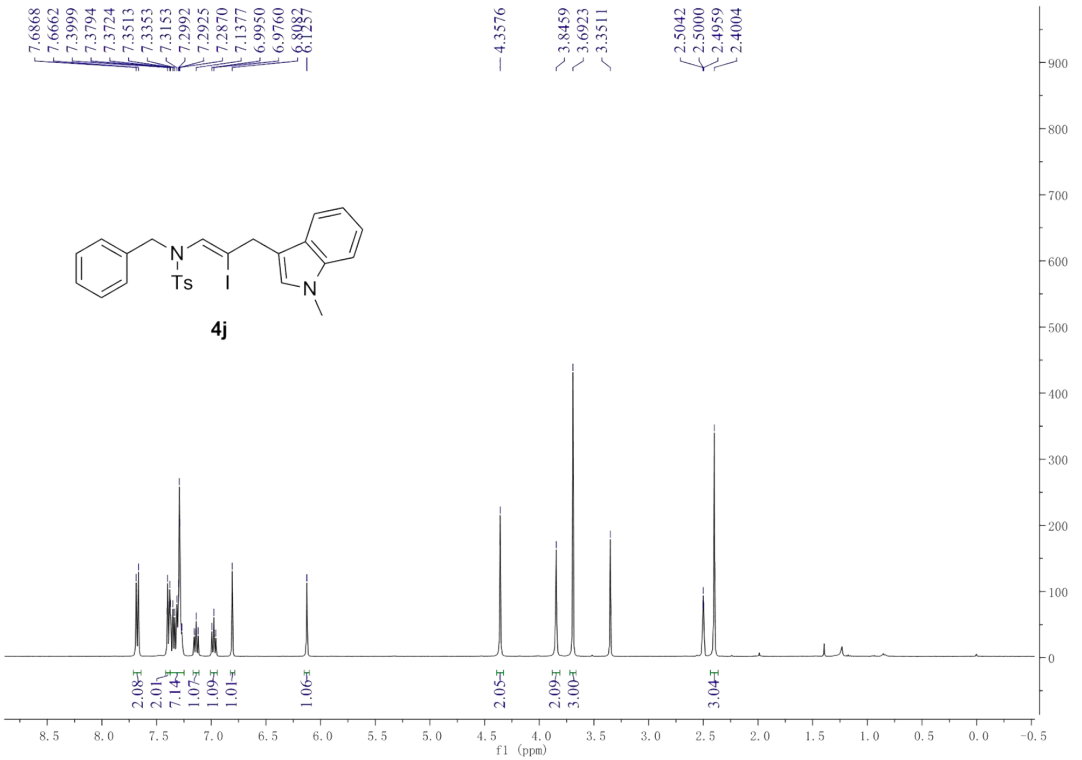
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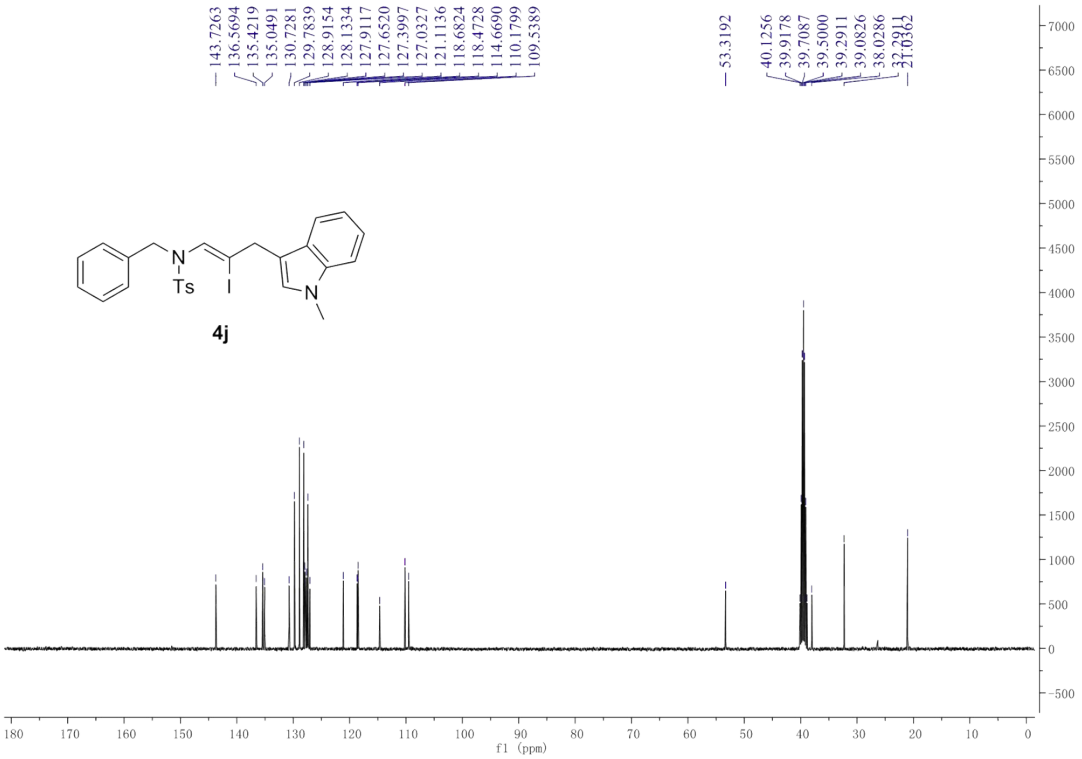
f1 (ppm)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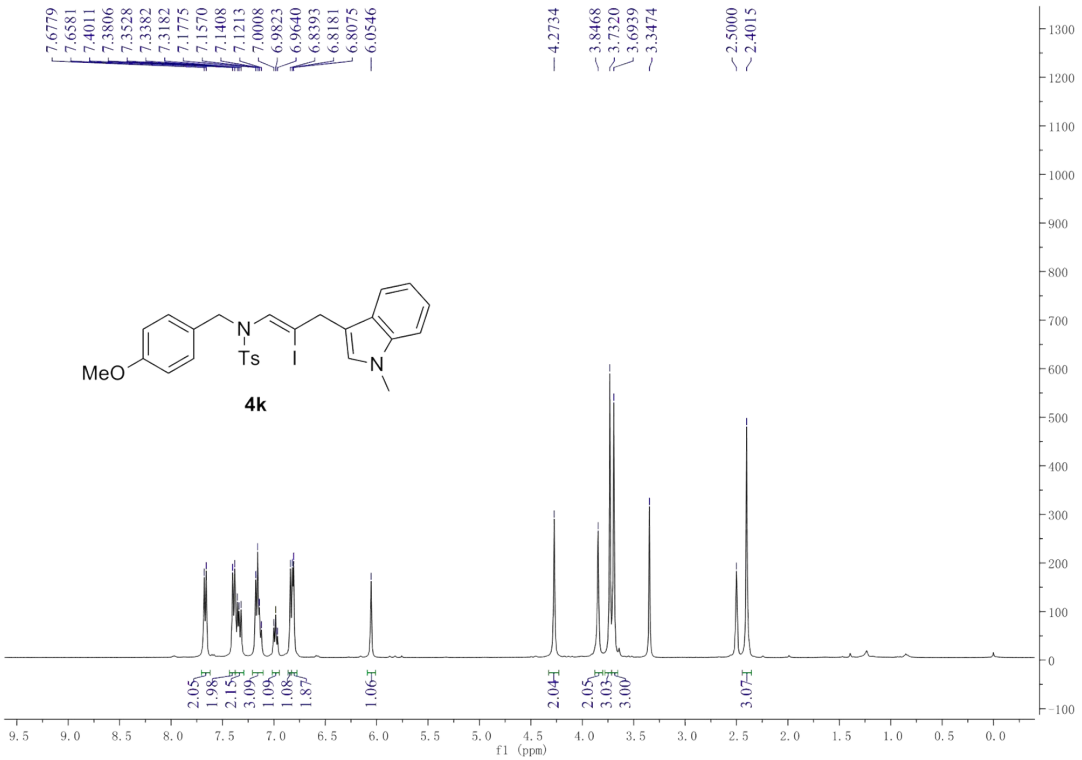
135.4219
135.0491
130.7281
129.7839
128.9154
128.1334
127.9117
127.6520
127.3997
127.0327
121.1136
118.6824
118.4728
114.6690
110.1799
109.5389
53.3192
40.1256
39.9178
39.7087
39.5000
39.2911
39.0826
38.0286
32.2911
21.0362
N
Ts
I
N
4j
f1 (ppm)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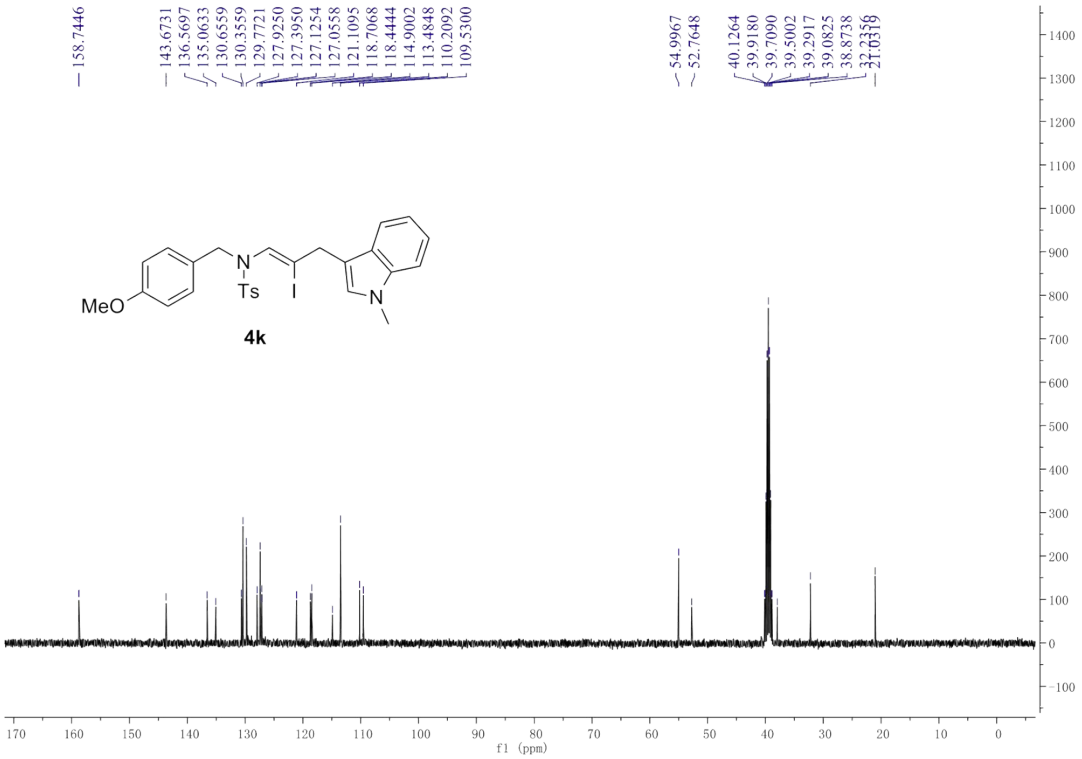
7.6581
7.4011
7.3806
7.3528
7.3382
7.3182
7.1775
7.1570
7.1408
7.1213
7.0008
6.9823
6.9640
6.8393
6.8181
6.8075
6.0546
4.2734
3.8468
3.7320
3.6939
3.3474
2.5000
2.4015
MeO
N
Ts
I
N
4k
2.05
1.98
2.15
3.09
1.09
1.08
1.87
1.06
2.04
2.05
3.03
3.00
3.07
f1 (ppm)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135.0633
130.6559
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129.7721
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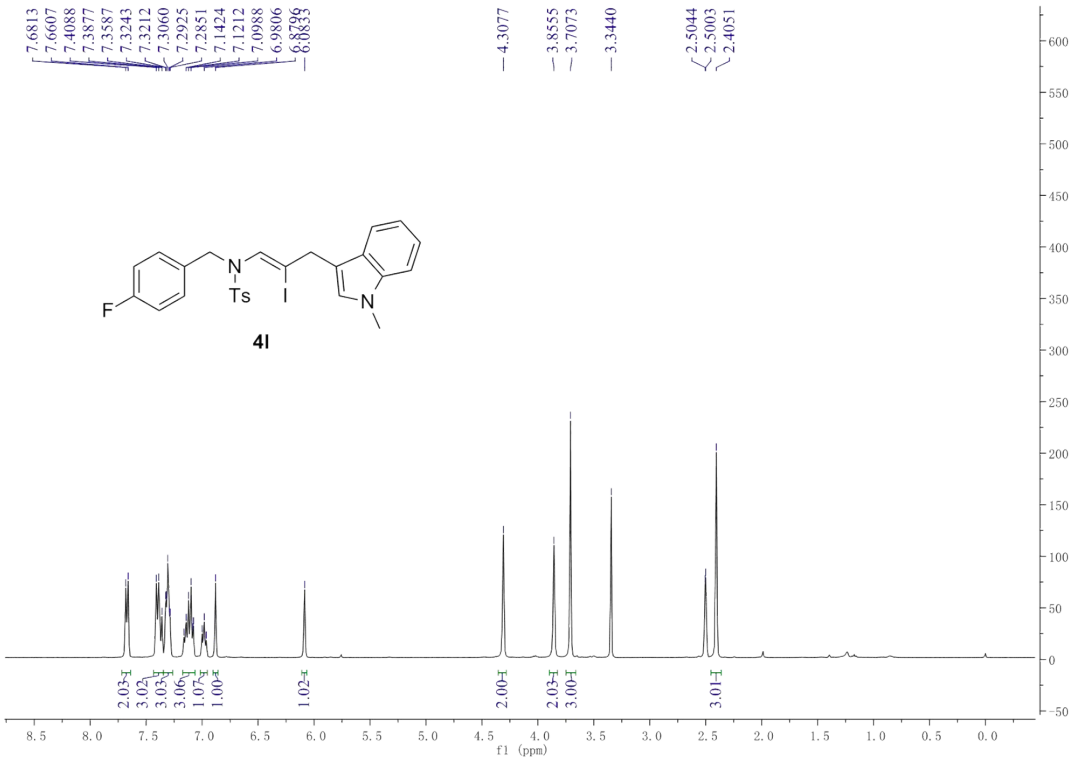
127.3950
127.1254
127.0558
121.1095
118.7068
118.4444
114.9002
113.4848
110.2092
109.5300
54.9967
52.7648
40.1264
39.9180
39.7090
39.5002
39.2917
39.0825
38.8738
32.2356
21.0319
MeO
N
Ts
I
N
4k
f1 (ppm)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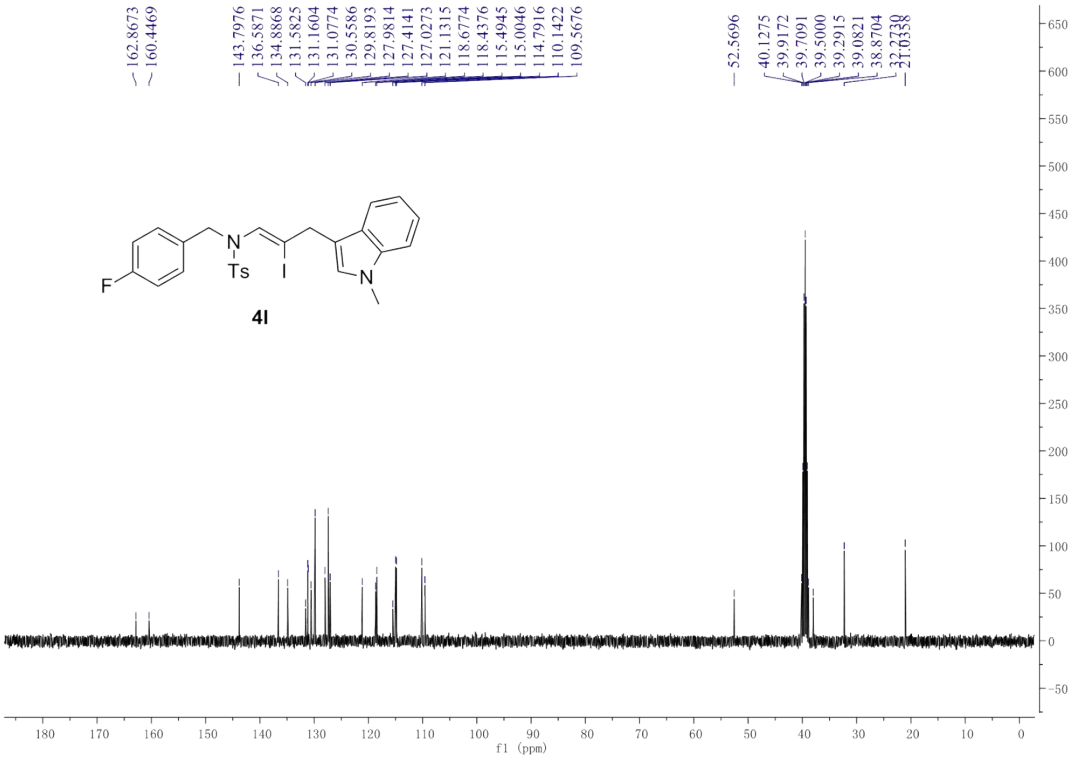
7.6607
7.4088
7.3877
7.3587
7.3243
7.3212
7.3060
7.2925
7.2851
7.1424
7.1212
7.0988
6.9806
6.8796
6.8633
4.3077
3.8555
3.7073
3.3440
2.5044
2.5003
2.4051
F
N
Ts
I
N
4l
2.03
3.02
3.03
3.06
1.07
1.00
1.02
2.00
2.03
3.00
3.01
f1 (ppm)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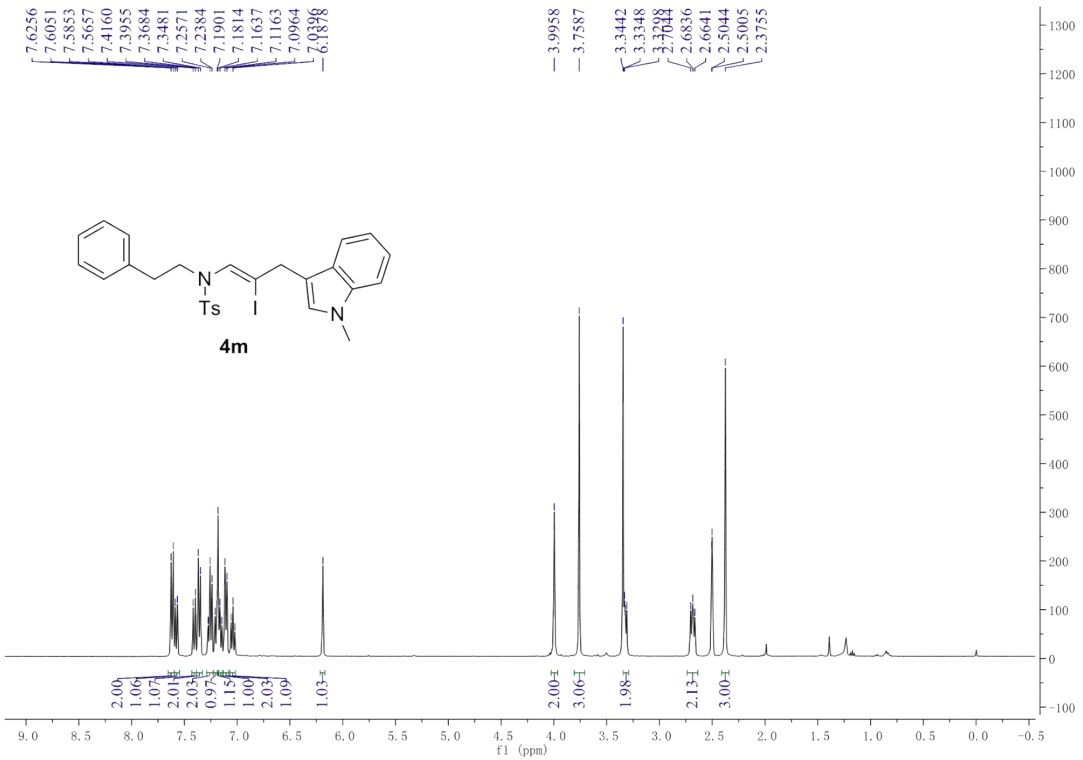
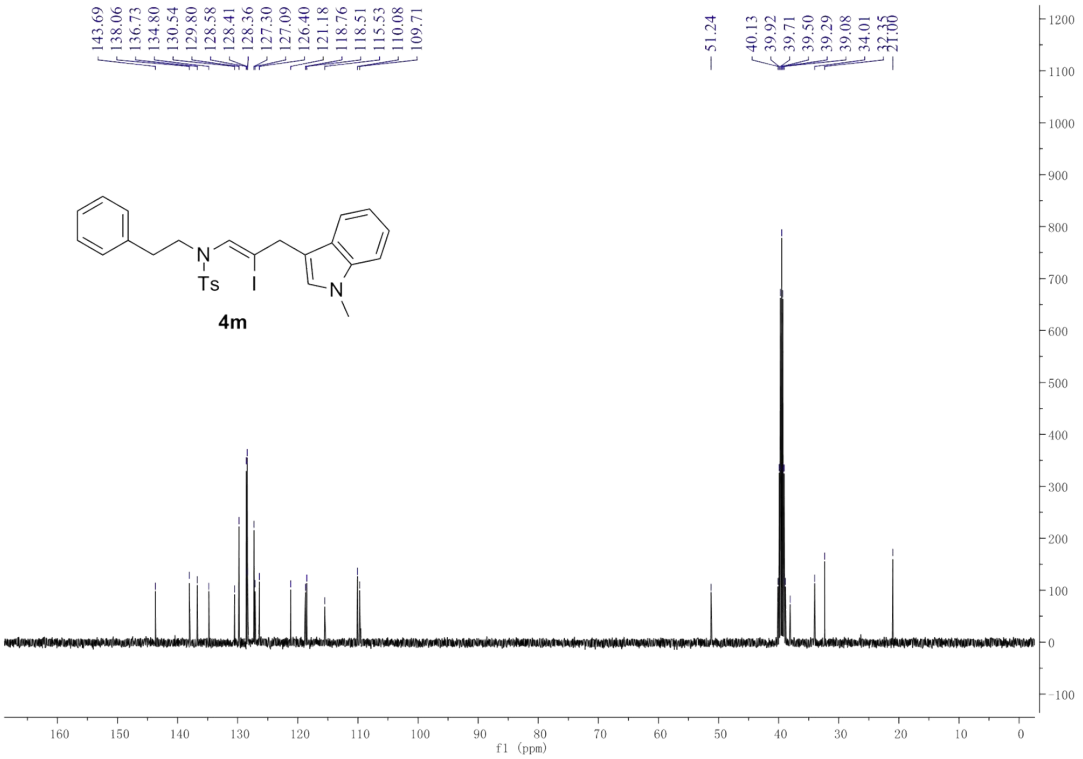
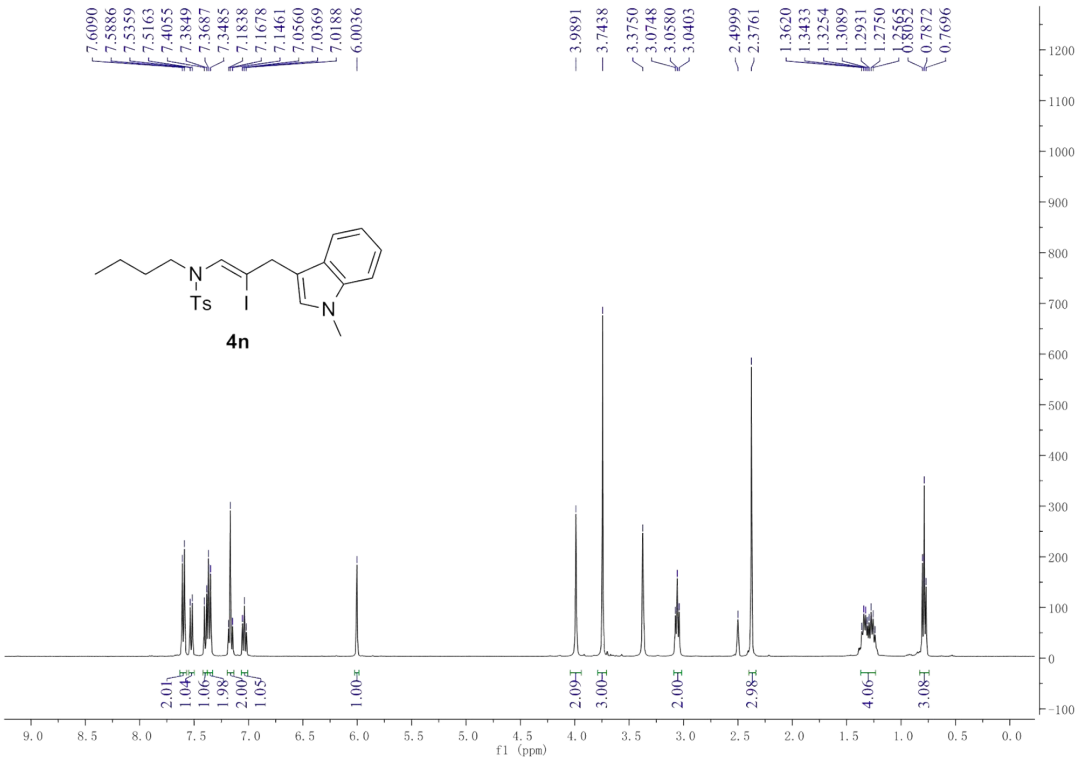
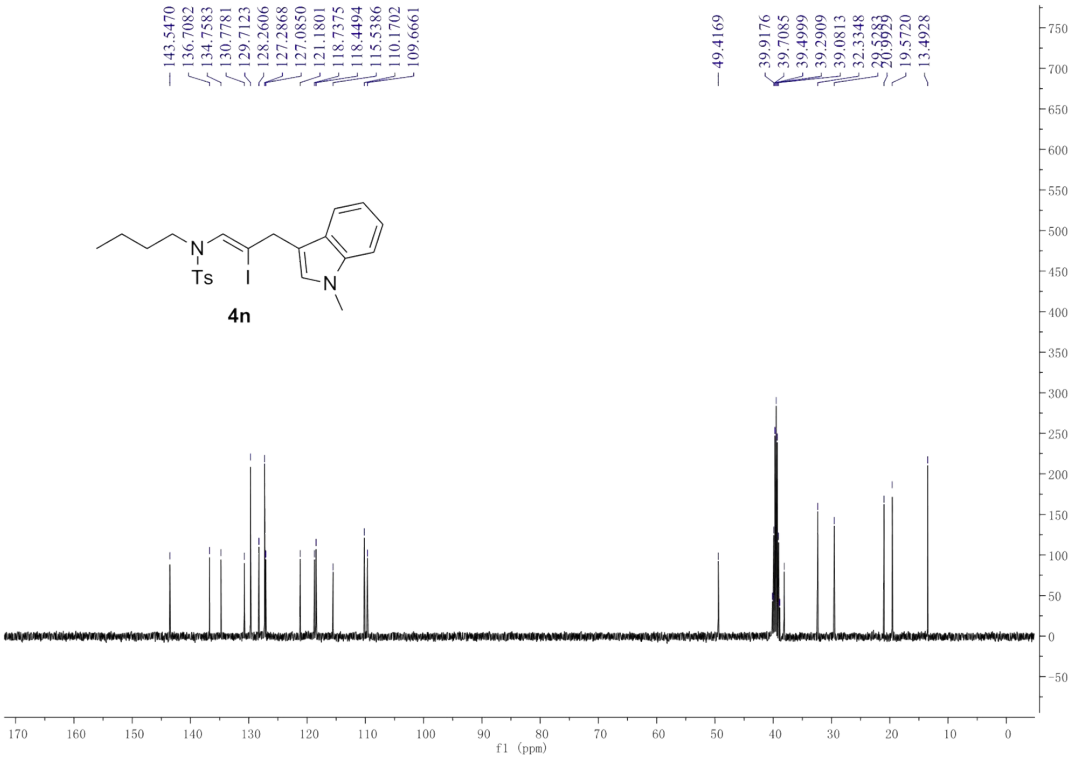
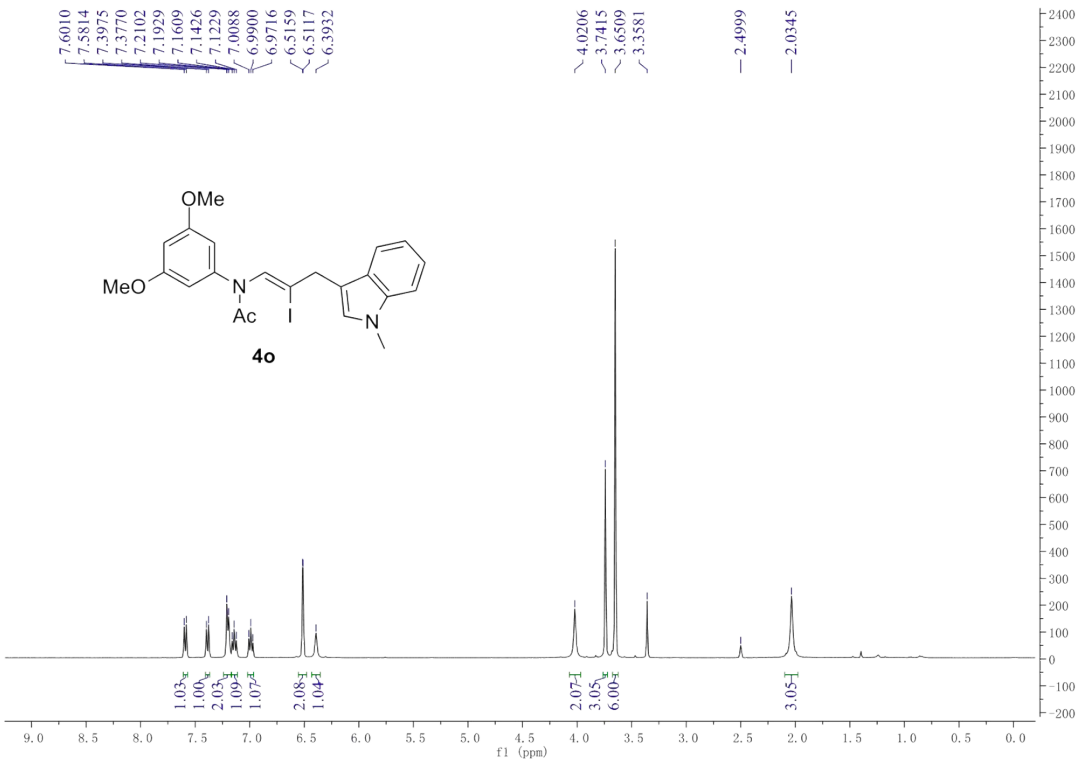
143.7976
136.5871
134.8868
131.5825
131.1604
131.0774
130.5586
129.8193
127.9814
127.4141
127.0273
121.1315
118.6774
118.4376
115.4945
115.0046
114.7916
110.1422
109.5676
52.5696
40.1275
39.9172
39.7091
39.5000
39.2915
39.0821
38.8704
32.2730
21.0358
F
N
Ts
I
N
4l
f1 (ppm)

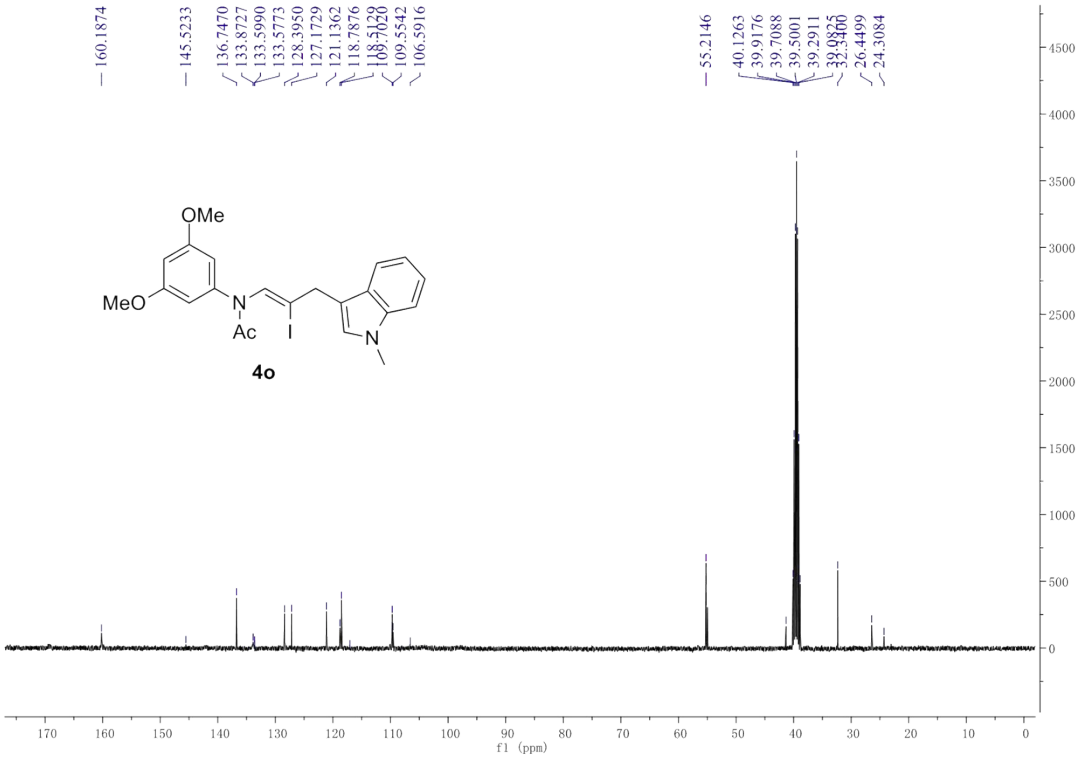

7.6256
7.6051
7.5853
7.5657
7.4160
7.3955
7.3684
7.3481
7.2571
7.2384
7.1901
7.1814
7.1637
7.1163
7.0964
6.8878
3.9958
3.7587
3.3442
3.3348
2.6836
2.6641
2.5044
2.5005
2.3755
Ts
I
N
4m
f1 (ppm)

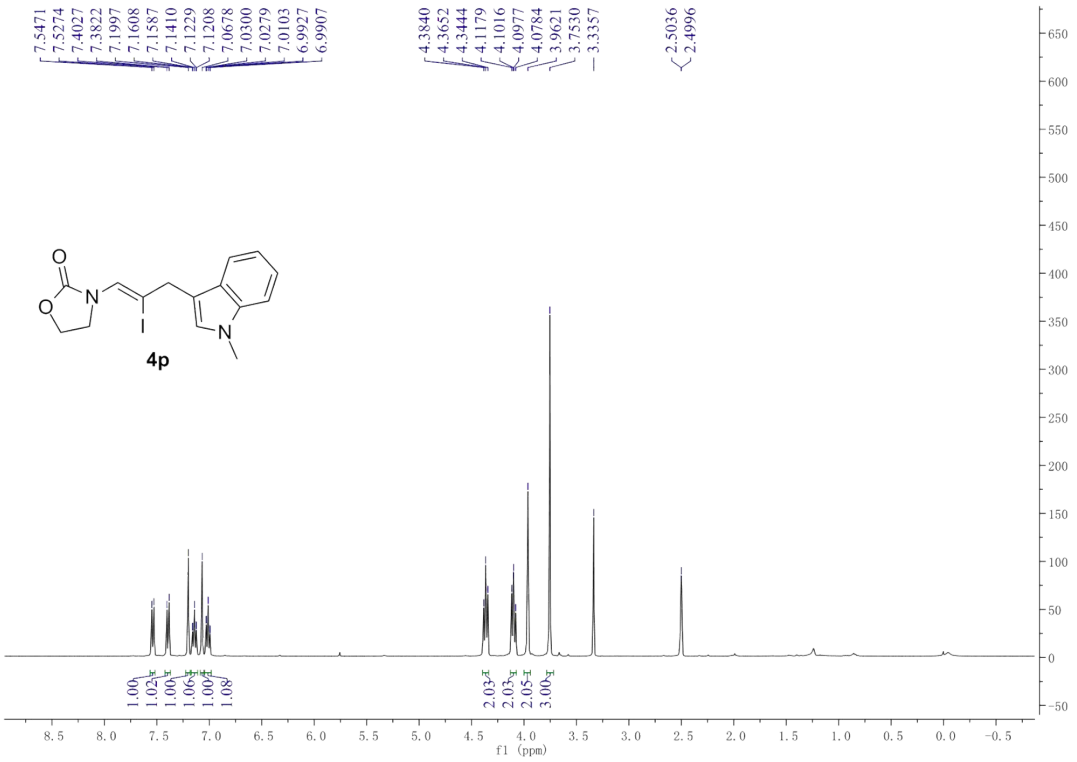

143.69
138.06
136.73
134.80
130.54
129.80
128.58
128.41
128.36
127.30
127.09
126.40
121.18
118.76
118.51
115.53
110.08
109.71
51.24
40.13
39.92
39.71
39.50
39.29
39.08
34.01
32.35
21.00
Ts
I
N
4m
f1 (ppm)

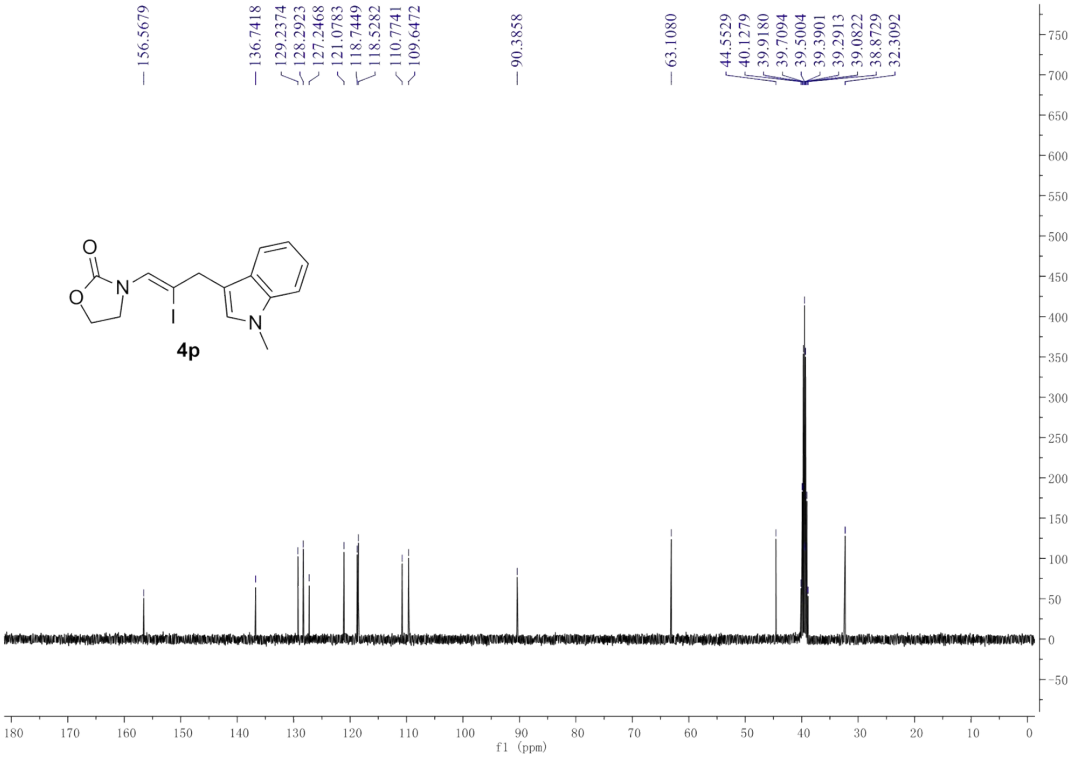

7.6090
7.5886
7.5359
7.5163
7.4055
7.3849
7.3687
7.3485
7.1838
7.1678
7.1461
7.0560
7.0369
7.0188
6.0036
3.9891
3.7438
3.3750
3.0748
3.0580
3.0403
2.4999
2.3761
1.3620
1.3433
1.3254
1.3089
1.2931
1.2750
0.8052
0.7872
0.7696
N
Ts
I
N
4n
2.01
1.04
1.06
1.98
2.00
1.05
1.00
2.09
3.00
2.00
2.98
4.06
3.08
f1 (ppm)


143.5470
136.7082
134.7583
130.7781
129.7123
128.2606
127.2868
127.0850
121.1801
118.7375
118.4494
115.5386
110.1702
109.6661
49.4169
39.9176
39.7085
39.4999
39.2909
39.0813
32.3348
20.6883
20.5929
19.5720
13.4928
N
Ts
I
N
4n
f1 (ppm)

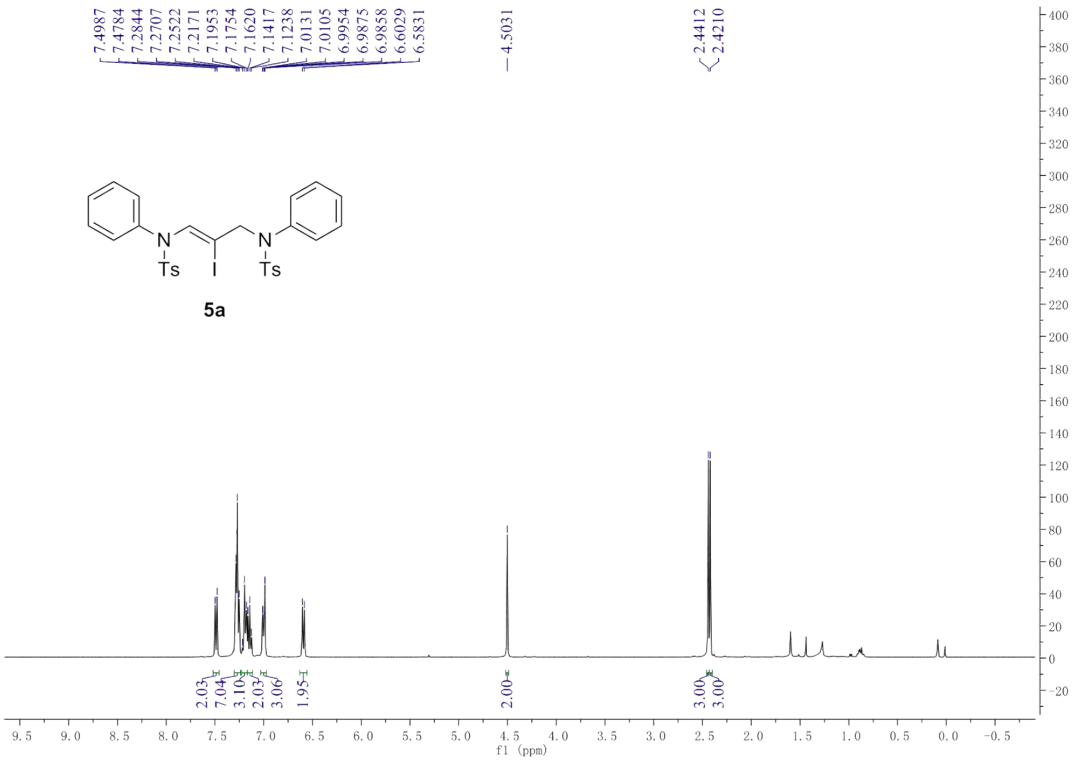

7.6010
7.5814
7.3975
7.3770
7.2102
7.1929
7.1609
7.1426
7.1229
7.0088
6.9900
6.9716
6.5159
6.5117
6.3932
4.0206
3.7415
3.6509
3.3581
2.4999
2.0345
OMe
MeO
N
Ac
I
N
4o
1.03
1.00
2.03
1.09
1.07
2.08
1.04
2.07
3.05
6.00
3.05
f1 (ppm)

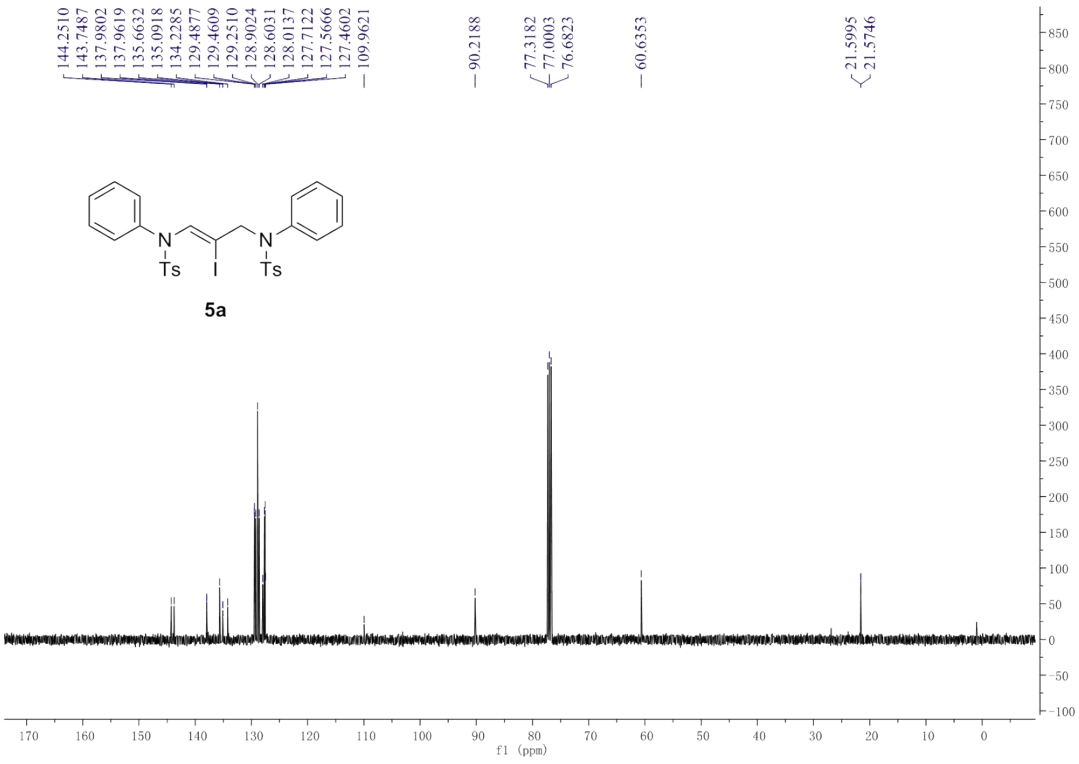

160.1874
145.5233
136.7470
133.8727
133.5990
133.5773
128.3950
127.1729
121.1362
118.7876
109.7020
109.5542
106.5916
55.2146
40.1263
39.9176
39.7088
39.5001
39.2911
32.9406
26.4499
24.3084
OMe
MeO
N
Ac
I
N
4o
f1 (ppm)

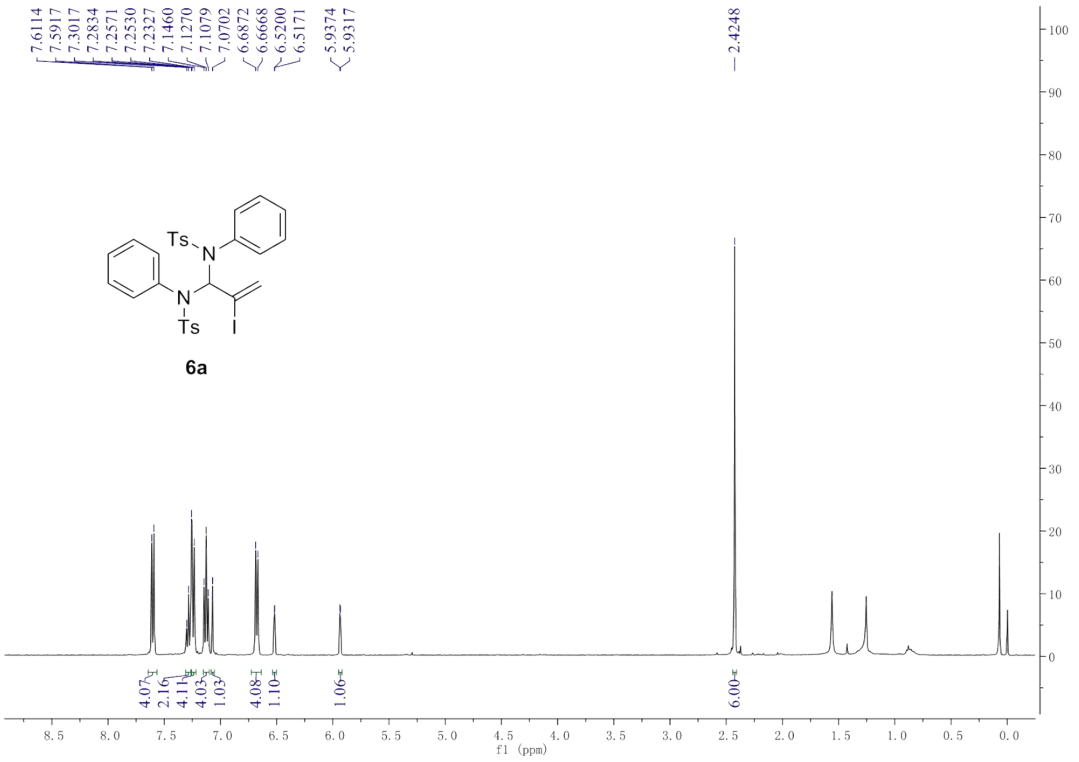

7.5471
7.5274
7.4027
7.3822
7.1997
7.1608
7.1587
7.1410
7.1229
7.1208
7.0678
7.0300
7.0279
7.0103
6.9927
6.9907
4.3840
4.3652
4.3444
4.1179
4.1016
4.0977
4.0784
3.9621
3.7530
3.3357
2.5036
2.4996
4p
1.00
1.02
1.00
1.06
1.00
1.08
2.03
2.03
2.05
3.00
f1 (ppm)

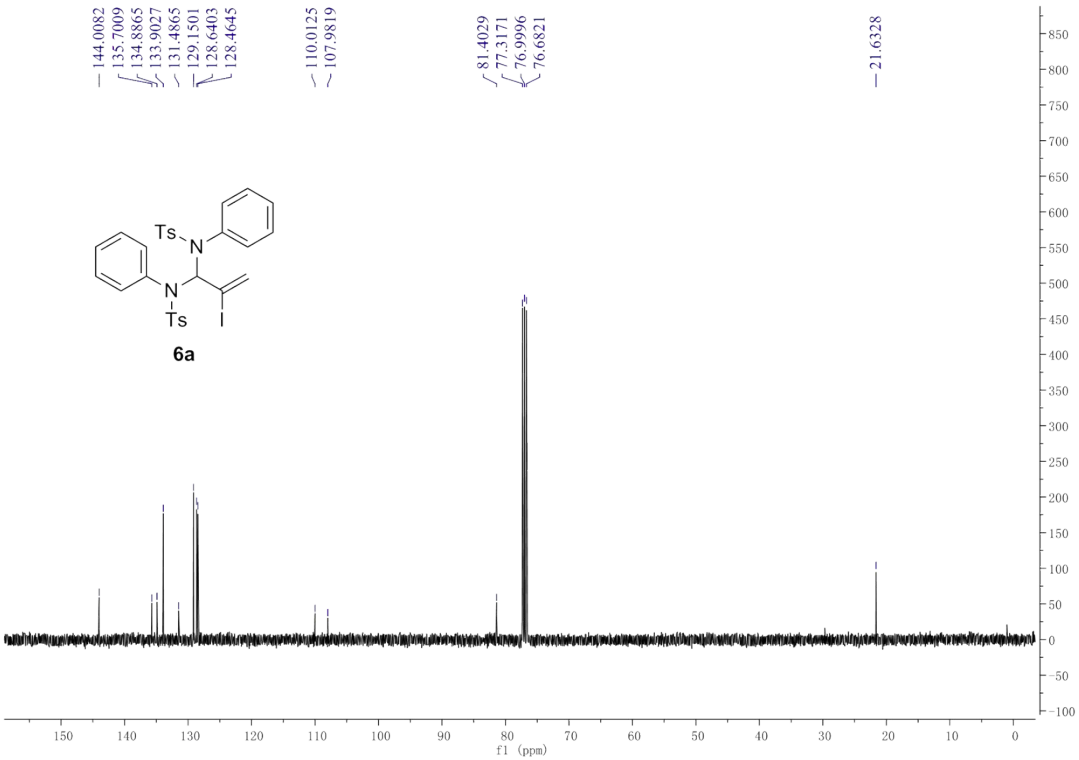

156.5679
136.7418
129.2374
128.2923
127.2468
121.0783
118.7449
118.5282
110.7741
109.6472
90.3858
63.1080
44.5529
40.1279
39.9180
39.7094
39.5004
39.3901
39.2913
39.0822
38.8729
32.3092
4p
f1 (ppm)

7. NMR Spectra for 5a and 6a

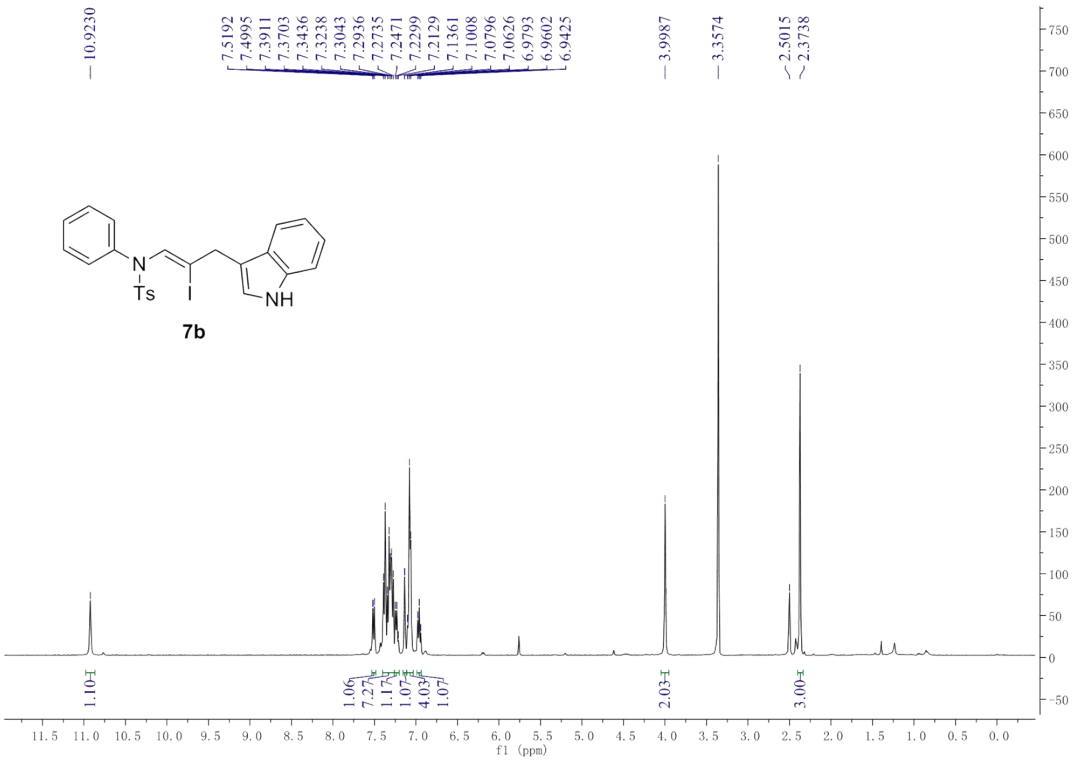


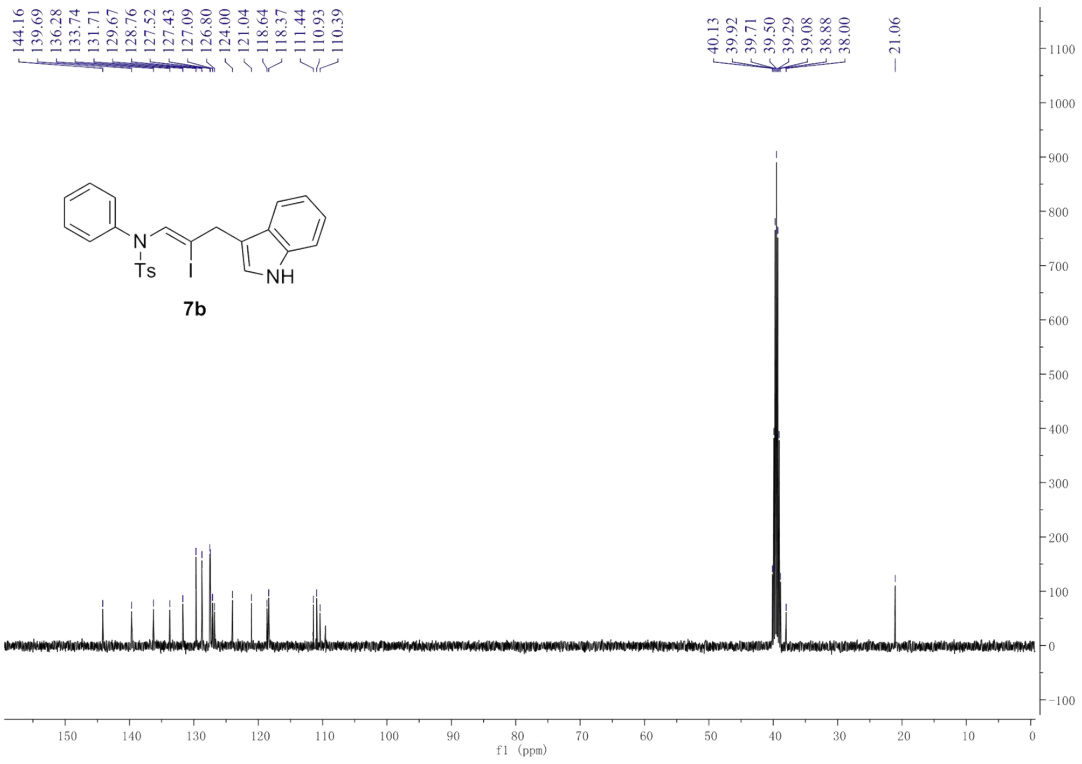


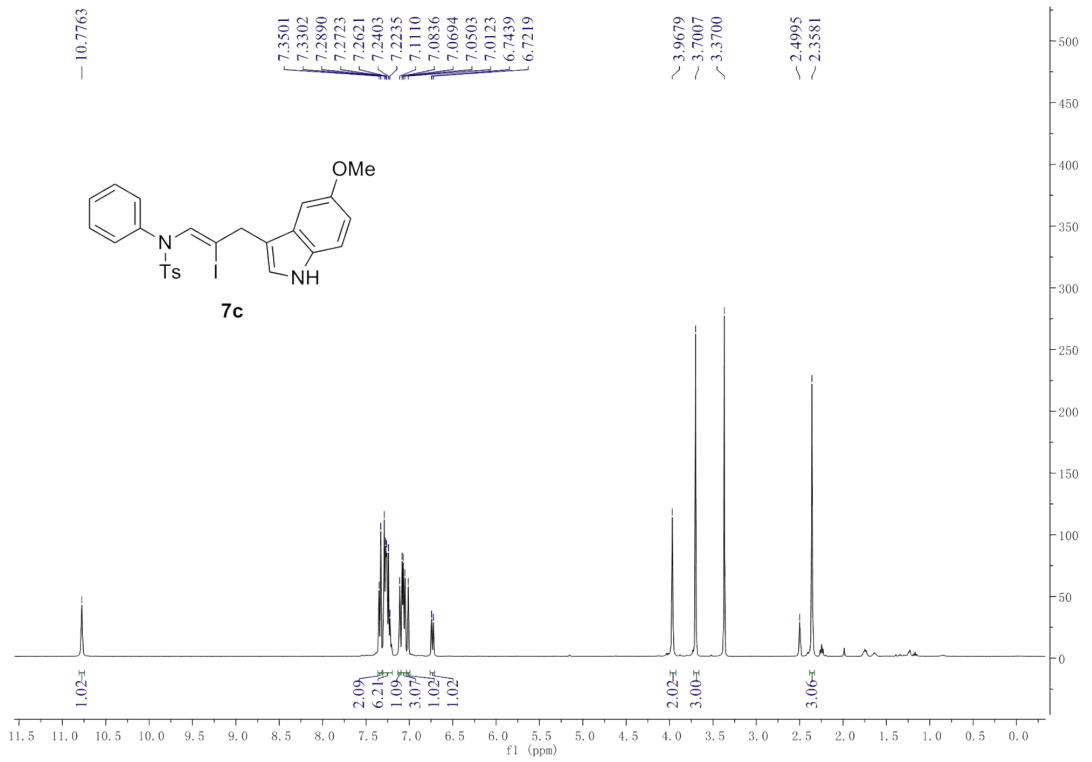

7.6114
7.5917
7.3017
7.2834
7.2571
7.2530
7.2327
7.1460
7.1270
7.1079
7.0702
6.6872
6.6668
6.5200
6.5171
5.9374
5.9317
2.4248
Ts
N
N
Ts
I
6a
4.07
2.16
4.11
4.03
1.03
4.08
1.10
1.06
6.00
f1 (ppm)

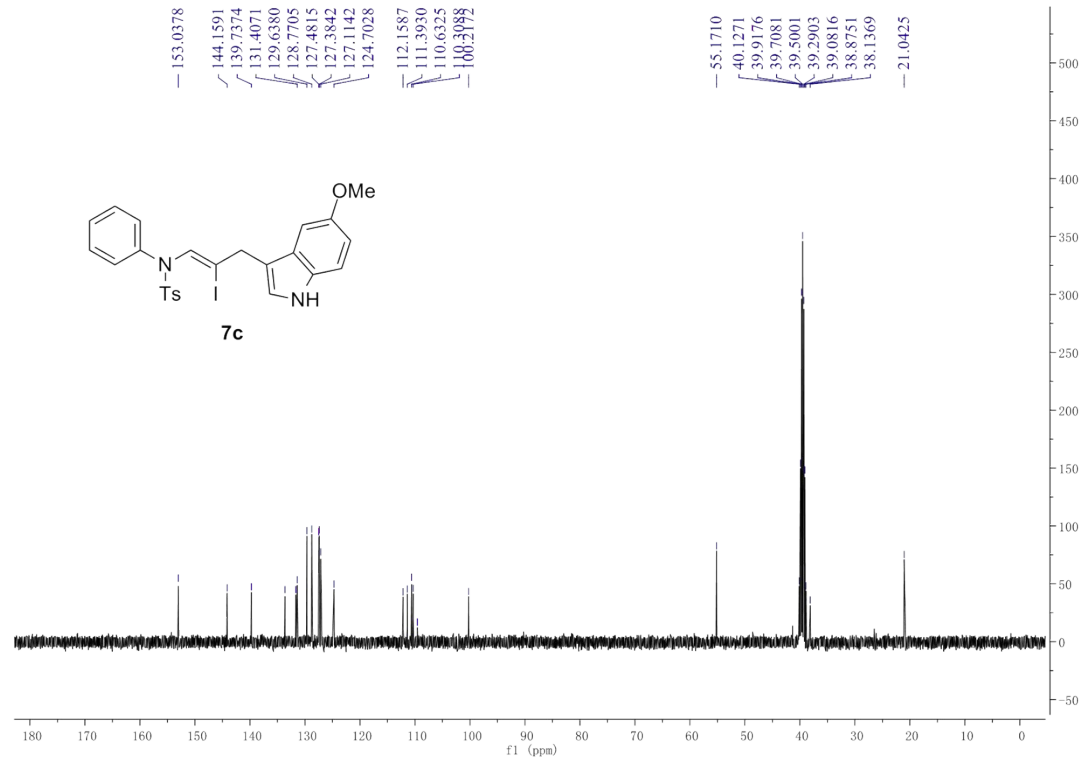

144.0082
135.7009
134.8865
133.9027
131.4865
129.1501
128.6403
128.4645
110.0125
107.9819
81.4029
77.3171
76.9996
76.6821
21.6328
Ts
N
N
Ts
I
6a
f1 (ppm)

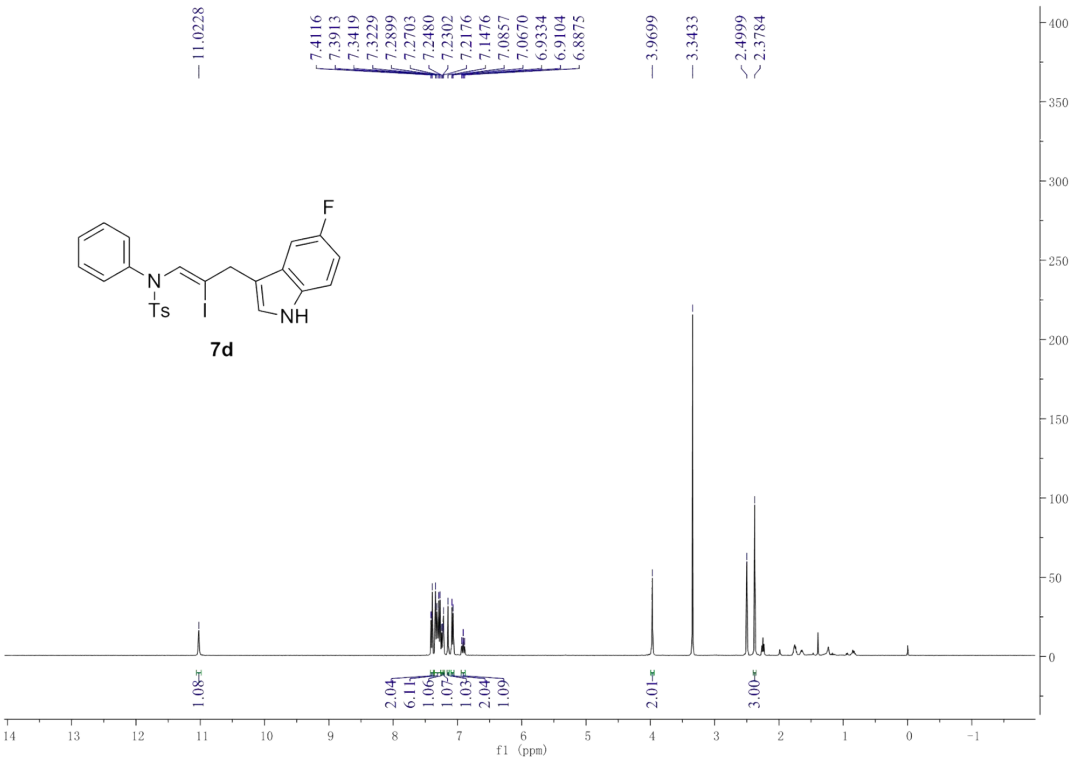
8. NMR Spectra for 7b – 7l

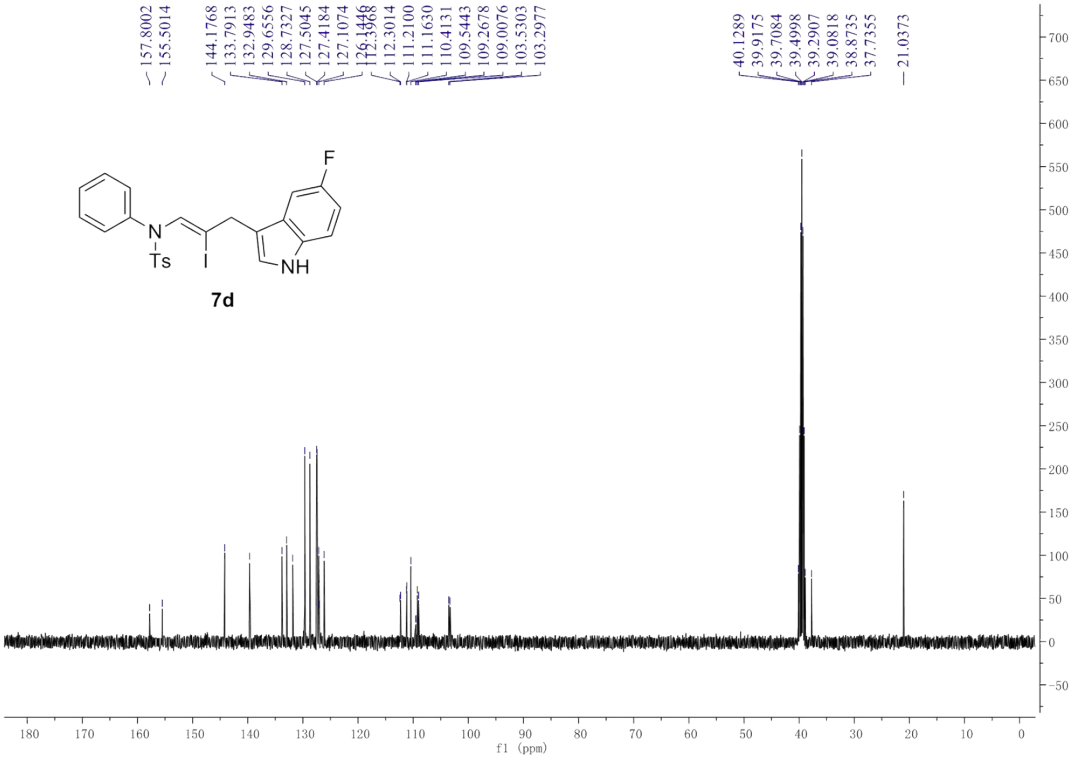


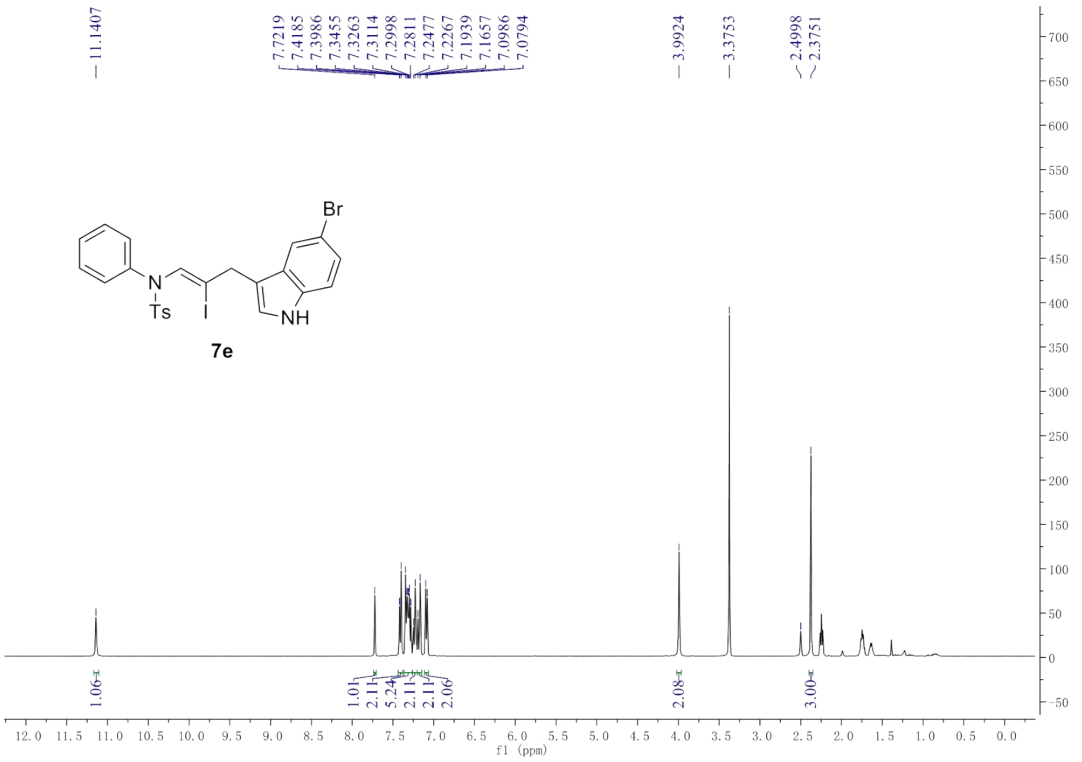


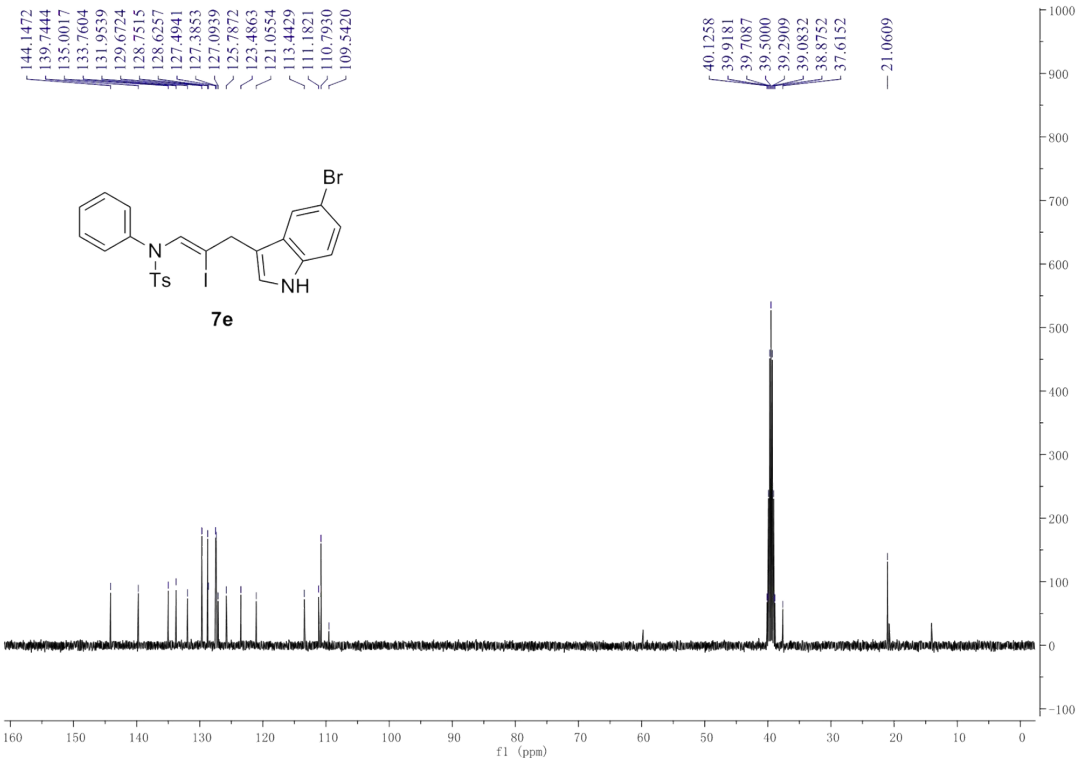

10.7763
7.3501
7.3302
7.2890
7.2723
7.2621
7.2403
7.2235
7.1110
7.0836
7.0694
7.0503
7.0123
6.7439
6.7219
3.9679
3.7007
3.3700
2.4995
2.3581
OMe
N
Ts
I
NH
7c
1.02
2.09
6.21
1.09
3.07
1.02
1.02
2.02
3.00
3.06
f1 (ppm)

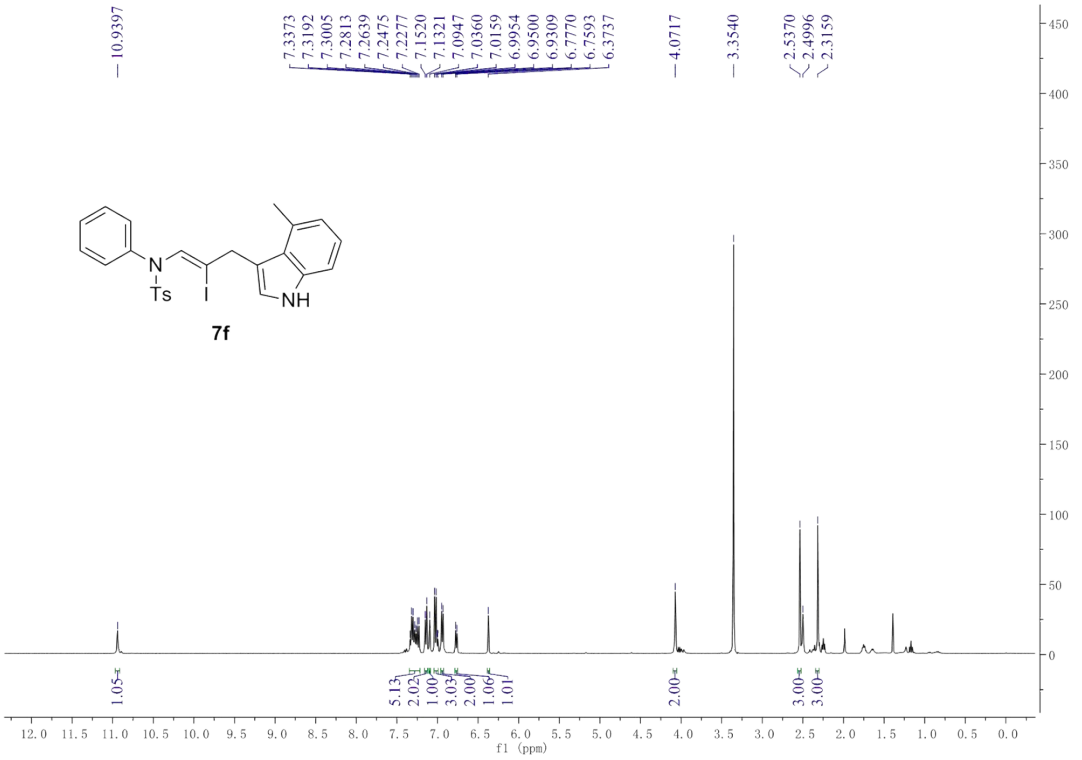

153.0378
144.1591
139.7374
131.4071
129.6380
128.7705
127.4815
127.3842
127.1142
124.7028
112.1587
111.3930
110.6325
55.1710
40.1271
39.9176
39.7081
39.5001
39.2903
39.0816
38.8751
38.1369
21.0425
OMe
N
Ts
I
NH
7c
f1 (ppm)

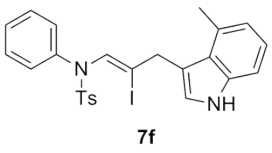

11.0228
7.4116
7.3913
7.3419
7.3229
7.2899
7.2703
7.2480
7.2302
7.2176
7.1476
7.0857
7.0670
6.9334
6.9104
6.8875
3.9699
3.3433
2.4999
2.3784
F
N
Ts
I
NH
7d
1.08
2.04
6.11
1.06
1.07
1.03
2.04
1.09
2.01
3.00
f1 (ppm)


157.8002
155.5014
144.1768
133.7913
132.9483
129.6556
128.7327
127.5045
127.4184
127.1074
112.3968
112.3014
111.2100
111.1630
110.4131
109.5443
109.2678
109.0076
103.5303
103.2977
40.1289
39.9175
39.7084
39.4998
39.2907
39.0818
38.8735
37.7355
21.0373
F
N
Ts
I
NH
7d
f1 (ppm)


11.1407
7.7219
7.4185
7.3986
7.3455
7.3263
7.3114
7.2998
7.2811
7.2477
7.2267
7.1939
7.1657
7.0986
7.0794
3.9924
3.3753
2.4998
2.3751
Br
N
Ts
I
NH
7e
1.06
1.01
2.11
5.24
2.11
2.11
2.06
2.08
3.00
f1 (ppm)


144.1472
139.7444
135.0017
133.7604
131.9539
129.6724
128.7515
128.6257
127.4941
127.3853
127.0939
125.7872
123.4863
121.0554
113.4429
111.1821
110.7930
109.5420
40.1258
39.9181
39.7087
39.5000
39.2909
39.0832
38.8752
37.6152
21.0609
Br
N
Ts
I
NH
7e
f1 (ppm)


10.9397
7.3373
7.3192
7.3005
7.2813
7.2639
7.2475
7.2277
7.1520
7.1321
7.0947
7.0360
7.0159
6.9954
6.9500
6.9309
6.7770
6.7593
6.3737
4.0717
3.3540
2.5370
2.4996
2.3159
1.05
5.13
2.02
1.00
3.03
2.00
1.06
1.01
2.00
3.00
3.00
f1 (ppm)

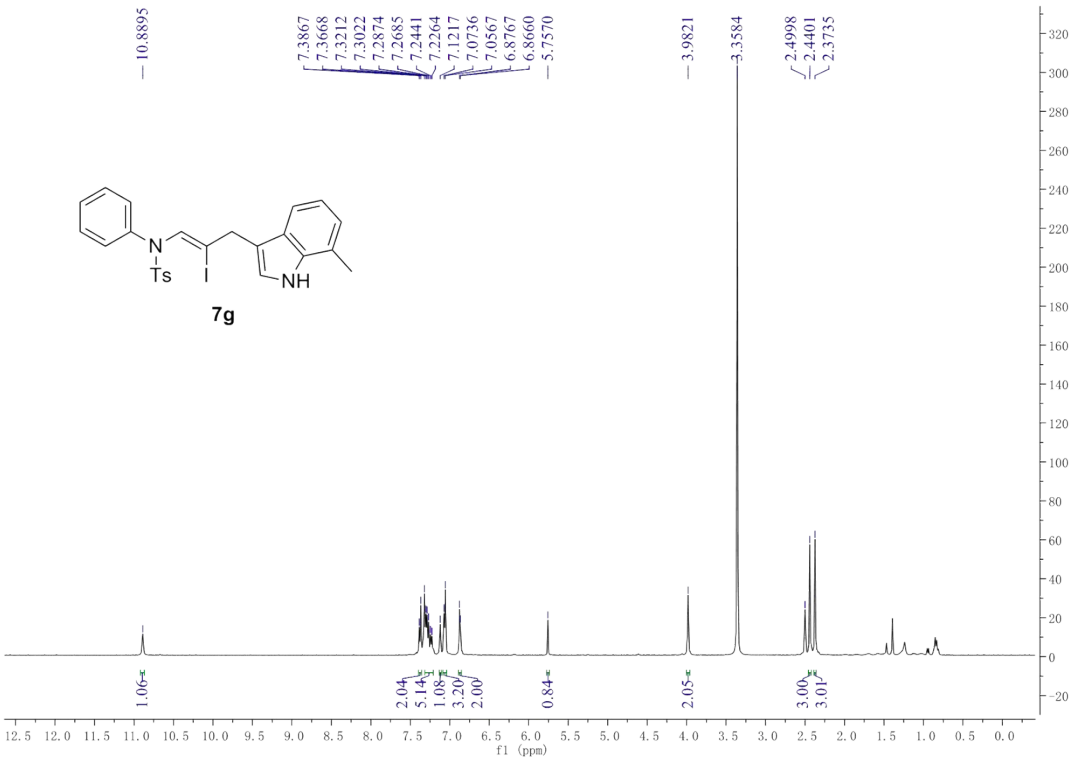

N
Ts
I
NH

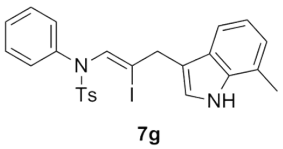
7f

144.0816
139.6998
136.7719
133.1493
131.9683
129.6082
129.5467
128.8270
127.3604
127.2701
125.2285
124.3889
121.3298
120.1743
111.9580
110.9747
109.5567
109.5294
40.1625
40.1254
39.9177
39.7085
39.5000
39.2914
39.0826
38.8722
21.0235
19.3874
f1 (ppm)

N
Ts
I
NH

7f


10.8895
7.3867
7.3668
7.3212
7.3022
7.2874
7.2685
7.2441
7.2264
7.1217
7.0736
7.0567
6.8767
6.8660
5.7570
3.9821
3.3584
2.4998
2.4401
2.3735
1.06
2.04
5.14
1.08
3.20
2.00
0.84
2.05
3.00
3.01
f1 (ppm)

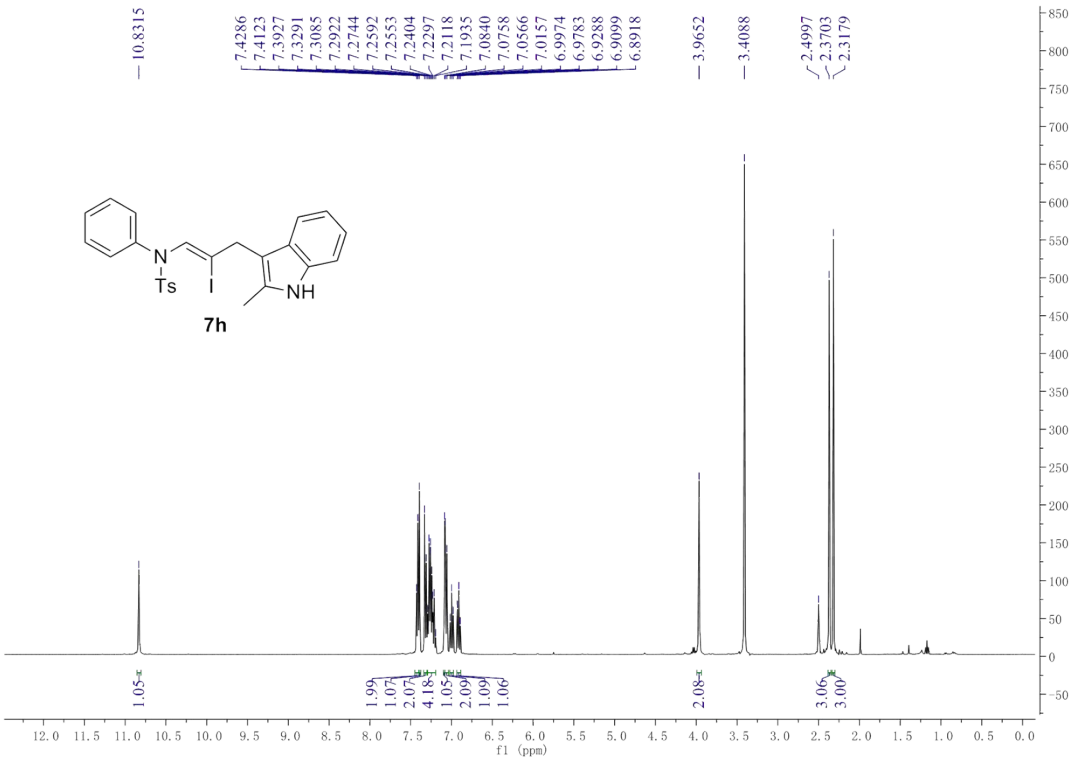

N
Ts
I
NH

7g

144.1380
139.7209
135.8253
133.7819
131.6928
129.6441
128.7399
127.5268
127.4230
127.0753
126.5062
123.7081
121.5817
120.4878
118.6255
116.2662
111.3842
110.5212
40.1267
39.9179
39.7094
39.5001
39.2921
39.0825
38.8745
38.1412
21.0517
16.7595
f1 (ppm)

N
Ts
I
NH

7g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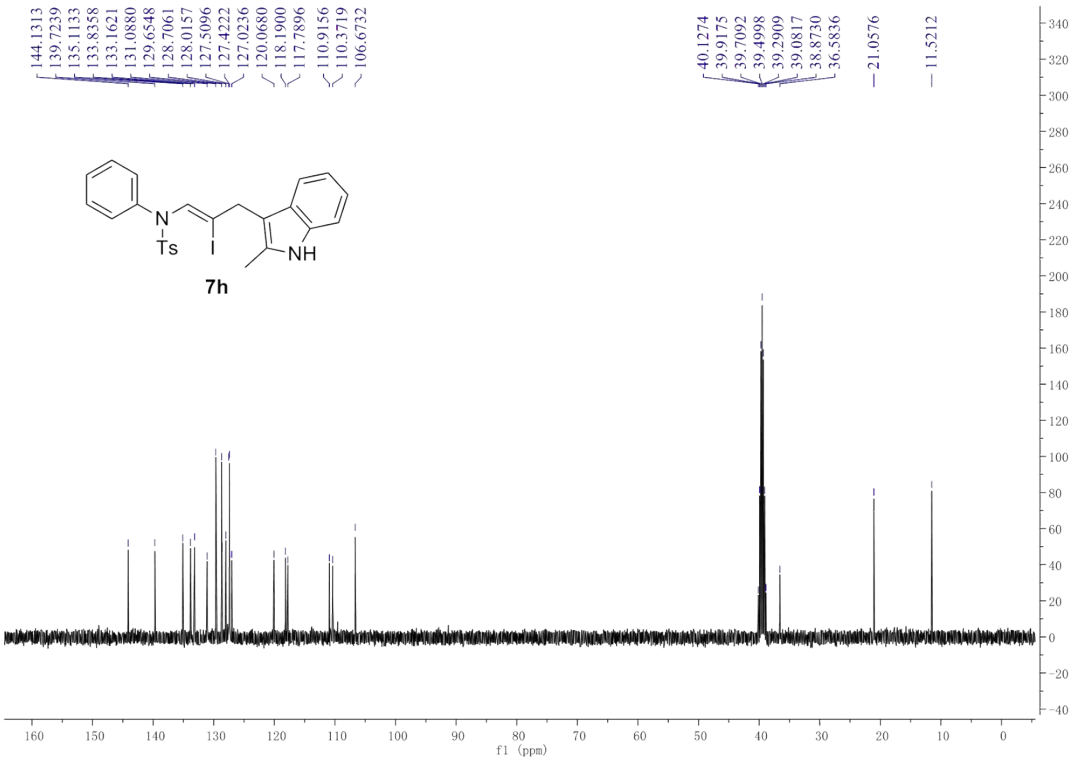
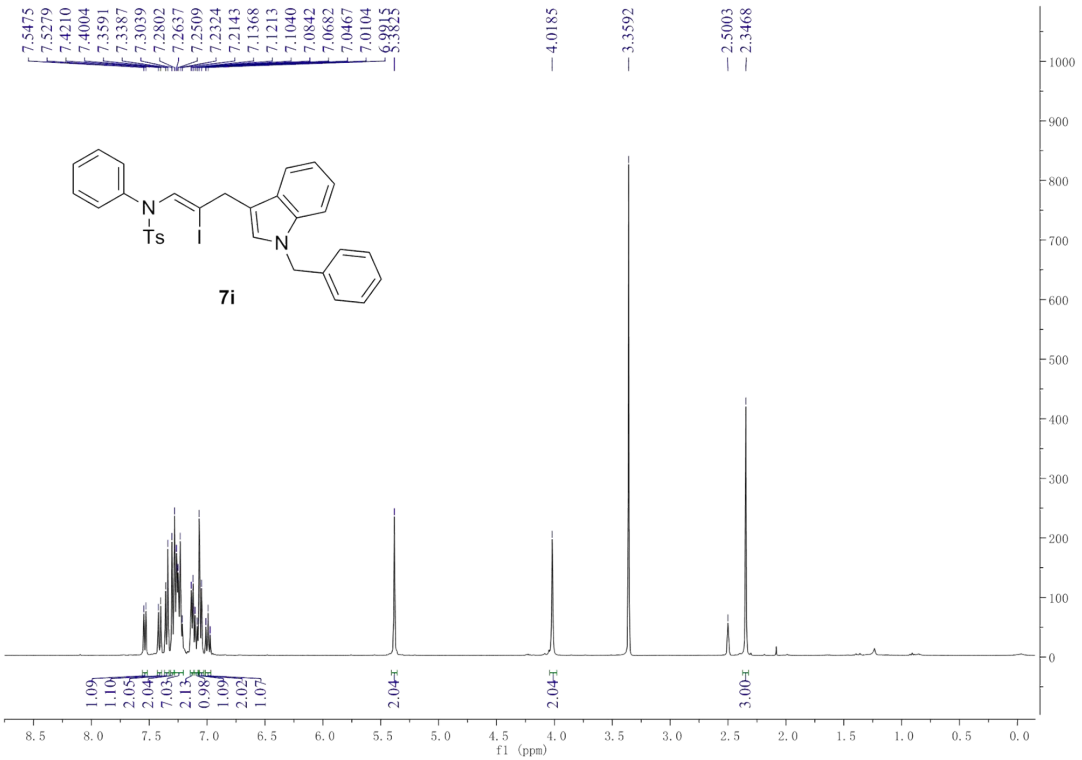
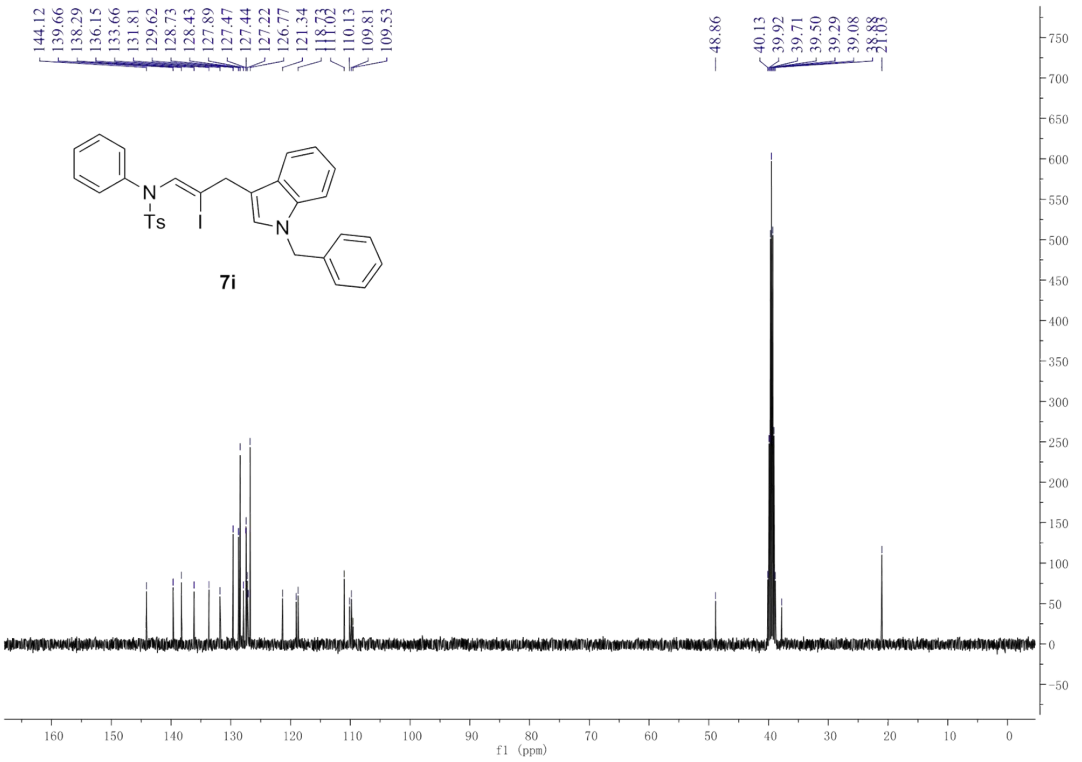
7.4286
7.4123
7.3927
7.3291
7.3085
7.2922
7.2744
7.2592
7.2553
7.2404
7.2297
7.2118
7.1935
7.0840
7.0758
7.0566
7.0157
6.9974
6.9783
6.9288
6.9099
6.8918
3.9652
3.4088
2.4997
2.3703
2.3179
1.05
1.99
1.07
2.07
4.18
1.05
2.09
1.09
1.06
2.08
3.06
3.00
f1 (ppm)
N
Ts
I
NH

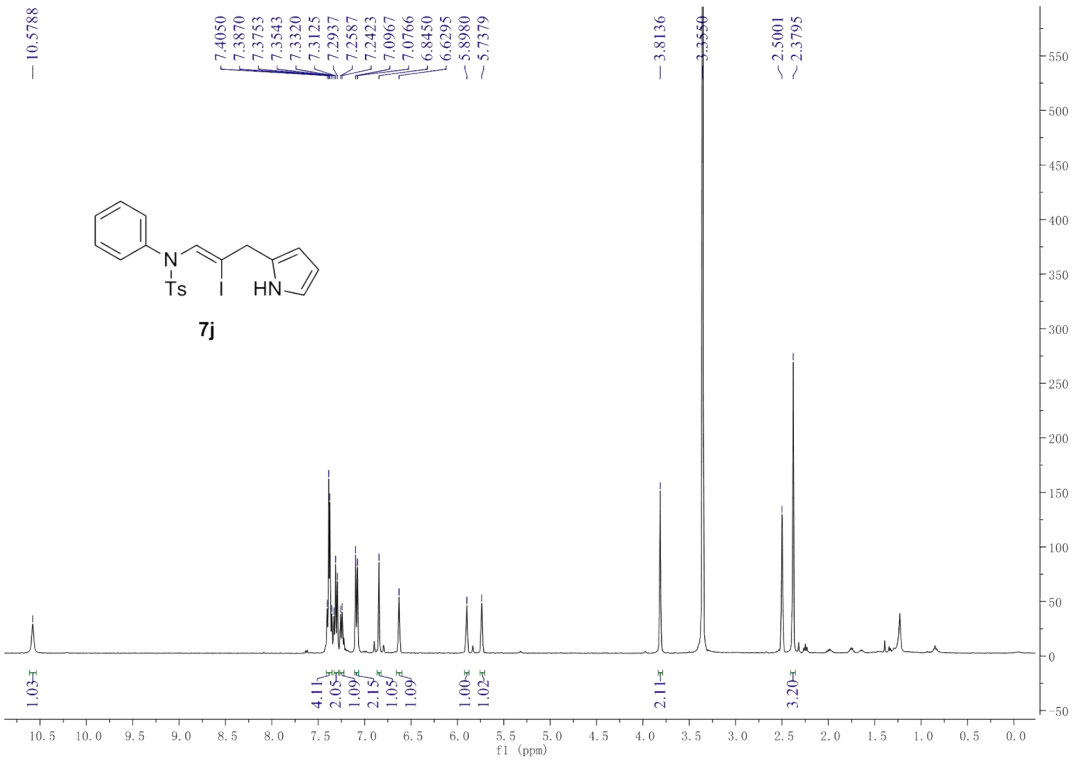
7h

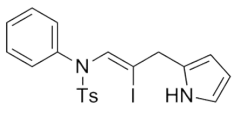

144.1313
139.7239
135.1133
133.8358
133.1621
131.0880
129.6548
128.7061
128.0157
127.5096
127.4222
127.0236
120.0680
118.1900
117.7896
110.9156
110.3719
106.6732
40.1274
39.9175
39.7092
39.4998
39.2909
39.0817
38.8730
36.5836
21.0576
11.5212
f1 (ppm)
N
Ts
I
NH

7h


7.5475
7.5279
7.4210
7.4004
7.3591
7.3387
7.3039
7.2802
7.2637
7.2509
7.2324
7.2143
7.1368
7.1213
7.1040
7.0842
7.0682
7.0467
7.0104
6.9815
5.3825
4.0185
3.3592
2.5003
2.3468
N
Ts
I
N
7i
1.09
1.10
2.05
2.04
7.03
2.13
0.98
1.09
2.02
1.07
2.04
2.04
3.00
f1 (ppm)


144.12
139.66
138.29
136.15
133.66
131.81
129.62
128.73
128.43
127.89
127.47
127.44
127.22
126.77
121.34
118.73
111.02
110.13
109.81
109.53
48.86
40.13
39.92
39.71
39.50
39.29
39.08
38.88
21.08
N
Ts
I
N
7i
f1 (ppm)


10.5788
7.4050
7.3870
7.3753
7.3543
7.3320
7.3125
7.2937
7.2587
7.2423
7.0967
7.0766
6.8450
6.6295
5.8980
5.7379
3.8136
3.3550
2.5001
2.3795
1.03
4.11
2.05
1.09
2.15
1.05
1.09
1.00
1.02
2.11
3.20
f1 (ppm)

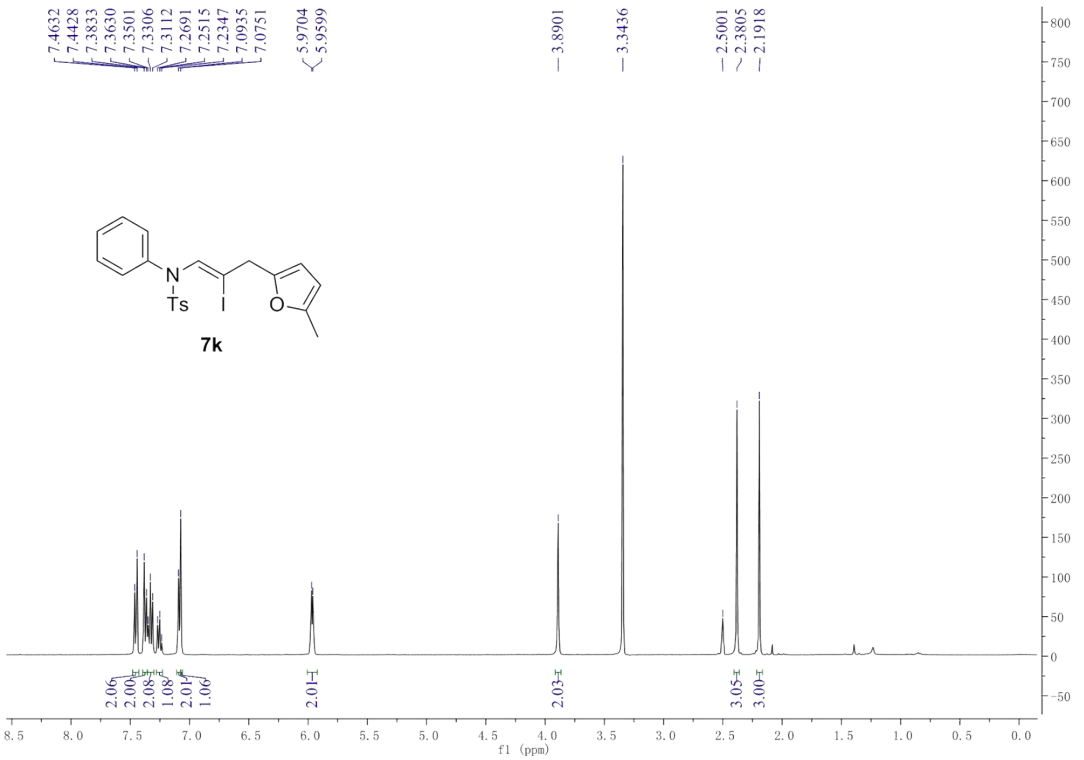

N
Ts
I
HN

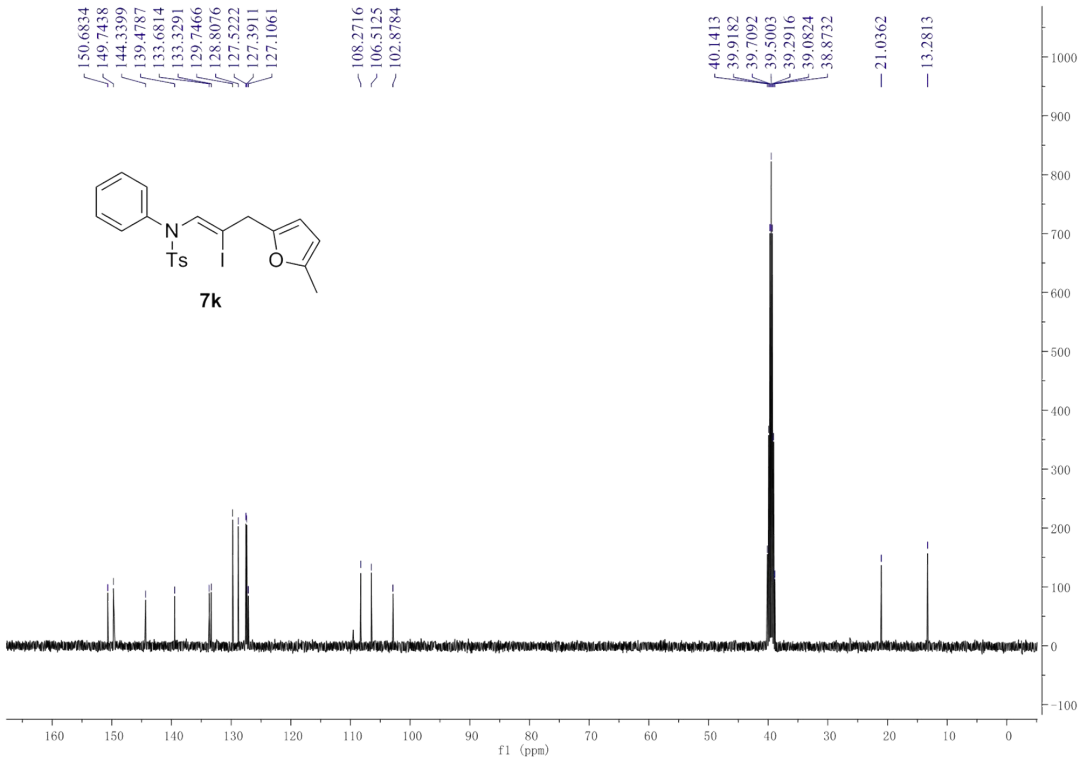
7j

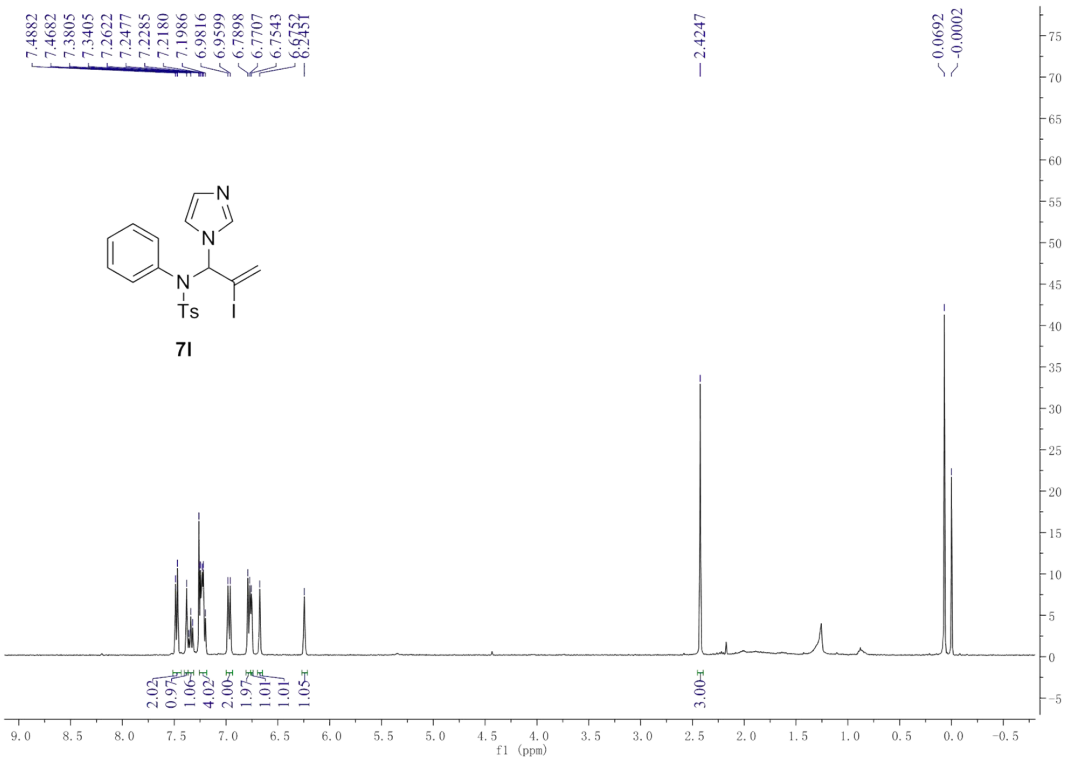
144.2808
139.6641
133.6127
132.0968
129.7521
128.7872
127.5544
127.4915
127.0953
117.0570
109.5746
107.4972
106.7607
106.4564
40.1967
40.1272
39.9176
39.7087
39.5000
39.2912
39.0823
38.8732
21.0652
f1 (ppm)

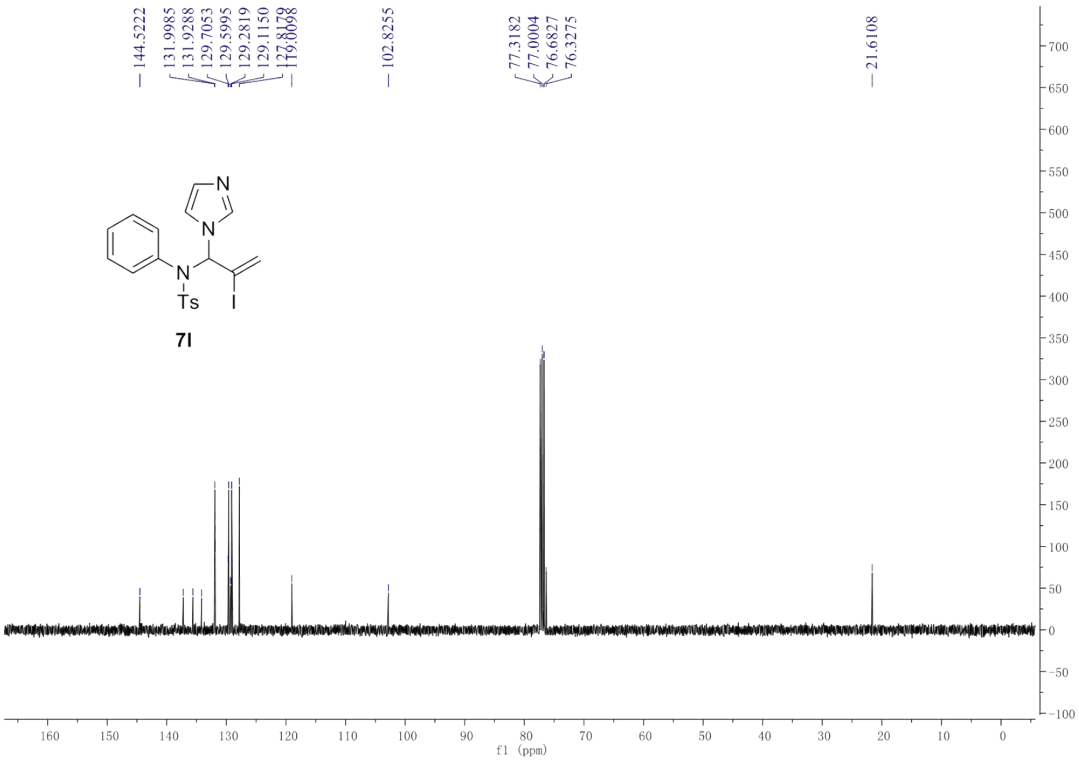
N
Ts
I
HN

7j


7.4632
7.4428
7.3833
7.3630
7.3501
7.3306
7.3112
7.2691
7.2515
7.2347
7.0935
7.0751
5.9704
5.9599
3.8901
3.3436
2.5001
2.3805
2.1918
N
Ts
I
O
7k
2.06
2.00
2.08
1.08
2.01
1.06
2.01
2.03
3.05
3.00
f1 (ppm)


150.6834
149.7438
144.3399
139.4787
133.6814
133.3291
129.7466
128.8076
127.5222
127.3911
127.1061
108.2716
106.5125
102.8784
40.1413
39.9182
39.7092
39.5003
39.2916
39.0824
38.8732
21.0362
13.2813
N
Ts
I
O
7k
f1 (ppm)


7.4882
7.4682
7.3805
7.3405
7.2622
7.2477
7.2285
7.2180
7.1986
6.9816
6.9599
6.7898
6.7707
6.7543
6.6752
6.6451
2.4247
0.0692
-0.0002
N
N
N
Ts
I
7l
2.02
0.97
1.06
4.02
2.00
1.97
1.01
1.01
1.05
3.00
f1 (ppm)


144.5222
131.9985
131.9288
129.7053
129.5995
129.2819
129.1150
127.8179
119.0098
102.8255
77.3182
77.0004
76.6827
76.3275
21.6108
N
N
N
Ts
I
7l
f1 (ppm)

9. **NMR Spectra for 9**