

Supporting Information  
For  
**Green and rapid acid-catalyzed ynamide skeletal  
rearrangement and stereospecific functionalization with  
anisole derivatives**

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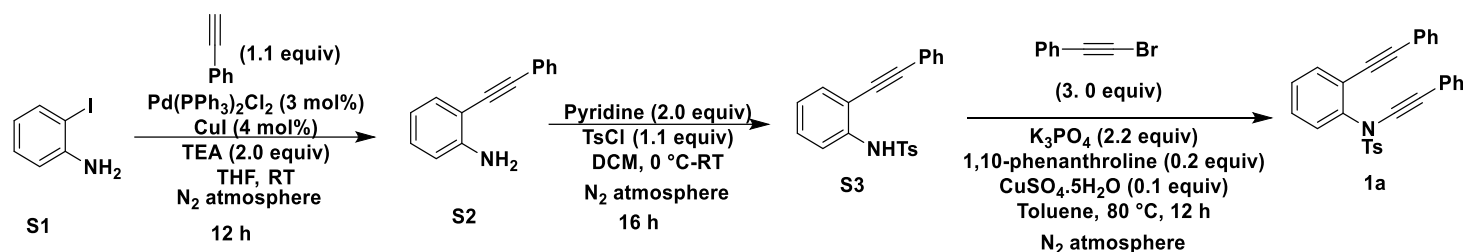
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## 1. General Information

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a 400 MHz Varian Unity Plus or Varian Mercury plus spectrometer. The chemical shift ( $\delta$ ) values are reported in parts per million (ppm), and the coupling constants ( $J$ ) are given in Hz. The spectra were recorded using  $\text{CDCl}_3$  as a solvent.  $^1\text{H}$  NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm).  $^{13}\text{C}$ NMR was referenced to  $\text{CDCl}_3$  (77.0 ppm). The abbreviations used are as follows: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublet; ddd, doublet of doublet; dt, doublet of triplets; td, a triplet of doublet; m, multiplet; brs, broad singlet and so on. Mass spectra and high-resolution mass spectra (HRMS) were measured using the LTQ Orbitrap XL (Thermo Fisher Scientific) Liquid chromatography-mass spectrometry at National Taiwan Normal University and National Sun Yat-sen University. All commercially available reagents were used without further purification unless noted otherwise. Commercially available reagents and solvents were obtained from Sigma-Aldrich, TCI, Acros, or Alfa Aesar. Melting points were determined on an EZ-Melt (Automated melting point apparatus). All the synthesized products showed  $^1\text{H}$ NMR spectra in agreement with the assigned structures. Reaction progress and product mixtures were routinely monitored by TLC using Merck TLC aluminum sheets (silica gel 60 F254). Column chromatography was carried out with 230-400 mesh silica gel 60 (Merck) using a mixture of hexane/ethyl acetate as the eluent.

## 2. Preparation of Starting Materials

### 2.1. General procedure (A) for the preparation of 2-alkynyl-ynamides derivatives (1)<sup>1</sup>



#### 2.1a. Procedure for the synthesis of 2-(phenylethynyl)aniline (S2)

To a dried schlenk flask equipped with a stir bar was charged with 2-iodoaniline (10 g, 45.65 mmol, 1.0 equiv) in THF. Next, the schlenk flask was evacuated and filled with nitrogen (three cycles), alkyne (5.12 g, 50.22 mmol, 1.1 equiv), freshly distilled Et<sub>3</sub>N (9.24 g, 91.31 mmol, 2.0 equiv), Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (0.96 g, 1.3697 mmol, 3 mol%) and CuI (0.34 g, 1.82 mmol, 4 mol%) were added under the nitrogen atmosphere. The resulting mixture was stirred at room temperature for 12 h. After the completion of the reaction by TLC, the reaction mixture was cooled to room temperature, diluted with water, and extracted with ethyl acetate. The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated to give the crude material. The crude material was purified by column chromatography using hexane-ethyl acetate (95:5%) as the eluent gave yellow solid 2-(phenylethynyl)aniline in 85% (7.50 g).

#### 2.1b. Procedure for the synthesis of 4-methyl-N-(2-(phenylethynyl)phenyl)benzenesulfonamide (S3)

To a dried schlenk flask equipped with a stir bar was charged with 2-(phenylethynyl)aniline (7 g, 36.22 mmol, 1.0 equiv) in DCM at 0 °C. Next, the schlenk flask was evacuated and filled with nitrogen (three cycles) followed by pyridine (5.73 g, 72.45 mmol, 2.0 equiv) and 4-methylbenzenesulfonyl chloride (7.59 g, 39.84 mmol, 1.1 equiv: The TsCl was added portion wise in 20 minutes) were added under nitrogen atmosphere. The resulting mixture was continued at room temperature for 16 h (if starting material was not consumed, heated at 40 °C (oil bath)). The solvent was removed under reduced pressure and the resulting solid was dissolved in DCM, washed with water and brine, and dried over MgSO<sub>4</sub>. The crude material was purified by column chromatography using hexane-ethyl acetate (90:10%) as the eluent gave yellow solid 4-methyl-N-(2-(phenylethynyl)phenyl)benzenesulfonamide in 63% (8.23 g).

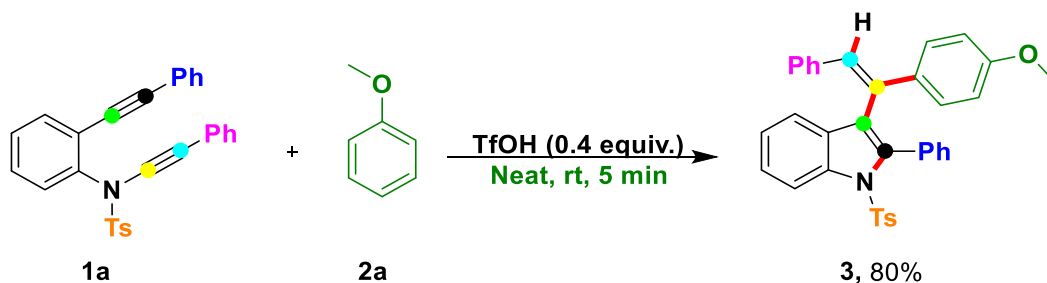
#### 2.1c. Procedure for the synthesis of 4-methyl-N-(phenylethynyl)-N-(2-(phenylethynyl)phenyl)benzenesulfonamide derivatives (1a)

To a dried flask was added 4-methyl-*N*-(2-(phenylethynyl)phenyl) (4 g, 11.52 mmol, 1.0 equiv), CuSO<sub>4</sub>·5H<sub>2</sub>O (288 mg, 1.15 mmol, 0.1 equiv), 1,10-phenanthroline (414 mg 2.30 mmol, 0.2 equiv), and K<sub>3</sub>PO<sub>4</sub> (5.38 g, 25.36 mmol, 2.2 equiv) in dry toluene. Next, the flask was evacuated and filled with nitrogen (three cycles) followed by addition of bromoalkyne (6.25 g, 34.58 mmol, 3.0 equiv) (note: need to prepare freshly before performing the reaction) and the mixture was stirred at 80 °C 12 h (Note: need vigorous stirring). The resulting mixture was filtered through silica gel and then concentrated in vacuum. The residue was purified by flash column chromatography on silica gel (Formation of the ynamide and side product; indole) is very close on TLC, so need to pack long silica and required long run) with hexane-ethyl acetate (99:1). A pale-yellow solid was obtained and washed with HPLC grade n-pentane gave the pure brown solid 4-methyl-*N*-(phenylethynyl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (3 g, 58%).

Note: Other ynamide derivatives were obtained (250 mg scale of respective **S1** starting material) through the procedure reported above. Compounds known in the literature were confirmed by comparing their <sup>1</sup>H and <sup>13</sup>C NMR spectra.<sup>1</sup>

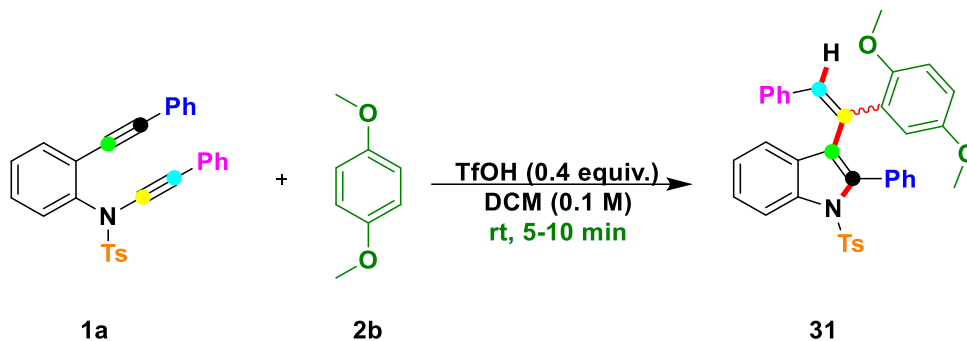
### 3. Experimental procedures

#### 3.1. General procedure (A) for the synthesis of (Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole derivatives (3-30)



An oven-dried screw-capped, 8 mL vial equipped with a magnetic stir bar was charged with 4-methyl-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (45 mg, 0.10 mmol, 1.0 equiv) in anisole (0.1 M) and trifluoromethanesulfonic acid (TfOH) (6 mg, 0.04 mmol, 0.4 equiv) was added. The resulting solution was stirred up to starting material completion (5-10 minutes) at room temperature. The progress of the reaction was monitored by TLC. After that, the crude reaction mixture was diluted with saturated sodium bicarbonate solution and extracted with ethyl acetate. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The crude material was purified by flash column chromatography using hexane-ethyl acetate (96:4) as the eluent gave the desired product (Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole as a white solid in 80% (44 mg). (Note: the minor product **3'** formation is very close to the major product on TLC. So, a long silica package is necessary in column purification).

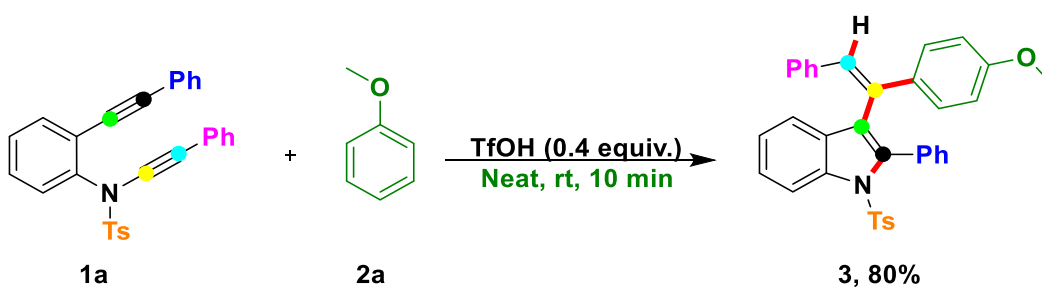
### 3.2. General procedure (B) for the synthesis of mixture of (*E/Z*) isomers of 3-(1-(2,5-dimethoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole derivatives (31-33)



An oven-dried screw-capped, 8 mL vial equipped with a magnetic stir bar was charged with 4-methyl-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (45 mg, 0.10 mmol, 1.0 equiv) in anisole (0.1 M) and trifluoromethanesulfonic acid (TfOH) (6 mg, 0.04 mmol, 0.4 equiv) was added. The resulting solution was stirred up to starting material completion (5-10 minutes) at room temperature. The progress of the reaction was monitored by TLC. After that, the crude reaction mixture was diluted with saturated sodium bicarbonate solution and extracted with ethyl acetate. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The crude material was purified by flash column chromatography using hexane-ethyl acetate (94:6) as the eluent gave mixture of two isomer product (*E/Z*=21:79) 3-(1-(2,5-dimethoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole as a white solid in 35% (21 mg).

### 3.3. Gram-scale synthesis

#### 3.3a. Gram-scale synthesis of (*Z*)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (3)

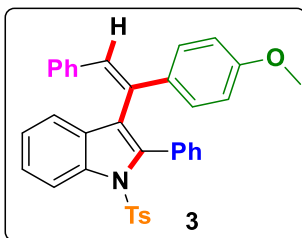


An oven-dried screw-capped, 8 mL vial equipped with a magnetic stir bar was charged with 4-methyl-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (1.0 g, 2.23 mmol, 1.0 equiv) in anisole (0.1 M) and trifluoromethanesulfonic acid (TfOH) (134 mg, 0.89 mmol, 0.4 equiv) was added. The resulting solution was stirred up to starting material completion (10 minutes) at room temperature. The progress of the reaction was monitored by TLC. After that, the crude reaction mixture was diluted with saturated sodium bicarbonate solution and extracted with ethyl acetate. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and

concentrated. The crude material was purified by flash column chromatography using hexane-ethyl acetate (96:4) as the eluent gave the desired product (Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole as a white solid in 80% (1.0 g).

#### 4. Characterization data

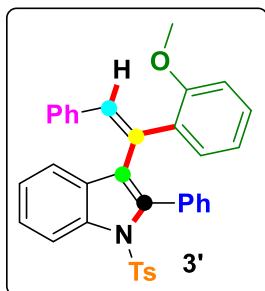
**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (3):** The title compound was prepared



according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (44 mg, yield = 80%); Mp. 187-188 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 8.4 Hz, 1H), 7.36 (dd, *J* = 11.4, 4.2 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 2H), 7.20 – 7.03 (m, 8H), 7.01 – 6.96 (m, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.86 (t, *J* = 7.6 Hz, 3H), 6.67 (d, *J* = 8.0 Hz, 2H), 6.64 (d, *J* = 8.8

Hz, 2H), 3.73 (s, 3H), 2.37 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 159.1, 144.4, 138.2, 138.0, 137.1, 134.8, 133.7, 131.7, 131.4, 130.9, 130.4, 129.7, 129.2, 128.2, 128.0, 127.8, 127.5, 126.9, 126.8, 126.5, 125.2, 124.6, 124.4, 120.5, 117.0, 113.5, 55.2, 21.6. HRMS (ESI) calcd for C<sub>36</sub>H<sub>30</sub>NO<sub>3</sub>S [M+H]<sup>+</sup> 556.1946; found: 556.1937.

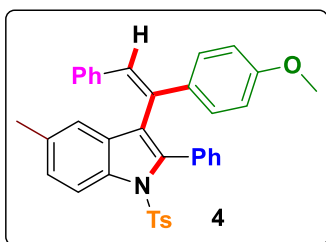
**(E)-3-(1-(2-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (3')**: The title compound was prepared



according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (97:3) to obtain as a white solid (6 mg, yield = 11%); Mp. 156-157 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.35 (d, *J* = 8.4 Hz, 1H), 7.38 – 7.28 (m, 3H), 7.18 (dt, *J* = 8.5, 4.3 Hz, 1H), 7.14 – 7.06 (m, 8H), 7.04 – 6.97 (m, 2H), 6.89 – 6.77 (m, 5H), 6.65 – 6.59 (m, 2H), 6.55 (t, *J* = 7.4 Hz, 1H), 3.34 (s, 3H), 2.36 (s, 3H). <sup>13</sup>C NMR (101

MHz, CDCl<sub>3</sub>) δ 156.8, 144.4, 137.7, 137.6, 137.2, 135.2, 134.1, 131.5, 131.3, 130.8, 130.7, 130.0, 129.1, 129.2, 128.4, 128.2, 127.9, 127.8, 127.0, 126.7, 126.6, 126.2, 124.7, 124.2, 120.1, 119.1, 116.6, 110.1, 55.1, 21.6. HRMS (ESI) calcd for C<sub>36</sub>H<sub>30</sub>NO<sub>3</sub>S [M+H]<sup>+</sup> 556.1946; found: 556.1953.

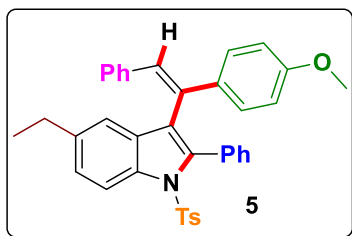
**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-5-methyl-2-phenyl-1-tosyl-indole (4):** The title compound was



prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (43 mg, yield = 75%); Mp. 139-140 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.25 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.17 (dd, *J* = 11.0, 8.1 Hz, 2H), 7.08 (dd, *J* = 16.5, 7.6 Hz, 4H), 7.04 – 6.91 (m, 5H), 6.91 – 6.77 (m, 5H), 6.66 (dd, *J* = 7.8, 5.4 Hz, 4H), 3.76 (s, 3H),

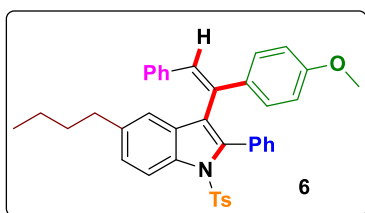
2.39 (s, 3H), 2.28 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 159.1, 144.3, 138.2, 137.2, 136.2, 134.9, 134.4, 133.7, 131.9, 131.8, 131.1, 130.4, 129.6, 129.2, 128.2, 127.1, 127.9, 127.4, 127.0, 126.8, 126.7, 126.5, 124.3, 120.3, 116.8, 113.6, 55.2, 21.6, 21.3. HRMS (ESI) calcd for C<sub>37</sub>H<sub>32</sub>NO<sub>3</sub>S [M+H]<sup>+</sup> 570.2103; found: 570.2107.

**(Z)-5-ethyl-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (5):** The title compound was



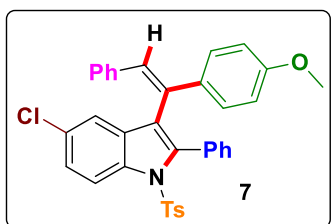
prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (42 mg, yield = 72%); Mp. 74-75 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.27 (d,  $J = 8.6$  Hz, 1H), 7.31 (d,  $J = 8.2$  Hz, 2H), 7.19 (dt,  $J = 15.7, 6.8$  Hz, 3H), 7.08 (dd,  $J = 16.9, 7.8$  Hz, 4H), 7.00 (d,  $J = 7.2$  Hz, 2H), 6.95 (d,  $J = 8.7$  Hz, 2H), 6.86 (t,  $J = 7.9$  Hz, 4H), 6.67 (dd,  $J = 16.6, 8.1$  Hz, 4H), 3.76 (s, 3H), 2.57 (q,  $J = 8.0$  Hz, 2H), 2.39 (s, 3H), 1.11 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 144.3, 140.7, 138.2, 137.2, 136.3, 134.1, 133.8, 131.1, 131.5, 131.1, 130.4, 129.7, 129.2, 128.2, 127.1, 127.8, 127.5, 127.0, 126.7, 126.4, 125.5, 124.5, 119.1, 116.7, 113.5, 55.2, 28.6, 21.6, 15.6. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{34}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  584.2259; found: 584.2260.

**(Z)-5-butyl-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (6):** The title compound was



prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (97:3) to obtain as a yellow gummy (36 mg, yield = 60%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.26 (d,  $J = 8.5$  Hz, 1H), 7.33 – 7.28 (m, 2H), 7.20 – 7.14 (m, 2H), 7.08 (dd,  $J = 13.9, 7.9$  Hz, 4H), 6.98 (dd,  $J = 13.3, 5.9$  Hz, 3H), 6.95 – 6.91 (m, 2H), 6.88 – 6.83 (m, 3H), 6.81 (d,  $J = 1.5$  Hz, 1H), 6.69 (d,  $J = 7.2$  Hz, 2H), 6.64 (d,  $J = 8.8$  Hz, 2H), 3.75 (s, 3H), 2.55 – 2.49 (m, 2H), 2.38 (s, 3H), 1.48 – 1.41 (m, 2H), 1.16 (dt,  $J = 14.6, 7.3$  Hz, 2H), 0.82 (t,  $J = 7.3$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 144.3, 139.4, 138.3, 137.2, 136.3, 134.9, 133.9, 132.0, 131.4, 131.2, 130.4, 129.6, 129.1, 128.2, 127.1, 127.8, 127.5, 127.0, 126.7, 126.4, 126.0, 124.6, 119.8, 116.7, 113.5, 55.2, 35.3, 33.6, 22.1, 21.6, 13.9. HRMS (ESI) calcd for  $\text{C}_{40}\text{H}_{38}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  612.2572; found: 612.2563.

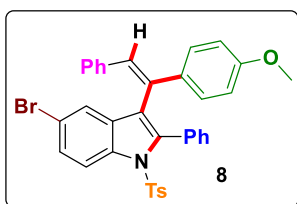
**(Z)-5-chloro-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (7):** The title compound was



prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (95:5) to obtain as a white solid (40 mg, yield = 70%); Mp. 163-164 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (d,  $J = 8.9$  Hz, 1H), 7.33 (dd,  $J = 8.9, 2.2$  Hz, 1H), 7.28 (d,  $J = 8.4$  Hz, 2H), 7.19 (t,  $J = 7.4$  Hz, 1H), 7.13 (d,  $J = 8.0$  Hz, 2H), 7.08 (t,  $J = 7.3$  Hz, 2H), 7.03 (d,  $J = 1.8$  Hz, 1H), 7.00 (d,  $J = 7.4$  Hz, 1H), 6.95 – 6.85 (m, 6H), 6.69 – 6.62 (m, 4H), 3.77 (s, 3H), 2.40 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 144.8, 139.6, 136.9, 136.4, 134.7, 133.3, 132.8, 131.1, 130.4, 130.1, 129.4, 128.3, 128.1, 127.9, 127.4, 126.1, 126.9, 126.7, 125.5, 123.6, 119.1, 118.2, 113.7, 55.21, 21.6. HRMS (ESI) calcd for  $\text{C}_{36}\text{H}_{29}\text{NO}_3\text{SCl}$   $[\text{M}+\text{H}]^+$  590.1557; found: 590.1578.

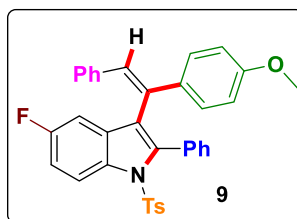


**(Z)-5-bromo-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (8):** The title compound was



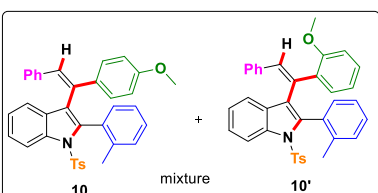
prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (95:5) to obtain as a white solid (38 mg, yield = 60%); Mp. 168-169 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.26 (d,  $J = 8.9$  Hz, 1H), 7.47 (dd,  $J = 8.9, 2.0$  Hz, 1H), 7.28 (d,  $J = 8.4$  Hz, 2H), 7.21-7.17 (m, 2H), 7.13 (d,  $J = 8.1$  Hz, 2H), 7.10-7.06 (m, 2H), 7.03-7.00 (m, 1H), 6.96 – 6.85 (m, 6H), 6.70 – 6.62 (m, 4H), 3.77 (s, 3H), 2.40 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 144.8, 139.4, 136.9, 136.8, 134.7, 133.2, 133.2, 131.0, 130.4, 130.1, 129.4, 128.4, 128.1, 127.9, 127.4, 126.1, 126.9, 126.7, 123.4, 123.0, 118.5, 118.2, 113.7, 55.2, 21.6. HRMS (ESI) calcd for  $\text{C}_{36}\text{H}_{29}\text{NO}_3\text{SBr}$   $[\text{M}+\text{H}]^+$  634.1052; found: 634.1055.

**(Z)-5-fluoro-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (9):** The title compound was



prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (95:5) to obtain as a white solid (42 mg, yield = 73%); Mp. 88-89 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (dd,  $J = 9.1, 4.5$  Hz, 1H), 7.30 – 7.27 (m, 2H), 7.21 – 7.16 (m, 1H), 7.15 – 7.10 (m, 3H), 7.09 – 7.06 (m, 2H), 7.03 – 6.86 (m, 7H), 6.85 (s, 1H), 6.70 (dd,  $J = 8.4, 2.6$  Hz, 1H), 6.68 – 6.63 (m, 4H), 3.76 (s, 3H), 2.40 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  161.6, 159.2, 144.7, 140.1, 136.9, 134.6, 134.2, 132.9, 132.8 (d,  $J_{\text{C-F}} = 9.9$  Hz), 132.3 (d,  $J_{\text{C-F}} = 211.0$  Hz), 130.63, 130.3, 129.1, 129.3, 128.3, 128.10, 127.93, 127.45, 126.99, 126.85, 126.63, 124.27 (d,  $J_{\text{C-F}} = 3.8$  Hz), 124.23, 118.4 (d,  $J_{\text{C-F}} = 9.1$  Hz), 118.3, 113.6, 113.2, 113.0, 106.2, 106.0, 55.2, 21.6. HRMS (ESI) calcd for  $\text{C}_{36}\text{H}_{29}\text{NO}_3\text{SF}$   $[\text{M}+\text{H}]^+$  574.1852; found: 574.1833.

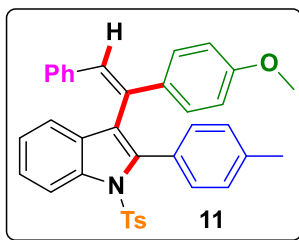
**Mixture of 3-(1-iodo-2-phenyl-2-tosylvinyl)-2-(4-methoxyphenyl)-1-tosylindole (10) and 3-(1-(2-methoxyphenyl)-2-phenylvinyl)-2-(o-tolyl)-1-tosyl-indole (10')**: The title



compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:5) to obtain mixture of regio-isomer products (**10:10'**=45:55) as a white solid (42 mg, yield = 71%); Mp.

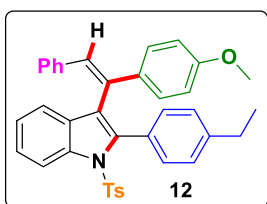
195-196 °C  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.42 (d,  $J = 8.4$  Hz, 1.05H), 8.38 (d,  $J = 8.5$  Hz, 0.66H), 7.43 (d,  $J = 8.2$  Hz, 2.36H), 7.41 – 7.35 (m, 2.08H), 7.32 (d,  $J = 8.2$  Hz, 1.43H), 7.20 (d,  $J = 7.7$  Hz, 0.60H), 7.18 – 7.08 (m, 9.38H), 7.05 – 6.95 (m, 4.66H), 6.94 – 6.87 (m, 5.62H), 6.87 – 6.78 (m, 7.96H), 6.78 – 6.72 (m, 1.32H), 6.68 – 6.63 (m, 3.23H), 6.63 – 6.56 (m, 3.20H), 3.78 (s, 1.85H), 3.71 (s, 3.32H), 2.39 (s, 5.71H), 2.09 (s, 3.22H), 1.74 (s, 1.84H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 158.9, 144.6, 144.5, 140.1, 139.4, 137.5, 137.2, 135.8, 134.5, 134.0, 132.3, 130.7, 130.4, 130.0, 129.7, 129.6, 129.4, 129.3, 129.3, 129.1, 128.8, 128.5, 128.4, 128.2, 128.0, 127.9, 127.6, 127.5, 127.0, 126.6, 126.5, 125.1, 125.1, 124.9, 124.6, 124.3, 124.2, 124.0, 120.5, 117.1, 116.2, 114.3, 113.5, 113.1, 55.2, 21.6, 20.6, 20.4. HRMS (ESI) calcd for  $\text{C}_{37}\text{H}_{32}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  570.2103; found: 570.2107.

**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-(p-tolyl)-1-tosyl-indole (11):** The title compound was prepared



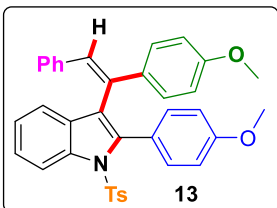
according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (43 mg, yield = 76%); Mp. 193-194 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (d,  $J = 8.4$  Hz, 1H), 7.38 – 7.34 (m, 1H), 7.32 (d,  $J = 8.4$  Hz, 2H), 7.17 – 7.13 (m, 1H), 7.10 (d,  $J = 8.3$  Hz, 2H), 7.05 (d,  $J = 7.7$  Hz, 1H), 7.01 – 6.84 (m, 10H), 6.70 (d,  $J = 7.6$  Hz, 2H), 6.67 – 6.63 (m, 2H), 3.75 (s, 3H), 2.38 (s, 3H), 2.28 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 144.4, 138.3, 138.0, 137.9, 137.2, 134.9, 133.9, 131.9, 131.5, 130.3, 129.7, 129.2, 128.2, 128.0, 127.8, 127.6, 127.5, 127.0, 126.5, 125.0, 124.6, 124.1, 120.3, 117.0, 113.5, 55.2, 21.6, 21.4. HRMS (ESI) calcd for  $\text{C}_{37}\text{H}_{32}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  570.2103; found: 570.2096.

**(Z)-2-(4-ethylphenyl)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-tosyl-indole (12):** The title compound was



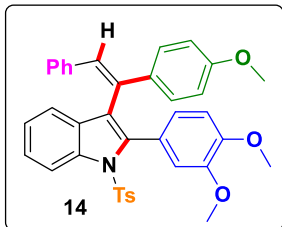
prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (46 mg, yield = 77%); Mp. 139-140 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.37 (d,  $J = 8.4$  Hz, 1H), 7.38 – 7.30 (m, 3H), 7.17-7.13 (m, 1H), 7.10 (d,  $J = 8.0$  Hz, 2H), 7.04 (d,  $J = 7.8$  Hz, 1H), 7.01-6.97 (m, 1H), 6.90 (ddd,  $J = 21.2, 10.4, 4.1$  Hz, 9H), 6.65 (dd,  $J = 12.3, 5.5$  Hz, 4H), 3.76 (s, 3H), 2.57 (q,  $J = 7.6$  Hz, 2H), 2.38 (s, 3H), 1.19 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) 159.1, 144.3, 144.1, 138.5, 138.0, 137.2, 134.9, 133.9, 132.0, 131.5, 129.7, 129.2, 128.2, 128.2, 127.8, 127.6, 127.0, 126.4, 126.3, 125.0, 124.6, 124.2, 120.4, 117.1, 113.5, 55.2, 28.7, 21.6, 15.4. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{34}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  584.2259; found: 584.2239.

**(Z)-2-(4-methoxyphenyl)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-tosyl-indole (13):** The title compound



was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (95:5) to obtain as a white solid (42 mg, yield = 70%); Mp. 188-189 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (d,  $J = 8.4$  Hz, 1H), 7.36 (ddd,  $J = 8.5, 7.2, 1.3$  Hz, 1H), 7.32 – 7.28 (m, 2H), 7.17 – 7.13 (m, 1H), 7.10 (d,  $J = 8.1$  Hz, 2H), 7.04 (d,  $J = 7.8$  Hz, 1H), 7.02 – 6.97 (m, 1H), 6.97 – 6.90 (m, 3H), 6.87 (dd,  $J = 10.2, 5.1$  Hz, 4H), 6.70 (d,  $J = 7.6$  Hz, 2H), 6.67 – 6.59 (m, 4H), 3.76 (s, 3H), 3.75 (s, 3H), 2.38 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.4, 159.1, 144.4, 138.2, 138.0, 137.2, 135.0, 133.8, 131.9, 131.7, 131.5, 129.6, 129.2, 128.2, 127.8, 127.5, 127.0, 126.5, 125.0, 124.6, 123.8, 123.3, 120.3, 117.1, 113.5, 112.4, 55.2, 55.1, 21.6. HRMS (ESI) calcd for  $\text{C}_{37}\text{H}_{32}\text{NO}_4\text{S}$   $[\text{M}+\text{H}]^+$  586.2052; found: 586.2062.

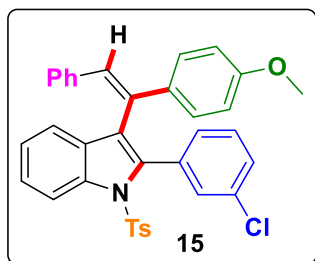
**(Z)-2-(3,4-dimethoxyphenyl)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-tosyl-indole (14):** The title



compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (51 mg, yield = 83%); Mp. 150-151 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.39 (d,  $J = 8.4$

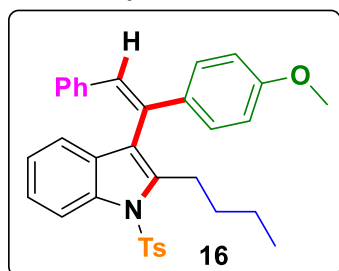
Hz, 1H), 7.37 (ddd,  $J = 8.4, 7.2, 1.3$  Hz, 1H), 7.32 (d,  $J = 8.3$  Hz, 2H), 7.17 (t,  $J = 7.5$  Hz, 1H), 7.11 – 7.07 (m, 3H), 7.03 – 6.96 (m, 3H), 6.89 (t,  $J = 7.6$  Hz, 3H), 6.72 (d,  $J = 7.7$  Hz, 2H), 6.69 – 6.61 (m, 4H), 6.38 (brs, 1H), 3.84 (s, 3H), 3.76 (s, 3H), 3.52 (s, 3H), 2.38 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 148.0, 147.3, 144.4, 138.0, 137.9, 137.2, 135.1, 133.8, 132.0, 131.4, 129.5, 129.1, 128.2, 127.9, 127.4, 127.0, 126.5, 125.1, 124.6, 123.4, 120.3, 117.0, 114.1, 113.6, 109.5, 55.7, 55.4, 55.2, 21.6. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{34}\text{NO}_5\text{S}$   $[\text{M}+\text{H}]^+$  616.2158; found: 616.2135.

**(Z)-2-(3-chlorophenyl)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-tosyl-indole (15):** The title compound was



prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (49 mg, yield = 84%); Mp. 74-75 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (d,  $J = 8.4$  Hz, 1H), 7.42 – 7.37 (m, 1H), 7.30 (d,  $J = 8.3$  Hz, 2H), 7.23 – 7.08 (m, 5H), 7.07 (ddd,  $J = 7.8, 1.3, 0.7$  Hz, 1H), 7.02 (t,  $J = 7.5$  Hz, 2H), 6.97 – 6.91 (m, 3H), 6.88 (d,  $J = 8.5$  Hz, 3H), 6.67 (d,  $J = 9.0$  Hz, 2H), 6.64 (d,  $J = 7.4$  Hz, 2H), 3.77 (s, 3H), 2.39 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 144.7, 138.1, 137.0, 136.4, 134.7, 133.5, 132.7, 131.6, 131.3, 130.0, 129.3, 128.1, 128.0, 128.0, 127.5, 126.9, 126.7, 125.5, 125.1, 124.7, 120.7, 117.0, 113.7, 55.2, 21.6. HRMS (ESI) calcd for  $\text{C}_{36}\text{H}_{29}\text{NO}_3\text{SCl}$   $[\text{M}+\text{H}]^+$  590.1557; found: 590.1536.

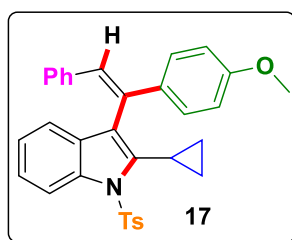
**(Z)-2-butyl-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-tosyl-indole (16):** The title compound was prepared



according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (97:3) to obtain as a white solid (30 mg, yield = 56%); Mp. 126-127 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 (d,  $J = 8.4$  Hz, 1H), 7.57 (d,  $J = 8.4$  Hz, 2H), 7.24 (ddd,  $J = 7.8, 7.0, 1.5$  Hz, 1H), 7.20 – 7.16 (m, 2H), 7.13 (t,  $J = 2.6$  Hz, 2H), 7.12 – 7.10 (m, 1H), 7.07 (ddd,  $J = 7.9, 7.0, 0.9$  Hz, 1H), 7.05 – 6.99

(m, 2H), 6.96 – 6.89 (m, 4H), 6.77 – 6.73 (m, 2H), 3.78 (s, 3H), 2.76 – 2.59 (m, 2H), 2.39 (s, 3H), 1.40-1.31 (m, 2H), 1.22-1.13 (m, 2H), 0.72 (t,  $J = 7.3$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.3, 144.4, 139.5, 137.3, 137.1, 136.1, 134.2, 132.3, 130.6, 129.7, 129.5, 128.5, 128.0, 127.7, 126.7, 126.4, 124.2, 123.9, 121.3, 119.9, 115.4, 113.7, 55.3, 31.9, 27.2, 23.0, 21.6, 13.6. HRMS (ESI) calcd for  $\text{C}_{34}\text{H}_{34}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  536.2259; found: 536.2261.

**(Z)-2-cyclopropyl-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-tosyl-indole (17):** The title compound was

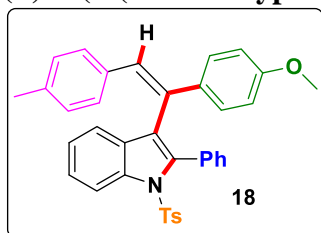


prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (97:3) to obtain as a yellow gummy (35 mg, yield = 68%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.26 (d,  $J = 8.5$  Hz, 1H), 7.66 (d,  $J = 8.3$  Hz, 2H), 7.27 (dd,  $J = 10.7, 3.5$  Hz, 1H), 7.22 (d,  $J = 8.1$  Hz, 2H), 7.15 (d,  $J = 8.8$  Hz, 2H), 7.10 (s, 1H), 7.07 – 7.02 (m, 1H), 7.01 – 6.91 (m, 6H), 6.78 (d,  $J = 8.8$  Hz, 2H), 3.79 (s, 3H),

2.41 (s, 3H), 1.63 – 1.57 (m, 1H), 0.79 – 0.74 (m, 1H), 0.70 (dd,  $J = 8.2, 3.5$  Hz, 2H), 0.59 – 0.51 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 144.4, 138.8, 137.6, 137.0, 136.9, 134.4, 132.7, 129.6, 129.4, 128.4, 128.0,

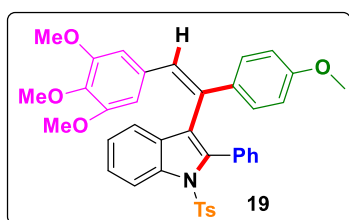
127.6, 126.6, 126.5, 124.6, 123.4, 120.4, 120.1, 114.6, 113.8, 55.2, 21.60, 9.4, 8.3, 8.1. HRMS (ESI) calcd for  $C_{33}H_{30}NO_3S$   $[M+H]^+$  520.1946; found: 520.1940.

**(Z)-3-(1-(4-methoxyphenyl)-2-(p-tolyl)vinyl)-2-phenyl-1-tosyl-indole (18):** The title compound was prepared



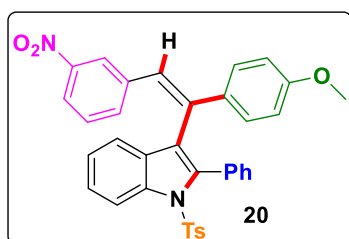
according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (39 mg, yield = 69%); Mp. 145-146 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.39 (d,  $J$  = 8.4 Hz, 1H), 7.37 (dd,  $J$  = 11.4, 4.2 Hz, 1H), 7.33 (d,  $J$  = 8.3 Hz, 2H), 7.21 – 6.99 (m, 9H), 6.92 (d,  $J$  = 8.8 Hz, 2H), 6.85 (s, 1H), 6.63 (dt,  $J$  = 14.7, 8.1 Hz, 6H), 3.74 (s, 3H), 2.39 (s, 3H), 2.21 (s, 3H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  158.9, 144.4, 138.1, 138.0, 136.3, 135.0, 134.3, 134.0, 131.4, 131.1, 130.8, 130.4, 129.8, 129.2, 128.6, 128.2, 128.1, 127.4, 127.0, 126.8, 125.2, 124.8, 124.6, 120.5, 117.0, 113.5, 55.20, 21.6, 21.2. HRMS (ESI) calcd for  $C_{37}H_{32}NO_3S$   $[M+H]^+$  570.2103; found: 570.2081.

**(Z)-3-(1-(4-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)vinyl)-2-phenyl-1-tosyl-indole (19):** The title



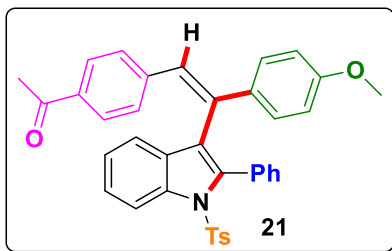
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (85:15) to obtain as a white solid (48 mg, yield = 74%); Mp. 167-168 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.34 (d,  $J$  = 8.4 Hz, 1H), 7.39 – 7.34 (m, 1H), 7.29 (d,  $J$  = 8.3 Hz, 2H), 7.21 (td,  $J$  = 7.2, 5.1 Hz, 2H), 7.15 – 7.08 (m, 5H), 7.02 – 6.89 (m, 4H), 6.79 (s, 1H), 6.70 (d,  $J$  = 8.8 Hz, 2H), 5.83 (s, 2H), 3.79 (s, 3H), 3.78 (s, 3H), 3.26 (s, 6H), 2.38 (s, 3H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ) 159.2, 152.4, 144.6, 138.2, 138.0, 136.7, 134.3, 133.4, 132.8, 132.2, 131.6, 131.0, 129.2, 127.9, 127.3, 126.9, 126.8, 125.3, 124.8, 124.5, 120.4, 117.1, 113.7, 105.1, 60.76, 55.30, 55.23, 21.59. HRMS (ESI) calcd for  $C_{39}H_{36}NO_6S$   $[M+H]^+$  646.2263; found: 646.2290.

**(Z)-3-(1-(4-methoxyphenyl)-2-(3-nitrophenyl)vinyl)-2-phenyl-1-tosyl-indole (20):** The title compound was



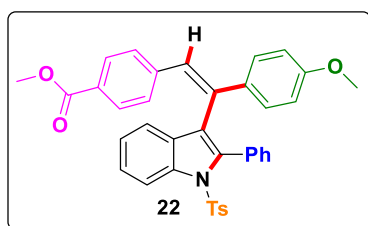
prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a pale-yellow solid (36 mg, yield = 61%); Mp. 195-196 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.39 (d,  $J$  = 8.4 Hz, 1H), 7.83 (dd,  $J$  = 8.1, 1.4 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.36 (s, 1H), 7.26 (d,  $J$  = 8.2 Hz, 2H), 7.23 – 7.07 (m, 5H), 7.07 – 6.92 (m, 6H), 6.85 (d,  $J$  = 7.8 Hz, 2H), 6.80 (s, 1H), 6.71 (t,  $J$  = 5.9 Hz, 2H), 3.80 (s, 3H), 2.38 (s, 3H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  159.8, 147.9, 144.6, 139.0, 138.6, 138.3, 135.2, 134.5, 133.3, 132.7, 131.4, 130.4, 129.1, 128.5, 128.3, 127.7, 126.9, 126.9, 126.4, 125.5, 124.9, 123.2, 123.2, 121.0, 120.3, 117.4, 113.8, 55.25, 21.60. HRMS (ESI) calcd for  $C_{36}H_{29}N_2O_5S$   $[M+H]^+$  601.1797; found: 601.1808.

**(Z)-1-(4-(2-(4-methoxyphenyl)-2-(2-phenyl-1-tosyl-indol-3-yl)vinyl)phenyl)ethan-1-one (21):** The title



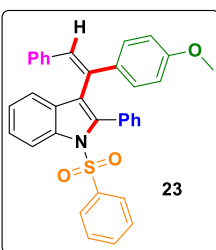
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (43 mg, yield = 72%); Mp. 188-189 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.41 (d,  $J$  = 8.4 Hz, 1H), 7.46 (d,  $J$  = 8.3 Hz, 2H), 7.39 (t,  $J$  = 7.8 Hz, 1H), 7.33 (d,  $J$  = 8.3 Hz, 2H), 7.21 – 7.01 (m, 8H), 6.96 (d,  $J$  = 8.8 Hz, 3H), 6.88 (s, 1H), 6.75 (d,  $J$  = 8.3 Hz, 2H), 6.66 (d,  $J$  = 8.8 Hz, 2H), 3.76 (s, 3H), 2.51 (s, 3H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  197.4, 159.5, 144.8, 142.0, 138.4, 138.1, 134.8, 134.7, 134.6, 133.2, 131.1, 130.8, 130.3, 129.3, 128.3, 128.2, 128.2, 128.0, 127.7, 127.0, 126.9, 125.4, 124.8, 124.0, 120.3, 117.2, 113.6, 55.22, 26.5, 21.6. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{32}\text{NO}_4\text{S}$   $[\text{M}+\text{H}]^+$  598.2052; found: 598.2044.

**methyl (Z)-4-(2-(4-methoxyphenyl)-2-(2-phenyl-1-tosyl-indol-3-yl)vinyl)benzoate (22):** The title compound



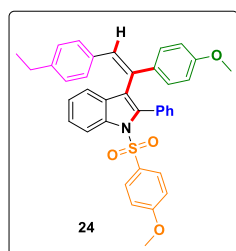
was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (90:10) to obtain as a white solid (52 mg, yield = 85%); Mp. 189-190 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.40 (d,  $J$  = 8.4 Hz, 1H), 7.52 (d,  $J$  = 8.4 Hz, 2H), 7.39 (dd,  $J$  = 11.4, 4.2 Hz, 1H), 7.33 (d,  $J$  = 8.3 Hz, 2H), 7.21 – 7.02 (m, 8H), 6.95 (d,  $J$  = 8.8 Hz, 3H), 6.89 (s, 1H), 6.74 (d,  $J$  = 8.4 Hz, 2H), 6.65 (d,  $J$  = 8.8 Hz, 2H), 3.87 (s, 3H), 3.75 (s, 3H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 159.5, 144.8, 141.8, 138.4, 138.0, 134.9, 134.5, 133.2, 131.0, 130.8, 130.3, 129.3, 129.3, 128.5, 128.2, 128.0, 127.7, 127.7, 127.0, 126.9, 125.4, 124.8, 124.1, 120.3, 117.2, 113.6, 55.2, 51.9, 21.6. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{32}\text{NO}_5\text{S}$   $[\text{M}+\text{H}]^+$  614.2001; found: 614.2005.

**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-1-(phenylsulfonyl)-indole (23):** The title compound



was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (41 mg, yield = 76%); Mp. 143-144 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.40 (d,  $J$  = 8.4 Hz, 1H), 7.56-7.52 (m, 1H), 7.46 – 7.41 (m, 2H), 7.41 – 7.36 (m, 1H), 7.34-7.30 (m, 2H), 7.19-7.15 (m, 2H), 7.10-7.06 (m, 3H), 6.99 (t,  $J$  = 7.3 Hz, 2H), 6.96 – 6.83 (m, 6H), 6.70 – 6.62 (m, 4H), 3.75 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 138.2, 138.0, 137.8, 137.1, 133.7, 133.5, 131.7, 131.4, 130.8, 130.4, 129.8, 128.6, 128.2, 128.1, 127.9, 127.5, 126.9, 126.8, 126.5, 125.3, 124.7, 124.5, 120.6, 117.0, 113.6, 55.23. HRMS (ESI) calcd for  $\text{C}_{35}\text{H}_{28}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  542.1790; found: 542.1763.

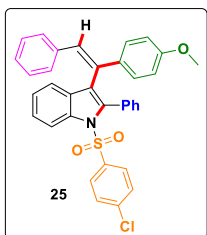
**(Z)-3-(2-(4-ethylphenyl)-1-(4-methoxyphenyl)vinyl)-1-((4-methoxyphenyl)sulfonyl)-2-phenyl-indole (24):**



The title compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (49 mg, yield = 82%); Mp. 137-138 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.40 (d,  $J$  = 8.4 Hz, 1H), 7.38 (dd,  $J$  = 11.0, 5.0 Hz, 3H), 7.16 (dd,  $J$  = 10.0, 4.6 Hz, 2H), 7.12 – 6.96 (m, 5H),

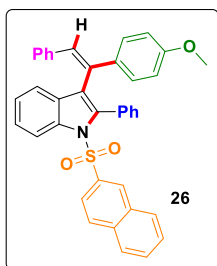
6.92 (d,  $J = 8.8$  Hz, 2H), 6.85 (s, 1H), 6.76 (d,  $J = 8.9$  Hz, 2H), 6.71 (d,  $J = 8.1$  Hz, 2H), 6.64 (d,  $J = 8.8$  Hz, 2H), 6.60 (d,  $J = 8.1$  Hz, 2H), 3.81 (s, 3H), 3.74 (s, 3H), 2.50 (q,  $J = 7.6$  Hz, 2H), 1.16 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  163.5, 158.9, 142.7, 138.2, 134.5, 134.0, 131.5, 131.1, 130.8, 130.4, 129.8, 129.4, 129.2, 128.2, 128.0, 127.4, 127.4, 126.8, 125.1, 124.8, 124.6, 120.5, 117.1, 113.7, 113.5, 55.5, 55.2, 28.5, 15.5. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{34}\text{NO}_4\text{S}$   $[\text{M}+\text{H}]^+$  599.2200; found: 600.2206.

**(Z)-1-((4-chlorophenyl)sulfonyl)-3-(2-(4-ethylphenyl)-1-(4-methoxyphenyl)vinyl)-2-phenyl-indole (25):**



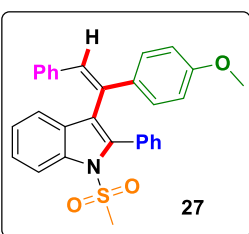
The title compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (95:5) to obtain as a white solid (44 mg, yield = 73%); Mp. 180-181 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (d,  $J = 8.4$  Hz, 1H), 7.42-7.39 (m, 1H), 7.34 (d,  $J = 8.7$  Hz, 2H), 7.28 (d,  $J = 8.7$  Hz, 2H), 7.20 (td,  $J = 7.5, 3.2$  Hz, 2H), 7.12-7.09 (m, 3H), 7.04-7.00 (m, 2H), 6.98 – 6.93 (brs, 1H), 6.92 – 6.87 (m, 5H), 6.69 (d,  $J = 8.8$  Hz, 2H), 6.66 (d,  $J = 7.6$  Hz, 2H), 3.77 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 140.2, 138.0, 137.0, 135.8, 133.5, 131.9, 131.5, 130.7, 129.9, 128.9, 128.4, 128.2, 128.1, 127.9, 127.4, 126.9, 126.7, 125.5, 125.1, 125.1, 120.7, 117.2, 113.7, 110.0, 55.23. HRMS (ESI) calcd for  $\text{C}_{35}\text{H}_{27}\text{ClNO}_3\text{S}$   $[\text{M}+\text{H}]^+$  576.1322; found: 576.1320.

**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-(naphthalen-2-ylsulfonyl)-2-phenyl-indole (26):** The title



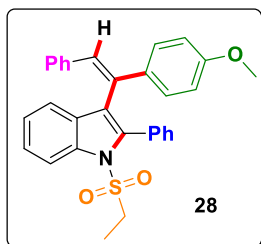
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (41 mg, yield = 70%); Mp. 241-242 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.48 (d,  $J = 8.4$  Hz, 1H), 7.93 (d,  $J = 1.6$  Hz, 1H), 7.87 (d,  $J = 8.2$  Hz, 1H), 7.73 (d,  $J = 8.8$  Hz, 2H), 7.67 – 7.62 (m, 1H), 7.58 – 7.53 (m, 1H), 7.43 – 7.38 (m, 2H), 7.18 (ddd,  $J = 15.1, 14.5, 7.3$  Hz, 2H), 7.09 (t,  $J = 7.6$  Hz, 2H), 7.05-6.93 (m, 3H), 6.86 (t,  $J = 7.4$  Hz, 1H), 6.78 (dt,  $J = 5.1, 2.8$  Hz, 3H), 6.70 (d,  $J = 7.9$  Hz, 2H), 6.59 (d,  $J = 7.3$  Hz, 2H), 6.41 (d,  $J = 8.8$  Hz, 2H), 3.68 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 138.2, 137.0, 135.2, 134.5, 133.6, 131.6, 131.6, 130.9, 130.5, 129.7, 129.5, 129.2, 128.7, 128.7, 128.1, 128.0, 127.8, 127.7, 127.6, 127.3, 126.8, 126.5, 125.3, 124.8, 124.7, 121.8, 120.5, 117.3, 113.5, 110.0, 55.2.

**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-1-(methylsulfonyl)-2-phenyl-indole (27):** The title compound



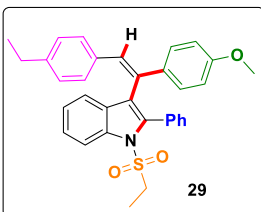
was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (97:3) to obtain as a white solid (36 mg, yield = 75%); Mp. 162-163 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.19 (d,  $J = 8.4$  Hz, 1H), 7.39 (ddd,  $J = 8.5, 6.5, 2.1$  Hz, 1H), 7.29 – 7.22 (m, 4H), 7.19 (t,  $J = 7.4$  Hz, 1H), 7.14 – 7.00 (m, 6H), 6.98 (s, 2H), 6.88 – 6.84 (m, 2H), 6.82 – 6.77 (m, 2H), 3.78 (s, 3H), 2.78 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.3, 137.6, 137.5, 137.5, 133.7, 131.9, 131.1, 130.6, 130.23, 130.1, 128.4, 128.3, 128.0, 127.6, 127.1, 126.8, 125.5, 124.7, 123.2, 120.9, 115.9, 113.8, 55.3, 39.9. HRMS (ESI) calcd for  $\text{C}_{30}\text{H}_{26}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  480.1633; found: 480.1637.

**(Z)-1-(ethylsulfonyl)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-indole (28):** The title compound was



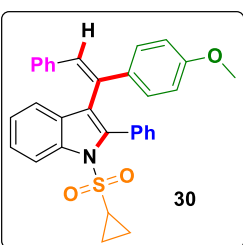
prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (93:3) to obtain as a white solid (33 mg, yield = 67%); Mp. 64-65 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.18 (d,  $J = 8.4$  Hz, 1H), 7.37 (t,  $J = 6.9$  Hz, 1H), 7.30 – 7.19 (m, 5H), 7.17 (d,  $J = 7.4$  Hz, 1H), 7.05 (dd,  $J = 14.9, 7.1$  Hz, 6H), 6.96 (s, 1H), 6.85 (d,  $J = 6.9$  Hz, 2H), 6.79 (d,  $J = 8.7$  Hz, 2H), 3.78 (s, 3H), 3.03 (dd,  $J = 14.6, 7.2$  Hz, 2H), 1.08 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.3, 137.9, 137.6, 134.0, 132.0, 131.5, 130.5, 130.4, 130.3, 130.2, 128.6, 128.4, 128.3, 128.0, 127.7, 127.6, 127.1, 126.9, 126.8, 125.2, 124.2, 122.2, 120.8, 115.4, 113.8, 55.3, 48.4, 7.7. HRMS (ESI) calcd for  $\text{C}_{31}\text{H}_{28}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  494.1790; found: 494.1793.

**(Z)-3-(2-(4-ethylphenyl)-1-(4-methoxyphenyl)vinyl)-1-(ethylsulfonyl)-2-phenyl-indole (29):** The title



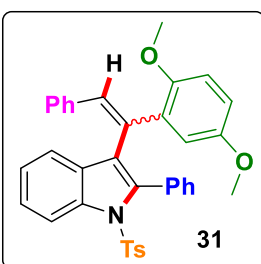
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (37 mg, yield = 71%); Mp. 124-125 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.19 (d,  $J = 8.4$  Hz, 1H), 7.37 (ddd,  $J = 8.5, 6.9, 1.6$  Hz, 1H), 7.31 – 7.14 (m, 6H), 7.07 (t,  $J = 7.3$  Hz, 2H), 6.99 (brs, 1H), 6.94 (s, 1H), 6.88 (d,  $J = 8.3$  Hz, 2H), 6.78 (d,  $J = 8.9$  Hz, 4H), 3.78 (s, 3H), 3.06 – 3.00 (m, 2H), 2.54 (q,  $J = 7.6$  Hz, 2H), 1.17 (t,  $J = 7.6$  Hz, 3H), 1.09 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 143.1, 137.9, 137.6, 134.9, 134.2, 131.0, 130.6, 130.5, 130.4, 130.2, 128.4, 128.2, 127.5, 126.9, 125.2, 124.3, 122.5, 120.9, 115.5, 113.8, 55.3, 48.3, 28.6, 15.6, 7.7. HRMS (ESI) calcd for  $\text{C}_{33}\text{H}_{32}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  522.2103; found: 522.2103.

**(Z)-1-(cyclopropylsulfonyl)-3-(1-(4-methoxyphenyl)-2-phenylvinyl)-2-phenyl-indole (30):** The title



compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a white solid (34 mg, yield = 67%); Mp. 63-64 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.23 (d,  $J = 8.4$  Hz, 1H), 7.39 – 7.35 (m, 1H), 7.27 (dd,  $J = 2.9, 1.6$  Hz, 1H), 7.25 (td,  $J = 1.8, 1.1$  Hz, 2H), 7.23 – 7.19 (m, 1H), 7.16 (t,  $J = 6.9$  Hz, 1H), 7.12 – 7.00 (m, 7H), 6.98 (s, 1H), 6.91 – 6.88 (m, 2H), 6.78 (d,  $J = 8.9$  Hz, 2H), 3.77 (s, 3H), 2.37 (tt,  $J = 8.0, 4.8$  Hz, 1H), 1.08 – 1.02 (m, 2H), 0.82 – 0.77 (m, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 138.0, 137.9, 137.5, 134.0, 132.0, 131.0, 130.9, 130.3, 130.1, 128.4, 128.1, 128.0, 127.6, 126.9, 126.7, 125.2, 124.4, 123.0, 120.7, 115.9, 113.8, 55.2, 30.5, 5.4, 5.2. HRMS (ESI) calcd for  $\text{C}_{32}\text{H}_{28}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  506.1790; found: 506.1805.

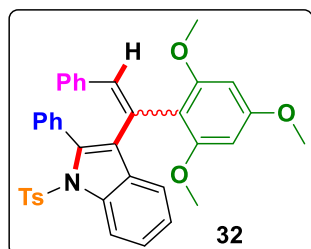
**(E/Z)-3-(1-(2,5-dimethoxyphenyl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (31):** The title compound was



prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (94:6) to obtain as a mixture of two isomer ( $E/Z=21:79$ ) white solid (21 mg, yield = 35%); Mp. 195-197 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (d,  $J = 8.4$  Hz, 1.96H), 7.39 – 7.30 (m, 7.08H), 7.24 – 6.95 (m, 23.63H), 6.86 (t,  $J = 7.7$

Hz, 4.53H), 6.80 (d,  $J = 10.5$  Hz, 2.40H), 6.77 – 6.70 (m, 3.74H), 6.47 (s, 0.20H), 6.05 (d,  $J = 4.2$  Hz, 1.62H), 5.98 (s, 0.34H), 2.97 (s, 2.23H), 2.91 (s, 2.78H), 2.85 (s, 0.59H), 2.80 (s, 0.56H), 2.33 (s, 3.02H), 2.32 (d,  $J = 2.9$  Hz, 3.01H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.7, 144.4, 139.1, 137.4, 137.3, 137.1, 135.4, 134.5, 134.4, 131.5, 131.4, 131.0, 130.9, 130.6, 130.5, 129.7, 129.2, 128.5, 128.4, 128.1, 127.9, 127.0, 126.8, 126.7, 125.3, 124.9, 124.1, 121.0, 116.4, 114.2, 114.0, 55.8, 21.6.

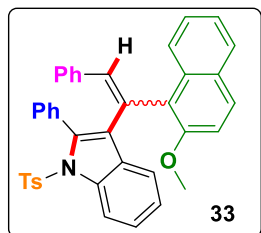
**(*E/Z*)-2-phenyl-3-(2-phenyl-1-(2,4,6-trimethoxyphenyl)vinyl)-1-tosyl-indole (32):** The title compound was



prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (85:15) to obtain mixture of two isomers ( $E/Z=33:67$ ) as a white solid (36 mg, yield = 58%); Mp. 183-184 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (d,  $J = 8.4$  Hz, 0.5H), 8.29 (d,  $J = 8.4$  Hz, 1H), 7.44 (d,  $J = 7.8$  Hz, 0.53H), 7.37 (d,  $J = 8.4$  Hz, 2.08H), 7.35 – 7.29 (m, 1.62H), 7.27 – 7.15 (m, 7.11H), 7.13 (d,  $J =$

8.2 Hz, 4.53H), 7.08 (d,  $J = 8.1$  Hz, 1.16H), 7.05 – 7.00 (m, 3.49H), 7.00 – 6.92 (m, 2.26H), 6.87 (d,  $J = 7.1$  Hz, 2.15H), 6.81 (t,  $J = 7.6$  Hz, 2.20H), 6.70 (s, 1H), 6.59 (s, 0.5H), 5.84 (s, 1H), 5.74 (s, 2H), 3.74 (s, 1.50H), 3.68 (s, 3H), 3.23 (s, 6H), 3.22 (s, 3H), 2.36 (s, 3H), 2.32 (s, 1.50H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  161.0, 160.0, 158.4, 158.3, 144.2, 144.2, 138.2, 137.6, 137.5, 137.1, 137.0, 136.2, 135.8, 135.4, 135.3, 134.6, 131.8, 131.7, 131.6, 130.8, 129.2, 129.1, 128.6, 127.9, 127.8, 127.7, 127.6, 127.5, 127.0, 126.9, 126.5, 126.4, 126.4, 126.3, 125.3, 124.4, 124.3, 123.8, 123.7, 121.6, 120.6, 116.4, 115.7, 113.8, 110.4, 90.8, 90.3, 55.2, 55.1, 55.1, 21.8. HRMS (ESI) calcd for  $\text{C}_{38}\text{H}_{34}\text{NO}_5\text{S}$   $[\text{M}+\text{H}]^+$  616.2158; found: 616.2162.

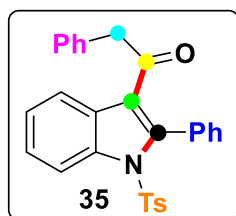
**(*E/Z*)-3-(1-(2-methoxynaphthalen-1-yl)-2-phenylvinyl)-2-phenyl-1-tosyl-indole (33):** The title compound



was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (90:10) to obtain mixture of two isomers ( $E/Z=23:77$ ) as a white solid (33 mg, yield = 55%); Mp. 179-180 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.37 (d,  $J = 8.5$  Hz, 0.27H), 8.32 (d,  $J = 8.4$  Hz, 1H), 7.92 (s, 0.82H), 7.70 (d,  $J = 8.1$  Hz, 0.37H), 7.61 (d,  $J = 9.5$  Hz, 0.57H), 7.56 (d,  $J = 13.9$  Hz, 2.04H), 7.44 (d,  $J = 8.5$  Hz,

0.37H), 7.42 – 7.33 (m, 2.28H), 7.32 – 7.26 (m, 2.17H), 7.23 – 7.10 (m, 6.39H), 7.10 – 6.98 (m, 0.51H), 6.92 (t,  $J = 6.9$  Hz, 5.22H), 6.88 – 6.78 (m, 2.86H), 6.72 (brs, 3.74H), 3.26 (s, 0.76H), 3.10 (brs, 2.51H), 2.38 (s, 3H), 2.33 (s, 0.9H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  154.1, 144.4, 137.5, 135.4, 131.2, 130.8, 130.1, 129.4, 129.3, 129.1, 129.0, 128.8, 128.2, 127.9, 127.6, 127.6, 127.4, 127.0, 126.8, 126.7, 126.1, 125.4, 125.0, 124.7, 124.5, 123.9, 123.1, 123.0, 120.6, 116.3, 115.6, 113.0, 55.5, 21.6. HRMS (ESI) calcd for  $\text{C}_{40}\text{H}_{32}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  606.2103; found: 606.2112.

**2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (35):** The title compound was prepared according to the

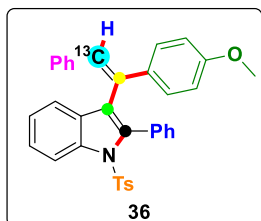


general modified procedure A (DCM solvent was used in absence of anisole solvent) via column chromatography of silica eluting hexane-ethyl acetate (96:4) to obtain as a colorless gummy (12 mg, yield = 26%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.36 (d,  $J = 8.4$  Hz,



1H), 8.10 (d,  $J = 8.0$  Hz, 1H), 7.56 (dd,  $J = 8.4, 6.5$  Hz, 1H), 7.49 – 7.41 (m, 3H), 7.37 – 7.33 (m, 3H), 7.31 (d,  $J = 8.4$  Hz, 2H), 7.22 – 7.13 (m, 3H), 7.10 (d,  $J = 8.1$  Hz, 2H), 6.85 (d,  $J = 6.2$  Hz, 2H), 3.30 (s, 2H), 2.34 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.8, 145.4, 143.0, 136.3, 135.4, 134.2, 131.8, 130.5, 130.2, 129.6, 129.4, 128.2, 128.0, 127.9, 126.9, 126.6, 125.9, 125.1, 122.9, 121.9, 115.1, 48.4, 21.6. HRMS (ESI) calcd for  $\text{C}_{29}\text{H}_{24}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  466.1477; found: 466.1468.

**(Z)-3-(1-(4-methoxyphenyl)-2-phenylvinyl-2- $^{13}\text{C}$ )-2-phenyl-1-tosyl-indole (36):** The title compound was



prepared according to the general procedure A via column chromatography of silica

eluting hexane-ethyl acetate (96:4) to obtain as a pale-yellow solid (42 mg, yield = 75%);

Mp. 187-188 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.39 (d,  $J = 8.4$  Hz, 1H), 7.40 – 7.35 (m,

1H), 7.31 (d,  $J = 8.3$  Hz, 2H), 7.17 (dt,  $J = 13.4, 6.7$  Hz, 2H), 7.13 – 7.03 (m, 6H), 6.99 (t,

$J = 7.3$  Hz, 2H), 6.94 (d,  $J = 8.8$  Hz, 2H), 6.86 (t,  $J = 7.7$  Hz, 2H), 6.73-6.64 (m, 5H),

3.75 (s, 3H), 2.38 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.1, 144.5, 138.1, 137.4, 136.8, 134.9, 134.2, 133.8,

132.2, 131.5, 131.0, 130.0, 129.8, 129.5, 129.4, 129.3, 129.2, 128.2, 128.2, 128.1, 127.9, 127.9, 127.5, 127.5,

127.0, 126.8, 126.5, 125.2, 124.7, 124.5, 120.5, 117.1, 113.5, 55.2, 21.6. HRMS (ESI) calcd for

$^{12}\text{C}_{35}^{13}\text{C}_1\text{H}_{30}\text{NO}_3\text{S}$   $[\text{M}+\text{H}]^+$  557.1980; found: 557.1969.

## 5. References

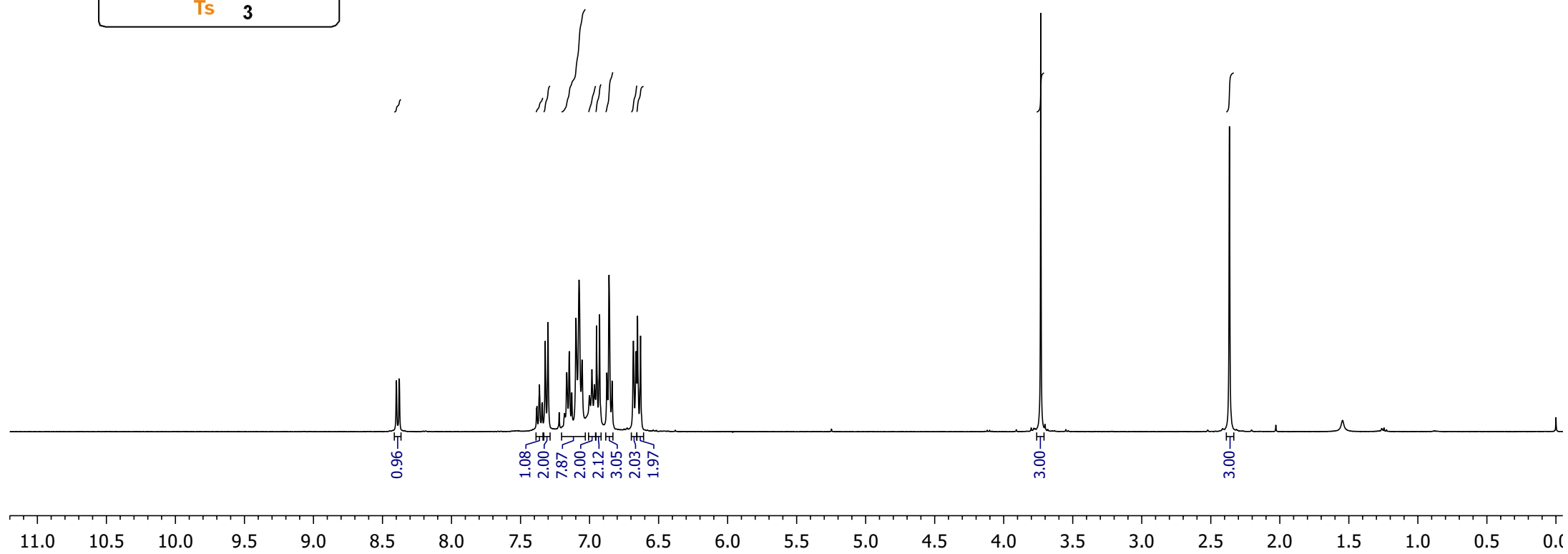
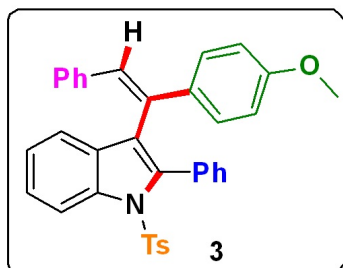
1. M. R. Mutra, J.-J Wang, *Nat. Commun.*, **2022**, 13, 2345.

Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$

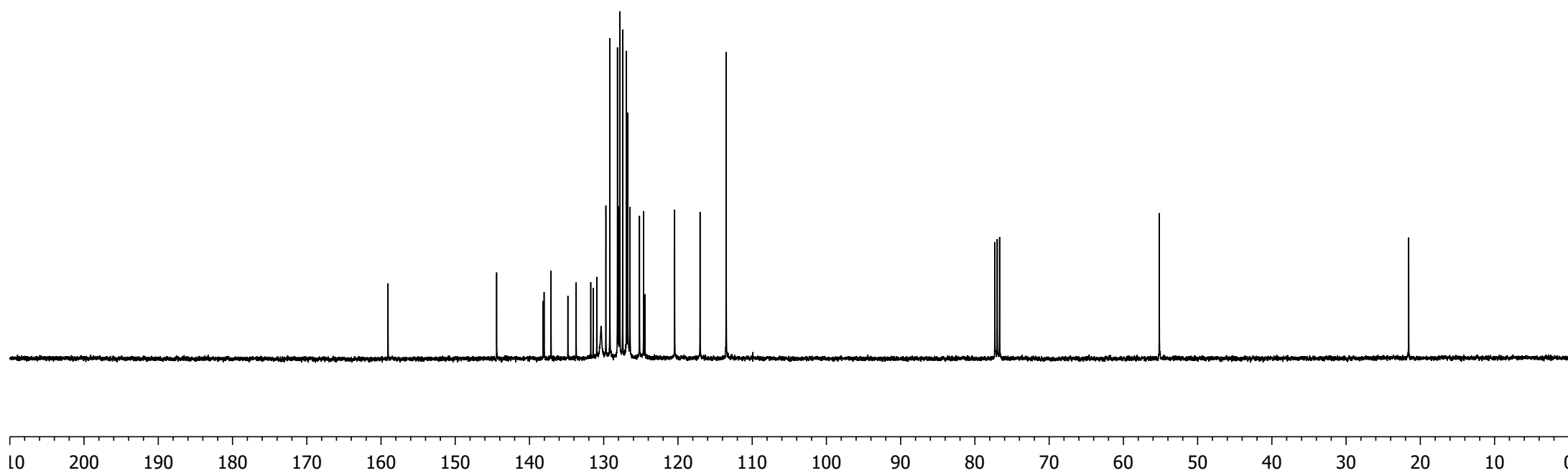
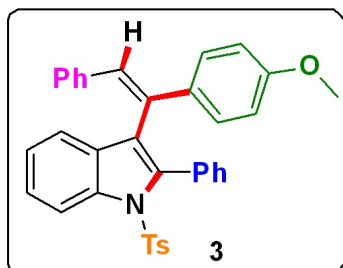
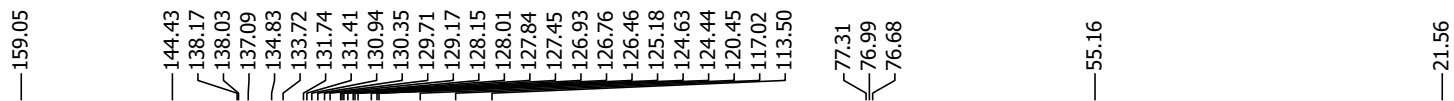
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3.73

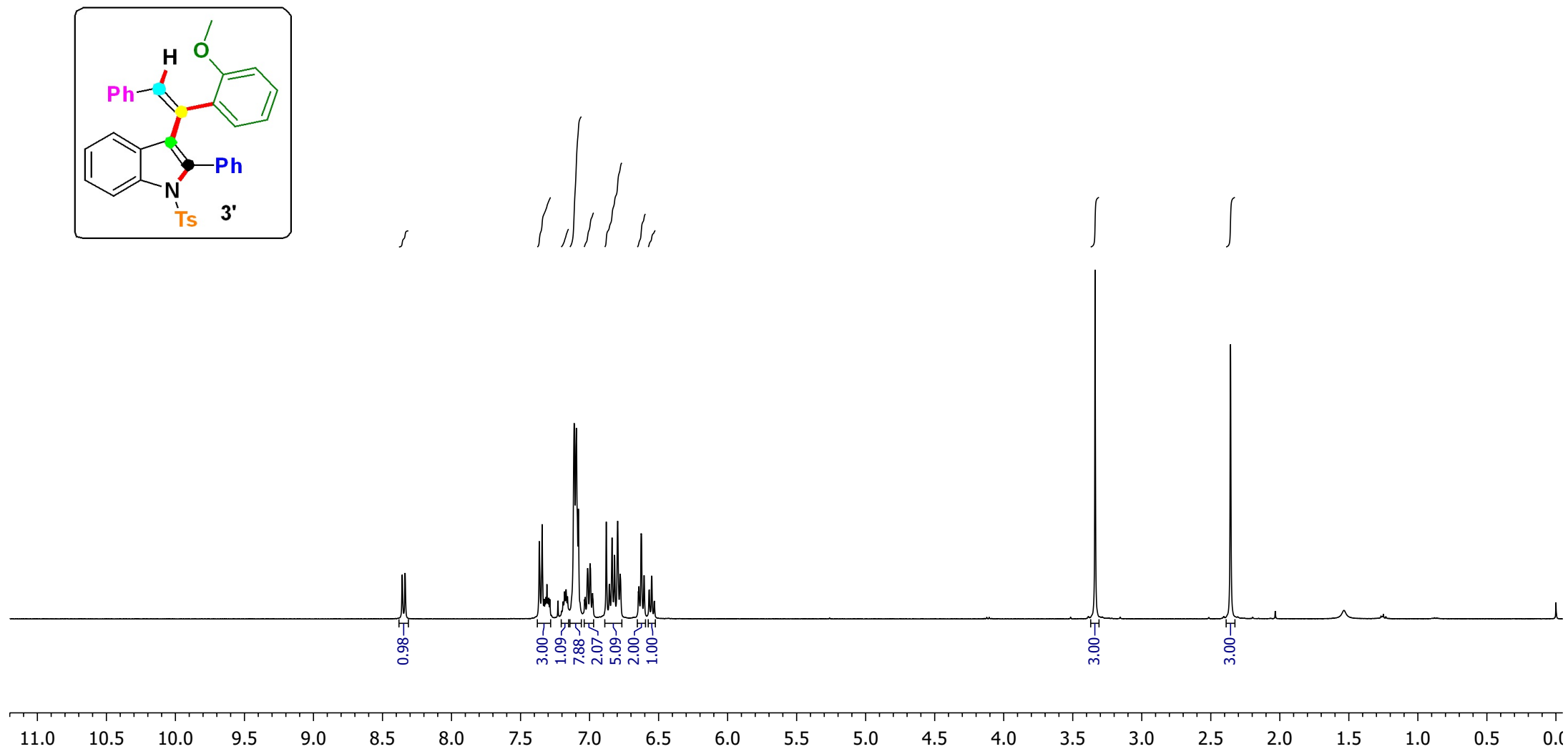
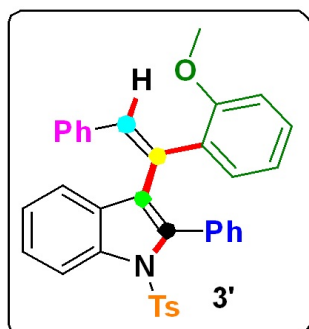
2.37



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 400.39  
Nucleus <sup>1</sup>H



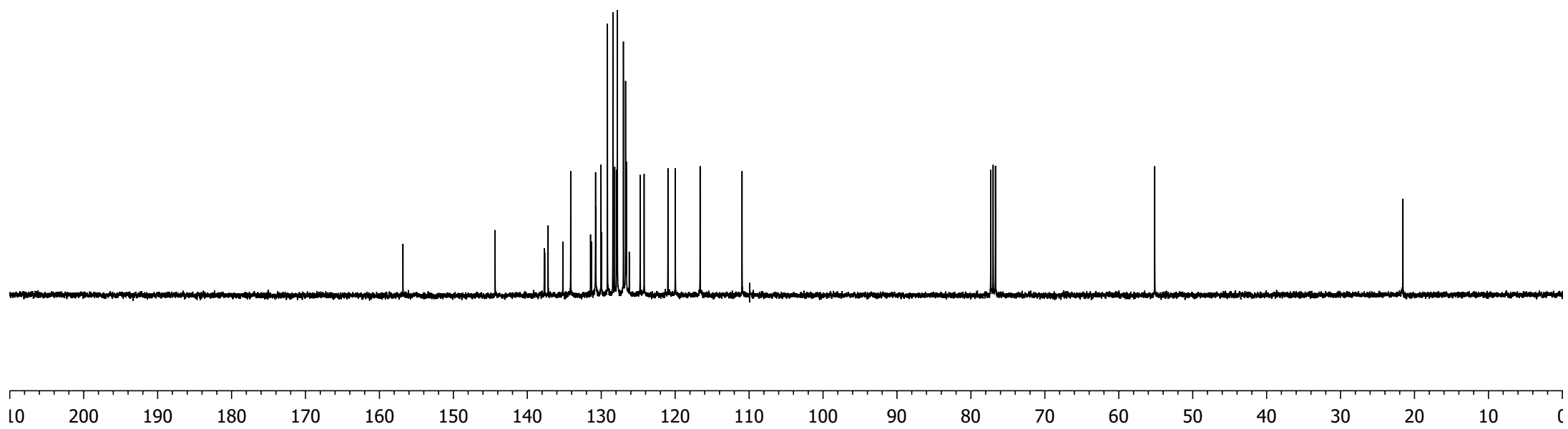
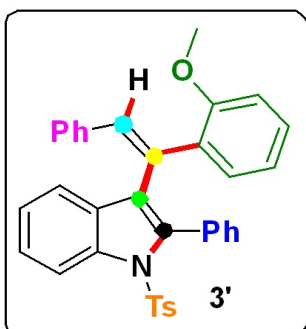
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Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

—156.82 —144.36  
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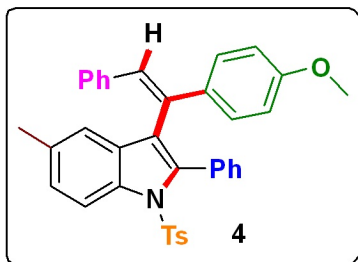
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—55.13

—21.56



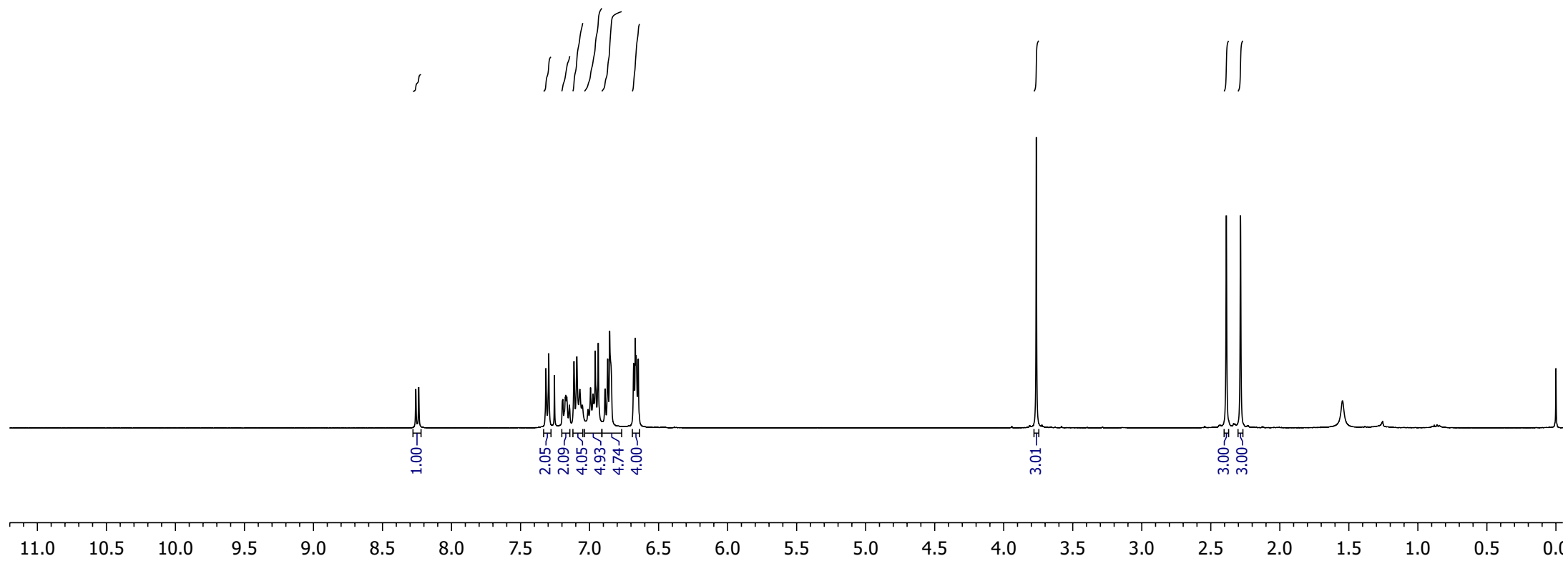
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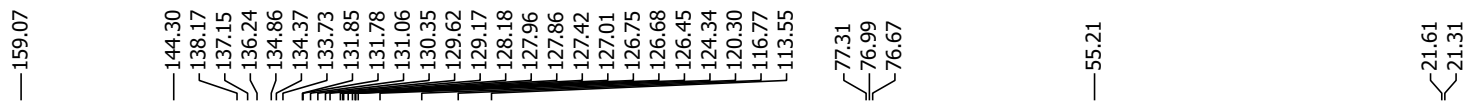


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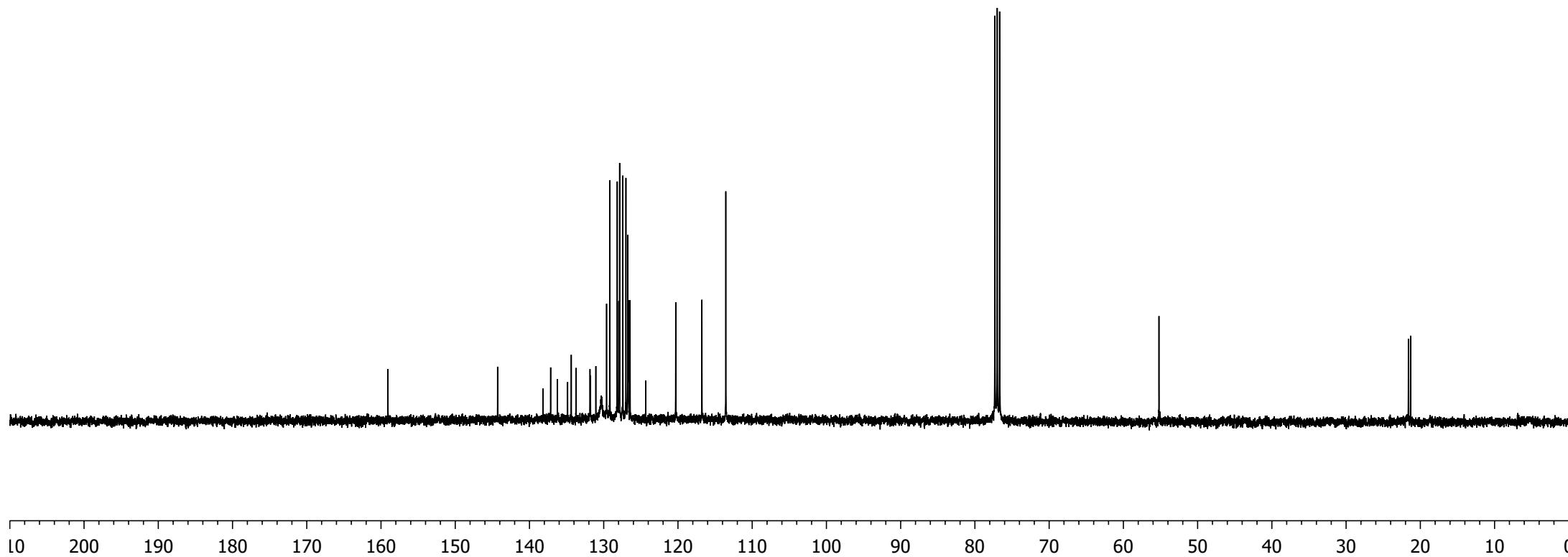
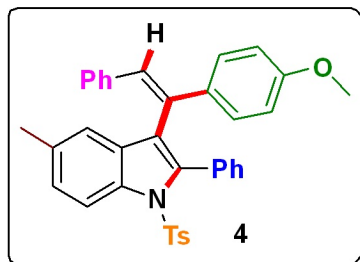
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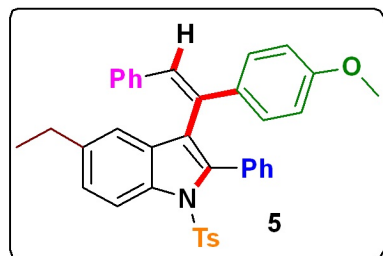




Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$

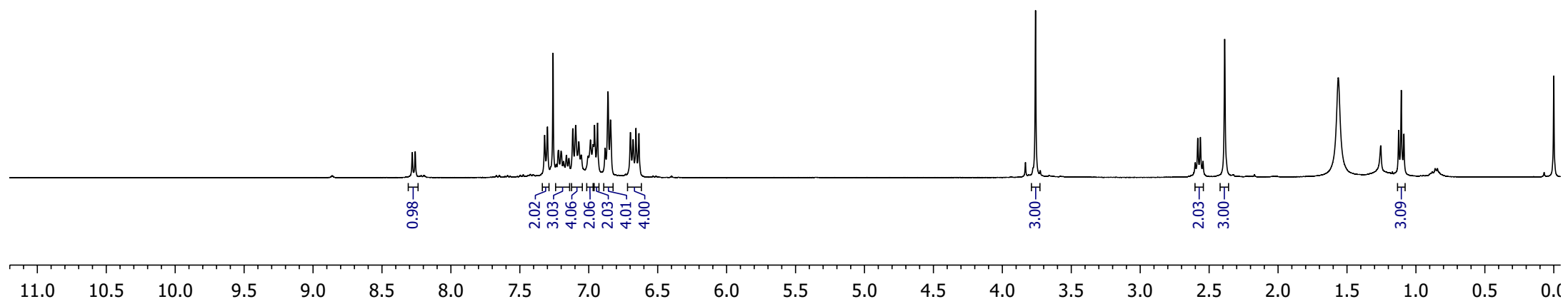


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7.07  
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6.97  
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3.76

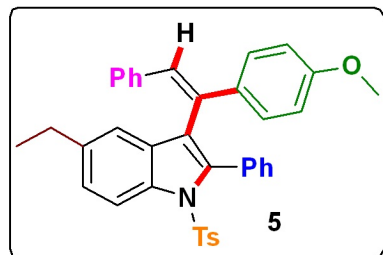
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Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



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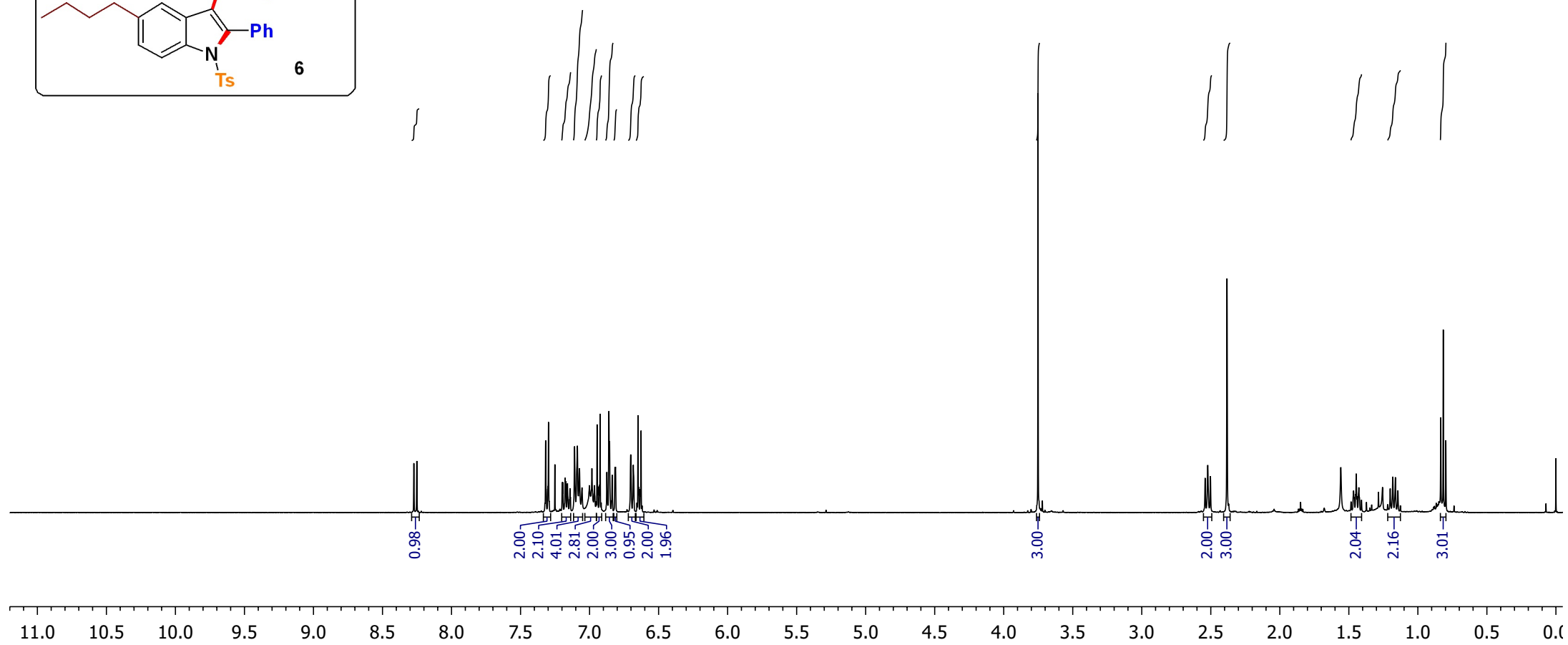
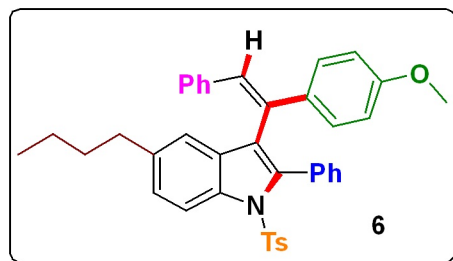
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Nucleus  $^1\text{H}$

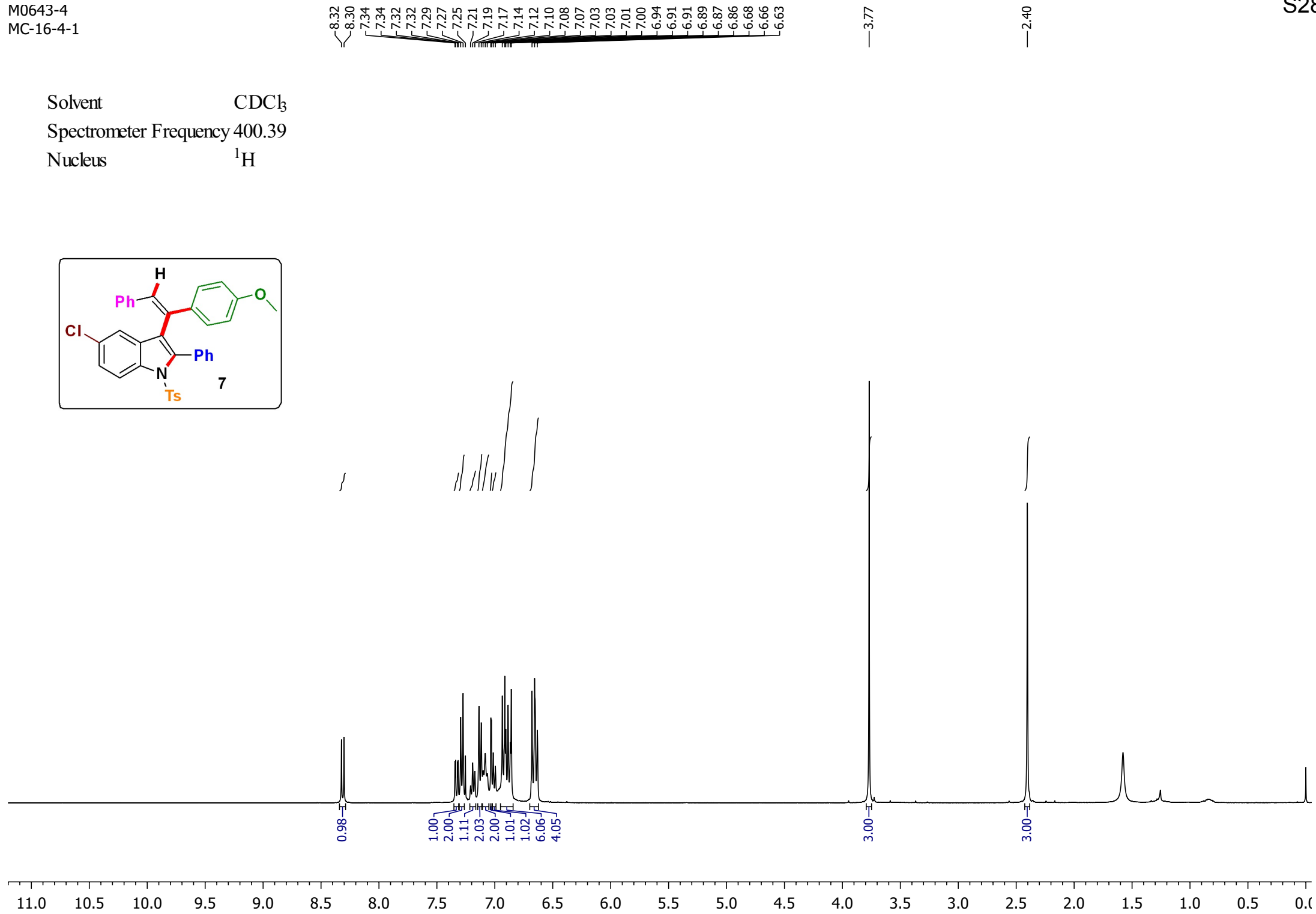
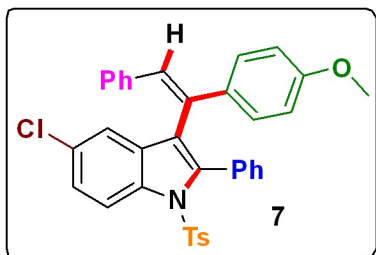
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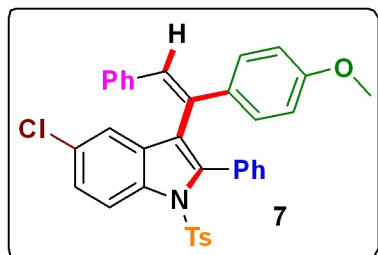




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Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
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Nucleus  $^{13}\text{C}$

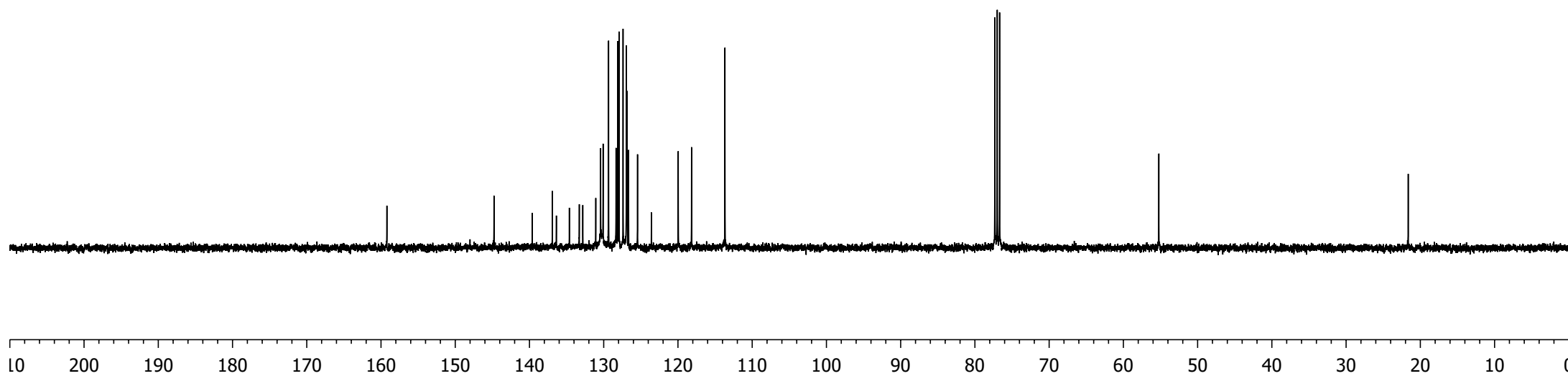


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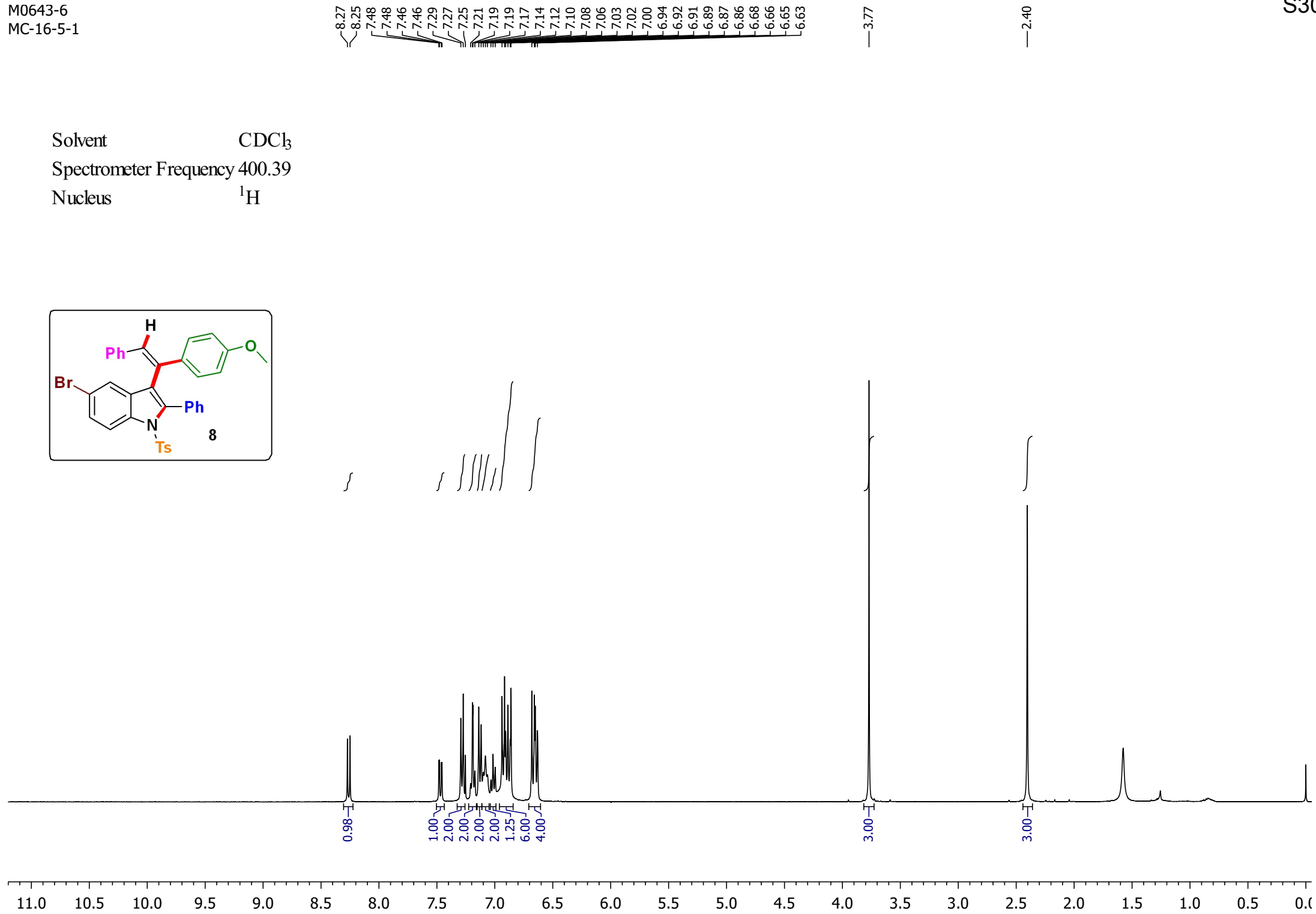
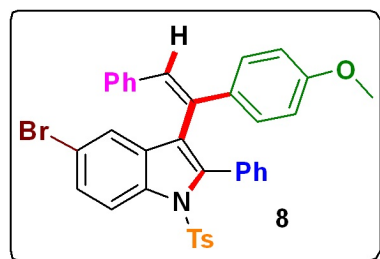
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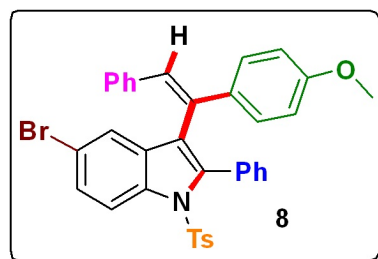
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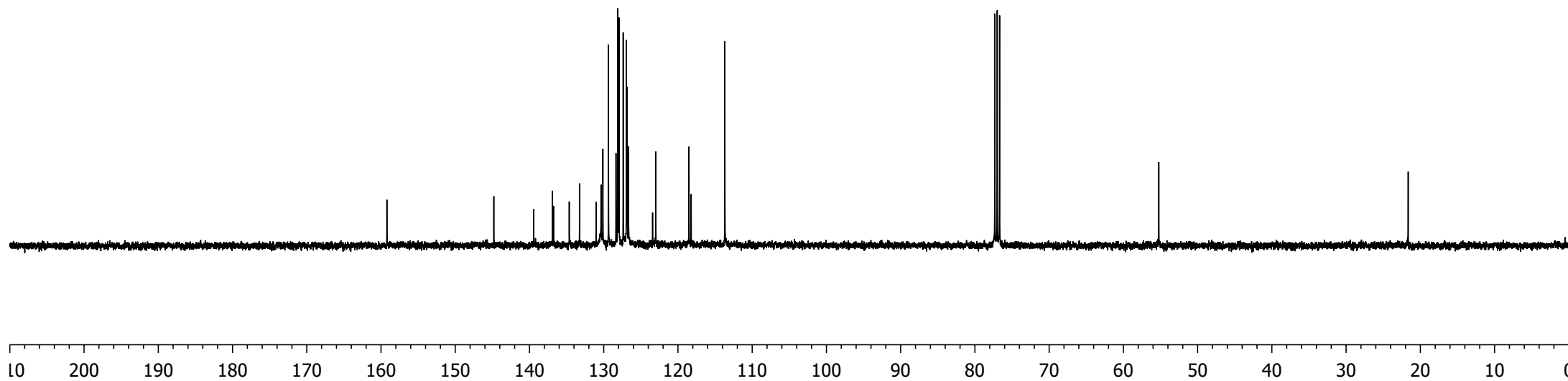


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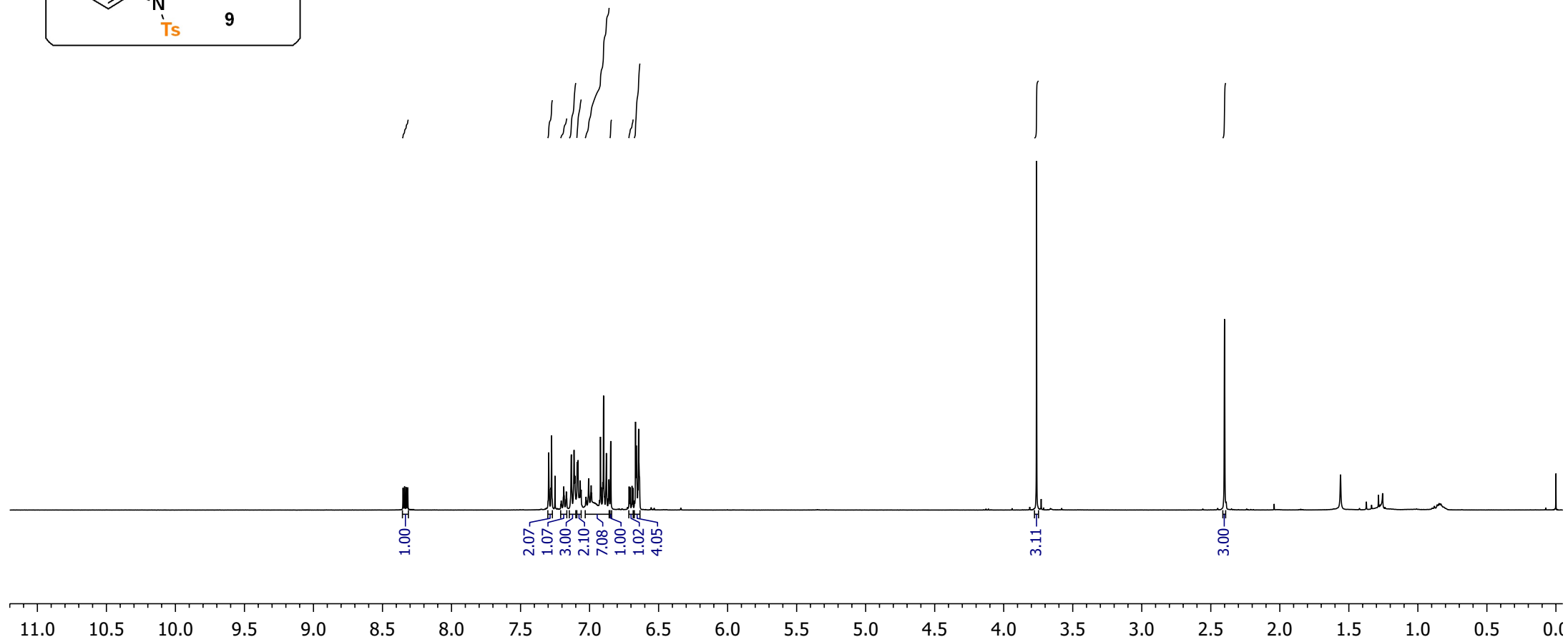
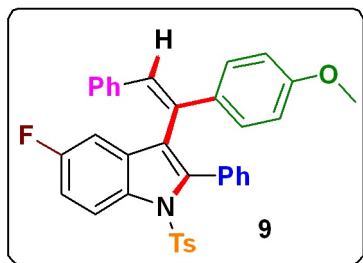
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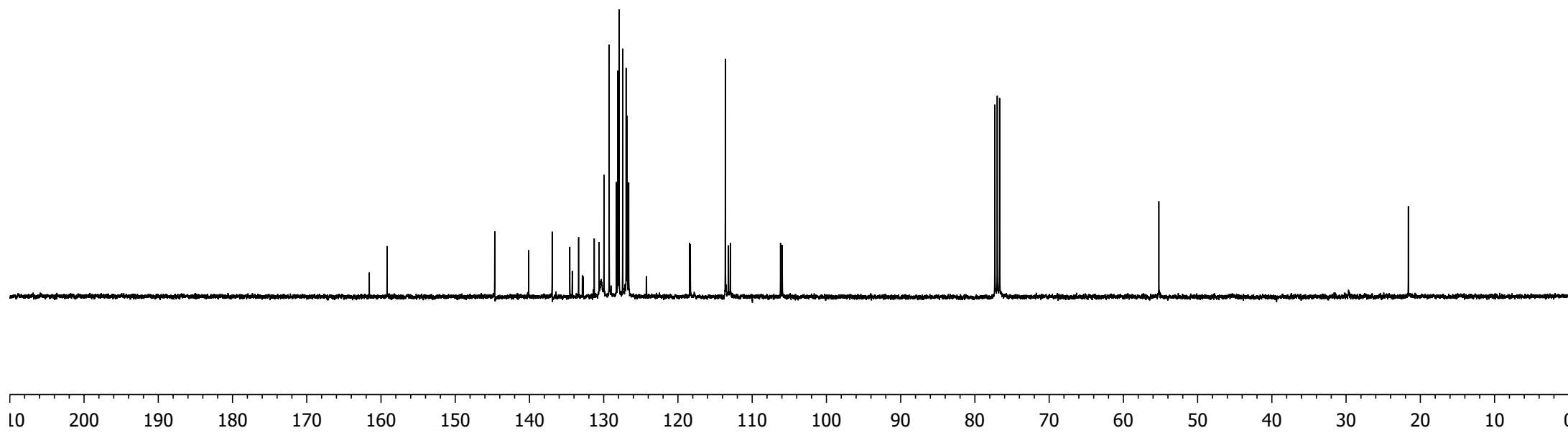
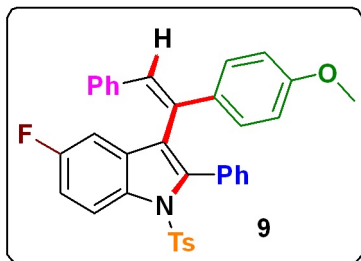
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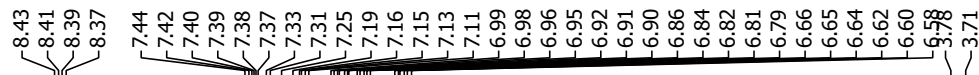




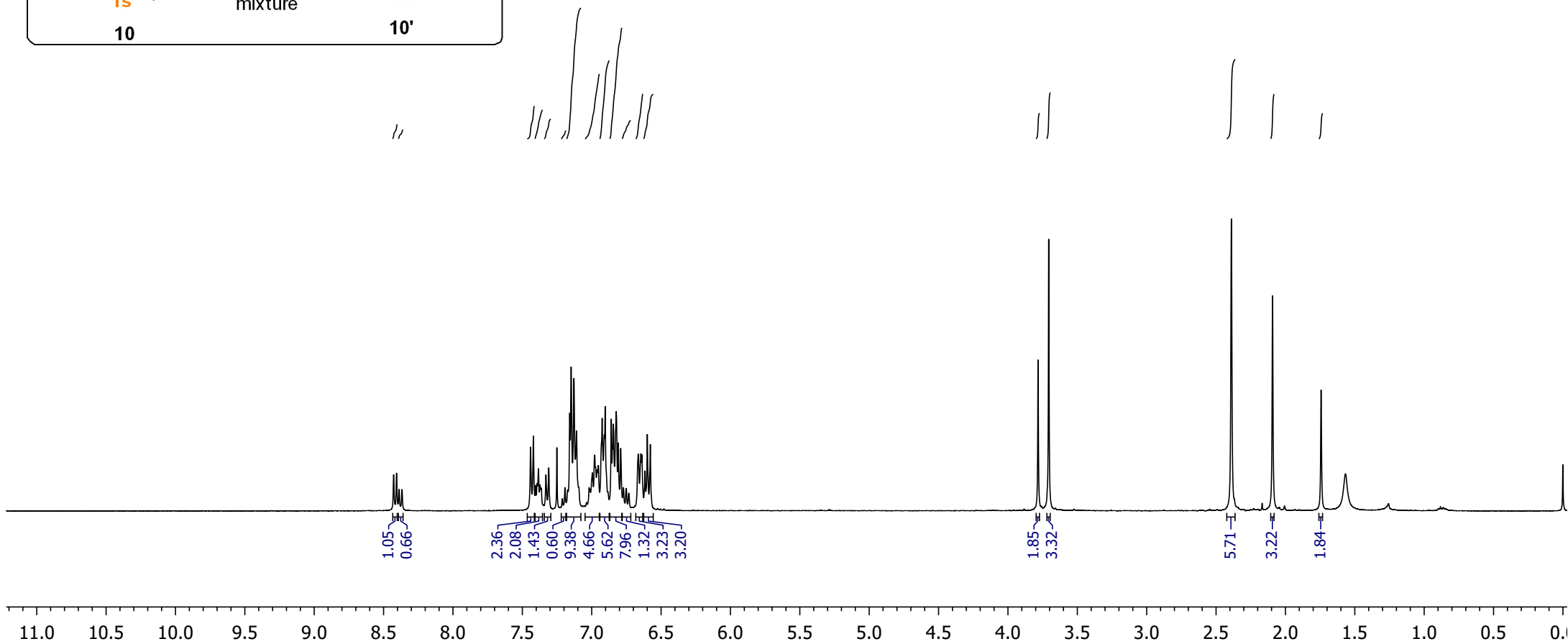
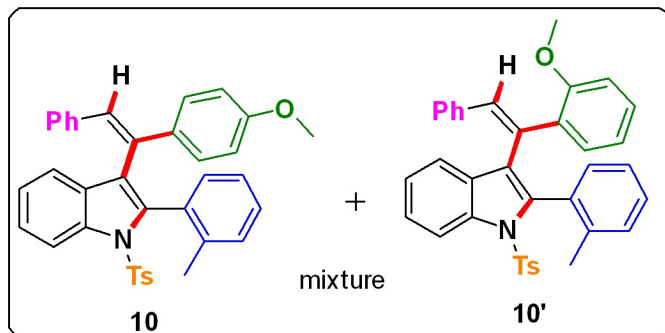


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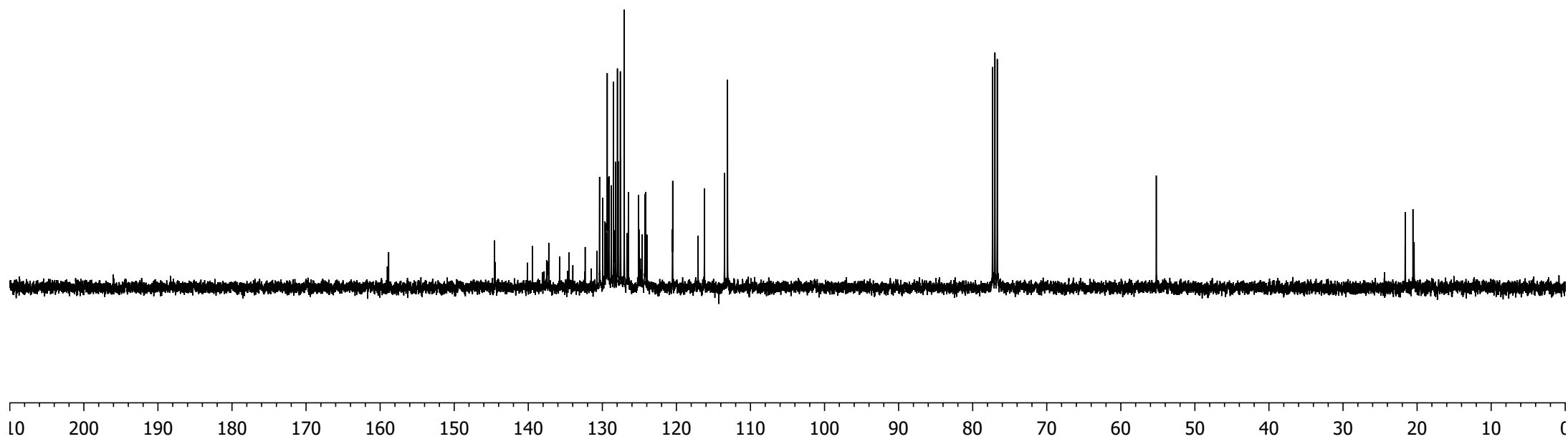
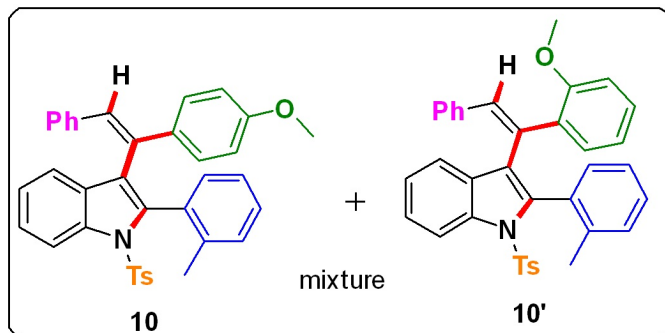
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Nucleus  $^1\text{H}$



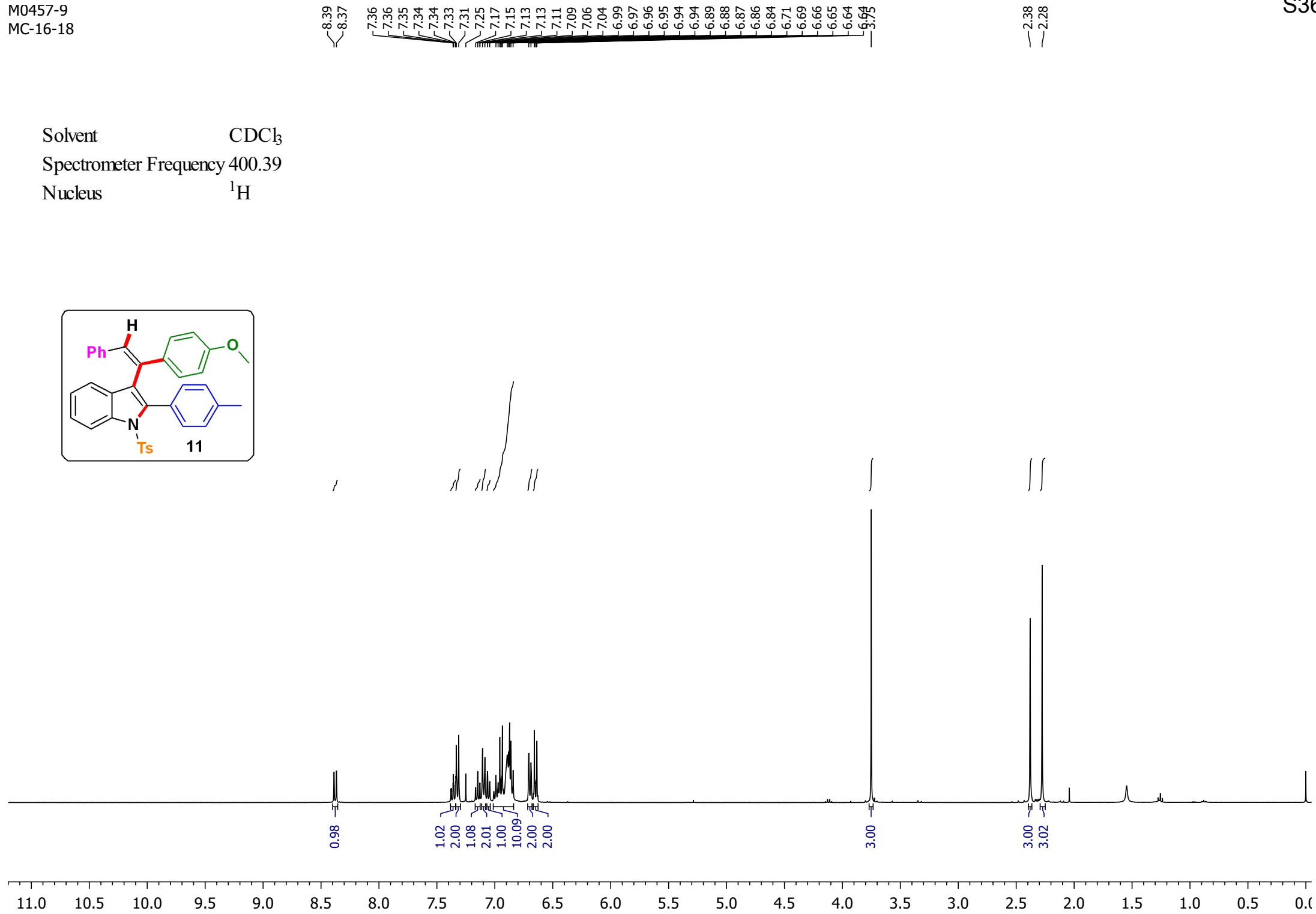
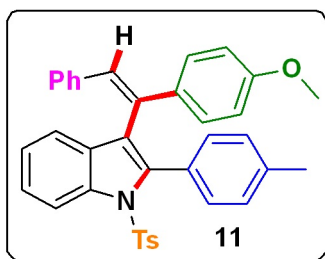
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55.21

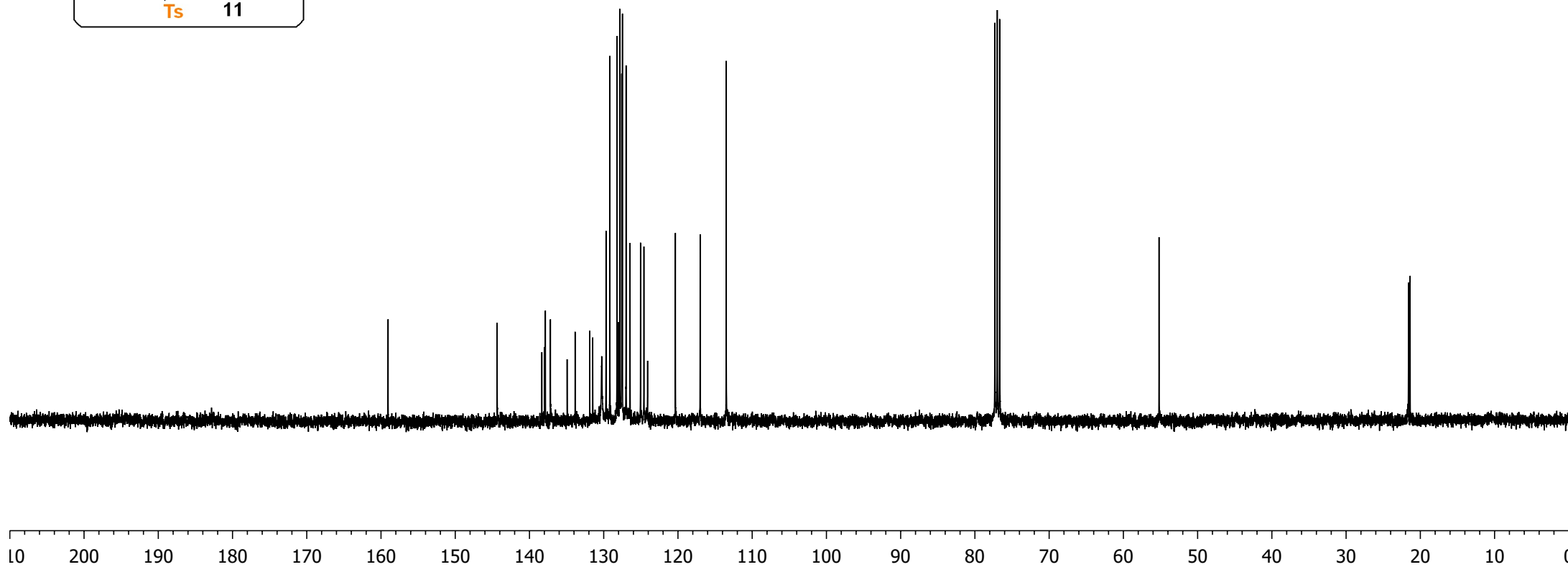
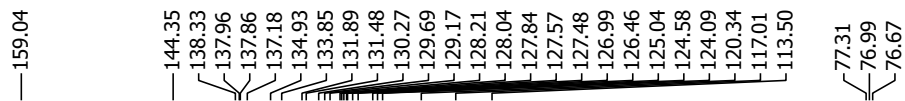
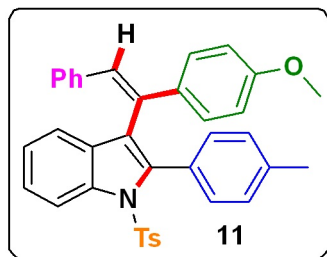
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Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



M0459-5  
MC-16-23

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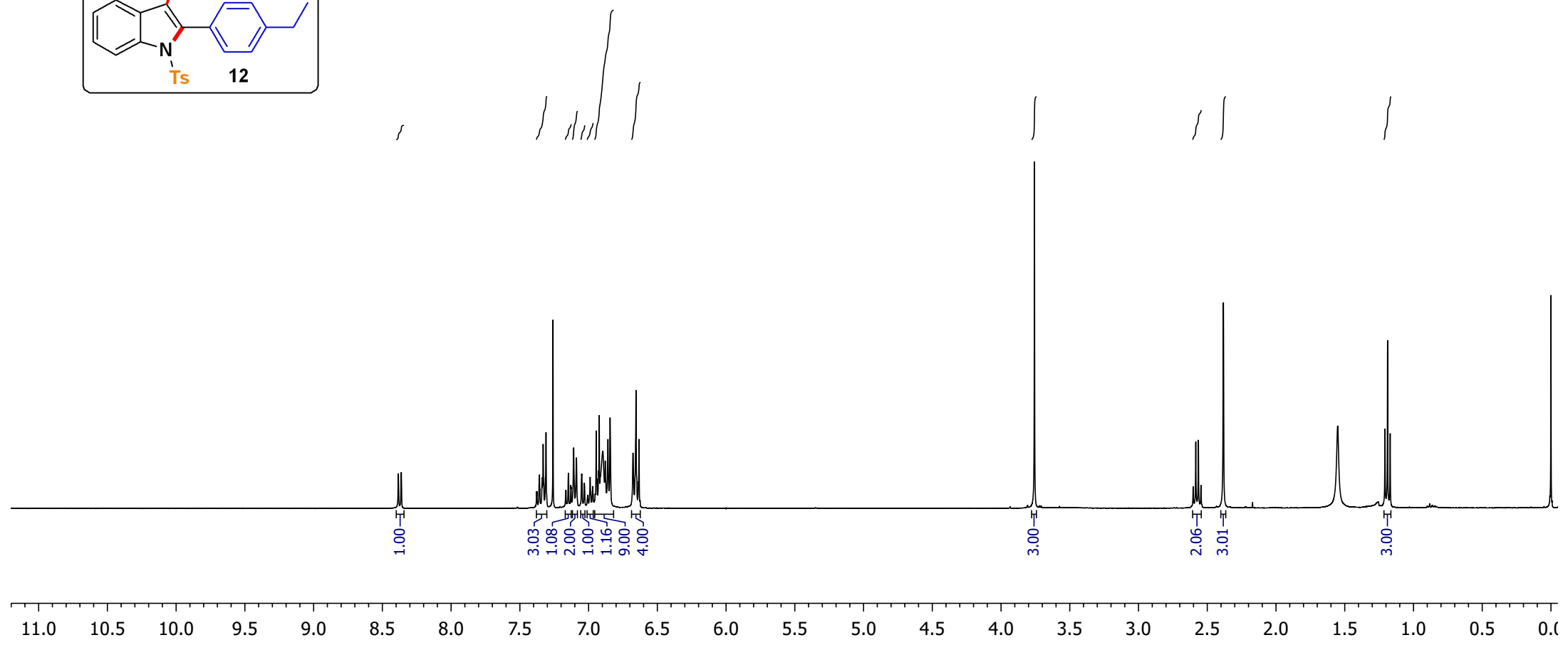
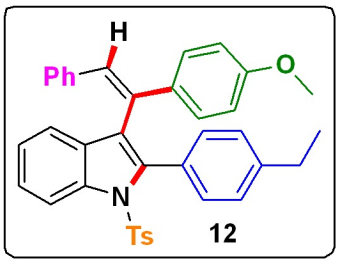
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1.55

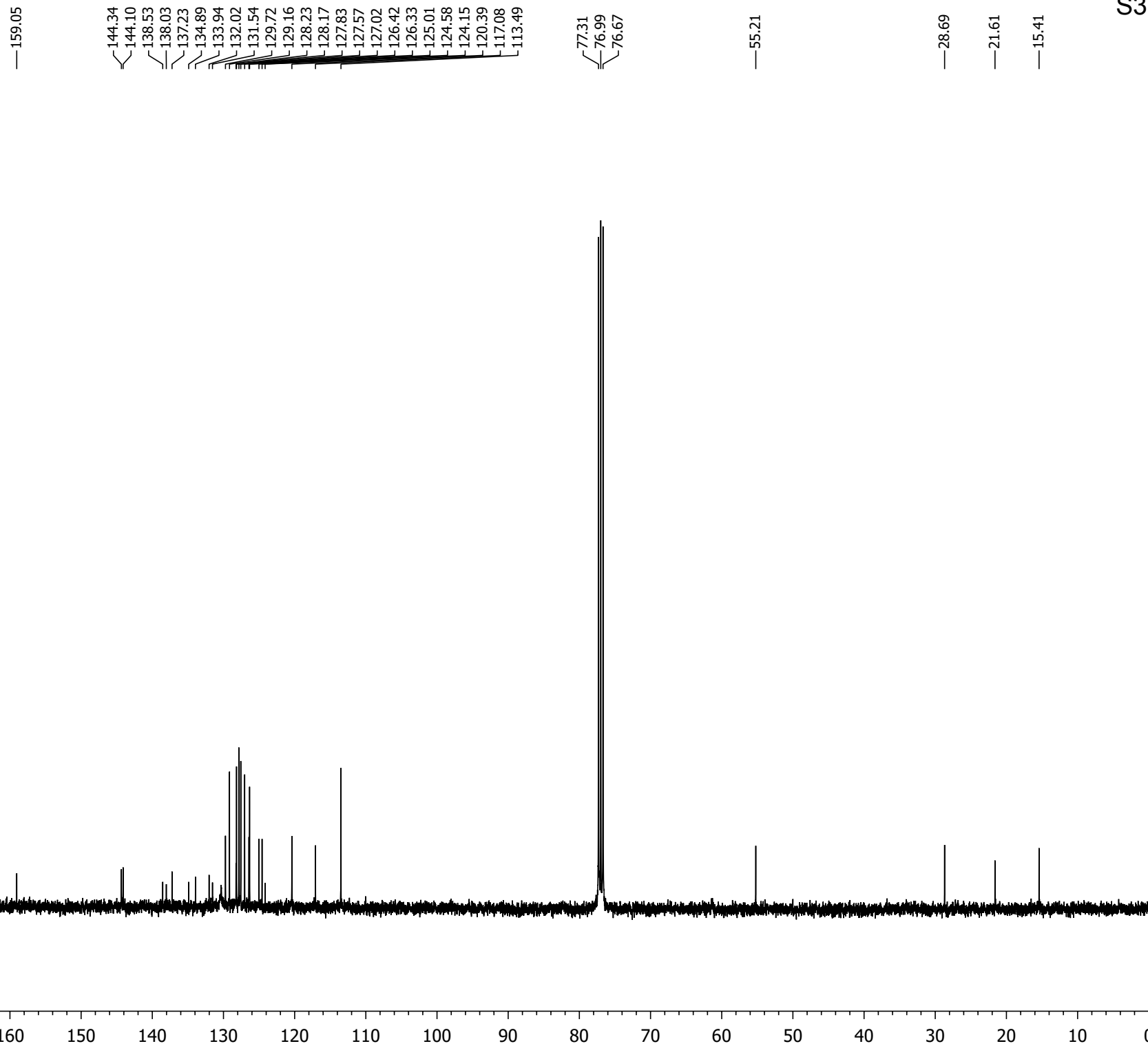
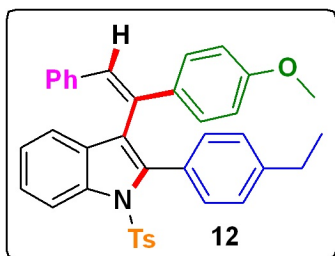
1.21  
1.19  
1.17

0.00  
-0.0038

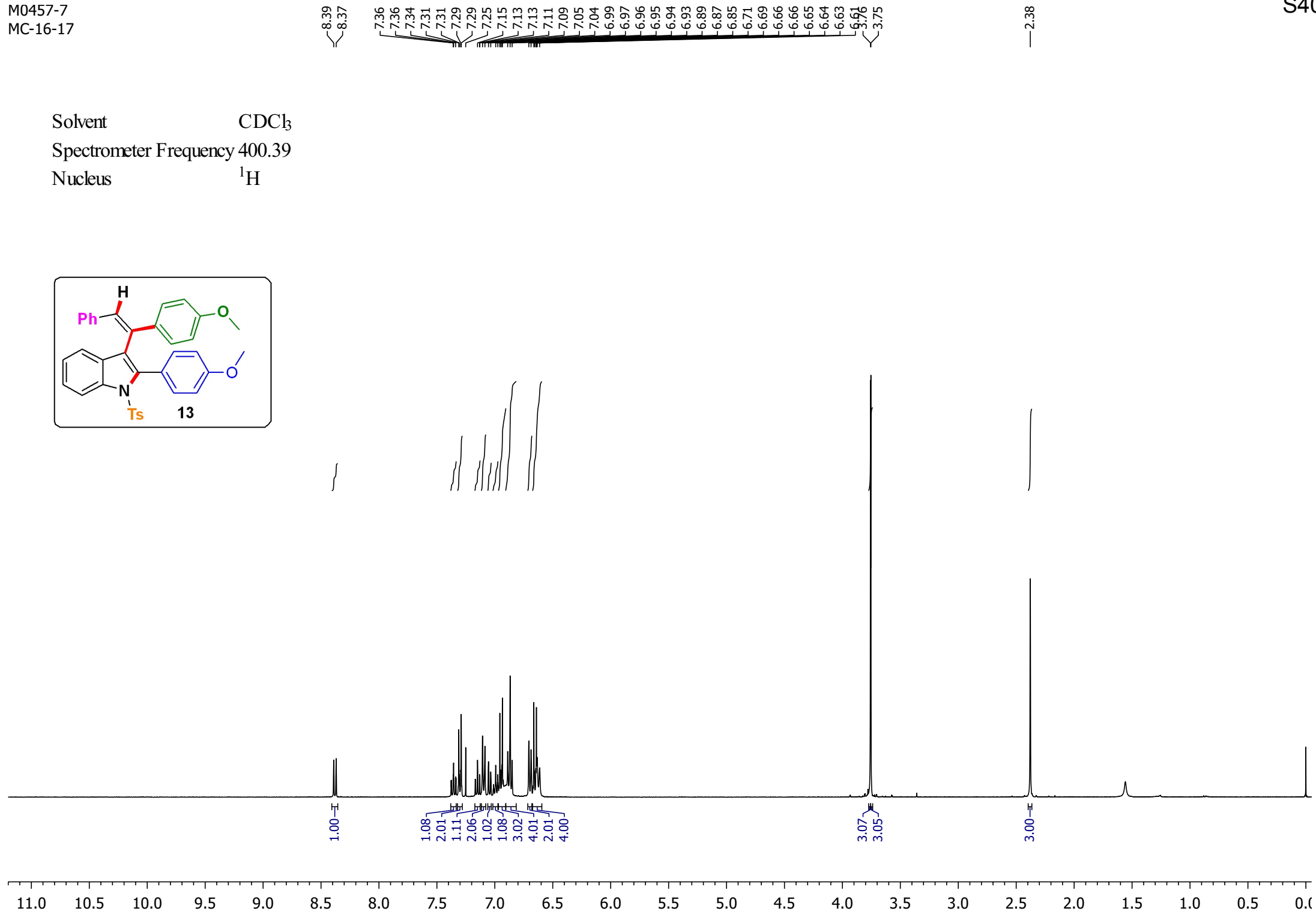
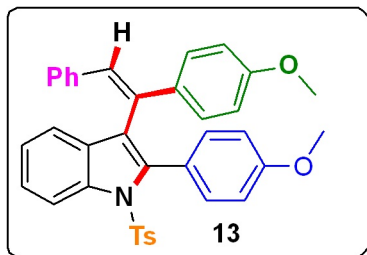
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

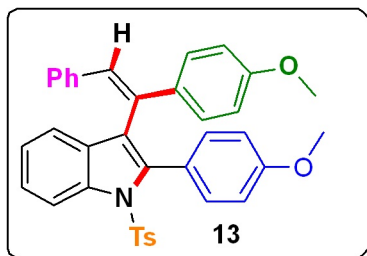


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$





Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

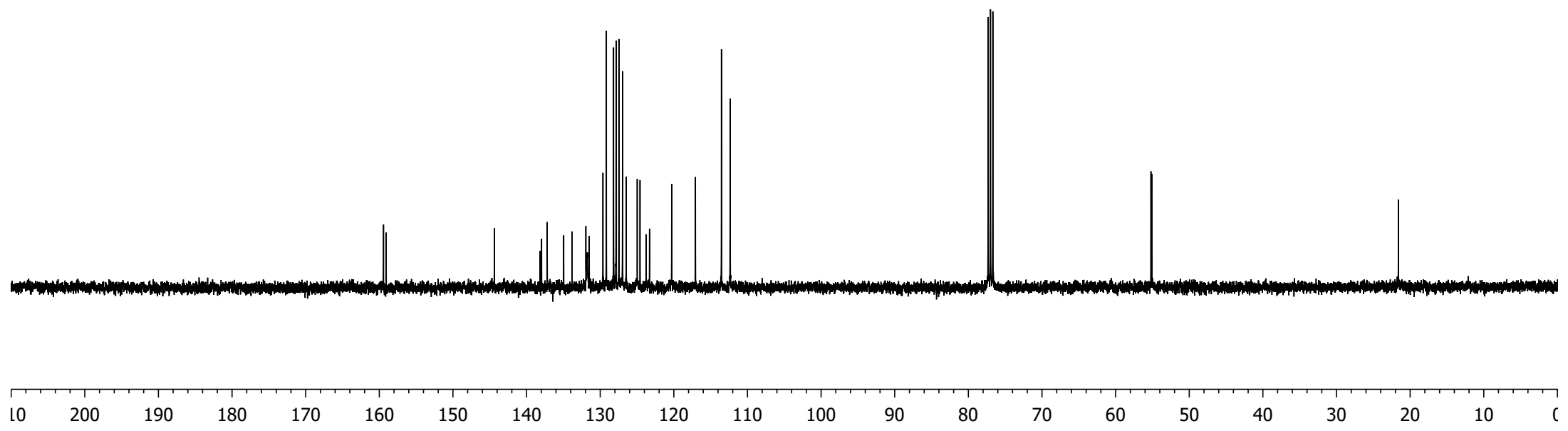


159.43  
159.07  
144.38  
138.15  
137.96  
137.19  
134.96  
133.82  
131.94  
131.74  
131.48  
129.62  
129.17  
128.19  
127.84  
127.46  
126.96  
126.47  
124.97  
124.59  
123.77  
123.30  
120.29  
117.06  
113.53  
112.35

77.31  
76.99  
76.67

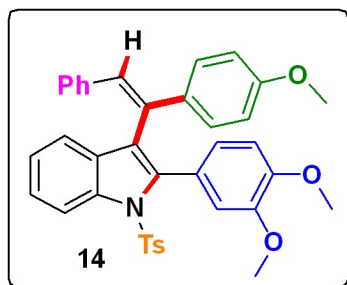
55.20  
55.10

21.60





Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

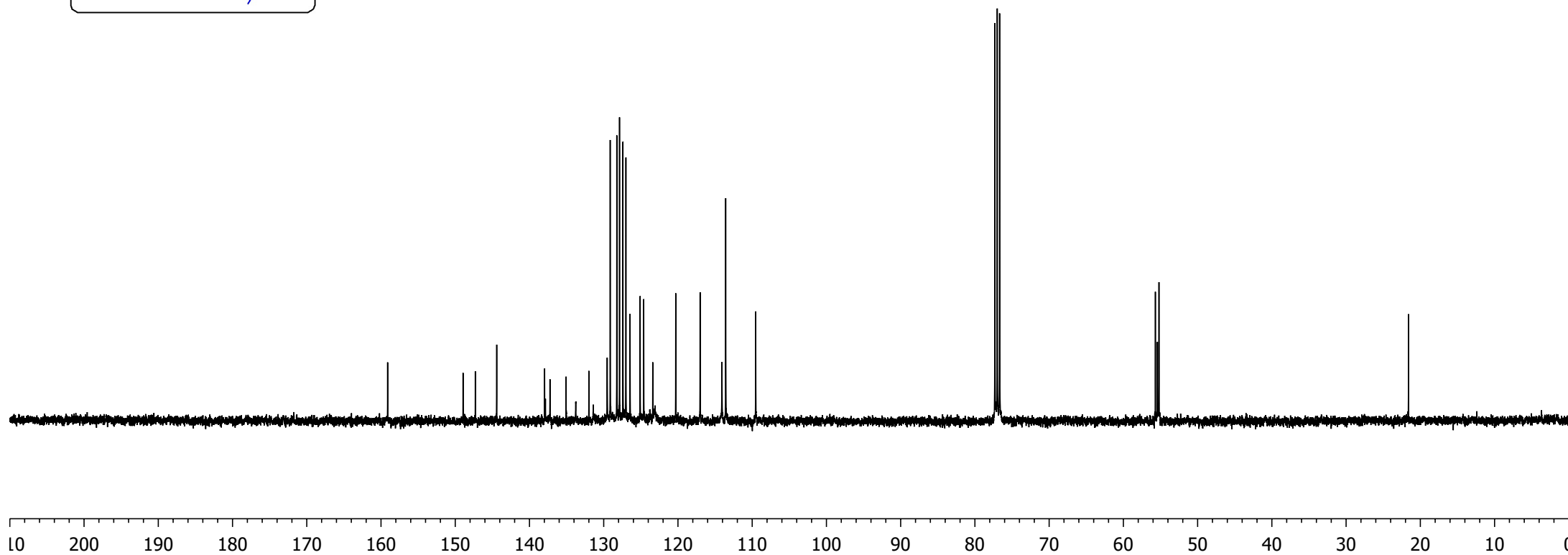


159.11  
148.95  
147.30  
144.41  
137.96  
137.85  
137.24  
135.08  
133.76  
132.00  
131.40  
129.53  
129.13  
128.24  
127.87  
127.41  
127.01  
126.45  
125.09  
124.61  
123.39  
120.30  
117.02  
114.08  
113.57  
109.53

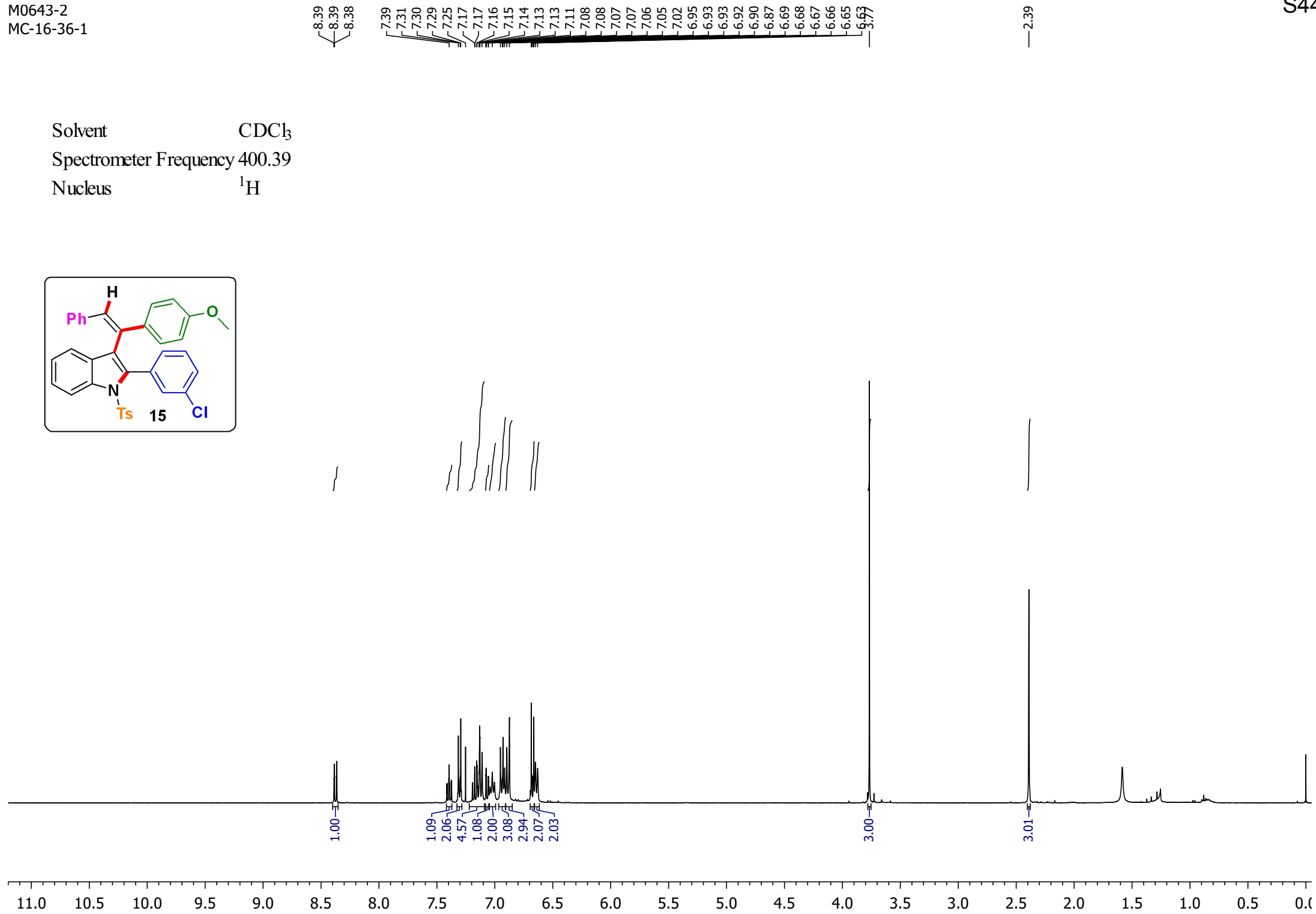
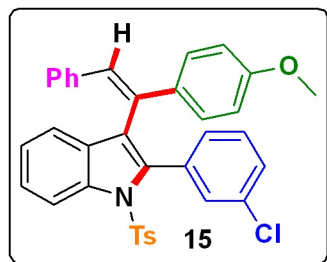
77.31  
76.99  
76.67

55.69  
55.42  
55.21

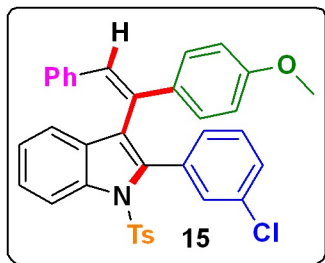
21.59



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

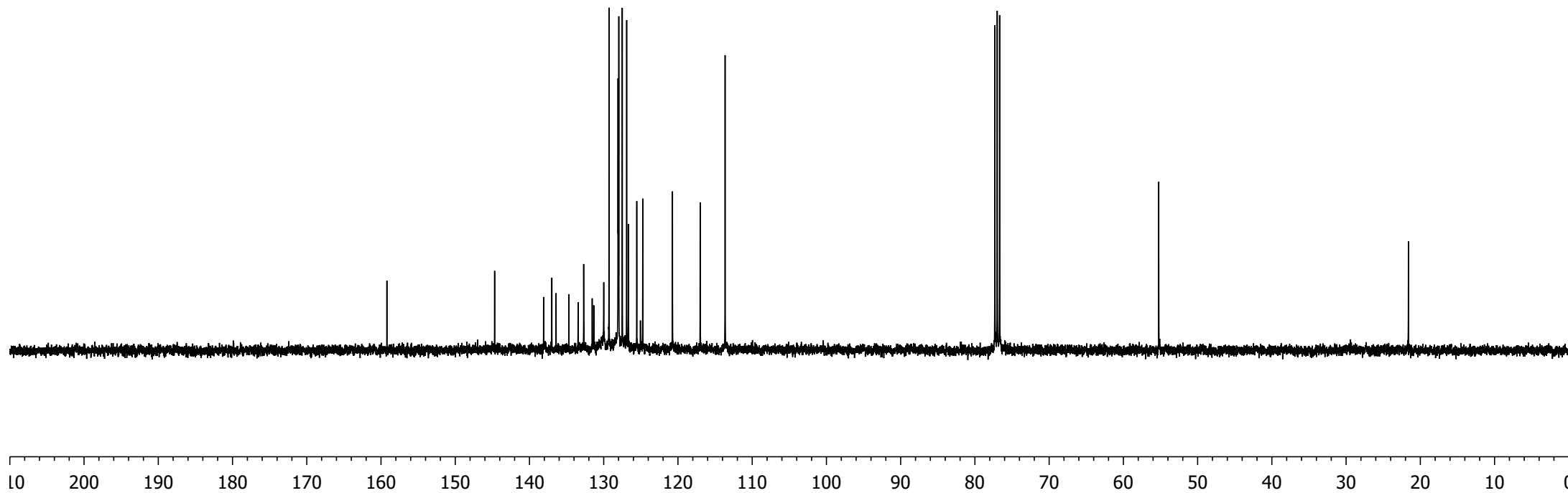


159.21  
144.69  
138.10  
136.99  
136.41  
134.69  
133.45  
132.70  
131.55  
131.34  
129.99  
129.29  
128.07  
128.03  
127.97  
127.50  
126.91  
126.67  
125.55  
125.06  
124.74  
120.74  
117.01  
113.65

77.31  
76.99  
76.68

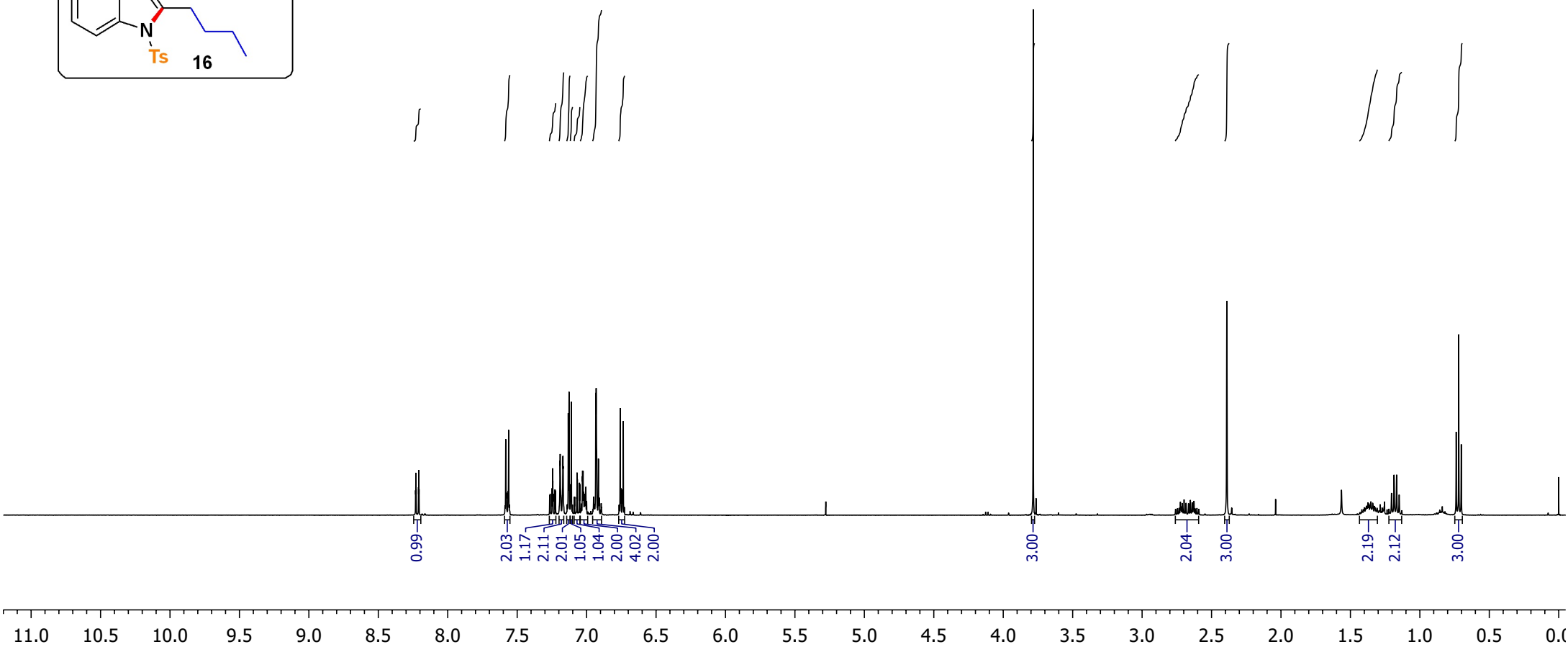
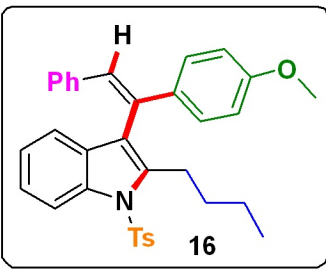
55.23

21.61

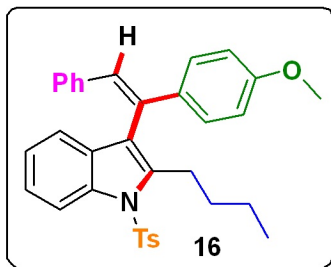


7.27  
7.26  
7.25  
7.24  
7.24  
7.23  
7.22  
7.19  
7.18  
7.17  
7.17  
7.14  
7.13  
7.13  
7.12  
7.11  
7.10  
7.09  
7.09  
7.07  
7.07  
7.05  
7.05  
7.04  
7.03  
7.03  
7.03  
7.02  
7.02  
7.01  
7.01  
7.01  
7.00  
6.95  
6.95  
6.93  
6.93  
6.91  
6.91  
6.89  
6.89  
6.77  
6.76  
6.75  
6.74  
6.74  
6.73  
3.78  
2.72  
2.72  
2.71  
2.70  
2.68  
2.67  
2.65  
2.64  
2.63  
2.63  
1.40  
1.38  
1.38  
1.37  
1.37  
1.36  
1.35  
1.34  
1.33  
1.32  
1.20  
1.19  
1.17  
1.15  
0.74  
0.74  
0.74

Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



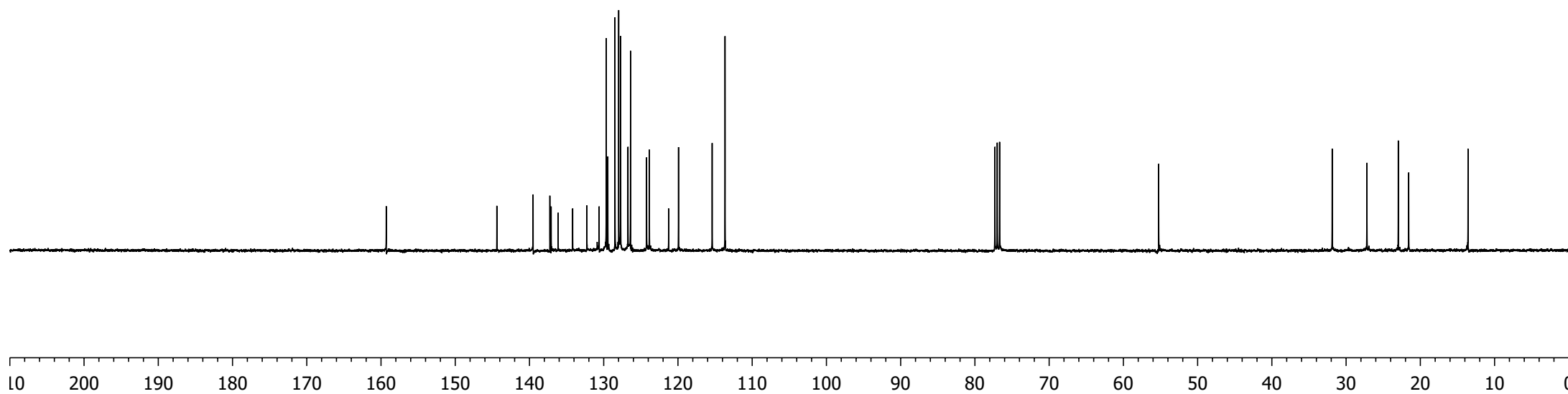
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137.08  
136.14  
134.18  
132.27  
130.62  
129.65  
129.45  
128.49  
127.98  
127.72  
126.73  
126.39  
124.22  
123.85  
121.25  
119.93  
115.39  
113.66

77.31  
76.99  
76.68

55.25

31.87  
27.20  
22.97  
21.57

13.57



M0459-9  
MC-16-25

8.27  
8.25  
7.67  
7.65  
7.28  
7.28  
7.26  
7.24  
7.24  
7.23  
7.21  
7.19  
7.16  
7.14  
7.10  
7.06  
7.04  
7.03  
7.01  
7.00  
6.98  
6.96  
6.94  
6.93  
6.93  
6.91  
6.79  
6.77

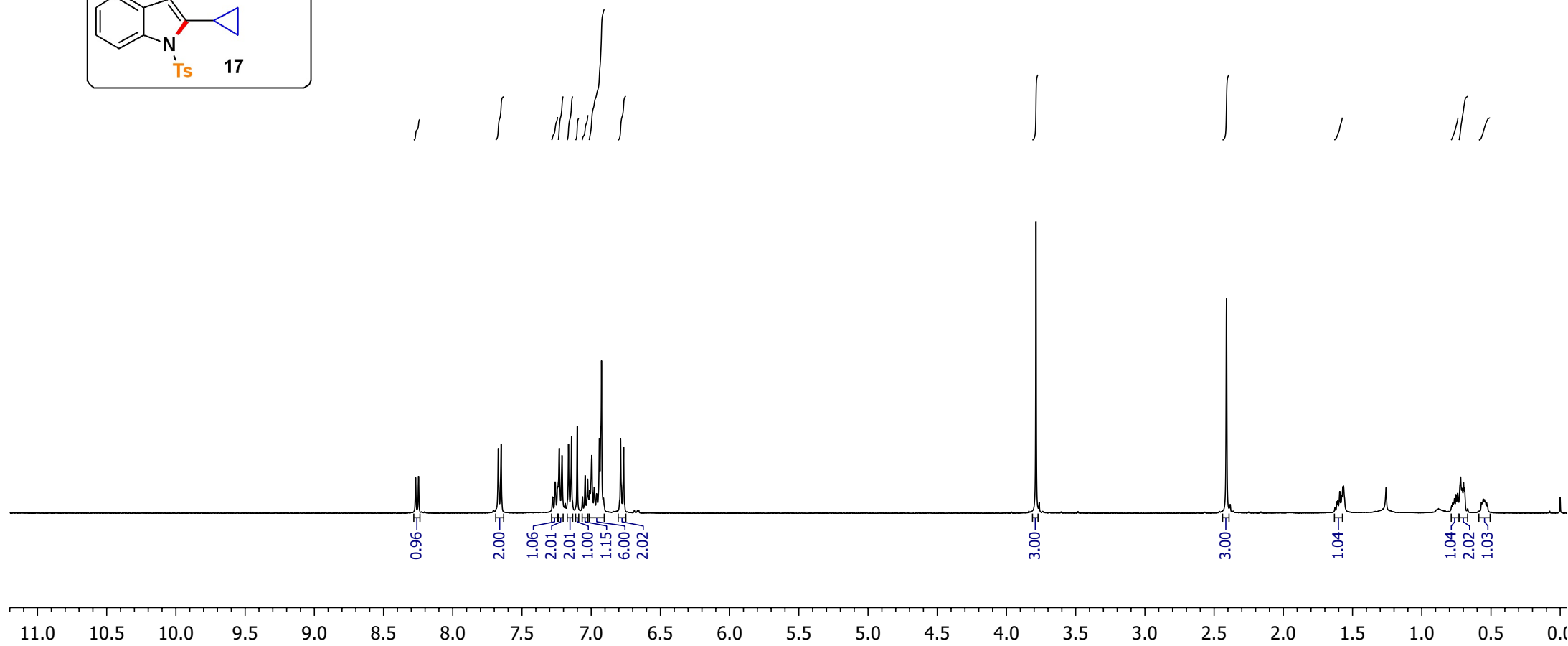
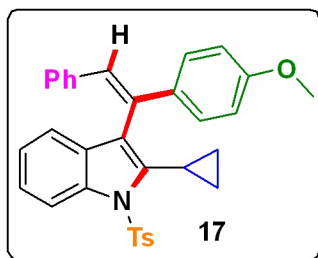
3.79

2.41

1.61  
1.61  
1.59  
1.58  
1.58

0.76  
0.75  
0.74  
0.72  
0.71  
0.70  
0.69  
0.58  
0.48

Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$





M0459-10  
MC-16-25

—159.24

—144.41

129.63

129.39

128.37

127.98

127.64

126.60

126.51

124.55

123.43

122.14

113.75

77.31

76.99

76.68

—55.23

—21.59

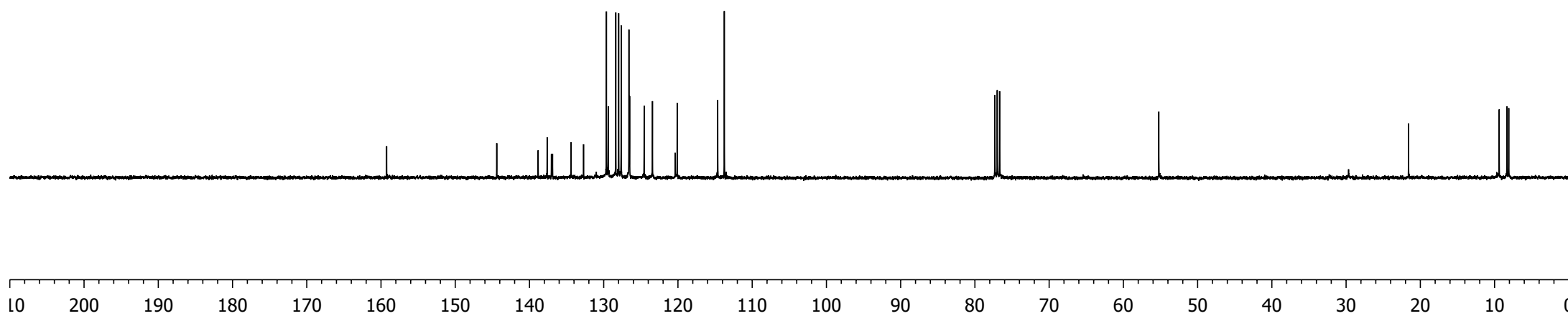
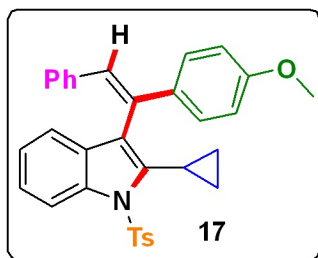
9.38

8.33

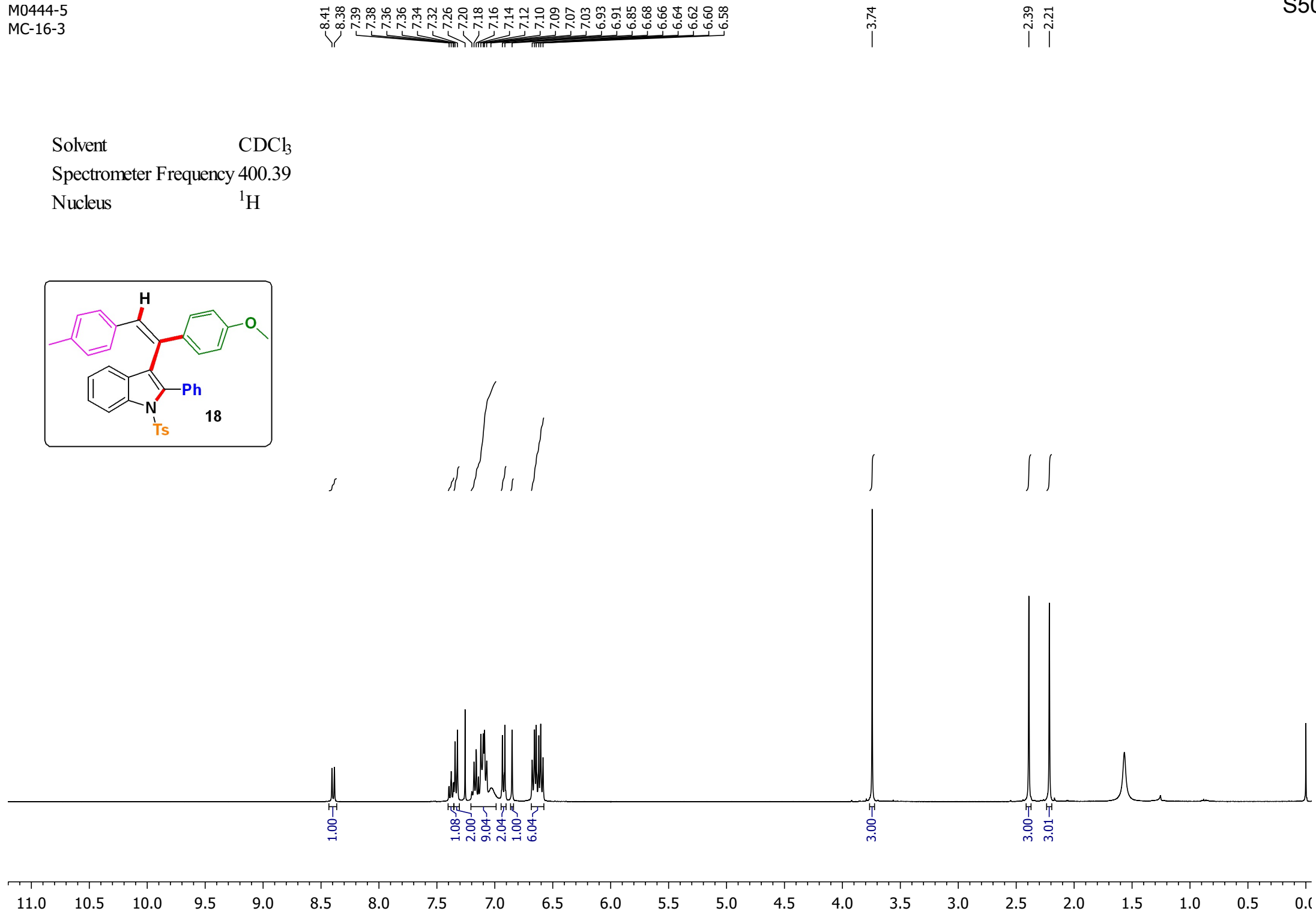
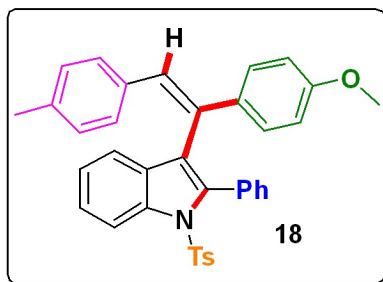
8.09

S49

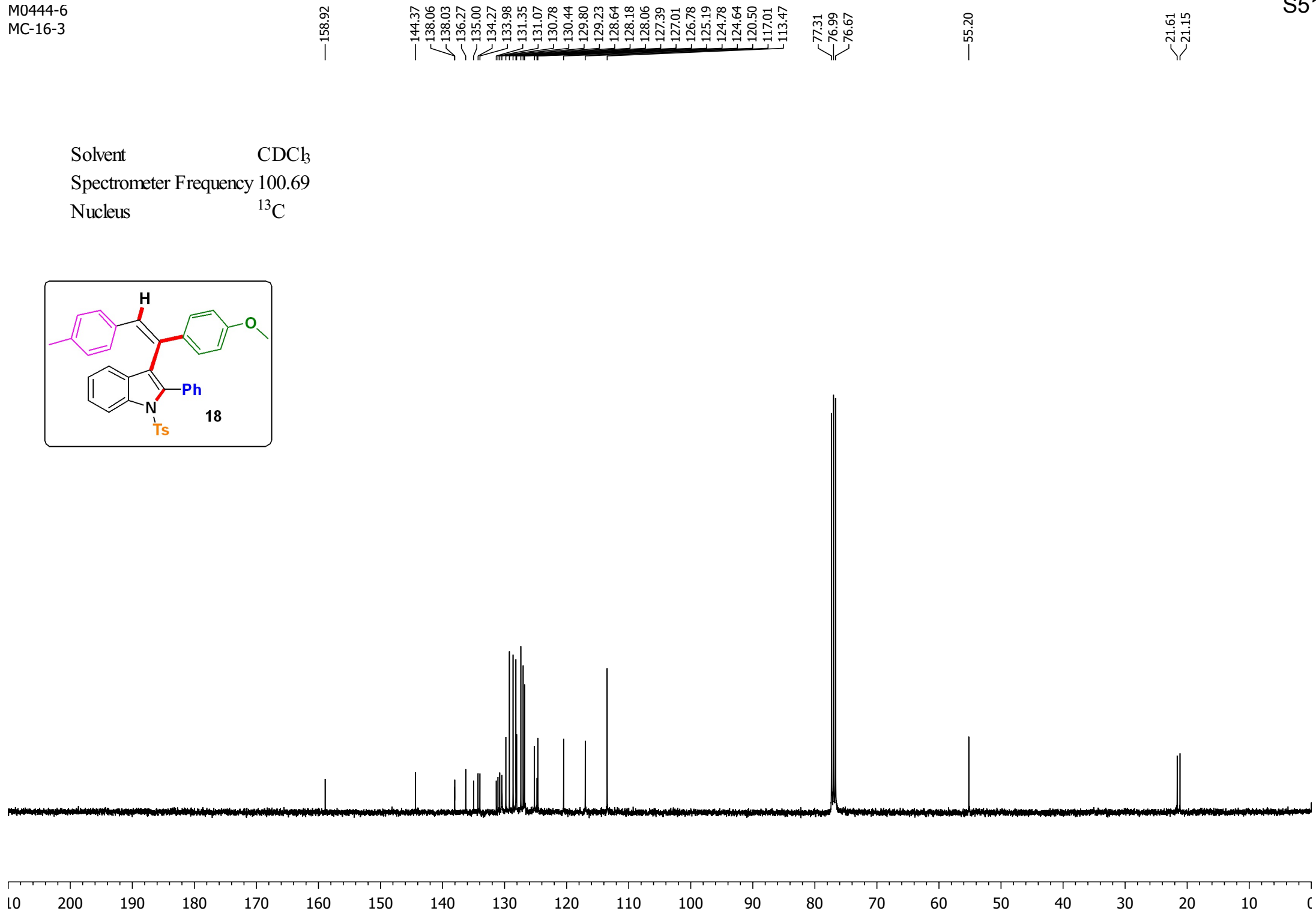
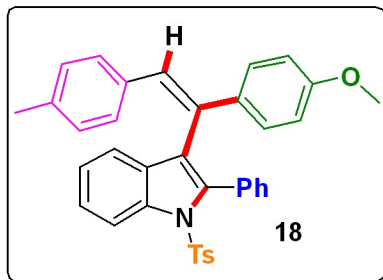
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



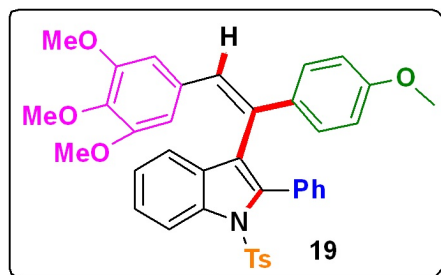
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$

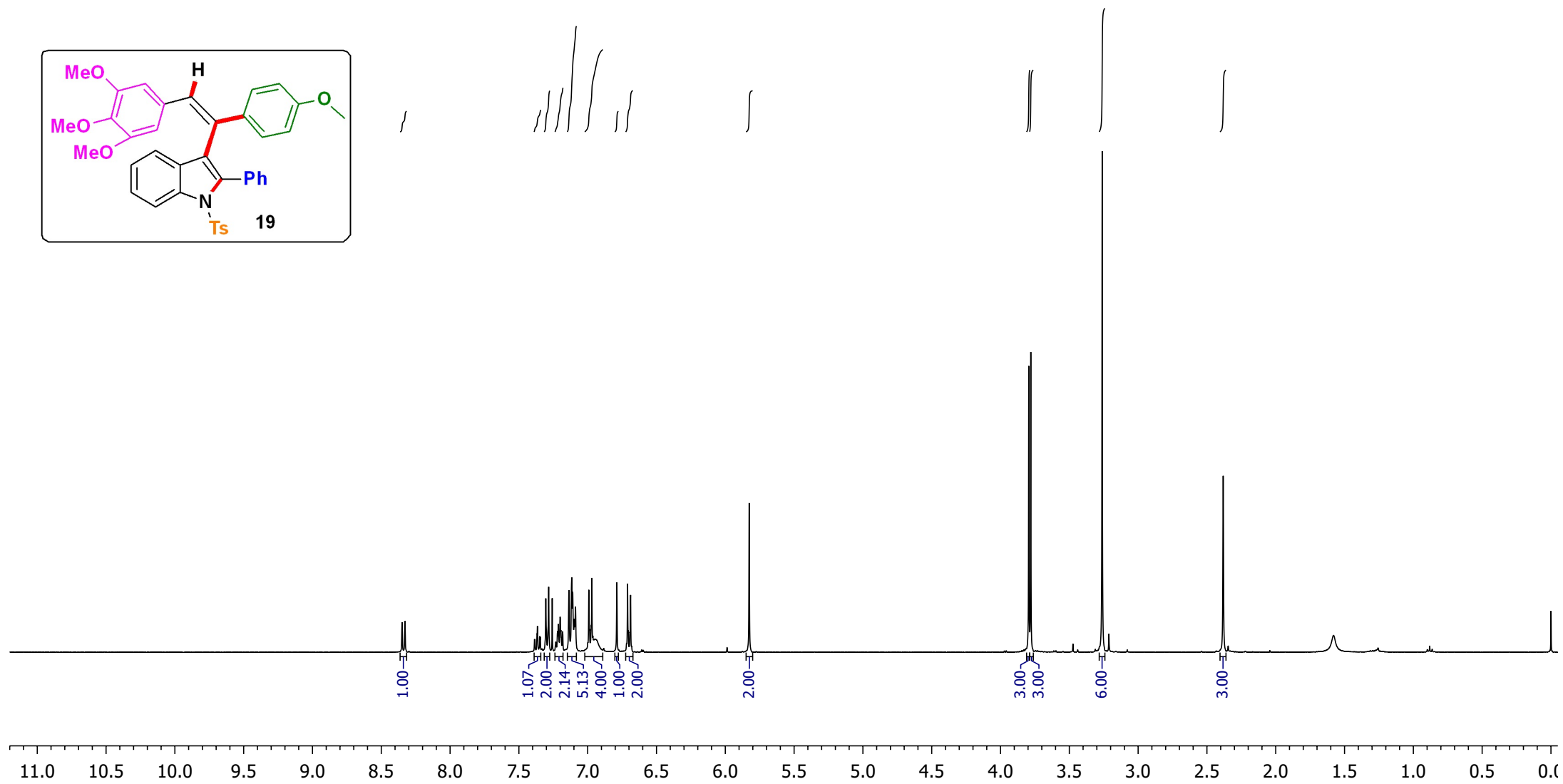


8.35  
8.33  
7.37  
7.30  
7.28  
7.21  
7.20  
7.14  
7.12  
7.11  
7.10  
7.09  
6.99  
6.99  
6.97  
6.97  
6.79  
6.71  
6.69

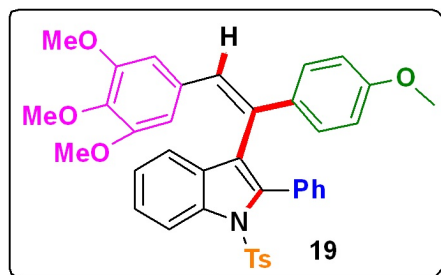
3.79  
3.78

3.26

2.38



Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 100.69  
Nucleus <sup>13</sup>C

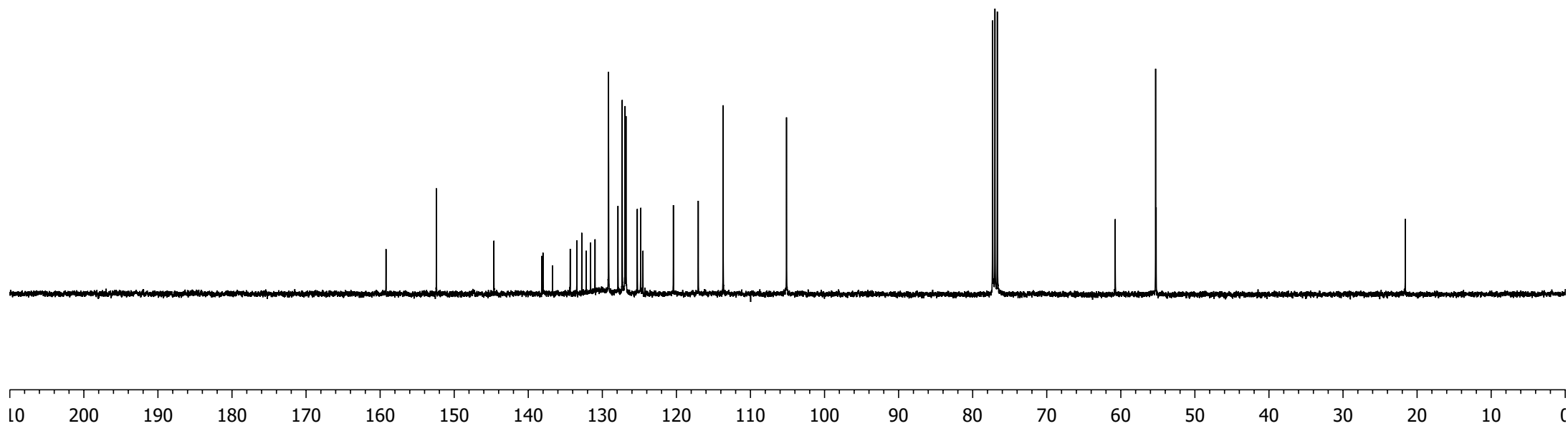


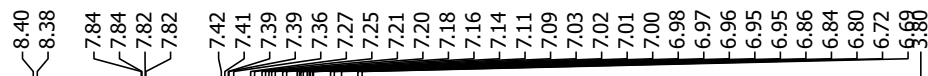
—159.21  
—152.41  
—144.64  
133.43  
132.78  
131.58  
130.98  
129.16  
127.88  
127.32  
126.92  
126.80  
125.28  
124.82  
120.41  
117.05  
103.64

77.31  
76.99  
76.67

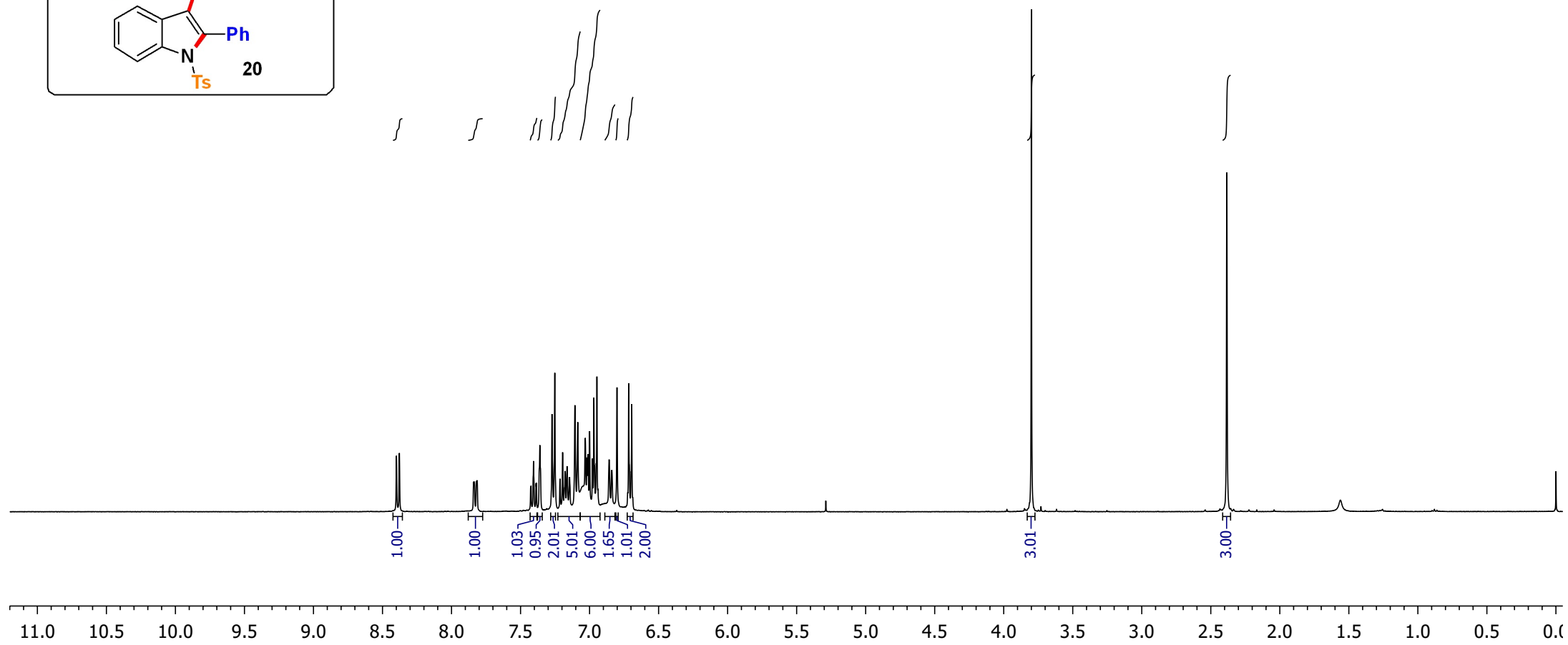
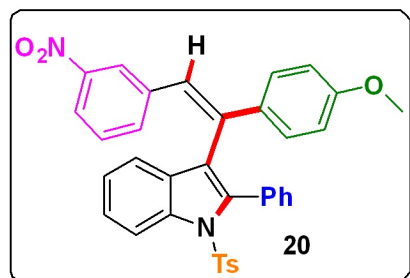
—60.76  
55.30  
55.23

—21.59

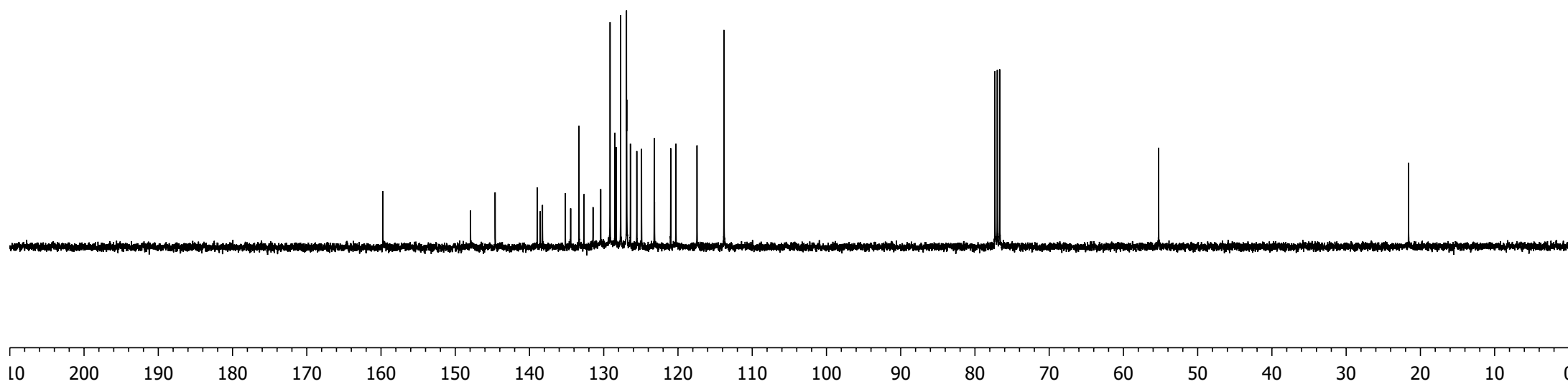
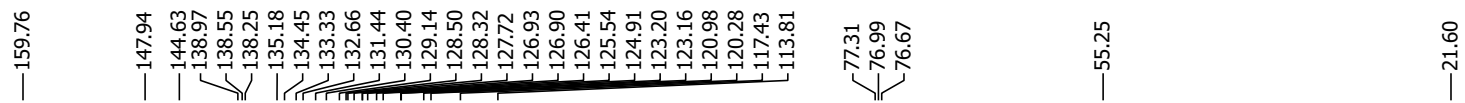
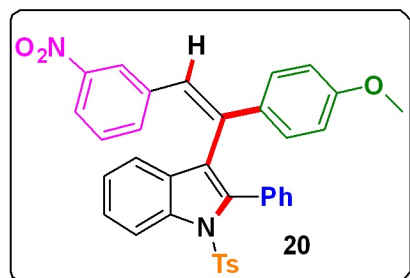




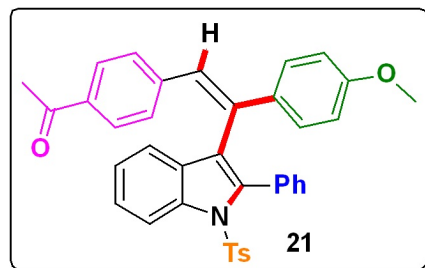
Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 400.39  
Nucleus <sup>1</sup>H



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



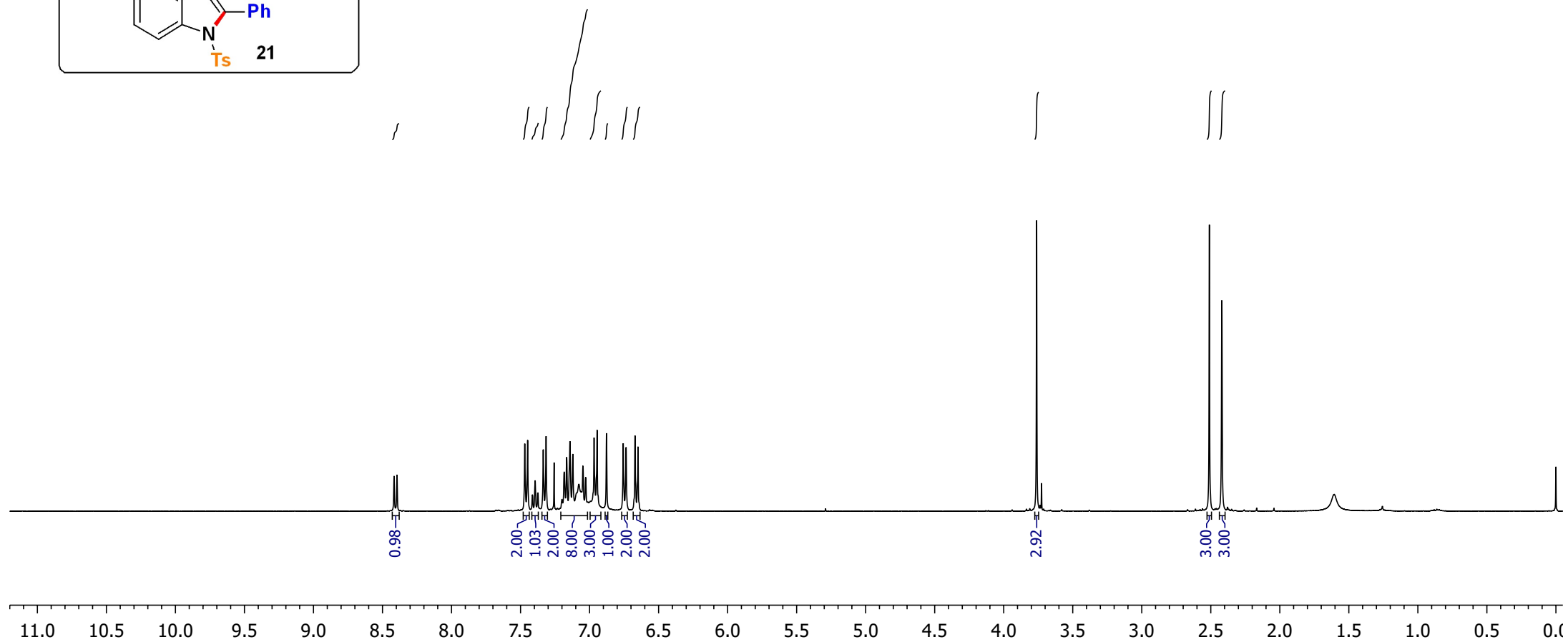
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



8.42  
8.39  
7.47  
7.45  
7.41  
7.39  
7.38  
7.34  
7.31  
7.26  
7.20  
7.18  
7.17  
7.14  
7.12  
7.08  
7.05  
7.03  
6.97  
6.95  
6.88  
6.76  
6.74  
6.67  
6.65

3.76

2.51  
2.42





M0444-14  
MC-16-33

—197.38

—159.50  
—144.81  
—142.00  
—138.43  
—138.06  
—134.78  
—134.73  
—134.60  
—133.16  
—131.09  
—130.77  
—130.30  
—129.27  
—128.26  
—128.23  
—128.18  
—128.04  
—127.72  
—126.98  
—126.91  
—125.43  
—124.80  
—124.02  
—120.30  
—117.19  
—113.63

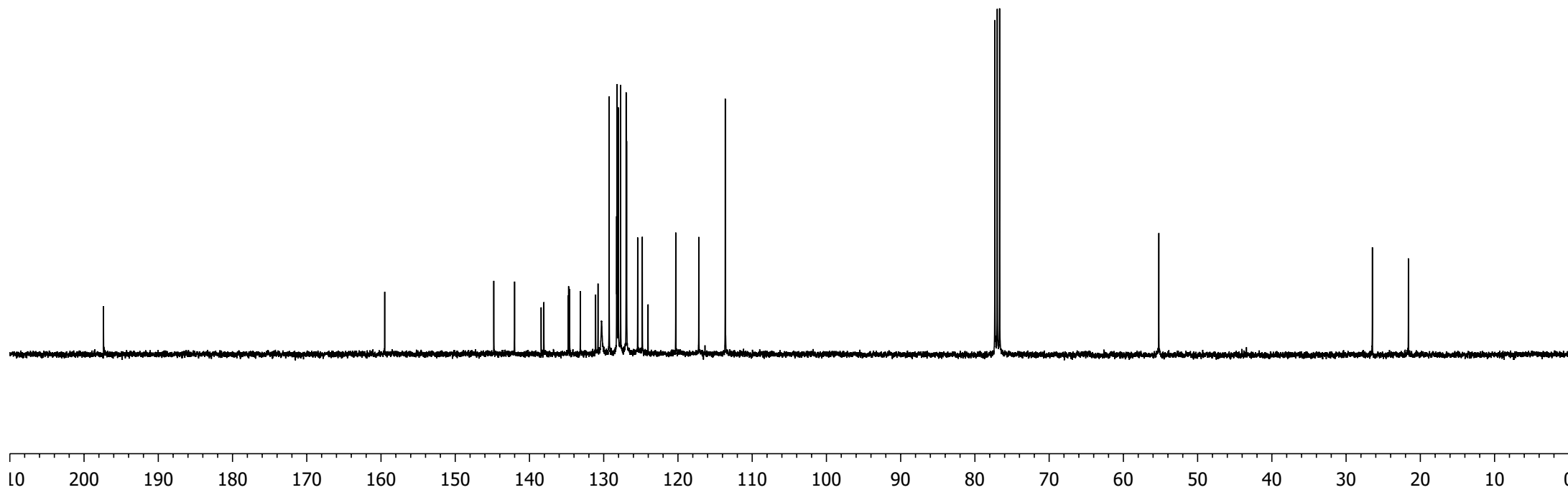
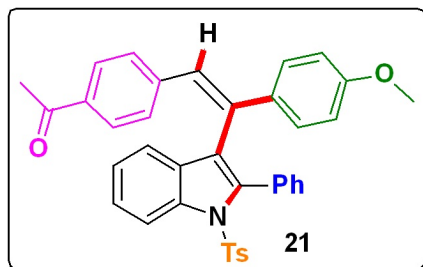
—77.31  
—76.99  
—76.68

—55.22

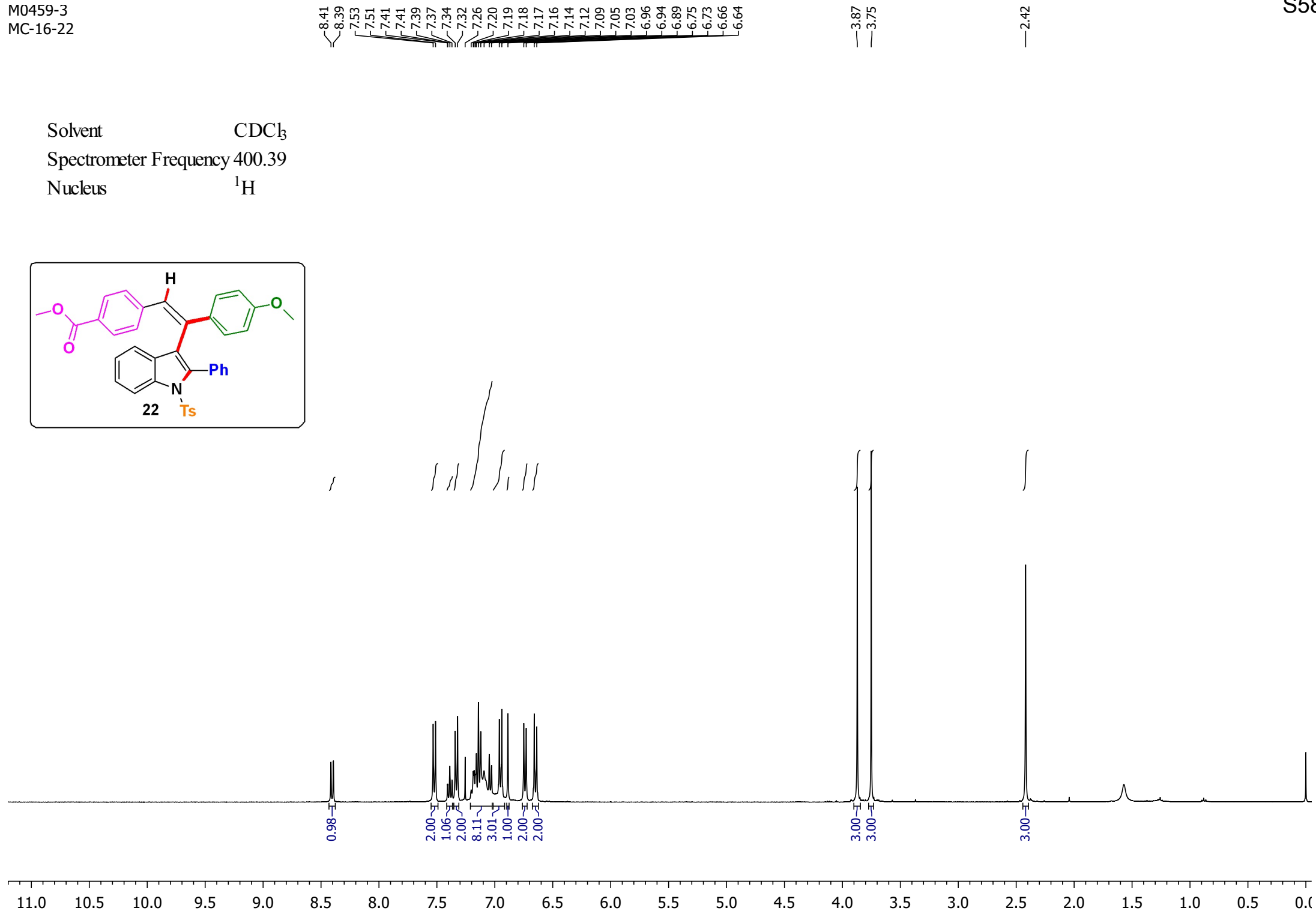
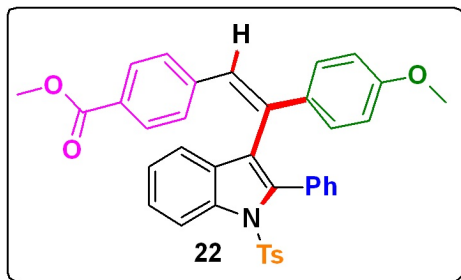
—26.46  
—21.61

S57

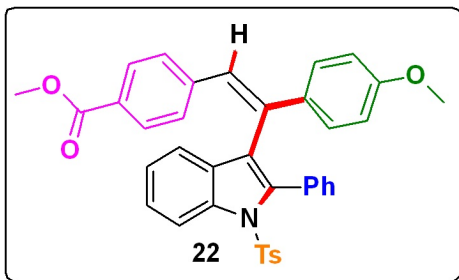
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

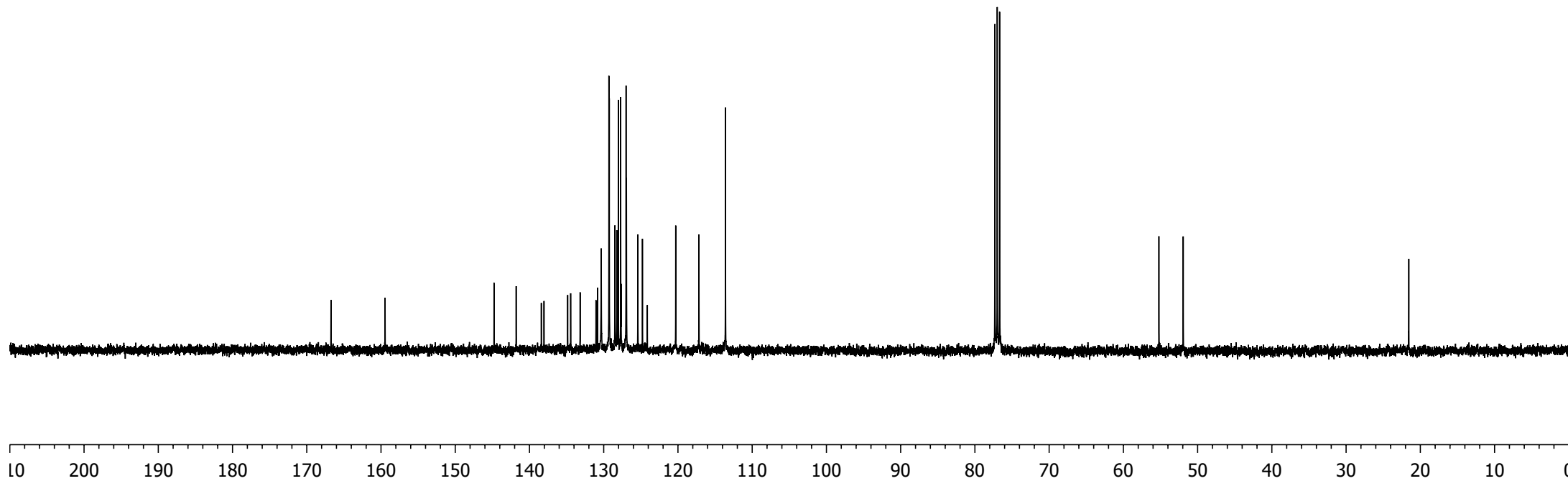


166.74  
159.45  
144.78  
141.79  
138.41  
138.04  
134.85  
134.45  
133.18  
131.04  
130.83  
130.34  
129.30  
129.25  
128.50  
128.24  
128.03  
127.71  
127.66  
126.99  
126.93  
125.41  
124.78  
124.12  
120.30  
117.17  
113.60

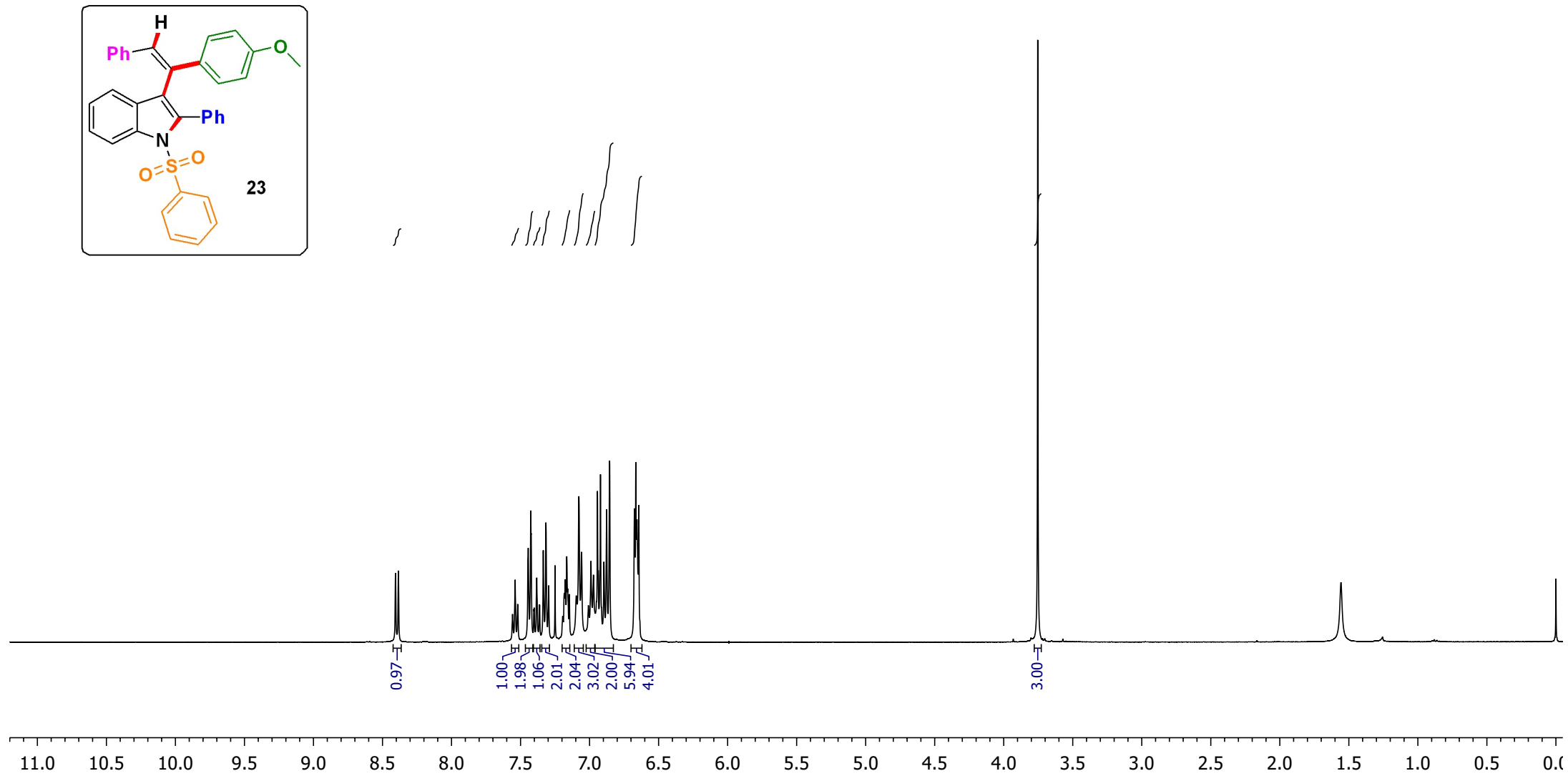
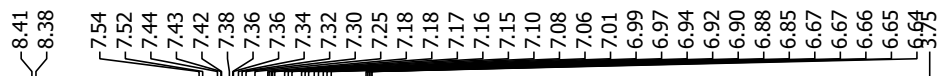
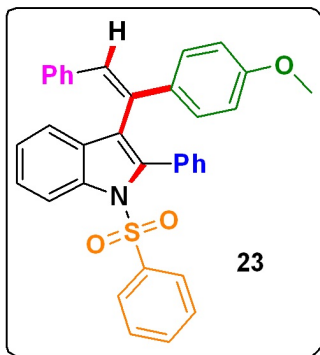
77.31  
76.99  
76.67

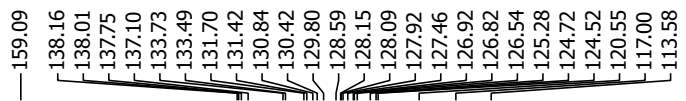
55.21  
51.94

21.55

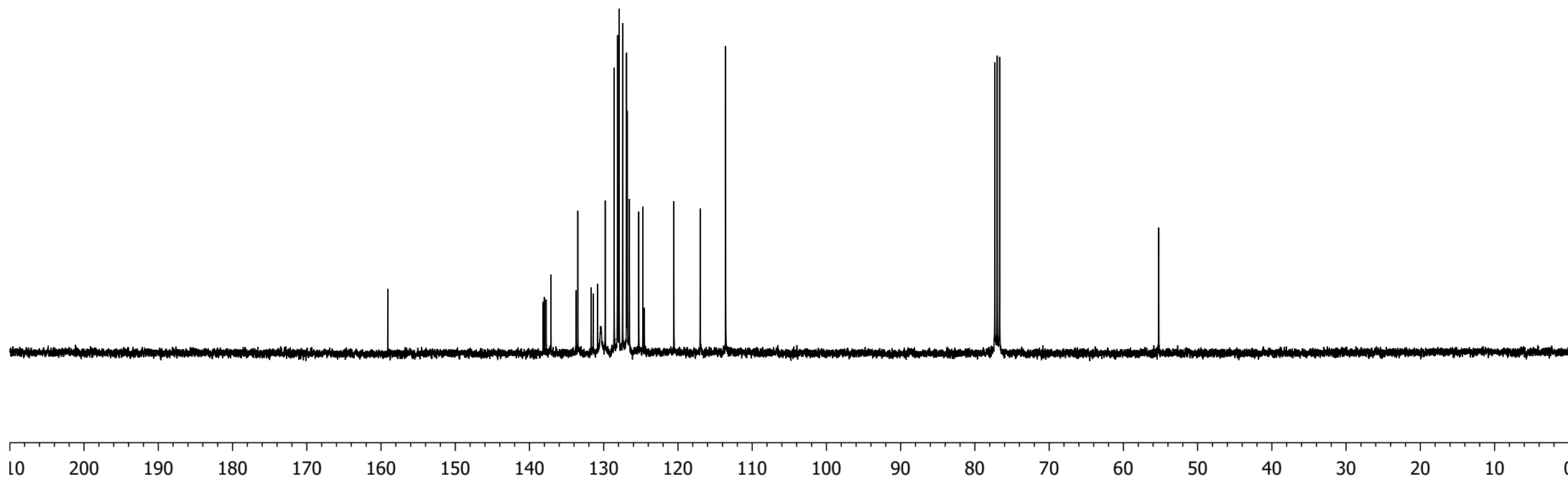
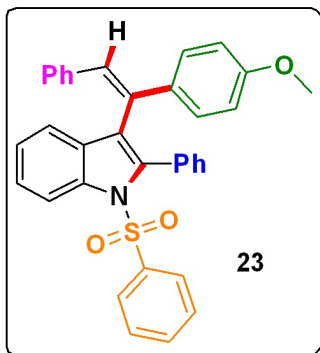


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$

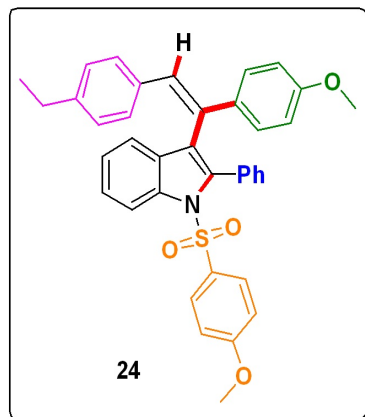




Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.28  
Nucleus  $^1\text{H}$

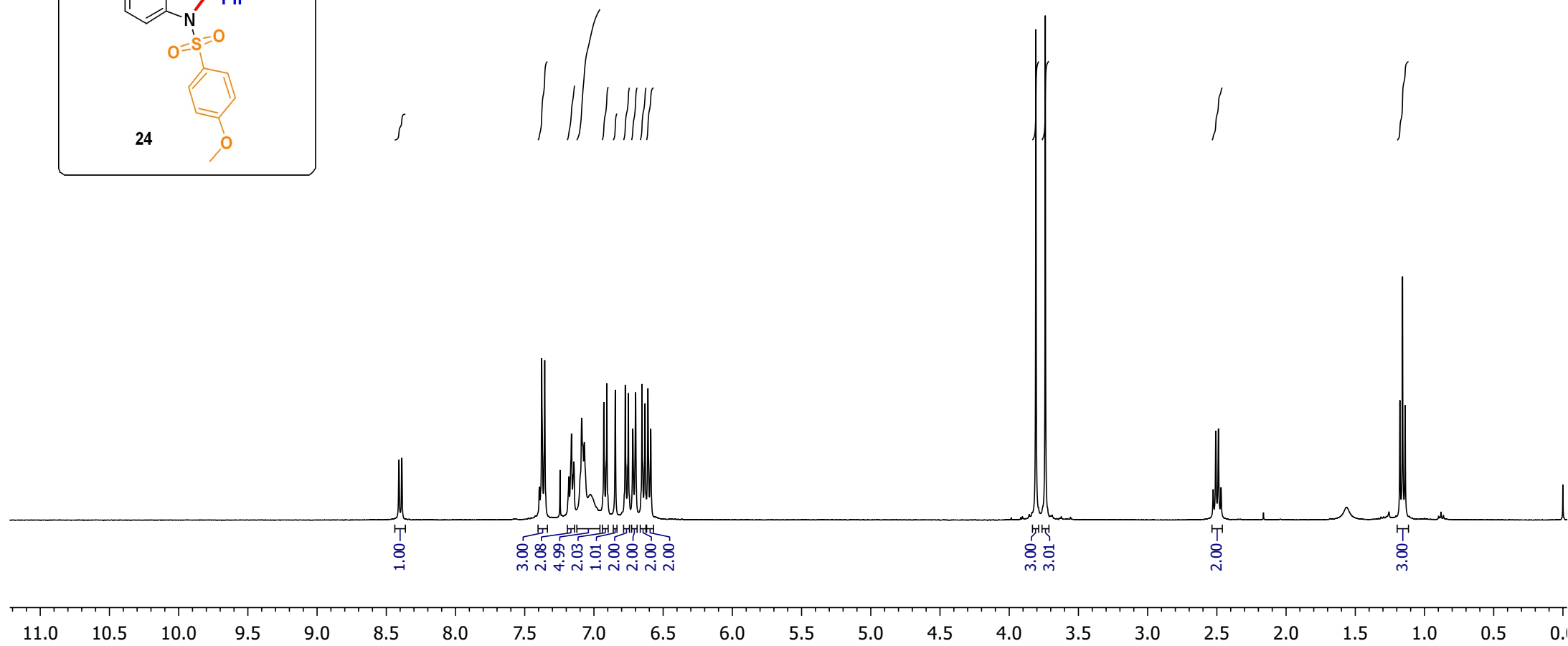


8.41  
8.39  
7.40  
7.39  
7.38  
7.36  
7.24  
7.18  
7.16  
7.15  
7.14  
7.09  
7.07  
7.03  
6.93  
6.91  
6.85  
6.77  
6.75  
6.72  
6.70  
6.65  
6.63  
6.61  
6.59

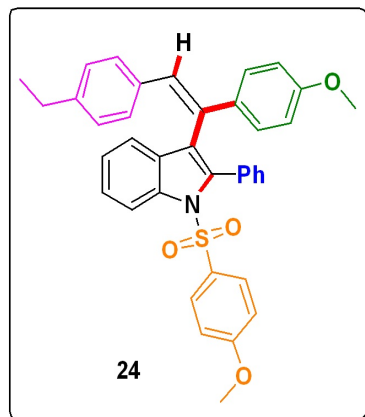
3.81  
3.74

2.53  
2.51  
2.49  
2.47

1.18  
1.16  
1.14



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.66  
Nucleus  $^{13}\text{C}$



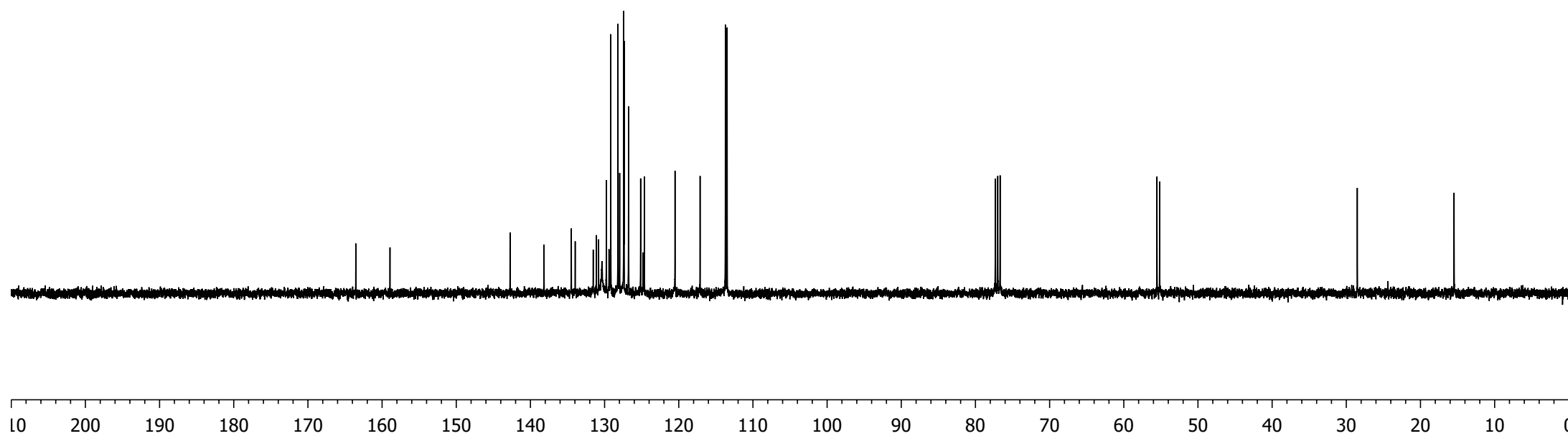
163.54  
158.93  
142.74  
138.16  
134.48  
133.96  
131.53  
131.11  
130.80  
130.36  
129.76  
129.41  
129.17  
128.19  
127.97  
127.43  
127.36  
126.77  
125.14  
124.82  
124.64  
120.50  
117.13  
113.71  
113.48

77.31  
76.99  
76.68

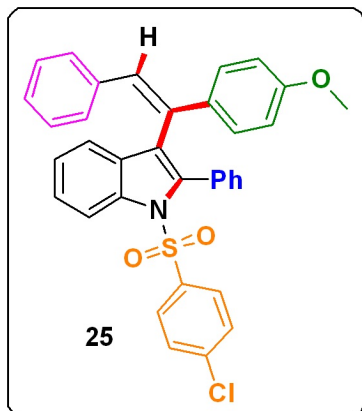
55.52  
55.17

28.52

15.47

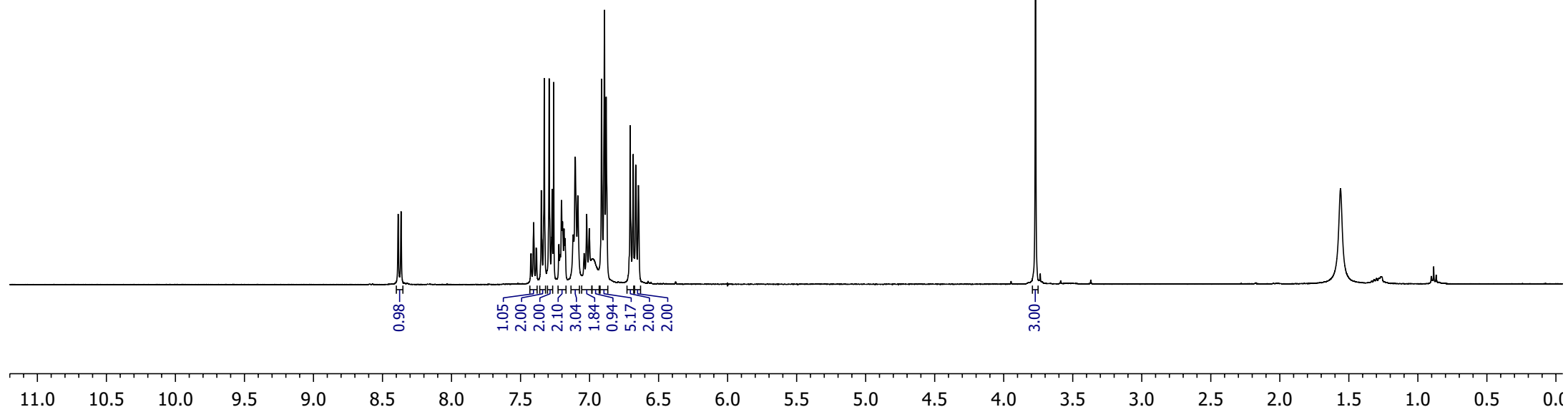


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



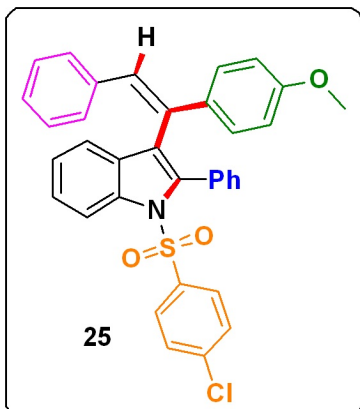
8.39  
8.37  
7.42  
7.40  
7.39  
7.35  
7.33  
7.29  
7.27  
7.26  
7.22  
7.21  
7.20  
7.20  
7.18  
7.18  
7.12  
7.10  
7.09  
7.04  
7.02  
7.00  
6.91  
6.89  
6.88

3.77





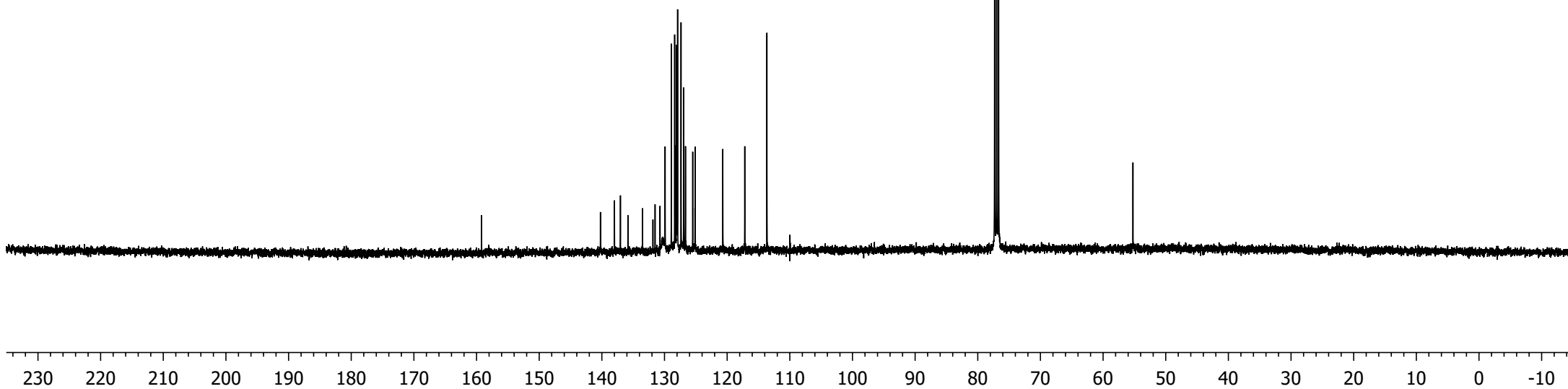
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



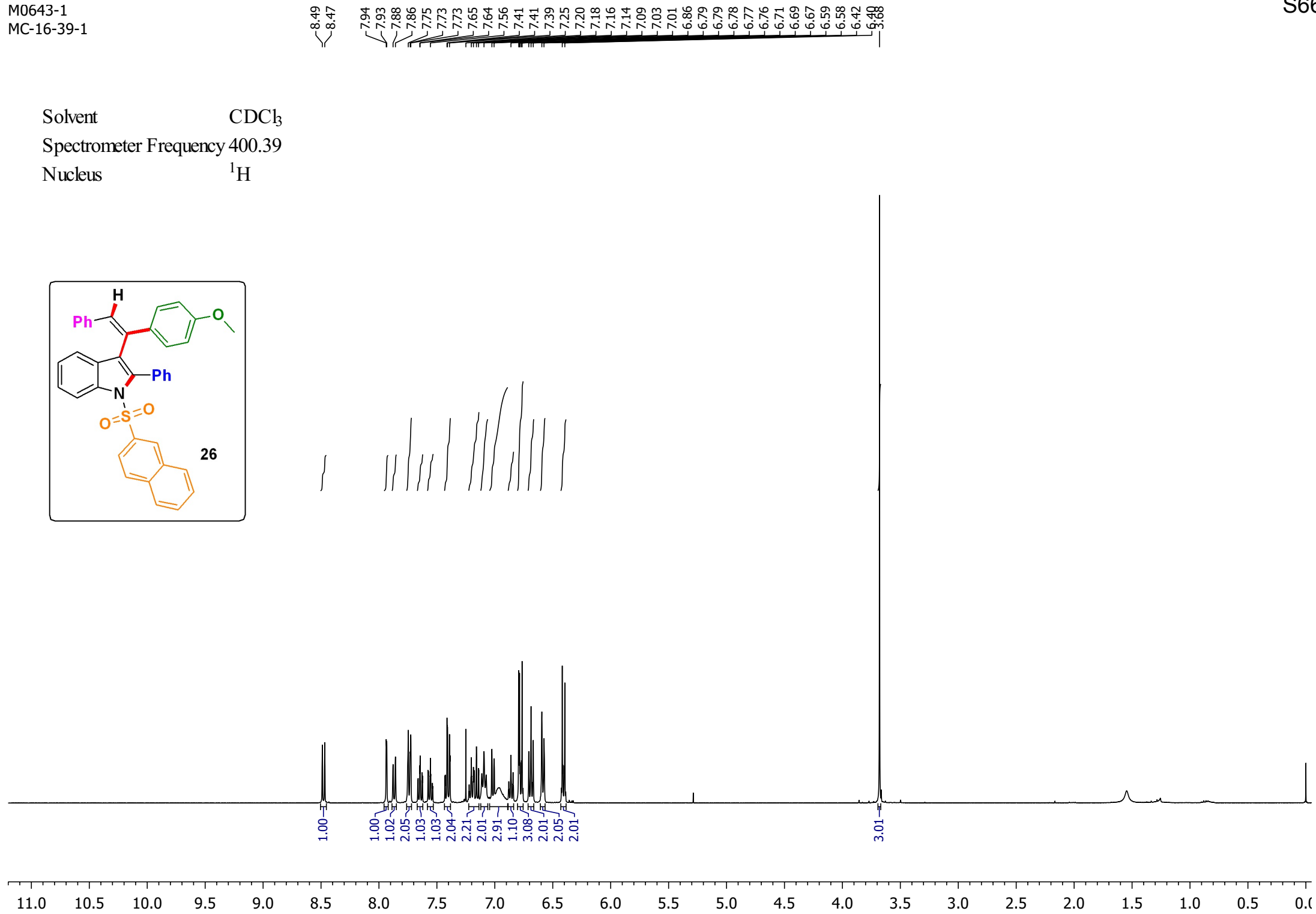
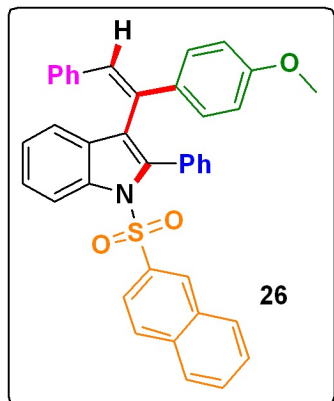
159.20  
140.23  
137.99  
137.03  
135.84  
133.51  
131.85  
131.50  
130.71  
129.90  
128.91  
128.38  
128.23  
128.07  
127.91  
127.36  
126.93  
126.65  
125.49  
125.14  
125.10  
120.69  
117.19  
113.66  
109.97

77.31  
76.99  
76.67

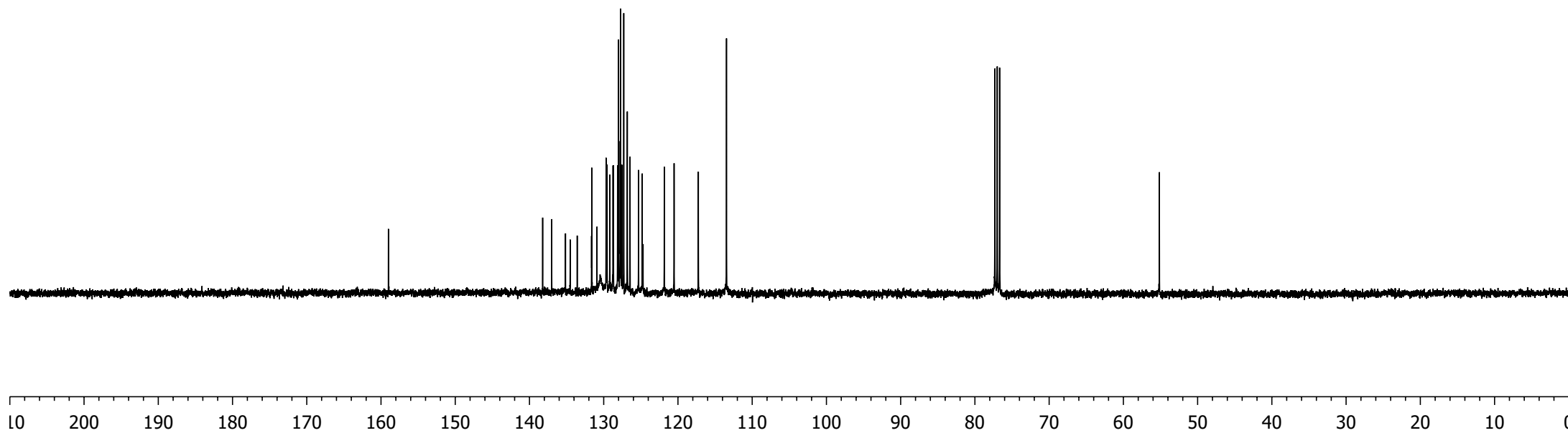
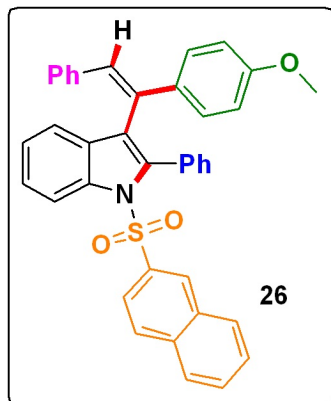
55.23



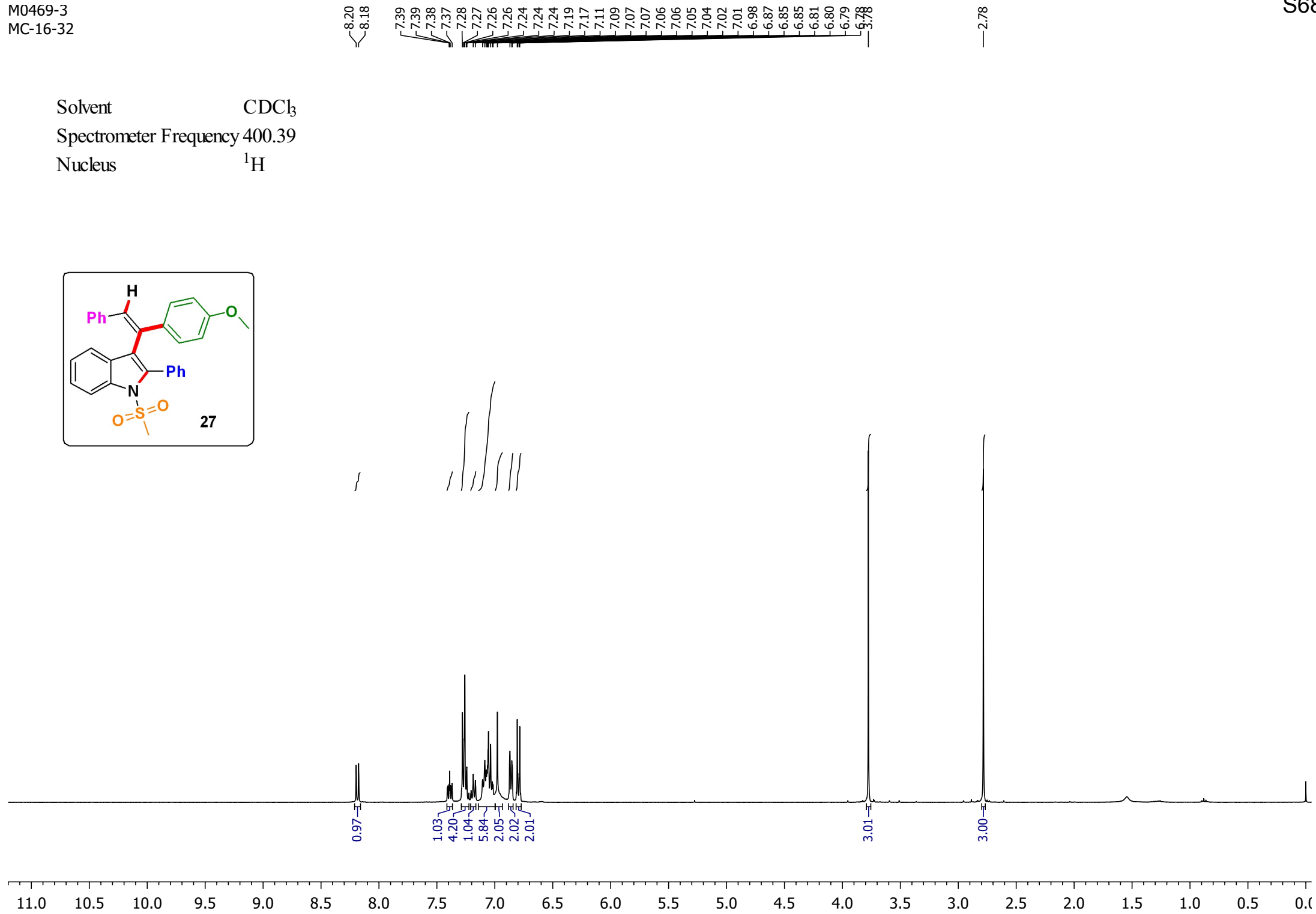
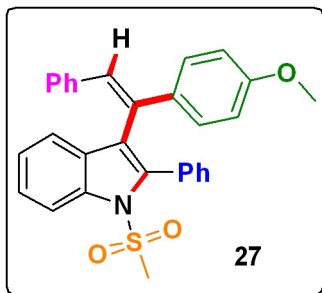
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



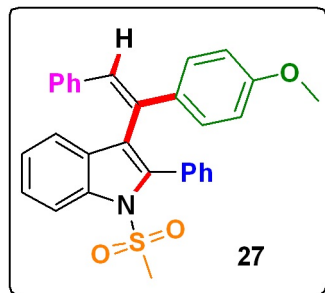
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

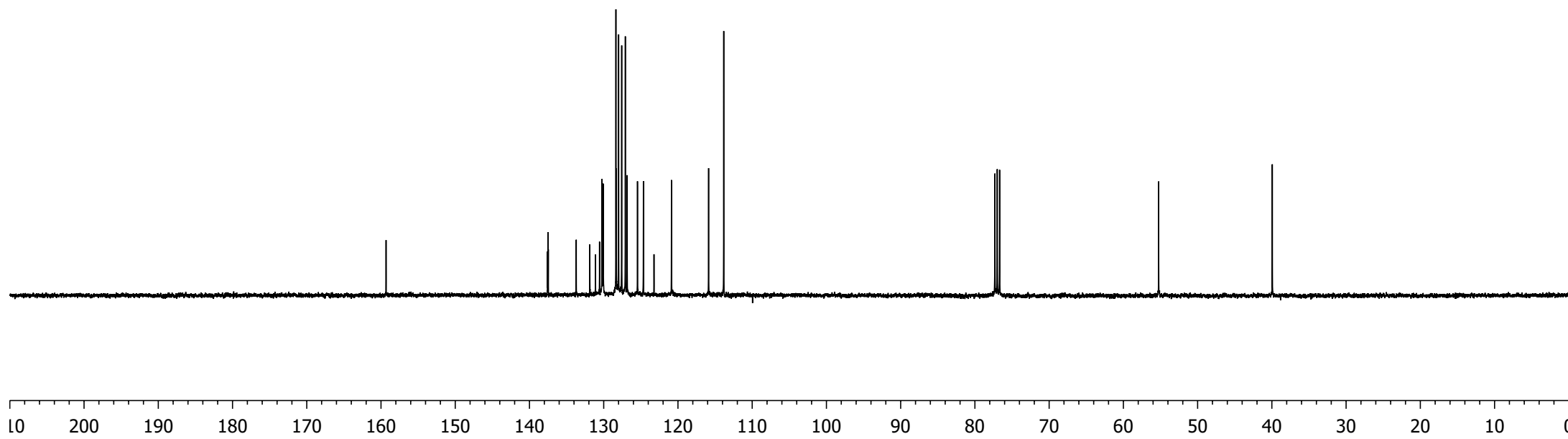


159.32  
137.50  
137.46  
133.70  
131.87  
130.56  
130.23  
130.08  
128.36  
128.30  
127.99  
127.58  
127.09  
126.84  
125.45  
124.65  
119.87  
115.87  
113.83

77.31  
76.99  
76.67

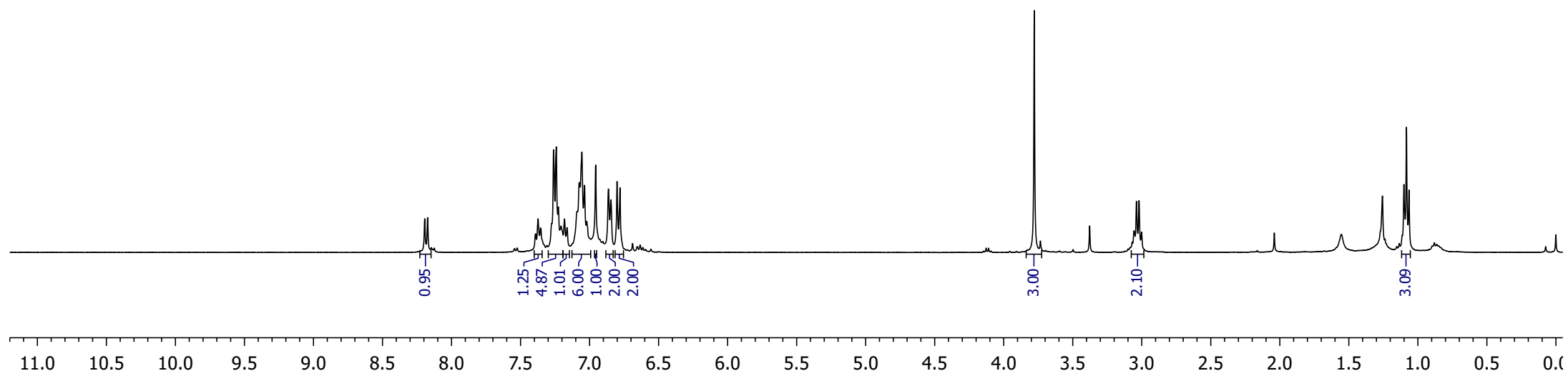
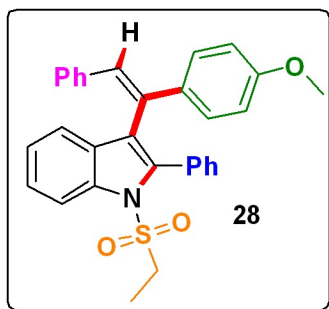
55.25

39.94

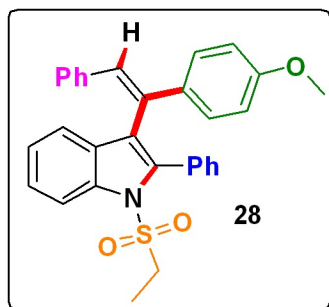




Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



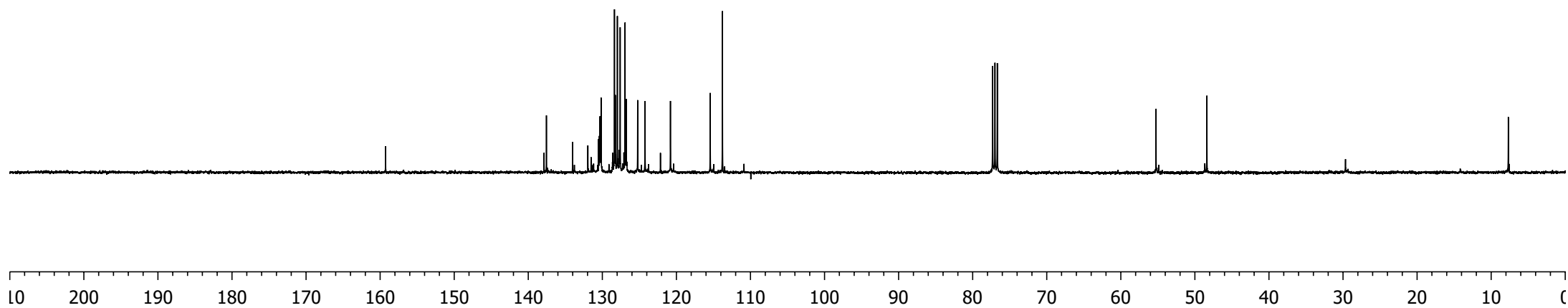
159.26  
137.55  
134.02  
131.95  
130.51  
130.40  
130.32  
130.17  
128.36  
128.25  
127.97  
127.59  
126.93  
126.78  
125.23  
124.24  
119.84  
115.84  
113.79

77.31  
76.99  
76.67

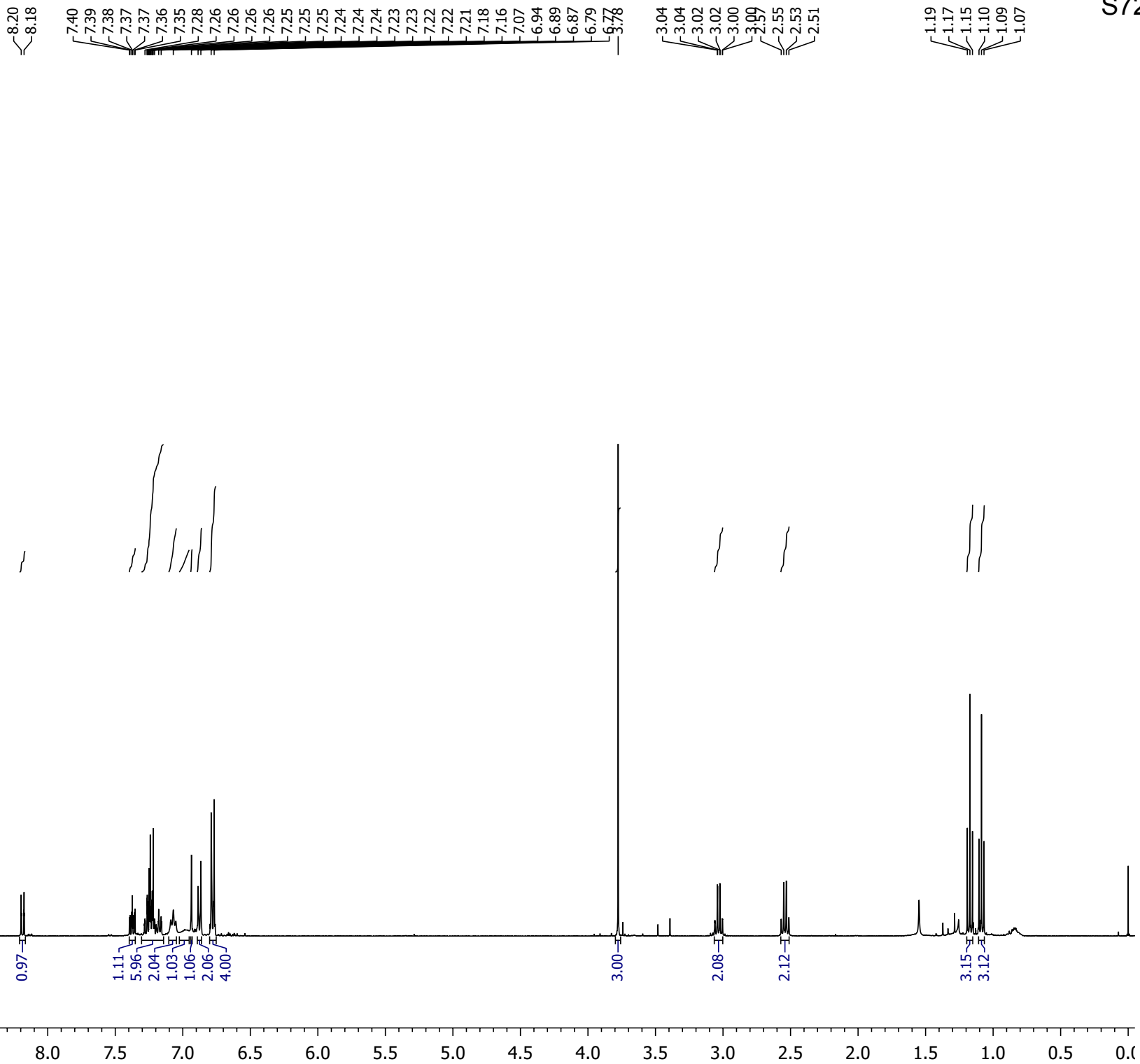
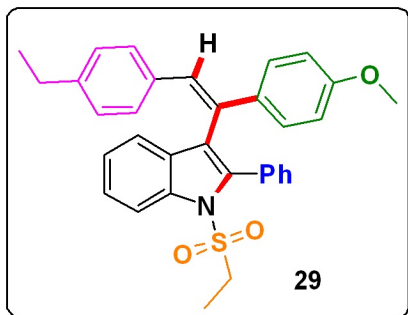
55.25

48.38

7.68



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$





—159.13  
—143.09  
—130.57  
—130.35  
—130.24  
—128.37  
—128.20  
—127.50  
—126.90  
—125.21  
—124.26  
—119.85  
—113.75

—77.31  
—76.99  
—76.67

—55.25

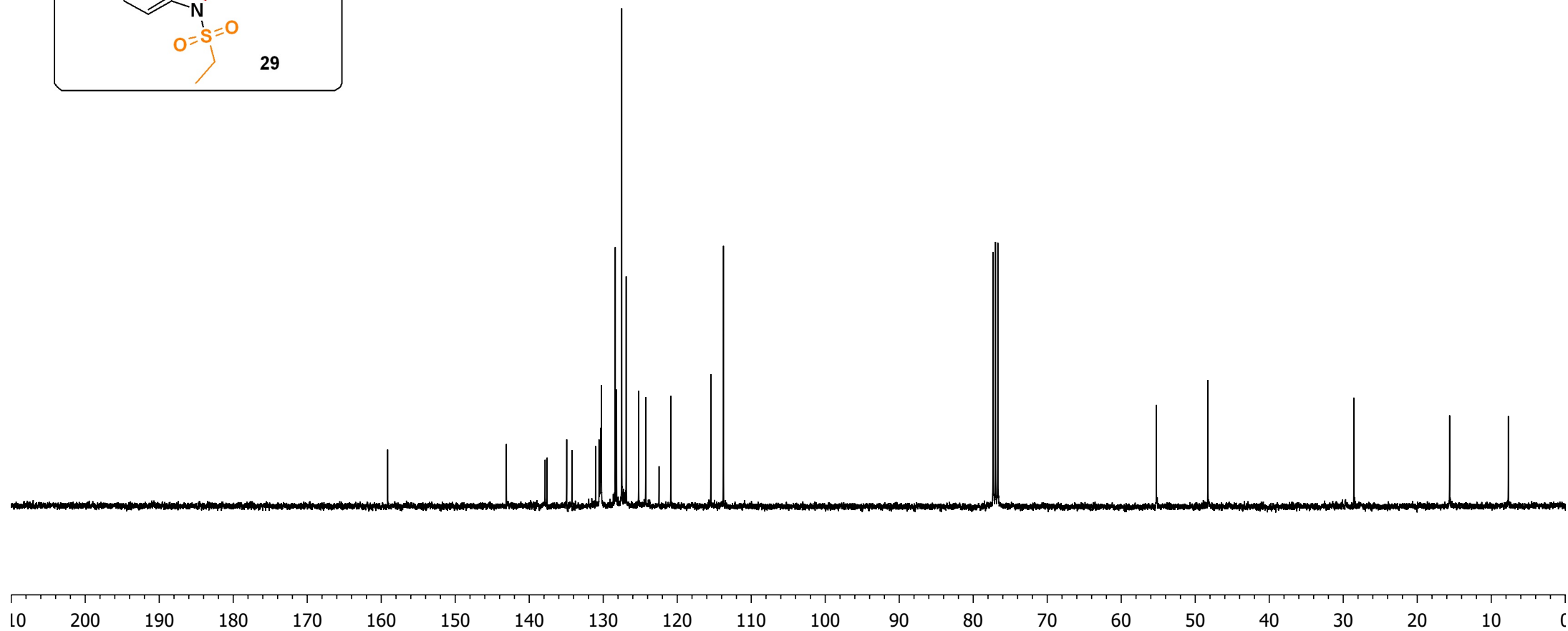
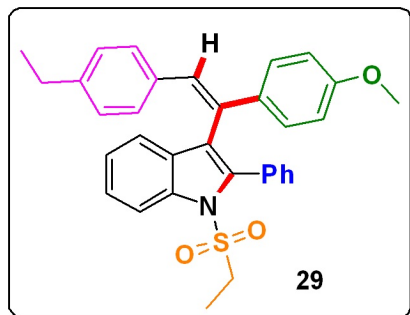
—48.30

—28.56

—15.62

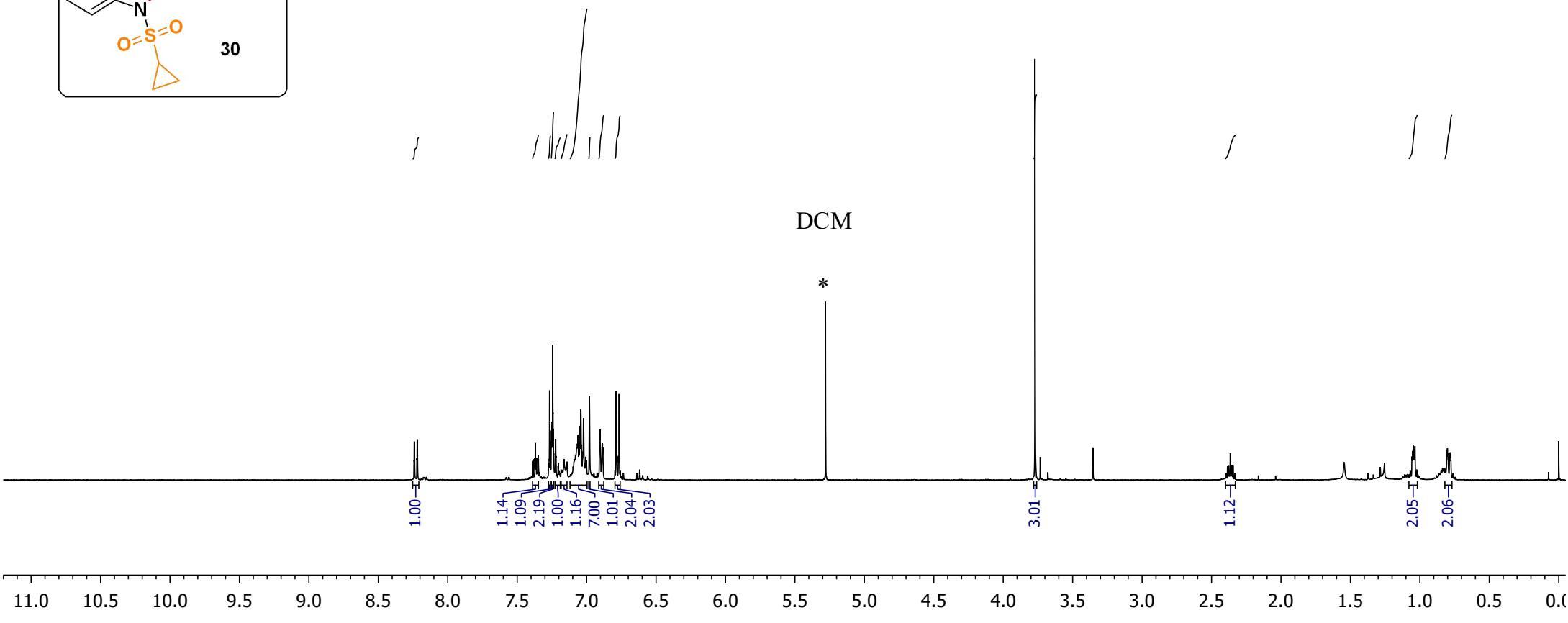
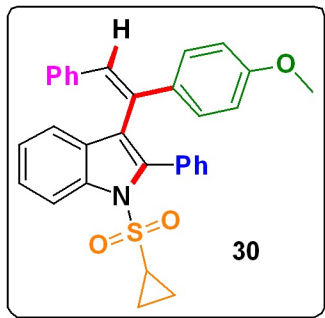
—7.69

Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



11.469  
11.467  
11.334  
11.331  
7.37  
7.37  
7.36  
7.35  
7.35  
7.27  
7.27  
7.27  
7.26  
7.25  
7.25  
7.25  
7.24  
7.24  
7.24  
7.22  
7.22  
7.22  
7.21  
7.20  
7.18  
7.16  
7.14  
7.14  
7.10  
7.09  
7.08  
7.08  
7.07  
7.07  
7.06  
7.05  
7.05  
7.05  
7.04  
7.04  
7.03  
7.02  
7.01  
7.01  
7.00  
6.98  
6.91  
6.90  
6.90  
6.89  
6.88  
6.88  
6.79  
6.77  
3.77  
2.40  
2.39  
2.38  
2.37  
2.37  
2.36  
2.35  
2.35  
2.35  
1.07  
1.06  
1.05  
1.05  
1.05  
1.04  
1.04  
1.04  
1.02  
0.86  
0.82  
0.81  
0.80  
0.80  
0.79  
0.78  
0.78  
0.74  
0.74

Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 400.39  
Nucleus <sup>1</sup>H



M0469-18  
MC-16-31

—159.24

137.96  
137.87  
137.48  
133.95  
132.02  
131.02  
130.87  
130.28  
130.08  
128.35  
128.10  
127.96  
127.56  
126.87  
126.74  
125.19  
124.39  
123.04  
120.71  
115.94  
113.76

77.31  
76.99  
76.67

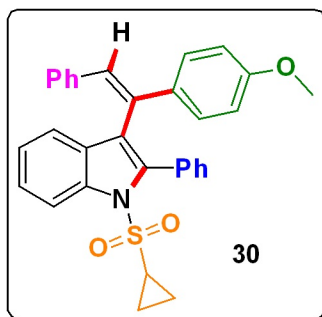
—55.24

—30.45

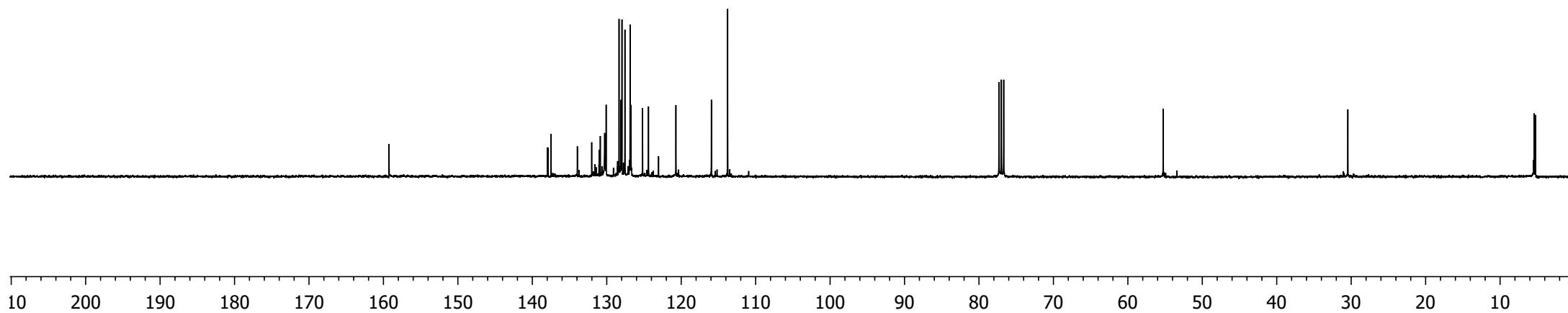
5.41  
5.24

S75

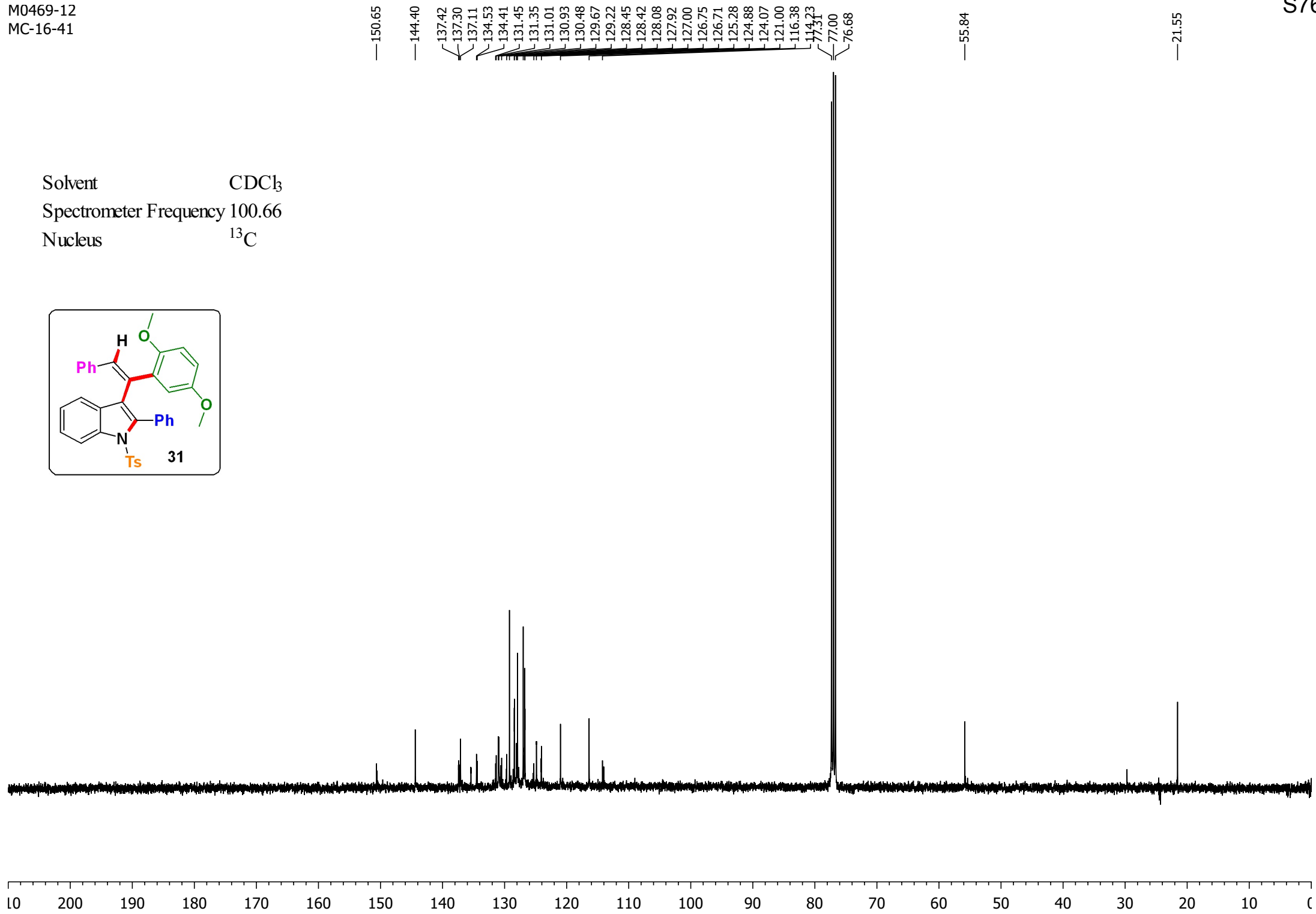
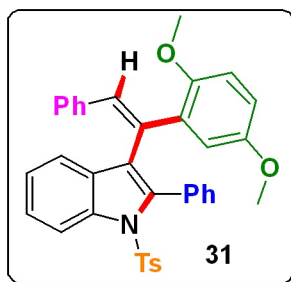
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



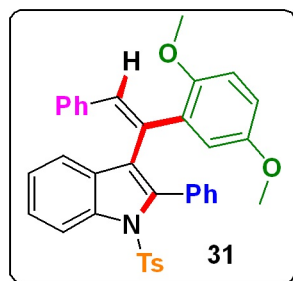
30



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.66  
Nucleus  $^{13}\text{C}$

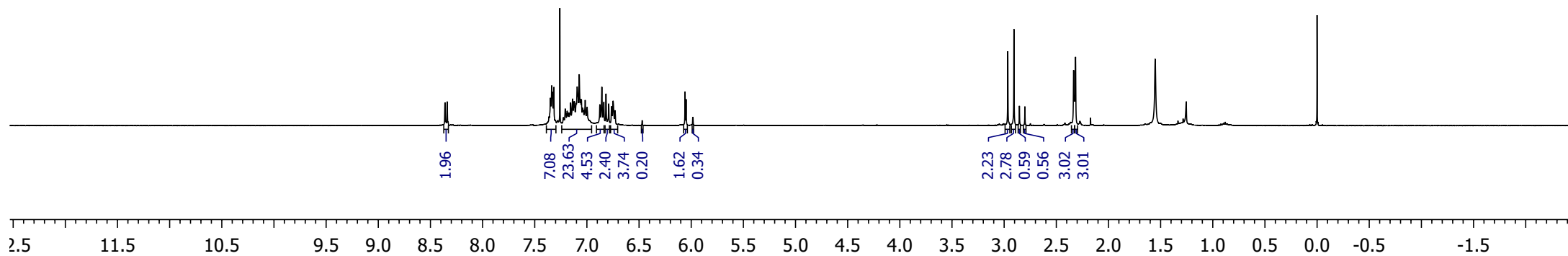


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.28  
Nucleus  $^1\text{H}$

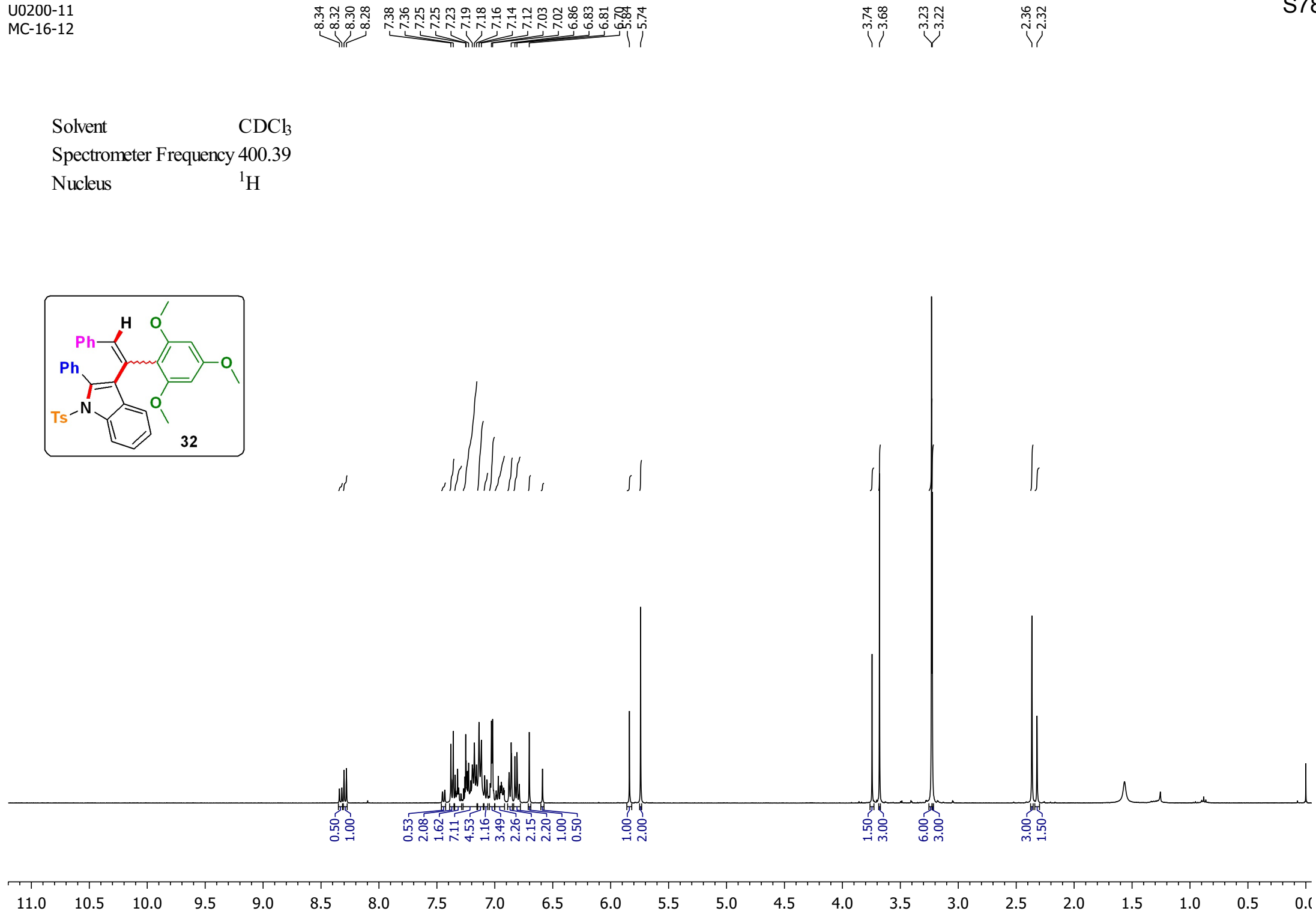
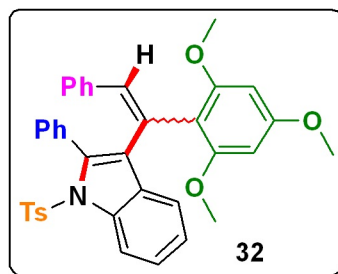


8.36  
8.34  
7.35  
7.34  
7.33  
7.32  
7.26  
7.14  
7.09  
7.07  
6.86  
6.86  
6.05  
5.98  
2.97  
2.91  
2.85  
2.80  
2.33  
2.32  
2.32

Handwritten annotations in the spectrum area, including a large bracket and several small marks.



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



160.95  
160.02  
158.35  
158.32

144.22  
144.17

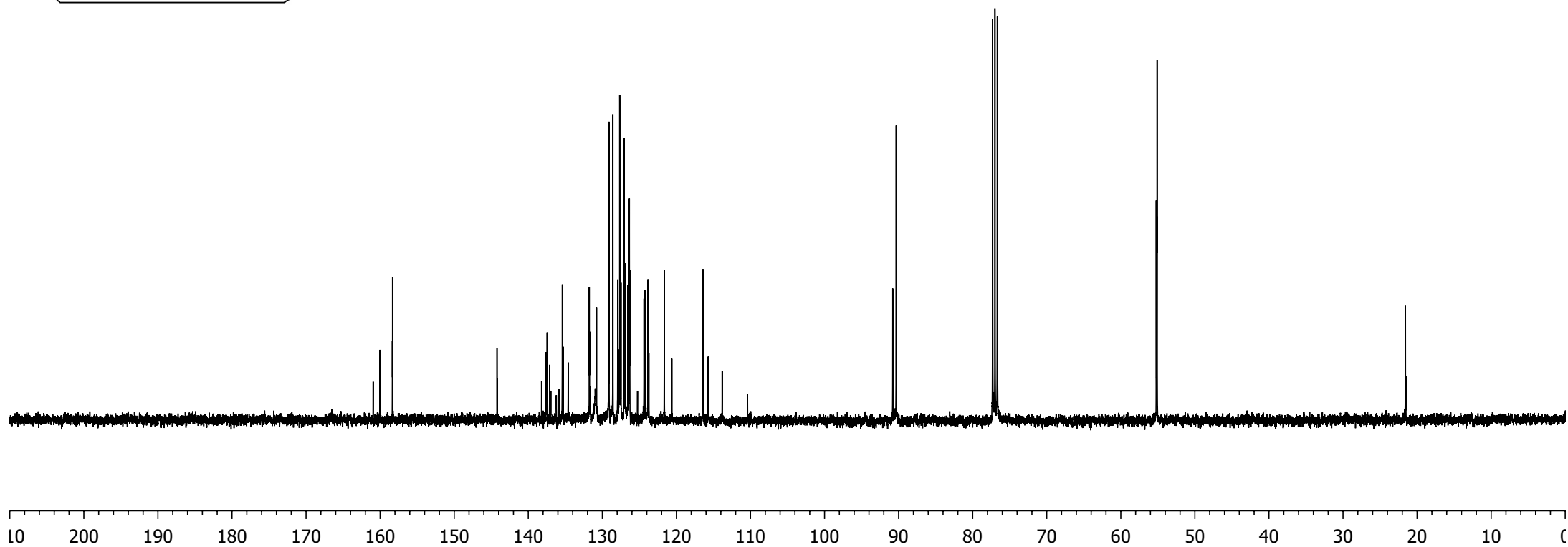
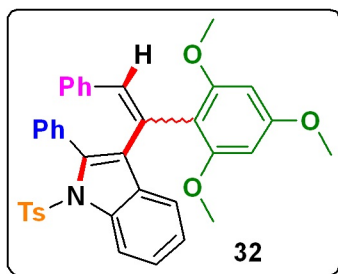
135.40  
131.76  
129.15  
129.09  
128.58  
127.91  
127.66  
127.56  
127.48  
127.04  
126.89  
126.54  
126.35  
126.30  
124.37  
124.25  
123.84  
121.64  
116.41  
90.79  
90.33

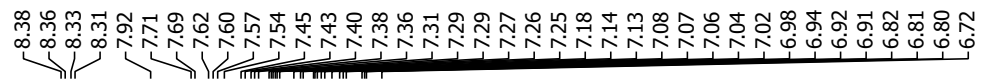
77.31  
76.99  
76.67

55.21  
55.12  
55.10

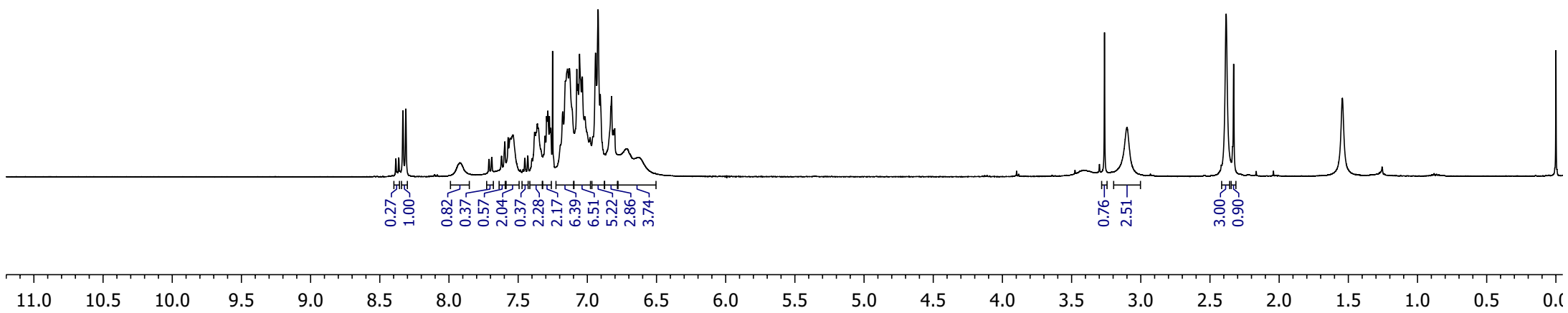
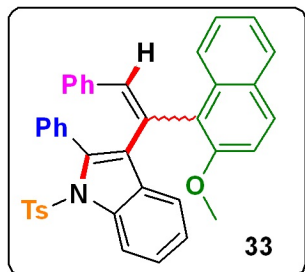
21.57

Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



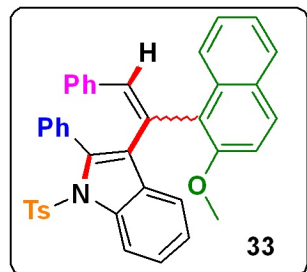


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$





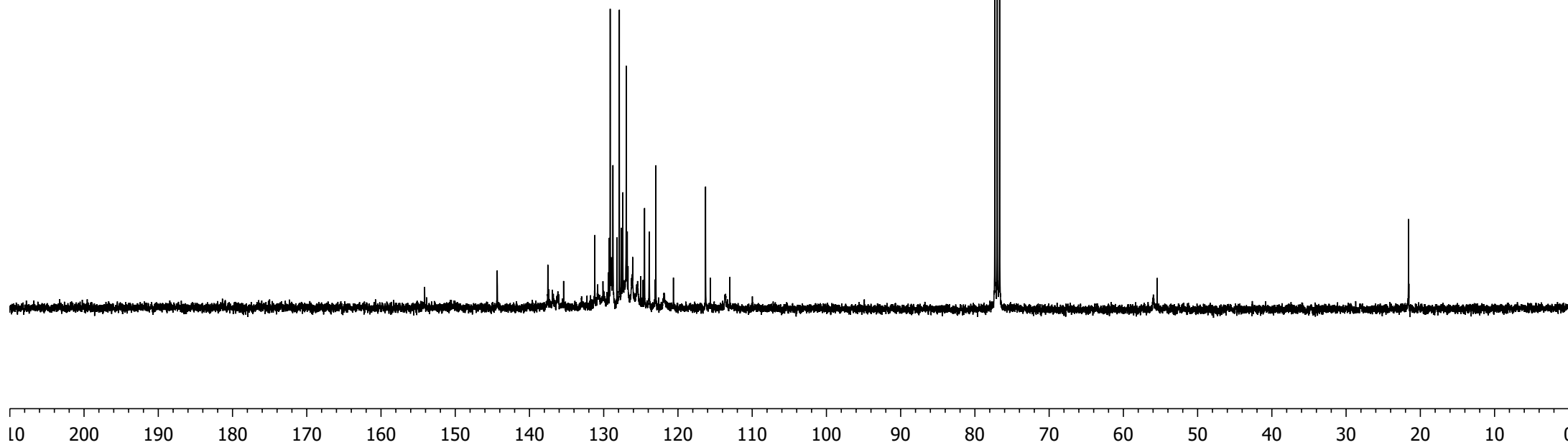
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$



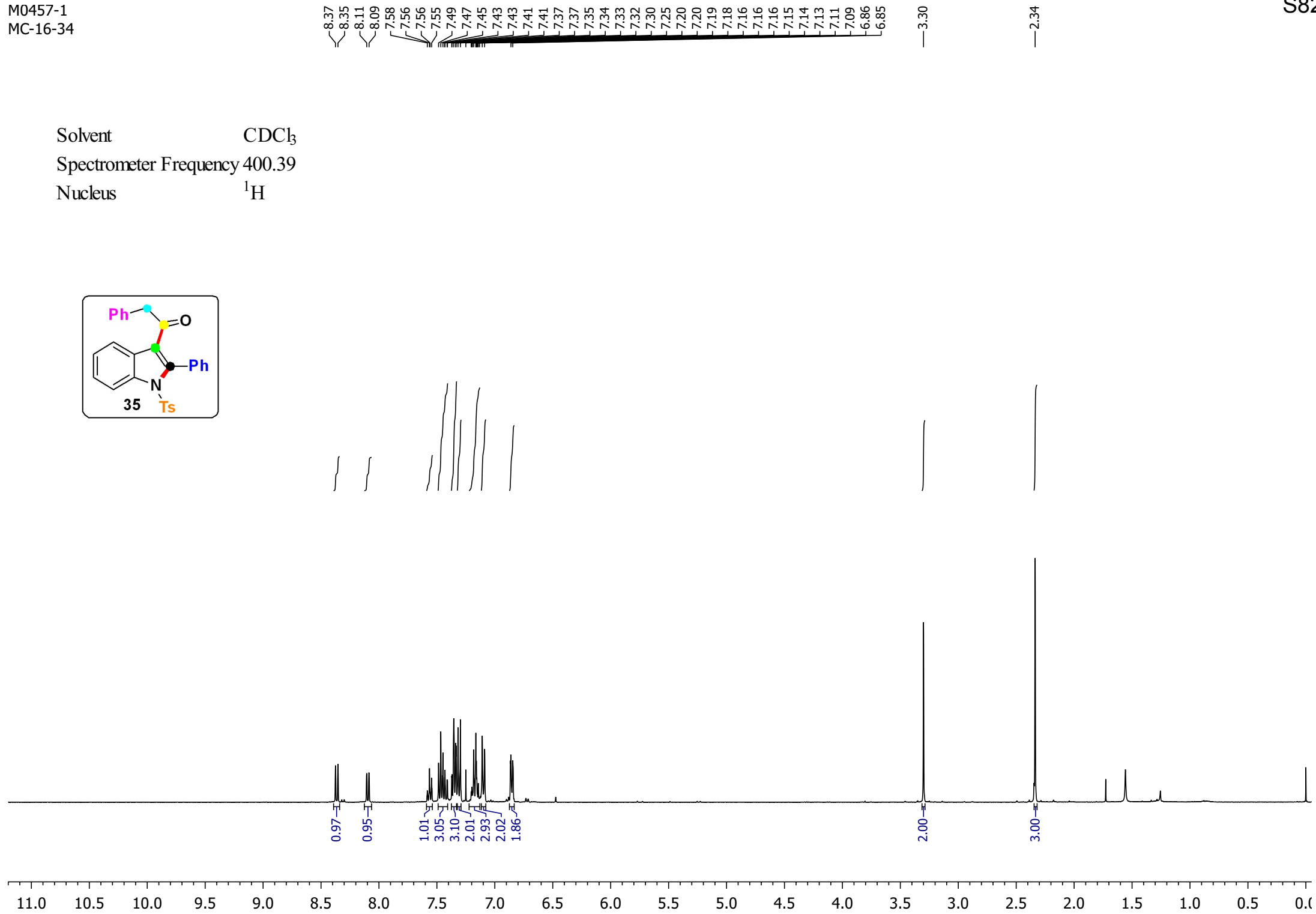
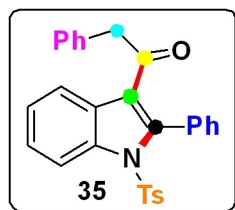
154.12  
144.35  
137.53  
131.20  
129.39  
129.25  
129.13  
128.96  
128.76  
128.23  
127.89  
127.64  
127.62  
127.43  
126.96  
126.82  
126.73  
126.10  
125.02  
124.50  
123.88  
123.07  
122.98  
120.61  
116.28  
115.64  
113.02  
77.31  
76.99  
76.67

55.45

21.59



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



M0457-2  
MC-16-34

—196.80

—145.40

—142.97

—131.76

—129.58

—129.37

—128.24

—127.86

—126.94

—126.64

—125.88

—125.06

—121.91

—115.14

—77.31

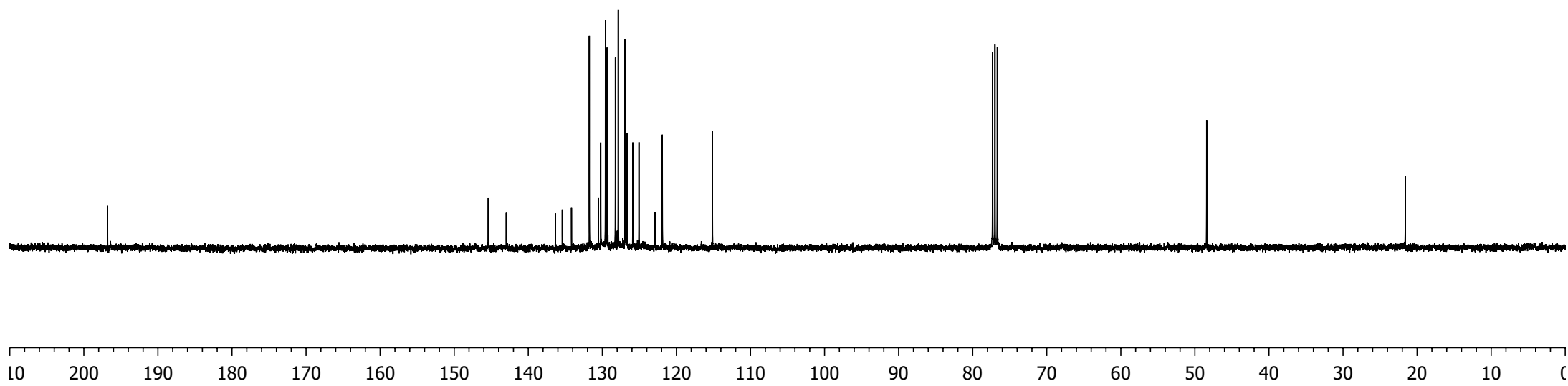
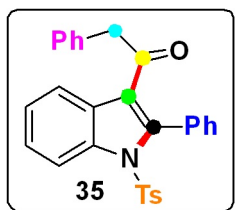
—76.99

—76.68

—48.41

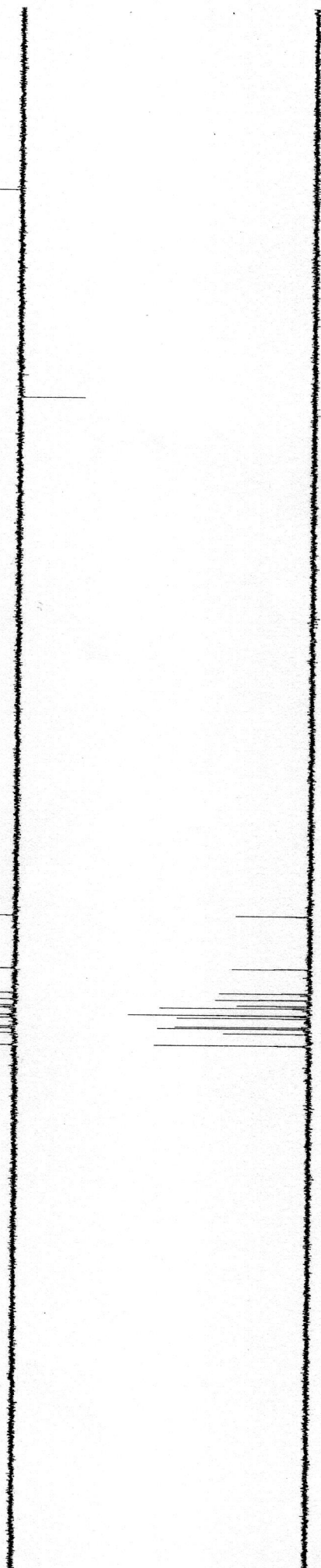
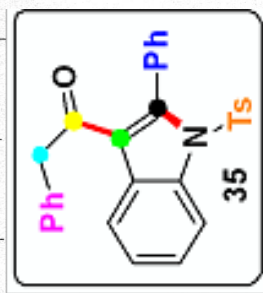
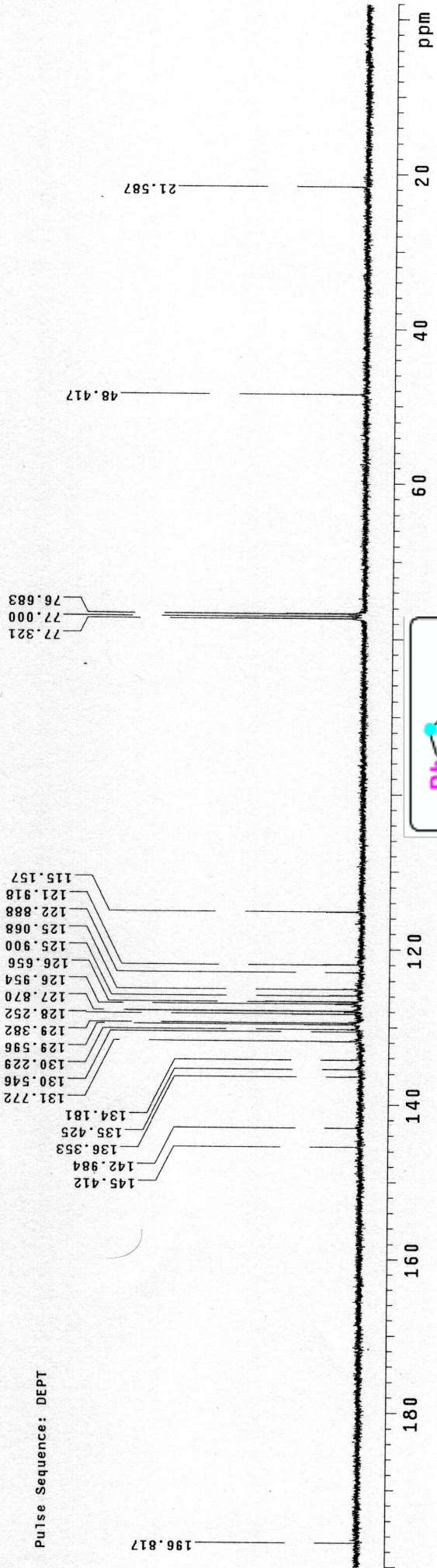
—21.58

Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69  
Nucleus  $^{13}\text{C}$

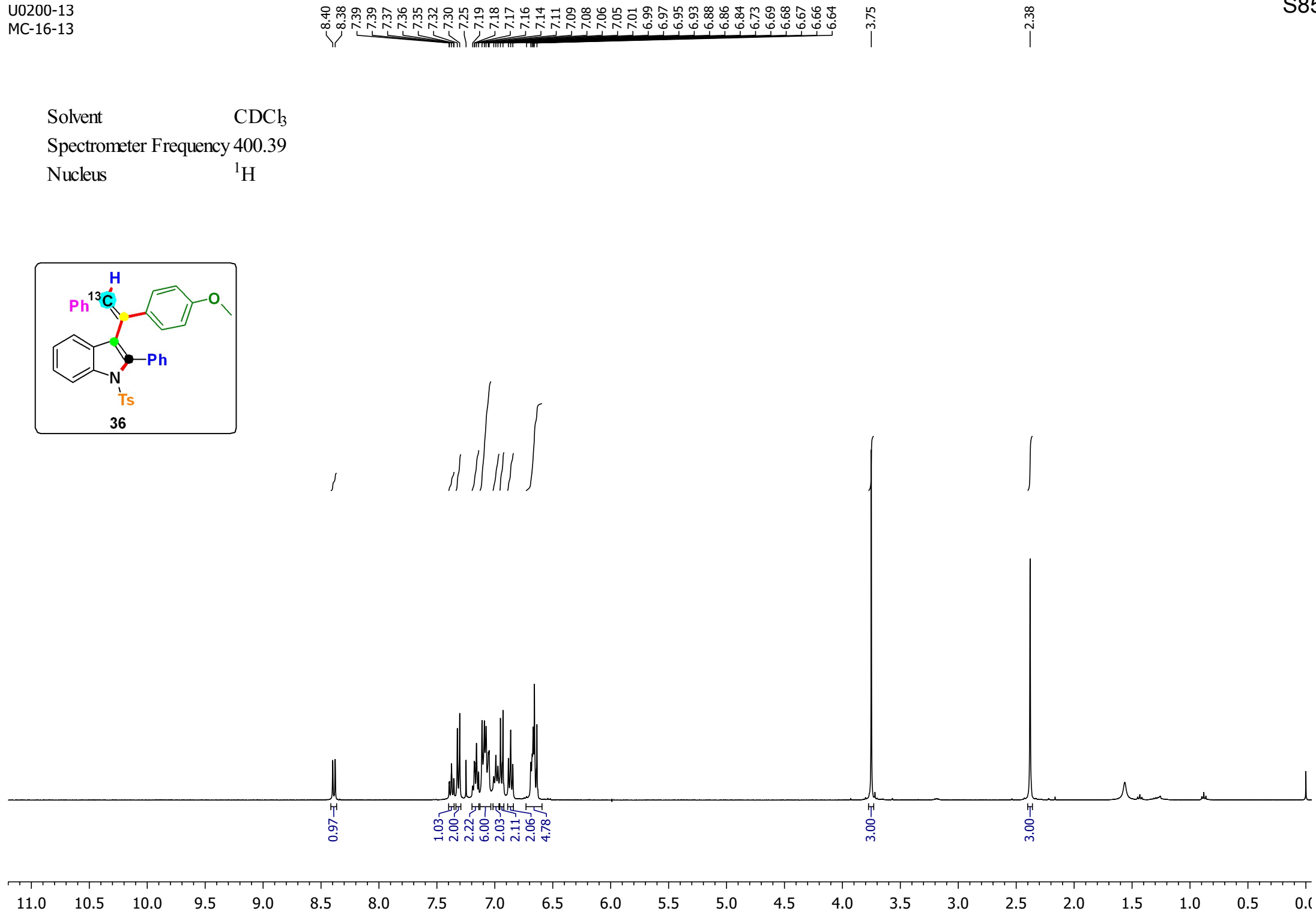
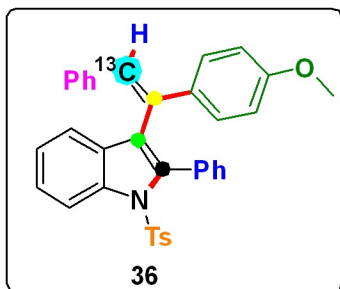


MC-16-34

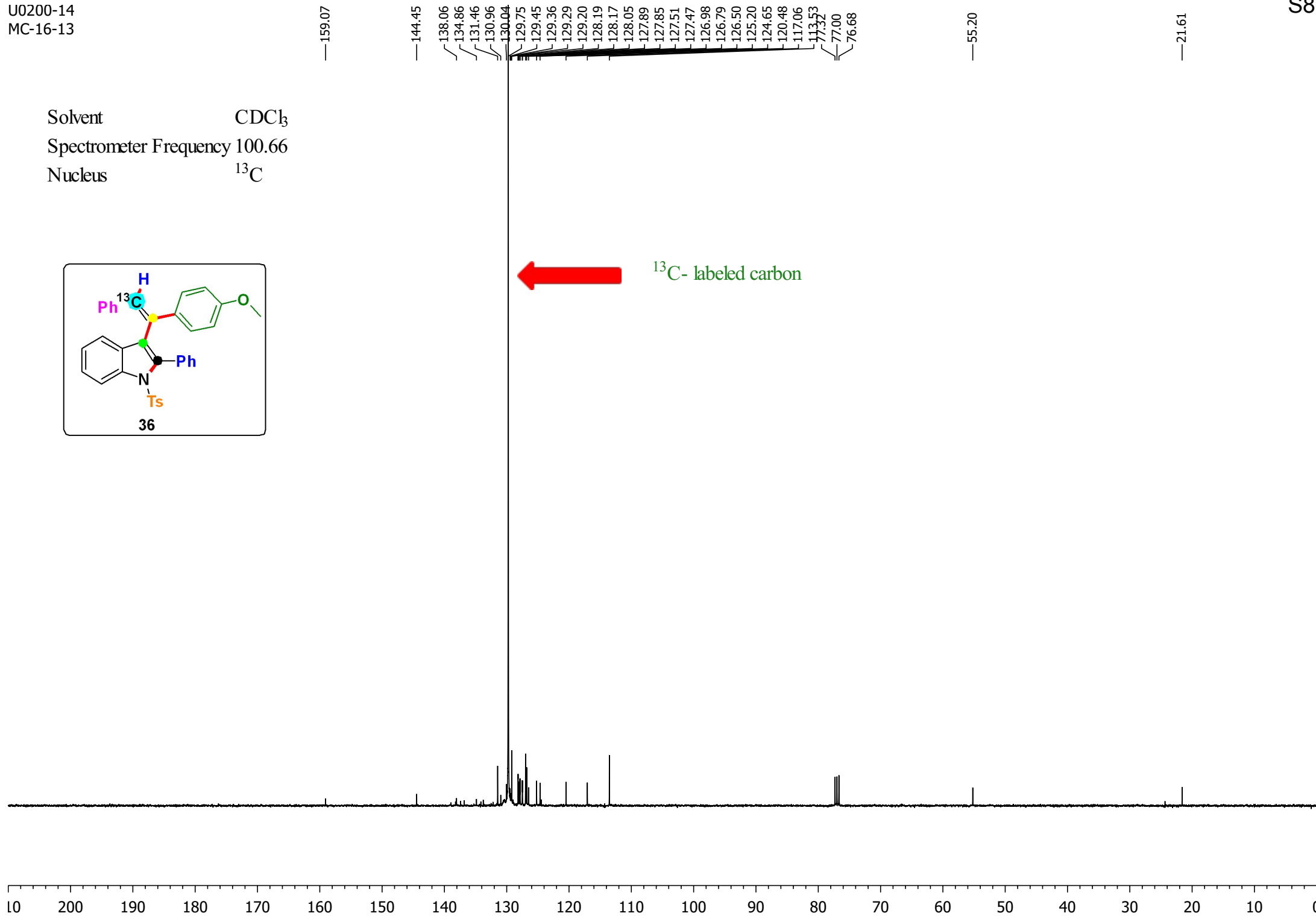
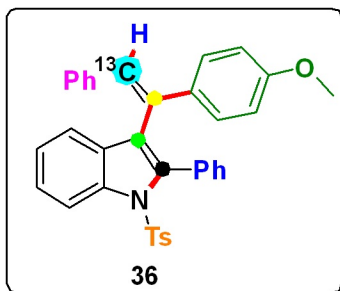
Pulse Sequence: DEPT



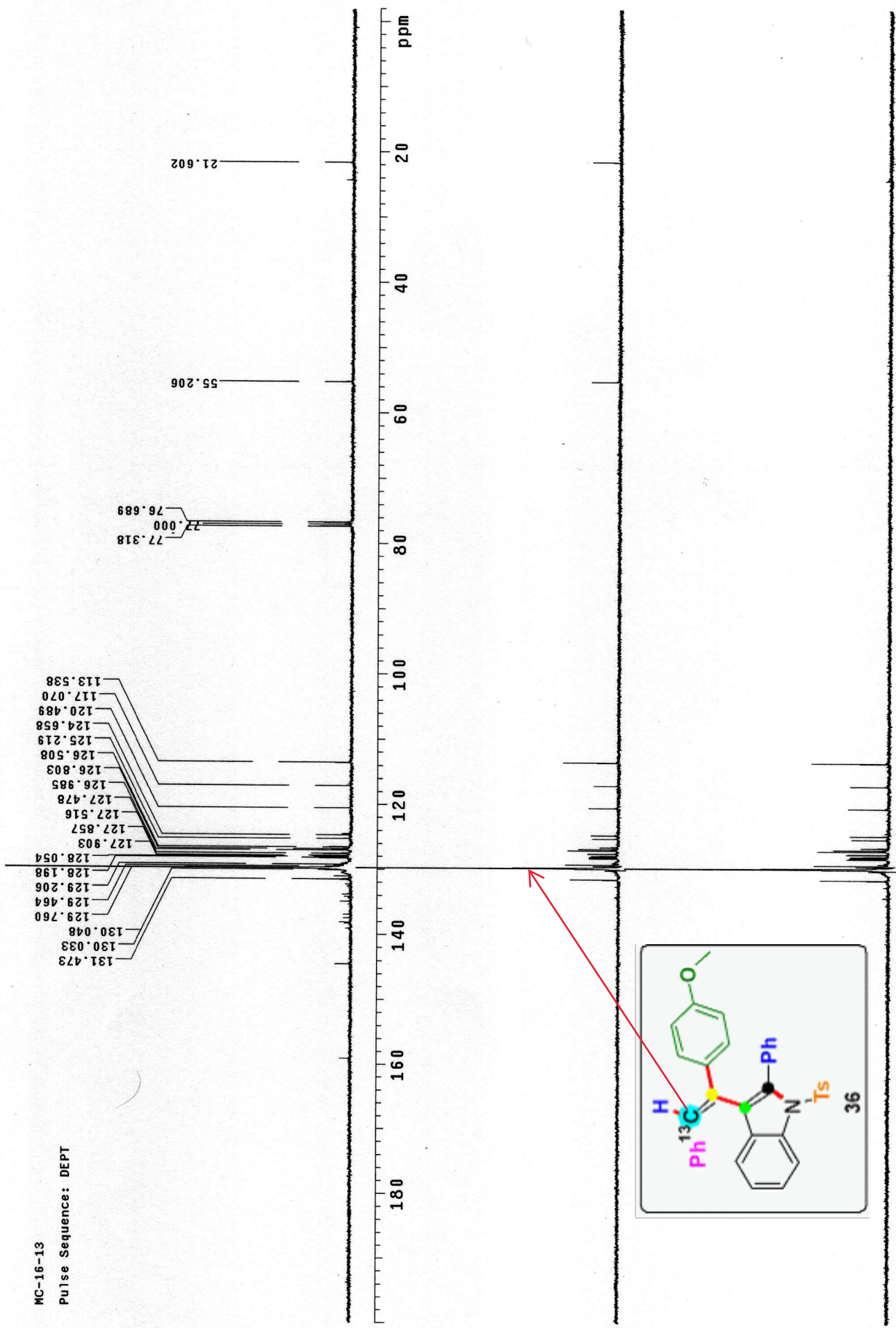
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.39  
Nucleus  $^1\text{H}$



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.66  
Nucleus  $^{13}\text{C}$



MC-16-13  
Pulse Sequence: DEPT







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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

---

● **Alert level C**

PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00511	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	10.804	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.594	17	Report

---

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	36	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	17	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

---

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check
- 
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 18/05/2022; check.def file version of 17/05/2022**

Datablock k11107-jjw-amr-y-tf\_auto - ellipsoid plot

