Supporting Information

For

Atom-economical and workup-free multiparticipation of *p*-TsOH in yne-ynamides skeletal reshuffle: access to regiospecific, chemospecific, and stereospecific (*E*)-alkenyl sulfonate/ketone–tethered indoles

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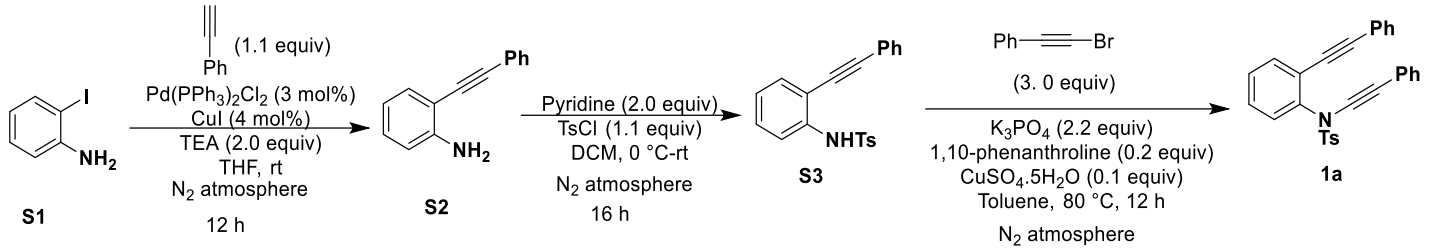
1. General Information

^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz Varian Unity Plus or Varian Mercury plus spectrometer. The chemical shift (δ) values are reported in parts per million (ppm), and the coupling constants (J) are given in Hz. The spectra were recorded using $CDCl_3$ as a solvent. ^{1}H NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm). ^{13}CNMR was referenced to $CDCl_3$ (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}HNMR 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 4-methyl-N-(phenylethynyl)-N-(2 (phenylethynyl)phenyl)benzenesulfonamide (1a)[1]



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_3N (9.24 g, 91.31 mmol, 2.0 equiv), $Pd(PPh_3)_2Cl_2$ (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_2SO_4, 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 $MgSO_4$. 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), $CuSO_4 \cdot 5H_2O$ (288 mg, 1.15 mmol, 0.1 equiv), 1,10-phenanthroline (414 mg 2.30 mmol, 0.2 equiv), and K_3PO_4 (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 ^oC 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 (300 mg scale of respective **S3** starting material) through the procedure reported above. Compounds known in the literature were confirmed by comparing their ^1H and ^{13}C NMR spectra.[1] The list of yne-ynamide (**1a-1x**) used in this transformation are shown below.

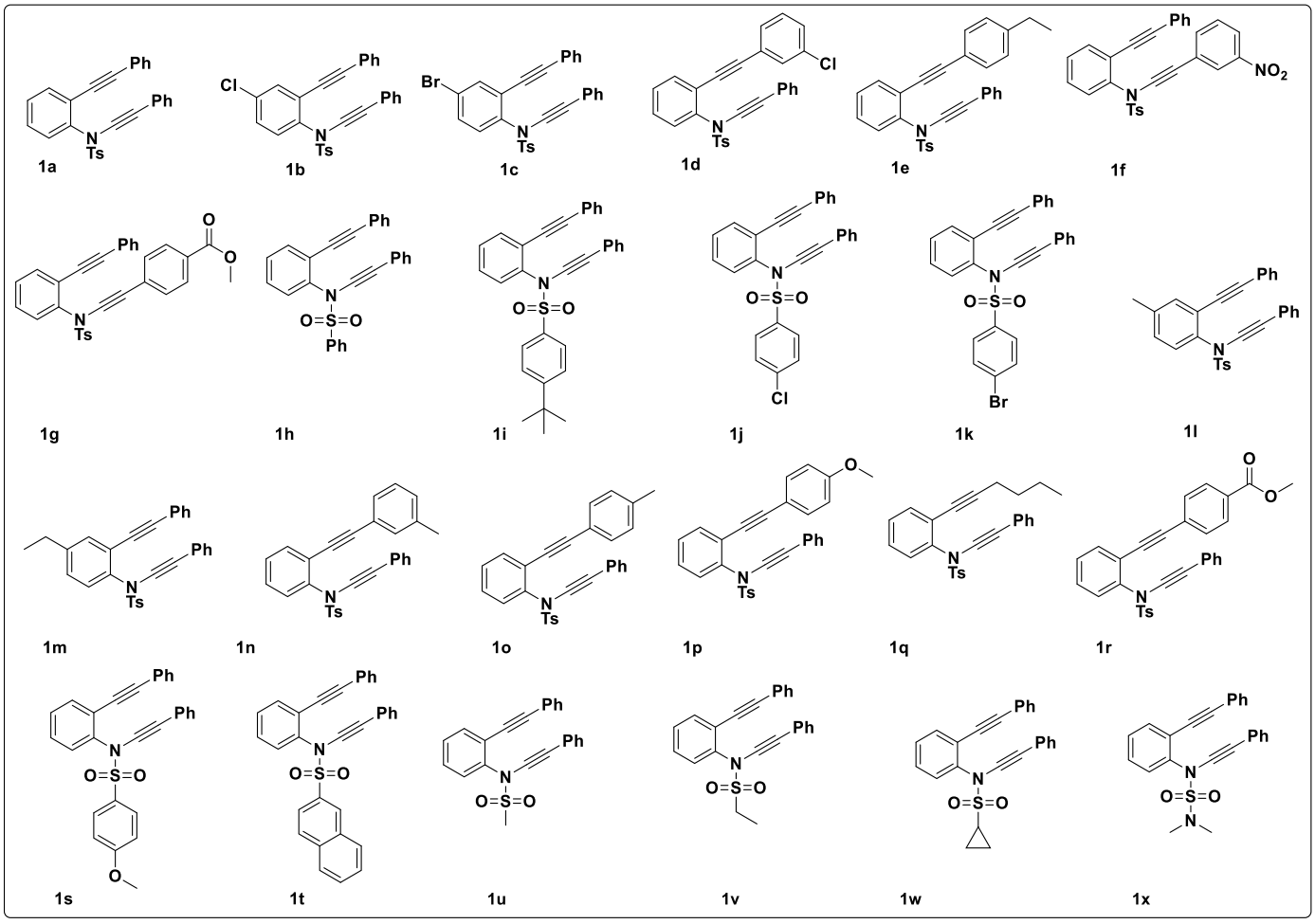
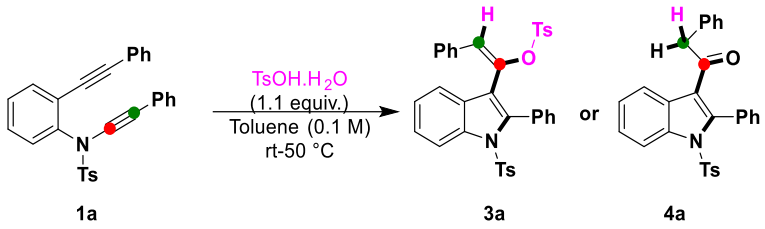


Table S1. Yne-ynamide synthesized and used in our transformations (**1a-1x**).

3. Control experiments

Investigation of the possible reaction intermediate with the help of LCMS.



1a 3a 4a

In a 15 mL dried Schlenk tube, 4-methyl-*N*-(phenylethynyl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (45 mg, 0.10 mmol, 1.0 equiv), *p*-Toluenesulfonic acid monohydrate (21 mg, 0.11 mmol, 1.1 equiv), toluene were added in sequence and stirred at room temperature for 1 h. And the resulting reaction mixture was stirred at 50 °C for respective time. With different interveal of the reaction time, the reaction crude was submitted to LCMS for analysis. From these outcome there may be formation of potential intermediates one of the intermediates (**I**/**II**/ **III** or **V**) due to the same molecular mass for all intermediates. The LCMS spectra are as follows.

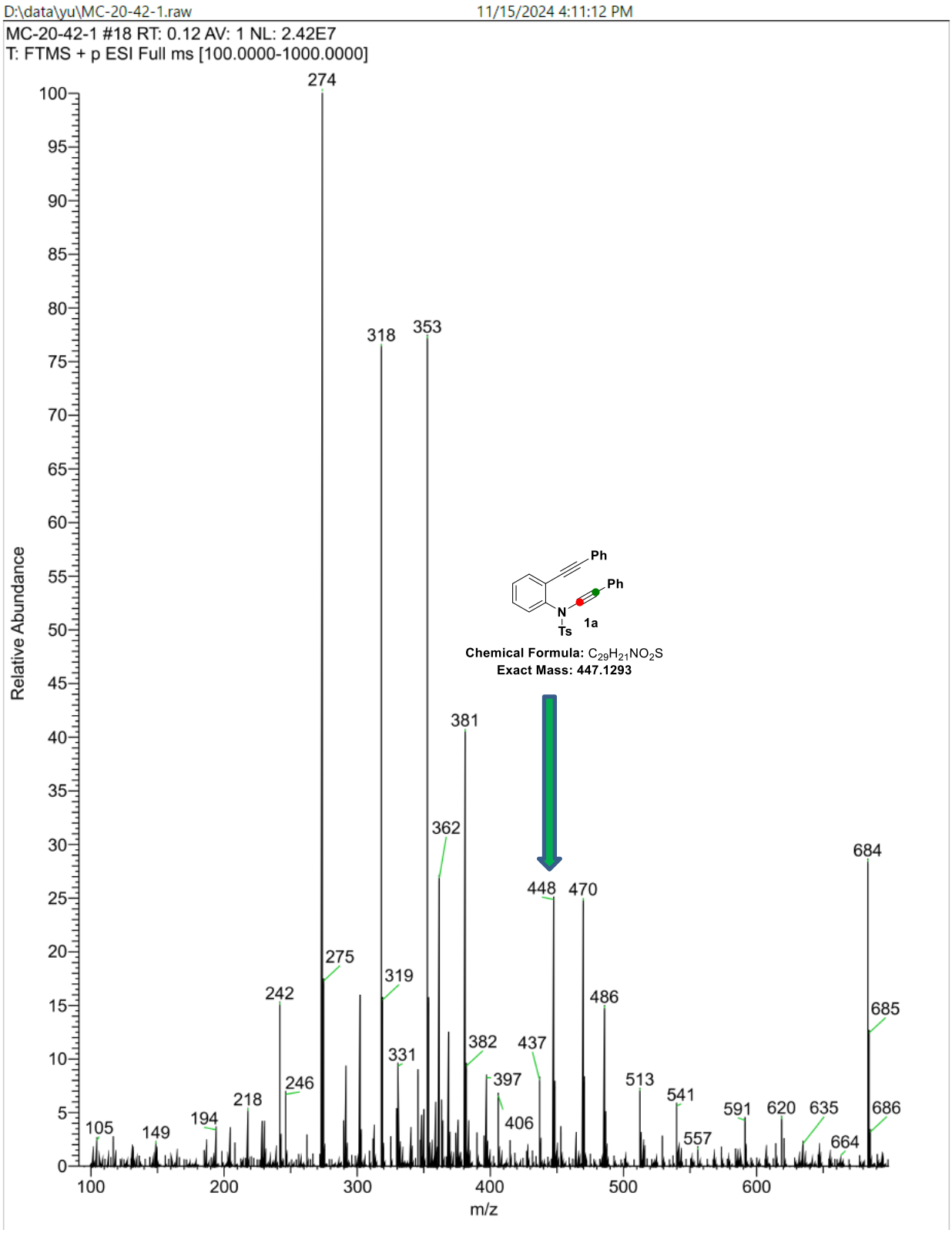


Table S2. LCMS spectra for crude reaction mixture after 1 h at room temperature.

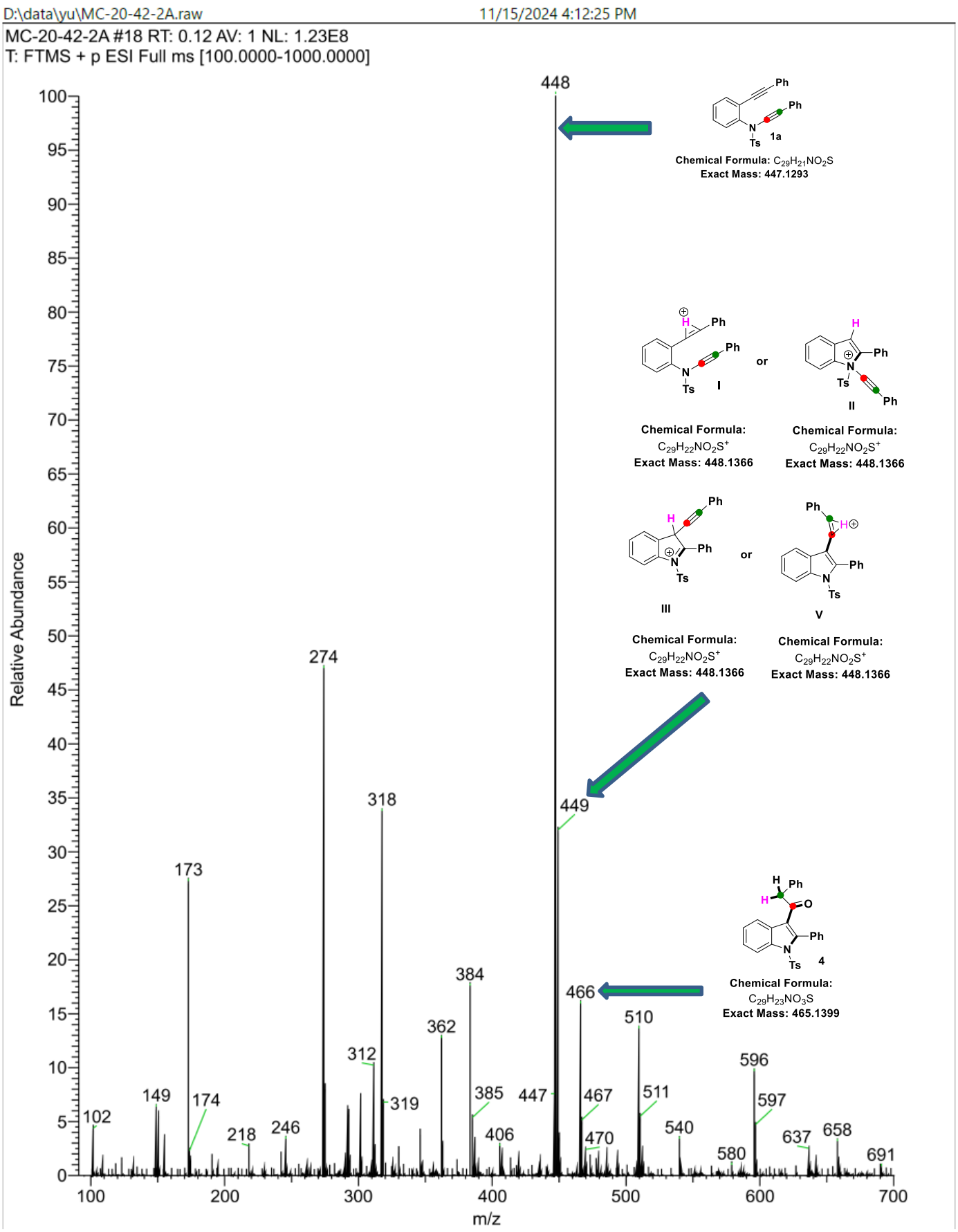
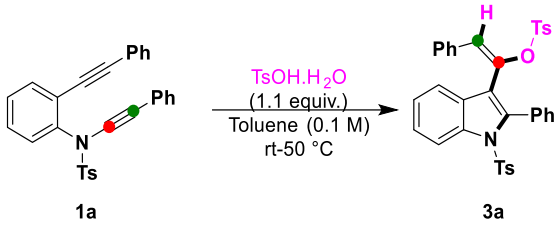


Table S3. LCMS spectra for crude reaction mixture after 1 h at 50°C.

4. Experimental procedures

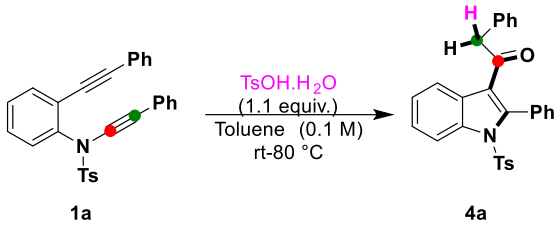
4.1. General procedure (A) for the synthesis of (*E*)-2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)vinyl 4-methylbenzenesulfonate derivatives (3a-3k)



1a 3a

In a 15 mL dried Schlenk tube, 4-methyl-*N*-(phenylethynyl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (45 mg, 0.10 mmol, 1.0 equiv), *p*-Toluenesulfonic acid monohydrate (21 mg, 0.11 mmol, 1.1 equiv), toluene were added in sequence. The resulting reaction mixture was stirred at 50 °C for respective time. The progress of reaction was monitored by TLC. After the reaction was complete, the reaction mixture was concentrated by rotary evaporation and purified by flash column chromatography using hexane-ethyl acetate (92:8) as the eluent gave the desired product (*E*)-2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)vinyl 4-methylbenzenesulfonate as a white solid in 79% (49 mg).

4.2. General procedure (B) for the synthesis of 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one derivatives (4a-4v)

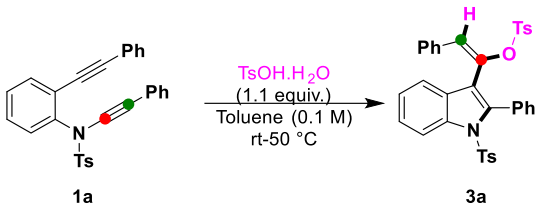


1a 4a

In a 15 mL dried Schlenk tube, 4-methyl-*N*-(phenylethynyl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (45 mg, 0.10 mmol, 1.0 equiv), *p*-toluenesulfonic acid monohydrate (21 mg, 0.11 mmol, 1.1 equiv), toluene were added in sequence. The resulting reaction mixture was stirred at 80 °C for respective time. The progress of reaction was monitored by TLC. After the reaction was complete, the reaction mixture was concentrated by rotary evaporation and purified by flash column chromatography using hexane-ethyl acetate (93:7) as the eluent gave the desired product 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one as a white solid in 80% (38 mg).

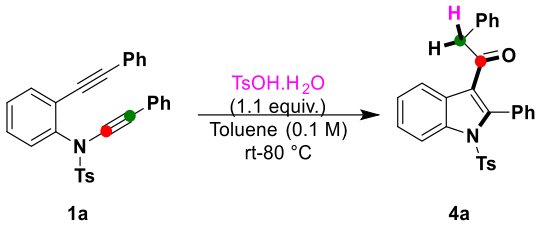
4.3. Gram-scale synthesis

4.3a. Gram-scale synthesis of (*E*)-2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)vinyl 4-methylbenzenesulfonate (3a)



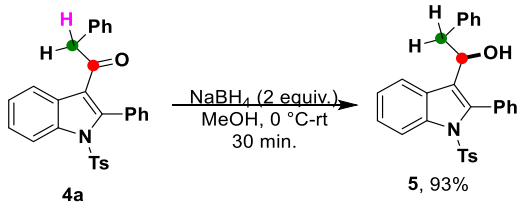
In a 50 mL dried Schlenk tube, 4-methyl-*N*-(phenylethynyl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (1.0 g, 2.23 mmol, 1.0 equiv), *p*-toluenesulfonic acid monohydrate (467 mg, 2.45 mmol, 1.1 equiv), Toluene were added in sequence. The resulting reaction mixture was stirred at 50 °C for respective time. The progress of reaction was monitored by TLC. After the reaction completion, the solvent (toulene) was recovered by rotary evaporator in 94% (21.0 mL) at 45°C water bath temperature and concentrated reaction mixture purified by flash column chromatography using hexane-ethyl acetate (92:8) as the eluent gave the desired product (*E*)-2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)vinyl 4-methylbenzenesulfonate as a white solid in 75% (1.04 g).

4.3b. Gram-scale synthesis of 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (4a)



In a 50 mL dried Schlenk tube, 4-methyl-*N*-(phenylethynyl)-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (1.0 g, 2.23 mmol, 1.0 equiv), *p*-toluenesulfonic acid monohydrate (467 mg, 2.45 mmol, 1.1 equiv), Toluene were added in sequence. The resulting reaction mixture was stirred at 80 °C for respective time. The progress of reaction was monitored by TLC. After the reaction completion, the reaction mixture was concentrated by rotary evaporation and purified by flash column chromatography using hexane-ethyl acetate (93:7) as the eluent gave the desired product 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one as a white solid in 78% (810 mg).

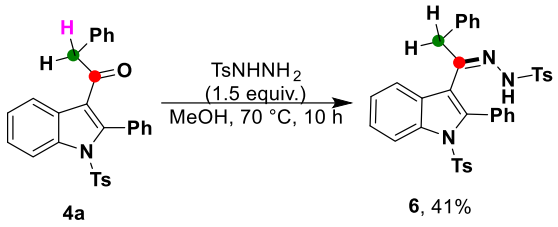
4.4. Synthesis of 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-ol (5) (procedure (C))



In a 15 mL dried Schlenk tube, 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (70 mg, 0.15 mmol, 1.0 equiv) in anhydrous MeOH (4 mL) was slowly added sodium borohydride (12 mg, 0.30 mmol) at 0°C. The resulting reaction mixture was stirred for 30 min at room temperature. The progress of reaction was monitored

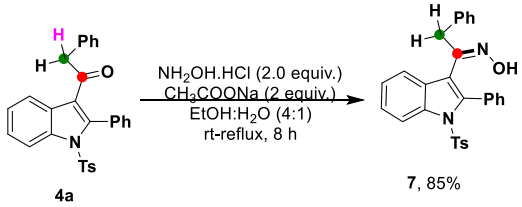
by TLC. After the reaction completion, the reaction mixture was concentrated by rotary evaporation and purified by flash column chromatography using hexane-ethyl acetate (86:14) as the eluent gave the desired product 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-ol as a white solid in 93% (66 mg).

4.5. Synthesis of 4-methyl-*N*'-(2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethylidene)benzenesulfonohydrazide (6) (procedure (D))



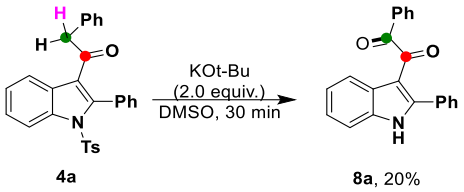
In a 15 mL dried Schlenk tube, solution of 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (70 mg, 0.15 mmol, 1.0 equiv) in anhydrous MeOH (4 ml) was added *p*-toluenesulfonyl hydrazide (42 mg, 0.22 mmol). The resulting reaction mixture was stirred at 70 °C for 10 h. The progress of reaction was monitored by TLC. After the reaction completion, the reaction mixture was concentrated by rotary evaporation and purified by flash column chromatography using hexane-ethyl acetate (85:14) as the eluent gave the desired product 4-methyl-*N*'-(2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethylidene)benzenesulfonohydrazide as a white solid in 41% (39 mg).

4.6. Synthesis of 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one oxime (7) (procedure (E))



A suspension of hydroxylamine hydrochloride (21 mg, 0.30 mmol, 2.0 equiv), and NaOAc (25 mg, 0.30 mmol 2.0 equiv) in ethanol:water (4:1) was stirred at room temperature for 30 min. To this solution, 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (70 mg, 0.15 mmol, 1.0 equiv) was added and the reaction mixture was heated refluxed for 8 h. After the reaction completion by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. Then the reaction mixture was diluted with water, extracted with ethyl acetate and evoporated under vacuum to get crude product. The crude material was purified by flash column chromatography using hexane-ethyl acetate (80:20) as the eluent gave product 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one oxime as a white solid in 85% (62 mg).

4.7. Synthesis of of 1-phenyl-2-(2-phenyl-indol-3-yl)ethane-1,2-dione (8) (procedure (F))



An oven-dried screw-capped, 8 mL vial equipped with a magnetic stir bar was charged with 2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (70 mg, 0.15 mmol, 1.0 equiv.) in dimethyl sulfoxide (0.1 M) and potassium *tert*-butoxide (KOt-Bu) (17 mg, 0.30 mmol, 2.0 equiv.) was added. The resulting solution was stirred up to starting material completion (30 minutes) at room temperature. The progress of reaction was monitored by TLC. After that, the crude reaction mixture was diluted with water and saturated solution of sodium chloride and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography using hexane-ethyl acetate (86:14) as the eluent gave the desired product 1-phenyl-2-(2-phenyl-indol-3-yl)ethane-1,2-dione as a white solid in 20% (10 mg).

5. Gram-scale synthesis and evaluation of green chemistry metrics in the synthesis of 3a

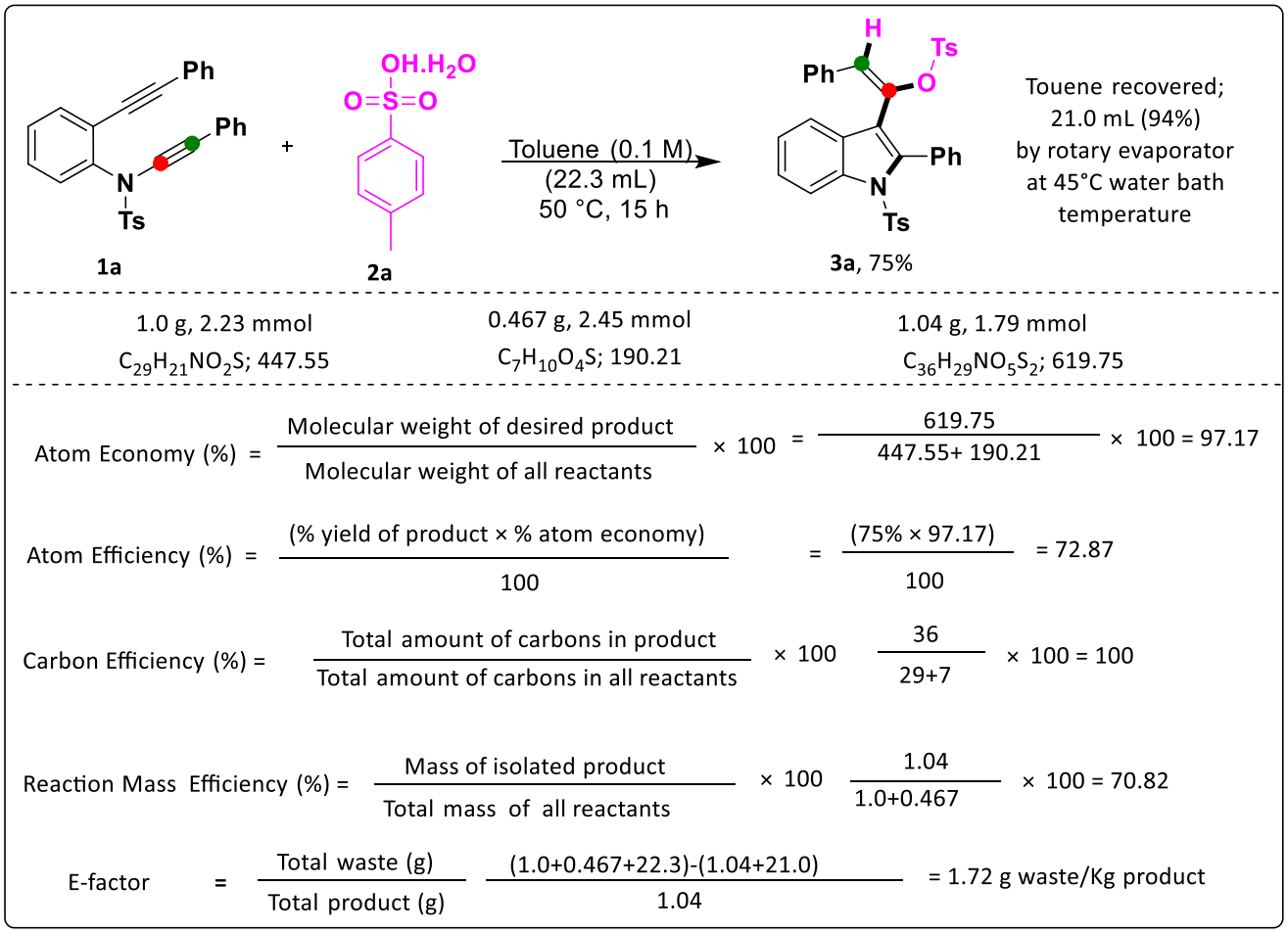
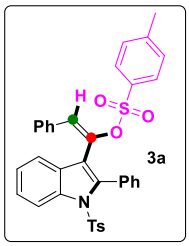


Table S4. Gram-scale synthesis and evaluation of green chemistry metrics in the synthesis of **3a**.

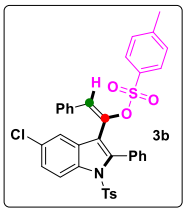
6. Characterization data

(*E*)-2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)vinyl 4-methylbenzenesulfonate (3a): The title compound was



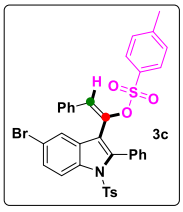
prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (49 mg, yield = 79%); Mp. 114-115 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.4 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.31 (ddd, *J* = 8.5, 7.1, 1.4 Hz, 2H), 7.29 – 7.20 (m, 6H), 7.13 – 7.01 (m, 6H), 6.95 (d, *J* = 7.9 Hz, 2H), 6.90 – 6.85 (m, 2H), 6.69 (d, *J* = 7.2 Hz, 2H), 6.66 (s, 1H), 2.33 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 144.6, 141.0, 139.1, 137.2, 134.9, 133.1, 132.7, 130.0, 129.3, 129.2, 129.0, 128.4, 128.3, 128.1, 127.8, 127.7, 127.3, 126.9, 126.7, 125.3, 124.5, 120.8, 118.0, 116.5, 21.6, 21.5. HRMS (ESI) calcd for $C_{36}H_{29}O_5NNaS_2$ $[M+Na]^+$ 642.1379; found: 642.1376.

(*E*)-1-(5-chloro-2-phenyl-1-tosyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3b): The title



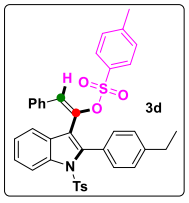
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (42 mg, yield = 63%); Mp. 142-143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.9 Hz, 1H), 7.42 – 7.32 (m, 2H), 7.31 – 7.21 (m, 7H), 7.15 – 7.05 (m, 4H), 6.99 (d, J = 8.0 Hz, 2H), 6.91 (t, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 2.1 Hz, 1H), 6.64 (d, *J* = 5.9 Hz, 3H), 2.35 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 144.9, 142.2, 138.7, 135.3, 134.7, 132.9, 132.5, 130.2, 129.6, 129.5, 129.4, 129.1, 128.3, 128.2, 127.9, 127.8, 127.3, 126.9, 126.8, 125.4, 120.1, 117.4, 21.6, 21.6. HRMS (ESI) calcd for $C_{36}H_{28}O_5NClNaS_2$ $[M+Na]^+$ 676.0989; found: 676.0986.

(*E*)-1-(5-bromo-2-phenyl-1-tosyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3c): The title



compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (51 mg, yield = 73%); Mp. 139-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.07 (m, 1H), 7.43 – 7.33 (m, 3H), 7.30 – 7.24 (m, 5H), 7.24 – 7.16 (m, 1H), 7.15 – 7.06 (m, 4H), 7.02 (d, *J* = 1.7 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.91 (t, *J* = 7.8 Hz, 2H), 6.66-6.62 (m, 3H), 2.35 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 144.9, 142.1, 138.7, 135.7, 134.8, 133.0, 132.5, 130.0, 129.5, 129.4, 129.3, 129.1, 128.2, 128.2, 128.0, 127.9, 127.8, 127.3, 126.9, 126.7, 123.1, 118.0, 117.7, 116.7, 21.6, 21.6. HRMS (ESI) calcd for $C_{36}H_{28}O_5NBrNaS_2$ $[M+Na]^+$ 720.0484; found: 720.0481.

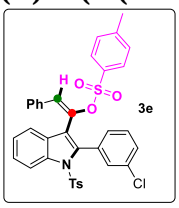
(*E*)-1-(2-(4-ethylphenyl)-1-tosyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3d): The title



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 (42 mg, yield = 64%); Mp. 149-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.4 Hz, 1H), 7.46 – 7.39 (m, 3H), 7.39 – 7.35 (m, 2H), 7.33 – 7.27 (m, 3H), 7.26 – 7.20 (m, 4H), 7.19 – 7.16 (m, 3H), 7.12 (ddd, *J* = 15.2, 7.1, 1.9 Hz, 3H), 6.73 (d, *J* = 8.0 Hz, 2H), 5.82 (s, 1H), 2.76 (q, *J* = 7.6 Hz, 2H), 2.33 (s, 3H), 2.23 (s, 3H),

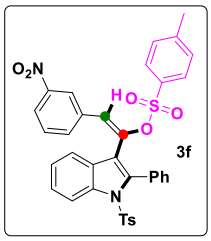
1.33 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 144.9, 144.5, 139.1, 138.8, 135.6, 133.2, 133.0, 131.5, 129.4, 129.1, 128.8, 128.7, 128.2, 127.9, 127.4, 127.1, 124.8, 124.6, 124.0, 120.5, 115.5, 28.8, 21.6, 21.4, 15.4. HRMS (ESI) calcd for $C_{38}H_{33}O_5NNaS_2$ $[M+Na]^+$ 670.1692; found: 670.1689.

(*E*)-1-(2-(3-chlorophenyl)-1-tosyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3e): The title



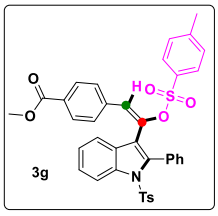
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (36 mg, yield = 55%); Mp. 69-70 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.3 Hz, 1H), 7.41 – 7.24 (m, 7H), 7.23 – 7.01 (m, 9H), 6.90 (t, *J* = 7.1 Hz, 2H), 6.62 (d, *J* = 7.4 Hz, 2H), 6.55 (s, 1H), 2.37 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 144.9, 139.1, 138.8, 137.3, 134.9, 133.2, 132.9, 132.61, 131.7, 129.5, 129.2, 128.9, 128.4, 128.2, 127.8, 126.8, 126.6, 125.6, 124.7, 120.9, 116.3, 21.6. HRMS (ESI) calcd for $C_{36}H_{28}O_5NClNaS_2$ $[M+Na]^+$ 676.0989; found: 676.0986.

(*E*)-2-(3-nitrophenyl)-1-(2-phenyl-1-tosyl-indol-3-yl)vinyl 4-methylbenzenesulfonate (3f): The title



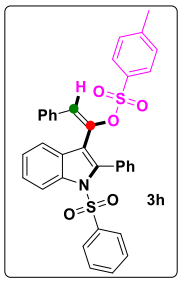
compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (89:11) to obtain as a white solid (50 mg, yield = 74%); Mp. 68-69 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.5 Hz, 1H), 7.89 (ddd, *J* = 8.2, 2.2, 1.0 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.39 – 7.31 (m, 4H), 7.31 – 7.23 (m, 4H), 7.15 – 7.12 (m, 2H), 7.12 – 7.07 (m, 3H), 7.04 (dd, *J* = 7.8, 7.0 Hz, 3H), 6.96 (d, *J* = 7.8 Hz, 1H), 6.59 (s, 1H), 2.36 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 145.1, 134.9, 133.7, 130.7, 129.5, 129.5, 129.3, 129.1, 129.0, 127.8, 127.7, 127.3, 126.8, 125.5, 124.5, 123.2, 123.1, 122.1, 120.3, 116.2, 21.6, 21.6. HRMS (ESI) calcd for $C_{36}H_{28}O_7N_2NaS_2$ $[M+Na]^+$ 687.1230; found: 687.1226.

methyl (*E*)-4-(2-(2-phenyl-1-tosyl-indol-3-yl)-2-(tosyloxy)vinyl)benzoate (3g): 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 (51 mg, yield = 75%); Mp. 168-169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.44 – 7.29 (m, 4H), 7.27 (d, *J* = 8.5 Hz, 3H), 7.19 (d, *J* = 8.3 Hz, 2H), 7.15 – 7.05 (m, 4H), 7.00 (d, *J* = 7.3 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 8.2 Hz, 2H), 6.72 (s, 1H), 3.86 (s, 3H), 2.38 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 145.2, 144.8, 141.2, 140.9, 137.4, 137.3, 134.7, 133.0, 129.9, 129.4, 129.4, 129.3, 129.0, 128.9, 128.2, 128.1, 127.7, 127.4, 126.9, 125.5, 125.5, 124.7, 120.5, 117.8, 116.7, 52.1, 21.5, 21.5. HRMS (ESI) calcd for $C_{38}H_{31}O_7NNaS_2$ $[M+Na]^+$ 700.1434; found: 700.1430.

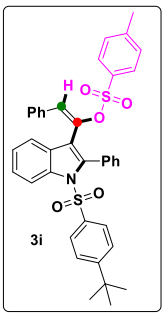
(*E*)-2-phenyl-1-(2-phenyl-1-(phenylsulfonyl)-indol-3-yl)vinyl 4-methylbenzenesulfonate (3h): The title



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 (49 mg, yield = 80%); Mp. 129-130 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.53-7.49 (ddt, *J* = 8.7, 7.6, 1.3, 1H), 7.42 – 7.22 (m, 11H), 7.13 – 7.06 (m, 2H), 7.06 – 7.02 (m, 2H), 6.96 (d, *J* = 8.0

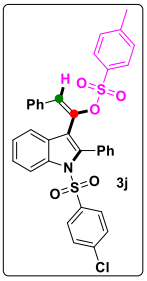
Hz, 2H), 6.89 (t, *J* = 7.8 Hz, 2H), 6.68 (d, *J* = 7.3 Hz, 2H), 6.65 (s, 1H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 140.9, 139.0, 137.8, 137.2, 133.8, 133.1, 132.7, 129.9, 129.2, 129.0, 128.7, 128.4, 128.3, 128.2, 127.8, 127.7, 127.3, 126.8, 126.8, 125.4, 124.6, 120.8, 118.1, 116.4, 21.6. HRMS (ESI) calcd for $C_{35}H_{27}O_5NNaS_2$ $[M+Na]^+$ 628.1222; found: 628.1220.

(*E*)-1-(1-((4-(*tert*-butyl)phenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3i):



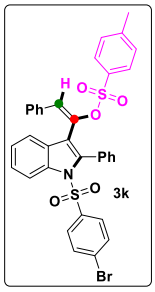
The title compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (40 mg, yield = 60%); Mp. 137-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.38 – 7.23 (m, 11H), 7.12 – 7.01 (m, 4H), 6.95 – 6.87 (m, 4H), 6.71 (d, *J* = 6.8 Hz, 1H), 6.62 (s, 1H), 2.32 (s, 3H), 1.24 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 144.6, 140.7, 139.4, 137.1, 135.3, 133.2, 132.8, 129.9, 129.0, 128.3, 128.2, 128.2, 127.9, 127.6, 127.2, 126.8, 126.5, 125.8, 125.2, 124.3, 120.7, 116.2, 35.2, 30.9, 21.5. HRMS (ESI) calcd for $C_{39}H_{35}O_5NNaS_2$ $[M+Na]^+$ 684.1848; found: 684.1846.

(*E*)-1-(1-((4-chlorophenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3j):



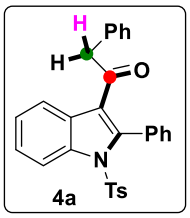
The title compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (42 mg, yield = 65%); Mp. 135-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.4 Hz, 1H), 7.42 – 7.32 (m, 3H), 7.32 – 7.24 (m, 8H), 7.17 – 7.07 (m, 4H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.92 (t, *J* = 7.8 Hz, 2H), 6.67 (d, *J* = 7.3 Hz, 2H), 6.65 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 140.7, 140.5, 138.8, 137.2, 136.0, 133.1, 132.6, 129.8, 129.3, 129.1, 129.0, 128.7, 128.3, 128.2, 128.2, 127.9, 127.8, 127.4, 126.9, 125.6, 124.9, 121.0, 118.6, 116.5, 21.56. HRMS (ESI) calcd for $C_{35}H_{26}O_5NClNaS_2$ $[M+Na]^+$ 662.0833; found: 662.0830.

(*E*)-1-(1-((4-bromophenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylvinyl 4-methylbenzenesulfonate (3k):



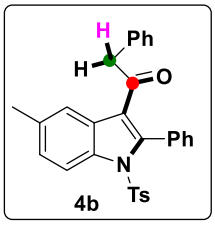
The title compound was prepared according to the general procedure A via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (47 mg, yield = 68%); Mp. 144-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.34 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 2H), 7.30 (s, 1H), 7.28 – 7.20 (m, 5H), 7.17 – 7.07 (m, 4H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.93 (t, *J* = 7.8 Hz, 2H), 6.67 (d, *J* = 7.4 Hz, 2H), 6.65 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 140.7, 138.8, 137.1, 136.5, 133.1, 132.6, 132.0, 129.8, 129.3, 129.2, 129.1, 128.7, 128.3, 128.3, 128.2, 127.9, 127.8, 127.4, 127.0, 125.6, 124.9, 121.0, 118.6, 116.5, 21.56. HRMS (ESI) calcd for $C_{35}H_{26}O_5NBrNaS_2$ $[M+Na]^+$ 706.0328; found: 706.0326.

2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (4a): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (38 mg, yield = 80%); Mp. 124-125 °C; ^{1}H NMR (400 MHz, $CDCl_3$)



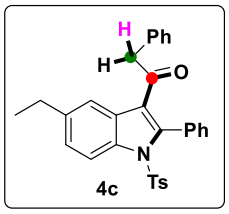
δ 8.37 (d, *J* = 8.4 Hz, 1H), 8.10 (d, *J* = 7.9 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.44 (ddd, *J* = 11.3, 8.6, 4.7 Hz, 3H), 7.38 – 7.28 (m, 5H), 7.22 – 7.14 (m, 3H), 7.10 (d, J = 8.4 Hz, 2H), 6.85 (d, J = 6.3 Hz, 2H), 3.30 (s, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.8, 145.4, 143.0, 136.3, 135.4, 134.2, 131.8, 130.5, 130.2, 129.6, 129.4, 128.2, 127.9, 126.9, 126.6, 125.9, 125.1, 122.9, 121.9, 115.1, 48.4, 21.6. HRMS (ESI) calcd for $C_{29}H_{23}O_3NNaS$ $[M+Na]^+$ 488.1290; found: 488.1290.

1-(5-methyl-2-phenyl-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4b): The title compound was prepared



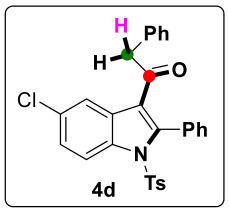
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (37 mg, yield = 75%); Mp. 156-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.6 Hz, 1H), 7.90 (s, 1H), 7.55 (ddd, *J* = 6.7, 4.0, 1.3 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.34 (d, *J* = 7.0 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.26 – 7.22 (m, 1H), 7.21 – 7.11 (m, 3H), 7.08 (d, J = 8.5 Hz, 2H), 6.86 (d, J = 6.3 Hz, 2H), 3.29 (s, 2H), 2.42 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 145.3, 143.1, 135.4, 134.9, 134.6, 134.2, 131.7, 130.6, 130.1, 129.5, 129.4, 128.2, 128.0, 127.8, 127.2, 126.9, 126.6, 122.8, 121.6, 114.8, 48.3, 21.5, 21.3. HRMS (ESI) calcd for $C_{30}H_{25}O_3NNaS$ $[M+Na]^+$ 502.1447; found: 502.1445.

1-(5-ethyl-2-phenyl-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4c): The title compound was prepared



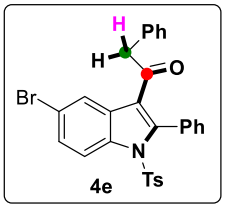
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (35 mg, yield = 70%); Mp. 103-104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.7 Hz, 1H), 7.94 (d, *J* = 1.2 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.49 – 7.44 (m, 2H), 7.35 – 7.26 (m, 5H), 7.22 – 7.12 (m, 3H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.86 (dd, *J* = 7.9, 1.6 Hz, 2H), 3.29 (s, 2H), 2.73 (q, *J* = 7.6 Hz, 2H), 2.34 (s, 3H), 1.26 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 145.3, 143.1, 141.4, 135.5, 134.7, 134.3, 131.8, 130.7, 130.2, 129.7, 129.4, 128.2, 128.0, 127.9, 127.0, 126.6, 126.3, 122.8, 120.6, 114.9, 48.4, 28.8, 21.6, 16.0. HRMS (ESI) calcd for $C_{31}H_{27}O_3NNaS$ $[M+Na]^+$ 516.1603; found: 516.1602.

1-(5-chloro-2-phenyl-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4d): The title compound was prepared



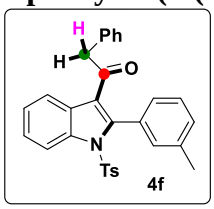
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (35 mg, yield = 69%); Mp. 161-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 9.0, 0.5 Hz, 1H), 8.16 (dd, *J* = 2.2, 0.5 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.50 – 7.45 (m, 2H), 7.39 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.33 (ddd, *J* = 7.4, 2.8, 1.6 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.22 – 7.14 (m, 3H), 7.12 (dd, *J* = 8.6, 0.7 Hz, 2H), 6.84 (dd, *J* = 7.8, 1.7 Hz, 2H), 3.27 (s, 2H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 145.7, 144.3, 135.2, 134.6, 133.9, 131.7, 131.0, 130.5, 130.0, 129.7, 129.4, 129.0, 128.3, 128.0, 127.0, 126.8, 126.2, 121.9, 121.8, 116.2, 48.24, 21.63. HRMS (ESI) calcd for $C_{29}H_{22}O_3NClNaS$ $[M+Na]^+$ 522.0901; found: 522.0900.

1-(5-bromo-2-phenyl-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4e): The title compound was prepared



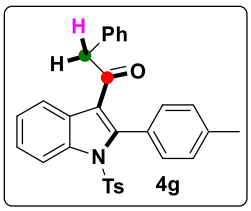
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (39 mg, yield = 70%); Mp. 147-148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.31 (m, 1H), 8.24 (d, *J* = 9.0 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.52 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.35 – 7.30 (m, 2H), 7.29 – 7.25 (m, 2H), 7.22 – 7.14 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.84 (dd, *J* = 7.8, 1.7 Hz, 2H), 3.27 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 145.7, 144.1, 135.2, 135.0, 133.9, 131.7, 130.5, 130.0, 129.7, 129.4, 129.4, 128.8, 128.3, 128.0, 127.0, 126.7, 124.8, 121.8, 118.8, 116.5, 48.2, 21.6. HRMS (ESI) calcd for $C_{29}H_{22}O_3NBrNaS$ $[M+Na]^+$ 566.0396; found: 566.0394.

2-phenyl-1-(2-(m-tolyl)-1-tosyl-indol-3-yl)ethan-1-one (4f): The title compound was prepared according to



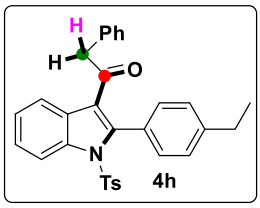
the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a colorless gummy compound (31 mg, yield = 63%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.41 – 7.31 (m, 4H), 7.28 – 7.11 (m, 6H), 6.99 (d, *J* = 6.7 Hz, 1H), 6.84 (d, *J* = 6.3 Hz, 2H), 3.33 – 3.22 (m, 2H), 2.35 (s, 3H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.2, 145.5, 142.9, 139.9, 136.2, 135.6, 134.2, 131.2, 130.5, 130.4, 130.2, 129.6, 129.4, 128.2, 127.9, 127.2, 126.6, 125.8, 125.2, 124.9, 122.3, 121.9, 114.8, 47.9, 21.6, 20.3. HRMS (ESI) calcd for $C_{30}H_{25}O_3NNaS$ $[M+Na]^+$ 502.1447; found: 502.1445.

2-phenyl-1-(2-(p-tolyl)-1-tosyl-indol-3-yl)ethan-1-one (4g): The title compound was prepared according to



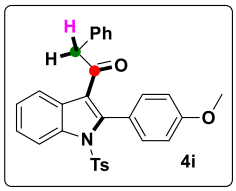
the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (35 mg, yield = 71%); Mp. 151-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 7.4 Hz, 1H), 7.42 (ddd, *J* = 8.6, 7.3, 1.4 Hz, 1H), 7.36 – 7.30 (m, 3H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.26 – 7.22 (m, 2H), 7.22 – 7.13 (m, 3H), 7.10 (d, *J* = 8.1 Hz, 2H), 6.87 (d, *J* = 6.3 Hz, 2H), 3.32 (s, 2H), 2.48 (s, 3H), 2.38 – 2.38 (m, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 145.3, 143.4, 140.5, 136.3, 135.4, 134.3, 131.6, 129.5, 129.4, 128.6, 128.2, 128.0, 127.5, 127.0, 126.6, 125.8, 125.0, 122.8, 121.9, 115.2, 48.4, 21.6, 21.6. HRMS (ESI) calcd for $C_{30}H_{25}O_3NNaS$ $[M+Na]^+$ 502.1447; found: 502.1445.

1-(2-(4-ethylphenyl)-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4h): The title compound was prepared



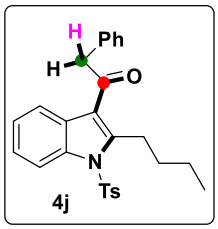
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (34 mg, yield = 69%); Mp. 126-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.4 Hz, 1H), 8.08 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.42 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.37 – 7.23 (m, 8H), 7.21 – 7.11 (m, 3H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.86 (dd, *J* = 7.8, 1.6 Hz, 2H), 3.31 (s, 2H), 2.78 (q, *J* = 7.6 Hz, 2H), 2.34 (s, 3H), 1.34 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 146.7, 145.3, 143.4, 136.4, 135.4, 134.3, 131.7, 129.5, 129.4, 128.2, 127.9, 127.6, 127.3, 127.0, 126.6, 125.8, 125.0, 122.8, 121.8, 115.2, 110.0, 48.3, 28.8, 21.6, 15.3. HRMS (ESI) calcd for $C_{31}H_{27}O_3NNaS$ $[M+Na]^+$ 516.1603; found: 516.1603.

1-(2-(4-methoxyphenyl)-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4i): The title compound was prepared



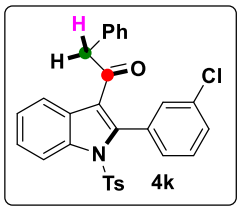
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (27 mg, yield = 53%); Mp. 131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.3 Hz, 1H), 8.07 (ddd, *J* = 7.9, 1.4, 0.7 Hz, 1H), 7.42 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.31 – 7.28 (m, 2H), 7.27 – 7.23 (m, 2H), 7.22 – 7.12 (m, 3H), 7.10 (s, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 6.88 (dd, *J* = 7.9, 1.6 Hz, 2H), 3.91 (s, 3H), 3.34 (s, 2H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 161.1, 145.3, 143.3, 136.4, 135.5, 134.3, 133.2, 129.5, 129.4, 128.2, 127.9, 126.9, 126.6, 125.8, 125.0, 122.3, 121.8, 115.2, 113.3, 55.4, 48.4, 21.6. HRMS (ESI) calcd for $C_{30}H_{25}O_4NNaS$ $[M+Na]^+$ 518.1396; found: 518.1394.

1-(2-butyl-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4j): The title compound was prepared according to the



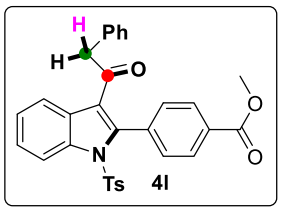
general procedure B via column chromatography of silica eluting hexane-ethyl acetate (94:6) to obtain as a white solid (20 mg, yield = 43%); Mp. 119-120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 5.6, 3.8 Hz, 1H), 7.85 (d, *J* = 9.2 Hz, 1H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.39 – 7.14 (m, 9H), 4.25 (s, 2H), 3.28 – 3.20 (m, 2H), 2.36 (s, 3H), 1.66 – 1.58 (m, 2H), 1.41 (dt, *J* = 14.9, 7.4 Hz, 2H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.1, 148.2, 145.3, 136.1, 136.0, 134.2, 130.0, 129.6, 128.5, 127.0, 126.9, 126.4, 124.6, 124.3, 120.5, 120.3, 115.1, 50.2, 33.2, 27.2, 22.9, 21.6, 13.7. HRMS (ESI) calcd for $C_{27}H_{27}O_3NNaS$ $[M+Na]^+$ 468.1603; found: 468.1601.

1-(2-(3-chlorophenyl)-1-tosyl-indol-3-yl)-2-phenylethan-1-one (4k): The title compound was prepared



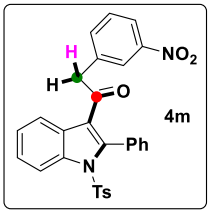
according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (35 mg, yield = 68%); Mp. 120-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.48 – 7.35 (m, 3H), 7.34 – 7.27 (m, 3H), 7.24 – 7.11 (m, 5H), 7.07 (s, 1H), 6.86 (d, *J* = 6.3 Hz, 2H), 3.38 (s, 2H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 145.7, 140.9, 136.5, 135.3, 133.8, 132.1, 131.5, 130.2, 130.1, 129.7, 129.3, 129.1, 128.4, 127.6, 126.9, 126.8, 126.2, 125.2, 123.0, 122.0, 115.2, 48.7, 21.6. HRMS (ESI) calcd for $C_{29}H_{23}O_3ClNS$ $[M+H]^+$ 500.1081; found: 500.1077.

methyl 4-(3-(2-phenylacetyl)-1-tosyl-indol-2-yl)benzoate (4l): The title compound was prepared according to

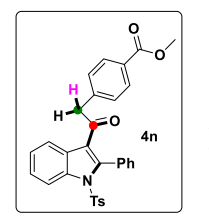


the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (37 mg, yield = 70%); Mp. 167-168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 2H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.41 (m, 3H), 7.39-7.35 (m, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 6.9 Hz, 3H), 7.12 (d, *J* = 8.5 Hz, 2H), 6.83 (dd, *J* = 7.2, 1.9 Hz, 2H), 4.00 (s, 3H), 3.33 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.4, 166.4, 145.7, 141.3, 136.4, 135.2, 135.2, 133.7, 131.8, 131.6, 129.7, 129.3, 128.9, 128.3, 127.8, 126.8, 126.8, 126.2, 125.3, 123.3, 122.0, 115.2, 52.5, 48.8, 21.6. HRMS (ESI) calcd for $C_{31}H_{26}O_5NS$ $[M+H]^+$ 524.1526; found: 524.1520.

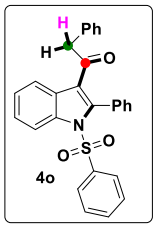
2-(3-nitrophenyl)-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one (4m): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (90:10) to obtain as a brown solid (37 mg, yield = 70%); Mp. 137-38 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.5 Hz, 1H), 8.19 – 8.12 (m, 1H), 8.02 (ddd, *J* = 8.2, 2.2, 1.0 Hz, 1H), 7.66 (s, 1H), 7.63 – 7.58 (m, 1H), 7.53 – 7.43 (m, 3H), 7.40 – 7.31 (m, 6H), 7.25 (dd, *J* = 4.5, 3.1 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 3.39 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.98, 147.9, 145.6, 143.6, 136.3, 136.1, 135.8, 135.4, 131.7, 130.5, 130.4, 129.7, 129.0, 128.1, 127.5, 127.0, 126.1, 125.2, 124.5, 122.2, 121.9, 121.8, 115.1, 47.5, 21.6. HRMS (ESI) calcd for $C_{29}H_{22}O_5N_2NaS$ $[M+Na]^+$ 533.1141; found: 533.1140.



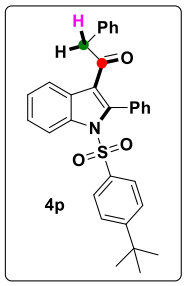
methyl 4-(2-oxo-2-(2-phenyl-1-tosyl-indol-3-yl)ethyl)benzoate (4n): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (91:9) to obtain as a white solid (41 mg, yield = 77%); Mp. 160-161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.4 Hz, 1H), 8.11 (dd, *J* = 7.9, 0.6 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.60 – 7.55 (m, 1H), 7.49 – 7.42 (m, 3H), 7.39 – 7.29 (m, 5H), 7.10 (d, *J* = 8.1 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H), 3.35 (s, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.8, 166.8, 145.5, 143.3, 139.5, 136.3, 135.4, 131.7, 130.4, 130.3, 129.6, 129.5, 129.4, 128.5, 127.9, 127.7, 126.9, 126.0, 125.1, 122.6, 121.9, 115.1, 52.0, 48.2, 21.6. HRMS (ESI) calcd for $C_{31}H_{25}O_5NNaS$ $[M+Na]^+$ 546.1345; found: 546.1344.



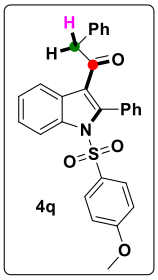
2-phenyl-1-(2-phenyl-1-(phenylsulfonyl)-indol-3-yl)ethan-1-one (4o): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (37 mg, yield = 80%); Mp. 155-156 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.11 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.59 – 7.49 (m, 2H), 7.48 – 7.29 (m, 10H), 7.22 – 7.12 (m, 3H), 6.85 (dd, *J* = 7.8, 1.7 Hz, 2H), 3.30 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.8, 142.9, 138.4, 136.4, 134.1, 131.8, 130.4, 130.3, 129.4, 129.0, 128.3, 127.9, 127.8, 126.9, 126.7, 126.0, 125.1, 123.0, 122.0, 115.1, 48.4. HRMS (ESI) calcd for $C_{28}H_{21}O_3NNaS$ $[M+Na]^+$ 474.1134; found: 474.1133.



1-(1-((4-(tert-butyl)phenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4p): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (32 mg, yield = 63%); Mp. 168-169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.10 (dd, *J* = 8.0, 0.7 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.48 – 7.41 (m, 3H), 7.38 – 7.29 (m, 7H), 7.21 – 7.11 (m, 3H), 6.86 (dd, *J* = 7.8, 1.6 Hz, 2H), 3.30 (s, 2H), 1.26 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 158.3, 142.9, 136.4, 135.4, 134.2, 131.8, 130.6, 130.2, 129.4, 128.2, 127.9, 127.8, 126.9, 126.7, 126.0, 125.9, 125.0, 122.8, 121.2, 115.1, 48.4, 35.3, 30.9. HRMS (ESI) calcd for $C_{32}H_{29}O_3NNaS$ $[M+Na]^+$ 530.1760; found: 530.1759.

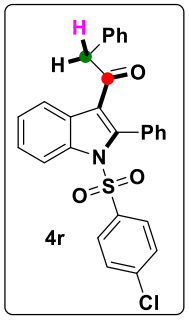


1-(1-((4-methoxyphenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4q): The title compound was



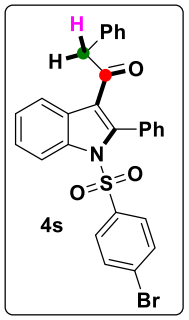
prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (24 mg, yield = 48%); Mp. 168-169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, J = 8.4 Hz, 1H), 8.10 (dd, J = 7.9, 0.7 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.50 – 7.41 (m, 3H), 7.39 – 7.32 (m, 5H), 7.22 – 7.11 (m, 3H), 6.85 (dd, J = 7.8, 1.6 Hz, 2H), 6.75 (d, J = 9.1 Hz, 2H), 3.79 (s, 3H), 3.30 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.80, 164.01, 142.96, 136.35, 134.21, 131.77, 130.62, 130.19, 129.89, 129.37, 129.27, 128.23, 127.86, 126.64, 125.84, 125.00, 122.78, 121.91, 115.14, 114.14, 77.31, 76.99, 76.67, 55.67, 48.41. HRMS (ESI) calcd for $C_{32}H_{29}O_3NNaS$ $[M+Na]^+$ 530.1760; found: 530.1759.

1-(1-((4-chlorophenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4r): The title compound was



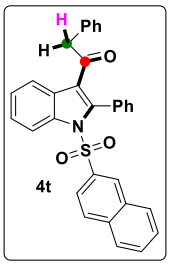
prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (33 mg, yield = 66%); Mp. 126-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.4 Hz, 1H), 8.09 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.50 – 7.42 (m, 3H), 7.41 – 7.26 (m, 7H), 7.22 – 7.10 (m, 3H), 6.85 (dd, *J* = 7.7, 1.7 Hz, 2H), 3.31 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 142.6, 141.0, 136.7, 136.3, 134.0, 131.8, 130.4, 130.2, 129.3, 128.3, 128.3, 128.0, 127.9, 126.7, 126.2, 125.3, 122.1, 115.1, 48.5. HRMS (ESI) calcd for $C_{28}H_{20}O_3NClNaS$ $[M+Na]^+$ 508.0744; found: 508.0743.

1-(1-((4-bromophenyl)sulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4s): The title compound was



prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to obtain as a white solid (38 mg, yield = 70%); Mp. 143-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1H NMR (400 MHz, CDCl3) δ 8.34 (d, *J* = 8.4 Hz, 1H), 8.12 – 8.07 (m, 1H), 7.60 – 7.55 (m, 1H), 7.50 – 7.42 (m, 5H), 7.40 – 7.31 (m, 3H), 7.27 – 7.23 (m, 2H), 7.22 – 7.12 (m, 3H), 6.85 (dd, *J* = 7.7, 1.7 Hz, 2H), 3.31 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 142.6, 137.2, 136.3, 134.0, 132.3, 131.8, 130.4, 130.2, 129.6, 129.3, 128.3, 128.3, 128.0, 127.9, 126.7, 126.2, 125.4, 123.3, 122.1, 115.1, 48.5. HRMS (ESI) calcd for $C_{28}H_{20}O_3NBrNaS$ $[M+Na]^+$ 552.0239; found: 552.0239.

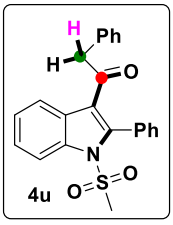
1-(1-(naphthalen-2-ylsulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4t): The title compound was



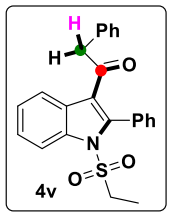
prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (89:10) to obtain as a white solid (38 mg, yield = 75%); Mp. 140-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.5 Hz, 1H), 8.12 (dd, J = 8.0, 0.6 Hz, 1H), 7.86 (d, *J* = 1.9 Hz, 1H), 7.83 – 7.80 (m, 1H), 7.74 (dd, *J* = 8.5, 2.6 Hz, 2H), 7.65 – 7.52 (m, 3H), 7.47 (ddd, *J* = 8.6, 7.3, 1.4 Hz, 1H), 7.42 – 7.34 (m, 4H), 7.26 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.20 – 7.09 (m, 3H), 6.86 – 6.79 (m, 2H), 3.28 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.6, 142.9, 136.5, 135.3, 135.1, 134.1, 131.9, 131.4, 130.3, 130.3, 129.6, 129.5, 129.4, 129.3, 129.3, 128.2, 127.9, 127.8, 127.8, 127.7, 126.6, 126.0,

125.1, 122.8, 122.0, 121.1, 115.1, 48.4. HRMS (ESI) calcd for $C_{32}H_{23}O_3NNaS$ $[M+Na]^+$ 524.1290; found: 524.1289.

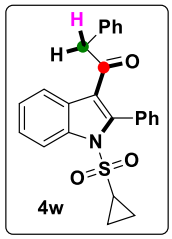
1-(1-(methylsulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4u): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (27 mg, yield = 68%); Mp. 168-169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.19 (m, 1H), 8.13 – 8.10 (m, 1H), 7.62 – 7.49 (m, 5H), 7.46 – 7.38 (m, 2H), 7.24 – 7.13 (m, 3H), 6.90 (dd, *J* = 7.9, 1.5 Hz, 2H), 3.39 (s, 2H), 2.95 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.5, 142.8, 135.9, 134.1, 131.1, 130.6, 130.4, 129.4, 128.3, 128.3, 127.9, 126.7, 126.1, 125.3, 122.7, 122.4, 114.4, 48.6, 41.8. HRMS (ESI) calcd for $C_{23}H_{19}O_3NNaS$ $[M+Na]^+$ 412.0977; found: 412.0975.



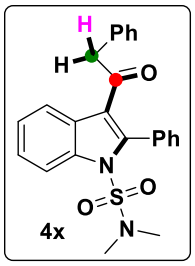
1-(1-(ethylsulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4v): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (25 mg, yield = 60%); Mp. 178-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.17 (m, 1H), 8.14 – 8.08 (m, 1H), 7.65 – 7.47 (m, 5H), 7.44 – 7.36 (m, 2H), 7.24 – 7.13 (m, 3H), 6.94 – 6.86 (m, 2H), 3.38 (s, 2H), 3.13 (q, *J* = 7.4 Hz, 2H), 1.12 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.6, 143.4, 136.2, 134.1, 131.3, 130.6, 130.3, 129.4, 128.3, 128.2, 127.6, 126.7, 126.0, 125.1, 122.3, 114.3, 114.3, 114.3, 49.5, 48.5, 7.6. HRMS (ESI) calcd for $C_{24}H_{21}O_3NNaS$ $[M+Na]^+$ 426.1134; found: 426.1131.



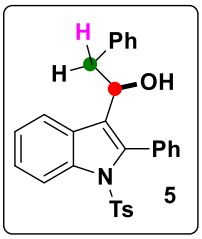
1-(1-(cyclopropylsulfonyl)-2-phenyl-indol-3-yl)-2-phenylethan-1-one (4w): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (93:7) to obtain as a white solid (28 mg, yield = 65%); Mp. 182-183 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.17 (m, 1H), 8.17 – 8.12 (m, 1H), 7.61 – 7.47 (m, 5H), 7.43 – 7.36 (m, 2H), 7.24 – 7.13 (m, 3H), 6.90 (dd, *J* = 7.9, 1.5 Hz, 2H), 3.38 (s, 2H), 2.45 (tt, *J* = 8.0, 4.8 Hz, 1H), 1.21 – 1.08 (m, 2H), 0.97 – 0.83 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 143.0, 136.2, 134.2, 131.5, 130.8, 130.3, 129.4, 128.3, 128.1, 127.8, 126.7, 125.9, 125.0, 122.5, 122.1, 114.5, 48.5, 32.1, 6.1. HRMS (ESI) calcd for $C_{25}H_{21}O_3NNaS$ $[M+Na]^+$ 438.1134; found: 438.1131.



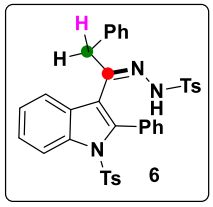
N,N-dimethyl-2-phenyl-3-(2-phenylacetyl)-indole-1-sulfonamide (4x): The title compound was prepared according to the general procedure B via column chromatography of silica eluting hexane-ethyl acetate (92:8) to as a white solid (26 mg, yield = 60%); Mp. 124-125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.15 (m, 2H), 7.56 – 7.52 (m, 4H), 7.44 – 7.31 (m, 3H), 7.23 – 7.14 (m, 4H), 6.94 – 6.88 (m, 2H), 3.34 (s, 2H), 2.50 (d, *J* = 1.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 131.4, 131.4, 130.1, 129.4, 129.0, 129.0, 128.2, 128.1, 128.0, 127.8, 126.6, 125.5, 124.5, 121.9, 114.9, 48.5, 37.4. HRMS (ESI) calcd for $C_{24}H_{22}O_3NNaS$ $[M+Na]^+$ 441.1243; found: 441.1241.



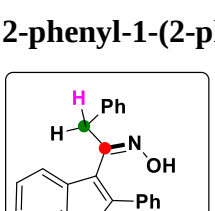
2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-ol (5): The title compound was prepared according to the procedure C via column chromatography of silica eluting hexane-ethyl acetate (86:14) to obtain as a white solid (66 mg, yield = 93%); Mp. 160-161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.30 (m, 4H), 7.30 – 7.11 (m, 6H), 7.08 (t, *J* = 7.5 Hz, 4H), 6.80 (d, *J* = 7.0 Hz, 2H), 6.27 (s, 1H), 4.63 (t, *J* = 6.7 Hz, 1H), 3.20 – 3.08 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 137.6, 137.2, 137.0, 135.5, 131.2, 130.2, 129.4, 129.4, 128.7, 128.3, 128.0, 127.2, 126.8, 126.3, 124.9, 123.8, 123.4, 121.3, 115.8, 69.7, 43.3, 21.5. HRMS (ESI) calcd for $C_{29}H_{25}O_3NNaS$ $[M+Na]^+$ 490.1447; found: 490.1445.



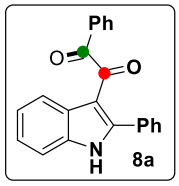
4-methyl-N'-(2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethylidene)benzenesulfonohydrazide (6): The title compound was prepared according to the procedure D via column chromatography of silica eluting hexane-ethyl acetate (85:15) to obtain as a white solid (39 mg, yield = 41%); Mp. 131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.5 Hz, 1H), 7.74 (s, 1H), 7.45 (ddd, *J* = 8.8, 4.8, 3.0 Hz, 3H), 7.37 – 7.27 (m, 7H), 7.26 – 7.17 (m, 3H), 7.16 – 7.11 (m, 2H), 7.06 (d, *J* = 8.1 Hz, 2H), 7.04 – 6.98 (m, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 7.1 Hz, 2H), 3.12 (s, 2H), 2.51 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.7, 145.2, 144.2, 139.5, 136.6, 135.2, 135.2, 133.8, 131.9, 130.5, 129.7, 129.5, 129.4, 128.3, 127.7, 127.6, 127.4, 126.9, 125.4, 124.1, 121.8, 121.0, 115.5, 35.7, 21.7, 21.6. HRMS (ESI) calcd for $C_{36}H_{31}O_4N_3NaS_2$ $[M+Na]^+$ 656.1648; found: 656.1644.



2-phenyl-1-(2-phenyl-1-tosyl-indol-3-yl)ethan-1-one oxime (7): The title compound was prepared according to the procedure E via column chromatography of silica eluting hexane-ethyl acetate (80:20) to obtain as a white solid (62 mg, yield = 85%); Mp. 159-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (brs, 1H), 8.30 (d, J = 8.4 Hz, 1H), 7.54 (dd, *J* = 7.9, 0.5 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.38 – 7.30 (m, 3H), 7.28 – 7.22 (m, 3H), 7.17 (dt, *J* = 8.4, 1.6 Hz, 2H), 7.09 – 6.99 (m, 5H), 6.79 (dd, *J* = 7.4, 2.1 Hz, 2H), 3.51 (s, 2H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.6, 144.8, 139.0, 136.8, 135.8, 135.1, 131.6, 130.5, 129.4, 129.1, 128.7, 128.2, 127.3, 126.8, 126.2, 125.3, 124.4, 120.3, 119.4, 115.8, 33.3, 21.5. HRMS (ESI) calcd for $C_{29}H_{24}O_3N_2NaS$ $[M+Na]^+$ 503.1399; found: 503.1398.



1-phenyl-2-(2-phenyl-1H-indol-3-yl)ethane-1,2-dione (8a)[2]: The title compound was prepared according to the procedure F via column chromatography of silica eluting hexane-ethyl acetate (86:14) to obtain as a pale-yellow solid (10 mg, yield = 20%); Mp. 198-199 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (brs, 1H), 8.17 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.64 (m, 3H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.50-7.46 (m, 2H), 7.40 – 7.28 (m, 5H), 7.23-7.19 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 193.6, 190.3, 148.7, 136.0, 134.2, 133.1, 130.5, 130.1, 129.7, 129.2, 128.8, 127.9, 126.8, 123.8, 122.9, 121.0, 112.3, 110.2. HRMS (ESI) calcd for $C_{22}H_{15}O_2NNa$ $[M+Na]^+$ 348.0995; found: 348.0993.



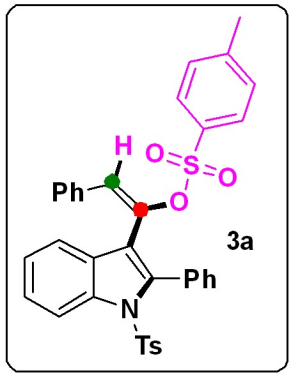
7. References

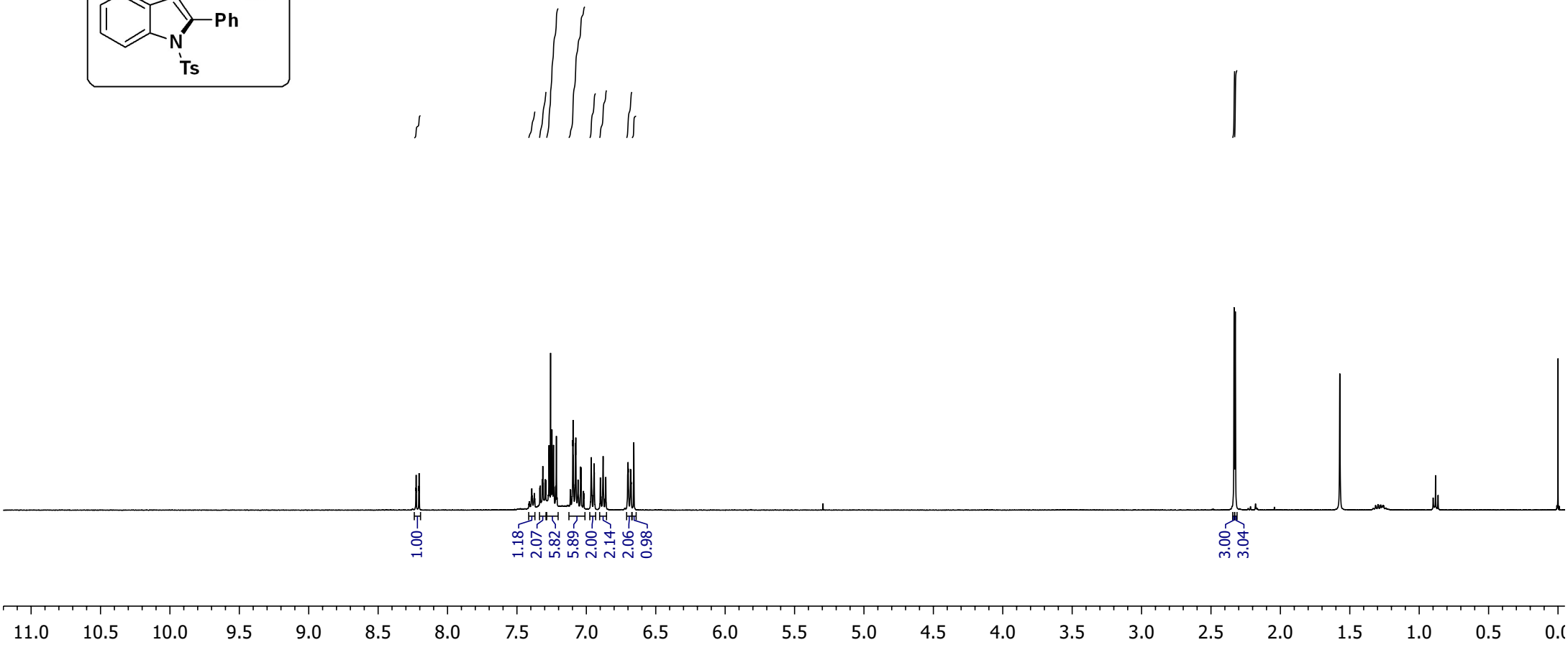
1. M. R. Mutra, J.-J Wang, *Nat. Commun*., 2022, **13**, 2345.

2. R.-Y. Tang, X.-K. Guo, J.-N. Xiang, and J.-H. Li, *J. Org. Chem*., 2013, **78**, 11163−11171.

8.23 8.21 7.41 7.41 7.39 7.37 7.37 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 7.23 7.22 7.22 7.21 7.12 7.11 7.10 7.10 7.09 7.08 7.08 7.06 7.04 7.04 7.04 7.04 7.02 7.02 7.02 7.02 6.96 6.94 6.90 6.90 6.88 6.86 6.86 6.70 6.68 6.66

Solvent	$CDCl_3$
Spectrometer Frequency	400.39
Nucleus	^1H





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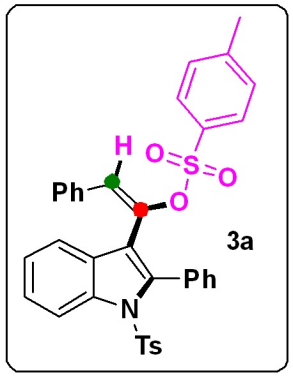
77.31 76.99 76.67

21.58 21.54

Solvent $CDCl_3$

Spectrometer Frequency 100.69

Nucleus ^{13}C



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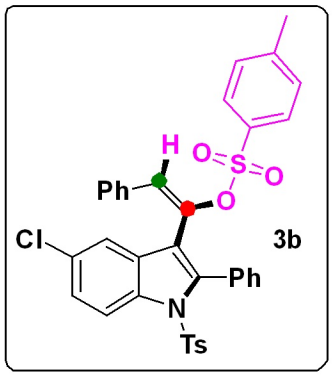
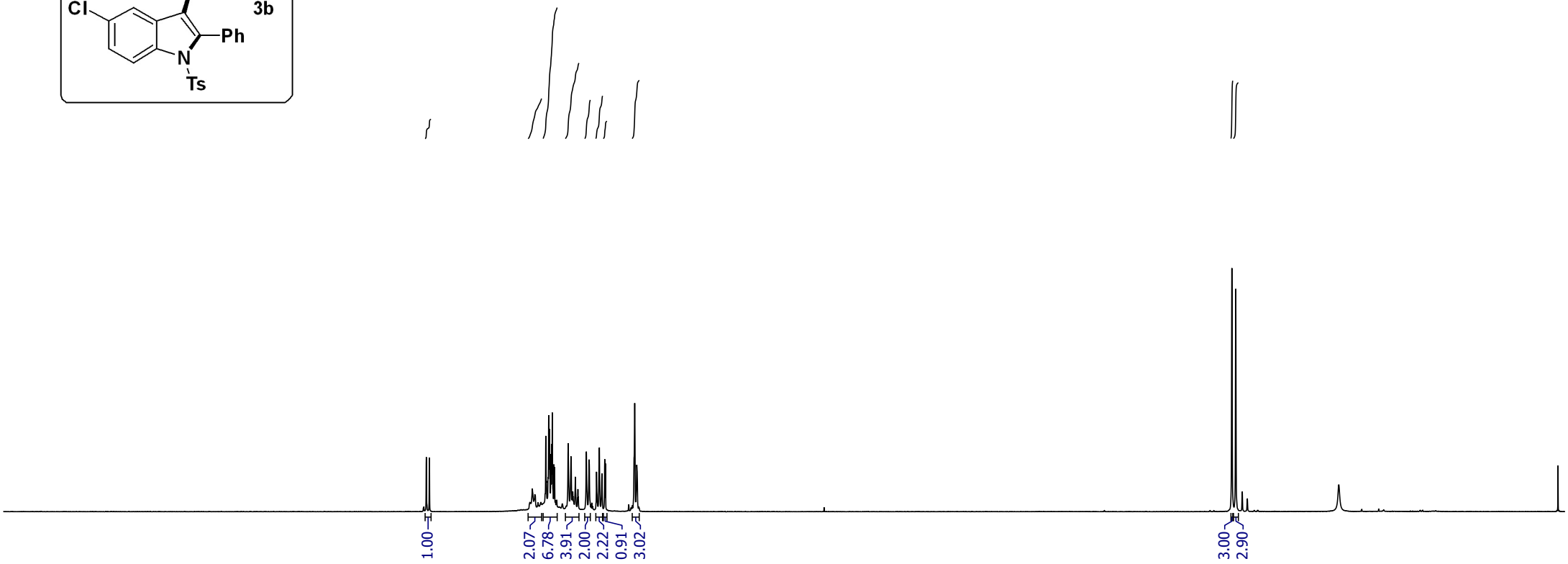
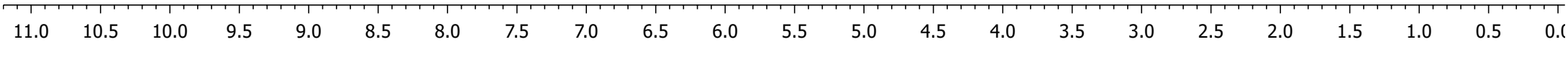
Solvent	$CDCl_3$
Spectrometer Frequency	400.39
Nucleus	^1H







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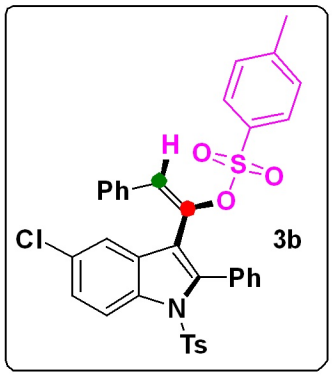
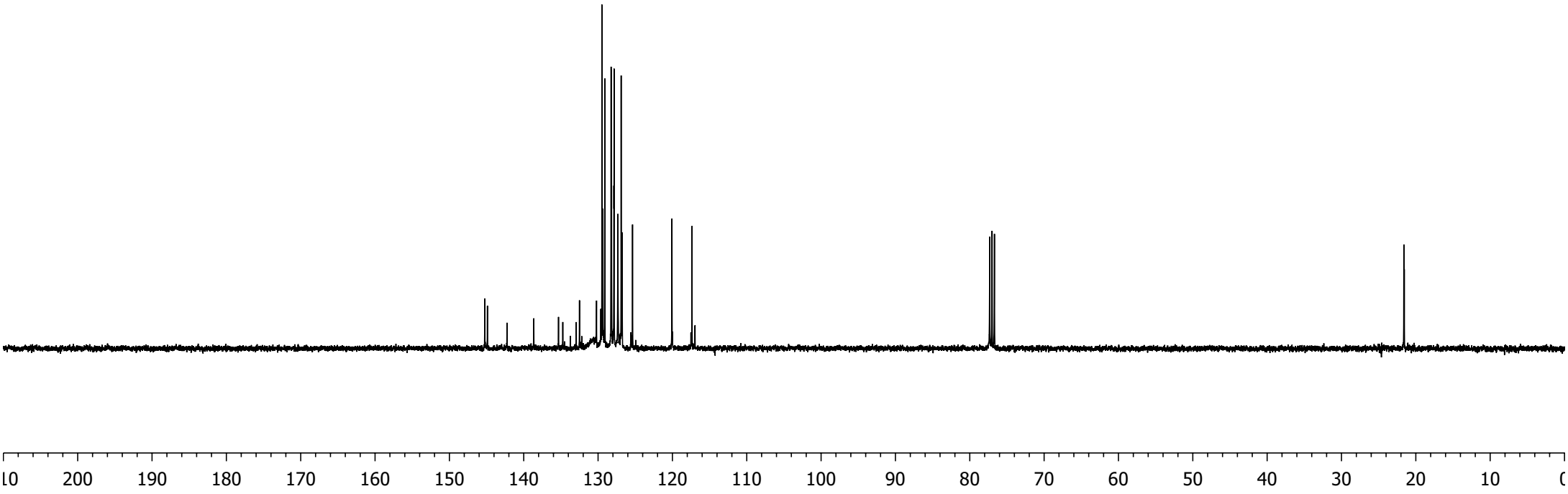
Spectrometer Frequency 100.66
Nucleus ^{13}C





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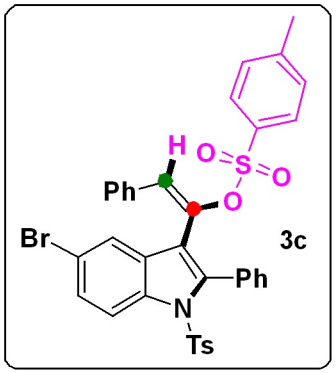
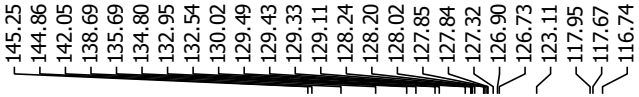
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



1.01 3.07 5.08 1.05 4.02 0.95 2.05 2.28 3.00 3.05 2.98

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0



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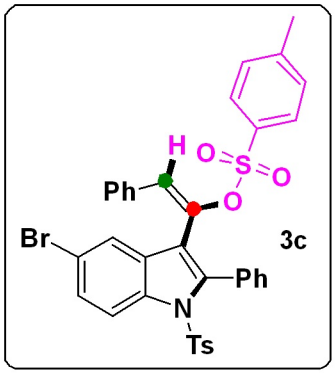
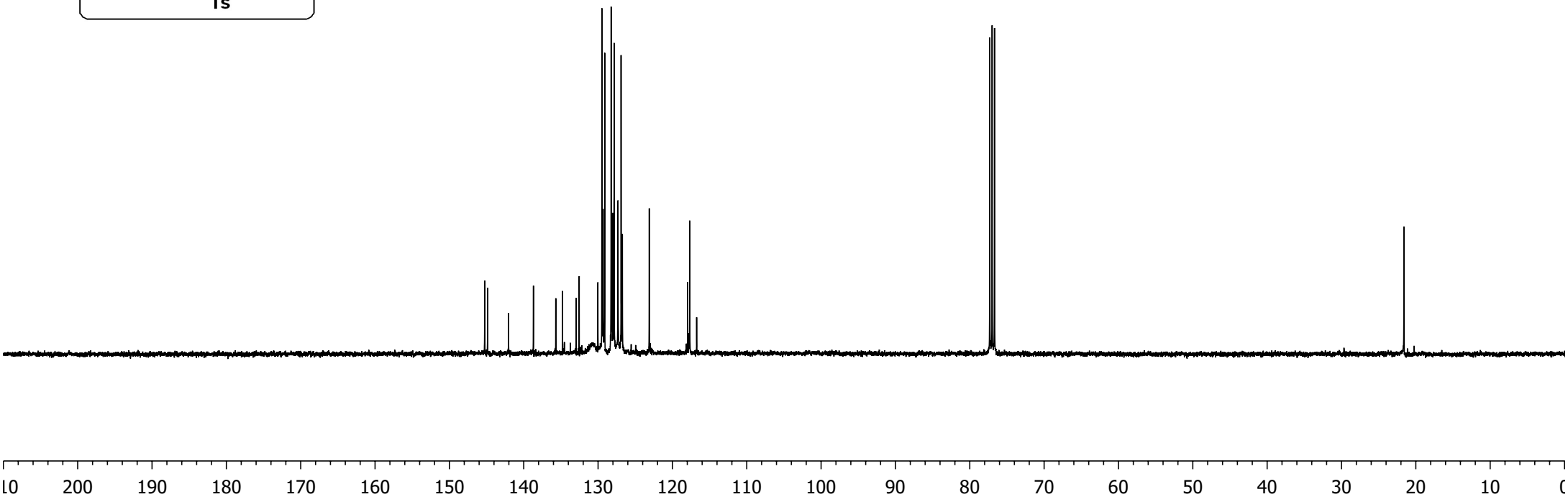
Spectrometer Frequency 100.69

Nucleus ^{13}C





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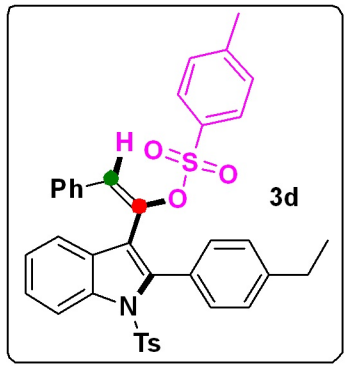
Spectrometer Frequency 400.39
Nucleus ^1H



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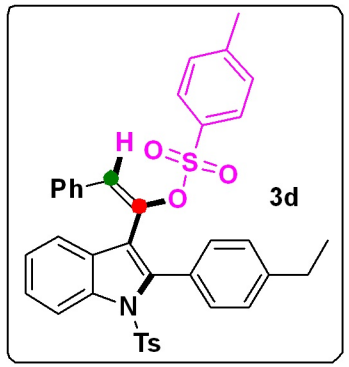
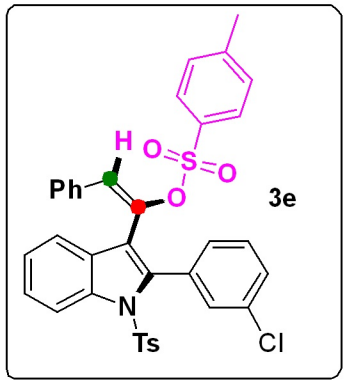
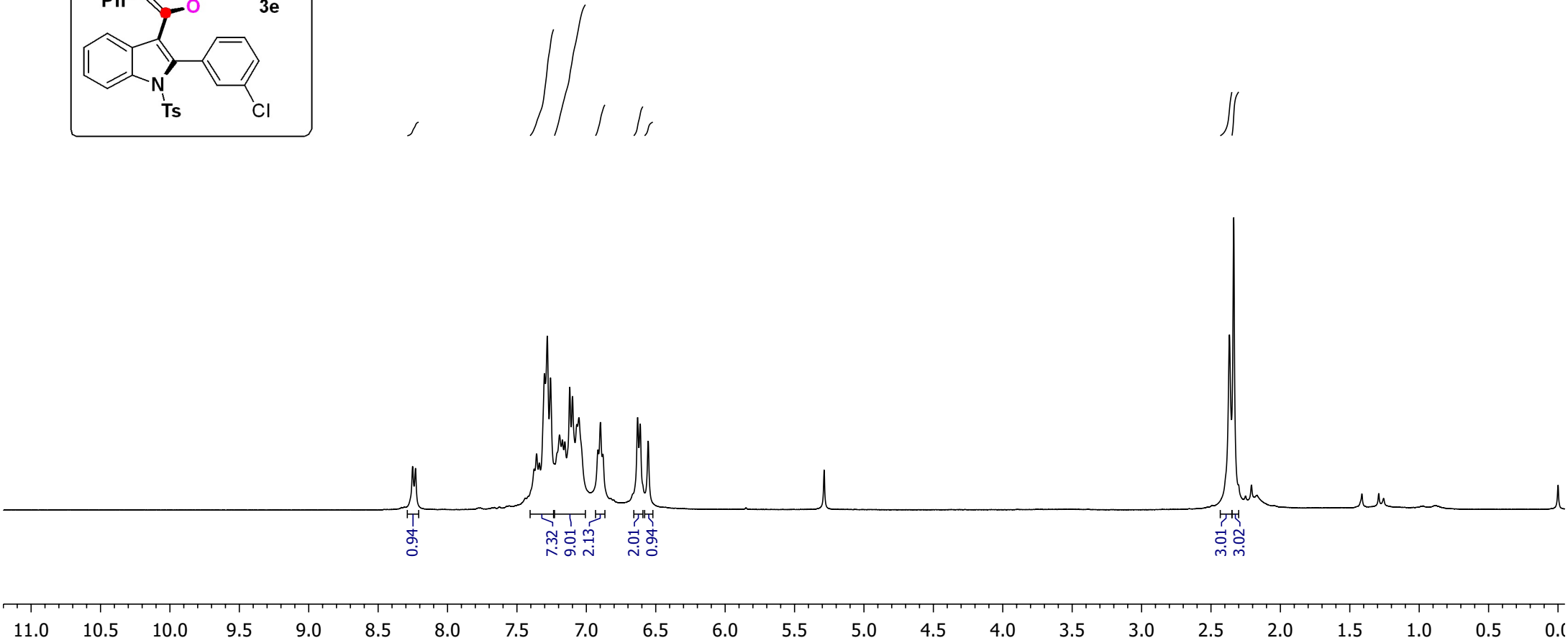
Spectrometer Frequency 100.69
Nucleus ^{13}C



8.25 8.23 7.38 7.36 7.34 7.30 7.28 7.26 7.19 7.17 7.15 7.12 7.10 7.07 7.05 6.92 6.90 6.88 6.63 6.61 6.55 2.37 2.34

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H





145.10
144.86
139.06
138.79
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134.87
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132.94
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131.65
129.45
129.23
128.94
128.41
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127.78
126.81
126.61
125.64
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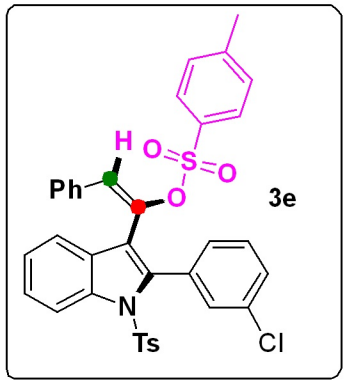
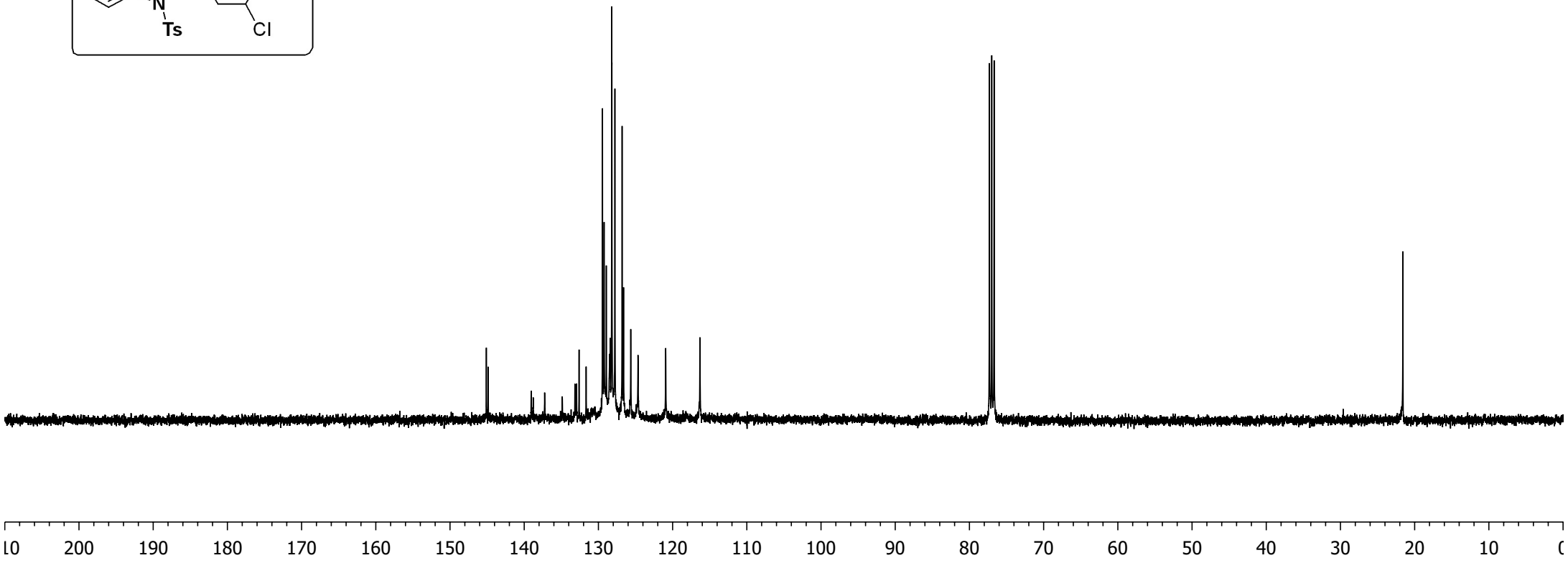
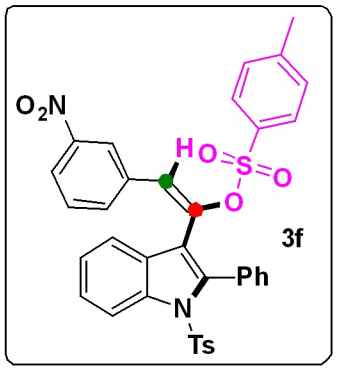
77.31
76.99
76.67
21.58

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



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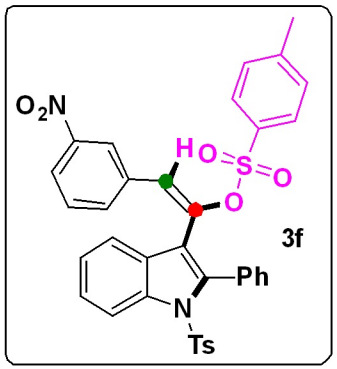
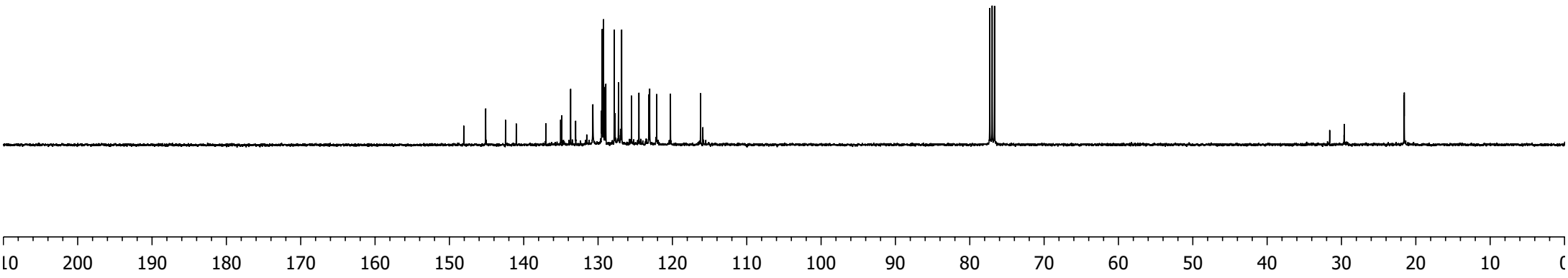
Nucleus ^{13}C





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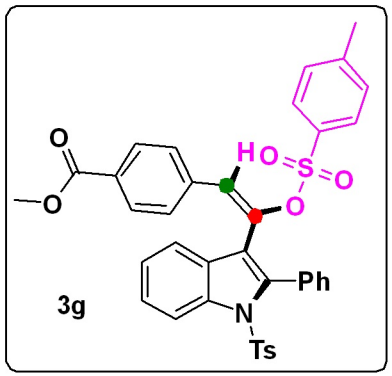
Spectrometer Frequency 400.39
Nucleus ^1H



166.36
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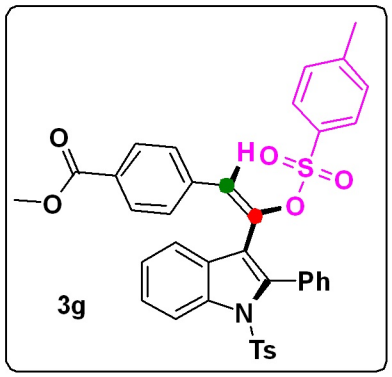
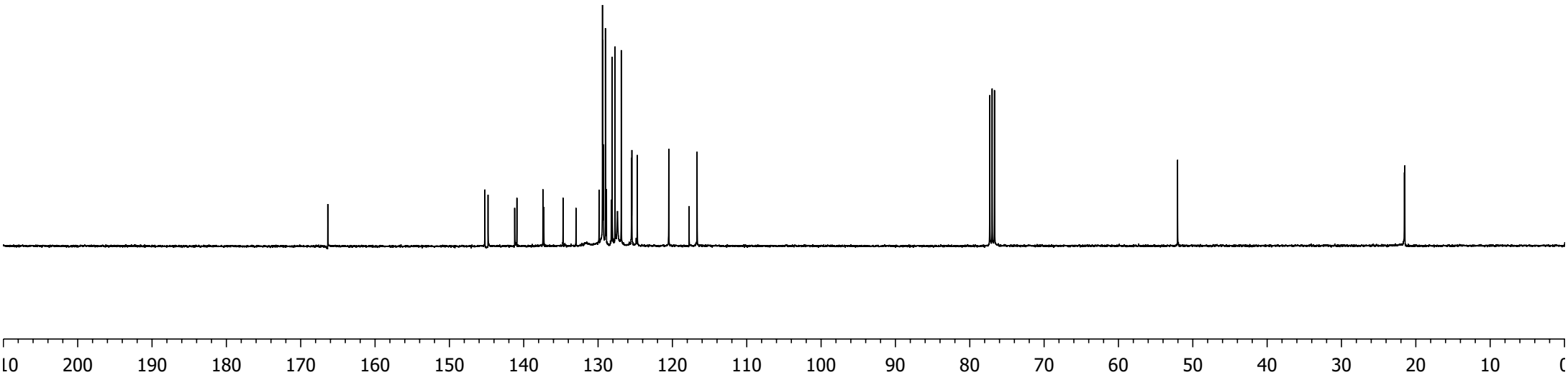
144.80
141.22
140.92
137.41
137.29
134.72
132.97
129.87
129.41
129.38
129.30
129.02
128.87
128.23
128.10
127.72
127.39
126.88
125.50
125.45
124.73
120.49
117.76
116.68
77.31
76.99
76.67
52.05
21.53
21.47

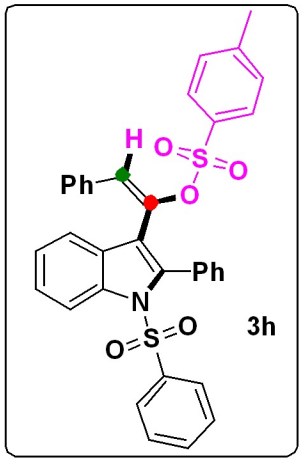
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





8.24 8.22 7.53 7.51 7.51 7.51 7.49 7.39 7.39 7.38 7.37 7.37 7.34 7.34 7.33 7.32 7.31 7.30 7.29 7.28 7.26 7.25 7.24 7.23 7.22 7.12 7.12 7.10 7.10 7.09 7.08 7.07 7.05 7.05 7.05 7.03 7.03 6.97 6.95 6.91 6.89 6.87 6.69 6.67 6.65 2.33

Solvent	$CDCl_3$
Spectrometer Frequency	400.39
Nucleus	^1H



1.00 1.10 11.02 1.82 1.95 1.96 2.14 2.01 0.94 2.97

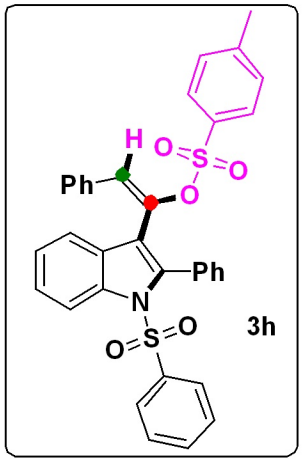
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

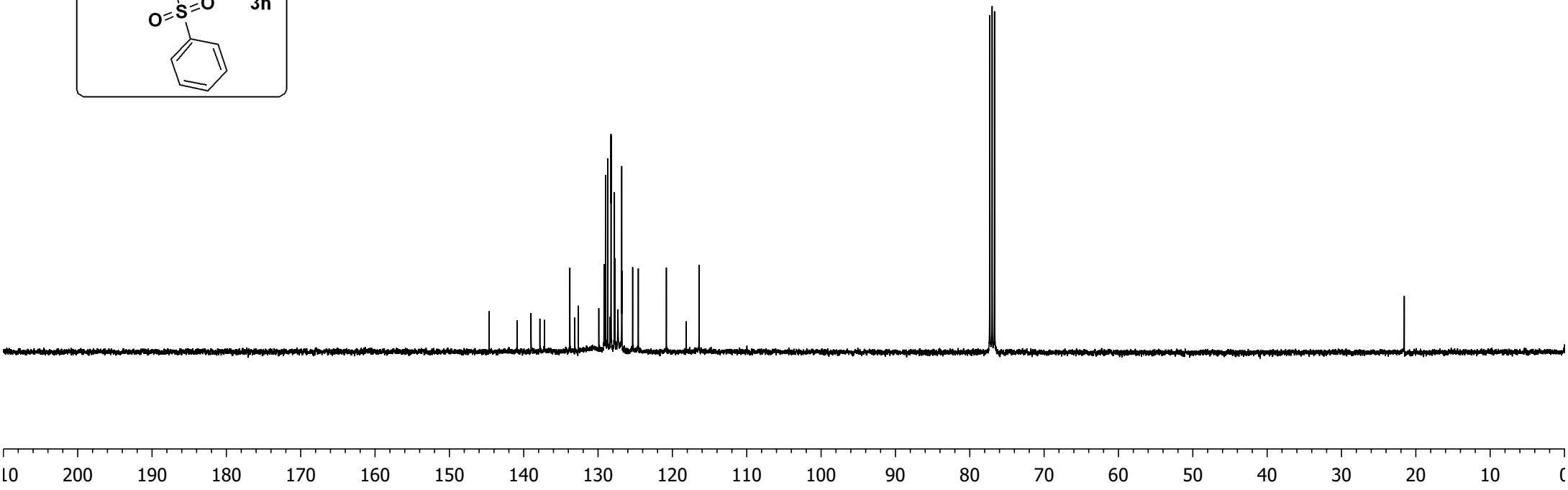
144.65
140.89
139.02
137.83
137.22
133.79
133.13
132.67
129.90
129.20
129.00
128.71
128.40
128.26
128.24
127.80
127.72
127.33
126.82
126.78
125.35
124.59
120.81
118.14
116.41

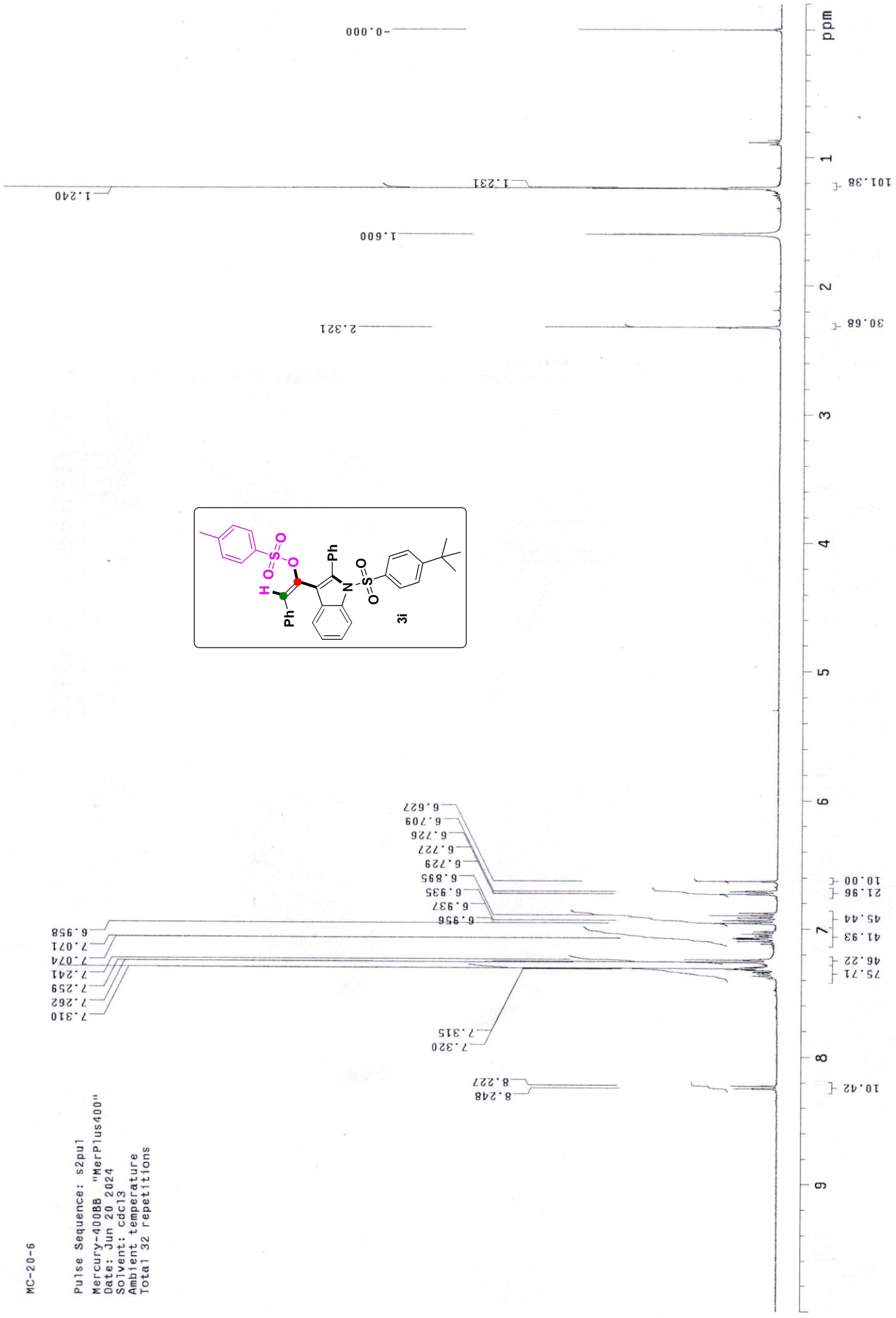
77.31
76.99
76.67

21.55

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C






MC-20-6
Pulse Sequence: s2pul
Mercury-400BB "MerPlus400"
Date: Jun 20 2024
Solvent: cdcl3
Ambient temperature
Total 32 repetitions
ppm
3i
-0.000
1.231
1.240
1.600
2.321
6.627
6.709
6.726
6.727
6.729
6.895
6.935
6.937
6.956
6.958
7.071
7.074
7.241
7.259
7.262
7.310
7.315
7.320
8.227
8.248
101.38
30.68
10.00
21.96
45.44
41.93
46.22
75.71
10.42

157.80 144.63 140.73 139.39 137.06 135.31 133.21 132.82 129.90 129.02 128.31 128.23 128.18 127.85 127.60 127.22 126.79 126.45 125.78 125.22 124.32 120.71 116.16

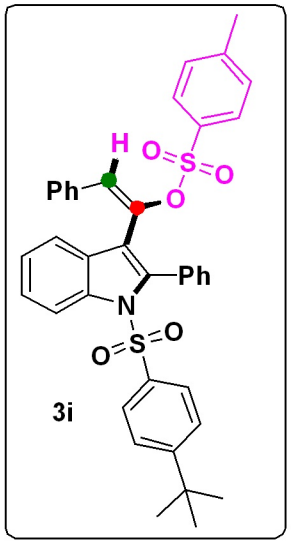
77.31 76.99 76.67

35.22 30.93 21.53

Solvent $CDCl_3$

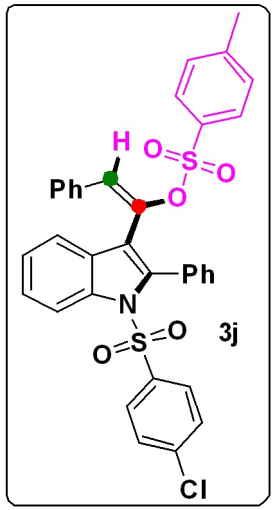
Spectrometer Frequency 100.69

Nucleus ^{13}C



8.21 8.19 7.40 7.38 7.36 7.36 7.35 7.34 7.34 7.33 7.32 7.31 7.30 7.29 7.28 7.28 7.28 7.27 7.27 7.26 7.26 7.26 7.25 7.25 7.25 7.15 7.15 7.13 7.13 7.11 7.11 7.11 7.11 7.11 7.09 7.09 7.07 7.01 6.99 6.94 6.92 6.90 6.68 6.66 6.65 2.34

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

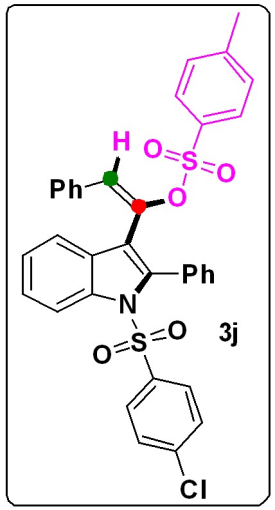


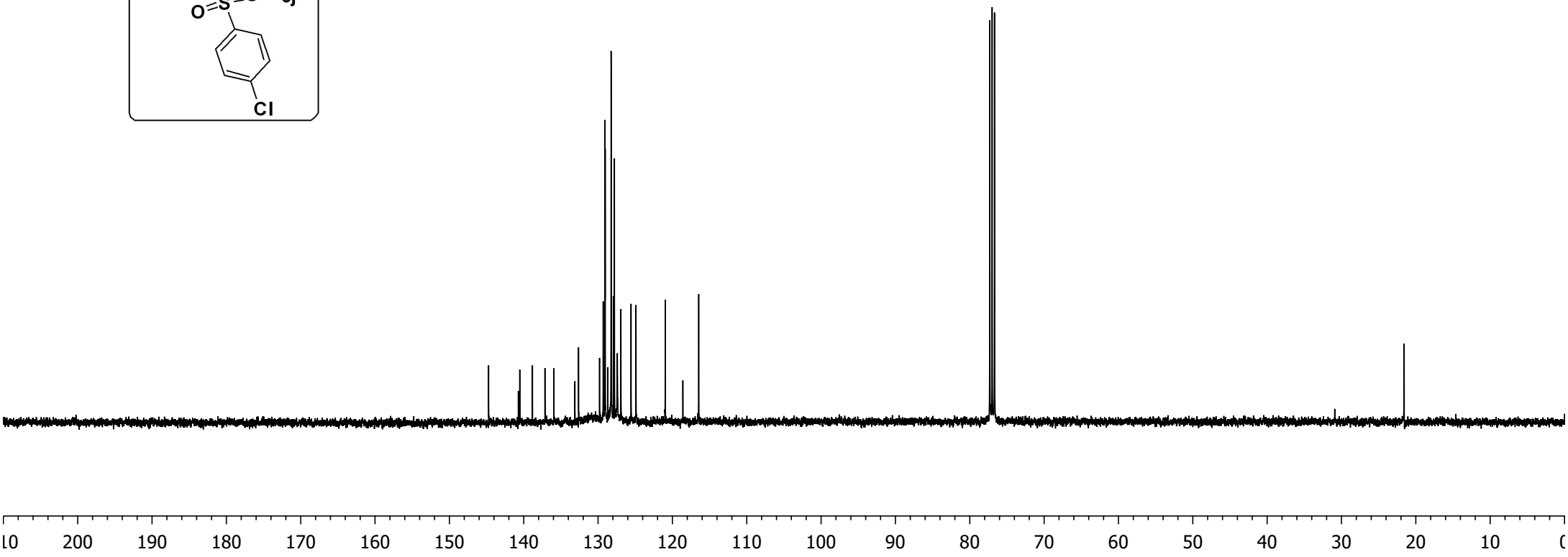
144.73
140.73
140.53
138.83
137.15
135.96
133.12
132.63
129.80
129.31
129.06
129.04
128.69
128.25
128.24
128.19
127.92
127.80
127.41
126.93
125.57
124.90
120.96
118.59
116.46

77.31
76.99
76.68

21.56

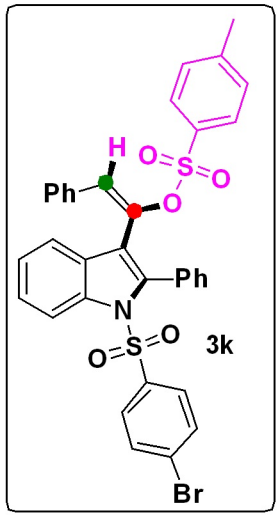
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





8.21 8.19 7.44 7.42 7.40 7.38 7.36 7.36 7.35 7.34 7.34 7.32 7.32 7.30 7.27 7.27 7.26 7.25 7.23 7.23 7.22 7.21 7.20 7.20 7.17 7.16 7.15 7.14 7.13 7.13 7.11 7.11 7.10 7.09 7.08 7.08 7.01 6.99 6.95 6.93 6.91 6.68 6.66 6.65 2.34

Solvent	$CDCl_3$
Spectrometer Frequency	400.39
Nucleus	^1H



0.99 2.13 1.01 1.77 0.89 5.19 3.98 2.01 2.20 2.01 0.93 3.00

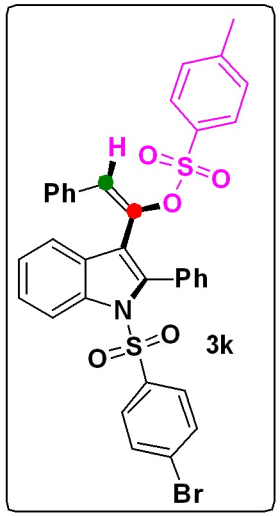
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

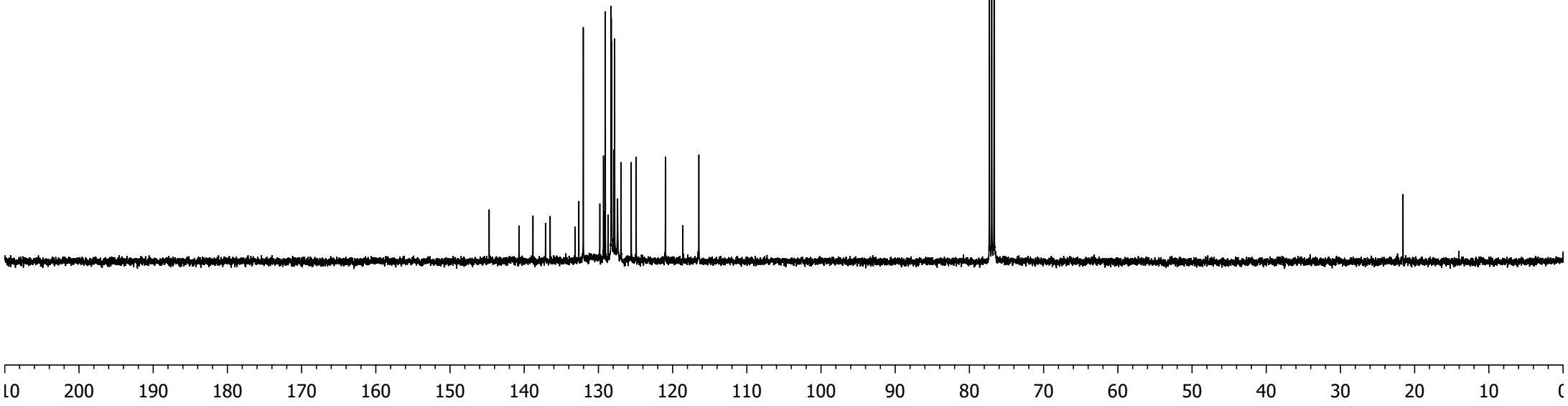
144.72
140.71
138.81
137.14
136.50
133.13
132.63
132.03
129.81
129.32
129.18
129.07
128.71
128.29
128.26
128.19
127.93
127.80
127.42
126.95
125.58
124.91
120.97
118.62
116.46

77.31
76.99
76.67

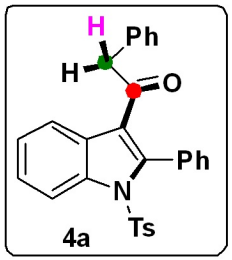
21.56

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





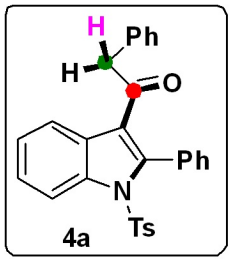
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



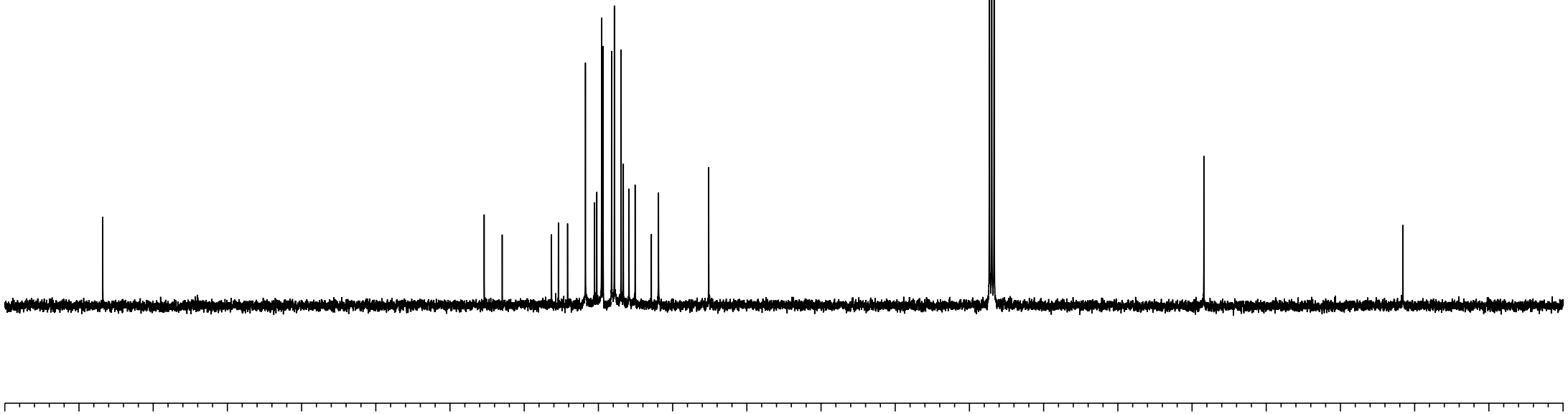
M0106-6
MC-18-2

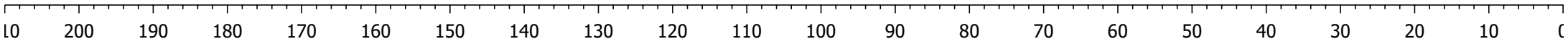
196.80
145.40
142.97
131.75
130.21
129.58
129.36
128.23
127.85
126.93
126.64
125.88
125.05
115.14
77.31
76.99
76.67
48.40
21.58

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C



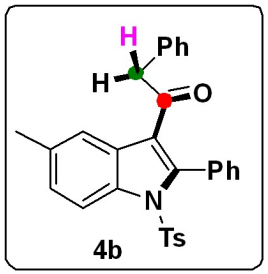
4a





8.24 8.22 7.90 7.57 7.56 7.55 7.55 7.54 7.53 7.53 7.48 7.46 7.44 7.35 7.34 7.30 7.28 7.25 7.25 7.25 7.23 7.23 7.22 7.20 7.20 7.19 7.18 7.16 7.16 7.15 7.15 7.14 7.09 7.07 6.86 6.85 3.29 2.42 2.32

Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H



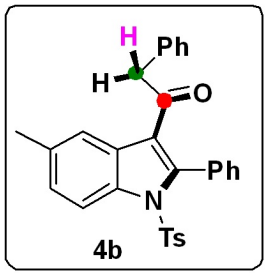
4b

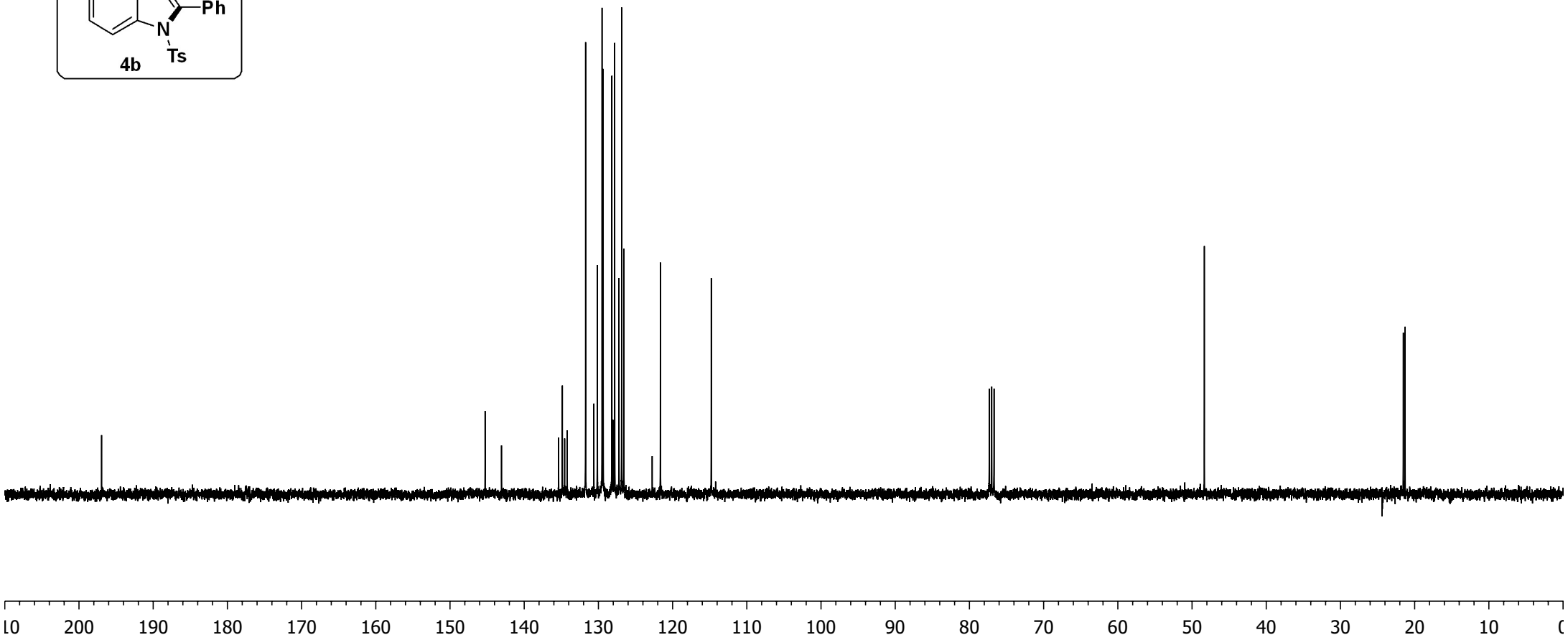
0.98 0.95 1.01 2.03 2.01 2.00 1.08 3.01 2.00 1.98 2.00 3.01 3.00

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

196.96
145.27
143.06
131.73
130.14
129.51
129.36
128.18
127.81
127.23
126.87
126.58
121.64
114.79
77.31
77.00
76.68
48.34
21.53
21.29

Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C



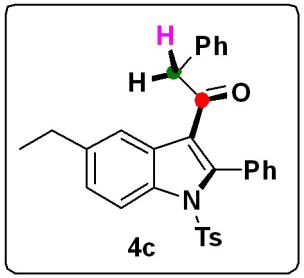


8.27 8.25 7.94 7.93 7.56 7.54 7.54 7.48 7.48 7.46 7.44 7.35 7.35 7.33 7.32 7.32 7.31 7.30 7.30 7.29 7.29 7.27 7.26 7.26 7.19 7.19 7.18 7.17 7.17 7.16 7.15 7.11 7.09 6.87 6.87 6.85 6.85 3.29 2.76 2.74 2.72 2.70 2.34 1.28 1.26 1.24

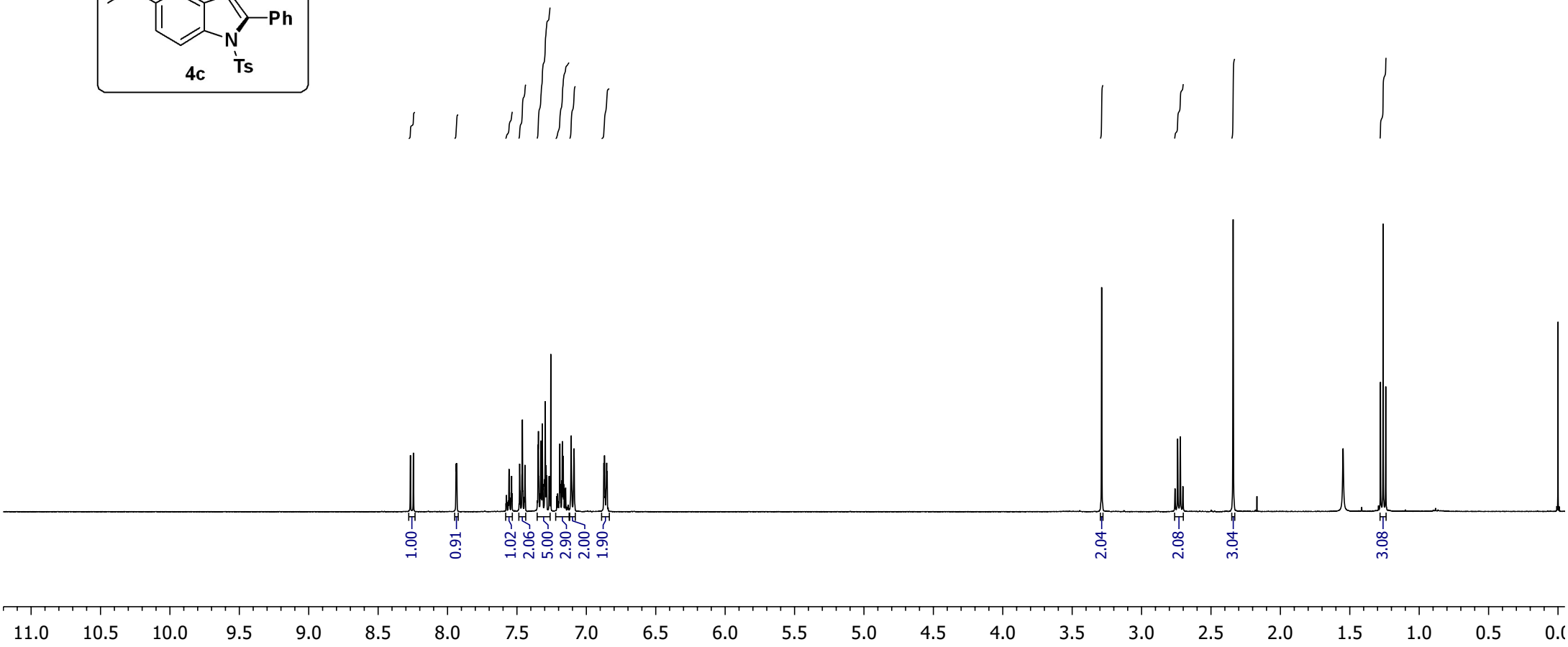
Solvent $CDCl_3$

Spectrometer Frequency 400.39

Nucleus 1H

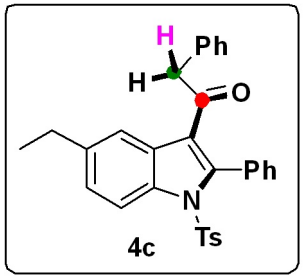


4c



196.94
145.30
143.10
141.41
131.76
129.56
129.43
128.22
127.85
126.96
126.62
126.26
120.55
114.91
77.31
76.99
76.67
48.41
28.84
21.59
15.98

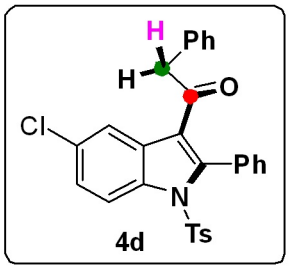
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C



4c

8.30 8.30 8.28 8.28 8.16 8.16 8.15 8.15 7.58 7.56 7.49 7.48 7.47 7.45 7.40 7.39 7.38 7.37 7.33 7.33 7.33 7.31 7.31 7.28 7.26 7.26 7.19 7.18 7.18 7.17 7.17 7.17 7.17 7.13 7.13 7.11 7.11 6.85 6.85 6.83 6.83 3.27 2.36

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



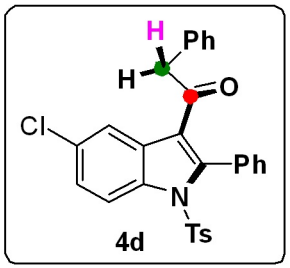
4d

1.00 0.80 1.02 2.06 1.00 2.00 1.98 2.90 2.00 1.90 2.04 3.03

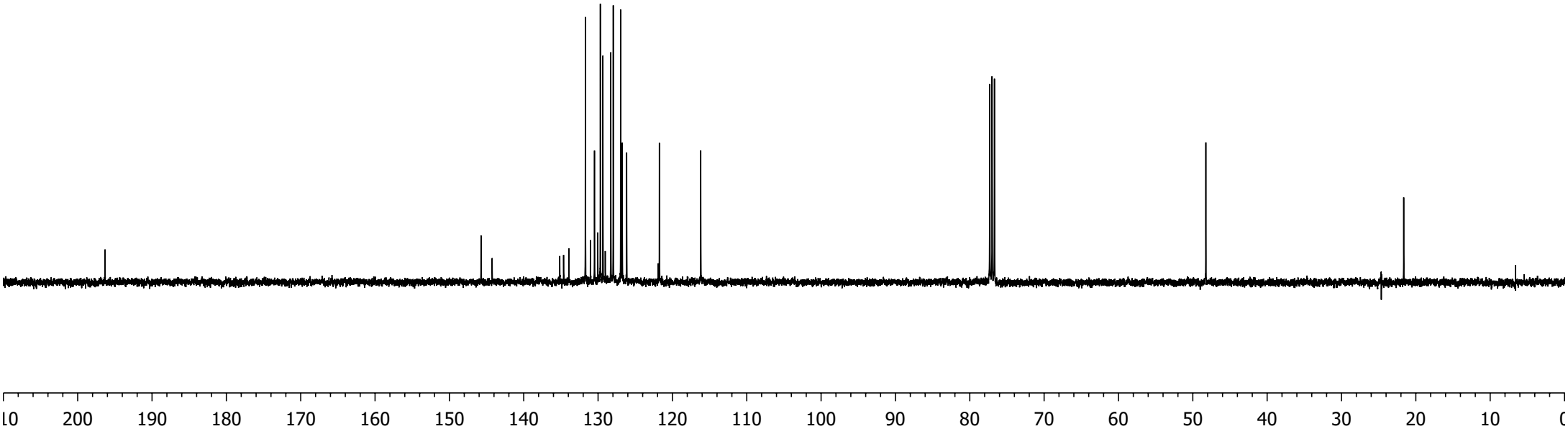
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

196.32
145.74
144.25
131.71
130.48
129.70
129.35
128.29
127.96
126.96
126.75
126.16
121.75
116.19
77.32
77.00
76.68
48.24
21.63

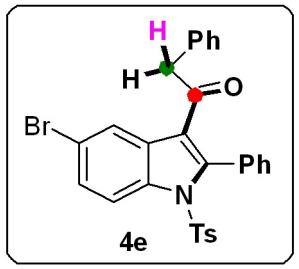
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C



4d



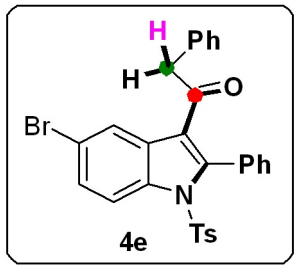
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

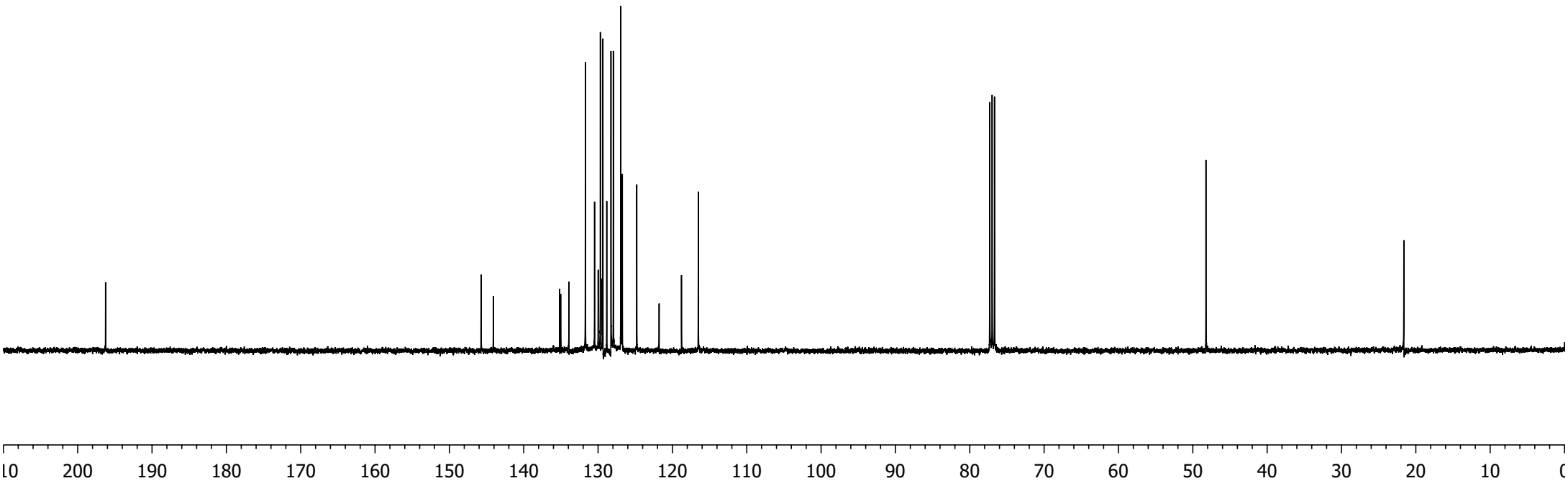


4e

196.25
145.74
144.09
135.16
135.03
133.92
131.71
130.47
129.99
129.69
129.44
129.35
128.83
128.27
127.95
126.95
126.73
124.79
121.78
118.78
116.52
77.31
76.99
76.67
48.23
21.61

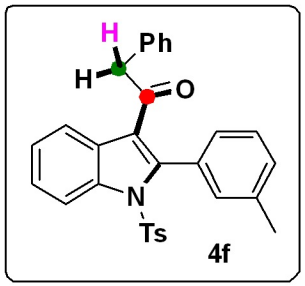
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





8.40 8.37 8.27 8.25 7.49 7.49 7.47 7.47 7.46 7.46 7.45 7.45 7.45 7.44 7.43 7.42 7.39 7.37 7.36 7.35 7.34 7.32 7.26 7.25 7.24 7.22 7.21 7.20 7.19 7.17 7.17 7.16 7.15 7.13 7.00 6.98 6.85 6.83 3.32 3.28 3.27 3.23 2.35 2.11

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



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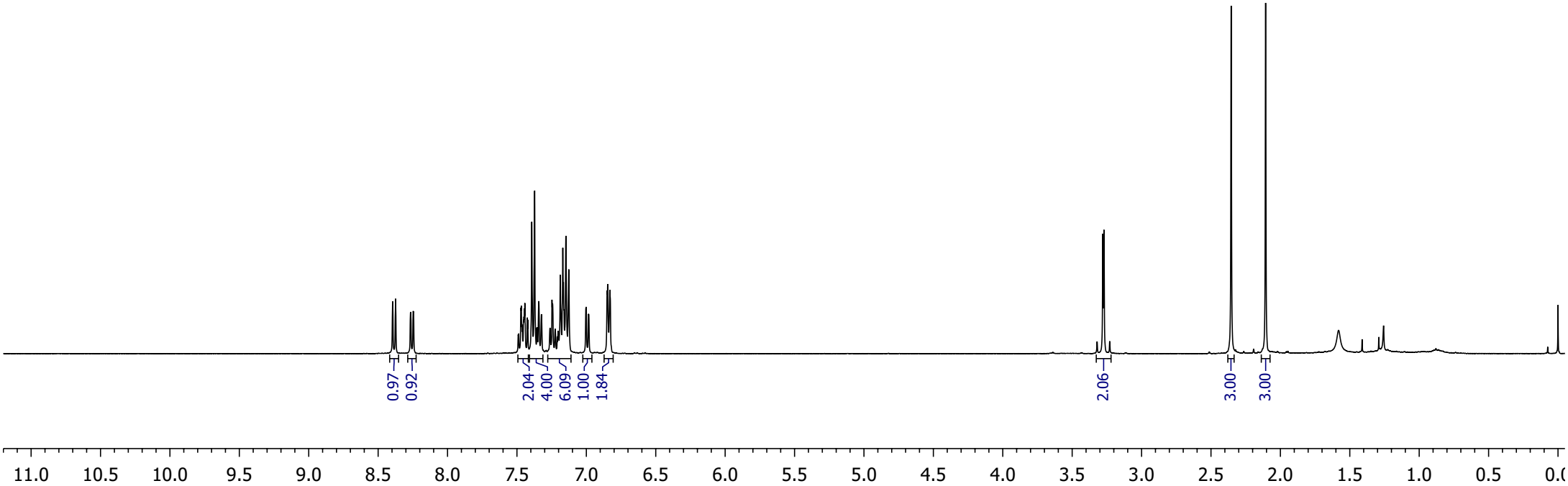
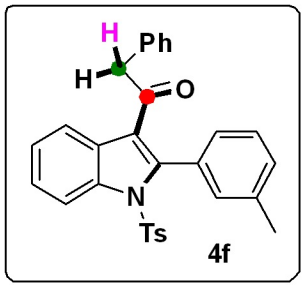
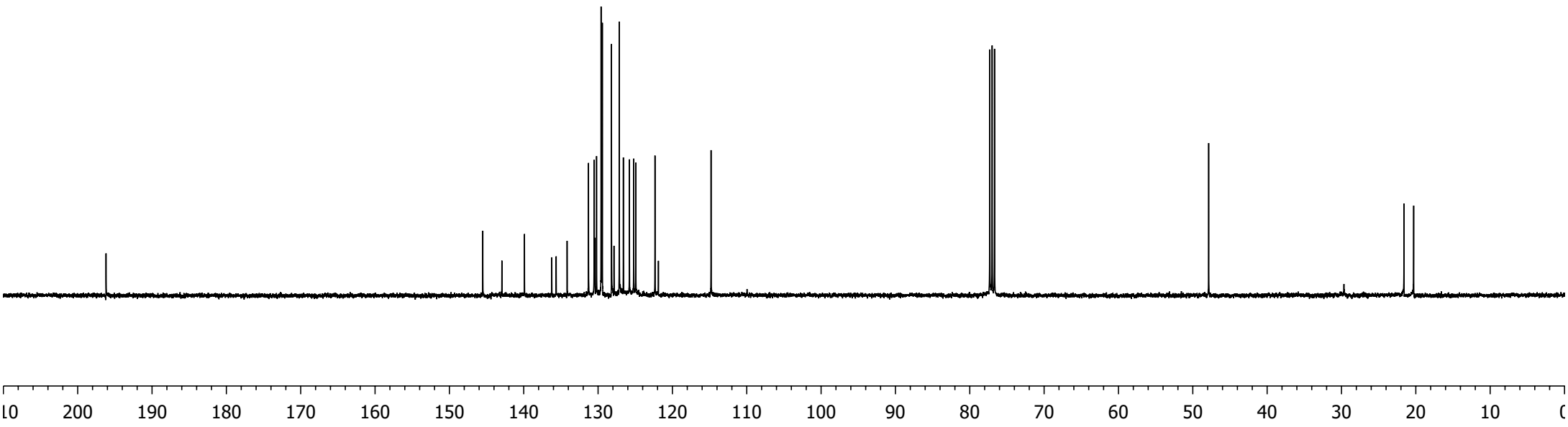


196.19
145.50
142.94
139.90
136.22
135.63
134.16
131.29
130.53
130.43
130.20
129.60
129.42
128.19
127.86
127.15
126.60
125.78
125.21
124.93
122.34
121.88
114.80
77.31
76.99
76.67
47.86
21.59
20.29

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C

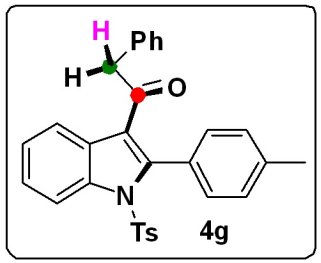


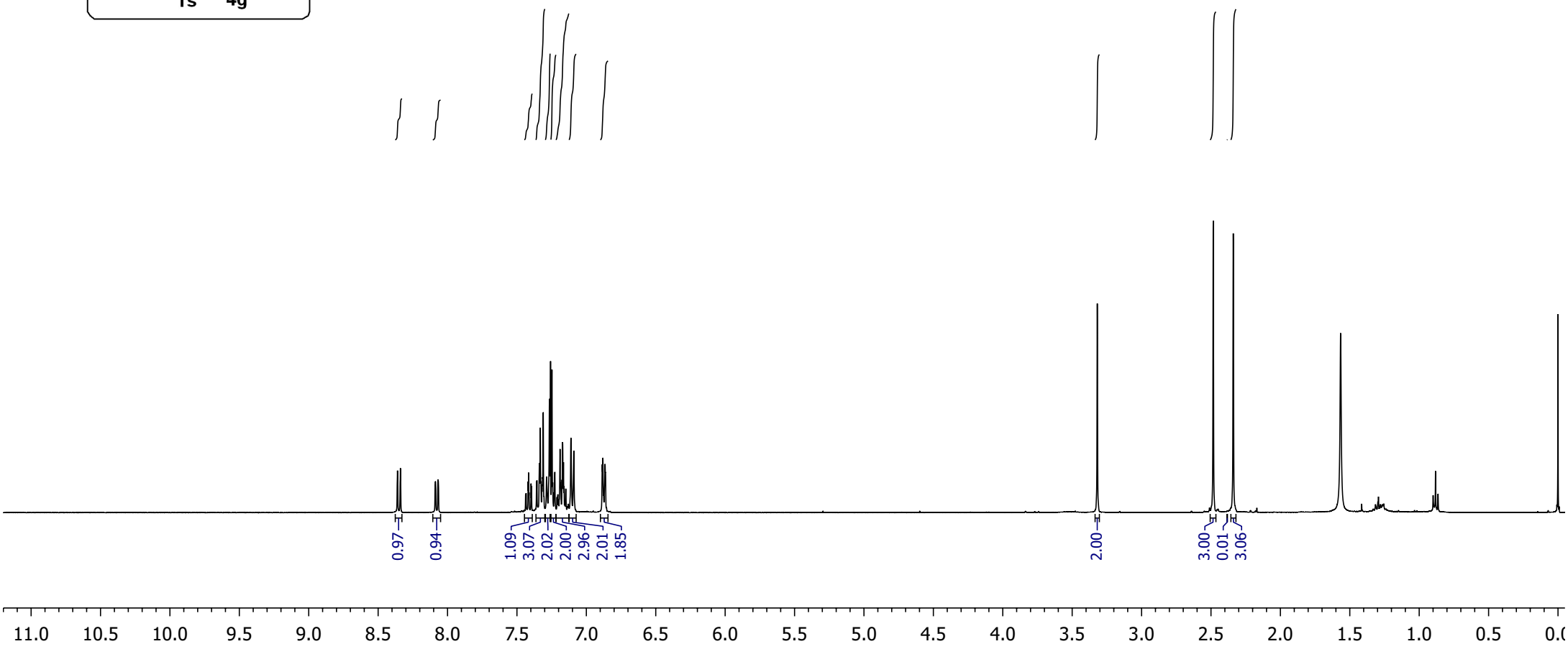
4f



8.36 8.34 8.09 8.07 7.44 7.43 7.42 7.42 7.41 7.40 7.39 7.36 7.36 7.34 7.33 7.32 7.31 7.29 7.27 7.26 7.25 7.24 7.23 7.21 7.21 7.20 7.19 7.19 7.18 7.17 7.16 7.16 7.16 7.15 7.11 7.09 6.88 6.87 3.32 2.48 2.34

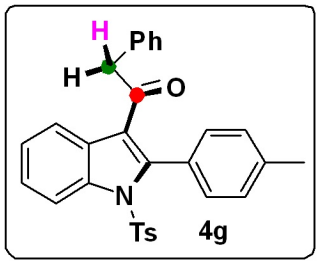
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H





196.95
145.34
143.42
140.45
136.32
135.43
134.33
131.61
129.54
129.42
128.61
128.23
127.98
127.52
126.96
126.63
125.77
125.03
122.81
121.87
115.18
77.31
76.99
76.68
48.39
21.62
21.59

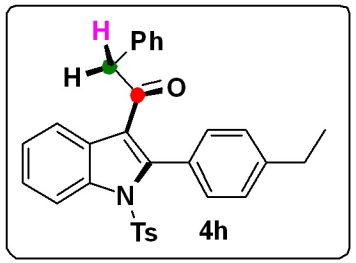
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C

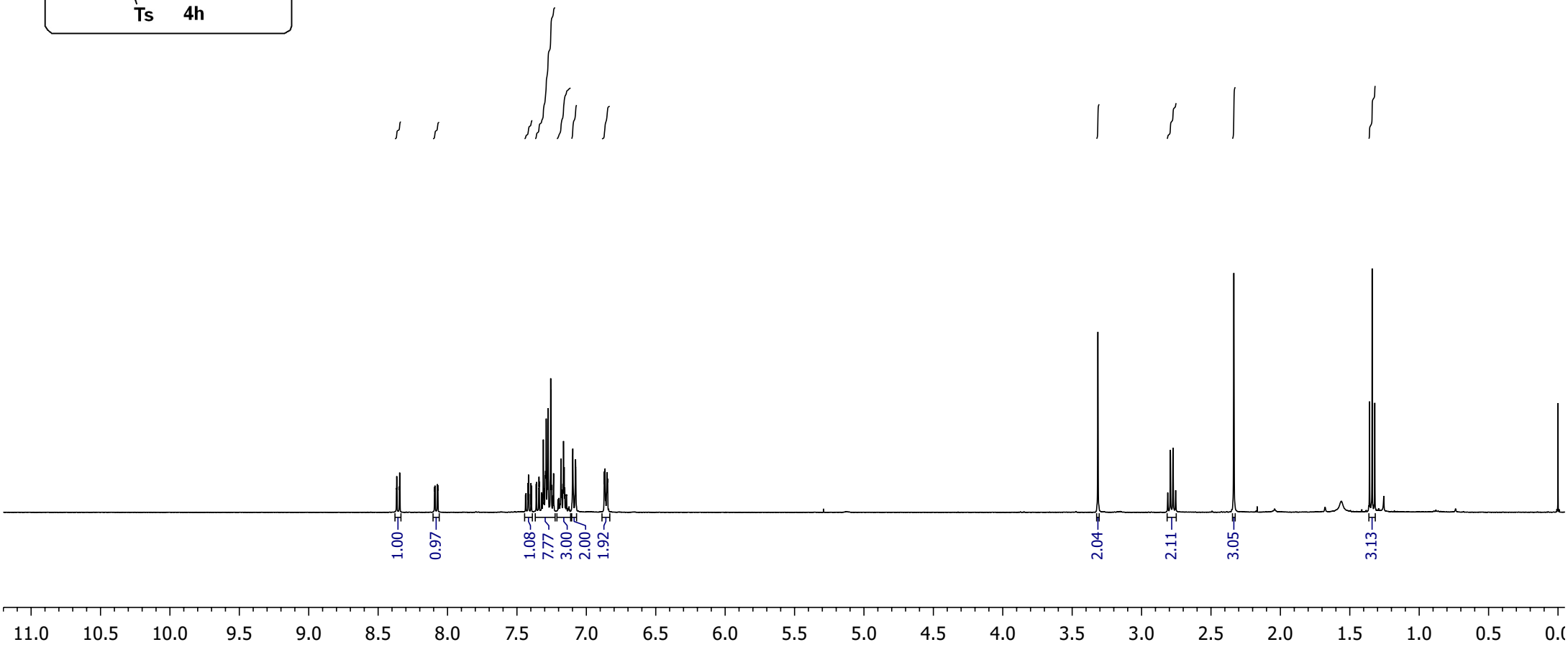


4g

8.37 8.34 8.09 8.09 8.07 8.07 7.42 7.42 7.40 7.40 7.36 7.36 7.34 7.34 7.34 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.28 7.26 7.25 7.25 7.24 7.18 7.18 7.17 7.16 7.16 7.16 7.10 7.08 6.87 6.87 6.85 6.85 3.31 2.81 2.79 2.77 2.75 2.34 1.36 1.34 1.32

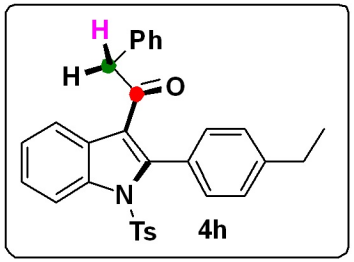
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



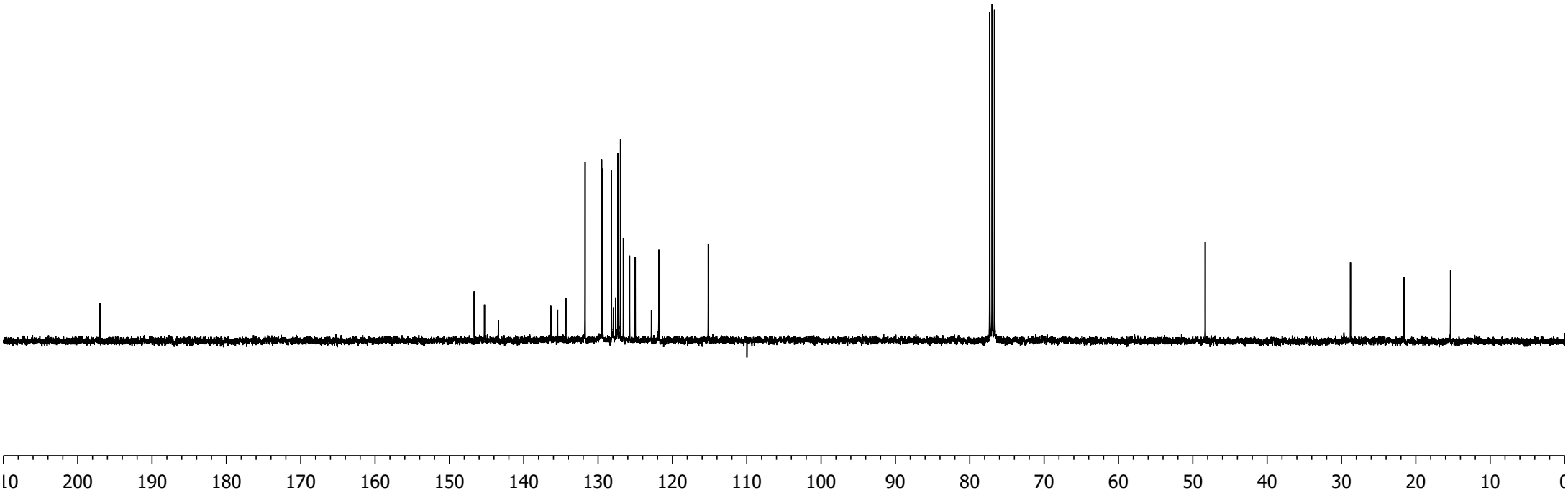


196.98
146.66
145.28
143.41
131.74
129.52
129.39
128.20
127.34
126.98
126.60
125.76
124.99
121.83
115.18
109.97
77.31
76.99
76.67
48.34
28.79
21.58
15.33

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C



4h

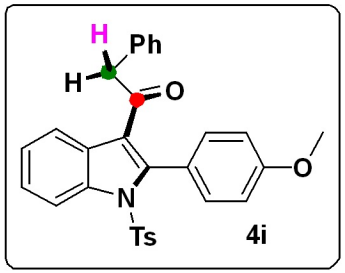


8.37 8.35 8.09 8.09 8.08 8.08 8.07 8.07 8.06 8.06 7.42 7.42 7.40 7.39 7.36 7.36 7.34 7.34 7.31 7.29 7.28 7.26 7.26 7.25 7.24 7.24 7.19 7.17 7.17 7.17 7.16 7.10 6.99 6.96 6.90 6.89 6.88 6.87 3.91 3.34 2.33

Solvent $CDCl_3$

Spectrometer Frequency 400.39

Nucleus ^1H

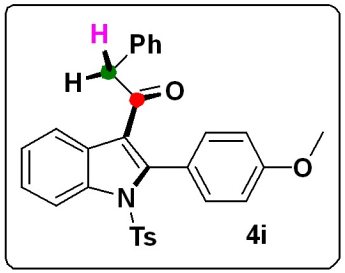


1.00 0.98 1.07 1.10 2.01 2.20 2.95 2.00 2.03 1.90 3.03 2.03 3.03

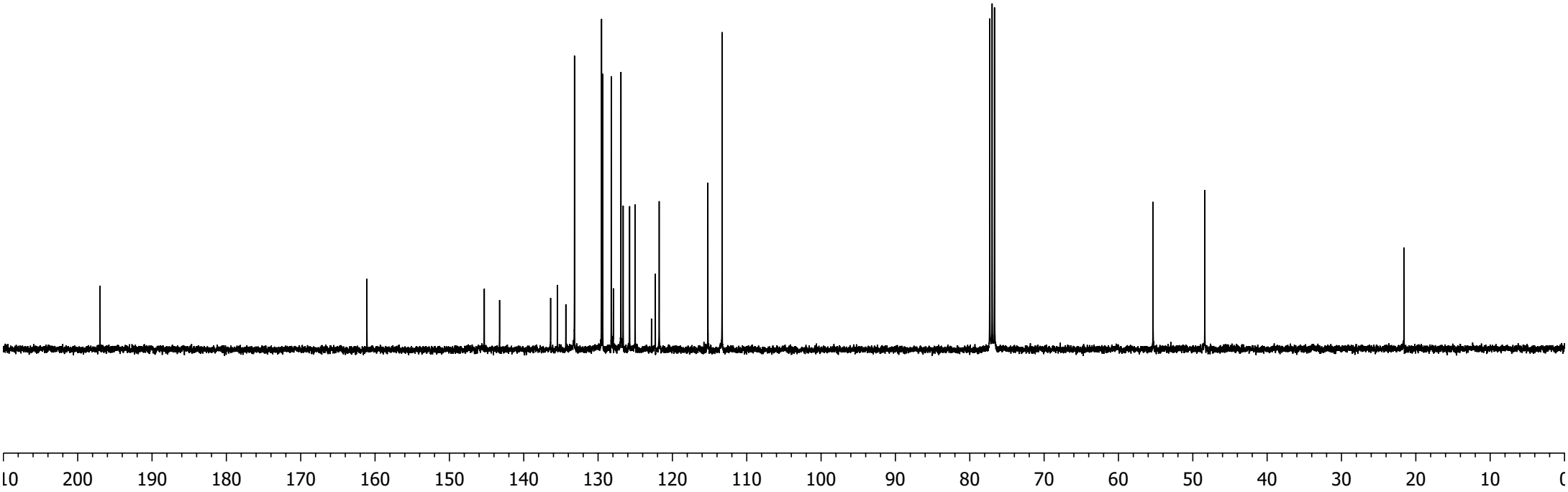
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

196.99 161.09 145.30 143.25 133.17 129.53 129.38 128.23 126.92 126.62 125.76 125.02 122.29 121.78 115.22 113.31 77.31 76.99 76.67 55.36 48.39 21.57

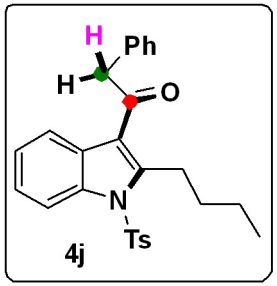
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C



4i



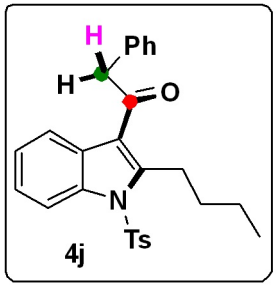
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



4j

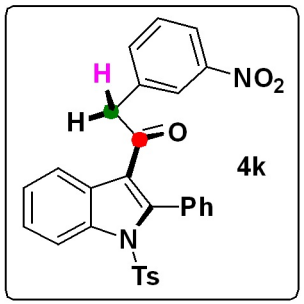
196.07
148.24
145.31
136.09
134.20
130.01
129.55
128.54
126.96
126.91
126.40
124.63
124.34
120.47
115.13
77.31
76.99
76.67
50.23
33.18
27.15
22.94
21.59
13.74

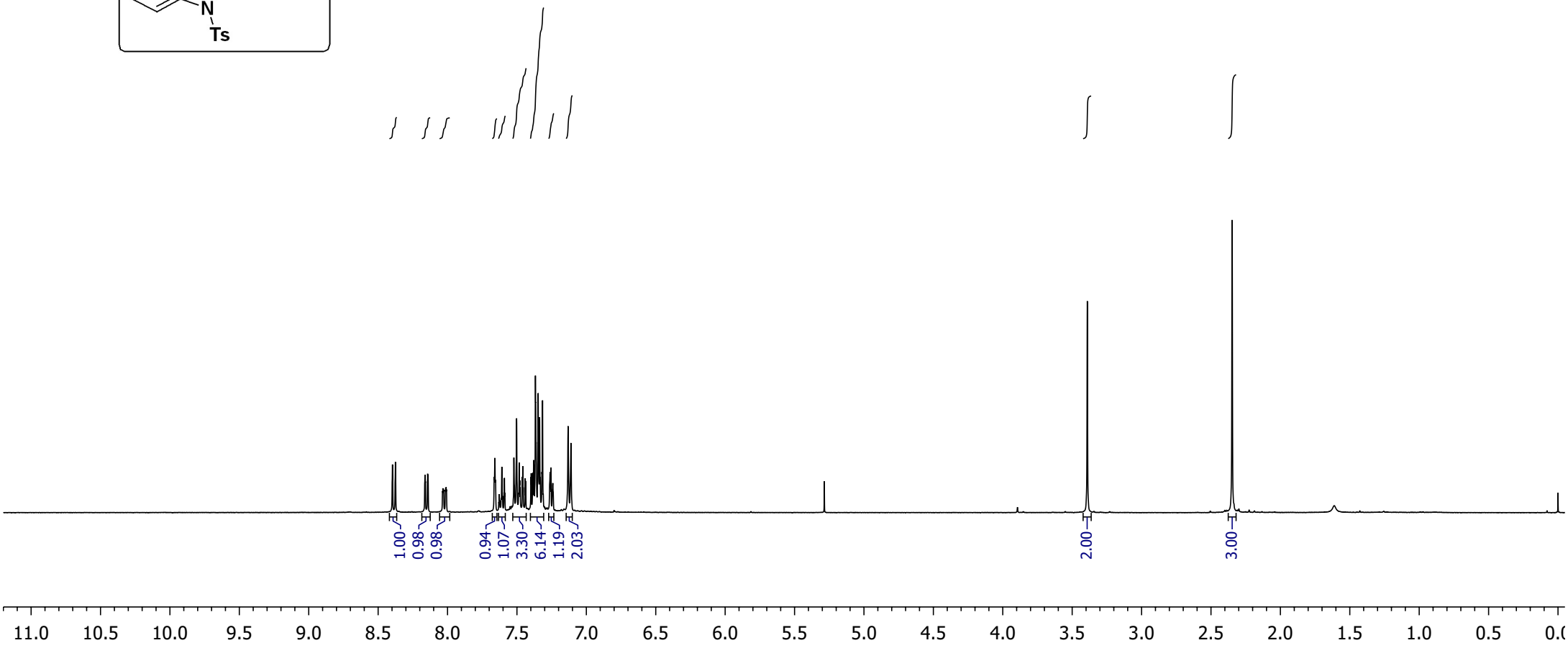
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C



4j

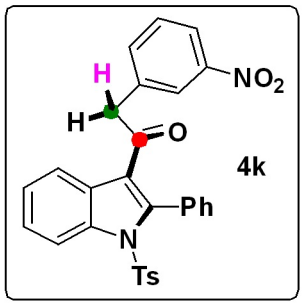
Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H

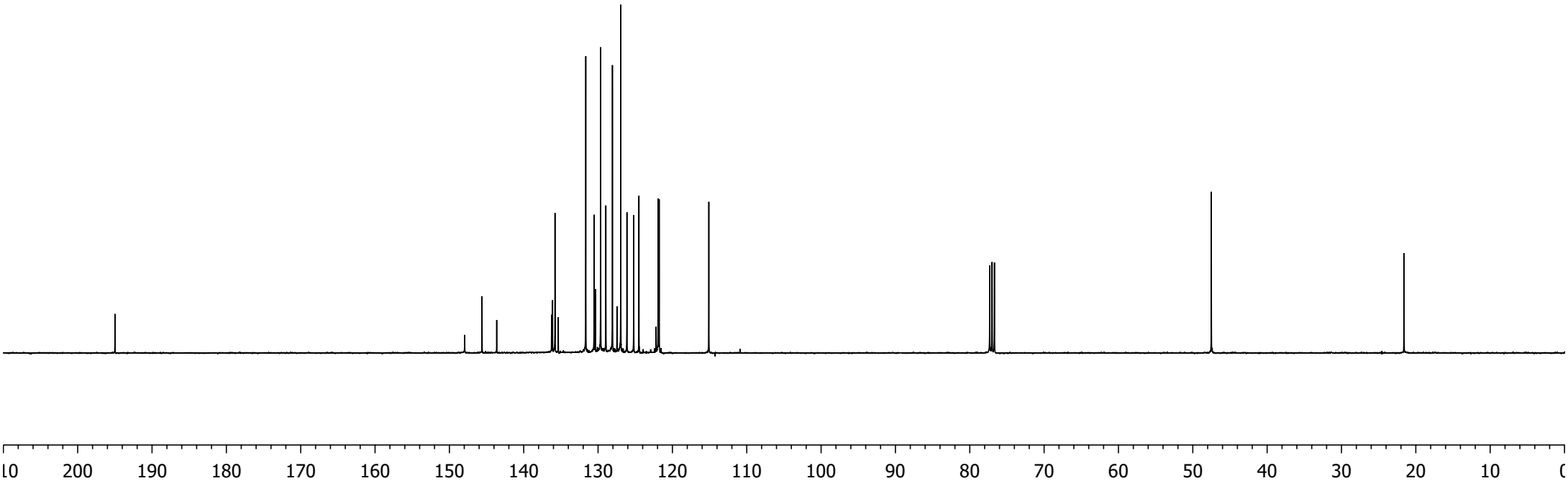




194.98
147.94
145.61
143.63
135.79
131.65
129.65
128.95
128.07
126.95
126.12
124.50
121.93
121.78
115.10
77.32
77.00
76.68
47.51
21.59

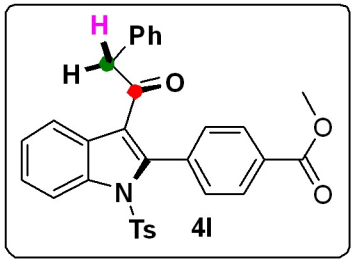
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C





8.37 8.35 8.15 8.13 8.08 8.06 7.44 7.42 7.30 7.26 7.17 7.13 6.84 6.84 6.83 6.82 4.00 3.33 2.35

Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H



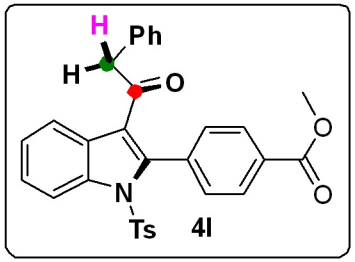
4l

1.00 2.00 1.00 3.06 1.08 2.00 2.98 2.03 1.93 3.01 2.06 3.01

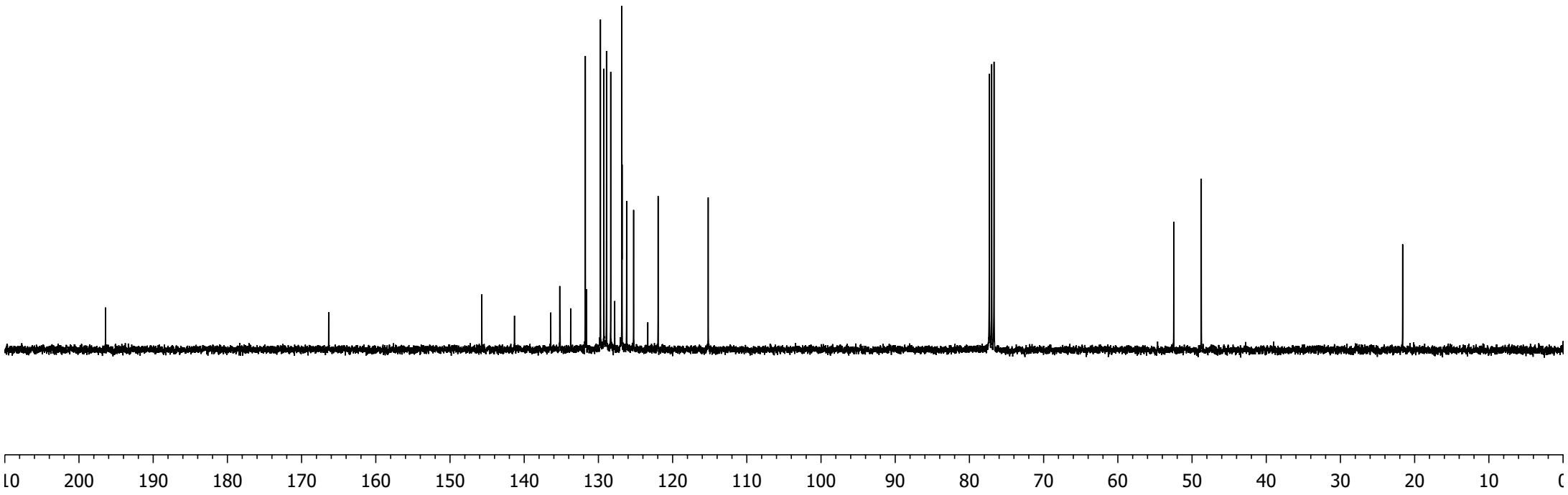
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

196.43 166.35 145.71 141.31 136.42 135.21 135.16 133.74 131.76 131.59 129.73 129.26 128.91 128.34 127.80 126.84 126.81 126.20 125.25 123.34 121.96 115.20 77.32 77.00 76.68 52.47 48.75 21.62

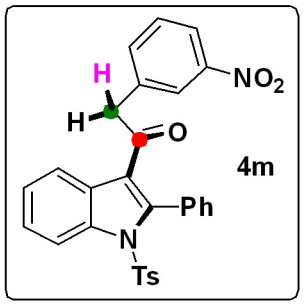
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C

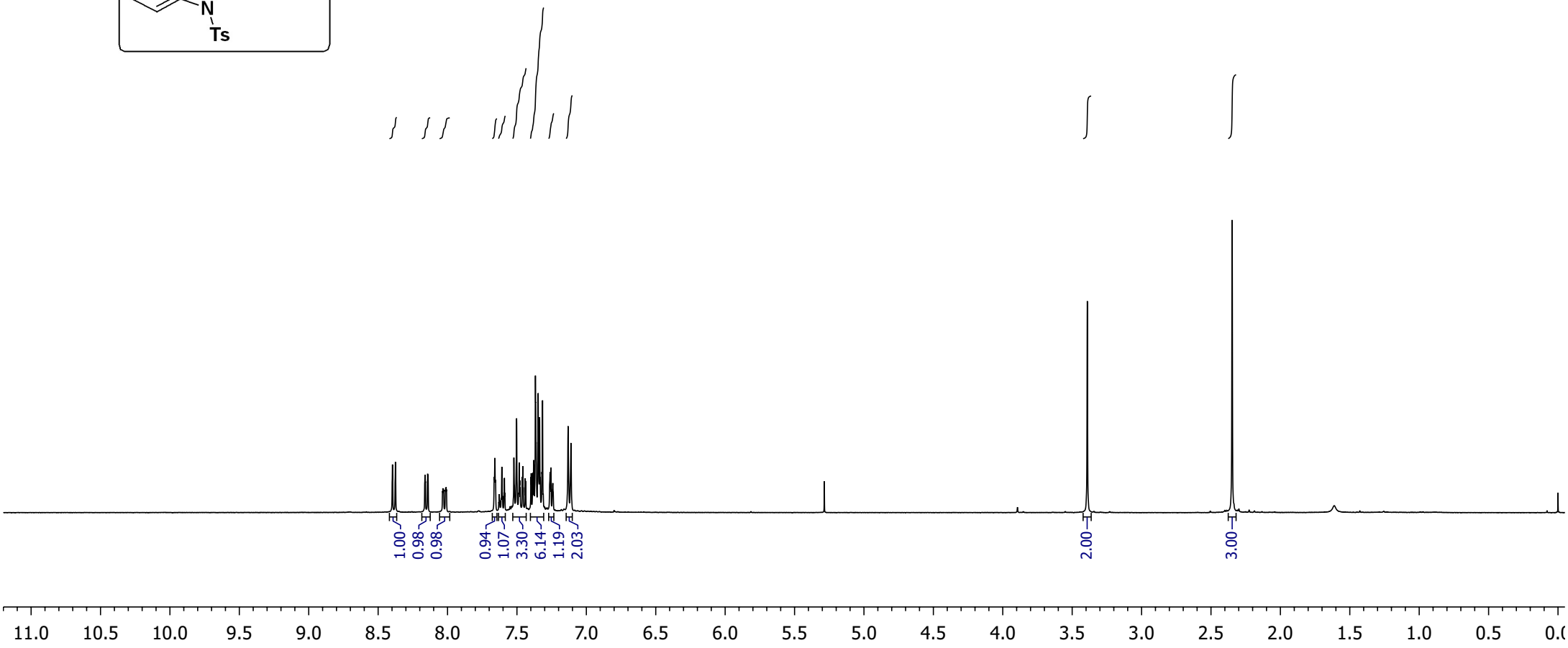


4l



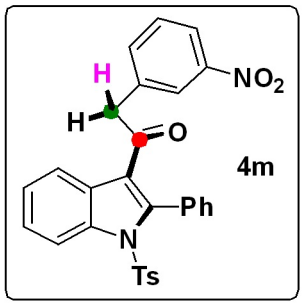
Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H

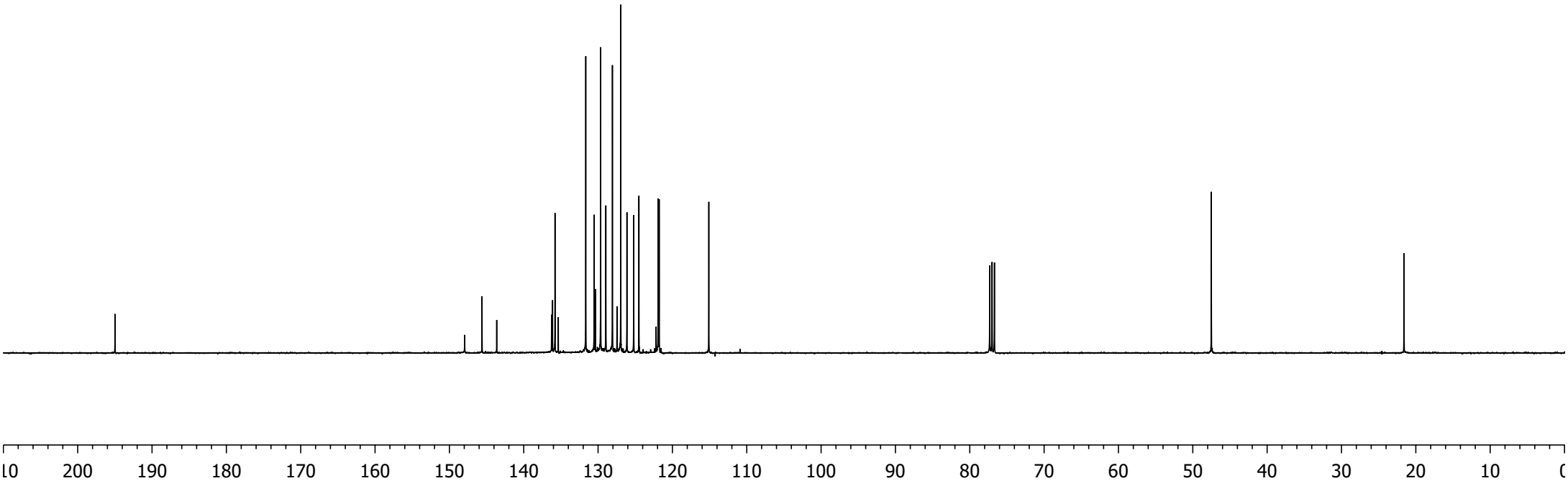




194.98
147.94
145.61
143.63
135.79
131.65
129.65
128.95
128.07
126.95
126.12
124.50
121.93
121.78
115.10
77.32
77.00
76.68
47.51
21.59

Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C

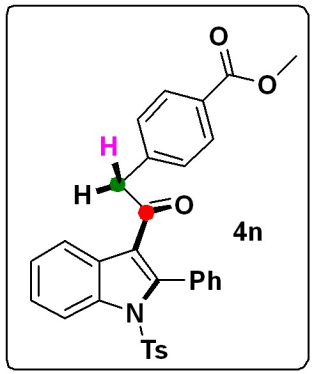




Solvent $CDCl_3$

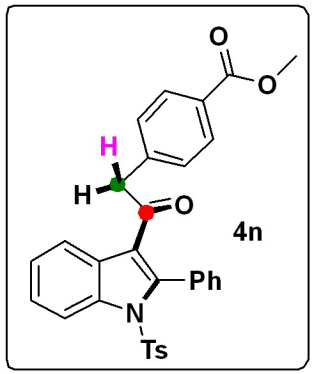
Spectrometer Frequency 400.39

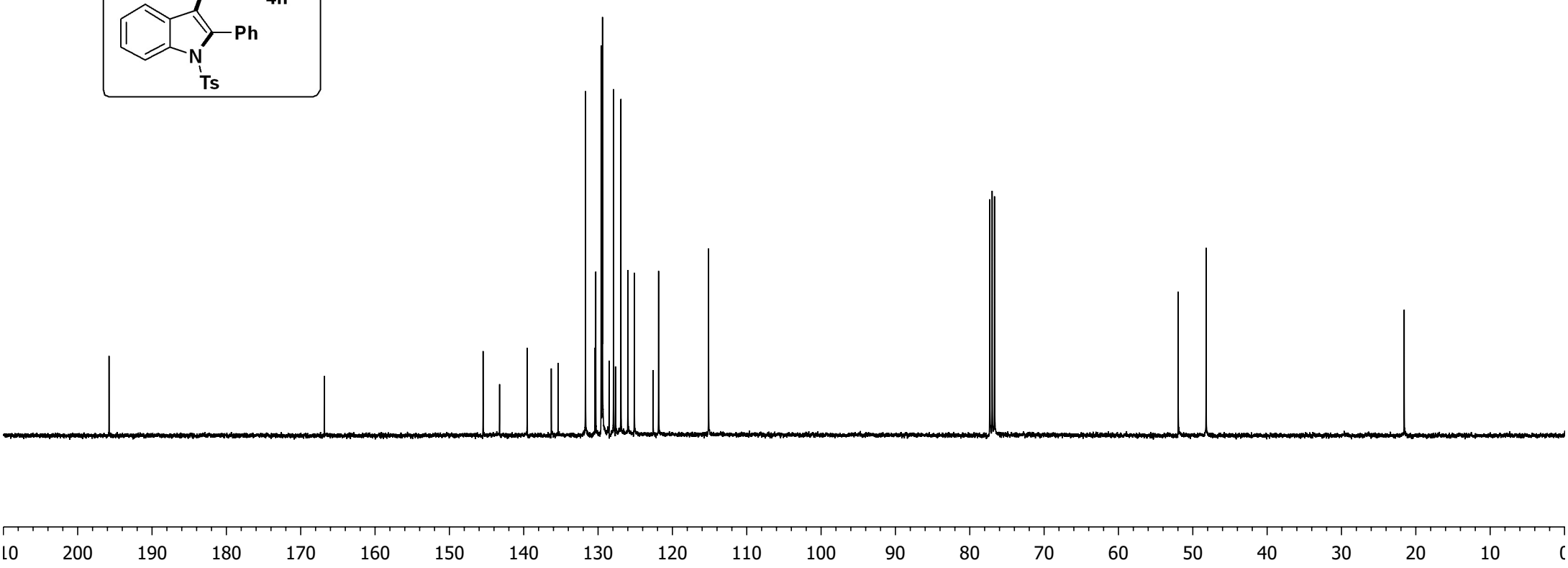
Nucleus ^1H



195.78 166.83 145.47 143.25 139.52 136.29 135.37 131.70 130.40 130.31 129.59 129.45 129.41 128.52 127.92 127.66 126.92 125.99 125.13 122.60 121.86 115.14 77.31 76.99 76.67 51.97 48.20 21.56

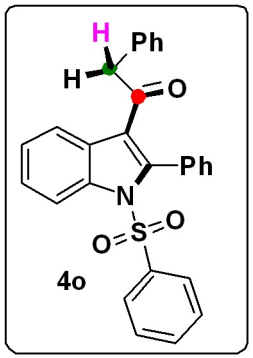
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C

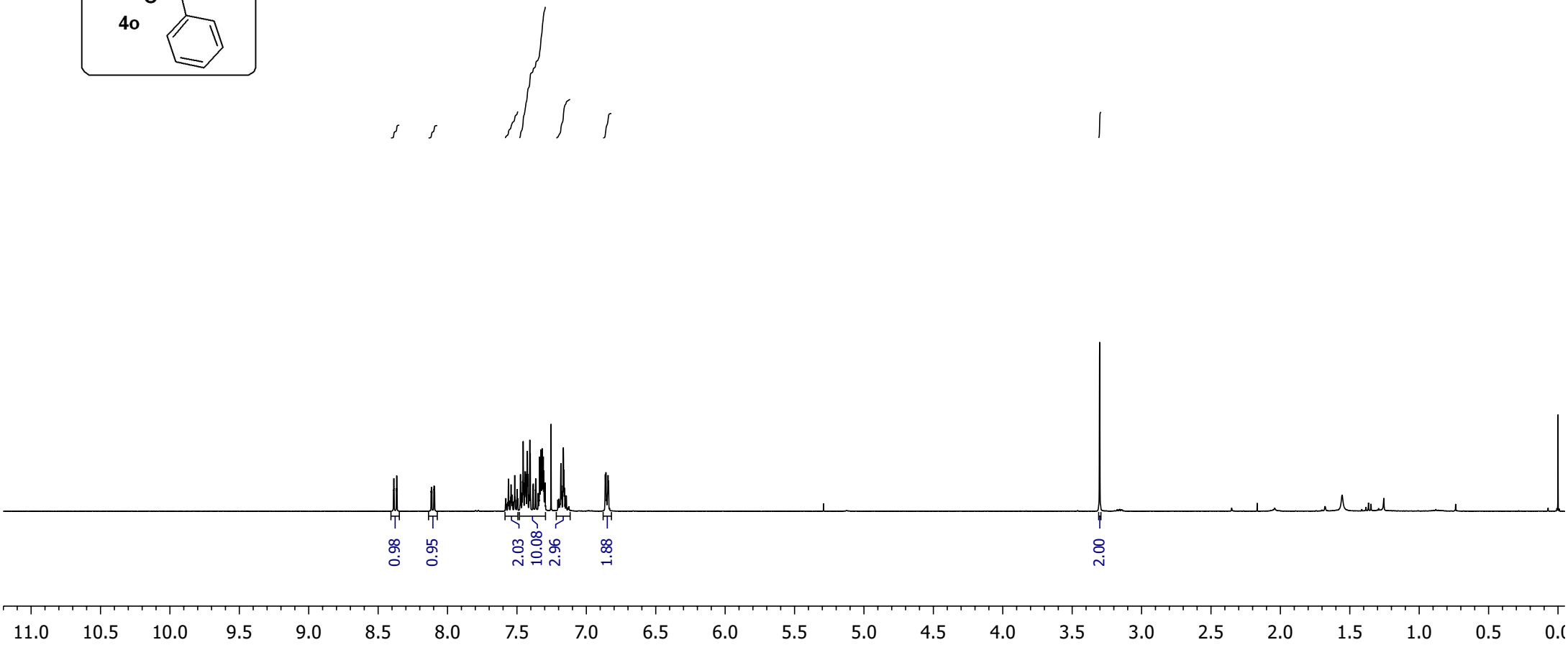




8.39 8.37 8.12 8.11 8.10 8.09 7.56 7.54 7.52 7.47 7.46 7.46 7.45 7.44 7.44 7.43 7.43 7.42 7.41 7.40 7.38 7.36 7.36 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.25 7.18 7.17 7.16 6.86 6.86 6.84 6.84 3.30

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H





M0474-2
MC-20-27-1

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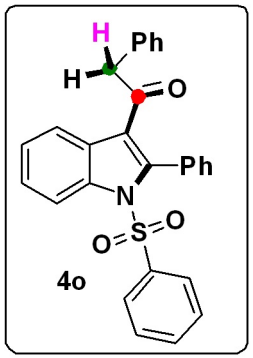
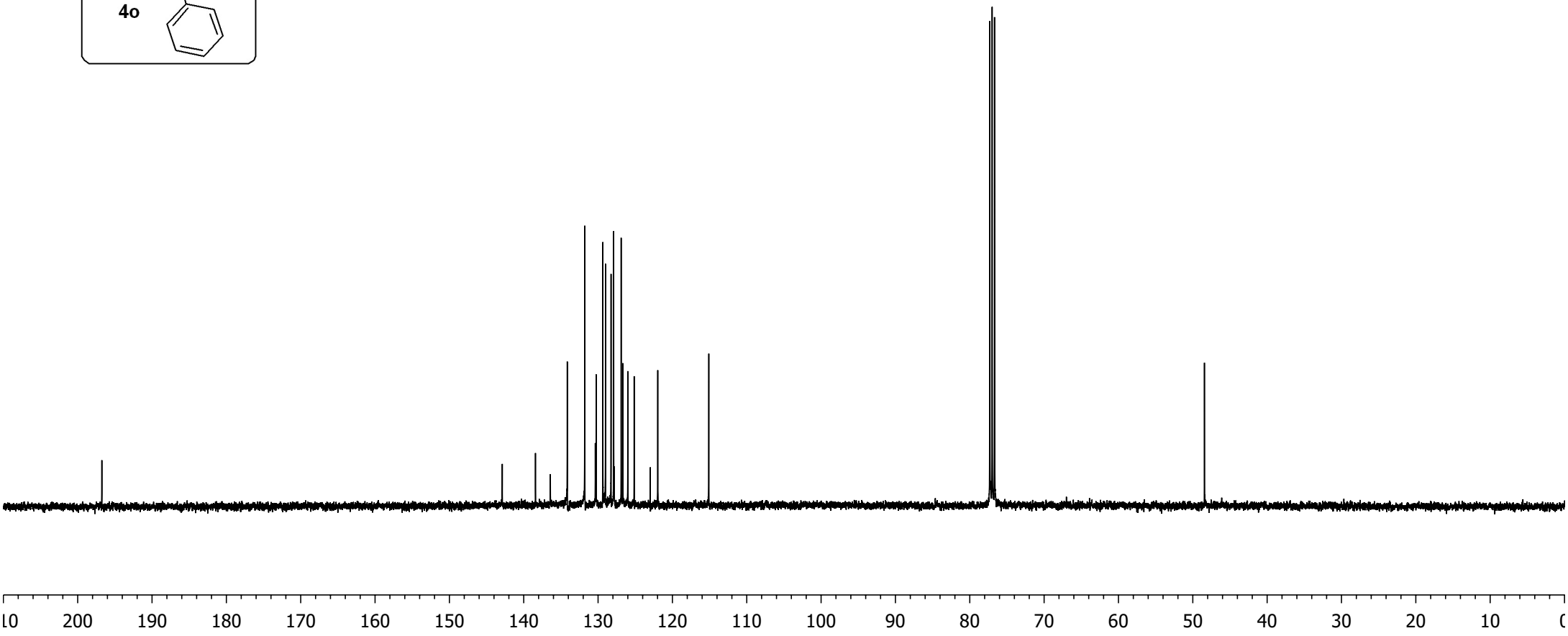
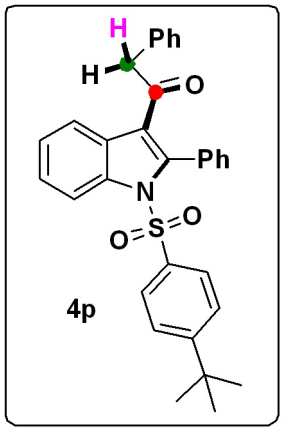
136.42
134.14
131.79
130.37
130.26
129.36
129.00
128.25
127.90
127.82
126.89
126.67
126.00
125.14
122.98
121.97
115.10
77.31
76.99
76.67
48.44

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

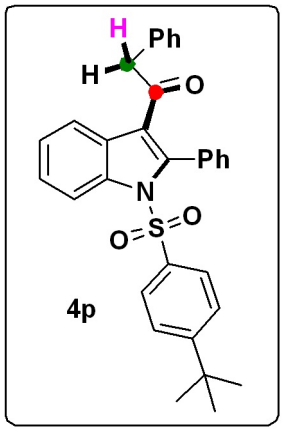


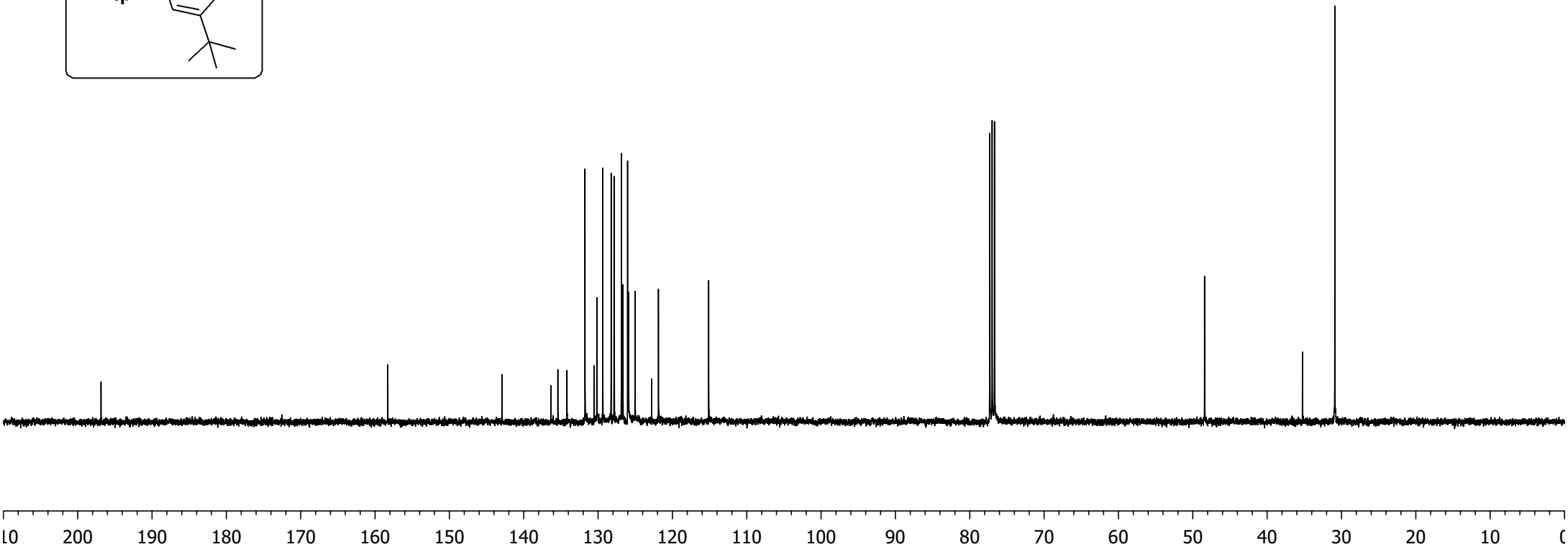
196.86 158.29 142.93 131.76 129.38 128.24 127.85 126.86 126.65 126.03 125.89 125.02 121.88 115.12 77.31 76.99 76.67 48.42 35.25 30.89

Solvent $CDCl_3$

Spectrometer Frequency 100.69

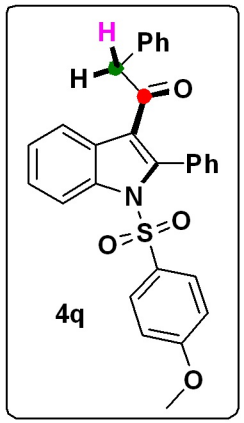
Nucleus ^{13}C

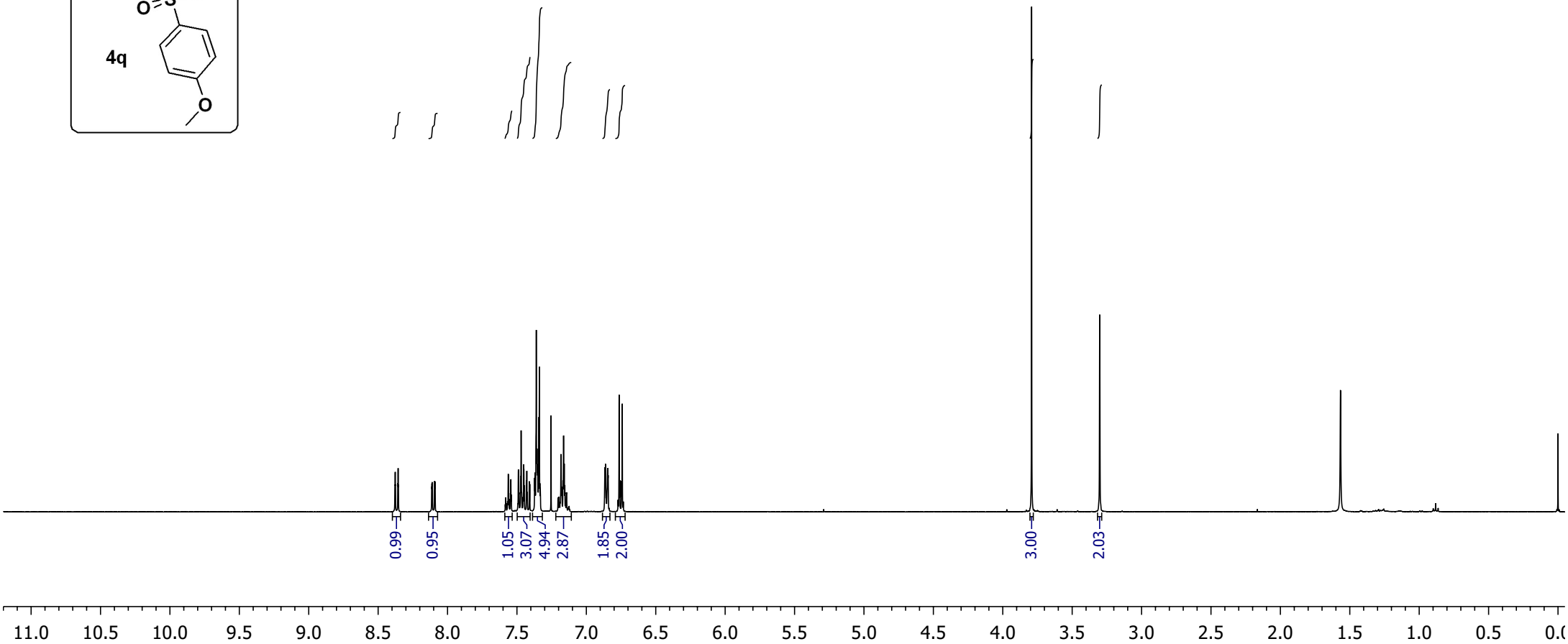




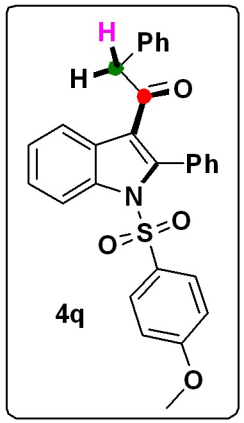
8.38 8.36 8.11 8.11 8.09 8.09 7.56 7.54 7.49 7.47 7.47 7.45 7.45 7.43 7.43 7.41 7.41 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.18 7.18 7.17 7.16 7.16 7.16 6.87 6.86 6.85 6.84 6.76 6.74 3.79 3.30

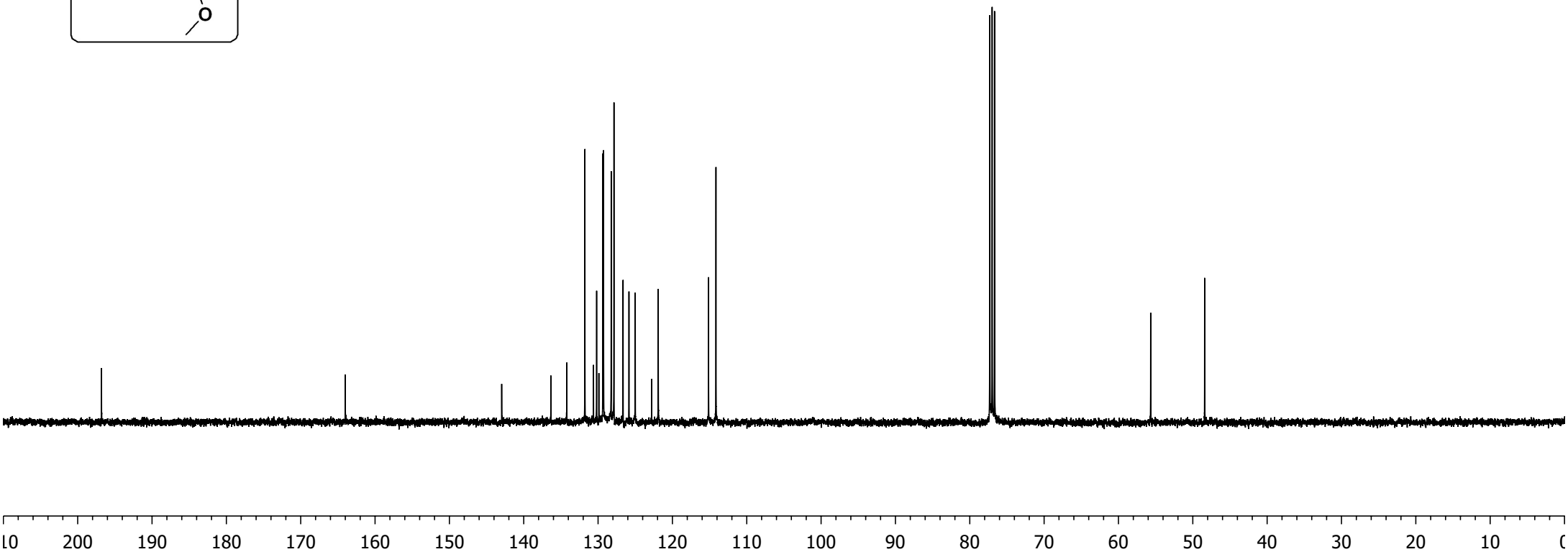
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H





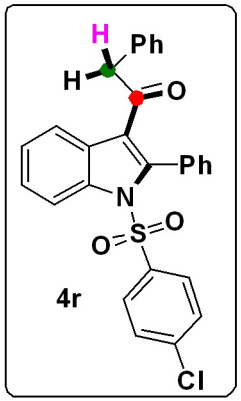
196.80
164.01
142.96
131.77
130.19
129.37
129.27
128.23
127.86
126.64
125.84
121.91
115.14
114.14
77.31
76.99
76.67
55.67
48.41

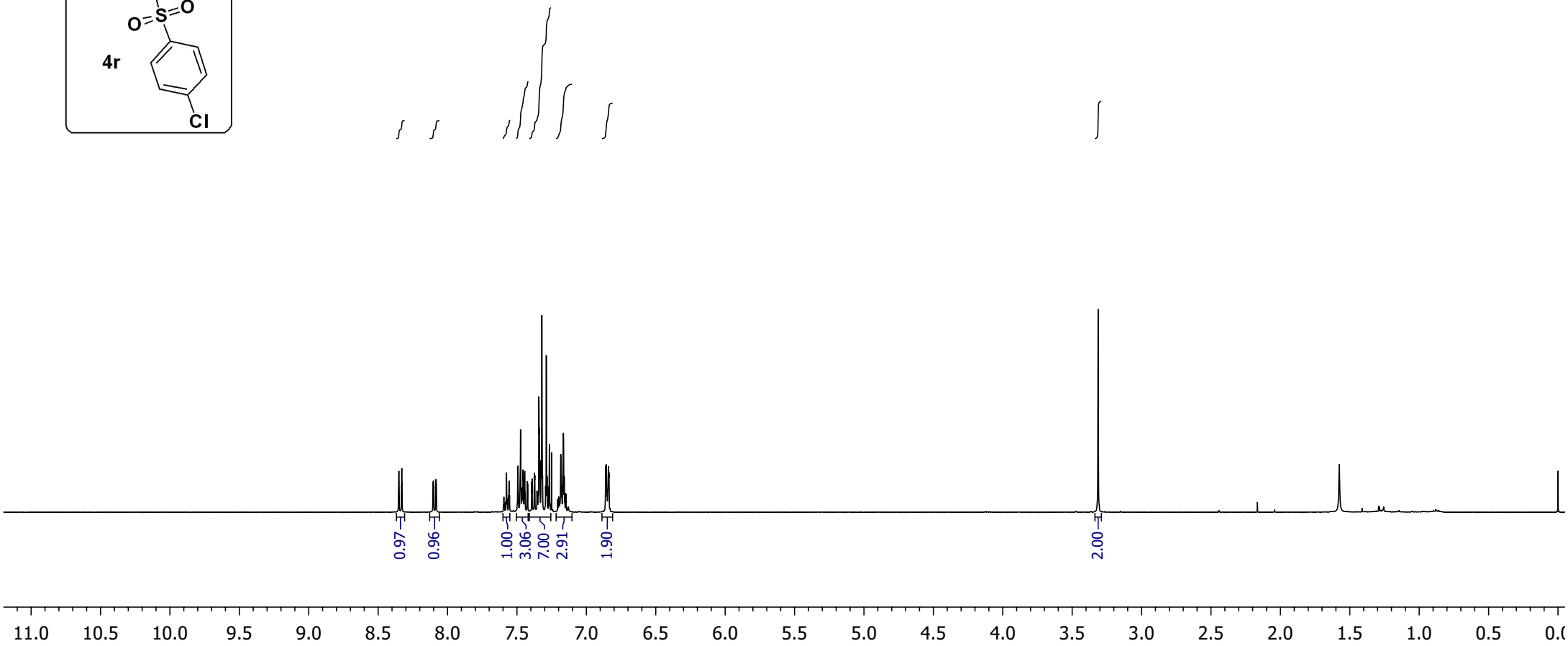




8.35 8.33 8.10 8.10 8.08 8.08 7.47 7.34 7.34 7.32 7.29 7.17 6.86 6.86 6.84 6.84 3.31

Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H

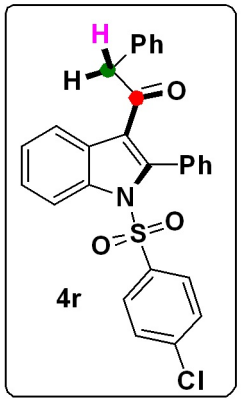


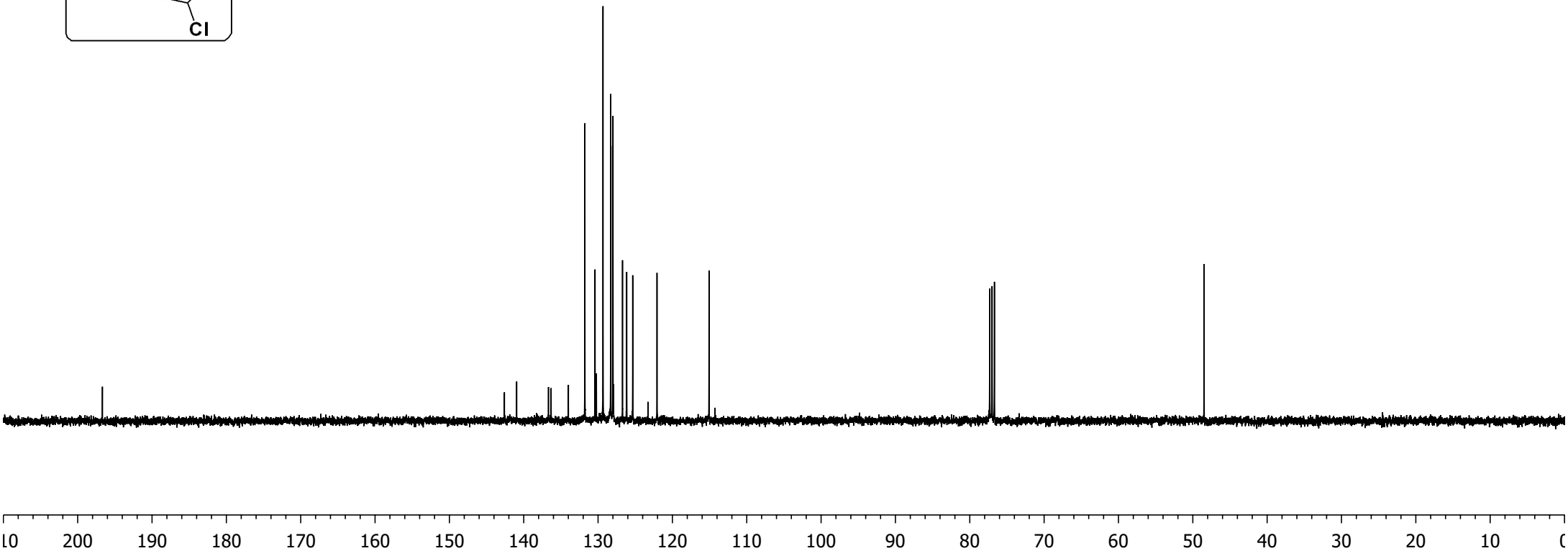


U0220-10
MC-20-14

196.68
142.60
140.95
136.67
136.32
133.99
131.77
130.41
130.22
129.34
128.31
128.27
127.99
127.91
126.71
126.15
125.34
122.07
115.08
77.32
77.00
76.68
48.48

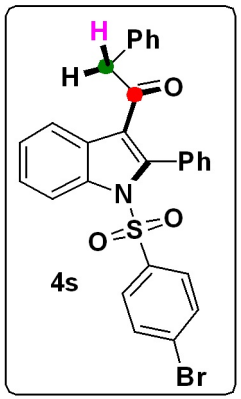
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C





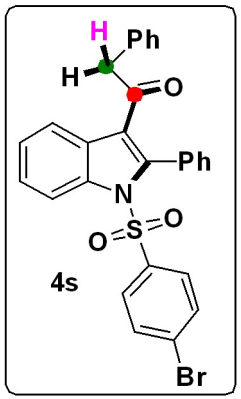
8.35 8.33 8.10 8.10 8.08 8.08 8.08 7.47 7.46 7.44 7.26 7.24 7.17 6.86 6.86 6.84 6.84 3.31

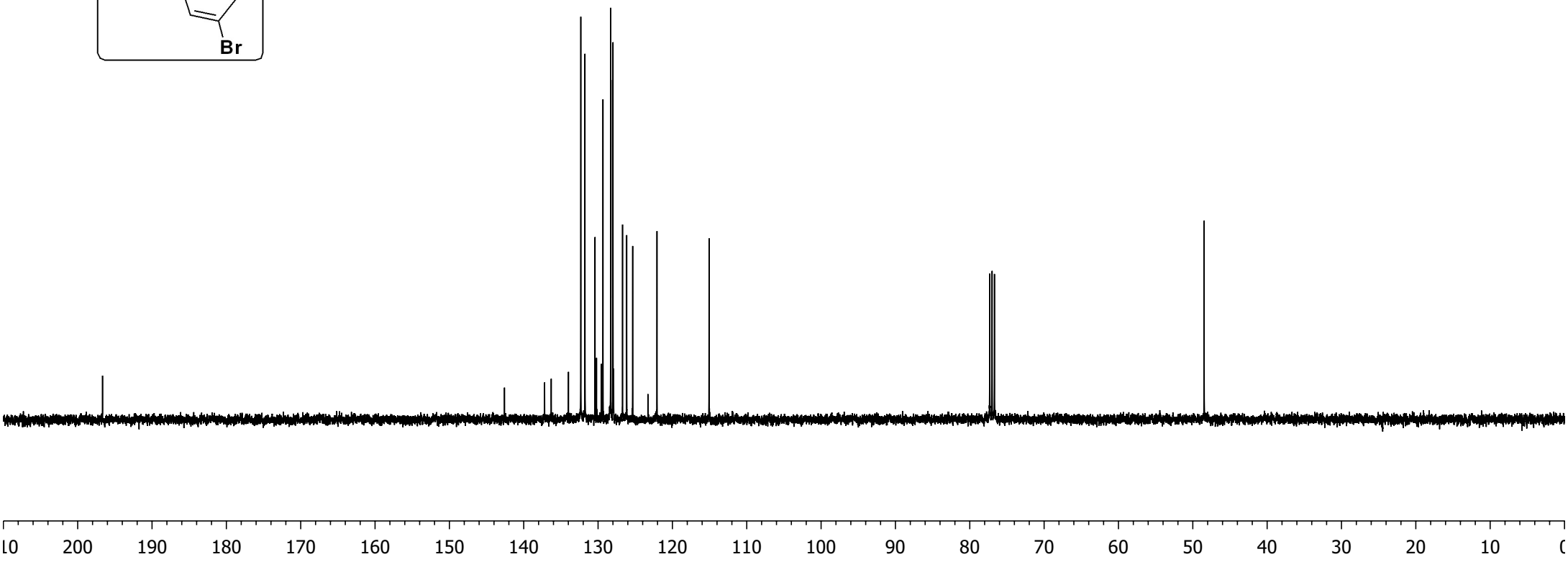
Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H



196.66
142.59
132.32
131.77
130.41
129.34
128.30
128.27
127.99
126.71
126.15
122.07
115.07
77.32
77.00
76.68
48.48

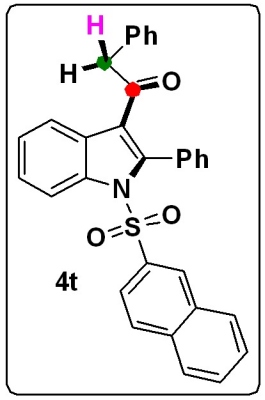
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C





8.48 8.46 8.13 8.13 8.11 8.11 7.86 7.86 7.81 7.81 7.75 7.73 7.73 7.63 7.63 7.57 7.57 7.55 7.47 7.47 7.45 7.41 7.41 7.39 7.39 7.38 7.37 7.37 7.37 7.36 7.27 7.27 7.25 7.25 7.16 7.14 7.14 7.14 7.13 3.28

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H



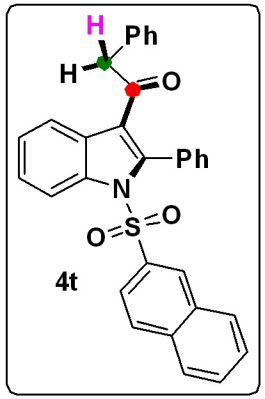
4t

1.00 0.98 0.99 1.00 2.04 3.17 1.07 4.12 2.19 2.89 1.91 2.03

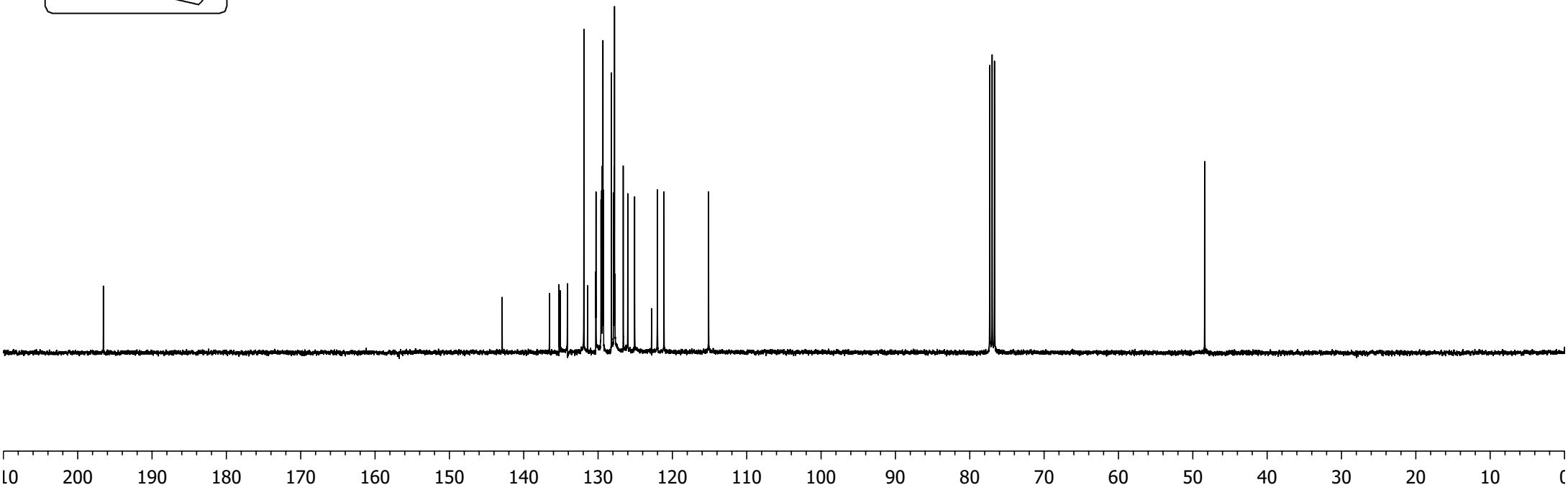
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

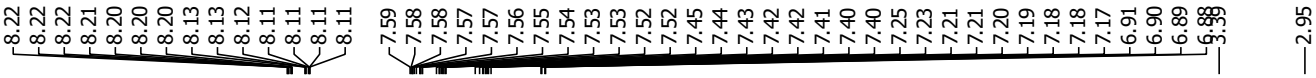
196.55 142.90 131.91 129.52 129.44 129.34 129.27 128.21 127.82 127.79 126.62 122.02 115.13 77.31 76.99 76.67 48.41

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C

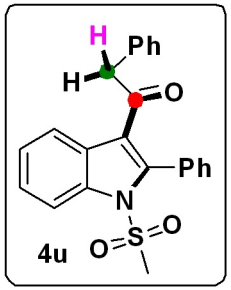


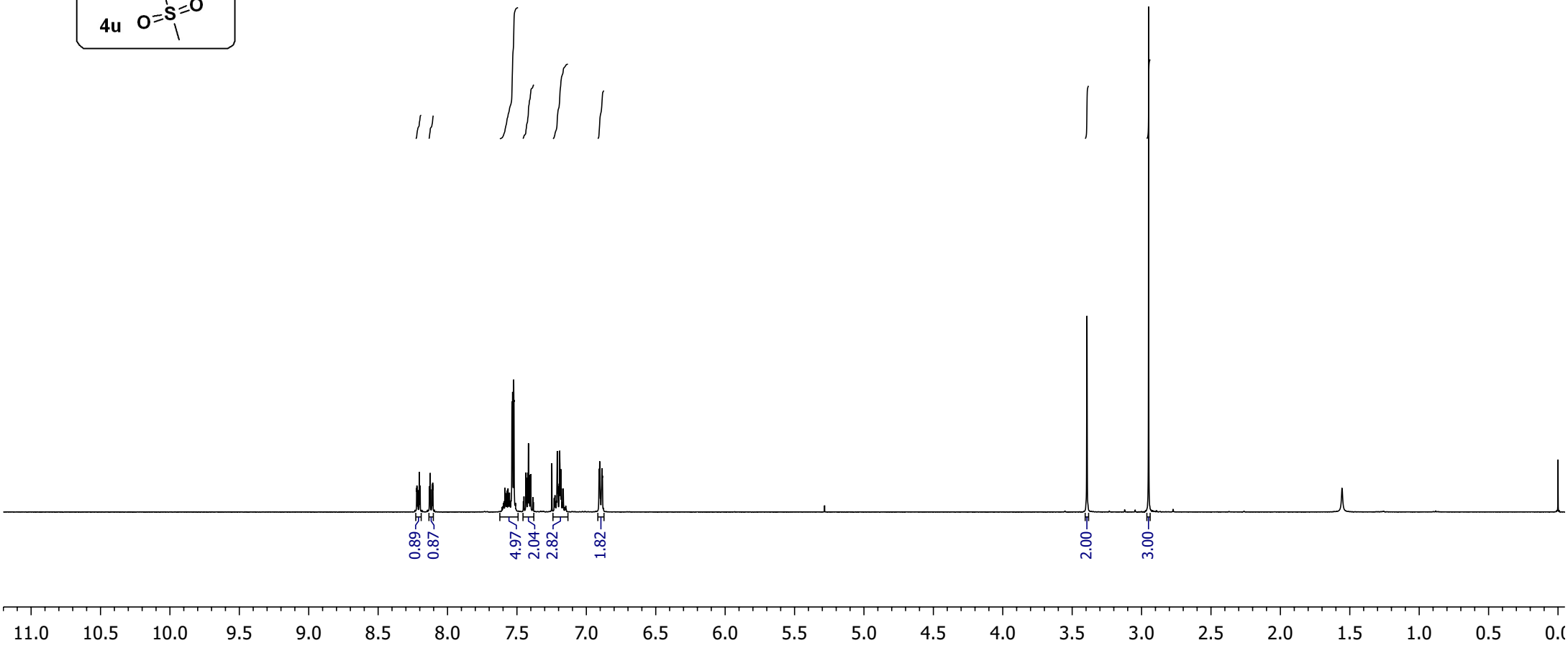
4t





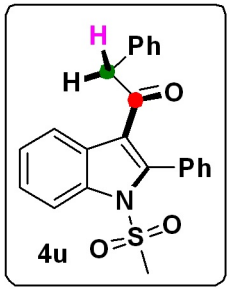
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

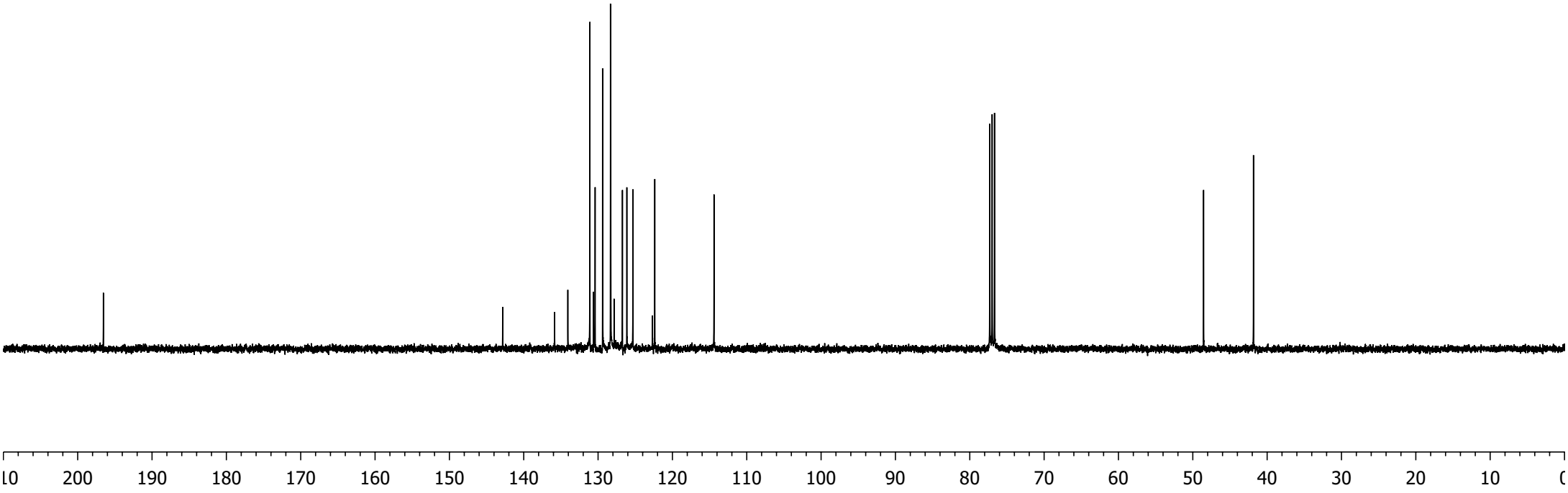


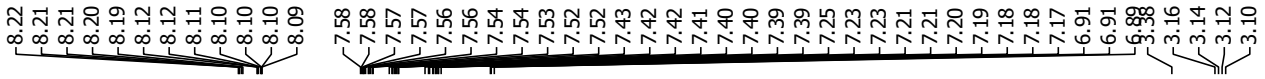


196.54 142.84 134.07 131.10 130.40 129.39 128.33 128.29 126.72 126.13 125.31 122.37 114.40 77.31 76.99 76.67 48.55 41.84

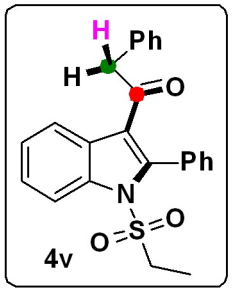
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C

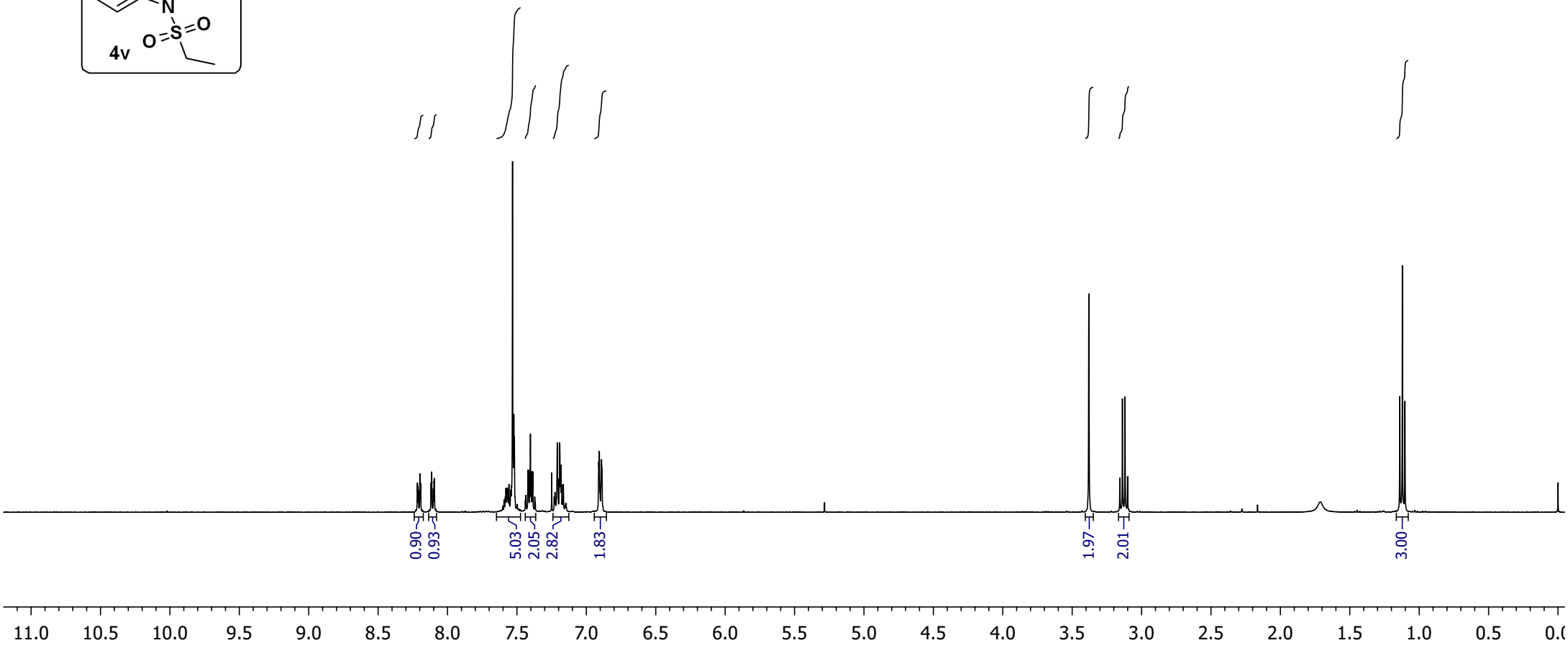






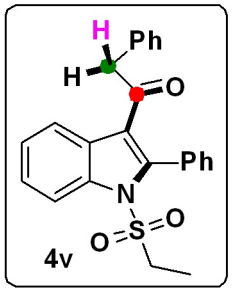
Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H

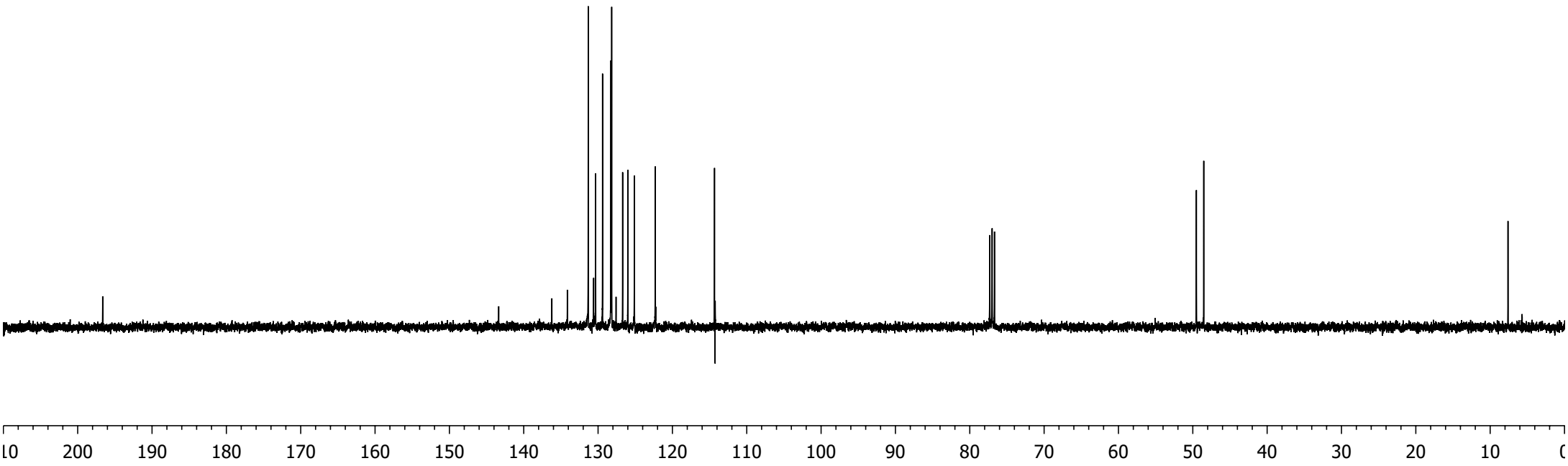




196.64 143.37 131.32 130.33 129.40 128.27 128.17 126.70 125.99 125.12 122.31 114.34 114.26 114.25 77.31 76.99 76.68 49.52 48.53 7.60

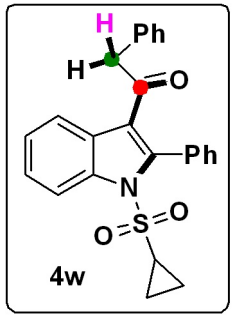
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C





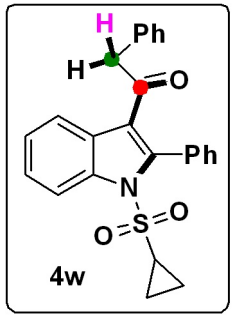
M0461-9
MC-20-20

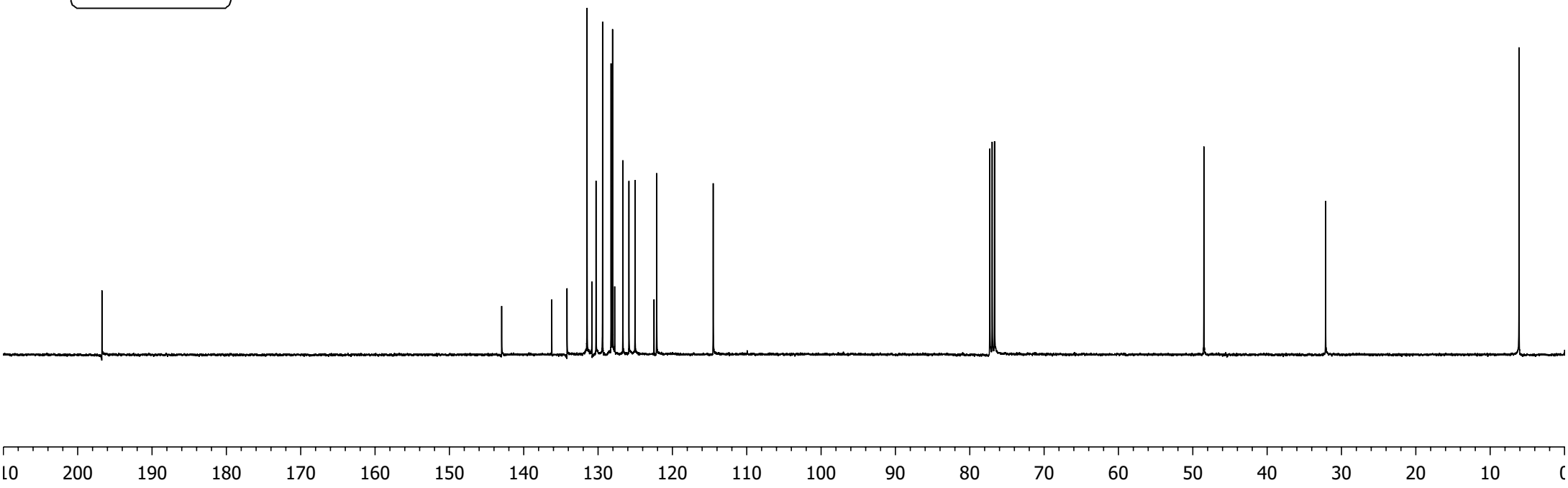
Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

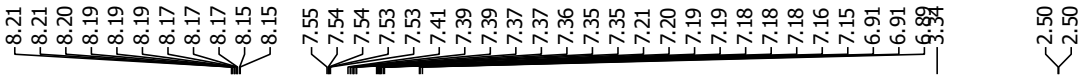


196.74 142.97 131.48 130.82 130.28 129.39 128.26 128.05 126.67 125.85 125.03 122.12 114.52 77.31 76.99 76.67 48.51 32.14 6.11

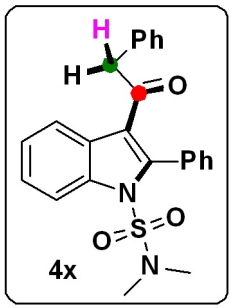
Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C





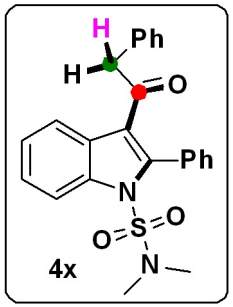


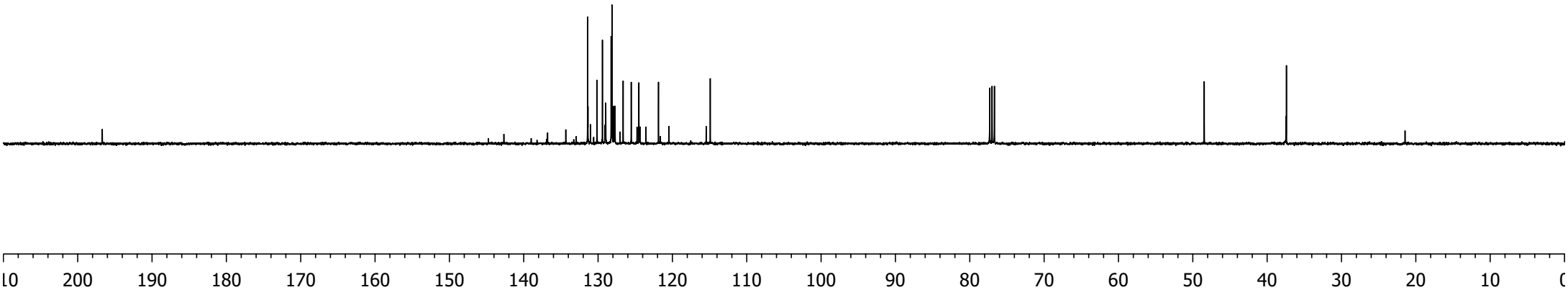
Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H



196.69
131.41
131.36
130.14
129.41
128.99
128.96
128.24
128.13
127.95
127.75
126.63
125.54
124.51
121.88
114.91
77.32
77.00
76.68
48.46
37.40

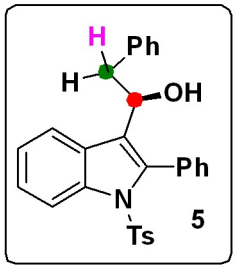
Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C





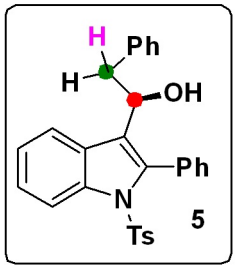
8.37 8.34 7.96 7.94 7.41 7.40 7.39 7.38 7.37 7.35 7.35 7.35 7.33 7.31 7.31 7.29 7.27 7.24 7.17 7.15 7.14 7.10 7.08 7.07 6.80 6.79 4.65 4.63 4.62 3.18 3.17 3.15 3.14 3.13 3.12 3.11 3.09 2.34

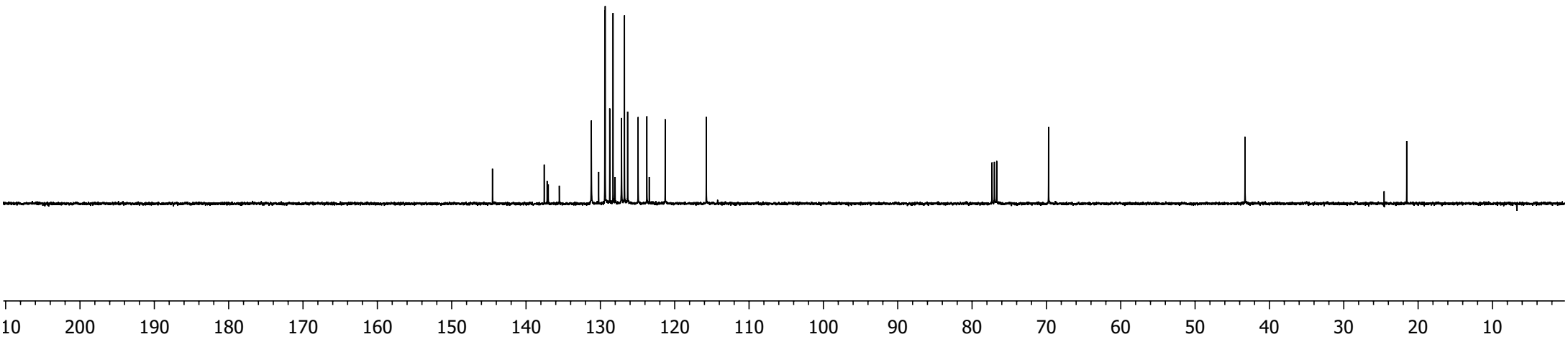
Solvent $CDCl_3$
Spectrometer Frequency 400.28
Nucleus ^1H



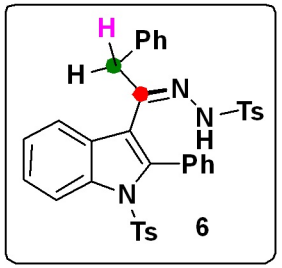
144.52
129.41
129.35
128.74
128.29
127.16
126.76
126.33
124.93
123.75
121.28
115.75
77.32
77.00
76.68
69.71
43.29
21.54

Solvent $CDCl_3$
Spectrometer Frequency 100.66
Nucleus ^{13}C



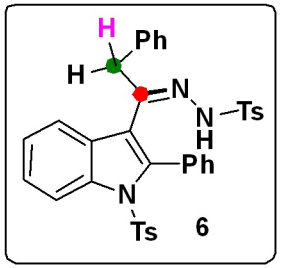


Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

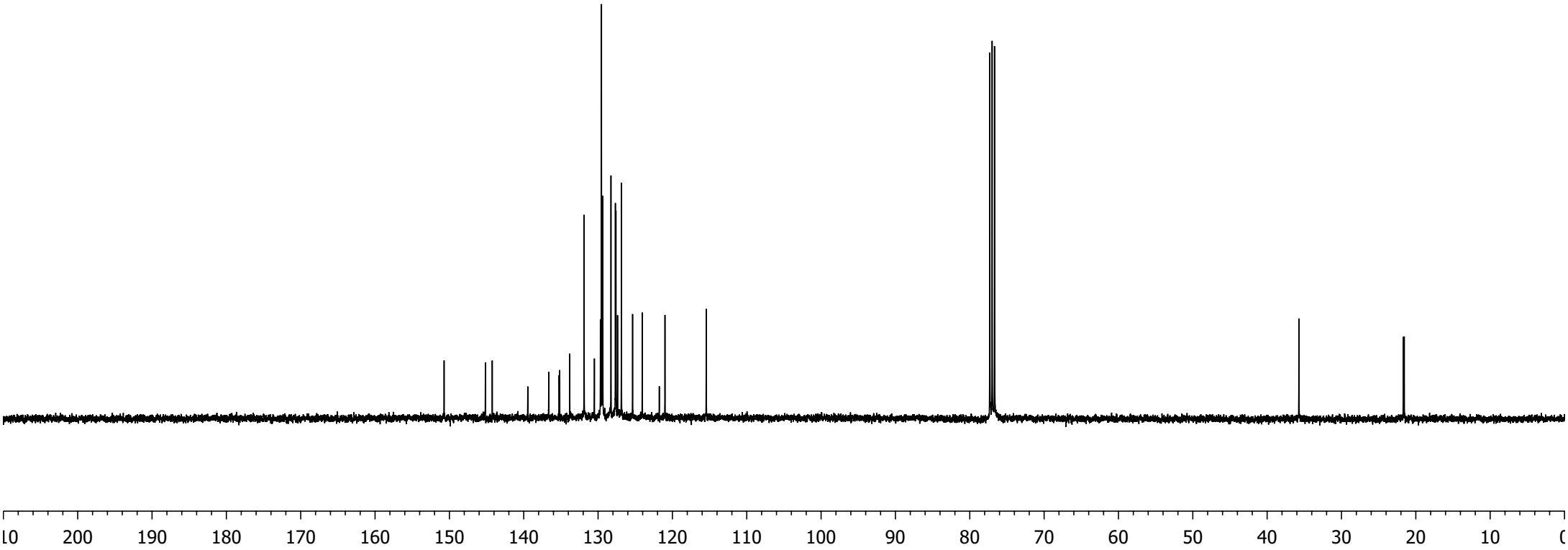


150.71
133.82
131.88
129.69
129.54
129.36
128.26
127.67
127.60
127.38
126.86
125.35
124.06
121.90
115.45
77.31
76.99
76.67
35.73
21.69
21.55

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C

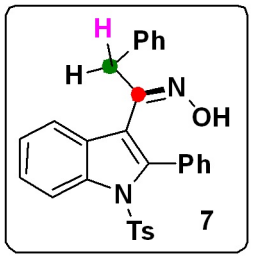


6

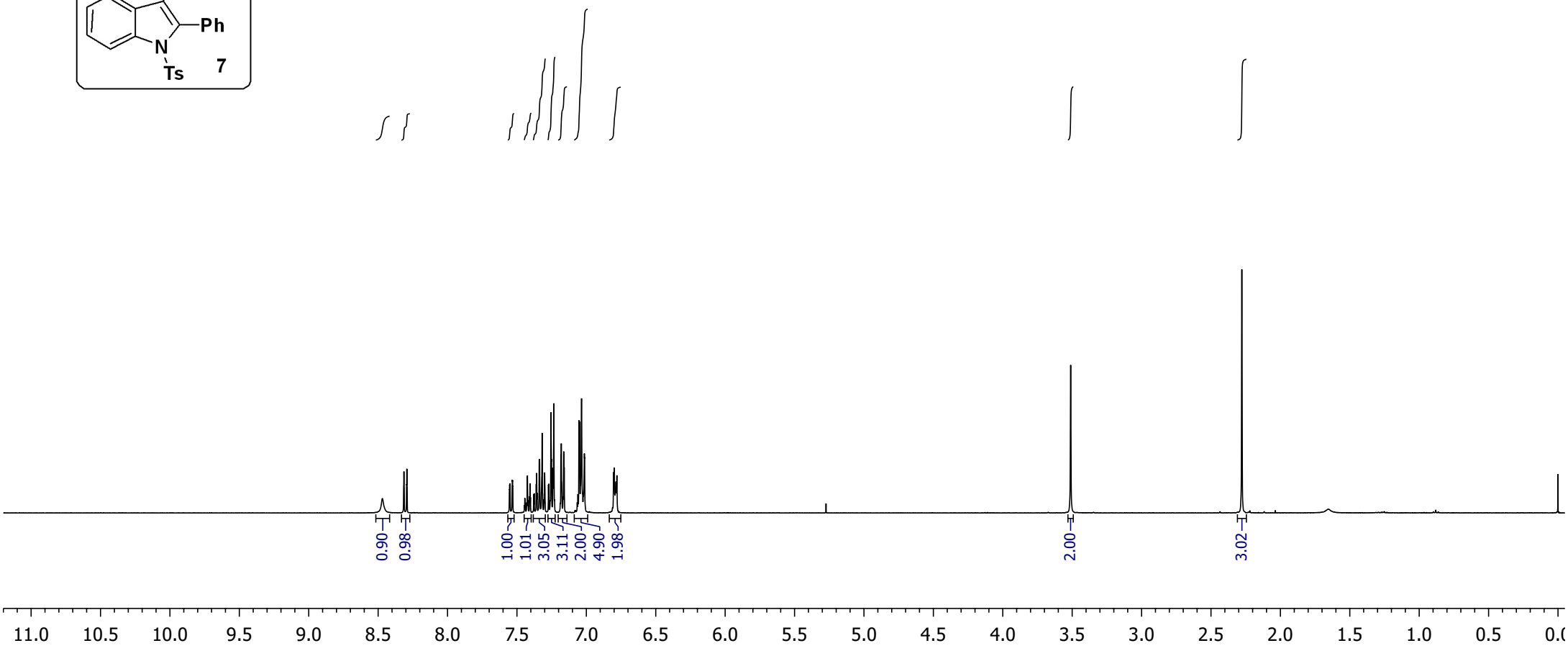


8.47 8.31 8.29 7.55 7.55 7.53 7.53 7.42 7.41 7.36 7.36 7.35 7.34 7.34 7.32 7.30 7.27 7.27 7.25 7.25 7.24 7.24 7.23 7.18 7.18 7.16 7.16 7.05 7.05 7.04 7.03 7.01 7.01 6.80 6.80 6.79 6.78 3.51 2.28

Solvent $CDCl_3$
Spectrometer Frequency 400.39
Nucleus ^1H

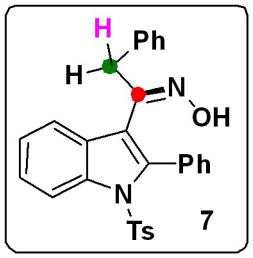


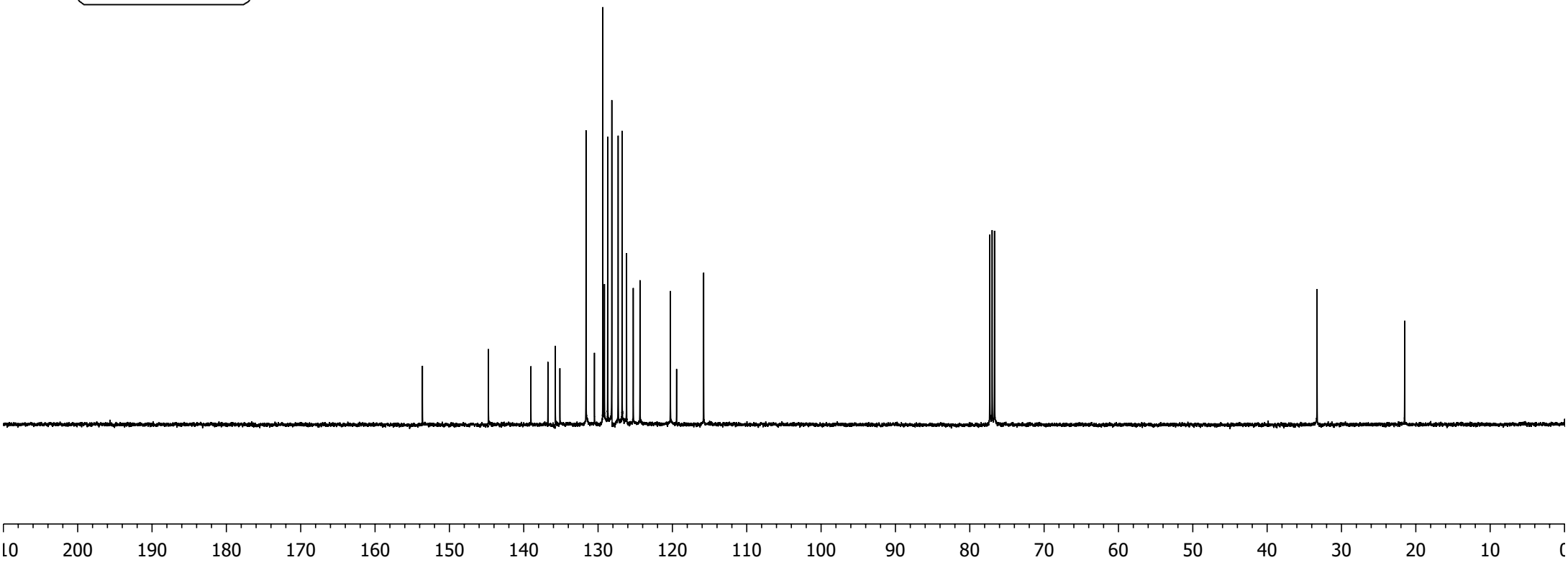
7



153.63
144.75
139.04
136.75
135.76
135.13
131.62
130.49
129.36
129.14
128.71
128.15
127.30
126.78
126.17
125.27
124.36
120.28
119.44
115.80
77.31
76.99
76.67
33.28
21.51

Solvent $CDCl_3$
Spectrometer Frequency 100.69
Nucleus ^{13}C



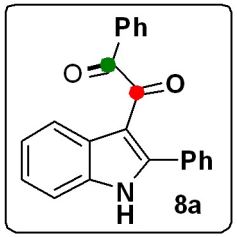


U0366-1
MC-20-39-2

12.63

8.17 8.16 7.69 7.67 7.67 7.67 7.66 7.64 7.54 7.52 7.50 7.48 7.46 7.38 7.37 7.35 7.35 7.34 7.34 7.32 7.32 7.30 7.28 7.23 7.21 7.19

Solvent DMSO-d_6
Spectrometer Frequency 400.28
Nucleus ^1H

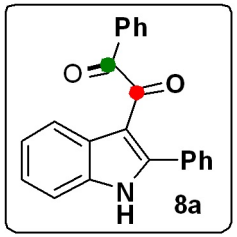


0.98 1.00 3.08 1.03 2.09 5.31 2.08

13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

193.55
190.33
148.70
135.98
134.21
133.14
130.45
130.13
129.70
129.15
128.83
127.86
126.80
123.82
122.88
121.04
112.27
110.15
40.13
39.92
39.71
39.50
39.29
39.09
38.88

Solvent DMSO-d_6
Spectrometer Frequency 100.66
Nucleus ^{13}C



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) k11301-jjw-a_auto

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: k11301-jjw-a_auto

```
Bond precision:   C-C = 0.0023 A           Wavelength=0.71073

Cell:           a=10.0336(2)       b=11.9429(2)      c=13.2152(2)
                alpha=87.388(1)    beta=78.345(1)    gamma=75.543(1)
Temperature:    130 K

                Calculated                 Reported
Volume          1501.80(5)                 1501.80(5)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  C36 H29 N O5 S2            C36 H29 N O5 S2
Sum formula     C36 H29 N O5 S2            C36 H29 N O5 S2
Mr              619.72                     619.72
Dx,g cm-3       1.370                      1.370
Z               2                          2
Mu (mm-1)       0.223                      0.223
F000            648.0                      648.0
F000'           648.78
h,k,lmax        12,15,17                   12,15,16
Nref            6785                       6361
Tmin,Tmax       0.923,0.956                0.815,1.000
Tmin'           0.894

Correction method= # Reported T Limits: Tmin=0.815 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.938           Theta(max)= 27.346

R(reflections)= 0.0369( 5508)                    wR2(reflections)=
                                                 0.1010( 6361)
S = 1.095                  Npar= 399
```

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

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         10 Report
               -4  1  0,   4  2  1,   0  5  2,   1 11  9,   0 10 10,   1 10 10,
                1 11 10,   2 11 10,   1 10 11,   2 10 11,
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        409 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
               -4  1  0,   0  5  2,   0 10 10,   2 15  2,   4  2  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       3.35 Note
             Predicted wR2: Based on SigI**2  3.02 or SHELX Weight  9.53
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         16 Info
```

---

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock k11301-jjw-a_auto - ellipsoid plot

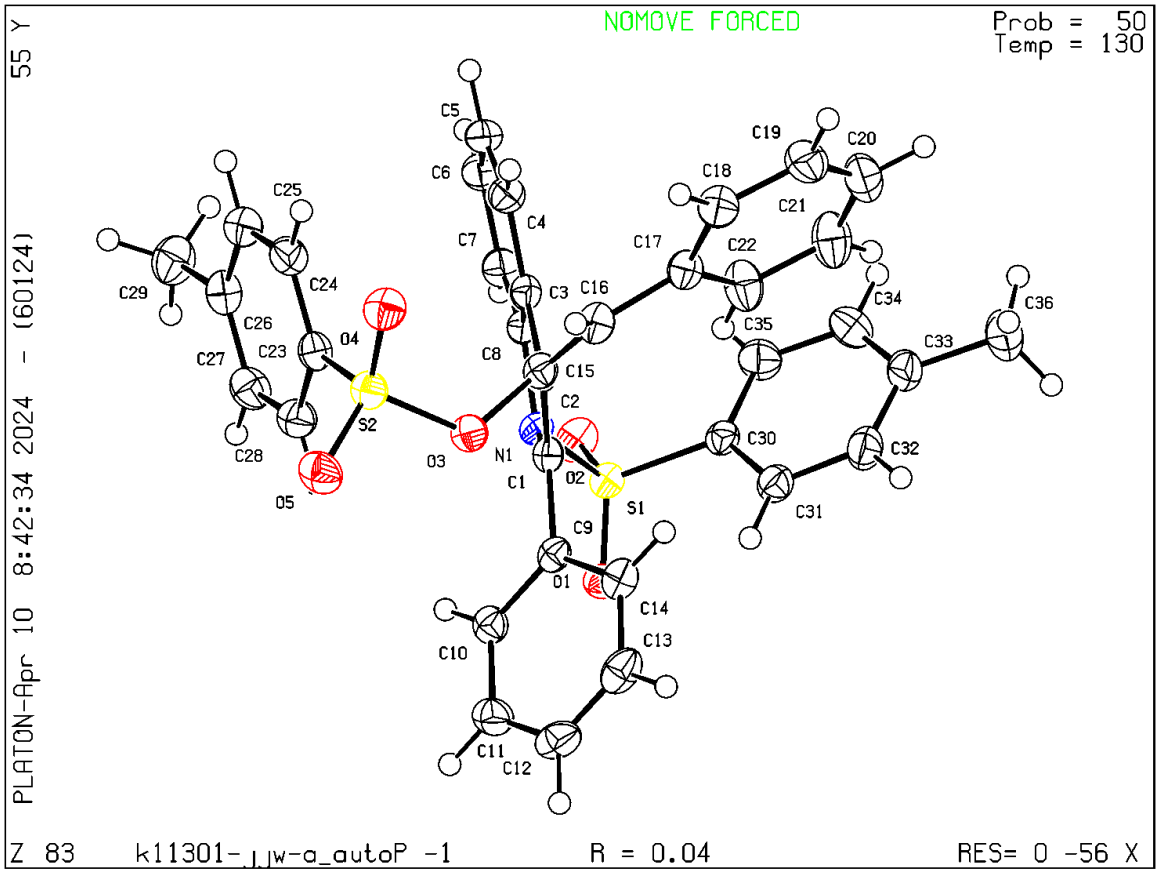
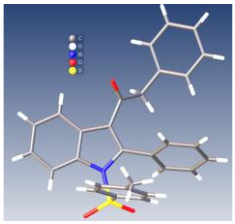


Table 1. Crystal data and structure refinement for d25047.



X-ray of **4a**

Identification code	d25047	
Empirical formula	C29 H23 N O3 S	
Formula weight	465.54	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 32.4449(14) Å	α= 90°.
	b = 8.4715(3) Å	β= 90°.
	c = 17.0615(7) Å	γ = 90°.
Volume	4689.5(3) $Å^3$	
Z	8	
Density (calculated)	1.319 Mg/m^3	
Absorption coefficient	0.170 mm^{-1}	
F(000)	1952	
Crystal size	0.43 x 0.30 x 0.16 mm^3	
Theta range for data collection	2.39 to 25.41°.	
Index ranges	-39<=h<=37, -9<=k<=10, -20<=l<=18	
Reflections collected	26420	
Independent reflections	4300 [R(int) = 0.0660]	
Completeness to theta = 25.41°	99.3 %	
Absorption correction	None	
Max. and min. transmission	0.9733 and 0.9305	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4300 / 0 / 308	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0425, wR2 = 0.1180	
R indices (all data)	R1 = 0.0551, wR2 = 0.1296	
Largest diff. peak and hole	0.196 and -0.371 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d25047. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5701(1)	1917(2)	5384(1)	34(1)
C(2)	5316(1)	1729(3)	5034(1)	45(1)
C(3)	4987(1)	2609(3)	5307(1)	51(1)
C(4)	5034(1)	3666(3)	5923(1)	46(1)
C(5)	4673(1)	4604(3)	6219(2)	70(1)
C(6)	5421(1)	3816(3)	6261(1)	48(1)
C(7)	5755(1)	2960(2)	5995(1)	42(1)
C(8)	6397(1)	3171(2)	4093(1)	33(1)
C(9)	6617(1)	4045(2)	4723(1)	33(1)
C(10)	6456(1)	5475(2)	4980(1)	41(1)
C(11)	6664(1)	6377(3)	5532(1)	50(1)
C(12)	7037(1)	5871(2)	5820(1)	51(1)
C(13)	7202(1)	4468(3)	5563(1)	53(1)
C(14)	6992(1)	3550(3)	5022(1)	44(1)
C(15)	6301(1)	3712(2)	3362(1)	33(1)
C(16)	6419(1)	5226(2)	2990(1)	39(1)
C(17)	6862(1)	5765(2)	3057(1)	44(1)
C(18)	6929(1)	7516(2)	2974(1)	38(1)
C(19)	7052(1)	8396(3)	3618(1)	51(1)
C(20)	7120(1)	10000(3)	3543(2)	63(1)
C(21)	7059(1)	10740(3)	2833(2)	62(1)
C(22)	6935(1)	9884(3)	2196(2)	55(1)
C(23)	6872(1)	8270(2)	2265(1)	44(1)
C(24)	6059(1)	2520(2)	2967(1)	36(1)
C(25)	5889(1)	2447(3)	2213(1)	47(1)
C(26)	5678(1)	1111(3)	2002(1)	60(1)
C(27)	5639(1)	-148(3)	2513(1)	67(1)
C(28)	5814(1)	-133(3)	3250(1)	55(1)
C(29)	6020(1)	1238(2)	3471(1)	37(1)
N(1)	6235(1)	1618(2)	4175(1)	35(1)
O(1)	5980(1)	-769(2)	4869(1)	48(1)

O(2)	6462(1)	1020(2)	5545(1)	46(1)
O(3)	6169(1)	5922(2)	2585(1)	56(1)
S(1)	6117(1)	791(1)	5045(1)	36(1)

Table 3. Bond lengths [Å] and angles [°] for d25047.

C(1)-C(7)	1.378(3)
C(1)-C(2)	1.395(3)
C(1)-S(1)	1.7528(19)
C(2)-C(3)	1.382(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.389(3)
C(3)-H(3)	0.9500
C(4)-C(6)	1.388(3)
C(4)-C(5)	1.505(3)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.380(3)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(15)	1.366(2)
C(8)-N(1)	1.424(2)
C(8)-C(9)	1.486(2)
C(9)-C(14)	1.387(3)
C(9)-C(10)	1.390(3)
C(10)-C(11)	1.389(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.376(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.374(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.385(3)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(24)	1.445(3)
C(15)-C(16)	1.481(3)
C(16)-O(3)	1.217(2)
C(16)-C(17)	1.514(3)
C(17)-C(18)	1.506(3)

C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(23)	1.381(3)
C(18)-C(19)	1.386(3)
C(19)-C(20)	1.383(4)
C(19)-H(19)	0.9500
C(20)-C(21)	1.378(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.367(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.388(3)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(29)	1.391(3)
C(24)-C(25)	1.401(3)
C(25)-C(26)	1.371(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.382(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.380(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.393(3)
C(28)-H(28)	0.9500
C(29)-N(1)	1.426(2)
N(1)-S(1)	1.6840(15)
O(1)-S(1)	1.4269(14)
O(2)-S(1)	1.4193(14)

C(7)-C(1)-C(2)	120.82(18)
C(7)-C(1)-S(1)	120.02(14)
C(2)-C(1)-S(1)	119.15(15)
C(3)-C(2)-C(1)	118.98(19)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	121.23(19)
C(2)-C(3)-H(3)	119.4

C(4)-C(3)-H(3)	119.4
C(3)-C(4)-C(6)	118.24(19)
C(3)-C(4)-C(5)	120.6(2)
C(6)-C(4)-C(5)	121.2(2)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(4)	121.68(19)
C(7)-C(6)-H(6)	119.2
C(4)-C(6)-H(6)	119.2
C(1)-C(7)-C(6)	119.04(18)
C(1)-C(7)-H(7)	120.5
C(6)-C(7)-H(7)	120.5
C(15)-C(8)-N(1)	108.35(15)
C(15)-C(8)-C(9)	127.09(17)
N(1)-C(8)-C(9)	124.51(15)
C(14)-C(9)-C(10)	118.52(18)
C(14)-C(9)-C(8)	122.45(17)
C(10)-C(9)-C(8)	118.84(17)
C(11)-C(10)-C(9)	120.73(19)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(12)-C(11)-C(10)	119.9(2)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	119.86(19)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	120.5(2)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(13)-C(14)-C(9)	120.5(2)
C(13)-C(14)-H(14)	119.8

C(9)-C(14)-H(14)	119.8
C(8)-C(15)-C(24)	108.42(16)
C(8)-C(15)-C(16)	128.51(17)
C(24)-C(15)-C(16)	123.06(16)
O(3)-C(16)-C(15)	119.40(17)
O(3)-C(16)-C(17)	121.92(18)
C(15)-C(16)-C(17)	118.34(16)
C(18)-C(17)-C(16)	115.23(17)
C(18)-C(17)-H(17A)	108.5
C(16)-C(17)-H(17A)	108.5
C(18)-C(17)-H(17B)	108.5
C(16)-C(17)-H(17B)	108.5
H(17A)-C(17)-H(17B)	107.5
C(23)-C(18)-C(19)	118.98(19)
C(23)-C(18)-C(17)	121.22(18)
C(19)-C(18)-C(17)	119.79(19)
C(20)-C(19)-C(18)	120.1(2)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(21)-C(20)-C(19)	120.4(2)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	120.0(2)
C(22)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0
C(21)-C(22)-C(23)	119.9(2)
C(21)-C(22)-H(22)	120.0
C(23)-C(22)-H(22)	120.0
C(18)-C(23)-C(22)	120.6(2)
C(18)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(29)-C(24)-C(25)	119.84(19)
C(29)-C(24)-C(15)	107.84(16)
C(25)-C(24)-C(15)	132.28(19)
C(26)-C(25)-C(24)	118.3(2)
C(26)-C(25)-H(25)	120.9

C(24)-C(25)-H(25)	120.9
C(25)-C(26)-C(27)	121.1(2)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(26)-C(27)-C(28)	122.0(2)
C(26)-C(27)-H(27)	119.0
C(28)-C(27)-H(27)	119.0
C(27)-C(28)-C(29)	116.9(2)
C(27)-C(28)-H(28)	121.6
C(29)-C(28)-H(28)	121.6
C(24)-C(29)-C(28)	121.82(18)
C(24)-C(29)-N(1)	107.50(16)
C(28)-C(29)-N(1)	130.64(19)
C(8)-N(1)-C(29)	107.86(15)
C(8)-N(1)-S(1)	123.66(12)
C(29)-N(1)-S(1)	122.52(13)
O(2)-S(1)-O(1)	119.95(9)
O(2)-S(1)-N(1)	107.12(8)
O(1)-S(1)-N(1)	105.72(8)
O(2)-S(1)-C(1)	109.52(9)
O(1)-S(1)-C(1)	109.41(9)
N(1)-S(1)-C(1)	103.84(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for d25047. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(1)	32(1)	36(1)	4(1)	2(1)	-4(1)
C(2)	41(1)	45(1)	48(1)	-7(1)	-2(1)	-5(1)
C(3)	35(1)	58(1)	61(1)	-2(1)	-2(1)	-4(1)
C(4)	42(1)	42(1)	55(1)	3(1)	12(1)	-1(1)
C(5)	52(2)	69(2)	88(2)	-4(2)	21(1)	8(1)
C(6)	48(1)	48(1)	48(1)	-8(1)	8(1)	-4(1)
C(7)	39(1)	47(1)	40(1)	-5(1)	-1(1)	-4(1)
C(8)	29(1)	31(1)	38(1)	-2(1)	2(1)	2(1)
C(9)	34(1)	30(1)	34(1)	0(1)	1(1)	0(1)
C(10)	42(1)	38(1)	43(1)	-2(1)	-1(1)	3(1)
C(11)	67(2)	34(1)	47(1)	-8(1)	-1(1)	0(1)
C(12)	68(2)	41(1)	43(1)	-1(1)	-14(1)	-13(1)
C(13)	53(1)	48(1)	58(1)	0(1)	-20(1)	-3(1)
C(14)	43(1)	38(1)	52(1)	-5(1)	-9(1)	3(1)
C(15)	30(1)	33(1)	37(1)	0(1)	-1(1)	2(1)
C(16)	37(1)	42(1)	37(1)	4(1)	-2(1)	2(1)
C(17)	36(1)	46(1)	48(1)	9(1)	-1(1)	-1(1)
C(18)	29(1)	42(1)	42(1)	1(1)	3(1)	-2(1)
C(19)	40(1)	70(2)	43(1)	-9(1)	2(1)	-2(1)
C(20)	44(1)	65(2)	80(2)	-38(2)	5(1)	-1(1)
C(21)	38(1)	36(1)	114(2)	-7(1)	6(1)	2(1)
C(22)	45(1)	44(1)	75(2)	13(1)	-3(1)	-5(1)
C(23)	44(1)	45(1)	44(1)	3(1)	-1(1)	-7(1)
C(24)	31(1)	39(1)	37(1)	-6(1)	1(1)	4(1)
C(25)	50(1)	52(1)	39(1)	-6(1)	-3(1)	8(1)
C(26)	68(2)	67(2)	44(1)	-19(1)	-12(1)	-3(1)
C(27)	84(2)	58(2)	58(1)	-22(1)	-7(1)	-20(1)
C(28)	72(2)	43(1)	49(1)	-11(1)	0(1)	-13(1)
C(29)	40(1)	36(1)	36(1)	-8(1)	4(1)	0(1)
N(1)	38(1)	30(1)	37(1)	-2(1)	0(1)	-2(1)
O(1)	58(1)	28(1)	59(1)	3(1)	2(1)	-1(1)

O(2)	42(1)	49(1)	46(1)	9(1)	-9(1)	5(1)
O(3)	45(1)	58(1)	66(1)	25(1)	-17(1)	-6(1)
S(1)	39(1)	31(1)	39(1)	4(1)	0(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d25047.

	x	y	z	U(eq)
H(2)	5279	1007	4613	53
H(3)	4724	2490	5069	62
H(5A)	4772	5492	6535	105
H(5B)	4497	3924	6542	105
H(5C)	4513	5005	5774	105
H(6)	5457	4525	6687	57
H(7)	6019	3089	6229	50
H(10)	6200	5839	4776	49
H(11)	6549	7343	5711	59
H(12)	7181	6489	6196	61
H(13)	7461	4126	5758	63
H(14)	7107	2575	4855	53
H(17A)	6970	5428	3573	52
H(17B)	7026	5219	2649	52
H(19)	7090	7897	4111	61
H(20)	7209	10595	3983	76
H(21)	7103	11845	2787	75
H(22)	6893	10394	1706	65
H(23)	6788	7678	1820	53
H(25)	5918	3302	1857	56
H(26)	5556	1048	1497	72
H(27)	5487	-1050	2351	80
H(28)	5795	-1018	3590	66