Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

For

Alkene Versus Alkyne Reactivity in Unactivated 1,6-Enynes: Regio- and Chemoselective Radical Cyclization with Chalcogens under metal- and oxidant-free conditions

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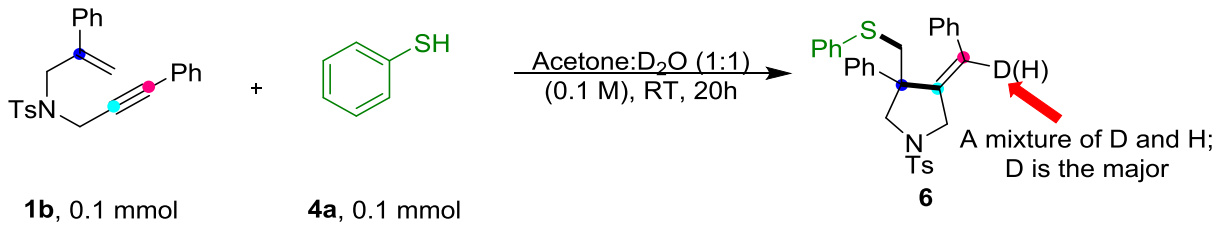
1. General Information

^{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 of doublet; dt, doublet of triplets; td, triplet of doublet; m, multiplet. Mass spectra and high-resolution mass spectra (HRMS) was measured using the LTQ Orbitrap XL (Thermo Fischer Scientific) Liquid chromatography–mass spectrometry at National Sun Yat-sen University. Melting points were determined on an EZ-Melt (Automated melting point apparatus). All IR (neat) λ max spectra were obtained as neat films with a Bruker FT-IR (neat) λ max SYSTEM and selected absorbance are reported in cm-1. 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. Control Experiments:

2.1 Procedure for the use of D_2O in experiment (5)



1b, 0.1 mmol **4a**, 0.1 mmol

2.2 Procedure for the 30 equivlance of D_2O in experiment (5ba')

To a overnight dried seal tube were added 1,6-enyne **1b** (0.1 mmol), **4a** (0.1 mmol) acetone:D_2O (1:1) (0.1 M). The resulting solution was stirred utpo starting material completion at room temperature. After that, the crude reaction mixture was diluted water and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to get **6** major.

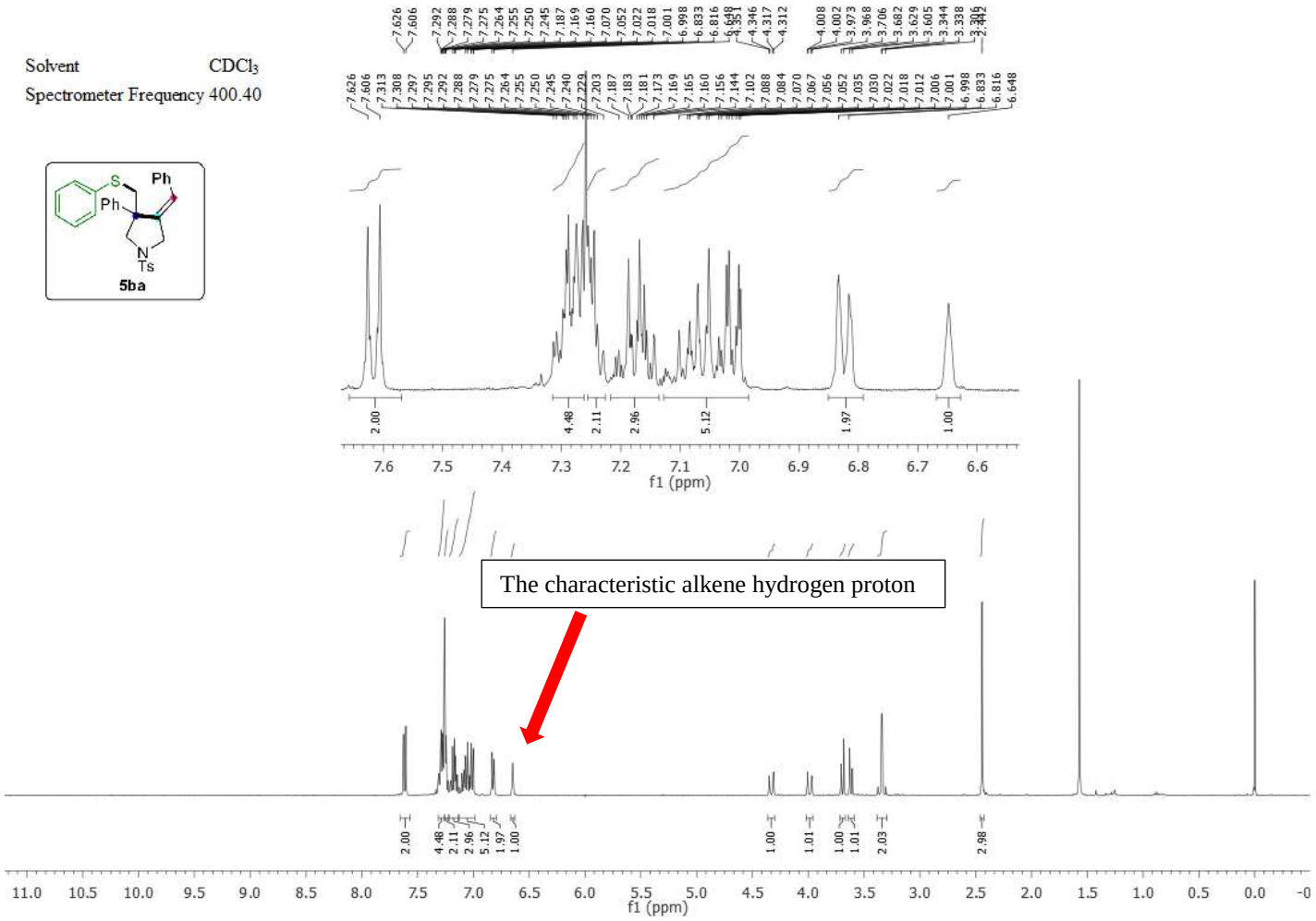


Figure S2. NMR spectra of the compound 5ba for reference

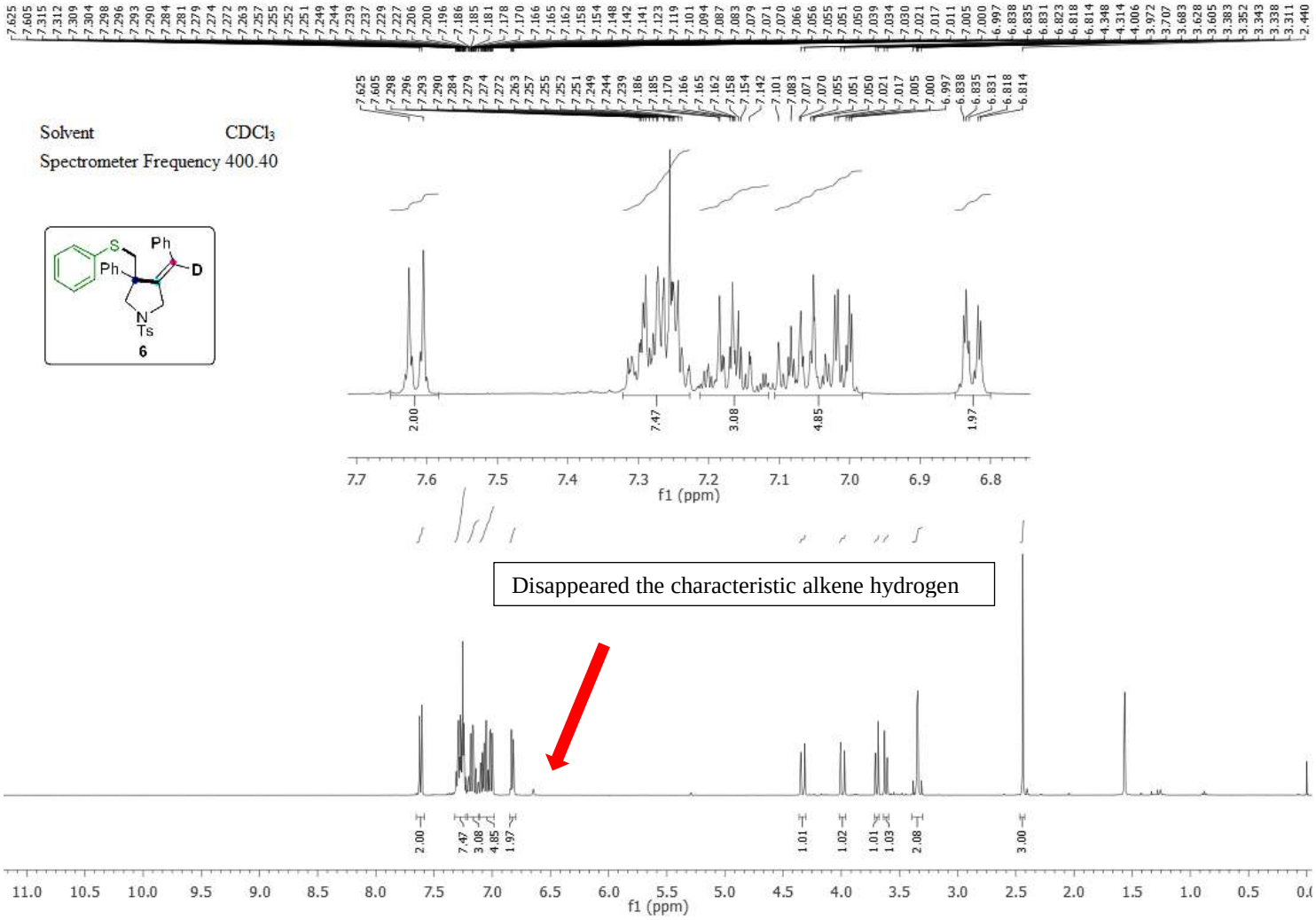


Figure S2. NMR spectra of the D_2O-mediated product

2.3 Reaction handling setup pictures:

Figure 1: Newly purched (99.5% + <= 0.1 ppm H_2O) dry acetone bottle

Figure 2: Bottle purged with nitrogen atomosphere

Figure 3: Acetone addition into the dry 4A° molecular sieves containing RB under nitrogen atomosphere

Figure 4: Acetone in RB under nitrogen atomosphere

Figure 5: Purging with nitrogen gas

Figure 6: starting material in vials for normal and dry reaction

Figure 7: Taking dry acetone from dry 4A° molecular sieves containing RB

Figure 8: Addition of dry solvent to reaction vial

Figure 1A: Previously used HPLC grade acetone

Figure 1B: Addition of normal acetone solvent to the vial

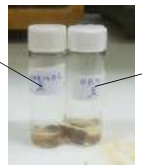


Figure 9: Normal solvent and dry solvent in reaction vials

Figure 10: vial under light irradiation

Figure 11: Vials under light irradiation in closed appearance

Figure 12: Reaction mixtures after 8.5 h

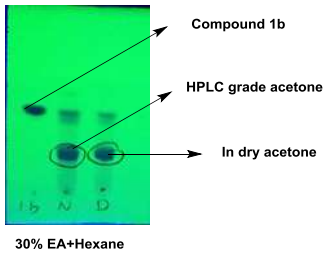
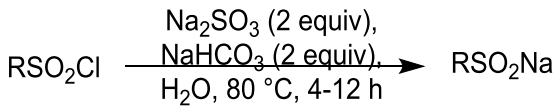


Figure 13: Both reactions progress on TLC

Reaction setup: Pictures represents the reactions setup while handling dry acetone and HPLC grade acetone

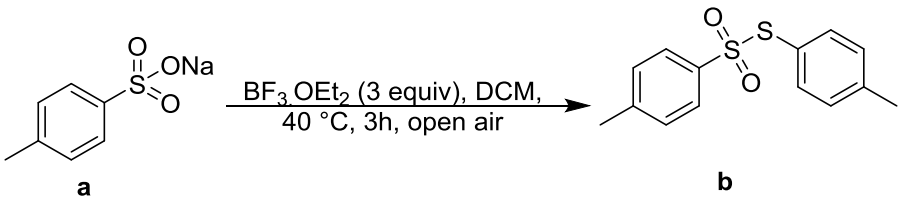
3. Preparation of Starting Materials

3.1 General procedure for the preparation of sodium sulfinates[1]



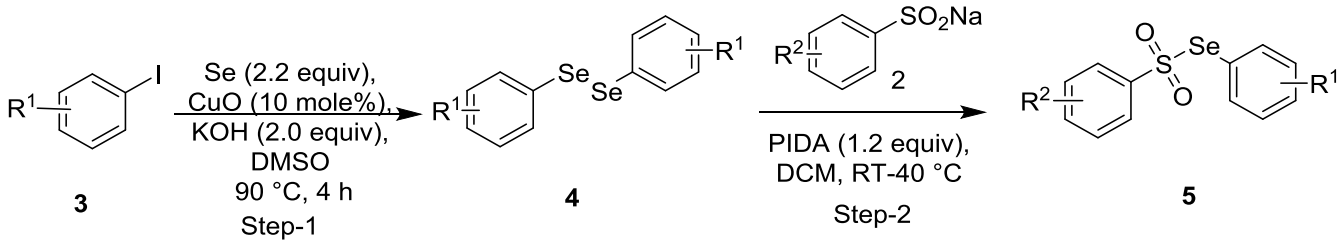
To a stirred solution of sodium sulfite (2 mmol), sodium bicarbonate (2 mmol) and the corresponding sulfonyl chloride (1 mmol) were dissolved in H_2O. After stirred at 80 °C for 4 h, the water was removed by a rotary evaporator. Then the remaining solid was extracted and recrystallized from ethanol to get the desired sodium sulfinate.

3.2 General procedure for the preparation of S-(p-tolyl) 4-methylbenzenesulfonothioate[2]



To a stirred solution of sodium sulfinate **a** (1 equiv), $BF_3{\cdot}OEt_2$ (3 equiv) in DCM (3 mL) was stirred at 40 °C under air for 3 h at open air. After completion of reaction in TLC, the reaction mixture was diluted with H_2O (15 mL) and extracted with DCM (3 × 15 mL). The organic extracts were dried over anhydrous Na_2SO_4. After filtration and evaporation of the solvents under reduced pressure, the crude product was purified by column chromatography on silica gel to afford desired product (**b**).

3.3 General procedure for the synthesis of selenosulfonates[3]

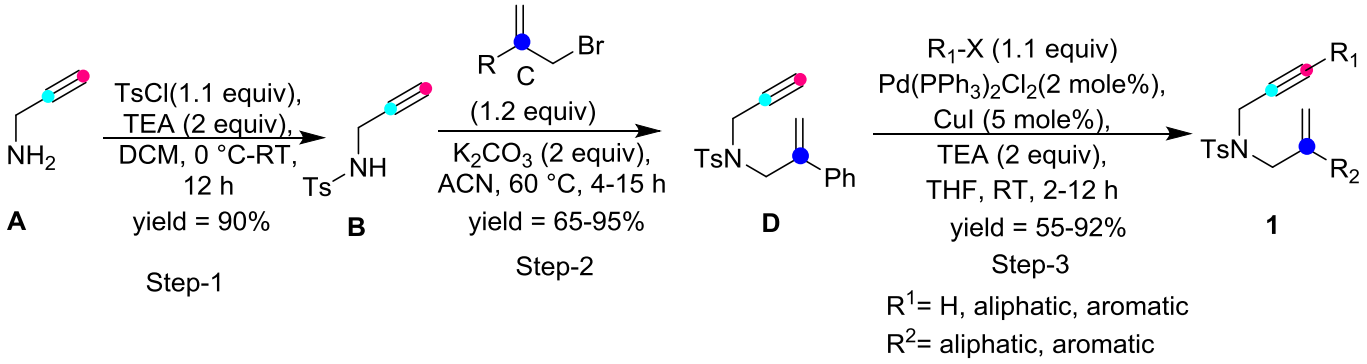


Step-1: To a stirred solution of Se metal (2.0 equiv) and halides (1.0 equiv.) in DMSO (10 mL) was added CuO nanoparticles (0.1 equiv.) followed by KOH (2.0 equiv.) under nitrogen atmosphere. The resulting reaction mixture was stirred at 90 C for 6 h. After the reaction was complete, the reaction mixture was allowed to cool, extraction with ethyl acetate. The combined organic layer was washed with brine, dried over Na_2SO_4, and

concentrated in vacuo. The crude product was purified by column chromatography on silica gel (PE:EA =100:1) to afford **4**.

Step-2: A suspension of appropriate sodium benzenesulfinates (4.0 equiv.) in CH_2Cl_2 (50 mL) containing **4** (1.0 equiv.) was cooled at 0 °C and [bis(trifluoroacetoxy)iodo]benzene (1.1 equiv.) in DCM was added dropwise. Then the mixture was stirred at room temperature to 40 °C for 4 h. The reaction mixture was washed with H_2O, dried over anhydrous Na_2SO_4. The solvent CH_2Cl_2 was removed under reduced pressure and the residue was purified by column chromatography on silica gel to afford compound **5**.

3.4 Preparation of Starting Materials 1,6-enynes[4]



3.5 General procedure for synthesis of 1,n-enynes (1)

General procedure for Step-1:

To a solution of prop-2-yn-1-amine (1 equiv) in DCM at 0 °C, TEA (2 equiv) and TsCl (1.1 equiv) were added. The resulting mixture was continued at room temperature for 16 h. The solvent was removed under reduced pressure and the resulting solid was dissolved in ethyl acetate, washed with water and brine and dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was carried out without further purification (**B**).

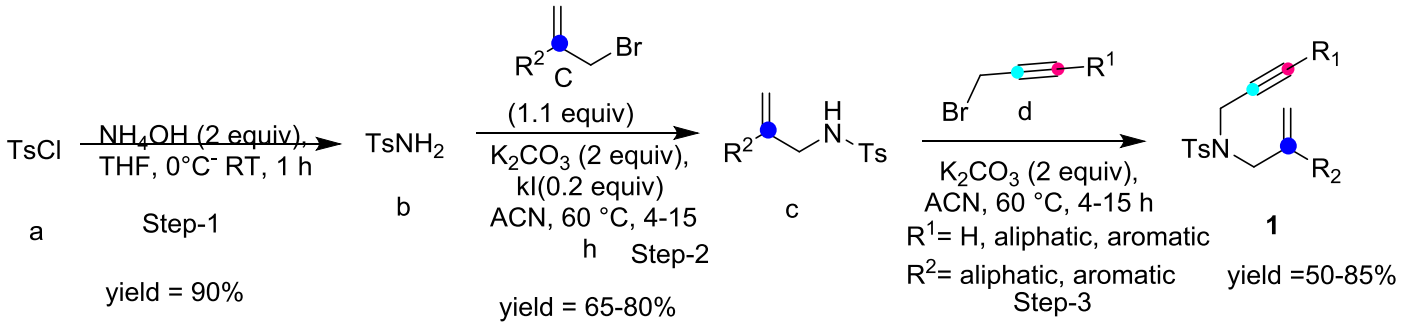
General procedure for Step-2:

To a solution of A (1 equiv) in ACN at 0 °C, K_2CO_3 (2 equiv) and allylbromide **C** (40.0 mmol) were added. The resulting mixture was heated under at 60 °C for 4-15 h. The reaction mixture cooled to RT and the solvent was removed under reduced pressure and the resulting solid was dissolved in ethyl acetate, washed with water and brine and dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified by chromatography to give compound (**D**).

General procedure for Step-3:

To a dried schlenk flask was added compound (**D**), iodoarene (1.1 equiv) followed by $Pd(PPh_3)_2Cl_2$ (2 mol%), CuI (5 mol %), in freshly distilled Et_3N under argon. The resulting mixture was stirred at RT for 2-12 h. After the completion of reaction by TLC, the reaction mixture was cooled to RT, diluted with water and extracted with ethyl acetate. The combined organic layer was dried over Na_2SO_4, filtered and concentrated to give crude material. The crude material was purified by column chromatography using hexane-ethyl acetate as the eluent (**1**).

3.6 Alternative route for the synthesis of compound (1)[5]



General procedure for Step-1:

To a stirred solution of ammonium hydroxide (30% aqueous solution) (2 equiv) in THF. the necessary sulfonyl chloride (1.0 equiv) or benzoyl chloride was added portion-wise at 0°C. The reaction mixture was stirred at r.t. for 1h, after which time the product had formed as a white solid precipitate, unless otherwise stated. The solid was collected by filtration, and washed with cold, water (3 x 10 mL). Subsequently, the product was recrystallised from ethyl acetate/hexanes and then dried in the vacuum oven overnight to get 4-methylbenzenesulfonamide.

General procedure for Step-2:

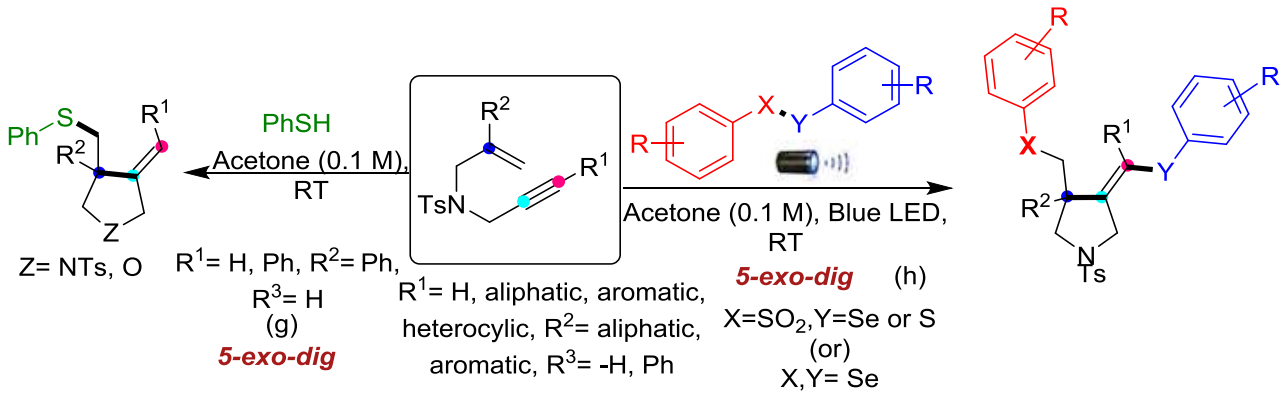
To a solution of A (1 equiv) in ACN at 0 °C, K_2CO_3 (2 equiv) and allylbromide **C** (1.1 equiv) were added. The resulting mixture was heated under at 60 °C for 4-15 h. The reaction mixture cooled to RT and the solvent was removed under reduced pressure and the resulting solid was dissolved in ethyl acetate, washed with water and brine and dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified by chromatography to give compound (**c**).

General procedure for Step-3:

To a solution of A (1 equiv) in ACN at 0 °C, K_2CO_3 (2 equiv) and allylbromide **C** (1.1 equiv) were added. The resulting mixture was heated under at 60 °C for 4-15 h. The reaction mixture cooled to RT and the solvent was removed under reduced pressure and the resulting solid was dissolved in ethyl acetate, washed with water and brine and dried over $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified by chromatography to give compound (**1)**.

4. Experimental procedures

4.1. General procedure for the Synthesis of N-heterocyclic compounds (3 and 5)



Scheme 1. Synthesis chalcongen containing Pyrrolidine

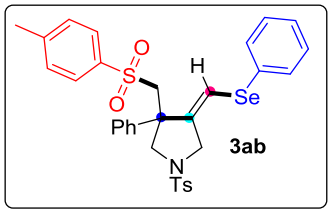
4.2 General procedure (A) for the synthesis of (Z)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-3-((phenylsulfonyl)methyl)-1-tosylpyrrolidine derivatives (3)

In an oven-dried screw-capped 5 mL vial equipped with a magnetic stir bar was charged with 1,6-enyne (1.0 equiv) chalcogen (1.0 equiv), acetone (0.1 M) was added. The resulting solution was stirred utpo starting material completion at room temperature under blue LED light. After that, the crude reaction mixture was diluted water and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography.

4.3 General procedure (B) for synthesis of (E)-4-benzylidene-3-phenyl-3-((phenylthio)methyl)-1-tosylpyrrolidine derivatives (5)

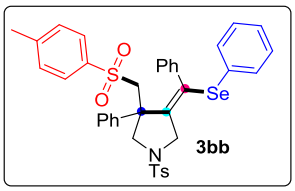
In an oven-dried screw-capped 5 mL vial equipped with a magnetic stir bar was charged with 1,6-enyne (1.0 equiv) aromatic thiols (1.0 equiv), acetone (0.1 M) was added. The resulting solution was stirred up to starting material completion at room temperature. After that, the crude reaction mixture was diluted water and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography.

(Z)-3-phenyl-4-((phenylselanyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3ab): The title compound



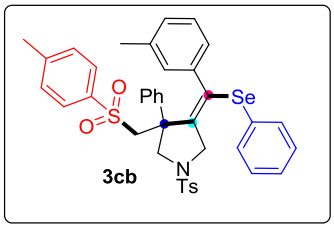
was prepared according to the general procedure A to obtain as a white solid (48 mg, yield = 75%); Mp. 150.5-151.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.38-7.31 (m, 6H), 7.28-7.26 (m, 3H), 7.20-7.18 (m, 2H), 7.11-7.08 (m, 3H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.43 (s, 1H), 4.62 (d, *J* = 10.4 Hz, 1H), 3.99 (d, *J* = 14.8 Hz, 1H), 3.70 (qd, J = 14.4, 2.4 Hz, 2H), 3.46 (d, *J* = 14.8 Hz, 1H), 3.37 (d, *J* = 10.4 Hz, 1H), 2.47 (s, 3H), 2.34 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 144.25, 143.91, 137.11, 136.98, 132.44, 132.15, 129.89, 129.53, 129.46, 128.47, 127.84, 127.71, 127.61, 127.19, 126.66, 114.89, 63.55, 55.85, 52.16, 50.61, 21.60, 21.50; IR (neat) λ max 3053, 2924, 1590, 1483, 1445, 1103, 1337, 1226, 1156, 1088, 1033, 821, 739 695, 669, 593, 557, 515, 466; HRMS (ESI) calcd for $C_{32}H_{32}NO_4S_2Se$ $[M+H]^+$ 638.0938; found: 638.0936.

(Z)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3bb): The title



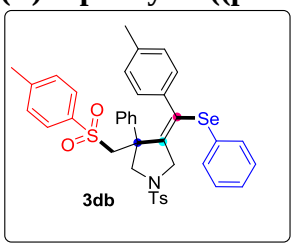
compound was prepared according to the general procedure A to obtain as a white solid (61 mg, yield = 82%); Mp. 165.8-166.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 8.4 Hz, 4H), 7.18 (d, *J* = 7.6 Hz, 2H), 7.13-7.07 (m, 8H), 7.01-6.97 (m, 2H), 6.91-6.87 (m, 1H), 6.79 (t, *J* = 8.0 Hz, 2H), 6.44 (s, 2H), 4.36 (d, *J* = 14.0 Hz, 1H), 4.10 (d, *J* = 14.4 Hz, 1H), 4.02 (d, *J* = 10 Hz, 1 H), 3.96 (d, *J* = 10.4 Hz, 1H), 3.48 (d, *J* = 14.8 Hz, 1H), 3.32 (d, *J* = 14.4 Hz, 1H), 2.50 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.35, 143.91, 142.70, 140.51, 138.31, 137.23, 135.63, 131.93, 130.05, 129.81, 129.63, 128.55, 128.20, 128.17, 128.01, 127.93, 127.35, 127.07, 17.00, 126.26, 61.58, 59.19, 54.58, 52.54; IR (neat) λ max 3055, 2931, 2589, 2309, 1904, 1808, 1739, 1592, 1330, 1158, 1084, 1030, 891, 743, 683, 561; HRMS (ESI) calcd for $C_{38}H_{36}NO_4S_2Se$ $[M+H]^+$ 714.1251; found: 714.1250.

(Z)-3-phenyl-4-((phenylselanyl)(m-tolyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3cb): The title



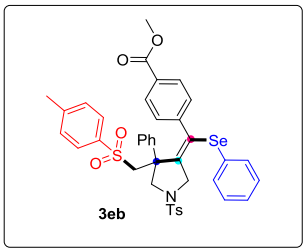
compound was prepared according to the general procedure A to obtain as a white solid (59 mg, yield = 80%); Mp. 147.5-147.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.13-7.09 (m, 8H), 7.01-6.98 (m, 2H), 6.71-6.67 (m, 2H), 6.32 (s, 1H), 6.03 (s, 1H), 4.37 (d, J = 14.0 Hz, 1H), 4.08 (d, J = 14.0 Hz, 1H), 4.02-3.96 (m, 2H), 3.48 (d, J = 14.8 Hz, 1H), 3.32 (d, J = 14.8 Hz, 1H), 2.49 (s, 3H), 2.39 (s, 3H), 1.86 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.36, 143.88, 143.15, 140.48, 138.41, 136.96, 136.48, 135.54, 131.84, 130.07, 130.03, 129.77, 129.63, 128.43, 128.16, 128.10, 128.06, 127.93, 127.72, 127.32, 126.92, 126.91, 126.15, 126.08, 61.33, 59.23, 54.61, 52.37, 21.64, 21.52, 20.92; IR (neat) λ max 3056, 2926, 1592, 1484, 1445, 1344, 1155, 1091, 824, 740, 697, 555; HRMS (EI) calcd for $C_{39}H_{38}NO_4S_2Se$ $[M+H]^+$ 728.1407; found: 728.1409.

(Z)-3-phenyl-4-((phenylselanyl)(p-tolyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3db): The title compound was prepared according to the general procedure A to obtain as a white solid (57 mg, yield = 78%); Mp. 176.1-176.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.2 Hz, 2H), 7.42-7.38 (m, 4H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.10-7.09 (m, 8H), 7.02-6.98 (m, 2H), 6.61 (d, *J* = 8.0 Hz, 2H), 6.36 (d, *J* = 6.8 Hz, 2H), 4.32 (d, *J* = 14.0 Hz, 1H), 4.08 (d, *J* = 14.4 Hz, 1H), 4.03 (d, *J* = 10.0 Hz, 1H), 3.92 (d, *J* = 10.4 Hz, 1H), 3.45 (d, *J* = 14.4 Hz, 1H), 3.31 (d, *J* = 14.8 Hz, 1H), 2.49 (s, 3H), 2.38 (s, 3H), 2.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.28, 143.85, 142.62, 140.83, 138.24, 136.89, 135.25, 134.47, 131.92, 129.90, 129.77, 129.55, 129.07, 128.54, 128.16, 128.10, 127.83, 127.72, 127.32, 126.97, 126.29, 61.63, 59.00, 54.55, 52.51, 21.63, 21.51, 20.98; IR (neat) λ max 3049, 2933, 1912, 1594, 1467, 1329, 1158, 1083, 900, 818, 742, 674, 553; HRMS (ESI) calcd for $C_{39}H_3{}_8NO_4S_2Se$ $[M+H]^+$ 728.1407; found: 728.1400.



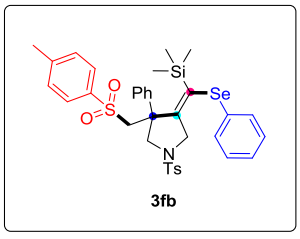
3db

(Z)-4-(((3-fluorophenyl)selanyl)(phenyl)methylene)-3-phenyl-1-tosyl-3-(tosylmethyl)pyrrolidine (3eb): The title compound was prepared according to the general procedure A to obtain as a white solid (52 mg, yield = 68%); Mp. 88.4-89.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.41 (d, J = 8.0 Hz, 4H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.13-7.07 (m, 6H), 7.03-6.98 (m, 4H), 6.44 (s, 2H), 4.48 (d, *J* = 14.0 Hz, 1H), 4.17 (d, *J* = 14.4 Hz, 1H), 4.11 (d, *J* = 10.0 Hz, 1H), 3. 87 (t, *J* = 4.0 Hz, 1 H), 3.82 (s, 3H), 3.46 (d, J = 14.4 Hz, 1H), 3.31 (d, J = 14.4 Hz, 1H), 2.49 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.38, 144.64, 144.00, 143.42, 142.14, 141.75, 138.33, 135.62, 131.73, 129.80, 129.11, 128.73, 128.35, 128.31, 128.17, 127.29, 127.19, 125.92, 61.01, 59.58, 55.11, 52.35, 52.04, 21.66, 21.55; IR (neat) λ max 3057, 1719, 1597, 1441, 1280, 1155, 1100, 822, 741, 597, 552; HRMS (ESI) calcd for $C_{40}H_{38}$ NO_6S_2Se $[M+H]^+$ 772.1306; found: 772.1306.



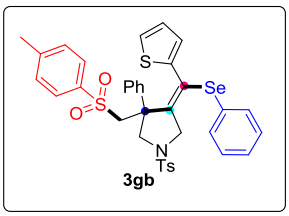
3eb

(Z)-3-phenyl-4-((phenylselanyl)(trimethylsilyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3fb): The title compound was prepared according to the general procedure A to obtain as a white solid (58 mg, yield = 81%); Mp. 171.6-172.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.45-7.41 (m, 4H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.29-7.24 (m, 6H), 7.21-7.19 (m, 5H), 4.30 (d, *J* = 15.6 Hz, 1H), 4.12 (d, *J* = 9.2 Hz, 1H), 3.90-3.85 (m, 3H), 3.43 (d, *J* = 9.2 Hz, 1H), 2.46 (s, 3H), 2.41 (s, 3H), 0.08 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.77, 144.80, 143.78, 143.50, 138.77, 132.47, 131.76, 130.99, 130.69, 130.03, 129.45, 129.19, 128.58, 128.00, 127.53, 127.45, 126.83, 126.35, 62.95, 61.68, 59.40, 53.46, 21.62, 21.59, 1.15; IR (neat) λ max 3057, 2955, 1590, 1483, 1443, 1344, 1251, 1155, 1089, 1029, 840, 672, 598, 556; HRMS (ESI) calcd for C35H39NO4S2NaSiSe $[M+H]^+$ 732.1153; found: 732.1152.



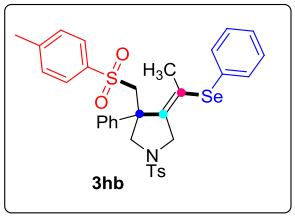
3fb

(Z)-3-phenyl-4-((phenylselanyl)(thiophen-2-yl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3gb): The title compound was prepared according to the general procedure A to obtain as a light brown solid (64 mg, yield = 88%); Mp. 94.6-95.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.24-7.14 (m, 10H), 7.10-7.05 (m, 2H), 6.92 (dd, *J* = 5.2, 1.2 Hz, 1H), 6.39 (dd, *J* = 5.2, 3.6 Hz, 1H), 5.93 (dd, *J* = 3.6, 1.2 Hz, 1H), 4.47 (d, *J* = 14.8 Hz, 1H), 4.09 (d, *J* = 10.0 Hz, 1H), 4.02 (d, *J* = 14.8 Hz, 1H), 3.92 (d, *J* = 10.0 Hz, 1H), 3.62 (d, *J* = 14.8 Hz, 1H), 3.55 (d, *J* = 14.8 Hz, 1H), 2.48 (s, 3H), 2.40 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 144.59, 144.51, 143.95, 143.52, 139.23, 138.11, 134.57, 132.69, 129.79, 129.67, 128.95, 128.79, 128.73, 128.54, 128.12, 127.90, 127.51, 127.29, 126.47, 126.10, 125.66, 60.16, 59.49, 55.78, 52.87, 21.64, 21.56; IR (neat) λ max 3057, 2935, 1919, 1802, 1593, 1457, 1328, 1158, 1083, 822, 687, 564; HRMS (ESI) calcd for $C_{36}H_{34}NO_4S_3Se$ $[M+H]^+$ 720.0815; found: 720.0815.



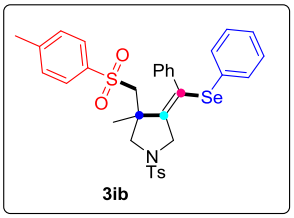
3gb

(Z)-3-phenyl-4-(1-(phenylselanyl)ethylidene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3hb): The title compound was prepared according to the general procedure A to obtain as a white solid (50 mg, yield = 77%); Mp. 94.8-95.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.41-7.38 (m, 3H), 7.35 (d, *J* = 5.6 Hz, 2H), 7.33 (s, 1H), 7.29-7.26 (m, 4H), 7.25-7.20 (m, 4H), 4.31 (dd, *J* = 13.6, 1.6 Hz, 1H), 4.16 (d, *J* = 9.6 Hz, 1H), 3.97-3.93 (m, 1H), 3.90 (d, *J* = 2.0 Hz, 2H), 3.53 (d, *J* = 9.6 Hz, 1H), 2.47 (s, 3H), 2.46 (s, 3H), 1.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.74, 143.89, 143.16, 139.42, 138.41, 134.23, 131.64, 129.98, 129.70, 129.15, 128.74, 128.67, 128.15, 127.80, 127.57, 127.30, 126.56, 125.83, 61.58, 60.94, 55.97, 52.24, 22.15, 21.65; IR (neat) λ max 3057, 2926, 1591, 1483, 1444, 1405, 1343, 1152, 1091, 1029, 824, 738, 697, 663, 592, 549; HRMS (ESI) calcd for $C_{33}H_{34}NO_4S_2Se$ $[M+H]^+$ 652.1094; found: 652.1095.



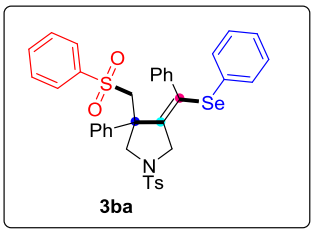
3hb

(Z)-3-methyl-4-(phenyl(phenylselanyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3ib): The title compound was prepared according to the general procedure A to obtain as a white solid (47 mg, yield = 72%); Mp. 69.5-70.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.26-7.23 (m, 2H), 7.14-7.11 (m, 3H), 7.09-6.99 (m, 5H), 6.73 – 6.71 (m, 2H), 4.13 (d, *J* = 14.4 Hz, 1H), 3.88 (d, *J* = 14.4 Hz, 1H), 3.59 (d, *J* = 10.0 Hz, 1H), 3.33 (d, *J* = 9.6 Hz, 1H), 3.00 (d, *J* = 14.4 Hz, 1H), 2.92 (d, *J* = 14.0 Hz, 1H), 2.48 (s, 3H), 2.41 (s, 3H), 1.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.43, 143.90, 141.11, 138.18, 137.52, 135.97, 131.65, 129.79, 129.71, 129.10, 128.62, 128.23, 128.15, 127.62, 127.49, 127.39, 127.25, 61.92, 59.45, 53.80, 46.31, 24.41, 21.61, 21.56; IR (neat) λ max 3056, 2979, 2934, 2863, 1812, 1731, 1593, 1454, 1329, 1156, 1086, 1049, 819, 740, 670, 572; HRMS (ESI) calcd for $C_{33}H_{34}NO_4S_2Se$ $[M+H]^+$ 652.1094; found: 652.1091.



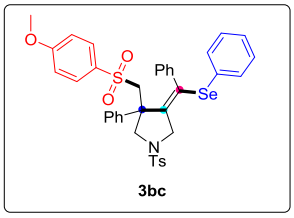
3ib

(Z)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-3-((phenylsulfonyl)methyl)-1-tosylpyrrolidine (3ba):



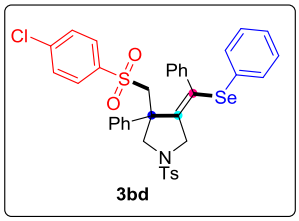
The title compound was prepared according to the general procedure A to obtain as a white solid (54 mg, yield = 77%); Mp. 165.2-166.25 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.55-7.51 (m, 3H), 7.42-7.37 (m, 4H), 7.13-7.07 (m, 8H), 7.00-6.97 (m, 2H), 6.90-6.86 (m, 1H), 6.79 (t, *J* = 7.6 Hz, 2H), 6.45 (s, 2H), 4.34 (d, *J* = 14.0 Hz, 1H), 4.12 (d, *J* = 14.4 Hz, 1H), 4.05 (d, *J* = 10.0 Hz, 1H), 3.95 (d, *J* = 10.2 Hz, 1H), 3.50 (d, *J* = 14.6 Hz, 1H), 3.34 (d, *J* = 14.6 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.92, 142.40, 141.13, 140.31, 137.16, 135.65, 133.36, 131.89, 130.14, 129.81, 129.21, 129.03, 128.55, 128.21, 128.14, 128.03, 127.85, 127.25, 127.11, 127.07, 126.26, 61.60, 59.14, 54.46, 52.55, 21.65; IR (neat) λ max 3477, 3058, 2930, 1895, 1746, 1590, 11448, 11335, 1155, 1088, 883, 826, 742, 693, 592, 552, 461; HRMS (ESI) calcd for $C_{37}H_{34}NO_4S_2Se$ $[M+H]^+$ 700.1094; found: 700.1087.

(Z)-3-(((4-methoxyphenyl)sulfonyl)methyl)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-1-tosylpyrrolidine (3bc):



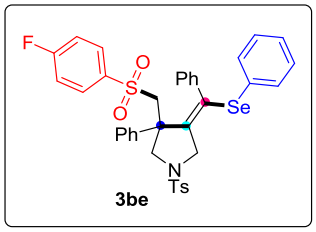
The title compound was prepared according to the general procedure A to obtain as a white solid (53 mg, yield = 73%); Mp. 173.8-174.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 9.2 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.13-7.06 (m, 8H), 7.00-6.97 (m, 2H), 6.92-6.88 (m, 1H), 6.85-6.78 (m, 4H), 6.45 (s, 2H), 4.34 (d, *J* = 14.4 Hz, 1H), 4.10 (d, *J* = 14.4 Hz, 1H), 4.03 (d, *J* = 10.4 Hz, 1H), 3.95 (d, *J* = 10.4 Hz, 1H), 3.83 (s, 3H), 3.47 (d, *J* = 14.8 Hz, 1H), 3.32 (d, *J* = 14.8 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.40, 143.91, 142.51, 140.48, 137.20, 135.63, 132.77, 131.87, 130.02, 129.81, 129.53, 129.25, 128.55, 128.19, 128.16, 128.01, 127.90, 127.07, 127.01, 126.30, 114.18, 61.84, 59.12, 55.65, 54.51, 52.52, 21.66; IR (neat) λ max 3468, 3057, 2933, 2584, 2509, 2404, 2305, 2050, 1898, 1805, 1745, 1589, 1447, 1328, 1154, 1091, 1030, 826, 741, 686, 559; HRMS (ESI) calcd for $C_{38}H_{36}NO_5S_2Se$ $[M+H]^+$ 730.1200; found: 730.1199.

(Z)-3-(((4-chlorophenyl)sulfonyl)methyl)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-1-tosylpyrrolidine (3bd):



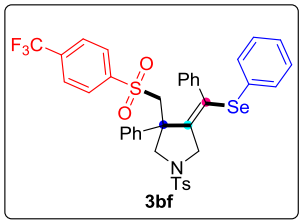
The title compound was prepared according to the general procedure A to obtain as a white solid (52 mg, yield = 71%); Mp. 142.6-114.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.44-7.40 (m, 4H), 7.38-7.31 (m, 2H), 7.13-7.07 (m, 8H), 7.01-6.90 (m, 3H), 6.83 (t, *J* = 8.0 Hz, 2H), 6.47 (s, 2H), 4.26 (d, J = 14.4 Hz, 1H), 4.12 (d, *J* = 10.4 Hz, 1H), 4.09 (d, *J* = 6.0 Hz, 1H), 3.87 (d, *J* = 10.4 Hz, 1H), 3.49 (d, *J* = 14.4 Hz, 1H), 3.33 (d, *J* = 14.4 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.00, 141.62, 140.08, 139.89, 139.39, 137.09, 135.78, 134.14, 131.89, 130.38, 129.85, 129.28, 129.26, 128.81, 128.57, 128.26, 128.14, 127.71, 127.21, 127.15, 126.39, 62.07, 58.90, 54.23, 52.61, 21.66; IR (neat) λ max 3060, 2929, 1898, 1745, 1647, 1583, 1397, 1334, 1158, 1088, 1025, 828, 753, 692, 597, 550, 4664; HRMS (ESI) calcd for $C_{37}H_{33}NO_4S_2ClSe$ $[M+H]^+$ 734.0705; found: 734.0713.

(Z)-3-(((4-fluorophenyl)sulfonyl)methyl)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-1-tosylpyrrolidine

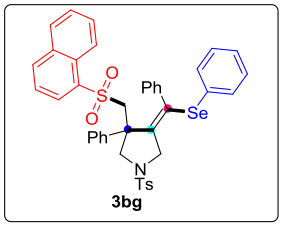


(3be): The title compound was prepared according to the general procedure A to obtain as a white solid (48 mg, yield = 68%); Mp. 148.9-149.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.53-7.50 (m, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.13-7.05 (m, 9H), 7.03-7.00 (m, 2H), 6.98-6.97 (m, 1H), 6.93-6.89 (m, 1H), 6.82 (t, *J* = 8.0 Hz, 2H), 6.47 (s, 2H), 4.27 (d, *J* = 14.4 Hz, 1H), 4.11 (t, *J* = 14.0 Hz, 2H), 3.89 (d, *J* = 10.0 Hz, 1H), 3.50 (d, *J* = 14.4 Hz, 1H), 3.34 (d, *J* = 14.8 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4 (d, J_{C-F} = 254.6 Hz) 143.99, 140.83 (d, J_{C-F} = 170.1 Hz), 137.12, 135.76, 131.89, 130.32, 130.25, 130.15, 129.84, 129.25, 128.57, 128.24, 128.13, 127.73, 127.17, 127.12, 126.39, 116.26 (d, J_{C-F} = 22.6 Hz) 62.10, 58.91, 54.25, 52.63, 21.65; IR (neat) λ max 3416, 3062, 2927, 1741, 1655, 1590, 11484, 1336, 1232, 1154, 1089, 833, 752, 681, 554, 550; HRMS (ESI) calcd for $C_{37}H_{33}NO_4S_2SeF$ $[M+H]^+$ 718.1000; found: 718.0999.

(Z)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-1-tosyl-3-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)pyrrolidine (3bf): The title compound was prepared according to the general procedure A to obtain as a white solid (53 mg, yield = 70%); Mp. 138.4-139.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.59 (s, 3H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.15 – 7.06 (m, 5H), 7.04 (d, *J* = 4.0 Hz, 4H), 7.02 – 6.98 (m, 2H), 6.95 (dt, *J* = 8.6, 1.3 Hz, 1H), 6.86 (t, *J* = 7.7 Hz, 2H), 6.50 (d, J = 6.1 Hz, 2H), 4.18 (dt, *J* = 23.5, 12.4 Hz, 3H), 3.84 (d, *J* = 10.3 Hz, 1H), 3.52 (t, *J* = 12.8 Hz, 1H), 3.36 (d, *J* = 14.8 Hz, 1H), 2.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.14, 142.46 (d, J_{C-F} = 318.2 Hz), 138.27 (d, J_{C-F} = 247.7 Hz), 135.90, 131.91, 130.58, 129.89, 129.31, 128.59, 128.27, 128.23, 128.04 (d, J_{C-F} = 100.0 Hz), 127.59, 127.31 s(d, J_{C-F} = 1.9 Hz), 127.21, 126.47, 126.10, 126.07, 62.28, 58.66, 53.99, 52.64, 21.67; IR (neat) λ max 3060, 2931, 1592, 1484, 1444, 1402, 1326, 1162, 1096, 1058, 832,745, 700, 664, 598, 550; HRMS (ESI) calcd for $C_{38}H_{33}NO_4S_2SeF_3$ $[M+H]^+$ 768.0968; found: 768.0962.



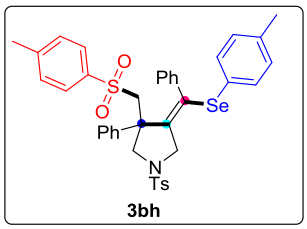
(Z)-3-((naphthalen-1-ylsulfonyl)methyl)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-1-tosylpyrrolidine



(3bg): The title compound was prepared according to the general procedure A to obtain as a white solid (49 mg, yield = 66%); Mp. 166.2-166.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 1.6 Hz, 1H), 7.88 (dd, *J* = 7.2, 4.0 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.79-7.77 (m, 2H), 7.67-7.59 (m, 2H), 7.49 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.11-7.07 (m, 5H), 7.02-6.96 (m, 5H), 6.90-6.86 (m, 1H), 6.79 (t, *J* = 8.0 Hz, 2H), 6.46 (s, 2H), 4.32 (d, *J* = 14.4 Hz, 1H), 4.14 (d, *J* = 4.4 Hz, 1H), 4.11 (d, *J* = 8.0 Hz, 1H), 3.97 (d, *J* = 10.4 Hz, 1H), 3.58 (d, *J* = 14.8 Hz, 1H), 3.40 (d, J = 14.6 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.91, 142.10, 140.29, 137.88, 137.17, 135.69, 135.00, 131.94, 131.87, 130.19, 129.82, 129.42, 129.35, 129.27, 129.22, 128.55, 128.14, 128.12, 128.05, 127.80, 127.58, 127.10, 126.31, 121.91, 61.78, 59.15, 54.40, 52.66, 21.66; IR (neat) λ max 3057, 2926, 1956,

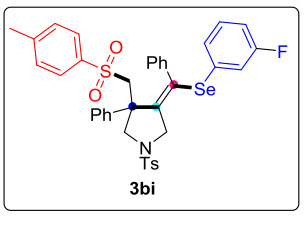
1815, 1743, 1592, 1482, 1452, 1331, 1156, 1085, 824, 752, 671, 596, 550, 490; HRMS (ESI) calcd for $C_{41}H_{36}NO_4S_2Se$ $[M+H]^+$ 750.1251; found: 750.1249.

(Z)-3-phenyl-4-(phenyl(p-tolylselanyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3bh): The title compound was prepared according to the general procedure A to obtain as a white solid (58 mg, yield = 80%); Mp. 135.8-136.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.43-7.41 (m, 4H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.11-7.06 (m, 5H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.92-6.88 (m, 1H), 6.82-6.78 (m, 4H), 6.44 (s, 2H), 4.33 (d, *J* = 14.0 Hz, 1H), 4.10 (d, *J* = 14.0 Hz, 1H), 4.03 (d, *J* = 10.4 Hz, 1H), 3.94 (d, *J* = 10.0 Hz, 1H), 3.47 (d, *J* = 14.4 Hz, 1H), 3.31 (d, *J* = 14.8 Hz, 1H), 2.49 (s, 3H), 2.38 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.31, 143.88, 142.52, 140.02, 138.29, 138.12, 137.26, 135.71, 131.93, 130.38, 129.78, 129.60, 129.34, 129.24, 128.15, 127.33, 127.03, 127.00, 126.94, 126.30, 124.21, 61.69, 59.11, 54.44, 52.53, 21.65, 21.52, 21.07; IR (neat) λ max 3050, 2929, 2301, 1909, 1742, 1597, 1472, 1330, 1156, 1088, 818, 679, 558; HRMS (ESI) calcd for $C_{39}H_{38}NO_4S_2Se$ $[M+H]^+$ 728.1407; found: 728.1406.



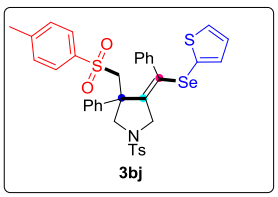
3bh

(Z)-4-(((3-fluorophenyl)selanyl)(phenyl)methylene)-3-phenyl-1-tosyl-3-(tosylmethyl)pyrrolidine (3bi): The title compound was prepared according to the general procedure A to obtain as a white solid (44 mg, yield = 62%); Mp. 141.6-142.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.17-7.05 (m, 5H), 7.01-6.90 (m, 3H), 6.84-6.81 (m, 4H), 6.47 (s, 2H), 4.39 (d, *J* = 14.0 Hz, 1H), 4.11 (d, *J* = 14.4 Hz, 1H), 4.02-3.97 (m, 2H), 3.48 (d, *J* = 14.4 Hz, 1H), 3.33 (d, *J* = 14.4 Hz, 1H), 2.49 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.89 (d, J_{C-F} = 247.9 Hz), 144.45, 144.01, 142.40 (d, J_{C-F} = 120.3 Hz) 137.70 (d, J_{C-F} = 116.4 Hz), 131.82, 130.86 (d, J_{C-F} = 3.1 Hz), 129.83, 129.74, 129.67, 129.57, 129.50, 129.24, 129.19, 128.23 (d, J_{C-F} = 13.6 Hz), 127.35, 127.32, 127.20, 127.12, 126.13, 122.05, 121.86, 115.14, 114.93, 61.27, 59.30, 54.82, 52.46, 21.66, 21.55; IR (neat) λ max 3056, 2937, 1919, 1588, 1464, 1328, 1158, 1080, 829, 746, 681, 558; HRMS (ESI) calcd for C_{38} $H_{35}NO_4S_2SeF$ $[M+H]^+$ 732.1157; found: 732.1151.s



3bi

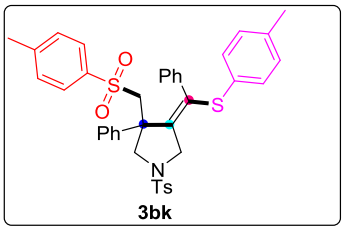
(Z)-3-phenyl-4-(phenyl(thiophen-2-ylselanyl)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3bj): The title compound was prepared according to the general procedure A to obtain as a yellow solid (47 mg, yield = 65%); Mp. 98.2-99.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.4 Hz, 2H), 7.43 (dd, *J* = 8.4, 2.0 Hz, 2H), 7.19-7.17 (m, 2H), 6.94 (t, *J* = 7.2 Hz, 2H), 6.85-6.83 (m, 2H), 6.69-6.65 (m, 2H), 6.44 (s, 2H), 4.36 (d, *J* = 14.4 Hz, 1H), 4.11 (d, *J* = 14.0 Hz, 1H), 4.03 (d, *J* = 10.4 Hz, 1H), 3.95 (d, *J* = 10.0 Hz, 1H), 3.47 (d, *J* = 14.8 Hz, 1H), 3.31 (d, *J* = 14.4 Hz, 1H), 2.50 (s, 3H), 2.39 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 144.36, 143.98, 142.29, 139.31, 138.28, 137.88, 136.32, 132.27, 132.02, 131.17, 129.85, 129.64, 129.28, 128.17, 127.55, 127.35, 127.21, 127.09, 127.00, 126.29, 121.33,



3bj

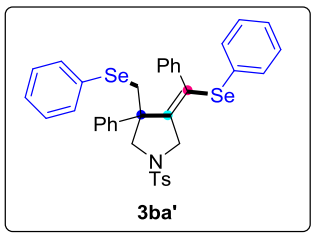
61.66, 58.98, 53.86, 52.65, 21.66, 21.54; IR (neat) λ max 3056, 2932, 1915, 1597, 1468, 1331, 1156, 1085, 1034, 902, 825, 702, 555; HRMS (ESI) calcd for $C_{36}H_{34}NO_4S_3Se$ $[M+H]^+$ 720.0815; found: 720.0814.

(Z)-3-phenyl-4-(phenyl(p-tolylthio)methylene)-1-tosyl-3-(tosylmethyl)pyrrolidine (3bk): The title compound was prepared according to the general procedure A to obtain as a white solid (53 mg, yield = 78%); Mp. 159.7-160.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.14-7.09 (m, 5H), 6.94-6.89 (m, 3H), 6.84-6.79 (m, 4H), 6.49 (d, J = 6.0 Hz, 2H), 4.50 (d, *J* = 14.4 Hz, 1H), 4.18 (d, *J* = 14.4 Hz, 1H), 3.99 (d, *J* = 10.0 Hz, 1H), 3.93 (d, *J* = 10.0 Hz, 1H), 3.47 (d, *J* = 14.4 Hz, 1H), 3.29 (d, *J* = 14.8 Hz, 1H), 2.49 (s, 3H), 2.40 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.39, 143.91, 143.40, 140.65, 138.37, 137.87, 136.23, 133.60, 131.87, 129.80, 129.71, 129.65, 129.25, 128.27, 128.22, 128.12, 127.38, 127.29, 127.12, 127.04, 126.18, 61.26, 59.28, 53.69, 52.14, 21.68, 21.56, 21.04; IR (neat) λ max 3046, 2933, 2586, 1910, 1798, 1713, 1596, 1476, 1332, 1156, 1084, 908, 819, 748, 676, 555; HRMS (ESI) calcd for $C_{39}H_{38}NO_4S_3$ $[M+H]^+$ 680.1963; found: 680.1963.



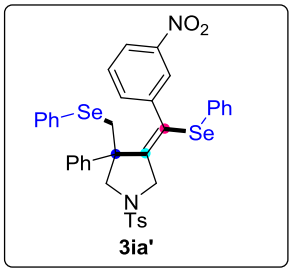
3bk

(Z)-3-phenyl-4-(phenyl(phenylselanyl)methylene)-3-((phenylselanyl)methyl)-1-tosylpyrrolidine (3ba'): The title compound was prepared according to the general procedure A to obtain as a lite yellow solid (55 mg, yield = 77%); Mp. 171.2-171.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.33-7.29 (m, 4H), 7.26-7.22 (m, 3H), 7.19-7.12 (m, 6H), 7.05-6.99 (m, 4H), 6.87 (tt, *J* = 8.8, 1.2 Hz, 1H), 6.74 (t, *J* = 8.0 Hz, 2H), 6.37 (s, 2H), 4.47 (d, *J* = 14.4 Hz, 1H), 4.06 (d, *J* = 14.4 Hz, 1H), 3.73 (d, *J* = 13.2 Hz, 1H), 3.57 (d, *J* = 9.2 Hz, 1H), 3.24 (d, *J* = 12.0 Hz, 1H), 3.03 (d, *J* = 12.0 Hz, 1H), 2.48 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 145.10, 143.70, 142.85, 137.43, 135.29, 132.66, 131.55, 131.33, 129.71, 129.48, 129.11, 128.94, 128.58, 128.16, 127.84, 127.04, 126.86, 126.80, 126.72, 126.23, 61.86, 56.15, 55.02, 35.88, 21.64; IR (neat) λ max 3442, 3057, 2926, 1740, 1672, 1586, 1447, 1346, 1161, 1094, 918, 880, 821, 743, 692, 592, 553, 505, 465; HRMS (ESI) calcd for $C_{37}H_{34}NO_2SSe_2$ $[M+H]^+$ 716.0641; found: 716.0643.



3ba'

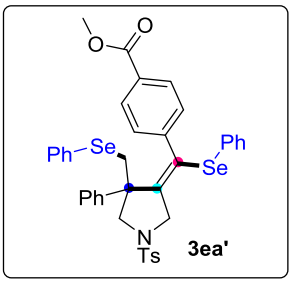
(Z)-4-((3-nitrophenyl)(phenylselanyl)methylene)-3-phenyl-3-((phenylselanyl)methyl)-1-tosylpyrrolidine (**3ia'**): The title compound was prepared according to the general procedure A to obtain as a yellow solid (38 mg, yield = 50%); Mp. 82.1-83.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.66 (ddd, *J* = 8.0, 2.4, 1.2 Hz, 1H), 7.42-7.37 (m, 4H), 7.28-7.26 (m, 3H), 7.15-7.11 (m, 3H), 7.09-7.07 (m, 3H), 7.03-6.98 (m, 2H), 6.95-6.92 (m, 2H), 6.88 (t, *J* = 8.0 Hz, 1H), 6.66 (s, 1H), 4.42 (d, *J* = 14.8 Hz, 1H), 4.20 (d, *J* = 14.8 Hz, 1H), 3.95 (d, *J* = 9.6 Hz, 1H), 3.56 (d, *J* = 9.6 Hz, 1H), 3.31 (d, *J* = 11.6 Hz, 1H), 3.06 (d, *J* = 12.0 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.59, 144.72, 144.03, 138.79, 135.93, 134.66, 133.24, 131.50, 130.72, 129.85, 129.29, 128.92, 128.61, 128.37, 128.22, 127.64, 127.48, 127.13, 127.05, 127.00, 126.19, 124.04, 121.43,



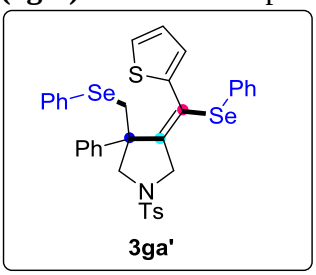
3ia'

61.78, 55.92, 55.16, 36.33, 21.68; IR (neat) λ max 3061, 2937, 2866, 1731, 1592, 1527, 1462, 1347, 1245, 1165, 1089, 1023, 918, 820, 737, 683, 554, 464; HRMS (ESI) calcd for $C_{37}H_{33}N_2O_4SSe_2$ $[M+H]^+$ 761.0491; found: 761.0497.

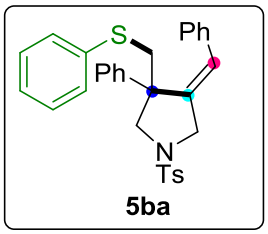
methyl(Z)-4-((4-phenyl-4-((phenylselanyl)methyl)-1-tosylpyrrolidin-3-ylidene)(phenylselanyl)methyl)benzoate (3ea'): The title compound was prepared according to the general procedure A to obtain as a white solid (43 mg, yield = 55%); Mp. 148.1-148.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.35-7.31 (m, 4H), 7.26 (d, *J* = 1.2, 1H), 7.25-7.24 (m, 2H), 7.16-7.12 (m, 6H), 7.03-6.99 (m, 4H), 6.38 (s, 2H), 4.50 (d, *J* = 14.6 Hz, 1H), 4.10 (d, *J* = 14.8 Hz, 1H), 3.82 (s, 3H), 3.79 (d, *J* = 9.6 Hz, 1H), 3.57 (d, *J* = 9.6 Hz, 1H), 3.22 (d, *J* = 12.0 Hz, 1H), 3.01 (d, *J* = 12.0 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 166.60, 144.82, 144.02, 143.83, 142.33, 135.41, 132.88, 131.55, 131.06, 129.76, 129.19, 128.93, 128.79, 128.29, 128.24, 128.19, 128.08, 127.59, 127.24, 126.95, 126.19, 61.92, 56.31, 54.99, 52.01, 35.97, 21.65; IR (neat) λ max 3056, 2941, 1720, 1593, 1443, 1347, 1279, 1167, 1103, 1026, 825, 744, 684, 592, 555, 467; HRMS (ESI) calcd for $C_{39}H_{36}NO_4SSe_2$ $[M+H]^+$ 774.0695; found: 774.0699.



(Z)-3-phenyl-4-((phenylselanyl)(thiophen-2-yl)methylene)-3-((phenylselanyl)methyl)-1-tosylpyrrolidine (3ga'): The title compound was prepared according to the general procedure A to obtain as a yellow solid (57 mg, yield = 79%); Mp. 164.2-164.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.32-7.27 (m, 6H), 7.25-7.19 (m, 5H), 7.17-7.14 (m, 3H), 7.12-7.08 (m, 2H), 6.94 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.40 (dd, *J* = 5.1, 3.6 Hz, 1H), 5.90 (dd, *J* = 3.6, 1.2 Hz, 1H), 4.52 (d, *J* = 15.1 Hz, 1H), 4.00 (d, *J* = 15.1 Hz, 1H), 3.71 (d, *J* = 9.2 Hz, 1H), 3.56 (d, *J* = 9.3 Hz, 1H), 3.33 (d, *J* = 12.2 Hz, 1H), 3.22 (d, *J* = 12.2 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.04, 145.18, 143.71, 139.44, 134.53, 132.73, 131.46, 131.43, 129.71, 129.13, 128.90, 128.77, 128.47, 128.43, 128.11, 127.85, 127.10, 126.97, 126.29, 126.20, 125.49, 121.88, 61.77, 56.90, 55.74, 35.15, 21.64; IR (neat) λ max 3061, 2937, 2866, 1731, 1592, 1527, 1462, 1347, 1245, 1165, 1089, 1023, 918, 820, 737, 683, 554, 464; HRMS (ESI) calcd for $C_{35}H_{32}NO_2S_2Se_2$ $[M+H]^+$ 722.0205; found: 722.0204.

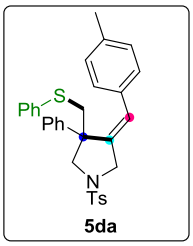


(E)-4-benzylidene-3-phenyl-3-((phenylthio)methyl)-1-tosylpyrrolidine (5ba): The title compound was prepared according to the general procedure B to obtain as a white solid (40 mg, yield = 80%); Mp. 140.2-140.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.31-7.26 (m, 4H), 7.25-7.22 (m, 2H), 7.20-7.14 (m, 3H), 7.02-6.99 (m, 5H), 6.82 (d, *J* = 6.8 Hz, 2H), 6.64 (s, 1H), 4.33 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.98 (dd, *J* = 14.0, 2.4 Hz, 1H), 3.69 (d, *J* = 9.6 Hz, 1H), 3.61 (d, *J* = 8.4 Hz, 1H), 3.37-3.30 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.34, 143.57, 141.10, 137.12, 135.49, 132.16, 129.63, 129.61, 128.82, 128.58, 128.47,



127.91, 127.71, 127.09, 127.07, 126.45, 126.22, 125.87, 61.04, 55.45, 54.06, 40.08, 21.57; IR (neat) λ max 3054, 2936, 2858, 1950, 1891, 1808, 1662, 1590, 1478, 1343, 1255, 1164, 1092, 1027, 917, 825, 750, 687, 592, 547, 492; HRMS (ESI) calcd for $C_{31}H_{30}NO_2S_2$ $[M+H]^+$ 512.1718; found: 512.1720.

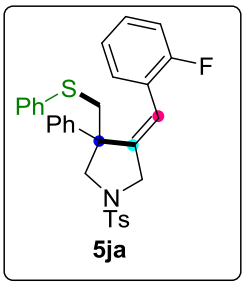
(E)-4-(4-methylbenzylidene)-3-phenyl-3-((phenylthio)methyl)-1-tosylpyrrolidine (**5da**)**:** The title compound



5da

was prepared according to the general procedure B to obtain as a white solid (32 mg, yield = 61%); Mp. 153.4-153.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.4 Hz, 2H), 7.33-7.24 (m, 7H), 7.20-7.12 (m, 3H), 7.00 (dt, *J* = 6.4, 1.6 Hz, 2H), 6.86 (d, *J* = 7.6 Hz, 2H), 6.72 (d, *J* = 8.0 Hz, 2H), 6.61 (s, 1H), 4.32 (dd, *J* = 15.6, 2.0 Hz, 1H), 3.96 (dd, *J* = 14.0, 2.4 Hz, 1H), 3.66 (d, *J* = 9.2 Hz, 1H), 3.61 (d, *J* = 9.6 Hz, 1H), 3.39 (d, *J* = 12.8 Hz, 1H), 3.32 (d, *J* = 12.8 Hz, 1H), 2.41 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.42, 143.52, 140.19, 137.25, 136.90, 132.54, 132.15, 129.58, 129.54, 128.77, 128.59, 128.43, 128.41, 127.88, 127.04, 126.46, 126.13, 125.85, 61.04, 55.49, 54.11, 39.87, 21.56, 21.08; IR (neat) λ max 3049, 2931, 2862, 1805, 1731, 1655, 1591, 1480, 1345, 1257, 1164, 1095, 1025, 820, 750, 668, 595, 548, 494; HRMS (ESI) calcd for $C_{32}H_{32}NO_2S_2$ $[M+H]^+$ 526.1874; found: 526.1876.

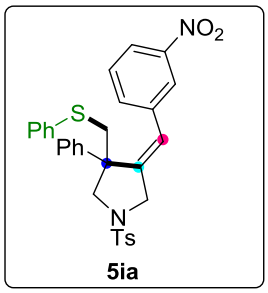
(E)-4-(2-fluorobenzylidene)-3-phenyl-3-((phenylthio)methyl)-1-tosylpyrrolidine (5ja): The title compound



5ja

was prepared according to the general procedure B to obtain as a white solid (23 mg, yield = 45%); Mp. 137.7-138.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.28-7.15 (m, 10H), 7.09-7.05 (m, 3H), 6.84 (td, *J* = 9.6, 0.8 Hz, 1H), 6.71 (td, *J* = 7.6, 0.8 Hz, 1H), 6.62-6.57 (m, 2H), 4.32 (dd, *J* = 14.0, 2.0 Hz, 1H), 4.01 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.73 (d, *J* = 9.6 Hz, 1H), 3.63 (d, *J* = 9.6 Hz, 1H), 3.41 (d, *J* = 12.8 Hz, 1H), 3.31 (d, *J* = 12.8 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.82 (d, J_{C-F} = 245.5 Hz), 143.67, 143.43, 136.99, 132.05, 129.98 (d, J_{C-F} = 2.7 Hz), 129.66, 129.58, 129.20, 129.12, 128.85, 128.50, 127.86, 126.67 (d, J_{C-F} = 84.1 Hz), 126.50, 123.24, 123.08, 123.04, 118.91, 118.88, 115.10, 114.88, 60.81, 55.11, 54.14, 40.05, 21.56; IR (neat) λ max 3055, 2942, 2859, 1930, 1802, 1589, 1471, 1341, 1240, 1166, 1088, 1031, 823, 679, 583, 556, 479; HRMS (ESI) calcd for $C_{31}H_{29}NO_2S_2F$ $[M+H]^+$ 530.1624; found: 530.1628.

(E)-4-(3-nitrobenzylidene)-3-phenyl-3-((phenylthio)methyl)-1-tosylpyrrolidine (5ia): The title compound

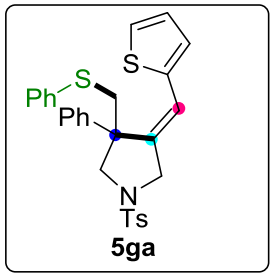


5ia

was prepared according to the general procedure B to obtain as a lite yellow solid (23 mg, yield = 42%); Mp. 74.2-74.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.58 (s, 1H), 7.31 (d, *J* = 4.0 Hz, 2H), 7.22-7.16 (m, 9H), 7.09-7.06 (m, 3H), 6.60 (s, 1H), 4.34 (dd, *J* = 14.0, 2.0 Hz, 1H), 4.07 (dd, *J* = 14.0, 2.4 Hz, 1H), 3.77 (d, *J* = 9.6 Hz, 1H), 3.57 (d, J = 9.6 Hz, 1H), 3.39 (d, *J* = 12.8 Hz, 1H), 3.27 (d, *J* = 12.8 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.44, 144.82, 143.87, 143.36, 136.86, 136.43, 134.23, 131.90, 129.92, 129.72, 128.96, 128.76, 128.45, 127.96, 127.42, 126.63, 126.29,

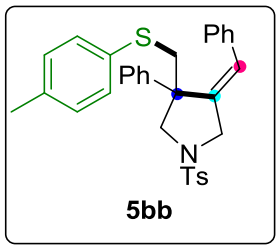
123.43, 123.40, 121.77, 109.97, 61.21, 55.50, 53.98, 40.24, 21.61; IR (neat) λ max 3064, 2932, 2861, 2294, 1950, 1805, 1729, 1590, 1527, 1471, 1345, 1164, 1092, 1029, 915, 821, 744, 689, 592, 548, 489; HRMS (ESI) calcd for $C_{31}H_{29}N_2O_4S_2$ $[M+H]^+$ 557.1569; found: 557.1570.

(E)-3-phenyl-3-((phenylthio)methyl)-4-(thiophen-2-ylmethylene)-1-tosylpyrrolidine (5ga): The title compound was prepared according to the general procedure B to obtain as a lite yellow solid (38 mg, yield = 74%); Mp. 63.3-64.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.35-7.26 (m, 8H), 7.23-7.14 (m, 3H), 7.10-7.07 (m, 3H), 6.73 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.66 (s, 1H), 6.44 (d, *J* = 3.6 Hz, 1H), 4.29 (dd, *J* = 13.6, 1.6 Hz, 1H), 4.00 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.79 (d, *J* = 13.2 Hz, 1H), 3.75 (d, *J* = 9.2 Hz, 1 H), 3.54 (d, *J* = 9.6 Hz, 1H), 3.50 (d, *J* = 13.2 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.70, 143.36, 140.68, 137.47, 137.03, 131.80, 129.90, 129.63, 128.84, 128.78, 128.04, 128.02, 127.26, 126.69, 126.59, 126.35, 118.50, 61.64, 56.13, 54.12, 39.64, 21.58; IR (neat) λ max 3057, 2931, 2860, 2299, 1888, 1679, 1591, 1463, 1341, 1254, 1165, 1092, 1032, 827, 696, 590, 549; HRMS (ESI) calcd for $C_{29}H_{28}NO_2S_3$ $[M+H]^+$ 518.1282; found: 518.1281.



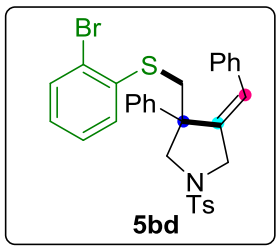
5ga

(E)-4-benzylidene-3-phenyl-3-((p-tolylthio)methyl)-1-tosylpyrrolidine (5bb): The title compound was prepared according to the general procedure B to obtain as a white solid (30 mg, yield = 58%); Mp. 151.1-151.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.29-7.23 (m, 7H), 7.10-7.03 (m, 3H), 7.00-6.98 (m, 2H), 6.93-6.91 (m, 2H), 6.82-6.80 (m, 2H), 6.63 (s, 1H), 4.32 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.98 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.71 (d, *J* = 9.2 Hz, 1H), 3.59 (d, *J* = 9.2 Hz, 1H), 3.34 (d, *J* = 12.8 Hz, 1H), 3.27 (d, *J* = 12.8 Hz, 1H), 2.44 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.43, 143.56, 141.07, 136.43, 135.51, 133.42, 132.17, 130.43, 129.59, 128.55, 128.48, 127.93, 127.68, 127.05, 127.01, 126.44, 125.80, 61.03, 55.49, 54.15, 40.88, 21.58, 20.97; IR (neat) λ max 3041, 2932, 2862, 2296, 1901, 1811, 1658, 1487, 1343, 1257, 1164, 1093, 1029, 922, 816, 753, 675, 592, 547, 497; HRMS (ESI) calcd for $C_{32}H_{32}NO_2S_2$ $[M+H]^+$ 526.1874; found: 526.1876.



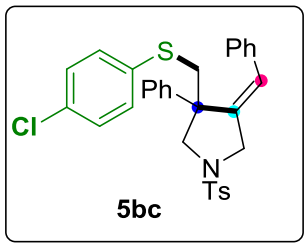
5bb

(E)-4-benzylidene-3-(((2-bromophenyl)thio)methyl)-3-phenyl-1-tosylpyrrolidine (5bd): The title compound was prepared according to the general procedure B to obtain as a white solid (45 mg, yield = 77%); Mp. 141.8-142.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.46 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.33-7.23 (m, 7H), 7.13-6.96 (m, 5H), 6.86 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.83-6.81 (m, 2H), 6.67 (s, 1H), 4.35 (dd, *J* = 14.0, 2.0 Hz, 1H), 4.00 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.71-3.65 (m, 2H), 3.31-3.25 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.31, 143.65, 140.90, 137.95, 135.46, 132.86, 132.02, 129.69, 129.61, 128.60, 128.41, 127.86, 127.66, 127.62, 127.17, 127.12, 127.05, 126.89, 126.34, 126.13, 124.80, 61.05, 58.78, 55.36, 53.50, 39.42, 21.54; IR (neat) λ max 3052, 2939, 2862, 2298, 1914, 1806, 1746, 1670, 1590, 1445, 1340, 1259, 1092, 1027, 922, 829, 743, 682, 584, 554; HRMS (ESI) calcd for $C_{31}H_{29}NO_2S_2Br$ $[M+H]^+$ 590.0823; found: 590.0823.



5bd

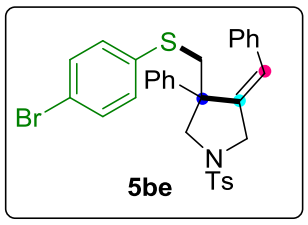
(E)-4-benzylidene-3-(((4-chlorophenyl)thio)methyl)-3-phenyl-1-tosylpyrrolidine (5bc): The title compound



5bc

was prepared according to the general procedure B to obtain as a white solid (32 mg, yield = 60%); Mp. 188.5-189.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.2 Hz, 2H), 7.28-7.25 (m, 7H), 7.14-7.05 (m, 5H), 6.93-6.90 (m, 2H), 6.81 (d, *J* = 7.1 Hz, 2H), 6.64 (s, 1H), 4.31 (dd, *J* = 14.0, 2.0 Hz, 1H), 3.99 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.62 (q, *J* = 9.2 Hz, 2H), 3.31 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.05, 143.65, 140.85, 135.54, 135.42, 132.25, 132.17, 131.01 (s), 129.60, 128.91, 128.64, 128.47, 127.88, 127.73, 127.16, 127.14, 126.42, 126.01, 61.00, 55.41, 54.08, 40.36, 21.57; IR (neat) λ max 3053, 2937, 2860, 1897, 1734, 1659, 1595, 1473, 1341, 1164, 1092, 1025, 922, 823, 747, 680, 588, 549, 497; HRMS (ESI) calcd for $C_{31}H_{29}NO_2S_2Cl$ $[M+H]^+$: 546.1328; found: 546.1328.

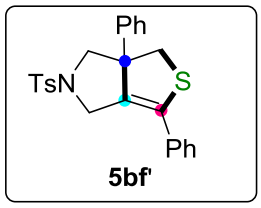
(E)-4-benzylidene-3-(((4-bromophenyl)thio)methyl)-3-phenyl-1-tosylpyrrolidine (5be): The title compound



5be

was prepared according to the general procedure B to obtain as a white solid (29 mg, yield = 50%); Mp. 183.9-184.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.28-7.23 (m, 9H), 7.10-7.02 (m, 3H), 6.86-6.60 (m, 4H), 6.64 (s, 1H), 4.31 (dd, *J* = 14.0, 2.0 Hz, 1H), 3.99 (dd, *J* = 13.6, 2.0 Hz, 1H), 3.65-3.59 (m, 2H), 3.35-3.28 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.99, 144.03, 143.65, 140.84, 136.24, 135.40, 132.16, 131.81, 131.13, 129.60, 128.64, 128.45, 127.87, 127.73, 127.16, 127.15, 126.41, 126.01, 120.09, 102.90, 61.00, 55.40, 54.06, 40.14, 21.57; IR (neat) λ max 3060, 2942, 2858, 2584, 2504, 2411, 2309, 1947, 1900, 1813, 1760, 1660, 1590, 1465, 1334, 1165, 1093, 1015, 825, 743, 604, 549; HRMS (ESI) calcd for $C_{31}H_{29}NO_2S_2Br$ $[M+H]^+$ 590.0823; found: 590.0822.

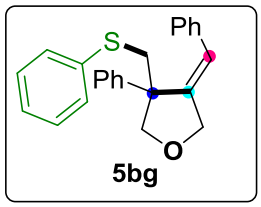
3,6a-diphenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (5bf'): The title compound was prepared



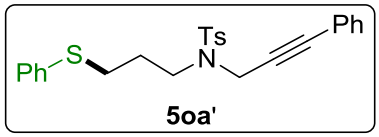
5bf'

according to the general procedure B to obtain as a white solid (22 mg, yield = 48%); Mp. 133.4-134.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.47 (m, 2H), 7.41-7.39 (m, 4H), 7.38-7.36 (m, 1H), 7.30-7.25 (m, 5H), 7.13-7.10 (m, 2H), 4.20 (d, *J* = 14.4 Hz, 1H), 4.16 (d, *J* = 9.2 Hz, 1H), 4.04 (d, *J* = 14.0 Hz, 1H), 3.74 (d, *J* = 10.8 Hz, 1H), 3.40 (d, *J* = 9.6 Hz, 1H), 3.10 (d, *J* = 11.2 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.34, 141.23, 135.35, 133.78, 132.49, 132.20, 129.58, 129.01, 128.83, 128.73, 128.15, 127.37, 127.11, 126.07, 102.90, 67.64, 59.61, 58.81, 47.76, 44.57, 21.45; IR (neat) λ max 3055, 2981, 2921, 2116, 1892, 1810, 1742, 1646, 1596, 1541, 1489, 1447, 1401, 1339, 1270, 1223, 1160, 1097, 1056, 1013, 913, 863, 815, 759, 688, 608, 542, 460; HRMS (ESI) calcd for $C_{25}H_{24}NO_2S_2$ $[M+H]^+$ 434.1248; found: 434.1247.

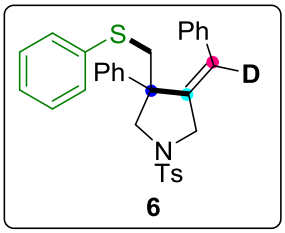
(E)-4-benzylidene-3-phenyl-3-((phenylthio)methyl)tetrahydrofuran (5bg): The title compound was prepared according to the general procedure B to obtain as a white solid (20 mg, yield = 55%); Mp. 109.4-110.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.36 (m, 5H), 7.32-7.28 (m, 2H), 7.25-7.19 (m, 2H), 7.18-7.18 (m, 2H), 7.14-7.05 (m, 4H), 6.62 (s, 1H), 4.79 (dd, *J* = 13.2, 2.0 Hz, 1H), 4.69 (dd, *J* = 12.8, 2.0 Hz, 1H), 4.38 (d, *J* = 8.8 Hz, 1H), 4.05 (d, *J* = 8.8 Hz, 1H), 3.54 (d, *J* = 12.4 Hz, 1H), 3.47 (d, *J* = 12.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.38, 145.05, 137.51, 135.91, 129.49, 128.80, 128.53, 128.48, 127.68, 126.77, 126.72, 126.56, 126.03, 122.72, 81.60, 75.20, 54.02, 39.04; IR (neat) λ max 3053, 2944, 2848, 1566, 1478, 1318, 1249, 1165, 1069, 939, 843, 704, 624, 499; HRMS (ESI) calcd for $C_{24}H_{23}OS$ $[M+H]^+$ 359.1470; found: 359.1472.



4-methyl-N-(3-phenylprop-2-yn-1-yl)-N-(3-(phenylthio)propyl)benzenesulfonamide (5oa'): The title compound was prepared according to the general procedure B to obtain as a white solid (27 mg, yield = 61%); Mp. 125.3-125.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.4 Hz, 2H), 7.32-7.25 (m, 8H), 7.21-7.16 (m, 3H), 7.08 (dt, *J* = 6.0, 1.6 Hz, 2H), 3.89 (d, *J* = 15.6 Hz, 1H), 3.44 (dd, *J* = 16.4, 2.0 Hz, 1H), 3.32 (dd, *J* = 11.6, 4.4 Hz, 1H), 3.12 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.84-2.80 (m, 1H), 2.43 (s, 3H), 1.06 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.55, 143.64, 139.73, 134.49, 133.15, 129.67, 129.17, 128.87, 128.05, 127.97, 127.67, 127.52, 126.41, 122.45, 49.58, 48.94, 36.98, 21.52, 17.82; IR (neat) λ max 3055, 2969, 2925, 2864, 1807, 1731, 1661, 1588, 1459, 1342, 1237, 1164, 1092, 1023, 940, 809, 754, 687, 561, 471; HRMS (ESI) calcd for $C_{25}H_{25}NO_2S_2$ $[M+H]^+$ 436.1426; found: 436.1451.



(E)-3-phenyl-4-(phenylmethylene-d)-3-((phenylthio)methyl)-1-tosylpyrrolidine (6): The title compound was prepared according to the general procedure B to obtain as a white solid (28 mg, yield = 58%); Mp. 140.8-141.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.23 (m, 7H), 7.21 – 7.11 (m, 3H), 7.11 – 6.98 (m, 5H), 6.85 – 6.80 (m, 2H), 4.33 (d, *J* = 13.7 Hz, 1H), 3.99 (d, *J* = 13.7 Hz, 1H), 3.70 (d, *J* = 9.5 Hz, 1H), 3.62 (d, *J* = 9.5 Hz, 1H), 3.39 – 3.30 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.33, 143.56, 140.97, 137.11, 135.41, 132.17, 129.64, 129.60, 128.81, 128.58, 128.48, 127.90, 127.70, 127.09, 127.07, 126.45, 126.22, 125.87, 61.05, 55.42, 54.03, 40.07, 21.57; IR (neat) λ max 3055, 2933, 2858, 1951, 1889, 1807, 1746, 1658, 1590, 1479, 1343, 1257, 1163, 1092, 1027, 914, 825, 692, 591, 546, 487; HRMS (ESI) calcd for $C_{31}H_{28}DNO_2S_2$ $[M+H]^+$ 513.1781; found: 513.1780.



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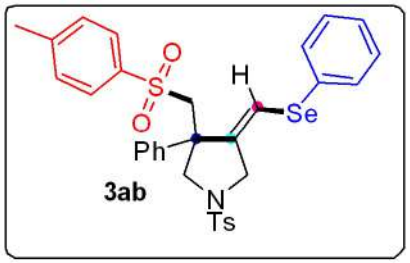

Solvent CDCl3

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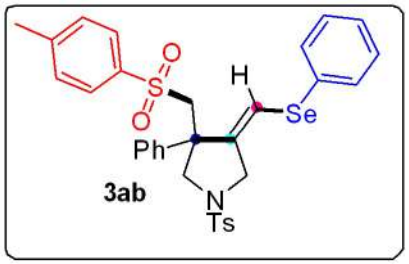

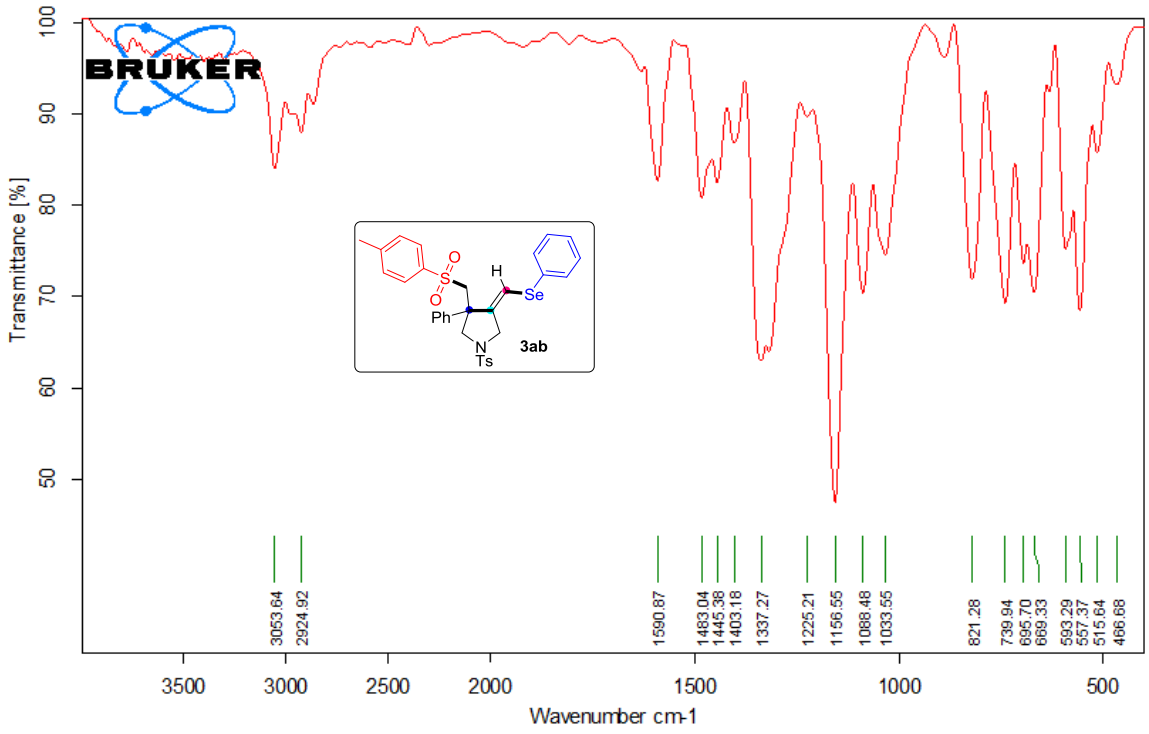
BRUKER
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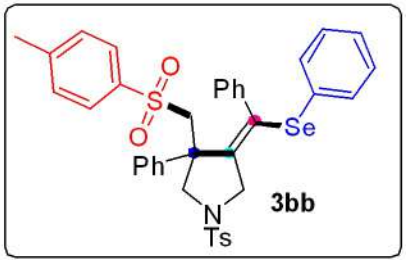
Solvent $CDCl_3$

Spectrometer Frequency 400.40



Solvent $CDCl_3$

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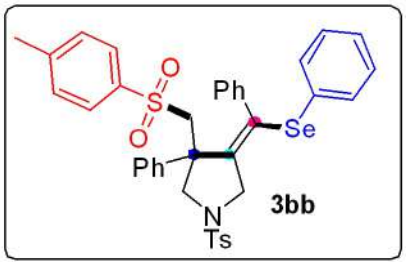
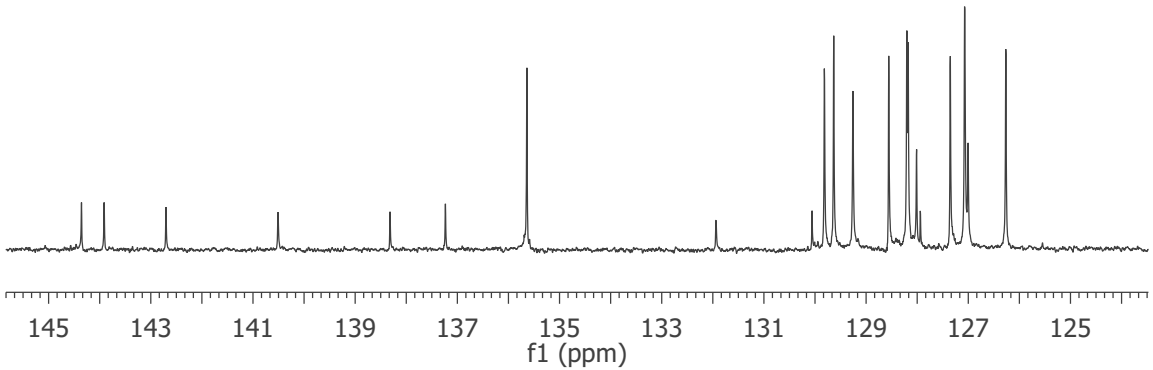
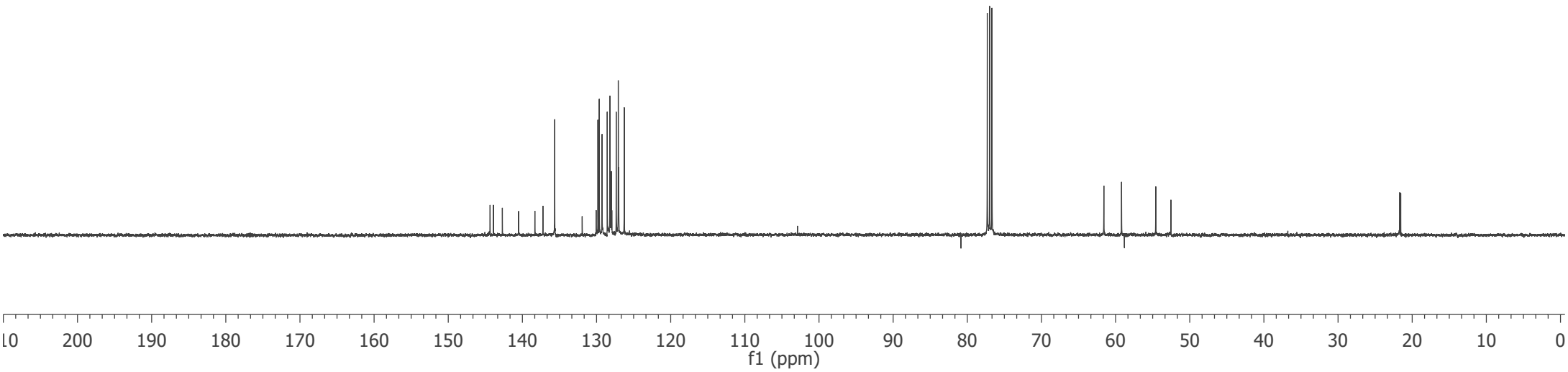
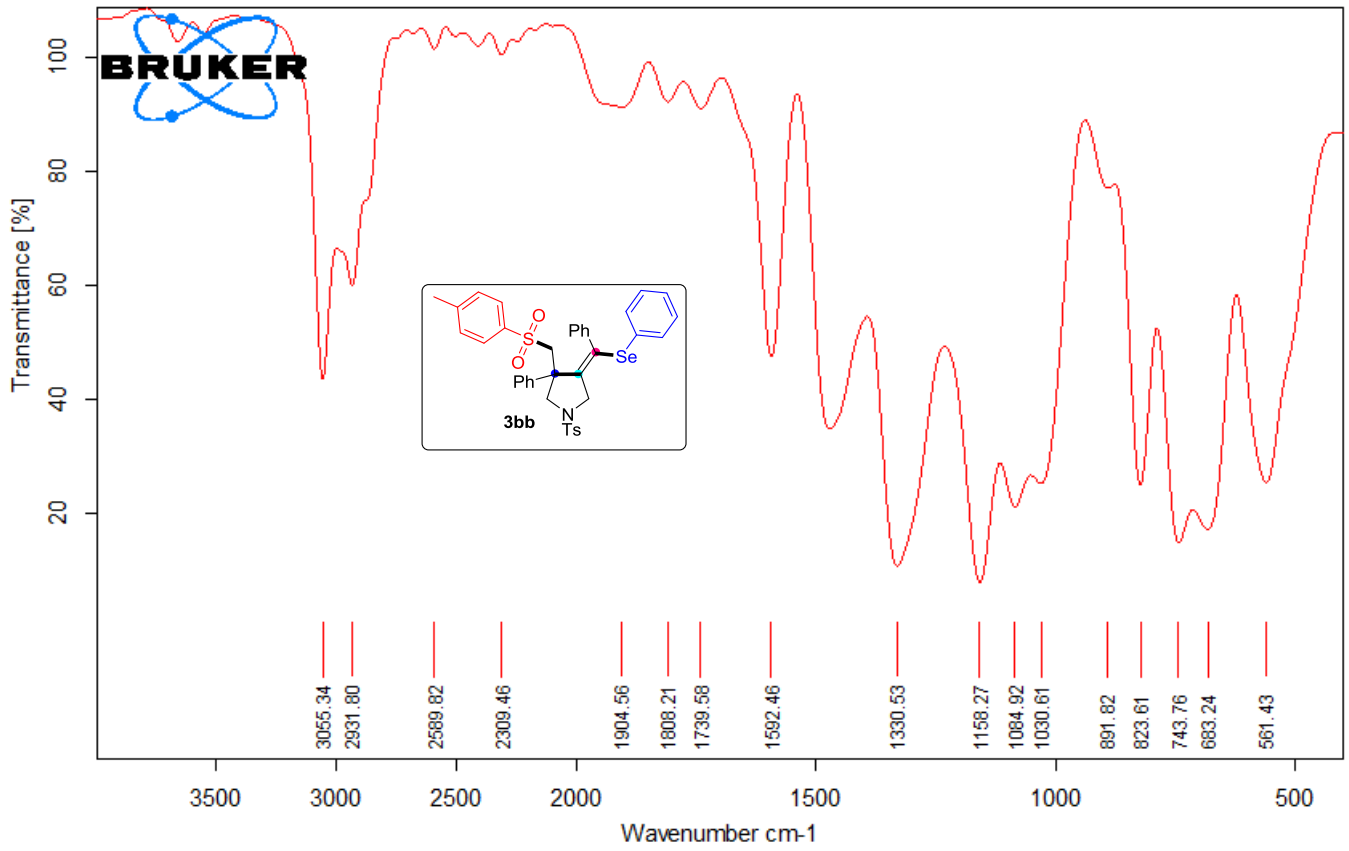


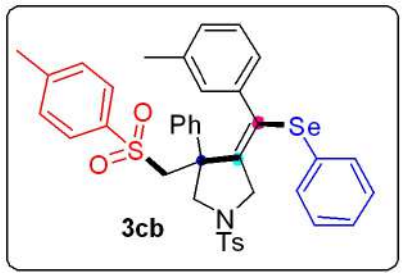





BRUKER
Transmittance [%]
100
80
60
40
20
3055.34
2931.80
2589.82
2309.46
1904.56
1808.21
1739.58
1592.46
1330.53
1158.27
1084.92
1030.61
891.82
823.61
743.76
683.24
561.43
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
Ph
Se
Ph
N
Ts
3bb

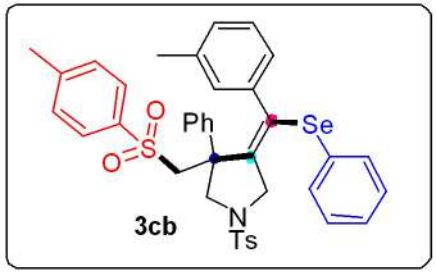
Solvent $CDCl_3$

Spectrometer Frequency 400.40



Solvent $CDCl_3$

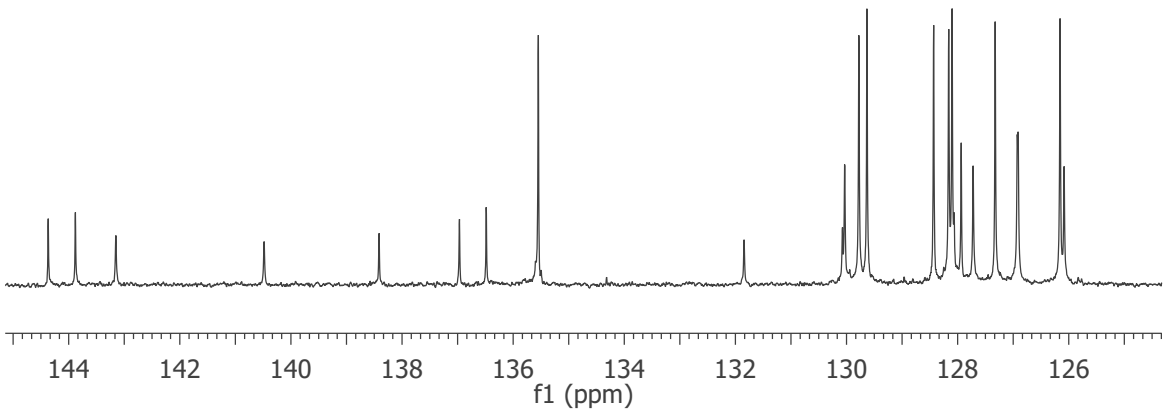
Spectrometer Frequency 100.69

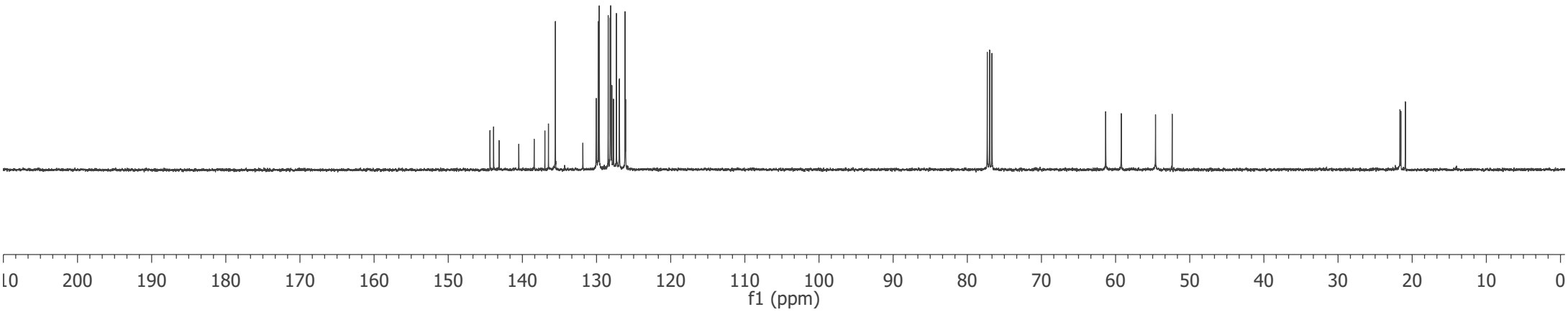


144.369
143.880
143.151
140.483
138.413
136.967
136.484
135.548
131.844
130.074
130.033
129.778
129.632
128.432
128.161
128.100
128.063
127.936
127.721
127.324
126.926
126.912
126.156
126.084

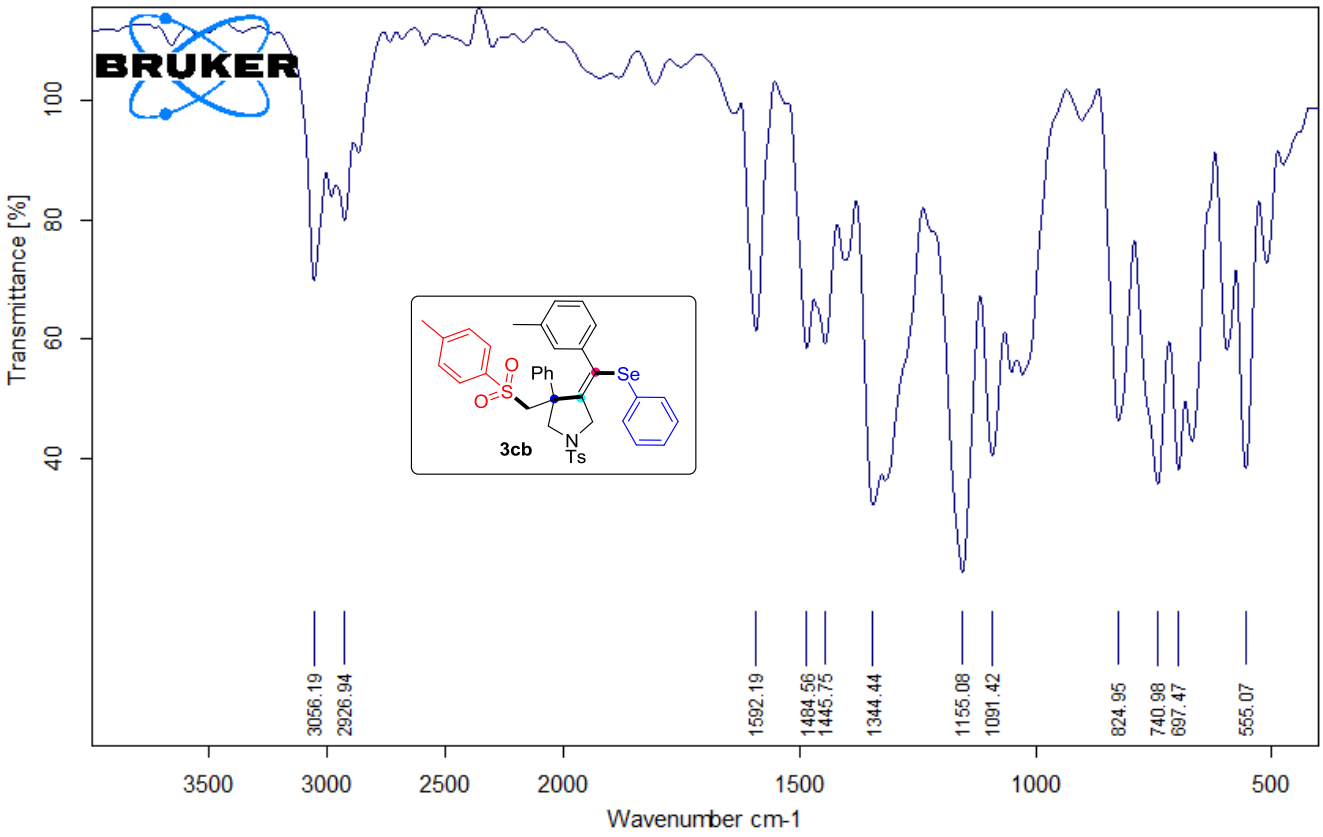
61.336
59.239
54.615
52.370

21.648
21.528
20.921



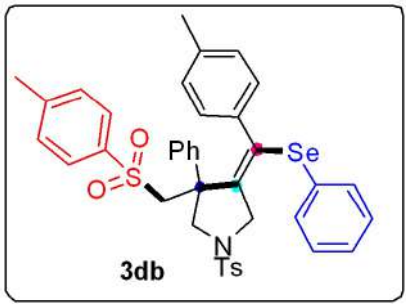


\


BRUKER
Transmittance [%]
100
80
60
40
Ph
Se
O
O
S
N
Ts
3cb
3056.19
2926.94
1592.19
1484.56
1445.75
1344.44
1155.08
1091.42
824.95
740.98
697.47
555.07
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

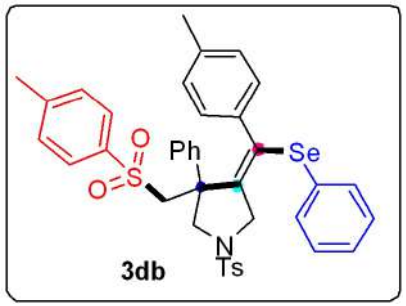
Solvent $CDCl_3$

Spectrometer Frequency 400.40



Solvent $CDCl_3$

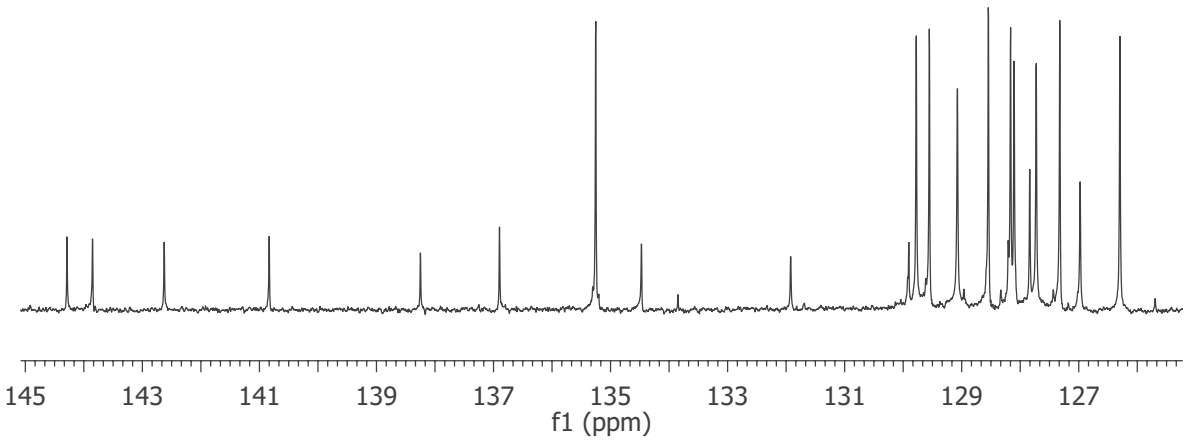
Spectrometer Frequency 100.69

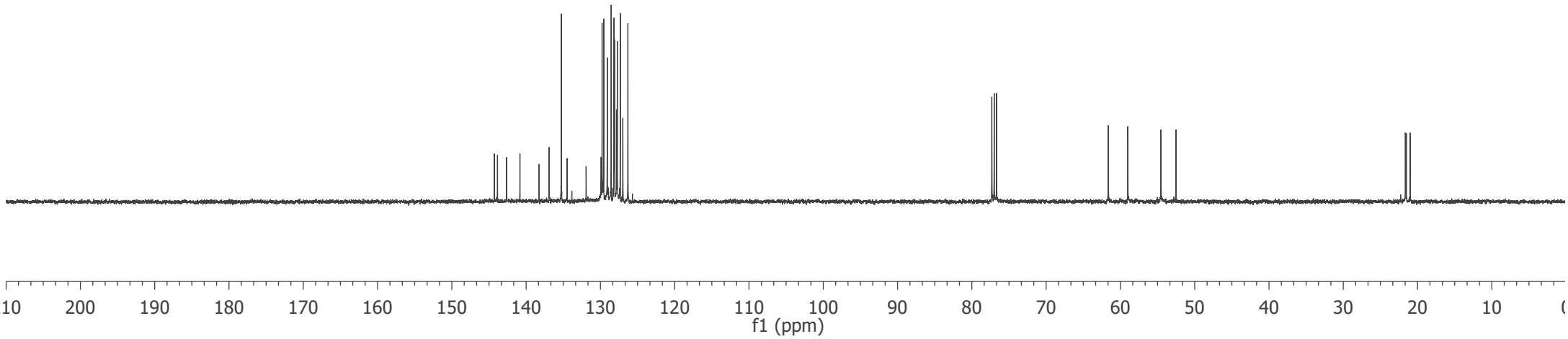


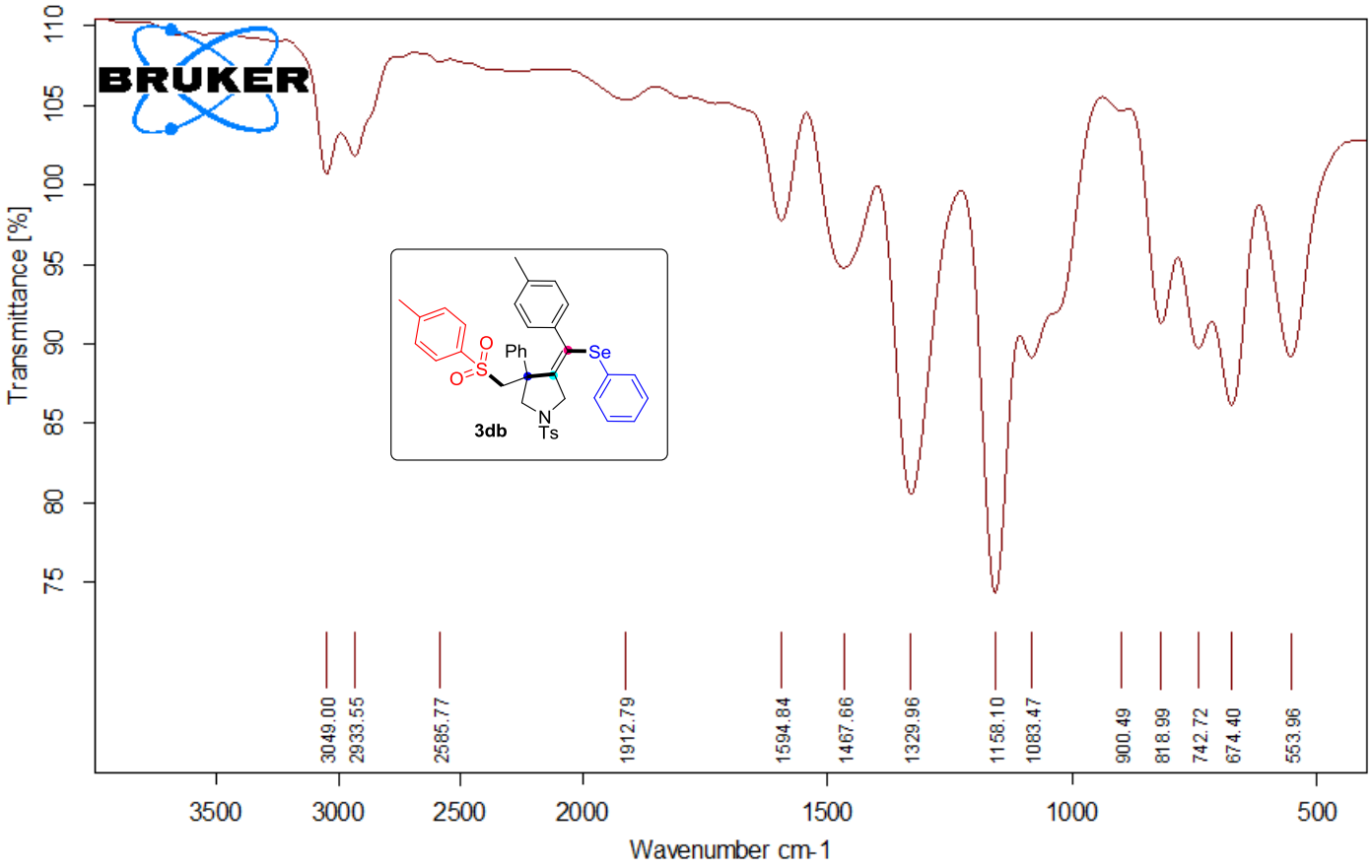
144.288
143.851
142.627
140.833
138.249
136.898
135.254
134.472
131.922
129.904
129.777
129.553
129.074
128.544
128.165
128.105
127.838
127.727
127.324
126.976
126.297

61.639
59.000
54.558
52.510

21.638
21.513
20.982

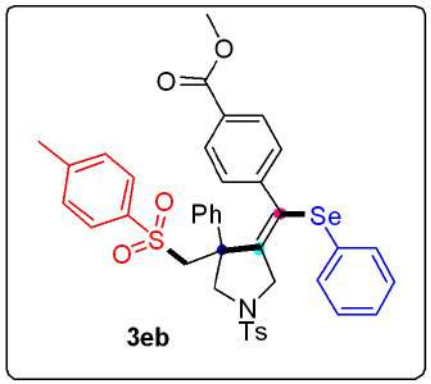





BRUKER
Transmittance [%]
110
105
100
95
90
85
80
75
3049.00
2933.55
2585.77
1912.79
1594.84
1467.66
1329.96
1158.10
1083.47
900.49
818.99
742.72
674.40
553.96
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
Ph
Se
O
O
S
N
Ts
3db

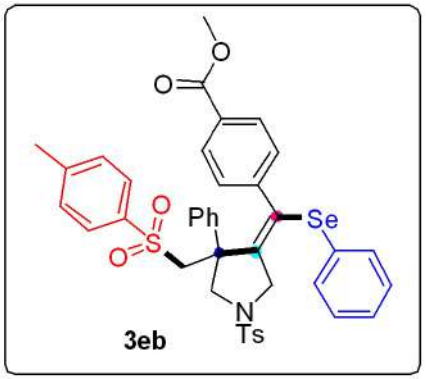
Solvent $CDCl_3$

Spectrometer Frequency 400.40



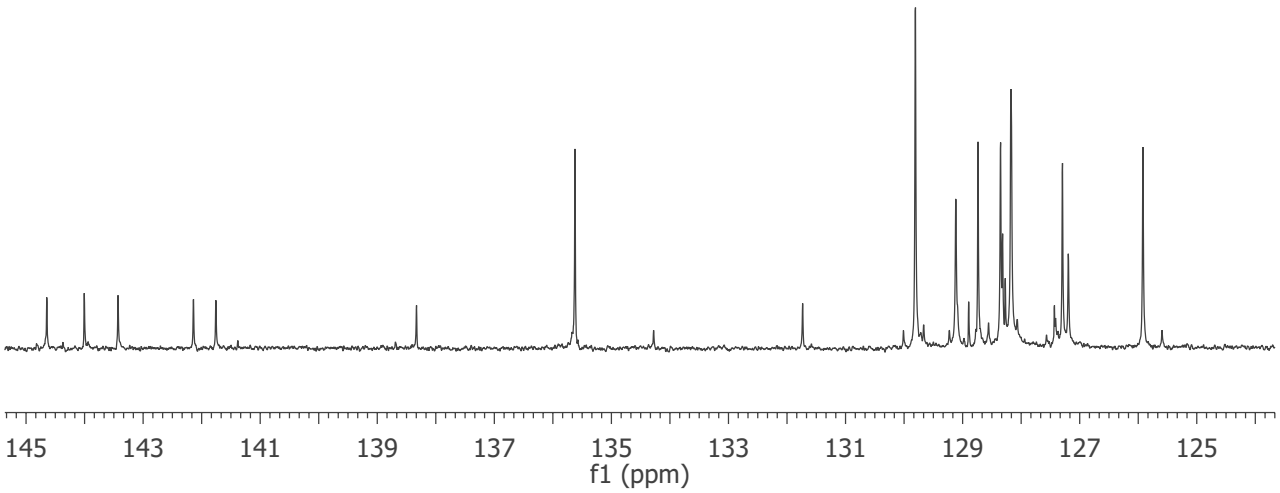
Solvent $CDCl_3$

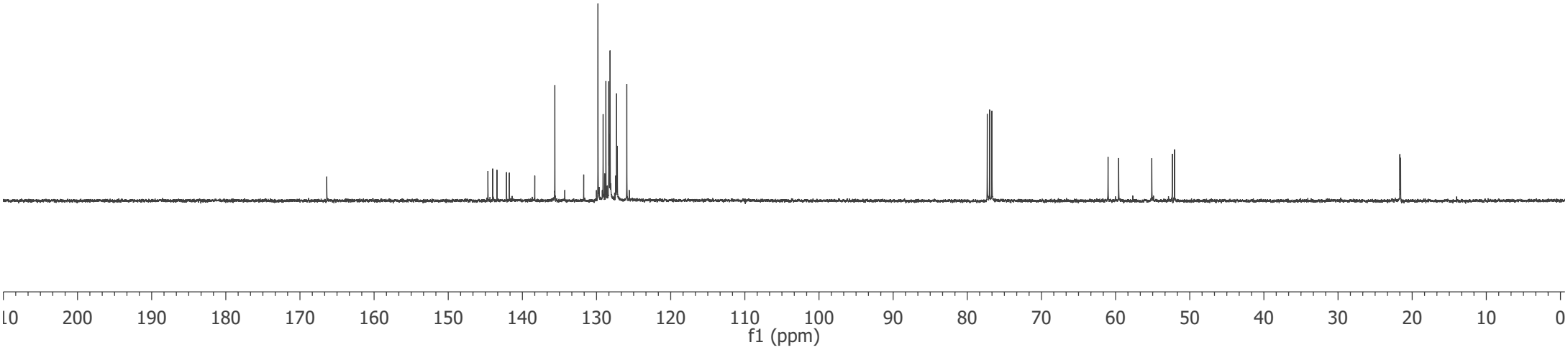
Spectrometer Frequency 100.69

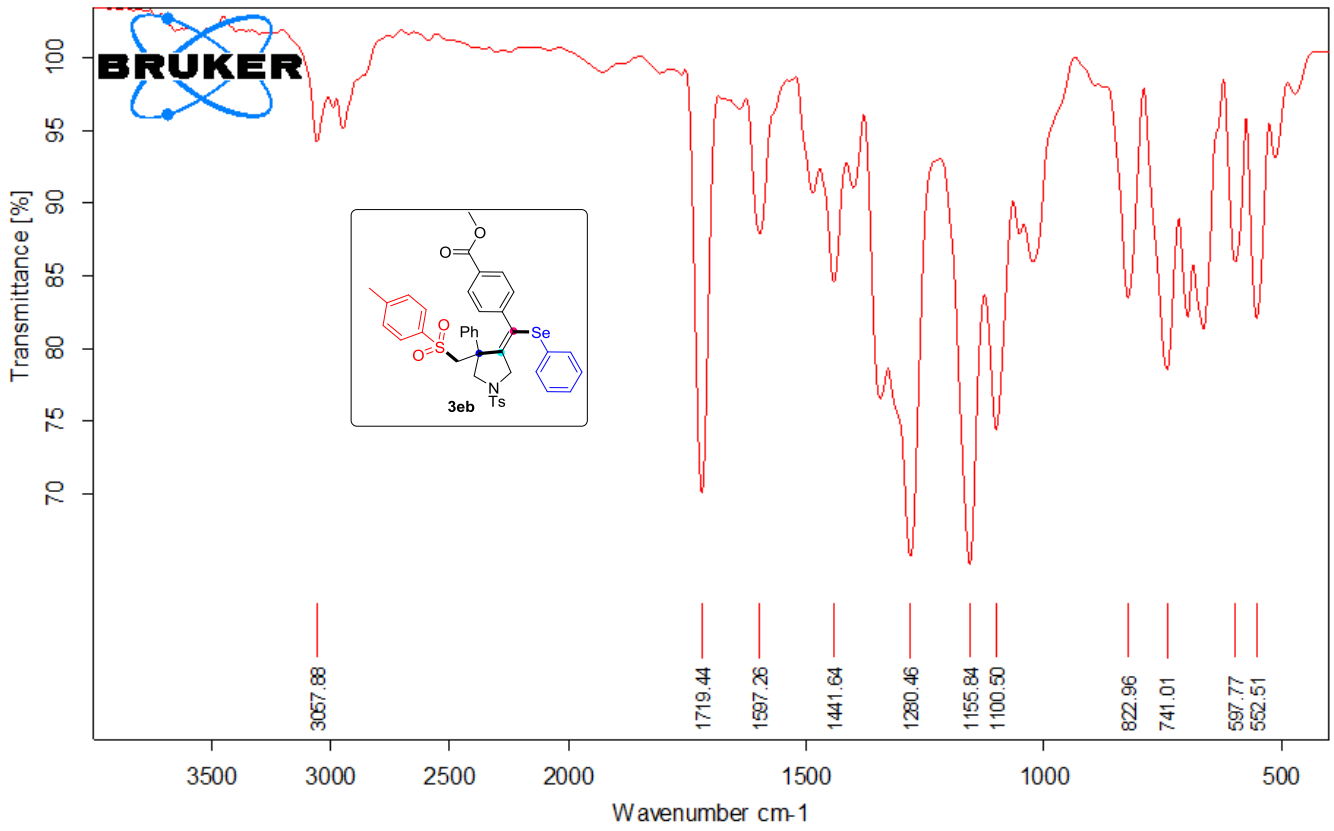


3eb

166.381
144.645
144.005
143.428
142.140
141.757
138.330
135.622
131.733
129.807
129.116
128.737
128.353
128.317
128.175
127.295
127.194
125.920
61.017
59.587
55.116
52.357
52.043
21.661
21.553

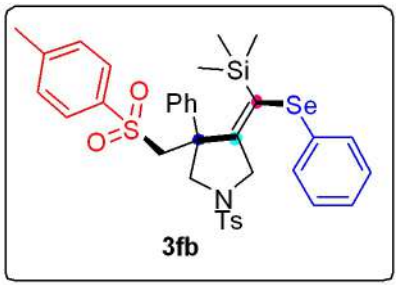





BRUKER
Transmittance [%]
100
95
90
85
80
75
70
3eb
Ph
Se
O
S
N
Ts
3057.88
1719.44
1597.26
1441.64
1280.46
1155.84
1100.50
822.96
741.01
597.77
552.51
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

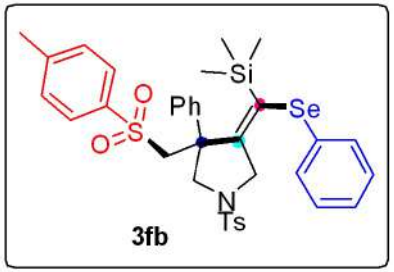
Spectrometer Frequency 400.40



3fb

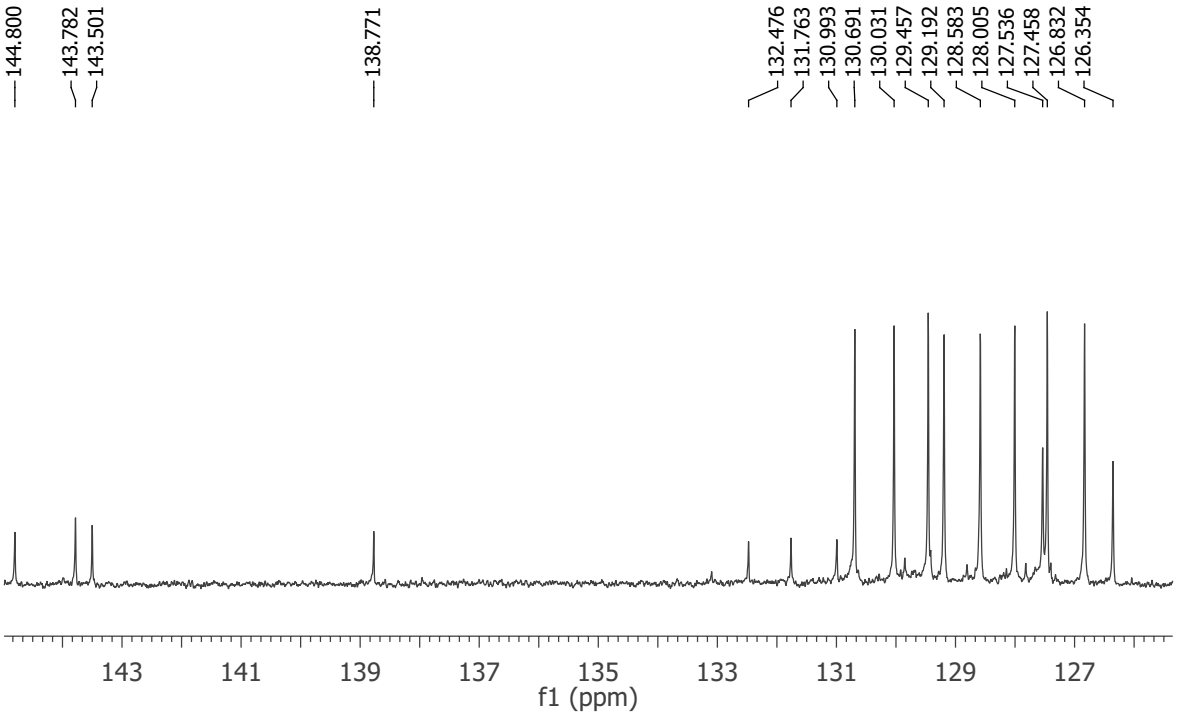
Solvent $CDCl_3$

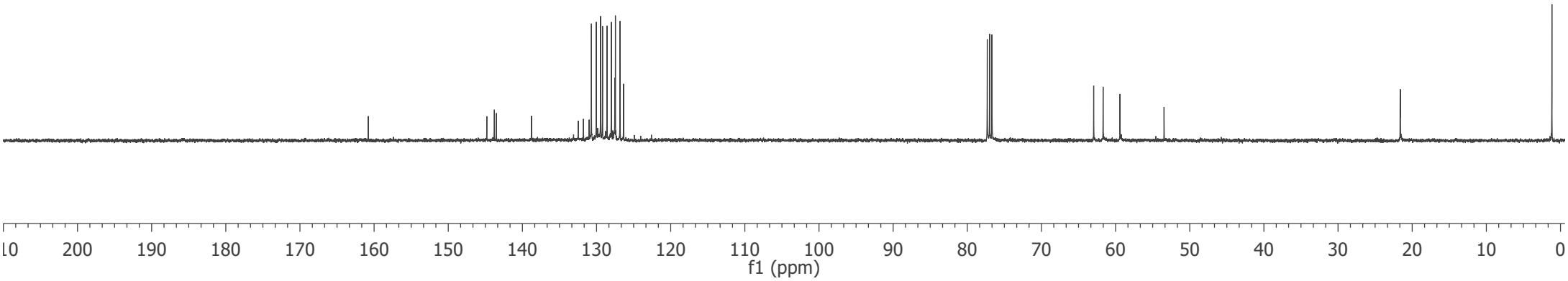
Spectrometer Frequency 100.69

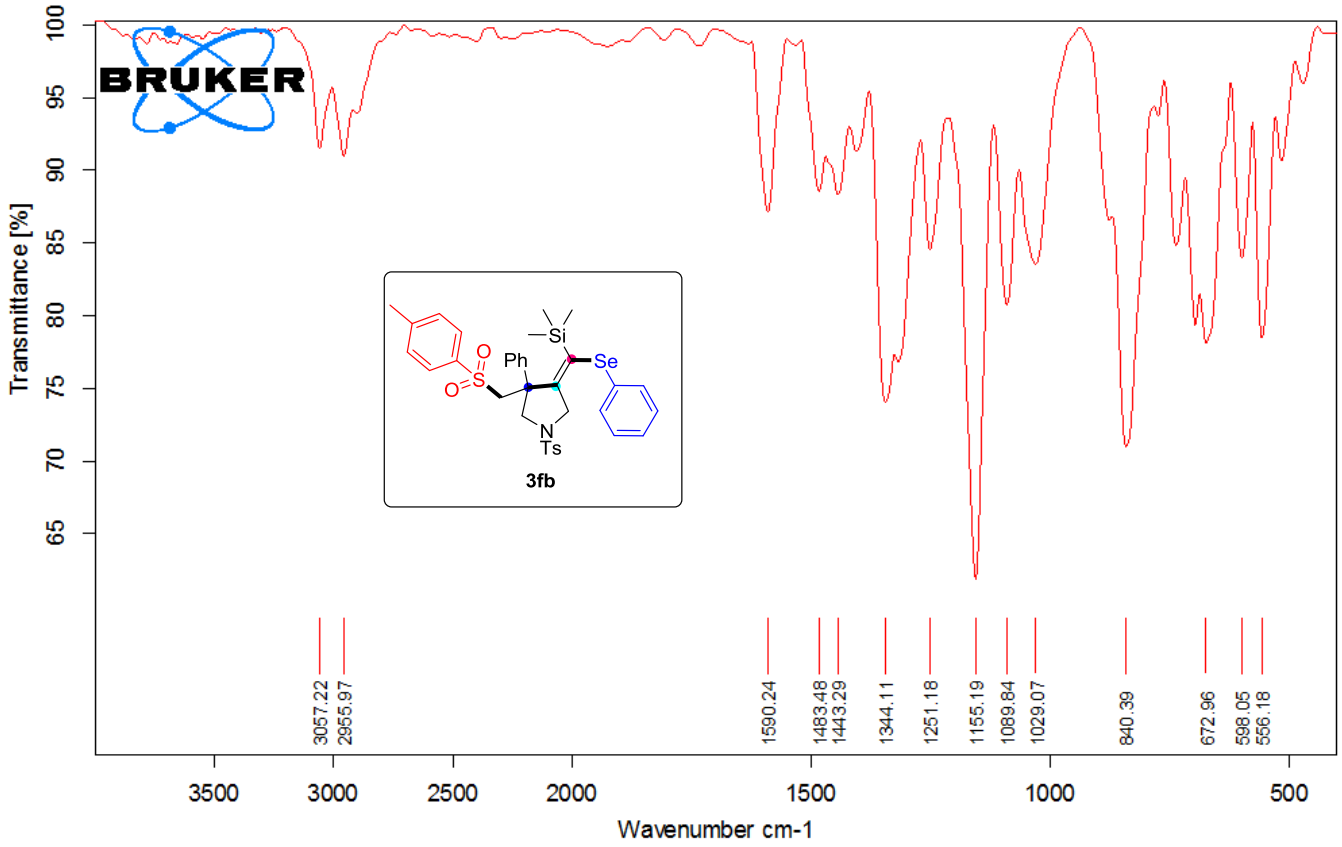


3fb

160.775
144.800
143.782
143.501
138.771
132.476
131.763
130.993
130.691
130.031
129.457
129.192
128.583
128.005
127.536
127.458
126.832
126.354
62.955
61.685
59.408
53.462
21.627
21.597
1.157

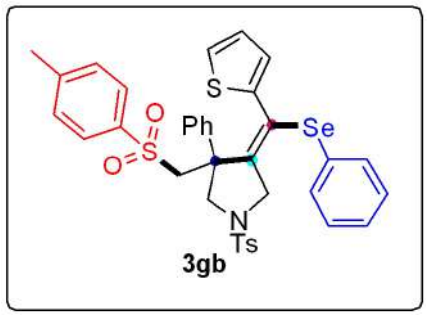





BRUKER
Transmittance [%]
100
95
90
85
80
75
70
65
Si
Ph
Se
O
O
S
N
Ts
3fb
3057.22
2955.97
1590.24
1483.48
1443.29
1344.11
1251.18
1155.19
1089.84
1029.07
840.39
672.96
598.05
556.18
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

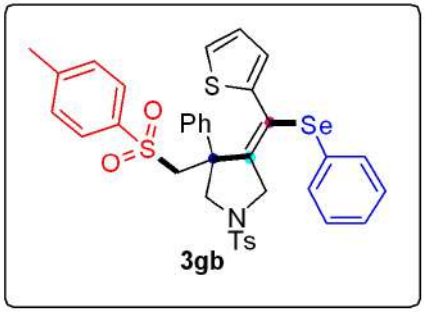
Spectrometer Frequency 400.40



3gb

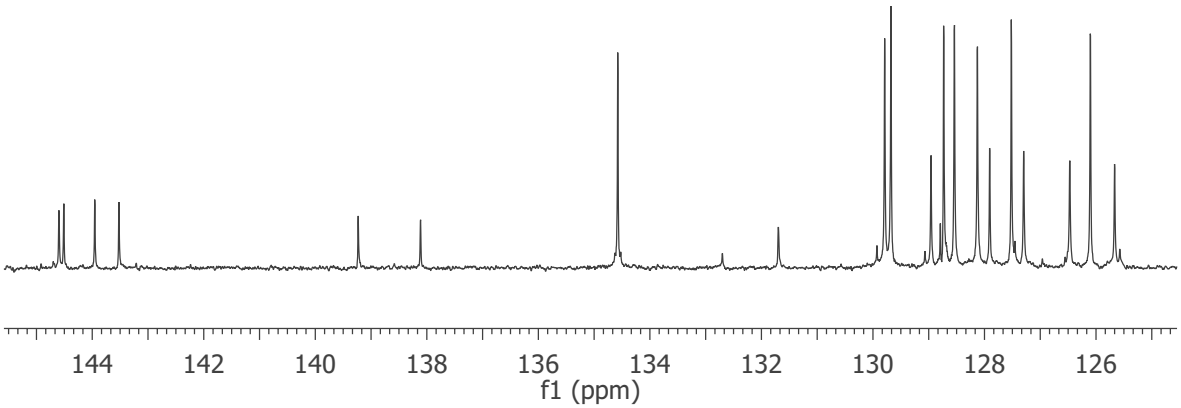
Solvent $CDCl_3$

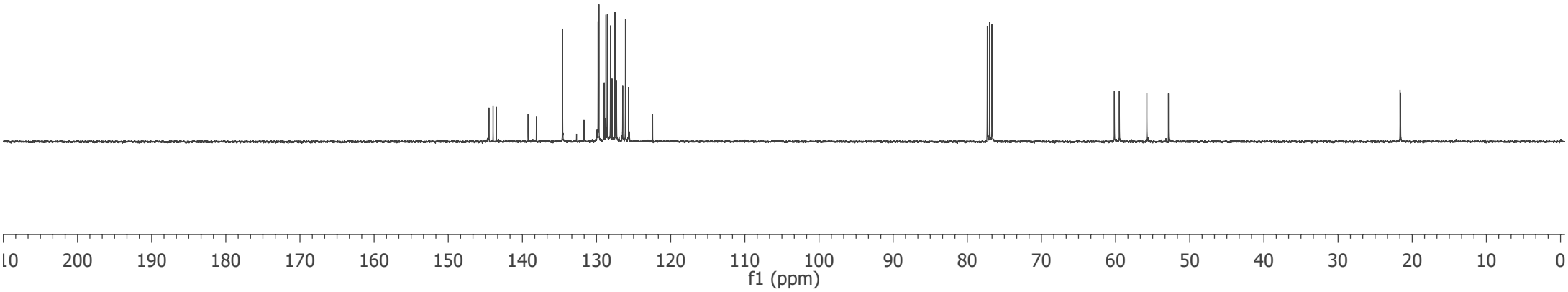
Spectrometer Frequency 100.69

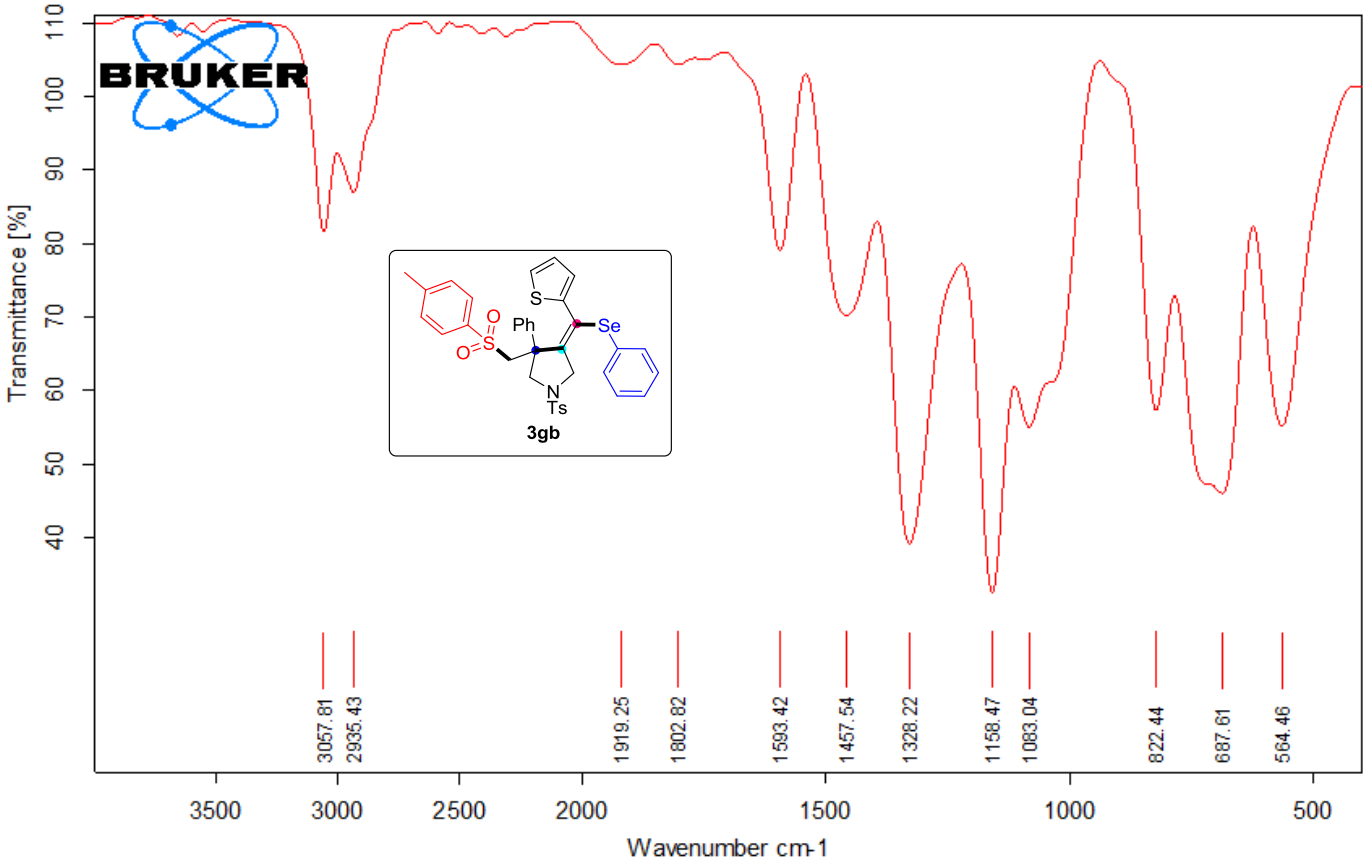


3gb

144.597
144.510
143.954
143.521
139.231
138.113
134.576
131.696
129.790
129.677
128.959
128.792
128.731
128.540
128.128
127.907
127.518
127.297
126.471
126.101
125.666
122.433
60.166
59.495
55.784
52.874
21.640
21.566

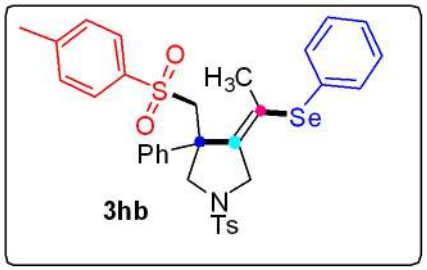





BRUKER
Transmittance [%]
110
100
90
80
70
60
50
40
3057.81
2935.43
1919.25
1802.82
1593.42
1457.54
1328.22
1158.47
1083.04
822.44
687.61
564.46
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
S
Ph
Se
O
O
S
N
Ts
3gb

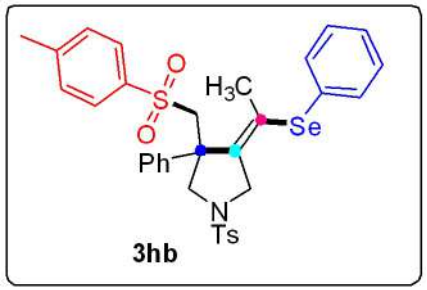
Solvent $CDCl_3$

Spectrometer Frequency 400.40



Solvent $CDCl_3$

Spectrometer Frequency 100.69

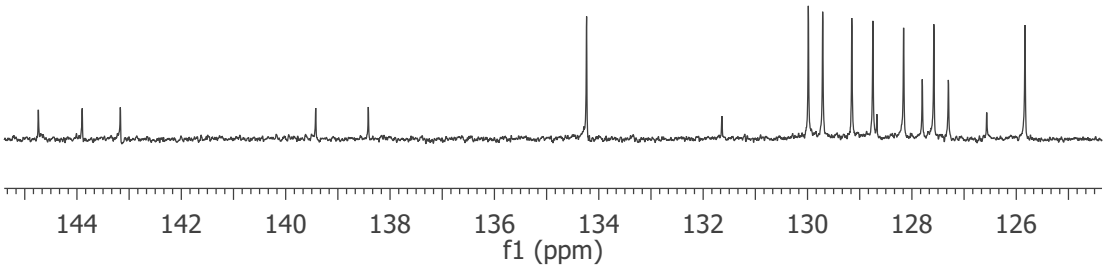


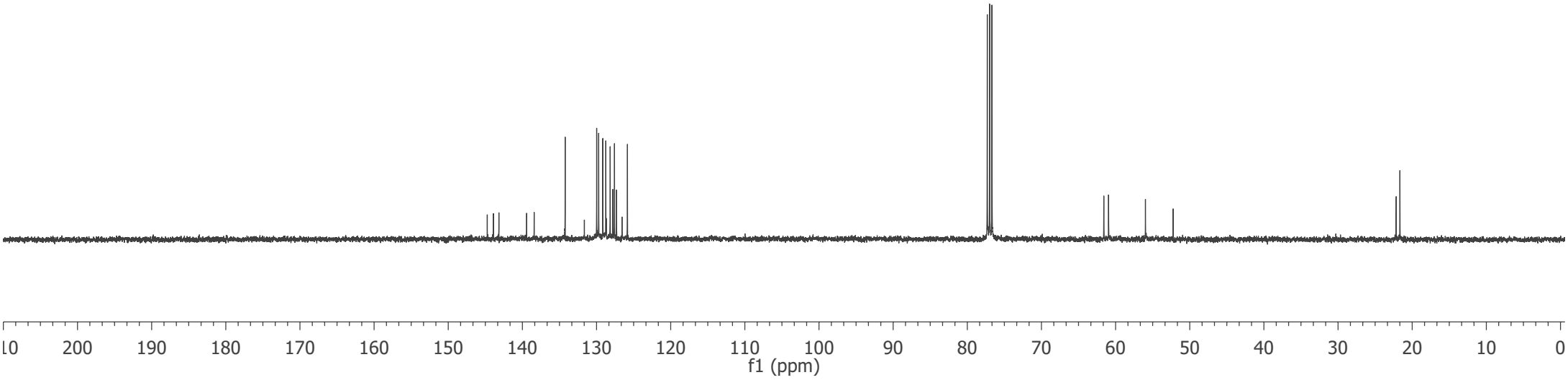
3hb

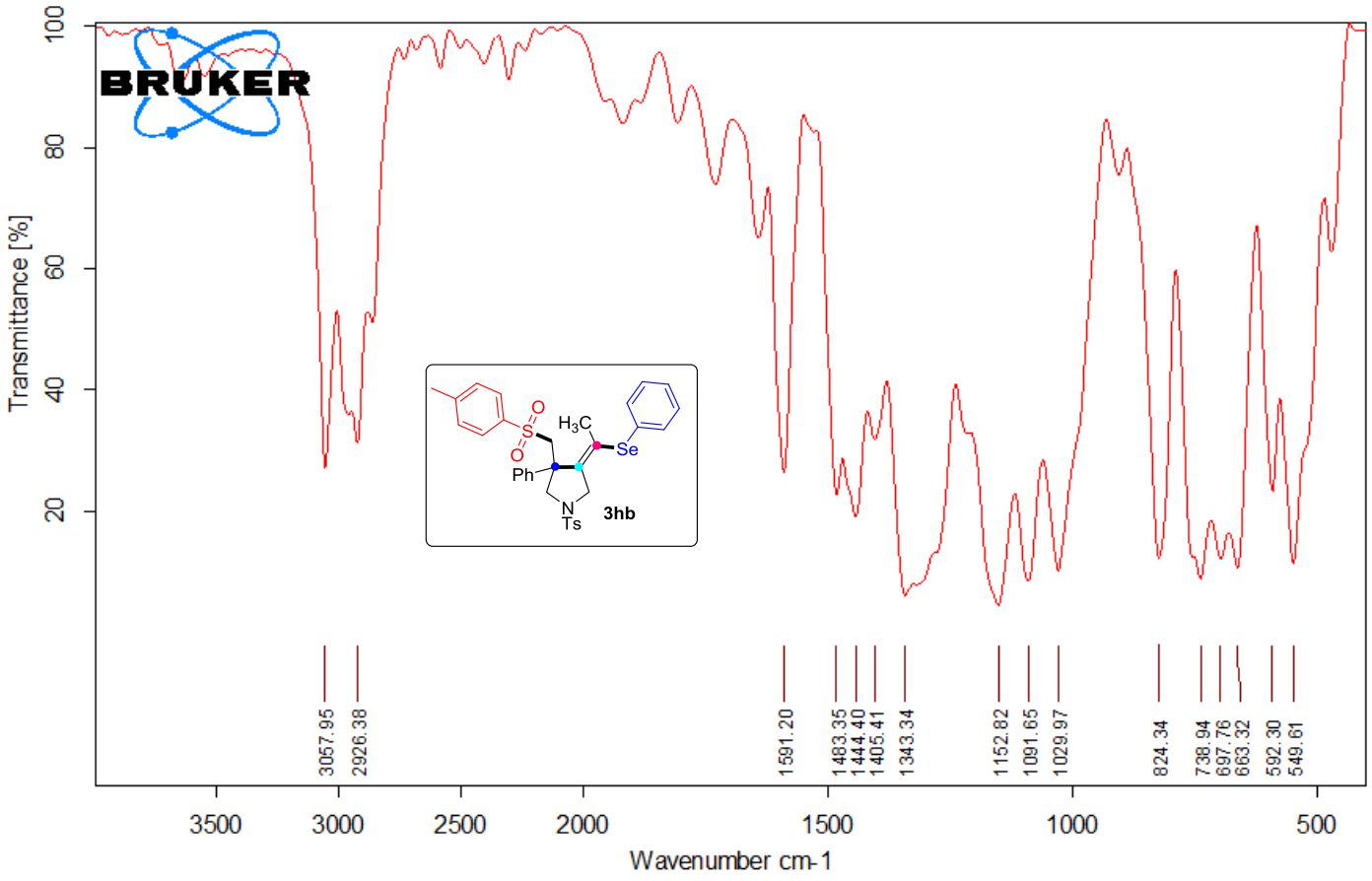
144.740 143.899 143.168 139.425 138.417 134.234 131.641 129.984 129.709 129.152 128.748 128.670 128.158 127.801 127.579 127.300 126.566 125.833

61.589 60.947 55.977 52.242

22.156 21.653

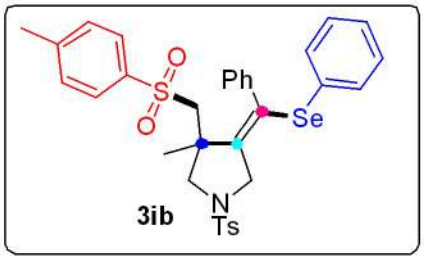





BRUKER
Transmittance [%]
100
80
60
40
20
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3057.95
2926.38
1591.20
1483.35
1444.40
1405.41
1343.34
1152.82
1091.65
1029.97
824.34
738.94
697.76
663.32
592.30
549.61
H3C
Se
Ph
N
Ts
3hb

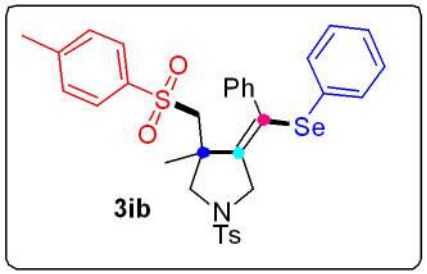
Solvent $CDCl_3$

Spectrometer Frequency 400.40

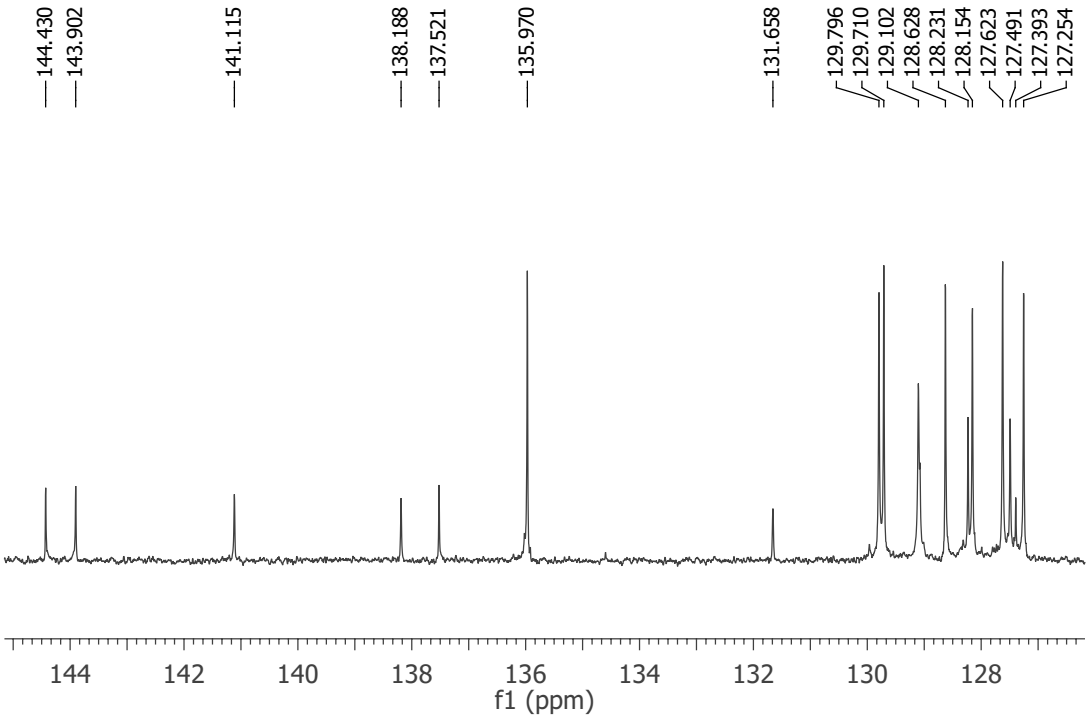


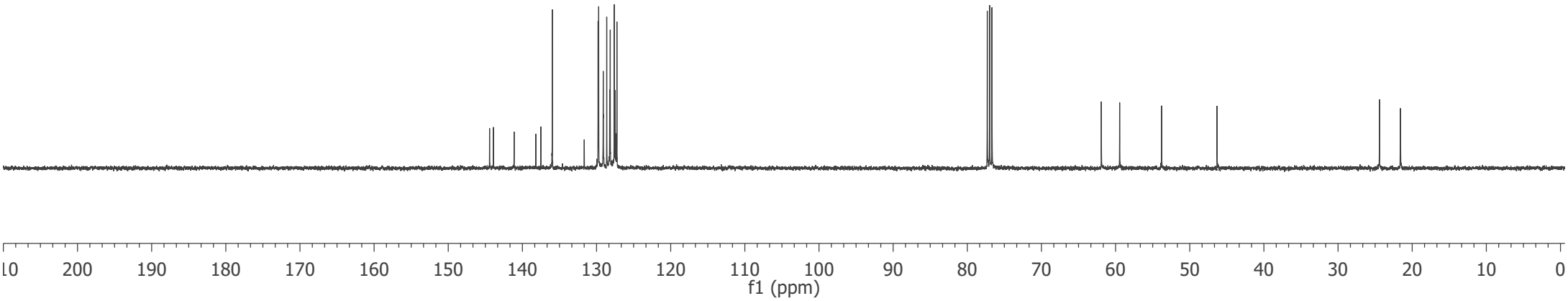
Solvent $CDCl_3$

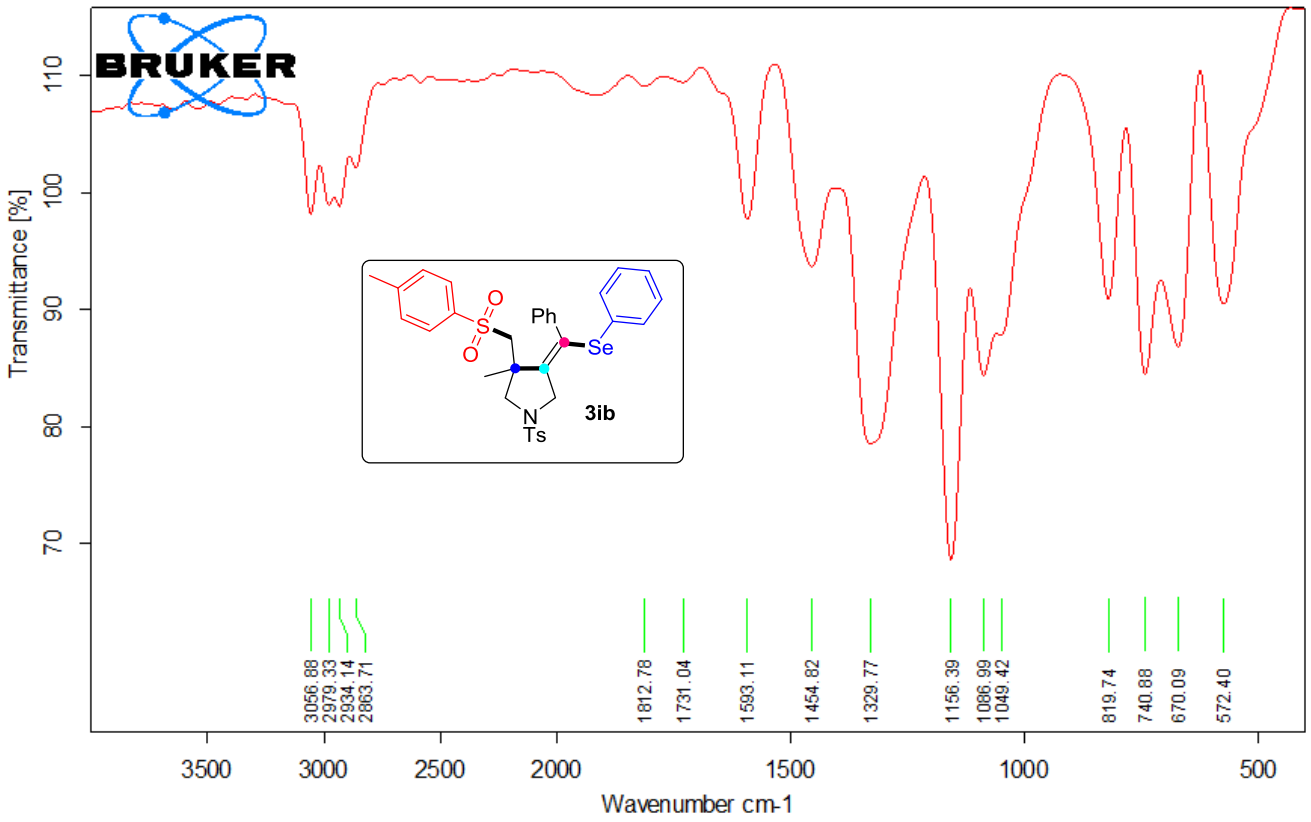
Spectrometer Frequency 100.69



144.430
143.902
141.115
138.188
137.521
135.970
131.658
129.796
129.710
129.102
128.628
128.231
128.154
127.623
127.491
127.393
127.254
61.924
59.455
53.804
46.315
24.417
21.613
21.568

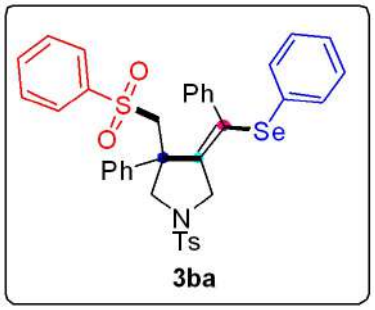




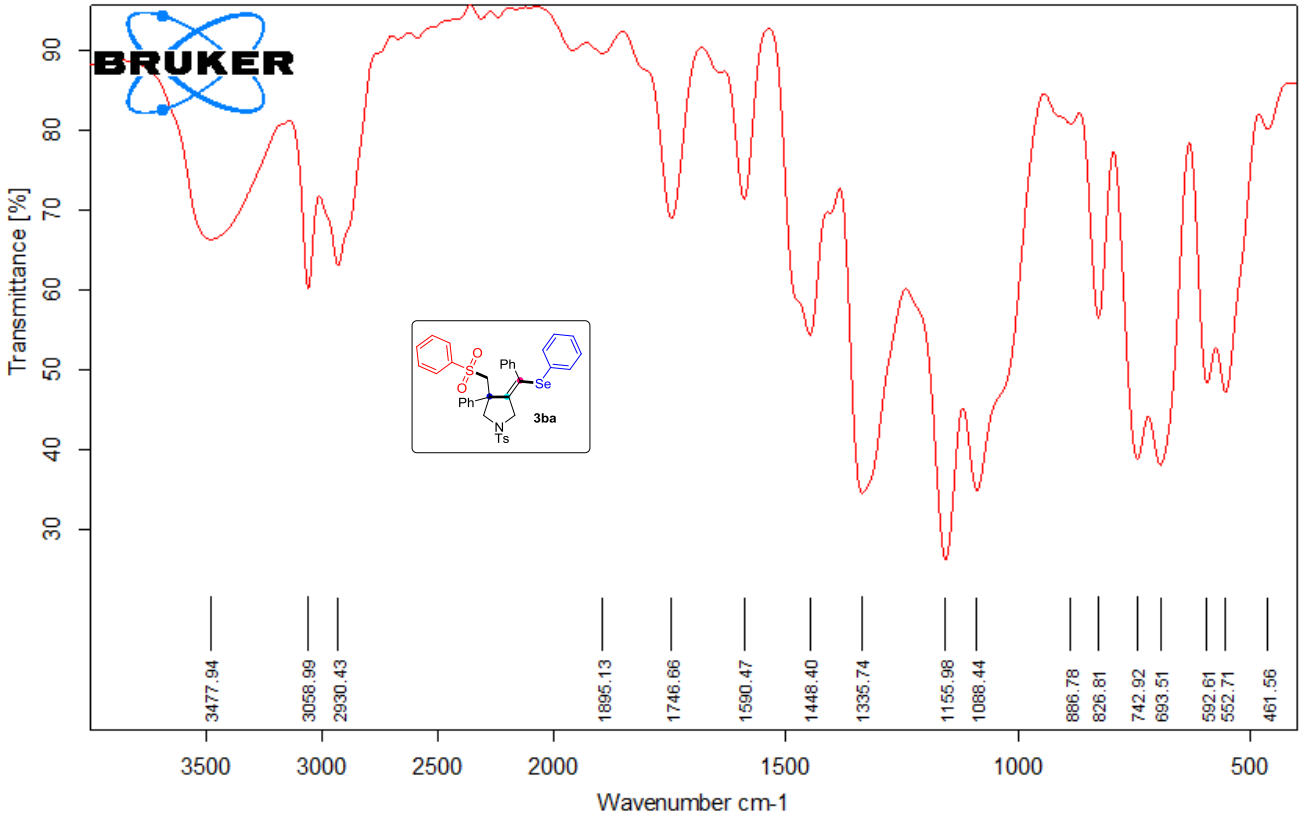

BRUKER
Transmittance [%]
110
100
90
80
70
Ph
Se
N
Ts
3ib
3056.88
2979.33
2934.14
2863.71
1812.78
1731.04
1593.11
1454.82
1329.77
1156.39
1086.99
1049.42
819.74
740.88
670.09
572.40
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

Spectrometer Frequency 400.40

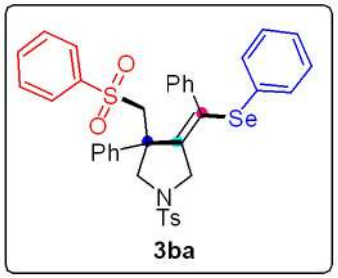


3ba


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
Ph
Se
Ph
N
Ts
O
O
S
3ba
3477.94
3058.99
2930.43
1895.13
1746.66
1590.47
1448.40
1335.74
1155.98
1088.44
886.78
826.81
742.92
693.51
592.61
552.71
461.56
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

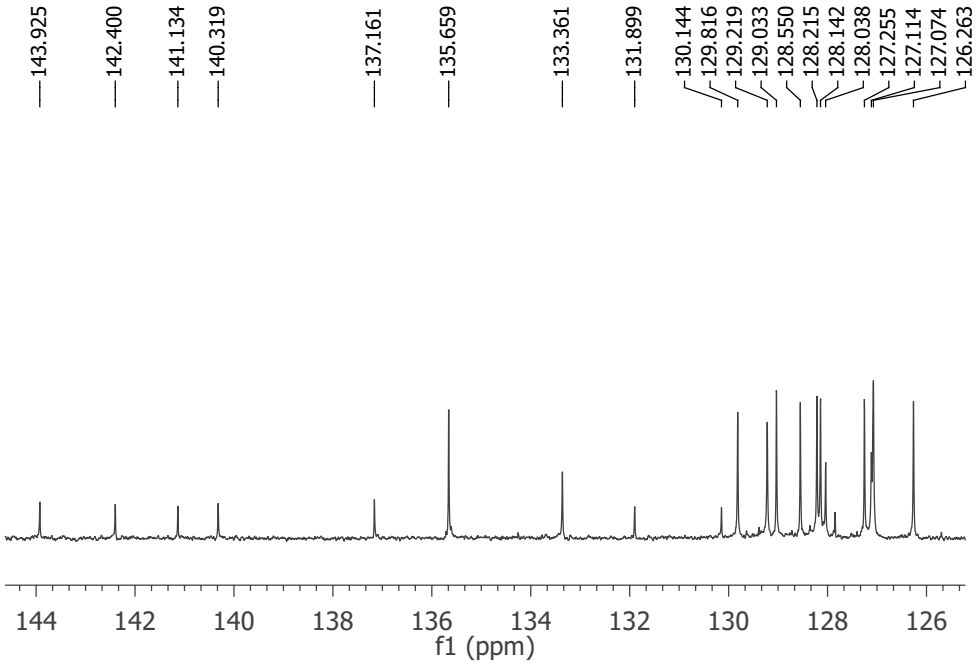
Spectrometer Frequency 100.69

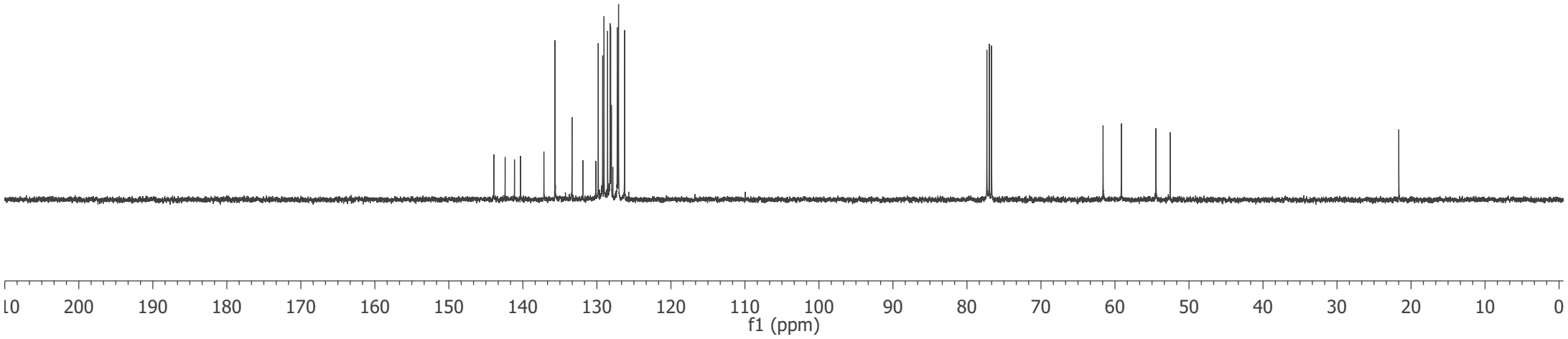


143.925 142.400 141.134 140.319 137.161 135.659 133.361 131.899 130.144 129.816 129.219 129.033 128.550 128.215 128.142 128.038 127.847 127.255 127.114 127.074 126.263

61.608 59.144 54.468 52.552

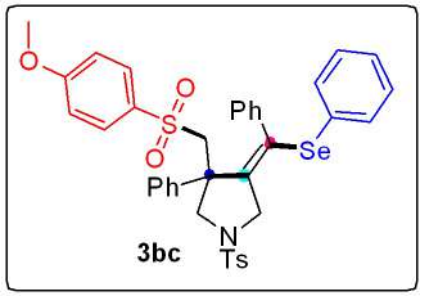
21.650





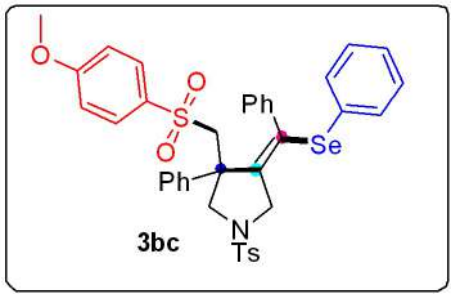
Solvent $CDCl_3$

Spectrometer Frequency 400.40

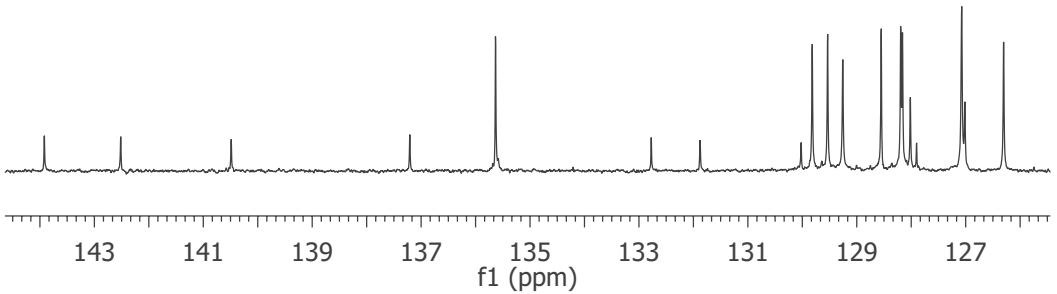


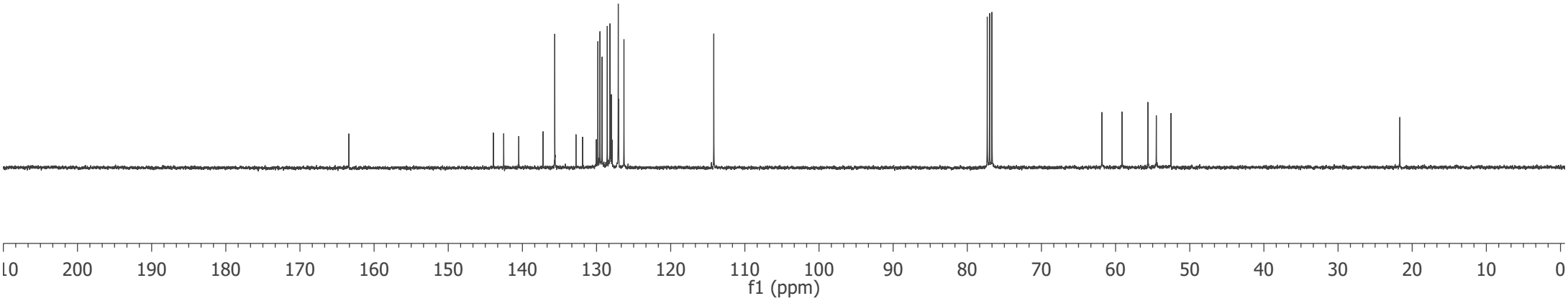
Solvent $CDCl_3$

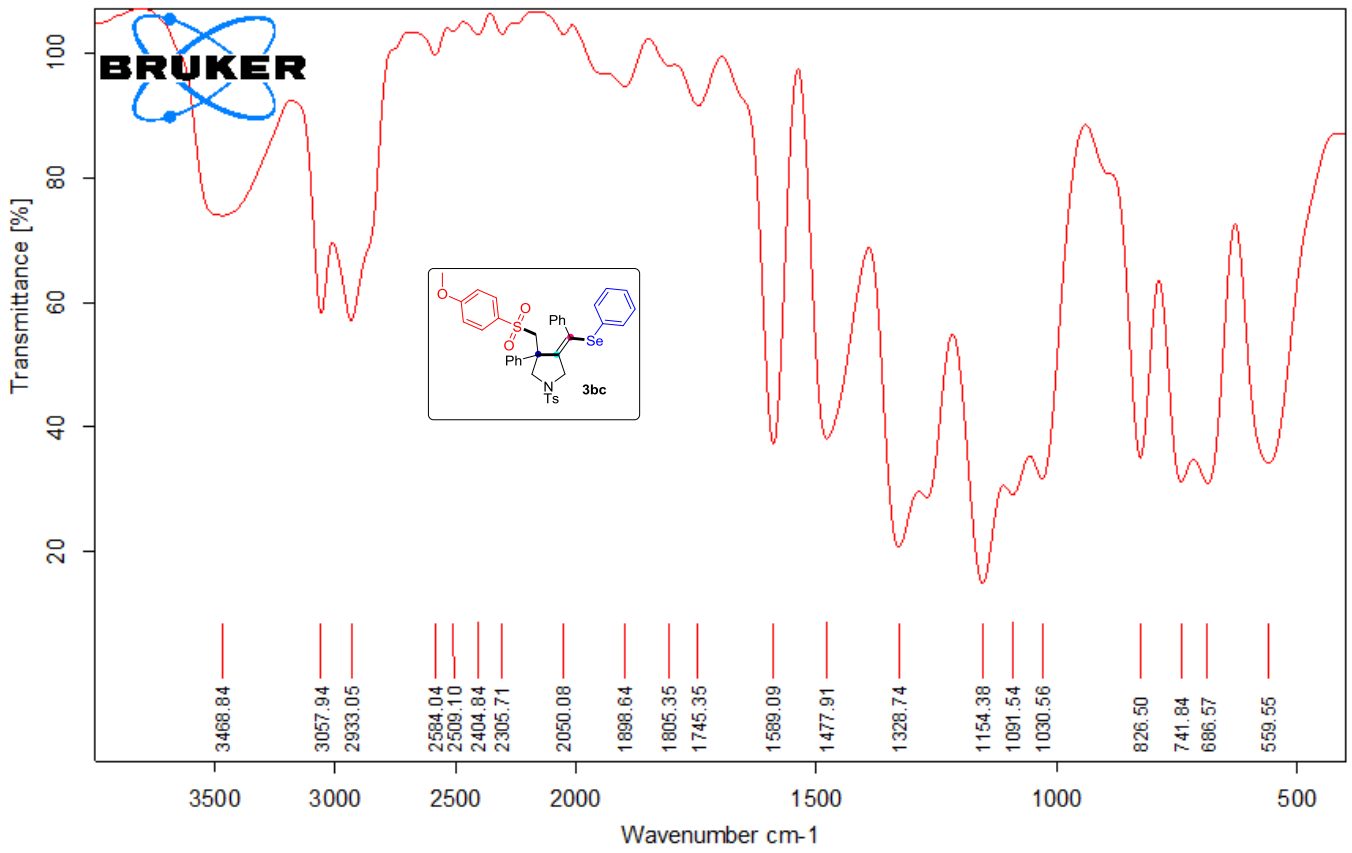
Spectrometer Frequency 100.69



163.407
143.919
142.516
140.487
137.208
135.633
132.774
131.877
130.021
129.818
129.535
129.257
128.551
128.193
128.160
128.017
127.073
127.015
126.303
114.186
61.844
59.124
55.653
54.512
52.528
21.664

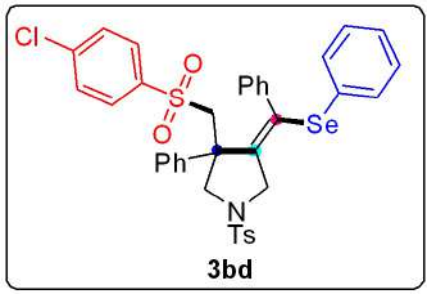





BRUKER
Transmittance [%]
100
80
60
40
20
3468.84
3057.94
2933.05
2584.04
2509.10
2404.84
2305.71
2050.08
1898.64
1805.35
1745.35
1589.09
1477.91
1328.74
1154.38
1091.54
1030.56
826.50
741.84
686.57
559.55
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3bc

Solvent $CDCl_3$

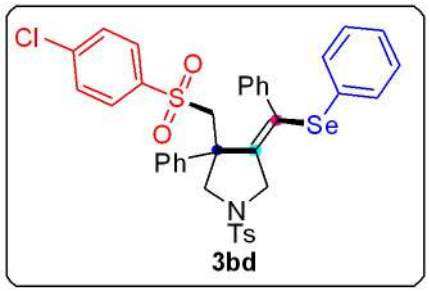
Spectrometer Frequency 400.40



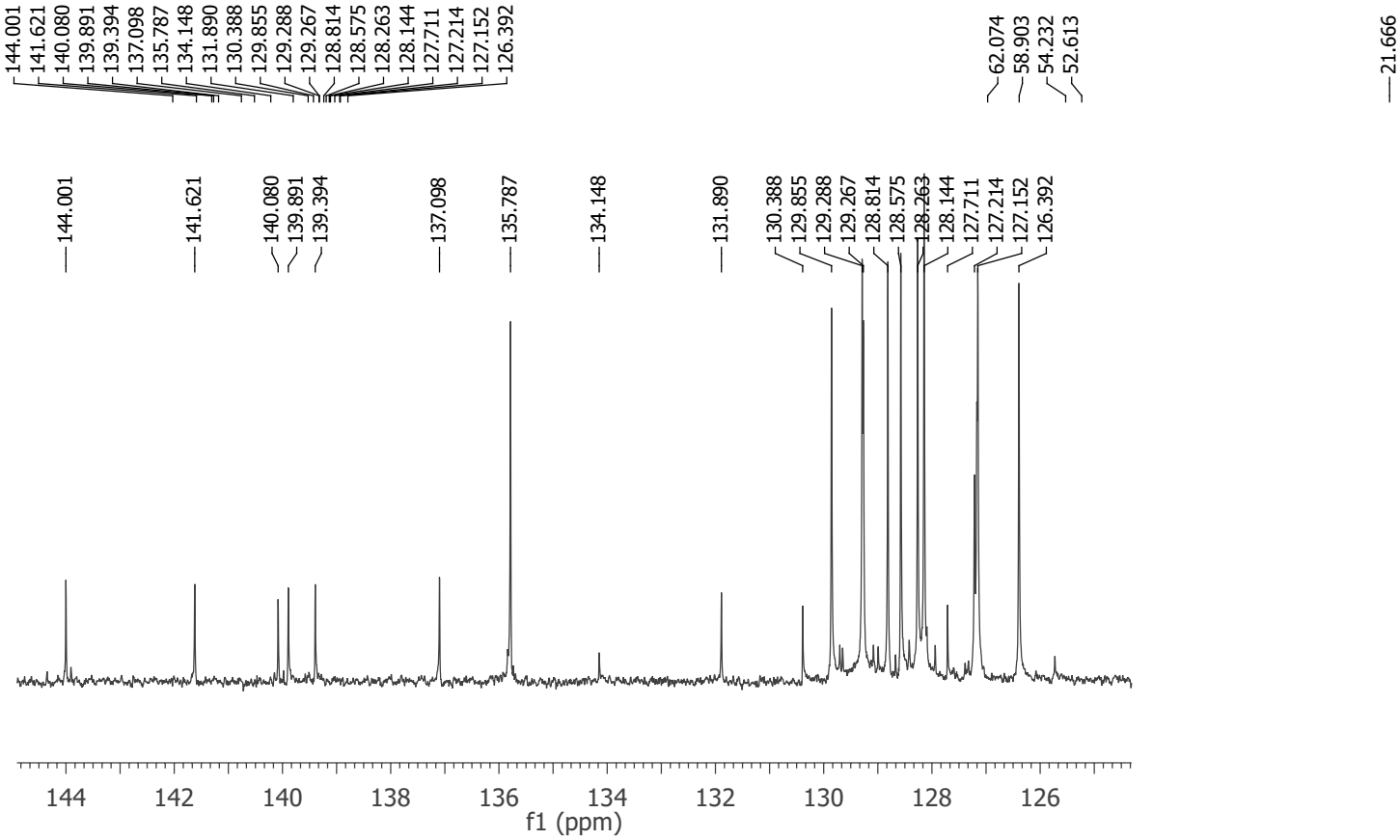
3bd

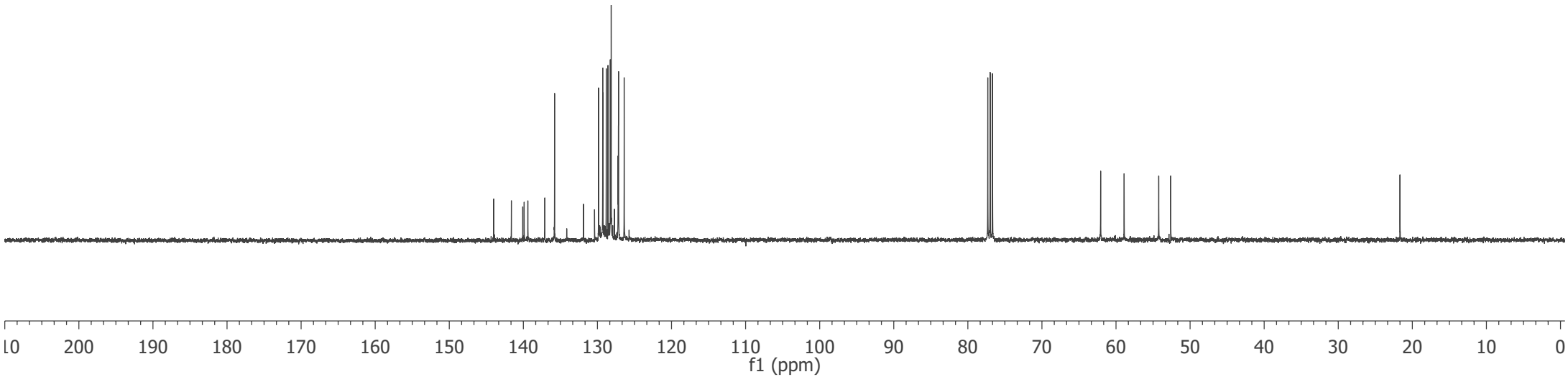
Solvent $CDCl_3$

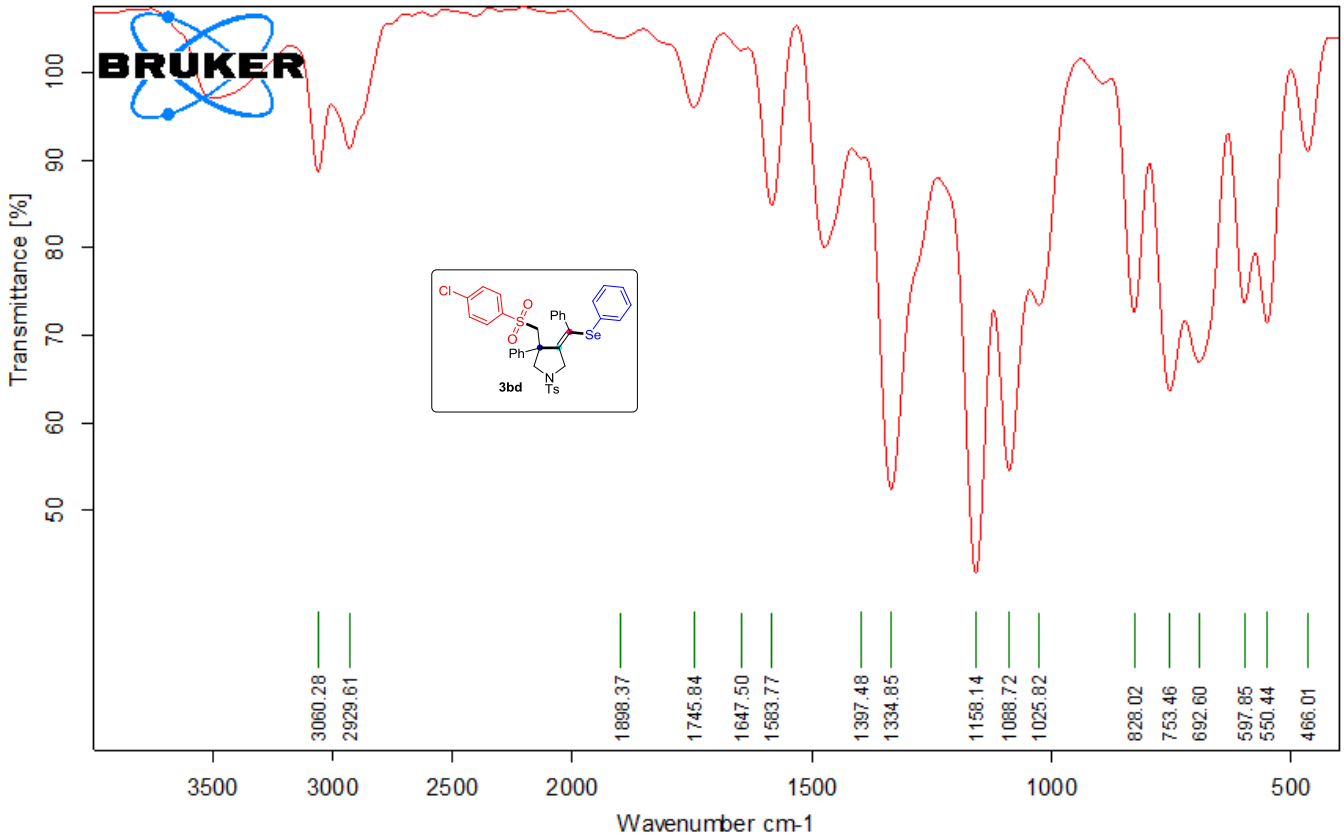
Spectrometer Frequency 100.69



3bd

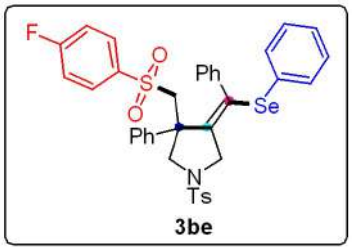





BRUKER
Transmittance [%]
100
90
80
70
60
50
3060.28
2929.61
1898.37
1745.84
1647.50
1583.77
1397.48
1334.85
1158.14
1088.72
1025.82
828.02
753.46
692.60
597.85
550.44
466.01
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
Cl
S
O
O
Ph
Se
Ph
N
Ts
3bd

Solvent $CDCl_3$

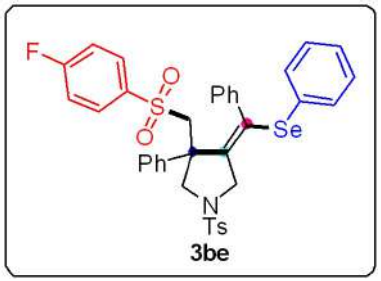
Spectrometer Frequency 400.40



3be

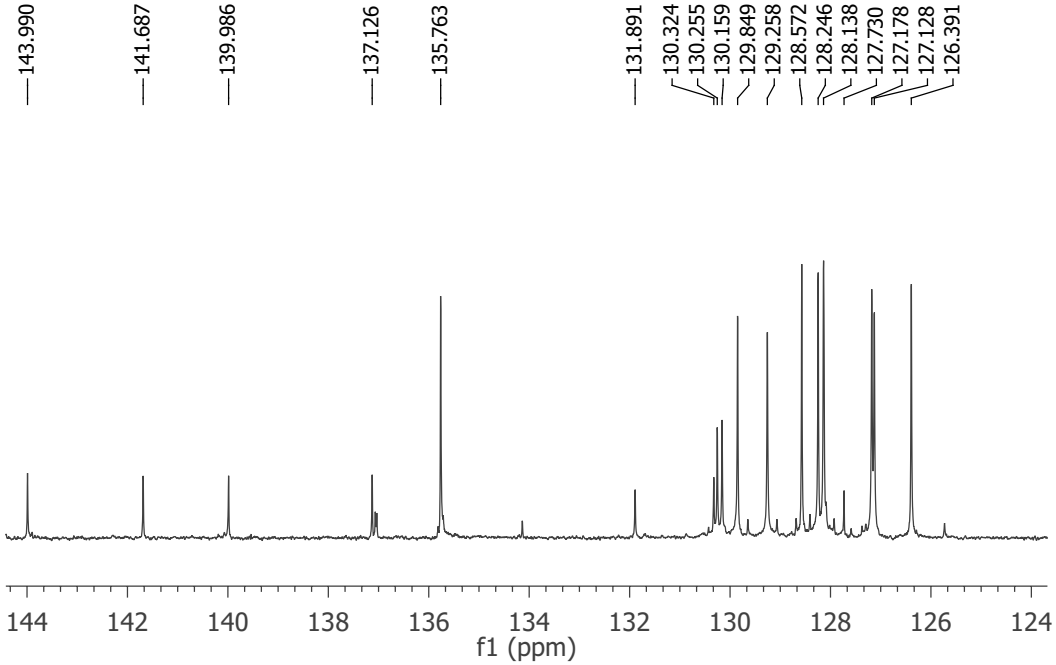
Solvent $CDCl_3$

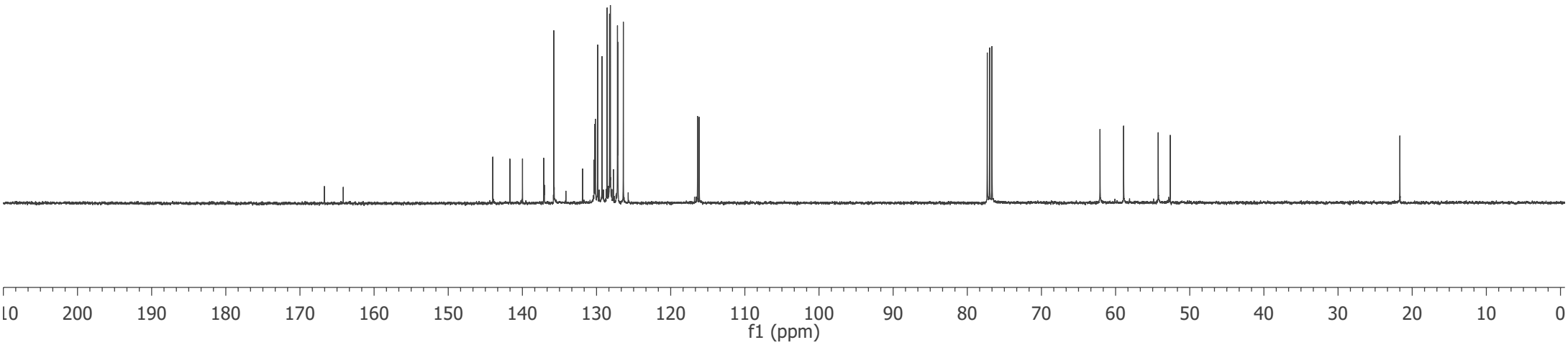
Spectrometer Frequency 100.69

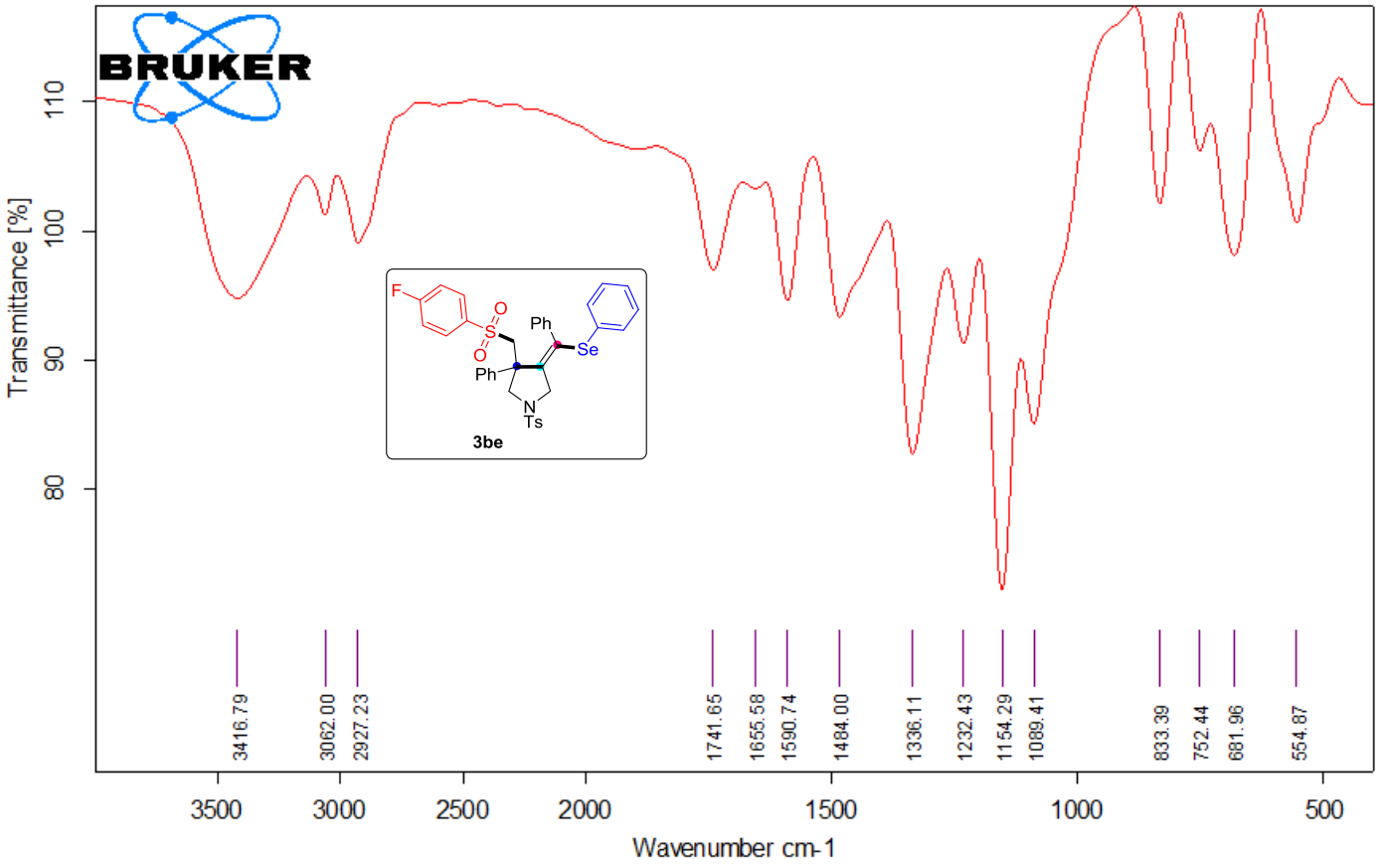


3be

166.704
164.158
143.990
141.687
139.986
137.126
135.763
131.891
130.324
130.255
130.159
129.849
129.258
128.572
128.246
128.138
127.178
127.128
126.391
116.381
116.155
62.100
58.918
54.251
52.631
21.658

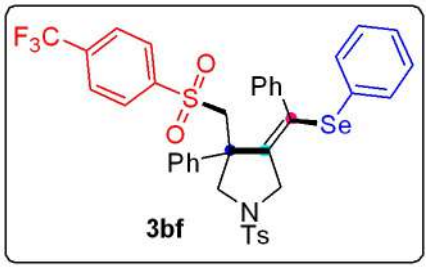


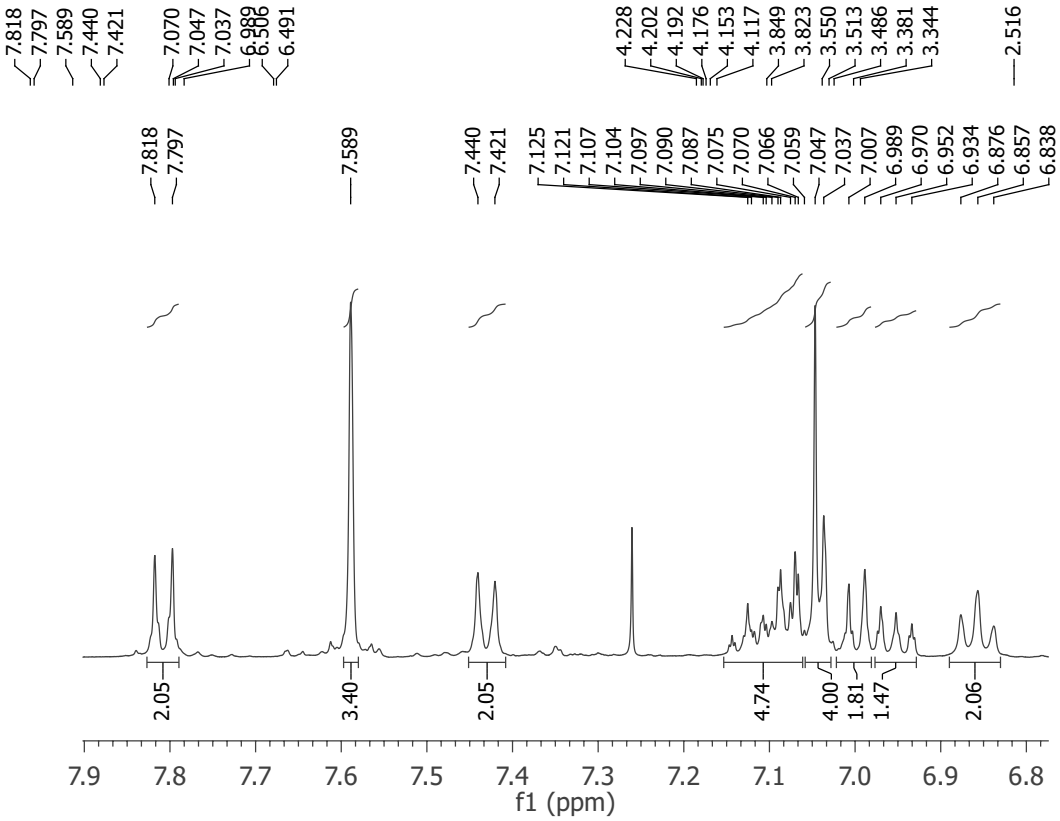


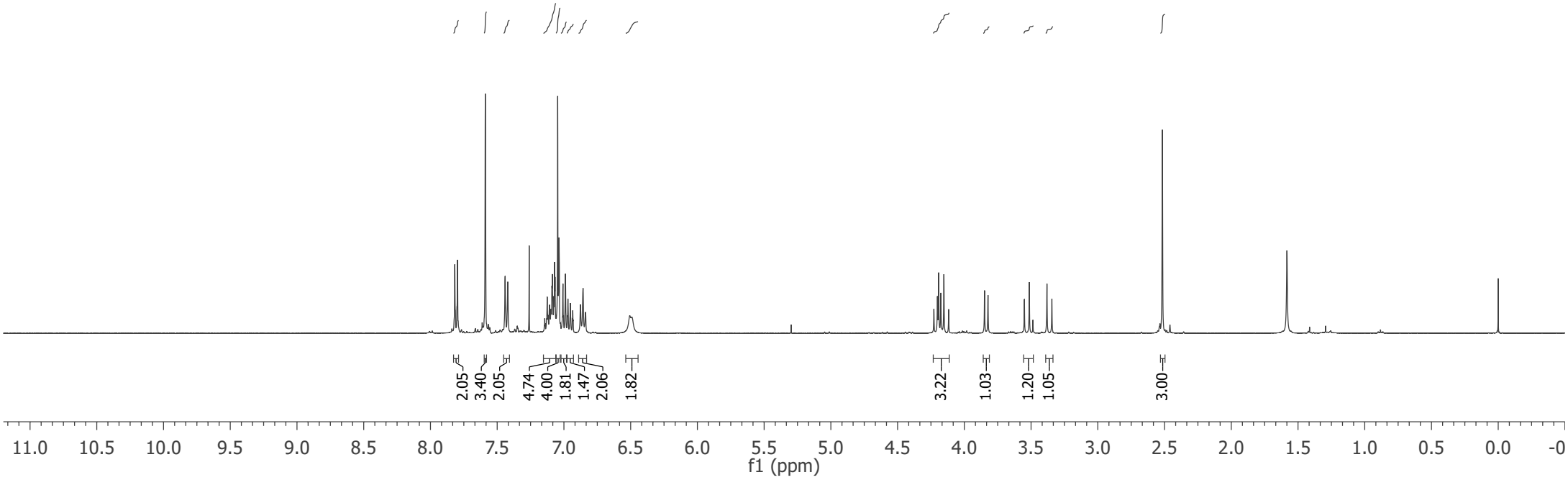

BRUKER
Transmittance [%]
110
100
90
80
F
O
S
O
Ph
Se
Ph
N
Ts
3be
3416.79
3062.00
2927.23
1741.65
1655.58
1590.74
1484.00
1336.11
1232.43
1154.29
1089.41
833.39
752.44
681.96
554.87
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

Spectrometer Frequency 400.40

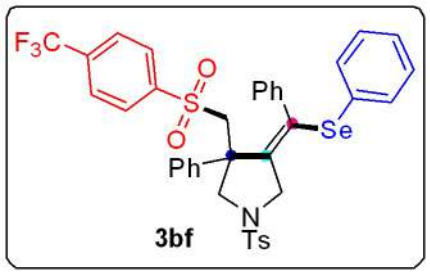




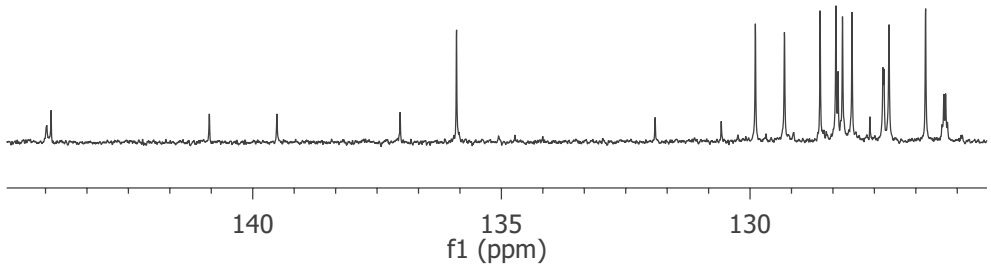


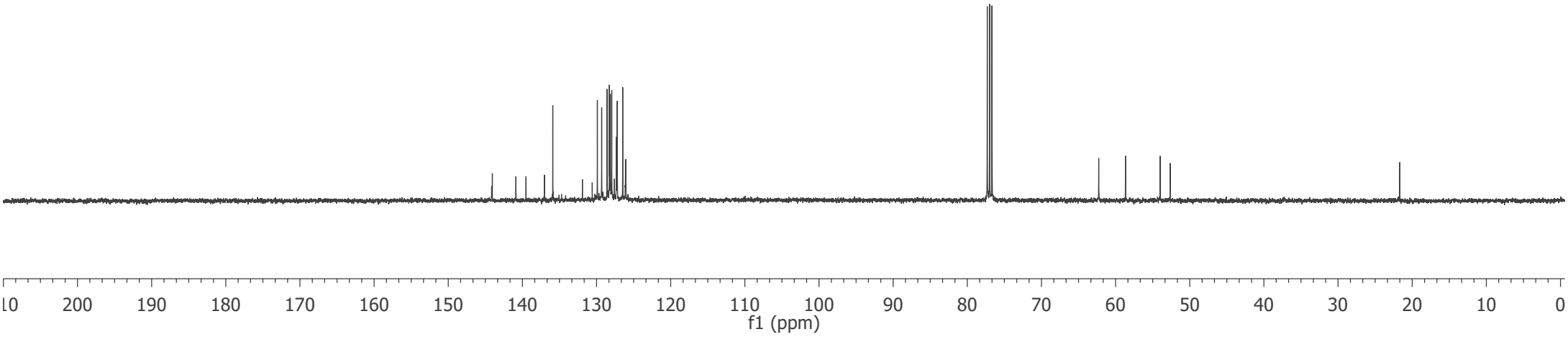
Solvent $CDCl_3$

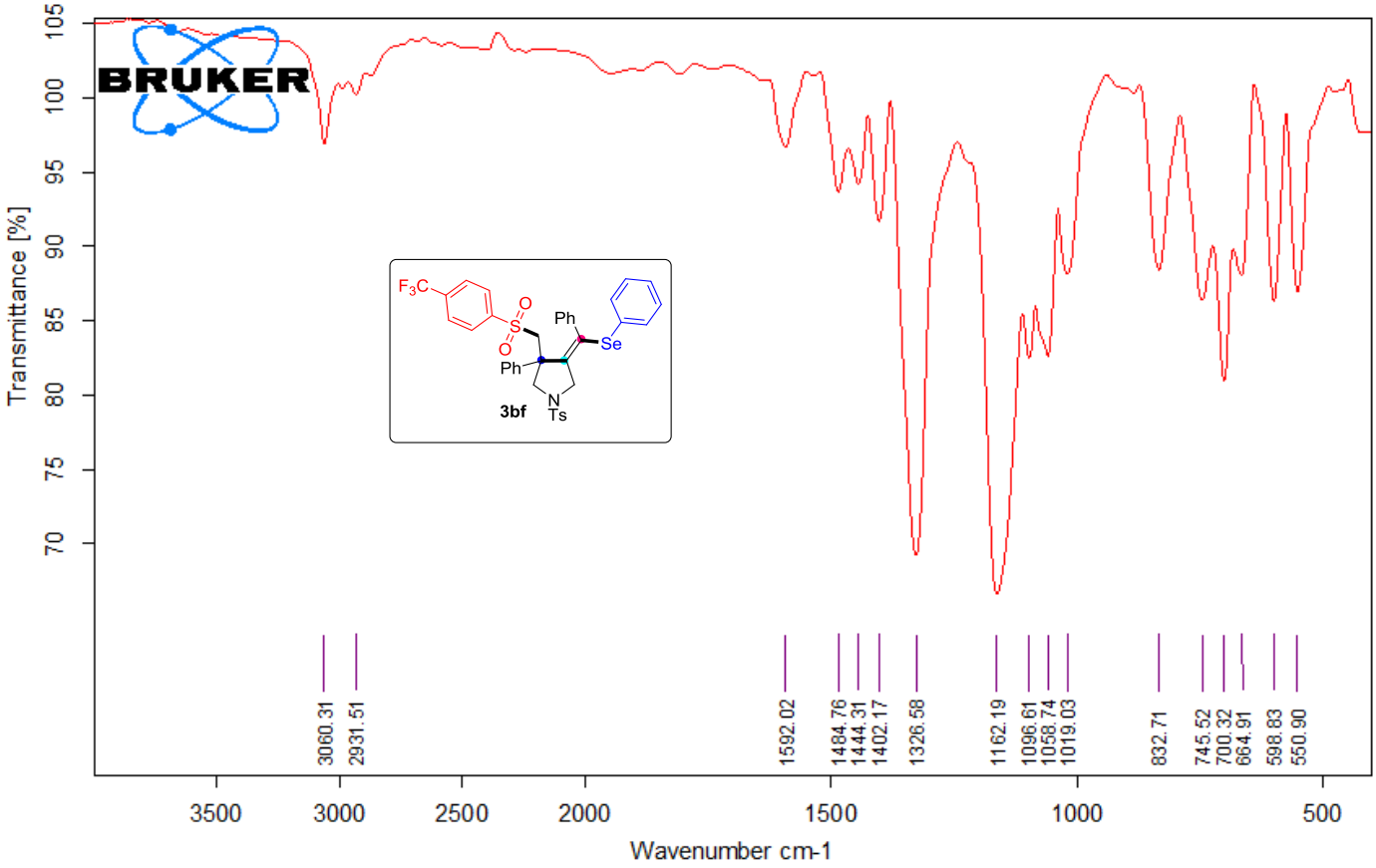
Spectrometer Frequency 100.69



144.142
144.055
140.873
139.513
137.036
135.903
131.909
130.580
129.893
129.308
128.591
128.273
128.231
128.141
127.950
127.590
127.327
127.308
127.206
126.471
126.103
126.067
62.275
58.664
53.991
52.643
21.671

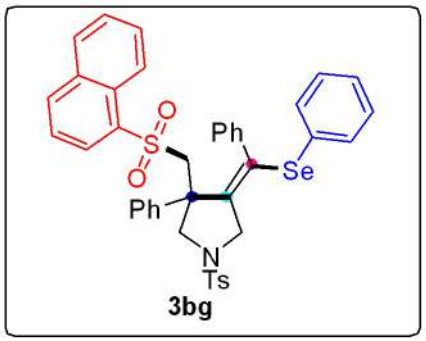





BRUKER
Transmittance [%]
105
100
95
90
85
80
75
70
F3C
O
S
O
Ph
Se
Ph
N
Ts
3bf
3060.31
2931.51
1592.02
1484.76
1444.31
1402.17
1326.58
1162.19
1096.61
1058.74
1019.03
832.71
745.52
700.32
664.91
598.83
550.90
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

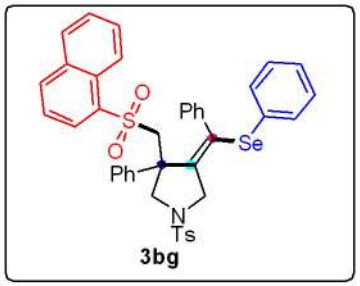
Spectrometer Frequency 400.40



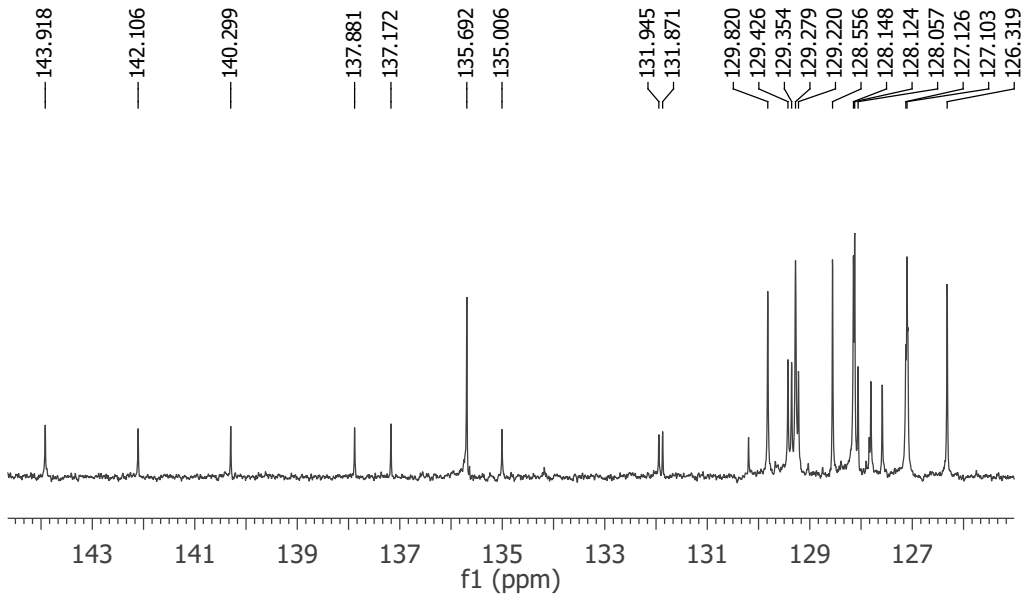
3bg

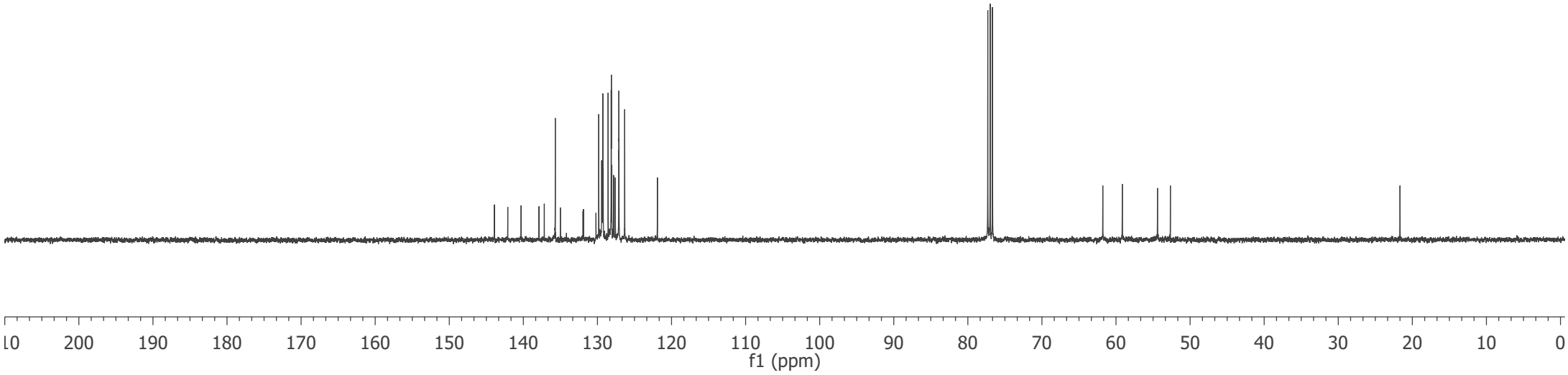
Solvent $CDCl_3$

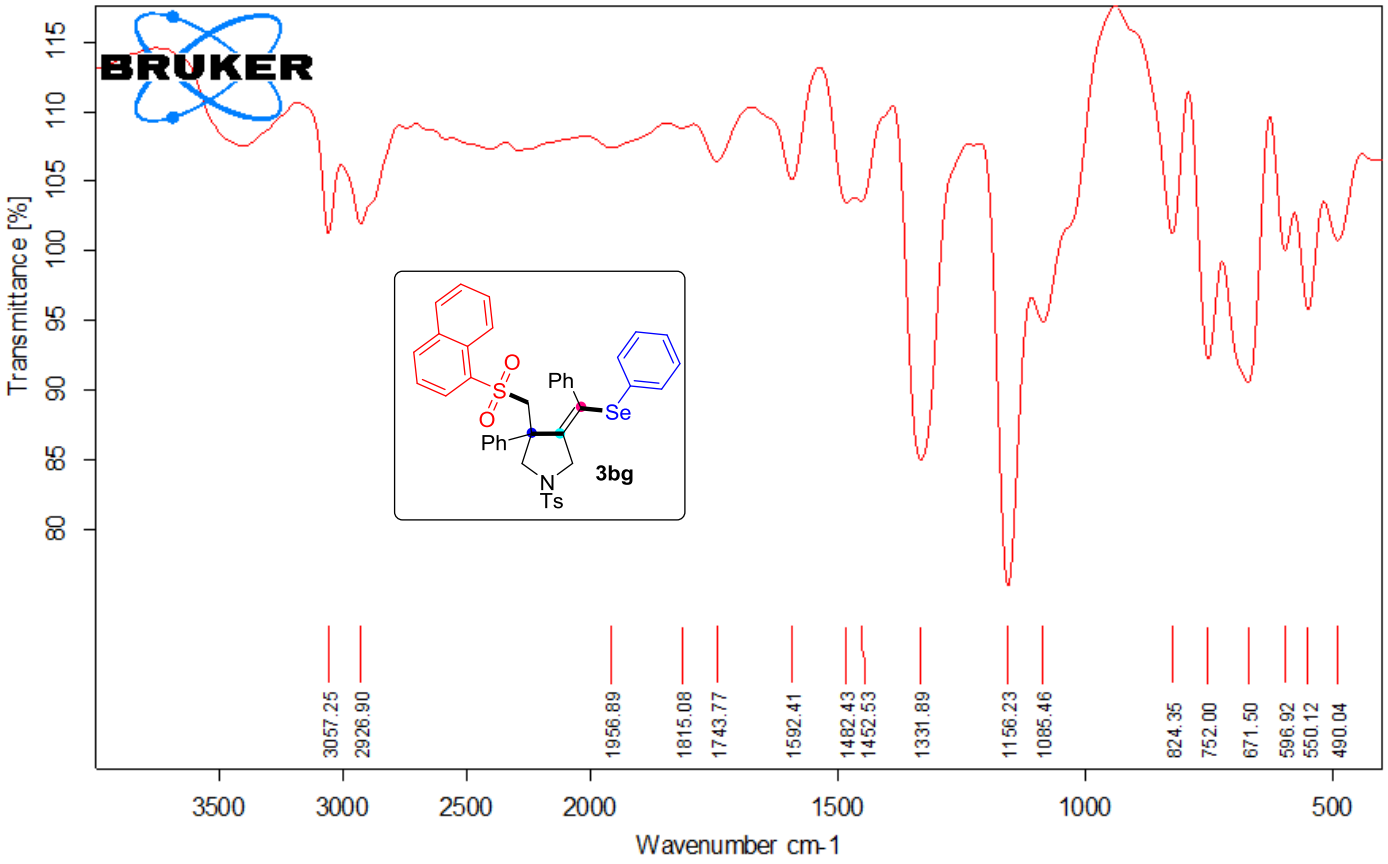
Spectrometer Frequency 100.69



143.918, 142.106, 140.299, 137.881, 137.172, 135.692, 135.006, 131.945, 131.871, 130.195, 129.820, 129.426, 129.354, 129.279, 129.220, 128.556, 128.148, 128.124, 128.057, 127.840, 127.808, 127.586, 127.126, 127.103, 126.319, 121.910, 61.783, 59.153, 54.403, 52.663, 21.662

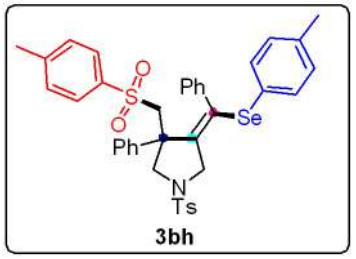





BRUKER
Transmittance [%]
115
110
105
100
95
90
85
80
Ph
Se
Ph
N
Ts
O
O
S
3bg
3057.25
2926.90
1956.89
1815.08
1743.77
1592.41
1482.43
1452.53
1331.89
1156.23
1085.46
824.35
752.00
671.50
596.92
550.12
490.04
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

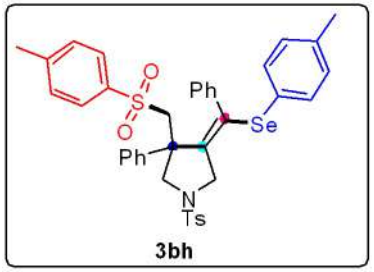
Solvent $CDCl_3$

Spectrometer Frequency 400.40

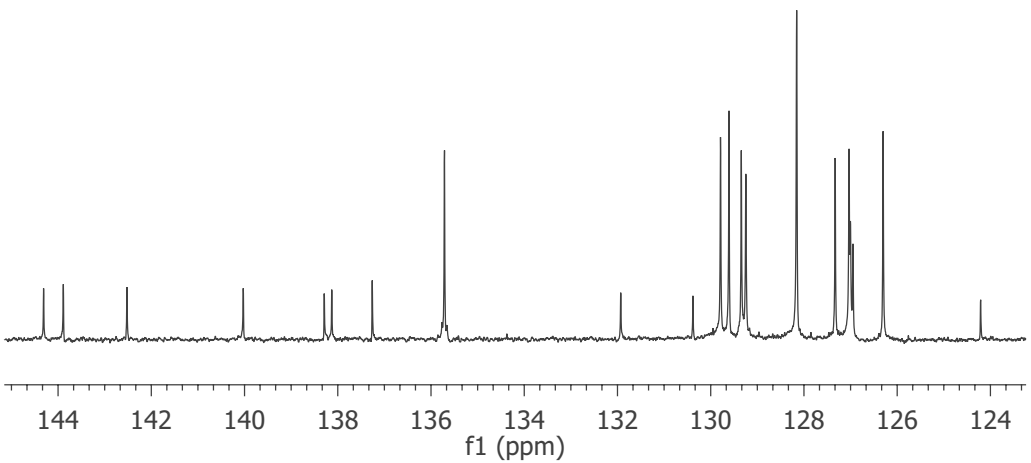


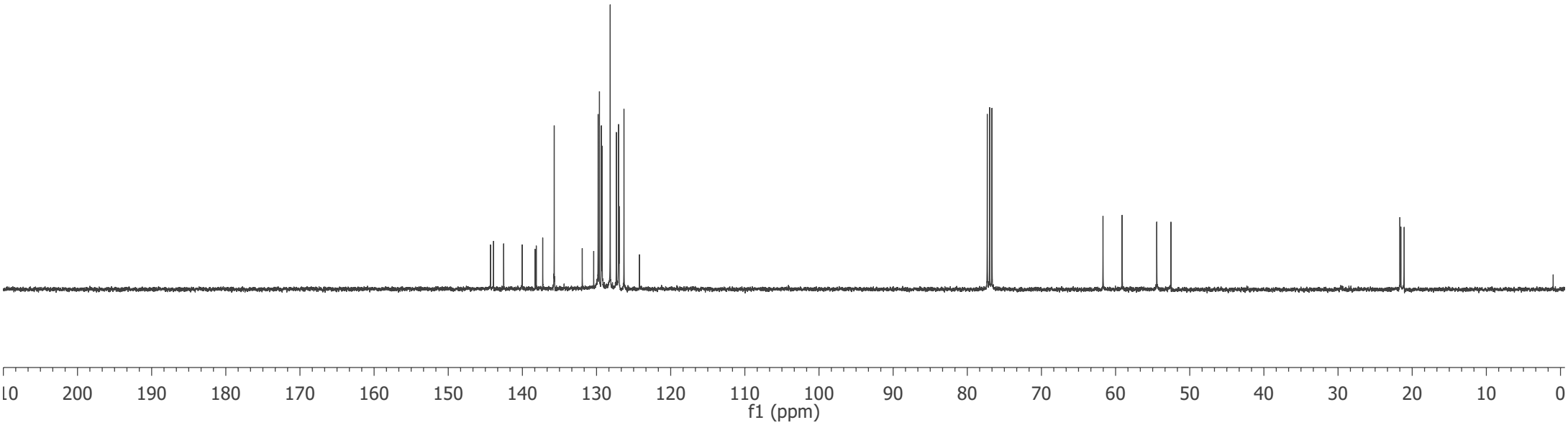
Solvent $CDCl_3$

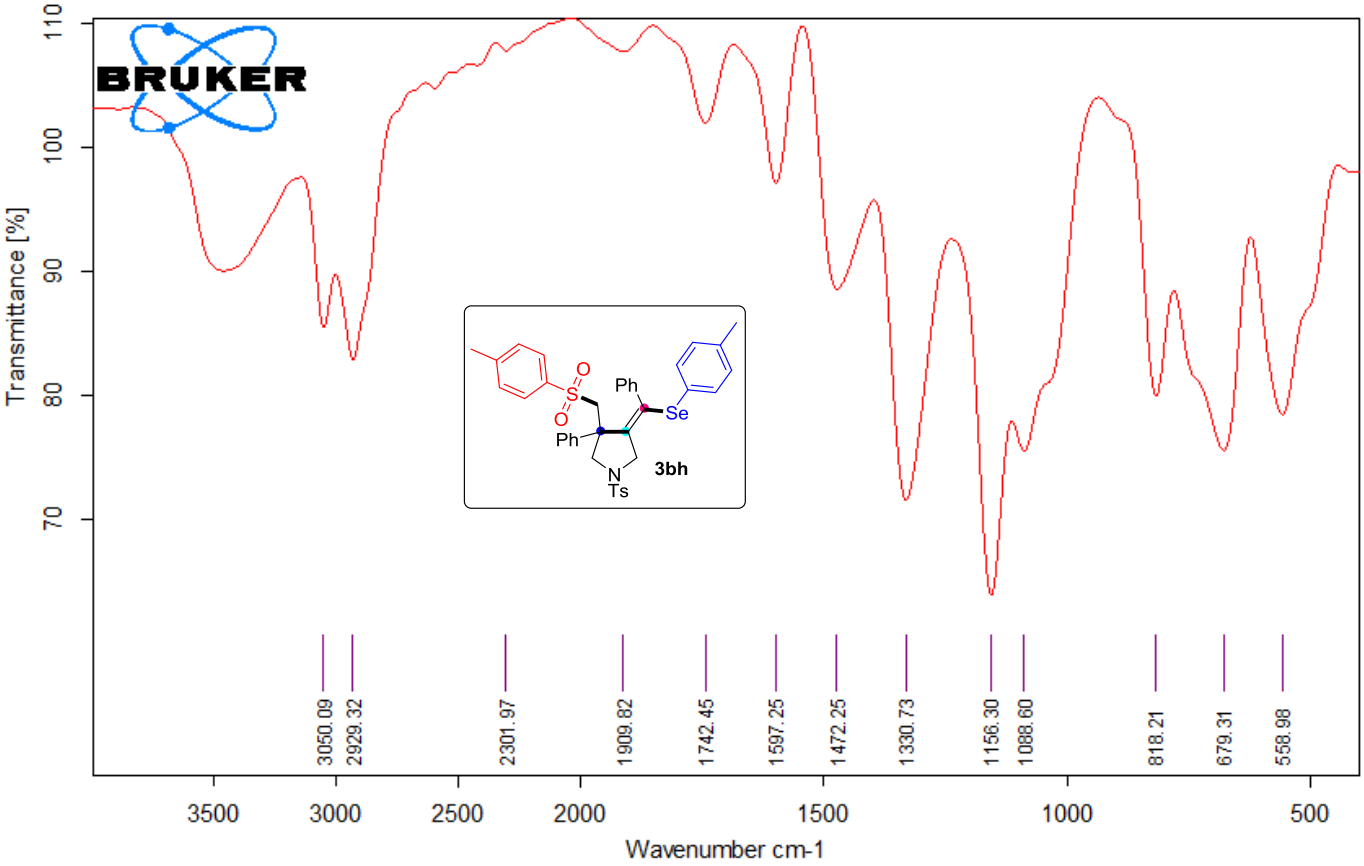
Spectrometer Frequency 100.69



144.310
143.887
142.522
140.027
138.290
138.129
137.260
135.712
131.930
130.381
129.789
129.608
129.344
129.246
128.156
127.330
127.032
127.002
126.948
126.302
124.211
61.699
59.116
54.447
52.535
21.658
21.528
21.077

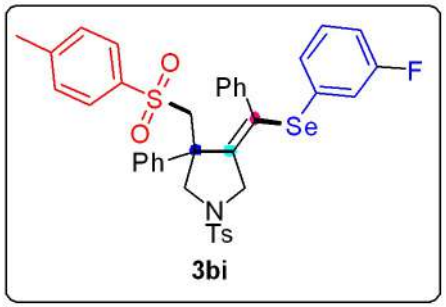





BRUKER
Transmittance [%]
110
100
90
80
70
3050.09
2929.32
2301.97
1909.82
1742.45
1597.25
1472.25
1330.73
1156.30
1088.60
818.21
679.31
558.98
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
O
S
O
Ph
Se
Ph
N
Ts
3bh

Solvent $CDCl_3$

Spectrometer Frequency 400.40



3bi

Solvent $CDCl_3$

Spectrometer Frequency 100.69

163.139
160.655
144.453
144.014
143.003
141.806
138.288
137.124
129.831
129.677
128.303
128.165
127.357
126.123
115.141
114.932
61.275
59.302
54.822
52.466
21.664
21.556

144.453
144.014
143.003
141.806
138.288
137.124
131.829
130.884
130.853
129.831
129.744
129.677
129.578
129.508
129.244
129.193
128.303
128.165
127.357
127.320
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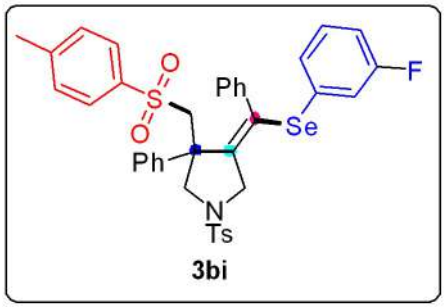
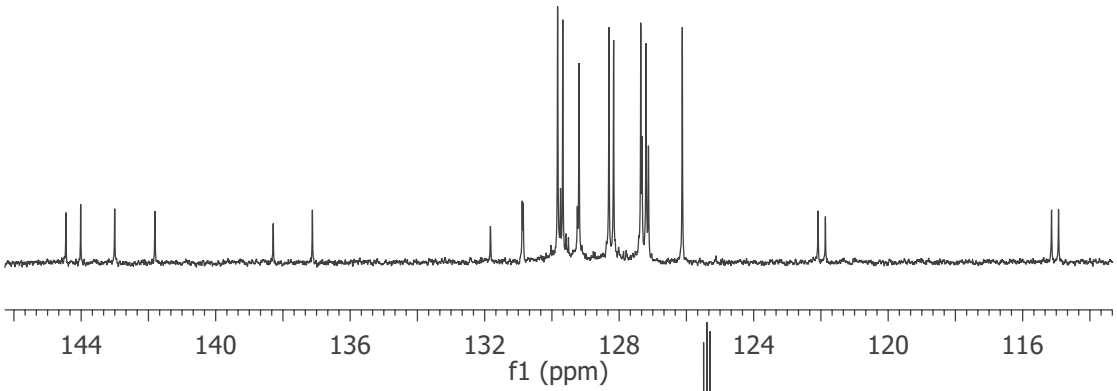
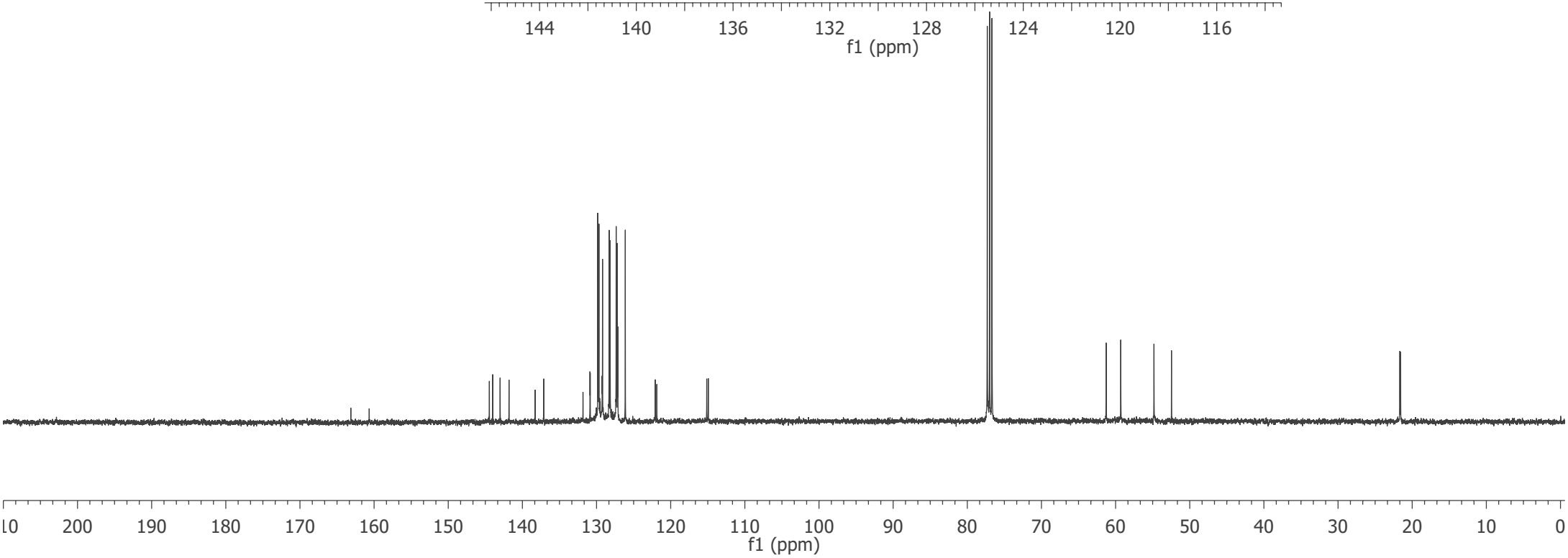
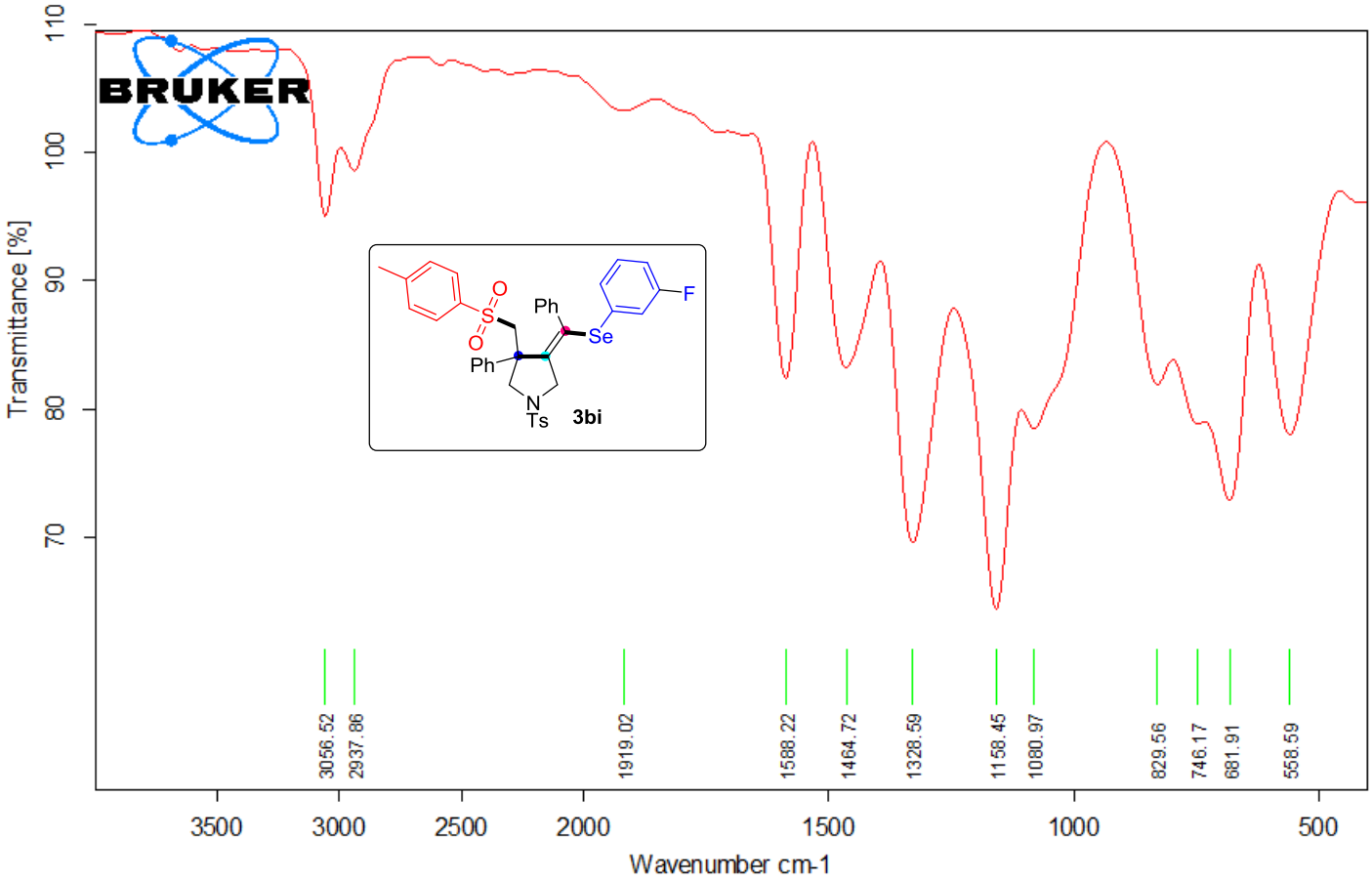
126.123
122.085
121.867
115.141
114.932



3bi

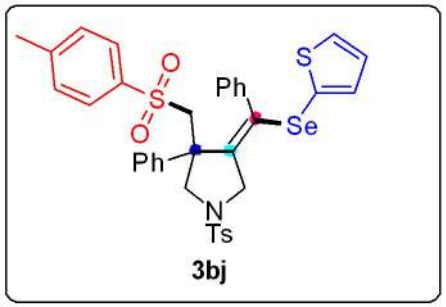





BRUKER
Transmittance [%]
110
100
90
80
70
Ph
Se
F
O
S
O
Ph
N
Ts
3bi
3056.52
2937.86
1919.02
1588.22
1464.72
1328.59
1158.45
1080.97
829.56
746.17
681.91
558.59
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

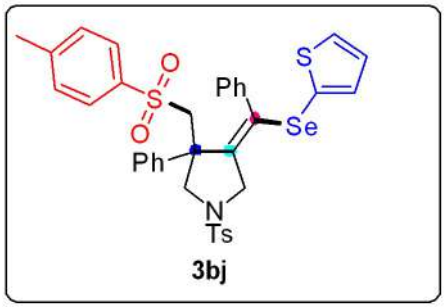
Spectrometer Frequency 400.28



3bj

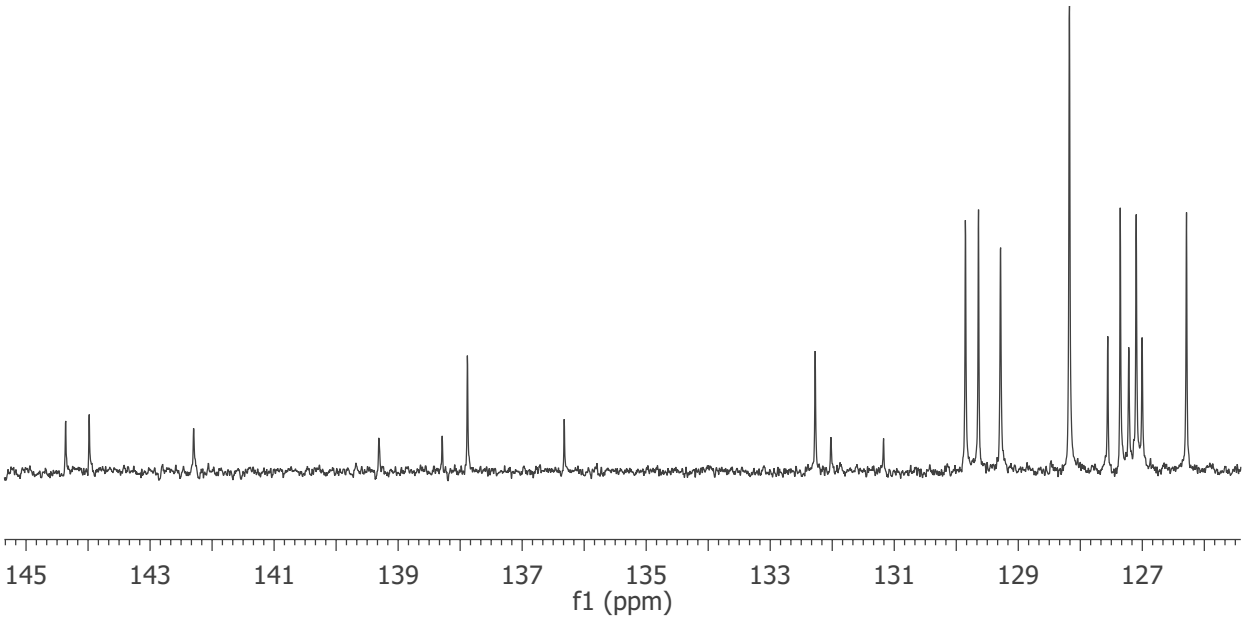
Solvent $CDCl_3$

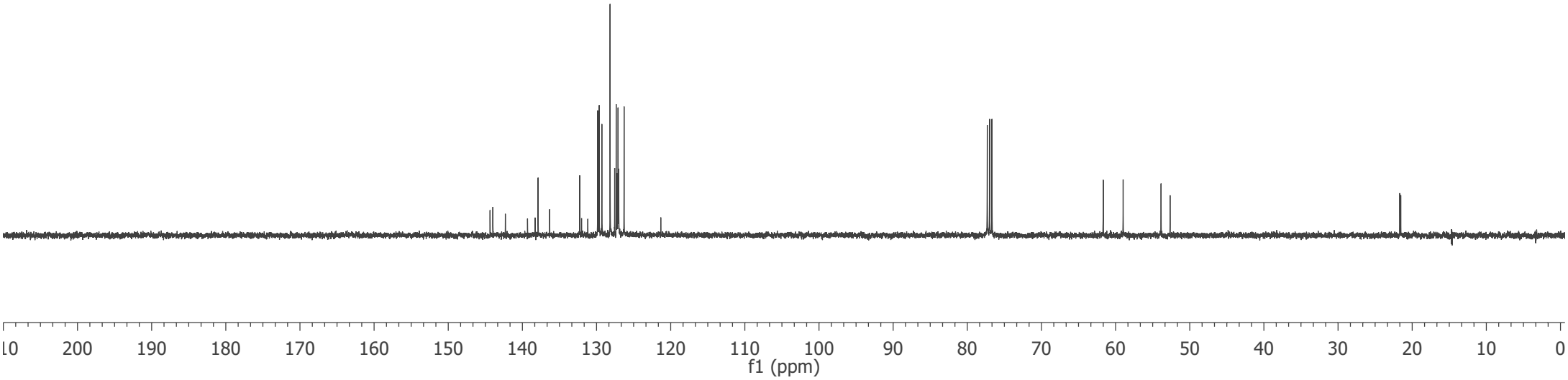
Spectrometer Frequency 100.66

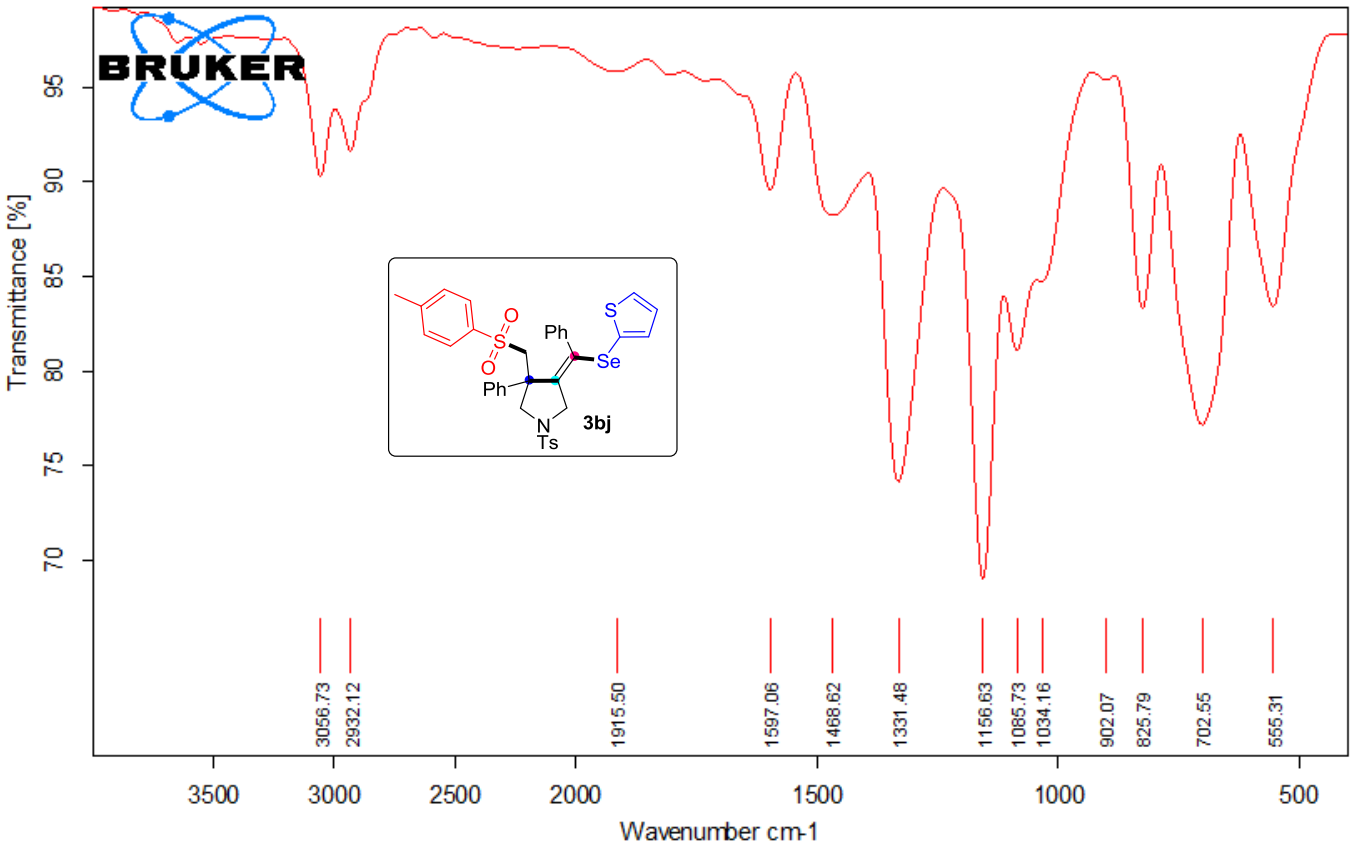


3bj

144.362 143.982 142.297 139.310 138.289 137.883 136.322 132.275 132.022 131.173 129.852 129.642 129.287 128.176 127.557 127.356 127.218 127.099 127.003 126.288 121.337 61.668 58.982 53.868 52.655 21.669 21.540

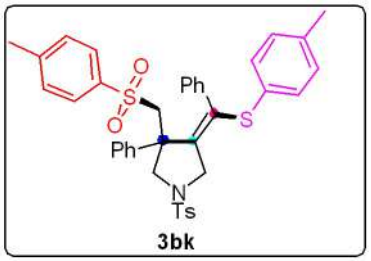





BRUKER
Transmittance [%]
95
90
85
80
75
70
3056.73
2932.12
1915.50
1597.06
1468.62
1331.48
1156.63
1085.73
1034.16
902.07
825.79
702.55
555.31
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
O
O
S
Ph
Se
S
Ph
N
Ts
3bj

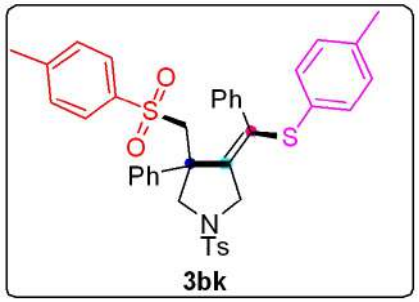
Solvent $CDCl_3$

Spectrometer Frequency 400.40



Solvent $CDCl_3$

Spectrometer Frequency 100.69



3bk

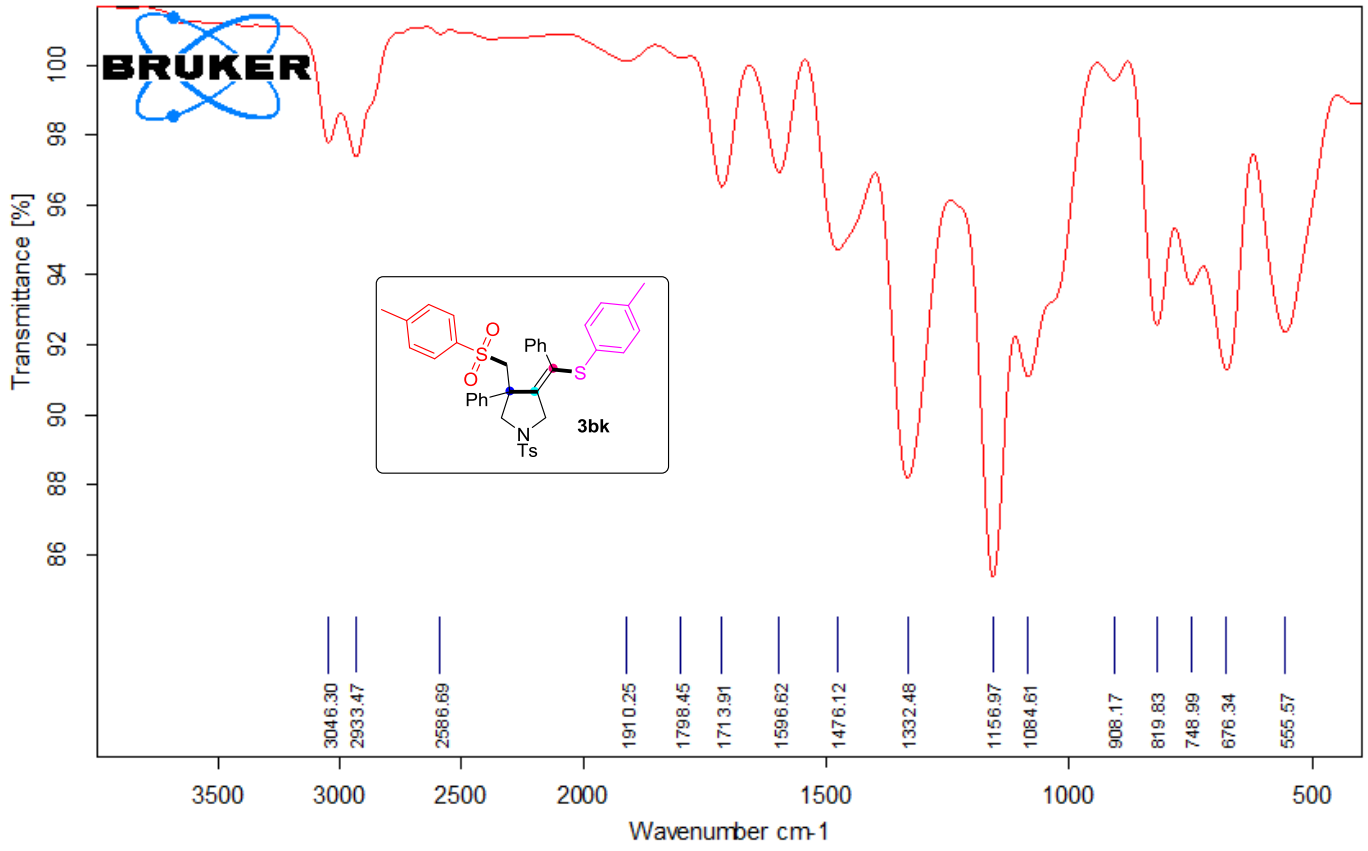
144.390 143.910 143.407 140.650 138.372 137.876 136.237 133.607 131.875 129.801 129.714 129.658 129.252 128.270 128.221 128.123 127.382 127.296 127.120 127.040 126.184

61.264 59.284 53.692 52.148

21.681 21.566 21.049

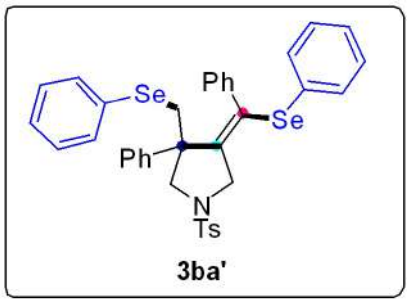
f1 (ppm)

f1 (ppm)


BRUKER
Transmittance [%]
100
98
96
94
92
90
88
86
Ph
S
O
O
Ph
N
Ts
3bk
3046.30
2933.47
2586.69
1910.25
1798.45
1713.91
1596.62
1476.12
1332.48
1156.97
1084.61
908.17
819.83
748.99
676.34
555.57
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

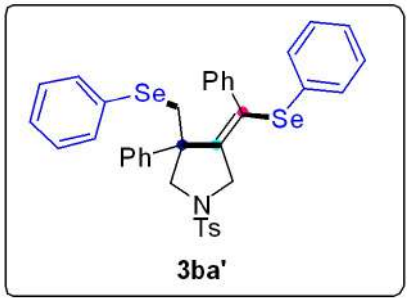
Spectrometer Frequency 400.40



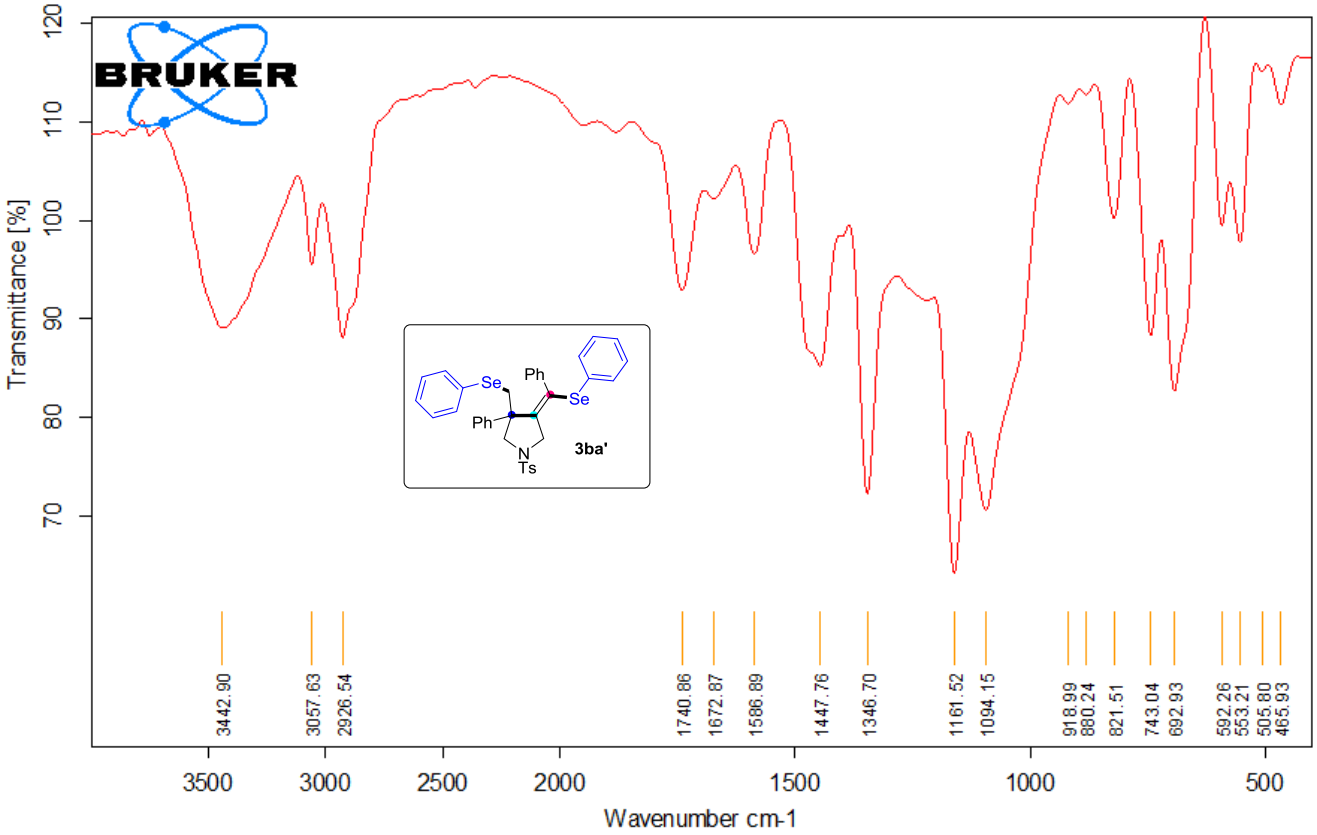
3ba'

Solvent $CDCl_3$

Spectrometer Frequency 100.69

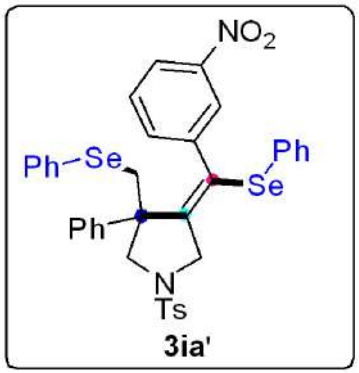


3ba'


BRUKER
Transmittance [%]
120
110
100
90
80
70
Se
Ph
Se
Ph
N
Ts
3ba'
3442.90
3057.63
2926.54
1740.86
1672.87
1586.89
1447.76
1346.70
1161.52
1094.15
918.99
880.24
821.51
743.04
692.93
592.26
553.21
505.80
465.93
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

Spectrometer Frequency 400.40

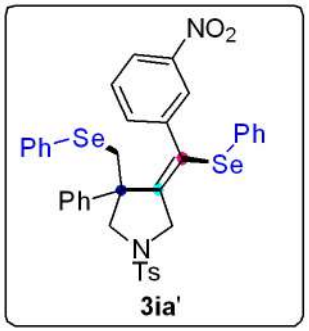


3ia'

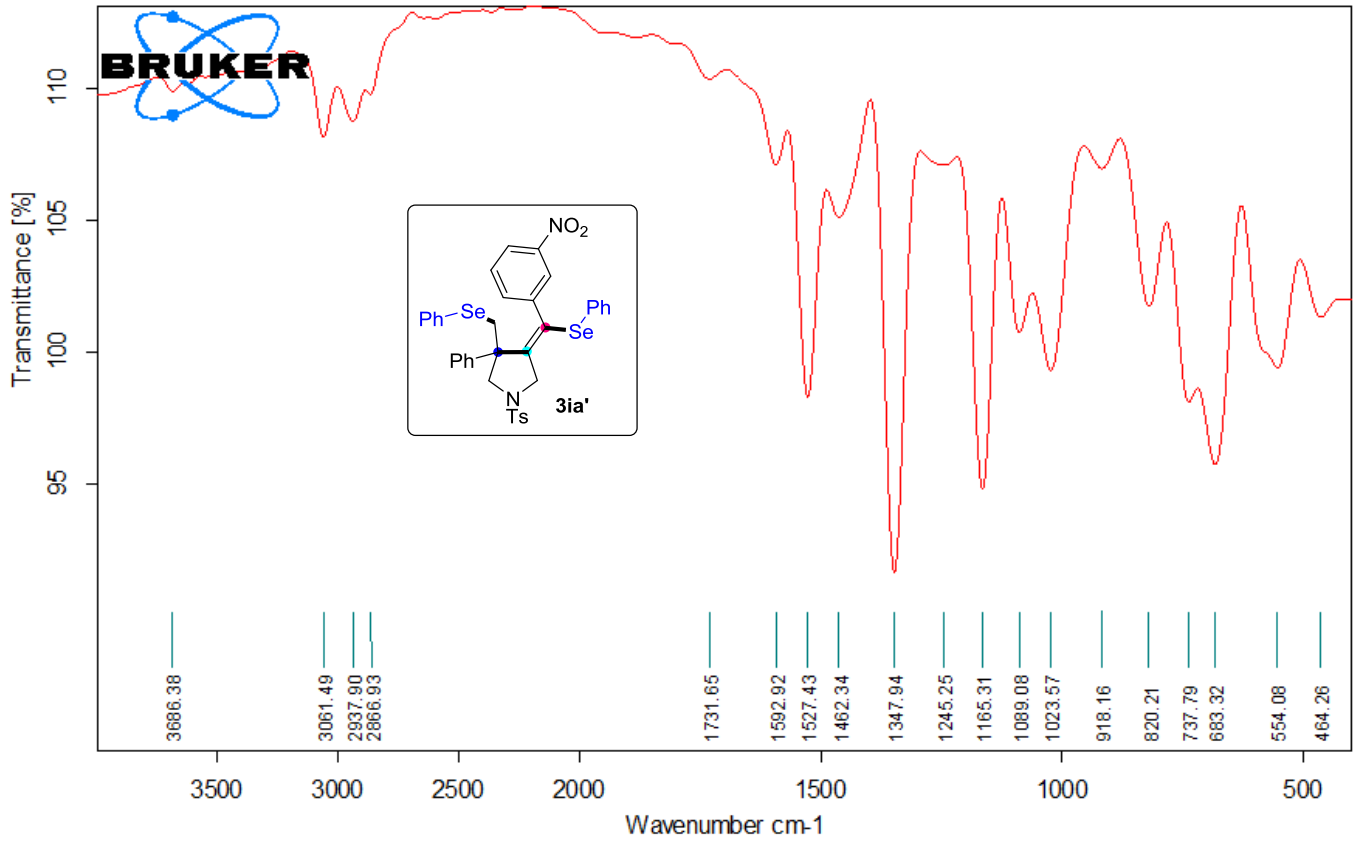
f1 (ppm)

Solvent $CDCl_3$

Spectrometer Frequency 100.69

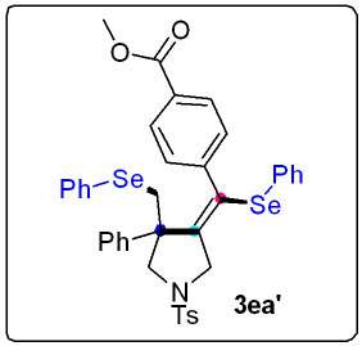


3ia'


BRUKER
Transmittance [%]
110
105
100
95
NO2
Ph
Se
Ph
Se
Ph
N
Ts
3ia'
3686.38
3061.49
2937.90
2866.93
1731.65
1592.92
1527.43
1462.34
1347.94
1245.25
1165.31
1089.08
1023.57
918.16
820.21
737.79
683.32
554.08
464.26
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

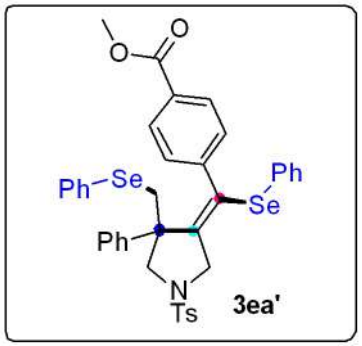
Solvent $CDCl_3$

Spectrometer Frequency 400.40



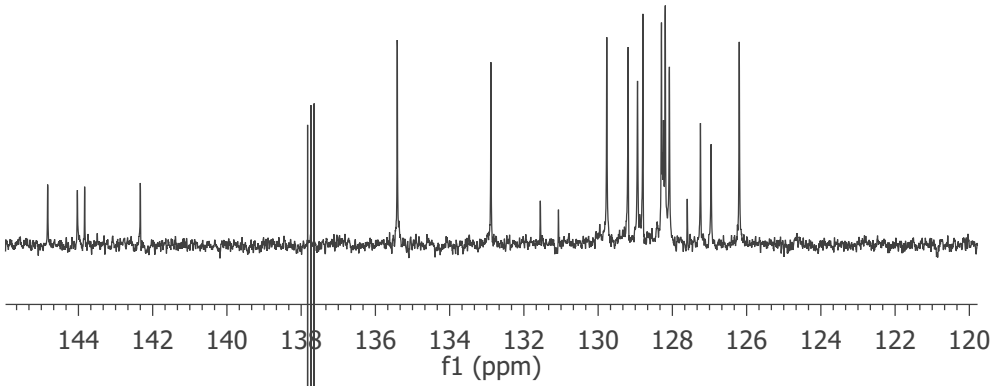
Solvent $CDCl_3$

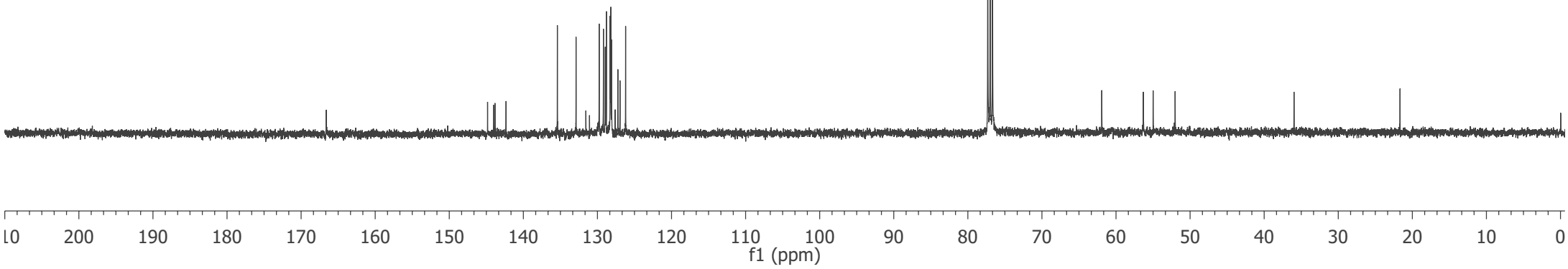
Spectrometer Frequency 100.69

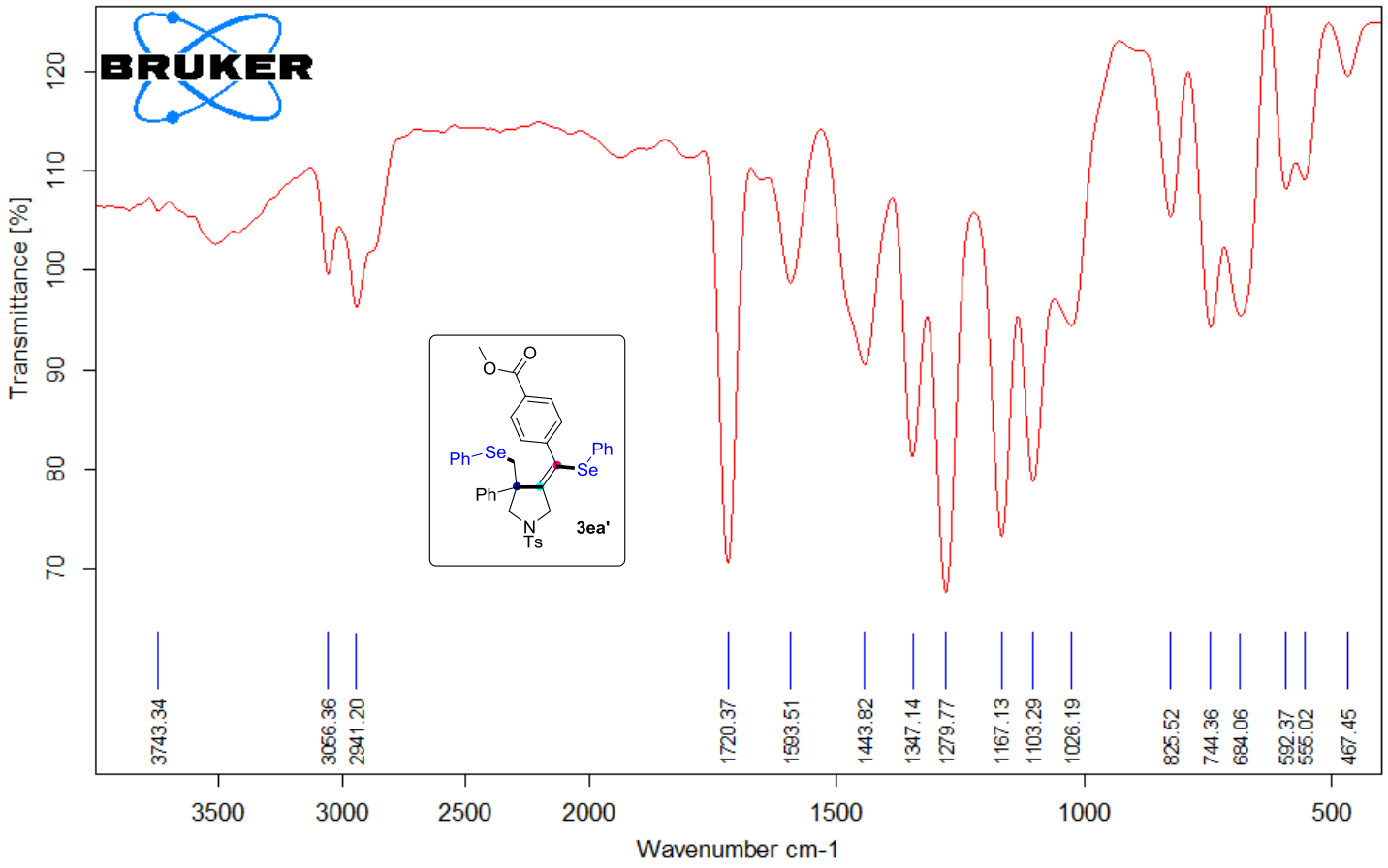


3ea'

166.601
144.828
144.029
143.833
142.333
135.411
132.888
131.557
131.069
129.767
129.192
128.939
128.794
128.294
128.240
128.192
128.081
127.599
127.244
126.957
126.198
61.920
56.310
54.993
52.019
35.971
21.658

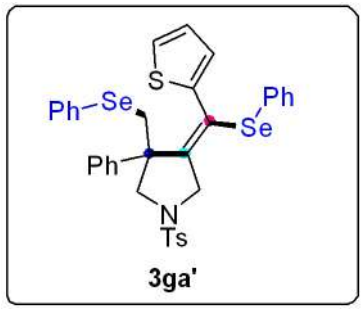





BRUKER
Transmittance [%]
120
110
100
90
80
70
3743.34
3056.36
2941.20
1720.37
1593.51
1443.82
1347.14
1279.77
1167.13
1103.29
1026.19
825.52
744.36
684.06
592.37
555.02
467.45
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
O
O
Ph
Se
Ph
Se
Ph
N
Ts
3ea'

Solvent $CDCl_3$

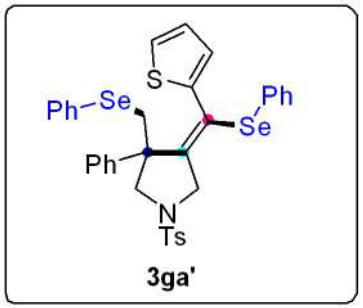
Spectrometer Frequency 400.40



3ga'

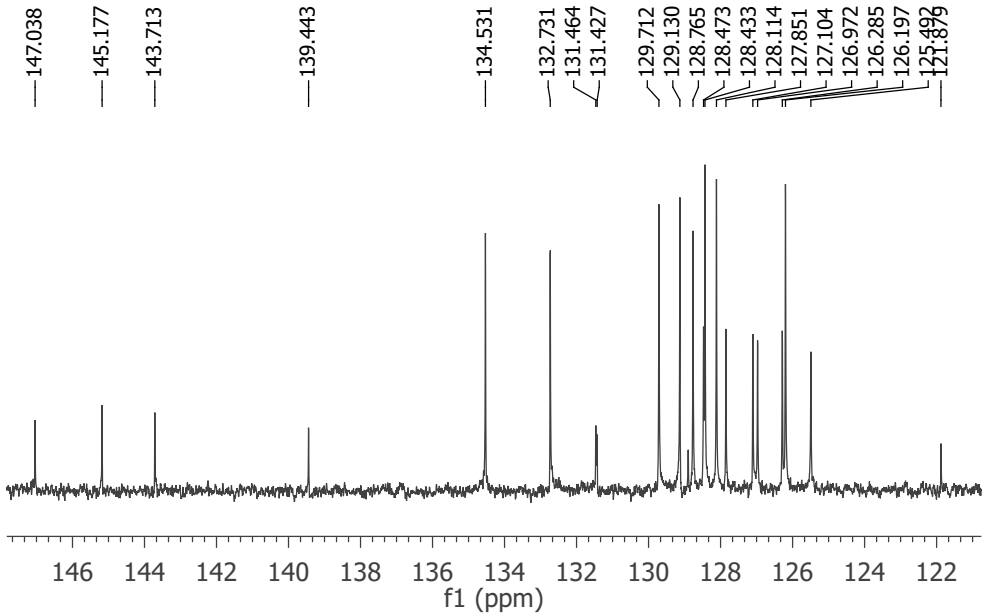
Solvent $CDCl_3$

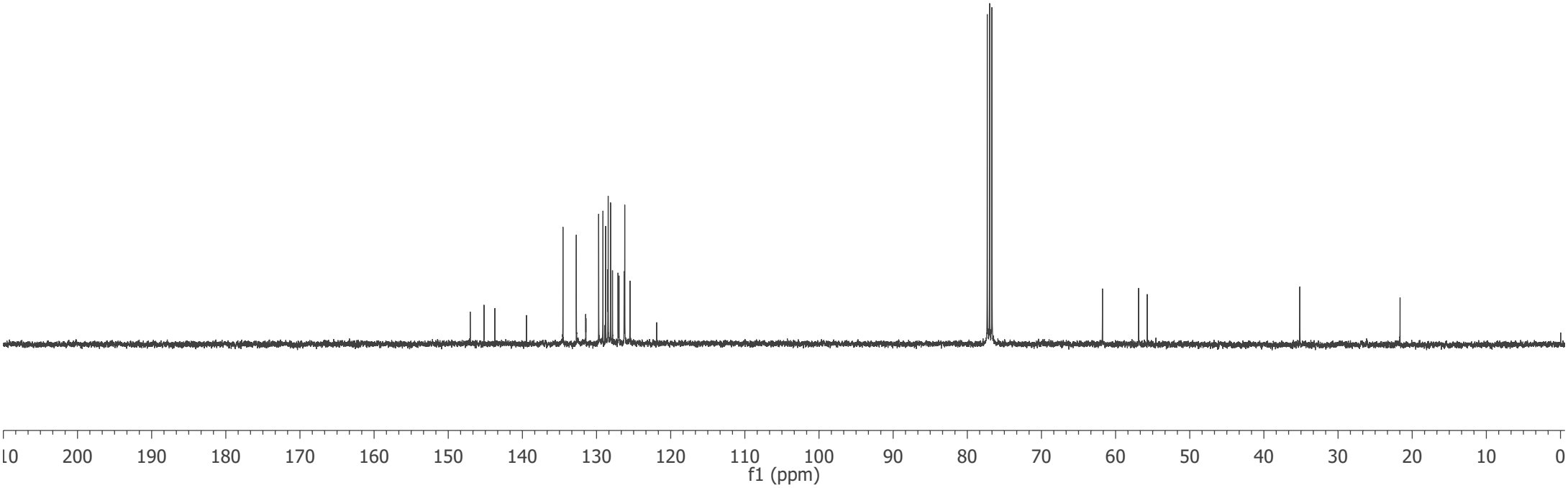
Spectrometer Frequency 100.69

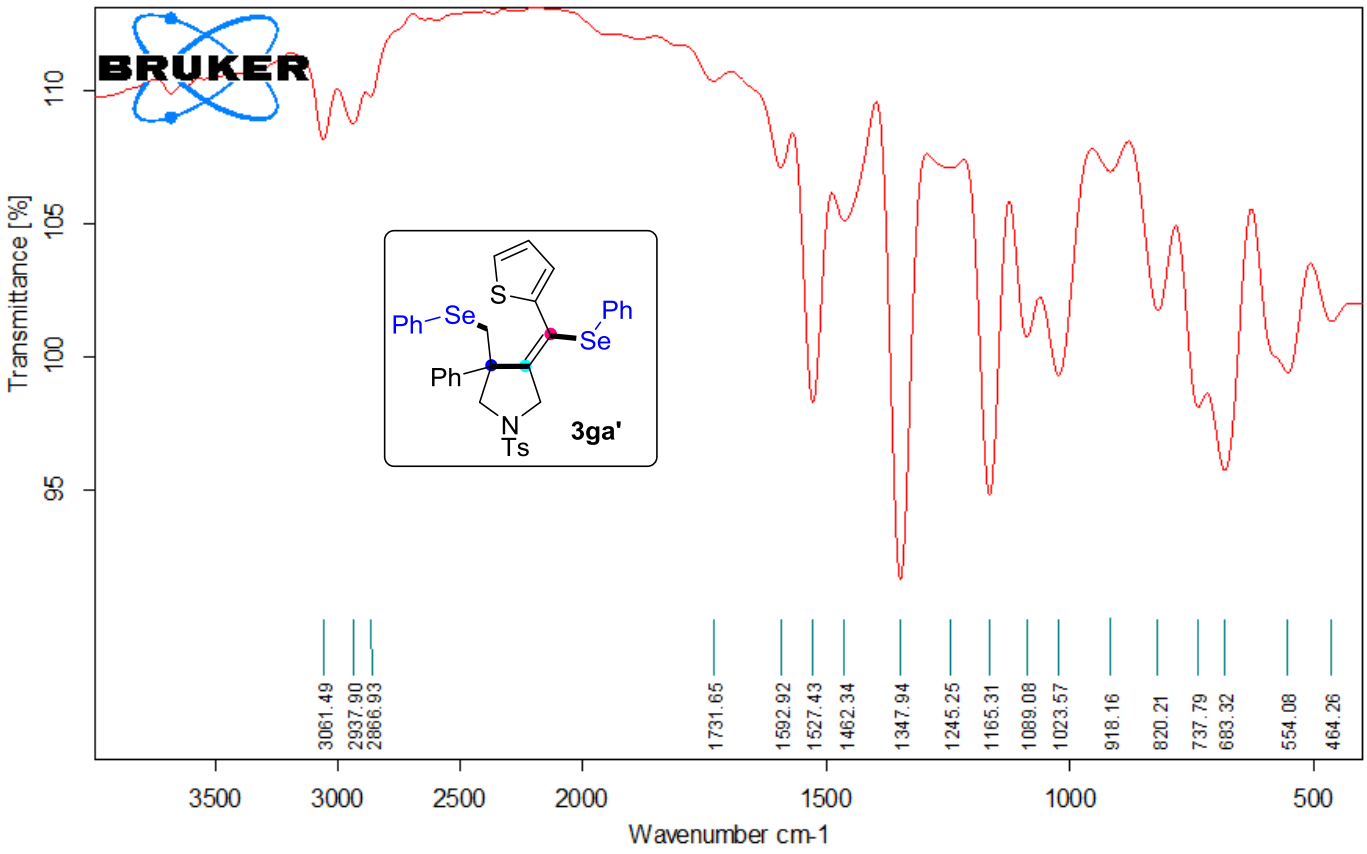


3ga'

147.038
145.177
143.713
139.443
134.531
132.731
131.464
131.427
129.712
129.130
128.899
128.765
128.473
128.433
128.114
127.851
127.104
126.972
126.285
126.197
125.492
121.879
61.771
56.896
55.742
35.153
21.637

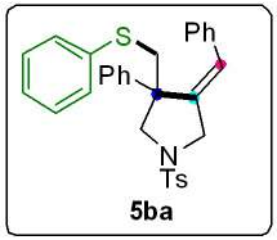





BRUKER
Transmittance [%]
110
105
100
95
S
Ph
Se
Ph
Se
Ph
N
Ts
3ga'
3061.49
2937.90
2866.93
1731.65
1592.92
1527.43
1462.34
1347.94
1245.25
1165.31
1089.08
1023.57
918.16
820.21
737.79
683.32
554.08
464.26
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

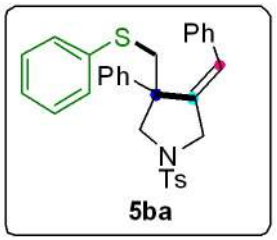
Spectrometer Frequency 400.40



5ba

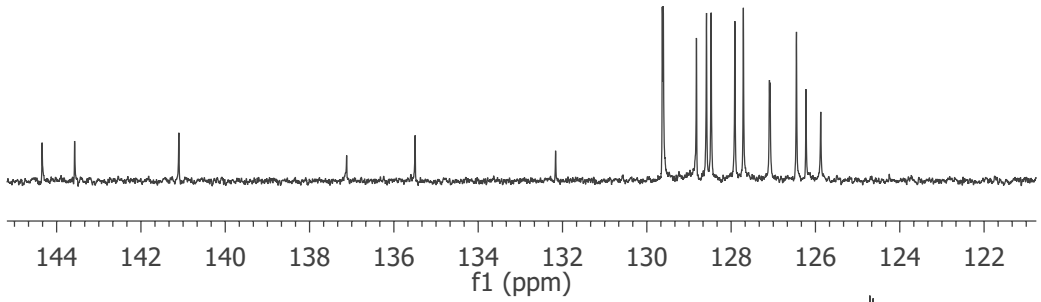
Solvent CDCl3

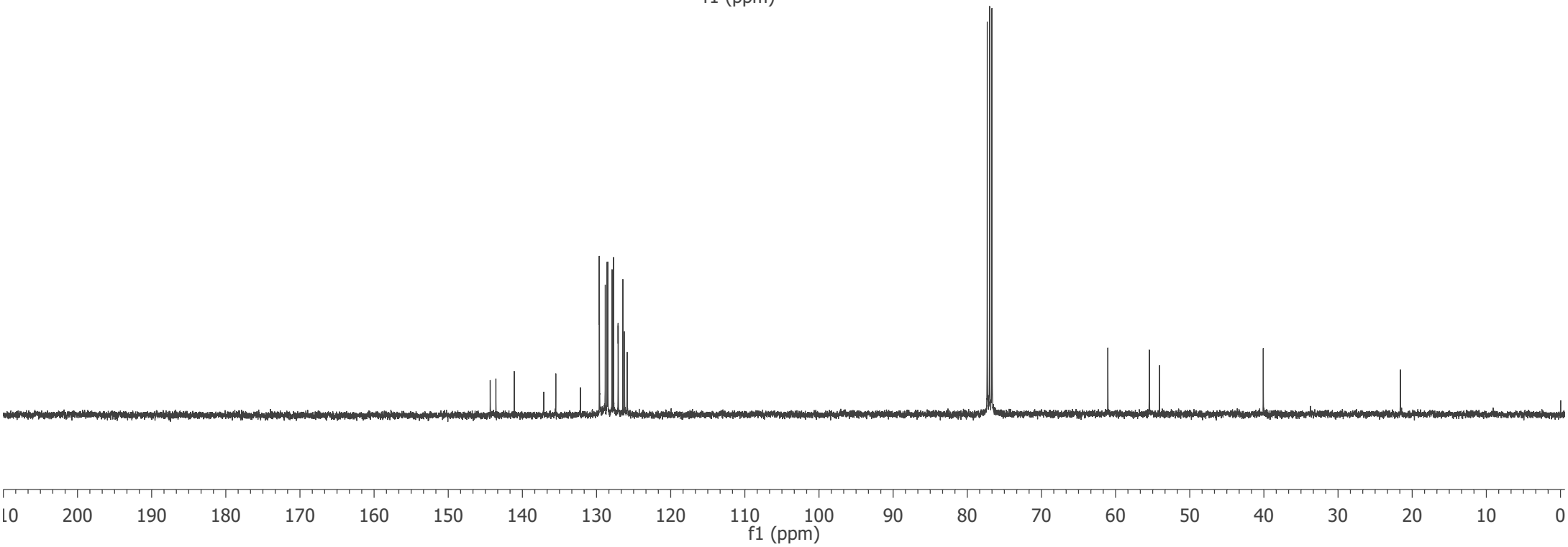
Spectrometer Frequency 100.69

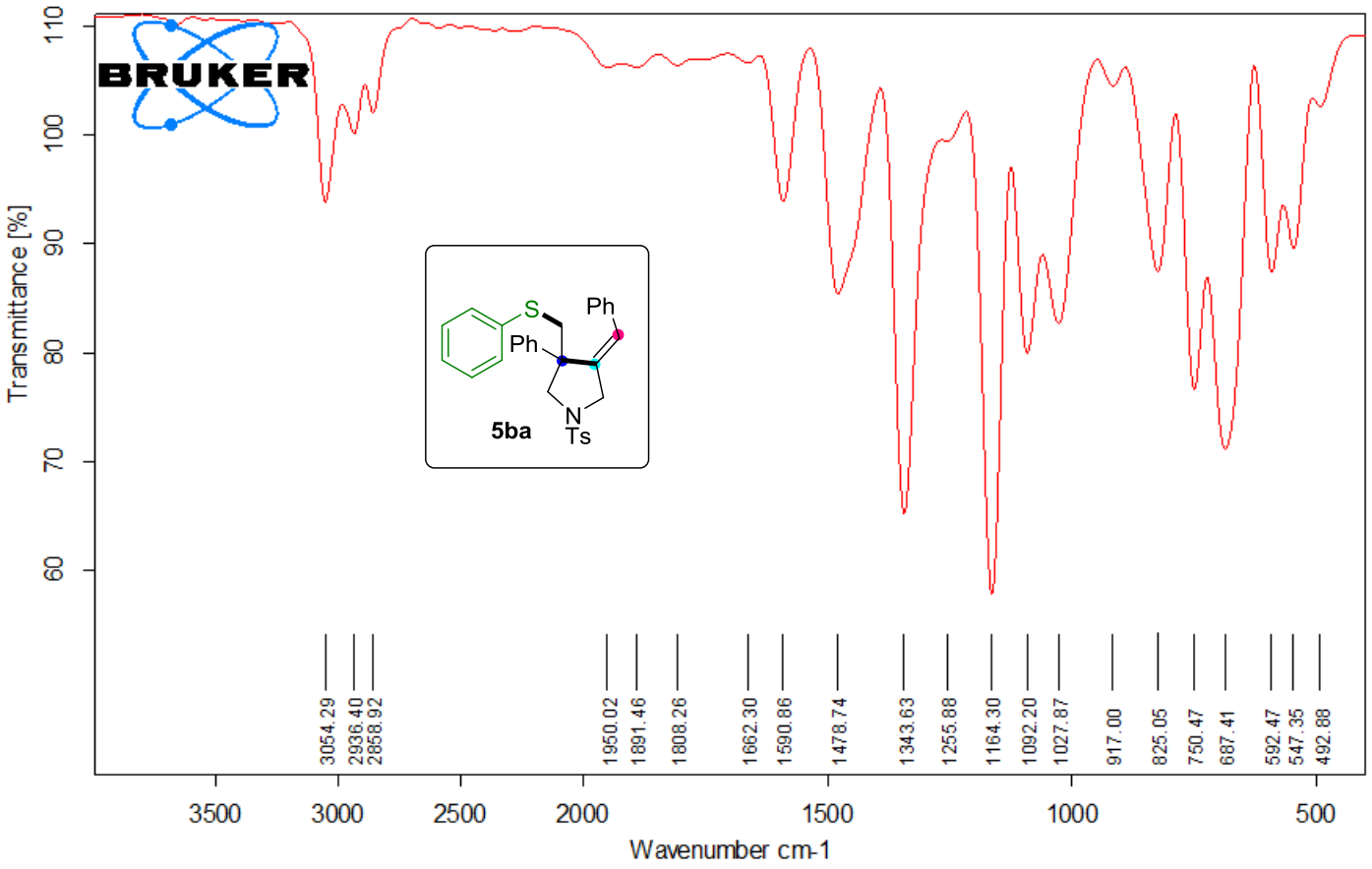


5ba

144.344
143.573
141.101
137.120
135.496
132.164
129.632
129.610
128.823
128.585
128.475
127.912
127.710
127.092
127.076
126.451
126.225
125.875
61.042
55.454
54.067
40.083
21.576

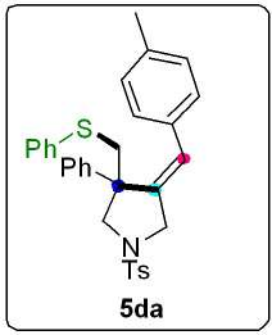





BRUKER
Transmittance [%]
110
100
90
80
70
60
S
Ph
Ph
N
Ts
5ba
3054.29
2936.40
2858.92
1950.02
1891.46
1808.26
1662.30
1590.86
1478.74
1343.63
1255.88
1164.30
1092.20
1027.87
917.00
825.05
750.47
687.41
592.47
547.35
492.88
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

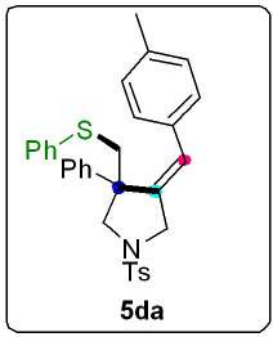
Spectrometer Frequency 400.40



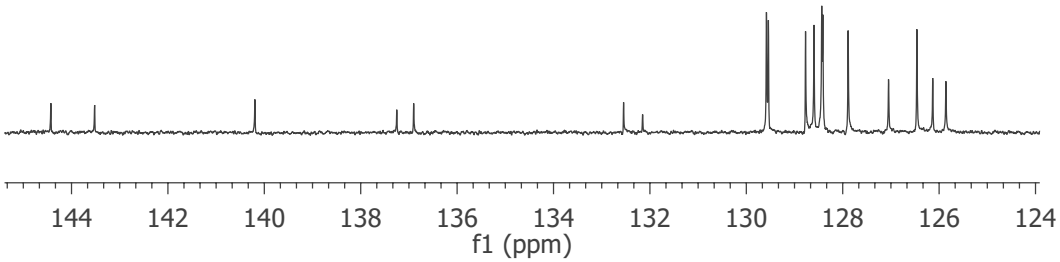
5da

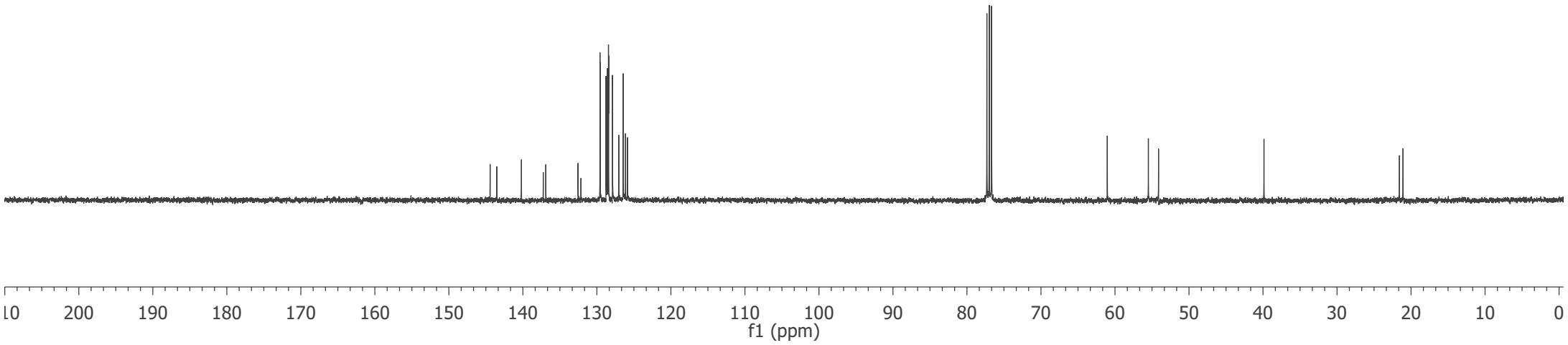
Solvent $CDCl_3$

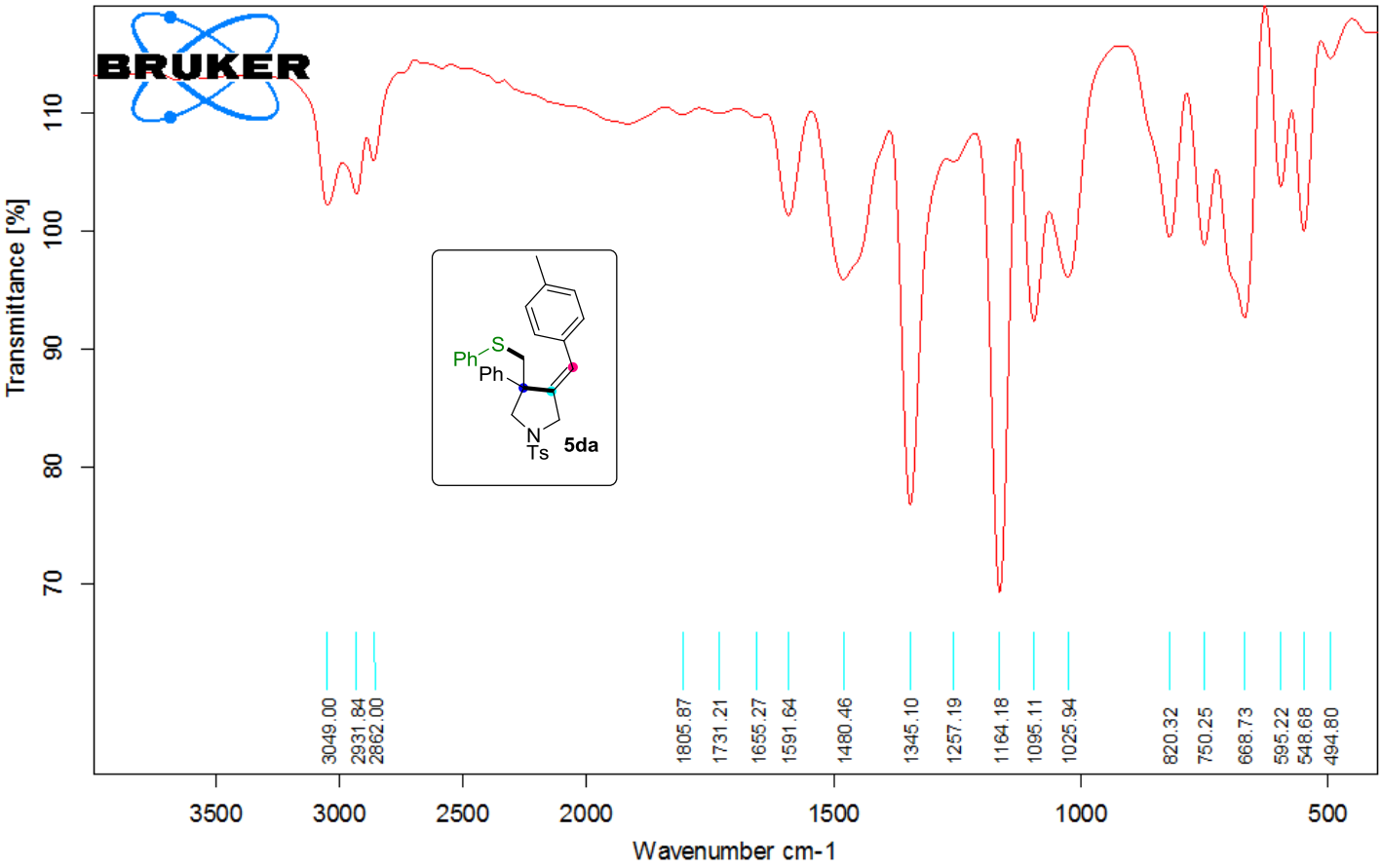
Spectrometer Frequency 100.69



144.429
143.521
140.195
137.252
136.901
132.546
132.151
129.582
129.542
128.771
128.595
128.435
128.412
127.887
127.049
126.461
126.132
125.859
61.041
55.491
54.116
39.870
21.566
21.081

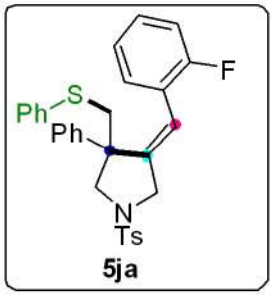





BRUKER
Transmittance [%]
110
100
90
80
70
Ph
S
Ph
N
Ts
5da
3049.00
2931.84
2862.00
1805.87
1731.21
1655.27
1591.64
1480.46
1345.10
1257.19
1164.18
1095.11
1025.94
820.32
750.25
668.73
595.22
548.68
494.80
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

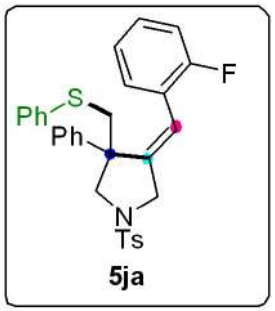
Spectrometer Frequency 400.40



5ja

Solvent $CDCl_3$

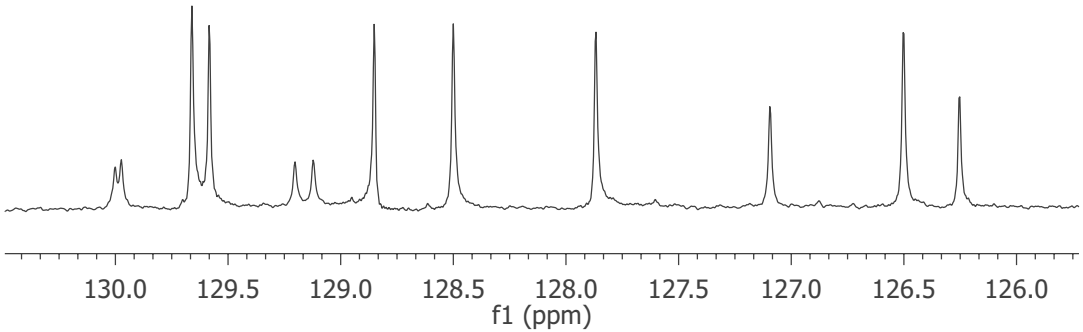
Spectrometer Frequency 100.69

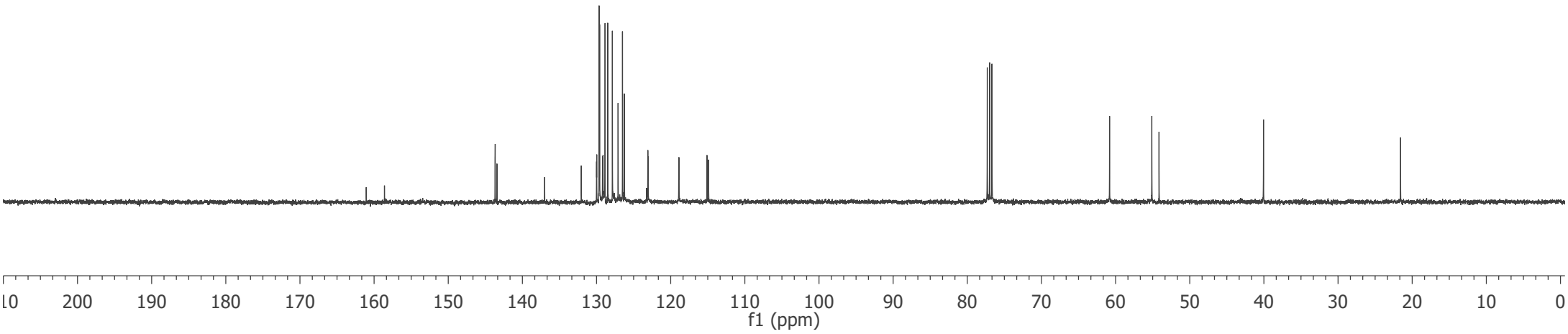


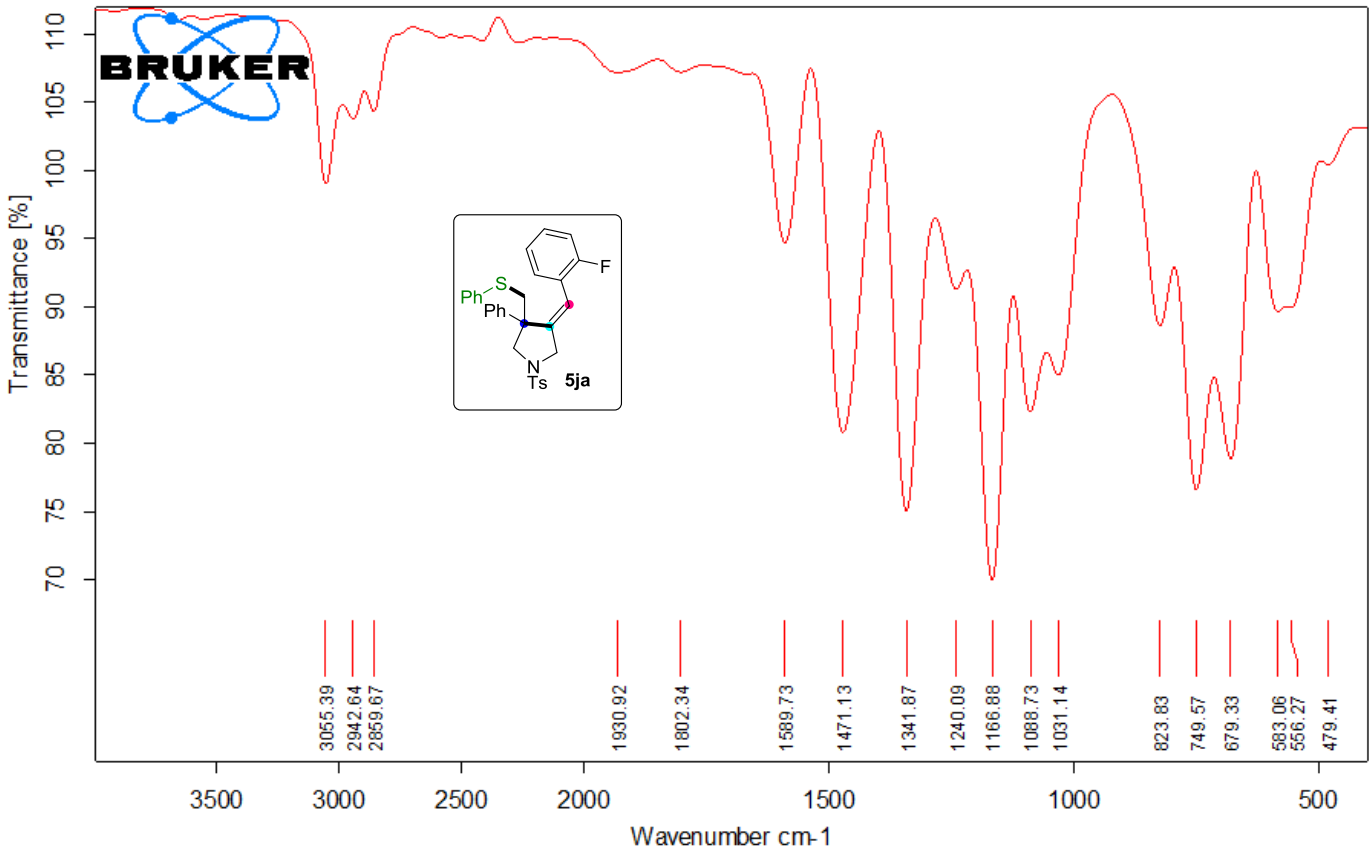
5ja

161.057, 158.602, 143.670, 143.431, 136.995, 132.054, 130.001, 129.974, 129.661, 129.583, 129.203, 129.122, 128.851, 128.500, 127.868, 127.094, 126.502, 126.253, 123.244, 123.082, 123.046, 118.915, 118.883, 115.105, 114.887, 60.813, 55.110, 54.142, 40.053, 21.563

130.001, 129.974, 129.661, 129.583, 129.203, 129.122, 128.851, 128.500, 127.868, 127.094, 126.502, 126.253

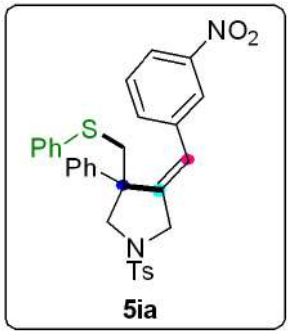





BRUKER
Transmittance [%]
110
105
100
95
90
85
80
75
70
Ph
S
Ph
F
N
Ts
5ja
3055.39
2942.64
2859.67
1930.92
1802.34
1589.73
1471.13
1341.87
1240.09
1166.88
1088.73
1031.14
823.83
749.57
679.33
583.06
556.27
479.41
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

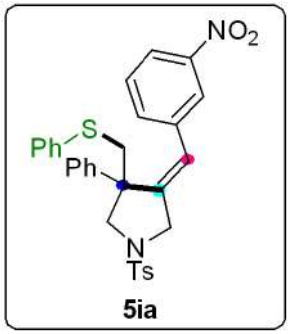
Spectrometer Frequency 400.40



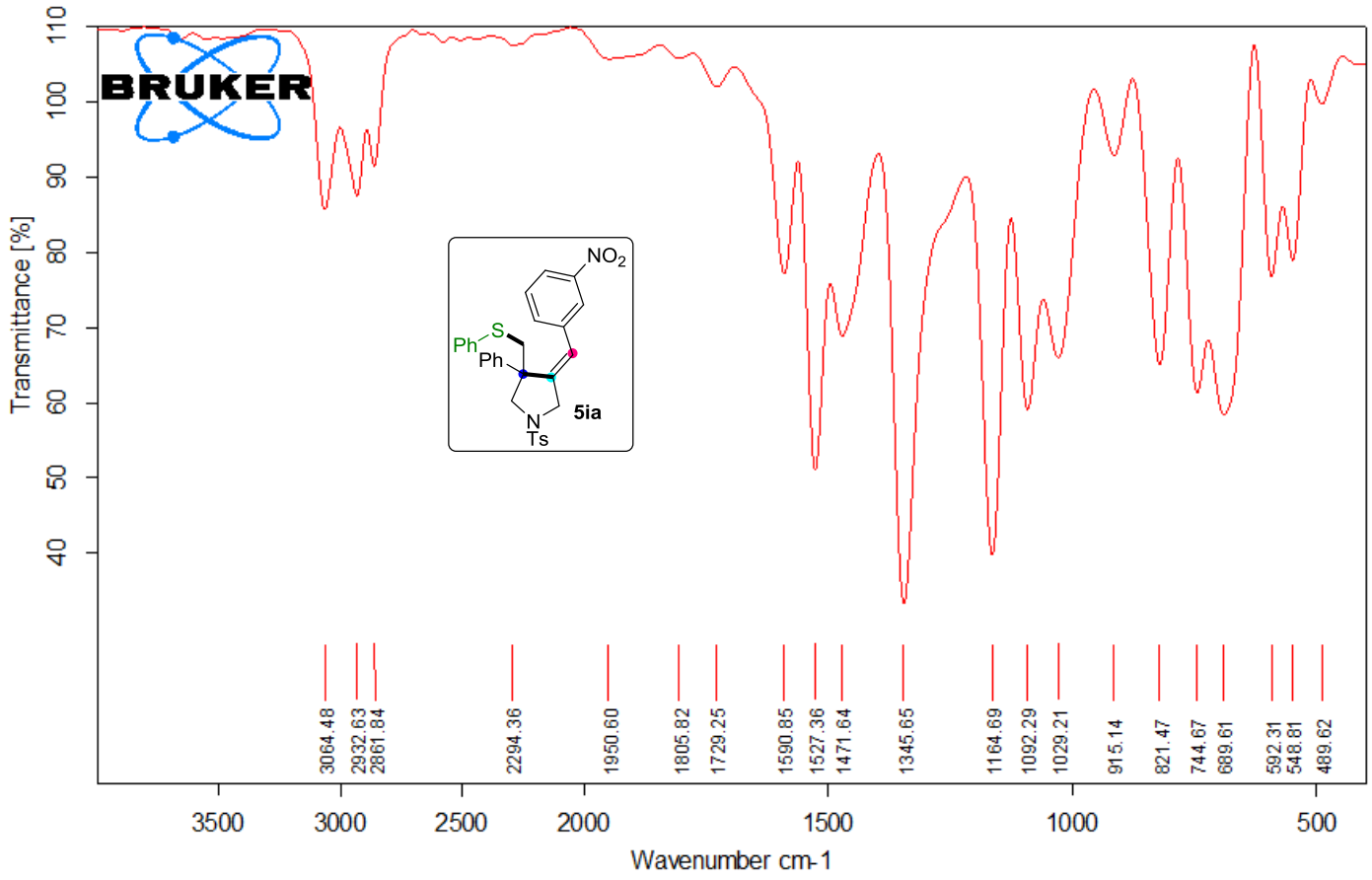
5ia

Solvent $CDCl_3$

Spectrometer Frequency 400.40

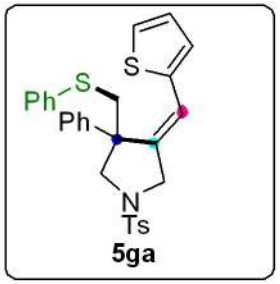


5ia


BRUKER
Transmittance [%]
110
100
90
80
70
60
50
40
NO2
Ph
S
Ph
N
Ts
5ia
3064.48
2932.63
2861.84
2294.36
1950.60
1805.82
1729.25
1590.85
1527.36
1471.64
1345.65
1164.69
1092.29
1029.21
915.14
821.47
744.67
689.61
592.31
548.81
489.62
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

Spectrometer Frequency 400.40

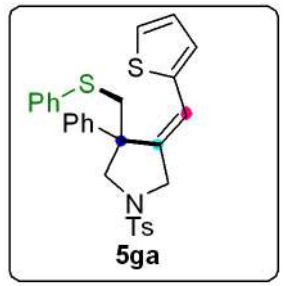


5ga

Solvent $CDCl_3$

Spectrometer Frequency 100.69

143.701
143.365
140.685
137.477
137.035
129.632
128.783
128.020
126.593
126.358
118.502
61.644
56.130
54.127
39.644
21.585

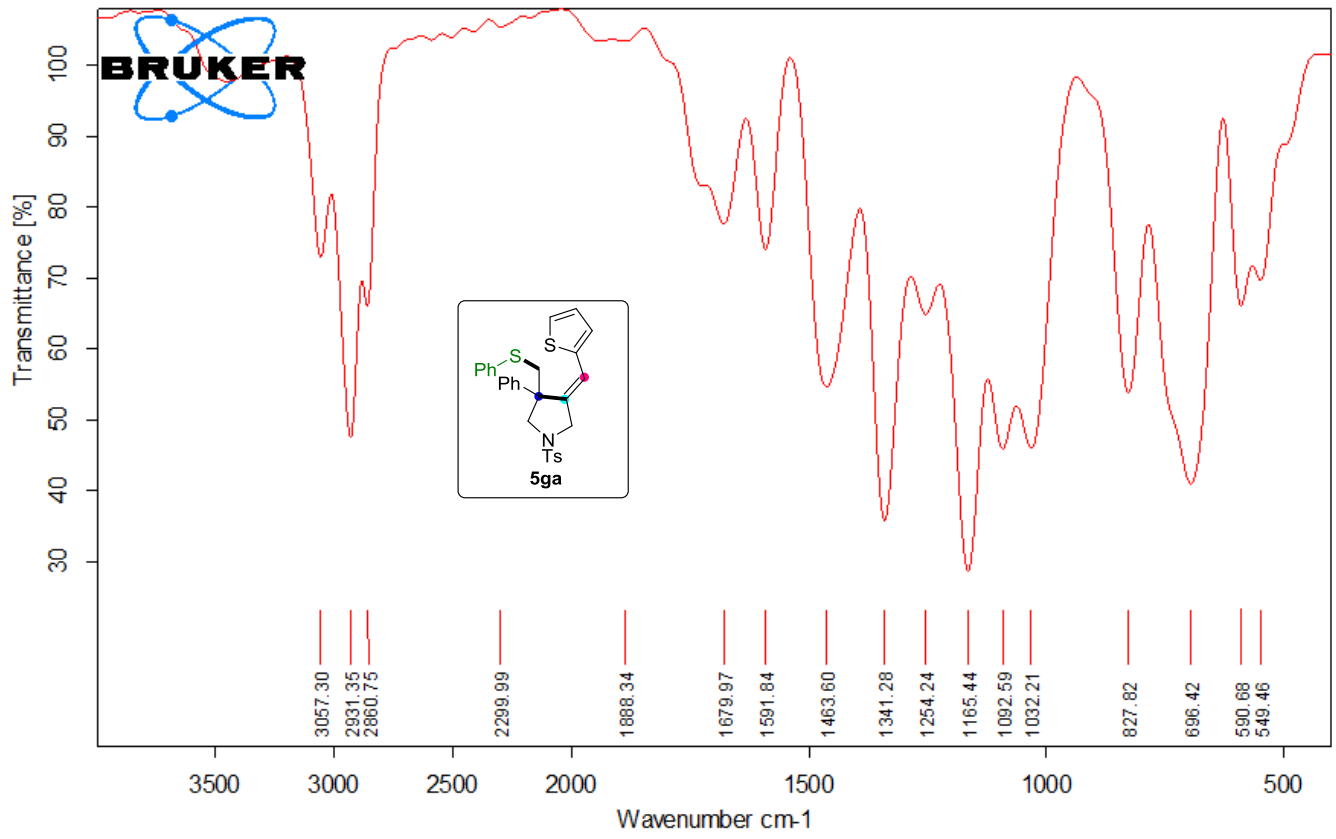


5ga

143.701
143.365
140.685
137.477
137.035
131.808
129.904
129.632
128.847
128.783
128.043
128.020
127.266
126.697
126.593
126.358

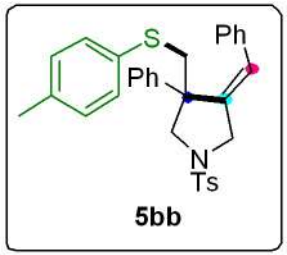
143 141 139 137 135 133 131 129 127
f1 (ppm)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


BRUKER
Transmittance [%]
100
90
80
70
60
50
40
30
Ph
S
Ph
S
N
Ts
5ga
3057.30
2931.35
2860.75
2299.99
1888.34
1679.97
1591.84
1463.60
1341.28
1254.24
1165.44
1092.59
1032.21
827.82
696.42
590.68
549.46
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

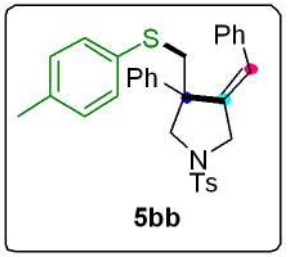
Spectrometer Frequency 400.40



5bb

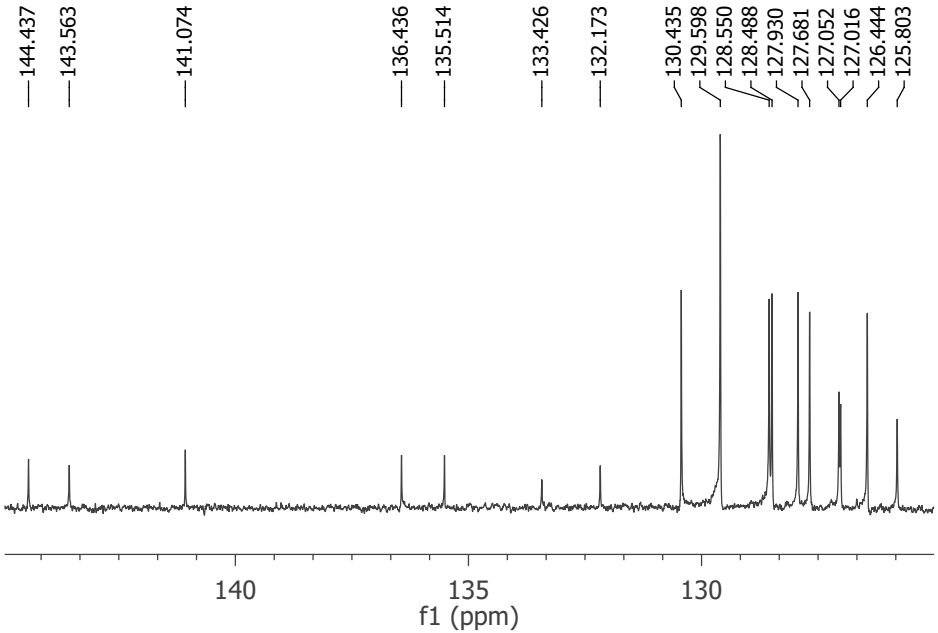
Solvent $CDCl_3$

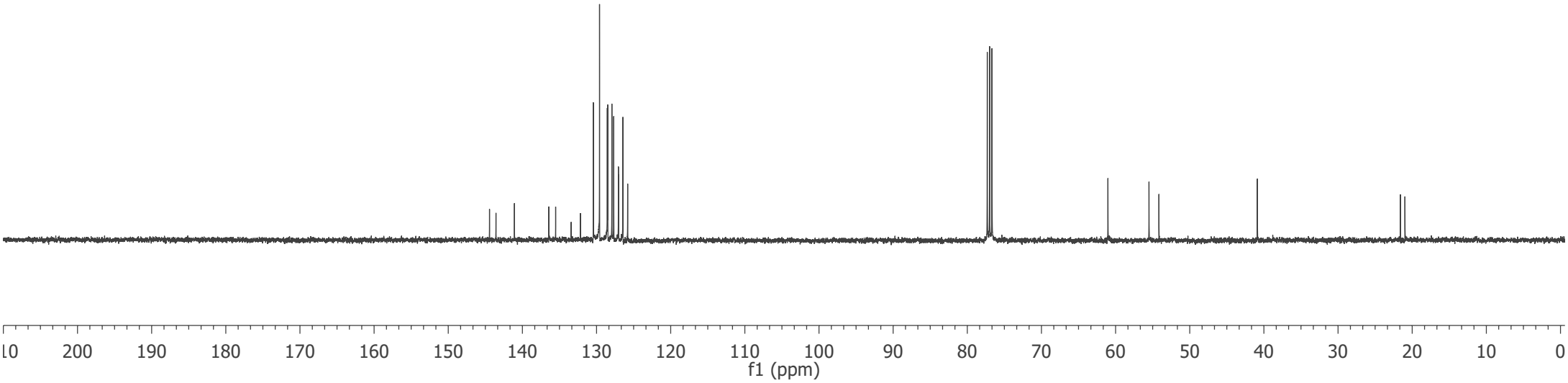
Spectrometer Frequency 100.69

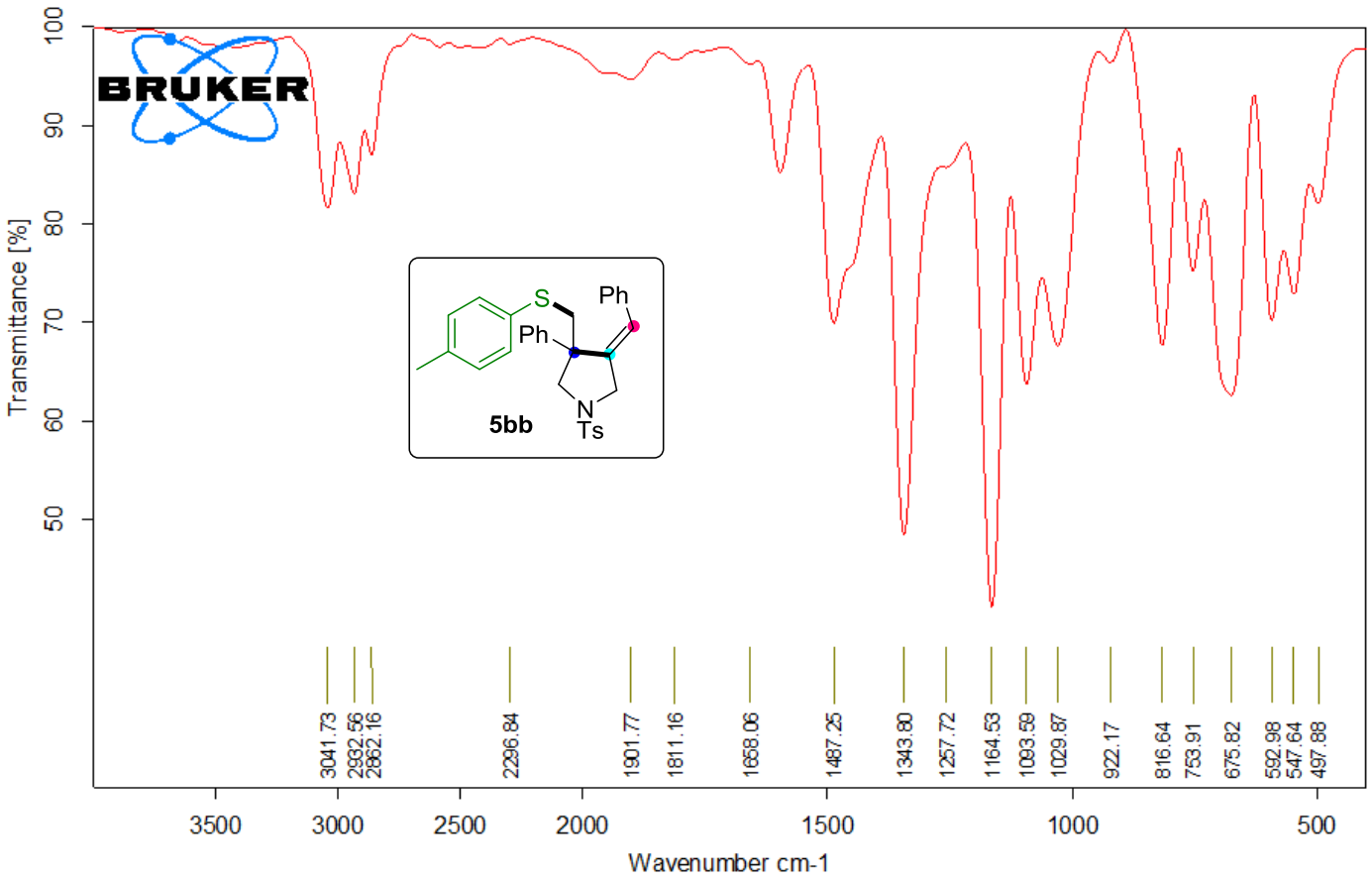


5bb

144.437
143.563
141.074
136.436
135.514
133.426
132.173
130.435
129.598
128.550
128.488
127.930
127.681
127.052
127.016
126.444
125.803
61.031
55.495
54.153
40.881
21.580
20.978

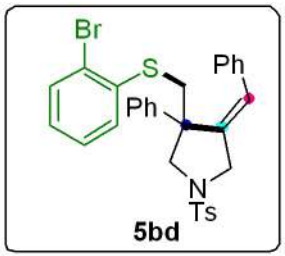





BRUKER
Transmittance [%]
100
90
80
70
60
50
S
Ph
Ph
N
Ts
5bb
3041.73
2932.56
2862.16
2296.84
1901.77
1811.16
1658.06
1487.25
1343.80
1257.72
1164.53
1093.59
1029.87
922.17
816.64
753.91
675.82
592.98
547.64
497.88
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

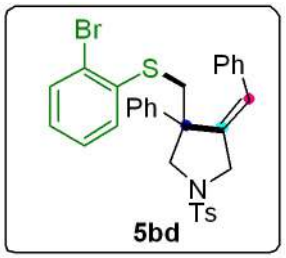
Spectrometer Frequency 400.40

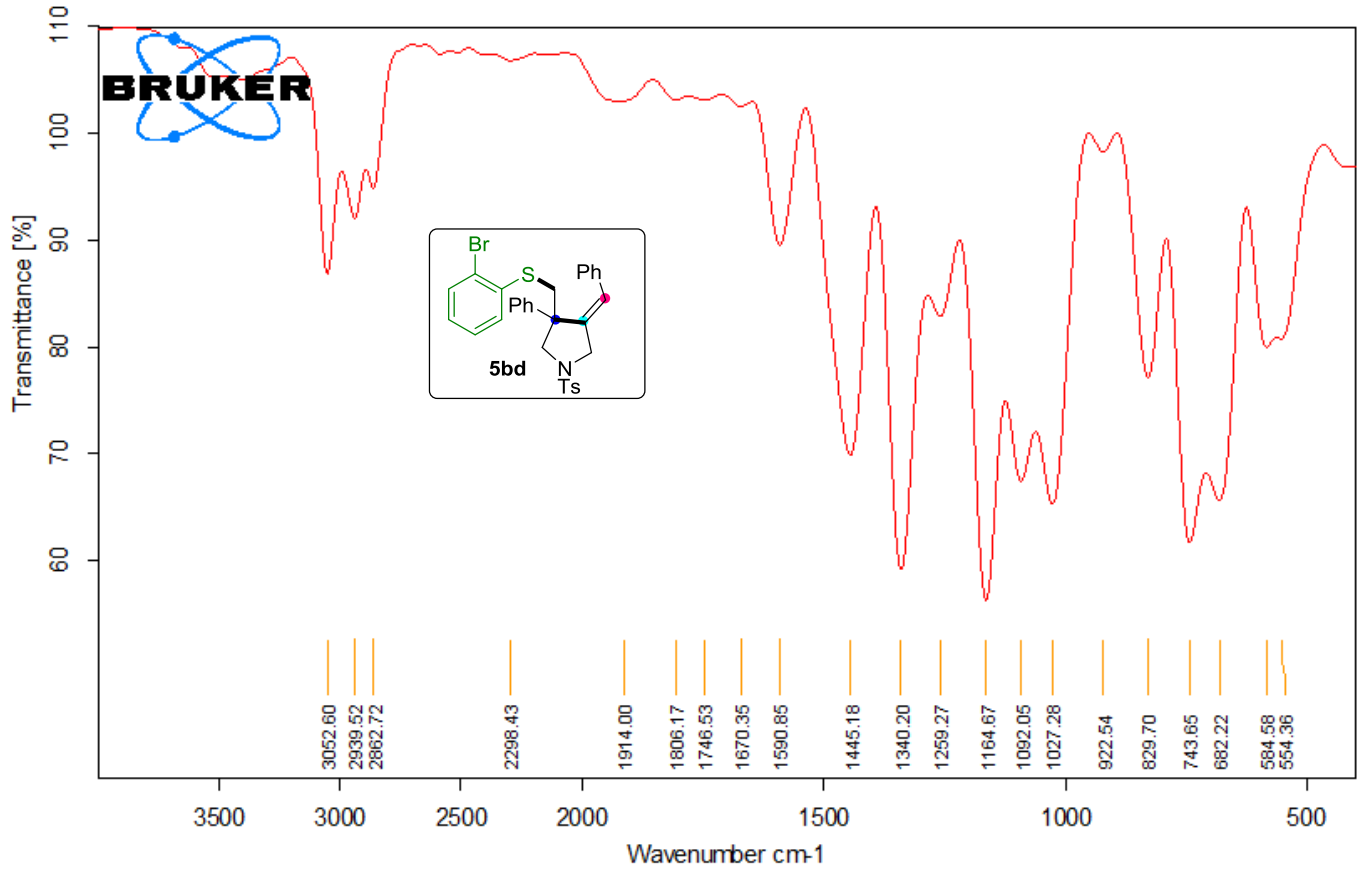


5bd

Solvent $CDCl_3$

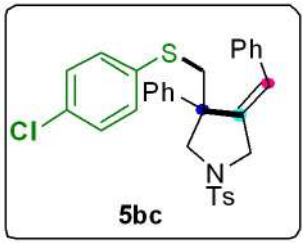
Spectrometer Frequency 100.69




BRUKER
Br
S
Ph
Ph
5bd
N
Ts
Transmittance [%]
110
100
90
80
70
60
3052.60
2939.52
2862.72
2298.43
1914.00
1806.17
1746.53
1670.35
1590.85
1445.18
1340.20
1259.27
1164.67
1092.05
1027.28
922.54
829.70
743.65
682.22
584.58
554.36
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

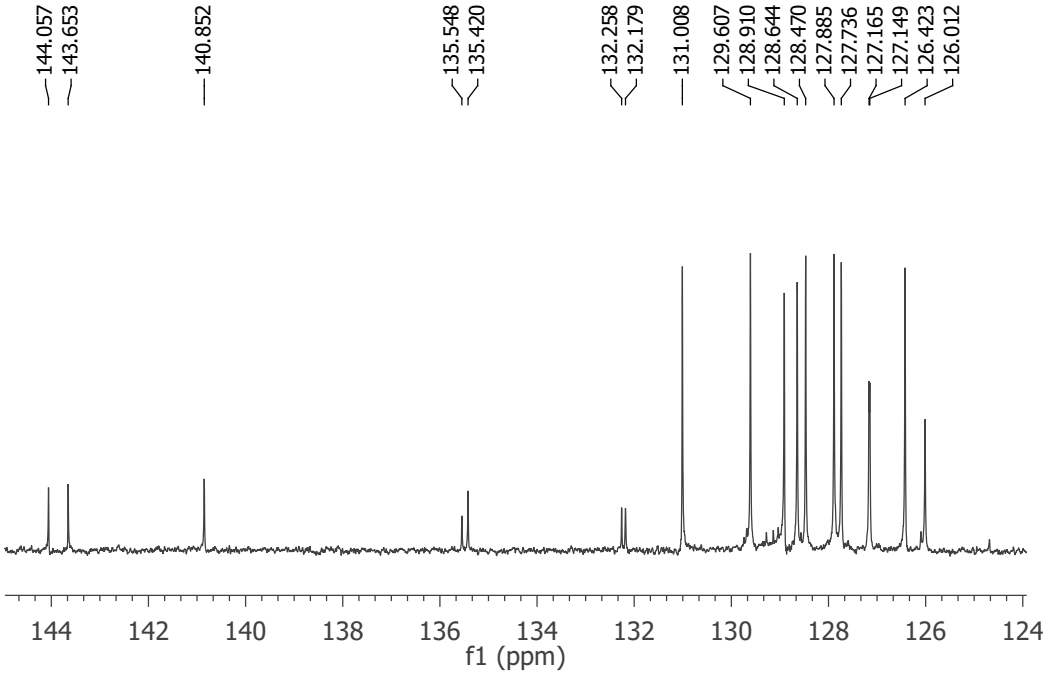
Solvent $CDCl_3$

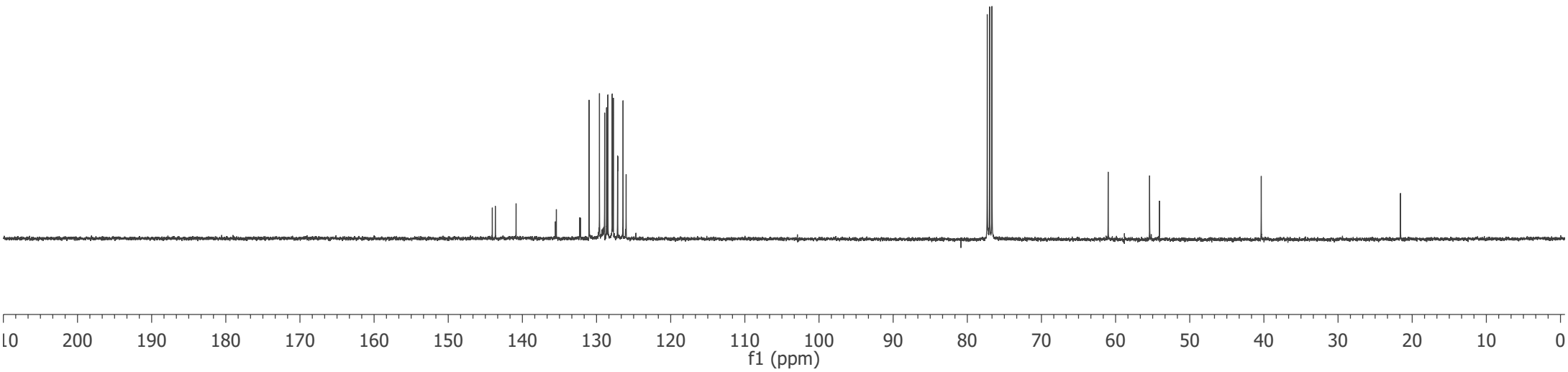
Spectrometer Frequency 100.69



5bc

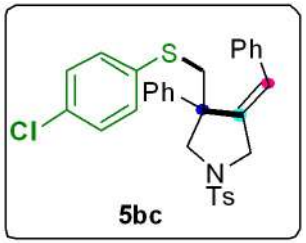
144.057
143.653
140.852
135.548
135.420
132.258
132.179
131.008
129.607
128.910
128.644
128.470
127.885
127.736
127.165
127.149
126.423
126.012
61.006
55.413
54.086
40.360
21.577



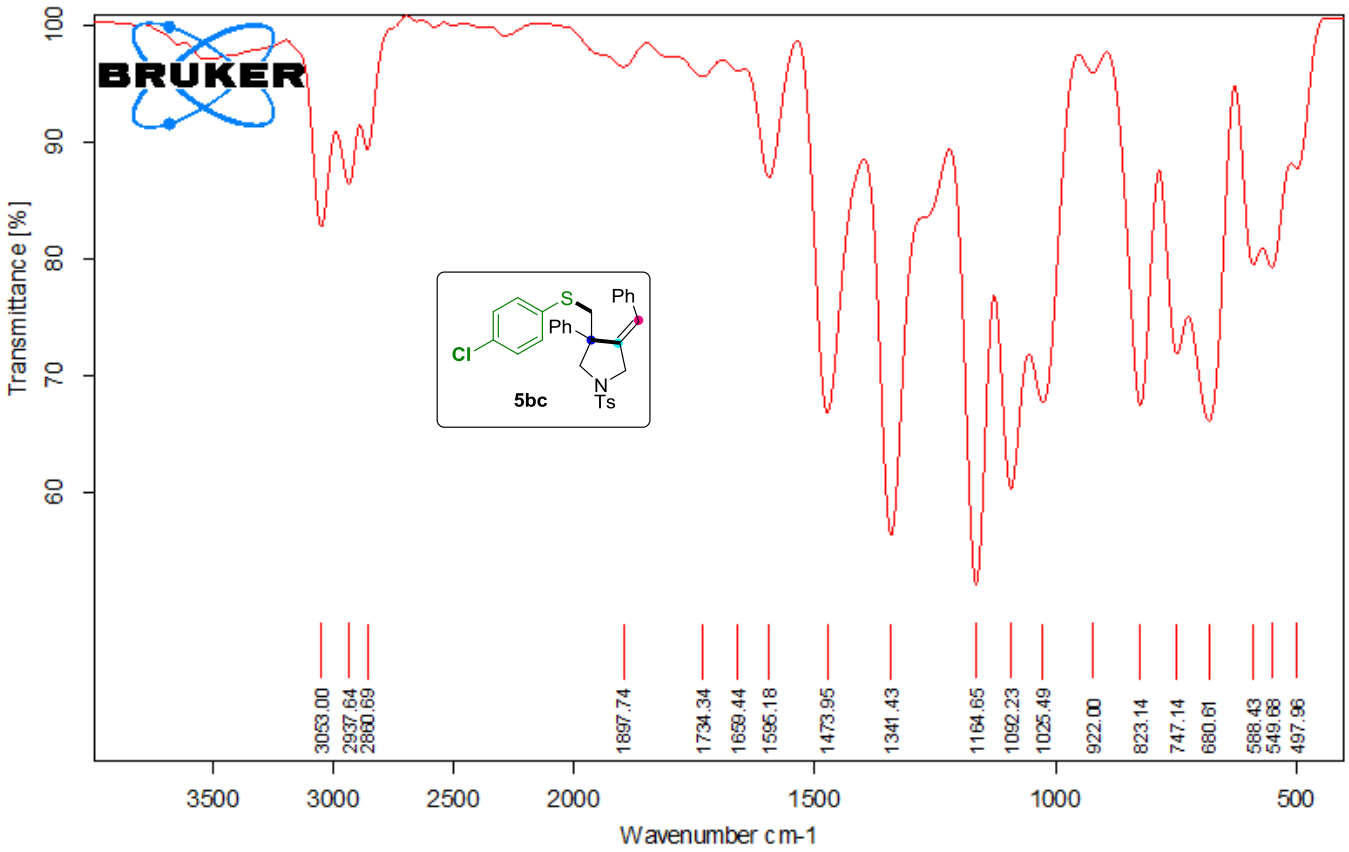


Solvent $CDCl_3$

Spectrometer Frequency 400.40

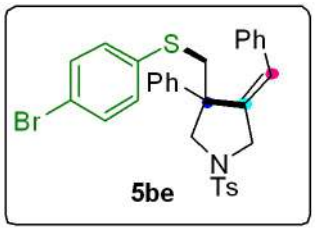


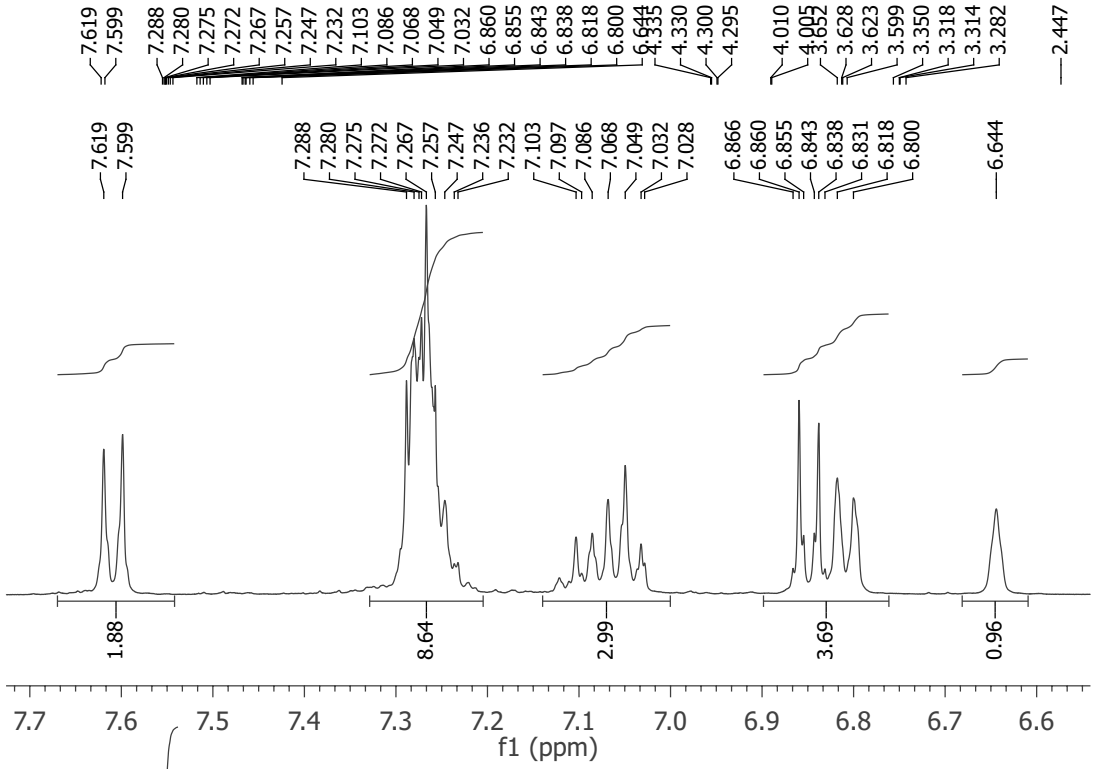
5bc

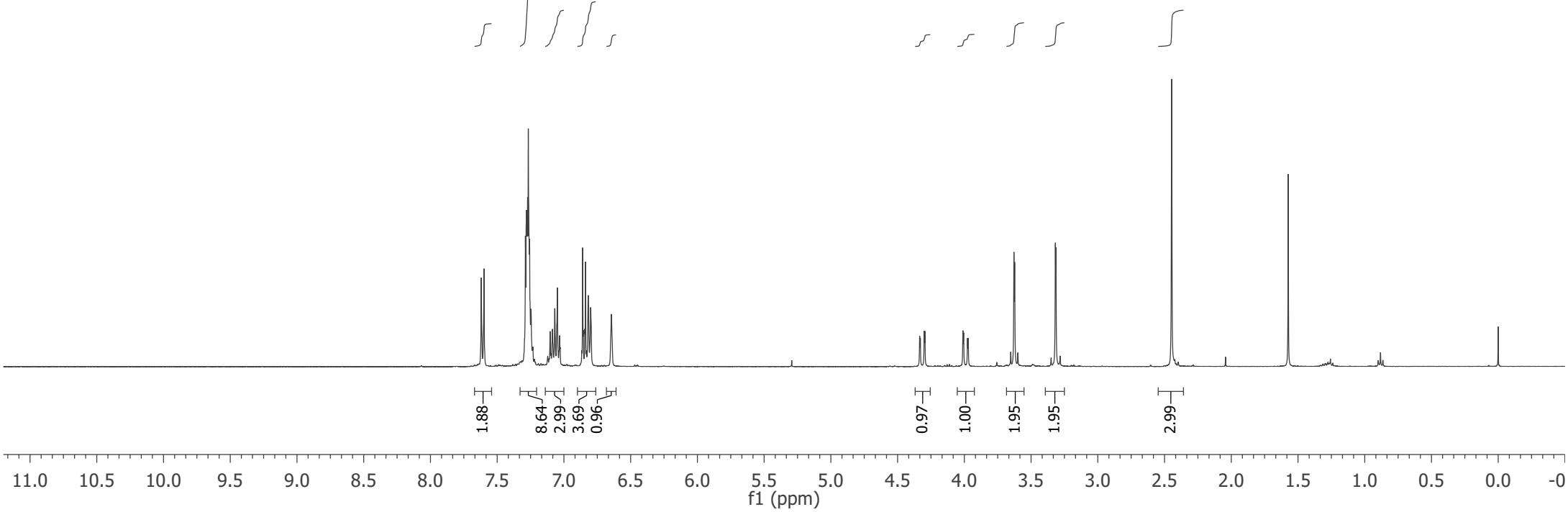

BRUKER
Transmittance [%]
100
90
80
70
60
Cl
S
Ph
Ph
N
Ts
5bc
3053.00
2937.64
2860.69
1897.74
1734.34
1659.44
1595.18
1473.95
1341.43
1164.65
1092.23
1025.49
922.00
823.14
747.14
680.61
588.43
549.68
497.96
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

Spectrometer Frequency 400.40

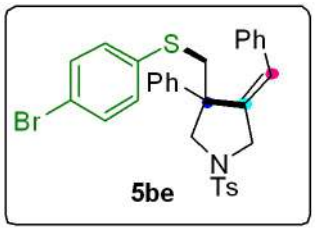




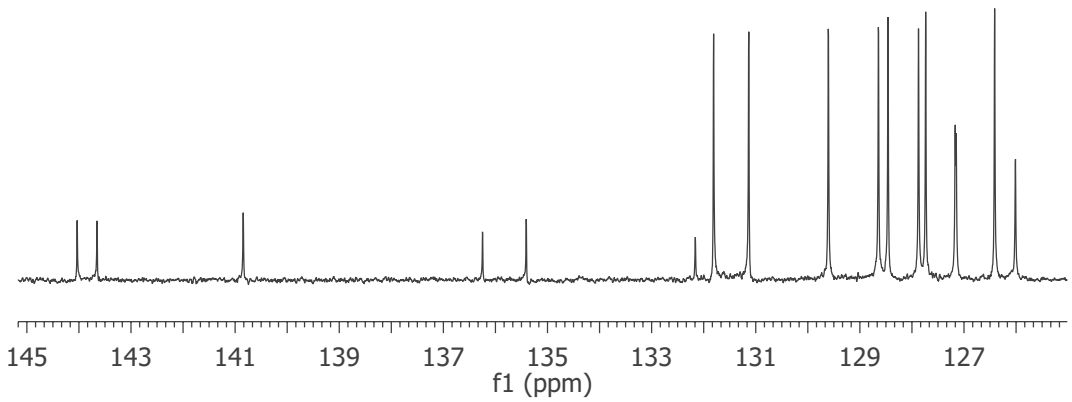


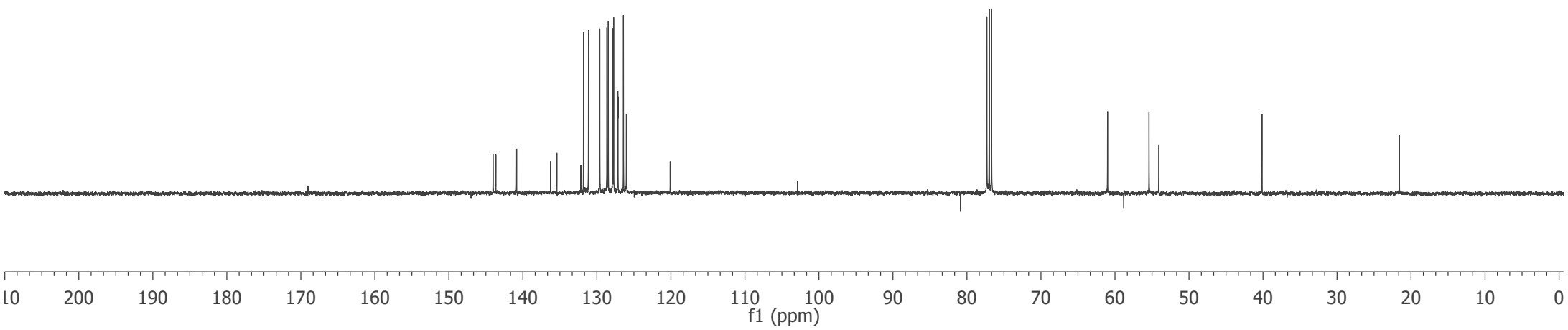
Solvent $CDCl_3$

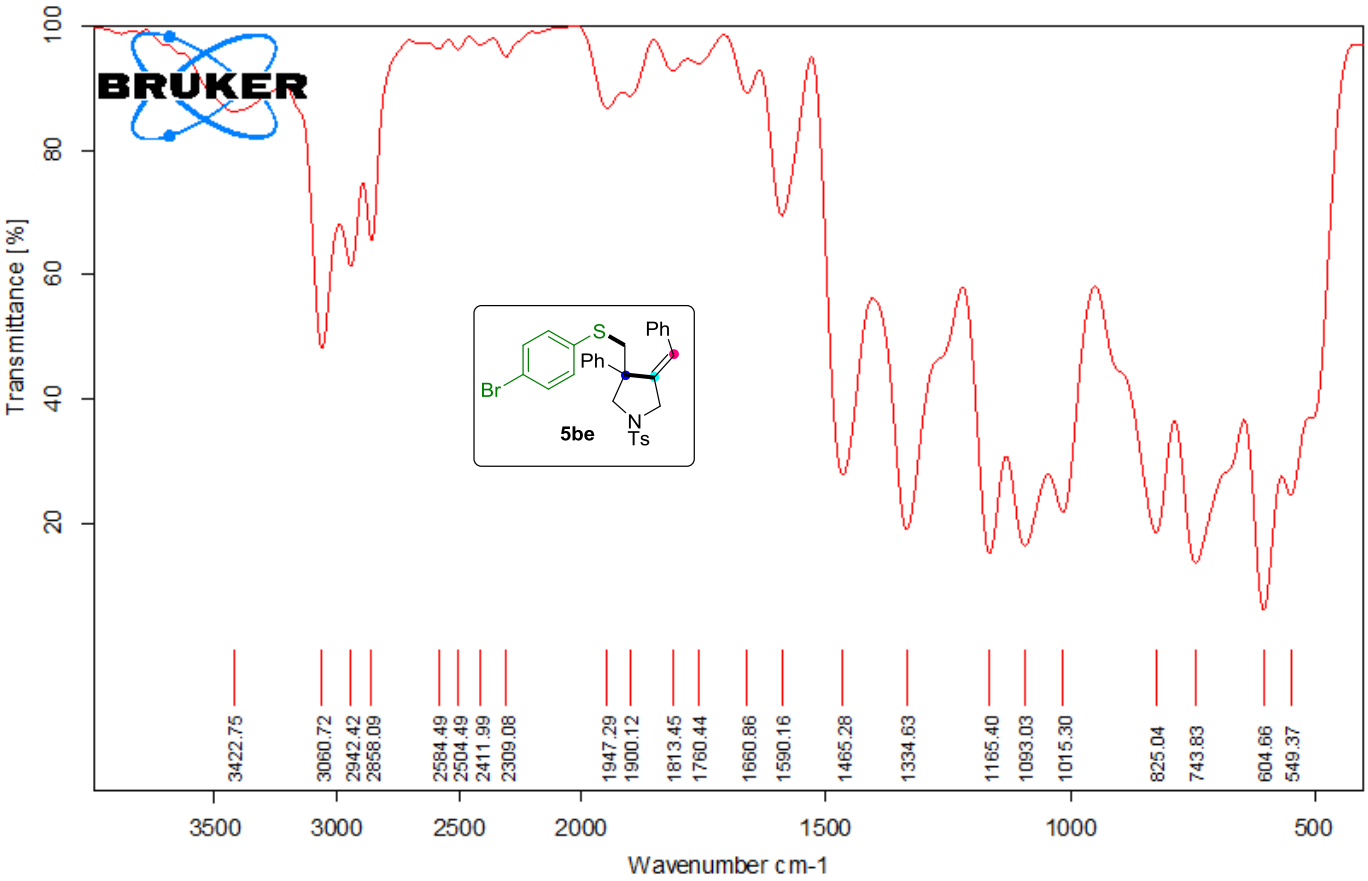
Spectrometer Frequency 100.69



146.994
144.034
143.652
140.844
136.247
135.408
132.161
131.810
131.135
129.605
128.643
128.459
127.874
127.736
127.169
127.151
126.412
126.013
120.094
102.901
61.002
55.401
54.063
40.140
21.577

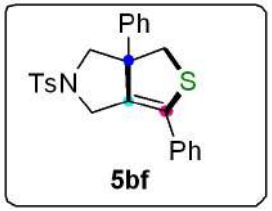


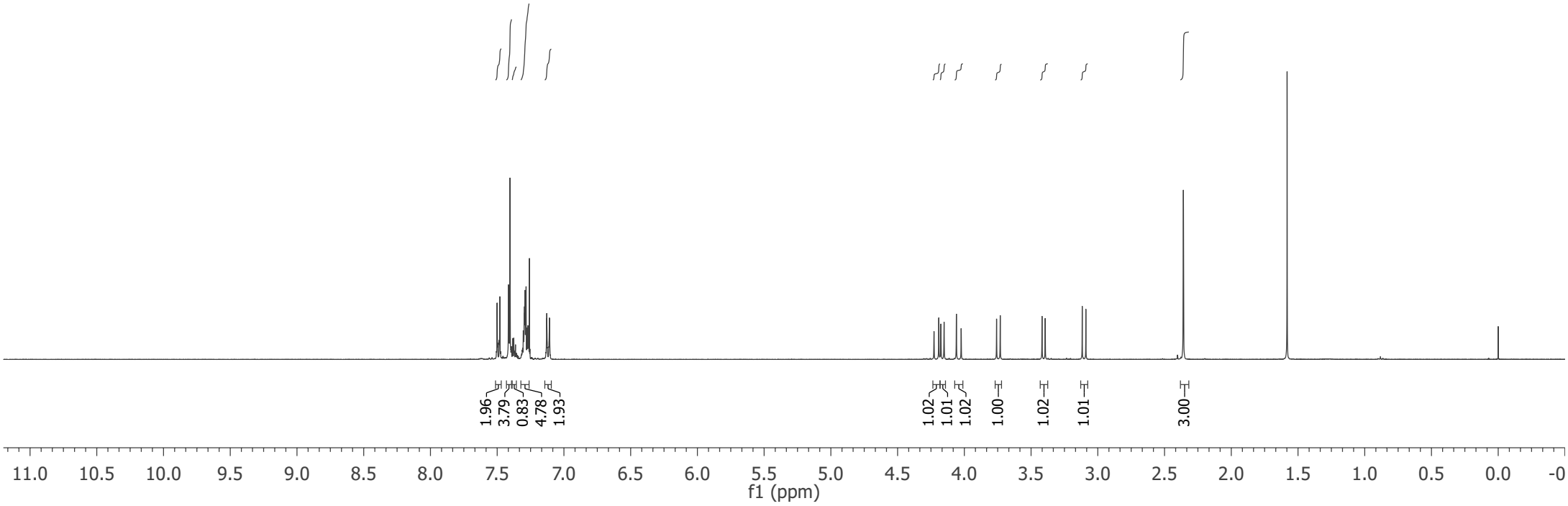



BRUKER
Transmittance [%]
100
80
60
40
20
Br
S
Ph
Ph
N
Ts
5be
3422.75
3060.72
2942.42
2858.09
2584.49
2504.49
2411.99
2309.08
1947.29
1900.12
1813.45
1760.44
1660.86
1590.16
1465.28
1334.63
1165.40
1093.03
1015.30
825.04
743.83
604.66
549.37
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

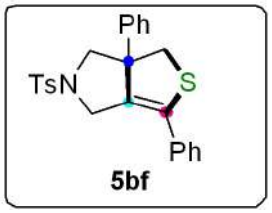
Spectrometer Frequency 400.40



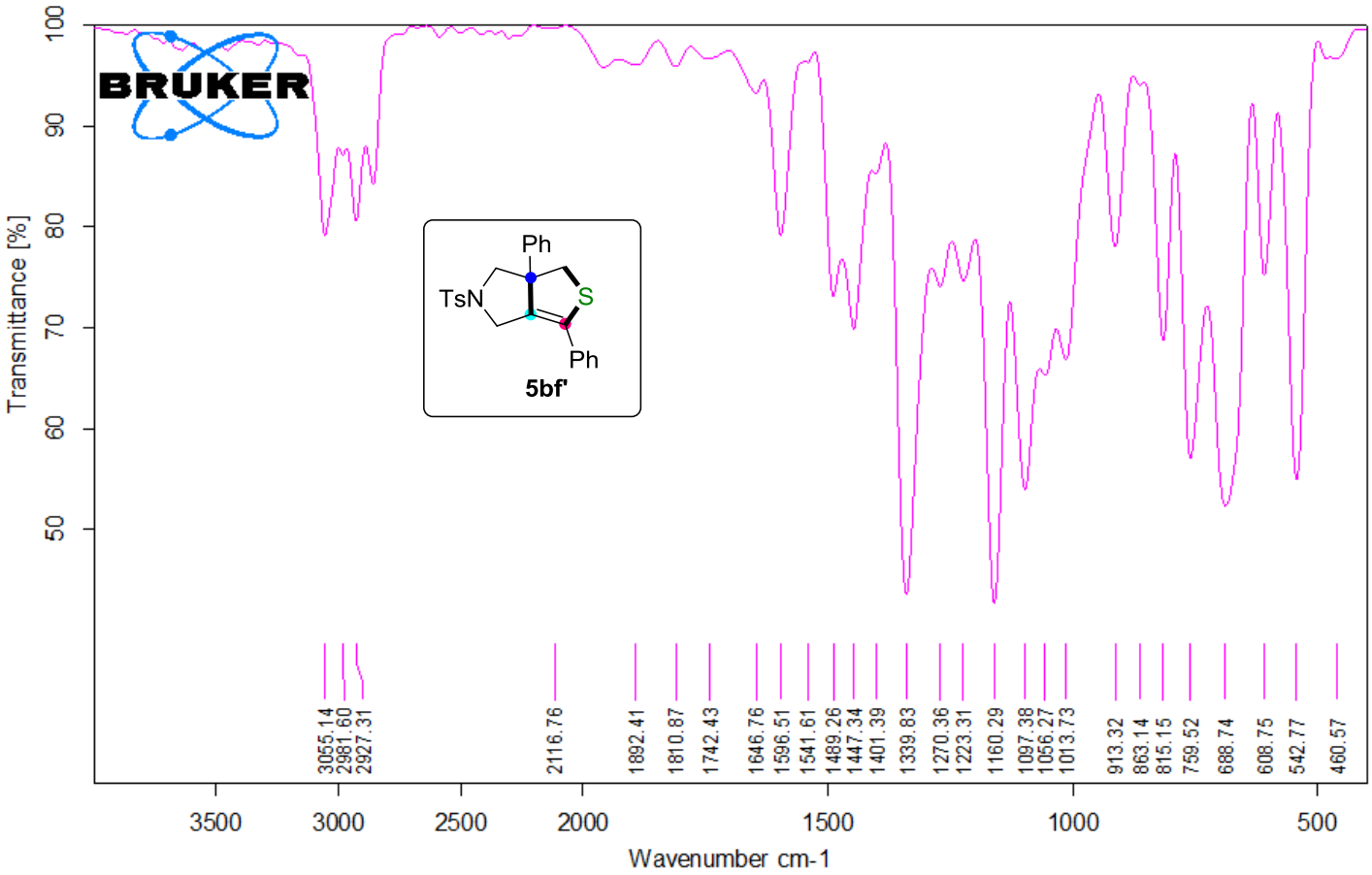


Solvent $CDCl_3$

Spectrometer Frequency 100.69

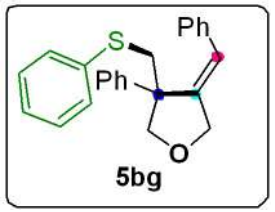


5bf


BRUKER
Transmittance [%]
100
90
80
70
60
50
Ph
TsN
S
Ph
5bf'
3055.14
2981.60
2927.31
2116.76
1892.41
1810.87
1742.43
1646.76
1596.51
1541.61
1489.26
1447.34
1401.39
1339.83
1270.36
1223.31
1160.29
1097.38
1056.27
1013.73
913.32
863.14
815.15
759.52
688.74
608.75
542.77
460.57
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

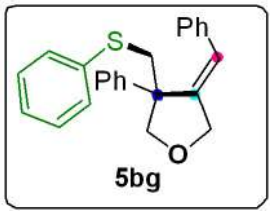
Solvent $CDCl_3$

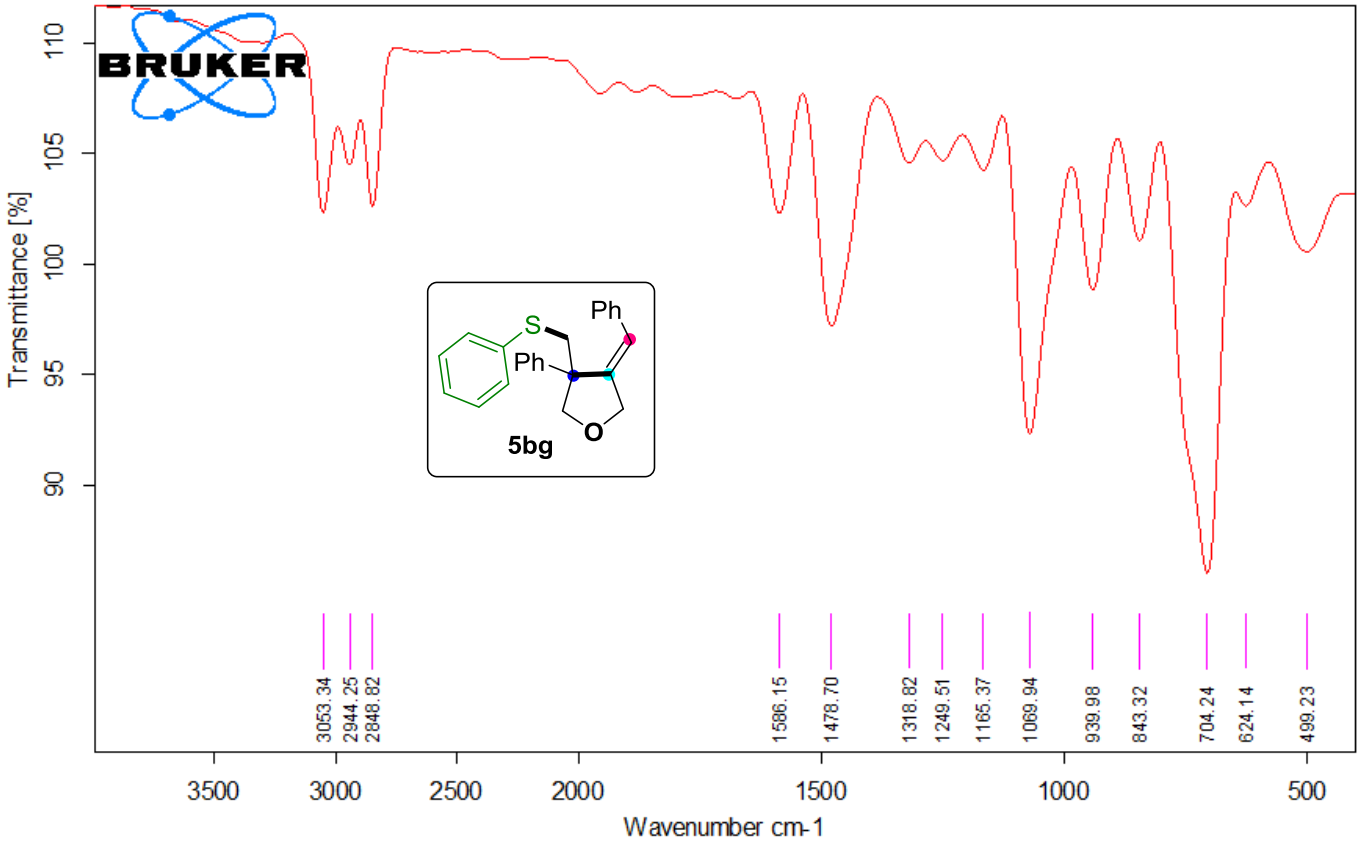
Spectrometer Frequency 400.40



Solvent $CDCl_3$

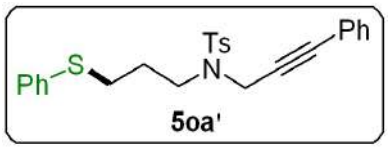
Spectrometer Frequency 100.69




BRUKER
Transmittance [%]
110
105
100
95
90
S
Ph
Ph
O
5bg
3053.34
2944.25
2848.82
1586.15
1478.70
1318.82
1249.51
1165.37
1069.94
939.98
843.32
704.24
624.14
499.23
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

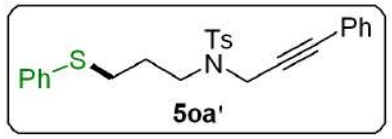
Spectrometer Frequency 400.40



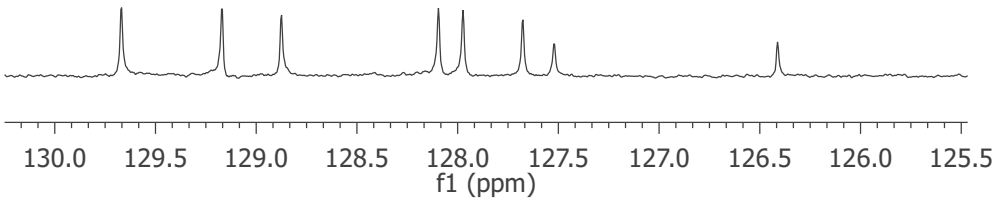
5oa'

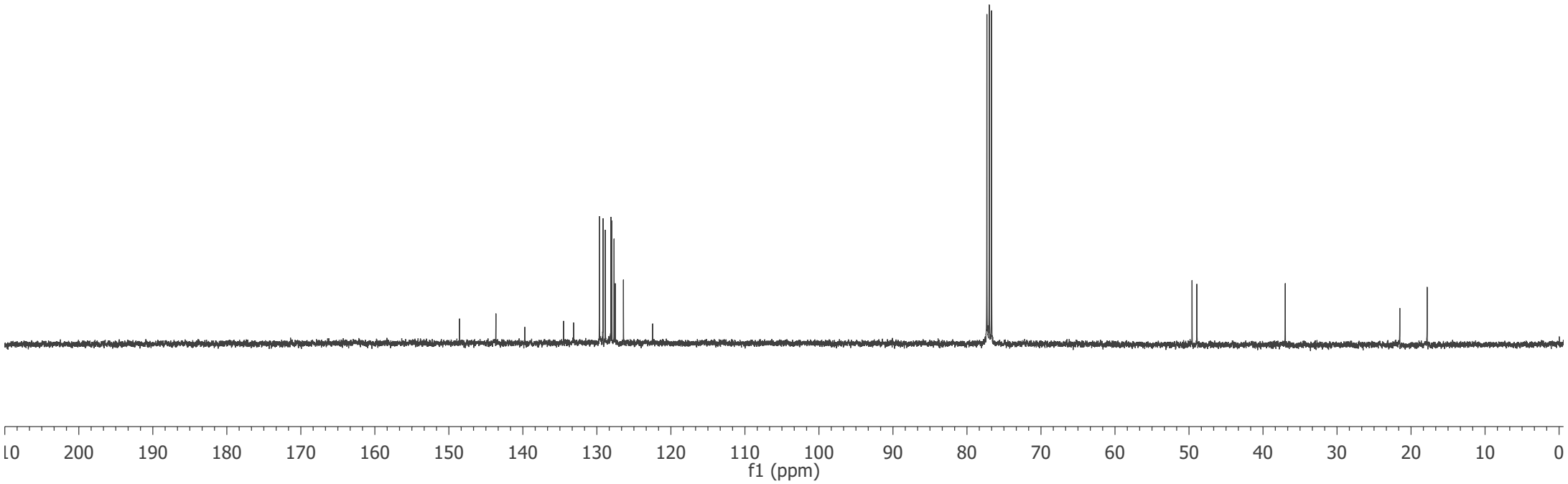
Solvent $CDCl_3$

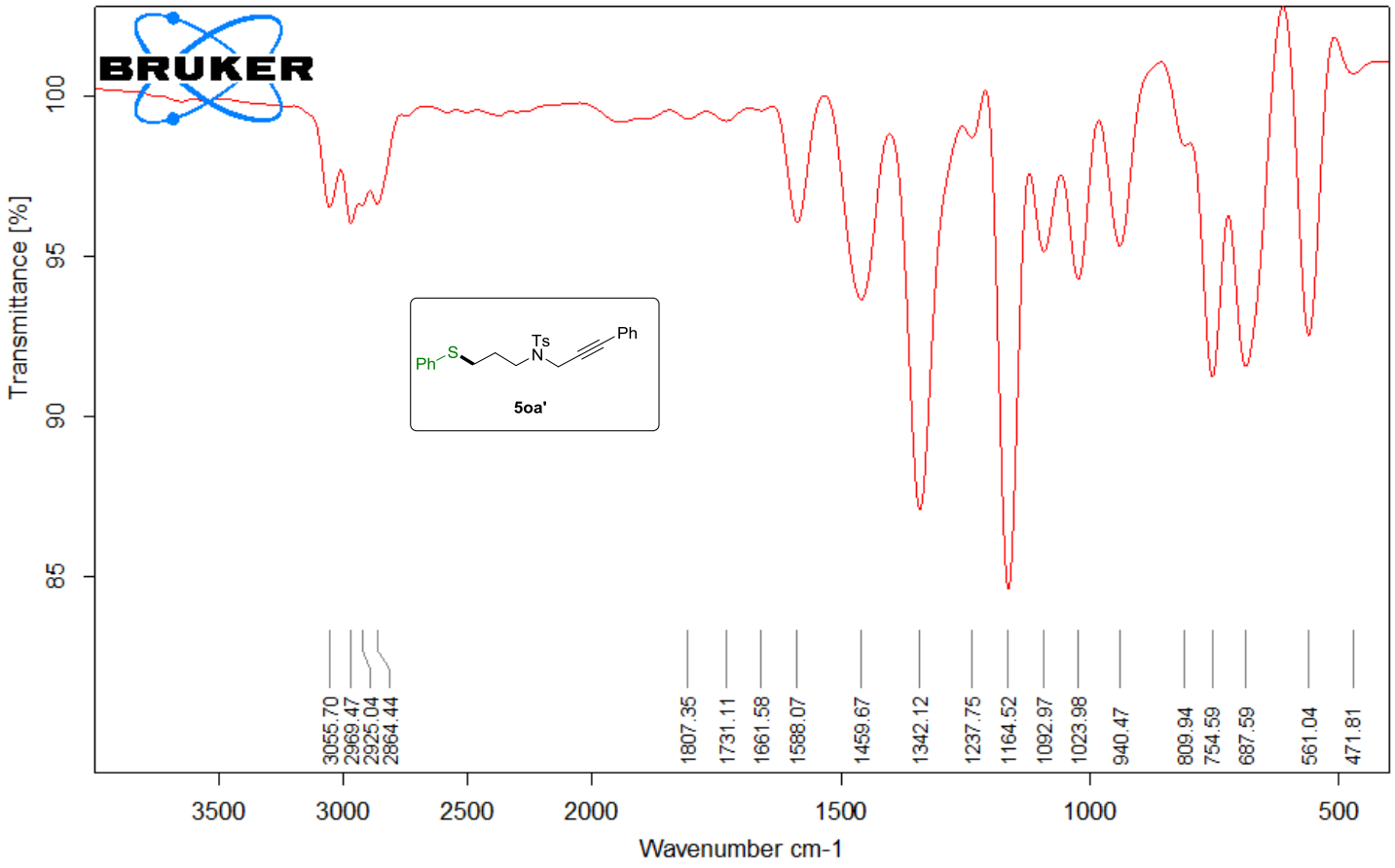
Spectrometer Frequency 100.69



148.550
143.647
139.739
134.495
133.153
129.670
129.170
128.875
128.095
127.973
127.677
127.521
126.412
122.459
49.587
48.943
36.989
21.522
17.827

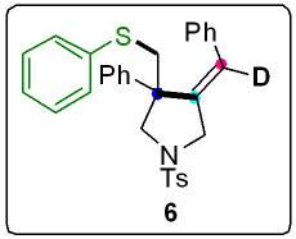





BRUKER
Transmittance [%]
100
95
90
85
Ph
S
Ts
N
Ph
5oa'
3055.70
2969.47
2925.04
2864.44
1807.35
1731.11
1661.58
1588.07
1459.67
1342.12
1237.75
1164.52
1092.97
1023.98
940.47
809.94
754.59
687.59
561.04
471.81
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Solvent $CDCl_3$

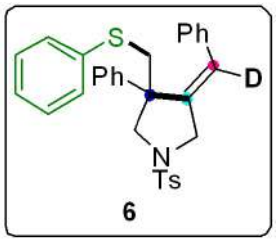
Spectrometer Frequency 400.40

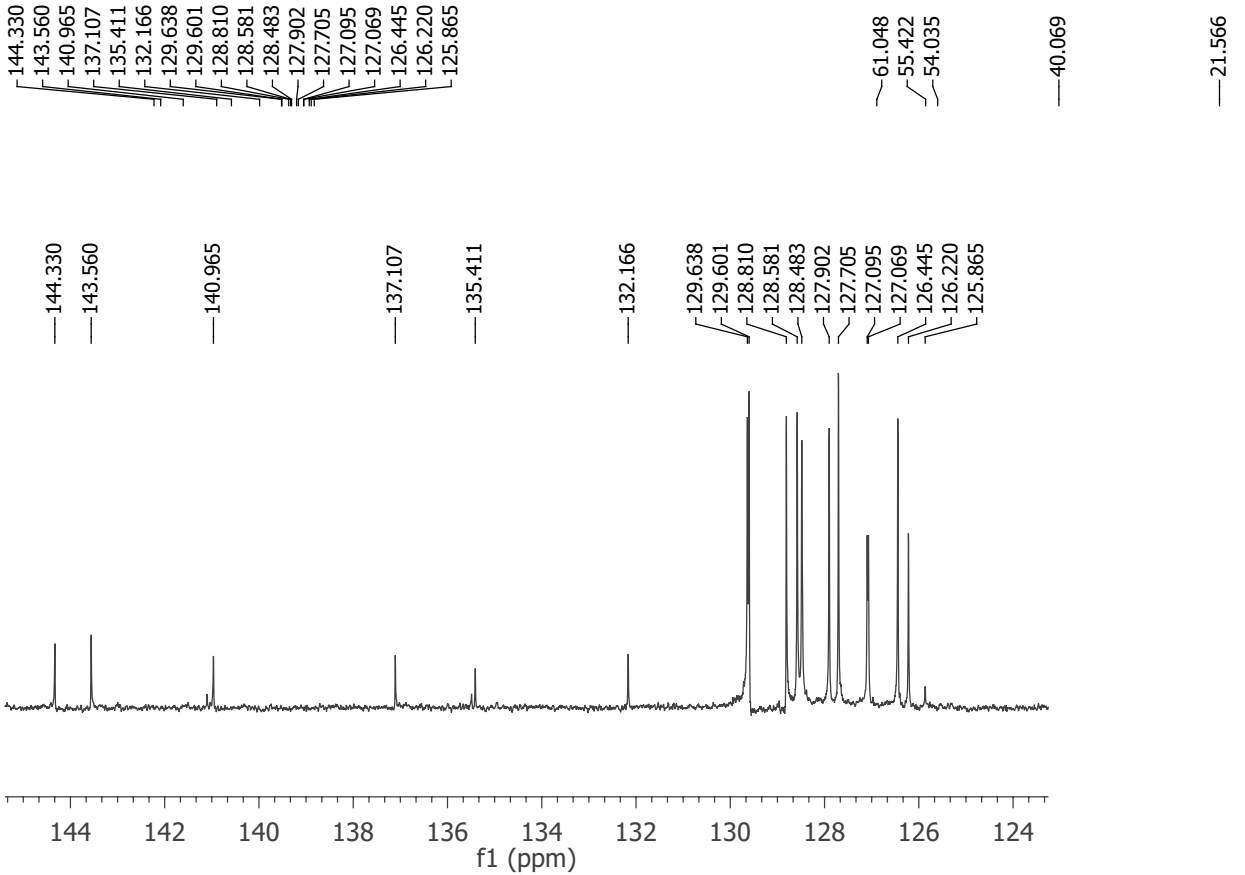


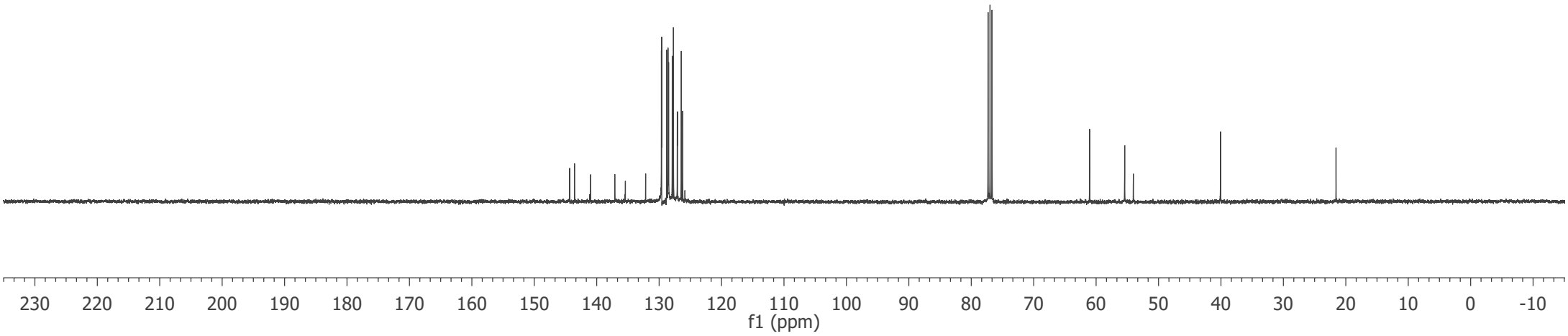
6

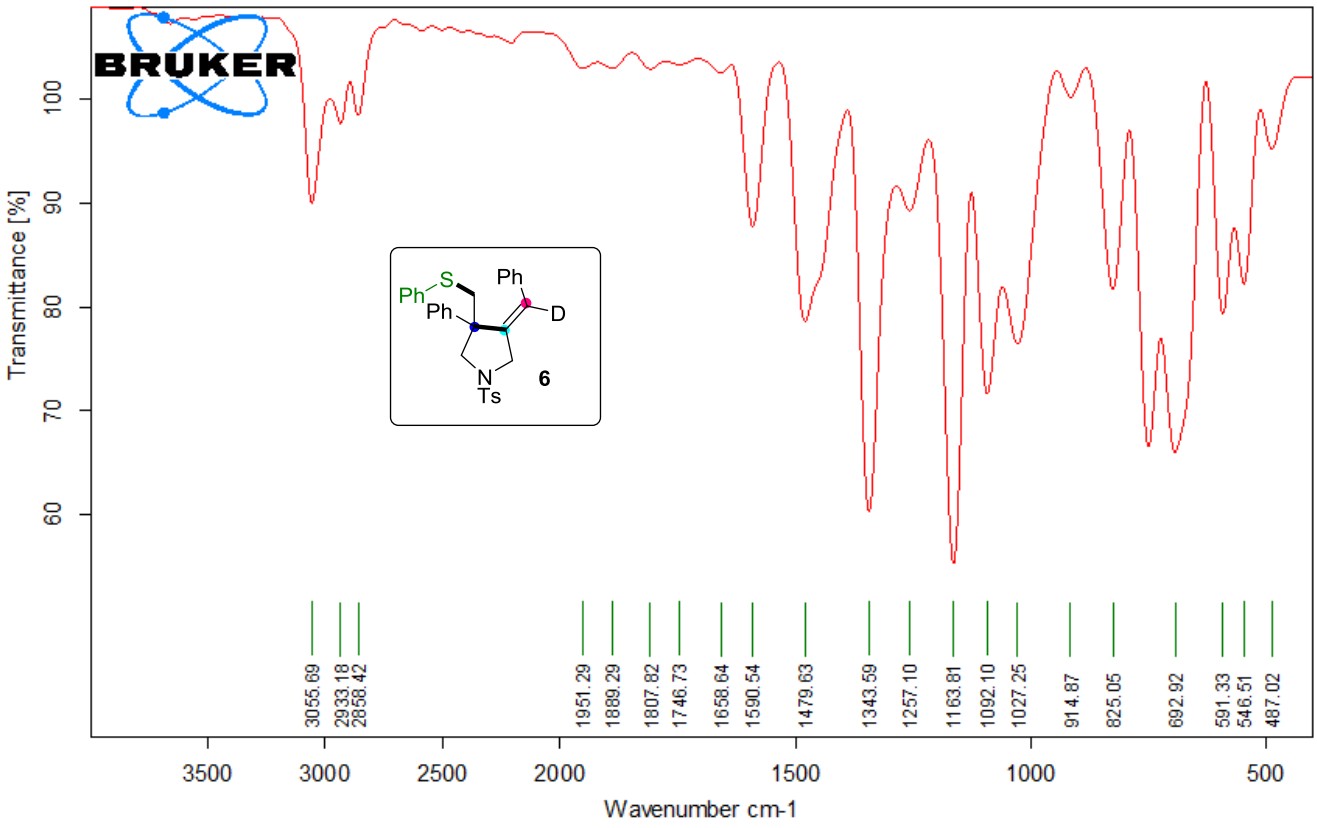
Solvent $CDCl_3$

Spectrometer Frequency 100.69








BRUKER
Transmittance [%]
100
90
80
70
60
Ph
S
Ph
Ph
D
N
Ts
6
3055.69
2933.18
2858.42
1951.29
1889.29
1807.82
1746.73
1658.64
1590.54
1479.63
1343.59
1257.10
1163.81
1092.10
1027.25
914.87
825.05
692.92
591.33
546.51
487.02
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mr-08

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mr-08

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=14.4315(3) b=11.9782(3) c=19.7756(5)
alpha=90 beta=95.022(2) gamma=90
Temperature: 113 K

	Calculated	Reported
Volume	3405.36(14)	3405.35(14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C38 H35 N O5 S2 Se	C38 H35 N O5 S2 Se
Sum formula	C38 H35 N O5 S2 Se	C38 H35 N O5 S2 Se
Mr	728.75	728.75
Dx,g cm-3	1.421	1.421
Z	4	4
Mu (mm-1)	1.270	1.270
F000	1504.0	1504.0
F000’	1505.19	
h,k,lmax	18,15,25	18,15,25
Nref	7513	7121
Tmin,Tmax	0.783,0.776	0.527,1.000
Tmin’	0.768	

Correction method= # Reported T Limits: Tmin=0.527 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.948 Theta(max)= 27.108

R(reflections)= 0.0348(5862) wR2(reflections)= 0.1218(7121)

S = 0.938 Npar= 426

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 A

PLAT902_ALERT_1_A No (Interpretable) Reflections Found in FCF .... Please Check

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 3.3 Ratio

Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT793_ALERT_4_G Model has Chirality at C16 (Centro SPGR) R Verify
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 19 Note

1 **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
3 **ALERT level G** = General information/check it is not something unexpected

2 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
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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

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Publication of your CIF in other journals

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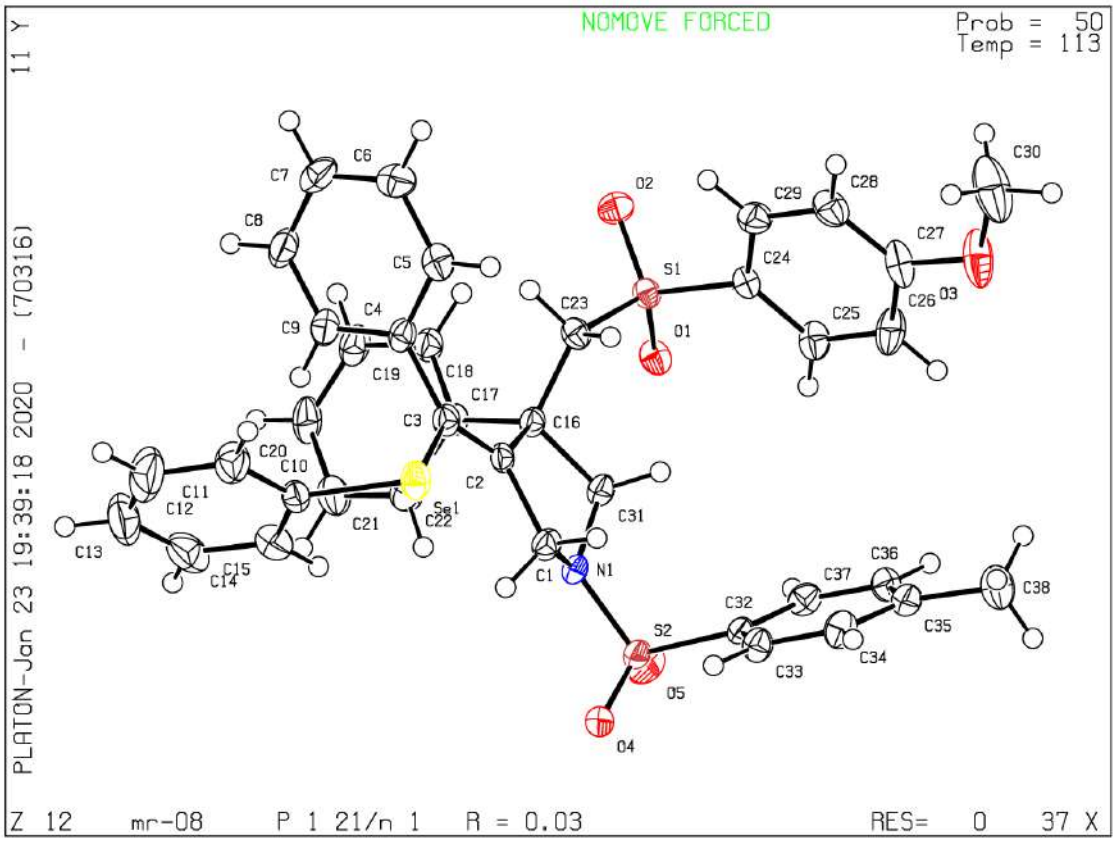
PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock mr-08 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_243

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: exp_243

```
Bond precision:  C-C = 0.0032 A          Wavelength=0.71073

Cell:           a=14.9578(4)    b=9.9529(2)         c=21.8477(4)
                alpha=90        beta=107.937(2)     gamma=90
Temperature:    113 K

                Calculated                Reported
Volume          3094.46(12)               3094.46(12)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C35 H31 N O2 S2 Se2       C35 H31 N O2 S2 Se2
Sum formula     C35 H31 N O2 S2 Se2       C35 H31 N O2 S2 Se2
Mr              719.65                    719.65
Dx,g cm-3       1.545                     1.545
Z               4                         4
Mu (mm-1)       2.558                     2.558
F000            1456.0                    1456.0
F000'           1456.71
h,k,lmax        19,12,27                  18,12,27
Nref            6809                      6488
Tmin,Tmax       0.533,0.600               0.401,1.000
Tmin'           0.522

Correction method= # Reported T Limits: Tmin=0.401 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.953          Theta(max)= 27.075

R(reflections)= 0.0279( 5594)     wR2(reflections)= 0.0647( 6488)

S = 1.039                 Npar= 380
```

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 A

PLAT902_ALERT_1_A No (Interpretable) Reflections Found in FCF .... Please Check

Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT793_ALERT_4_G Model has Chirality at C3 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

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0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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Publication of your CIF in other journals

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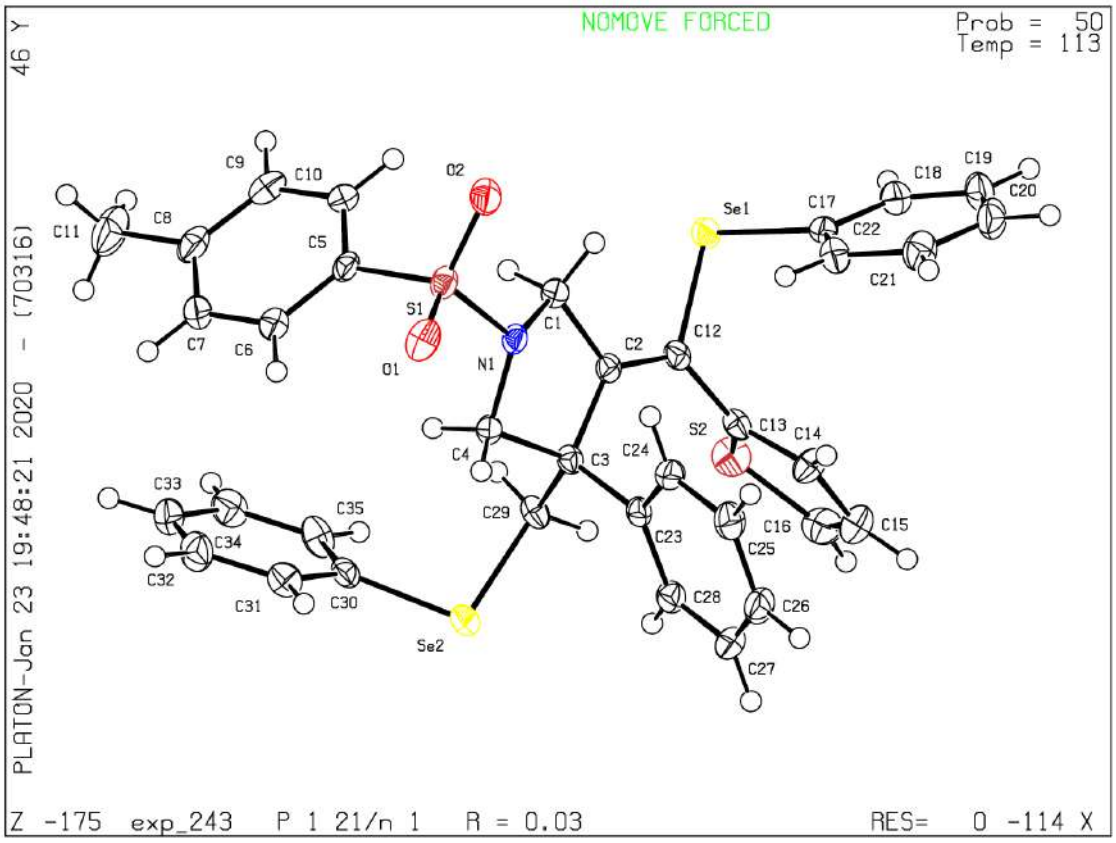
PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock exp_243 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mr0878

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mr0878

Bond precision: C-C = 0.0088 A Wavelength=0.71073

Cell: a=12.7099(13) b=16.6188(17) c=13.6736(16)
alpha=90 beta=104.205(6) gamma=90
Temperature: 287 K

	Calculated	Reported
Volume	2799.9(5)	2799.9(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C31 H28 Br N O2 S2	C31 H28 Br N O2 S2
Sum formula	C31 H28 Br N O2 S2	C31 H28 Br N O2 S2
Mr	590.56	590.57
Dx,g cm-3	1.401	1.401
Z	4	4
Mu (mm-1)	1.646	1.646
F000	1216.0	1216.0
F000’	1216.25	
h,k,lmax	16,22,18	16,21,18
Nref	7013	6777
Tmin,Tmax	0.596,0.807	0.705,0.928
Tmin’	0.585	

Correction method= # Reported T Limits: Tmin=0.705 Tmax=0.928
AbsCorr = MULTI-SCAN

Data completeness= 0.966 Theta(max)= 28.386

R(reflections)= 0.0834(4228) wR2(reflections)= 0.3108(6777)

S = 1.061 Npar= 334

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

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.31 Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C22 --C23 .	5.4 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C21 --C22 .	0.18 Ang.
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of	C22 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C18 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00878 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-6.741 Report
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-0.599 Report
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	7 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	47 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	33 Note
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1 Check

Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.17 Report
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C7 Check
PLAT793_ALERT_4_G	Model has Chirality at C9 (Centro SPGR)	S Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT898_ALERT_4_G	Second Reported H-M Symbol in CIF Ignored	! Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	172 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1 Check

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PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock mr0878 - ellipsoid plot