Supplementary Information

Formation of Chalcogen-Bonding Interactions and their Role in the *Trans-Trans* Conformation of Thiourea

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Content:

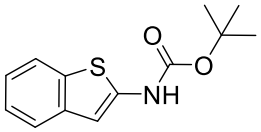
General methods

Uncorrected melting points were measured by using a Büchi Melting Point M-565. NMR spectra were obtained with a Bruker UltraShield 300, or a Bruker Ascend 500 spectrometer. Chemical shifts are given in units of ppm (^{1}H NMR in $CDCl_3$: tetramethylsilane as the internal standard at 0 ppm, and $CDCl_3$ as the internal standard at 7.26 ppm; ^{13}C NMR in $CDCl_3$: $CDCl_3$ as the internal standard at 77.0 ppm; ^{1}H NMR in DMSO-d_6: DMSO-d_6 as the internal standard at 2.50 ppm; ^{13}C NMR in DMSO-d_6: DMSO-d_6 as the internal standard at 39.5 ppm; ^{1}H NMR in THF-d_8: THF-d_8 as the internal standard at 3.58 ppm). Spin-spin coupling constants are in Hz. NOE experiments were carried out with a JNM ECA 600 (600 MHz) spectrometer. IR spectra were recorded on a JASCO FT-IR 4200 spectrometer. HRMS was recorded on a JEOL GCmate II (for EI). UV/Vis spectra were recorded on a JASCO V-550 UV/Vis spectrophotometer. The crystal structure was obtained by X-ray crystallographic analysis with Rigaku/XtaLAB Synergy-DW X-ray diffractometer.

Column chromatography on silica gel was carried out using silica gel 60 N (spherical, neutral, 63–210 μm, Kanto Chemical Co., Inc.). TLC analysis and preparative TLC analysis were performed on commercial glass plates bearing a 0.25 mm layer or 0.5 mm layer of Merck Kiesel-gel 60 F254, respectively. All chemicals and reagents were commercially available and used without further purification.

Synthetic procedures

tert-Butyl(benzo[b]thiophen-2-yl)carbamate (**5a**)

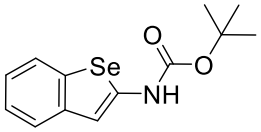


5a

To a solution of the benzo[b]thiophen-2-carboxylic acid (**4a**) (3.0 g, 16.8 mmol, 1.0 equiv.) in *t*-BuOH (30 mL), Et_3N (7.0 mL, 50.5 mmol, 3.0 equiv.) and DPPA (5.4 mL, 25.3 mmol, 1.5 equiv.) were added at rt under N_2 atmosphere. The mixture was heated and stirred for 23 h under reflux. The reaction was quenched with sat. aq. NH_4Cl, and extracted with AcOEt. The organic layer was washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane/AcOEt = 9/1) to afford **5a** (3.6 g, 85%).

Brown solid; M.p. 167–168 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.55 (9H, s), 6.74 (1H, s), 7.06 (1H, br s), 7.18–7.23 (1H, m), 7.27–7.32 (1H, m), 7.54–7.59 (1H, m), 7.67–7.73 (1H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 28.3, 82.0, 105.8, 121.8, 121.9, 122.8, 124.5, 134.8, 138.0, 140.5, 152.2; IR (ATR): 1692, 2978, 3294 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{13}H_{15}NO_2S$ $[M]^+$ 249.0823, found 249.0821.

tert-Butyl(benzo[b]selenophen-2-yl)carbamate (**5b**)

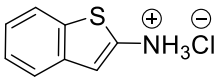


5b

To a solution of the benzo[b]selenophen-2-carboxylic acid[1)] (**4b**) (290 mg, 1.29 mmol, 1.0 equiv.) in *t*-BuOH (7 mL), Et_3N (540 μL, 3.87 mmol, 3.0 equiv.) and DPPA (556 μL, 2.58 mmol, 2.0 equiv.) were added at rt under N_2 atmosphere. The mixture was heated and stirred for 23 h under reflux. The reaction was quenched with sat. aq. NH_4Cl, and extracted with AcOEt. The organic layer was washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane/AcOEt = 10/1) to afford **5b** (305 mg, 80%).

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.55 (9H, s), 6.73 (1H, s), 7.10–7.16 (1H, m), 7.26–7.33 (2H, m), 7.53–7.56 (1H, m), 7.77 (1H, d, J = 7.8 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 28.3, 82.1, 106.8, 122.7, 123.3, 124.7, 124.8, 137.0, 140.1, 141.0, 152.5; IR (ATR): 1686, 2978, 3292 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{13}H_{15}NO_2Se$ $[M]^+$ 297.0268, found 297.0284.

Benzo[b]thiophen-2-aminium chloride (**6a**)

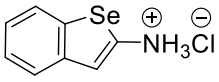


6a

tert-Butyl(benzo[b]thiophen-2-yl)carbamate (**5a**) (2.0 g, 8.2 mmol) and 4 M HCl in dioxane (82 mL) were mixed, and stirred for 2 h at rt. The mixture was cooled to 0 °C, and diluted with *n*-hexane to form a precipitate. The resulting precipitate was collected by filtration, washed with *n*-hexane, and dried under vacuum to afford **6a** (1.3 g, 85%).

Colorless amorphous; ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.02 (1H, s), 6.92 (1H, t, J = 7.6 Hz), 7.11 (1H, t, J = 7.5 Hz), 7.29 (1H, d, J = 7.9 Hz), 7.54 (1H, d, J = 7.9 Hz); IR (ATR): 1225, 1437, 1504, 2520, 2691 cm^{-1}; HRMS (EI): *m/z* calcd for C_8H_7NS (NH_2 form) $[M]^+$ 149.0299, found 149.0299. The ^{13}C NMR signals could not be assigned, because they were quite complex. This might be due to aggregation of **6a**.

Benzo[b]selenophen-2-aminium chloride (**6b**)

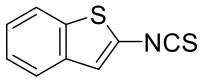


6b

tert-Butyl(benzo[b]selenophen-2-yl)carbamate (**5b**) (305 mg, 1.0 mmol) and 4 M HCl in dioxane (10 mL) were mixed, and stirred for 2 h at rt. The mixture was cooled to 0 °C, and diluted with *n*-hexane to form a precipitate. The resulting precipitate was collected by filtration, washed with *n*-hexane, and dried under vacuum to afford **6b** (209 mg, 88%).

Yellow amorphous; ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.07 (1H, s), 6.81–6.87 (1H, m), 7.06–7.12 (1H, m), 7.23–7.27 (1H, m), 7.59 (1H, d, J = 7.9 Hz); IR (ATR): 1222, 1436, 1504, 2517 cm^{-1}; HRMS (EI): *m/z* calcd for C_8H_7NSe (NH_2 form) $[M]^+$ 196.9744, found 196.9746. The ^{13}C NMR signals could not be assigned, because they were quite complex. This might be due to aggregation of **6b**.

2-Isothiocyanatobenzo[b]thiophene (**7a**)



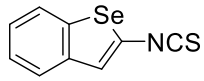
7a

To a solution of benzo[b]thiophen-2-aminium chloride (**6a**) (93.0 mg, 501 μmol, 1.0 equiv.) and ^{i}Pr$_2$EtN (349 μL, 2.0 mmol, 4.0 equiv.) in anhydrous CH_2Cl_2 (7 mL) was added thiophosgene (76.8 μL, 1.0 mmol, 2.0 equiv.) dropwise at 0 °C under N_2 atmosphere. After being stirred for 3 h at 0 °C,

the reaction was quenched with water, and extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give a residue. The residue was purified by flash column chromatography (SiO_2, *n*-hexane/AcOEt = 3/1) to obtain **7a** (37.7 mg, 39%).

Brown amorphous; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.06 (1H, s), 7.33–7.40 (2H, m), 7.64–7.73 (2H, m). Compound **7a** was thought to be relatively unstable. Therefore, **7a** was immediately used for the thiourea formation after ^{1}H NMR measurement.

2-Isothiocyanatobenzo[b]selenophene (**7b**)

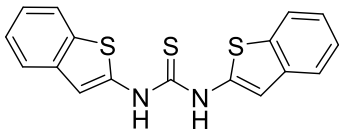


7b

To a solution of benzo[b]selenophen-2-aminium chloride (**6b**) (116.9 mg, 503 μmol, 1.0 equiv.) and ^{i}Pr$_2$EtN (350 μL, 2.0 mmol, 4.0 equiv.) in anhydrous CH_2Cl_2 (10 mL) was added thiophosgene (77.0 μL, 1.0 mmol, 2.0 equiv.) dropwise at 0 ℃ under N_2 atmosphere. After being stirred for 2 h at 0 ℃, the reaction was quenched with water, and extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give a residue. The residue was purified by flash column chromatography (SiO_2, *n*-hexane/AcOEt = 3/1) to obtain **7b** (64.0 mg, 54%).

Brown amorphous; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (1H, s), 7.30 (1H, t, J = 7.5 Hz), 7.36 (1H, t, J = 7.6 Hz), 7.69 (1H, d, J = 7.6 Hz), 7.73 (1H, d, J = 7.8 Hz). Compound **7b** was thought to be relatively unstable. Therefore, **7b** was immediately used for the thiourea formation after ^{1}H NMR measurement.

1,3-Bis(benzo[b]thiophen-2-yl)thiourea (**3a**)

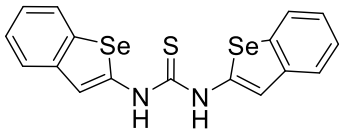


3a

To a solution of 2-isothiocyanatobenzo[b]thiophene (**7a**) (57.1 mg, 299 μmol, 1.0 equiv.) in anhydrous CH_2Cl_2 (1.0 mL), a mixed solution of benzo[b]thiophen-2-aminium chloride (**6a**) (66.5 mg, 358 μmol, 1.2 equiv.) and ^{i}Pr$_2$EtN (156 μL, 896 μmol, 3.0 equiv.) in anhydrous CH_2Cl_2 (2.0 mL) was added slowly at –20 ℃ under N_2 atmosphere. After being stirred for 20 h at –20 ℃, the reaction was quenched with sat. aq. NH_4Cl, and extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give a residue. The resulting solid was collected by filtration, washed with $CHCl_3$, and dried under vacuum to afford **3a** (35.7 mg, 35%).

Red-brown solid; M.p. 191-192 ℃, ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.14 (2H, s), 7.25 (2H, t, J = 7.6 Hz), 7.32 (2H, t, J = 7.5 Hz), 7.69 (2H, d, J = 7.9 Hz), 7.85 (2H, d, J = 7.9 Hz), 11.19 (2H, s); ^{1}H NMR (600 MHz, THF-d_8) δ 7.06 (2H, s), 7.17 (2H, t, J = 7.8 Hz), 7.23 (2H, t, J = 7.8 Hz), 7.56 (2H, d, J = 8.4 Hz), 7.71 (2H, d, J = 7.8 Hz), 10.86 (2H, s); ^{13}C NMR (75 MHz, DMSO-d_6) δ 110.2, 122.3, 122.4, 123.6, 124.9, 135.2, 137.0, 142.4, 174.9; IR (ATR): 1574, 1597, 3074, 3208 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{17}H_{12}N_2S_3$ $[M]^+$ 340.0163, found 340.0151.

1,3-Bis(benzo[b]selenophen-2-yl)thiourea (**3b**)



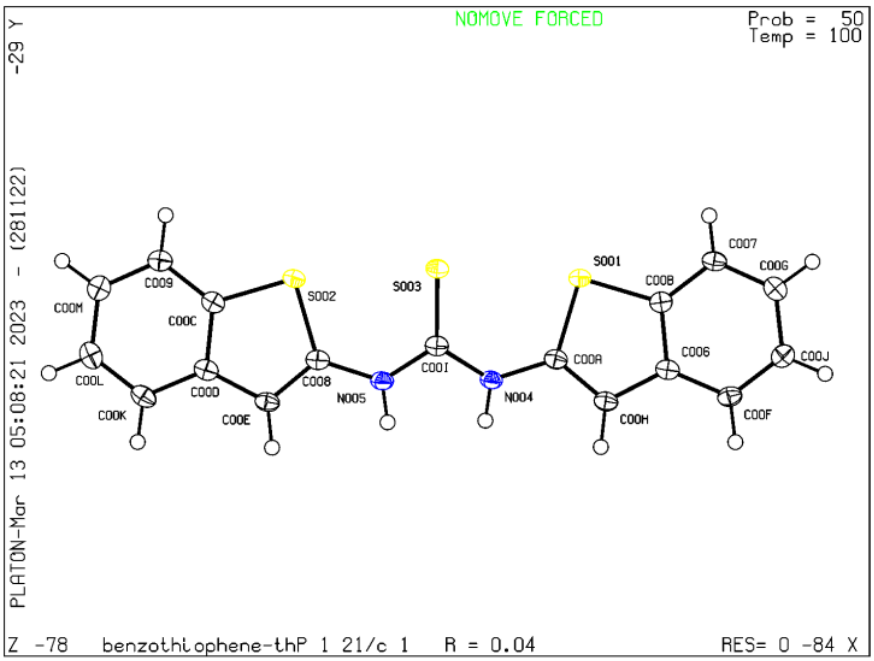
3b

To a solution of 2-isothiocyanatobenzo[b]selenophene (**7b**) (55.7 mg, 234 μmol, 1.0 equiv.) in anhydrous CH_2Cl_2 (4.5 mL), a mixed solution of benzo[b]selenophen-2-aminium chloride (**6b**) (65.3 mg, 281 μmol, 1.2 equiv.) and ^{i}Pr$_2$EtN (122 μL, 702 μmol, 3.0 equiv.) in anhydrous CH_2Cl_2 (5.6 mL) was added slowly at –20 ℃ under N_2 atmosphere. After being stirred for 21.5 h at –20 ℃, the reaction was quenched with sat. aq. NH_4Cl, and extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give a residue. The resulting solid was diluted with MeOH/Ether (1:1) and collected by filtration, washed with Toluene and MeOH, and dried under vacuum to afford **3b** (35.9 mg, 35%).

Brown solid; M.p. 201 ℃, ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.17 (2H, t, J = 7.3 Hz), 7.24 (2H, s), 7.31 (2H, t, J = 7.7 Hz), 7.67 (2H, d, J = 8.2 Hz), 7.92 (2H, d, J = 7.3 Hz), 11.44 (2H, s); ^{13}C NMR (126 MHz, DMSO-d_6) 111.4, 123.5, 123.8, 125.14, 125.15, 137.8, 139.1, 142.9, 173.6; IR (ATR): 1555, 1573, 1589, 2334 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{17}H_{12}N_2SSe_2$ $[M]^+$ 435.9051, found 435.9047.

Crystal structure of 3a

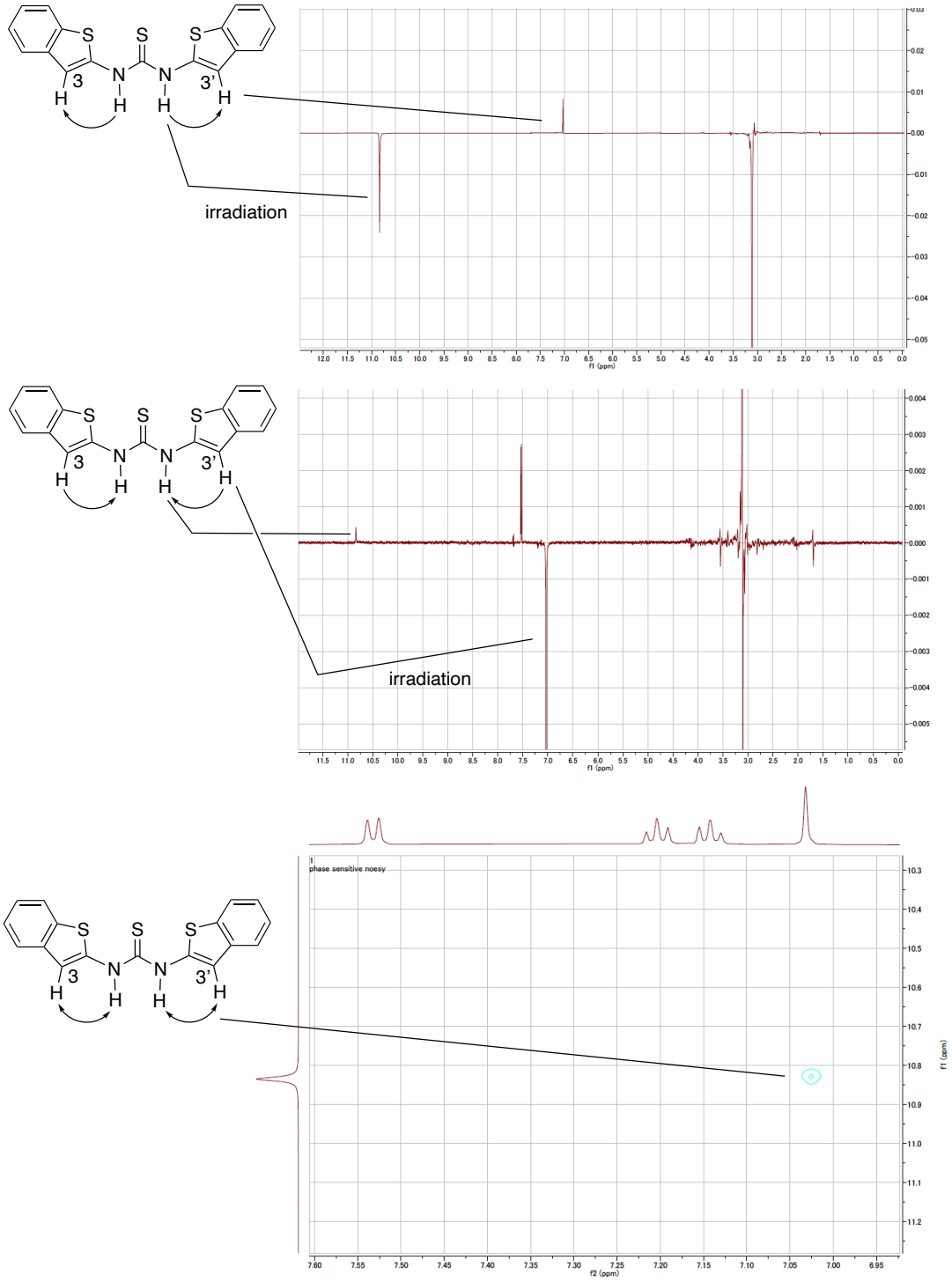
Crystallographic data for the single crystal of **3a** obtained by recrystallization from acetone: $C_{17}H_{12}N_2S_3$, M = 340.47, 0.17 × 0.08 × 0.04 mm^3, monoclinic, $P2_1/c$, a = 5.60550(10) Å, b = 7.63800(10) Å, c = 34.1020(6) Å, α = 90º, β = 91.472(2)º, γ = 90º, V = 1459.59(4) Å^3, Z = 4, ρ_{calcd} = 1.549 gcm^{-3}, T = 100.00(10) K, 14469 reflections measured, 2954 unique. The final R_1 and wR were 0.0397 and 0.0953 (all data). These data have been deposited with the Cambridge Crystallographic Data Center as CCDC 2348537.



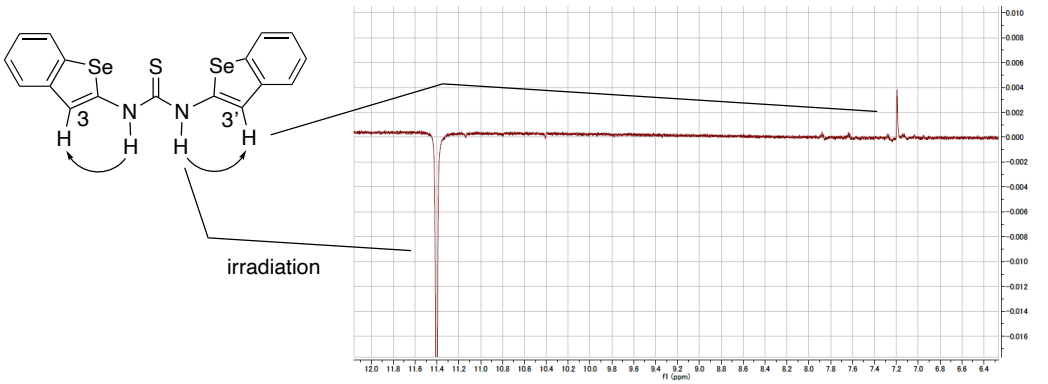
ORTEP diagram of the crystal structure of **3a** (50% probability).

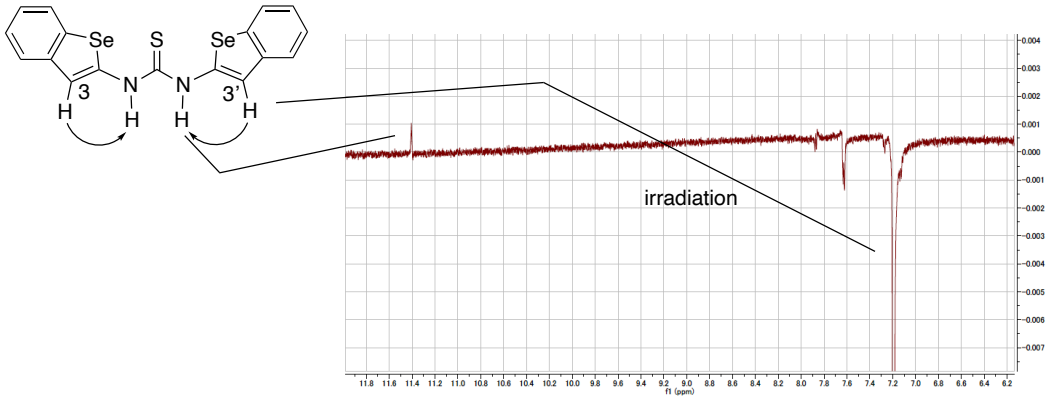
NOE correlations

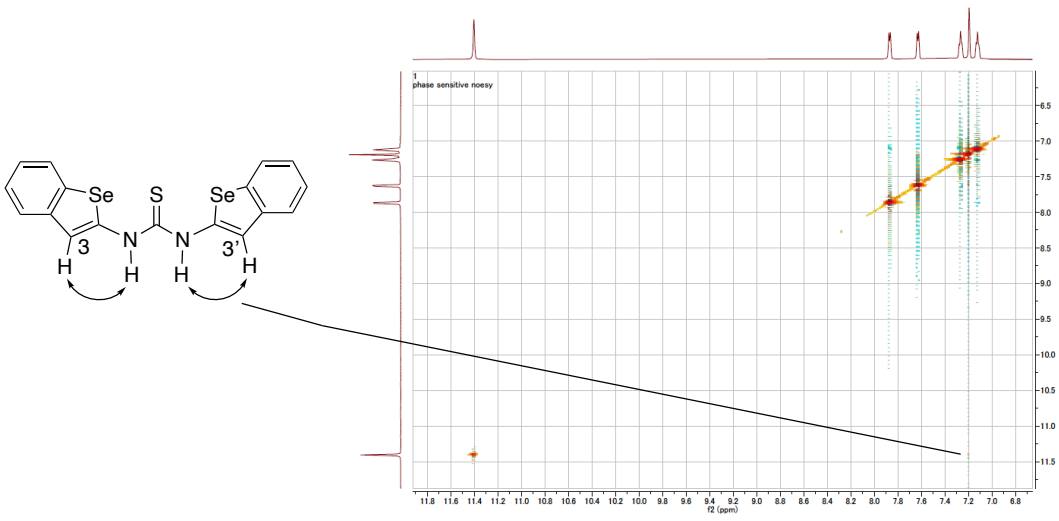
1) Differential NOE and NOESY spectra for **3a** in THF-d_8



2) Differential NOE and NOESY spectra for **3b** in DMSO-d_6



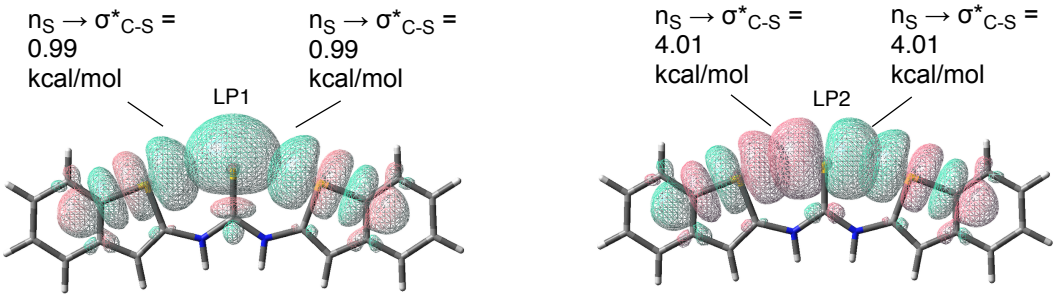




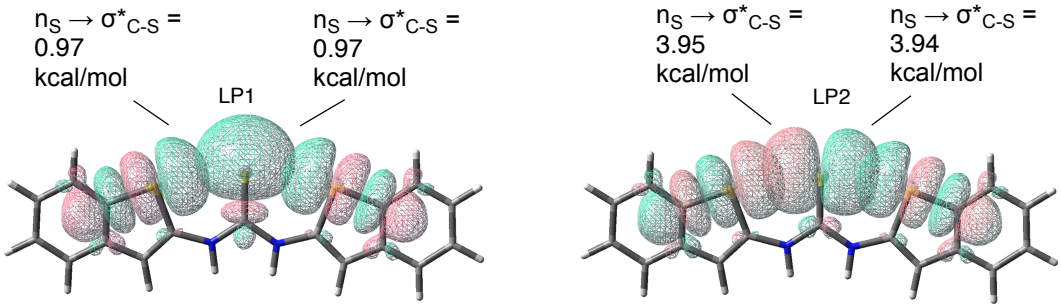
NBO analysis

The NBO analysis[2] of the intramolecular chalcogen-bonding interactions was performed at the *ω*B97XD/6-311G(d,p) level of theory[3] using the Gaussian 16 program[4] with SMD(DMSO) and with SMD(THF) conditions, based on their optimized structure at the *ω*B97XD/6-311G(d,p) level with the corresponding solvation conditions.

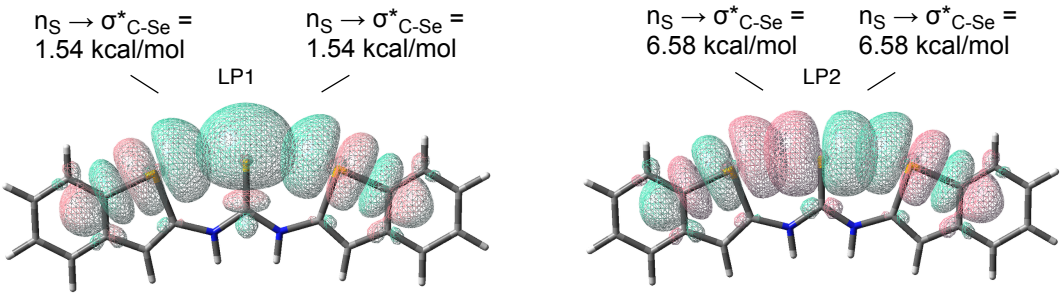
(1) NBO analysis for the optimized structure of **3a** with SMD(DMSO)



(2) NBO analysis for the optimized structure of **3a** with SMD(THF)



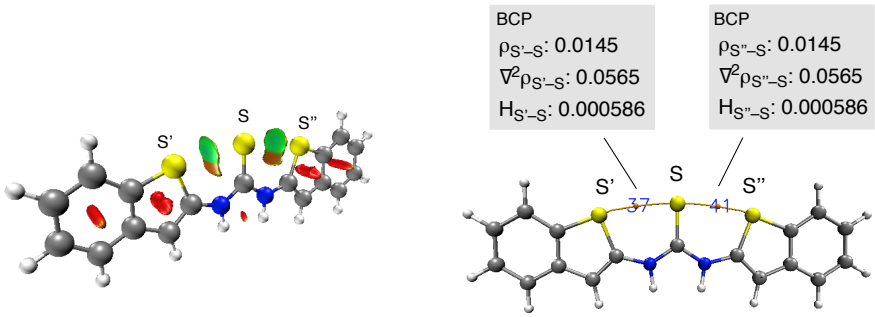
(3) NBO analysis for the optimized structure of **3b** with SMD(THF)



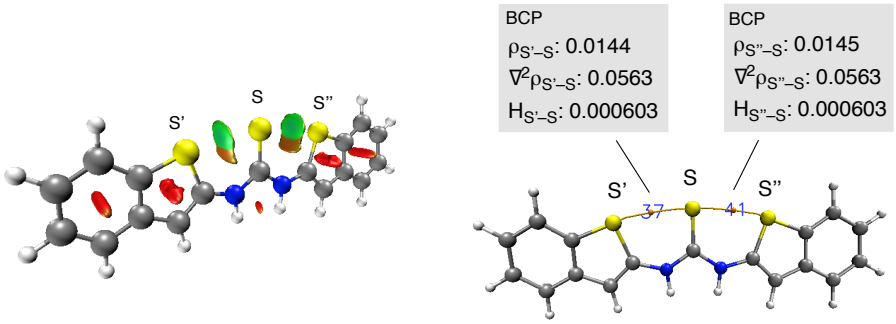
NCI plot index and QTAIM analyses

Non-covalent interaction (NCI) plot index analysis[5] and the quantum theory of atoms in molecules (QTAIM) analysis[6] were carried out with the X-ray crystal structure of **3a** and the optimized structures of **3a** and **3b** at the *ω*B97XD/6-311G(d,p) level of theory with SMD(DMSO) and SMD(THF) using the Gaussian 16 program. The cubic files for NCI plot index analysis were generated with Multiwfn program,[7] and the results were visualized with the VMD program.[8] QTAIM analyses were also carried out by using the Multiwfn program.

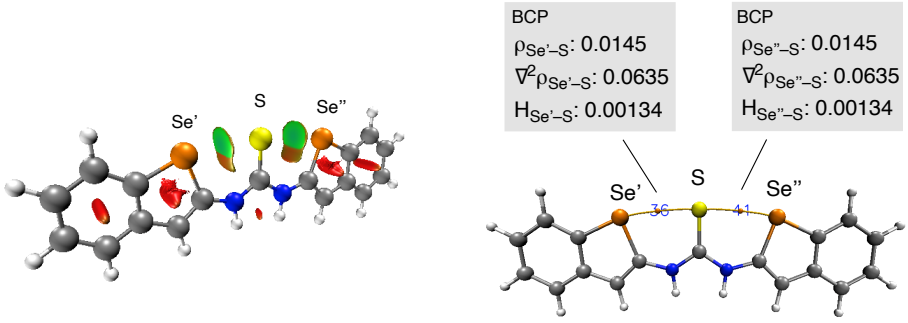
(1) The results of NCI and QTAIM analysis in the optimized structure of **3a** with SMD(DMSO) conditions.



(2) The results of NCI and QTAIM analysis in the optimized structure of **3a** with SMD(THF) conditions.

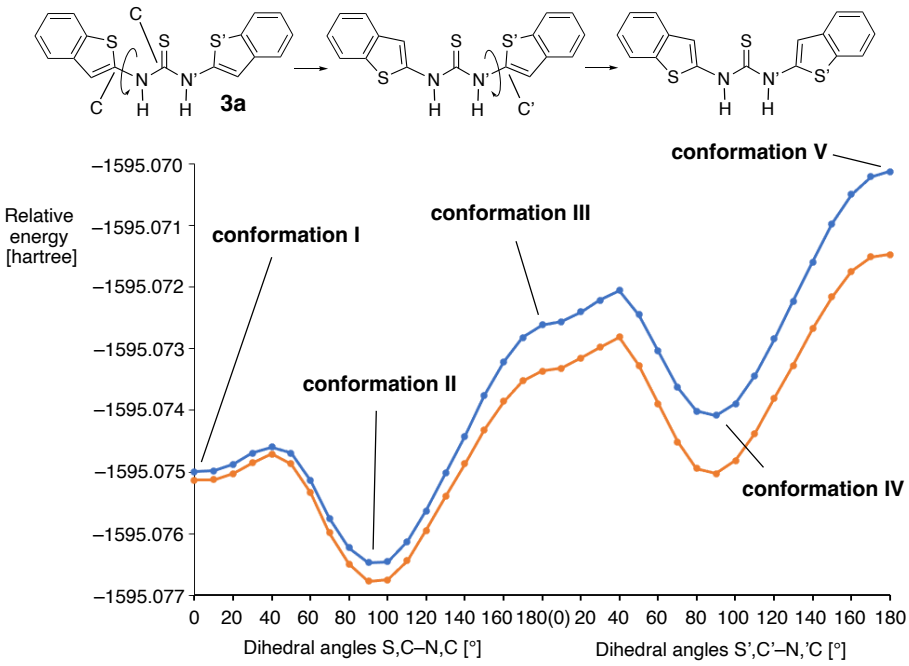


(3) The results of NCI and QTAIM analysis in the optimized structure of **3b** with SMD(THF) conditions.



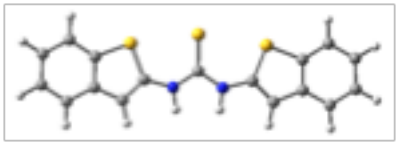
Conformational analysis of *trans-trans* 3a

Density functional theory (DFT) calculations were performed at *ω*B97XD/6-311G(d,p) with SMD(DMSO) or SMD(THF). All of the Gibbs free energy values reported in this paper were calculated for a temperature of 298.15 K. The relative energies of the conformations generated through the rotation of the C–N bond of **3a** were calculated. Subsequently, the relative energies of the conformations generated through the rotation of the C'–N' bond were determined after fixation of the bond rotation of the C–N bond at ϕ S,C–N,C = 180°. The conformation I, II, and IV were optimized at *ω*B97XD/6-311G(d,p) with the corresponding solvation conditions, and re-calculated their Gibbs free energies.



1) The energies and the coordinates of each conformation of *trans-trans* **3a** with SMD(DMSO) (blue line)

Conformation I



Calculation Method = R*ω*B97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –1959.075 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –1959.075 Hartree

Zero-point Energy Correction = 0.252054 Hartree

Thermal Correction to Energy = 0.270303 Hartree

Thermal Correction to Enthalpy = 0.271247 Hartree

Thermal Correction to Free Energy = 0.202181 Hartree

EE + Zero-point Energy = –1958.8229 Hartree

EE + Thermal Energy Correction = –1959.8047 Hartree

EE + Thermal Enthalpy Correction = –1958.8037 Hartree

EE + Thermal Free Energy Correction = –1959.8728 Hartree

E (Thermal) = 169.617 kcal/mol

Heat Capacity (Cv) = 71.423 cal/mol-kelvin

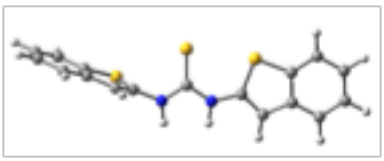
Entropy (S) = 145.362 cal/mol-kelvin

0 1

S	-3.10508300	-1.10211700	-0.02835700
S	3.10508400	-1.10211900	0.02823500
N	1.12388400	0.87766900	-0.04161100
N	-1.12388900	0.87767600	0.04136400
C	-4.76651700	0.92716400	0.03303200
C	0.00000400	0.11688700	0.00002100
C	-3.44685000	1.48437600	0.05947800
C	2.47358200	0.53696100	-0.02983700
C	4.76651300	0.92717500	-0.03295600
C	3.44684500	1.48438300	-0.05932400
C	4.74300400	-0.47661700	0.01817400
C	-5.91478200	-1.23202900	-0.05333900
C	-2.47358400	0.53696200	0.02988900

C	-4.74300800	-0.47661700	-0.01830900
C	-6.00606600	1.58511700	0.04873700
C	6.00606100	1.58512700	-0.04861600
C	-7.12609500	-0.56169900	-0.03699400
C	5.91478000	-1.23203400	0.05304700
C	-7.16946600	0.83974400	0.01425900
C	7.12609300	-0.56170200	0.03675100
C	7.16946300	0.83974800	-0.01429600
H	0.99283600	1.88232200	-0.08882300
H	-0.99283100	1.88232300	0.08868800
H	-3.23508100	2.54581000	0.09492800
H	3.23505100	2.54581200	-0.09478300
H	-5.88149400	-2.31518600	-0.09303600
H	-6.04185700	2.66846600	0.08763600
H	6.04185400	2.66848200	-0.08735900
H	-8.05030500	-1.12775200	-0.06374100
H	5.88149000	-2.31519600	0.09261100
H	-8.12999400	1.34284600	0.02622800
H	8.05030200	-1.12776100	0.06339000
H	8.12999100	1.34285100	-0.02623200
S	0.00001400	-1.55939600	0.00036700

Conformation II



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –1959.0765 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –1959.07565 Hartree

Zero-point Energy Correction = 0.252121 Hartree

Thermal Correction to Energy = 0.27033 Hartree

Thermal Correction to Enthalpy = 0.271275 Hartree

Thermal Correction to Free Energy = 0.202598 Hartree

EE + Zero-point Energy = –1958.8244 Hartree

EE + Thermal Energy Correction = –1958.8062 Hartree

EE + Thermal Enthalpy Correction = –1958.8052 Hartree

EE + Thermal Free Energy Correction = –1958.8739 Hartree

E (Thermal) = 169.635 kcal/mol

Heat Capacity (Cv) = 71.4 cal/mol-kelvin

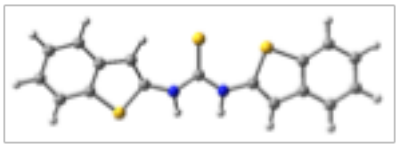
Entropy (S) = 144.543 cal/mol-kelvin

0 1

S	-2.96965000	-1.11252800	-0.12874700
S	3.28009400	0.72358100	-1.36989000
N	1.10184100	1.14699200	0.23935800
N	-1.15014600	0.99373200	0.19051700
C	-4.78679100	0.76087100	0.14250200
C	0.02638700	0.32671700	0.10513300
C	-3.51470400	1.41247100	0.24433800
C	2.43944100	0.72694600	0.17641400
C	4.55746200	0.02008100	0.79716300
C	3.22090800	0.35169000	1.20842100
C	4.74188800	0.17510500	-0.59036500
C	-5.76061000	-1.45887100	-0.18954400
C	-2.46976900	0.55407300	0.12090800
C	-4.65212000	-0.62232600	-0.06207200
C	-6.07434400	1.31382900	0.21958500
C	5.63408400	-0.41643400	1.58312300
C	-7.02122300	-0.89195600	-0.11000900
C	5.96863400	-0.09429200	-1.20004500
C	-7.17530300	0.48766200	0.09346100
C	7.01389400	-0.52355500	-0.40261800
C	6.84819500	-0.68415100	0.98174200
H	0.94610100	2.14095200	0.36490700

H	-1.09143500	1.99510900	0.34099300
H	-3.38735100	2.47604400	0.40385700
H	2.86529800	0.30070600	2.22934100
H	-5.64148800	-2.52512300	-0.34692000
H	-6.19572200	2.38007000	0.37737400
H	5.50361200	-0.54087400	2.65251400
H	-7.89789500	-1.52251300	-0.20581200
H	6.10038300	0.02793000	-2.26889200
H	-8.17268500	0.90916200	0.15262200
H	7.97488100	-0.73935500	-0.85582800
H	7.68431100	-1.02287000	1.58300100
S	0.16917900	-1.32927000	-0.13543100

Conformation III



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –1959.0726 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

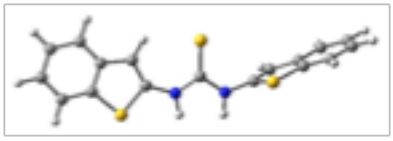
Pressure = 1 atm

00 1

S	3.12504700	-1.17376700	0.06270000
S	-3.58377700	1.79061500	0.13048300
N	-1.11343900	0.80127300	0.04258200
N	1.13279200	0.79286700	-0.06207800
C	4.77510200	0.86146400	-0.07316300
C	0.01181600	0.03012600	0.02486100
C	3.45235500	1.41077400	-0.10605000

C	-2.45666500	0.43601000	0.02423100
C	-4.51622000	-0.63253800	-0.06934500
C	-3.08221400	-0.76222000	-0.07318700
C	-4.94633200	0.70064300	0.03472600
C	5.93534500	-1.28831000	0.06960300
C	2.48418500	0.45965700	-0.04068100
C	4.75929800	-0.54022900	0.02027600
C	6.01111900	1.52488700	-0.11784100
C	-5.48140300	-1.64528700	-0.15700500
C	7.14296200	-0.61284500	0.02373400
C	-6.29547400	1.04639500	0.05377800
C	7.17857300	0.78670200	-0.06993700
C	-7.22933700	0.02711500	-0.03460200
C	-6.82327200	-1.31014900	-0.13934200
H	-0.95664800	1.80149600	0.07046400
H	0.99622300	1.79304300	-0.16053600
H	3.23450600	2.46946000	-0.17325000
H	-2.57161000	-1.70725200	-0.14743500
H	5.90797700	-2.36993400	0.14229900
H	6.04099800	2.60672700	-0.18963800
H	-5.16900900	-2.68064600	-0.23822600
H	8.07032100	-1.17318400	0.06021600
H	-6.60846700	2.08104500	0.13440100
H	8.13635800	1.29397400	-0.10456900
H	-8.28585600	0.26947100	-0.02251600
H	-7.57245600	-2.09096600	-0.20785000
S	0.02892900	-1.64218500	0.10386600

Conformation IV



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –1959.0741 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –1959.0741 Hartree

Zero-point Energy Correction = 0.252014 Hartree

Thermal Correction to Energy = 0.269431 Hartree

Thermal Correction to Enthalpy = 0.270375 Hartree

Thermal Correction to Free Energy = 0.204174 Hartree

EE + Zero-point Energy = –1958.8221 Hartree

EE + Thermal Energy Correction = –1958.8046 Hartree

EE + Thermal Enthalpy Correction = –1958.8052 Hartree

EE + Thermal Free Energy Correction = –1958.8699 Hartree

E (Thermal) = 169.071 kcal/mol

Heat Capacity (Cv) = 69.562 cal/mol-kelvin

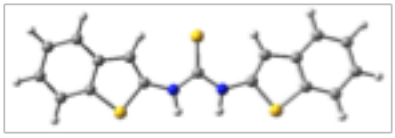
Entropy (S) = 149.333 cal/mol-kelvin

0 1

S	-3.31743300	-0.56003000	-1.43072300
S	3.67761600	-1.71957600	0.20657700
N	1.13490800	-0.92596500	0.08825000
N	-1.11658200	-1.08191500	0.11661500
C	-4.56910900	-0.01362900	0.79585000
C	-0.04429200	-0.24689600	0.04610100
C	-3.22608300	-0.36652600	1.16599300
C	2.44787300	-0.46144800	0.05656600
C	4.41808600	0.76348500	-0.04856800
C	2.97840500	0.77894600	-0.06868200
C	4.95090400	-0.52845700	0.09374800
C	-6.00673400	0.23241100	-1.17025900
C	-2.45675500	-0.66582000	0.10053900
C	-4.77114500	-0.07344900	-0.59662000
C	-5.63674500	0.36315600	1.62391500

C	5.30128900	1.84696000	-0.15220700
C	-7.04270500	0.60171700	-0.33177200
C	6.32294400	-0.76555800	0.13424100
C	-6.85944200	0.66689200	1.05815000
C	7.17444000	0.32205200	0.02978700
C	6.66522000	1.62001900	-0.11226100
H	1.04873900	-1.93229100	0.16045700
H	-0.95787900	-2.08130100	0.18199400
H	-2.85716400	-0.38389300	2.18331100
H	2.39292700	1.67658700	-0.17266300
H	-6.15220600	0.18417800	-2.24318200
H	-5.49256700	0.41371200	2.69757800
H	4.90905100	2.85207500	-0.26216800
H	-8.01012400	0.84484400	-0.75655300
H	6.71585600	-1.76983100	0.24419100
H	-7.68870400	0.95998500	1.69200300
H	8.24652600	0.16414600	0.05856900
H	7.35116400	2.45595700	-0.19174000
S	-0.20460800	1.41884800	-0.07416500

Conformation V



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –1959.0701 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

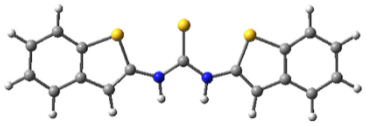
Pressure = 1 atm

0 1

S	-3.12504700	-1.17376700	-0.06270000
S	3.58377700	1.79061500	-0.13048300
N	1.11343900	0.80127300	-0.04258200
N	-1.13279200	0.79286700	0.06207800
C	-4.77510200	0.86146400	0.07316300
C	-0.01181600	0.03012600	-0.02486100
C	-3.45235500	1.41077400	0.10605000
C	2.45666500	0.43601000	-0.02423100
C	4.51622000	-0.63253800	0.06934500
C	3.08221400	-0.76222000	0.07318700
C	4.94633200	0.70064300	-0.03472600
C	-5.93534500	-1.28831000	-0.06960300
C	-2.48418500	0.45965700	0.04068100
C	-4.75929800	-0.54022900	-0.02027600
C	-6.01111900	1.52488700	0.11784100
C	5.48140300	-1.64528700	0.15700500
C	-7.14296200	-0.61284500	-0.02373400
C	6.29547400	1.04639500	-0.05377800
C	-7.17857300	0.78670200	0.06993700
C	7.22933700	0.02711500	0.03460200
C	6.82327200	-1.31014900	0.13934200
H	0.95664800	1.80149600	-0.07046400
H	-0.99622300	1.79304300	0.16053600
H	-3.23450600	2.46946000	0.17325000
H	2.57161000	-1.70725200	0.14743500
H	-5.90797700	-2.36993400	-0.14229900
H	-6.04099800	2.60672700	0.18963800
H	5.16900900	-2.68064600	0.23822600
H	-8.07032100	-1.17318400	-0.06021600
H	6.60846700	2.08104500	-0.13440100
H	-8.13635800	1.29397400	0.10456900
H	8.28585600	0.26947100	0.02251600
H	7.57245600	-2.09096600	0.20785000
S	-0.02892900	-1.64218500	-0.10386600

2) The energies and the coordinates of each conformation of *trans-trans* **3a** with SMD(THF) (orange line)

Conformation I



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = – 1959.0751 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = – 1959.0751 Hartree

Zero-point Energy Correction = 0.252136 Hartree

Thermal Correction to Energy = 0.270338 Hartree

Thermal Correction to Enthalpy = 0.271282 Hartree

Thermal Correction to Free Energy = 0.202871 Hartree

EE + Zero-point Energy = – 1958.823 Hartree

EE + Thermal Energy Correction = –1958.8048 Hartree

EE + Thermal Enthalpy Correction = –1958.8039 Hartree

EE + Thermal Free Energy Correction = –1958.8723 Hartree

E (Thermal) = 169.639 kcal/mol

Heat Capacity (Cv) = 71.45 cal/mol-kelvin

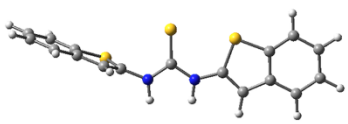
Entropy (S) = 143.982 cal/mol-kelvin

0 1

S	3.10266800	-1.09599900	0.09522500
S	-3.10265100	-1.09613200	-0.09346600

N	-1.12450500	0.88058000	0.04601200
N	1.12449900	0.88073800	-0.04331200
C	4.76840400	0.92415100	-0.07132600
C	0.00000100	0.11683000	0.00024600
C	3.44932700	1.48130700	-0.12160300
C	-2.47466800	0.53827900	0.04147300
C	-4.76842700	0.92418100	0.07086900
C	-3.44936600	1.48135400	0.12131700
C	-4.74129700	-0.47494800	-0.05047200
C	5.91143500	-1.23040300	0.11796000
C	2.47464800	0.53832300	-0.04059000
C	4.74130600	-0.47488200	0.05114300
C	6.00935100	1.57689400	-0.12467600
C	-6.00938800	1.57699800	0.12302500
C	7.12412300	-0.56531600	0.06421000
C	-5.91140900	-1.23047500	-0.11751900
C	7.17084000	0.83145000	-0.05669500
C	-7.12411100	-0.56532100	-0.06490600
C	-7.17085800	0.83153300	0.05496700
H	-0.99338900	1.88364000	0.10222900
H	0.99341500	1.88392000	-0.09746200
H	3.24205000	2.54075700	-0.20782800
H	-3.24214800	2.54085600	0.20702100
H	5.87514700	-2.31005400	0.21168900
H	6.04860800	2.65677700	-0.21841700
H	-6.04867200	2.65695300	0.21592400
H	8.04704700	-1.13163900	0.11601800
H	-5.87509800	-2.31019200	-0.21048800
H	8.13252500	1.33073400	-0.09720000
H	-8.04702100	-1.13166000	-0.11681500
H	-8.13255100	1.33087400	0.09457100
S	0.00002500	-1.55474000	-0.00192700

Conformation II



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –1959.0768 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –1959.0768 Hartree

Zero-point Energy Correction = 0.25211 Hartree

Thermal Correction to Energy = 0.270332 Hartree

Thermal Correction to Enthalpy = 0.271276 Hartree

Thermal Correction to Free Energy = 0.202679 Hartree

EE + Zero-point Energy = –1958.8247 Hartree

EE + Thermal Energy Correction = –1958.8065 Hartree

EE + Thermal Enthalpy Correction = –1958.8055 Hartree

EE + Thermal Free Energy Correction = –1958.8741 Hartree

E (Thermal) = 169.636 kcal/mol

Heat Capacity (Cv) = 71.463 cal/mol-kelvin

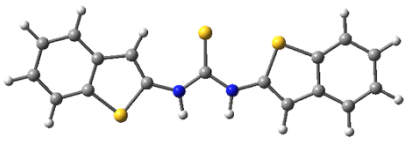
Entropy (S) = 144.374 cal/mol-kelvin

0 1

S	2.97038700	1.10977600	-0.13729400
S	-3.27961700	-0.73580200	-1.36484800
N	-1.10227800	-1.14277200	0.24983200
N	1.15070000	-0.99006300	0.20243400
C	4.78868900	-0.76112700	0.14816800
C	-0.02593100	-0.31865800	0.11533800
C	3.51640500	-1.41078900	0.25953800
C	-2.44080700	-0.72467800	0.18157700
C	-4.55897400	-0.01068200	0.79367300
C	-3.22237300	-0.33626800	1.20867700
C	-4.74260800	-0.18307000	-0.59172000
C	5.76057100	1.45467900	-0.20934400

C	2.47154600	-0.55283400	0.12970700
C	4.65251600	0.61961000	-0.07038000
C	6.07659800	-1.31238100	0.22759300
C	-5.63660700	0.43398000	1.57343800
C	7.02142500	0.88954600	-0.12759200
C	-5.96985500	0.07610400	-1.20451700
C	7.17675400	-0.48749900	0.08988800
C	-7.01616100	0.51267700	-0.41308400
C	-6.85099900	0.69136600	0.96890700
H	-0.94626000	-2.13619400	0.37003300
H	1.08936400	-1.99018300	0.35332700
H	3.39043800	-2.47301800	0.42915200
H	-2.86493100	-0.26905600	2.22793800
H	5.64041800	2.51907300	-0.37754200
H	6.19993600	-2.37677900	0.39614700
H	-5.50686400	0.57404900	2.64096900
H	7.89747800	1.51940800	-0.23274200
H	-6.10056200	-0.05865000	-2.27194600
H	8.17443300	-0.90796200	0.15070800
H	-7.97737600	0.72117700	-0.86914800
H	-7.68757300	1.03688400	1.56556400
S	-0.16880700	1.33172800	-0.12457900

Conformation III



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –1959.0734 Hartree

Imaginary Freq = 0

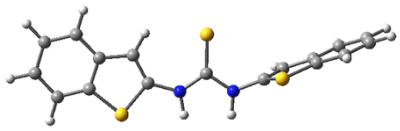
Temperature = 298.15 Kelvin

Pressure = 1 atm

0 1

S	3.12469400	-1.17206900	0.05735900
S	-3.58558100	1.79085400	0.12673800
N	-1.11417500	0.80145100	0.04254600
N	1.13359900	0.79432700	-0.05959900
C	4.77721200	0.86188500	-0.07111000
C	0.01166700	0.02850000	0.02729900
C	3.45463700	1.41191800	-0.10125500
C	-2.45848300	0.43616900	0.02456500
C	-4.51697200	-0.63272200	-0.06737300
C	-3.08284400	-0.76197600	-0.06980000
C	-4.94805100	0.70024300	0.03233200
C	5.93414300	-1.28923600	0.06400400
C	2.48577100	0.46110200	-0.03897400
C	4.75903800	-0.53981800	0.01688000
C	6.01406200	1.52341800	-0.11316700
C	-5.48164500	-1.64576800	-0.15246100
C	7.14256300	-0.61578200	0.02094200
C	-6.29711700	1.04520600	0.04903700
C	7.18030200	0.78376500	-0.06759600
C	-7.23036800	0.02543900	-0.03696000
C	-6.82351100	-1.31158000	-0.13699500
H	-0.95946500	1.80101900	0.07209600
H	0.99736900	1.79324900	-0.15915400
H	3.24135400	2.47185700	-0.16373000
H	-2.56984200	-1.70595000	-0.13944400
H	5.90472300	-2.37097900	0.13292200
H	6.04641500	2.60548900	-0.18083100
H	-5.16868500	-2.68117400	-0.22992600
H	8.06908000	-1.17753800	0.05577100
H	-6.61068900	2.07990500	0.12626900
H	8.13876400	1.28980500	-0.10005200
H	-8.28702300	0.26716800	-0.02655500
H	-7.57207600	-2.09309500	-0.20343100
S	0.03036800	-1.63970800	0.10710500

Conformation IV



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –1959.075 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –1959.075 Hartree

Zero-point Energy Correction = 0.252161 Hartree

Thermal Correction to Energy = 0.269542 Hartree

Thermal Correction to Enthalpy = 0.270486 Hartree

Thermal Correction to Free Energy = 0.20461 Hartree

EE + Zero-point Energy = –1958.8229 Hartree

EE + Thermal Energy Correction = –1958.8055 Hartree

EE + Thermal Enthalpy Correction = –1958.8045 Hartree

EE + Thermal Free Energy Correction = –1958.8704 Hartree

E (Thermal) = 169.14 kcal/mol

Heat Capacity (Cv) = 69.517 cal/mol-kelvin

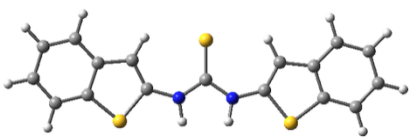
Entropy (S) = 138.648 cal/mol-kelvin

0 1

S	-3.31660400	-0.56504100	-1.42517500
S	3.67654600	-1.71936200	0.20766400
N	1.13524400	-0.91873900	0.09110500
N	-1.11672100	-1.07317700	0.13009700
C	-4.57342700	-0.00901900	0.79594700

C	-0.04325700	-0.23535000	0.04913400
C	-3.22981000	-0.35464800	1.16974000
C	2.45029800	-0.45803300	0.05691600
C	4.42261200	0.76154300	-0.05004500
C	2.98284100	0.78041300	-0.06973300
C	4.95288200	-0.53117600	0.09326000
C	-6.00879000	0.21816200	-1.17334800
C	-2.45829000	-0.66026400	0.10754100
C	-4.77292500	-0.07930800	-0.59619300
C	-5.64378100	0.36960000	1.61941500
C	5.30833700	1.84251200	-0.15464900
C	-7.04742300	0.58892500	-0.33937000
C	6.32412300	-0.77107600	0.13352500
C	-6.86665700	0.66436000	1.05013600
C	7.17801600	0.31431800	0.02795000
C	6.67158600	1.61289500	-0.11498900
H	1.04808600	-1.92387700	0.16756500
H	-0.95709300	-2.07132800	0.19460700
H	-2.86024800	-0.35985500	2.18687900
H	2.39718900	1.67790200	-0.17377700
H	-6.15190000	0.16322000	-2.24621900
H	-5.50165500	0.42988900	2.69283300
H	4.91837500	2.84836800	-0.26525800
H	-8.01493600	0.82593100	-0.76731500
H	6.71496900	-1.77602200	0.24442800
H	-7.69773300	0.95932900	1.68067000
H	8.24974900	0.15418800	0.05662100
H	7.35914700	2.44737200	-0.19531700
S	-0.20441900	1.42472800	-0.07971200

Conformation V



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2S_3$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –1959.0715 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

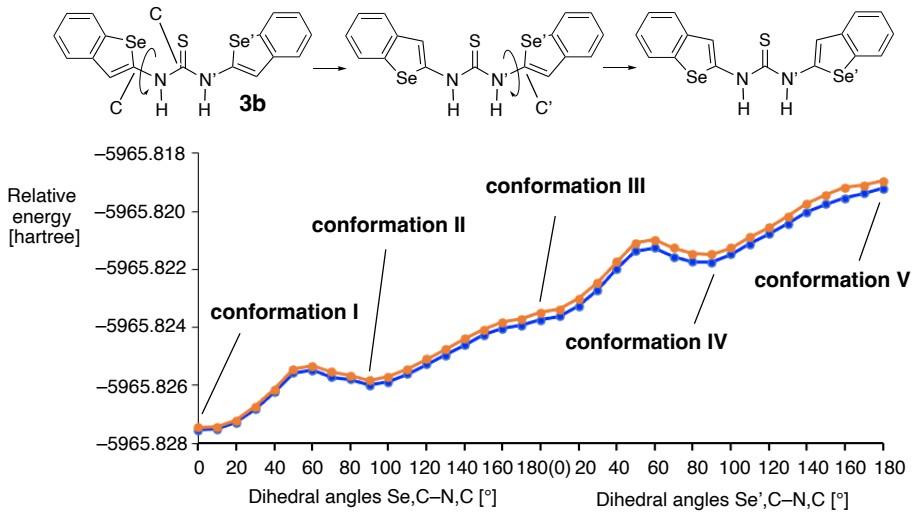
0 1

S	-3.58523700	1.71986100	0.12090500
S	3.58703700	1.71872700	-0.14434300
N	1.12363200	0.71214900	-0.04099300
N	-1.12316800	0.70738500	0.07073200
C	-4.53925800	-0.69756300	-0.03092400
C	0.00019500	-0.06667700	-0.01412100
C	-3.10643300	-0.84062900	-0.03059800
C	2.47029700	0.35625900	-0.02497100
C	4.53799900	-0.69563900	0.06632500
C	3.10503100	-0.83601100	0.07723900
C	4.95840900	0.63953900	-0.04765400
C	-6.30380800	0.99780300	0.06615100
C	-2.47013500	0.35284800	0.04531100
C	-4.95788600	0.64053400	0.05026100
C	-5.51322000	-1.70305600	-0.09837100
C	5.51057900	-1.70086000	0.15429200
C	-7.24640700	-0.01466900	-0.00217200
C	6.30481600	0.99417700	-0.07505300
C	-6.85197100	-1.35666300	-0.08391100
C	7.24609200	-0.01795800	0.01415300
C	6.84983300	-1.35706800	0.12788500
H	0.96369900	1.71011100	-0.09038300
H	-0.96342300	1.70094100	0.17740500
H	-2.60216900	-1.79016100	-0.08198900
H	2.60020600	-1.78332700	0.15717700
H	-6.60794200	2.03624600	0.12929700
H	-5.20973300	-2.74224500	-0.16166100

H	5.20571300	-2.73785300	0.24230600
H	-8.30081100	0.23671300	0.00777900
H	6.61038700	2.03040400	-0.16294200
H	-7.60778000	-2.13223200	-0.13673700
H	8.30084300	0.23145600	-0.00457800
H	7.60454500	-2.13248700	0.19628100
S	0.00060100	-1.73424500	-0.07926000

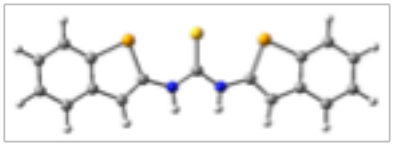
Conformation analysis of *trans-trans* 3b

Density functional theory (DFT) calculations were performed using the Gaussian 16 software package at ωB97XD/6-311G(d,p) with SMD(DMSO) or SMD(THF). All of the Gibbs free energy values reported in this paper were calculated for a temperature of 298.15 K. The relative energies of the conformations generated through the rotation of the C–N bond of **3b** were calculated. Subsequently, the relative energies of the conformations generated through the rotation of the C'–N' bond were determined after fixation of the bond rotation of the C–N bond at ϕ Se,C–N,C = 180°. The conformation I, II, and IV were optimized at ωB97XD/6-311G(d,p) with the corresponding solvation conditions, and re-calculated their Gibbs free energies.



1) The energies and the coordinates of each conformation of *trans-trans* **3b** with SMD(DMSO) (blue line)

Conformation I



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –5965.8275 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –5965.8275 Hartree

Zero-point Energy Correction = 0.249893 Hartree

Thermal Correction to Energy = 0.268863 Hartree

Thermal Correction to Enthalpy = 0.269807 Hartree

Thermal Correction to Free Energy = 0.199022 Hartree

EE + Zero-point Energy = –5965.5776 Hartree

EE + Thermal Energy Correction = –5965.5587 Hartree

EE + Thermal Enthalpy Correction = –5965.5577 Hartree

EE + Thermal Free Energy Correction = –5965.6285 Hartree

E (Thermal) = 168.714 kcal/mol

Heat Capacity (Cv) = 73.038 cal/mol-kelvin

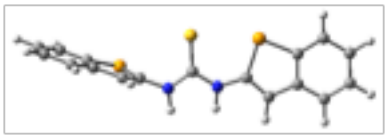
Entropy (S) = 148.979 cal/mol-kelvin

0 1

N	-1.12598700	1.08052100	0.03580000
N	1.12598500	1.08049700	-0.03595200
C	4.79029300	1.13843100	-0.03748900
C	-0.00000600	0.32691800	0.00000900
C	3.44967000	1.65656900	-0.06079100
C	-2.47045600	0.71979900	0.02916800
C	-4.79029700	1.13843000	0.03750700
C	-3.44967800	1.65658100	0.06080500
C	-4.86152600	-0.26376200	-0.01503000
C	6.08367600	-0.93232400	0.04558300
C	2.47045500	0.71977800	-0.02919600
C	4.86153400	-0.26376400	0.01497000
C	5.98410700	1.87611400	-0.05825400
C	-5.98411600	1.87610100	0.05834300
C	7.25047000	-0.18471500	0.02450500
C	-6.08366200	-0.93233300	-0.04563000
C	7.19833800	1.21456300	-0.02764700

C	-7.25046300	-0.18473500	-0.02449200
C	-7.19834200	1.21454100	0.02772700
H	-1.00011500	2.08670000	0.07460900
H	1.00012300	2.08667700	-0.07478100
H	3.23364500	2.71858000	-0.09622800
H	-3.23366300	2.71859400	0.09624100
H	6.12215400	-2.01526900	0.08596500
H	5.94565500	2.95965000	-0.09789600
H	-5.94567200	2.95963600	0.09804200
H	8.21043900	-0.68824700	0.04858600
H	-6.12213100	-2.01527700	-0.08605400
H	8.12105600	1.78408500	-0.04328100
H	-8.21042800	-0.68827400	-0.04857500
H	-8.12106500	1.78405400	0.04340900
S	-0.00002900	-1.35422300	0.00019400
Se	3.14103700	-1.05600400	0.03336600
Se	-3.14102200	-1.05598500	-0.03344300

Conformation II



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = – 5965.826 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –5965.826 Hartree

Zero-point Energy Correction = 0.249623 Hartree

Thermal Correction to Energy = 0.268712 Hartree

Thermal Correction to Enthalpy = 0.269656 Hartree

Thermal Correction to Free Energy = 0.198054 Hartree

EE + Zero-point Energy = –5965.5763 Hartree

EE + Thermal Energy Correction = –5965.5572 Hartree

EE + Thermal Enthalpy Correction = –5965.5563 Hartree

EE + Thermal Free Energy Correction = –5965.6279 Hartree

E (Thermal) = 168.619 kcal/mol

Heat Capacity (Cv) = 73.213 cal/mol-kelvin

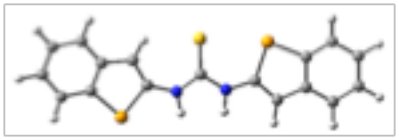
Entropy (S) = 150.701 cal/mol-kelvin

0 1

N	1.09819200	1.07346500	0.59164600
N	-1.15936900	1.01333800	0.47096500
C	-4.82259700	0.89124200	0.36320900
C	0.00074900	0.33789000	0.28944000
C	-3.51397400	1.44761500	0.57685300
C	2.42646100	0.63767900	0.44354200
C	4.55206700	-0.17736200	1.02382500
C	3.20198900	0.13559600	1.42146800
C	4.83677600	0.10604500	-0.32548900
C	-5.99317700	-1.13273200	-0.34466500
C	-2.48217100	0.61022300	0.31177300
C	-4.81186100	-0.43917600	-0.08874100
C	-6.05708700	1.52963800	0.55843600
C	5.56296700	-0.71730100	1.83193800
C	-7.20158500	-0.48378500	-0.14496800
C	6.09648500	-0.14149900	-0.87036200
C	-7.23078900	0.84302700	0.30450300
C	7.07798500	-0.67522100	-0.05211000
C	6.81255800	-0.96184800	1.29371600
H	0.97624100	2.03612000	0.88479700
H	-1.08129300	1.97115900	0.79620600
H	-3.35926400	2.46308200	0.92450100
H	2.83185200	-0.02317000	2.42752800
H	-5.96892500	-2.15965800	-0.69229000
H	-6.08211900	2.55682300	0.90687400

H	5.35525400	-0.93906400	2.87324800
H	-8.13070100	-1.00812500	-0.33892600
H	6.30333200	0.07898800	-1.91117000
H	-8.18502000	1.33585100	0.45515000
H	8.06315200	-0.87308500	-0.45959600
H	7.59546200	-1.37955200	1.91663300
S	0.09253700	-1.25499300	-0.24708000
Se	-3.04739600	-1.10321100	-0.28114200
Se	3.33859900	0.82534900	-1.21362700

Conformation III



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –5965.8237 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

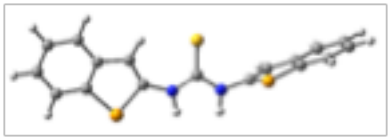
Pressure = 1 atm

0 1

N	-1.10641000	0.74422700	-0.00860600
N	1.14571900	0.83822100	-0.06394100
C	4.80728900	1.03540300	-0.06415200
C	0.05366800	0.03182300	-0.01215300
C	3.44814700	1.50323900	-0.09659100
C	-2.43372800	0.32106300	-0.01057300
C	-4.43721900	-0.91157000	-0.05854900
C	-2.99340300	-0.90965400	-0.06821200
C	-5.03237800	0.35941300	0.00871100

C	6.17561500	-0.98508000	0.05658400
C	2.50328300	0.53195000	-0.04641500
C	4.92994500	-0.36208300	0.01463100
C	5.97358500	1.81559800	-0.10015200
C	-5.26982400	-2.03843400	-0.11094200
C	7.31450500	-0.19618600	0.02001000
C	-6.41419400	0.52631000	0.02383000
C	7.21107600	1.19916400	-0.05834100
C	-7.21634100	-0.60333500	-0.02915800
C	-6.64467400	-1.87939200	-0.09606800
H	-1.00307600	1.75130700	-0.02100100
H	0.97847900	1.83809400	-0.12059000
H	3.19352000	2.55575400	-0.15392500
H	-2.42128400	-1.82160600	-0.12019600
H	6.25327100	-2.06505500	0.11743100
H	5.89628000	2.89612000	-0.16033000
H	-4.82881400	-3.02818100	-0.16314300
H	8.29240200	-0.66355500	0.05248200
H	-6.85352100	1.51584500	0.07579200
H	8.11262900	1.80126500	-0.08560800
H	-8.29500500	-0.49440200	-0.01855300
H	-7.28698300	-2.75206900	-0.13649200
S	0.15069800	-1.64255600	0.04953800
Se	3.24008600	-1.21640700	0.05185900
Se	-3.72762600	1.71760900	0.07210000

Conformation IV



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –5965.8218 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –5965.8218 Hartree

Zero-point Energy Correction = 0.250118 Hartree

Thermal Correction to Energy = 0.269149 Hartree

Thermal Correction to Enthalpy = 0.270094 Hartree

Thermal Correction to Free Energy = 0.197356 Hartree

EE + Zero-point Energy = –5965.5716 Hartree

EE + Thermal Energy Correction = –5965.5526 Hartree

EE + Thermal Enthalpy Correction = –5965.5517 Hartree

EE + Thermal Free Energy Correction = –5965.6244 Hartree

E (Thermal) = 168.894 kcal/mol

Heat Capacity (Cv) = 73.01 cal/mol-kelvin

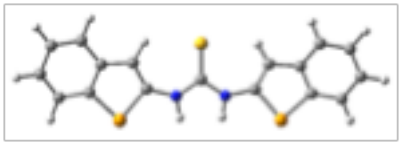
Entropy (S) = 153.089 cal/mol-kelvin

0 1

N	1.12008100	-0.71459200	0.19783500
N	-1.12559800	-0.89728500	0.29746200
C	-4.62666600	0.04987700	1.02229200
C	-0.06793000	-0.05018200	0.18803300
C	-3.25623600	-0.27414000	1.33094900
C	2.43079700	-0.24908200	0.12323200
C	4.38177600	1.05394200	-0.05961100
C	2.93943200	0.99533400	-0.02815300
C	5.03004200	-0.18615000	0.07013500
C	-6.20467300	0.34398700	-0.82070200
C	-2.47646900	-0.51406700	0.26138400
C	-4.92386100	0.05010600	-0.35396100
C	-5.64584200	0.35121700	1.93718800
C	5.16618600	2.20693900	-0.20417400
C	-7.19406500	0.63876900	0.10235800
C	6.41747200	-0.29712400	0.05895600

C	-6.91602300	0.64230500	1.47588400
C	7.17132100	0.85782200	-0.08516000
C	6.54644400	2.10349900	-0.21609000
H	1.04761000	-1.72018800	0.29080100
H	-0.94744800	-1.89525800	0.31446800
H	-2.87464000	-0.31691800	2.34429600
H	2.32581800	1.87711300	-0.11883500
H	-6.42167300	0.34216400	-1.88261700
H	-5.42811900	0.35408600	2.99987000
H	4.68374600	3.17330900	-0.30567100
H	-8.19541300	0.86965500	-0.24371400
H	6.89875400	-1.26300100	0.16068000
H	-7.70551700	0.87614600	2.18118000
H	8.25352300	0.79254400	-0.09596100
H	7.15110600	2.99668100	-0.32765400
S	-0.25440700	1.61515400	0.06787300
Se	-3.41016700	-0.38191200	-1.38963300
Se	3.78343700	-1.58820400	0.25183100

Conformation V



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(DMSO)

E(RωB97XD) = –5965.8192 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

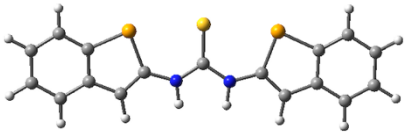
0 1

N	1.12151100	0.43856400	-0.04957900

N	-1.12145200	0.43503600	0.09111700
C	-4.54333600	-1.00862400	-0.10137100
C	0.00029200	-0.33854300	0.00693300
C	-3.10228600	-1.09305800	-0.09002900
C	2.47070800	0.09783900	-0.02474900
C	4.54373500	-1.00674900	0.11533400
C	3.10260900	-1.08983800	0.12185500
C	5.06429000	0.28892400	-0.04316400
C	-6.43461000	0.53529200	0.04427100
C	-2.47075400	0.09562700	0.05060700
C	-5.06455600	0.28903000	0.03718600
C	-5.43881500	-2.07903800	-0.23579700
C	5.43987100	-2.07630200	0.25224300
C	-7.29993200	-0.53986700	-0.09077700
C	6.43437100	0.53403200	-0.06700400
C	-6.80222700	-1.84078400	-0.23007000
C	7.30036500	-0.54023700	0.07082200
C	6.80330100	-1.83916100	0.22962300
H	0.95537300	1.43543900	-0.11175100
H	-0.95529400	1.42896600	0.18897400
H	-2.58346200	-2.03263900	-0.18696900
H	2.58443500	-2.02771900	0.23749100
H	-6.81745600	1.54362600	0.15204900
H	-5.05467400	-3.08782900	-0.34391000
H	5.05622000	-3.08354200	0.37550300
H	-8.37048600	-0.36834600	-0.08839500
H	6.81675300	1.54084100	-0.18967100
H	-7.49318200	-2.66992200	-0.33469600
H	8.37094700	-0.36956700	0.05544800
H	7.49477900	-2.66761900	0.33617000
S	0.00116400	-2.01258500	-0.02674800
Se	-3.68290100	1.56105300	0.20035600
Se	3.68169100	1.55992400	-0.20707700

2) The energies and the coordinates of each conformation of *trans-trans* **3b** with SMD(THF) (orange line)

Conformation I



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –5965.8274 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –5965.8274 Hartree

Zero-point Energy Correction = 0.249987 Hartree

Thermal Correction to Energy = 0.26897 Hartree

Thermal Correction to Enthalpy = 0.269915 Hartree

Thermal Correction to Free Energy = 0.198912 Hartree

EE + Zero-point Energy = –5965.5775 Hartree

EE + Thermal Energy Correction = –5965.5585 Hartree

EE + Thermal Enthalpy Correction = –5965.5575 Hartree

EE + Thermal Free Energy Correction = –5965.6285 Hartree

E (Thermal) = 168.781 kcal/mol

Heat Capacity (Cv) = 73.064 cal/mol-kelvin

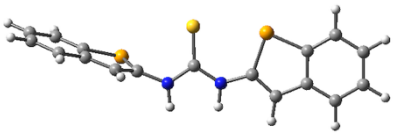
Entropy (S) = 149.437 cal/mol-kelvin

0 1

N	-1.12643100	1.08324900	0.04180100
N	1.12642100	1.08326000	-0.04030600

C	4.79246700	1.13679400	-0.04860200
C	-0.00001700	0.32690000	0.00031200
C	3.45262500	1.65685500	-0.07786000
C	-2.47163600	0.72229500	0.03620800
C	-4.79248600	1.13679700	0.04835000
C	-3.45266100	1.65688900	0.07796100
C	-4.85953900	-0.26470700	-0.01912300
C	6.08011900	-0.93565700	0.05773000
C	2.47162200	0.72225800	-0.03563900
C	4.85956000	-0.26470300	0.01901400
C	5.98821600	1.87069300	-0.07598600
C	-5.98825700	1.87067800	0.07524900
C	7.24869300	-0.19182100	0.03010700
C	-6.08007200	-0.93568400	-0.05823900
C	7.20047200	1.20668500	-0.03683700
C	-7.24866700	-0.19186600	-0.03108500
C	-7.20048900	1.20664800	0.03574900
H	-0.99976100	2.08812200	0.08445400
H	0.99979900	2.08819800	-0.08156100
H	3.24209200	2.71960100	-0.12380400
H	-3.24220200	2.71965300	0.12383300
H	6.11655300	-2.01820200	0.10978300
H	5.95375100	2.95392300	-0.12697700
H	-5.95382900	2.95391500	0.12613900
H	8.20721600	-0.69762600	0.06085800
H	-6.11646600	-2.01823400	-0.11020700
H	8.12470800	1.77350800	-0.05720300
H	-8.20717200	-0.69768800	-0.06211700
H	-8.12473900	1.77345900	0.05575000
S	-0.00006100	-1.34985300	-0.00054000
Se	3.13779300	-1.05267200	0.04396800
Se	-3.13775200	-1.05264800	-0.04351600

Conformation II



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –5965.8258 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –5965.8258 Hartree

Zero-point Energy Correction = 0.249708 Hartree

Thermal Correction to Energy = 0.268777 Hartree

Thermal Correction to Enthalpy = 0.269721 Hartree

Thermal Correction to Free Energy = 0.198485 Hartree

EE + Zero-point Energy = –5965.5761 Hartree

EE + Thermal Energy Correction = –5965.557 Hartree

EE + Thermal Enthalpy Correction = –5965.5561 Hartree

EE + Thermal Free Energy Correction = –5965.6273 Hartree

E (Thermal) = 168.66 kcal/mol

Heat Capacity (Cv) = 73.223 cal/mol-kelvin

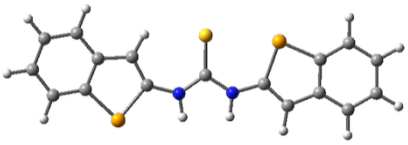
Entropy (S) = 149.929 cal/mol-kelvin

0 1

N	1.09897100	1.03669600	0.65675600
N	-1.15889800	0.98790300	0.51692600
C	-4.82292600	0.88056200	0.38419100
C	0.00074800	0.31343800	0.31515300
C	-3.51426400	1.42679100	0.62170800
C	2.42828100	0.61342100	0.48113400
C	4.55679300	-0.23164300	1.00553900
C	3.20800000	0.05579800	1.42494500
C	4.83614900	0.12990400	-0.32589100
C	-5.99230900	-1.11849000	-0.39053300
C	-2.48283300	0.59527700	0.33676900

C	-4.81107900	-0.43565400	-0.10696600
C	-6.05740300	1.51483000	0.59088500
C	5.57095300	-0.81745900	1.77646900
C	-7.20059900	-0.47401600	-0.17875100
C	6.09397400	-0.08457900	-0.88846000
C	-7.23052900	0.83851800	0.31004600
C	7.07867200	-0.66407300	-0.10661800
C	6.81853400	-1.02911000	1.22085900
H	0.97449100	1.98237800	0.99696900
H	-1.07909100	1.93464500	0.86972100
H	-3.36231000	2.43078200	1.00235500
H	2.83941700	-0.16594800	2.41950800
H	-5.96859000	-2.13462000	-0.76865600
H	-6.08376300	2.53134900	0.96939800
H	5.36706800	-1.10174300	2.80324200
H	-8.12929400	-0.99073400	-0.39379100
H	6.29743400	0.19434400	-1.91581900
H	-8.18482800	1.32831400	0.46962700
H	8.06212900	-0.83770400	-0.52891500
H	7.60352900	-1.48325500	1.81486800
S	0.09298200	-1.25103300	-0.28434500
Se	-3.04691800	-1.09655500	-0.31068700
Se	3.33264200	0.89289100	-1.16659600

Conformation III



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –5965.8237 Hartree

Imaginary Freq = 0

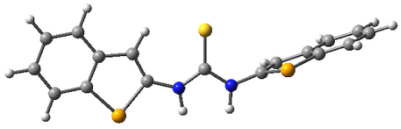
Temperature = 298.15 Kelvin

Pressure = 1 atm

0 1

N	-1.10611700	0.74487300	-0.01270200
N	1.14710200	0.83892200	-0.07555700
C	4.81000700	1.03499900	-0.06833200
C	0.05458800	0.02998800	-0.02087400
C	3.45119500	1.50317500	-0.10790000
C	-2.43440500	0.32073300	-0.01186300
C	-4.43816600	-0.91094100	-0.05843500
C	-2.99414900	-0.90876200	-0.07060600
C	-5.03451000	0.35890100	0.01218400
C	6.17461100	-0.98598100	0.06887700
C	2.50544000	0.53289500	-0.05522900
C	4.92983400	-0.36196300	0.01878300
C	5.97748700	1.81298500	-0.10440400
C	-5.27068900	-2.03731400	-0.11241800
C	7.31457500	-0.19937900	0.03218300
C	-6.41578500	0.52608100	0.02901800
C	7.21370300	1.19538000	-0.05435500
C	-7.21744000	-0.60355600	-0.02609900
C	-6.64533300	-1.87877000	-0.09624100
H	-1.00383400	1.75150300	-0.02829500
H	0.97939100	1.83735900	-0.13383600
H	3.20092900	2.55649200	-0.17148900
H	-2.42047400	-1.81946500	-0.12487500
H	6.25142100	-2.06565000	0.13640200
H	5.90297300	2.89336300	-0.17088100
H	-4.82958500	-3.02676700	-0.16701900
H	8.29157300	-0.66801400	0.07126000
H	-6.85638000	1.51489500	0.08355600
H	8.11627100	1.79590100	-0.08152500
H	-8.29607300	-0.49510100	-0.01452800
H	-7.28721900	-2.75161300	-0.13814700
S	0.15151800	-1.64030800	0.04001200
Se	3.23935300	-1.21413800	0.05438500
Se	-3.72894000	1.71603900	0.07712200

Conformation IV



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –5965.8215 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

Electronic Energy (EE) = –5965.8215 Hartree

Zero-point Energy Correction = 0.250122 Hartree

Thermal Correction to Energy = 0.269155 Hartree

Thermal Correction to Enthalpy = 0.270099 Hartree

Thermal Correction to Free Energy = 0.197923 Hartree

EE + Zero-point Energy = –5965.5714 Hartree

EE + Thermal Energy Correction = –5965.5523 Hartree

EE + Thermal Enthalpy Correction = –5965.5514 Hartree

EE + Thermal Free Energy Correction = –5965.6236 Hartree

E (Thermal) = 168.897 kcal/mol

Heat Capacity (Cv) = 73.07 cal/mol-kelvin

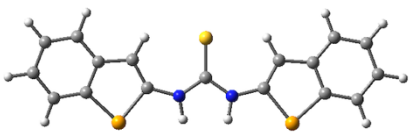
Entropy (S) = 151.908 cal/mol-kelvin

0 1

N	1.12203600	-0.72191600	0.15168900
N	-1.12557400	-0.89810700	0.25722800
C	-4.62377200	0.01418200	1.03783900
C	-0.06478300	-0.05114100	0.14371600
C	-3.24939200	-0.31202500	1.32408400

C	2.43433900	-0.25524700	0.09744300
C	4.38675400	1.05127800	-0.03088600
C	2.94413500	0.99125100	-0.02046100
C	5.03499500	-0.19011600	0.08047100
C	-6.21677800	0.36609500	-0.78133700
C	-2.47637300	-0.51132600	0.24112300
C	-4.93144900	0.06059800	-0.33509700
C	-5.63736200	0.27859600	1.96987200
C	5.17218100	2.20729100	-0.13699300
C	-7.20037100	0.62314800	0.15858600
C	6.42197600	-0.30036100	0.08856800
C	-6.91217500	0.57926300	1.52902400
C	7.17654700	0.85796800	-0.01761100
C	6.55231000	2.10530200	-0.12971200
H	1.04770200	-1.72696200	0.24183700
H	-0.95059000	-1.89504600	0.29198700
H	-2.85794800	-0.38474600	2.33190300
H	2.32954400	1.87338400	-0.09852700
H	-6.44235300	0.40276600	-1.84082400
H	-5.41183800	0.24705800	3.03045100
H	4.69032400	3.17526100	-0.22344700
H	-8.20506600	0.86237800	-0.17166000
H	6.90381100	-1.26733200	0.17589300
H	-7.69705100	0.78483800	2.24806700
H	8.25880300	0.79386000	-0.01292200
H	7.15745200	3.00134400	-0.21090700
S	-0.24968400	1.60889000	0.01883600
Se	-3.42350300	-0.32657700	-1.39582400
Se	3.78621600	-1.59570000	0.21237000

Conformation V



Calculation Method = RωB97XD

Formula = $C_{17}H_{12}N_2SSe_2$

Basis Set = 6-311G(d,p)

Charge = 0

Spin = Singlet

Solvation = SMD(THF)

E(RωB97XD) = –5965.8192 Hartree

Imaginary Freq = 0

Temperature = 298.15 Kelvin

Pressure = 1 atm

0 1

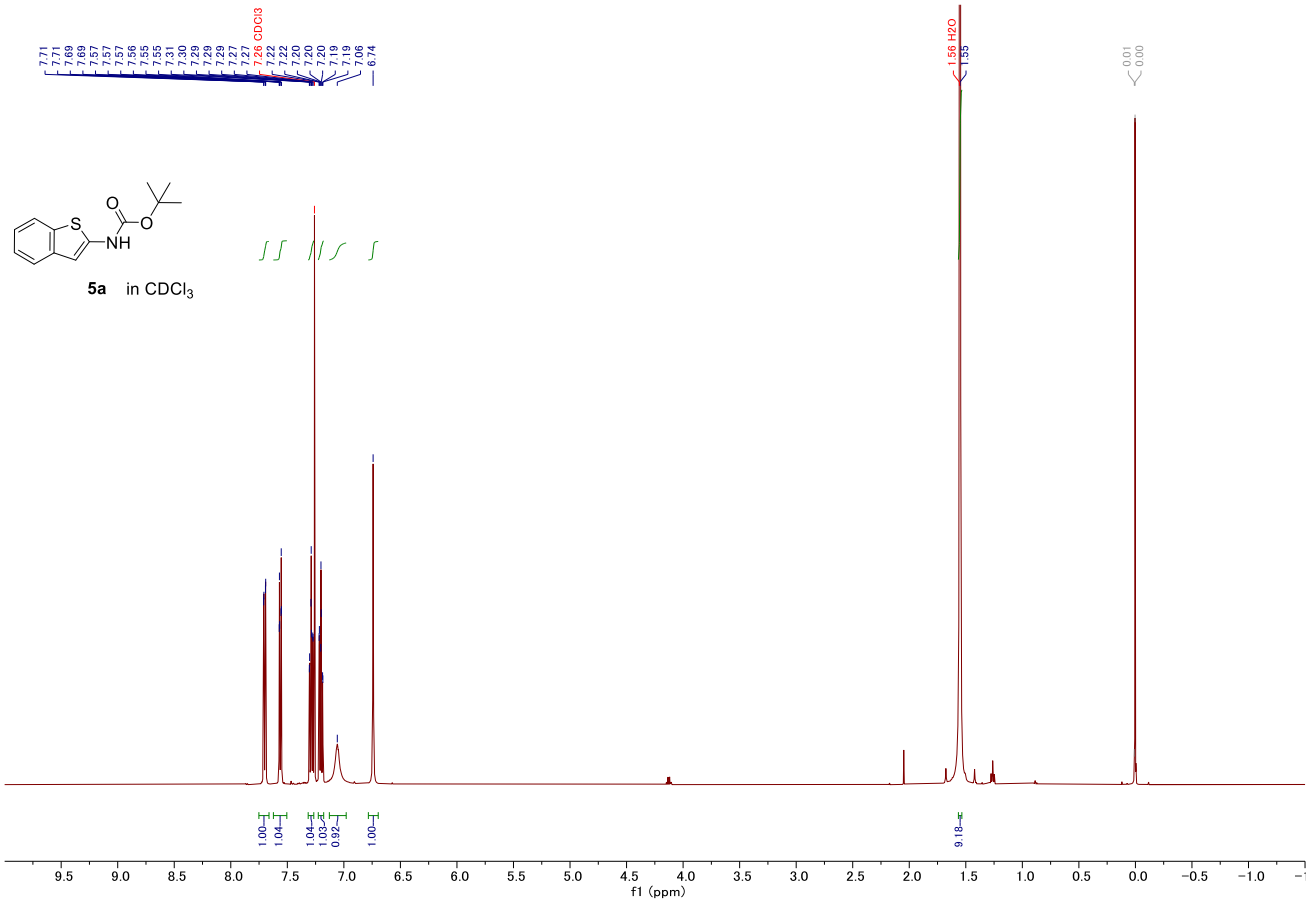
N	1.12153500	0.42568000	-0.03672100
N	-1.12160100	0.42296700	0.09427900
C	-4.54960600	-1.00632300	-0.09924200
C	0.00031900	-0.35494200	0.01891700
C	-3.10872700	-1.09659600	-0.08365100
C	2.47299700	0.09035800	-0.01801100
C	4.55143600	-1.00439600	0.10624700
C	3.11047300	-1.09420100	0.11795200
C	5.06669700	0.29389000	-0.04549000
C	-6.43570200	0.54531200	0.03307100
C	-2.47305500	0.08900600	0.05225700
C	-5.06711800	0.29338300	0.03077000
C	-5.44893000	-2.07342900	-0.22982600
C	5.45283200	-2.07029100	0.23236300
C	-7.30453600	-0.52726200	-0.09817700
C	6.43507000	0.54561400	-0.07280000
C	-6.81123500	-1.83022100	-0.22886200
C	7.30597100	-0.52574200	0.05460300
C	6.81492500	-1.82727300	0.20635800
H	0.95279700	1.42056600	-0.10204300
H	-0.95287000	1.41461600	0.19614100
H	-2.59128800	-2.03768700	-0.17315700
H	2.59481300	-2.03410800	0.22806100
H	-6.81616700	1.55521800	0.13440200
H	-5.06836500	-3.08415200	-0.33117300
H	5.07404100	-3.07991700	0.34998900
H	-8.37439700	-0.35181800	-0.09936400

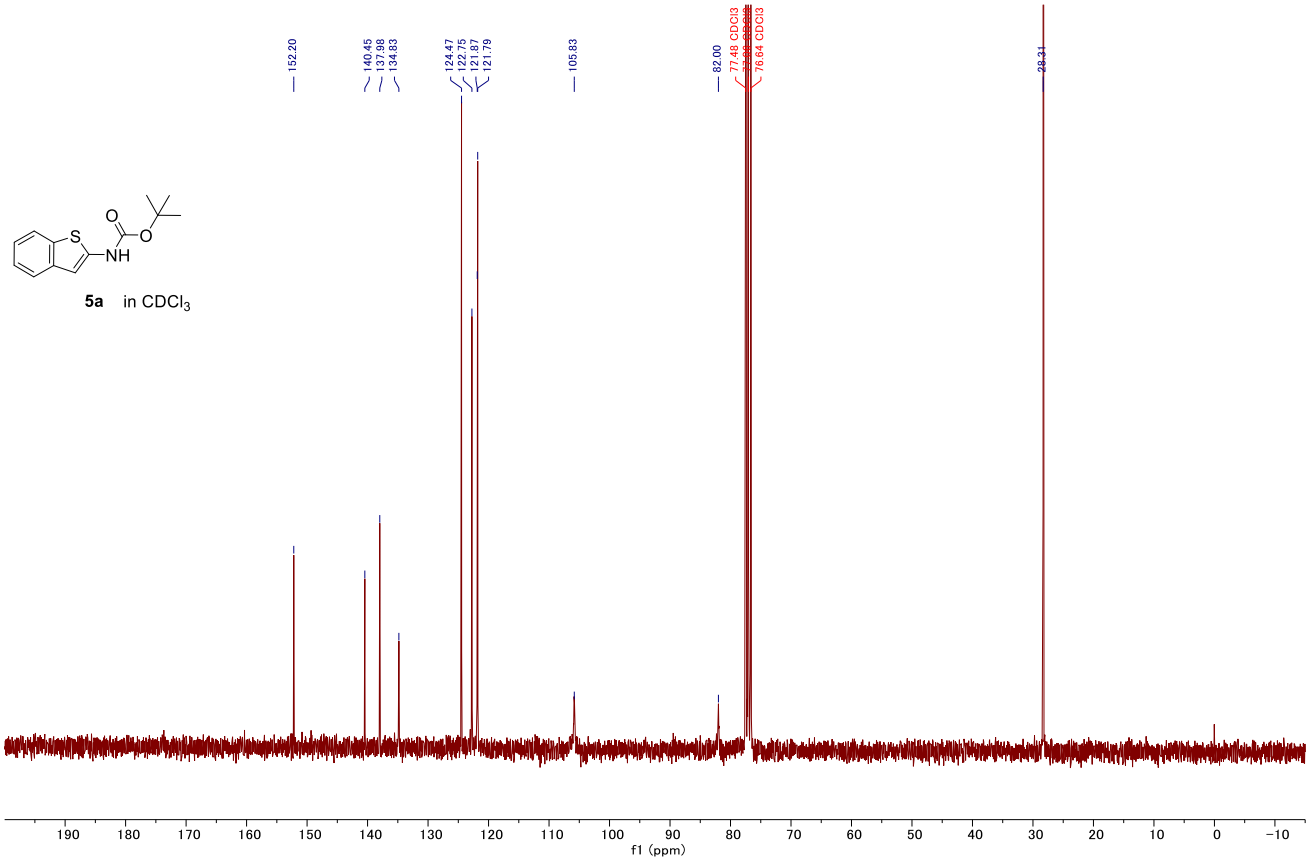
H	6.81381300	1.55442200	-0.19024400
H	-7.50480200	-2.65745700	-0.33051000
H	8.37570500	-0.35045000	0.03641700
H	7.51010400	-2.65356200	0.30464400
S	0.00131300	-2.02495900	-0.00658200
Se	-3.68013800	1.56066000	0.19085500
Se	3.67705600	1.55939300	-0.19613800

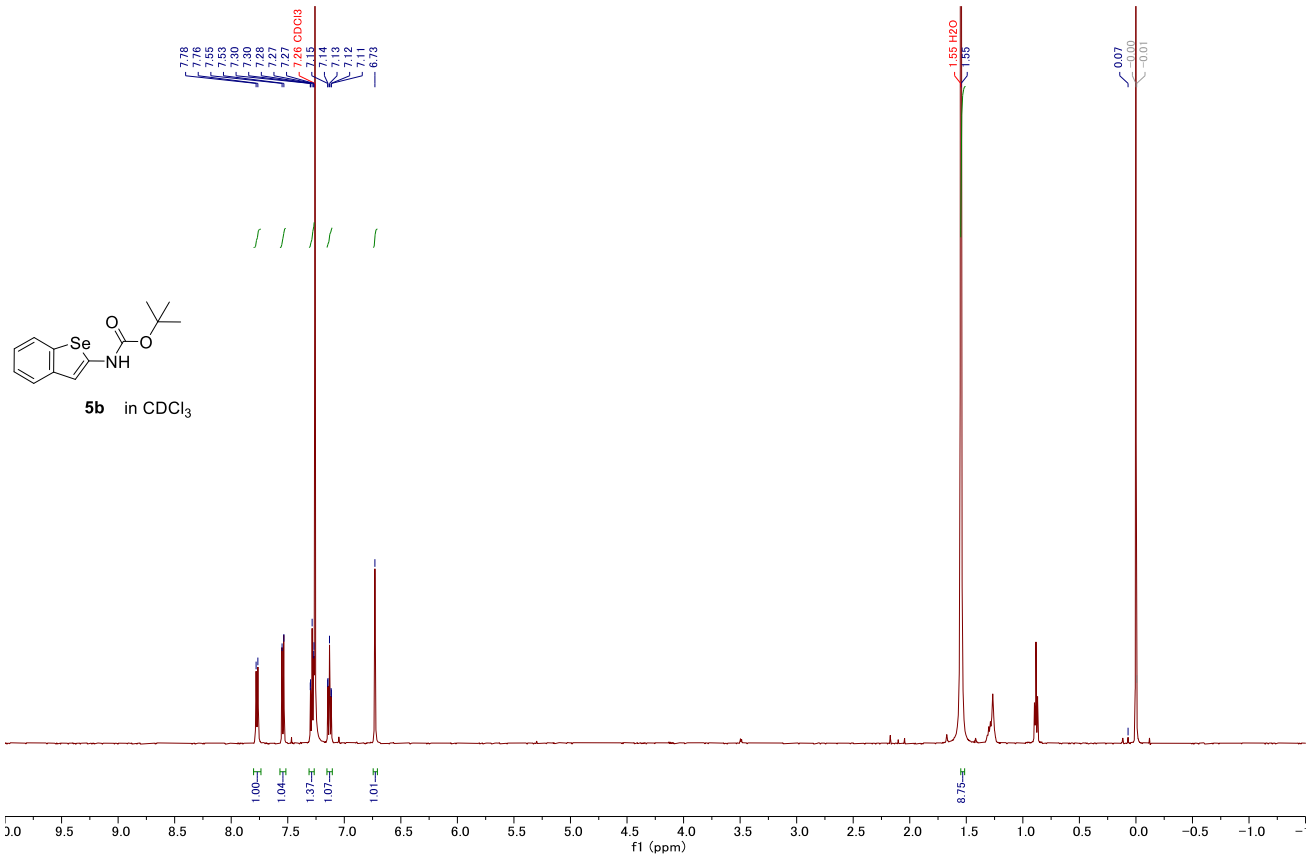
References

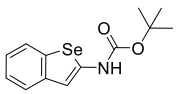
1) T. Inoue, M. Ota, Y. Amijima, H. Takahashi, S. Hamada, S. Nakamura, Y. Kobayashi, T. Sasamori, T. Furuta, *Chem. Eur. J.* **2023**, e202302139.
2) (a) A. E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev*. **1988**, *88*, 899. (b) F. Weinhold, *J. Comput. Chem.* **2012**, *33*, 2363.
3) J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615.
4) Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
5) (a) E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-Garciá, A. J. Cohen, W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498. (b) J. Contreas-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan, W. Yang, *J. Chem. Theory Comput.* **2011**, *7*, 625.
6) R. F. W. Bader, *Atoms in Molecules, A Quantum Theory,* Oxford University Press, Oxford, **1990**. See, also, W. Humphrey, A. Dalke, K. Schulten, *J. Mol. Graphics* **1996**, *14*, 33.
7) T. Lu, F. W. Chen, *J. Comput. Chem.* **2012**, *33*, 580.
8) W. Humphrey, A. Dalke, K. Schulten, *J. Mol. Graphics* **1996**, *14*, 33.

^{1}H and ^{13}C NMR spectra



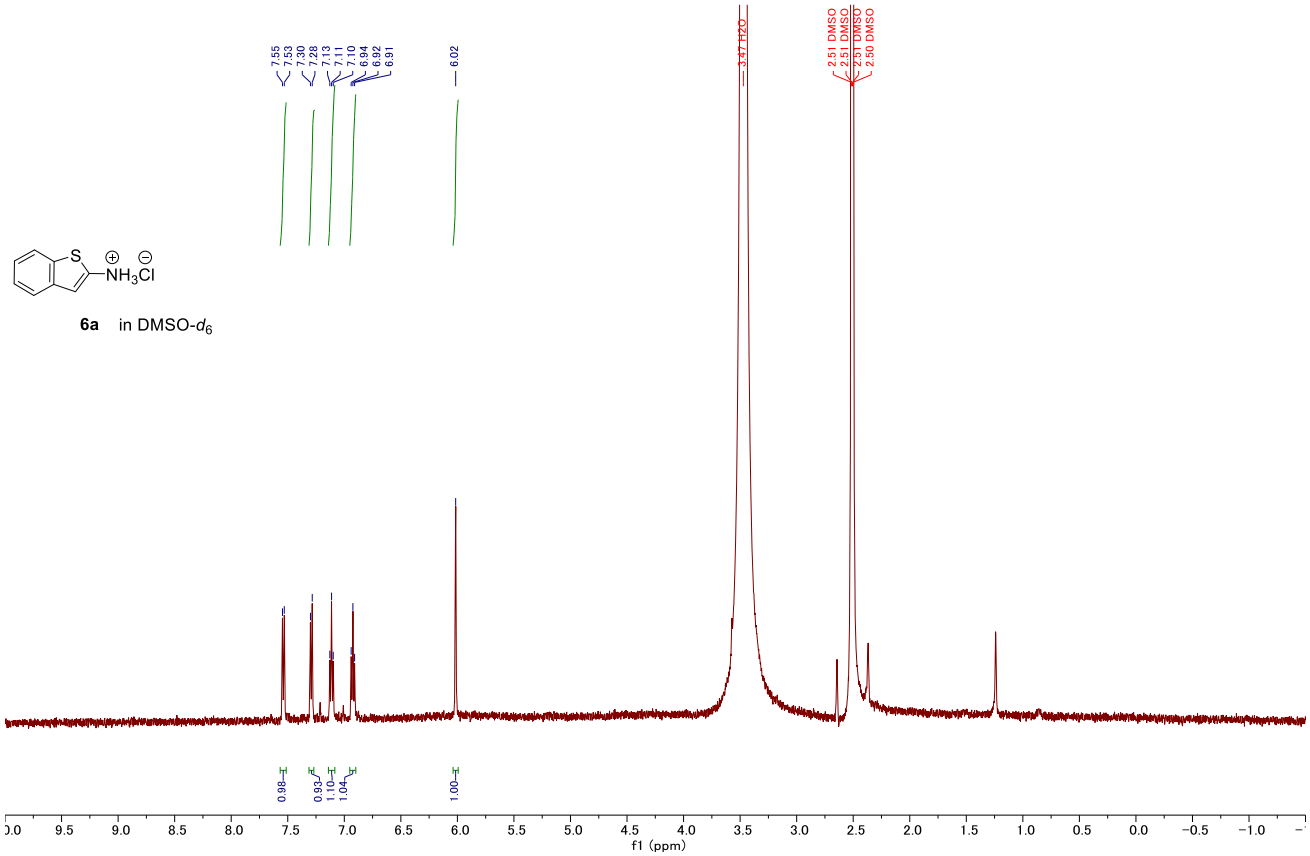






5b in $CDCl_3$

5b in $CDCl_3$



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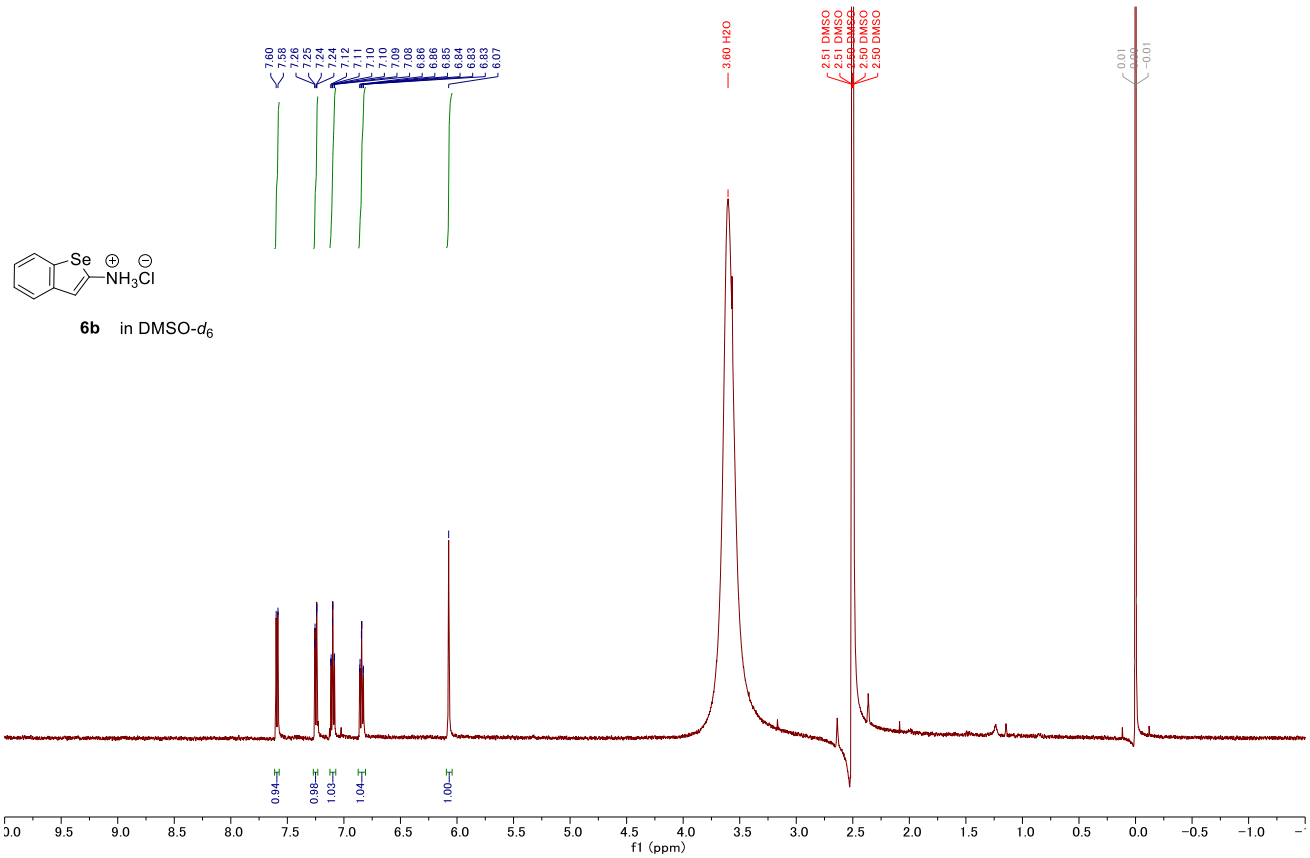

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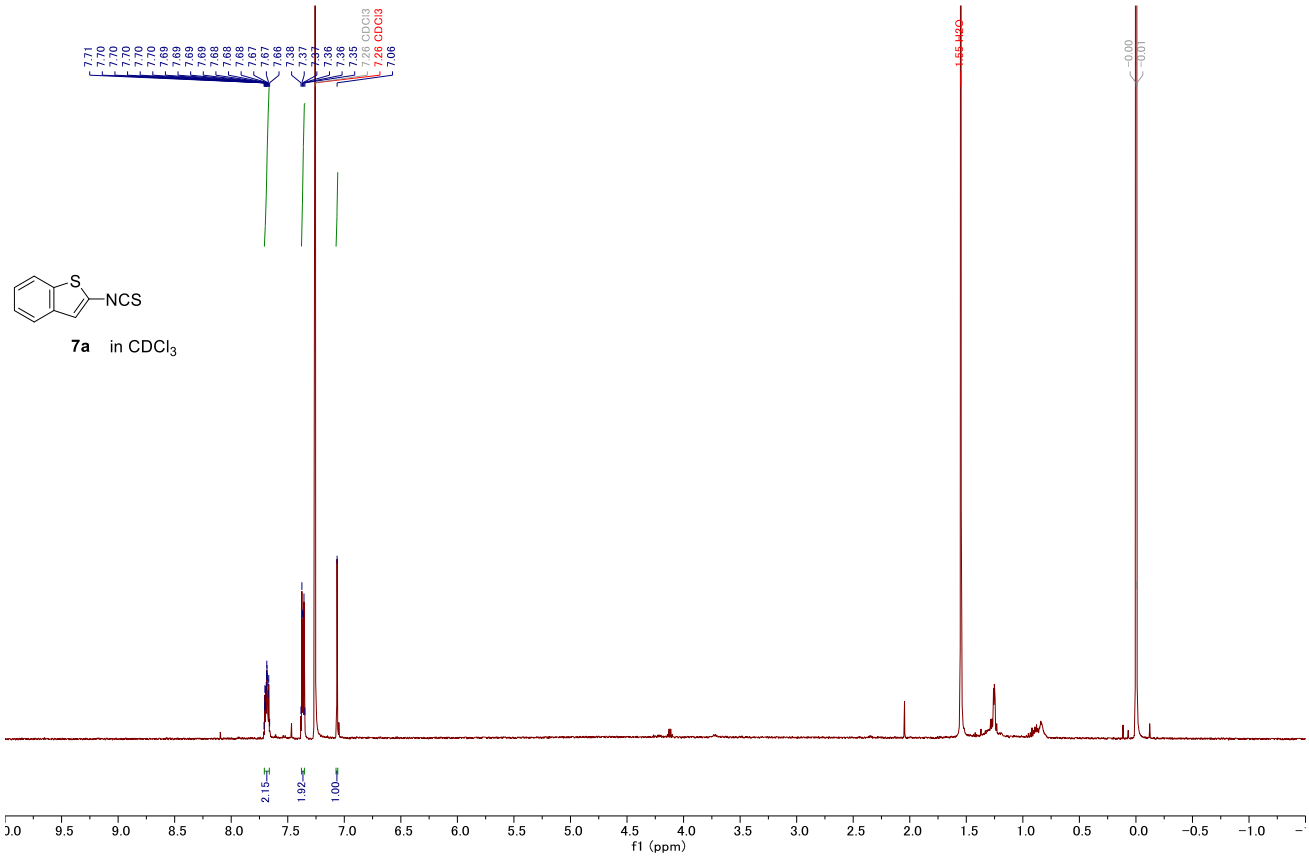

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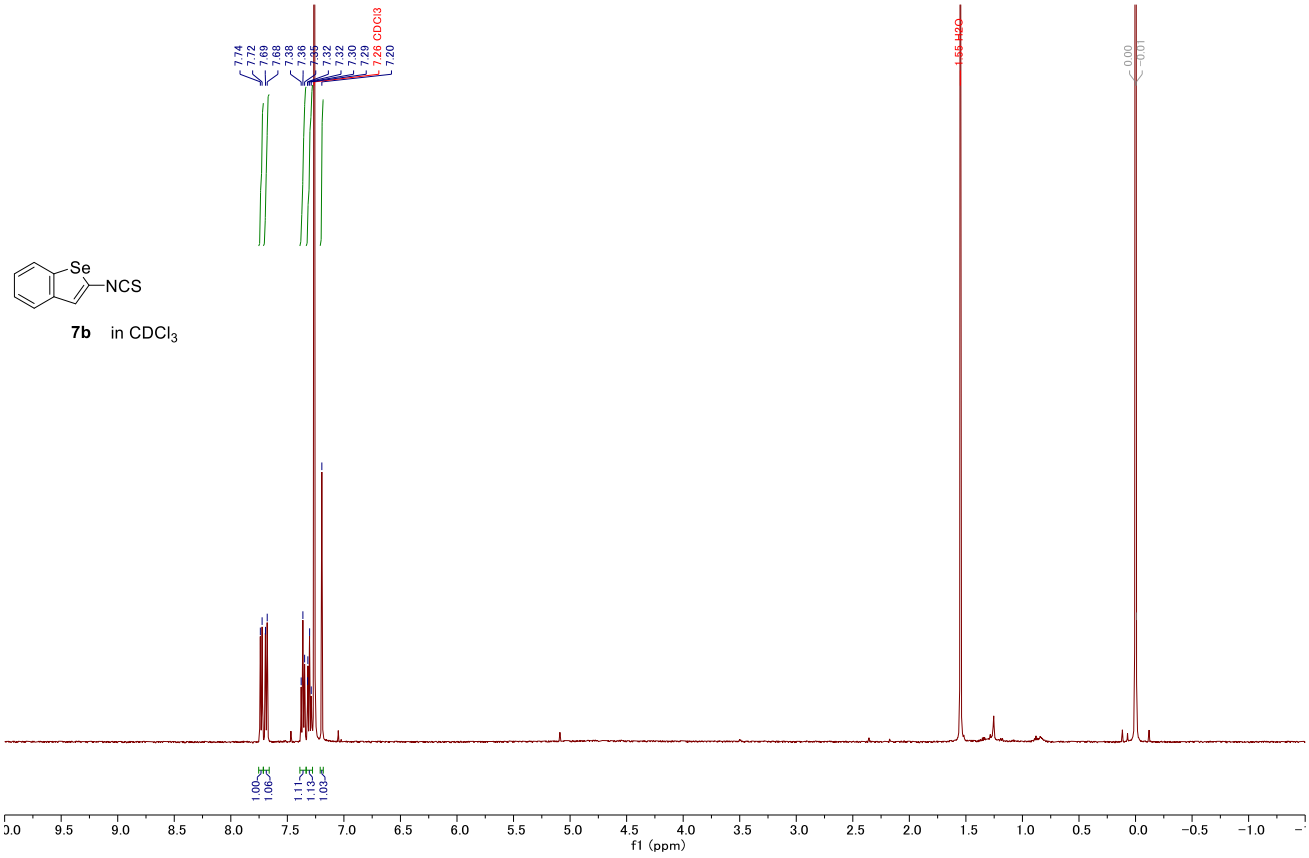

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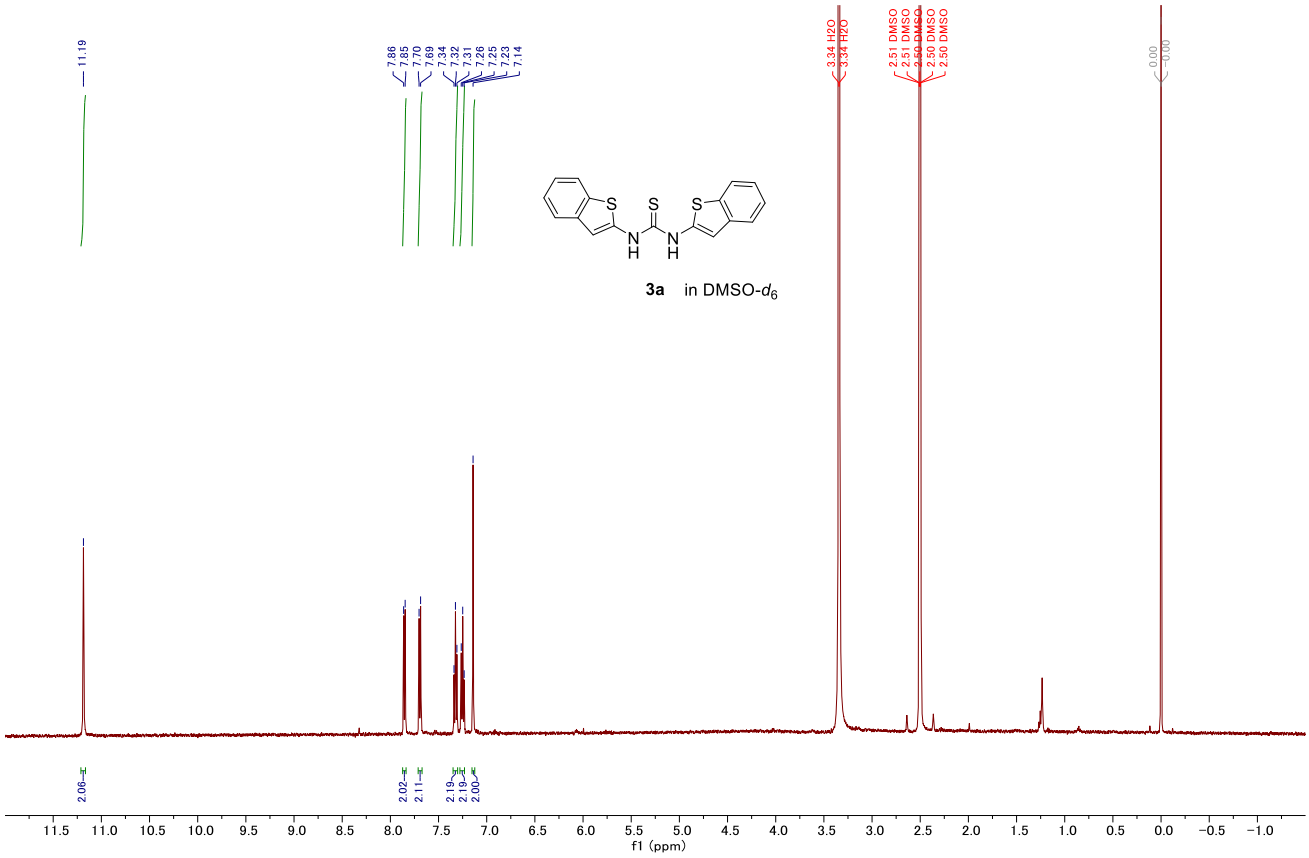

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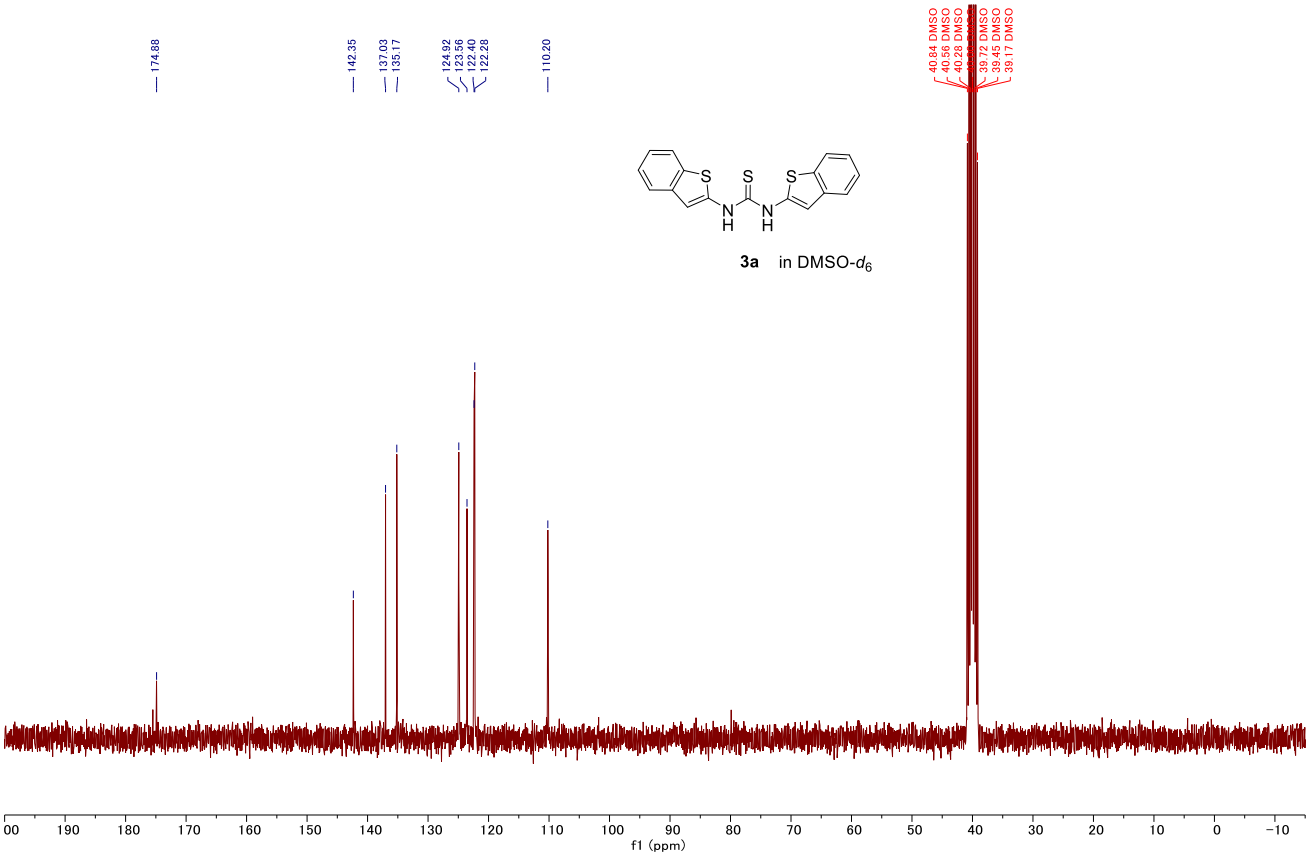

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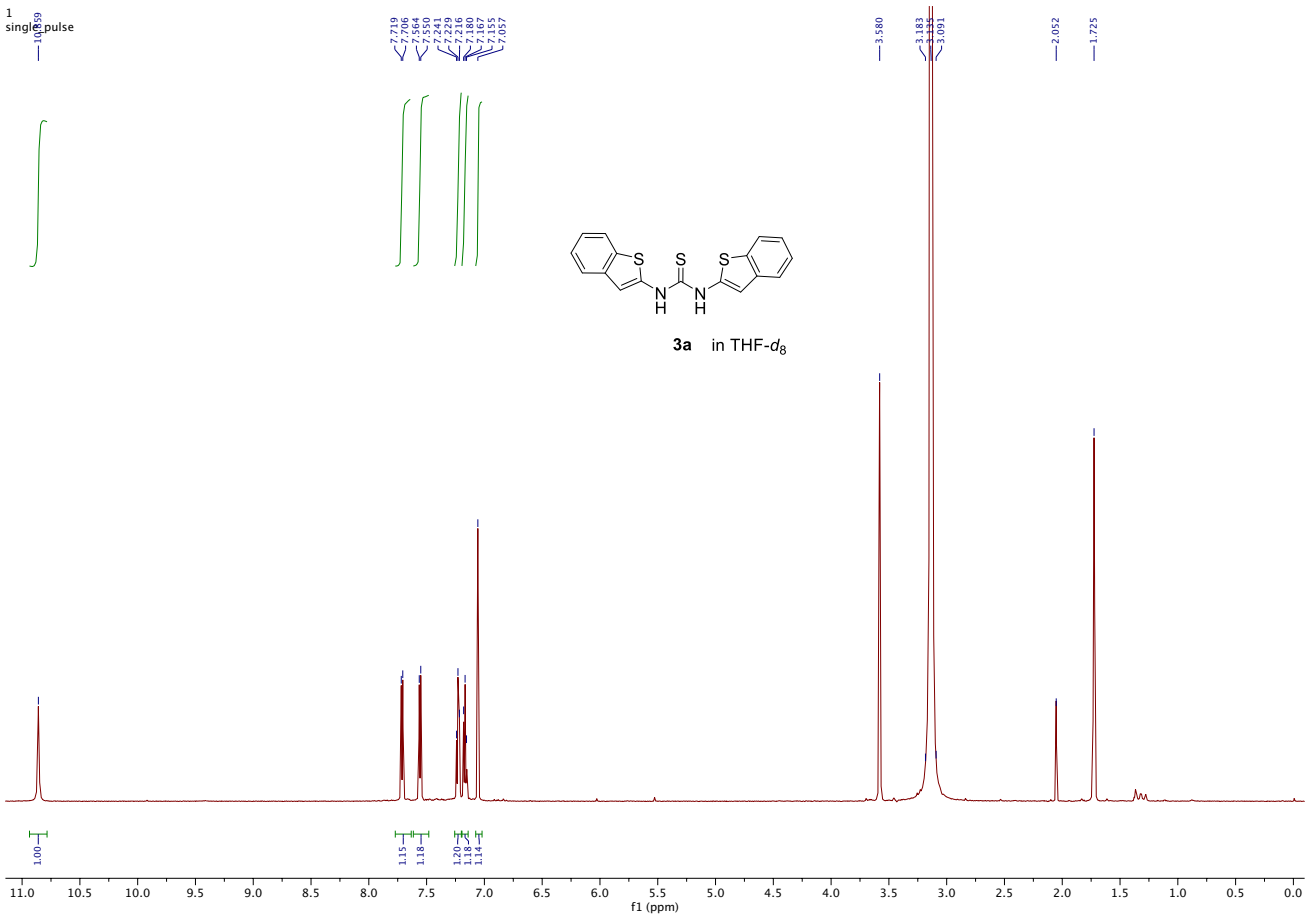
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single pulse
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7.057
3.580
3.183
3.135
3.091
2.052
1.725
S
S
S
N
H
N
H
1.00
1.15
1.18
1.20
1.18
1.14
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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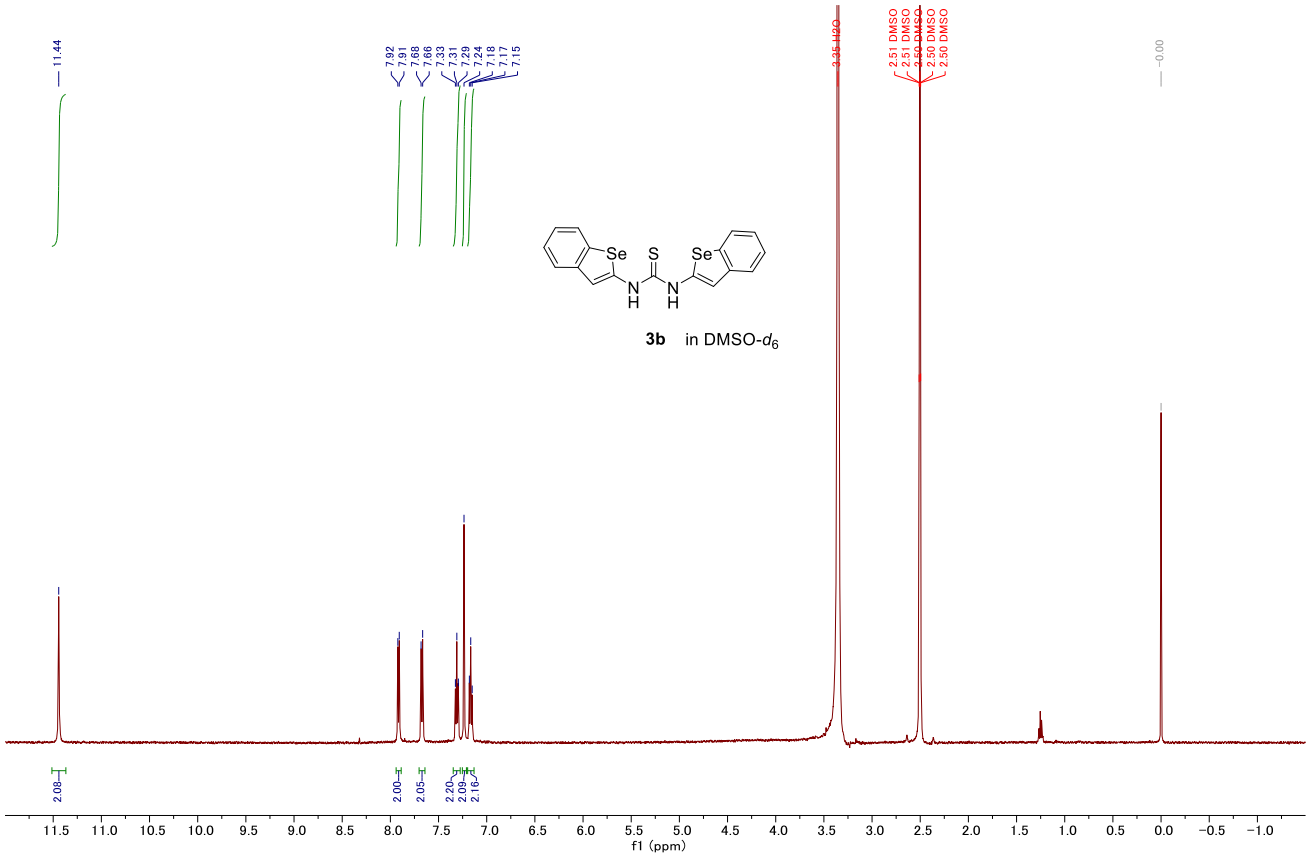
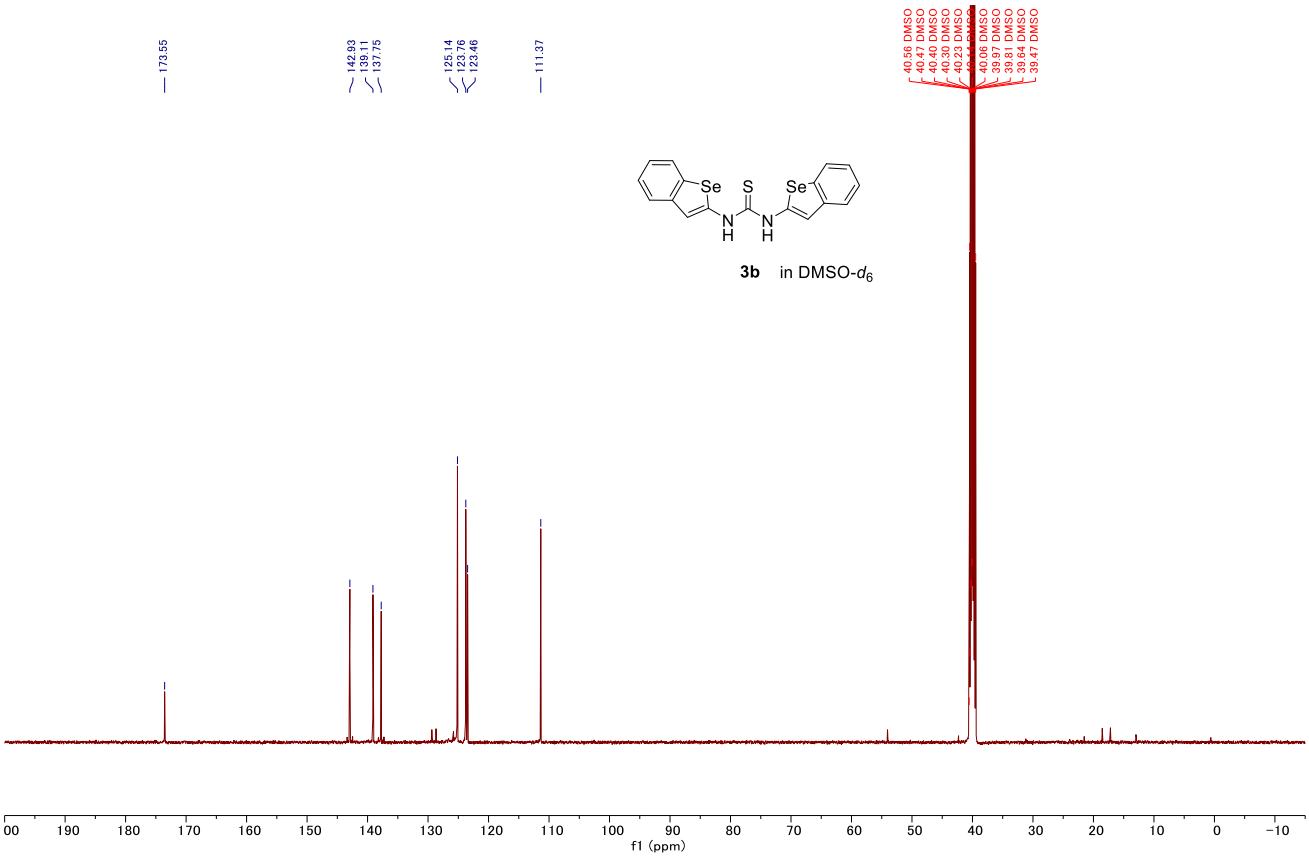
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3a in THF-d_8



3b in DMSO-d_6



3b in DMSO-d_6