Supporting Information

Singlet Oxygen Driven Stereoselective Iodothiocyanation and Iodoselenocyanation of Alkynes

Mahima Gupta, Ashwini Vishwasrao Katkar, Vaibhav Pramod Charpe*, and Kuo Chu Hwang*

Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, R. O. C.

E-mail: kchwang@mx.nthu.edu.tw, vaib.charpe@gmail.com

Table of contents

Experimental section	S3
Mechanistic studies	S6
Green metrics and Eco-scale evaluation for **4a**	S16
^{1}H NMR, ^{13}C NMR, ^{19}F NMR, and HRMS data	S18
References	S34
^{1}H NMR, ^{13}C NMR, and ^{19}F-NMR spectra	S35
ORTEP diagram and X-ray Data of compound **2c**	S75
ORTEP diagram and X-ray Data of compound **2e'**	S82
ORTEP diagram and X-ray Data of compound **4a**	S88
ORTEP diagram and X-ray Data of compound **4h'**	S96
ORTEP diagram and X-ray Data of compound **4k'**	S103
ORTEP diagram and X-ray Data of compound **4m'**	S111

ORTEP diagram and X-ray Data of compound **6b** S117

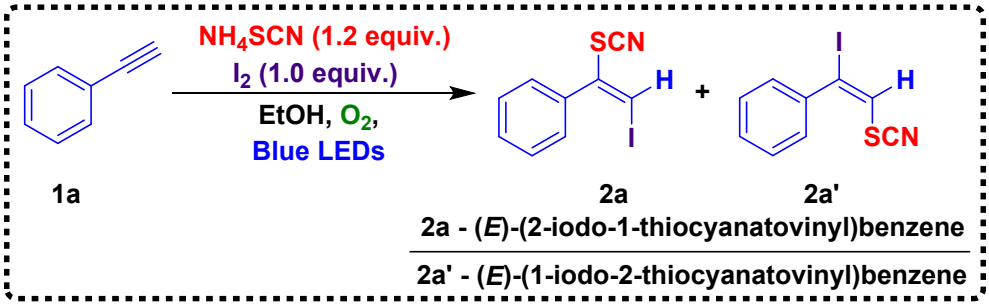
ORTEP diagram and X-ray Data of compound **6c** and **6c'** S126

ORTEP diagram and X-ray Data of compound **9a** S138

Experimental section

General: All reactions were conducted in oven-dried glassware using a blue light-emitting diode (LED) array (power density: 150 mW/cm^2 at 460 nm) as the visible-light source under air (O_2) atmosphere. All solvents were dried according to known methods and distilled prior to use. Starting materials were commercially available (Sigma-Aldrich or Alfa-Aesar or TCI-chemicals) and used as received. ^{1}H NMR and ^{13}C NMR spectra were recorded at 700/400 and 175/100 MHz using deuterated $CDCl_3$ as a solvent, respectively. Chemical shifts (δ) were reported as parts per million (ppm) and the following abbreviations were used to identify the multiplicities: s= singlet, d= doublet, t= triplet, q= quartet, m= multiplet, b= broad and all combinations thereof can be explained by their integral parts. Unless otherwise specified, the proton/carbon signal of 2 residual solvent peaks (at δ 7.24 or 2.50 and δ 77.00 or 39.51 ppm, respectively) were used as the internal references.

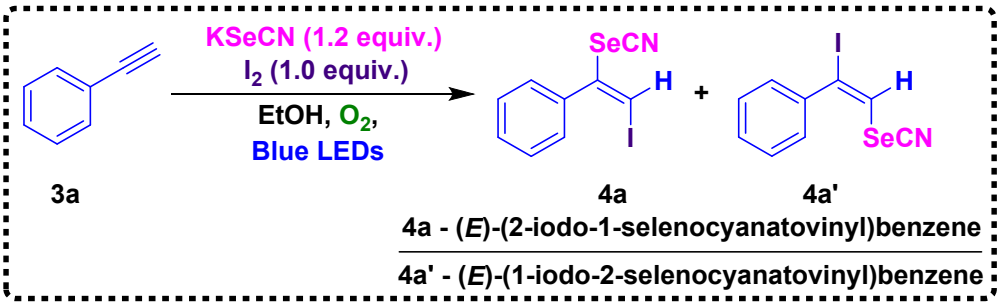
General procedure for the synthesis of *(E)*-(2-iodo-1-thiocyanatovinyl)benzene:



Scheme S1: Photochemical process for the synthesis of *(E)*-(2-iodo-1-thiocyanatovinyl)benzene.

To a dry test tube (20 mL) containing 1.2 equiv. NH_4SCN, 1.0 equiv. molecular I_2 and alkyne (0.5 mmol), was added 3 mL of ethanol. The reaction mixture was then irradiated with blue LEDs (150 mW/cm^2 at 460 nm) under O_2 atmosphere (O_2 balloon) at room temperature (25-28^{o}C) until completion of the reaction (monitored by TLC). The reaction mixture was then concentrated, and the residue was purified by column chromatography on silica gel.

General procedure for the synthesis of *(E)*-(2-iodo-1-selenocyanatovinyl)benzene:

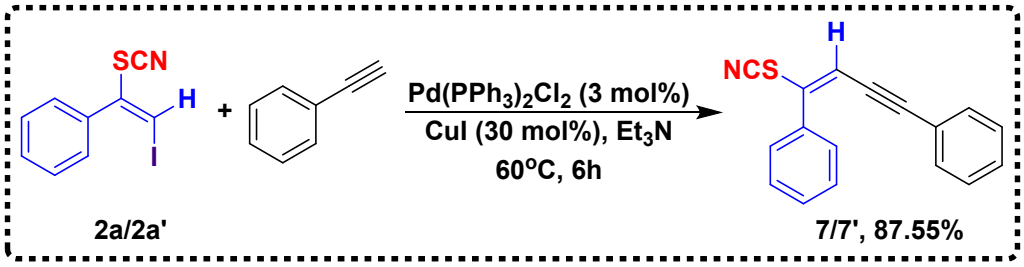


Scheme S2: Photochemical process for the synthesis of *(E)*-(2-iodo-1-selenocyanatovinyl)benzene.

To a dry test tube (20 mL) containing 1.2 equiv. KSeCN, 1.0 equiv. molecular I_2 and alkyne (0.5 mmol), was added 3 mL of ethanol. The reaction mixture was then irradiated with blue LEDs (150 mW/cm^2 at 460 nm) under O_2 atmosphere (O_2 balloon) at room temperature (25-28^{o}C) until completion of the reaction (monitored by TLC). The reaction mixture was then concentrated, and the residue was purified by column chromatography on silica gel.

Procedures for the Synthesis of late-stage functionalization of Iodo-vinyl-thiocyanates:

A) Synthesis of *(E)*-(1-thiocyanatobut-1-en-3-yne-1,4-diyl)dibenzene (7/7')

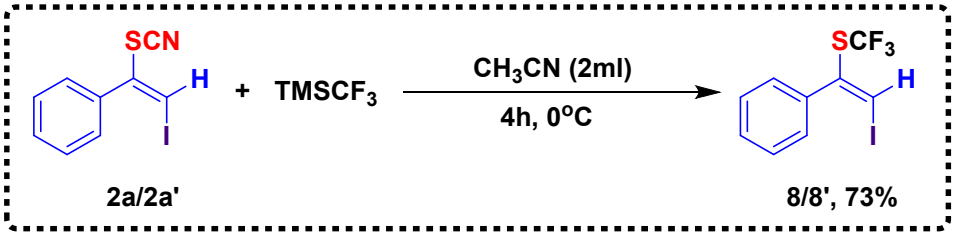


Scheme S3: Reaction scheme for the synthesis of *(E)*-(1-thiocyanatobut-1-en-3-yne-1,4-diyl)dibenzene

Into a 25 mL Schlenk flask 144 mg of **2a**/**2a'** (0.5 mmol) was loaded. The vessel was then degassed and loaded with 11 mg (3 mol%) of palladium catalyst, 29 mg (30 mol%) of copper catalyst and 5ml of anhydrous triethylamine (Et_3N) solvent. To this reaction mixture ethynylbenzene (1.2 equiv., 62 mg) was then added at once. The reaction was stirred at 60 °C for 6 h. The reaction

mixture was then concentrated, and the residue was purified by column chromatography on silica gel to directly afford the pure product **7/7'** in 96 mg (87.55% yield).

B) Synthesis of *(E)*-(2-iodo-1-phenylvinyl)(trifluoromethyl)sulfane (8/8')



Scheme S4: Reaction scheme for the synthesis of *(E)*-(2-iodo-1-phenylvinyl) (trifluoromethyl)sulfane.

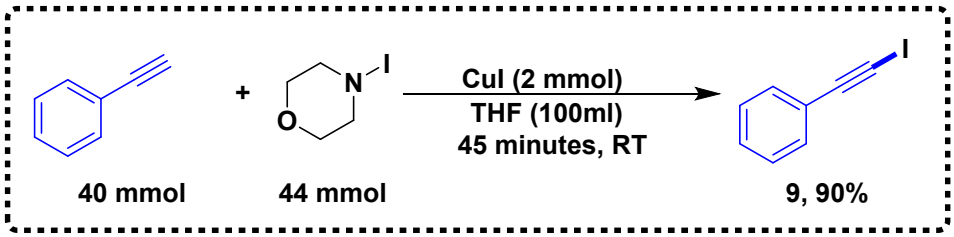
Into a 25 mL Schlenk flask 144 mg of **2a**/**2a'** (0.5 mmol) was loaded. Followed by addition of 143 mg (2 equiv.) of $TMSCF_3$. The reaction mixture was stirred at 0 ºC for 4 h. After the starting material was consumed as judged by TLC, the solvent was removed under reduced pressure. The reaction mixture was then concentrated, and the residue was purified by column chromatography on silica gel to directly afford the pure product **8/8'** in 120.42 mg (73% yield).

Mechanistic studies

Reactions with (iodoethynyl)benzene

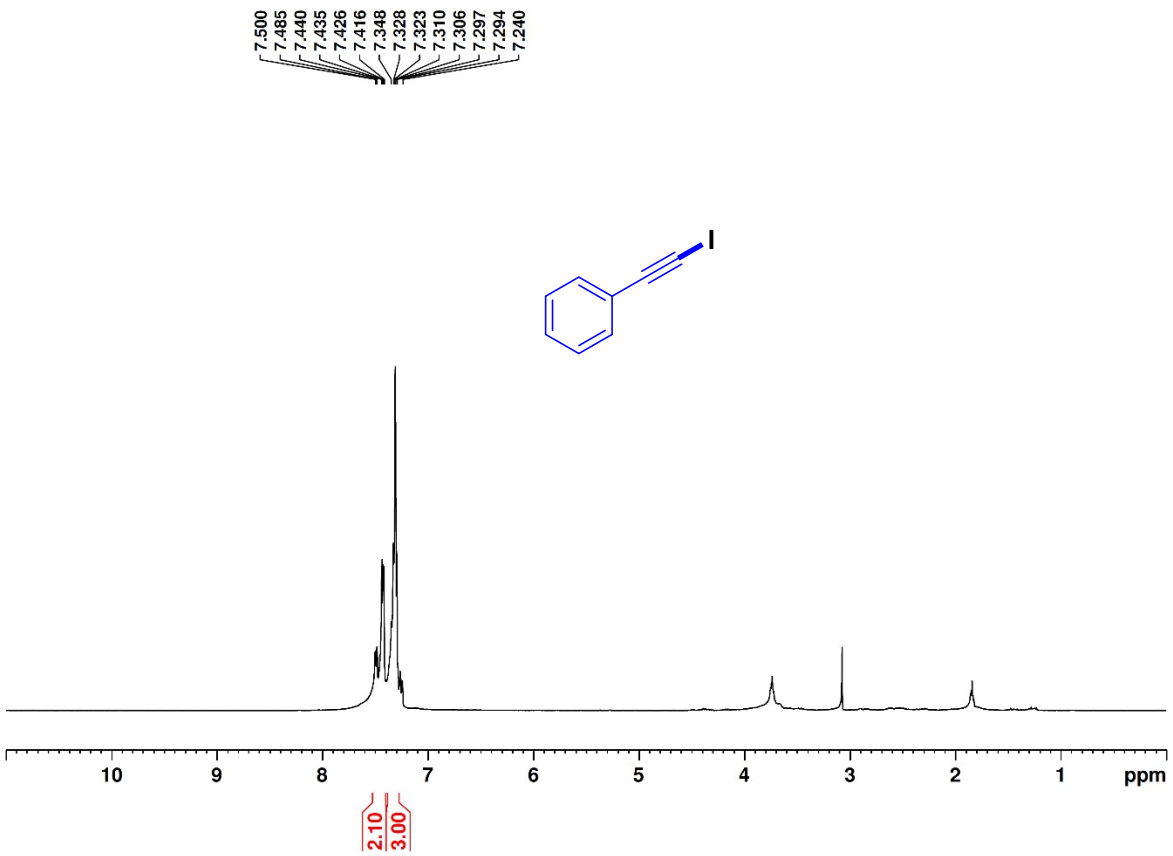
A) Procedure for synthesis of (iodoethynyl)benzene (9)[S1]:

Phenylacetylene (4.08 g, 40.00 mmol) was dissolved in THF (100 mL) and treated with CuI (0.38 g, 2.00 mmol) and N-iodomorpholine[S2] (15.00 g, 44.00 mmol). The reaction mixture was stirred at room temperature for 45 minutes, after which a fine white precipitate had formed. The suspension was poured onto a pad of neutral alumina (400 mL), and the filtrate was collected under vacuum. The solid phase was washed with DCM (2x20 mL) and the combined organic fractions were pooled and concentrated by evaporation, giving (iodoethynyl)benzene (8.21 g, 90%) as a yellow oil. This material was used without further purification.

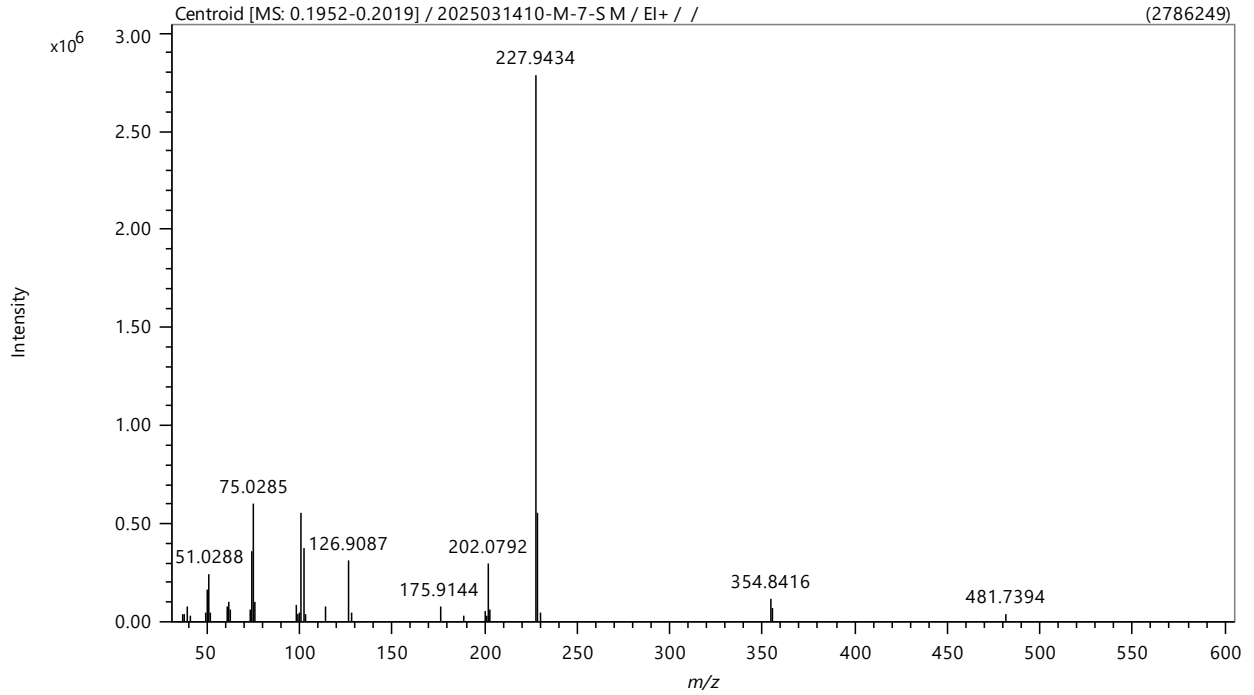


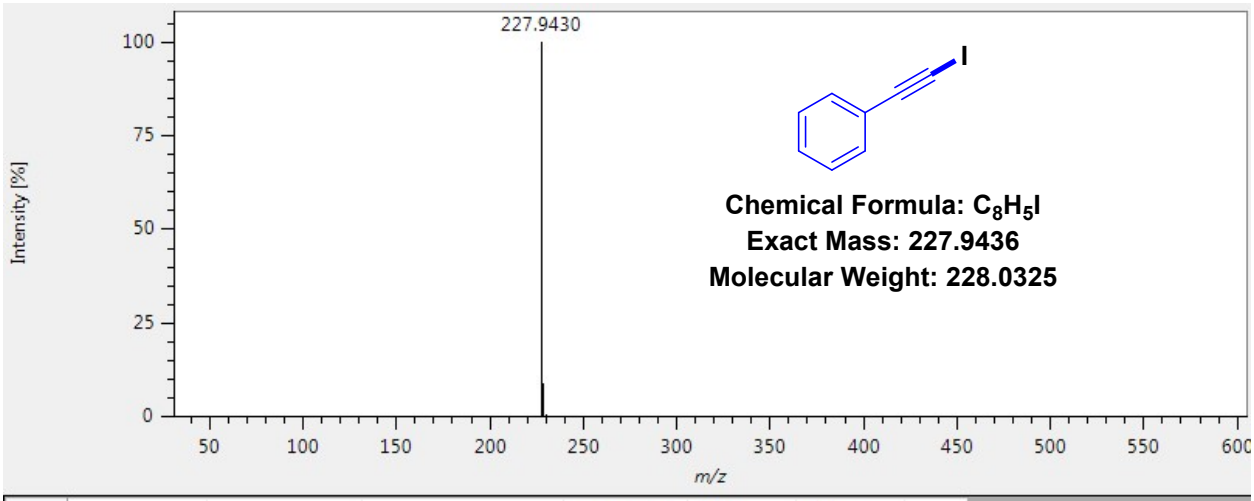
Scheme S5: Reaction scheme for the synthesis (iodoethynyl)benzene

^{1}H NMR


7.500
7.485
7.440
7.435
7.426
7.416
7.348
7.328
7.323
7.310
7.306
7.297
7.294
7.240
I
10
9
8
7
6
5
4
3
2
1
ppm
2.10
3.00

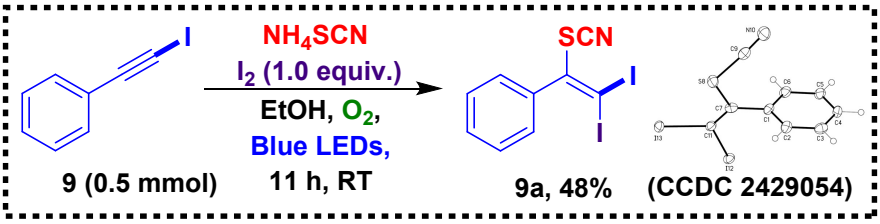
EI Mass Data





Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
227.94340	2786249.30	C8 H5 I	227.94304	0.35	1.55	6.0

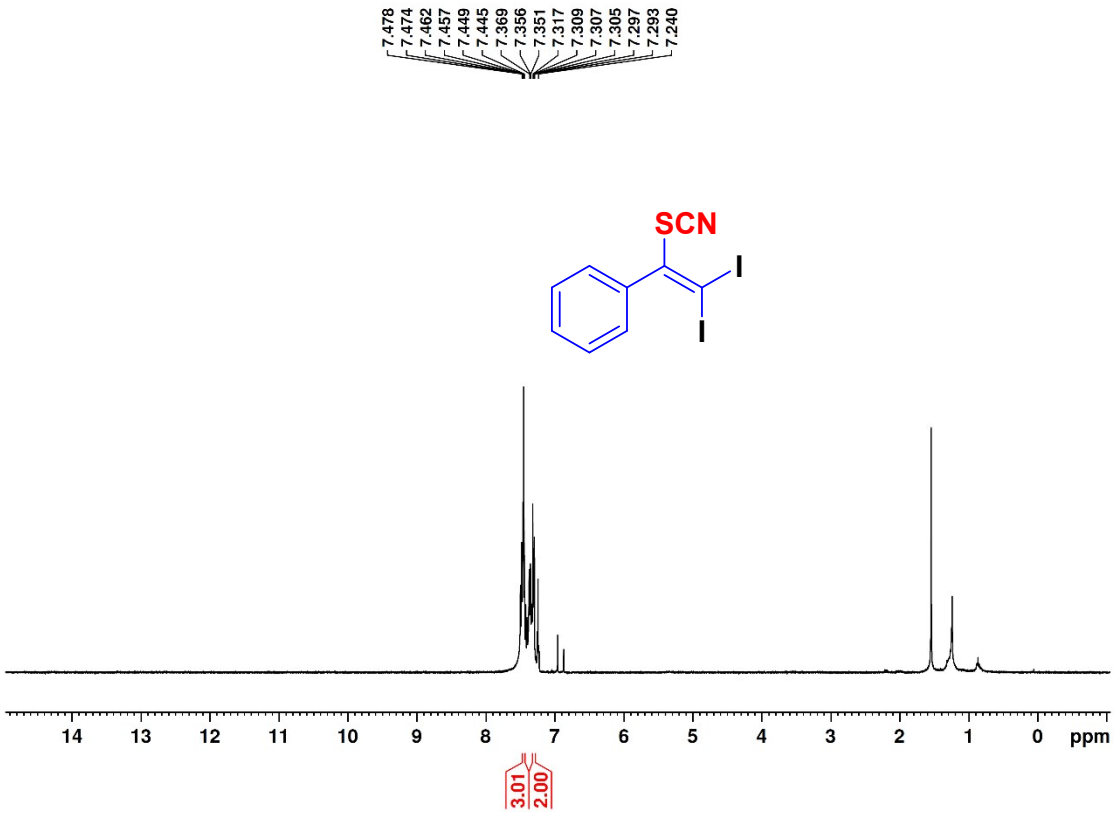
B) Reaction of (iodoethynyl)benzene in presence of Iodine:



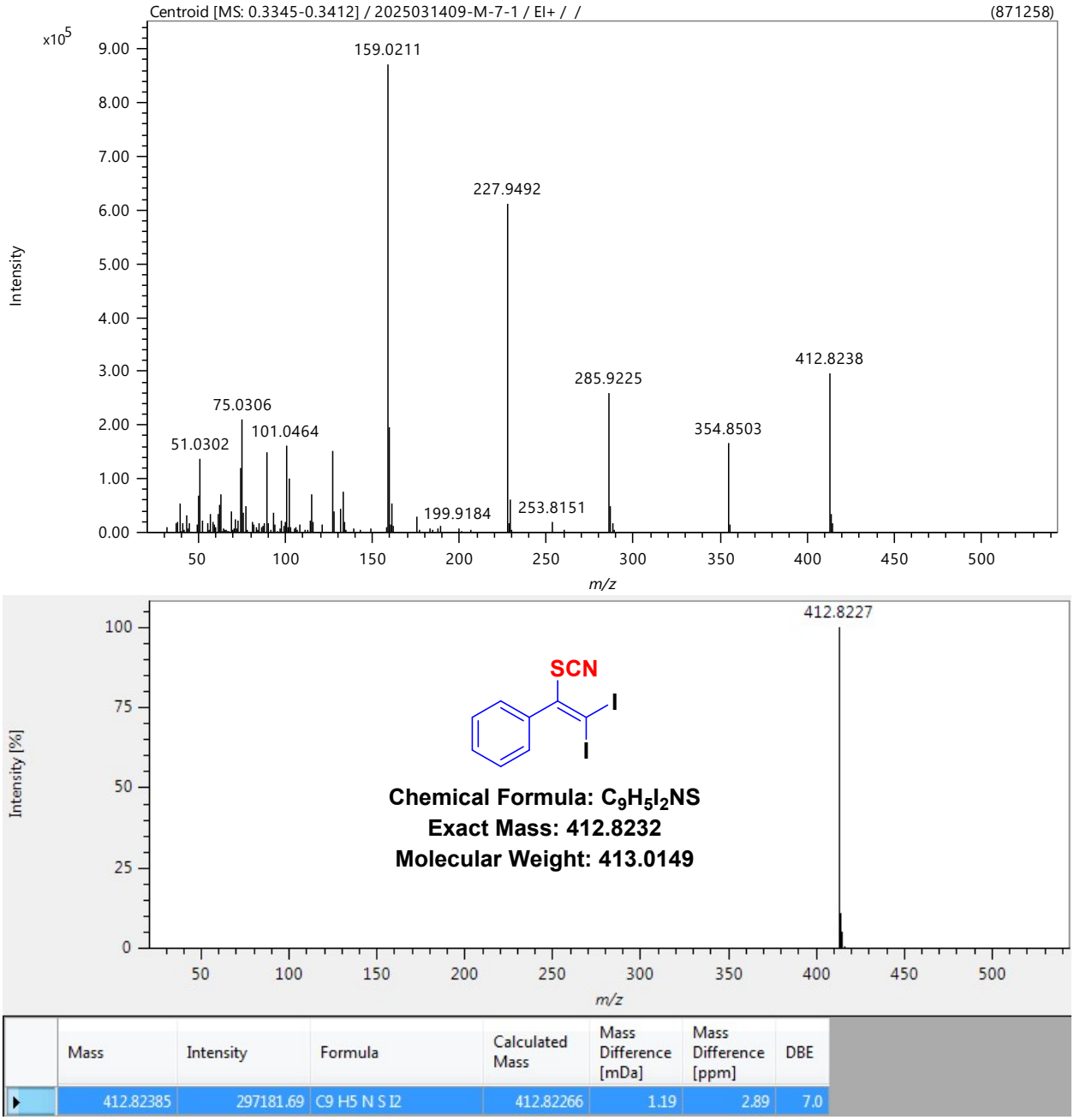
Scheme S6: Control Reaction of (iodoethynyl)benzene in presence of Iodine

To a dry test tube (20 mL) containing 1.2 equiv. NH_4SCN, 1.0 equiv. molecular I_2 and (iodoethynyl)benzene **(9)** (0.5 mmol), was added 3 mL of ethanol. The reaction mixture was then irradiated with blue LEDs (150 mW/cm^2 at 460 nm) under O_2 atmosphere (O_2 balloon) at room temperature (25-28 ^{o}C) until completion of the reaction (monitored by TLC; 11 h). The reaction mixture was then concentrated, and the residue was purified by column chromatography on silica gel to directly afford the pure product **(9a)** in 99.12 mg (48% yield).

^{1}H NMR

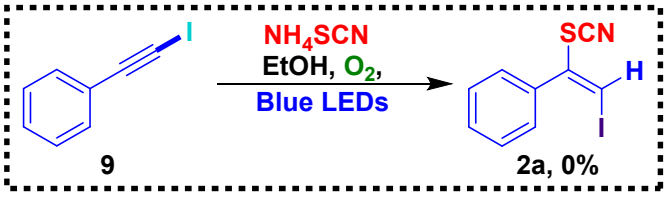


EI Mass Data



	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▶	412.82385	297181.69	C9 H5 N S I2	412.82266	1.19	2.89	7.0

C) Reaction of (iodoethynyl)benzene in the absence of Iodine:

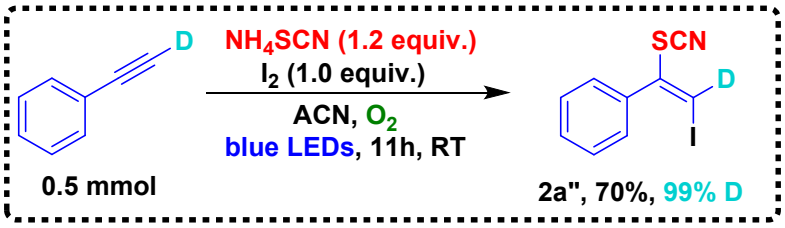


Scheme S7: Control Reaction of (iodoethynyl)benzene in the **absence of iodine**

To a dry test tube (20 mL) containing 1.2 equiv. NH_4SCN, and (iodoethynyl)benzene **(9)** (0.5 mmol), was added 3 mL of ethanol. The reaction mixture was then irradiated with blue LEDs (150 mW/cm^2 at 460 nm) under O_2 atmosphere (O_2 balloon) at room temperature (25-28 ^oC) for 11h. In this case we did not observe product **2a**. Thus, confirming that Iodine is required for the reaction to proceed.

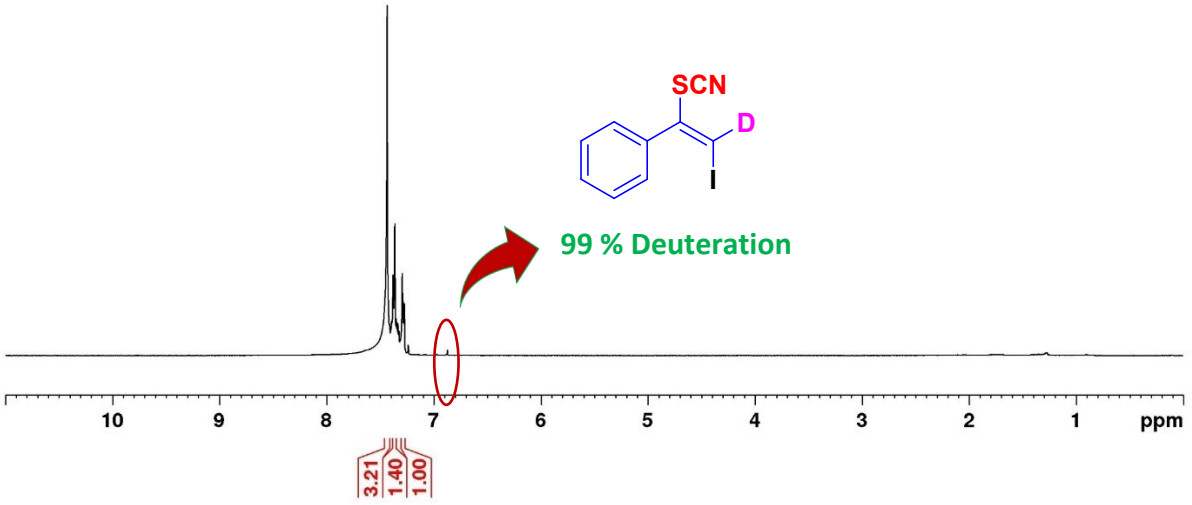
Deuterium labeling experiments

D) For Iodothiocyanates:

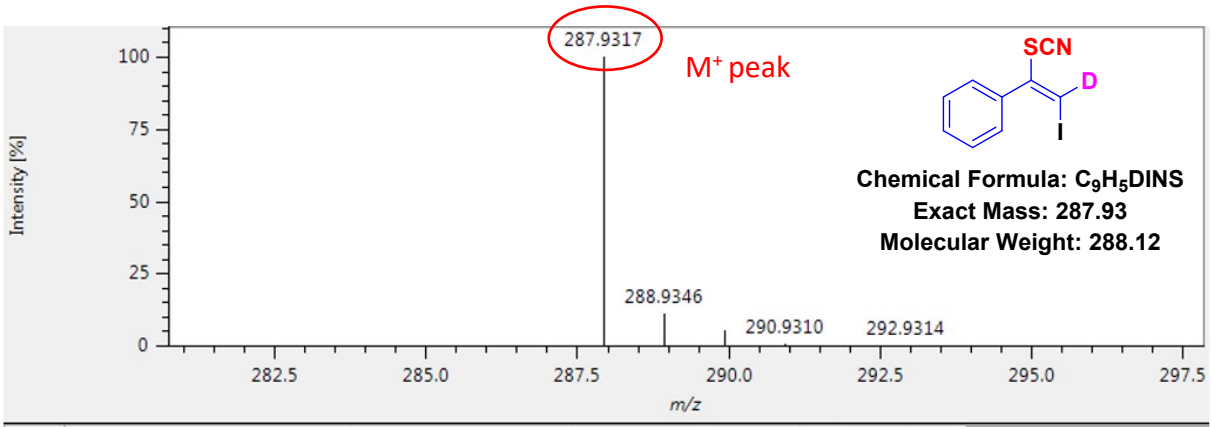


Scheme S8: Reaction of D1-phenylacetylene with ammonium thiocyanate

^{1}H NMR



EI Mass Spectrum

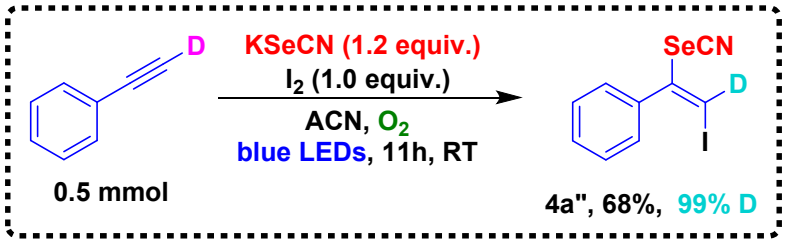


	Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
▸	287.93127	300509.01	C9 H5 N S I D	287.93174	-0.47	-1.64	7.5

No.	m/z	Intensity	Intensity [%]	Saturated
81	286.92507	11170.06	0.92	
82	287.93127	300509.01	24.71	

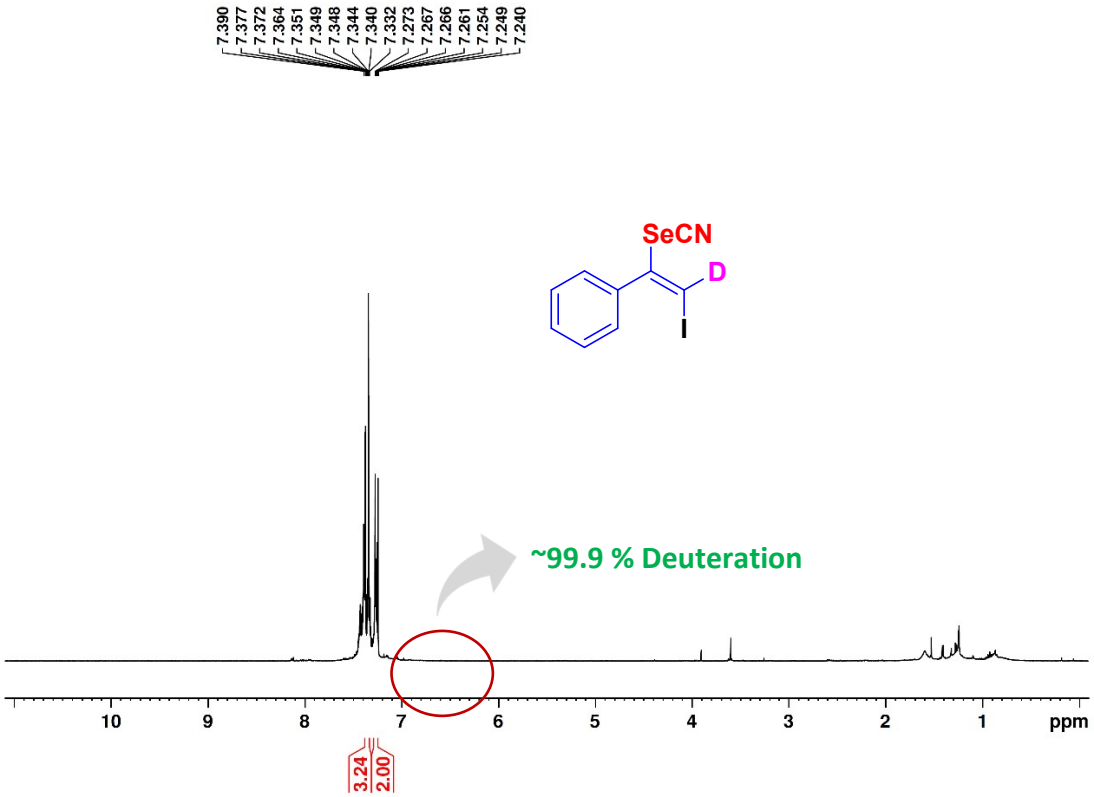
96.42% Deuteration

E) For Idoselenocyanates:

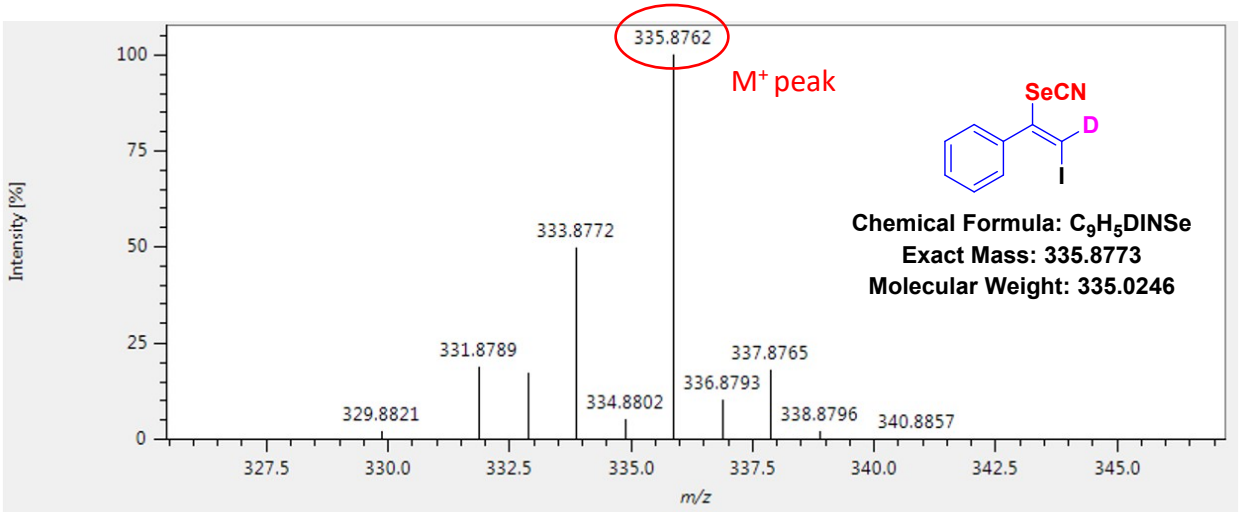


Scheme S9: Reaction of D1-phenylacetylene with potassium selenocyanate.

^{1}H NMR



EI Mass Spectrum



Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
335.87730	1862.69	C9 H5 N Se I D	335.87619	1.10	3.29	8.5

EPR Experiment to detect the $^1O_2$ and I$^{\cdot}$

EPR measurements: EPR spectra were recorded at room temperature on a Bruker ESP-300E(X band, 9.8 GHz) with parameters setting as shown below: receiver gain=30n; receiver phase=0deg; receiver harmonic=1; field modulation frequency=100000 Hz; microwave frequency[Hz]= 9.660469e^{+09}; field modulation amplitude [T]= 0.00016; receiver time constant[S] = 0.32768; microwave power= 0.015 W; receiver offset [%FS]=0; TEMP (2,2,6,6-tetramethylpiperidin-4-one hydrochloride) was employed as a radical trapping agent for singlet oxygen and (DMPO) 5,5-dimethyl-1-pyrroline N-oxide as trapping agent for iodine radical[S3].

The reaction under standard condition (**1**, NH_4SCN, I_2, O_2) in ACN was irradiated with blue LED light for 1 hr in the presence of TEMP and DMPO to obtain the EPR signals shown in **Figure S1** correspond to singlet oxygen and iodine radical, respectively. This result indicates that singlet oxygen and iodine radical were formed in the reaction solution. No singlet oxygen and iodine radical EPR signals were observed from the reaction solution under standard condition without irradiation.

EPR spectra of the reaction mixture

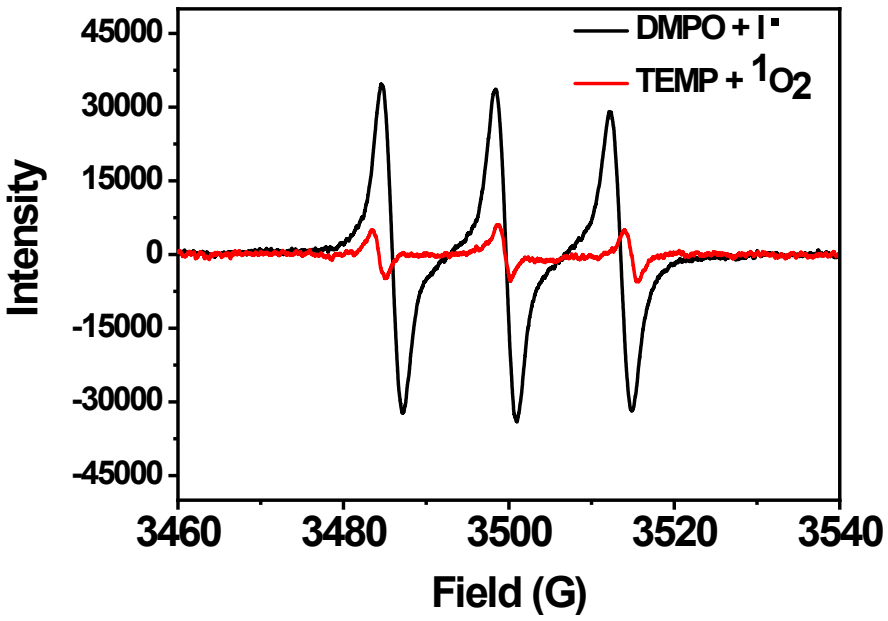


Figure S1: EPR spectra of the reaction mixture after irradiation.

Green chemistry metrics and EcoScale evaluation[S4, S5]

Table S1. Evaluation of green chemistry metrics of current protocol for synthesis of **4a** (*(E)*-(2-iodo-1-selenocyanatovinyl)benzene)

$$\text{Atom economy (\%) (AE)} = \frac{\text{Molecular mass of desired product}}{\text{Molecular mass of all reactants}} \times 100$$

$$\text{Reaction mass efficiency (\%) (RME)} = \frac{\text{Mass of desired product}}{\text{Mass of all reactants}} \times 100$$

Reactant 1	Phenylacetylene	1.02g	10.0 mmol	FW 102.13
Reactant 2	KSeCN	1.73g	12.0 mmol	FW 144.07
Reactant 3	I_2	2.53g	10.0 mmol	FW 253.81
Solvent	EtOH (15mL)	11.83g	----	----
Auxiliary	----	----	----	----
Recycled Solvent	EtOH (9.3mL)	7.34g	----	----
Product	(*E*)-(2-iodo-1-selenocyanatovinyl)benzene 4a/4a' = 5.3:1	1.74g	5.20 mmol	FW 334.02

Product yield = 52.16%

$$\text{E-factor} = \frac{1.02 + 1.73 + 2.53 + 11.83 - (7.34+1.74)}{1.74\text{g}} = 4.61 \text{ Kg waste/1 Kg of product}$$

$$\text{Atom economy} = \frac{334.02}{373.10} \times 100 = 89.53\%$$

$$\text{Atom efficiency} = 52.16\% \times 89.53\% / 100 = 46.7\%$$

$$\text{Carbon efficiency} = \frac{9}{8+1} \times 100 = 100\%$$

$$\text{Reaction mass efficiency} = \frac{1.74\text{g}}{1.02\text{g}+1.73\text{g}+2.53\text{g}} \times 100 = 67.44\%$$

Table S2. Eco scale calculation of current photochemical method for the synthesis of **4a** (*(E)*-(2-iodo-1-selenocyanatovinyl)benzene)

EcoScale = 100 - Sum of individual penalties

Score on EcoScale: >75, Excellent; >50, Acceptable; <50, Inadequate

A) Calculation of penalty points:

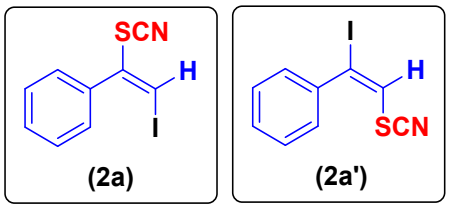
Parameters		Penalty points
1. Yield	(100-%yield)/2 = (100-52.16)/2 = 23.92	23.92
2. Price of reaction components (To obtain 10 mmol of end product)		
a. Phenylacetylene	= 1.02g = $0.82	
b. KSeCN	= 1.73g = $8.30	
c. Iodine	= 2.53g = $0.17	
d. Ethanol	= 15mL = $0.01	
Total price (USD) = $9.30		
Thus, expensive (> $10 and < $50)		0
3. Safety		
Solvent : Ethanol		
Toxic (T)		0
Highly flammable (F)		5
4. Technical Setup		
Inconventional activation technique (Photochemical activation)		2
5. Temperature and time		
Room temperature and <24h		1
6. Workup and purification		
Removal of solvent with bp <150^{o}C		0
Classical Chromatography		10
Total Penalty Points		41.92

B) EcoScale calculation:

EcoScale = 100- 41.92 = 58.08 (an acceptable synthesis)

Spectroscopic Data

(E)-(2-iodo-1-thiocyanatovinyl)benzene (2a)



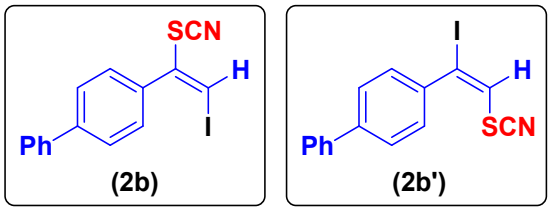
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45-7.39 (m, 2H), 7.33-7.32 (m, 1H), 7.29-7.27 (m, 2H), 6.87 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 138.8, 135.9, 130.8, 130.2, 130.0, 129.7, 129.0, 128.9, 128.7, 128.0, 127.9, 118.7, 109.6, 109.2, 107.7, 98.6 and 81.3;

EI-HREI calcd for C_9H_6INS (M+): 286.9266, found: 286.9255.

(E)-4-(2-iodo-1-thiocyanatovinyl)-1,1'-biphenyl (2b)



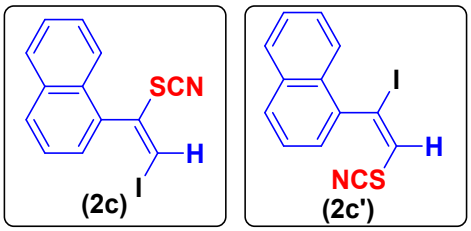
The product obtained as a pale-yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61-7.55 (m, 5H), 7.45 (t, *J*= 7.2 Hz, 2H), 7.39-7.35 (m, 2H), 6.90 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 142.9, 142.6, 139.7, 138.6, 137.6, 128.9, 128.6, 128.5, 128.0, 127.9, 127.5, 127.3, 127.1, 127.0, 122.7, 118.7, 109.7, 109.3, 107.4 and 98.5;

EI-HRFD calcd for $C_{15}H_{10}INS$ (M+): 362.9579, found: 362.9573.

(E)-1-(2-iodo-1-thiocyanatovinyl)naphthalene (2c)



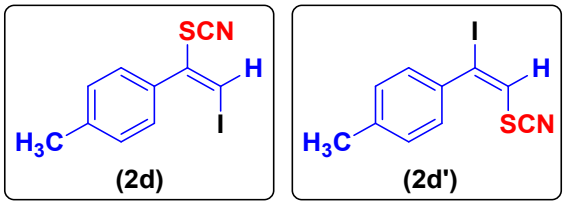
The product obtained as a pale-yellow powder.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96-7.87 (m, 2H), 7.65-7.53 (m, 2H), 7.49 (t, *J*= 9.2 Hz, 1H), 7.45-7.38 (m, 2H), 7.13 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 135.9, 133.9, 133.7, 133.5, 130.8, 130.4, 129.6, 129.3, 128.9, 128.7, 128.6, 127.9, 127.4, 127.2, 127.0, 126.8, 126.7, 125.7, 125.5, 125.3, 124.5, 124.1, 122.1, 109.2, 109.1, 95.2 and 83.9;

EI-HRFD calcd for $C_{13}H_8INS$ (M+): 336.9422, found: 336.9417.

(E)-1-(2-iodo-1-thiocyanatovinyl)-4-methylbenzene (2d)



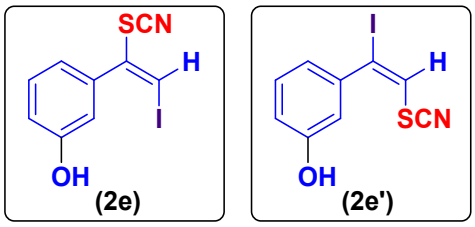
The product obtained as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17-7.13 (m, 4H), 6.82 (s, 1H), 2.35 (s, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 140.3, 135.9, 129.5, 129.3, 128.9, 127.9, 121.7, 118.0, 109.4, 99.0, 80.4 and 21.3;

EI-HRFD calcd for $C_{10}H_8INS$ (M+): 300.9422, found: 300.9417.

(E)-3-(2-iodo-1-thiocyanatovinyl)phenol (2e)



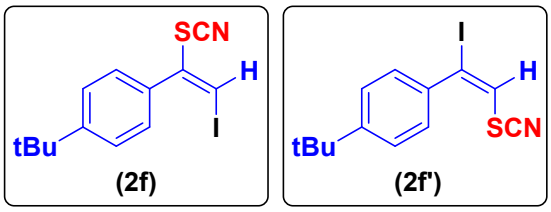
The product obtained as a yellow powder.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.19 (m, 2H), 6.97-6.88 (m, 3H), 6.83 (s, 1H), 6.00 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 156.1, 155.2, 144.5, 131.0, 129.9, 129.8, 124.6, 120.9, 116.1, 115.3, 114.9, 95.3, 94.3 and 80.9;

EI-HREI calcd for C_9H_6INOS (M+): 302.9215, found: 302.9209.

(E)-1-(tert-butyl)-4-(2-iodo-1-thiocyanatovinyl)benzene (2f)



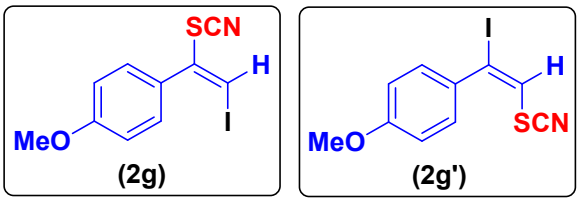
The product obtained as a pale-yellow oil.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.38 (d, *J*= 8.4 Hz, 2H), 7.19 (d, *J*= 8.4 Hz, 2H), 7.14 (s, 1H), 1.30 (s, 9H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 153.5, 153.4, 135.8, 132.6, 130.7, 128.8, 127.9, 127.8, 125.8, 125.6, 121.9, 118.0, 109.5, 99.1, 80.1 and 31.1;

EI-HRFD calcd for $C_{13}H_{14}INS$ (M+): 342.9892, found: 342.9886.

(E)-1-(2-iodo-1-thiocyanatovinyl)-4-methoxybenzene (2g)



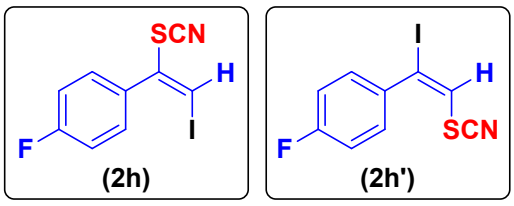
The product obtained as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (d, *J*= 8.4 Hz, 2H), 6.88 (d, *J*= 8.8 Hz, 2H), 6.81 (s, 2H), 3.85 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 160.8, 160.6, 132.6, 131.1, 130.8, 130.7, 129.7, 129.4, 127.8, 120.6, 117.5, 114.2, 113.9, 109.9, 109.5, 99.1, 79.8 and 55.4;

EI-HRFD calcd for $C_{10}H_8INOS$ (M+): 316.9371, found: 316.9366.

(E)-1-fluoro-4-(2-iodo-1-thiocyanatovinyl)benzene (2h)



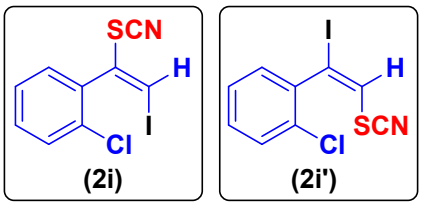
The product obtained as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.26 (m, 2H), 7.09-7.04 (m, 2H), 6.87 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 163.9 ($J_{C\text{-}F}$= 249.9 Hz), 163.7 ($J_{C\text{-}F}$= 250.6 Hz), 136.1, 134.9, 131.2, 130.1 ($J_{C\text{-}F}$= 8.6 Hz), 129.8 ($J_{C\text{-}F}$= 8.4 Hz), 123.1, 119.1, 116.1 ($J_{C\text{-}F}$= 21.9 Hz), 115.7 ($J_{C\text{-}F}$= 21.9 Hz), 109.4, 108.9, 106.0, 97.3 and 82.3;

EI-HRFD calcd for C_9H_5FINS (M+): 304.9171, found: 304.9166.

(E)-1-chloro-2-(2-iodo-1-thiocyanatovinyl)benzene (2i)



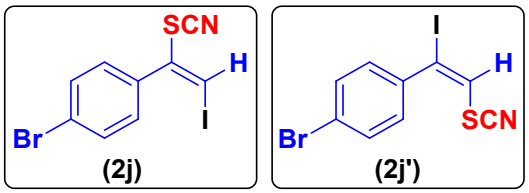
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.40 (m, 1H), 7.32-7.31 (m, 2H), 7.22-7.21 (m, 1H), 6.97 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 137.2, 131.8, 131.2, 130.7, 130.4, 130.3, 129.3, 127.5, 127.4, 127.0, 122.0, 108.7 and 94.5;

EI-HRFD calcd for C_9H_5ClINS (M+): 320.8876, found: 320.8870.

(E)-1-bromo-4-(2-iodo-1-thiocyanatovinyl)benzene (2j)



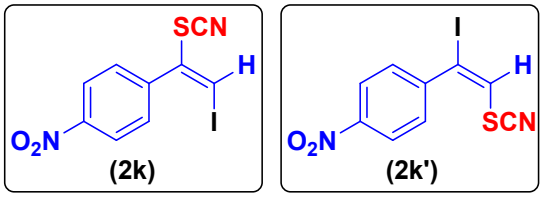
The product obtained as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J*= 8.4 Hz, 2H), 7.31 (d, *J*= 8.4 Hz, 2H), 6.88 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 137.7, 134.8, 132.3, 132.2, 131.8, 130.6, 129.5, 129.4, 124.6, 124.3, 123.8, 119.4, 108.8, 97.1 and 82.9;

EI-HRFD calcd for C_9H_5BrINS (M+): 364.8371, found: 364.8365.

(E)-1-(2-iodo-1-thiocyanatovinyl)-4-nitrobenzene (2k)



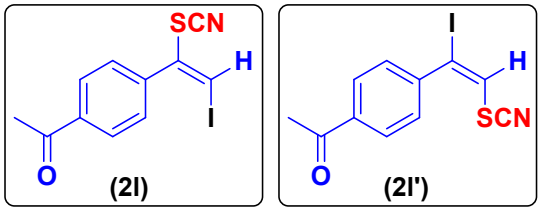
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J*= 9.2 Hz, 2H), 7.48 (d, *J*= 8.8 Hz, 2H), 7.02 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 148.1, 144.9, 130.3, 129.1, 128.9, 127.5, 124.2, 123.9, 121.2, 108.8, 108.1, 103.2, 95.3 and 86.4;

EI-HREI calcd for $C_9H_5IN_2O_2S$ (M+): 331.9116, found: 331.9111.

(E)-1-(4-(2-iodo-1-thiocyanatovinyl)phenyl)ethan-1-one (2l)



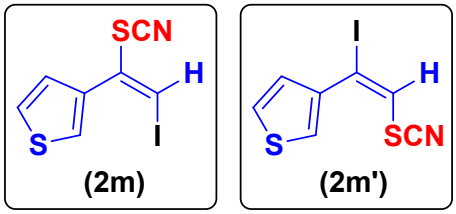
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J*= 8.4 Hz, 2H), 7.37 (d, *J*= 8.0 Hz, 2H), 6.93 (s, 1H), 2.58 (s, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 196.9, 196.8, 143.5, 143.1, 140.4, 137.7, 137.5, 129.4, 128.8, 128.6, 128.3, 125.4, 120.0, 109.2, 108.7, 105.5, 97.0, 84.0 and 26.6;

EI-HRFD calcd for $C_{11}H_8INOS$ (M+): 328.9371, found: 328.9366.

(E)-3-(2-iodo-1-thiocyanatovinyl)thiophene (2m)



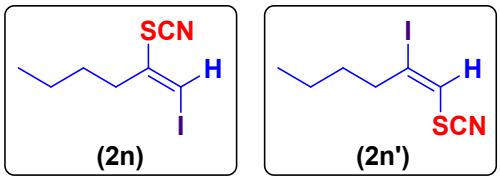
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.38 (m, 2H), 7.15-7.14 (m, 1H), 6.83 (s, 2H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 140.8, 138.9, 135.6, 128.2, 127.9, 127.4, 127.2, 126.8, 126.5, 126.3, 125.1, 118.1, 109.2, 91.8 and 80.9;

EI-HREI calcd for $C_7H_4INS_2$ (M+): 292.8830, found: 292.8824.

(E)-1-iodo-2-thiocyanatohex-1-ene (2n)



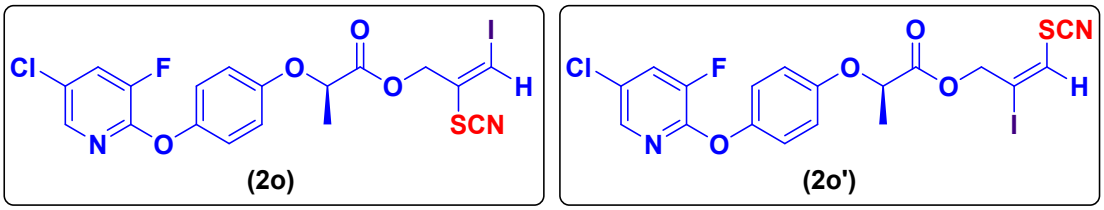
The product obtained as a light brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.86 (s, 1H), 2.58-2.50 (m, 2H), 1.60-1.47 (m, 2H), 1.41-1.28 (m, 2H), 0.94 (t, *J*= 7.2 Hz, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 132.1, 115.1, 112.7, 109.2, 109.0, 82.3, 78.8, 44.3, 39.8, 37.0, 30.7, 30.2, 28.9, 21.8, 21.3, 13.9 and 13.7;

EI-HRFD calcd for $C_7H_{10}INS$ (M+): 266.9579, found: 266.9573.

(E)-3-iodo-2-thiocyanatoallyl (R)-2-(4-((5-chloro-3-fluoropyridin-2-yl)oxy)phenoxy)propan-oate (2o)



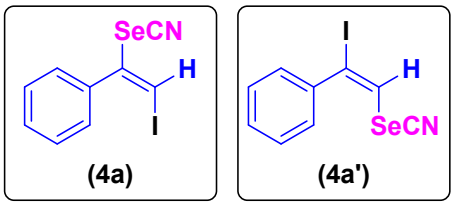
The product obtained as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84-7.82 (m, 1H), 7.48-7.45 (m, 1H), 7.07-7.03 (m, 2H), 6.92-6.89 (m, 2H), 5.03-4.94 (m, 1H), 4.91-4.77 (m, 2H), 1.67 (s, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 171.7, 171.5, 166.2, 154.5 ($J_{C\text{-}F}$= 250.6 Hz), 151.3, 151.2, 148.2($J_{C\text{-}F}$= 28.4 Hz) , 147.2, 145.6, 140.0 ($J_{C\text{-}F}$= 24.9 Hz), 125.1, 125.0, 122.6, 122.5 ($J_{C\text{-}F}$= 8.4 Hz), 121.7, 116.5, 109.0, 94.4, 85.3, 84.4, 75.7, 73.0, 72.8, 72.0, 67.2, 67.1 and 18.5;

EI-HRFD calcd for $C_{18}H_{13}ClFIN_2O_4S$ (M+): 533.9313, found: 533.9308.

(E)-(2-iodo-1-selenocyanatovinyl)benzene (4a)



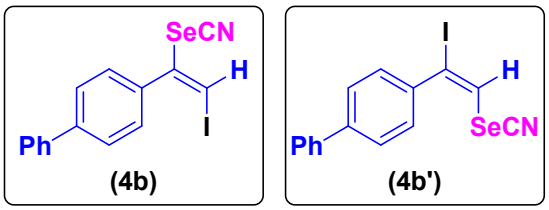
The product obtained as a light brown crystal.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.28 (m, 3H), 7.26-7.24 (m, 2H), 7.17 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 140.2, 137.2, 130.1, 130.0, 129.6, 129.2, 129.0, 128.9, 128.7, 128.4, 127.8, 127.4, 123.2, 116.4, 100.2, 95.7 and 81.7;

EI-HRFD calcd for C_9H_6INSe (M+): 334.8710, found: 334.8705.

(E)-4-(2-iodo-1-selenocyanatovinyl)-1,1'-biphenyl (4b)



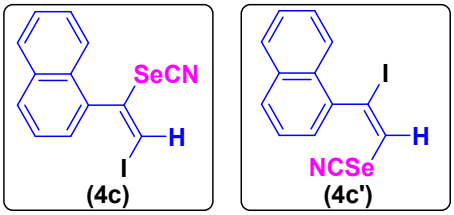
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.47 (m, 5H), 7.36 (t, *J*= 7.7 Hz, 3H), 7.25 (d, *J*= 8.4 Hz, 2H), 7.12 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 142.9, 139.6, 139.0, 129.4, 128.9, 128.3, 128.1, 128.0, 127.9, 127.7, 127.6, 127.3, 127.1, 127.0, 123.0, 116.3, 100.2, 95.6 and 81.8;

EI- HRFD calcd for $C_{15}H_{10}INSe$ (M+): 410.9023, found: 410.9018.

(E)-1-(2-iodo-1-selenocyanatovinyl)naphthalene (4c)



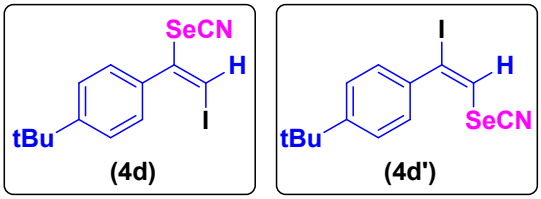
The product obtained as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94-7.90 (m, 3H), 7.63 (t, *J*= 8.8 Hz, 1H), 7.58-7.52 (m, 1H), 7.46 (s, 1H), 7.44-7.40 (s, 2H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 140.9, 137.0, 134.0, 133.9, 133.8, 131.8, 130.6, 130.5, 130.0, 129.2, 128.9, 128.7, 128.5, 128.4, 128.1, 127.6, 127.3, 127.1, 126.8, 126.7, 126.2, 125.5, 125.4, 125.0, 119.5, 118.3, 100.1, 94.2 and 92.6;

EI-HRFD calcd for $C_{13}H_8INSe$ (M+H): 384.8867, found: 384.8861.

(E)-1-(tert-butyl)-4-(2-iodo-1-selenocyanatovinyl)benzene (4d)



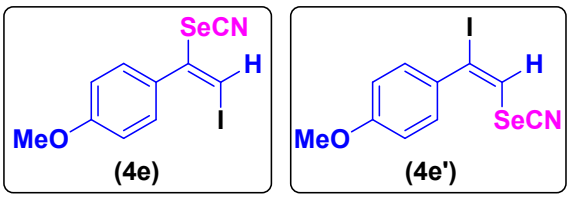
The product obtained as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (d, *J*= 8.4 Hz, 2H), 7.27 (d, *J*= 8.4 Hz, 2H), 6.88 (s, 1H), 1.36 (s, 9H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 137.3, 128.7, 127.6, 127.3, 126.1, 125.9, 125.7, 115.7, 102.8, 100.5, 96.0, 34.9, 31.1 and 31.0;

EI-HRFD calcd for $C_{13}H_{14}INSe$ (M+): 390.9336, found: 390.9331.

(E)-1-(2-iodo-1-selenocyanatovinyl)-4-methoxybenzene (4e)



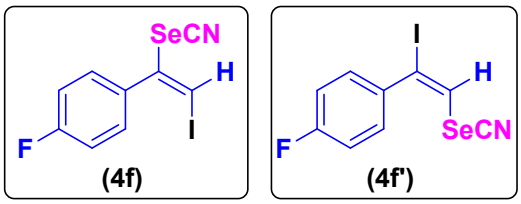
The product obtained as a reddish-brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 (d, *J*= 8.4 Hz, 2H), 7.17 (s, 1H), 6.86 (d, *J*= 8.4 Hz, 2H), 3.81 (s, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 159.7, 135.2, 130.2, 113.6, 96.6, 79.8 and 53.3;

EI-HRFD calcd for $C_{10}H_8INOSe$ (M+): 364.8816, found: 364.8811.

(E)-1-fluoro-4-(2-iodo-1-selenocyanatovinyl)benzene (4f)



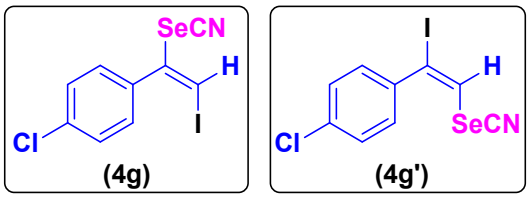
The product obtained as a reddish-brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (m, 2H), 7.18 (s, 1H), 7.09-7.05 (m, 2H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 163.8 ($J_{C\text{-}F}$= 250.7 Hz), 162.4, 136.3, 131.1, 131.0, 129.6 ($J_{C\text{-}F}$= 8.6 Hz), 123.3, 116.8, 116.4 ($J_{C\text{-}F}$= 22.0 Hz), 116.1, 115.7 ($J_{C\text{-}F}$= 21.9 Hz), 106.8, 101.1, 99.8, 94.6 and 82.9;

EI-HRFD calcd for C_9H_5FINSe (M+): 352.8616, found: 352.8611.

(E)-1-chloro-4-(2-iodo-1-selenocyanatovinyl)benzene (4g)



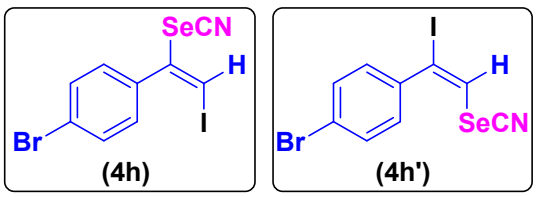
The product obtained as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (d, *J*= 7.7 Hz, 2H), 7.21 (d, *J*= 8.4 Hz, 2H), 7.19 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 138.7, 138.6, 136.1, 135.7, 129.4, 129.0, 128.9, 128.8, 124.1, 117.0, 106.6, 101.1, 99.8 and 94.4;

EI-HRFD calcd for $C_9H_5ClINSe$ (M+): 368.8320, found: 368.8312.

(E)-1-bromo-4-(2-iodo-1-selenocyanatovinyl)benzene (4h)



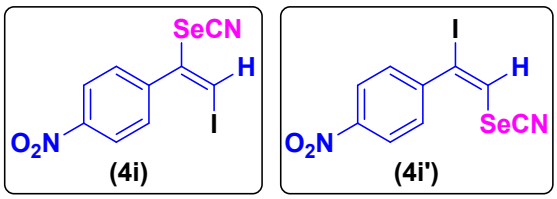
The product obtained as a pale-yellow oil.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.52 (d, *J*= 8.4 Hz, 2H), 7.19 (s, 1H), 7.14 (d, *J*= 8.4 Hz, 2H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 139.1, 132.4, 131.8, 129.2, 129.0, 124.4, 124.1, 117.0, 99.7 and 94.5;

EI-HRFD calcd for $C_9H_5BrINSe$ (M+): 412.7815, found: 412.7806.

(E)-1-(2-iodo-1-selenocyanatovinyl)-4-nitrobenzene (4i)



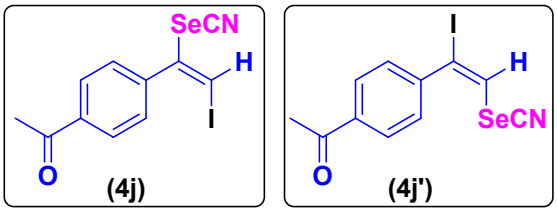
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, *J*= 8.8 Hz, 2H), 7.47 (d, *J*= 8.8 Hz, 2H), 7.34 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 148.2, 146.2, 128.7, 128.1, 124.4, 124.0, 118.6, 99.0 and 93.4;

EI-HRFD calcd for $C_9H_5IN_2O_2Se$ (M+): 379.8561, found: 379.8556.

(E)-1-(4-(2-iodo-1-selenocyanatovinyl)phenyl)ethan-1-one (4j)



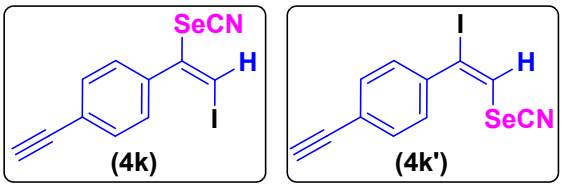
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J*= 8.4 Hz, 2H), 7.37 (d, *J*= 8.4 Hz, 2H), 7.26 (s, 1H), 2.60 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 196.7, 144.4, 137.9, 129.1, 128.7, 128.3, 128.0, 127.8, 125.9, 117.5, 99.6, 94.6 and 26.7;

EI-HRFD calcd for $C_{11}H_8INOSe$ (M+): 376.8816, found: 376.8811.

(E)-1-ethynyl-4-(2-iodo-1-selenocyanatovinyl)benzene (4k)



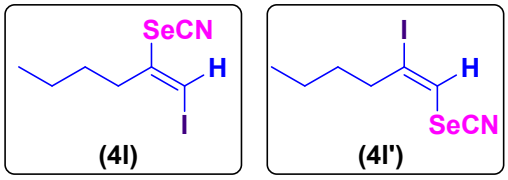
The product obtained as a light brown solid.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.49 (d, *J*= 7.7 Hz, 2H), 7.22 (d, *J*= 7.7 Hz, 2H), 7.20 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 140.3, 140.0, 132.7, 132.6, 132.3, 128.9, 127.7, 127.5, 124.4, 124.0, 123.4, 116.9, 107.2, 101.1, 99.9, 94.8, 82.4 and 79.4;

EI-LRFD calcd for $C_{11}H_6INSe$ (M+): 358.8710, found: 358.8705.

(E)-1-iodo-2-selenocyanatohex-1-ene (4l)



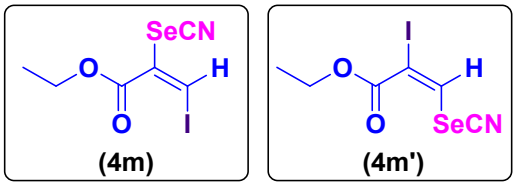
The product obtained as a brown oil.

^{1}H NMR (700 MHz, $CDCl_3$): δ 6.78 (s, 1H), 2.49 (t, *J*= 7.0 Hz, 2H), 1.52-1.48 (m, 2H), 1.36-1.33 (m, 2H),0.96-0.92 (m, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 131.2, 111.7, 104.4, 100.7, 84.2, 78.8, 44.4, 41.9, 39.0, 30.8, 30.3, 29.4, 21.9, 21.4, 14.0 and 13.8;

ESI-HRMS calcd for $C_7H_{10}INSe$ (M+): 314.9023, found: 314.9023.

ethyl (E)-3-iodo-2-selenocyanatoacrylate (4m)



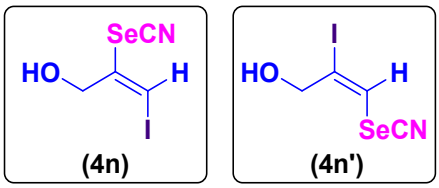
The product obtained as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (s, 1H), 4.32 (q, *J*= 7.2 Hz, 2H), 1.38-1.33 (m, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 166.2, 163.8, 142.7, 105.4, 86.6, 86.1, 76.2, 64.5, 62.9, 14.0 and 13.9;

EI-HRFD calcd for $C_6H_6INO_2Se$ (M+): 330.8608, found: 330.8603.

(E)-3-iodo-2-selenocyanatoprop-2-en-1-ol (4n)



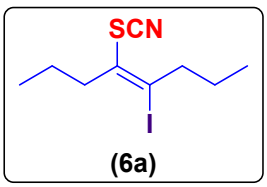
The product obtained as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.01 (s, 1H), 4.25 (s, 2H), 2.13 (s, 1H),;

^{13}C NMR (175 MHz, $CDCl_3$): δ 104.0, 79.8 and 70.7;

EI-HRFD calcd for C_4H_4INOSe (M+): 288.8503, found: 288.8500.

(E)-4-iodo-5-thiocyanatooct-4-ene (6a)



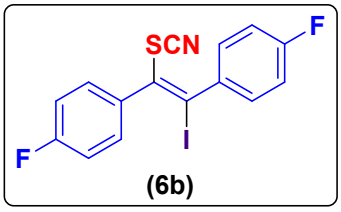
The product obtained as a brown oil.

^{1}H NMR (700 MHz, $CDCl_3$): δ 2.74-2.69 (m, 4H), 1.66 (q, *J*= 7.7 Hz, 2H), 1.58 (q, *J*= 7.0 Hz, 2H), 0.97 (t, *J*= 7.0 Hz, 3H), 0.89 (t, *J*= 7.7 Hz, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 125.0, 112.5, 1096, 101.9, 52.4, 45.5, 44.4, 22.3, 21.5, 20.7, 13.2, 12.7 and 12.6;

EI-HRFD calcd for $C_9H_{14}INS$ (M+): 294.9892, found: 294.9886.

(E)-4,4'-(1-iodo-2-thiocyanatoethene-1,2-diyl)bis(fluorobenzene) (6b)



(6b)

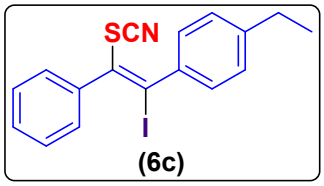
The product obtained as a pale-yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02-7.45 (m, 1H), 7.44-7.38 (m, 1H), 7.37-7.35 (m, 1H), 7.20-7.15 (m, 2H), 7.14-7.08 (m, 2H), 7.07-6.7 (m, 1H);

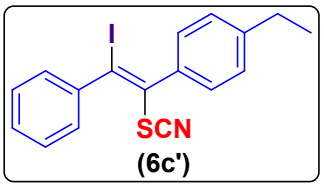
^{13}C NMR (175 MHz, $CDCl_3$): δ 167.5, 166.1, 163.8 (J_{C-F}= 200.4 Hz), 163.6, 162.7, 162.4 (J_{C-F}= 199.9 Hz), 162.2, 161.9, 138.4, 138.3, 137.9, 136.1, 135.9, 132.7 (J_{C-F}= 186.9 Hz), 131.6, 131.3 (J_{C-F}= 185.7 Hz) , 131.2 (J_{C-F}= 45.9 Hz), 130.2 (J_{C-F}= 46.1 Hz), 129.3, 128.5, 166.4, 116.1, 116.1, 115.9 (J_{C-F}= 21.9 Hz), 115.4 (J_{C-F}= 21.8 Hz), 109.8, 108.8, 100.9 and 100.3;

EI-HRFD calcd for $C_{15}H_8F_2INS$ (M+): 398.9390, found: 398.9385.

(E)-1-ethyl-4-(1-iodo-2-phenyl-2-thiocyanatovinyl)benzene (6c)



(6c)



(6c')

The product obtained as a pale-yellow crystal.

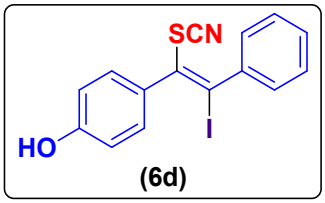
^{1}H NMR (700 MHz, $CDCl_3$): δ 7.52-7.50 (m, 1H), 7.47-7.43 (m, 2H), 7.40-7.39 (m, 2H), 7.34-7

31 (m, 2H), 7.27-7.26 (m, 1H), 2.75-2.69 (m, 2H), 1.31-1.27 (m, 3H);

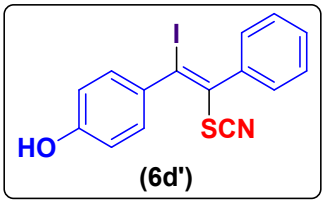
^{13}C NMR (175 MHz, $CDCl_3$): δ 146.0, 142.2, 140.4, 139.4, 137.6, 129.7, 129.2, 129.1, 128.9, 128.4, 128.3, 128.1, 109.4, 109.3, 101.3, 100.6, 28.7, 15.1 and 15.0;

EI-HRFD calcd for $C_{17}H_{14}INS$ (M+): 390.9892, found: 390.9886.

(E)-4-(2-iodo-2-phenyl-1-thiocyanatovinyl)phenol (6d)



(6d)



(6d')

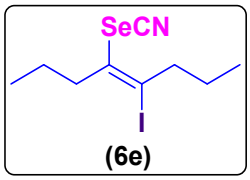
The product obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.25 (m, 2H), 7.24-7.22 (m, 3H), 7.21-7.20 (m, 2H), 6.99-6.80 (m, 2H), 3.73 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 157.9, 142.1, 131.1, 130.6, 129.2, 129.0, 128.7, 127.9, 127.8, 115.3, 115.1, 109.7, 99.6, 49.0, 48.8 and 48.3;

EI-HRFD calcd for $C_{15}H_{10}INOS$ (M+): 378.9528, found: 378.9522.

(E)-4-iodo-5-selenocyanatooct-4-ene (6e)



(6e)

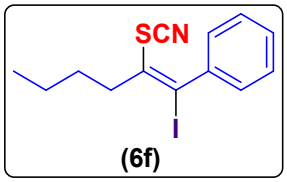
The product obtained as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.78-2.68 (m, 2H), 1.65 (q, *J*= 7.7 Hz, 2H), 1.60 (q, *J*= 7.0 Hz, 2H), 0.98 (t, *J*= 7.0 Hz, 3H), 0.90 (t, *J*= 7.7 Hz, 3H);

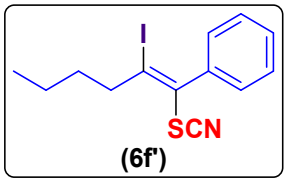
^{13}C NMR (175 MHz, $CDCl_3$): δ 125.1, 109.9, 101.9, 100.9, 52.5, 47.8, 46.6, 41.6, 22.3, 21.6, 21.1, 13.2, 12.8 and 12.7;

EI-HRFD calcd for $C_9H_{14}INSe$ (M+): 342.9336, found: 342.9886.

(E)-(1-iodo-2-thiocyanatohex-1-en-1-yl)benzene (6f)



(6f)



(6f')

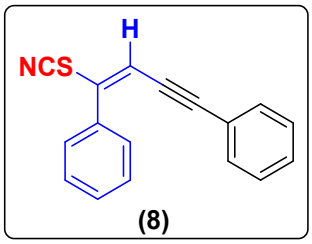
The product obtained as a light brown liquid.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.36-7.27 (m, 3H), 7.19 (t, *J*= 8.4 Hz, 2H), 2.91 (t, *J*= 7.7 Hz, 2H), 1.73 (t, *J*= 7.7 Hz, 2H), 1.51 (t, *J*= 7.0 Hz, 2H), 1.01 (t, *J*= 7.7 Hz, 3H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 142.4, 136.7, 129.2, 129.1, 128.8, 128.5, 128.0, 127.9, 109.6, 98.8, 41.6, 29.5, 22.0 and 13.9;

EI-HRFD calcd for $C_{13}H_{14}INS$ (M+): 342.9892, found: 342.9886.

(E)-(1-thiocyanatobut-1-en-3-yne-1,4-diyl)dibenzene (8)



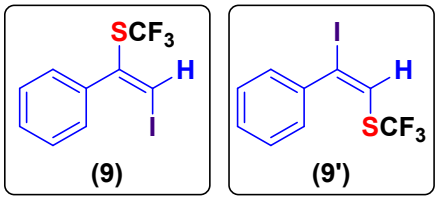
The product obtained as a pale yellow oil.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.39-7.37 (m, 2H), 7.36-7.34 (m, 5H), 7.28-7.24 (m, 3H), 6.87 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 138.9, 135.9, 130.8, 130.2, 130.0, 129.1, 128.9, 128.0, 118.8, 109.3, 109.2 98.6, and 81.2;

EI-HRFD calcd for $C_{17}H_{11}NS$ (M+): 261.0612, found: 342.0607.

(E)-(2-iodo-1-phenylvinyl)(trifluoromethyl)sulfane (9)



The product obtained as a yellow liquid.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.45-7.41 (m, 1H), 7.40-7.27 (m, 4H), 6.87 (s, 1H);

^{13}C NMR (175 MHz, $CDCl_3$): δ 139.7, 138.7 ($J_{C\text{-}F}$= 34.9 Hz), 135.8, 130.7, 130.1, 129.9, 129.6, 129.7, 128.9, 128.8, 128.6, 127.9, 122.9, 118.6 ($J_{C\text{-}F}$= 329.9 Hz), 109.2, 109.1 ($J_{C\text{-}F}$= 8.4 Hz), 98.6 and 81.3;

EI-HRFD calcd for $C_9H_6F_3IS$ (M+): 329.9187, found: 329.9182.

References:

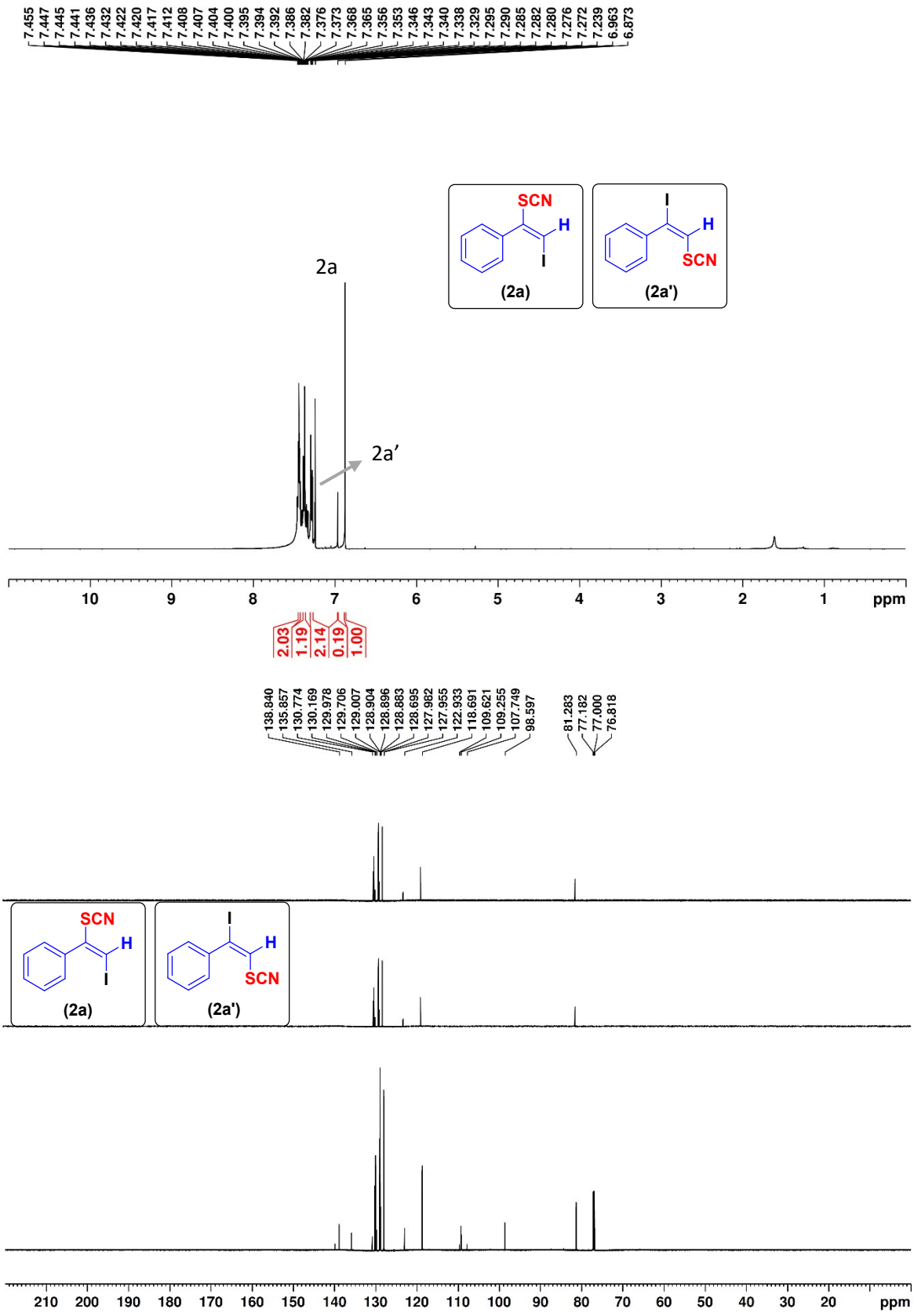
S1. J. E. Hein, J. C. Tripp, L. B. Krasnova, K. B. Sharpless, and V. V. Fokin, *Angew. Chem. Int. Ed.,* 2009, **48**, 8018 –8021.

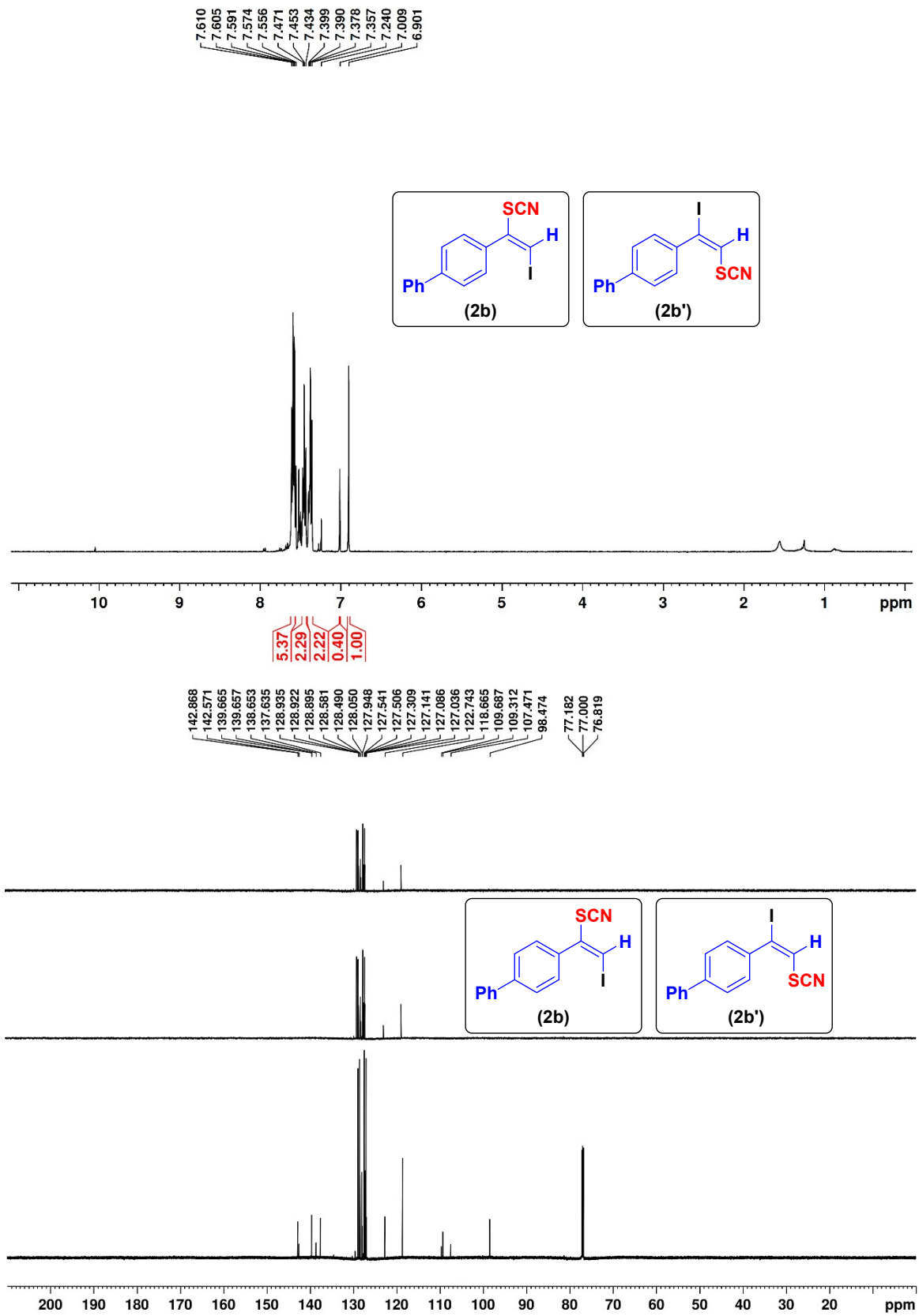
S2. M. Koyama, N. Ohtani, F. Kai, I. Moriguchi, and S. Inouye, *J. Med. Chem.,* 1987, **30**, 552-562.

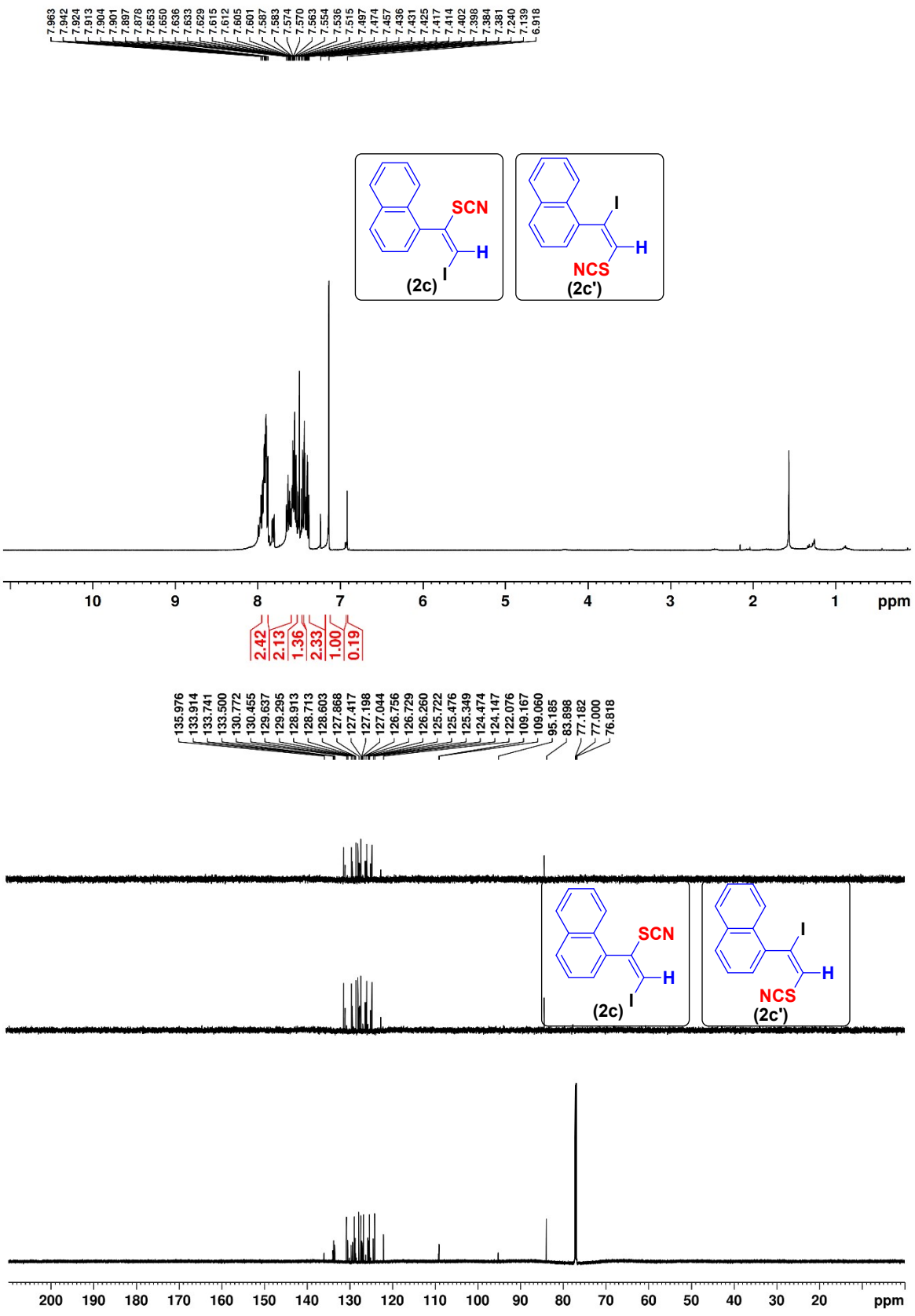
S3. A. Fernando, S. Parajuli, K. K. Barakoti, W. Miao, and M. A. Alpuche-Aviles, *J. Mex. Chem. Soc.,* 2019, **63**, 3.

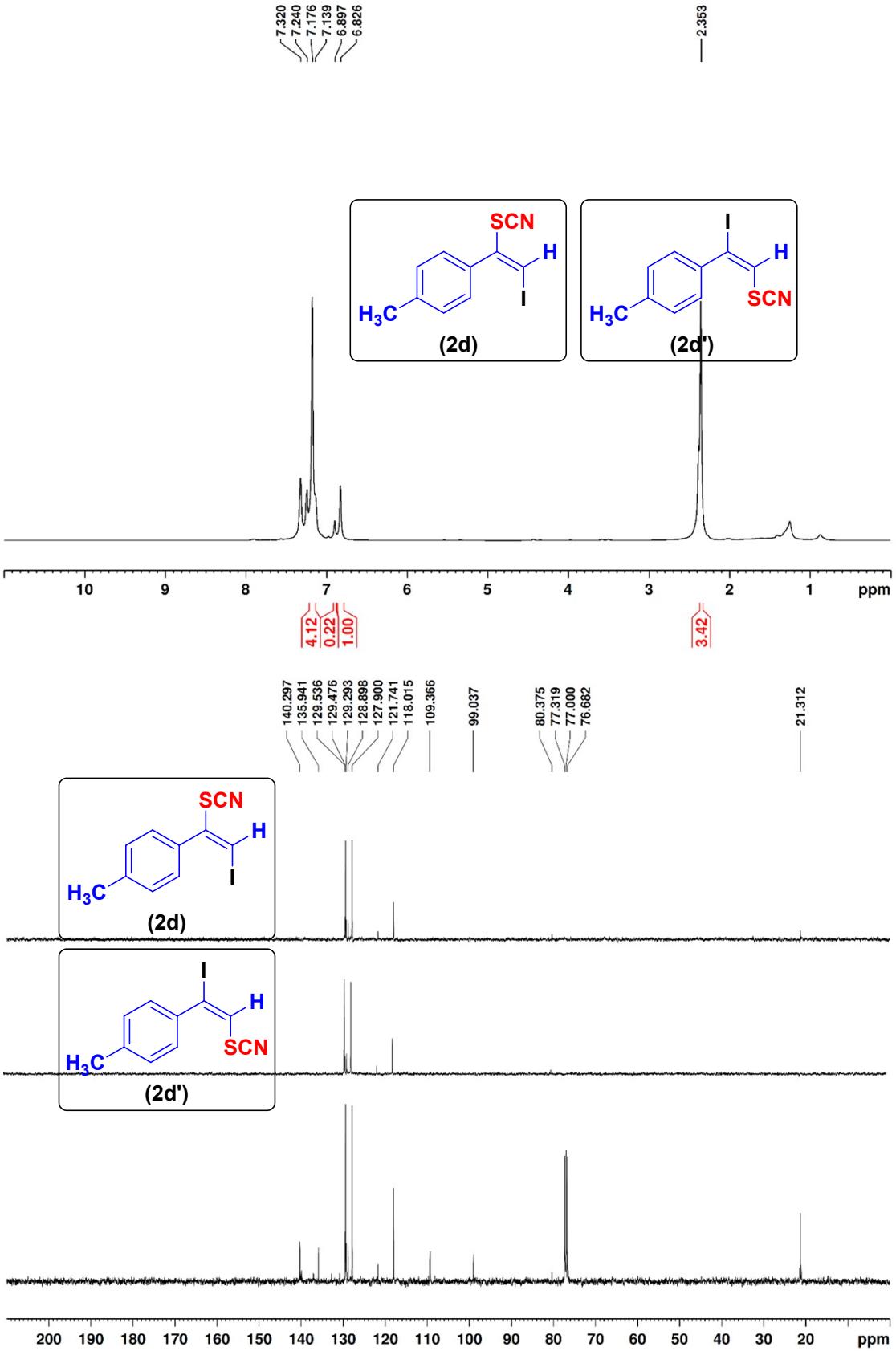
S4. (a) V. P. Charpe, A. Sagadevan, K. C. Hwang, *Green Chem.,* 2020, **22**, 4426–4432; (b) V. P. Charpe, A. Ragupathi, A. Sagadevan, Y. S. Ho, M. J. Cheng and K. C. Hwang, *Chem. Eur. J.,* 2023, **29**, e202300110; (c) V. P. Charpe, M. Gupta and K. C. Hwang, *ChemSusChem.,* 2022, **15**, e202200957.

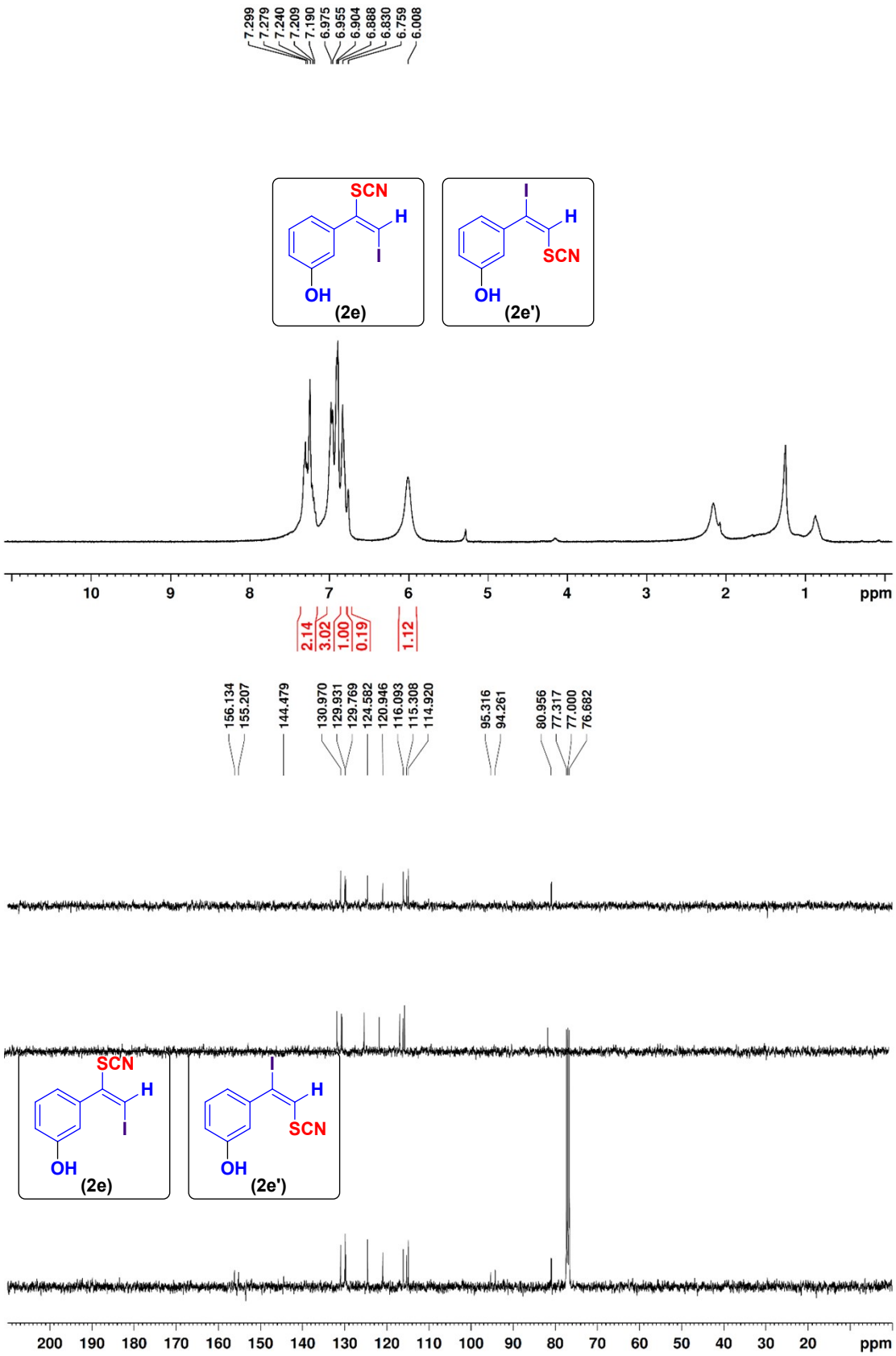
S5. (a) V. P. Charpe, M. Gupta and K. C. Hwang, *Green Chem.,* 2024, **26**, 1329; (b) M. Gupta, V. P. Charpe, and K. C. Hwang, *ACS Sustainable Chem. Eng.,* 2024, **12**, 16297-16307.

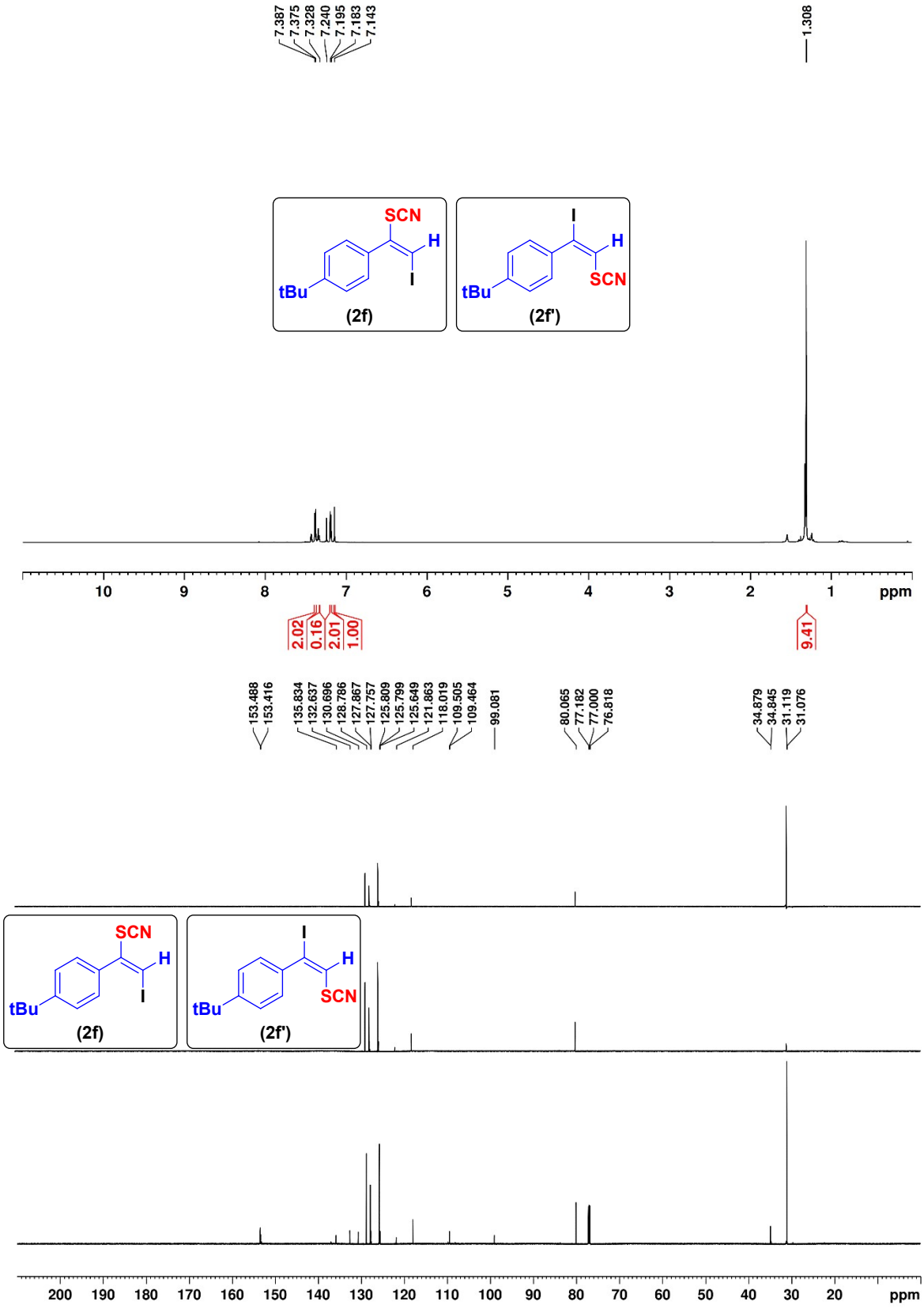

7.455
7.447
7.445
7.441
7.436
7.432
7.422
7.420
7.417
7.412
7.408
7.407
7.404
7.400
7.395
7.394
7.392
7.386
7.382
7.376
7.373
7.368
7.365
7.356
7.353
7.346
7.343
7.340
7.338
7.329
7.295
7.290
7.285
7.282
7.280
7.276
7.272
7.239
6.963
6.873
SCN
H
I
(2a)
I
H
SCN
(2a')
2a
2a’
10
9
8
7
6
5
4
3
2
1
ppm
2.03
1.19
2.14
0.19
1.00
138.840
135.857
130.774
130.169
129.978
129.706
129.007
128.904
128.896
128.883
128.695
127.982
127.955
122.933
118.691
109.621
109.255
107.749
98.597
81.283
77.182
77.000
76.818
SCN
H
I
(2a)
I
H
SCN
(2a')
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

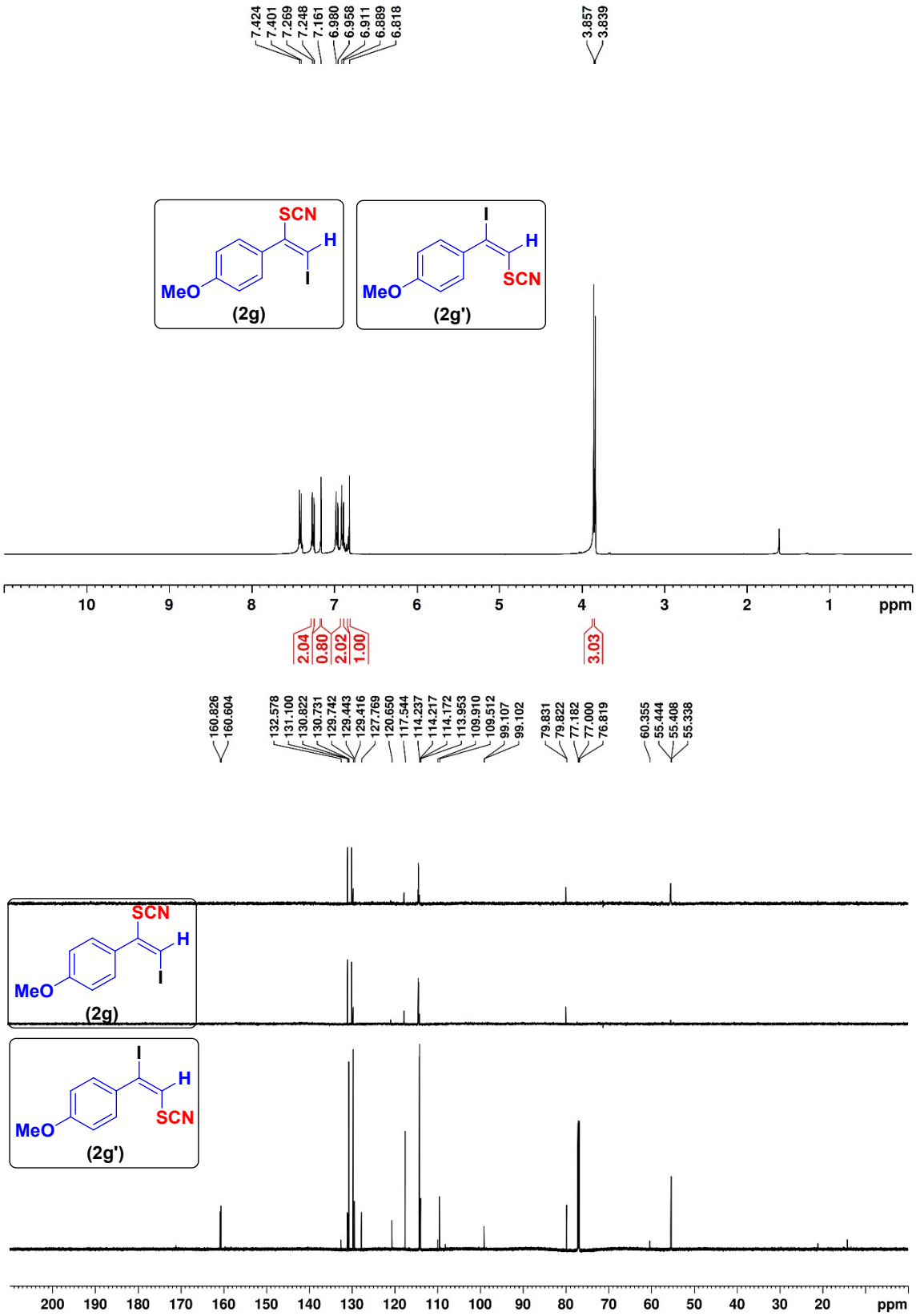

7.610
7.605
7.591
7.574
7.556
7.471
7.453
7.434
7.399
7.390
7.378
7.357
7.240
7.009
6.901
SCN
H
Ph
I
(2b)
I
H
Ph
SCN
(2b')
10
9
8
7
6
5
4
3
2
1
ppm
5.37
2.29
2.22
0.40
1.00
142.868
142.571
139.665
139.657
138.653
137.635
128.935
128.922
128.895
128.581
128.490
128.050
127.948
127.541
127.506
127.309
127.141
127.086
127.036
122.743
118.665
109.687
109.312
107.471
98.474
77.182
77.000
76.819
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

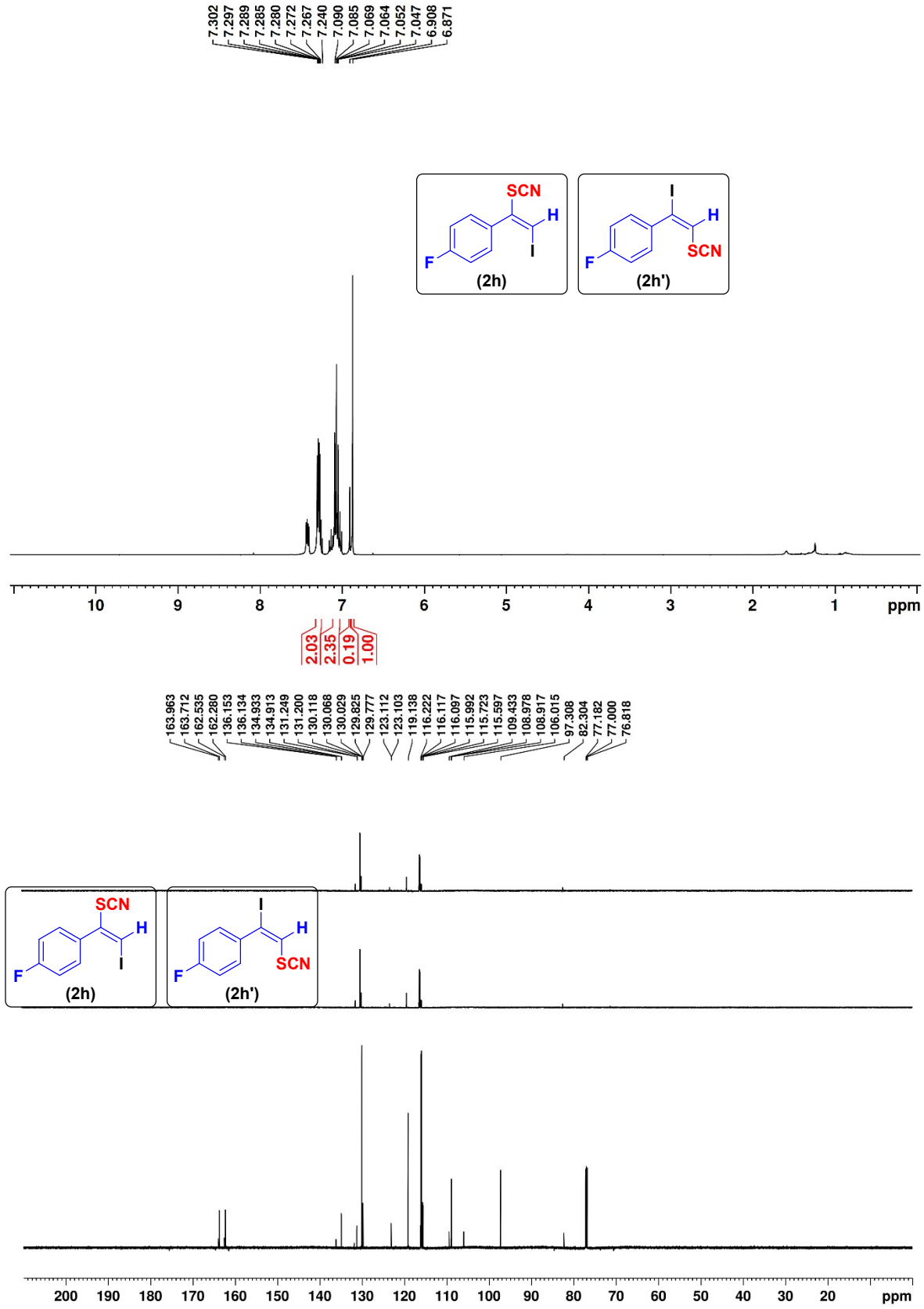

7.963
7.942
7.924
7.913
7.904
7.901
7.897
7.878
7.653
7.650
7.636
7.633
7.629
7.615
7.612
7.605
7.601
7.587
7.583
7.574
7.570
7.563
7.554
7.536
7.515
7.497
7.474
7.457
7.436
7.431
7.425
7.417
7.414
7.402
7.398
7.384
7.381
7.240
7.139
6.918
SCN
H
I
(2c)
I
H
NCS
(2c')
10
9
8
7
6
5
4
3
2
1
ppm
2.42
2.13
1.36
2.33
1.00
0.19
135.976
133.914
133.741
133.500
130.772
130.455
129.637
129.295
128.913
128.713
128.603
127.868
127.417
127.198
127.044
126.756
126.729
126.260
125.722
125.476
125.349
124.474
124.147
122.076
109.167
109.060
95.185
83.898
77.182
77.000
76.818
SCN
H
I
(2c)
I
H
NCS
(2c')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

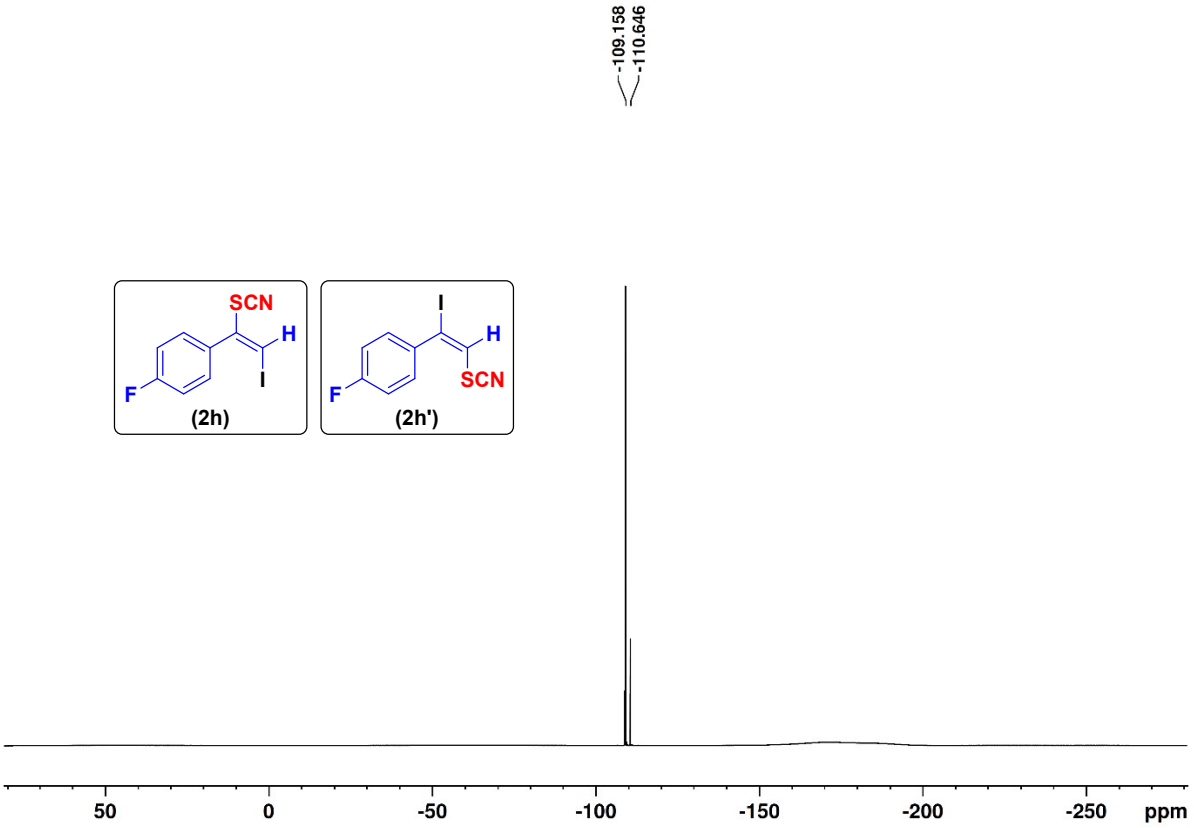

7.320
7.240
7.176
7.139
6.897
6.826
2.353
SCN
H
I
H3C
(2d)
I
H
SCN
H3C
(2d')
10
9
8
7
6
5
4
3
2
1
ppm
4.12
0.22
1.00
3.42
140.297
135.941
129.536
129.476
129.293
128.898
127.900
121.741
118.015
109.366
99.037
80.375
77.319
77.000
76.682
21.312
SCN
H
I
H3C
(2d)
I
H
SCN
H3C
(2d')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

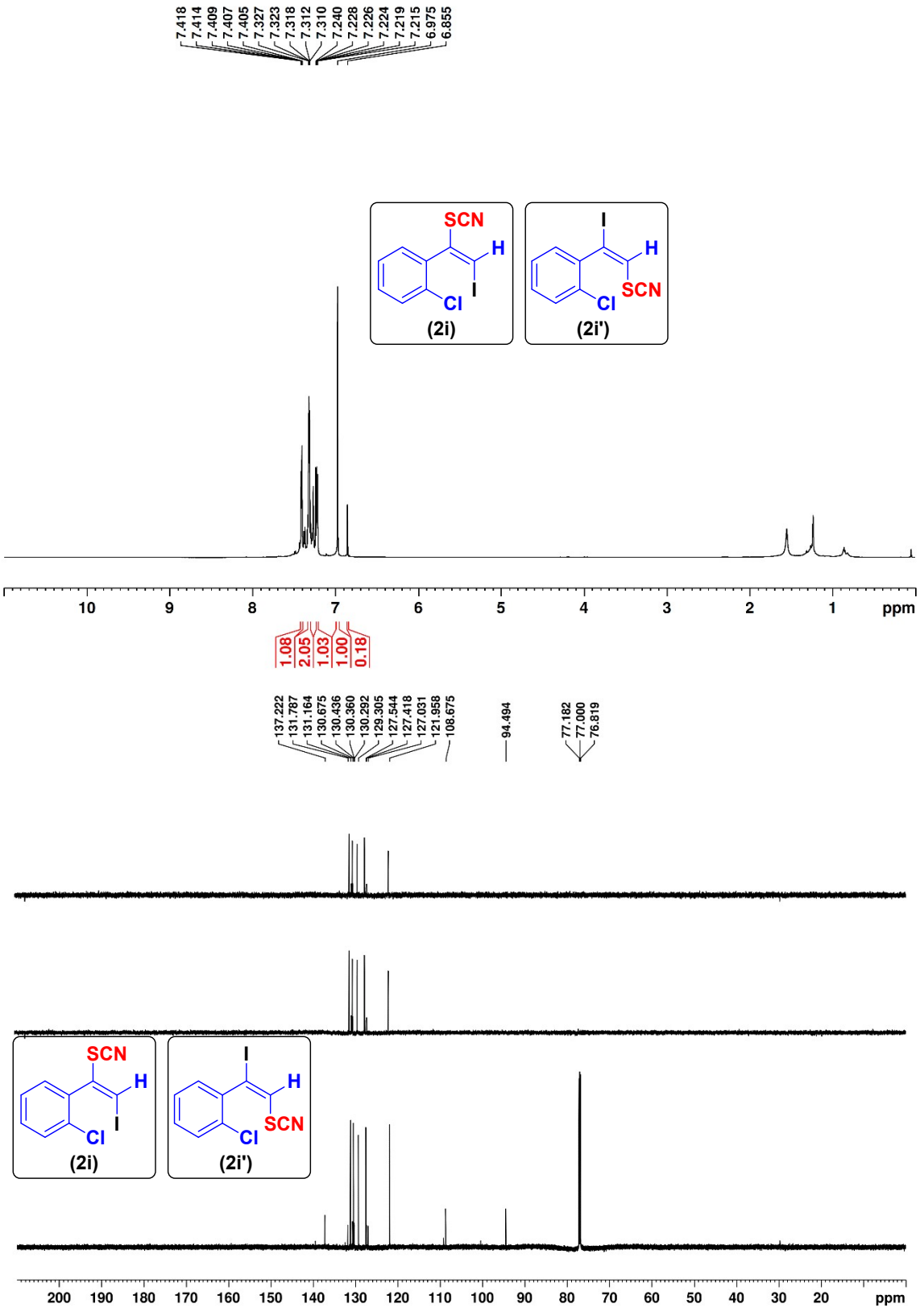

7.299
7.279
7.240
7.209
7.190
6.975
6.955
6.904
6.888
6.830
6.759
6.008
SCN
H
I
OH
(2e)
I
H
SCN
OH
(2e')
10
9
8
7
6
5
4
3
2
1
ppm
2.14
3.02
1.00
0.19
1.12
156.134
155.207
144.479
130.970
129.931
129.769
124.582
120.946
116.093
115.308
114.920
95.316
94.261
80.956
77.317
77.000
76.682
SCN
H
I
OH
(2e)
I
H
SCN
OH
(2e')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

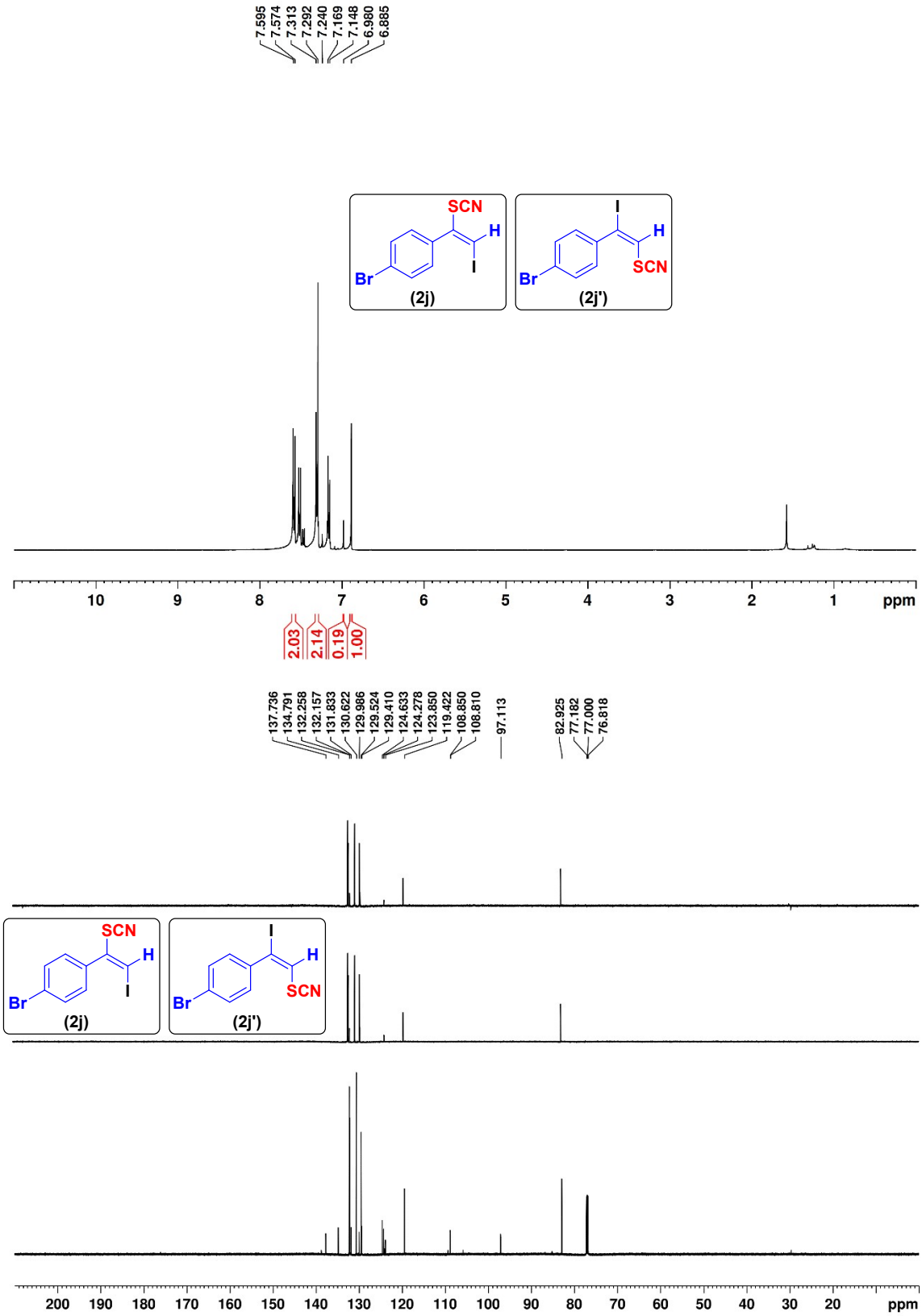

7.387
7.375
7.328
7.240
7.195
7.183
7.143
1.308
SCN
H
I
tBu
(2f)
I
H
SCN
tBu
(2f')
10
9
8
7
6
5
4
3
2
1
ppm
2.02
0.16
2.01
1.00
9.41
153.488
153.416
135.834
132.637
130.696
128.786
127.867
127.757
125.809
125.799
125.649
121.863
118.019
109.505
109.464
99.081
80.065
77.182
77.000
76.818
34.879
34.845
31.119
31.076
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

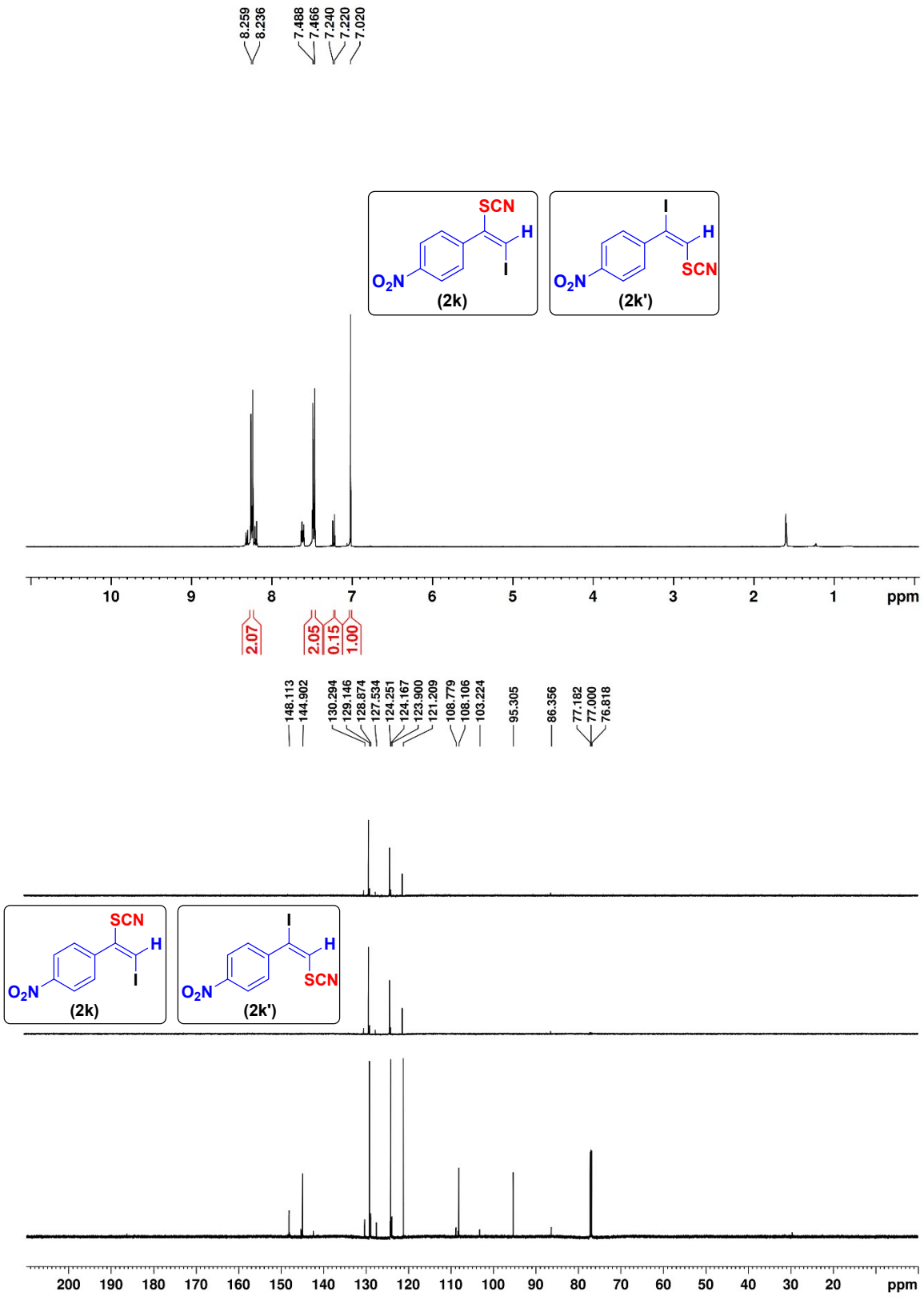

7.424
7.401
7.269
7.248
7.161
6.980
6.958
6.911
6.889
6.818
3.857
3.839
SCN
H
I
MeO
(2g)
I
H
SCN
MeO
(2g')
10
9
8
7
6
5
4
3
2
1
ppm
2.04
0.80
2.02
1.00
3.03
160.826
160.604
132.578
131.100
130.822
130.731
129.742
129.443
129.416
127.769
120.650
117.544
114.237
114.217
114.172
113.953
109.910
109.512
99.107
99.102
79.831
79.822
77.182
77.000
76.819
60.355
55.444
55.408
55.338
SCN
H
I
MeO
(2g)
I
H
SCN
MeO
(2g')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

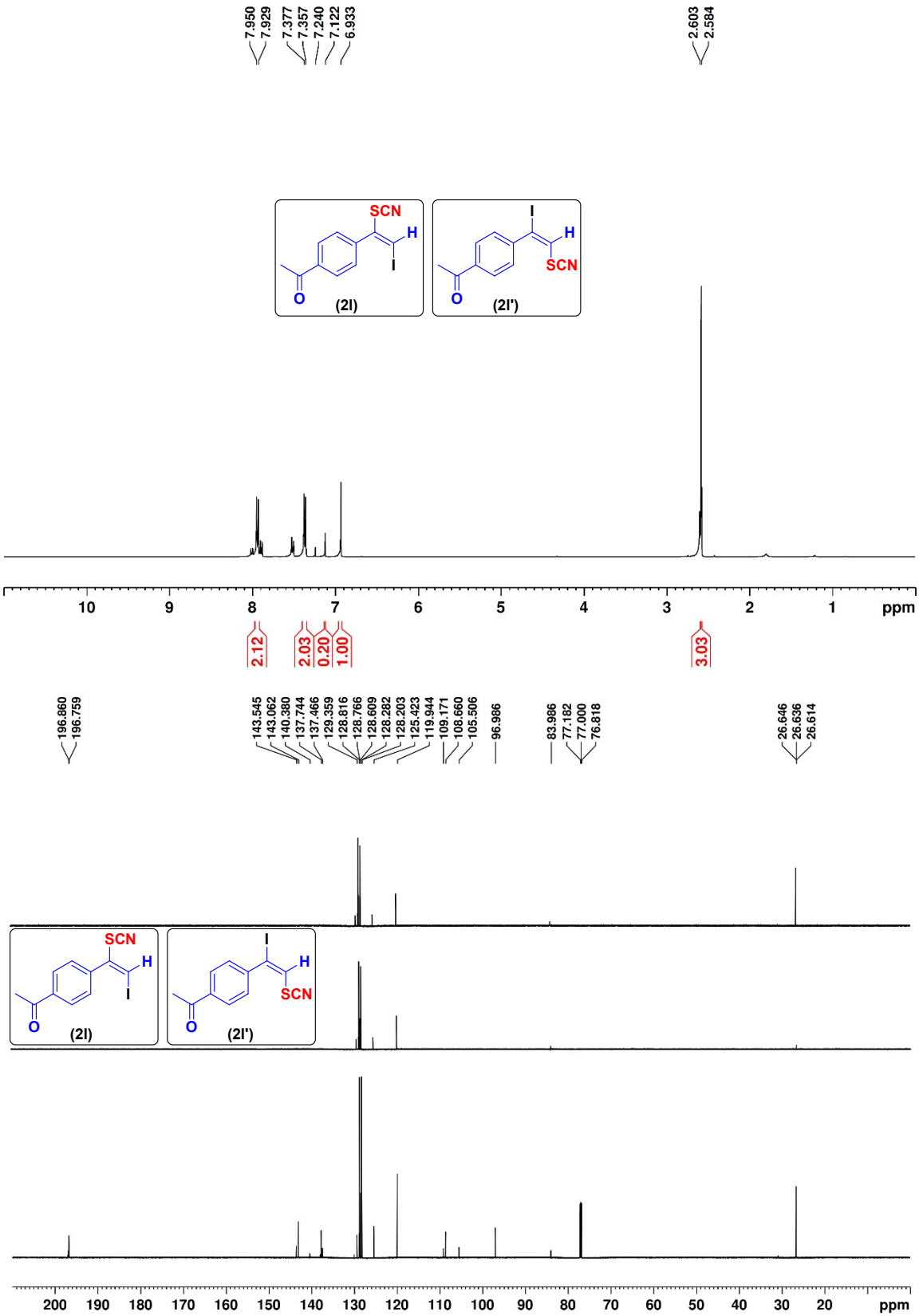

7.302
7.297
7.289
7.285
7.280
7.272
7.267
7.240
7.090
7.085
7.069
7.064
7.052
7.047
6.908
6.871
SCN
H
F
I
(2h)
I
H
SCN
F
(2h')
10
9
8
7
6
5
4
3
2
1
ppm
2.03
2.35
0.19
1.00
163.963
163.712
162.535
162.280
136.153
136.134
134.933
134.913
131.249
131.200
130.118
130.068
130.029
129.825
129.777
123.112
123.103
119.138
116.222
116.117
116.097
115.992
115.723
115.597
109.433
108.978
108.917
106.015
97.308
82.304
77.182
77.000
76.818
SCN
H
F
I
(2h)
I
H
SCN
F
(2h')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

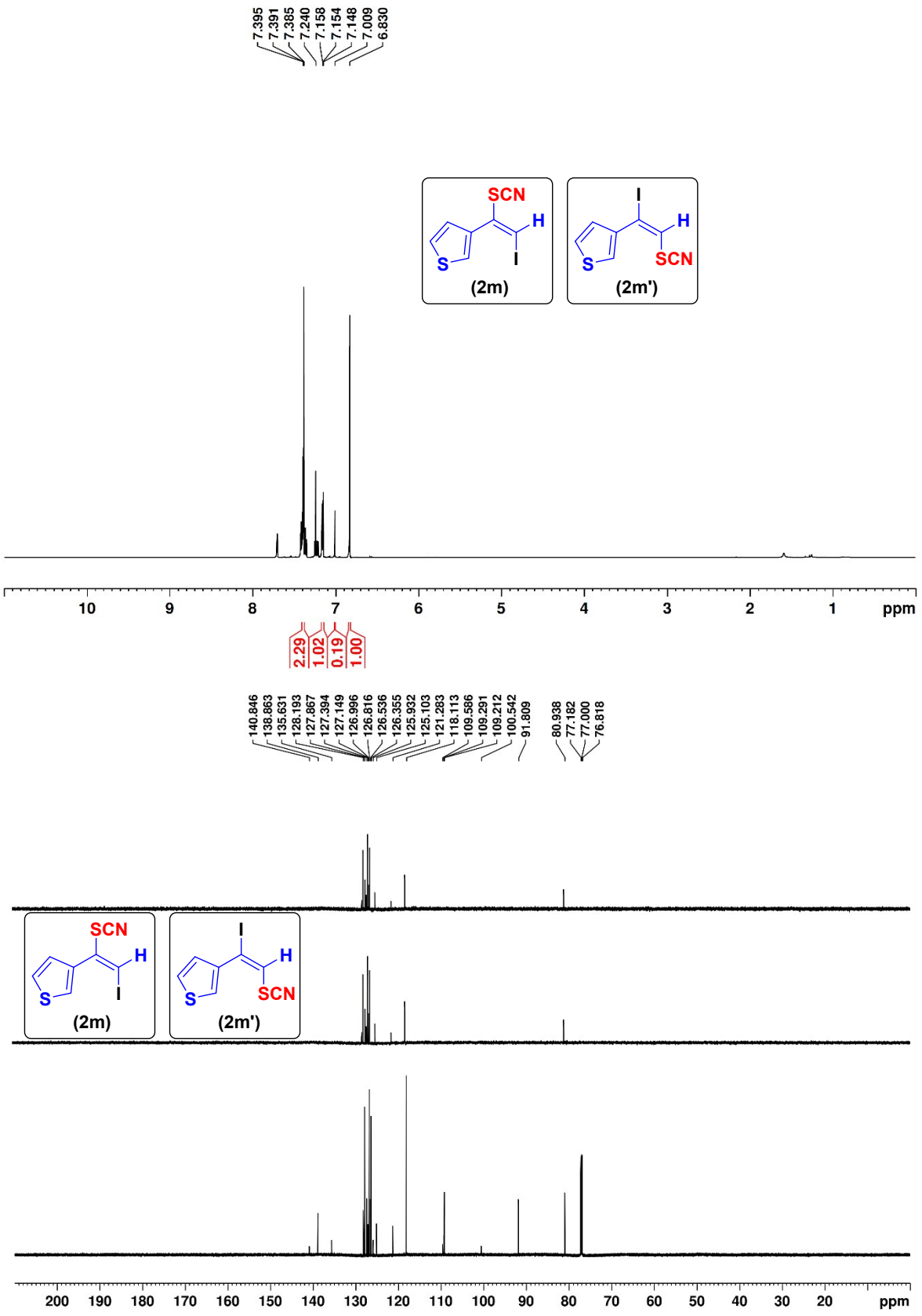

-109.158
-110.646
SCN
H
F
I
(2h)
I
H
F
SCN
(2h')
50
0
-50
-100
-150
-200
-250
ppm

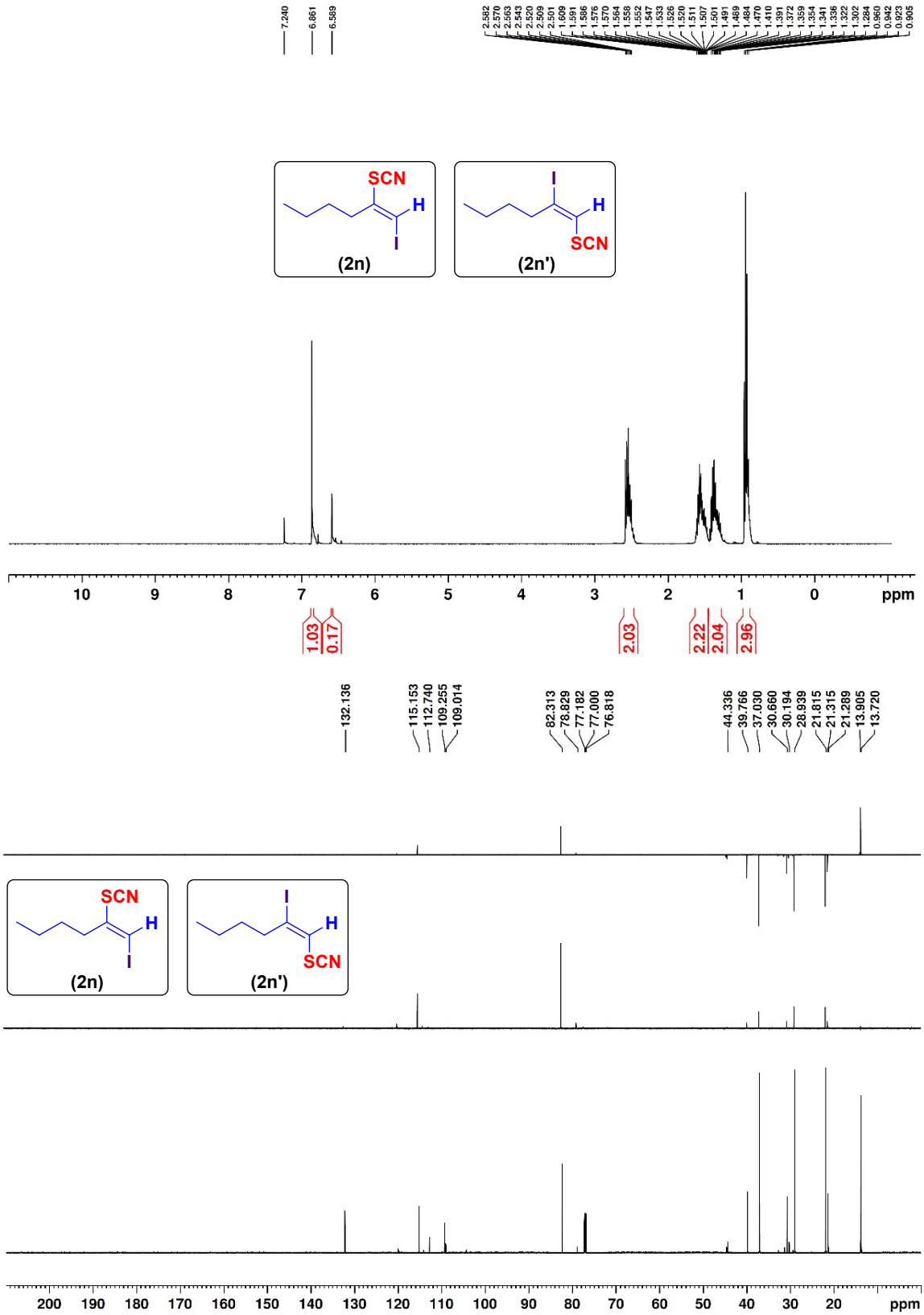

7.418
7.414
7.409
7.407
7.405
7.327
7.323
7.318
7.312
7.310
7.240
7.228
7.226
7.224
7.219
7.215
6.975
6.855
SCN
H
I
Cl
(2i)
I
H
SCN
Cl
(2i')
10
9
8
7
6
5
4
3
2
1
ppm
1.08
2.05
1.03
1.00
0.18
137.222
131.787
131.164
130.675
130.436
130.360
130.292
129.305
127.544
127.418
127.031
121.958
108.675
94.494
77.182
77.000
76.819
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

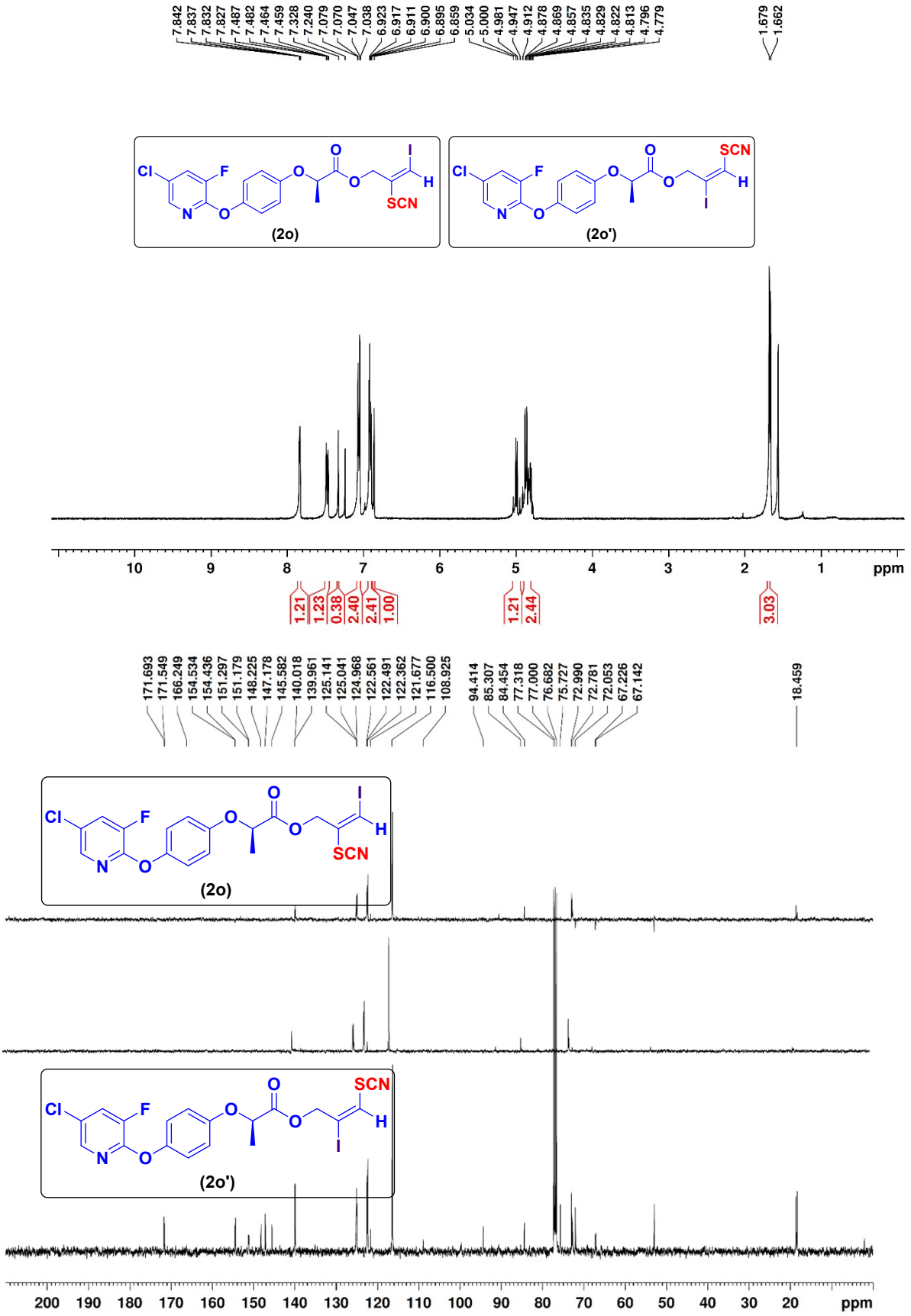

7.595
7.574
7.313
7.292
7.240
7.169
7.148
6.980
6.885
SCN
H
I
Br
(2j)
I
H
SCN
Br
(2j')
10
9
8
7
6
5
4
3
2
1
ppm
2.03
2.14
0.19
1.00
137.736
134.791
132.258
132.157
131.833
130.622
129.986
129.524
129.410
124.633
124.278
123.850
119.422
108.850
108.810
97.113
82.925
77.182
77.000
76.818
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

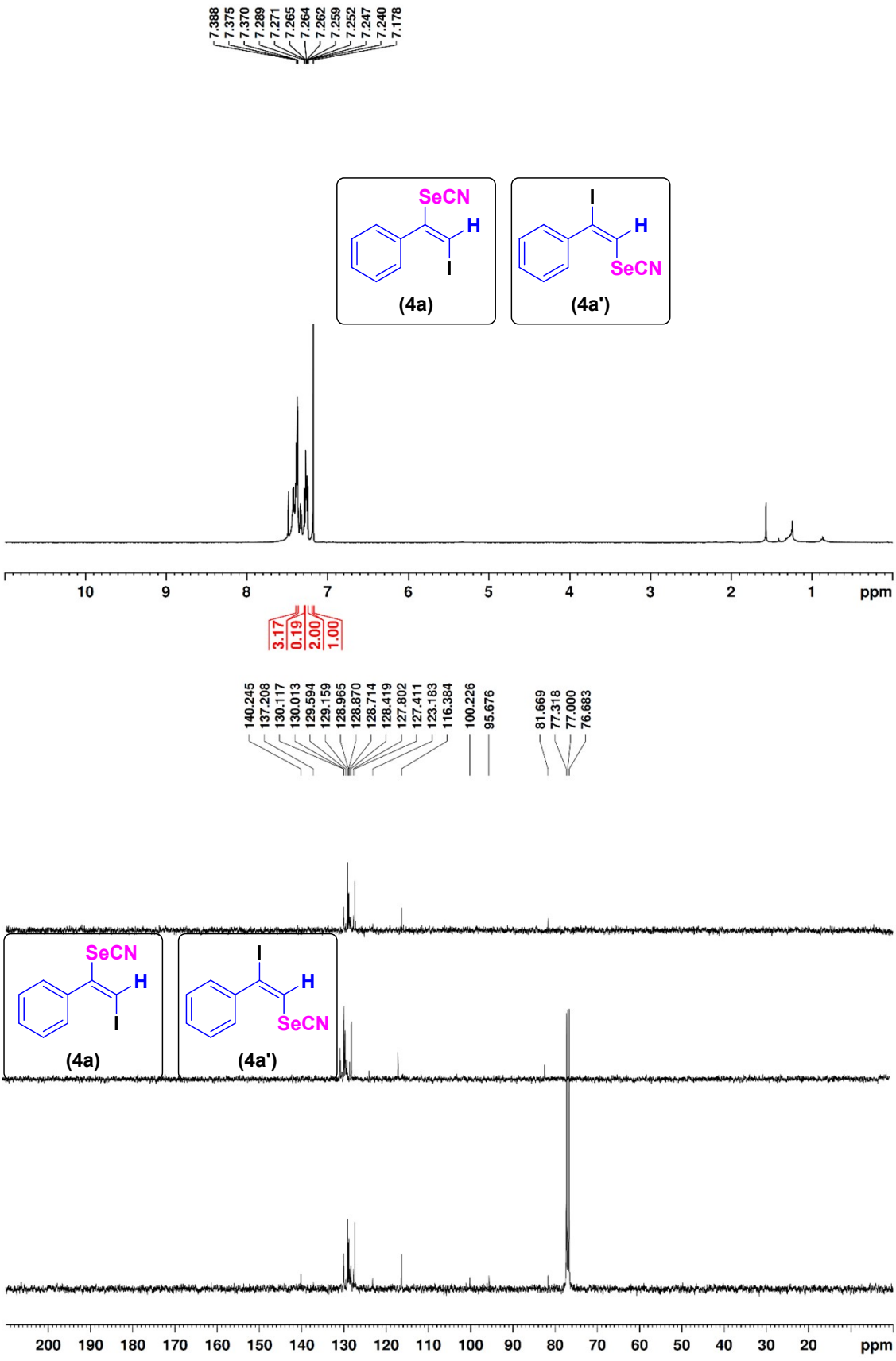

8.259
8.236
7.488
7.466
7.240
7.220
7.020
SCN
H
I
O2N
(2k)
I
H
SCN
O2N
(2k')
10
9
8
7
6
5
4
3
2
1
ppm
2.07
2.05
0.15
1.00
148.113
144.902
130.294
129.146
128.874
127.534
124.251
124.167
123.900
121.209
108.779
108.106
103.224
95.305
86.356
77.182
77.000
76.818
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

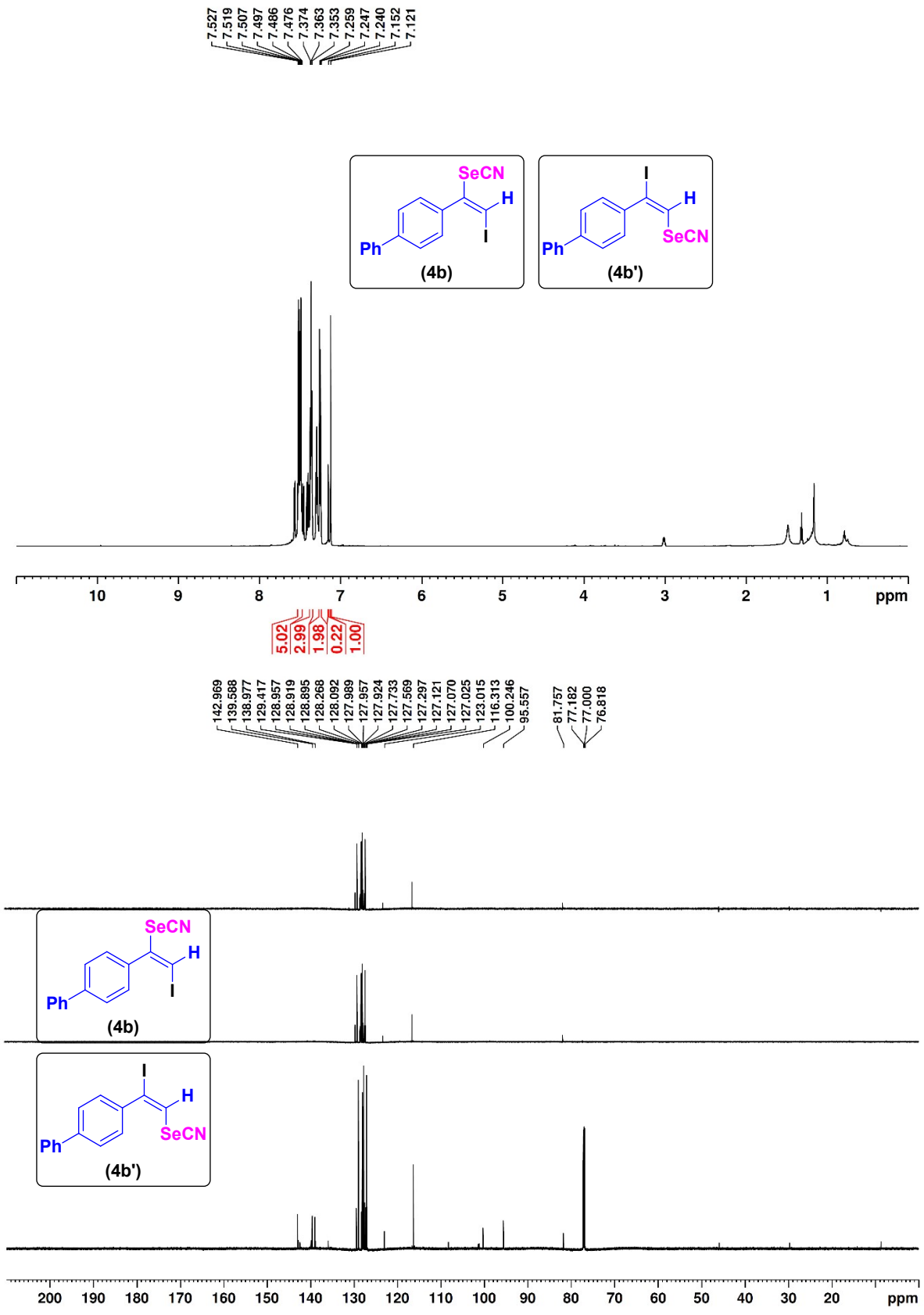

7.950
7.929
7.377
7.357
7.240
7.122
6.933
2.603
2.584
SCN
H
I
O
(2l)
I
H
SCN
O
(2l')
10
9
8
7
6
5
4
3
2
1
ppm
2.12
2.03
0.20
1.00
3.03
196.860
196.759
143.545
143.062
140.380
137.744
137.466
129.359
128.816
128.766
128.609
128.282
128.203
125.423
119.944
109.171
108.660
105.506
96.986
83.986
77.182
77.000
76.818
26.646
26.636
26.614
SCN
H
I
O
(2l)
I
H
SCN
O
(2l')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

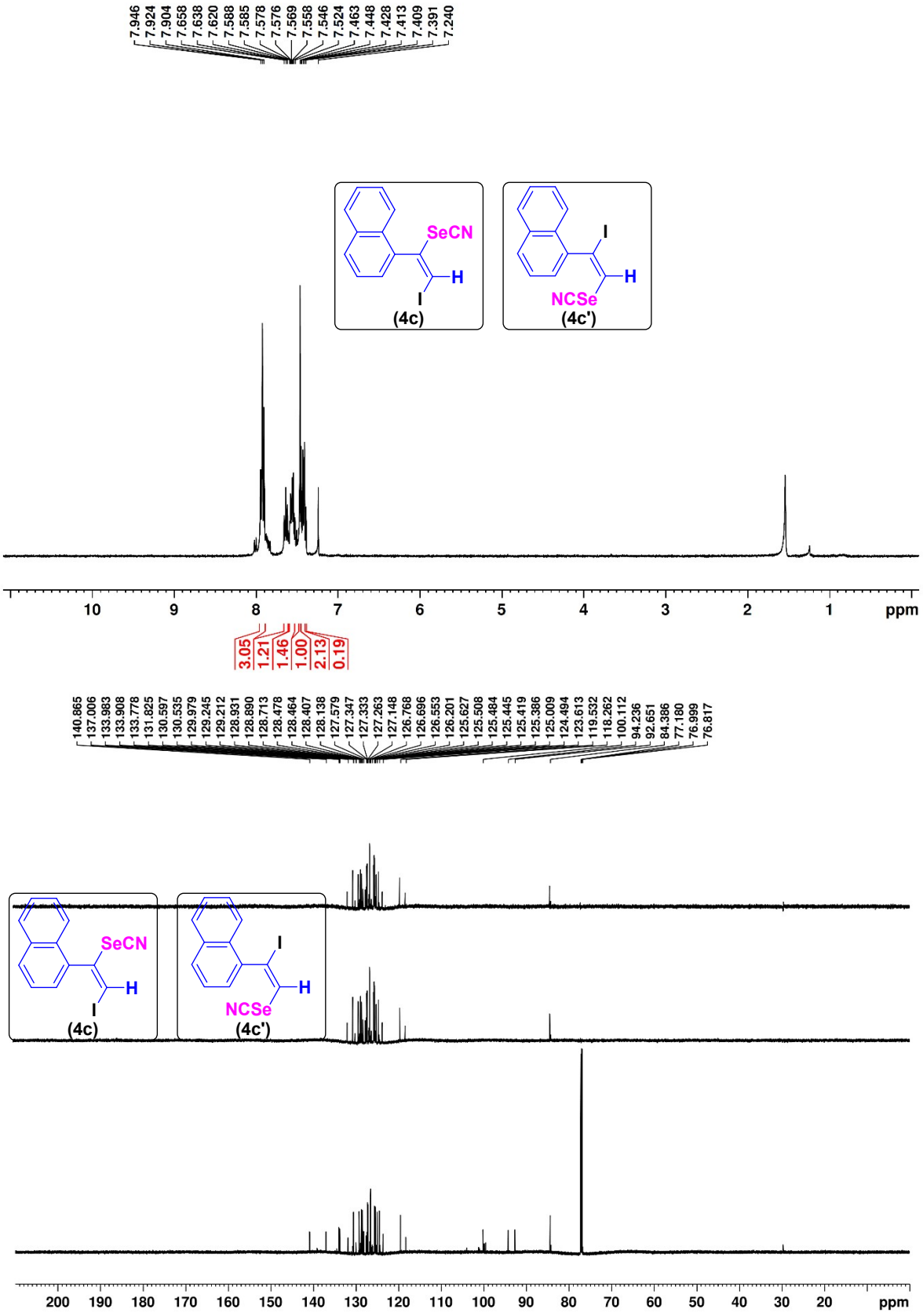

7.395
7.391
7.385
7.240
7.158
7.154
7.148
7.009
6.830
SCN
H
S
I
(2m)
I
H
S
SCN
(2m')
10
9
8
7
6
5
4
3
2
1
ppm
2.29
1.02
0.19
1.00
140.846
138.863
135.631
128.193
127.867
127.394
127.149
126.996
126.816
126.536
126.355
125.932
125.103
121.283
118.113
109.586
109.291
109.212
100.542
91.809
80.938
77.182
77.000
76.818
SCN
H
S
I
(2m)
I
H
S
SCN
(2m')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

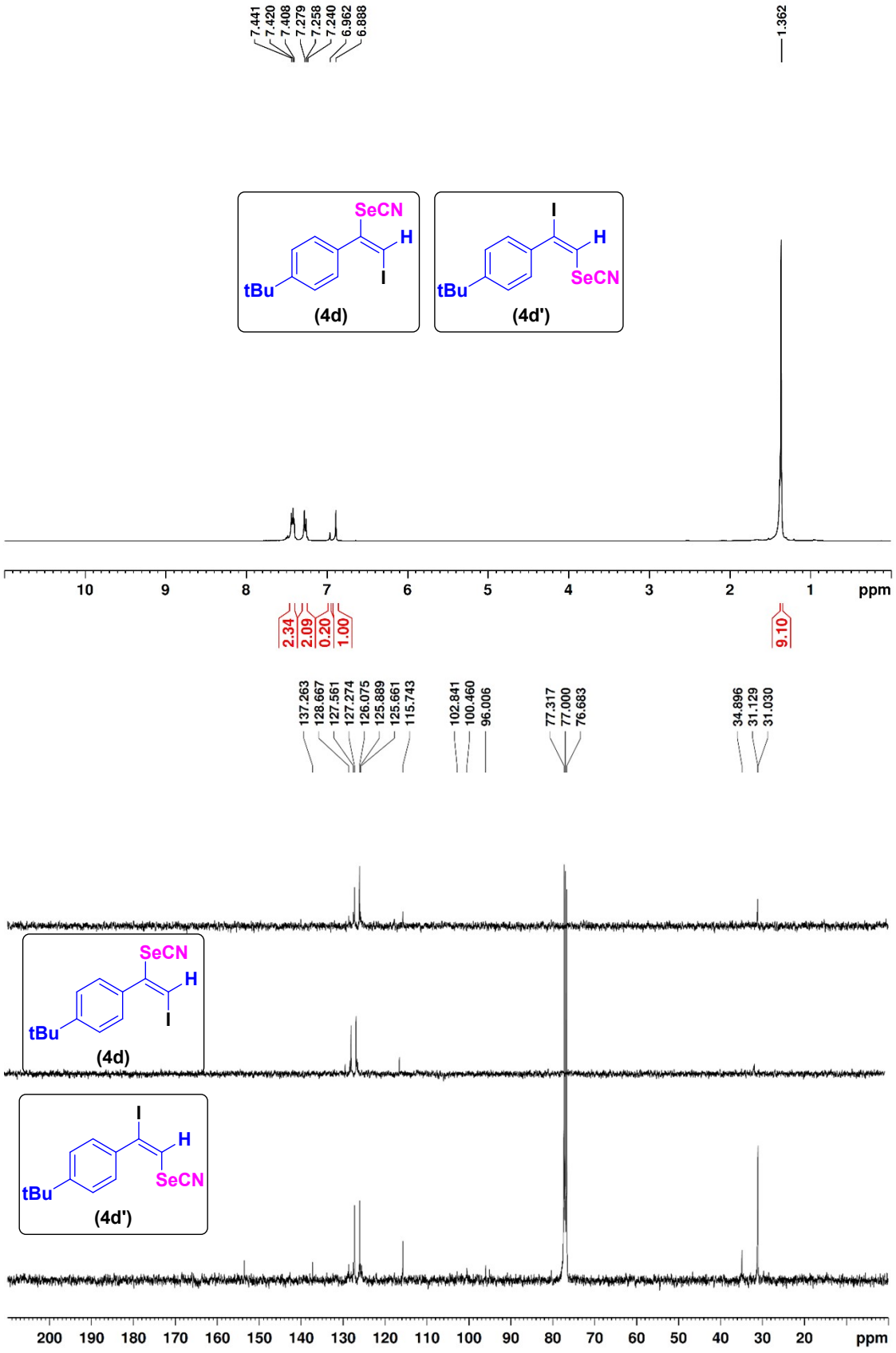

7.240
6.861
6.589
2.582
2.570
2.563
2.543
2.520
2.509
2.501
1.609
1.591
1.586
1.575
1.570
1.564
1.558
1.552
1.547
1.533
1.526
1.520
1.511
1.507
1.501
1.491
1.489
1.484
1.470
1.410
1.391
1.372
1.359
1.354
1.341
1.336
1.322
1.302
1.284
0.960
0.942
0.923
0.905
SCN
H
I
(2n)
I
H
SCN
(2n')
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
0.17
2.03
2.22
2.04
2.96
132.136
115.153
112.740
109.255
109.014
82.313
78.829
77.182
77.000
76.818
44.336
39.766
37.030
30.660
30.194
28.939
21.815
21.315
21.289
13.905
13.720
SCN
H
I
(2n)
I
H
SCN
(2n')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

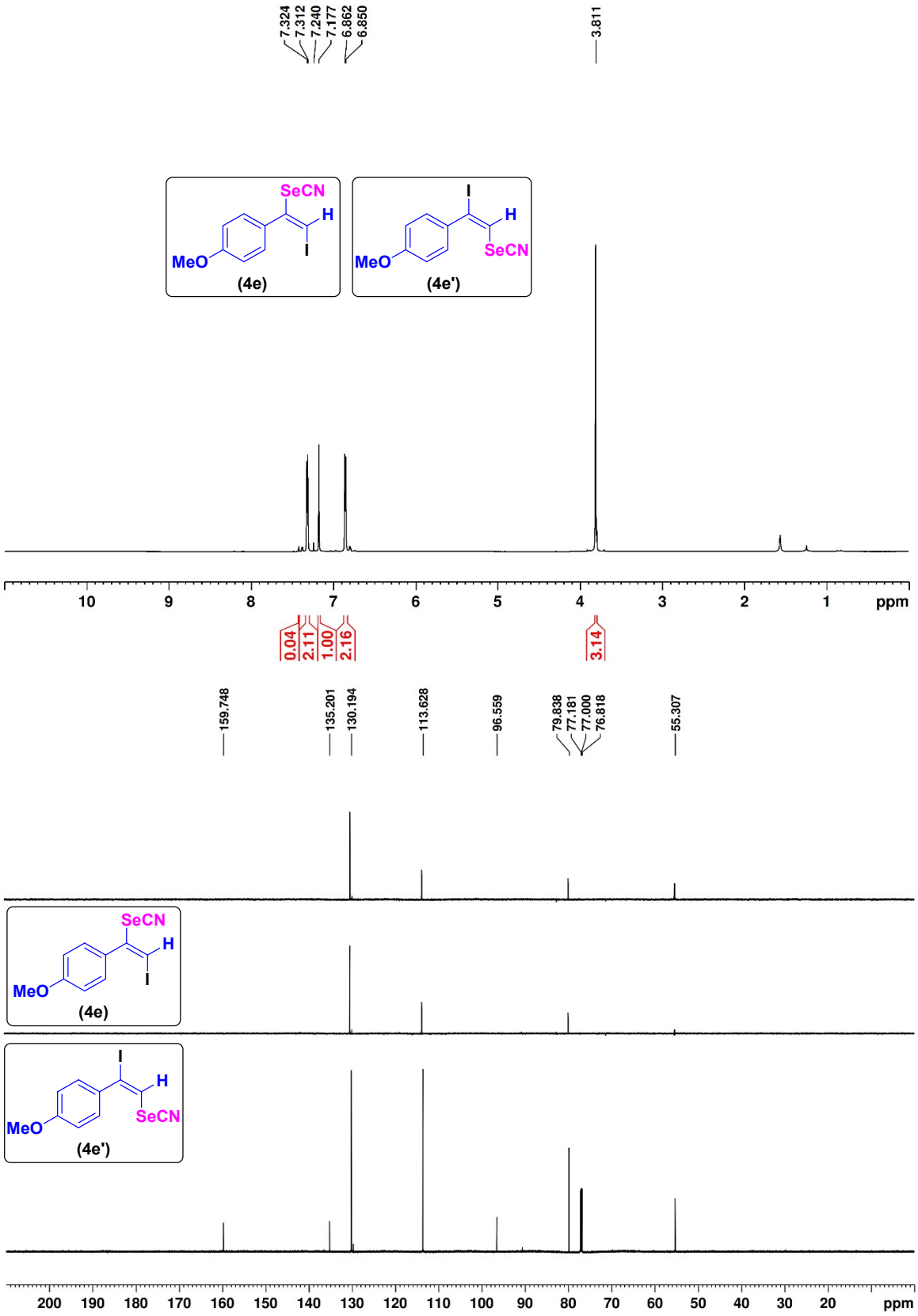

7.842
7.837
7.832
7.827
7.487
7.482
7.464
7.459
7.328
7.240
7.079
7.070
7.047
7.038
6.923
6.917
6.911
6.900
6.895
6.859
5.034
5.000
4.981
4.947
4.912
4.878
4.869
4.857
4.835
4.829
4.822
4.813
4.796
4.779
1.679
1.662
(2o)
(2o')
10
9
8
7
6
5
4
3
2
1
ppm
1.21
1.23
0.38
2.40
2.41
1.00
1.21
2.44
3.03
171.693
171.549
166.249
154.534
154.436
151.297
151.179
148.225
147.178
145.582
140.018
139.961
125.141
125.041
124.968
122.561
122.491
122.362
121.677
116.500
108.925
94.414
85.307
84.454
77.318
77.000
76.682
75.727
72.990
72.781
72.053
67.226
67.142
18.459
(2o)
(2o')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

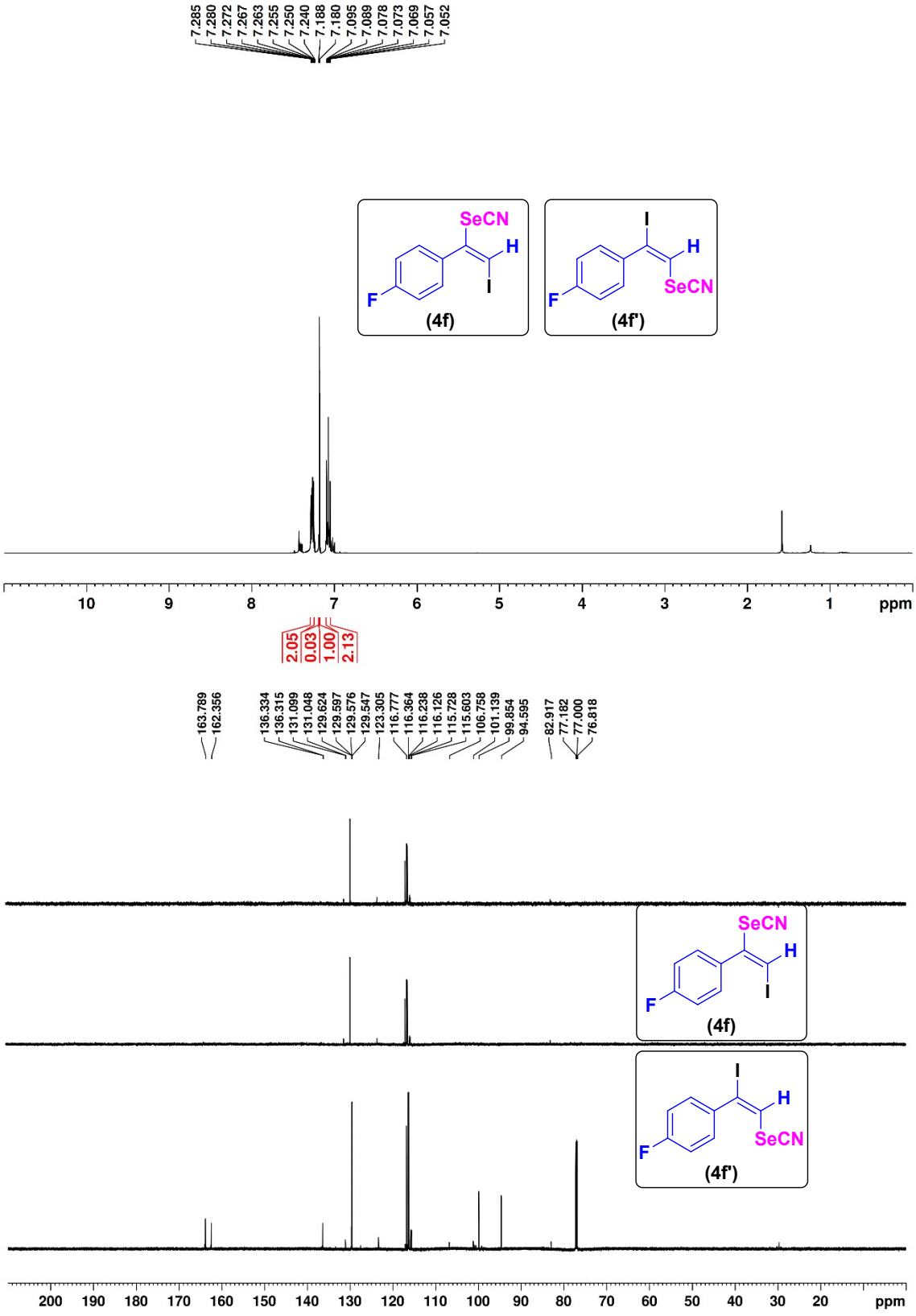

7.388
7.375
7.370
7.289
7.271
7.265
7.264
7.262
7.259
7.252
7.247
7.240
7.178
SeCN
H
I
(4a)
I
H
SeCN
(4a')
10
9
8
7
6
5
4
3
2
1
ppm
3.17
0.19
2.00
1.00
140.245
137.208
130.117
130.013
129.594
129.159
128.965
128.870
128.714
128.419
127.802
127.411
123.183
116.384
100.226
95.676
81.669
77.318
77.000
76.683
SeCN
H
I
(4a)
I
H
SeCN
(4a')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

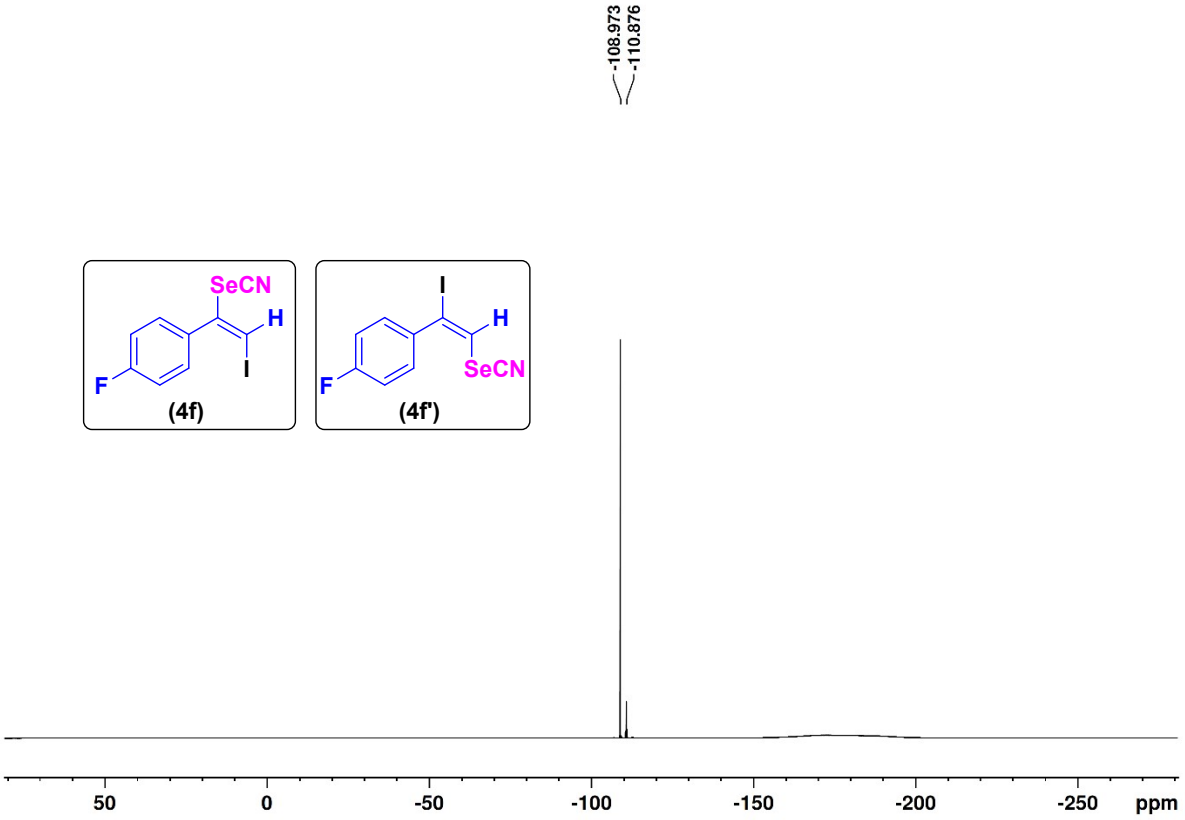

7.527
7.519
7.507
7.497
7.486
7.476
7.374
7.363
7.353
7.259
7.247
7.240
7.152
7.121
SeCN
H
I
Ph
(4b)
I
H
SeCN
Ph
(4b')
10
9
8
7
6
5
4
3
2
1
ppm
5.02
2.99
1.98
0.22
1.00
142.969
139.588
138.977
129.417
128.957
128.919
128.895
128.268
128.092
127.989
127.957
127.924
127.733
127.569
127.297
127.121
127.070
127.025
123.015
116.313
100.246
95.557
81.757
77.182
77.000
76.818
SeCN
H
I
Ph
(4b)
I
H
SeCN
Ph
(4b')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

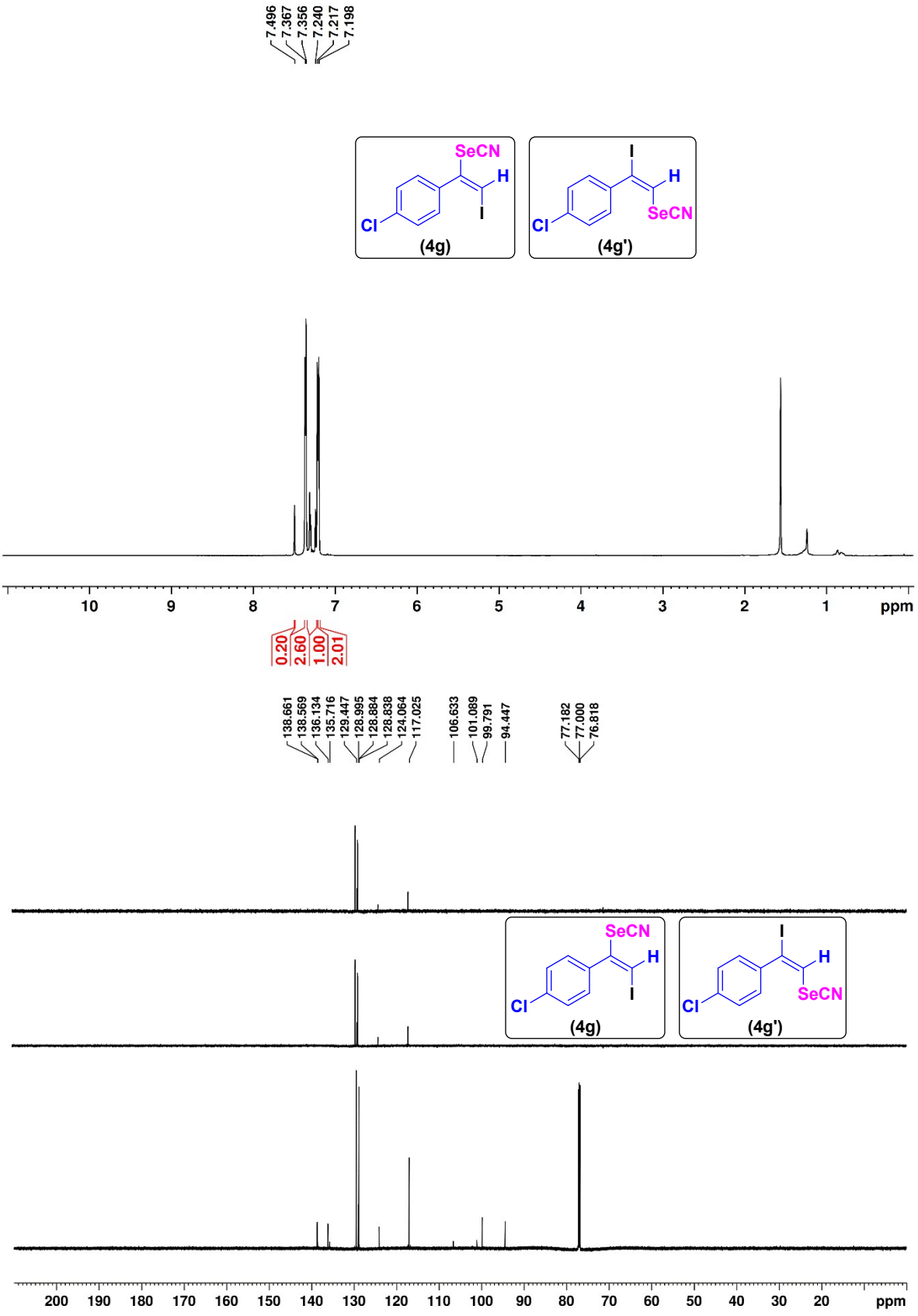

7.946
7.924
7.904
7.658
7.638
7.620
7.588
7.585
7.578
7.576
7.569
7.558
7.546
7.524
7.463
7.448
7.428
7.413
7.409
7.391
7.240
SeCN
H
I
(4c)
I
H
NCSe
(4c')
10
9
8
7
6
5
4
3
2
1
ppm
3.05
1.21
1.46
1.00
2.13
0.19
140.865
137.006
133.983
133.908
133.778
131.825
130.597
130.535
129.979
129.245
129.212
128.931
128.890
128.713
128.478
128.464
128.407
128.138
127.579
127.347
127.333
127.263
127.148
126.768
126.696
126.553
126.201
125.627
125.508
125.484
125.445
125.419
125.386
125.009
124.494
123.613
119.532
118.262
100.112
94.236
92.651
84.386
77.180
76.999
76.817
SeCN
H
I
(4c)
I
H
NCSe
(4c')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

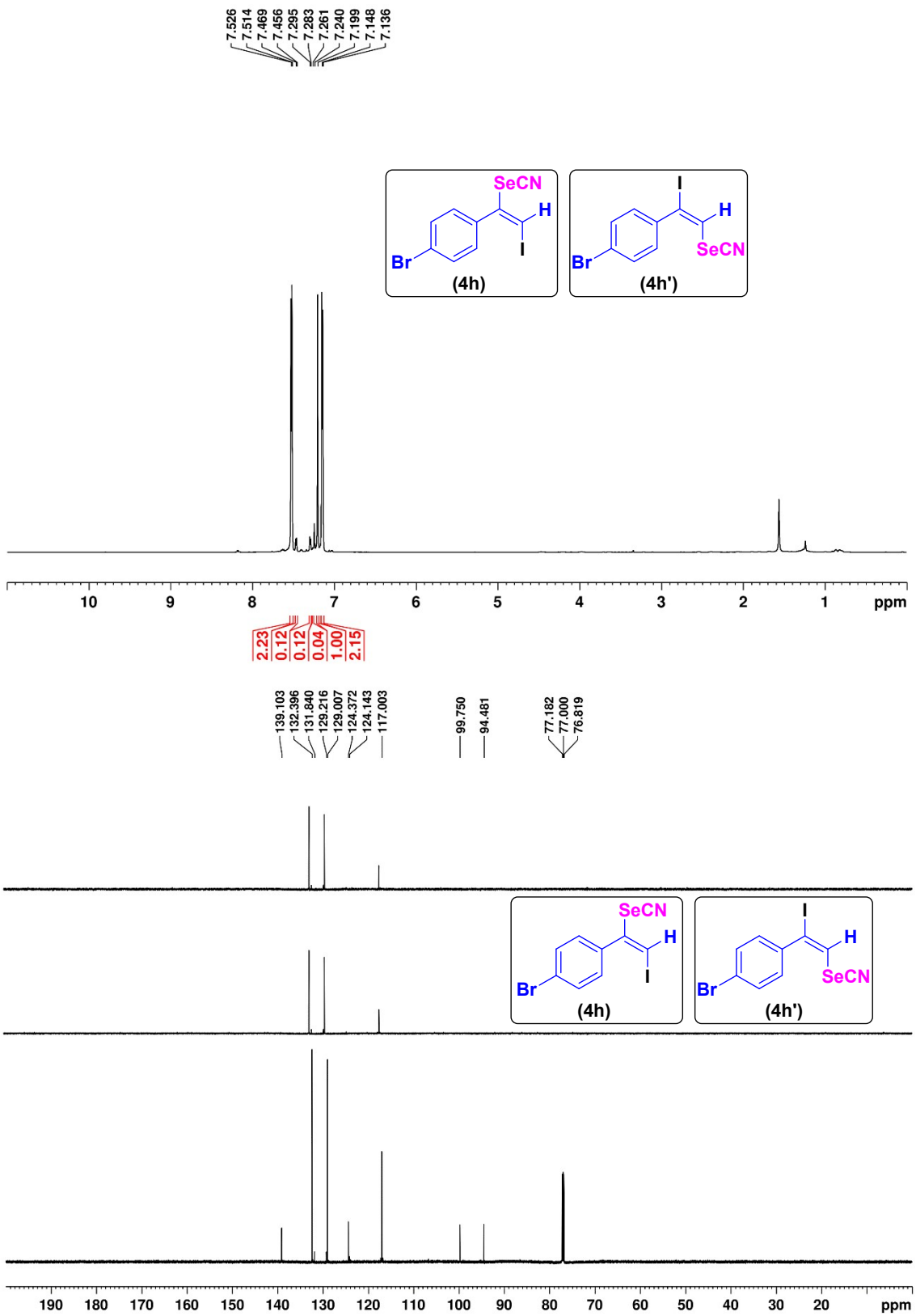

7.441
7.420
7.408
7.279
7.258
7.240
6.962
6.888
1.362
SeCN
H
I
tBu
(4d)
I
H
SeCN
tBu
(4d')
10
9
8
7
6
5
4
3
2
1
ppm
2.34
2.09
0.20
1.00
9.10
137.263
128.667
127.561
127.274
126.075
125.889
125.661
115.743
102.841
100.460
96.006
77.317
77.000
76.683
34.896
31.129
31.030
SeCN
H
I
tBu
(4d)
I
H
SeCN
tBu
(4d')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

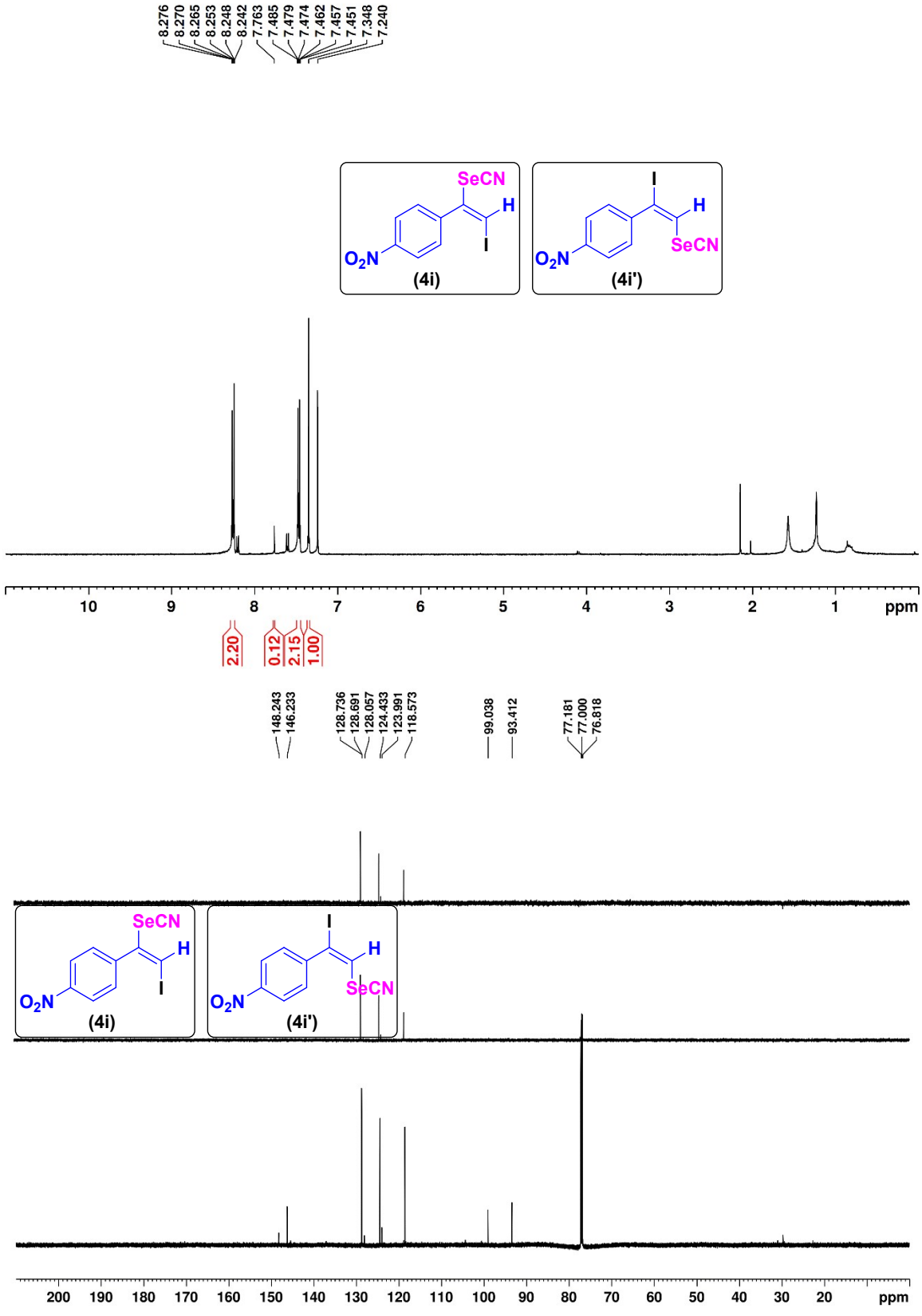

7.324
7.312
7.240
7.177
6.862
6.850
3.811
SeCN
H
I
MeO
(4e)
I
H
SeCN
MeO
(4e')
10
9
8
7
6
5
4
3
2
1
ppm
0.04
2.11
1.00
2.16
3.14
159.748
135.201
130.194
113.628
96.559
79.838
77.181
77.000
76.818
55.307
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

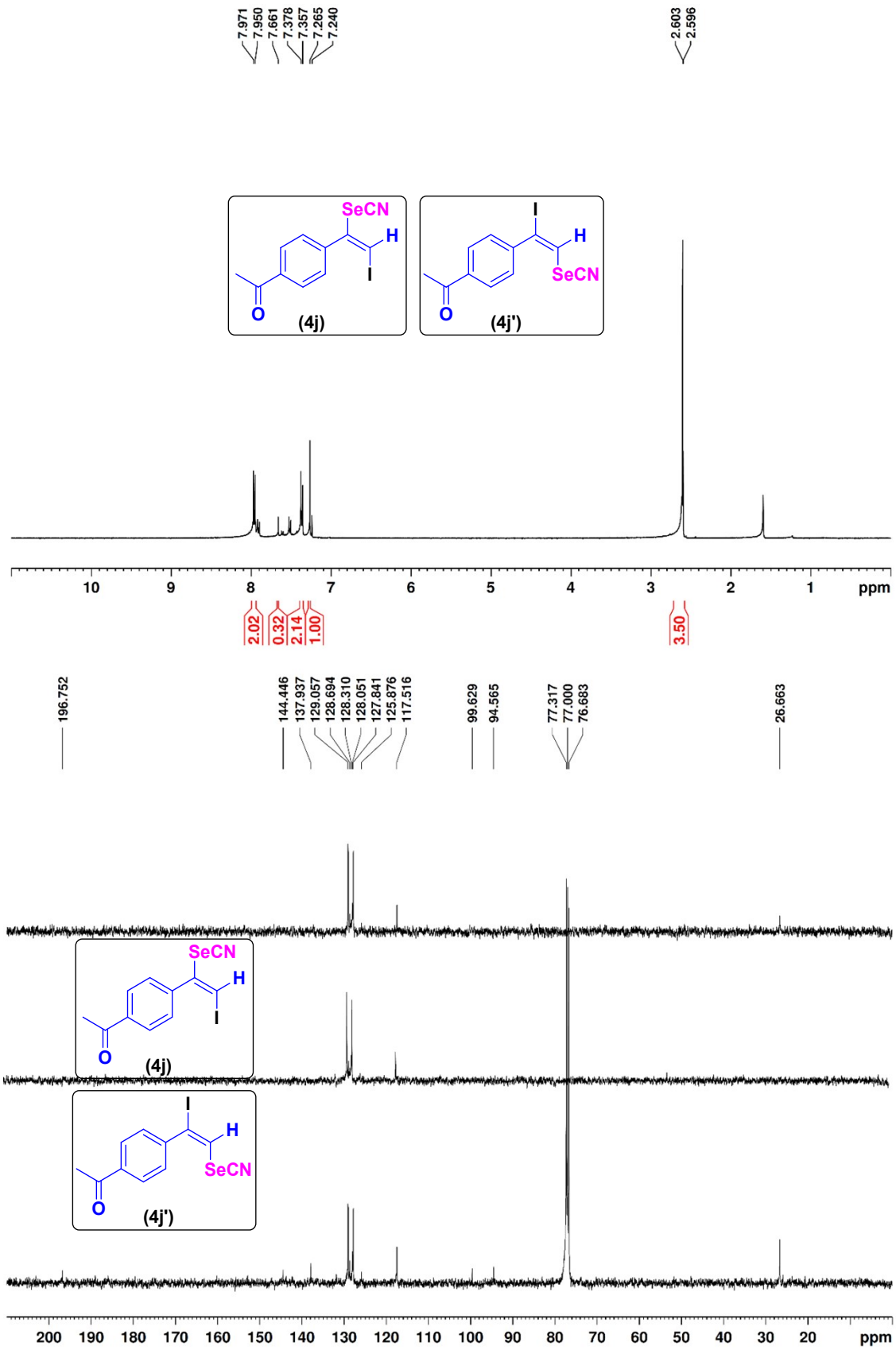

7.285
7.280
7.272
7.267
7.263
7.255
7.250
7.240
7.188
7.180
7.095
7.089
7.078
7.073
7.069
7.057
7.052
SeCN
H
I
F
(4f)
I
H
SeCN
F
(4f')
10
9
8
7
6
5
4
3
2
1
ppm
2.05
0.03
1.00
2.13
163.789
162.356
136.334
136.315
131.099
131.048
129.624
129.597
129.576
129.547
123.305
116.777
116.364
116.238
116.126
115.728
115.603
106.758
101.139
99.854
94.595
82.917
77.182
77.000
76.818
SeCN
H
I
F
(4f)
I
H
SeCN
F
(4f')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

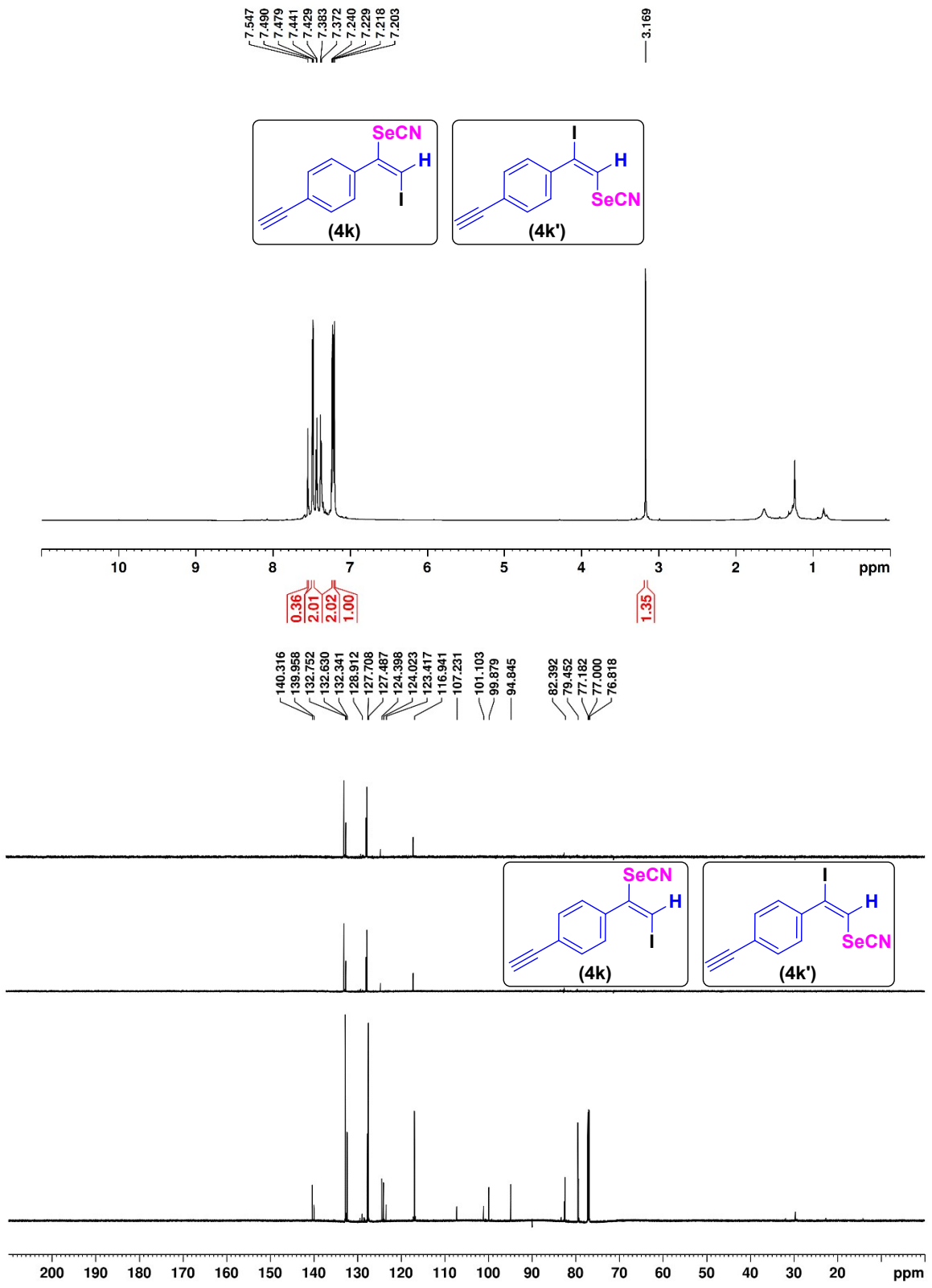

-108.973
-110.876
SeCN
H
F
I
(4f)
I
H
F
SeCN
(4f')
50
0
-50
-100
-150
-200
-250
ppm

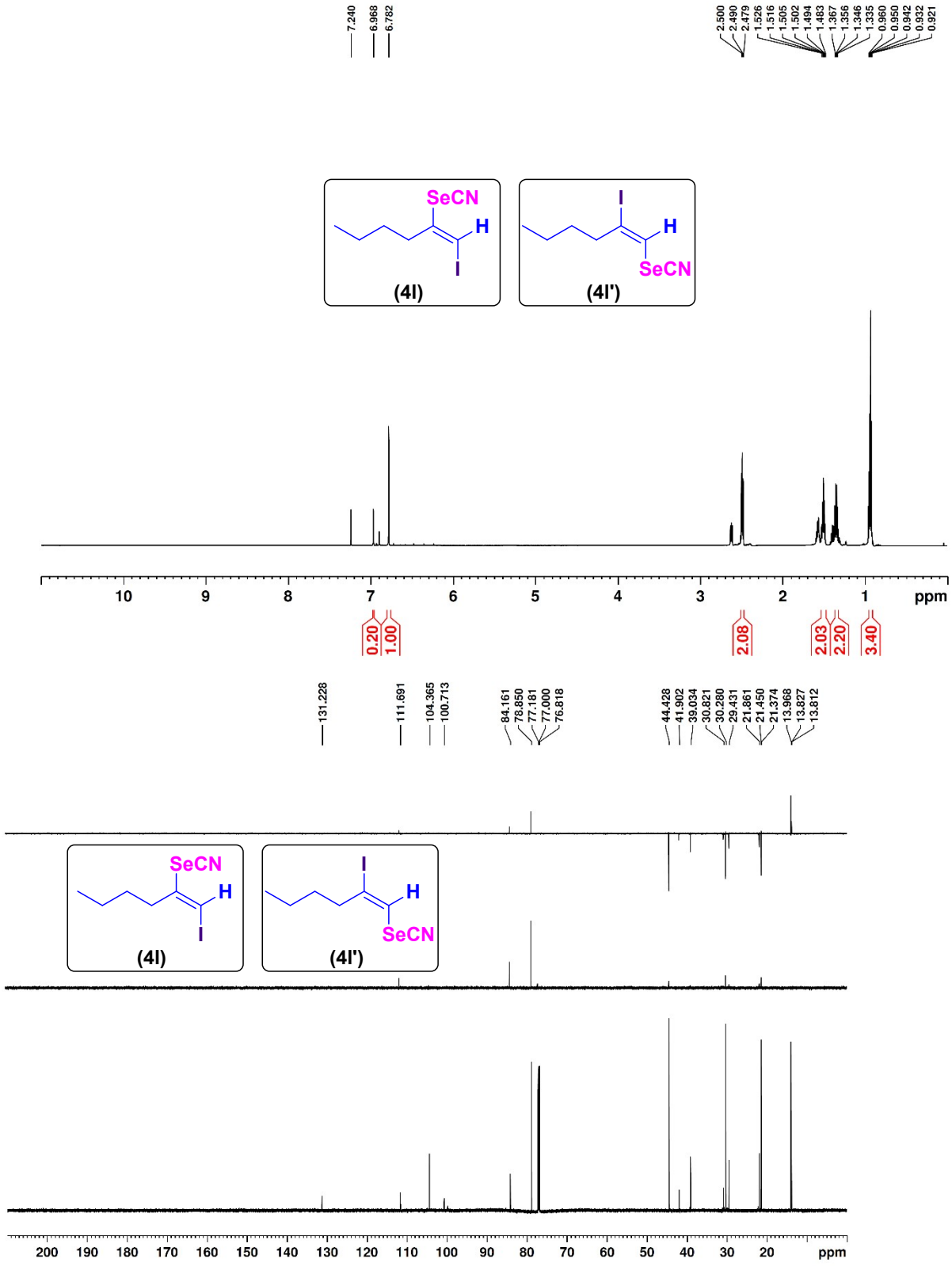

7.496
7.367
7.356
7.240
7.217
7.198
SeCN
H
Cl
I
(4g)
I
H
Cl
SeCN
(4g')
10
9
8
7
6
5
4
3
2
1
ppm
0.20
2.60
1.00
2.01
138.661
138.569
136.134
135.716
129.447
128.995
128.884
128.838
124.064
117.025
106.633
101.089
99.791
94.447
77.182
77.000
76.818
SeCN
H
Cl
I
(4g)
I
H
Cl
SeCN
(4g')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

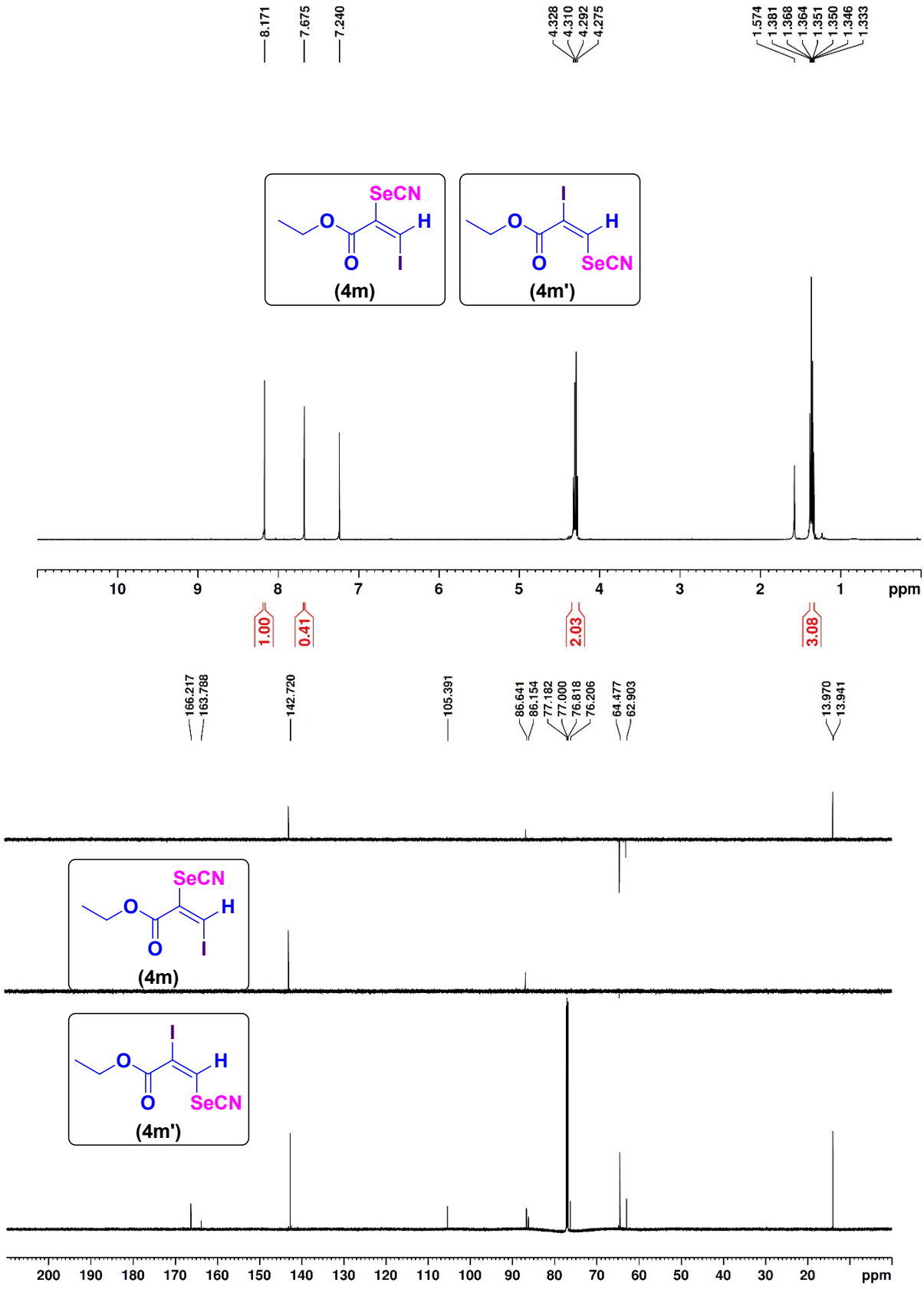

7.526
7.514
7.469
7.456
7.295
7.283
7.261
7.240
7.199
7.148
7.136
SeCN
H
I
Br
(4h)
I
H
SeCN
Br
(4h')
10
9
8
7
6
5
4
3
2
1
ppm
2.23
0.12
0.12
0.04
1.00
2.15
139.103
132.396
131.840
129.216
129.007
124.372
124.143
117.003
99.750
94.481
77.182
77.000
76.819
SeCN
H
I
Br
(4h)
I
H
SeCN
Br
(4h')
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

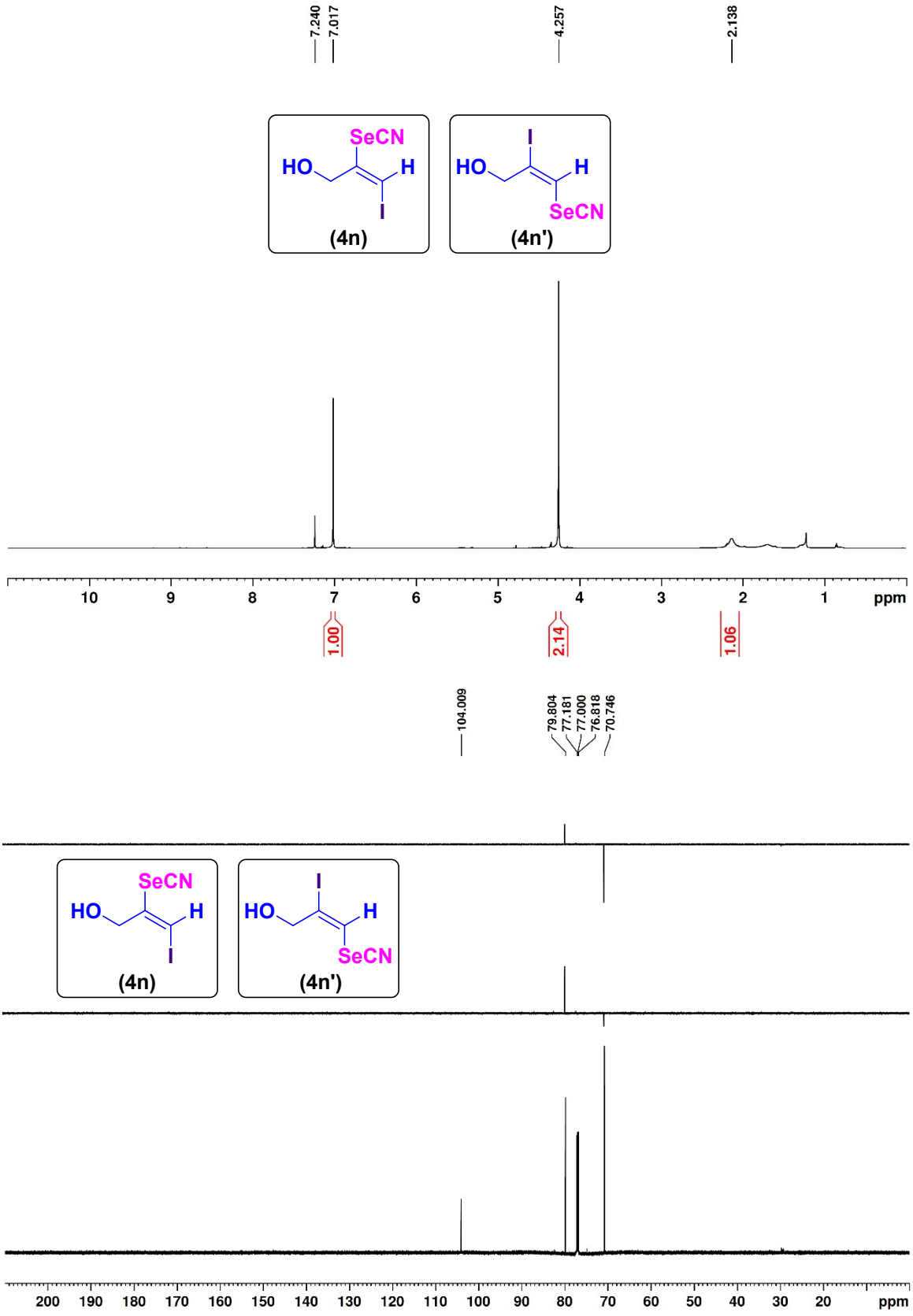

8.276
8.270
8.265
8.253
8.248
8.242
7.763
7.485
7.479
7.474
7.462
7.457
7.451
7.348
7.240
SeCN
H
I
O2N
(4i)
I
H
SeCN
O2N
(4i')
10
9
8
7
6
5
4
3
2
1
ppm
2.20
0.12
2.15
1.00
148.243
146.233
128.736
128.691
128.057
124.433
123.991
118.573
99.038
93.412
77.181
77.000
76.818
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

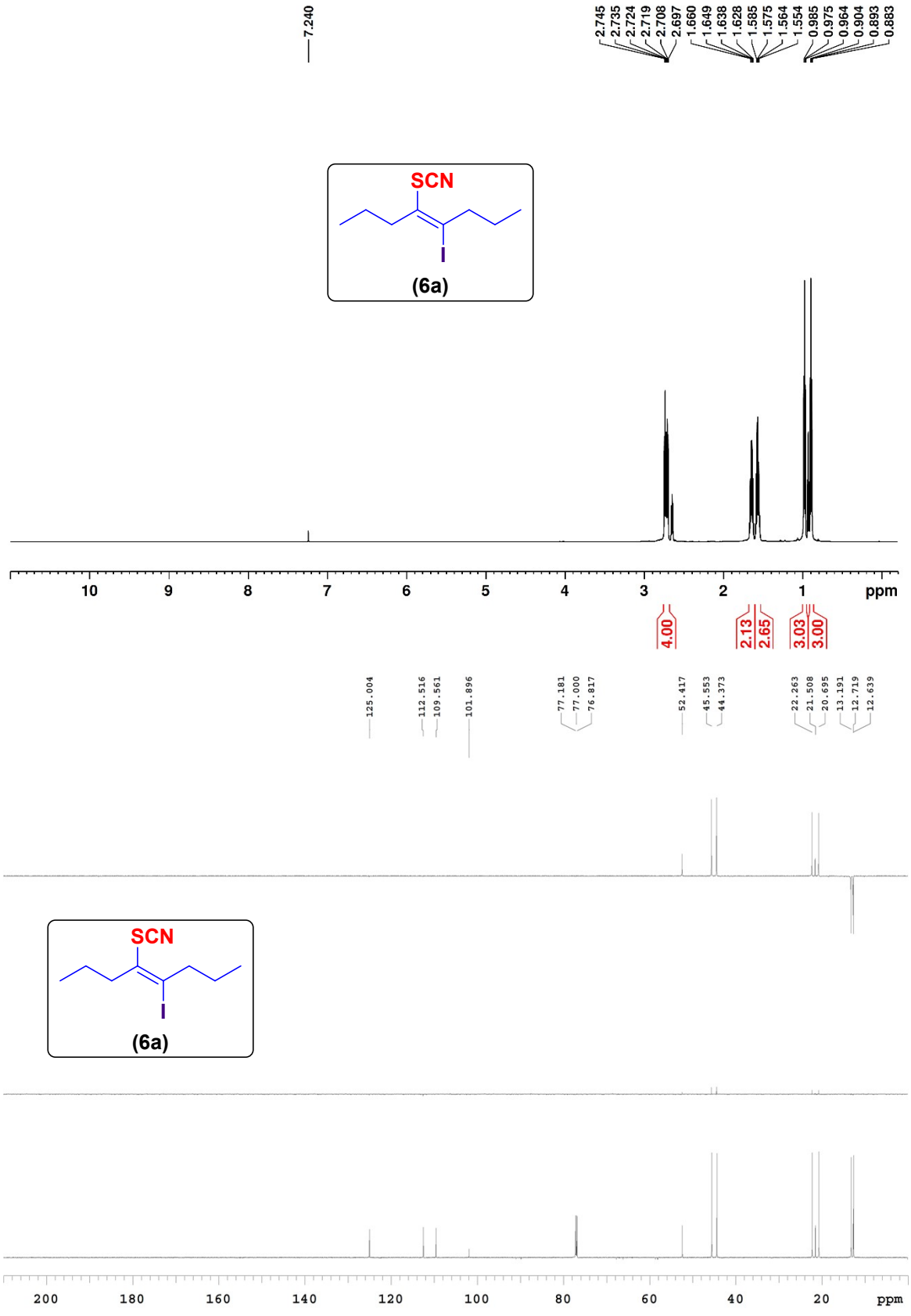

7.971
7.950
7.661
7.378
7.357
7.265
7.240
2.603
2.596
SeCN
H
I
O
(4j)
I
H
SeCN
O
(4j')
10
9
8
7
6
5
4
3
2
1
ppm
2.02
0.32
2.14
1.00
3.50
196.752
144.446
137.937
129.057
128.694
128.310
128.051
127.841
125.876
117.516
99.629
94.565
77.317
77.000
76.683
26.663
SeCN
H
I
O
(4j)
I
H
SeCN
O
(4j')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

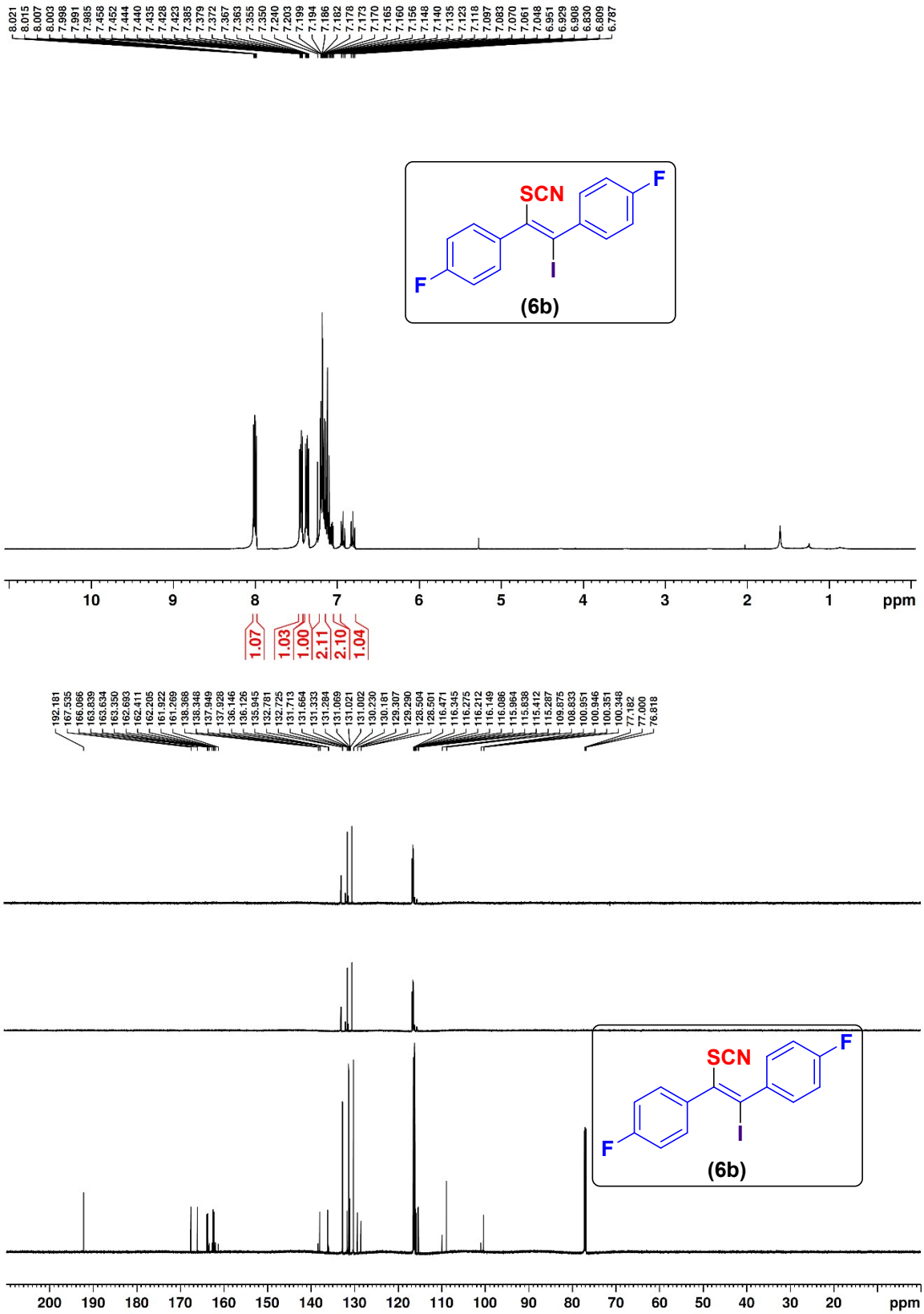

7.547
7.490
7.479
7.441
7.429
7.383
7.372
7.240
7.229
7.218
7.203
3.169
SeCN
H
I
(4k)
I
H
SeCN
(4k')
10
9
8
7
6
5
4
3
2
1
ppm
0.36
2.01
2.02
1.00
1.35
140.316
139.958
132.752
132.630
132.341
128.912
127.708
127.487
124.398
124.023
123.417
116.941
107.231
101.103
99.879
94.845
82.392
79.452
77.182
77.000
76.818
SeCN
H
I
(4k)
I
H
SeCN
(4k')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

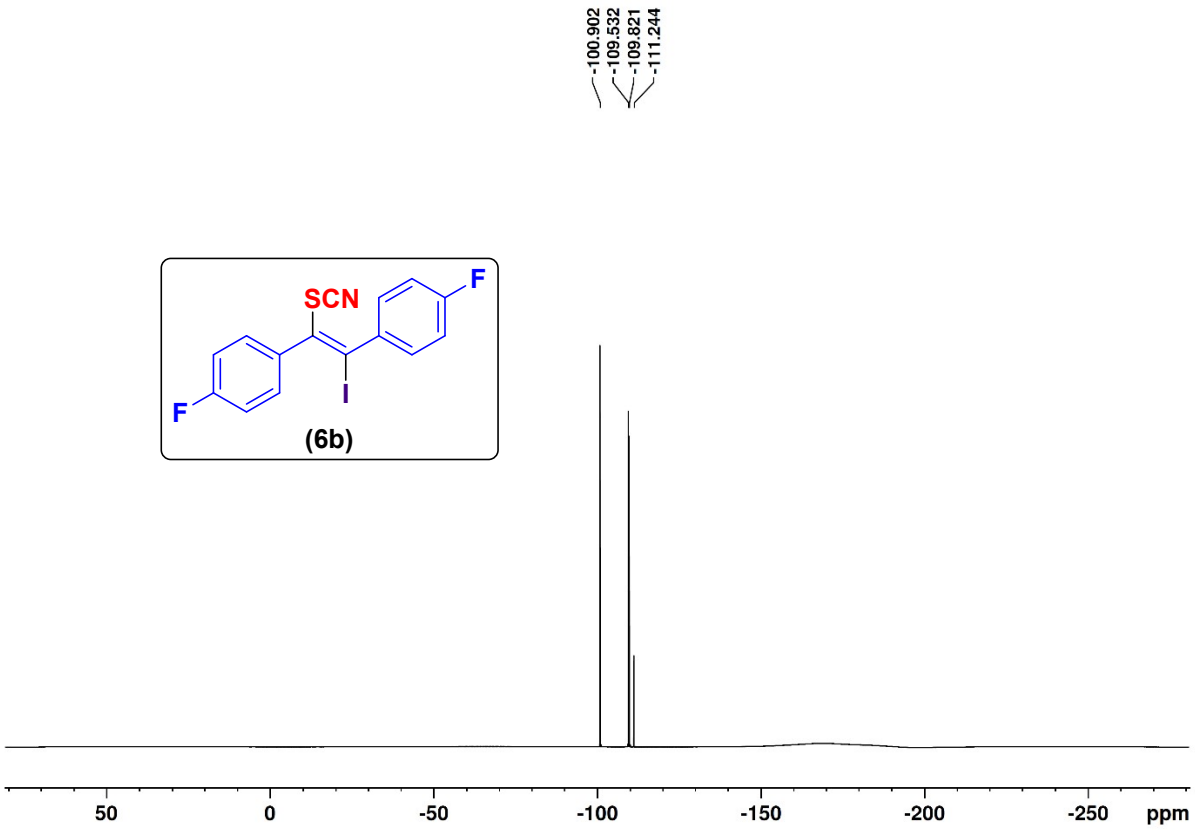

7.240
6.968
6.782
2.500
2.490
2.479
1.526
1.516
1.505
1.502
1.494
1.483
1.367
1.356
1.346
1.335
0.960
0.950
0.942
0.932
0.921
SeCN
H
I
(4l)
I
H
SeCN
(4l')
10
9
8
7
6
5
4
3
2
1
ppm
0.20
1.00
2.08
2.03
2.20
3.40
131.228
111.691
104.365
100.713
84.161
78.850
77.181
77.000
76.818
44.428
41.902
39.034
30.821
30.280
29.431
21.861
21.450
21.374
13.968
13.827
13.812
SeCN
H
I
(4l)
I
H
SeCN
(4l')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

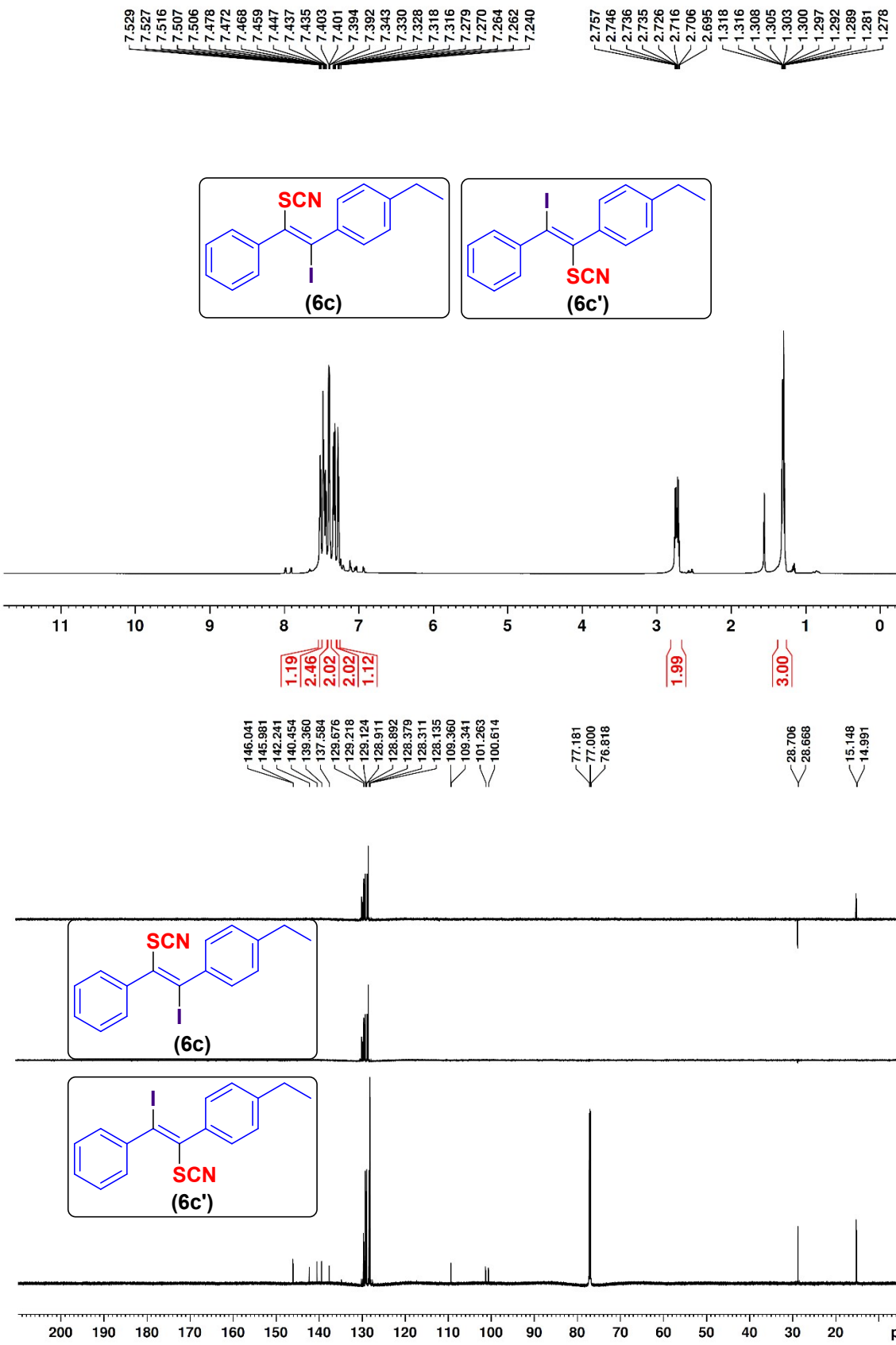

8.171
7.675
7.240
4.328
4.310
4.292
4.275
1.574
1.381
1.368
1.364
1.351
1.350
1.346
1.333
SeCN
O
H
O
I
(4m)
I
O
H
O
SeCN
(4m')
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.41
2.03
3.08
166.217
163.788
142.720
105.391
86.641
86.154
77.182
77.000
76.818
76.206
64.477
62.903
13.970
13.941
SeCN
O
H
O
I
(4m)
I
O
H
O
SeCN
(4m')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

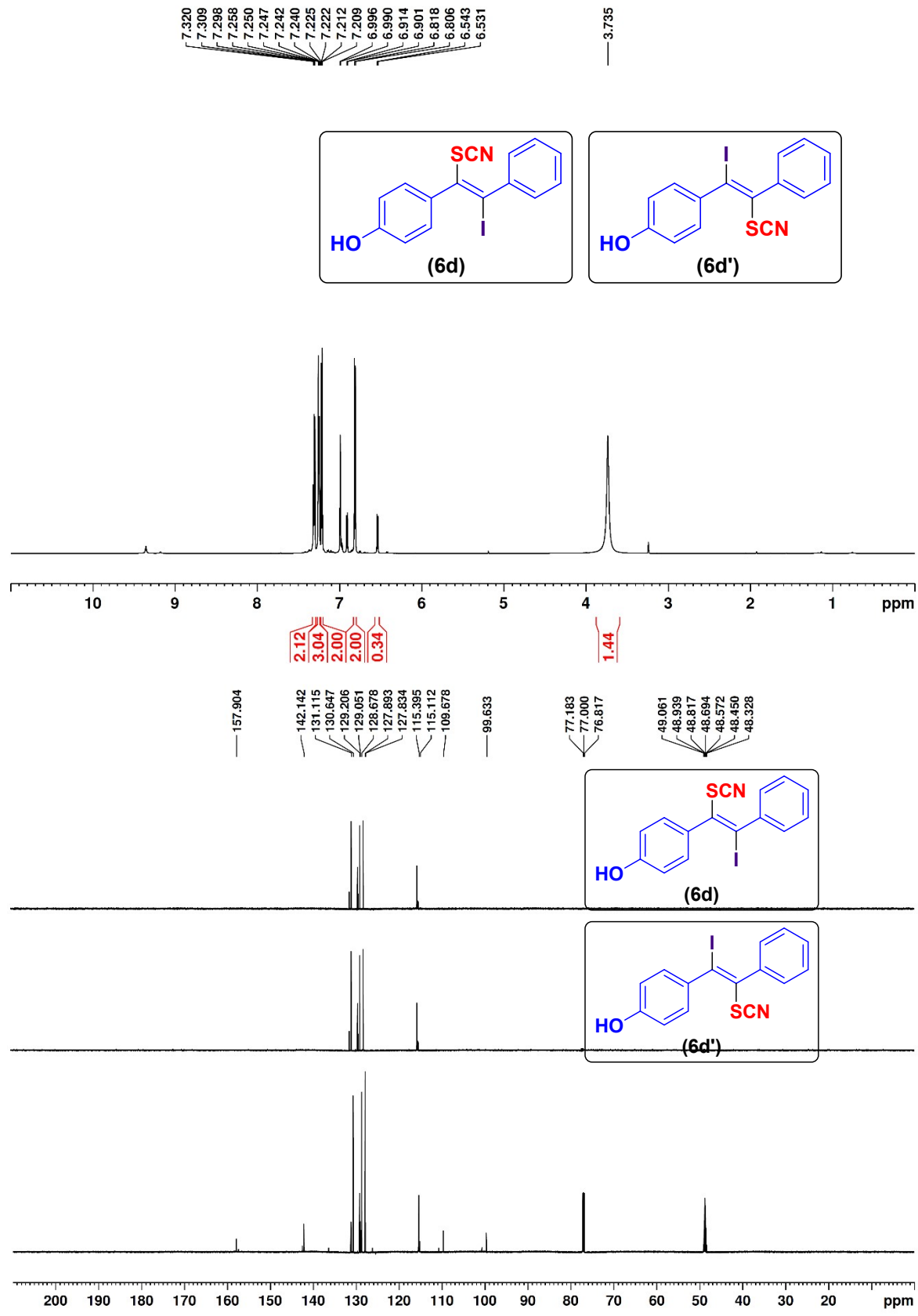

7.240
7.017
4.257
2.138
SeCN
HO
H
I
(4n)
I
HO
H
SeCN
(4n')
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.14
1.06
104.009
79.804
77.181
77.000
76.818
70.746
SeCN
HO
H
I
(4n)
I
HO
H
SeCN
(4n')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

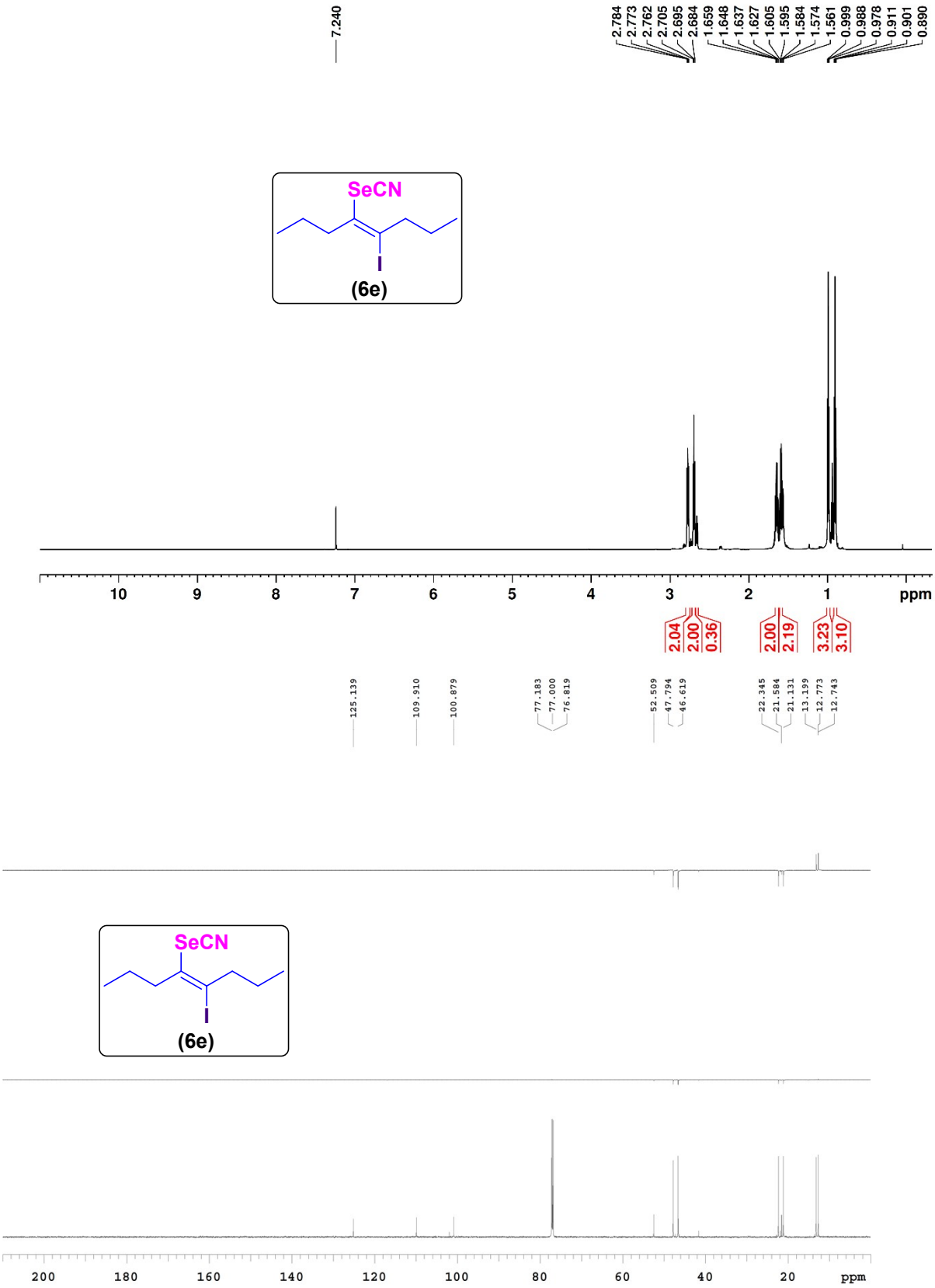

7.240
2.745
2.735
2.724
2.719
2.708
2.697
1.660
1.649
1.638
1.628
1.585
1.575
1.564
1.554
0.985
0.975
0.964
0.904
0.893
0.883
SCN
I
(6a)
10
9
8
7
6
5
4
3
2
1
ppm
4.00
2.13
2.65
3.03
3.00
125.004
112.516
109.561
101.896
77.181
77.000
76.817
52.417
45.553
44.373
22.263
21.508
20.695
13.191
12.719
12.639
SCN
I
(6a)
200
180
160
140
120
100
80
60
40
20
ppm

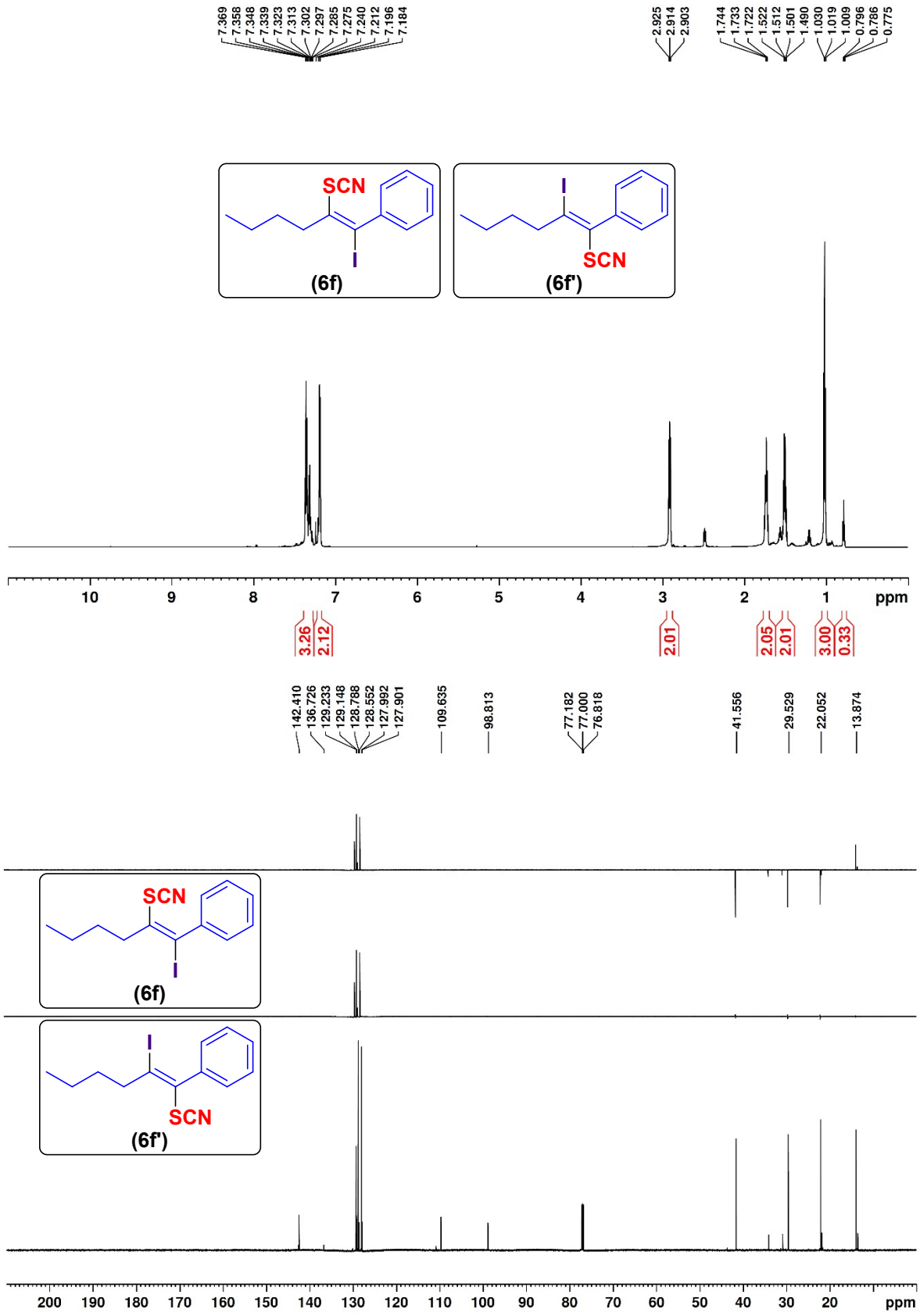

8.021
8.015
8.007
8.003
7.998
7.991
7.985
7.458
7.452
7.444
7.440
7.435
7.428
7.423
7.385
7.379
7.372
7.367
7.363
7.355
7.350
7.240
7.203
7.199
7.194
7.186
7.182
7.178
7.173
7.170
7.165
7.160
7.156
7.148
7.140
7.135
7.123
7.118
7.097
7.083
7.070
7.061
7.048
6.951
6.929
6.908
6.830
6.809
6.787
SCN
F
F
I
(6b)
10
9
8
7
6
5
4
3
2
1
ppm
1.07
1.03
1.00
2.11
2.10
1.04
192.181
167.535
166.086
163.839
163.634
163.350
162.693
162.411
162.205
161.922
161.269
138.368
138.348
137.949
137.928
136.146
136.126
135.945
132.781
132.725
131.713
131.664
131.333
131.284
131.069
131.021
131.002
130.230
130.181
129.307
129.290
128.504
128.501
116.471
116.345
116.275
116.212
116.149
116.086
115.964
115.838
115.412
115.287
109.875
108.833
100.951
100.946
100.351
100.348
77.182
77.000
76.818
SCN
F
F
I
(6b)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

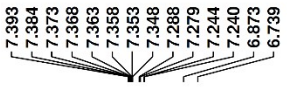

-100.902
-109.532
-109.821
-111.244
SCN
F
F
I
(6b)
50
0
-50
-100
-150
-200
-250
ppm

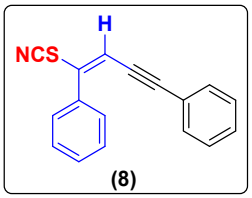

7.529
7.527
7.516
7.507
7.506
7.478
7.472
7.468
7.459
7.447
7.437
7.435
7.403
7.401
7.394
7.392
7.343
7.330
7.328
7.318
7.316
7.279
7.270
7.264
7.262
7.240
2.757
2.746
2.736
2.735
2.726
2.716
2.706
2.695
1.318
1.316
1.308
1.305
1.303
1.300
1.297
1.292
1.289
1.281
1.278
SCN
I
(6c)
I
SCN
(6c')
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.19
2.46
2.02
2.02
1.12
1.99
3.00
146.041
145.981
142.241
140.454
139.360
137.584
129.676
129.218
129.124
128.911
128.892
128.379
128.311
128.135
109.360
109.341
101.263
100.614
77.181
77.000
76.818
28.706
28.668
15.148
14.991
SCN
I
(6c)
I
SCN
(6c')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.320
7.309
7.298
7.258
7.250
7.247
7.242
7.240
7.225
7.222
7.212
7.209
6.996
6.990
6.914
6.901
6.818
6.806
6.543
6.531
3.735
SCN
I
HO
(6d)
I
SCN
HO
(6d')
10
9
8
7
6
5
4
3
2
1
ppm
2.12
3.04
2.00
2.00
0.34
1.44
157.904
142.142
131.115
130.647
129.206
129.051
128.678
127.893
127.834
115.395
115.112
109.678
99.633
77.183
77.000
76.817
49.061
48.939
48.817
48.694
48.572
48.450
48.328
SCN
I
HO
(6d)
I
SCN
HO
(6d')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

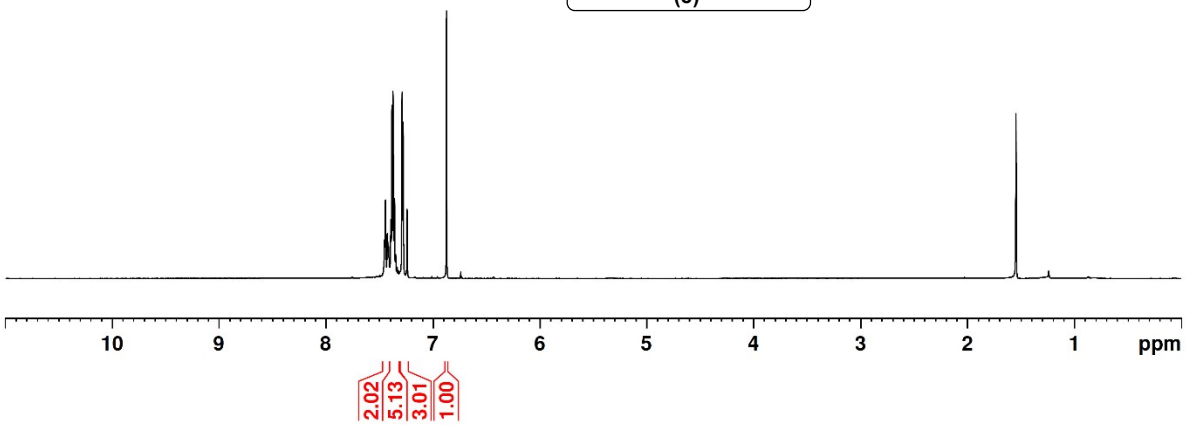

7.240
2.784
2.773
2.762
2.705
2.695
2.684
1.659
1.648
1.637
1.627
1.605
1.595
1.584
1.574
1.561
0.999
0.988
0.978
0.911
0.901
0.890
SeCN
(6e)
10
9
8
7
6
5
4
3
2
1
ppm
2.04
2.00
0.36
2.00
2.19
3.23
3.10
125.139
109.910
100.879
77.183
77.000
76.819
52.509
47.794
46.619
22.345
21.584
21.131
13.199
12.773
12.743
SeCN
(6e)
200
180
160
140
120
100
80
60
40
20
ppm

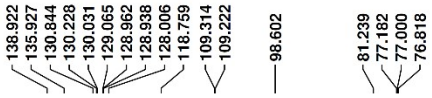

7.369
7.358
7.348
7.339
7.323
7.313
7.302
7.297
7.285
7.275
7.240
7.212
7.196
7.184
2.925
2.914
2.903
1.744
1.733
1.722
1.522
1.512
1.501
1.490
1.030
1.019
1.009
0.796
0.786
0.775
SCN
I
(6f)
I
SCN
(6f')
10
9
8
7
6
5
4
3
2
1
ppm
3.26
2.12
2.01
2.05
2.01
3.00
0.33
142.410
136.726
129.233
129.148
128.788
128.552
127.992
127.901
109.635
98.813
77.182
77.000
76.818
41.556
29.529
22.052
13.874
SCN
I
(6f)
I
SCN
(6f')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

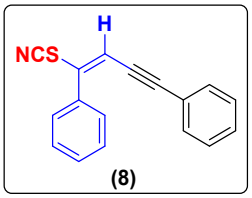

7.393
7.384
7.373
7.368
7.363
7.358
7.353
7.348
7.288
7.279
7.244
7.240
6.873
6.739


H
NCS

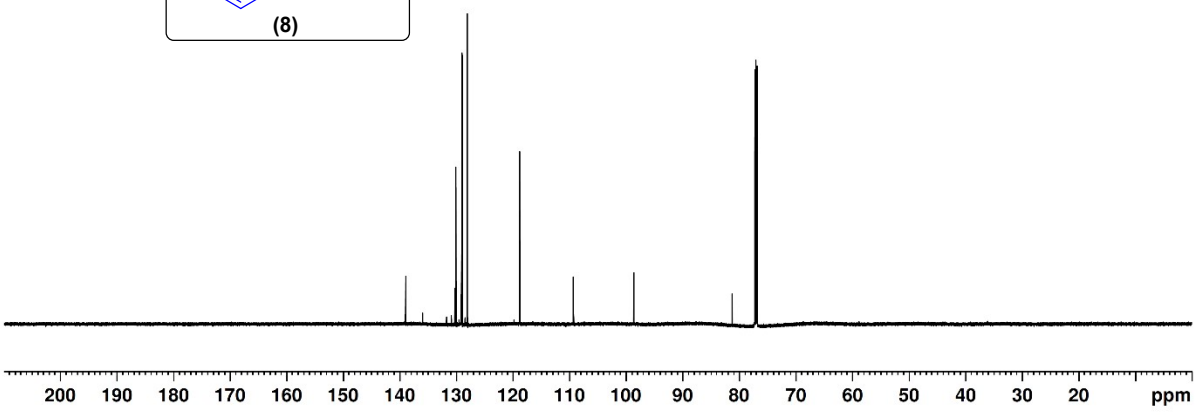
(8)

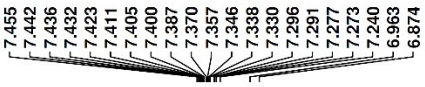

10
9
8
7
6
5
4
3
2
1
ppm
2.02
5.13
3.01
1.00

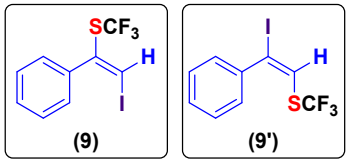

138.922
135.927
130.844
130.228
130.031
129.065
128.962
128.938
128.006
118.759
109.314
109.222
98.602
81.239
77.182
77.000
76.818

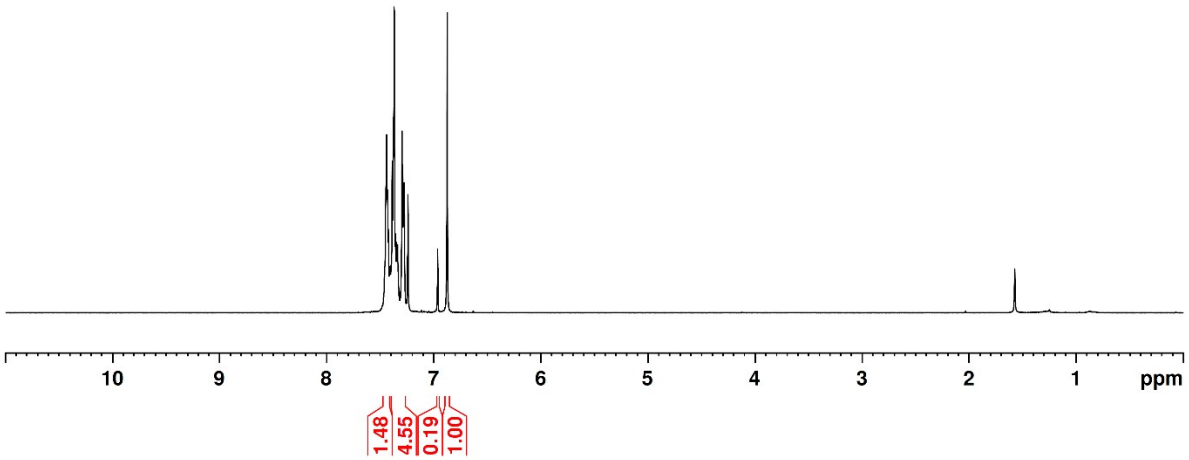

H
NCS

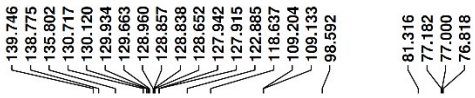
(8)

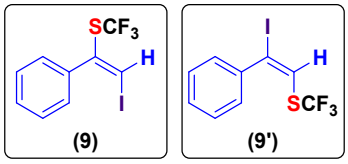

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.455
7.442
7.436
7.432
7.423
7.411
7.405
7.400
7.387
7.370
7.357
7.346
7.338
7.330
7.296
7.291
7.277
7.273
7.240
6.963
6.874


SCF3
H
I
(9)
I
H
SCF3
(9')


10
9
8
7
6
5
4
3
2
1
ppm
1.48
4.55
0.19
1.00


139.746
138.775
135.802
130.717
130.120
129.934
129.663
128.960
128.857
128.838
128.652
127.942
127.915
122.885
118.637
109.204
109.133
98.592
81.316
77.182
77.000
76.818


SCF3
H
I
(9)
I
H
SCF3
(9')

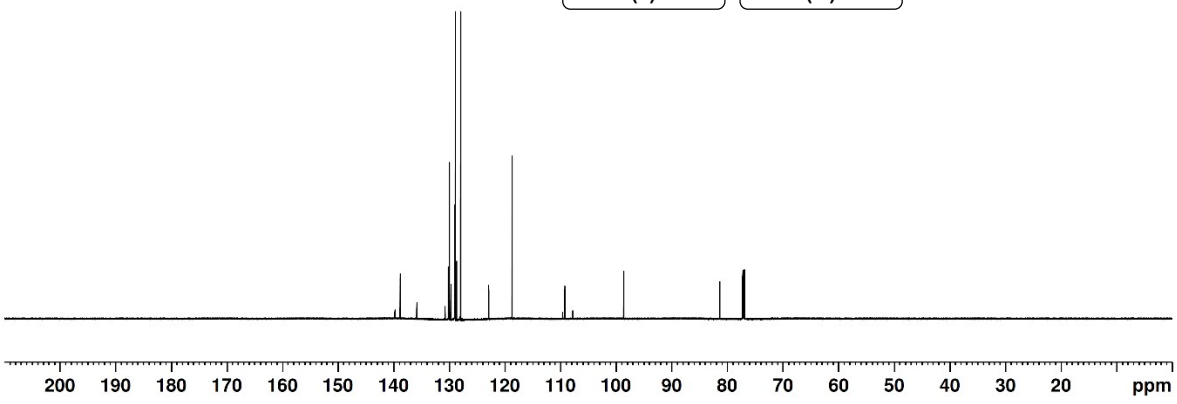

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

Figure S2: ORTEP diagram of compound **2c (CCDC No.2426651)**

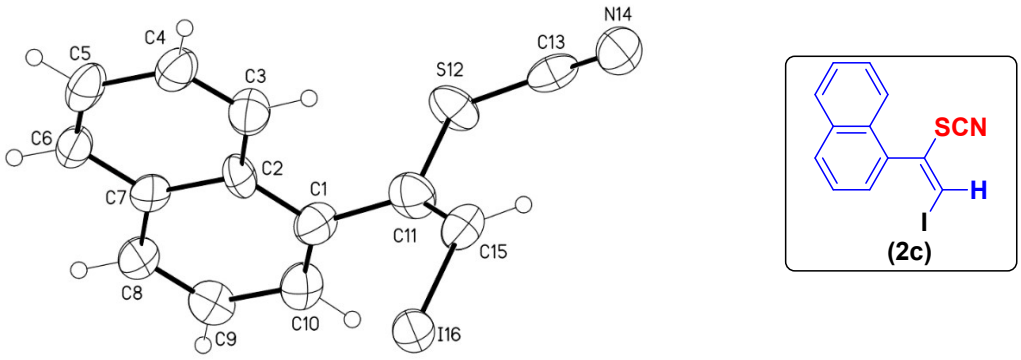


Table S3 Crystal data and structure refinement for 240204lt_auto.

Identification code	240204lt_auto
Empirical formula	$C_{13}H_8INS$
Formula weight	337.16
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	15.8497(6)
b/Å	10.5227(4)
c/Å	7.2426(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1207.93(8)
Z	4
ρ_{calc}g/cm^3	1.854
μ/mm^{-1}	22.192
F(000)	648.0
Crystal size/mm^3	0.16 × 0.03 × 0.03

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.09 to 134.07
Index ranges	$-18 \leq h \leq 17$, $-12 \leq k \leq 12$, $-8 \leq l \leq 8$
Reflections collected	7726
Independent reflections	2110 [R_{int} = 0.0459, R_{sigma} = 0.0422]
Data/restraints/parameters	2110/1/145
Goodness-of-fit on F^2	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.1254
Final R indexes [all data]	R_1 = 0.0545, wR_2 = 0.1290
Largest diff. peak/hole / e $Å^{-3}$	2.56/-1.80
Flack parameter	-0.012(14)

Table S4 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240204lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	4484(9)	2848(13)	3790(20)	40(4)
C2	4074(7)	1693(12)	3230(30)	34(3)
C3	3223(8)	1414(13)	3600(30)	44(3)
C4	2863(9)	309(13)	3075(19)	43(3)
C5	3346(10)	-608(16)	2057(19)	45(3)
C6	4158(9)	-360(13)	1638(19)	37(3)
C7	4550(8)	789(13)	2208(15)	32(3)
C8	5417(9)	1048(14)	1814(16)	38(3)
C9	5789(8)	2144(15)	2380(20)	39(3)
C10	5311(8)	3046(12)	3420(30)	41(3)
C11	3961(10)	3915(16)	4590(20)	47(4)

Table S4 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240204lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S12	3596(2)	4968(4)	2827(5)	45.3(8)
C13	2893(9)	5906(15)	3925(15)	38(3)
N14	2428(8)	6530(14)	4693(17)	48(3)
C15	3785(10)	4116(15)	6260(20)	50(4)
I16	4193.6(5)	2837.4(7)	8417.5(19)	41.8(3)

Table S5 Anisotropic Displacement Parameters (Å^2×10^3) for 240204lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	35(6)	50(8)	36(12)	-8(7)	4(6)	-4(6)
C2	38(6)	33(5)	32(9)	-2(7)	9(7)	10(4)
C3	45(6)	41(7)	47(9)	-6(9)	3(8)	-1(6)
C4	51(7)	44(7)	34(9)	-4(6)	-4(6)	-3(6)
C5	66(10)	42(8)	26(6)	-8(6)	-2(6)	-4(7)
C6	51(8)	29(7)	31(7)	-2(6)	-5(6)	0(6)
C7	47(7)	36(7)	14(5)	5(5)	-4(5)	2(6)
C8	51(8)	47(8)	16(6)	-2(6)	1(5)	7(6)
C9	37(7)	48(9)	33(9)	8(6)	9(5)	1(6)
C10	55(7)	43(6)	25(5)	2(9)	5(9)	1(5)
C11	54(9)	42(8)	44(9)	11(7)	-3(7)	4(7)
S12	50.0(17)	49.5(19)	36.4(17)	18.1(15)	1.4(14)	13.2(16)
C13	45(7)	54(9)	17(7)	7(5)	-4(5)	-13(7)
N14	57(7)	55(8)	33(6)	-3(6)	3(6)	6(7)

Table S5 Anisotropic Displacement Parameters ($Å^2×10^3$) for 240204lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15	55(9)	44(9)	50(10)	-11(7)	-9(7)	-5(7)
I16	58.3(5)	46.3(5)	20.7(4)	1.6(6)	-2.8(6)	12.3(3)

Table S6 Bond Lengths for 240204lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.437(19)	C7	C8	1.431(19)
C1	C10	1.354(19)	C8	C9	1.36(2)
C1	C11	1.51(2)	C9	C10	1.43(2)
C2	C3	1.406(18)	C11	S12	1.785(15)
C2	C7	1.420(19)	C11	C15	1.26(2)
C3	C4	1.350(18)	S12	C13	1.688(16)
C4	C5	1.43(2)	C13	N14	1.132(18)
C5	C6	1.35(2)	C15	I16	2.161(17)
C6	C7	1.420(19)			

Table S7 Bond Angles for 240204lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C11	119.3(12)	C6	C7	C2	119.3(12)
C10	C1	C2	120.9(13)	C6	C7	C8	121.6(12)
C10	C1	C11	119.5(13)	C9	C8	C7	121.2(13)
C3	C2	C1	123.8(13)	C8	C9	C10	119.6(12)
C3	C2	C7	118.0(13)	C1	C10	C9	121.0(13)
C7	C2	C1	118.2(12)	C1	C11	S12	111.4(11)
C4	C3	C2	122.1(15)	C15	C11	C1	127.9(15)

Table S7 Bond Angles for 240204lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	C4	C5	119.9(13)	C15	C11	S12	120.7(14)
C6	C5	C4	119.7(14)	C13	S12	C11	103.9(7)
C5	C6	C7	121.1(13)	N14	C13	S12	178.7(12)
C2	C7	C8	119.1(12)	C11	C15	I16	121.6(13)

Table S8 Torsion Angles for 240204lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	-178.9(16)	C5	C6	C7	C8	178.4(13)
C1	C2	C7	C6	-180.0(14)	C6	C7	C8	C9	-179.2(13)
C1	C2	C7	C8	1(2)	C7	C2	C3	C4	2(3)
C1	C11	S12	C13	169.8(11)	C7	C8	C9	C10	1(2)
C1	C11	C15	I16	-2(2)	C8	C9	C10	C1	-2(2)
C2	C1	C10	C9	3(3)	C10	C1	C2	C3	178.5(18)
C2	C1	C11	S12	-89.9(16)	C10	C1	C2	C7	-3(2)
C2	C1	C11	C15	91(2)	C10	C1	C11	S12	82.8(17)
C2	C3	C4	C5	-2(3)	C10	C1	C11	C15	-96(2)
C2	C7	C8	C9	-0.5(19)	C11	C1	C2	C3	-9(3)
C3	C2	C7	C6	-1(2)	C11	C1	C2	C7	170.0(14)
C3	C2	C7	C8	-179.9(15)	C11	C1	C10	C9	-169.3(14)
C3	C4	C5	C6	0(2)	S12	C11	C15	I16	178.7(8)
C4	C5	C6	C7	1(2)	C15	C11	S12	C13	-11.1(16)
C5	C6	C7	C2	0(2)					

Table S9. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240204lt_auto**.**

Atom	*x*	*y*	*z*	U(eq)
H3	2891.23	2022.97	4238.72	53
H4	2291.01	138.3	3380.06	52
H5	3093.99	-1385.09	1680.69	54
H6	4474.14	-964.49	950.89	45
H8	5739.6	443.9	1141.72	45
H9	6362.94	2308.94	2093.99	47
H10	5577.27	3796.06	3858.27	49
H15	3465.52	4846.86	6578.87	60

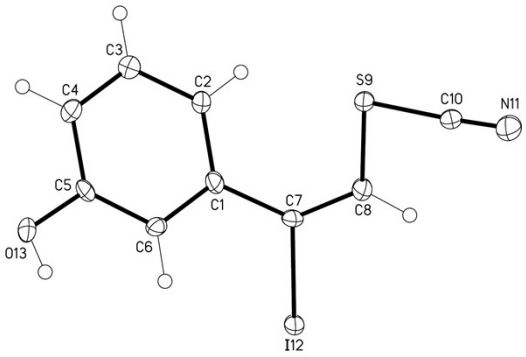
240204lt_auto

Table S10. Crystal data and structure refinement for 240204lt_auto**.**

Identification code	240204lt_auto
Empirical formula	$C_{13}H_8INS$
Formula weight	337.16
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	15.8497(6)
b/Å	10.5227(4)
c/Å	7.2426(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1207.93(8)
Z	4

ρ_{calc}g/cm^3	1.854
μ/mm^{-1}	22.192
F(000)	648.0
Crystal size/mm^3	0.16 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.09 to 134.07
Index ranges	$-18 \leq h \leq 17$, $-12 \leq k \leq 12$, $-8 \leq l \leq 8$
Reflections collected	7726
Independent reflections	2110 [R_{int} = 0.0459, R_{sigma} = 0.0422]
Data/restraints/parameters	2110/1/145
Goodness-of-fit on F^2	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.1254
Final R indexes [all data]	R_1 = 0.0545, wR_2 = 0.1290
Largest diff. peak/hole / e Å^{-3}	2.56/-1.80
Flack parameter	-0.012(14)

Figure S3: ORTEP diagram of compound **2e' (CCDC No.2415478)**



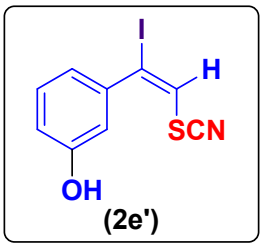


Table S11. Crystal data and structure refinement for 240426lt_auto**.**

Identification code	240426lt_auto
Empirical formula	C_9H_6INOS
Formula weight	303.11
Temperature/K	100.00(10)
Crystal system	tetragonal
Space group	$I4_1/a$
a/Å	30.1435(4)
b/Å	30.1435(4)
c/Å	4.27580(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3885.12(14)
Z	16
ρ_{calc}g/cm^3	2.073
μ/mm^{-1}	27.576
F(000)	2304.0
Crystal size/mm^3	0.18 × 0.04 × 0.04

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.296 to 134.14
Index ranges	$-34 \leq h \leq 36$, $-36 \leq k \leq 34$, $-4 \leq l \leq 5$
Reflections collected	11258
Independent reflections	1732 [R_{int} = 0.0667, R_{sigma} = 0.0316]
Data/restraints/parameters	1732/0/119
Goodness-of-fit on F^2	1.120
Final R indexes [I>=2σ (I)]	R_1 = 0.0294, wR_2 = 0.0811
Final R indexes [all data]	R_1 = 0.0304, wR_2 = 0.0818
Largest diff. peak/hole / e Å^{-3}	1.13/-0.70

Table S12. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240426lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor**.**

Atom	***x***	***y***	***z***	**U(eq)**
I12	5707.1(2)	2026.1(2)	264.9(6)	16.27(14)
S9	5624.9(3)	588.8(3)	4299(2)	17.3(2)
O13	7361.1(9)	1619.3(9)	6092(7)	20.2(6)
N11	4840.9(12)	478.4(12)	7893(8)	22.9(8)
C1	6333.3(13)	1260.5(13)	2259(9)	15.9(8)
C2	6482.1(12)	869.0(13)	843(10)	16.5(8)
C3	6923.8(13)	741.4(13)	1206(10)	19.4(8)
C4	7214.5(13)	997.1(13)	2950(9)	18.4(8)
C5	7062.4(13)	1385.1(13)	4379(9)	16.1(8)
C6	6625.7(12)	1520.4(12)	3994(9)	14.7(7)
C7	5859.8(13)	1384.3(12)	1990(9)	13.9(7)
C8	5517.9(13)	1125.8(13)	2743(9)	16.4(8)

Table S12. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240426lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor**.**

Atom	*x*	*y*	*z*	U(eq)
C10	5152.1(13)	533.5(12)	6424(10)	18.2(8)

Table S13 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240426lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I12	11.58(17)	10.38(17)	26.8(2)	2.83(8)	-1.24(9)	0.08(8)
S9	11.6(4)	10.2(4)	30.1(5)	2.4(4)	1.9(4)	0.5(3)
O13	9.4(12)	20.0(14)	31.3(16)	-7.1(12)	-0.2(12)	-1.0(11)
N11	18.9(18)	17.6(17)	32(2)	3.7(14)	1.3(15)	1.6(14)
C1	11.2(19)	11.5(18)	25(2)	4.0(15)	1.0(14)	-2.4(15)
C2	10.4(17)	13.8(18)	25(2)	0.4(16)	-0.8(15)	-0.4(14)
C3	15.0(18)	15.9(18)	27(2)	-2.1(16)	2.8(17)	-0.3(15)
C4	12.0(18)	16(2)	27(2)	1.6(16)	0.2(15)	2.5(15)
C5	13.0(18)	10.3(18)	25(2)	2.8(15)	1.8(15)	-4.6(15)
C6	13.8(17)	10.1(16)	20.0(19)	0.6(15)	6.5(16)	0.6(14)
C7	14.0(18)	8.0(17)	19.9(18)	0.4(14)	-1.7(14)	0.8(14)
C8	11.6(18)	13.5(18)	24(2)	2.1(15)	-1.0(15)	0.2(15)
C10	13.7(19)	10.4(17)	31(2)	0.9(16)	-1.0(18)	1.7(15)

Table S14. Bond Lengths for 240426lt_auto**.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I12	C7	2.121(4)	C1	C7	1.480(5)

Table S14. Bond Lengths for 240426lt_auto**.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S9	C8	1.780(4)	C2	C3	1.395(5)
S9	C10	1.699(4)	C3	C4	1.385(6)
O13	C5	1.358(5)	C4	C5	1.397(6)
N11	C10	1.141(5)	C5	C6	1.388(5)
C1	C2	1.400(6)	C7	C8	1.332(6)
C1	C6	1.393(6)			

Table S15. Bond Angles for 240426lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	S9	C8	97.89(18)	O13	C5	C6	122.7(3)
C2	C1	C7	119.2(3)	C6	C5	C4	120.4(4)
C6	C1	C2	120.1(4)	C5	C6	C1	119.9(3)
C6	C1	C7	120.7(4)	C1	C7	I12	117.8(3)
C3	C2	C1	119.4(4)	C8	C7	I12	116.7(3)
C4	C3	C2	120.7(4)	C8	C7	C1	125.5(3)
C3	C4	C5	119.6(4)	C7	C8	S9	118.8(3)
O13	C5	C4	117.0(3)	N11	C10	S9	177.0(4)

Table S16. Torsion Angles for 240426lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
I12	C7	C8	S9	-178.38(18)	C3	C4	C5	C6	-1.6(6)
O13	C5	C6	C1	-178.7(3)	C4	C5	C6	C1	2.1(6)
C1	C2	C3	C4	0.1(6)	C6	C1	C2	C3	0.4(6)

Table S16. Torsion Angles for 240426lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C7	C8	S9	1.6(5)	C6	C1	C7	I12	55.7(4)
C2	C1	C6	C5	-1.5(6)	C6	C1	C7	C8	-124.2(4)
C2	C1	C7	I12	-126.6(3)	C7	C1	C2	C3	-177.2(4)
C2	C1	C7	C8	53.4(5)	C7	C1	C6	C5	176.1(3)
C2	C3	C4	C5	0.5(6)	C10	S9	C8	C7	152.6(3)
C3	C4	C5	O13	179.2(4)					

Table S17. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240426lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H13	7226.41	1801.37	7236.44	30
H2	6284.04	692.08	-353.13	20
H3	7026.41	476.28	246.08	23
H4	7515.45	909.19	3174.15	22
H6	6526.43	1789.74	4911.52	18
H8	5222.02	1226.26	2454.27	20

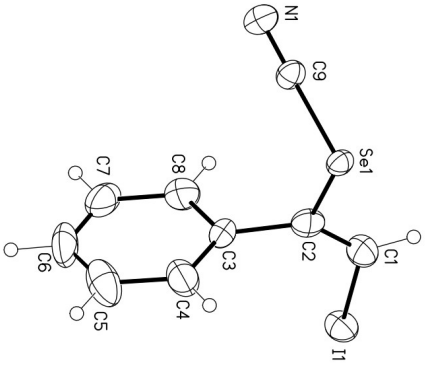
240426lt_auto

Table S18 Crystal data and structure refinement for 240426lt_auto**.**

Identification code	240426lt_auto
Empirical formula	C_9H_6INOS
Formula weight	303.11
Temperature/K	100.00(10)
Crystal system	tetragonal

Space group	$I4_1/a$
a/Å	30.1435(4)
b/Å	30.1435(4)
c/Å	4.27580(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3885.12(14)
Z	16
ρ_{calc}g/cm^3	2.073
μ/mm^{-1}	27.576
F(000)	2304.0
Crystal size/mm^3	0.18 × 0.04 × 0.04
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.296 to 134.14
Index ranges	$-34 \leq h \leq 36$, $-36 \leq k \leq 34$, $-4 \leq l \leq 5$
Reflections collected	11258
Independent reflections	1732 [R_{int} = 0.0667, R_{sigma} = 0.0316]
Data/restraints/parameters	1732/0/119
Goodness-of-fit on F^2	1.120
Final R indexes [I>=2σ (I)]	R_1 = 0.0294, wR_2 = 0.0811
Final R indexes [all data]	R_1 = 0.0304, wR_2 = 0.0818
Largest diff. peak/hole / e Å^{-3}	1.13/-0.70

Figure S4: ORTEP diagram of compound **4a (CCDC No.2415348)**



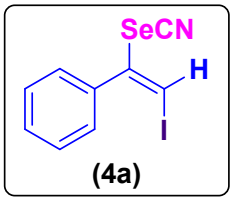


Table S19 Crystal data and structure refinement for 240212LT_auto**.**

Identification code	240212LT_auto
Empirical formula	C_9H_6INSe
Formula weight	334.01
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	5.8525(2)
b/Å	8.8084(5)
c/Å	10.7100(5)
α/°	93.190(4)
β/°	103.729(4)
γ/°	104.690(4)
Volume/Å^3	514.85(4)
Z	2
ρ_{calc}g/cm^3	2.155
μ/mm^{-1}	28.042

F(000)	308.0
Crystal size/mm^3	0.16 × 0.13 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.564 to 134.128
Index ranges	-6 ≤ h ≤ 6, -10 ≤ k ≤ 10, -12 ≤ l ≤ 12
Reflections collected	4493
Independent reflections	1794 [R_{int} = 0.0320, R_{sigma} = 0.0343]
Data/restraints/parameters	1794/137/166
Goodness-of-fit on F^2	1.092
Final R indexes [I>=2σ (I)]	R_1 = 0.0339, wR_2 = 0.0924
Final R indexes [all data]	R_1 = 0.0352, wR_2 = 0.0931
Largest diff. peak/hole / e Å^{-3}	0.81/-1.34

Table S20 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240212LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor**.**

Atom	***x***	***y***	***z***	**U(eq)**
C3	7327(9)	3439(7)	7451(6)	32.0(13)
C4	6972(12)	4500(7)	8328(6)	42.1(15)
C5	8557(15)	6004(8)	8670(7)	54.7(19)
C6	10466(14)	6455(8)	8115(8)	59(2)
C7	10859(12)	5431(9)	7250(9)	55(2)
C8	9280(11)	3913(8)	6904(7)	46.4(16)
I1	2972.4(6)	2318.2(4)	4575.3(3)	32.72(16)

Table S20 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240212LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor**.**

Atom	*x*	*y*	*z*	U(eq)
Se1	6190(50)	490(40)	8470(30)	22.4(18)
N1	11590(60)	950(70)	8850(60)	24(3)
C1	3993(12)	1086(8)	6132(7)	26.2(15)
C2	5741(12)	1772(8)	7196(7)	23.3(15)
C9	9500(60)	780(80)	8550(80)	24(2)
C2A	4790(80)	1010(60)	6820(50)	25(4)
C1A	5330(70)	2100(50)	6460(40)	25(4)
I1A	3540(130)	3530(90)	5360(70)	36(6)
Se1A	6161(12)	465(10)	8616(9)	22.3(6)
C9A	9369(17)	580(18)	8598(19)	24.5(15)
N1A	11351(19)	628(19)	8606(15)	28.3(18)

Table S21 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240212LT_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	20(3)	27(3)	43(3)	-2(2)	3(2)	2(2)
C4	47(4)	30(3)	46(4)	1(3)	9(3)	9(3)
C5	82(5)	33(4)	36(4)	2(3)	-2(3)	9(4)
C6	52(4)	25(4)	74(5)	17(4)	-15(4)	-9(3)
C7	29(3)	43(4)	91(6)	33(4)	9(3)	6(3)

Table S21 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240212LT_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C8	33(3)	39(4)	70(5)	7(3)	16(3)	12(3)
I1	39.4(3)	31.9(2)	26.0(2)	2.69(15)	2.57(16)	13.96(17)
Se1	18(2)	27(3)	24(4)	4(3)	9(2)	7(2)
N1	22(4)	27(6)	25(6)	-2(6)	10(5)	8(5)
C1	22(3)	27(3)	26(4)	-2(3)	1(3)	7(2)
C2	18(3)	26(3)	26(4)	-3(3)	7(3)	6(3)
C9	20(3)	27(3)	25(3)	3(3)	9(3)	6(3)
C2A	20(7)	26(7)	28(7)	-7(7)	1(6)	9(6)
C1A	20(6)	28(6)	26(7)	-4(6)	3(6)	10(6)
I1A	38(8)	35(8)	34(8)	1(7)	8(7)	11(7)
Se1A	18.6(6)	25.8(6)	23.4(14)	6.9(9)	7.4(7)	5.1(5)
C9A	22(2)	27(3)	25(3)	3(3)	8.4(19)	5(2)
N1A	25(3)	30(4)	26(4)	-7(3)	3(3)	6(3)

Table S22 Bond Lengths for 240212LT_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C3	C4	1.376(8)	Se1	C9	1.865(16)
C3	C8	1.388(8)	N1	C9	1.157(18)
C3	C2	1.496(8)	C1	C2	1.329(10)
C3	C1A	1.57(4)	C2A	C1A	1.06(8)
C4	C5	1.382(9)	C2A	Se1A	2.03(5)

Table S22 Bond Lengths for 240212LT_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C5	C6	1.370(12)	C1A	I1A	2.08(9)
C6	C7	1.355(12)	I1A	I1A[1]	2.97(15)
C7	C8	1.391(9)	Se1A	C9A	1.859(7)
I1	C1	2.090(7)	C9A	N1A	1.148(9)
Se1	C2	1.83(4)			

[1]1-X,1-Y,1-Z

Table S23 Bond Angles for 240212LT_auto**.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	C3	C8	118.9(6)	C3	C2	Se1	118.1(11)
C4	C3	C2	119.4(5)	C1	C2	C3	127.3(7)
C4	C3	C1A	127.5(15)	C1	C2	Se1	114.6(11)
C8	C3	C2	121.5(6)	N1	C9	Se1	167(7)
C8	C3	C1A	106.9(16)	C1A	C2A	Se1A	127(5)
C3	C4	C5	120.4(7)	C3	C1A	I1A	98(3)
C6	C5	C4	120.0(7)	C2A	C1A	C3	115(5)
C7	C6	C5	120.8(7)	C2A	C1A	I1A	136(5)
C6	C7	C8	119.7(7)	C1A	I1A	I1A[1]	119(4)
C3	C8	C7	120.3(7)	C9A	Se1A	C2A	101.7(13)
C2	Se1	C9	94(2)	N1A	C9A	Se1A	178.5(14)
C2	C1	I1	122.5(6)				

[1]1-X,1-Y,1-Z

Table S24 Torsion Angles for 240212LT_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C3	C4	C5	C6	1.3(10)	C8	C3	C1A	I1A	-87(3)
C4	C3	C8	C7	0.6(9)	I1	C1	C2	C3	-3.4(9)
C4	C3	C2	Se1	-71.2(14)	I1	C1	C2	Se1	176.5(12)
C4	C3	C2	C1	108.7(8)	C2	C3	C4	C5	173.9(6)
C4	C3	C1A	C2A	-87(4)	C2	C3	C8	C7	-174.1(6)
C4	C3	C1A	I1A	63(3)	C2	Se1	C9	N1	145(23)
C4	C5	C6	C7	-1.5(11)	C9	Se1	C2	C3	-56(3)
C5	C6	C7	C8	1.2(11)	C9	Se1	C2	C1	124(3)
C6	C7	C8	C3	-0.8(10)	C1A	C3	C4	C5	-148(2)
C8	C3	C4	C5	-0.9(9)	C1A	C3	C8	C7	154.1(18)
C8	C3	C2	Se1	103.4(14)	Se1A	C2A	C1A	C3	-3(6)
C8	C3	C2	C1	-76.7(9)	Se1A	C2A	C1A	I1A	-138(5)
C8	C3	C1A	C2A	123(4)					

Table S25 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240212LT_auto**.**

Atom	*x*	*y*	*z*	U(eq)
H4	5629.71	4197.41	8701.37	51
H5	8322.6	6724.38	9289.91	66
H6	11526.96	7498.39	8337.6	71
H7	12206.89	5748.48	6883.16	66
H8	9539.74	3196.88	6290.34	56

Table S25 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240212LT_auto**.**

Atom	*x*	*y*	*z*	U(eq)
H1	3176.2	-4.75	6076.06	31
H2A	3524.55	198.95	6248.05	30

Table S26 Atomic Occupancy for 240212LT_auto.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
I1	0.9949(9)	Se1	0.19(6)	N1	0.19(6)
C1	0.863(12)	H1	0.863(12)	C2	0.863(12)
C9	0.19(6)	C2A	0.137(12)	H2A	0.137(12)
C1A	0.137(12)	I1A	0.0051(9)	Se1A	0.81(6)
C9A	0.81(6)	N1A	0.81(6)		

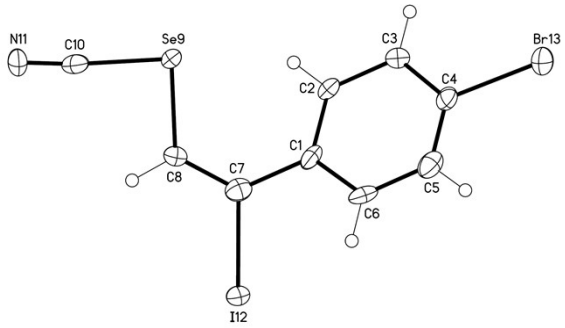
240212LT_auto

Table S27 Crystal data and structure refinement for 240212LT_auto**.**

Identification code	240212LT_auto
Empirical formula	C_9H_6INSe
Formula weight	334.01
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	5.8525(2)
b/Å	8.8084(5)
c/Å	10.7100(5)

α/°	93.190(4)
β/°	103.729(4)
γ/°	104.690(4)
Volume/Å^3	514.85(4)
Z	2
ρ_{calc}g/cm^3	2.155
μ/mm^{-1}	28.042
F(000)	308.0
Crystal size/mm^3	0.16 × 0.13 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.564 to 134.128
Index ranges	-6 ≤ h ≤ 6, -10 ≤ k ≤ 10, -12 ≤ l ≤ 12
Reflections collected	4493
Independent reflections	1794 [R_{int} = 0.0320, R_{sigma} = 0.0343]
Data/restraints/parameters	1794/137/166
Goodness-of-fit on F^2	1.092
Final R indexes [I>=2σ (I)]	R_1 = 0.0339, wR_2 = 0.0924
Final R indexes [all data]	R_1 = 0.0352, wR_2 = 0.0931
Largest diff. peak/hole / e Å^{-3}	0.81/-1.34

Figure S5: ORTEP diagram of compound **4h' (CCDC No. 2415349)**



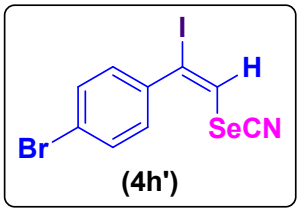


Table S28 Crystal data and structure refinement for 240427lt_auto**.**

Identification code	240427lt_auto
Empirical formula	$C_9H_5BrINSe$
Formula weight	412.91
Temperature/K	99.98(11)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	15.1846(2)
b/Å	17.1716(3)
c/Å	4.14080(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1079.69(4)
Z	4
ρ_{calc}g/cm^3	2.540
μ/mm^{-1}	31.115

F(000)	752.0
Crystal size/mm^3	0.16 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.772 to 134.044
Index ranges	-18 ≤ h ≤ 18, -20 ≤ k ≤ 20, -4 ≤ l ≤ 4
Reflections collected	12033
Independent reflections	1889 [R_{int} = 0.0391, R_{sigma} = 0.0208]
Data/restraints/parameters	1889/1/119
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.1158
Final R indexes [all data]	R_1 = 0.0454, wR_2 = 0.1159
Largest diff. peak/hole / e Å^{-3}	1.88/-1.05
Flack parameter	0.011(14)

Table S29 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240427lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
I12	1913.2(4)	7207.0(4)	1548(3)	21.0(3)
Br13	649.7(8)	3146.0(7)	3841(4)	29.9(4)
Se9	4232.2(7)	5553.9(6)	5525(3)	18.6(3)
N11	5635(7)	6545(6)	8480(40)	33(3)
C1	2187(8)	5504(6)	3490(30)	19(2)
C2	2551(7)	4834(7)	2150(30)	22(2)

Table S29 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240427lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C3	2109(8)	4112(7)	2290(30)	22(3)
C4	1298(7)	4100(7)	3830(30)	22(2)
C5	940(8)	4741(7)	5250(30)	24(2)
C6	1372(8)	5446(7)	5110(30)	21(2)
C7	2658(8)	6267(7)	3280(30)	20(2)
C8	3505(8)	6388(6)	3900(30)	22(2)
C10	5087(8)	6201(7)	7330(30)	29(3)

Table S30 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240427lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I12	16.9(4)	17.1(4)	29.1(5)	-0.9(3)	-3.5(3)	3.6(2)
Br13	20.0(6)	23.6(7)	45.9(8)	3.4(6)	1.1(6)	-5.4(4)
Se9	11.2(5)	16.0(6)	28.5(7)	0.8(5)	-0.5(5)	1.3(4)
N11	20(5)	20(5)	60(8)	0(6)	-11(5)	-6(4)
C1	9(5)	26(6)	22(7)	4(5)	0(5)	0(4)
C2	10(5)	22(5)	33(7)	1(5)	-1(4)	2(4)
C3	18(5)	17(6)	30(7)	-1(5)	-1(5)	3(4)
C4	14(5)	21(5)	30(6)	4(5)	-7(5)	-1(4)
C5	17(5)	30(6)	24(6)	8(5)	-1(5)	0(5)

Table S30 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240427lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C6	16(5)	25(5)	21(6)	4(5)	2(5)	11(4)
C7	21(6)	23(6)	17(6)	4(4)	1(4)	4(4)
C8	19(5)	14(5)	33(6)	0(5)	-4(5)	3(4)
C10	19(6)	19(6)	48(9)	5(6)	1(6)	7(5)

Table S31 Bond Lengths for 240427lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I12	C7	2.098(11)	C1	C7	1.495(16)
Br13	C4	1.911(11)	C2	C3	1.410(17)
Se9	C8	1.929(11)	C3	C4	1.387(17)
Se9	C10	1.865(13)	C4	C5	1.362(19)
N11	C10	1.127(18)	C5	C6	1.379(17)
C1	C2	1.392(17)	C7	C8	1.328(19)
C1	C6	1.410(17)			

Table S32 Bond Angles for 240427lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	Se9	C8	95.5(5)	C5	C4	C3	122.7(11)
C2	C1	C6	118.6(10)	C4	C5	C6	120.1(12)
C2	C1	C7	120.7(10)	C5	C6	C1	120.0(11)
C6	C1	C7	120.6(10)	C1	C7	I12	115.8(8)

Table S32 Bond Angles for 240427lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	C2	C3	121.5(11)	C8	C7	I12	117.9(8)
C4	C3	C2	117.0(11)	C8	C7	C1	126.1(10)
C3	C4	Br13	118.2(9)	C7	C8	Se9	120.4(8)
C5	C4	Br13	119.1(9)	N11	C10	Se9	175.1(11)

Table S33 Torsion Angles for 240427lt_auto**.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
I12	C7	C8	Se9	179.6(6)	C2	C3	C4	C5	-1.8(19)
Br13	C4	C5	C6	-176.2(10)	C3	C4	C5	C6	2(2)
C1	C2	C3	C4	-0.4(19)	C4	C5	C6	C1	0(2)
C1	C7	C8	Se9	-4.6(18)	C6	C1	C2	C3	2.3(19)
C2	C1	C6	C5	-2.1(19)	C6	C1	C7	I12	-51.9(15)
C2	C1	C7	I12	129.5(11)	C6	C1	C7	C8	132.3(14)
C2	C1	C7	C8	-46.4(19)	C7	C1	C2	C3	-179.0(12)
C2	C3	C4	Br13	176.4(9)	C7	C1	C6	C5	179.2(12)

Table S34 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240427lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H2	3109.22	4863.04	1127.75	26
H3	2355.34	3655.57	1363.45	26
H5	390.59	4702.51	6339.97	28

Table S34 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240427lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H6	1121.91	5892.85	6104.03	25
H8	3754.69	6887.97	3545.93	27

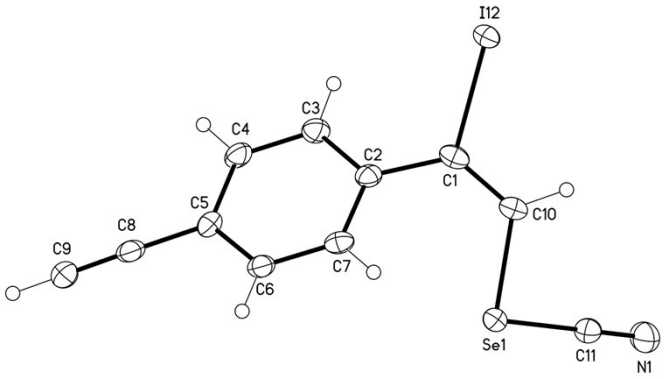
240427lt_auto

Table S35 Crystal data and structure refinement for 240427lt_auto**.**

Identification code	240427lt_auto
Empirical formula	$C_9H_5BrINSe$
Formula weight	412.91
Temperature/K	99.98(11)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	15.1846(2)
b/Å	17.1716(3)
c/Å	4.14080(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1079.69(4)
Z	4
ρ_{calc}g/cm^3	2.540
μ/mm^{-1}	31.115
F(000)	752.0

Crystal size/mm^3	0.16 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.772 to 134.044
Index ranges	$-18 \leq h \leq 18$, $-20 \leq k \leq 20$, $-4 \leq l \leq 4$
Reflections collected	12033
Independent reflections	1889 [R_{int} = 0.0391, R_{sigma} = 0.0208]
Data/restraints/parameters	1889/1/119
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.1158
Final R indexes [all data]	R_1 = 0.0454, wR_2 = 0.1159
Largest diff. peak/hole / e $Å^{-3}$	1.88/-1.05
Flack parameter	0.011(14)

Figure S6: ORTEP diagram of compound **4k' (CCDC No. 2415484)**



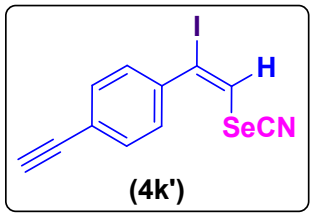


Table S36 Crystal data and structure refinement for 240424lt2_auto**.**

Identification code	240424lt2_auto
Empirical formula	$C_{11}H_6INSe$
Formula weight	358.03
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	4.13040(10)
b/Å	24.4751(7)
c/Å	10.7813(3)
α/°	90
β/°	97.051(2)
γ/°	90
Volume/Å^3	1081.66(5)
Z	4
ρ_{calc}g/cm^3	2.199
μ/mm^{-1}	26.761

F(000)	664.0
Crystal size/mm^3	0.47 × 0.036 × 0.019
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.224 to 134.116
Index ranges	-4 ≤ h ≤ 2, -29 ≤ k ≤ 26, -12 ≤ l ≤ 12
Reflections collected	6202
Independent reflections	1922 [R_{int} = 0.0341, R_{sigma} = 0.0330]
Data/restraints/parameters	1922/0/131
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0345, wR_2 = 0.1043
Final R indexes [all data]	R_1 = 0.0355, wR_2 = 0.1052
Largest diff. peak/hole / e Å^{-3}	2.01/-1.01

Table S37 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240424lt2_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
I12	7638.0(7)	5744.9(2)	3920.4(3)	18.56(19)
Se1	5107.2(12)	6033.9(2)	8118.5(4)	18.9(2)
N1	1975(13)	4969.0(19)	8652(5)	31.3(10)
C1	6490(11)	6110(2)	5587(5)	18.6(10)
C2	5855(11)	6705(2)	5570(4)	18.4(9)
C3	3812(12)	6952(2)	4586(5)	21.4(10)
C4	2981(13)	7495(2)	4667(5)	22.1(10)

Table S37 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240424lt2_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C5	4114(12)	7814(2)	5703(4)	18.8(9)
C6	6321(12)	7575(2)	6648(4)	19.9(10)
C7	7135(12)	7029(2)	6581(4)	19.5(9)
C8	3058(12)	8365(2)	5798(4)	21.7(10)
C9	2000(13)	8823(2)	5887(5)	25.6(11)
C10	6314(13)	5777.8(19)	6549(5)	19.4(10)
C11	3221(12)	5374(2)	8453(5)	21.7(10)
I12A	8110(30)	6028(7)	3773(11)	18.56(19)

Table S38 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240424lt2_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$**.**

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I12	19.2(3)	19.1(3)	17.9(2)	-4.22(12)	4.45(15)	-0.51(11)
Se1	23.3(3)	16.6(3)	17.0(3)	-1.52(17)	3.2(2)	-0.59(17)
N1	41(3)	23(2)	31(2)	-2.2(19)	11(2)	-7.3(19)
C1	14(2)	23(2)	19(2)	-7.9(18)	-0.5(18)	-4.0(17)
C2	18(2)	22(2)	16(2)	0.9(18)	6.2(17)	1.2(17)
C3	24(2)	23(2)	16(2)	-1.8(19)	-1.4(18)	-2.5(18)
C4	26(3)	24(3)	15(2)	2.8(18)	-3.1(18)	-2.0(19)
C5	19(2)	20(2)	18(2)	4.4(18)	3.4(18)	0.0(17)

Table S38 Anisotropic Displacement Parameters ($Å^2×10^3$) for 240424lt2_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C6	23(3)	22(2)	14(2)	0.2(19)	3.3(18)	-2.5(18)
C7	19(2)	26(2)	13(2)	-0.8(18)	0.0(17)	-3.1(18)
C8	27(2)	25(3)	13(2)	1.6(19)	4.5(18)	-2(2)
C9	33(3)	24(3)	19(2)	2(2)	0(2)	6(2)
C10	19(3)	22(3)	17(3)	-4.8(17)	3.1(19)	1.0(16)
C11	25(3)	22(2)	19(2)	-0.3(19)	5.5(19)	2.2(19)
I12A	19.2(3)	19.1(3)	17.9(2)	-4.22(12)	4.45(15)	-0.51(11)

Table S39 Bond Lengths for 240424lt2_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I12	C1	2.112(5)	C2	C7	1.398(7)
Se1	C10	1.927(5)	C3	C4	1.378(7)
Se1	C11	1.847(5)	C4	C5	1.396(7)
N1	C11	1.150(7)	C5	C6	1.409(7)
C1	C2	1.480(7)	C5	C8	1.424(7)
C1	C10	1.326(8)	C6	C7	1.381(7)
C1	I12A	2.153(13)	C8	C9	1.213(8)
C2	C3	1.408(7)			

Table S40 Bond Angles for 240424lt2_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

Table S40 Bond Angles for 240424lt2_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	Se1	C10	92.8(2)	C3	C4	C5	121.9(5)
C2	C1	I12	117.6(3)	C4	C5	C6	118.0(4)
C2	C1	I12A	98.9(6)	C4	C5	C8	120.8(4)
C10	C1	I12	116.4(4)	C6	C5	C8	121.2(5)
C10	C1	C2	125.9(5)	C7	C6	C5	120.3(4)
C10	C1	I12A	134.9(6)	C6	C7	C2	121.2(4)
C3	C2	C1	121.4(4)	C9	C8	C5	176.6(6)
C7	C2	C1	120.0(4)	C1	C10	Se1	122.1(4)
C7	C2	C3	118.6(4)	N1	C11	Se1	178.4(5)
C4	C3	C2	119.8(5)				

Table S41 Torsion Angles for 240424lt2_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
I12	C1	C2	C3	46.1(6)	C4	C5	C6	C7	-4.5(7)
I12	C1	C2	C7	-137.8(4)	C5	C6	C7	C2	1.3(7)
I12	C1	C10	Se1	-177.2(2)	C7	C2	C3	C4	-3.4(7)
C1	C2	C3	C4	172.7(5)	C8	C5	C6	C7	175.3(5)
C1	C2	C7	C6	-173.5(4)	C10	C1	C2	C3	-131.8(6)
C2	C1	C10	Se1	0.8(8)	C10	C1	C2	C7	44.3(7)
C2	C3	C4	C5	0.2(8)	I12A	C1	C2	C3	53.6(6)
C3	C2	C7	C6	2.7(7)	I12A	C1	C2	C7	-130.3(5)

Table S41 Torsion Angles for 240424lt2_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C3	C4	C5	C6	3.8(8)	I12A	C1	C10	Se1	173.2(6)
C3	C4	C5	C8	-176.1(5)					

Table S42 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240424lt2_auto**.**

Atom	*x*	*y*	*z*	U(eq)
H3	3010.02	6744.81	3868.5	26
H4	1595.07	7656.52	3998.36	26
H6	7254.12	7789.52	7333.91	24
H7	8590.23	6871.22	7234.29	23
H9	1171.04	9182.8	5955.71	31
H10	6799.05	5401.42	6460.46	23

Table S43 Atomic Occupancy for 240424lt2_auto**.**

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
I12	0.9733(11)	I12A	0.0267(11)		

240424lt2_auto

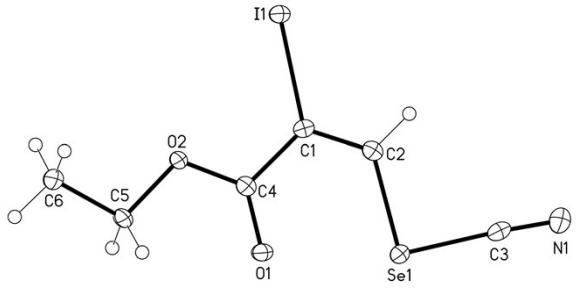
Table S44 Crystal data and structure refinement for 240424lt2_auto**.**

Identification code	240424lt2_auto
Empirical formula	$C_{11}H_6INSe$
Formula weight	358.03
Temperature/K	100.00(10)

Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	4.13040(10)
b/Å	24.4751(7)
c/Å	10.7813(3)
α/°	90
β/°	97.051(2)
γ/°	90
Volume/Å^3	1081.66(5)
Z	4
ρ_{calc}g/cm^3	2.199
μ/mm^{-1}	26.761
F(000)	664.0
Crystal size/mm^3	0.47 × 0.036 × 0.019
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.224 to 134.116
Index ranges	$-4 \leq h \leq 2$, $-29 \leq k \leq 26$, $-12 \leq l \leq 12$
Reflections collected	6202
Independent reflections	1922 [R_{int} = 0.0341, R_{sigma} = 0.0330]
Data/restraints/parameters	1922/0/131
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0345, wR_2 = 0.1043
Final R indexes [all data]	R_1 = 0.0355, wR_2 = 0.1052

Largest diff. peak/hole / e $Å^{-3}$ 2.01/-1.01

Figure S7: ORTEP diagram of compound **4m' (CCDC No. 2415490)**



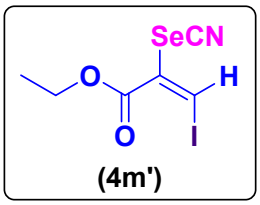


Table S45 Crystal data and structure refinement for 2405112lt_Mo_auto**.**

Identification code	2405112lt_Mo_auto
Empirical formula	$C_6H_6INO_2Se$
Formula weight	329.98
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.9161(3)
b/Å	7.3338(2)
c/Å	13.8985(5)
α/°	90
β/°	98.850(3)
γ/°	90
Volume/Å^3	897.99(5)
Z	4
ρ_{calc}g/cm^3	2.441
μ/mm^{-1}	7.571

F(000)	608.0
Crystal size/mm^3	0.09 × 0.09 × 0.02
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.94 to 52.736
Index ranges	-10 ≤ h ≤ 11, -9 ≤ k ≤ 9, -17 ≤ l ≤ 14
Reflections collected	6738
Independent reflections	1832 [R_{int} = 0.0231, R_{sigma} = 0.0220]
Data/restraints/parameters	1832/0/101
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0200, wR_2 = 0.0461
Final R indexes [all data]	R_1 = 0.0224, wR_2 = 0.0470
Largest diff. peak/hole / e Å^{-3}	1.47/-0.46

Table S46 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2405112lt_Mo_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
$I_{(1)}$	2367.7(2)	3769.8(2)	5264.8(2)	17.85(8)
$Se_{(1)}$	3722.4(3)	9342.5(4)	3773.7(2)	17.06(9)
$O_{(1)}$	2256(3)	9571(3)	5208.2(15)	22.9(5)
$O_{(2)}$	1438(2)	7499(3)	6199.0(14)	17.5(4)
$N_{(1)}$	5373(4)	8213(4)	2130(2)	29.8(7)
$C_{(1)}$	2701(3)	6494(4)	4909(2)	15.7(6)
$C_{(2)}$	3430(3)	6894(4)	4169(2)	16.1(6)

Table S46 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 2405112lt_Mo_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
$C_{(3)}$	4742(4)	8593(4)	2756(2)	21.2(7)
$C_{(4)}$	2113(3)	7997(4)	5456(2)	16.1(6)
$C_{(5)}$	839(4)	9015(4)	6712(2)	19.5(7)
$C_{(6)}$	-72(4)	8213(4)	7434(2)	19.8(6)

Table S47 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2405112lt_Mo_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$I_{(1)}$	25.35(12)	10.32(11)	20.13(12)	1.21(7)	10.67(8)	1.12(7)
$Se_{(1)}$	24.31(17)	11.83(15)	17.19(16)	1.57(11)	10.04(12)	0.41(11)
$O_{(1)}$	36.5(14)	10.0(10)	27.2(12)	1.1(8)	20.6(10)	0.6(9)
$O_{(2)}$	27.1(12)	10.1(10)	18.4(11)	0.1(8)	13.9(9)	2.0(8)
$N_{(1)}$	47.8(19)	21.8(14)	24.7(15)	3.1(12)	20.4(14)	3.4(13)
$C_{(1)}$	21.1(16)	10.9(14)	15.8(14)	1.6(11)	5.4(12)	-0.1(11)
$C_{(2)}$	20.0(15)	12.1(13)	17.2(15)	-0.8(11)	6.2(12)	1.6(12)
$C_{(3)}$	31.3(18)	12.6(15)	21.6(17)	5.0(11)	9.9(14)	0.2(12)
$C_{(4)}$	20.5(15)	12.5(14)	16.8(14)	-0.7(11)	7.1(12)	1.3(12)
$C_{(5)}$	28.4(18)	11.6(14)	22.3(17)	-1.1(12)	16.2(14)	3.4(12)
$C_{(6)}$	27.8(17)	14.0(14)	20.5(15)	0.8(12)	13.1(13)	0.6(13)

Table S48 Bond Lengths for 2405112lt_Mo_auto**.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
$I_{(1)}$	$C_{(1)}$	2.090(3)	$O_{(2)}$	$C_{(5)}$	1.465(3)
$Se_{(1)}$	$C_{(2)}$	1.907(3)	$N_{(1)}$	$C_{(3)}$	1.141(4)
$Se_{(1)}$	$C_{(3)}$	1.878(3)	$C_{(1)}$	$C_{(2)}$	1.331(4)
$O_{(1)}$	$C_{(4)}$	1.217(4)	$C_{(1)}$	$C_{(4)}$	1.480(4)
$O_{(2)}$	$C_{(4)}$	1.324(3)	$C_{(5)}$	$C_{(6)}$	1.504(4)

Table S49 Bond Angles for 2405112lt_Mo_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$C_{(3)}$	$Se_{(1)}$	$C_{(2)}$	92.58(12)	$N_{(1)}$	$C_{(3)}$	$Se_{(1)}$	177.1(3)
$C_{(4)}$	$O_{(2)}$	$C_{(5)}$	114.5(2)	$O_{(1)}$	$C_{(4)}$	$O_{(2)}$	124.2(3)
$C_{(2)}$	$C_{(1)}$	$I_{(1)}$	119.8(2)	$O_{(1)}$	$C_{(4)}$	$C_{(1)}$	120.0(3)
$C_{(2)}$	$C_{(1)}$	$C_{(4)}$	119.1(3)	$O_{(2)}$	$C_{(4)}$	$C_{(1)}$	115.8(2)
$C_{(4)}$	$C_{(1)}$	$I_{(1)}$	121.0(2)	$O_{(2)}$	$C_{(5)}$	$C_{(6)}$	107.6(2)
$C_{(1)}$	$C_{(2)}$	$Se_{(1)}$	122.3(2)				

Table S50 Torsion Angles for 2405112lt_Mo_auto**.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
$I_{(1)}$	$C_{(1)}$	$C_{(2)}$	$Se_{(1)}$	177.97(14)	$C_{(4)}$	$O_{(2)}$	$C_{(5)}$	$C_{(6)}$	172.2(3)
$I_{(1)}$	$C_{(1)}$	$C_{(4)}$	$O_{(1)}$	-176.5(2)	$C_{(4)}$	$C_{(1)}$	$C_{(2)}$	$Se_{(1)}$	-1.0(4)
$I_{(1)}$	$C_{(1)}$	$C_{(4)}$	$O_{(2)}$	2.9(4)	$C_{(5)}$	$O_{(2)}$	$C_{(4)}$	$O_{(1)}$	0.7(4)
$C_{(2)}$	$C_{(1)}$	$C_{(4)}$	$O_{(1)}$	2.4(5)	$C_{(5)}$	$O_{(2)}$	$C_{(4)}$	$C_{(1)}$	-178.7(2)
$C_{(2)}$	$C_{(1)}$	$C_{(4)}$	$O_{(2)}$	-178.2(3)					

Table S51 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2405112lt_Mo_auto.

Atom	*x*	*y*	*z*	U(eq)
$H_{(2)}$	3819.35	5925.99	3826.22	19
$H_{(5A)}$	187.38	9805.23	6243.63	23
$H_{(5B)}$	1682.26	9761.25	7053.03	23
$H_{(6A)}$	-917.56	7502.17	7086.71	30
$H_{(6B)}$	-470.78	9196.52	7798.85	30
$H_{(6C)}$	579.02	7415.99	7885.43	30

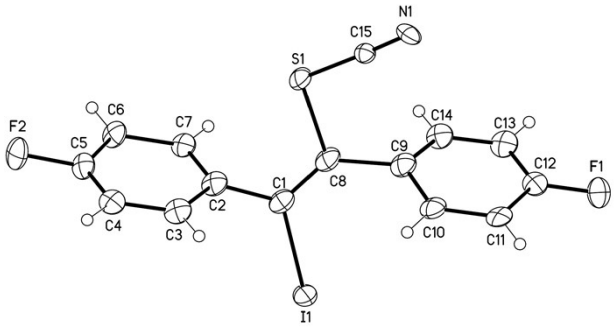
2405112lt_Mo_auto

Table S52 Crystal data and structure refinement for 2405112lt_Mo_auto**.**

Identification code	2405112lt_Mo_auto
Empirical formula	$C_6H_6INO_2Se$
Formula weight	329.98
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.9161(3)
b/Å	7.3338(2)
c/Å	13.8985(5)
α/°	90
β/°	98.850(3)
γ/°	90
Volume/Å^3	897.99(5)

Z	4
ρ_{calc}g/cm^3	2.441
μ/mm^{-1}	7.571
F(000)	608.0
Crystal size/mm^3	0.09 × 0.09 × 0.02
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.94 to 52.736
Index ranges	$-10 \leq h \leq 11$, $-9 \leq k \leq 9$, $-17 \leq l \leq 14$
Reflections collected	6738
Independent reflections	1832 [R_{int} = 0.0231, R_{sigma} = 0.0220]
Data/restraints/parameters	1832/0/101
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0200, wR_2 = 0.0461
Final R indexes [all data]	R_1 = 0.0224, wR_2 = 0.0470
Largest diff. peak/hole / e Å^{-3}	1.47/-0.46

Figure S8: ORTEP diagram of compound **6b (CCDC No. 2415489)**



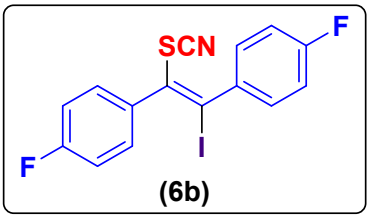


Table S53 Crystal data and structure refinement for 240495lt_auto.

Identification code	240495lt_auto
Empirical formula	$C_{15}H_8F_2INS$
Formula weight	399.18
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	7.67880(10)
b/Å	9.3435(2)
c/Å	10.3948(2)
α/°	90
β/°	96.971(2)
γ/°	90
Volume/Å^3	740.28(2)
Z	2
ρ_{calc}g/cm^3	1.791
μ/mm^{-1}	18.423
F(000)	384.0
Crystal size/mm^3	0.07 × 0.03 × 0.03

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.57 to 134.158
Index ranges	$-8 \le h \le 9$, $-11 \le k \le 11$, $-12 \le l \le 11$
Reflections collected	7744
Independent reflections	2659 [R_{int} = 0.0303, R_{sigma} = 0.0308]
Data/restraints/parameters	2659/226/214
Goodness-of-fit on F^2	1.290
Final R indexes [I>=2σ (I)]	R_1 = 0.0482, wR_2 = 0.1173
Final R indexes [all data]	R_1 = 0.0486, wR_2 = 0.1175
Largest diff. peak/hole / e $Å^{-3}$	0.95/-1.51
Flack parameter	0.16(3)

Table S54 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240495lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
I1	7712.6(18)	3733.8(13)	1721.5(17)	30.0(3)
S1	2568(8)	5819(7)	2855(6)	29.7(13)
F2	285(11)	-66(10)	999(9)	48(2)
F1	9451(11)	10066(9)	4085(10)	47(2)
C3	3870(19)	1948(16)	2695(13)	33(3)
C10	7365(16)	6630(15)	4092(13)	32(3)
C13	7119(19)	9164(15)	2685(14)	38(3)
C11	8503(17)	7715(15)	4468(14)	31(3)
C2	3866(16)	3173(15)	1908(12)	29(2)
C1	5156(17)	4321(16)	2230(13)	34(3)
C9	6085(17)	6796(15)	3028(12)	30(2)

Table S54 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240495lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C12	8375(16)	8998(14)	3733(13)	31(3)
C5	1512(18)	1024(18)	1288(13)	37(3)
C8	4808(17)	5592(16)	2675(12)	30(2)
N1	2970(20)	7992(16)	4745(15)	28(3)
C6	1407(19)	2169(17)	495(14)	37(3)
C7	2621(16)	3278(13)	813(12)	27(2)
C14	5935(19)	8085(16)	2343(13)	34(3)
C4	2701(18)	845(17)	2384(14)	35(3)
C15	2830(20)	7092(17)	3991(15)	19(3)
I1A	2226(4)	6262(2)	3191(3)	30.0(3)
S1A	7429(15)	4192(15)	2148(12)	37(3)
C15A	7110(40)	2910(30)	1000(30)	31(5)
N1A	6970(50)	2040(30)	220(30)	49(8)

Table S55 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240495lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	21.3(5)	24.9(6)	45.9(7)	-1.3(5)	12.9(4)	-1.0(4)
S1	18(2)	30(3)	43(3)	-14(3)	10(2)	-4(2)
F2	38(4)	40(5)	68(6)	-11(4)	14(4)	-17(4)
F1	37(4)	27(4)	80(6)	-5(4)	13(4)	-8(4)
C3	25(6)	39(6)	37(6)	4(5)	9(5)	0(5)
C10	17(5)	39(6)	39(6)	-3(5)	6(5)	2(5)

Table S55 Anisotropic Displacement Parameters ($Å^2×10^3$) for 240495lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C13	35(6)	33(6)	51(7)	16(5)	25(5)	-3(5)
C11	20(5)	32(6)	44(6)	-4(5)	14(5)	6(5)
C2	25(5)	32(5)	31(5)	3(4)	8(4)	0(4)
C1	23(5)	47(6)	32(5)	10(5)	2(4)	-5(5)
C9	26(5)	33(6)	32(5)	6(5)	7(4)	-4(5)
C12	27(5)	18(7)	50(6)	-4(5)	21(5)	0(4)
C5	30(6)	42(7)	44(6)	-14(6)	17(5)	-11(5)
C8	19(5)	42(5)	31(5)	10(5)	8(4)	-8(5)
N1	29(5)	22(5)	34(5)	-6(4)	6(4)	7(4)
C6	31(6)	40(6)	40(6)	-4(5)	1(5)	-3(5)
C7	27(5)	22(5)	33(5)	3(4)	7(4)	-1(4)
C14	30(6)	33(6)	40(6)	17(5)	5(5)	2(5)
C4	30(6)	33(6)	45(6)	1(5)	18(5)	0(5)
C15	18(4)	19(4)	20(4)	2(3)	5(3)	0(3)
I1A	21.3(5)	24.9(6)	45.9(7)	-1.3(5)	12.9(4)	-1.0(4)
S1A	22(4)	45(6)	44(5)	-7(4)	1(4)	-10(4)
C15A	19(8)	36(9)	39(9)	3(8)	7(8)	-11(8)
N1A	44(15)	42(15)	59(15)	-13(13)	-1(13)	-2(13)

Table S56 Bond Lengths for 240495lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	C1	2.165(14)	C2	C7	1.399(18)
S1	C8	1.765(14)	C1	C8	1.314(15)
S1	C15	1.671(15)	C1	S1A	1.762(17)

Table S56 Bond Lengths for 240495lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F2	C5	1.395(16)	C9	C8	1.508(18)
F1	C12	1.318(16)	C9	C14	1.397(19)
C3	C2	1.41(2)	C5	C6	1.35(2)
C3	C4	1.38(2)	C5	C4	1.38(2)
C10	C11	1.364(19)	C8	I1A	2.206(14)
C10	C9	1.396(18)	N1	C15	1.145(18)
C13	C12	1.37(2)	C6	C7	1.406(19)
C13	C14	1.38(2)	S1A	C15A	1.69(2)
C11	C12	1.419(19)	C15A	N1A	1.15(2)
C2	C1	1.471(18)			

Table S57 Bond Angles for 240495lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C15	S1	C8	97.2(8)	F1	C12	C11	119.3(12)
C4	C3	C2	121.1(13)	C13	C12	C11	121.2(12)
C11	C10	C9	120.6(13)	C6	C5	F2	117.3(13)
C12	C13	C14	120.1(12)	C6	C5	C4	125.9(14)
C10	C11	C12	118.3(13)	C4	C5	F2	116.8(14)
C3	C2	C1	120.5(12)	C1	C8	S1	112.9(8)
C7	C2	C3	118.9(12)	C1	C8	C9	127.3(11)
C7	C2	C1	120.6(12)	C1	C8	I1A	124.7(8)
C2	C1	I1	111.4(10)	C9	C8	S1	119.9(11)
C2	C1	S1A	125.6(12)	C9	C8	I1A	107.9(9)
C8	C1	I1	123.0(8)	C5	C6	C7	116.9(13)

Table S57 Bond Angles for 240495lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8	C1	C2	125.4(10)	C2	C7	C6	120.5(12)
C8	C1	S1A	108.9(9)	C13	C14	C9	119.3(12)
C10	C9	C8	119.0(12)	C3	C4	C5	116.7(14)
C10	C9	C14	120.4(13)	N1	C15	S1	177.8(17)
C14	C9	C8	120.5(12)	C15A	S1A	C1	91.3(14)
F1	C12	C13	119.4(12)	N1A	C15A	S1A	177(3)

Table S58 Torsion Angles for 240495lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
I1	C1	C8	S1	174.2(7)	C9	C10	C11	C12	-1.4(19)
I1	C1	C8	C9	-6.1(15)	C12	C13	C14	C9	-3(2)
F2	C5	C6	C7	178.4(11)	C5	C6	C7	C2	0(2)
F2	C5	C4	C3	-177.6(12)	C8	C1	S1A	C15A	-156.0(15)
C3	C2	C1	I1	76.5(13)	C8	C9	C14	C13	-179.9(12)
C3	C2	C1	C8	-108.5(15)	C6	C5	C4	C3	1(2)
C3	C2	C1	S1A	68.6(17)	C7	C2	C1	I1	-103.3(12)
C3	C2	C7	C6	-0.8(19)	C7	C2	C1	C8	71.7(16)
C10	C11	C12	F1	179.4(11)	C7	C2	C1	S1A	-111.1(14)
C10	C11	C12	C13	1.4(19)	C14	C13	C12	F1	-176.9(12)
C10	C9	C8	S1	112.4(13)	C14	C13	C12	C11	1.1(19)
C10	C9	C8	C1	-67.3(17)	C14	C9	C8	S1	-64.3(16)
C10	C9	C8	I1A	108.0(12)	C14	C9	C8	C1	116.0(15)
C10	C9	C14	C13	3(2)	C14	C9	C8	I1A	-68.7(14)
C11	C10	C9	C8	-177.7(12)	C4	C3	C2	C1	-178.1(12)

Table S58 Torsion Angles for 240495lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C11	C10	C9	C14	-1(2)	C4	C3	C2	C7	2(2)
C2	C3	C4	C5	-2(2)	C4	C5	C6	C7	0(2)
C2	C1	C8	S1	-0.3(14)	C15	S1	C8	C1	155.5(9)
C2	C1	C8	C9	179.5(14)	C15	S1	C8	C9	-24.3(12)
C2	C1	C8	I1A	4.9(15)	S1A	C1	C8	C9	1.9(14)
C2	C1	S1A	C15A	26.5(18)	S1A	C1	C8	I1A	-172.6(8)
C1	C2	C7	C6	179.0(12)					

Table S59 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240495lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H3	4691.23	1879.9	3453.06	40
H10	7443.86	5753.94	4558.86	38
H13	7067.79	10024.85	2196.33	45
H11	9357.94	7613.69	5203.15	37
H6	551.79	2224.82	-245.3	45
H7	2594.87	4105.85	279.41	33
H14	5024.11	8214.98	1648.19	41
H4	2712.55	4.32	2898.68	41

Table S60 Atomic Occupancy for 240495lt_auto.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
I1	0.638(3)	S1	0.638(3)	N1	0.638(3)
C15	0.638(3)	I1A	0.362(3)	S1A	0.362(3)
C15A	0.362(3)	N1A	0.362(3)		

240495lt_auto

Table S61 Crystal data and structure refinement for 240495lt_auto.

Identification code	240495lt_auto
Empirical formula	$C_{15}H_8F_2INS$
Formula weight	399.18
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	7.67880(10)
b/Å	9.3435(2)
c/Å	10.3948(2)
α/°	90
β/°	96.971(2)
γ/°	90
Volume/Å^3	740.28(2)
Z	2
ρ_{calc}g/cm^3	1.791
μ/mm^{-1}	18.423
F(000)	384.0
Crystal size/mm^3	0.07 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.57 to 134.158
Index ranges	$-8 \leq h \leq 9$, $-11 \leq k \leq 11$, $-12 \leq l \leq 11$
Reflections collected	7744
Independent reflections	2659 [R_{int} = 0.0303, R_{sigma} = 0.0308]
Data/restraints/parameters	2659/226/214

Goodness-of-fit on F^2	1.290
Final R indexes [I>=2σ (I)]	$R_1 = 0.0482$, $wR_2 = 0.1173$
Final R indexes [all data]	$R_1 = 0.0486$, $wR_2 = 0.1175$
Largest diff. peak/hole / e $Å^{-3}$	0.95/-1.51
Flack parameter	0.16(3)

Figure S9: ORTEP diagram of compound **6c and 6c' (CCDC No. 2415491)**

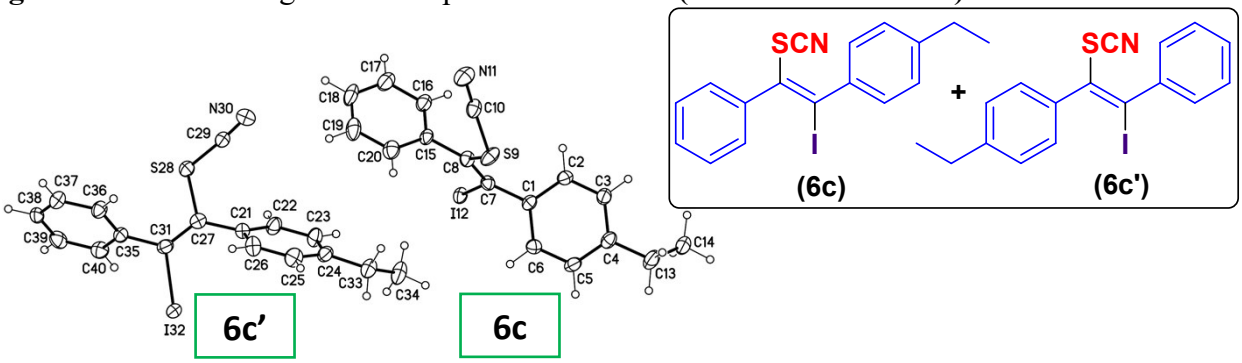


Table S62 Crystal data and structure refinement for 240507lt_auto.

Identification code	240507lt_auto
Empirical formula	$C_{34}H_{28}I_2N_2S_2$
Formula weight	782.50
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.4074(2)
b/Å	9.5738(2)
c/Å	18.6802(3)
α/°	90.5660(10)
β/°	93.8530(10)
γ/°	111.035(2)
Volume/Å^3	1565.72(6)
Z	2
ρ_{calc}g/cm^3	1.660
μ/mm^{-1}	17.214
F(000)	768.0
Crystal size/mm^3	0.05 × 0.05 × 0.03

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.496 to 134.152
Index ranges	$-11 \leq h \leq 11$, $-7 \leq k \leq 11$, $-22 \leq l \leq 22$
Reflections collected	16745
Independent reflections	5552 [R_{int} = 0.0320, R_{sigma} = 0.0351]
Data/restraints/parameters	5552/0/363
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0253, wR_2 = 0.0619
Final R indexes [all data]	R_1 = 0.0287, wR_2 = 0.0632
Largest diff. peak/hole / e Å^{-3}	0.92/-0.78

Table S63 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 240507lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
I12	2163.9(2)	-244.1(2)	5457.8(2)	22.66(7)
S9	3062.0(10)	4816.6(8)	5101.3(4)	31.62(18)
N11	1408(4)	6266(3)	5841.5(17)	39.1(7)
C1	2816(3)	2013(3)	4271.5(16)	21.1(6)
C2	1793(3)	2304(3)	3772.0(17)	24.9(6)
C3	2045(4)	2370(3)	3049.2(17)	25.7(6)
C4	3332(4)	2185(3)	2800.6(17)	25.8(6)
C5	4355(4)	1911(3)	3303.3(18)	27.7(6)
C6	4101(3)	1805(3)	4025.2(17)	24.7(6)
C7	2528(3)	1896(3)	5042.7(16)	21.5(6)
C8	2482(4)	2989(3)	5478.1(17)	23.7(6)
C10	2041(4)	5618(3)	5556.7(17)	28.6(7)

Table S63 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240507lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C13	3595(4)	2276(4)	2008.3(18)	37.0(8)
C14	2274(4)	1167(5)	1539.3(19)	44.7(9)
C15	2121(4)	2903(3)	6244.0(16)	23.6(6)
C16	643(4)	2102(3)	6424.2(17)	28.5(7)
C17	297(5)	2061(4)	7137.7(19)	36.0(8)
C18	1437(5)	2793(4)	7668.2(18)	37.8(8)
C19	2917(5)	3575(4)	7492.1(19)	38.5(8)
C20	3259(4)	3653(4)	6779.7(18)	32.0(7)
I32	10144.5(2)	2576.8(2)	9779.7(2)	29.22(7)
S28	5085.8(9)	1975.0(10)	10123.0(4)	34.50(18)
N30	3629(4)	3655(4)	9334.6(18)	45.6(8)
C21	6923(4)	2733(3)	8948.7(17)	26.0(6)
C22	5943(4)	1696(4)	8445.4(17)	29.9(7)
C23	6037(4)	1948(4)	7718.3(18)	32.2(7)
C24	7111(4)	3249(4)	7475.4(17)	28.3(7)
C25	8049(4)	4294(4)	7984.0(19)	33.9(7)
C26	7961(4)	4055(4)	8707.6(18)	32.0(7)
C27	6899(4)	2451(3)	9727.6(17)	28.2(7)
C29	4279(4)	3013(4)	9638.2(18)	34.1(7)
C31	8034(3)	2391(3)	10177.8(17)	25.9(6)
C33	7312(4)	3567(4)	6690.4(18)	32.0(7)
C34	6520(5)	2247(4)	6172.2(19)	39.9(8)
C35	7998(3)	2191(3)	10965.5(16)	23.9(6)

Table S63 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 240507lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C36	7935(4)	3331(3)	11419.7(17)	27.7(6)
C37	7959(4)	3159(4)	12156.0(17)	29.4(7)
C38	8016(4)	1845(4)	12443.1(17)	28.3(7)
C39	8050(4)	709(4)	11992.7(19)	31.9(7)
C40	8057(4)	880(3)	11258.8(19)	29.9(7)

Table S64 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240507lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I12	31.26(11)	19.48(10)	19.49(10)	-0.12(7)	2.40(7)	11.82(7)
S9	47.6(5)	20.6(3)	29.9(4)	1.5(3)	16.4(4)	13.9(3)
N11	59(2)	30.0(14)	38.8(17)	5.5(12)	15.0(15)	26.1(14)
C1	24.2(14)	17.6(13)	20.4(15)	-3.1(11)	3.4(11)	6.0(11)
C2	24.3(15)	27.3(15)	24.8(16)	-1.2(12)	3.9(12)	11.3(12)
C3	25.8(15)	28.9(15)	21.4(15)	0.6(12)	2.5(12)	8.6(12)
C4	26.0(15)	23.9(14)	22.7(16)	-3.8(12)	4.8(12)	2.8(12)
C5	25.1(15)	31.4(16)	27.3(16)	-3.2(13)	7.9(13)	10.1(13)
C6	24.7(15)	25.9(14)	25.6(16)	-0.1(12)	1.7(12)	11.6(12)
C7	24.0(14)	20.4(13)	21.8(15)	1.7(11)	0.1(11)	10.2(11)
C8	28.1(15)	21.6(14)	22.4(15)	1.9(11)	2.1(12)	9.9(12)
C10	42.5(18)	23.1(14)	22.1(15)	2.5(12)	2.8(14)	14.1(14)
C13	38.6(19)	45.4(19)	24.0(18)	1.3(14)	10.6(14)	10.2(16)
C14	34.0(19)	78(3)	21.8(18)	-3.5(17)	3.2(14)	20.3(19)

Table S64 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 240507lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15	34.9(17)	23.6(14)	17.4(15)	-2.7(11)	1.7(12)	17.1(13)
C16	34.9(17)	29.7(15)	23.1(16)	-0.9(12)	4.0(13)	13.9(14)
C17	51(2)	38.5(18)	28.0(18)	7.6(14)	13.2(16)	26.2(16)
C18	70(3)	36.6(18)	17.8(16)	1.3(13)	7.5(16)	32.3(18)
C19	62(2)	33.6(17)	23.3(17)	-7.1(14)	-5.9(16)	23.4(17)
C20	39.8(19)	28.2(16)	28.6(18)	-3.8(13)	0.7(14)	13.6(14)
I32	25.89(11)	42.56(12)	21.71(11)	-1.64(8)	4.27(8)	15.01(9)
S28	27.2(4)	55.5(5)	23.1(4)	9.7(3)	7.6(3)	16.4(4)
N30	36.4(17)	70(2)	39.2(18)	2.1(16)	1.4(14)	30.2(17)
C21	25.9(15)	32.6(16)	21.4(15)	1.2(12)	1.1(12)	12.9(13)
C22	30.0(16)	33.6(16)	22.7(16)	3.8(13)	6.9(13)	6.2(13)
C23	37.4(18)	35.1(17)	22.0(16)	-4.3(13)	0.0(13)	11.0(14)
C24	36.2(17)	32.1(16)	23.1(16)	3.4(12)	7.2(13)	19.2(14)
C25	36.8(18)	28.8(16)	34.0(19)	4.5(14)	5.5(15)	8.8(14)
C26	38.1(18)	28.9(16)	26.6(17)	1.5(13)	-2.2(14)	9.9(14)
C27	27.4(16)	32.3(16)	26.6(17)	0.5(13)	4.3(13)	12.4(13)
C29	27.2(16)	56(2)	21.3(16)	-3.0(15)	2.2(13)	17.2(16)
C31	24.7(15)	28.6(15)	25.9(16)	-1.0(12)	5.5(12)	10.9(13)
C33	42.7(19)	30.4(16)	23.9(17)	2.0(13)	5.7(14)	14.0(14)
C34	64(3)	36.9(18)	21.5(17)	-0.2(14)	4.3(16)	21.0(17)
C35	22.8(15)	27.5(15)	21.1(15)	3.1(12)	3.5(12)	8.4(12)
C36	36.6(17)	25.6(15)	23.8(16)	4.3(12)	5.8(13)	13.9(13)
C37	33.6(17)	31.2(16)	23.9(16)	-1.1(13)	5.0(13)	11.8(14)

Table S64 Anisotropic Displacement Parameters ($Å^2×10^3$) for 240507lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C38	23.0(15)	41.3(17)	21.0(15)	7.6(13)	2.6(12)	11.7(13)
C39	32.2(17)	30.3(16)	35.9(19)	11.2(14)	1.8(14)	14.6(14)
C40	31.3(17)	25.8(15)	32.7(18)	-3.2(13)	1.6(13)	10.7(13)

Table S65 Bond Lengths for 240507lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I12	C7	2.116(3)	I32	C31	2.116(3)
S9	C8	1.801(3)	S28	C27	1.811(3)
S9	C10	1.692(3)	S28	C29	1.688(4)
N11	C10	1.151(4)	N30	C29	1.142(5)
C1	C2	1.397(4)	C21	C22	1.388(5)
C1	C6	1.400(4)	C21	C26	1.393(5)
C1	C7	1.481(4)	C21	C27	1.483(4)
C2	C3	1.385(4)	C22	C23	1.385(5)
C3	C4	1.393(4)	C23	C24	1.395(5)
C4	C5	1.393(5)	C24	C25	1.385(5)
C4	C13	1.515(4)	C24	C33	1.511(4)
C5	C6	1.384(5)	C25	C26	1.376(5)
C7	C8	1.334(4)	C27	C31	1.332(5)
C8	C15	1.489(4)	C31	C35	1.487(4)
C13	C14	1.526(5)	C33	C34	1.514(5)
C15	C16	1.392(5)	C35	C36	1.396(4)
C15	C20	1.397(5)	C35	C40	1.392(5)
C16	C17	1.391(5)	C36	C37	1.387(5)

Table S65 Bond Lengths for 240507lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C17	C18	1.388(6)	C37	C38	1.390(5)
C18	C19	1.387(6)	C38	C39	1.379(5)
C19	C20	1.387(5)	C39	C40	1.382(5)

Table S66 Bond Angles for 240507lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	S9	C8	101.11(15)	C29	S28	C27	100.92(16)
C2	C1	C6	118.5(3)	C22	C21	C26	118.6(3)
C2	C1	C7	120.7(3)	C22	C21	C27	121.5(3)
C6	C1	C7	120.8(3)	C26	C21	C27	119.9(3)
C3	C2	C1	120.4(3)	C23	C22	C21	120.5(3)
C2	C3	C4	121.4(3)	C22	C23	C24	120.9(3)
C3	C4	C13	120.6(3)	C23	C24	C33	123.6(3)
C5	C4	C3	117.8(3)	C25	C24	C23	117.9(3)
C5	C4	C13	121.6(3)	C25	C24	C33	118.5(3)
C6	C5	C4	121.6(3)	C26	C25	C24	121.6(3)
C5	C6	C1	120.3(3)	C25	C26	C21	120.4(3)
C1	C7	I12	114.60(19)	C21	C27	S28	117.6(2)
C8	C7	I12	119.1(2)	C31	C27	S28	114.1(2)
C8	C7	C1	126.3(3)	C31	C27	C21	128.1(3)
C7	C8	S9	115.1(2)	N30	C29	S28	174.6(3)
C7	C8	C15	128.2(3)	C27	C31	I32	119.7(2)
C15	C8	S9	116.6(2)	C27	C31	C35	126.7(3)
N11	C10	S9	174.7(3)	C35	C31	I32	113.6(2)

Table S66 Bond Angles for 240507lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	C13	C14	113.1(3)	C24	C33	C34	115.5(3)
C16	C15	C8	120.0(3)	C36	C35	C31	120.2(3)
C16	C15	C20	120.1(3)	C40	C35	C31	120.4(3)
C20	C15	C8	120.0(3)	C40	C35	C36	119.4(3)
C17	C16	C15	119.9(3)	C37	C36	C35	119.9(3)
C18	C17	C16	119.8(4)	C36	C37	C38	120.3(3)
C19	C18	C17	120.6(3)	C39	C38	C37	119.8(3)
C20	C19	C18	119.9(3)	C38	C39	C40	120.5(3)
C19	C20	C15	119.8(3)	C39	C40	C35	120.2(3)

Table S67 Torsion Angles for 240507lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
I12	C7	C8	S9	171.90(14)	I32	C31	C35	C36	111.1(3)
I12	C7	C8	C15	-3.4(5)	I32	C31	C35	C40	-67.6(3)
S9	C8	C15	C16	115.7(3)	S28	C27	C31	I32	170.53(15)
S9	C8	C15	C20	-62.9(3)	S28	C27	C31	C35	-9.1(4)
C1	C2	C3	C4	-1.5(4)	C21	C22	C23	C24	-0.3(5)
C1	C7	C8	S9	-8.1(4)	C21	C27	C31	I32	-4.1(4)
C1	C7	C8	C15	176.6(3)	C21	C27	C31	C35	176.3(3)
C2	C1	C6	C5	1.0(4)	C22	C21	C26	C25	-2.6(5)
C2	C1	C7	I12	115.7(3)	C22	C21	C27	S28	-53.8(4)
C2	C1	C7	C8	-64.3(4)	C22	C21	C27	C31	120.6(4)
C2	C3	C4	C5	0.8(4)	C22	C23	C24	C25	-1.7(5)
C2	C3	C4	C13	-179.4(3)	C22	C23	C24	C33	177.7(3)

Table S67 Torsion Angles for 240507lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C3	C4	C5	C6	0.9(4)	C23	C24	C25	C26	1.5(5)
C3	C4	C13	C14	-56.6(4)	C23	C24	C33	C34	-12.9(5)
C4	C5	C6	C1	-1.8(5)	C24	C25	C26	C21	0.6(5)
C5	C4	C13	C14	123.2(4)	C25	C24	C33	C34	166.4(3)
C6	C1	C2	C3	0.6(4)	C26	C21	C22	C23	2.4(5)
C6	C1	C7	I12	-63.0(3)	C26	C21	C27	S28	127.1(3)
C6	C1	C7	C8	117.0(3)	C26	C21	C27	C31	-58.5(5)
C7	C1	C2	C3	-178.1(3)	C27	C21	C22	C23	-176.7(3)
C7	C1	C6	C5	179.7(3)	C27	C21	C26	C25	176.6(3)
C7	C8	C15	C16	-69.1(4)	C27	C31	C35	C36	-69.2(4)
C7	C8	C15	C20	112.3(4)	C27	C31	C35	C40	112.1(4)
C8	C15	C16	C17	-178.0(3)	C29	S28	C27	C21	-34.4(3)
C8	C15	C20	C19	179.8(3)	C29	S28	C27	C31	150.4(3)
C10	S9	C8	C7	151.7(3)	C31	C35	C36	C37	-177.6(3)
C10	S9	C8	C15	-32.5(3)	C31	C35	C40	C39	178.9(3)
C13	C4	C5	C6	-179.0(3)	C33	C24	C25	C26	-177.9(3)
C15	C16	C17	C18	-1.4(5)	C35	C36	C37	C38	-1.2(5)
C16	C15	C20	C19	1.2(4)	C36	C35	C40	C39	0.1(5)
C16	C17	C18	C19	0.5(5)	C36	C37	C38	C39	0.0(5)
C17	C18	C19	C20	1.2(5)	C37	C38	C39	C40	1.2(5)
C18	C19	C20	C15	-2.1(5)	C38	C39	C40	C35	-1.3(5)
C20	C15	C16	C17	0.6(4)	C40	C35	C36	C37	1.1(5)

Table S68 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240507lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H2	919.07	2458.27	3929.09	30
H3	1324.84	2545.17	2715.62	31
H5	5247.54	1795.13	3146.77	33
H6	4802.47	1589.78	4355.1	30
H13A	4540.25	2080.86	1933.39	44
H13B	3750.57	3304.22	1855.11	44
H14A	2513.79	1263.3	1035.5	67
H14B	1342.18	1379.43	1595.25	67
H14C	2116.51	145.11	1685.83	67
H16	-128.16	1584.67	6060.48	34
H17	-715.15	1533.72	7261.6	43
H18	1202.31	2758.08	8155.95	45
H19	3694.79	4056.35	7859.24	46
H20	4263.22	4215.23	6656.1	38
H22	5201.95	805.51	8601	36
H23	5361.51	1225.85	7380.44	39
H25	8771.19	5197.97	7829.78	41
H26	8611.78	4795.56	9044.82	38
H33A	8417.54	3946.35	6619.63	38
H33B	6924.79	4376.35	6566.66	38
H34A	6795.66	2534.91	5684.02	60
H34B	5411.32	1939.06	6190.9	60
H34C	6840.87	1411.46	6306.36	60
H36	7876.12	4223	11224.51	33
H37	7935.23	3942.61	12465.56	35

Table S68 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 240507lt_auto.

H38	8031.6	1729.48	12947.76	34
H39	8069.71	-196.65	12188.2	38
H40	8102.55	99.6	10953.56	36

240507lt_auto

Table S69 Crystal data and structure refinement for 240507lt_auto.

Identification code	240507lt_auto
Empirical formula	$C_{34}H_{28}I_2N_2S_2$
Formula weight	782.50
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.4074(2)
b/Å	9.5738(2)
c/Å	18.6802(3)
α/°	90.5660(10)
β/°	93.8530(10)
γ/°	111.035(2)
Volume/Å^3	1565.72(6)
Z	2
ρ_{calc}g/cm^3	1.660
μ/mm^{-1}	17.214
F(000)	768.0
Crystal size/mm^3	0.05 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184)

2Θ range for data collection/°	9.496 to 134.152
Index ranges	$-11 \leq h \leq 11$, $-7 \leq k \leq 11$, $-22 \leq l \leq 22$
Reflections collected	16745
Independent reflections	5552 [R_{int} = 0.0320, R_{sigma} = 0.0351]
Data/restraints/parameters	5552/0/363
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0253, wR_2 = 0.0619
Final R indexes [all data]	R_1 = 0.0287, wR_2 = 0.0632
Largest diff. peak/hole / e $Å^{-3}$	0.92/-0.78

Figure S10: ORTEP diagram of compound **9a (CCDC No. 2429054)**

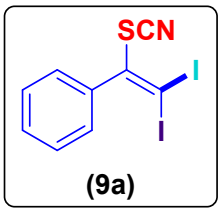


Table S70 Crystal data and structure refinement for 2502056lt_auto.

Identification code	2502056lt_auto
Empirical formula	$C_9H_5I_2NS$
Formula weight	413.00
Temperature/K	99.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.6916(2)
b/Å	8.6661(2)
c/Å	17.4852(4)
α/°	84.454(2)
β/°	87.571(2)
γ/°	73.493(2)
Volume/Å^3	1112.09(5)
Z	4
ρ_{calc}g/cm^3	2.467
μ/mm^{-1}	45.807
F(000)	752.0
Crystal size/mm^3	0.06 × 0.02 × 0.01
Radiation	Cu Kα (λ = 1.54184)

2Θ range for data collection/°	10.166 to 145.654
Index ranges	$-9 \leq h \leq 9$, $-7 \leq k \leq 10$, $-21 \leq l \leq 21$
Reflections collected	13749
Independent reflections	4258 [R_{int} = 0.0408, R_{sigma} = 0.0445]
Data/restraints/parameters	4258/0/235
Goodness-of-fit on F^2	0.996
Final R indexes [I>=2σ (I)]	R_1 = 0.0352, wR_2 = 0.0884
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0911
Largest diff. peak/hole / e Å^{-3}	1.65/-1.41

Table S71 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2502056lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
I12	16306.4(5)	-6208.8(5)	1085.7(2)	20.03(11)
I13	11887.9(5)	-6609.1(4)	898.6(2)	20.14(11)
S8	10393(2)	-2759.3(18)	1235.5(10)	24.8(3)
N10	10022(8)	590(7)	955(4)	30.5(13)
C1	13920(8)	-2495(7)	1442(4)	19.2(13)
C2	14026(9)	-2215(8)	2204(4)	24.4(14)
C3	15066(9)	-1230(7)	2394(4)	24.0(14)
C4	15942(9)	-518(7)	1829(4)	24.6(14)
C5	15839(9)	-788(8)	1068(4)	23.3(14)
C6	14816(8)	-1776(7)	864(4)	22.8(14)
C7	12823(8)	-3568(7)	1232(3)	19.5(13)
C9	10254(9)	-761(8)	1069(4)	25.2(14)
C11	13494(8)	-5091(7)	1090(3)	19.0(13)

Table S71 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 2502056lt_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
I25	13080.6(6)	-1263.3(5)	4653.3(2)	25.03(12)
I26	9580.1(5)	-1684.9(5)	3497.1(2)	21.83(11)
S21	9165(2)	2122.6(19)	2814.5(9)	24.9(3)
N23	8178(9)	5434(7)	3101(4)	42.1(17)
C14	11943(8)	2407(7)	3723(3)	19.3(13)
C15	11730(10)	3078(8)	4421(4)	27.8(15)
C16	12769(9)	4081(8)	4578(4)	26.7(14)
C17	14014(9)	4412(8)	4035(4)	27.5(15)
C18	14204(9)	3758(8)	3332(4)	29.8(16)
C19	13168(9)	2748(8)	3172(4)	24.2(14)
C20	10834(8)	1319(7)	3553(3)	19.4(13)
C22	8609(9)	4108(9)	2996(4)	28.5(16)
C24	11051(9)	-172(8)	3842(4)	23.5(14)

Table S72 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2502056lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I12	14.45(19)	22.8(2)	22.1(2)	-0.53(15)	-1.97(14)	-4.32(15)
I13	16.9(2)	21.3(2)	23.8(2)	-2.28(16)	-1.54(15)	-7.63(16)
S8	14.6(7)	21.1(8)	38.9(9)	-3.1(7)	-1.6(6)	-4.7(6)
N10	21(3)	32(3)	40(3)	-2(3)	1(3)	-9(3)
C1	14(3)	22(3)	21(3)	-3(2)	-3(2)	-5(3)
C2	21(3)	27(3)	27(3)	-1(3)	-3(3)	-10(3)

Table S72 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2502056lt_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	26(4)	27(3)	17(3)	-3(3)	-2(3)	-4(3)
C4	21(3)	21(3)	34(4)	-1(3)	-9(3)	-10(3)
C5	19(3)	28(4)	25(3)	5(3)	-4(3)	-12(3)
C6	17(3)	27(3)	25(3)	1(3)	-4(3)	-7(3)
C7	16(3)	22(3)	17(3)	0(2)	1(2)	-1(3)
C9	20(3)	32(4)	25(3)	-3(3)	-2(3)	-7(3)
C11	16(3)	22(3)	19(3)	1(2)	-3(2)	-6(3)
I25	27.7(2)	24.0(2)	23.5(2)	0.98(16)	-10.18(17)	-7.08(17)
I26	22.8(2)	25.1(2)	20.2(2)	0.00(16)	-2.69(15)	-11.27(17)
S21	25.5(8)	25.7(8)	24.9(8)	0.4(6)	-11.6(6)	-8.6(7)
N23	35(4)	27(3)	67(5)	-6(3)	-22(3)	-11(3)
C14	17(3)	20(3)	17(3)	2(2)	-6(2)	0(3)
C15	28(4)	38(4)	20(3)	2(3)	-2(3)	-14(3)
C16	26(4)	32(4)	22(3)	-3(3)	-8(3)	-5(3)
C17	25(4)	24(3)	35(4)	-3(3)	-13(3)	-7(3)
C18	21(3)	32(4)	36(4)	2(3)	0(3)	-8(3)
C19	24(3)	29(4)	23(3)	-5(3)	2(3)	-12(3)
C20	20(3)	25(3)	16(3)	3(2)	-6(2)	-12(3)
C22	24(4)	34(4)	30(4)	8(3)	-16(3)	-15(3)
C24	20(3)	28(3)	24(3)	-1(3)	-4(3)	-8(3)

Table S73 Bond Lengths for 2502056lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I12	C11	2.104(6)	I25	C24	2.106(6)

Table S73 Bond Lengths for 2502056lt_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I13	C11	2.100(6)	I26	C24	2.102(6)
S8	C7	1.800(6)	S21	C20	1.806(6)
S8	C9	1.701(7)	S21	C22	1.709(7)
N10	C9	1.133(8)	N23	C22	1.132(9)
C1	C2	1.386(9)	C14	C15	1.386(9)
C1	C6	1.396(8)	C14	C19	1.389(9)
C1	C7	1.500(8)	C14	C20	1.496(8)
C2	C3	1.394(8)	C15	C16	1.389(9)
C3	C4	1.368(9)	C16	C17	1.388(10)
C4	C5	1.383(9)	C17	C18	1.388(10)
C5	C6	1.394(8)	C18	C19	1.394(9)
C7	C11	1.317(8)	C20	C24	1.308(8)

Table S74 Bond Angles for 2502056lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	S8	C7	98.9(3)	C22	S21	C20	98.1(3)
C2	C1	C6	120.6(6)	C15	C14	C19	120.6(6)
C2	C1	C7	120.1(5)	C15	C14	C20	120.0(6)
C6	C1	C7	119.3(6)	C19	C14	C20	119.4(6)
C1	C2	C3	119.5(6)	C14	C15	C16	119.9(6)
C4	C3	C2	120.1(6)	C17	C16	C15	119.9(6)
C3	C4	C5	120.7(6)	C16	C17	C18	120.1(6)
C4	C5	C6	120.2(6)	C17	C18	C19	120.2(6)
C5	C6	C1	118.8(6)	C14	C19	C18	119.3(6)

Table S74 Bond Angles for 2502056lt_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	C7	S8	117.6(4)	C14	C20	S21	115.4(4)
C11	C7	S8	117.2(5)	C24	C20	S21	117.9(5)
C11	C7	C1	125.0(6)	C24	C20	C14	126.5(6)
N10	C9	S8	174.8(6)	N23	C22	S21	177.2(6)
I13	C11	I12	114.9(3)	I26	C24	I25	115.3(3)
C7	C11	I12	121.4(4)	C20	C24	I25	120.6(5)
C7	C11	I13	123.6(5)	C20	C24	I26	124.0(5)

Table S75 Torsion Angles for 2502056lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S8	C7	C11	I12	-179.0(3)	S21	C20	C24	I25	176.0(3)
S8	C7	C11	I13	-1.5(7)	S21	C20	C24	I26	0.1(8)
C1	C2	C3	C4	1.4(10)	C14	C15	C16	C17	0.2(10)
C1	C7	C11	I12	-3.4(9)	C14	C20	C24	I25	1.6(10)
C1	C7	C11	I13	174.1(4)	C14	C20	C24	I26	-174.3(5)
C2	C1	C6	C5	0.8(10)	C15	C14	C19	C18	0.9(10)
C2	C1	C7	S8	75.5(7)	C15	C14	C20	S21	111.4(6)
C2	C1	C7	C11	-100.0(8)	C15	C14	C20	C24	-74.1(9)
C2	C3	C4	C5	-1.2(10)	C15	C16	C17	C18	0.8(10)
C3	C4	C5	C6	0.9(10)	C16	C17	C18	C19	-1.0(10)
C4	C5	C6	C1	-0.7(10)	C17	C18	C19	C14	0.1(10)
C6	C1	C2	C3	-1.2(10)	C19	C14	C15	C16	-1.1(10)
C6	C1	C7	S8	-104.0(6)	C19	C14	C20	S21	-67.8(7)
C6	C1	C7	C11	80.5(8)	C19	C14	C20	C24	106.7(8)

Table S75 Torsion Angles for 2502056lt_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C7	C1	C2	C3	179.3(6)	C20	C14	C15	C16	179.7(6)
C7	C1	C6	C5	-179.7(6)	C20	C14	C19	C18	-179.8(6)
C9	S8	C7	C1	26.1(5)	C22	S21	C20	C14	-34.1(5)
C9	S8	C7	C11	-158.0(5)	C22	S21	C20	C24	150.9(6)

Table S76 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2502056lt_auto.

Atom	*x*	*y*	*z*	U(eq)
H2	13395.59	-2692.16	2594.19	29
H3	15165.42	-1051.62	2915.65	29
H4	16628.62	169.13	1961.23	30
H5	16468.16	-298.19	681.86	28
H6	14730.59	-1956.4	341.65	27
H15	10874.09	2852.97	4790.88	33
H16	12627.1	4540.53	5056.43	32
H17	14735.98	5086.06	4145.15	33
H18	15043.73	4000.29	2958.16	36
H19	13298.41	2297.25	2691.48	29

2502056lt_auto

Table S77 Crystal data and structure refinement for 2502056lt_auto**.**

Identification code	2502056lt_auto
Empirical formula	$C_9H_5I_2NS$
Formula weight	413.00
Temperature/K	99.99(10)

Crystal system	triclinic
Space group	P-1
a/Å	7.6916(2)
b/Å	8.6661(2)
c/Å	17.4852(4)
α/°	84.454(2)
β/°	87.571(2)
γ/°	73.493(2)
Volume/Å^3	1112.09(5)
Z	4
ρ_{calc}g/cm^3	2.467
μ/mm^{-1}	45.807
F(000)	752.0
Crystal size/mm^3	0.06 × 0.02 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.166 to 145.654
Index ranges	-9 ≤ h ≤ 9, -7 ≤ k ≤ 10, -21 ≤ l ≤ 21
Reflections collected	13749
Independent reflections	4258 [R_{int} = 0.0408, R_{sigma} = 0.0445]
Data/restraints/parameters	4258/0/235
Goodness-of-fit on F^2	0.996
Final R indexes [I>=2σ (I)]	R_1 = 0.0352, wR_2 = 0.0884
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0911
Largest diff. peak/hole / e Å^{-3}	1.65/-1.41