

SUPPORTING INFORMATION

Diaryliodonium as a Double σ -Hole Donor: The Dichotomy of Thiocyanate Halogen Bonding Provides Divergent Solid State Arylation by Diaryliodonium Cations

Natalia S. Soldatova¹, Pavel S. Postnikov^{2,3}, Vitalii V. Suslonov¹, Troyana Yu. Kissler¹, Daniil M. Ivanov¹, Mekhman S. Yusubov^{2*}, Bartomeu Galmés⁴, Antonio Frontera^{4*}, Vadim Yu. Kukushkin^{1,5*}

- 1 Institute of Chemistry, Saint Petersburg State University, Saint Petersburg 199034, Russian Federation
 - 2 Research School of Chemistry and Applied Biomedical Sciences, Tomsk Polytechnic University, Tomsk 634034, Russian Federation
 - 3 Department of Solid State Engineering, Institute of Chemical Technology, Prague 16628, Czech Republic
 - 4 Department of Chemistry, Universitat de les Illes Balear, Crta. de Valldemossa km 7.7, 07122 Palma de Mallorca (Balears), Spain
 - 5 South Ural State University, 76, Lenin Av., Chelyabinsk, 454080, Russian Federation.
- * Correspondence: yusubov@mail.ru, toni.frontera@uib.es, v.kukushkin@spbu.ru

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Table S1. Crystal data and structure refinement for **3–7**.

Identification code	3	4	5	6	7
CCDC number	2000276	2000277	2000278	2000279	2000280
Empirical formula	C ₁₃ H ₁₀ INS	C ₁₆ H ₁₆ INO ₃ S	C ₁₆ H ₁₅ FINO ₃ S	C ₁₆ H ₁₆ INOS	C ₁₈ H ₂₀ INO ₃ S
Formula weight	339.18	429.26	447.25	397.26	457.31
Temperature/K	100(2)	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	monoclinic	triclinic	triclinic
Space group	P2 ₁ /n	P-1	P2 ₁ /c	P-1	P-1
a/Å	7.5458(5)	7.9290(4)	9.8222(4)	7.9702(4)	8.68740(10)
b/Å	11.1302(8)	10.6799(5)	23.0680(10)	9.5118(4)	9.16050(10)
c/Å	15.0196(10)	10.9498(9)	8.0455(4)	11.5477(5)	11.76420(10)
α/°	90	99.640(5)	90	102.282(4)	95.5680(10)
β/°	91.316(6)	102.654(6)	108.998(5)	90.743(4)	93.4270(10)
γ/°	90	107.017(4)	90	107.413(4)	99.6570(10)
Volume/Å ³	1261.11(15)	838.04(9)	1723.64(14)	813.44(7)	915.821(17)
Z	4	2	4	2	2
ρ _{calc} g/cm ³	1.786	1.701	1.724	1.622	1.658
μ/mm ⁻¹	2.676	2.046	2.001	2.092	14.934
F(000)	656.0	424.0	880.0	392.0	456.0
Crystal size/mm ³	0.21 × 0.19 × 0.18	0.25 × 0.21 × 0.18	0.19 × 0.18 × 0.15	0.20 × 0.18 × 0.16	0.214 × 0.195 × 0.142
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2θ range for data collection/°	5.426 to 64.412	5.604 to 64.364	5.632 to 54.99	5.374 to 55	7.574 to 129.992
Index ranges	-10 ≤ h ≤ 10, -16 ≤ k ≤ 10, -12 ≤ l ≤ 22	-10 ≤ h ≤ 11, -15 ≤ k ≤ 14, -16 ≤ l ≤ 15	-12 ≤ h ≤ 12, -27 ≤ k ≤ 29, -10 ≤ l ≤ 8	-9 ≤ h ≤ 10, -12 ≤ k ≤ 11, -14 ≤ l ≤ 14	-10 ≤ h ≤ 9, -10 ≤ k ≤ 10, -13 ≤ l ≤ 13
Reflections collected	7469	9033	9191	6571	11872
Independent reflections	3991 [R _{int} = 0.0313, R _{sigma} = 0.0495]	5289 [R _{int} = 0.0318, R _{sigma} = 0.0538]	3968 [R _{int} = 0.0242, R _{sigma} = 0.0319]	3730 [R _{int} = 0.0246, R _{sigma} = 0.0407]	3114 [R _{int} = 0.0556, R _{sigma} = 0.0416]
Data/restraints/parameters	3991/0/145	5289/0/202	3968/0/211	3730/0/184	3114/0/204
Goodness-of-fit on F ²	1.020	1.039	1.072	1.034	1.055
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0287, wR ₂ = 0.0496	R ₁ = 0.0302, wR ₂ = 0.0622	R ₁ = 0.0227, wR ₂ = 0.0462	R ₁ = 0.0236, wR ₂ = 0.0488	R ₁ = 0.0348, wR ₂ = 0.0885
Final R indexes [all data]	R ₁ = 0.0399, wR ₂ = 0.0541	R ₁ = 0.0370, wR ₂ = 0.0661	R ₁ = 0.0265, wR ₂ = 0.0476	R ₁ = 0.0267, wR ₂ = 0.0500	R ₁ = 0.0352, wR ₂ = 0.0889
Largest diff. peak/hole / e·Å ⁻³	0.80/-0.80	0.75/-0.90	0.47/-0.48	0.49/-0.41	1.16/-2.04

Table S2. Crystal data and structure refinement for **8** and **9**.

Identification code	8	9
CCDC number	2000281	2000282
Empirical formula	C ₁₆ H ₁₅ ClINO ₃ S	C ₁₆ H ₁₅ BrINO ₃ S
Formula weight	463.70	508.16
Temperature/K	100(2)	100(2)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	8.4080(3)	8.3448(5)
b/Å	10.5039(4)	10.7012(8)
c/Å	11.2572(4)	11.2708(9)
α/°	67.872(3)	67.245(7)
β/°	70.296(3)	70.464(6)
γ/°	82.896(3)	83.175(5)
Volume/Å ³	867.04(6)	874.64(12)
Z	2	2
ρ _{calc} g/cm ³	1.776	1.930
μ/mm ⁻¹	2.134	18.294
F(000)	456.0	492.0
Crystal size/mm ³	0.19 × 0.17 × 0.13	0.16 × 0.15 × 0.1
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2θ range for data collection/°	5.482 to 54.996	8.962 to 140.866
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14	-10 ≤ h ≤ 10, -13 ≤ k ≤ 9, -13 ≤ l ≤ 13
Reflections collected	14517	8682
Independent reflections	3975 [R _{int} = 0.0278, R _{sigma} = 0.0257]	3323 [R _{int} = 0.0524, R _{sigma} = 0.0565]
Data/restraints/parameters	3975/0/211	3323/0/211
Goodness-of-fit on F ²	1.039	1.027
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0164, wR ₂ = 0.0374	R ₁ = 0.0375, wR ₂ = 0.0951
Final R indexes [all data]	R ₁ = 0.0180, wR ₂ = 0.0382	R ₁ = 0.0402, wR ₂ = 0.0968
Largest diff. peak/hole / e·Å ⁻³	0.40/-0.31	0.97/-1.18

Additional interactions observed in the crystal packing of **3** and **8**

In Figure S1 we show partial views the X-ray packing of compounds **3** (a) and **8** (b), where the thiocyanate anions have been omitted for clarity. Both compounds exhibit different packing architectures and interactions governing them. In compound **3**, the packing is dominated (among others) by π - π stacking interactions (red dashed lines) and also C-H \cdots π involving the aromatic C-H atoms (see blue dashed lines). In compound **8**, the presence of the methoxy groups directs the formation of multiple CH₃ \cdots π interactions (represented as blue dashed lines) in addition to C-H \cdots π also involving aromatic C-H groups. Moreover, I \cdots π interactions are also established (blue dashed lines). This analysis of the crystal packing of **3** and **8** clearly supports that the negligible difference between the stabilities of the two different types of heterotetrameric motifs, can be easily overcome by packing effects since a multitude of noncovalent interactions are established. These interactions likely govern the formation of four or eight-membered supramolecular rings in the solid state.

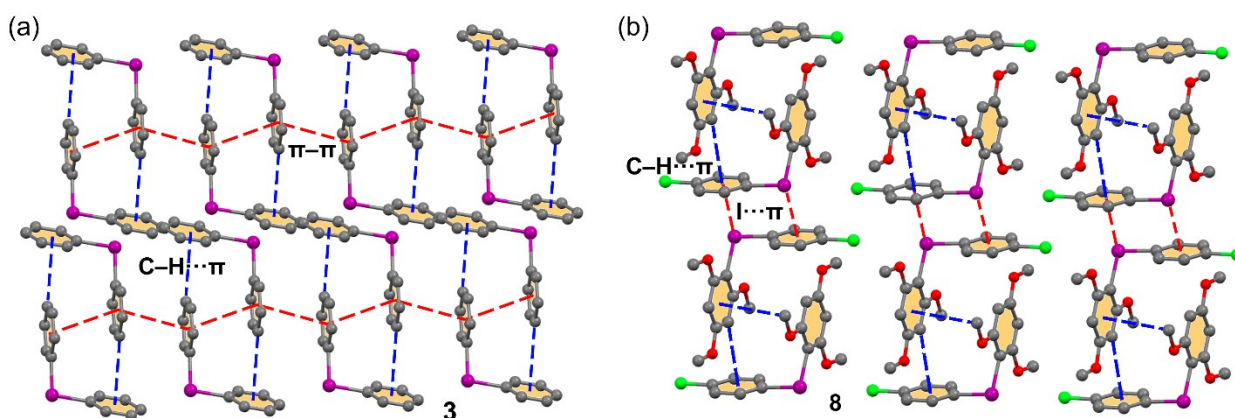
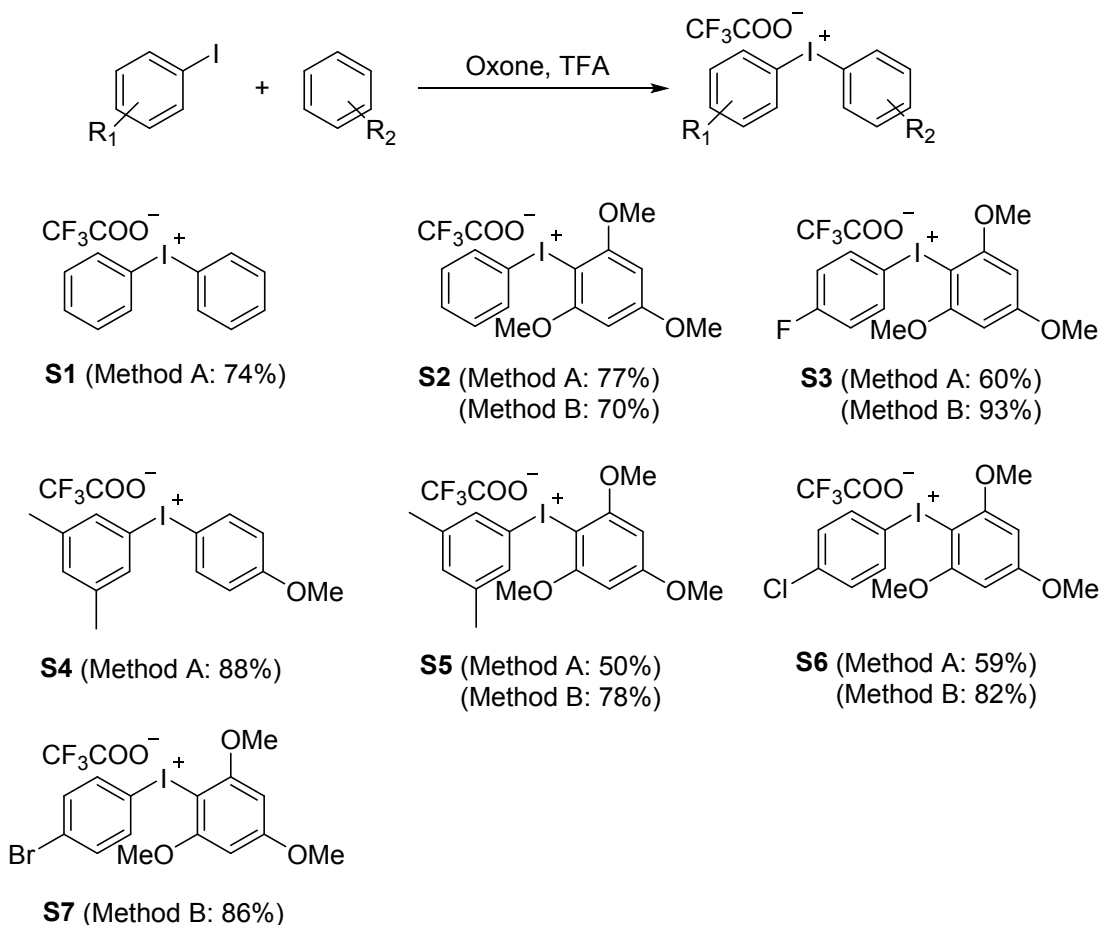


Figure S1. (a) Partial view of the X-ray of **3** with indication of the π - π stacking (red dashed lines) and C-H \cdots π (blue dashed lines) interactions. (b) Partial view of the X-ray of **8** with indication of the CH₃- π and C-H \cdots π (blue dashed lines) interactions and I \cdots π interactions (red dashed lines).

Synthesis of diaryliodonium trifluoroacetates

Diaryliodonium trifluoroacetates **S1–S7** were obtained by Method A¹ or Method B:



Method A

Diaryliodonium trifluoroacetates **S1–S6** were prepared by the previously reported procedure in flow.¹

Reagent mixture **1**: Iodoarene (0.898 mmol, 100 μ L) and TFA (1.39 mL) were dissolved CH_2Cl_2 to achieve a total volume of 10 mL.

Reagent mixture **2**: Arene (1.037–1.087 mmol) or boronic acid (1.087 mmol) and TFA (1.53 mL) were dissolved CH_2Cl_2 to achieve a total volume of 11 mL.

Reagent mixture **1** was pumped through the Oxone-filled cartridge using a syringe pump at a flow rate of 0.11 mL/min. After 15.5 minutes, reagent mixture **2** was started to pump with a second syringe pump with 0.11 mL/min. After the reagent mixture **1** addition, the syringe with a mixture of reagents was immediately replaced with a syringe with CH_2Cl_2 (10 mL) and CH_2Cl_2 was pumped with 0.11 mL/min until the end of the pumping reagent mixture **2**. Then flow rate was increased to 0.22 mL/min for 5 min, then and addition continued until the end of the CH_2Cl_2 in the syringe with 0.5 mL/min flow rate. The solvent was removed from the resulting solution *in vacuo* at 40 °C and the residue was diluted with water (5 mL). The product was extracted with

CH₂Cl₂ (3 × 5 mL). The organic layer was dried with Na₂SO₄ and the solvent was removed *in vacuo*. Then diethyl ether (5 mL) was added to the residue and a precipitate was formed, the suspension was stirred for 10 min, then the product was filtered off and washed with diethyl ether (3×5 mL) and hexane (10 mL). The obtained product was dried *in vacuo* (10 mbar) at ambient temperature.

Method B

This batch procedure for synthesis of **S2–S3**, **S5–S7** is based on previously reported flow synthesis of diaryliodonium trifluoroacetates.¹

Oxone (1.234 g, 2 mmol) and iodoarene (2 mmol) were added to mixture of DCM and TFA (3 mL, 1:1 v/v). The reaction mixture was stirred for 20 min at ambient temperature. Reaction was monitored by TLC (Eluent: Hexane:EtOAc 10:1 v/v), whereupon the solvent was evaporated to dryness at 40 °C, and solid residue was suspended in DCM (25 mL) and stirred for 30 min. The suspension was filtered off and an inorganic residue was washed with 25 mL of DCM. The solvent was removed to 3–5 mL residue in a flask and trifluoroethanol (TFE) (1.5 mL) and 1,3,5-trimethoxybenzene (2.1 mmol, 353 mg) were added to the mixture and stirring was continued for 30 min at ambient temperature. The solvent was evaporated at 40 °C and cold Et₂O (10 mL) was added to the residue. Product was filtered off and washed with cold Et₂O (3×5 mL). The product was dried *in vacuo* (10 mbar) at ambient temperature.

Diphenyliodonium trifluoroacetate (S1).¹ Obtained in 74% yield (Method A). ¹H NMR (400 MHz, DMSO-*d*₆) δ: 8.24 (d, *J* = 7.6 Hz, 4H), 7.67 (t, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 4H).

Phenyl(2,4,6-trimethoxyphenyl)iodonium trifluoroacetate (S2).^{1,2} Obtained in 77% yield (Method A) and 70% (Method B). ¹H NMR (400 MHz, DMSO-*d*₆) δ: 7.91 (d, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.46 (s, 2H), 3.94 (s, 6H), 3.87 (s, 3H).

(4-fluorophenyl)(2,4,6-trimethoxyphenyl)iodonium trifluoroacetate (S3).^{1,2} Obtained in 60% yield (Method A) and 93% (Method B). ¹H NMR (400 MHz, DMSO-*d*₆) δ: 8.00–7.93 (m, 2H), 7.33 (t, *J* = 8.8 Hz, 2H), 6.46 (s, 2H), 3.94 (s, 6H), 3.87 (s, 3H).

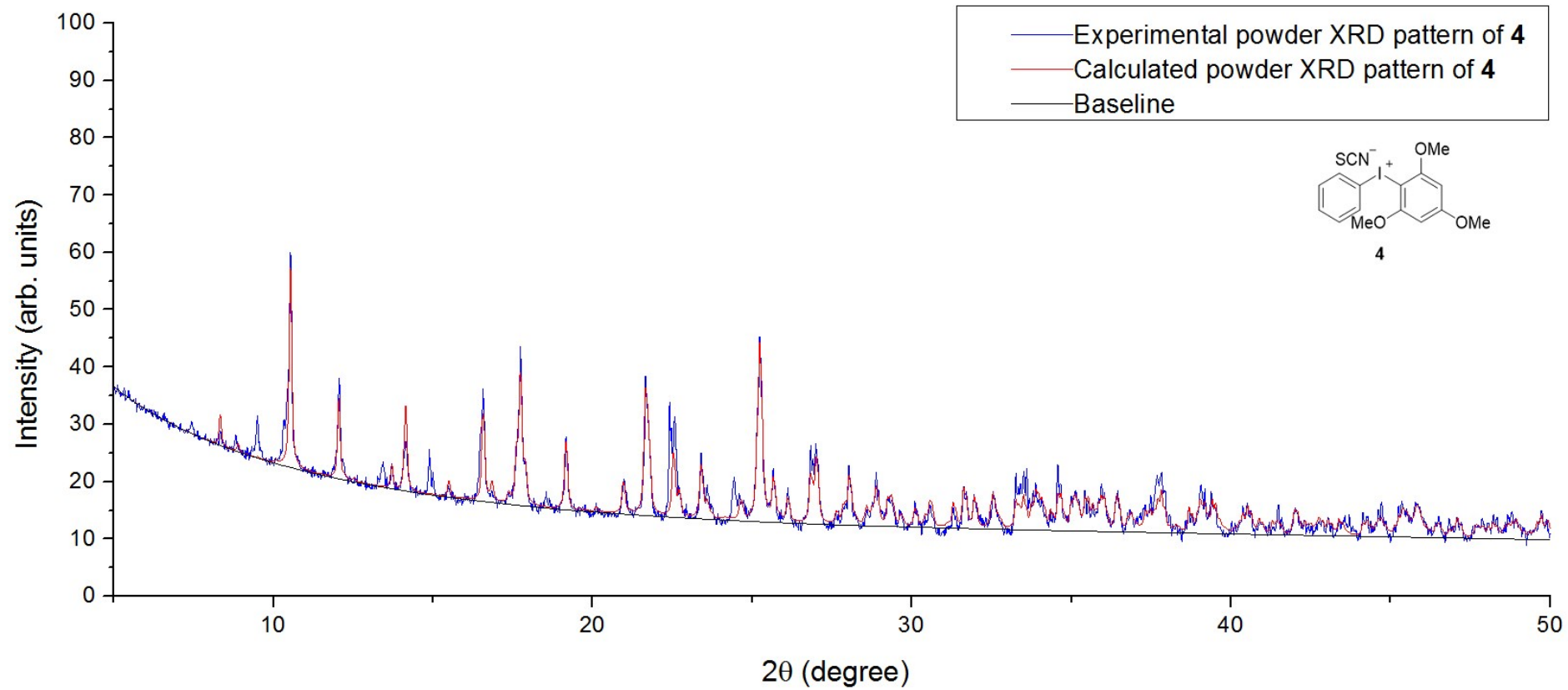
(3,5-Dimethylphenyl)(4-methoxyphenyl)iodonium trifluoroacetate (S4).¹ Obtained in 88% yield (Method A). ¹H NMR (400 MHz, CDCl₃) δ: 7.85 (d, *J* = 8.0 Hz, 2H), 7.51 (s, 2H), 7.12 (s, 1H), 6.89 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H), 2.29 (s, 6H).

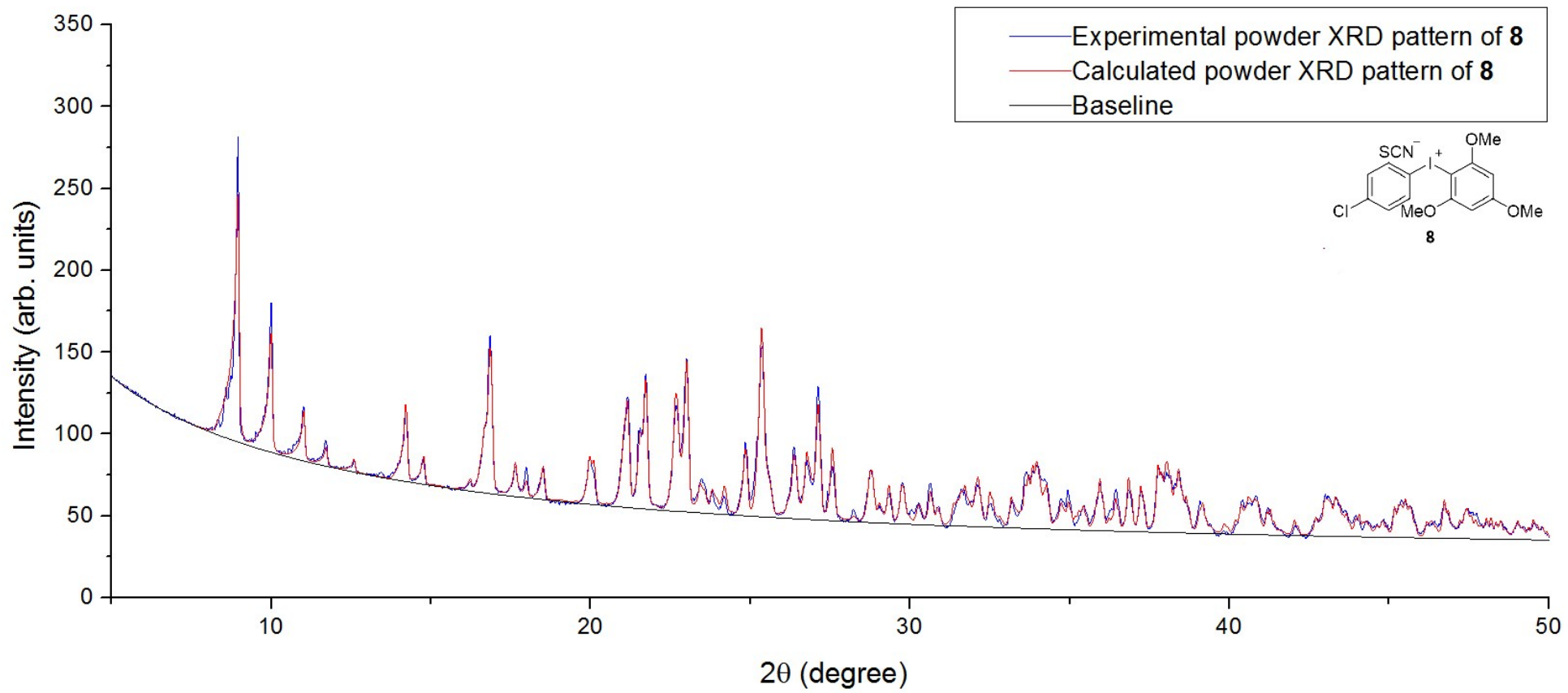
(3,5-dimethylphenyl)(2,4,6-trimethoxyphenyl)iodonium trifluoroacetate (S5).¹ Obtained in 50% yield (Method A) and 78% (Method B). ¹H NMR (400 MHz, CDCl₃) δ: 7.51 (s, 2H), 7.07 (s, 1H), 6.16 (s, 2H), 3.88 (s, 6H), 3.86 (s, 3H), 2.28 (s, 6H).

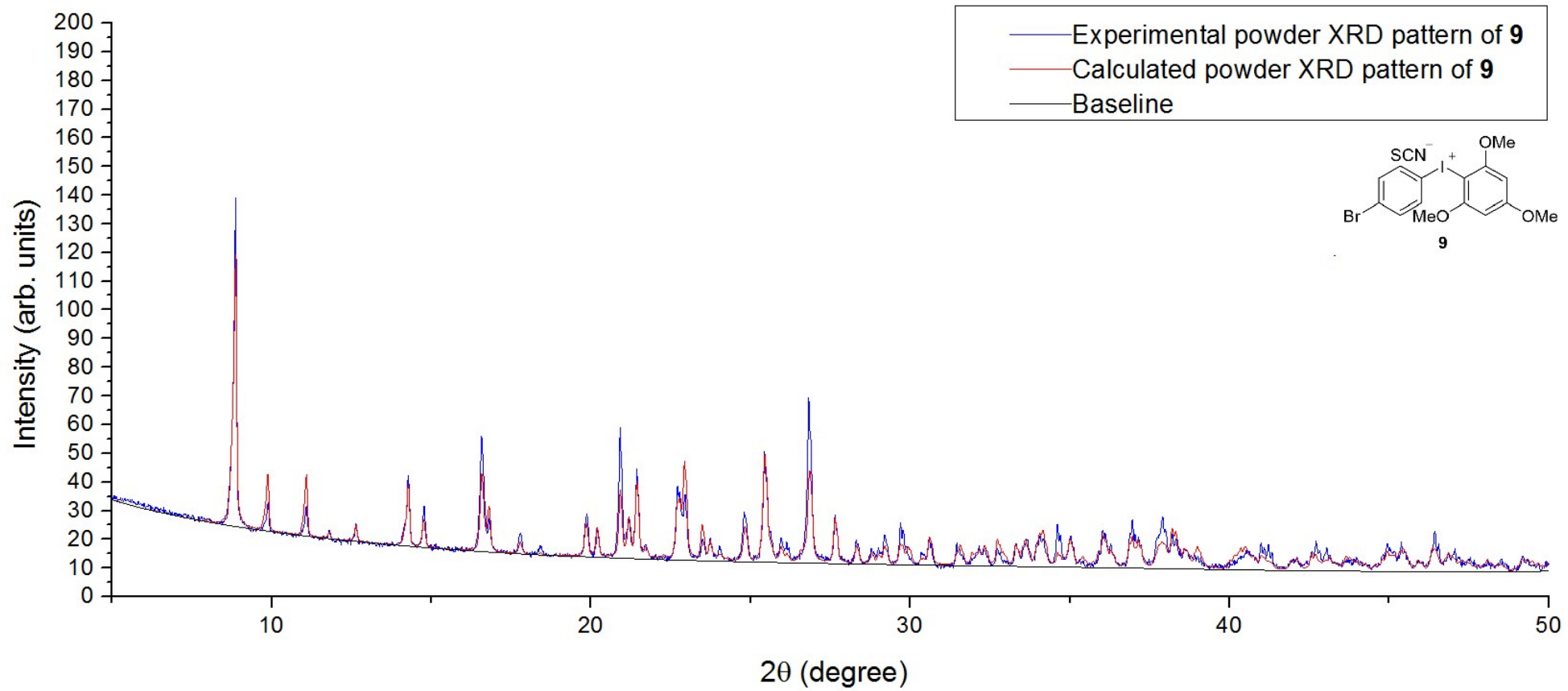
(4-chlorophenyl)(2,4,6-trimethoxyphenyl)iodonium trifluoroacetate (S6).^{1,2} Obtained in 59% yield (Method A) and 82% (Method B). ¹H NMR (400 MHz, CDCl₃) δ: 7.84 (d, *J* = 8.8 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 6.17 (s, 2H), 3.89 (s, 6H), 3.86 (s, 3H).

(4-bromophenyl)(2,4,6-trimethoxyphenyl)iodonium trifluoroacetate (S7).² Obtained in 86% (Method B). ¹H NMR (400 MHz, DMSO-*d*₆) δ: 7.83 (d, *J* = 8.8 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 6.47 (s, 2H), 3.94 (s, 6H), 3.87 (s, 3H).

Powder XRD data

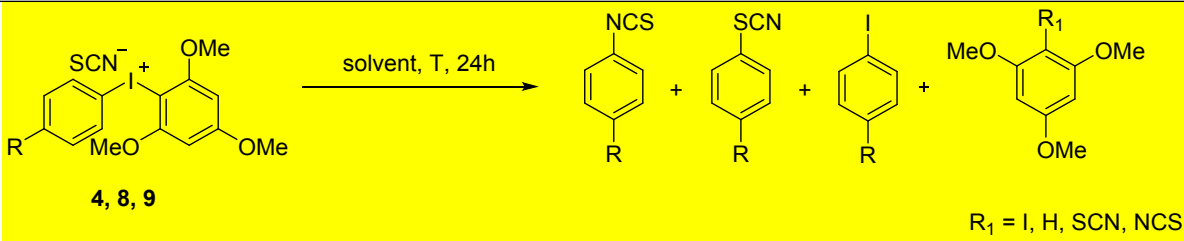






Thermolysis of diaryliodonium thiocyanates **4**, **8–9**

Table S3. Detailed ratio of thermolysis products^a

														
Entry	Substrate	Products ratio, %												
		ArNCS		ArSCN		ArI		TMPI		TMP		TMPSCN		TMPNCS
		GCMS ^c	NMR ^b	GCMS ^c	NMR ^b	GCMS ^c	NMR ^b	GCMS ^c	NMR ^b	GCMS ^c	NMR ^b	GCMS ^c	NMR ^b	GCMS ^c
1	4	2	2	29	38	4	6	59	46	5	6	2	2	–
2	4	–	1	31	31	15	15	32	29	12	11	10	13	–
3	8	24	27	13	18	3	5	52	43	2	2	5	5	1
4	8	–	–	15	19	20	21	31	26	8	8	25	26	<1
5	9	25	28	18	22	2	1	53	47	–	–	<1	<1	<1
6	9	–	–	23	27	21	20	30	24	6	7	21	22	–

^a Reactions were performed in a sealed NMR tube; ^b Calculated by NMR spectra; ^c According to the GCMS analysis;

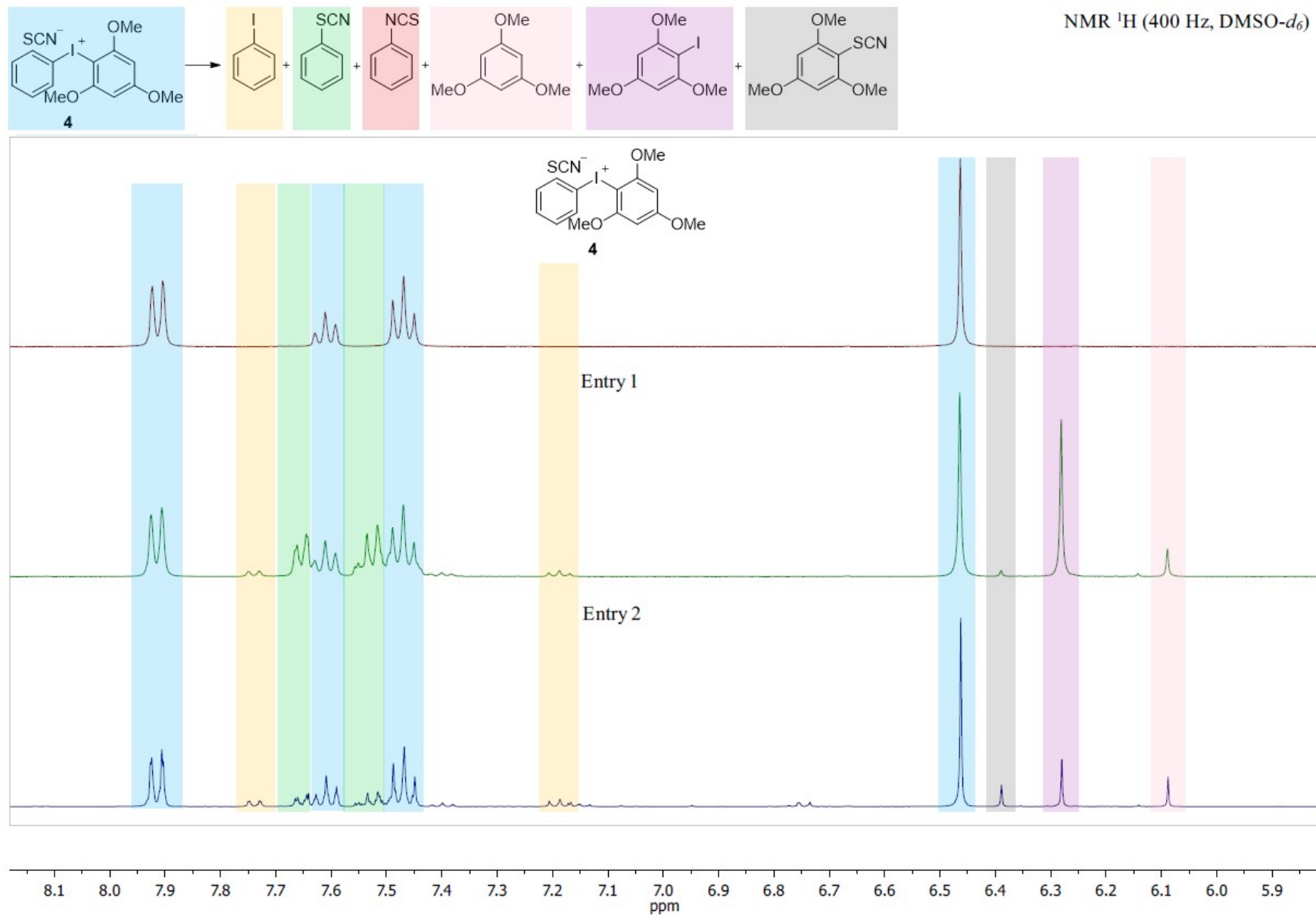
Consistence of the solid phase composition of **4**, **8–9** to the single crystal XRD data was checked by powder XRD (see Powder XRD data). Powder of **8** (or **9**) obtained by the anion metathesis was used; powder of **4** was obtained by the recrystallization **4** in acetone (Table 3).

Thermolysis of **4, **8–9** in solid state (Entry 1, 3, 5).** Diaryliodonium thiocyanate (0.02 mmol) was heated in neat in an NMR tube at 100 °C for 24 h, whereupon the residue was diluted with DMSO-*d*₆ (0.6 mL) and monitored by ¹H NMR.

Thermolysis of **4, **8–9** in solution (Entry 2, 4, 6).** Diaryliodonium thiocyanate (0.02 mmol) was heated in a solution of DMSO-*d*₆ in an NMR tube at 100 °C for 24 h. Then reaction mixture was then monitored by ¹H NMR.

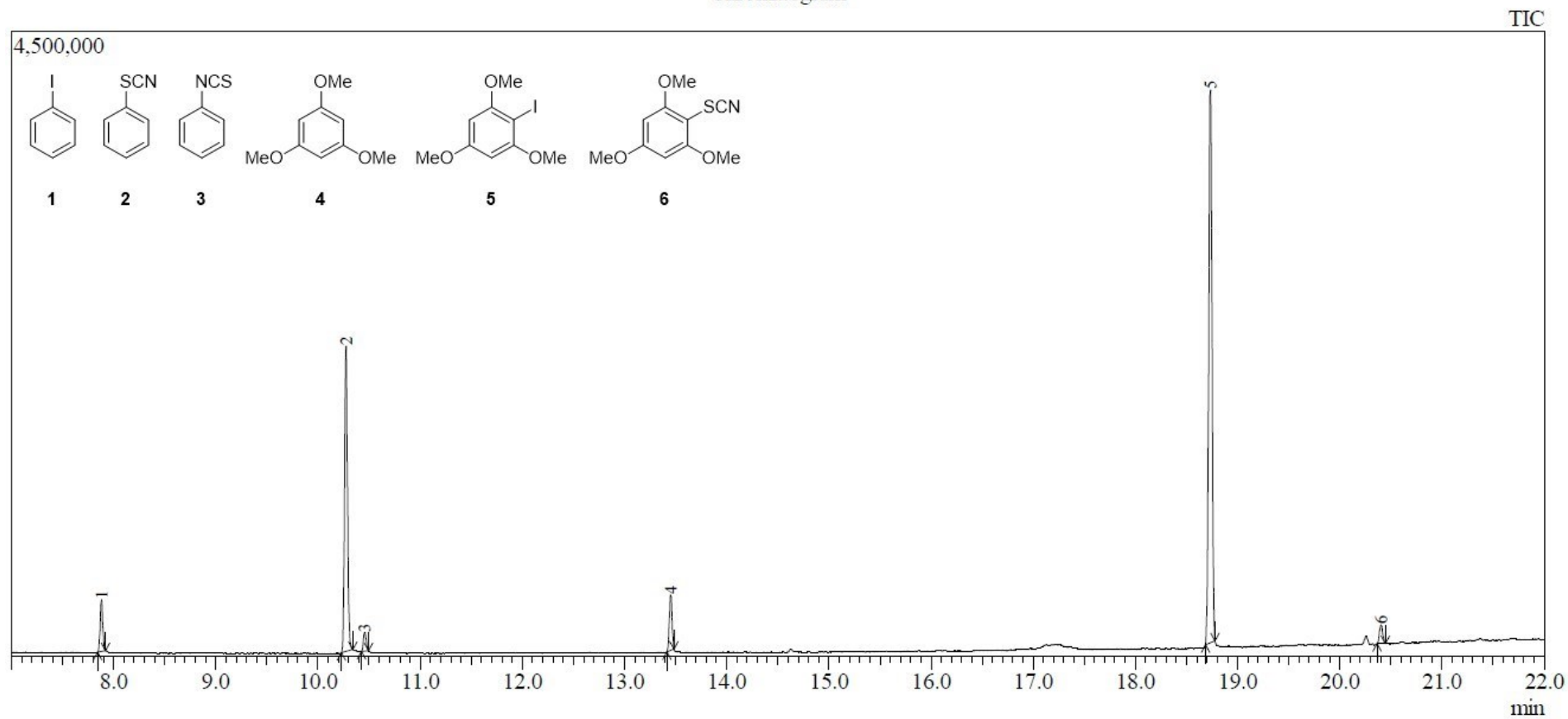
Preparation of samples for GS-MS monitoring (Entry 1–6). The reaction mixture in DMSO-*d*₆ was diluted with water (2 mL) and products were extracted with EtOAc (3×2 mL). The extract was dried over Na₂SO₄ and flushed off through silica column (0.25 g). Additionally, silica column was washed with EtOAc (2 mL). Resulting solution in EtOAc was analyzed by GCMS.³

Final products ratio was calculated by using GCMS data and thus obtained values agree with the ¹H NMR data. According to ¹H NMR spectroscopy, the products in cases of Entries 2, 4, and 6 contain traces of the identified byproduct. However, side processes do not affect a ratio between ArSCN and ArNSC.



Entry 1

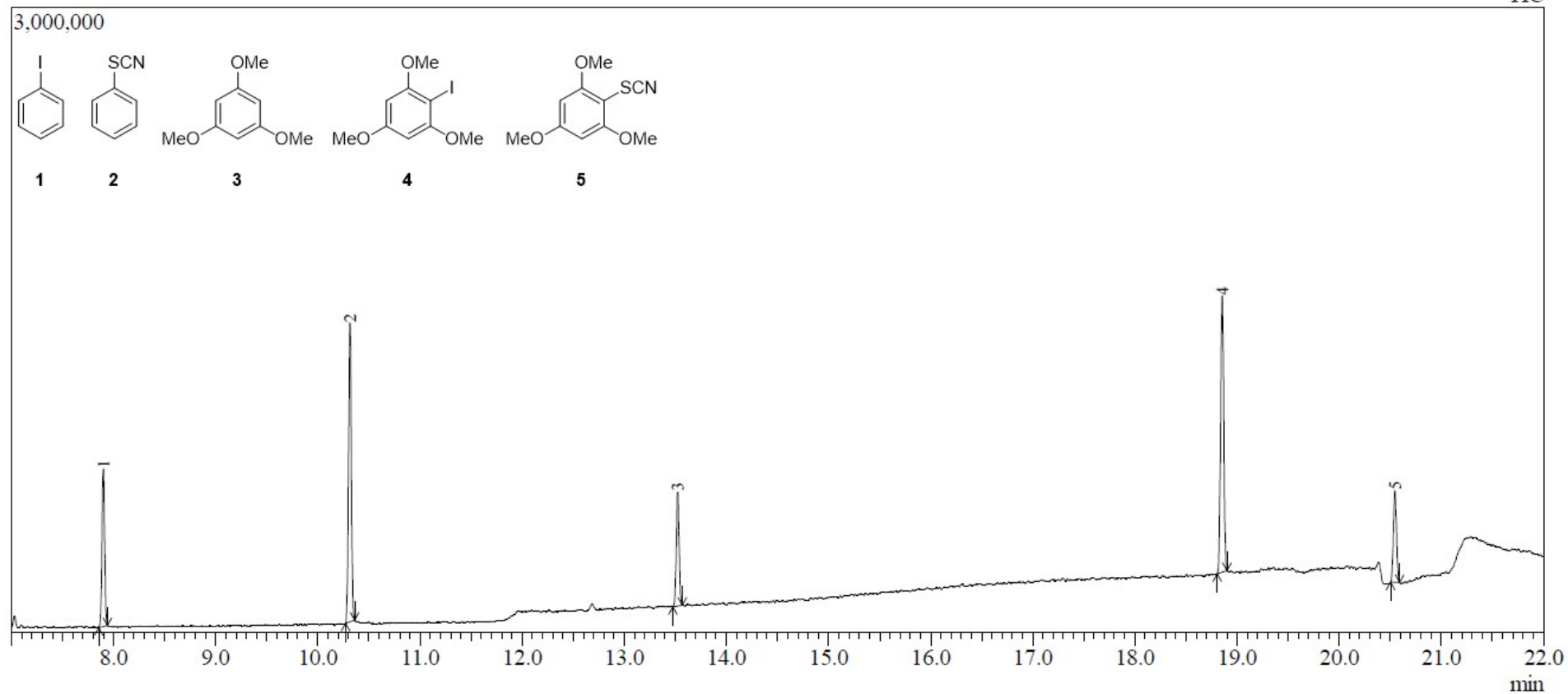
Chromatogram



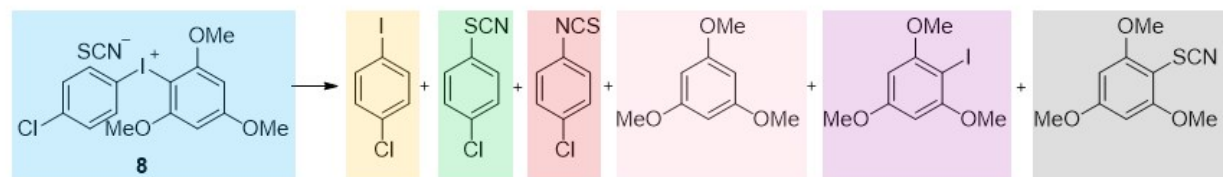
Peak#	R. Time	Area	Area%	Height	Height%	A/H
1	7.880	665588	4.34	372484	5.15	1.79
2	10.274	4384009	28.59	2200171	30.45	1.99
3	10.457	261601	1.71	135334	1.87	1.93
4	13.452	753110	4.91	400139	5.54	1.88
5	18.733	8974286	58.52	3983591	55.13	2.25
6	20.404	296291	1.93	134365	1.86	2.21
		15334885	100.00	7226084	100.00	

Entry 2

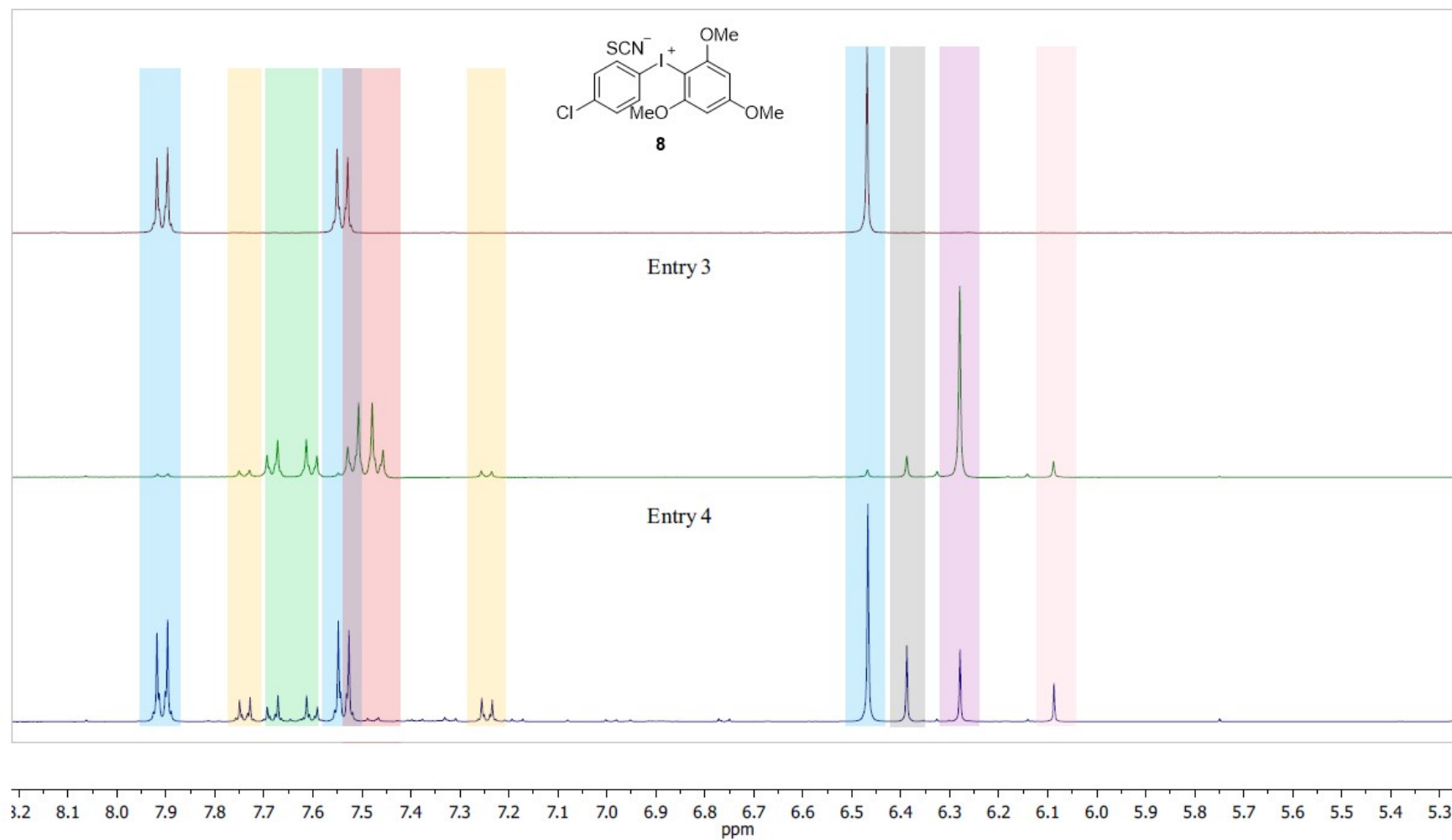
Chromatogram



Peak#	R.Time	Area	Area%	Peak Report TIC		A/H
				Height	Height%	
1	7.899	1360525	15.24	756041	16.79	1.80
2	10.315	2732089	30.60	1432825	31.82	1.91
3	13.523	1076220	12.05	545715	12.12	1.97
4	18.854	2833943	31.74	1326642	29.47	2.14
5	20.545	926678	10.38	441045	9.80	2.10
		8929455	100.00	4502268	100.00	

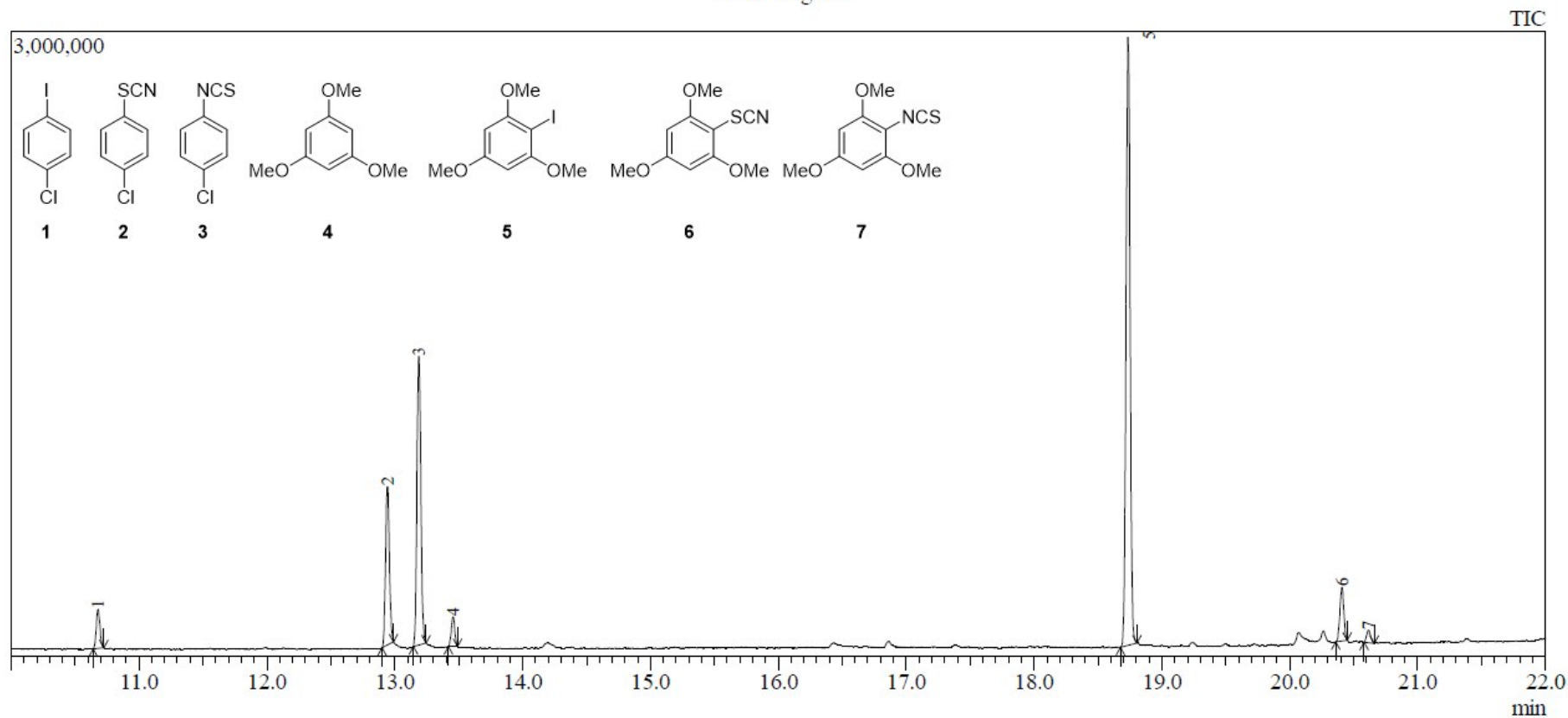


NMR ^1H (400 Hz, $\text{DMSO-}d_6$)



Entry 3

Chromatogram

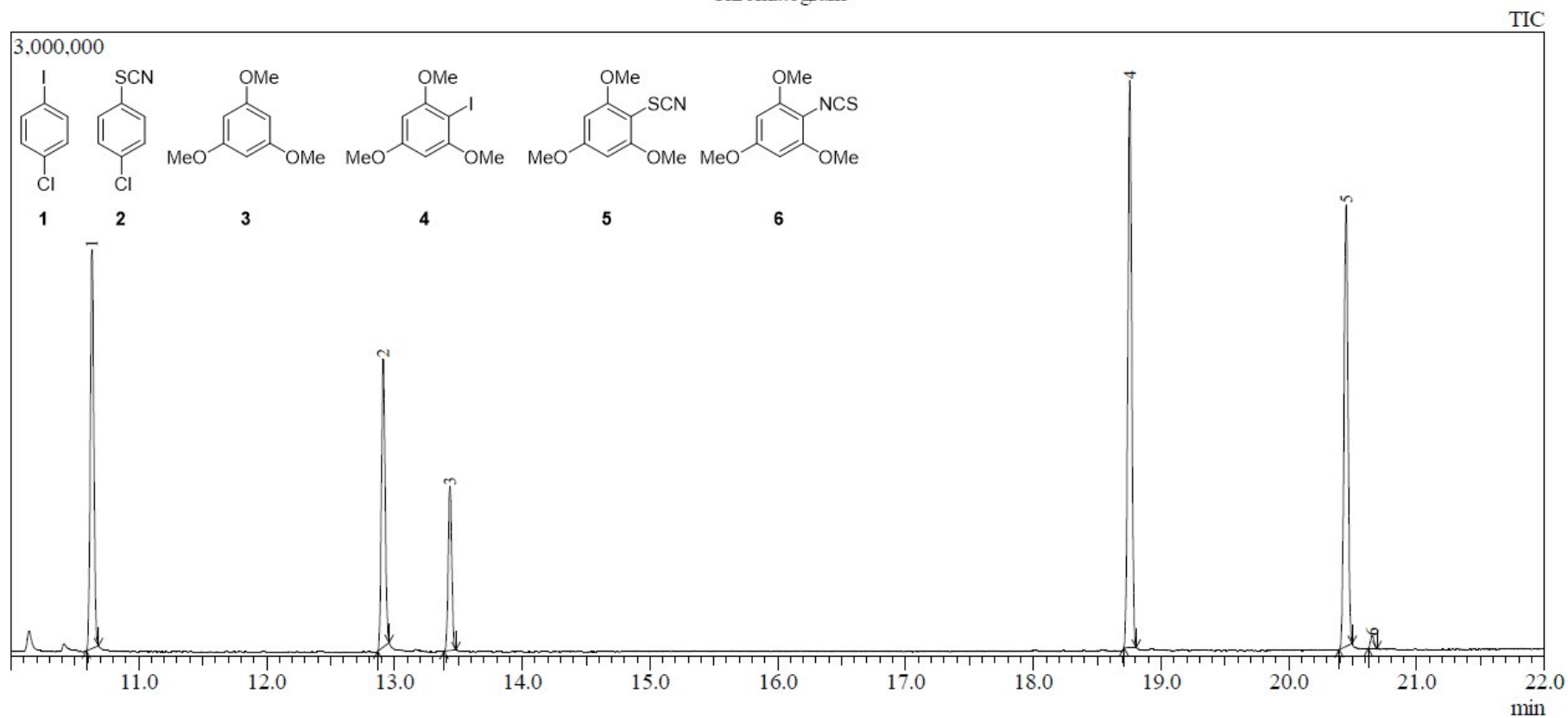


Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H
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2	12.942	1585034	12.90	759102	13.30	2.09
3	13.187	2930473	23.86	1382350	24.23	2.12
4	13.456	272790	2.22	143448	2.51	1.90
5	18.736	6434364	52.38	2914320	51.08	2.21
6	20.408	560227	4.56	259064	4.54	2.16
7	20.616	128947	1.05	60247	1.06	2.14

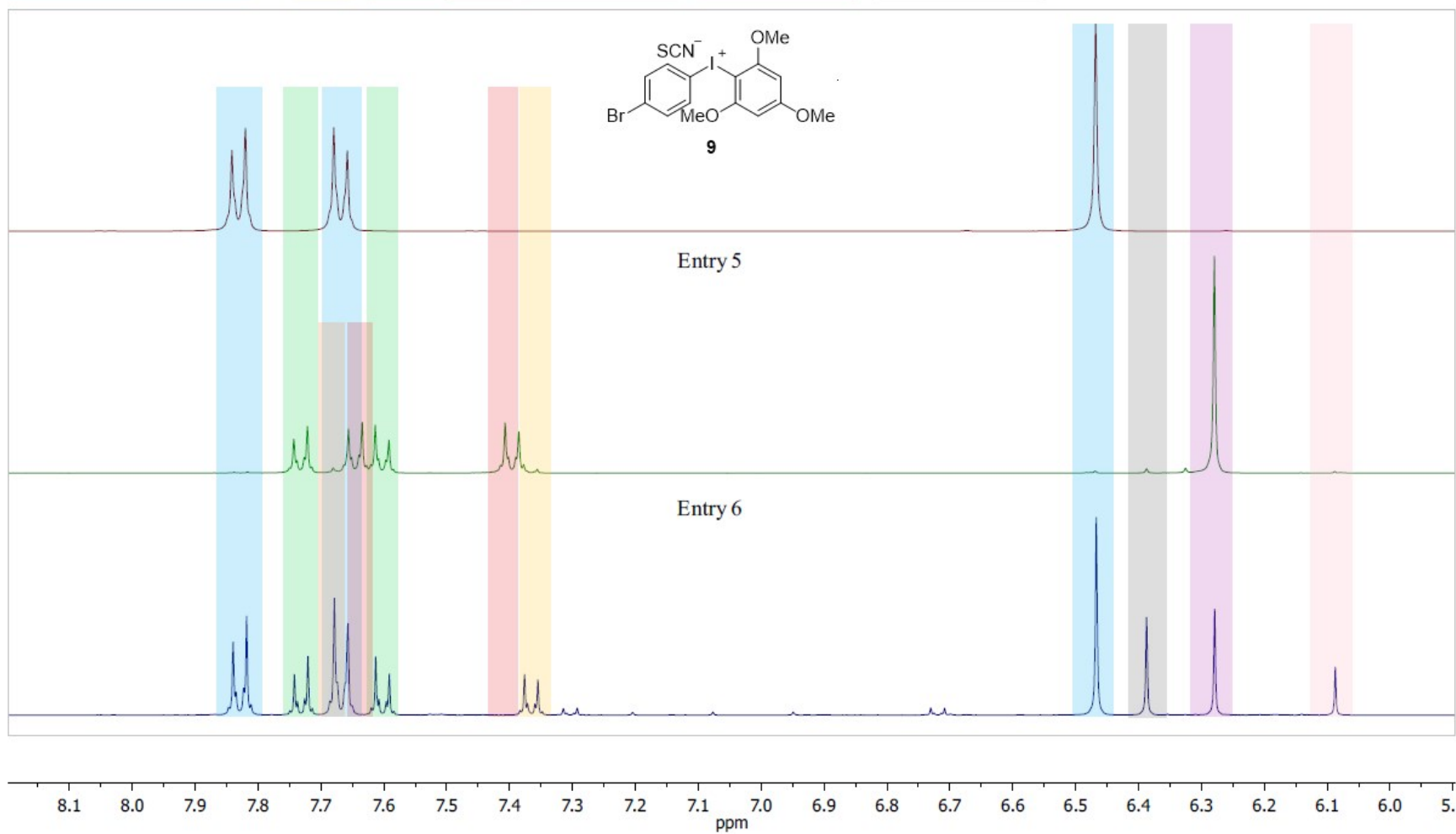
Entry 4

Chromatogram



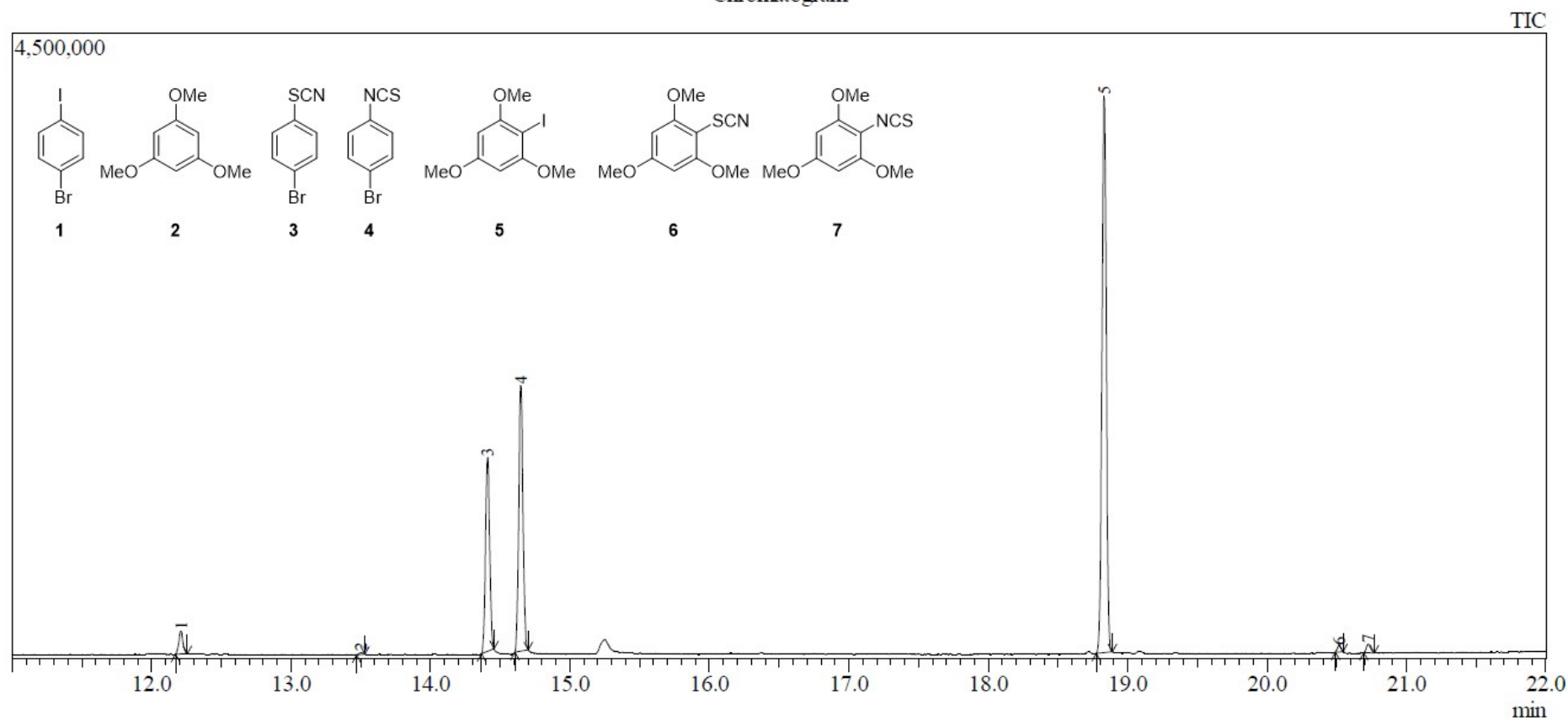
Peak#	R.Time	Area	Area%	Peak Report TIC		A/H
				Height	Height%	
1	10.633	3671864	19.96	1914135	21.31	1.92
2	12.912	2801889	15.23	1384802	15.41	2.02
3	13.434	1528770	8.31	788390	8.78	1.94
4	18.755	5657692	30.76	2719870	30.27	2.08
5	20.448	4609361	25.06	2118072	23.58	2.18
6	20.653	122406	0.67	58988	0.66	2.08
		18391982	100.00	8984257	100.00	

NMR ^1H (400 Hz, $\text{DMSO-}d_6$)



Entry 5

Chromatogram



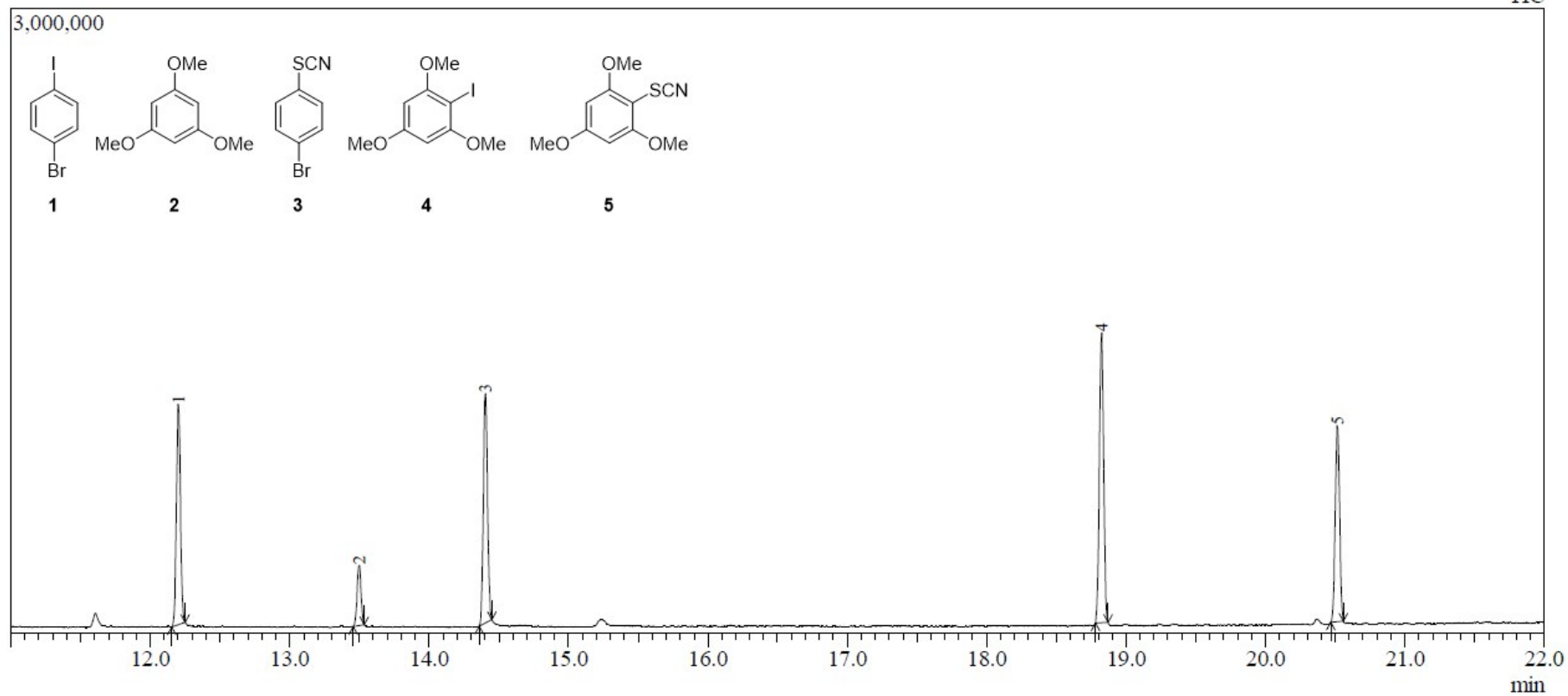
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H
1	12.209	341063	2.12	166784	2.19	2.04
2	13.502	24989	0.16	14086	0.19	1.77
3	14.409	2882980	17.91	1394799	18.34	2.07
4	14.647	4026786	25.01	1913294	25.16	2.10
5	18.832	8612191	53.49	4004661	52.67	2.15
6	20.517	82555	0.51	46764	0.62	1.77
7	20.726	129482	0.80	62989	0.83	2.06

Entry 6

Chromatogram

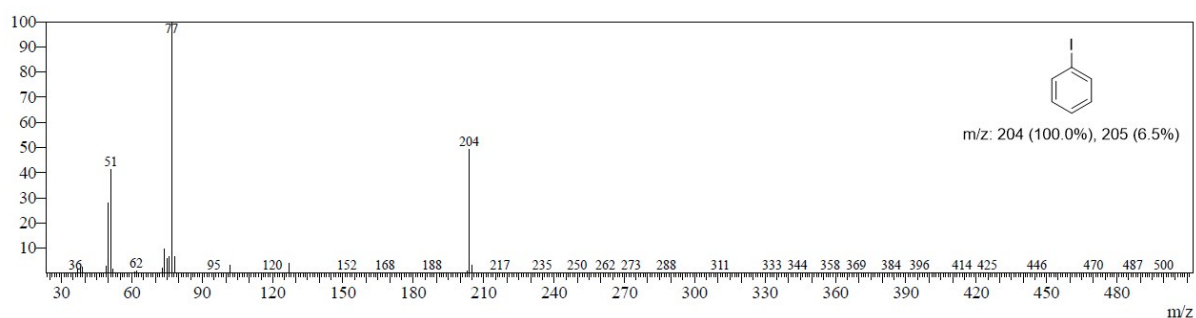
TIC



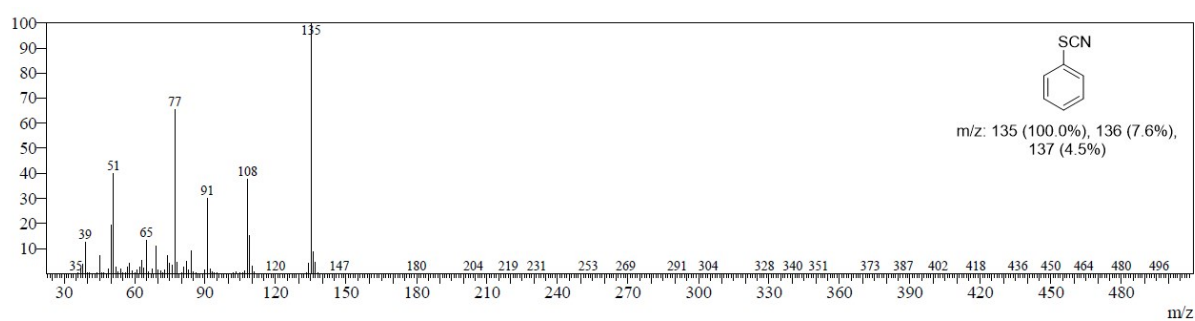
Peak Report TIC						
Peak#	R.Time	Area	Area%	Height	Height%	A/H
1	12.202	2145771	21.50	1056637	22.11	2.03
2	13.498	563869	5.65	288669	6.04	1.95
3	14.404	2273595	22.78	1099429	23.01	2.07
4	18.824	2948675	29.54	1391740	29.12	2.12
5	20.516	2050058	20.54	942240	19.72	2.18
		9981968	100.00	4778715	100.00	

Mass-spectrum (EI) of thermolysis products of 4, 8–9

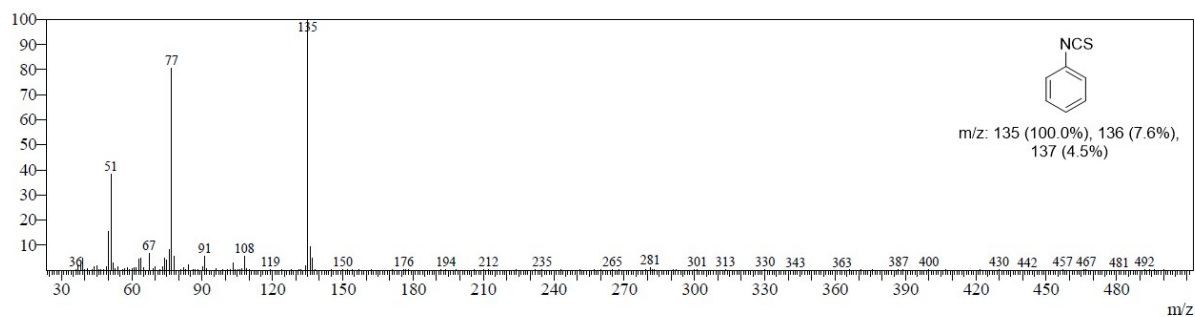
Iodobenzene⁴



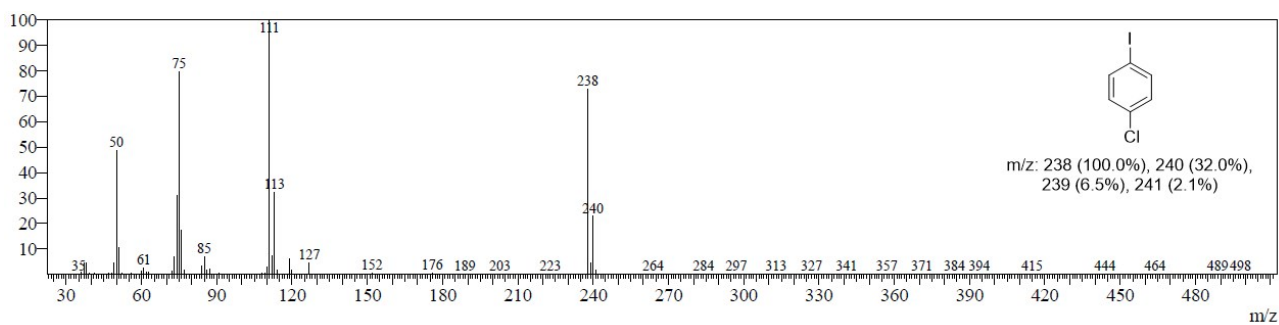
Thiocyanatobenzene⁵



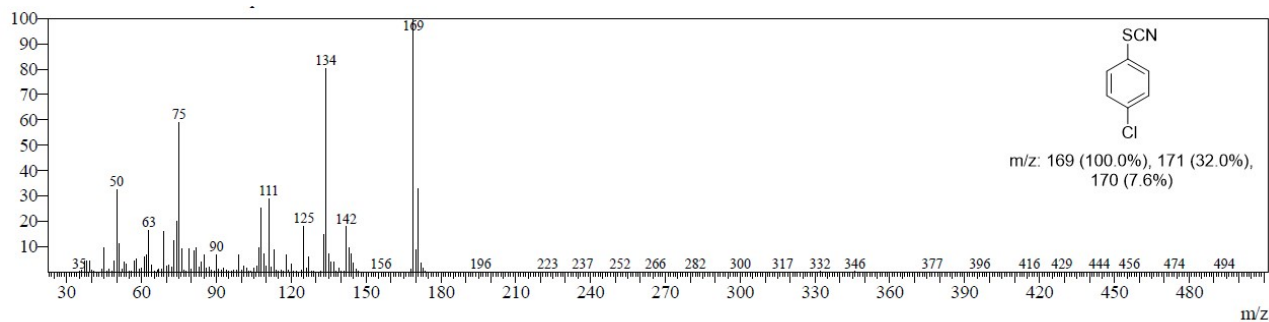
Isothiocyanatobenzene⁴



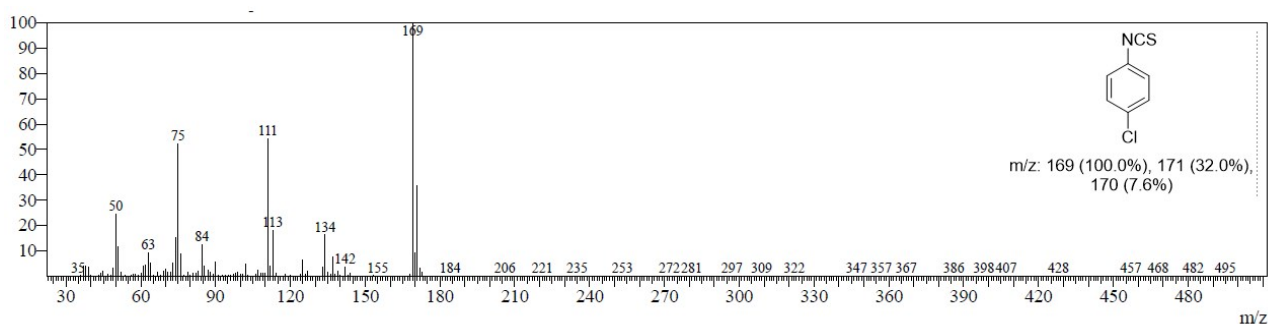
1-chloro-4-iodobenzene⁴



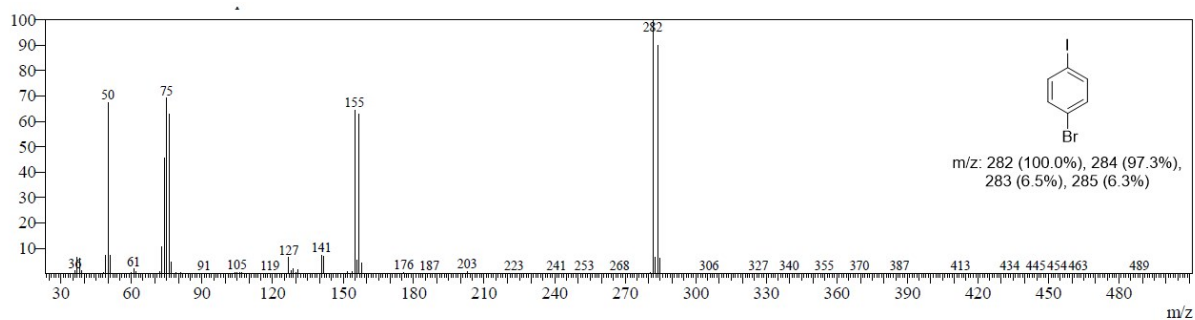
1-chloro-4-thiocyanatobenzene⁵



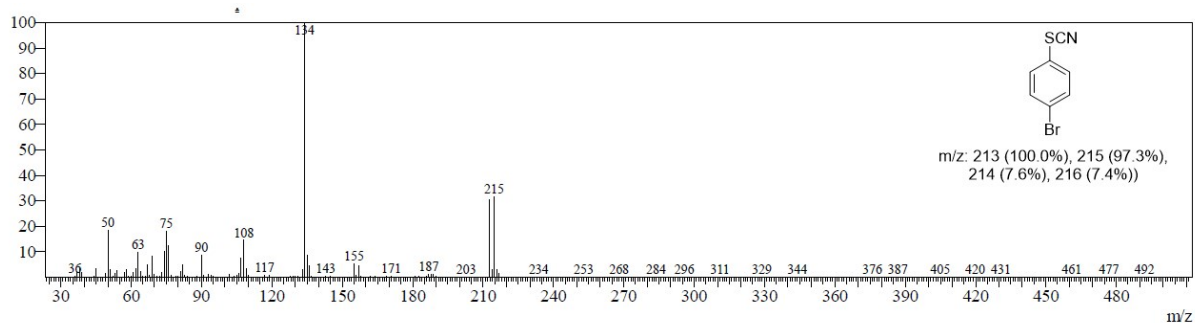
1-chloro-4-isothiocyanatobenzene⁴



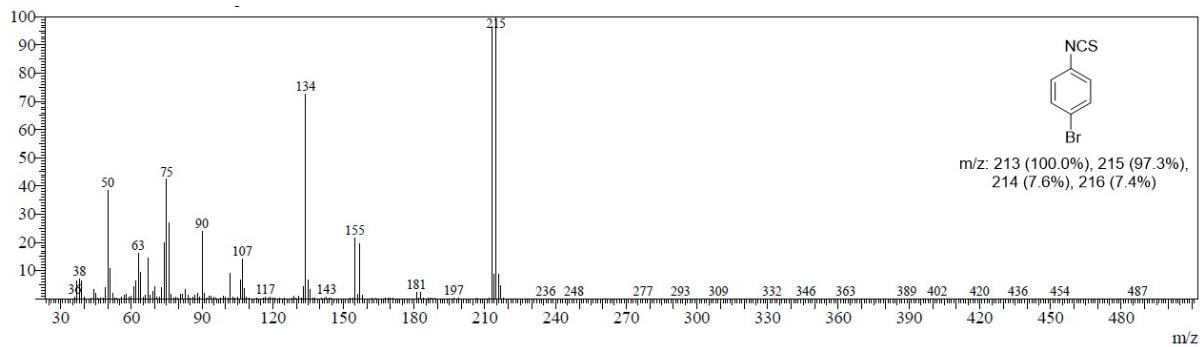
1-bromo-4-iodobenzene⁴



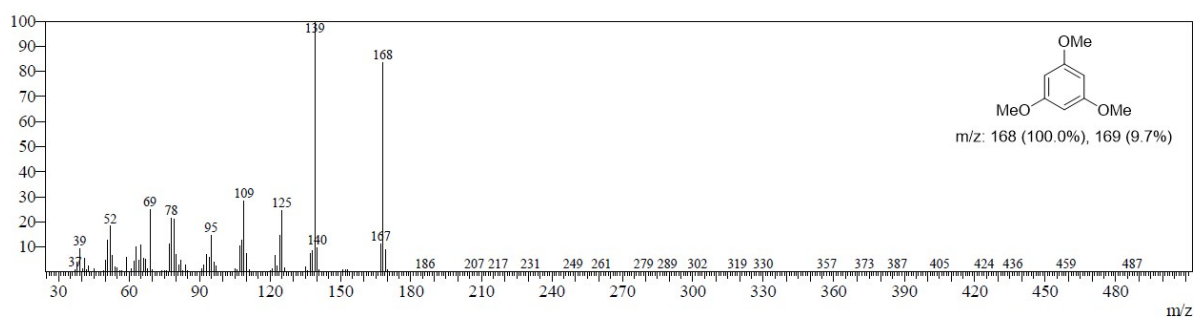
1-bromo-4-thiocyanatobenzene⁵



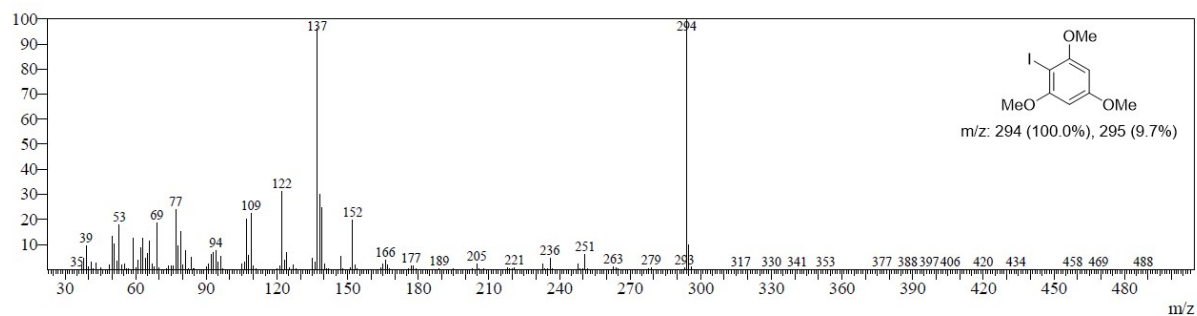
1-bromo-4-isothiocyanatobenzene⁴



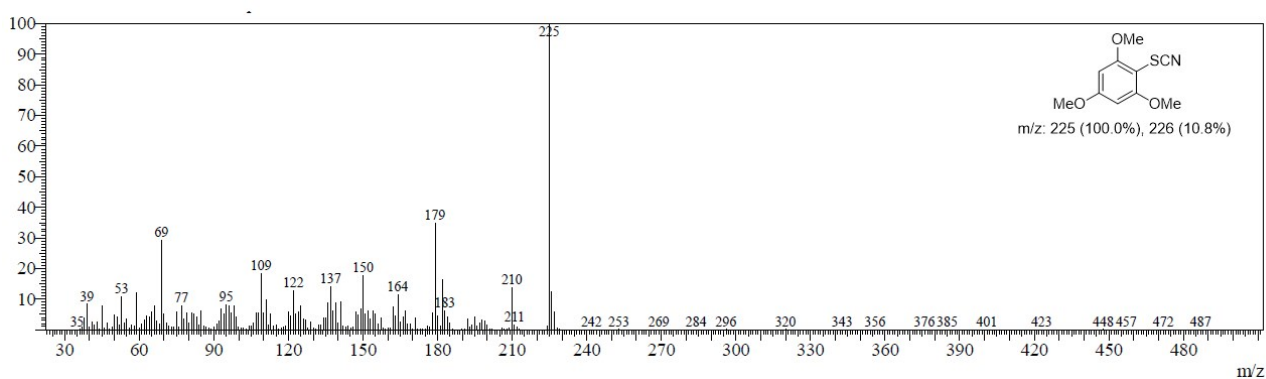
1,3,5-trimethoxybenzene⁴



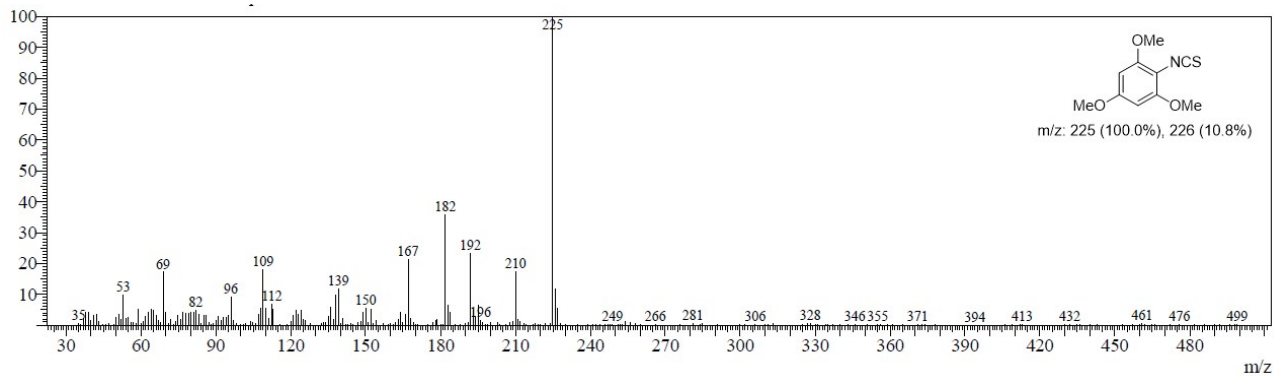
2-iodo-1,3,5-trimethoxybenzene⁶



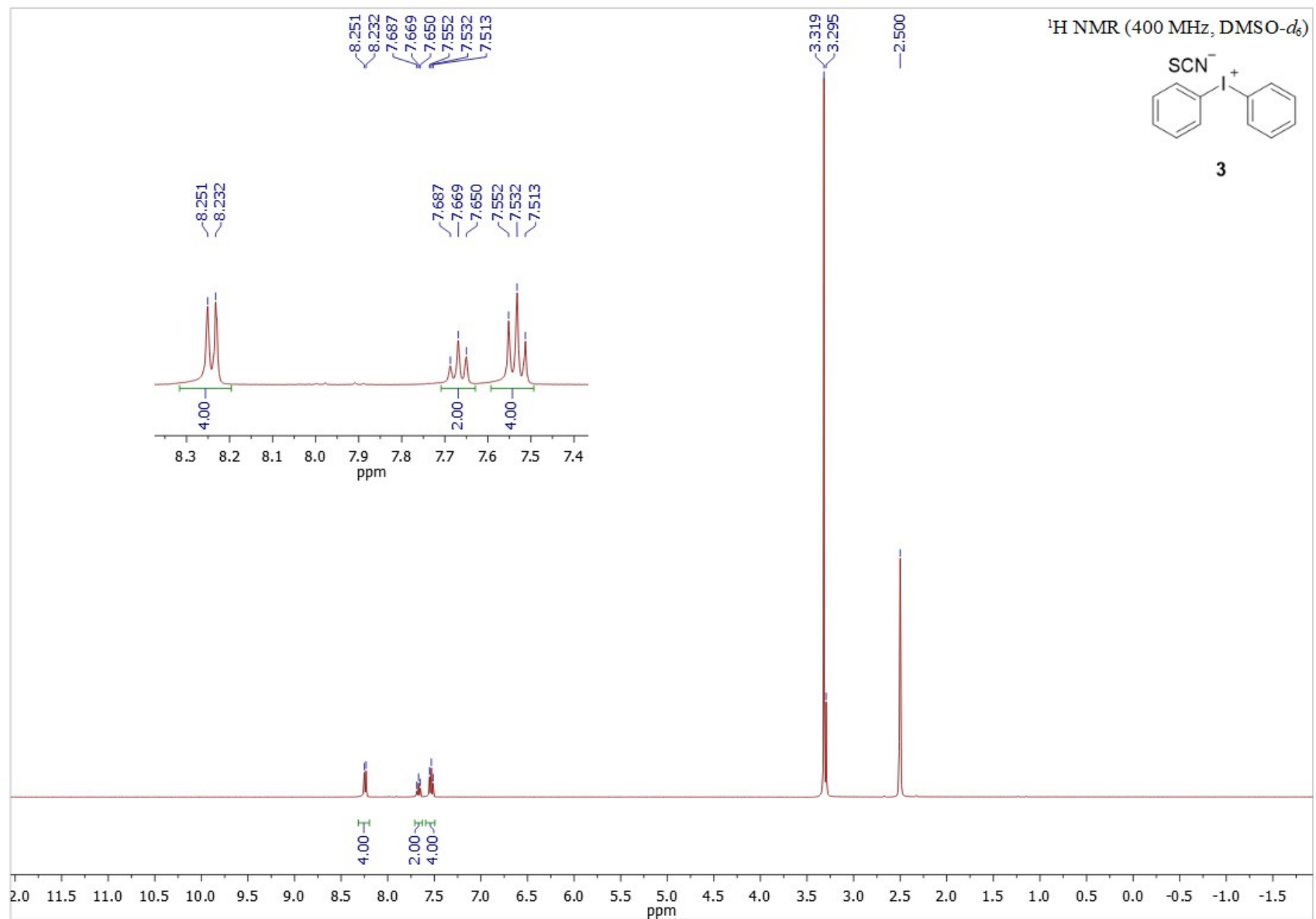
1,3,5-trimethoxy-2-thiocyanatobenzene⁷

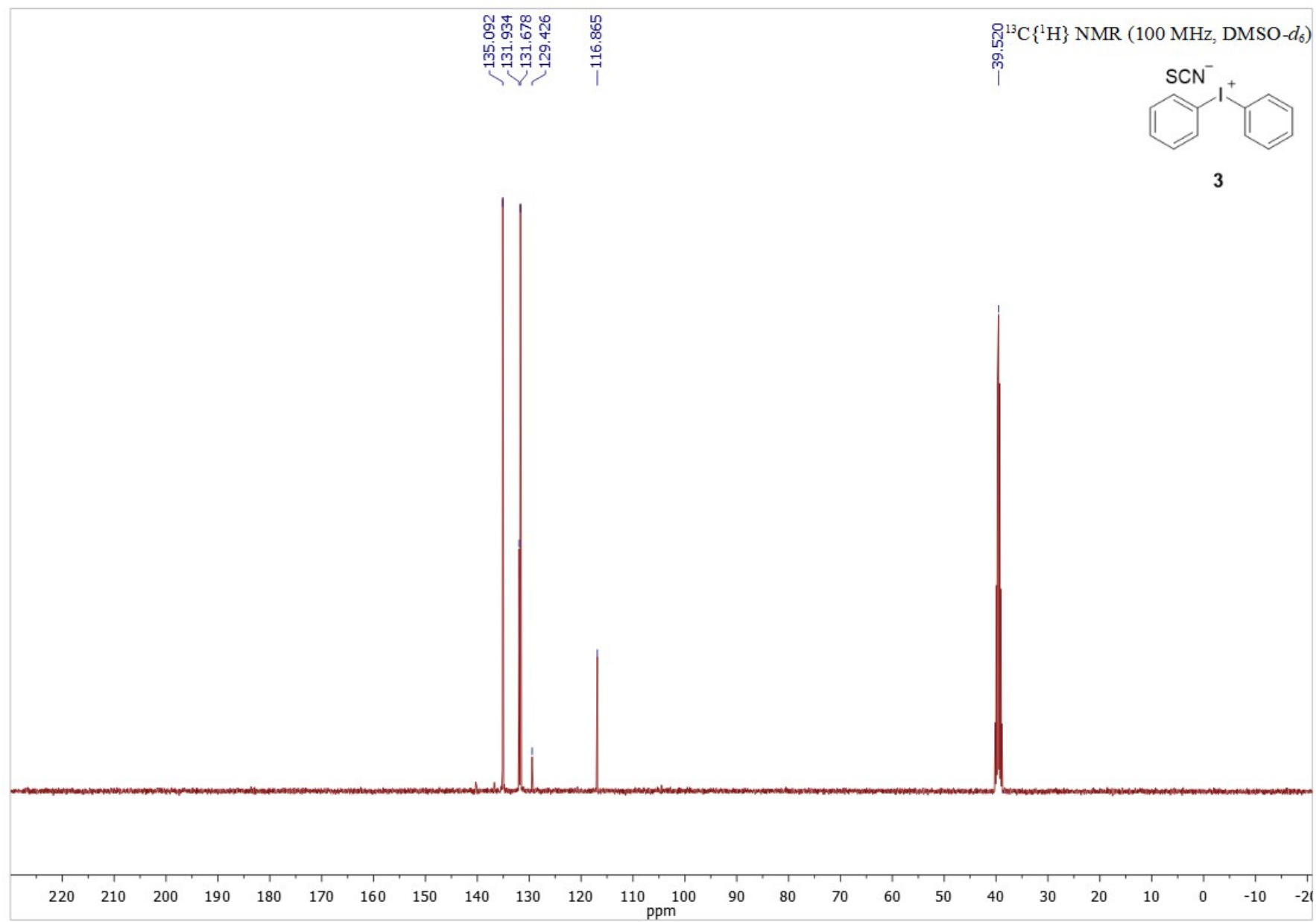


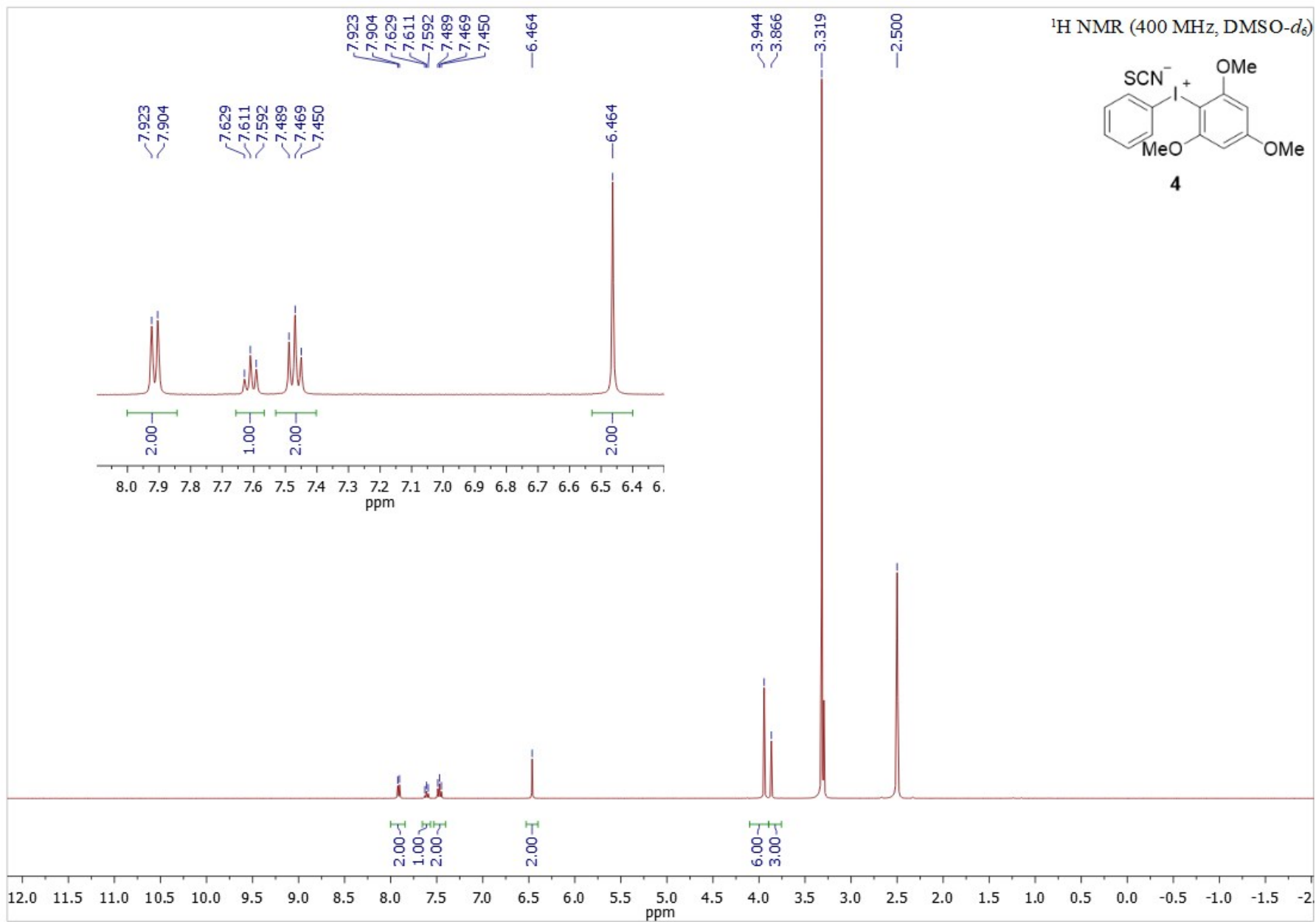
1,3,5-trimethoxy-2-isothiocyanatobenzene

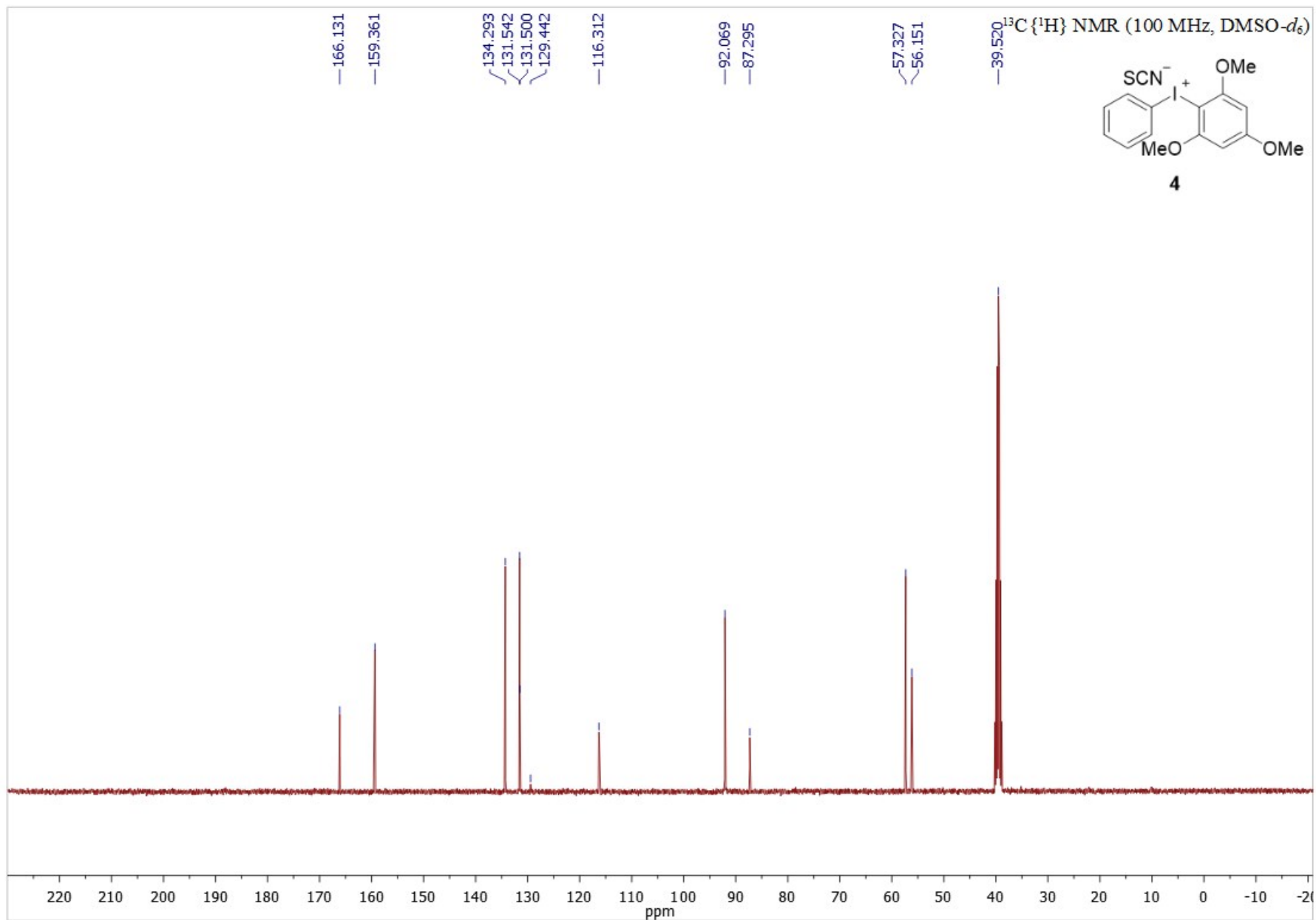


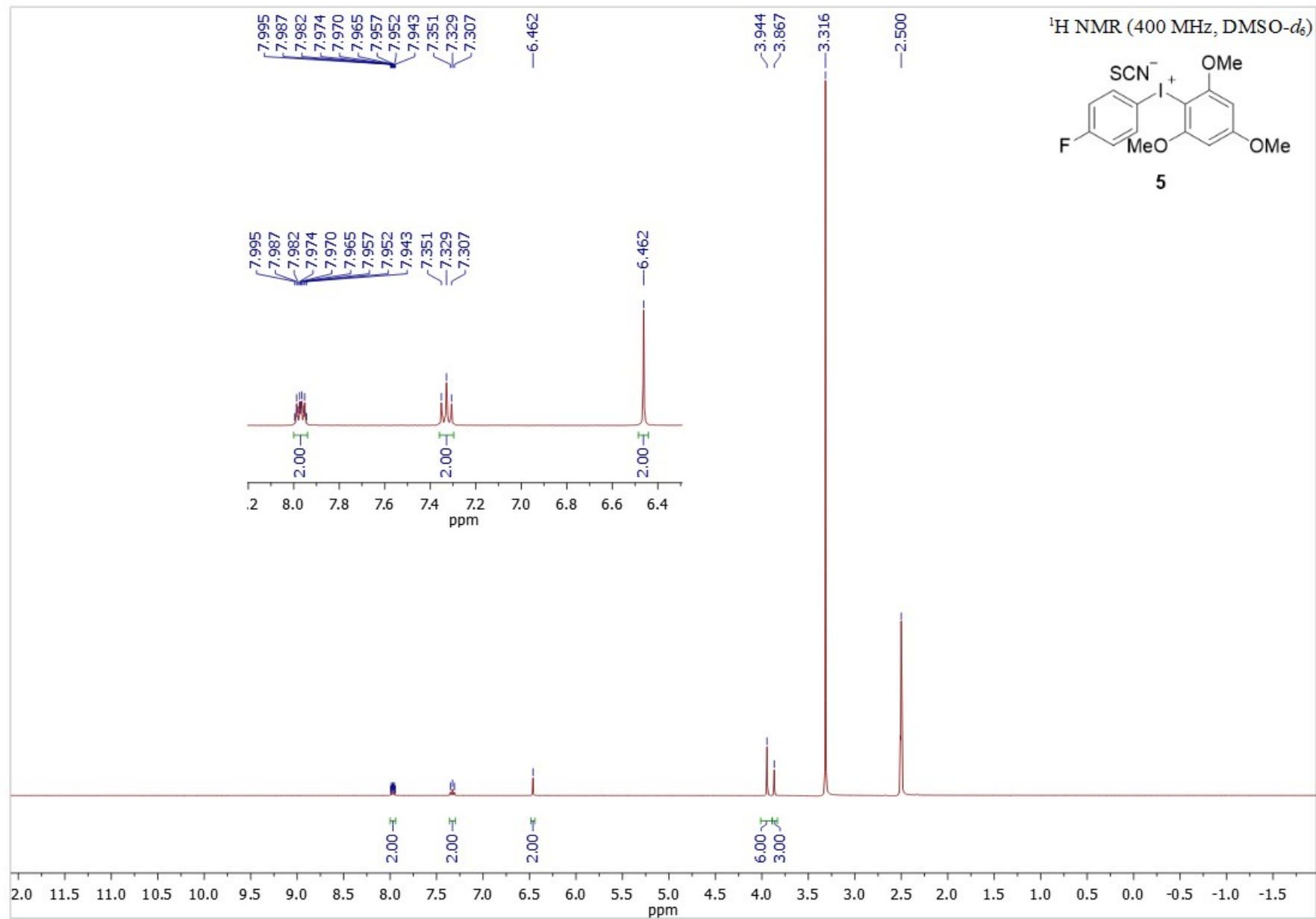
NMR spectra of products 3-9

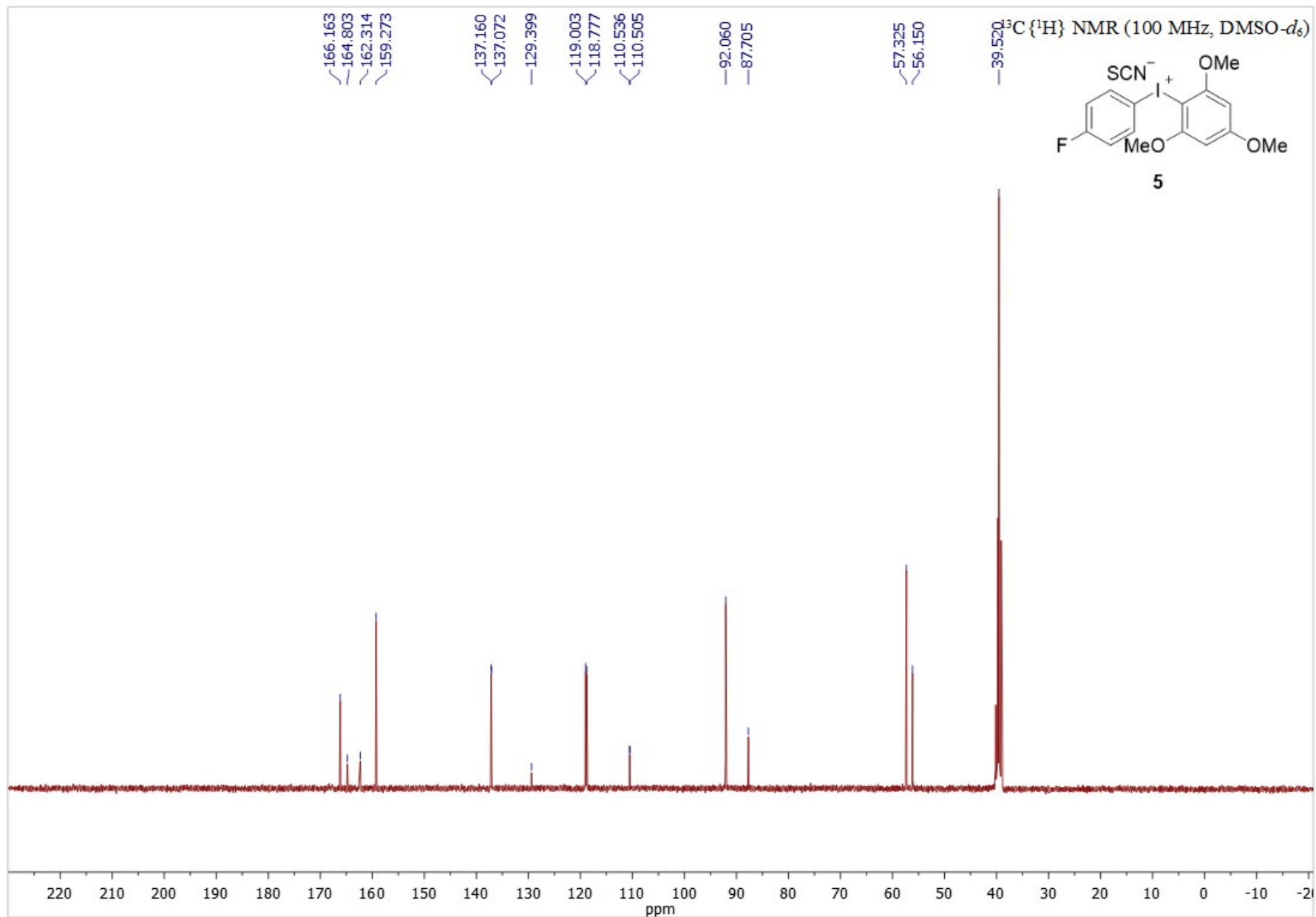


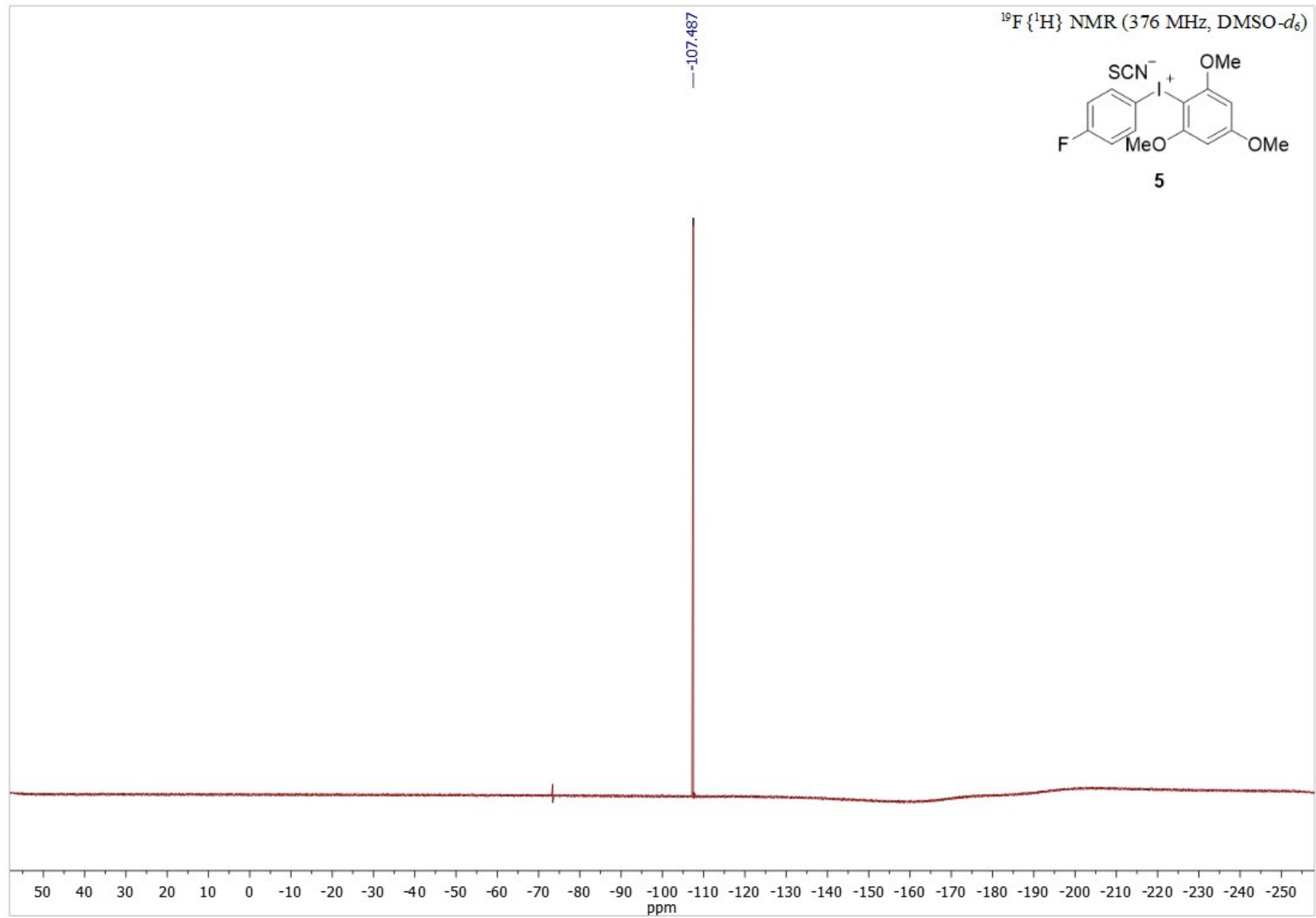


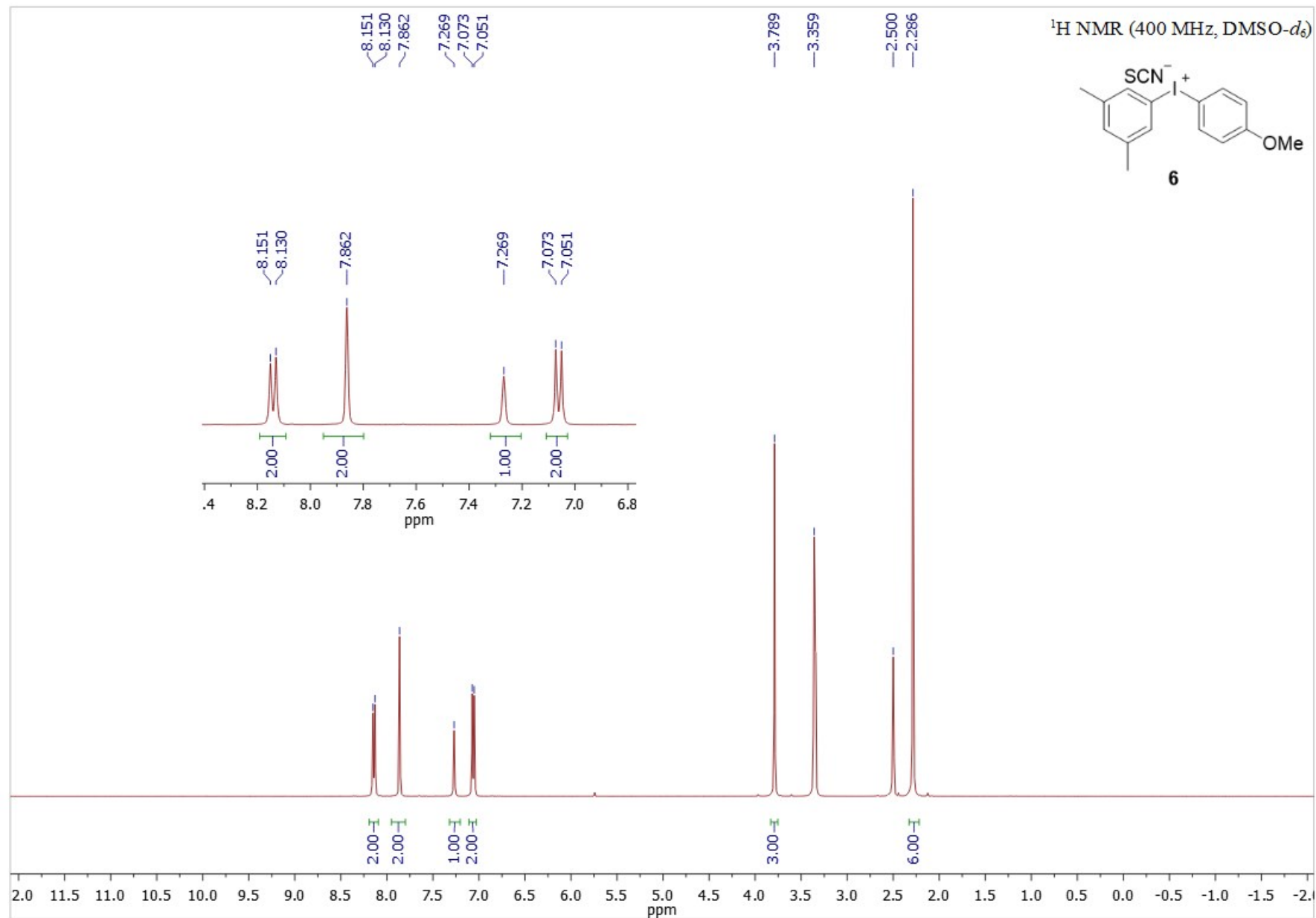


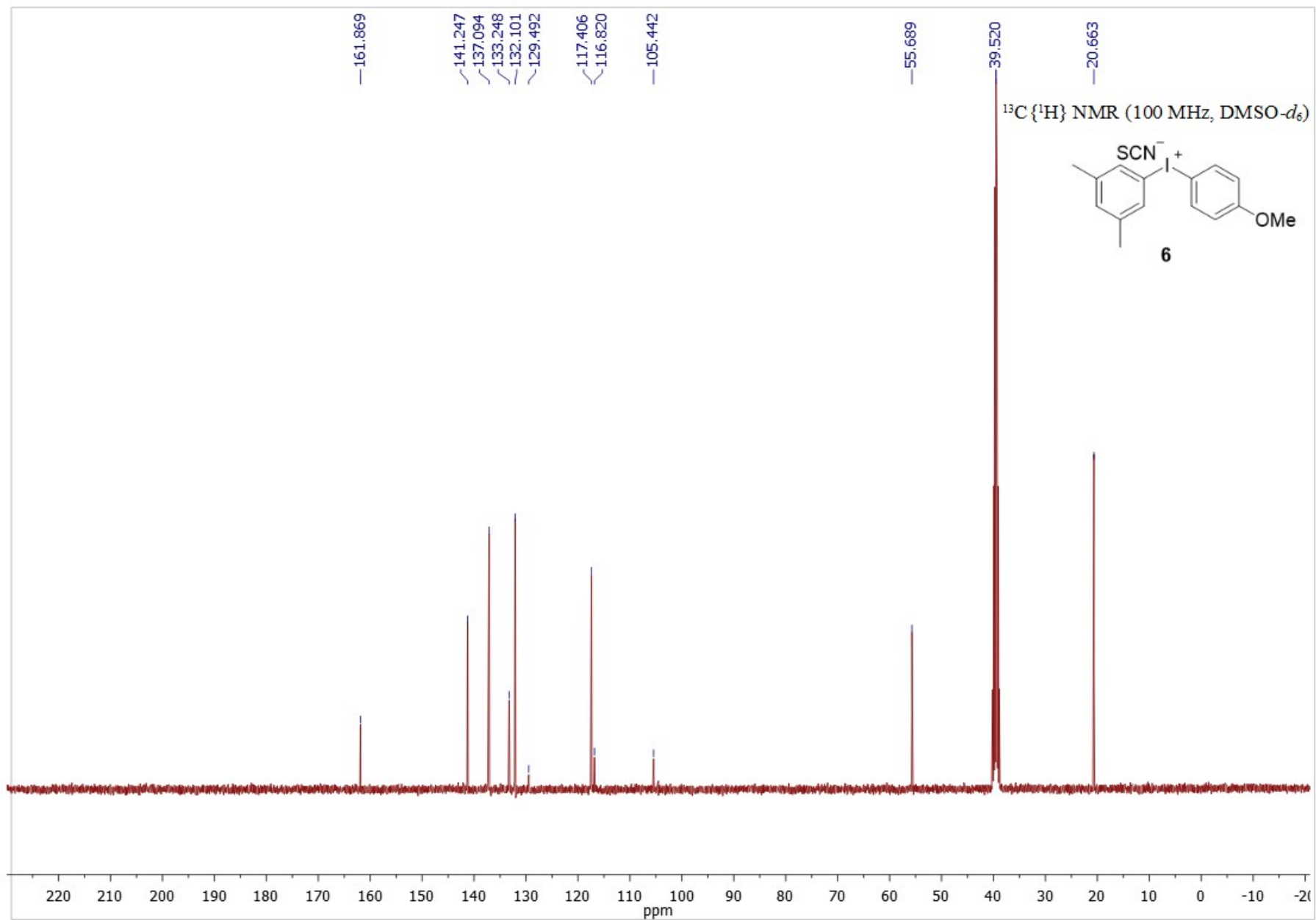


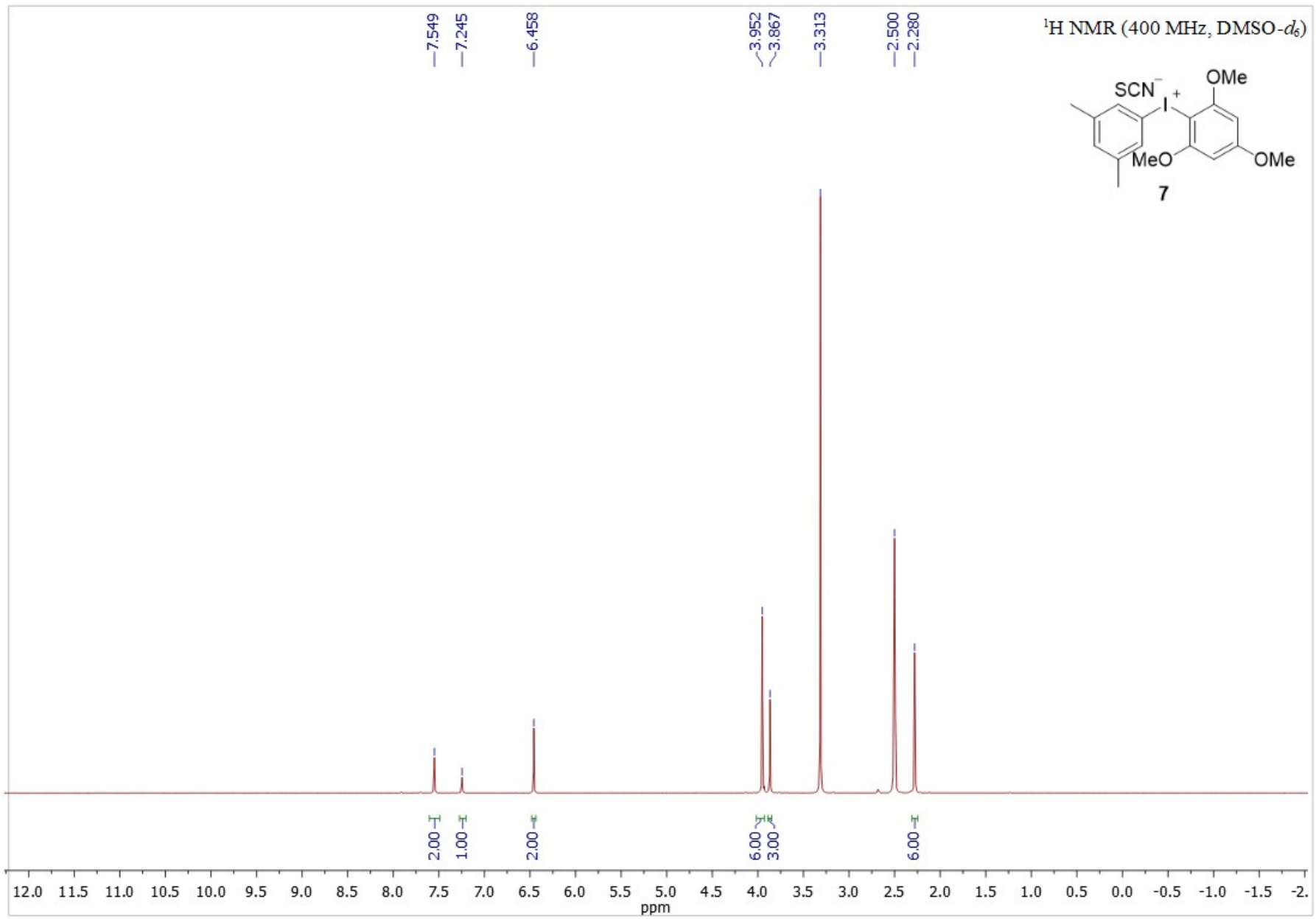


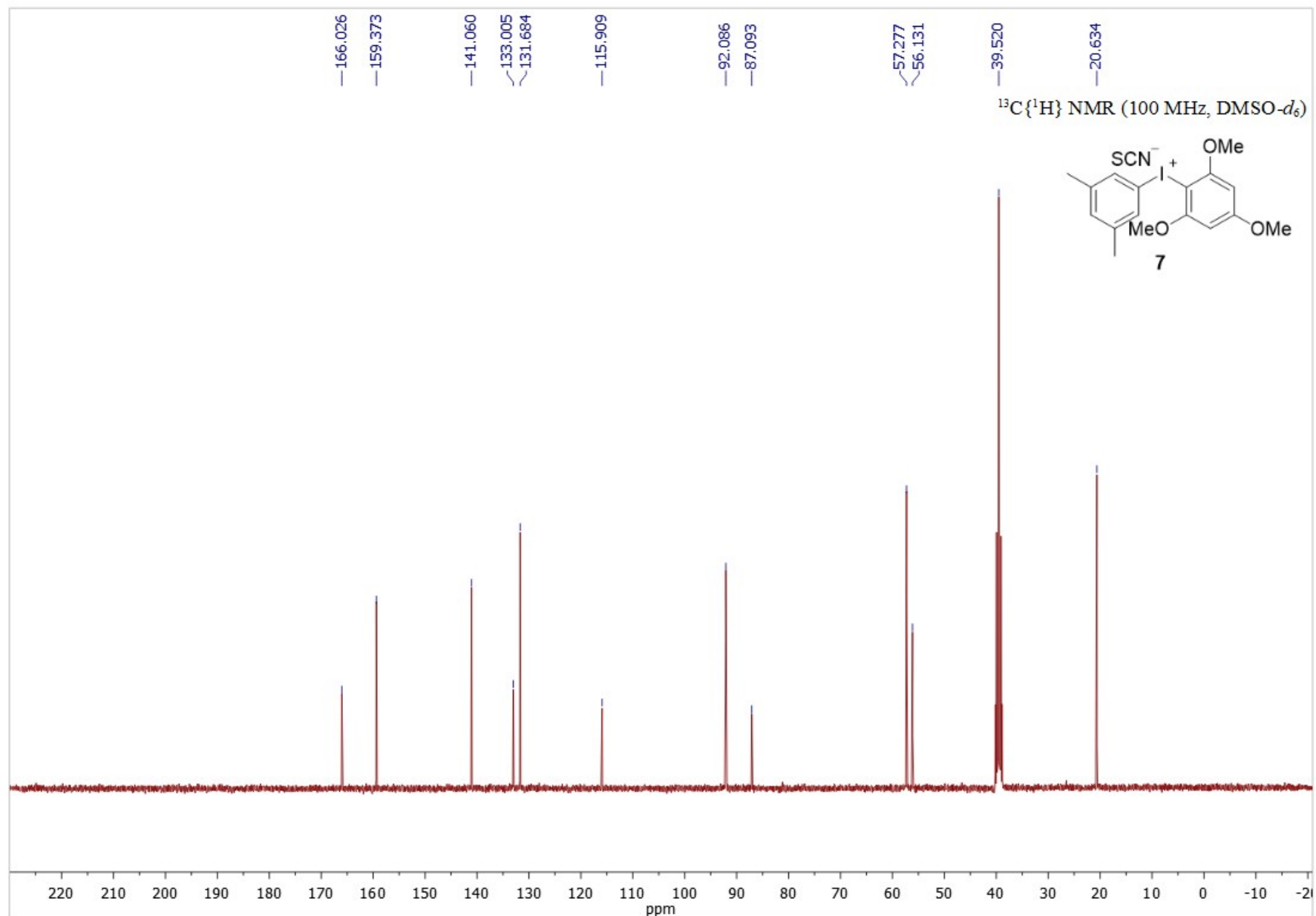


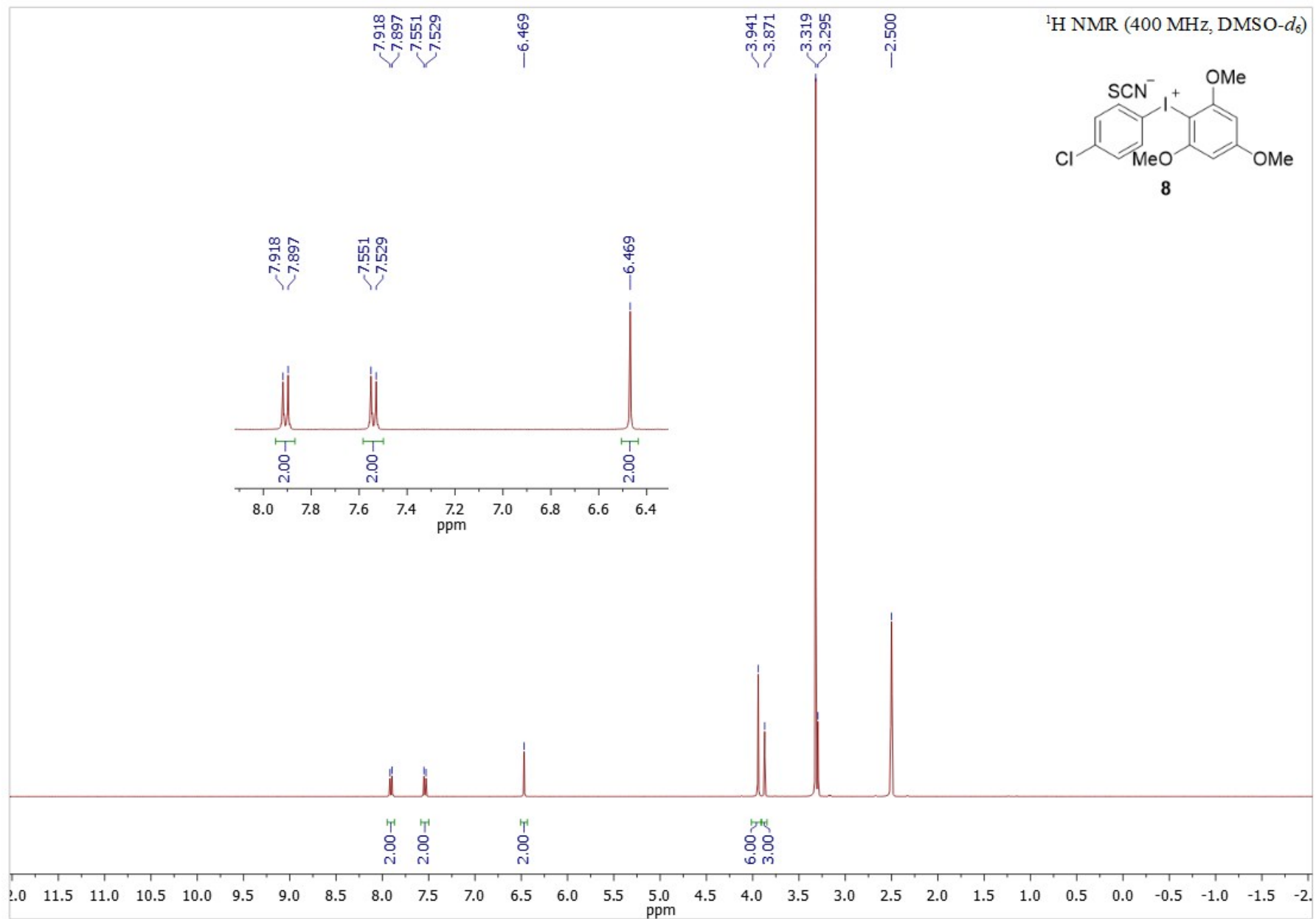


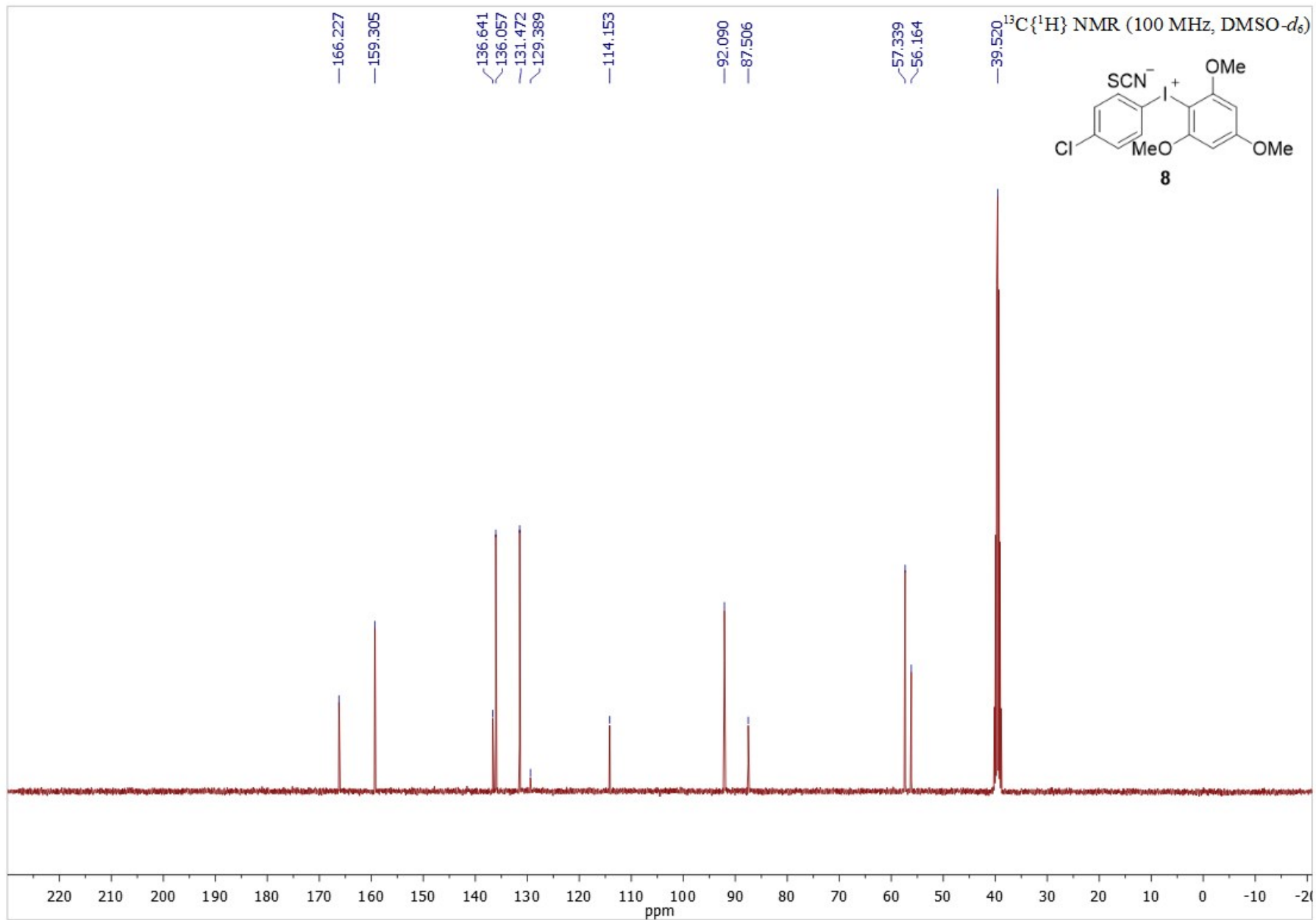




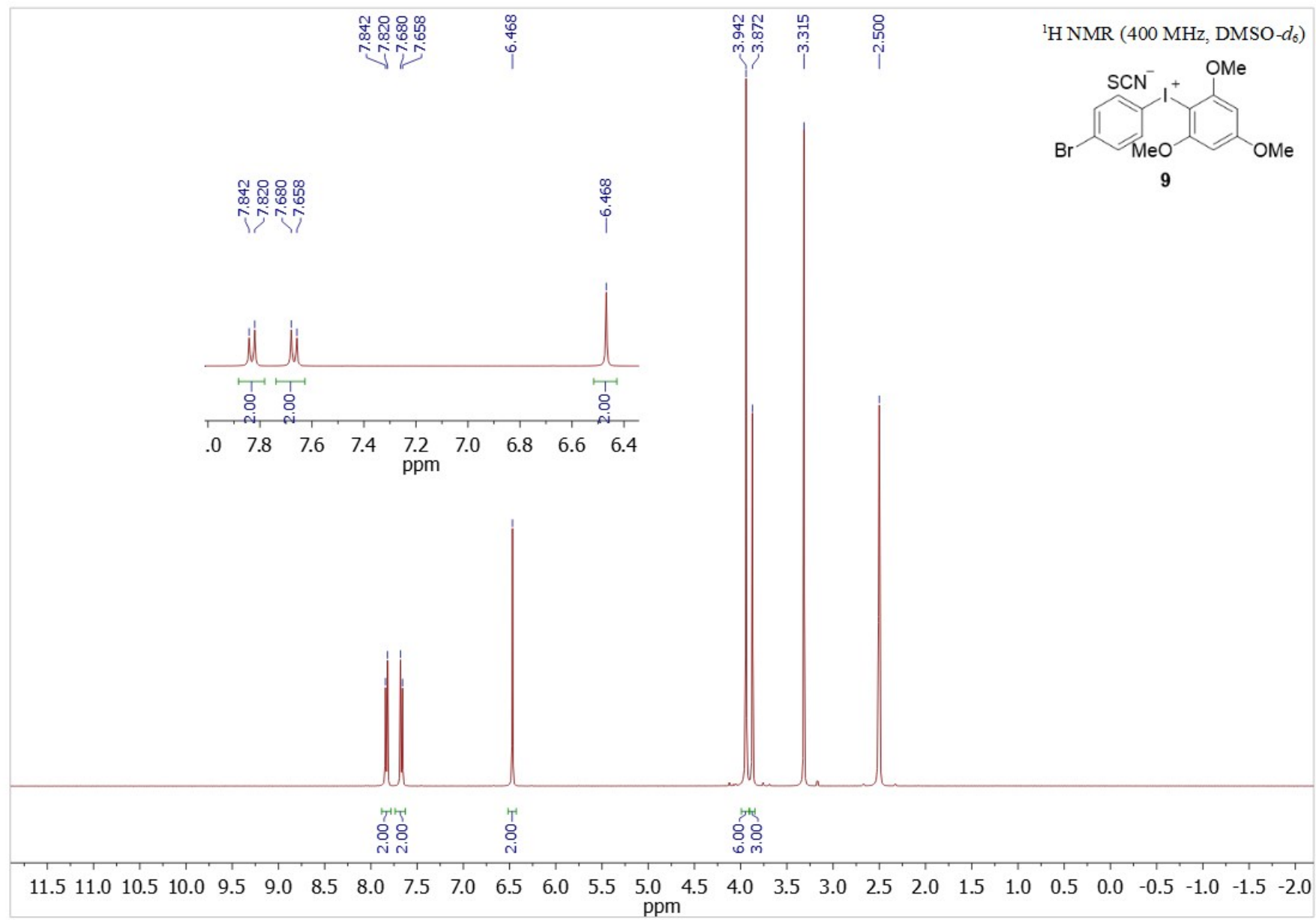


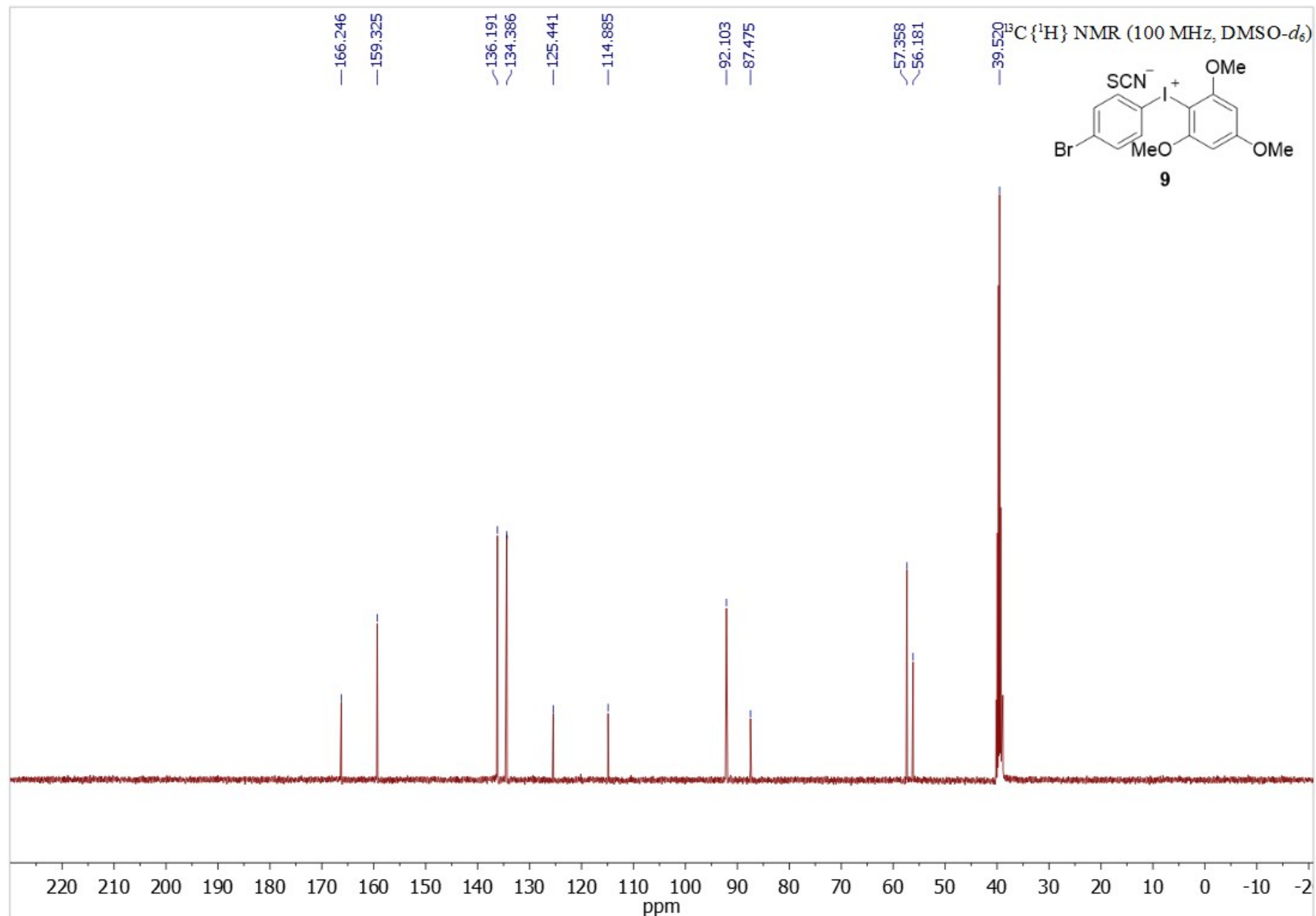






S37





Cartesian coordinates of the compounds used in the DFT study

Compound 3 (SCN N-coordinated)

I	0.12995092	-0.84995597	-0.21454707
C	2.22908085	-0.68981645	-0.07535772
C	2.85560719	-1.49037896	0.86840940
H	2.36402293	-2.07146571	1.40286438
C	4.23231373	-1.40161143	0.99548536
H	4.67816386	-1.94115654	1.60850908
C	-0.27467829	1.20512520	0.02099817
C	-0.60937033	1.64949859	1.28514619
H	-0.59666122	1.06994278	2.01245845
C	2.91966875	0.18401423	-0.88738958
H	2.47778101	0.69281730	-1.52705530
C	4.94388297	-0.51138057	0.21421513
H	5.86555007	-0.44265129	0.31571236
C	4.29338902	0.28078925	-0.72086311
H	4.78065373	0.87967229	-1.23847250
C	-0.25769987	2.04625314	-1.08400366
H	-0.02851566	1.72335532	-1.92521838
C	-0.96284647	2.97287355	1.44169243
H	-1.20796864	3.28897154	2.28180995
C	-0.59192749	3.37695641	-0.89909757
H	-0.57250860	3.96359570	-1.62110642
C	-0.95544473	3.83983386	0.35710325
H	-1.19477625	4.73021485	0.47335909
S	-5.50208653	-1.38841976	-0.06014399
N	-2.73450917	-0.95283912	0.15153165
C	-3.86834064	-1.12233012	0.06528111

Compound 3 (SCN S-coordinated)

I	0.18902575	-0.70092656	-0.03034262
C	0.50303855	1.38539783	-0.02698270
C	1.34943092	1.88832041	0.95016663
H	1.75902858	1.32213586	1.56386349
C	1.56835465	3.25575484	0.98946465
H	2.14598684	3.61586476	1.62377629
C	-1.91607206	-0.61784982	0.03466854
C	-2.52264721	-0.74684150	1.26876109
H	-2.01422702	-0.80778923	2.04517841
C	-0.12338947	2.18890088	-0.95534589
H	-0.66820272	1.82373939	-1.61348964
C	0.92840917	4.08566878	0.08894393
H	1.06466300	5.00446493	0.13070707
C	0.08399755	3.55825146	-0.87741353
H	-0.34517339	4.12550108	-1.47578418
C	-2.64199010	-0.49877017	-1.14332829
H	-2.21048397	-0.41271257	-1.96236868
C	-3.89986960	-0.78326319	1.32077414
H	-4.32833848	-0.88640957	2.14027123
C	-4.02413598	-0.51267215	-1.06491236
H	-4.53249313	-0.41851565	-1.83855769
C	-4.65464022	-0.66616141	0.16119786
H	-5.58244987	-0.69129243	0.20714302
S	3.40631982	-0.73057969	-0.12312644
N	3.21231222	-3.53339370	-0.13450290
C	3.30051758	-2.38721059	-0.12950028

Compound 4 (SCN N-coordinated)

I	0.78543024	-0.41572762	-0.78435751
O	-5.26454186	-0.64514369	0.44951404
O	-0.84765200	-2.25114848	1.01881763
O	-1.51240448	1.46165766	-1.73847142
C	1.17956782	0.99938166	0.73588459
C	-1.25227912	-0.44589026	-0.40254503
C	1.00326414	0.60906482	2.05557876
H	0.72664094	-0.25457452	2.26106706
C	-3.47029230	0.45383850	-0.72930507
H	-4.04821771	1.06337892	-1.12971025
C	-2.10257096	0.50363270	-0.97805238
C	-1.76211620	-1.41334322	0.47758806
C	-3.11683618	-1.45644157	0.74735870
H	-3.46320691	-2.09310820	1.33022578
C	1.24759588	1.53492855	3.06169311
H	1.12875820	1.29352610	3.95090331
C	-3.95576796	-0.52671321	0.13100318
C	-6.19221933	0.24593987	-0.18963169
H	-5.99182351	1.15014598	0.06082405
H	-7.08606490	0.02704418	0.08509207

H	-6.11941423	0.15298844	-1.14248550
C	1.59487492	2.27428548	0.39804165
H	1.71400285	2.51520299	-0.49256161
C	1.82815836	3.18649057	1.41744833
H	2.09570535	4.05238052	1.20945059
C	-1.29088200	-3.17725904	2.02141874
H	-0.53683575	-3.65813486	2.36884235
H	-1.91394480	-3.79625732	1.63234765
H	-1.72014521	-2.69676516	2.73271808
C	1.66612955	2.81579609	2.74478586
H	1.83950177	3.42794478	3.42245358
C	-2.36478124	2.53112653	-2.19299379
H	-1.82946884	3.21703639	-2.59836531
H	-2.84296011	2.89783388	-1.44520463
H	-2.98971288	2.19009279	-2.83667836
S	6.19288895	-1.24628377	-0.64205662
N	3.60586571	-0.17236857	-0.91299322
C	4.66796914	-0.60666655	-0.80043868

Compound 4 (SCN S-coordinated)

I	-1.34776399	0.47177243	-0.42590222
O	4.62414094	-0.49213100	0.83285703
O	0.30000511	0.96953431	2.08890553
O	0.86913301	-0.83964314	-2.18104044
C	-1.92177040	-1.48298879	0.13840264
C	0.66240193	0.12427197	-0.05519155
C	-1.79481879	-1.84346199	1.47218122
H	-1.47288436	-1.23606398	2.09831588
C	2.82988980	-0.66829749	-0.76912177
H	3.38733236	-1.03289880	-1.41887965
C	1.47824252	-0.46413928	-1.02677537
C	1.18533249	0.45327252	1.20529867
C	2.52238555	0.23372442	1.47730532
H	2.87712285	0.44740866	2.31010277
C	-2.15753658	-3.12947274	1.85139081
H	-2.07340381	-3.39079128	2.73893046
C	3.33055899	-0.31581315	0.48083170
C	5.52460688	-1.00468467	-0.16191554
H	5.24999957	-1.88765741	-0.41769906
H	6.41410685	-1.03671676	0.19879511
H	5.51241300	-0.42931423	-0.93046683
C	-2.40198073	-2.36129313	-0.81552457
H	-2.48629096	-2.09881956	-1.70400996
C	-2.75352946	-3.64343879	-0.41772402
H	-3.06643171	-4.25225619	-1.04704383
C	0.74685716	1.20609617	3.43192613
H	0.00833590	1.50342279	3.96738267
H	1.43119097	1.88019573	3.42751491
H	1.10178984	0.39317621	3.79835747
C	-2.64255006	-4.02334621	0.91225589
H	-2.89485634	-4.87898789	1.17347678
C	1.67212187	-1.59277890	-3.11103818
H	1.11579151	-1.92329919	-3.81998856
H	2.08135728	-2.33159546	-2.65387911
H	2.35408600	-1.02520042	-3.47703402
S	-0.19256144	3.43697218	-0.79993030
N	-2.71275299	4.43893917	-0.04887345
C	-1.67756885	4.03389144	-0.35494058

Compound 5 (SCN N-coordinated)

I	0.67615512	-0.98759744	0.49404655
O	-1.31814379	0.35322699	2.46759310
F	1.99844052	4.76727170	-1.32718409
O	-1.23374499	-1.52059758	-1.81845151
O	-5.40056922	0.12707491	0.06767812
C	1.19234641	0.95385211	-0.15669177
C	-1.36195895	-0.61014094	0.33013375
C	-2.05872621	0.00612712	1.37790588
C	0.82416116	1.35623167	-1.43356956
H	0.39215181	0.76668402	-2.00823886
C	-3.41759654	0.24586090	1.25502376
H	-3.89132653	0.65509444	1.94378556
C	-2.01386718	-0.97118397	-0.85300634
C	1.86424498	1.79967708	0.71412459
H	2.11768732	1.50074087	1.55795233
C	1.11173642	2.65176576	-1.83933794
H	0.87719494	2.94785702	-2.68892104
C	-3.37807735	-0.73248129	-0.98385043
H	-3.82632301	-0.96454074	-1.76441923
C	-2.01415114	1.03124454	3.53084791
H	-2.74949168	0.48989464	3.82671715

H	-2.34515703	1.87335810	3.20966694
H	-1.41234271	1.18145909	4.26244516
C	-1.85708134	-1.91487936	-3.05332335
H	-2.52520763	-2.58053380	-2.87631955
H	-1.19472113	-2.27731967	-3.64434211
H	-2.26718220	-1.14987087	-3.46326539
C	-4.06199002	-0.13708063	0.07966341
C	1.75159926	3.48465534	-0.95640106
C	2.15484875	3.09182097	0.31303644
H	2.60623923	3.67833764	0.87585984
C	-6.13024299	-0.19274036	-1.11770442
H	-6.10298782	-1.14079282	-1.26393886
H	-5.73570061	0.25867400	-1.86691640
H	-7.04163560	0.09024785	-1.01843516
S	5.99480944	-1.99456747	-0.23942754
N	3.46862226	-1.05848894	0.58549992
C	4.51125024	-1.43726283	0.23920625

Compound 5 (SCN S-coordinated)

I	-0.54783434	1.36835772	0.14725557
O	0.27552189	-0.52533300	2.47232421
F	-5.32926983	-2.46528656	-0.64324093
O	1.10854249	0.12315590	-2.08553262
O	3.40875614	-3.39080877	0.36310027
C	-2.21742814	0.11247006	-0.15989729
C	0.77551888	-0.23452106	0.19984507
C	0.99368286	-0.93926066	1.39099743
C	-2.27313344	-0.66471717	-1.30914204
H	-1.60536075	-0.60377864	-1.95319906
C	1.88263386	-2.00156333	1.41049142
H	2.03555802	-2.47785469	2.19537725
C	1.42780645	-0.59964789	-0.98183178
C	-3.21258846	0.06675461	0.80589499
H	-3.16270909	0.61157312	1.55844131
C	-3.34145283	-1.53332623	-1.48225501
H	-3.40450579	-2.06515230	-2.24229220
C	2.32099804	-1.66606074	-0.96995973
H	2.76147095	-1.92303526	-1.74714125
C	0.45508824	-1.27305281	3.69023876
H	1.38473279	-1.27496342	3.92915586
H	0.15656253	-2.17590872	3.55753243
H	-0.05542542	-0.86681034	4.39331430
C	1.75633589	-0.20874779	-3.32614474
H	2.70475598	-0.09731844	-3.23179562
H	1.43477800	0.37014361	-4.01959444
H	1.56167383	-1.12049353	-3.55483570
C	2.54348948	-2.34401134	0.23178097
C	-4.30289768	-1.58727209	-0.50479880
C	-4.28078834	-0.79650544	0.63651617
H	-4.96239513	-0.84516320	1.26704765
C	4.09484245	-3.83648965	-0.80757969
H	4.66351974	-3.13465836	-1.13157011
H	3.45476427	-4.06837515	-1.48380914
H	4.62594394	-4.60633698	-0.59347813
S	2.14374010	2.99046147	0.49260410
N	0.73078203	5.13403731	-0.66800015
C	1.31912687	4.25611722	-0.18471063

Compound 6 (SCN N-coordinated)

I	0.42676010	-1.42341509	-0.03851391
O	-5.61491172	-0.17858698	0.42759110
C	-1.65771473	-1.21203447	-0.00504374
C	0.71926786	0.66964561	0.04150943
C	-3.66368920	-0.39967583	-1.01754280
H	-4.12114428	-0.07240910	-1.75763406
C	-4.32538843	-0.55889073	0.19923337
C	-3.66547220	-1.10767394	1.29215555
H	-4.12538353	-1.25736514	2.08652218
C	-2.32276581	-0.72937699	-1.11686647
H	-1.87316896	-0.62723270	-1.92463289
C	-2.32284521	-1.42998419	1.19641129
H	-1.87154824	-1.78862438	1.92736120
C	0.95712073	1.24736877	1.27159390
H	1.00752167	0.72512777	2.04111922
C	-6.26218889	0.57192147	-0.60058998
H	-5.73307081	1.34300177	-0.81595355
H	-7.12820731	0.85274803	-0.29590039
H	-6.36044108	0.02361428	-1.38335586
C	0.61202837	1.39347226	-1.13029248
H	0.45653873	0.96602802	-1.94142550
C	0.74241873	2.78219911	-1.06776561

C	1.12089008	2.63594391	1.33612576
C	1.00291860	3.37610641	0.16954154
H	1.10102937	4.30026918	0.21199909
C	1.42195239	3.29534680	2.65643707
H	1.23795206	2.68038528	3.37044648
H	0.87192146	4.07603982	2.75678376
H	2.34712145	3.54978366	2.68358635
C	0.58804918	3.61982776	-2.31305444
H	0.53699565	3.04560842	-3.08071543
H	1.34352470	4.20481203	-2.40135340
H	-0.21536479	4.14137708	-2.25017698
S	6.08139162	-1.19642539	-0.37296640
N	3.30936652	-1.16185742	0.07705601
C	4.44856872	-1.15713931	-0.10820100

Compound 6 (SCN S-coordinated)

I	-0.82617667	-1.13539780	-0.05504455
O	-0.09297163	4.97456204	0.57697608
C	-0.79342598	0.95760942	0.04027340
C	1.28554384	-1.24833713	-0.02768016
C	-0.17976696	3.05559515	-0.92455453
H	0.08973760	3.56151167	-1.65634652
C	-0.36663167	3.66441794	0.31566960
C	-0.83119515	2.92721589	1.39818761
H	-1.00114894	3.34853988	2.20969610
C	-0.39560822	1.69477967	-1.05960024
H	-0.27421001	1.28002175	-1.88318735
C	-1.03944517	1.56523518	1.26651167
H	-1.34094026	1.06301507	1.99001371
C	1.91008138	-1.47206626	1.18200739
H	1.41218770	-1.59034711	1.96018260
C	0.57511461	5.71466232	-0.44542276
H	1.38345030	5.26077621	-0.69340062
H	0.78775411	6.59220245	-0.11924027
H	0.00228023	5.78854795	-1.21315866
C	1.96996535	-1.04402762	-1.21020706
H	1.51195070	-0.90185980	-2.00697131
C	3.36583708	-1.05582423	-1.18060176
C	3.30870839	-1.51717524	1.21255859
C	4.00860363	-1.30092394	0.03524871
H	4.93851235	-1.32009144	0.05543680
C	4.02212475	-1.79949250	2.50870931
H	3.41049953	-1.69070015	3.24077627
H	4.75495587	-1.18734822	2.61031146
H	4.35544945	-2.69963184	2.50117259
C	4.15785769	-0.79255905	-2.43741947
H	3.56360969	-0.76836352	-3.19102520
H	4.80319109	-1.49172208	-2.56176750
H	4.60998667	0.05065084	-2.35984532
S	-4.01300379	-0.75973594	0.03548627
N	-3.82056765	-3.50962128	-0.50154140
C	-3.91844611	-2.38119136	-0.28002779

Compound 7 (SCN N-coordinated)

I	-0.53703768	-0.98832651	0.61731895
O	1.65879600	-0.10530233	2.62672571
O	5.48689586	0.22591393	-0.14245208
O	1.15745441	-0.89222122	-1.96130802
C	1.46611248	-0.48504093	0.32432732
C	3.62331821	0.07930686	1.22330964
H	4.16688666	0.30889899	1.94201134
C	2.01294777	-0.56784434	-0.96309436
C	3.36749145	-0.33258114	-1.16790270
H	3.73732878	-0.38526227	-2.01953933
C	2.28598757	-0.16839655	1.42037379
C	-1.34462390	0.93171993	0.09056162
C	-2.22948757	1.50123059	0.97134442
H	-2.45644958	1.07008118	1.76318689
C	4.15954886	-0.01539668	-0.06004159
C	2.47068468	0.23790723	3.75765683
H	3.16847611	-0.41266549	3.86103017
H	1.92810259	0.25356916	4.54882161
H	2.86020885	1.10474791	3.61959866
C	-1.53487251	2.74344158	-1.44219332
C	-2.78177328	2.74585898	0.65305071
C	-2.41854312	3.34403817	-0.55355417
H	-2.77985654	4.17405853	-0.77025749
C	1.66694065	-0.94088059	-3.30899682
H	2.37048335	-1.59231085	-3.36237142
H	2.01069833	-0.07831007	-3.55215687
H	0.95934083	-1.18443465	-3.90991320

C	-0.98476740	1.50599369	-1.11132002
H	-0.39028303	1.07968452	-1.68563250
C	6.12158692	0.12280816	-1.42230287
H	5.94593066	-0.74426199	-1.79728893
H	7.06849119	0.24168821	-1.32089447
H	5.77449173	0.79970463	-2.00716599
C	-1.20857284	3.39525869	-2.76240124
H	-1.90740482	3.20805420	-3.39264921
H	-0.37751282	3.04887203	-3.09301441
H	-1.13439245	4.34486957	-2.63997403
C	-3.71366465	3.43578660	1.60987100
H	-4.21479197	2.77927982	2.09876302
H	-4.31709532	3.99921961	1.11957401
H	-3.20418858	3.97142627	2.22313230
S	-4.82622885	-2.96558260	-1.11275469
N	-3.22821329	-1.68464585	0.81162798
C	-3.85056035	-2.23169102	0.00727674

Compound 7 (SCN S-coordinated)

I	0.51558023	1.26197527	-0.01918508
O	-0.93040717	0.26811698	2.54216202
O	-4.05375750	-2.83591931	0.79801757
O	-0.89013138	-0.57564405	-2.06295290
C	-0.95321948	-0.19523189	0.24713390
C	-2.52585762	-1.32993004	1.66821221
H	-2.87862078	-1.50231167	2.51115590
C	-1.46386906	-0.86692886	-0.87152603
C	-2.51046629	-1.77086158	-0.73144151
H	-2.85417785	-2.22069210	-1.46924553
C	-1.50039283	-0.42707305	1.52017266
C	2.18790900	-0.08674261	-0.04206968
C	3.23778912	0.20428854	0.79229060
H	3.21266043	0.95088953	1.34579903
C	-3.03343009	-1.98559587	0.54750931
C	-1.45726526	0.03182075	3.85461997
H	-2.38905184	0.26051935	3.87235436
H	-0.98348749	0.57027710	4.49194385
H	-1.35190449	-0.89606013	4.07853527
C	3.27538060	-2.01522587	-0.91741267
C	4.34658754	-0.64776470	0.79354628
C	4.34001804	-1.74666516	-0.06553721
H	5.07343897	-2.31984173	-0.06750496
C	-1.35115085	-1.27943064	-3.23357433
H	-2.28803716	-1.11115603	-3.36050046
H	-1.20835193	-2.22144014	-3.11716707
H	-0.86443560	-0.97455221	-4.00251775
C	2.17208639	-1.16319290	-0.90509398
H	1.44450006	-1.31732191	-1.46352783
C	-4.65040192	-3.53006725	-0.30364284
H	-4.93911805	-2.89412658	-0.96356917
H	-5.40565217	-4.03444047	0.00659671
H	-4.00637128	-4.12478172	-0.69385820
C	3.32808684	-3.18185590	-1.87160470
H	3.83594467	-2.93706109	-2.64799384
H	2.43692991	-3.42077217	-2.13372660
H	3.74661192	-3.92989881	-1.43856828
C	5.49802954	-0.40239623	1.72837372
H	5.59503667	0.54085520	1.87673653
H	6.30497706	-0.75018349	1.34126110
H	5.33036899	-0.84245010	2.56551629
S	-1.71376400	3.53748216	0.10505728
N	-0.98499157	4.59865648	-2.39303694
C	-1.24441346	4.16737345	-1.35368598

Compound 8 (SCN N-coordinated, A)

I	-0.31026437	-1.54645596	-0.75367538
Cl	-6.02129535	1.30674320	0.86882664
O	0.90669624	-0.92306589	1.95628421
O	0.65489551	0.94087084	-2.31531763
O	2.95853716	3.29313470	1.24253622
C	0.79712149	0.09317686	-0.14297611
C	1.11236873	1.10841591	-1.04874921
C	-2.18128459	-0.66363232	-0.29919465
C	1.24480920	0.14043640	1.19051237
C	-2.47816541	0.58870404	-0.81715900
H	-1.88994157	1.01317140	-1.39996208
C	1.85002123	2.20942160	-0.62394617
H	2.06955478	2.89419231	-1.21275262
C	-3.67233171	1.19500174	-0.44664798

H	-3.89660217	2.03544507	-0.77755078
C	2.25214368	2.25545248	0.71331565
C	-3.02707056	-1.32746765	0.57180623
H	-2.80136270	-2.16554226	0.90576893
C	-4.52331548	0.53336534	0.41971311
C	1.96719986	1.23166589	1.61850326
H	2.26245424	1.28516858	2.49846121
C	-4.22099859	-0.71611360	0.93729762
H	-4.80792324	-1.13992822	1.52035770
C	1.42906801	-0.96182196	3.29520947
H	1.16549049	-1.78218840	3.71778777
H	1.08286518	-0.21892246	3.79487536
H	2.38659496	-0.90985439	3.26642740
C	1.04734763	1.91104234	-3.30306129
H	0.68722492	1.66196919	-4.15744508
H	2.00516949	1.94326354	-3.35664485
H	0.71198522	2.77523367	-3.05439311
C	3.38305436	4.32974723	0.35227571
H	3.90416457	3.94763722	-0.35851554
H	3.91649806	4.96587350	0.83357777
H	2.61358381	4.77055654	-0.01519172
S	4.26185519	-1.62224531	0.64808059
N	2.33166845	-2.79711446	-1.00826553
C	3.14067922	-2.30745013	-0.31848421

Compound 8 (SCN N-coordinated B)

I	-0.38715975	-1.34978220	0.17519105
Cl	-2.82826864	4.76252668	-0.08900647
O	1.47932713	-0.63236073	2.45883341
O	1.52193672	-0.84540816	-2.20346658
O	5.43079735	0.70984258	0.20490171
C	1.57061995	-0.67721347	0.12617318
C	2.23416889	-0.52600034	-1.09339782
C	-1.23320877	0.58746615	0.04133727
C	2.21758071	-0.40833543	1.34682697
C	-0.82871527	1.42914499	-0.98469070
H	-0.23634037	1.13133461	-1.63756144
C	3.54713991	-0.06502123	-1.11358944
H	4.00455920	0.04122278	-1.91563603
C	-1.32709080	2.72589275	-1.01592450
H	-1.07179555	3.31266695	-1.69169019
C	4.15857526	0.23266414	0.10691076
C	-2.10994696	0.99175296	1.03257695
H	-2.36210034	0.40688953	1.71021816
C	-2.20752273	3.13311462	-0.03026350
C	3.51350130	0.05662172	1.33230262
H	3.95349489	0.24943755	2.12828715
C	-2.60615992	2.28988212	0.99469221
H	-3.19708274	2.58743446	1.64763268
C	2.13478514	-0.46649576	3.72767491
H	1.52916192	-0.70234203	4.43382198
H	2.40513211	0.44880712	3.83041356
H	2.90701307	-1.03450860	3.76525597
C	2.20250433	-0.80439357	-3.47076075
H	1.60135013	-1.08112323	-4.16626905
H	2.95826560	-1.39566020	-3.44708041
H	2.50232477	0.09058433	-3.64469389
C	6.19540741	0.81404846	-1.00002848
H	6.23233446	-0.04376844	-1.43081226
H	7.08539168	1.10485613	-0.78972042
H	5.78137474	1.45048564	-1.58735694
S	-5.66654735	-2.35679677	-0.71995870
N	-3.13004029	-2.10889927	0.44393306
C	-4.19072167	-2.20918806	-0.04103388

Compound 9 (SCN N-coordinated, A)

I	-0.33184079	-1.66505983	0.74661831
Br	5.81256736	0.80533240	-0.52959001
O	-1.32852896	-0.82057725	-1.99980584
O	-3.07665492	3.51779348	-1.17940127
O	-1.14435206	0.83412413	2.36359600
C	-1.25413428	0.08892094	0.15148962
C	-1.52787026	1.08954668	1.09398679
C	3.26675376	0.76140513	0.73193658
H	3.54372847	1.56206755	1.11481969
C	-1.62116726	0.22974836	-1.18850002
C	4.10228601	0.06662793	-0.13724848
C	-1.79919094	-0.75143442	-3.35806054
H	-1.60705391	-1.57849744	-3.80582092
H	-1.35792866	-0.03042428	-3.81332192
H	-2.74768421	-0.59973092	-3.36000799

C	-2.15923898	2.27599139	0.67563939
H	-2.35311788	2.95467674	1.28107190
C	-2.48243282	2.40110220	-0.65994923
C	-1.52449982	1.80051395	3.37958231
H	-1.22082721	1.49796914	4.23903808
H	-2.48020021	1.89155574	3.39224667
H	-1.12490978	2.65010370	3.17973029
C	3.71491225	-1.11181449	-0.73828031
H	4.29040187	-1.55238624	-1.32204485
C	-2.22893888	1.39953431	-1.60782345
H	-2.46448602	1.51916493	-2.50038591
C	2.44835298	-1.63659181	-0.46355390
H	2.16116517	-2.42790993	-0.85887875
C	1.63257009	-0.94006543	0.41918416
C	-3.50326886	4.53574976	-0.24926185
H	-4.02371113	4.13219307	0.44888106
H	-4.03579829	5.18751960	-0.70976020
H	-2.73318693	4.96337470	0.13252500
C	2.01892387	0.24184969	1.01512481
H	1.44688682	0.68315499	1.60093916
S	-4.79728391	-1.28110579	-0.90443909
N	-3.09521172	-2.67183446	0.83587493
C	-3.80410043	-2.09133142	0.11750722

Compound 9 (SCN N-coordinated B)

I	0.24765194	-1.70303755	0.21404771
Br	-3.68679060	3.76682455	-0.07932486
O	1.88866823	-0.49887826	2.47379321
O	5.39543297	1.70308195	0.14904785
O	1.94560954	-0.77179877	-2.18812759
C	1.97642288	-0.56854756	0.13964689
C	2.57195352	-0.28195109	-1.09635064
C	-1.67945019	1.98656207	-1.01516446
H	-1.58127767	2.60366120	-1.70358701
C	2.54234173	-0.13316852	1.33977137
C	-2.62146052	2.19038954	-0.01147973
C	2.51172060	-0.16407149	3.72713650
H	2.00432527	-0.54359475	4.44821300
H	2.54223136	0.79062411	3.82438029
H	3.40482489	-0.51724542	3.74416961
C	3.74995103	0.48770403	-1.13163402
H	4.16552763	0.69083248	-1.93834728
C	4.26978122	0.93098248	0.06719239
C	2.60650811	-0.59275787	-3.46945785
H	2.08148578	-1.00353022	-4.16085662
H	3.47439896	-1.00237258	-3.44128870
H	2.70106239	0.34458816	-3.65346244
C	-2.77842385	1.30644335	1.03447719
H	-3.41081464	1.47079300	1.69715652
C	3.69199887	0.63561296	1.31008713
H	4.07378745	0.95020618	2.09858587
C	-1.97653427	0.16237942	1.09041511
H	-2.05967090	-0.44779751	1.78734794
C	-1.05255616	-0.03539216	0.07206937
C	6.13307721	1.93176869	-1.07036887
H	6.29244450	1.09310421	-1.50896394
H	6.97165032	2.34962881	-0.86387858
H	5.62431642	2.50385506	-1.64961851
C	-0.89233905	0.85268574	-0.97051683
H	-0.26284979	0.68984959	-1.63563550
S	-4.59516768	-4.02388591	-0.74497996
N	-2.21508884	-3.12657176	0.43397532
C	-3.20610853	-3.49889523	-0.05052831

Tetramers (Figure 7, left)

I	-1.7610133	-1.7477485	-1.1921710
C	-3.6970138	-1.8657695	-2.0334916
C	-4.6955258	-1.0322825	-1.5573385
H	-4.4816220	-0.3014010	-0.7877612
C	-5.9665276	-1.1293024	-2.1071176
H	-6.7551404	-0.4808628	-1.7437292
C	-1.8773228	-3.8040391	-0.6352925
C	-3.0221523	-4.2709658	-0.0114621
H	-3.8566589	-3.6093719	0.1885852
C	-3.9367171	-2.7836220	-3.0440068
H	-3.1452210	-3.4307116	-3.4029187
C	-6.2249070	-2.0468452	-3.1148940
H	-7.2191127	-2.1171126	-3.5405937
C	-5.2117546	-2.8717142	-3.5830845
H	-5.4094000	-3.5848193	-4.3748926

C	-0.8010190	-4.6318816	-0.9018545
H	0.0968662	-4.2370848	-1.3588750
C	-3.0910453	-5.6099071	0.3456328
H	-3.9810960	-5.9863822	0.8364525
C	-0.8839968	-5.9689917	-0.5371686
H	-0.0470999	-6.6277087	-0.7380150
C	-2.0247073	-6.4578199	0.0822344
H	-2.0818226	-7.5024047	0.3652910
S	2.1686577	-1.2023035	2.1267284
N	0.6549386	-2.0219208	-0.0894512
C	1.2783766	-1.6840957	0.8402605
S	-2.0532868	1.1910576	-2.0450019
N	-0.6887988	1.9583858	0.2840671
C	-1.2501465	1.6442832	-0.6929653
I	1.7793968	1.7235419	1.2724174
C	3.7569950	1.8780622	2.0061396
C	4.7400122	1.0557264	1.4809268
H	4.4948996	0.3171007	0.7281756
C	6.0376299	1.1745673	1.9595652
H	6.8145228	0.5349756	1.5573080
C	1.8285571	3.7794001	0.7063093
C	2.9192315	4.2616668	0.0024383
H	3.7471436	3.6116439	-0.2553152
C	4.0381195	2.8063213	2.9961120
H	3.2580849	3.4445876	3.3938682
C	6.3372021	2.1023848	2.9462638
H	7.3519976	2.1895012	3.3166402
C	5.3393026	2.9160342	3.4640716
H	5.5695105	3.6372616	4.2395611
C	0.7612924	4.5917442	1.0467515
H	-0.0960131	4.1849064	1.5668903
C	2.9422917	5.6004591	-0.3611165
H	3.7893308	5.9889005	-0.9147155
C	0.7978105	5.9288319	0.6749521
H	-0.0326679	6.5755744	0.9331883
C	1.8843396	6.4328549	-0.0245436
H	1.9052794	7.4772953	-0.3130550
tetramer Figure 7, right			
I	1.4601579	0.2467561	1.2894465
C	1.9073391	-0.5899257	3.1759885
C	3.1323783	-1.2089313	3.3693434
C	4.6856043	2.9730395	2.3082102
H	4.9360143	3.6074727	3.1504441
C	0.9485343	-0.5242340	4.1721381
C	5.5104525	2.9329453	1.1915494
C	3.4046612	-1.7683998	4.6079129
H	4.3592545	-2.2530760	4.7763509
C	2.4559658	-1.7178195	5.6208274
C	5.1856082	2.1257323	0.1125996
H	5.8180399	2.1000618	-0.7666938
C	1.2331501	-1.1029770	5.4021283
H	0.4850175	-1.0708034	6.1851862
C	4.0393365	1.3420823	0.1422703
H	3.7857042	0.7231137	-0.7094916
C	3.2295611	1.4010995	1.2632878
C	3.5287532	2.2103773	2.3483757
H	2.8796756	2.2422672	3.2152883
S	2.6284762	1.2856333	-3.3482773
N	0.8218512	1.2687611	-1.2163998
C	1.5851412	1.2852333	-2.1209629
S	-2.7201813	-1.0035942	3.3885931
N	-0.8918697	-1.2213123	1.2857699
C	-1.6652390	-1.1377043	2.1782615
I	-1.5044257	-0.2246514	-1.2440832
C	-1.8997693	0.5819865	-3.1531492
C	-3.1030673	1.2313100	-3.3808991
C	-4.6884269	-2.9716673	-2.3420174
H	-4.9216924	-3.5959132	-3.1967182
C	-0.9277412	0.4655837	-4.1315406
C	-5.5260897	-2.9584107	-1.2345063
C	-3.3391326	1.7680785	-4.6367590
H	-4.2761112	2.2762490	-4.8325472
C	-2.3763716	1.6657773	-5.6325240
C	-5.2231520	-2.1632151	-0.1403033
H	-5.8673804	-2.1561928	0.7307990
C	-1.1751568	1.0224600	-5.3793784
H	-0.4145929	0.9530283	-6.1478216
C	-4.0857989	-1.3660908	-0.1444200
H	-3.8510857	-0.7551799	0.7189858

C	-3.2627737	-1.3987302	-1.2569594
C	-3.5406222	-2.1944542	-2.3575075
H	-2.8823082	-2.2046786	-3.2180282
H	3.8674363	-1.2493605	2.5742802
H	2.6713250	-2.1653746	6.5840120
H	-0.0141385	-0.0568694	4.0035615
H	6.4084342	3.5389562	1.1623594
H	0.0184715	-0.0226638	-3.9339346
H	-2.5634234	2.0961797	-6.6093722
H	-3.8485041	1.3130271	-2.5989072
H	-6.4172894	-3.5749817	-1.2247677

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