

Support Information

Synthesis of 2,3-bis-organochalcogenyl-benzo[*b*]chalcogenophenes promoted by Oxone[®]

Gelson Perin,^{*a} Liane K. Soares,^a Paola S. Hellwig,^a Marcio S. Silva,^a José S. S. Neto,^a Juliano A. Roehrs,^b Thiago Barcellos^c and Eder J. Lenardão^{*a}

^aLASOL-CCQFA, Universidade Federal de Pelotas – UFPel; P.O. Box 354 - 96010-900, Pelotas, RS, Brazil. <http://wp.ufpel.edu.br/lasol>.

^bInstituto Federal Sul-Rio-Grandense, Campus Pelotas - Praça Vinte de Setembro 96015-360, RS, Brazil.

^cLaboratory of Biotechnology of Natural and Synthetic Products – Universidade de Caxias do Sul – UCS, Caxias do Sul, 95070-560, RS, Brazil.

Corresponding authors: gelson_perin@ufpel.edu.br (G. Perin) and lenardao@ufpel.edu.br (E. J. Lenardão)

Selected spectra

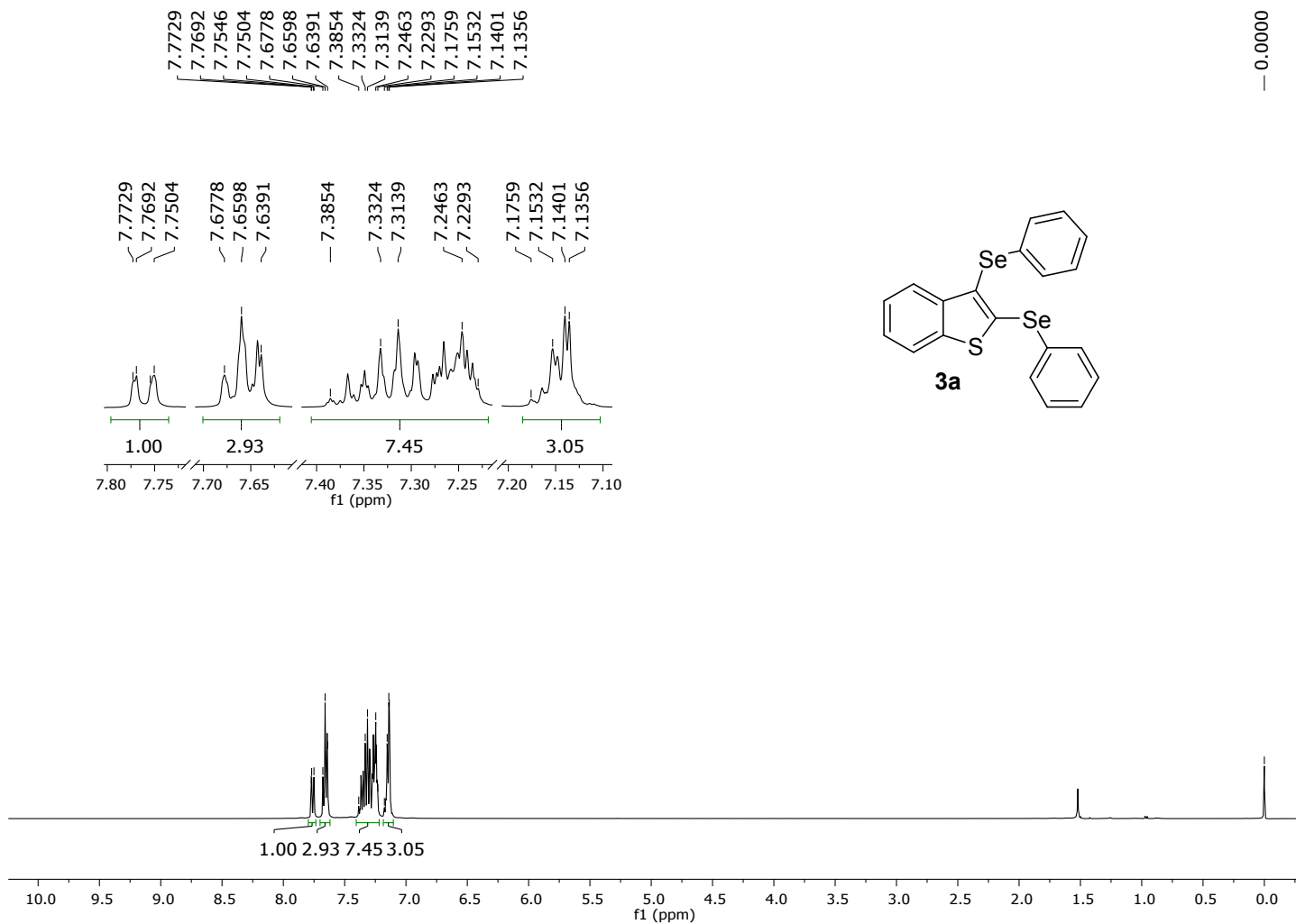


Figure S1: ^1H NMR (400 MHz, CDCl_3) spectrum 2,3-bis(phenylselanyl)benzo[*b*]thiophene **3a**.

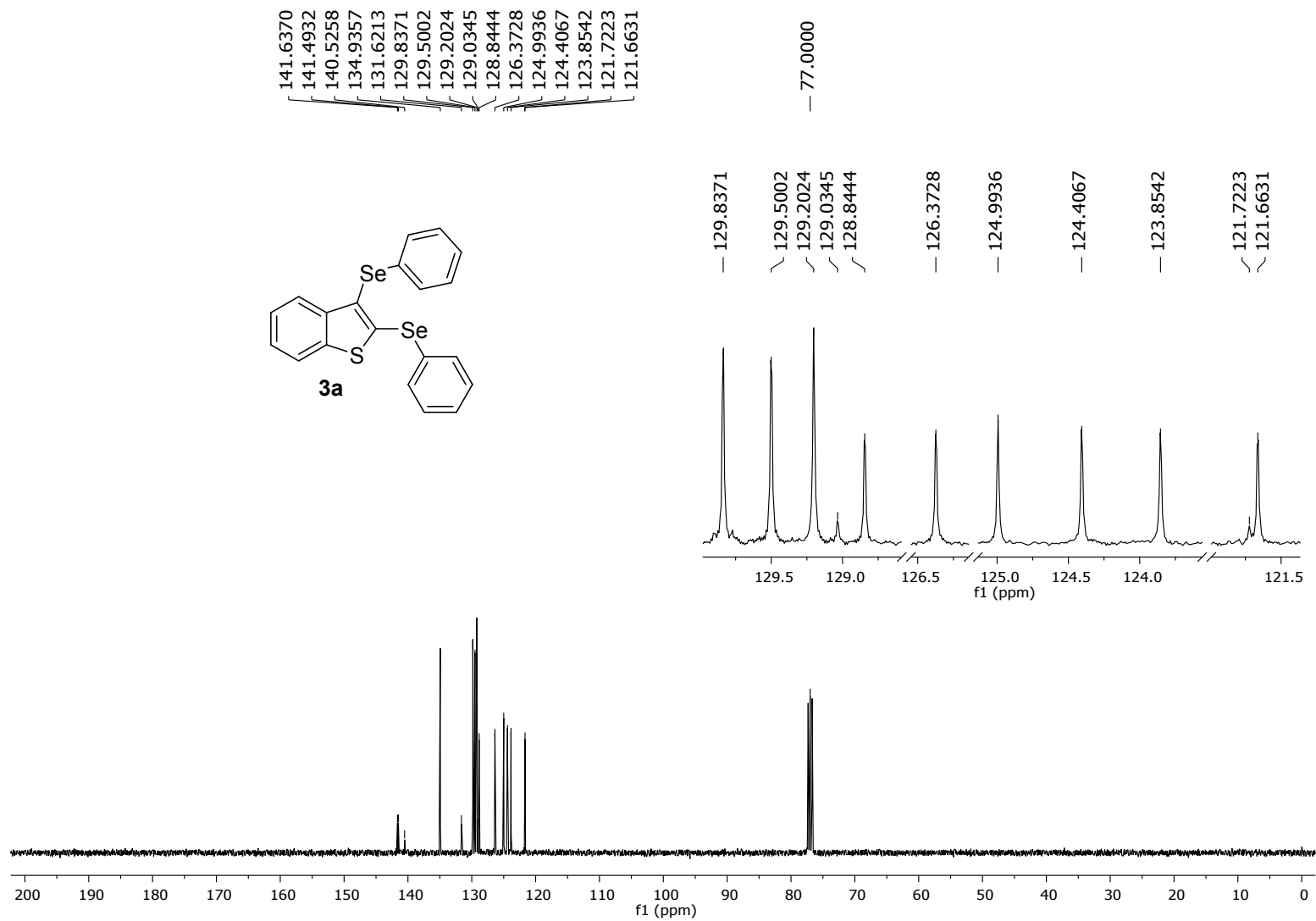


Figure S2: ¹³C NMR (100 MHz, CDCl₃) spectrum 2,3-bis(phenylselanyl)benzo[*b*]thiophene **3a**.

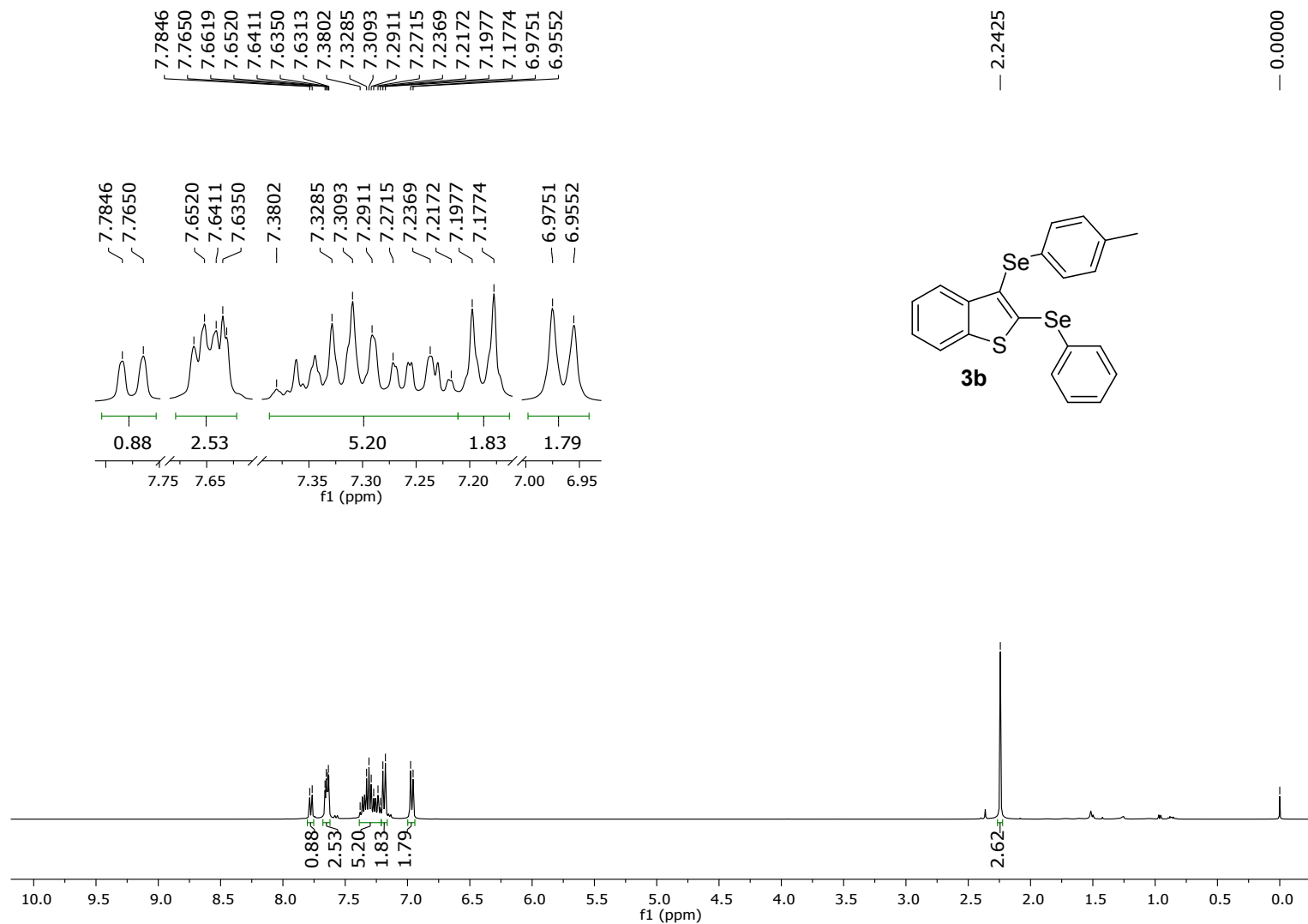


Figure S3: ^1H NMR (400 MHz, CDCl_3) spectrum 2-(phenylselanyl)-3-(4-tolylselanyl)benzo[*b*]thiophene **3b**.

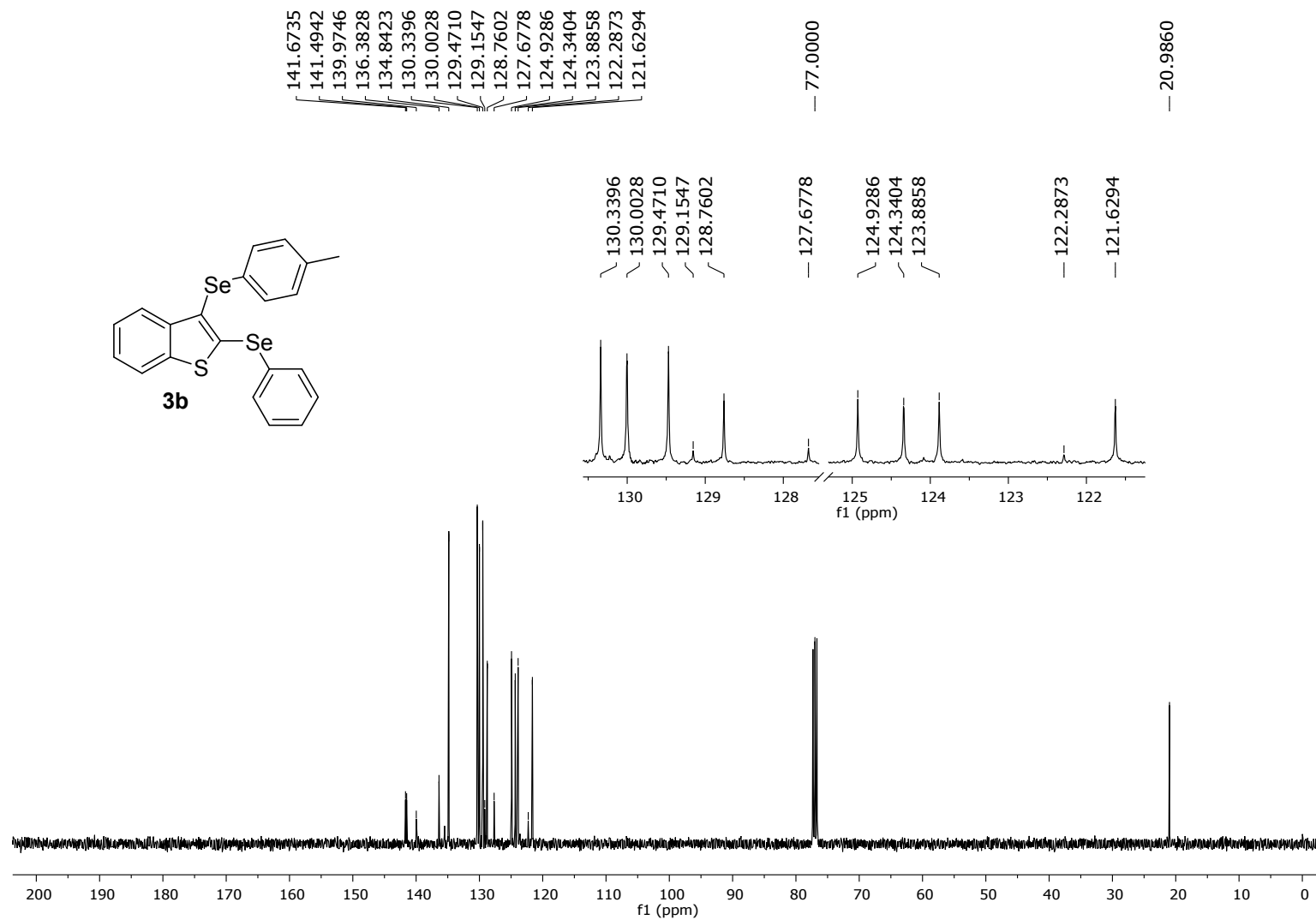


Figure S4: ¹³C NMR (100 MHz, CDCl₃) spectrum 2-(phenylselanyl)-3-(4-tolylselanyl)benzo[*b*]thiophene **3b**.

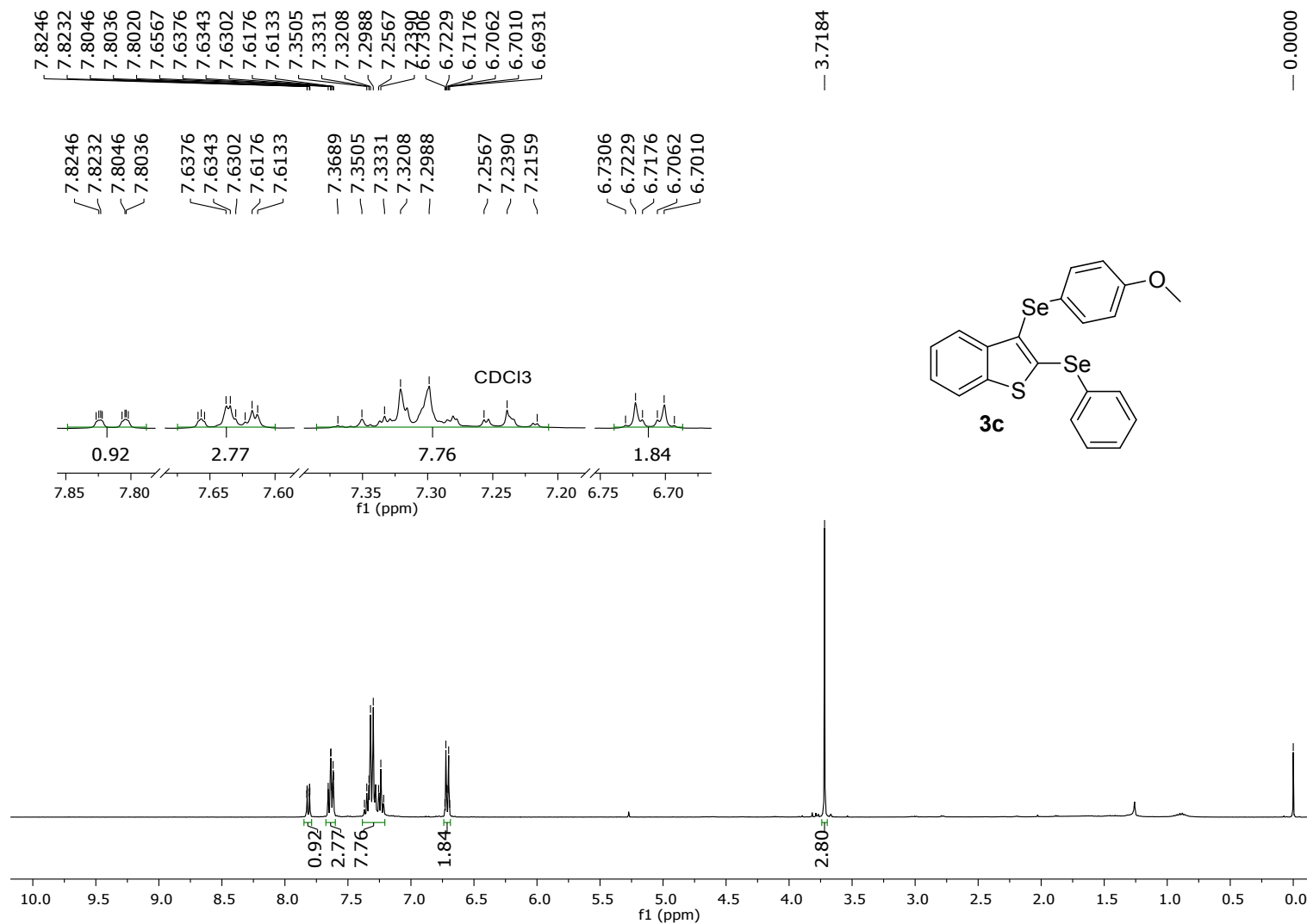


Figure S5: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-methoxyphenyl)selanyl]-2-(phenylselanyl)benzo[*b*]thiophene **3c**.

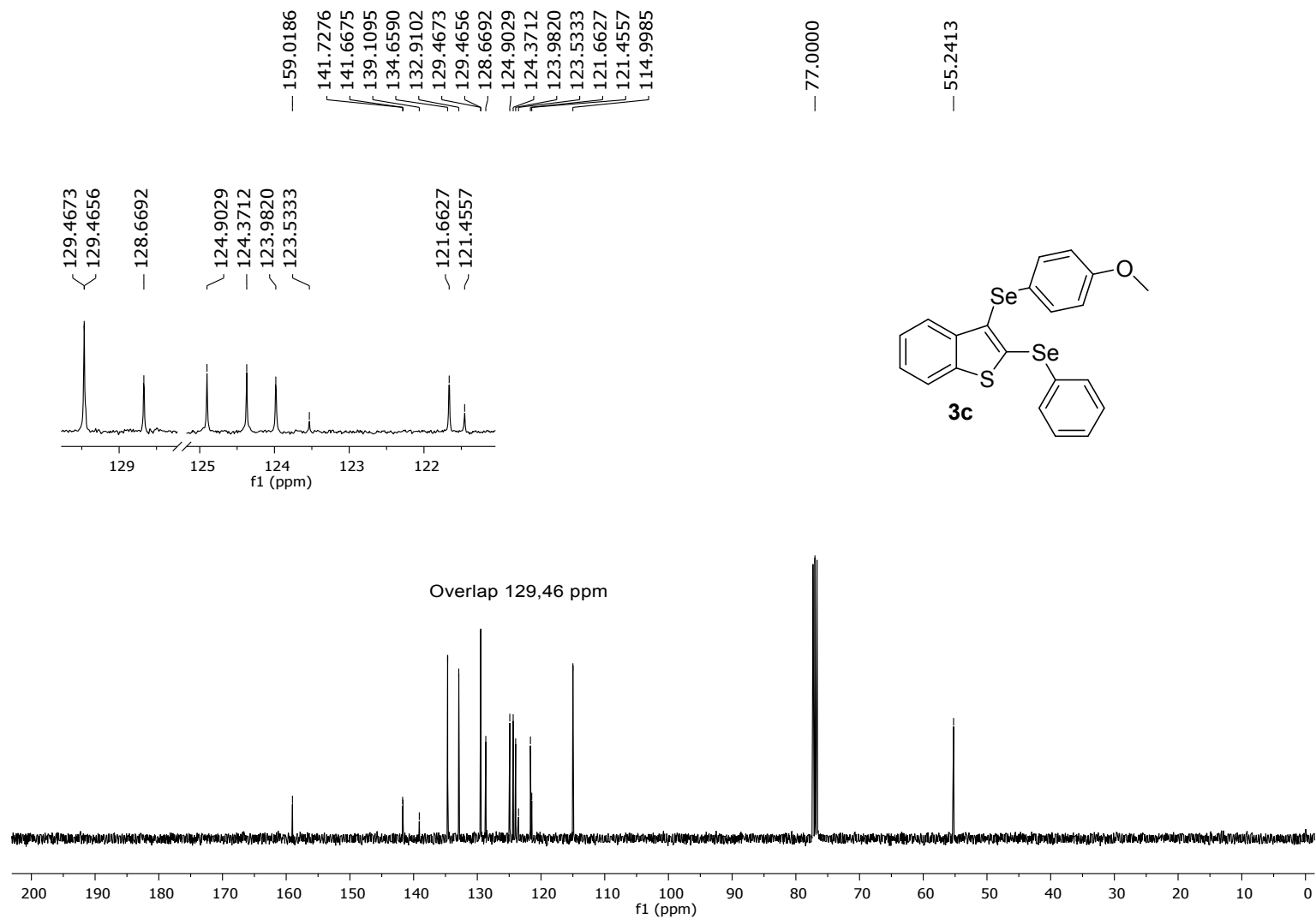


Figure S6: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-methoxyphenyl)selanyl]-2-(phenylselanyl)benzo[*b*]thiophene **3c**.

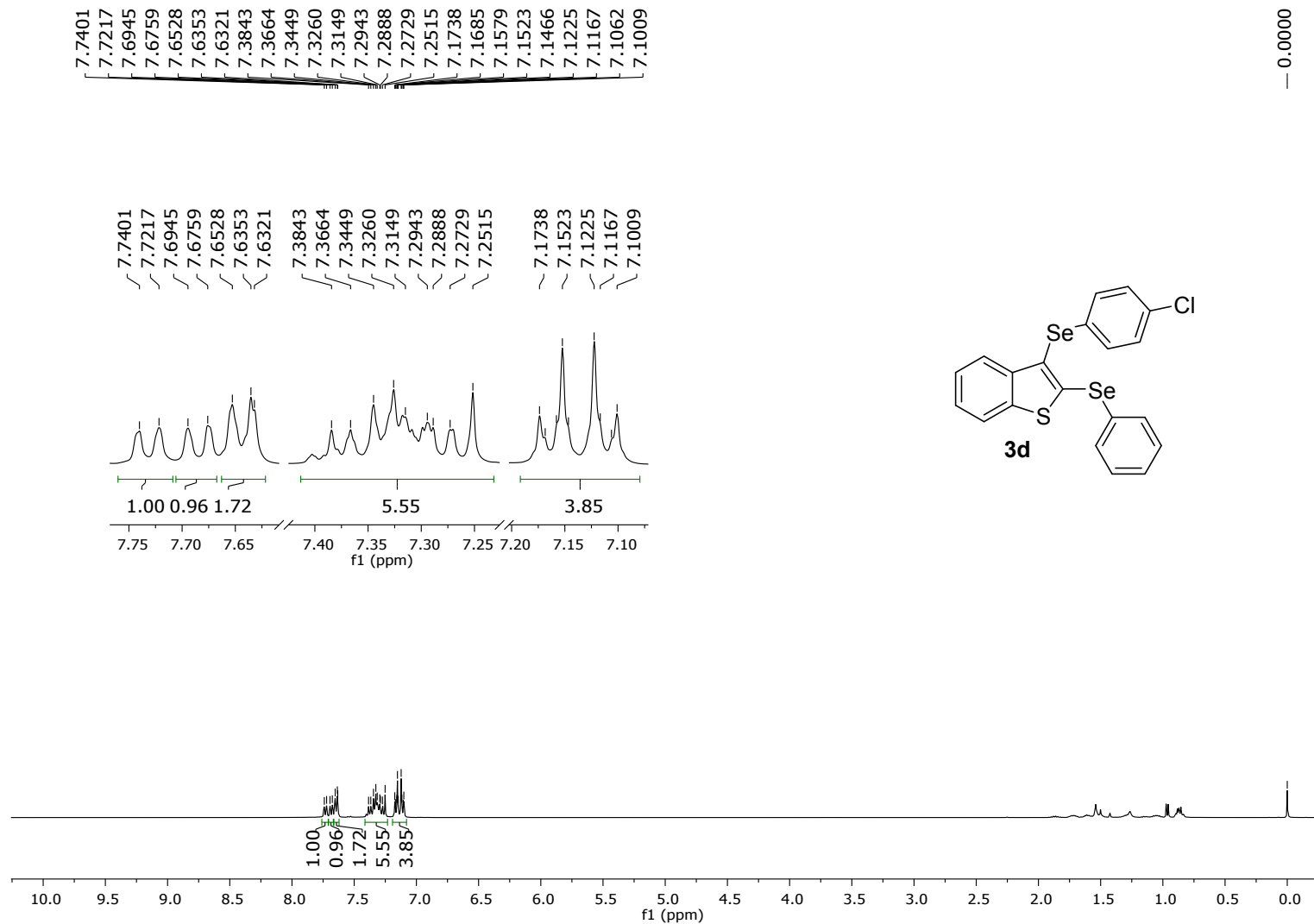


Figure S7: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-Chlorophenyl)selenyl]-2-(phenylselenyl)benzo[*b*]thiophene **3d**.

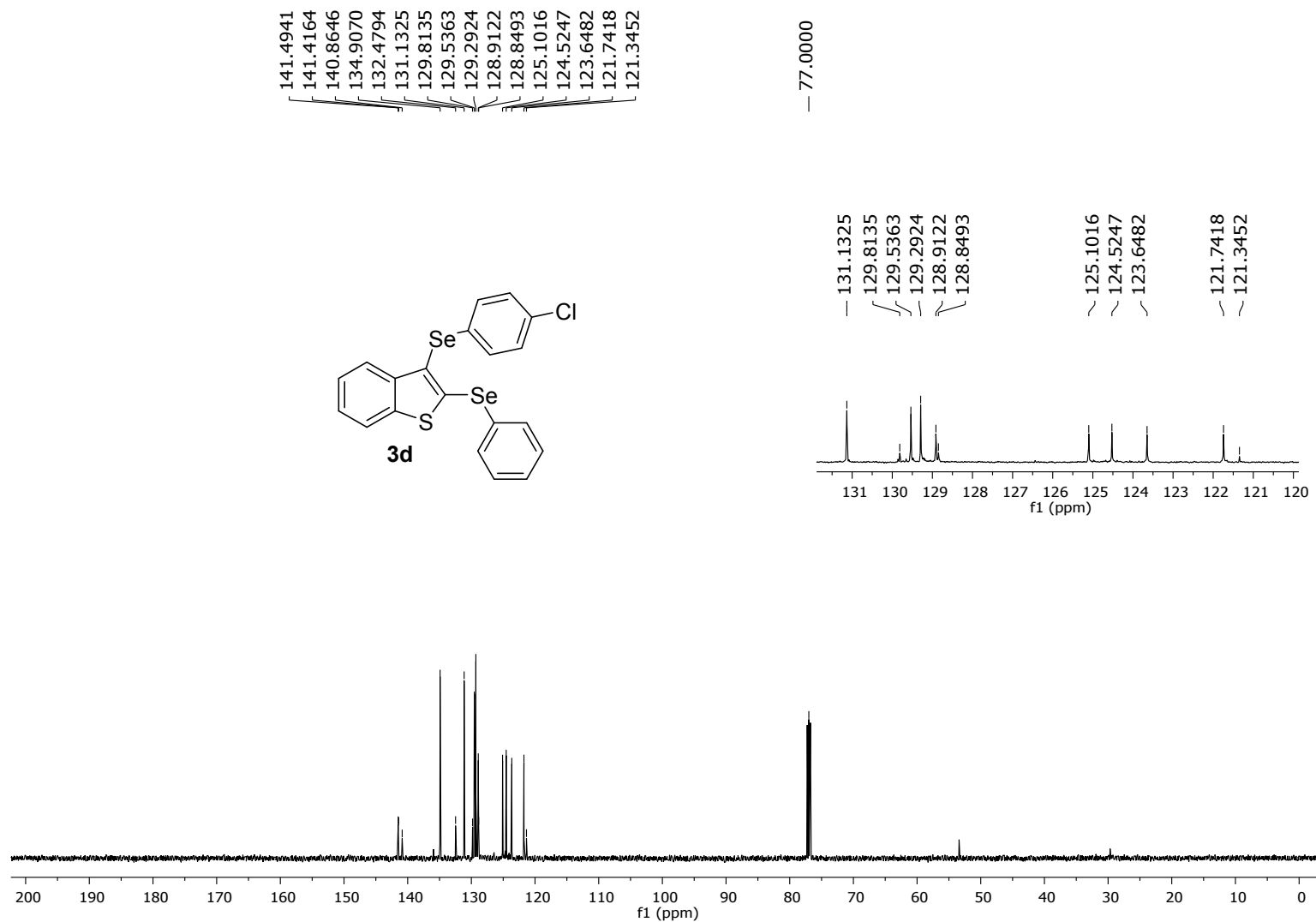


Figure S8: ^{13}C NMR (100 MHz, CDCl_3) spectrum 3-[(4-Chlorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]thiophene **3d**.

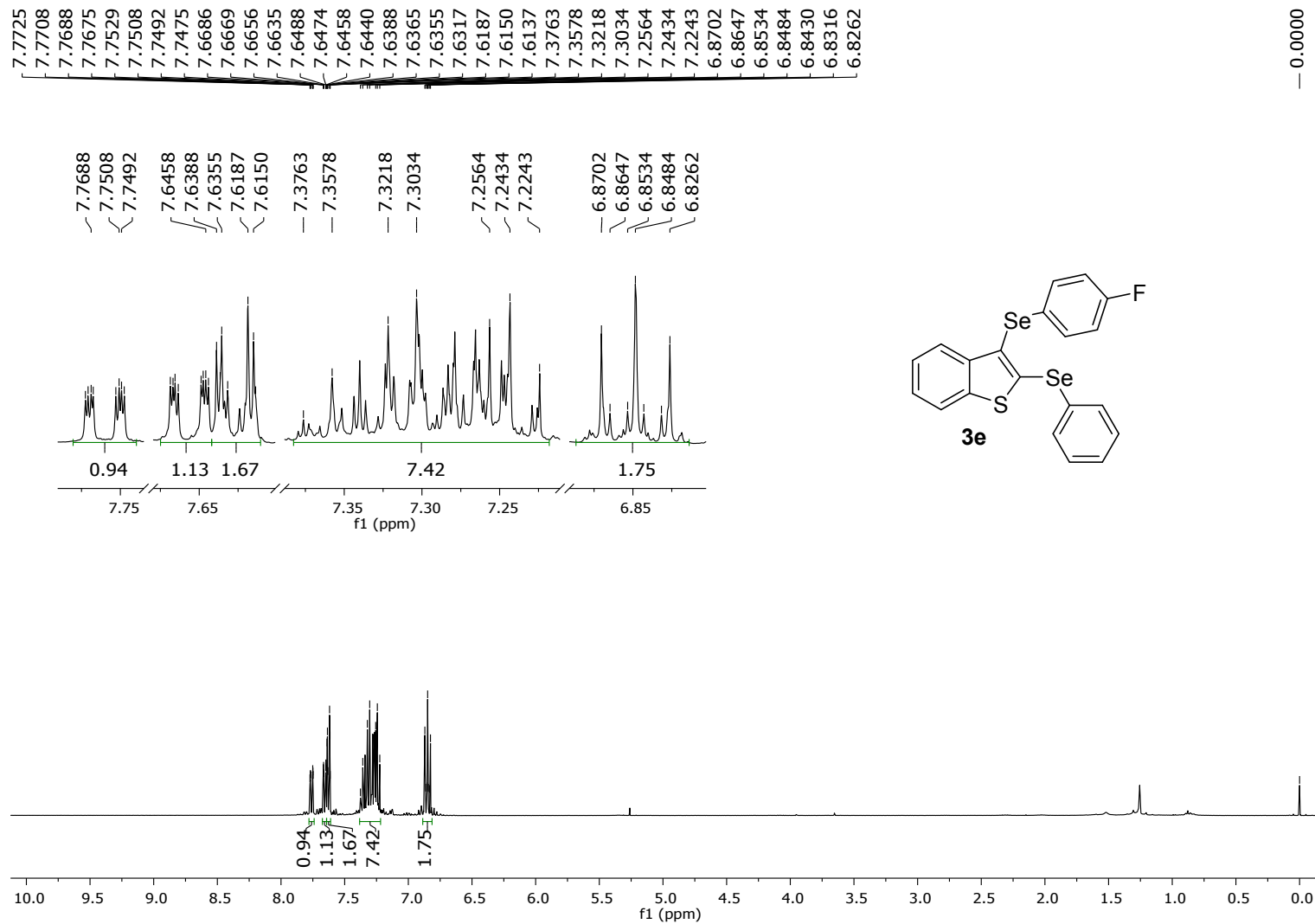


Figure S9: $^1\text{H NMR}$ (400 MHz, CDCl_3) spectrum 3-[(4-fluorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]thiophene **3e**.

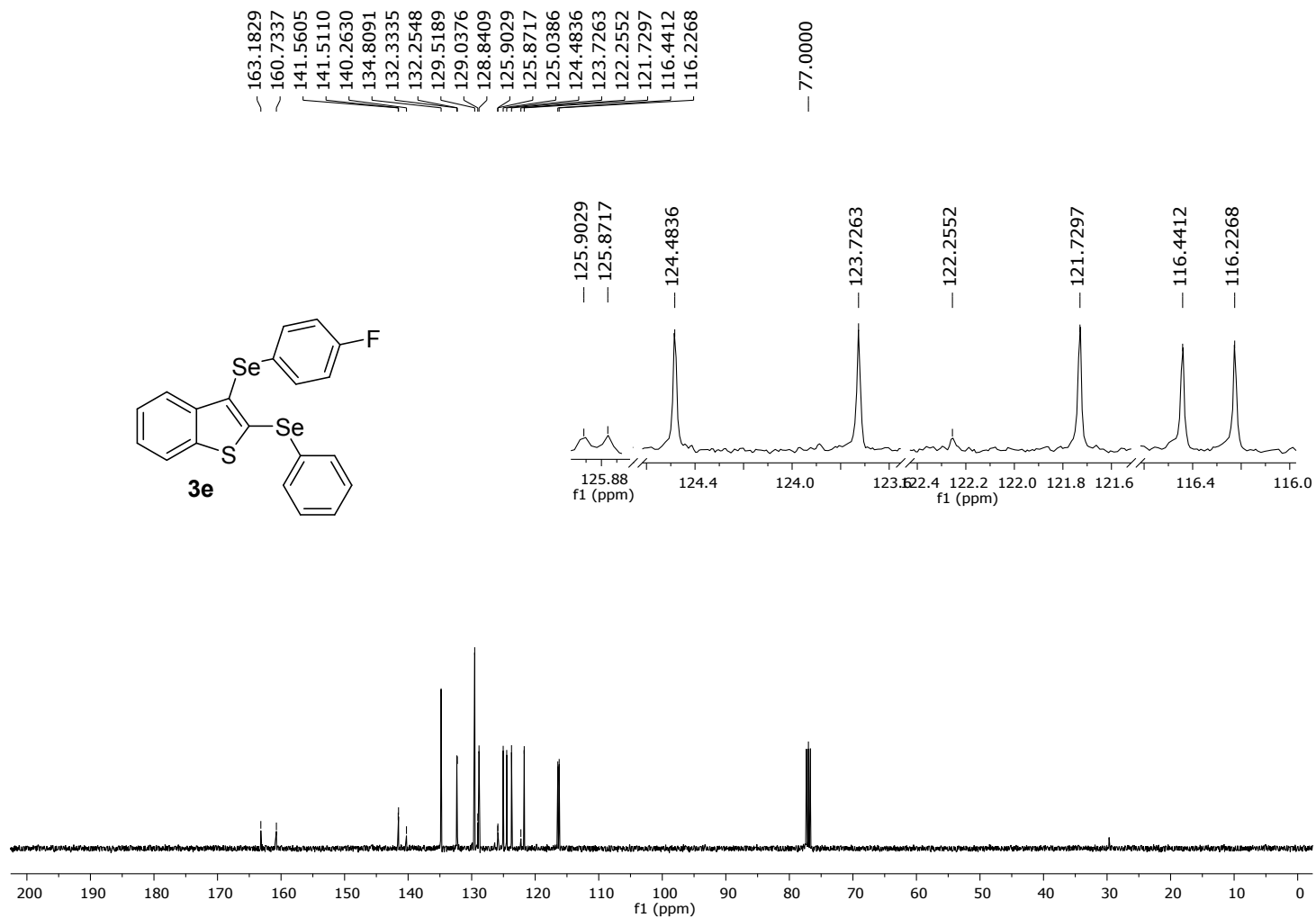


Figure S10: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-fluorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]thiophene **3e**.

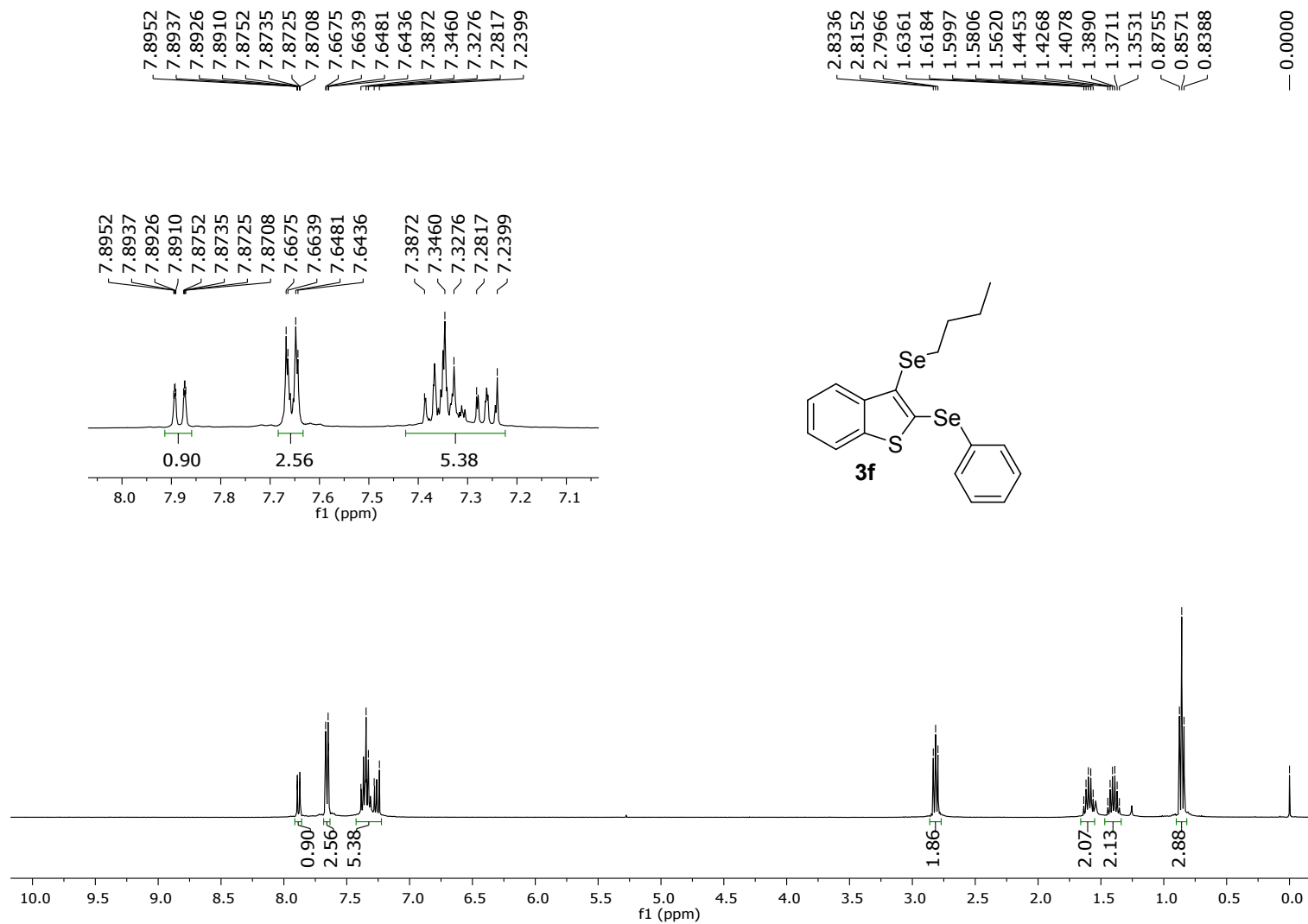


Figure S11: ¹H NMR (400 MHz, CDCl₃) spectrum 3-(butylselanyl)-2-(phenylselanyl)benzo[b]thiophene **3f**.

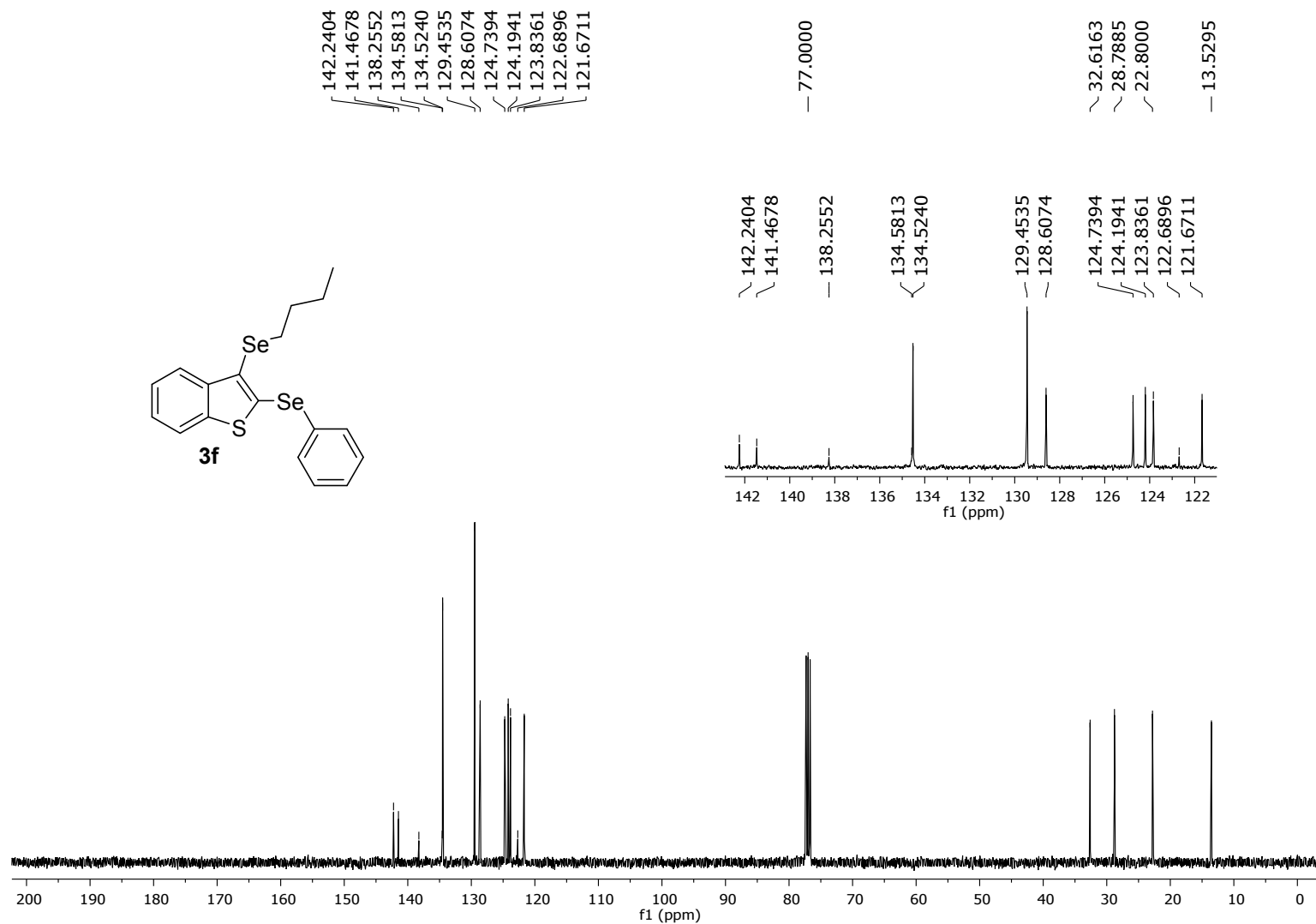


Figure S12: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-(butylselanyl)-2-(phenylselanyl)benzo[*b*]thiophene **3f**.

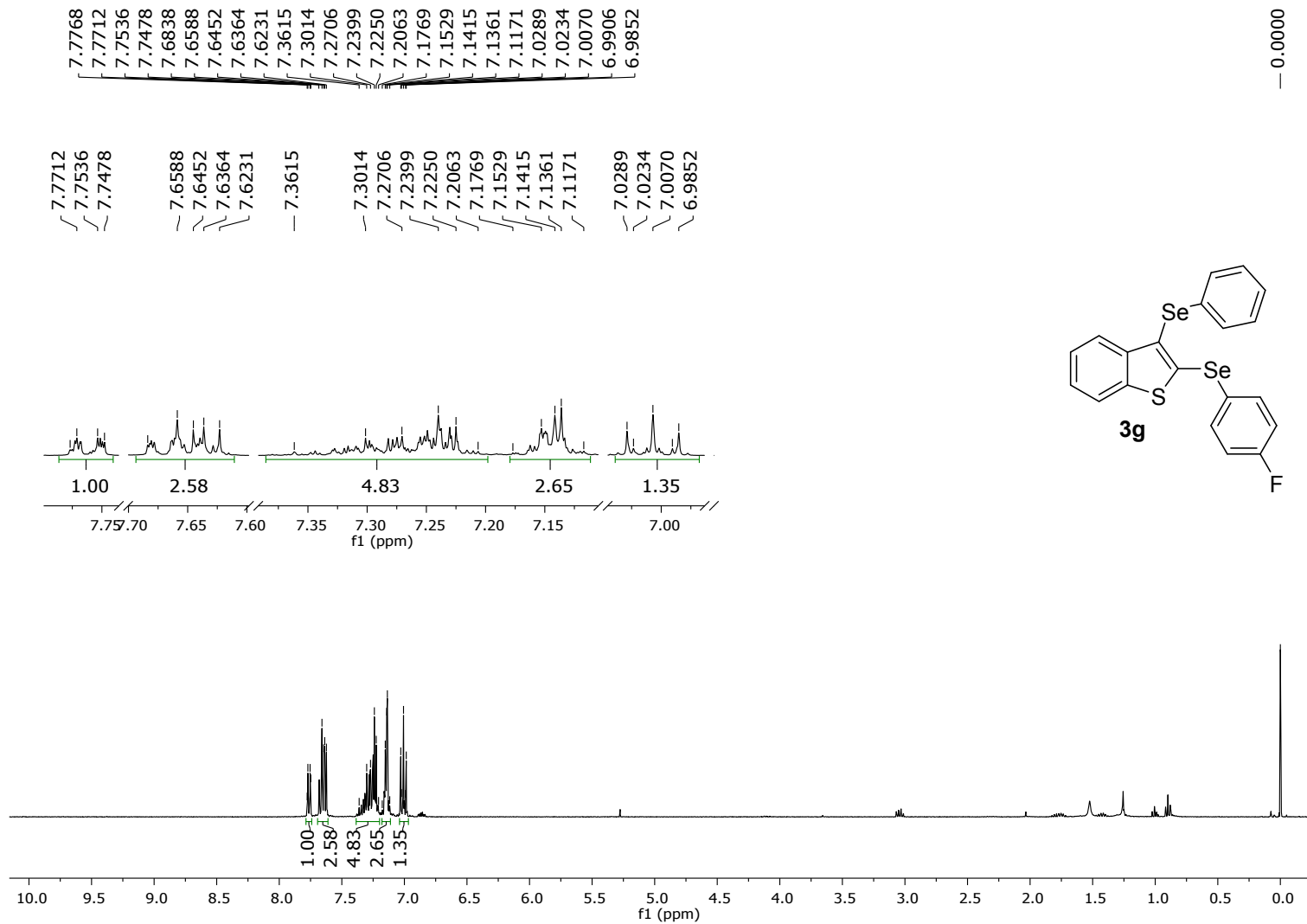


Figure S13: ¹H NMR (400 MHz, CDCl₃) spectrum 2-[(4-fluorophenyl)selanyl]-3-(phenylselanyl)benzo[*b*]thiophene **3g**.

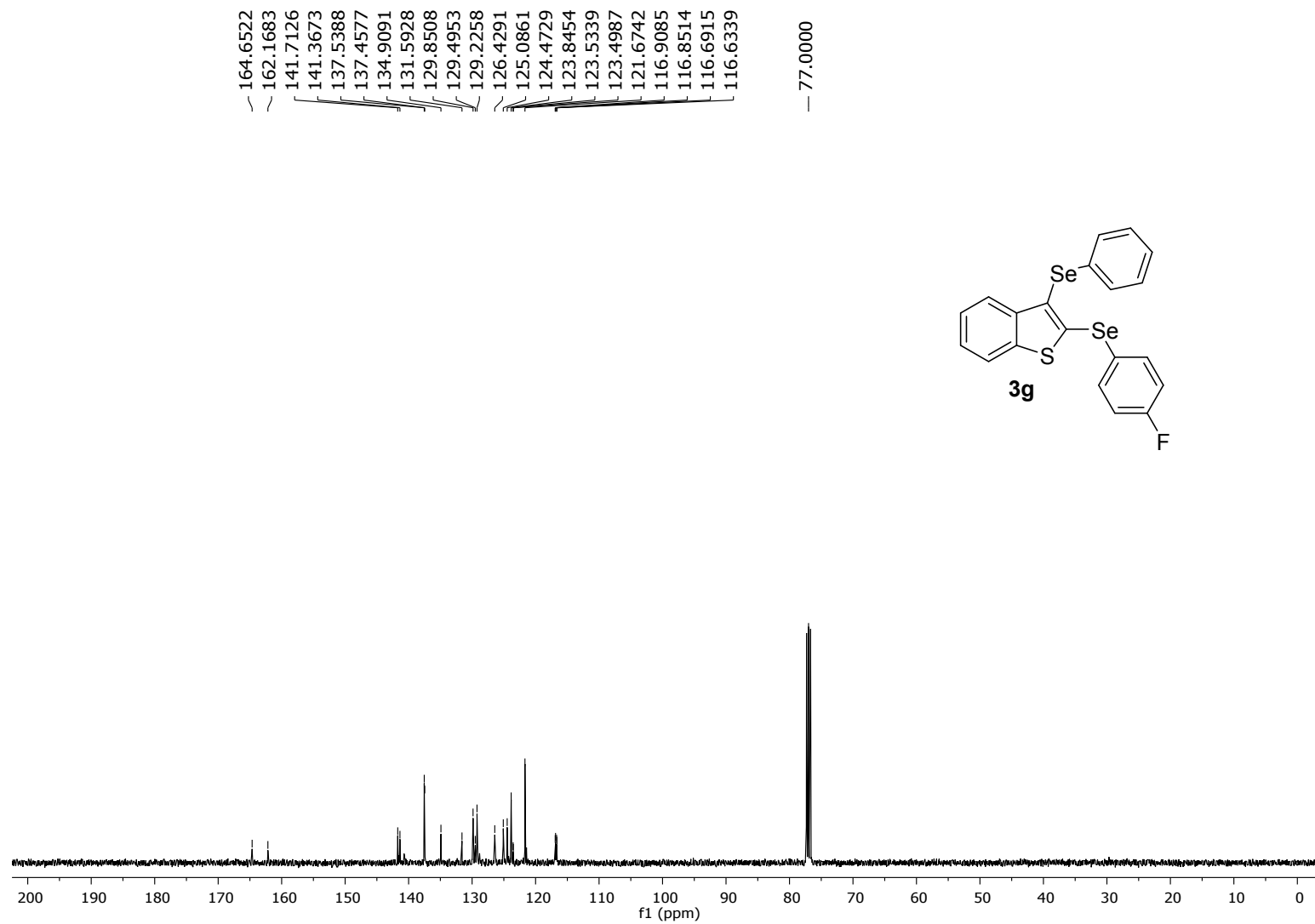


Figure S14: ¹³C NMR (100 MHz, CDCl₃) spectrum 2-[4-fluorophenyl]selanyl]-3-(phenylselanyl)benzo[*b*]thiophene **3g**.

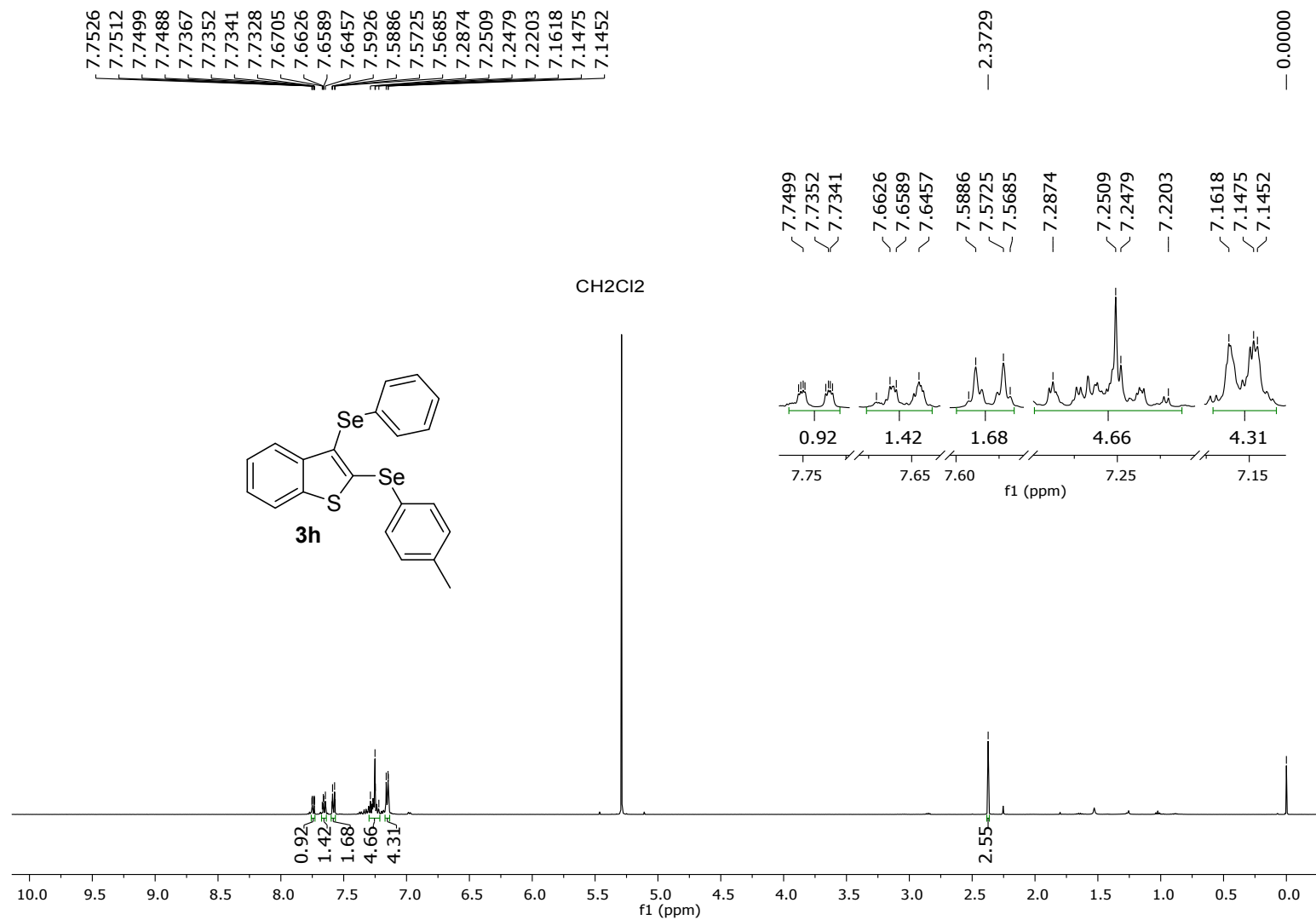


Figure S15: ^1H NMR (400 MHz, CDCl_3) spectrum 3-(phenylselanyl)-2-(4-tolylselanyl)benzo[*b*]thiophene **3h**.

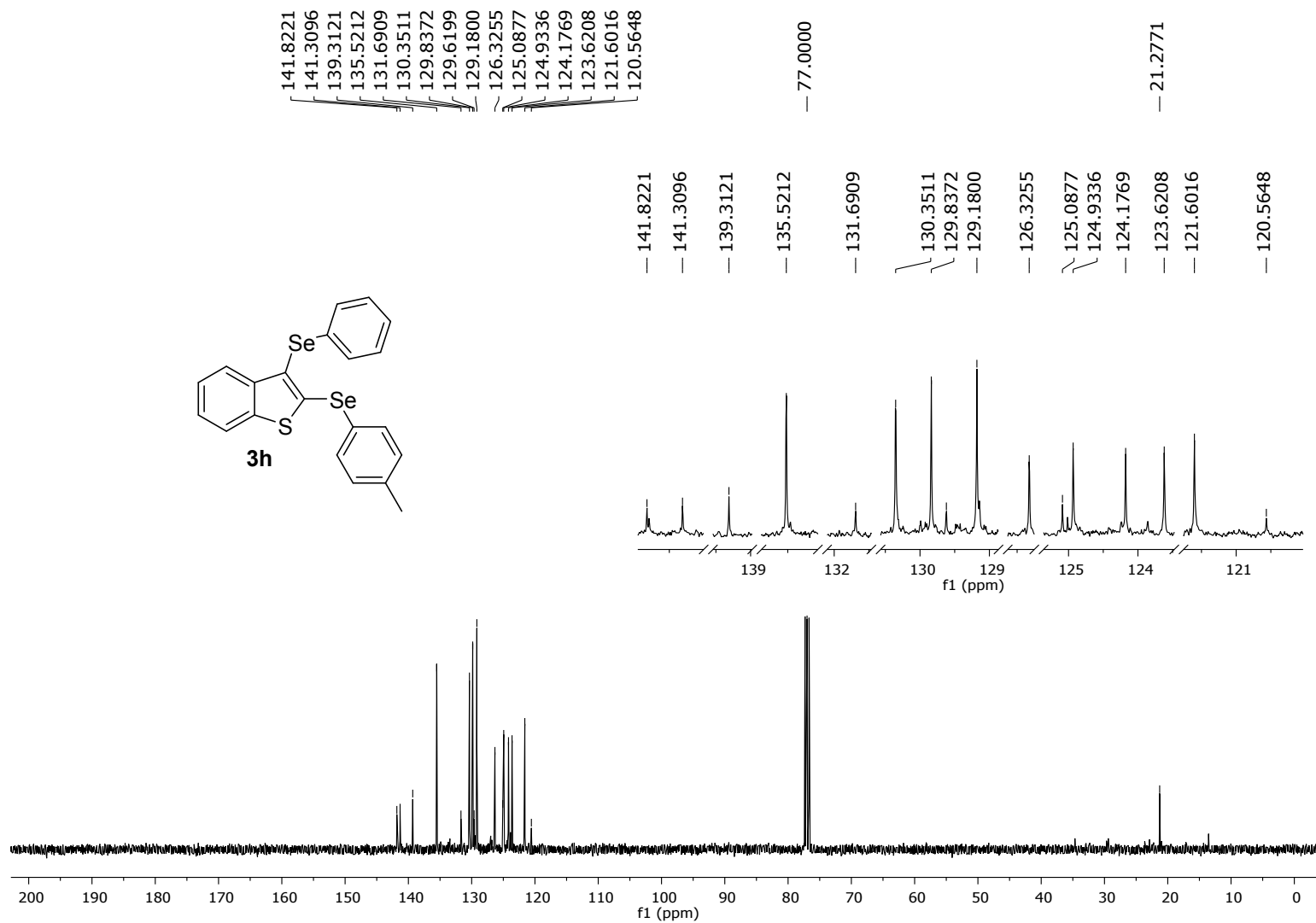


Figure S16: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-(phenylselanyl)-2-(4-tolylselanyl)benzo[*b*]thiophene **3h**.

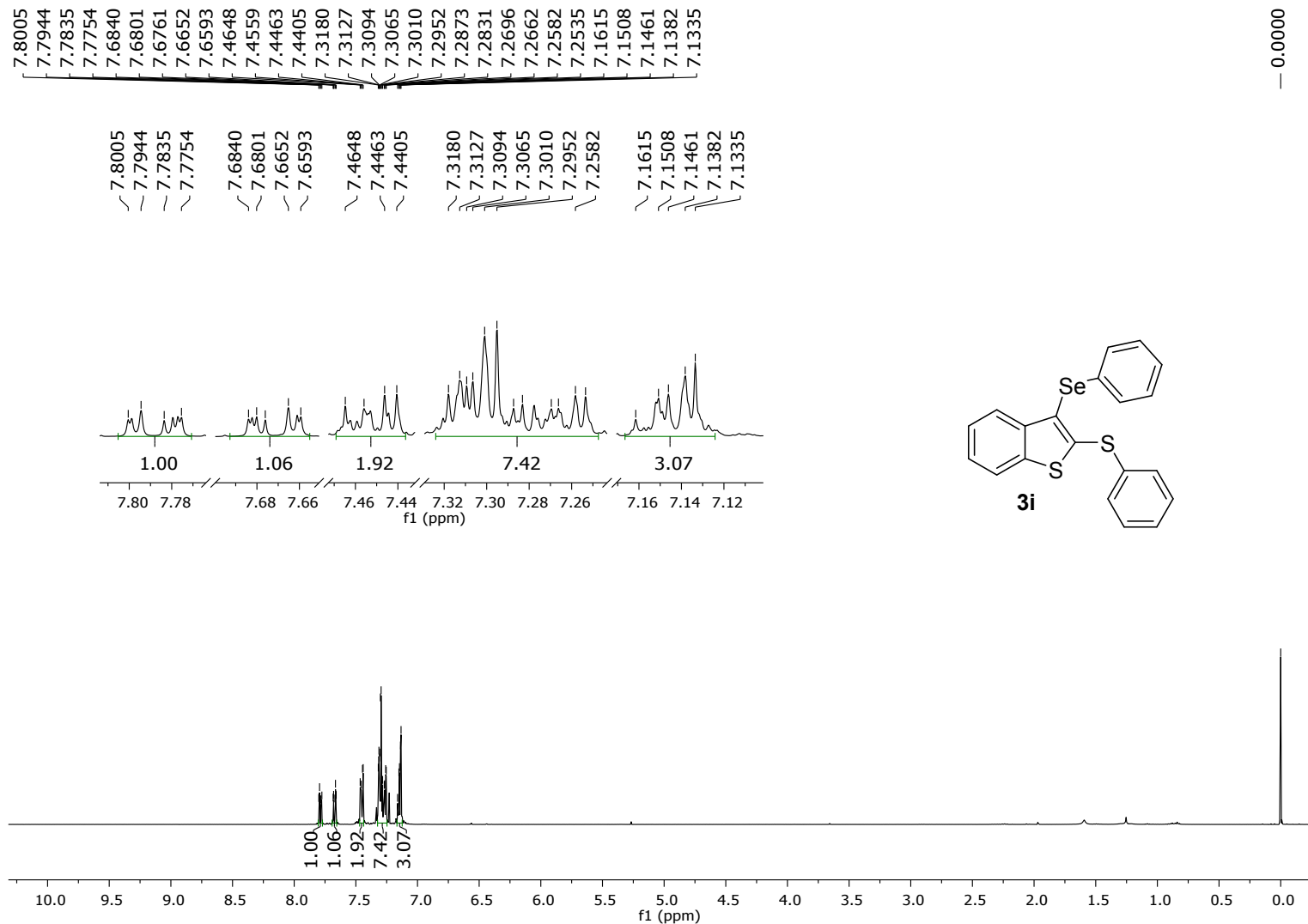


Figure S17: ¹H NMR (400 MHz, CDCl₃) spectrum 3-(phenylselanyl)-2-(phenylsulfanyl)benzo[b]thiophene **3i**.

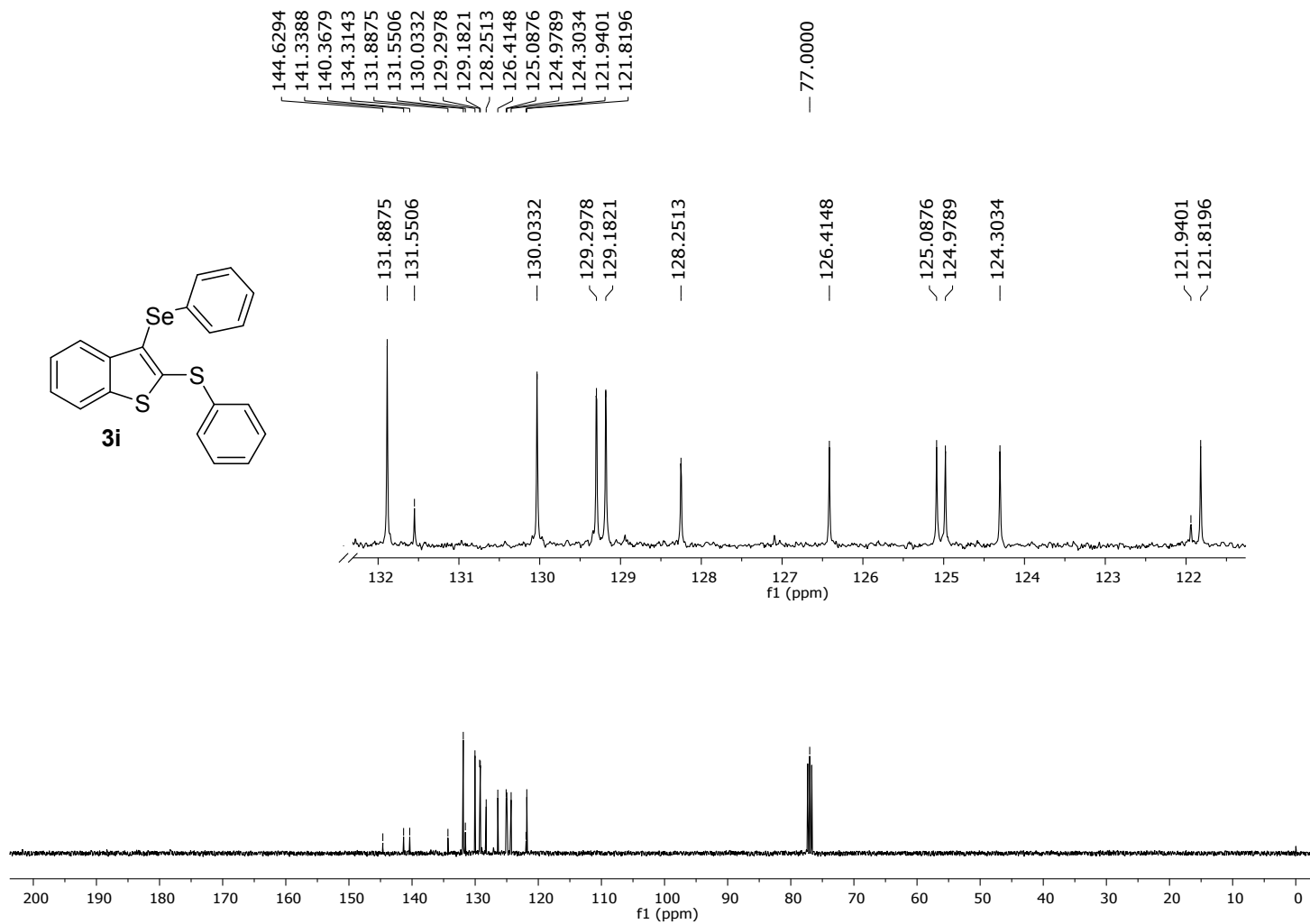


Figure S18: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-(phenylselanyl)-2-(phenylsulfanyl)benzo[*b*]thiophene **3i**.

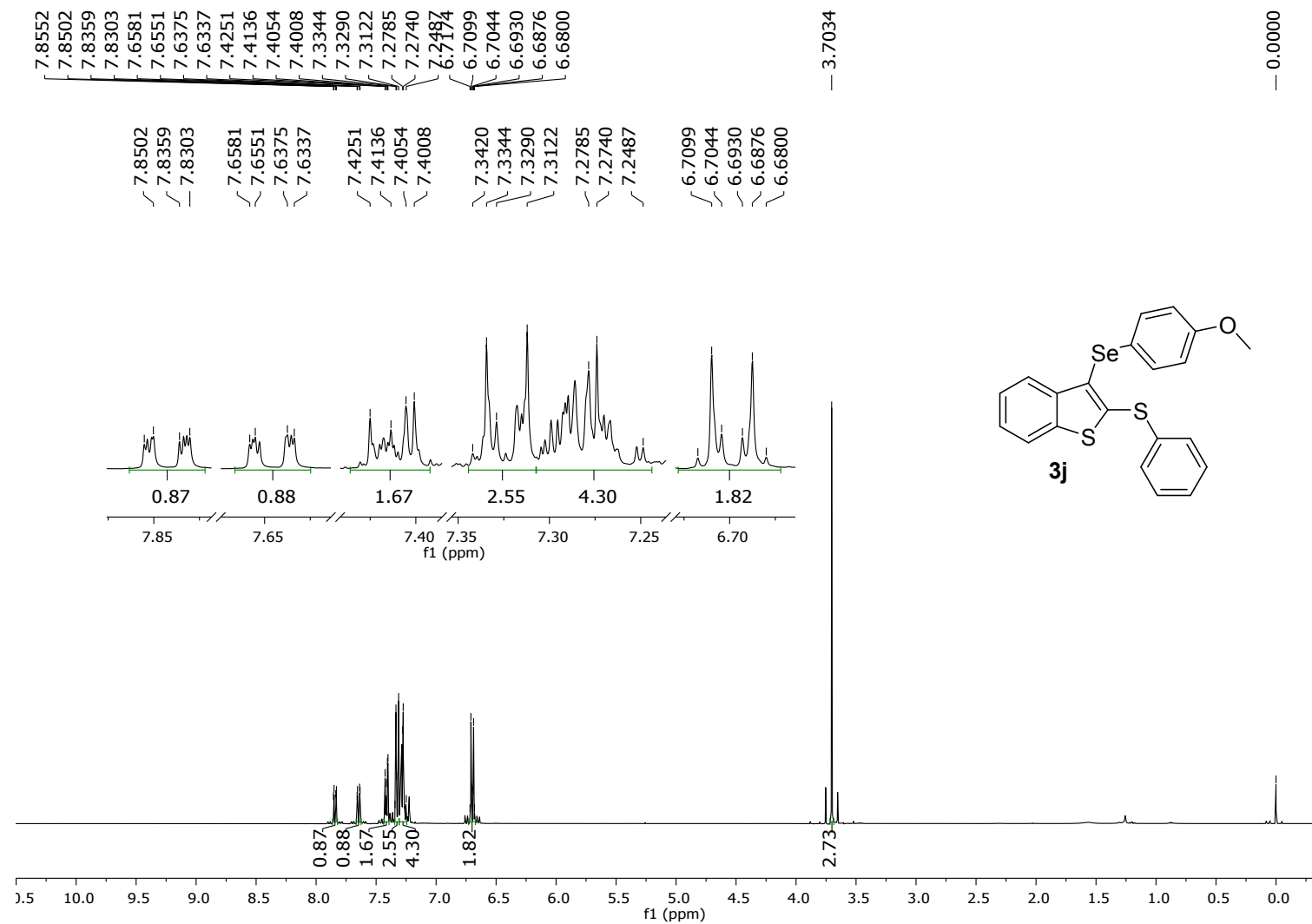


Figure S19: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-methoxyphenyl)selanyl]-2-(phenylsulfanyl)benzo[*b*]thiophene **3j**.

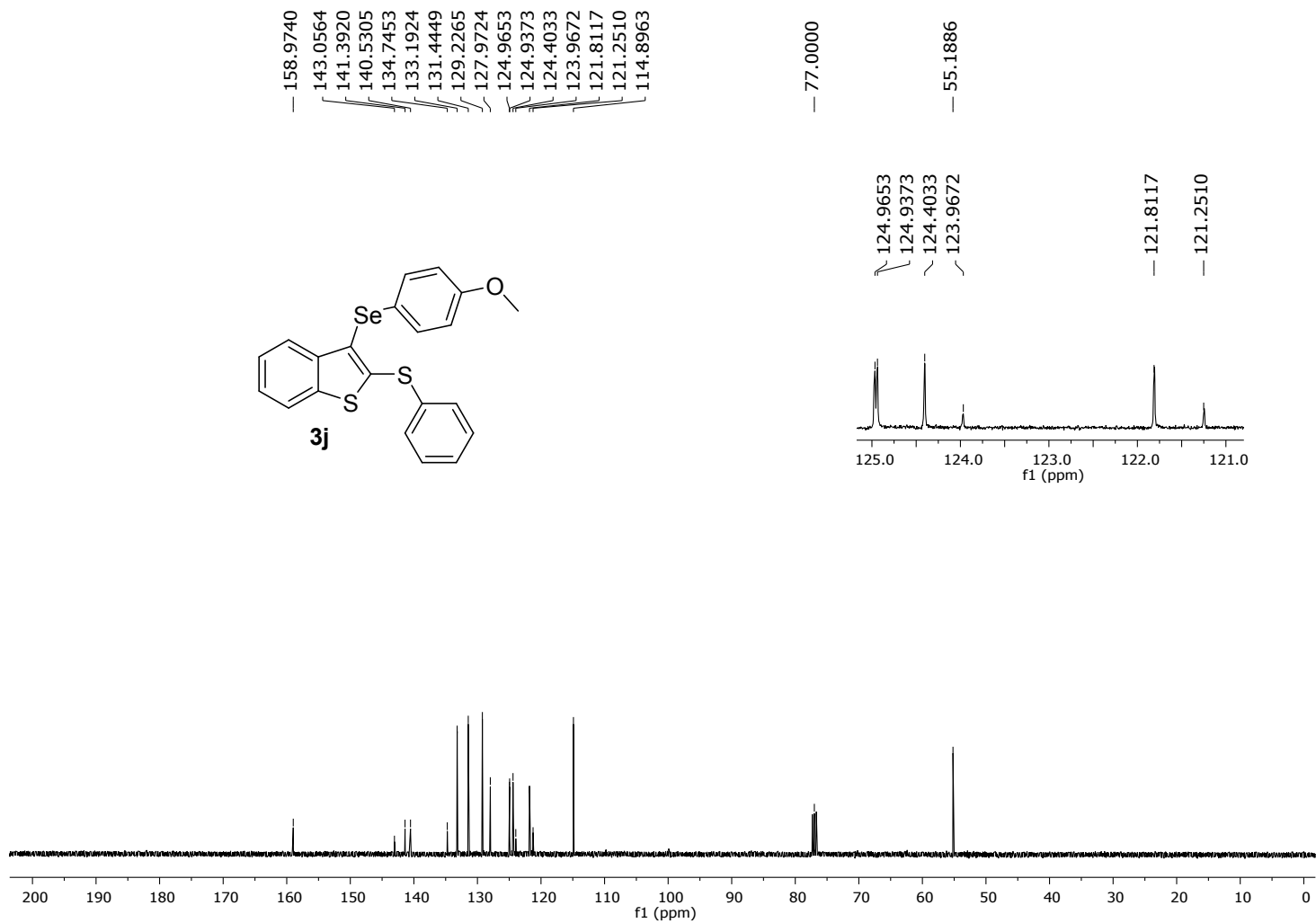


Figure S20: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-methoxyphenyl)selanyl]-2-(phenylsulfanyl)benzo[*b*]thiophene **3j**.

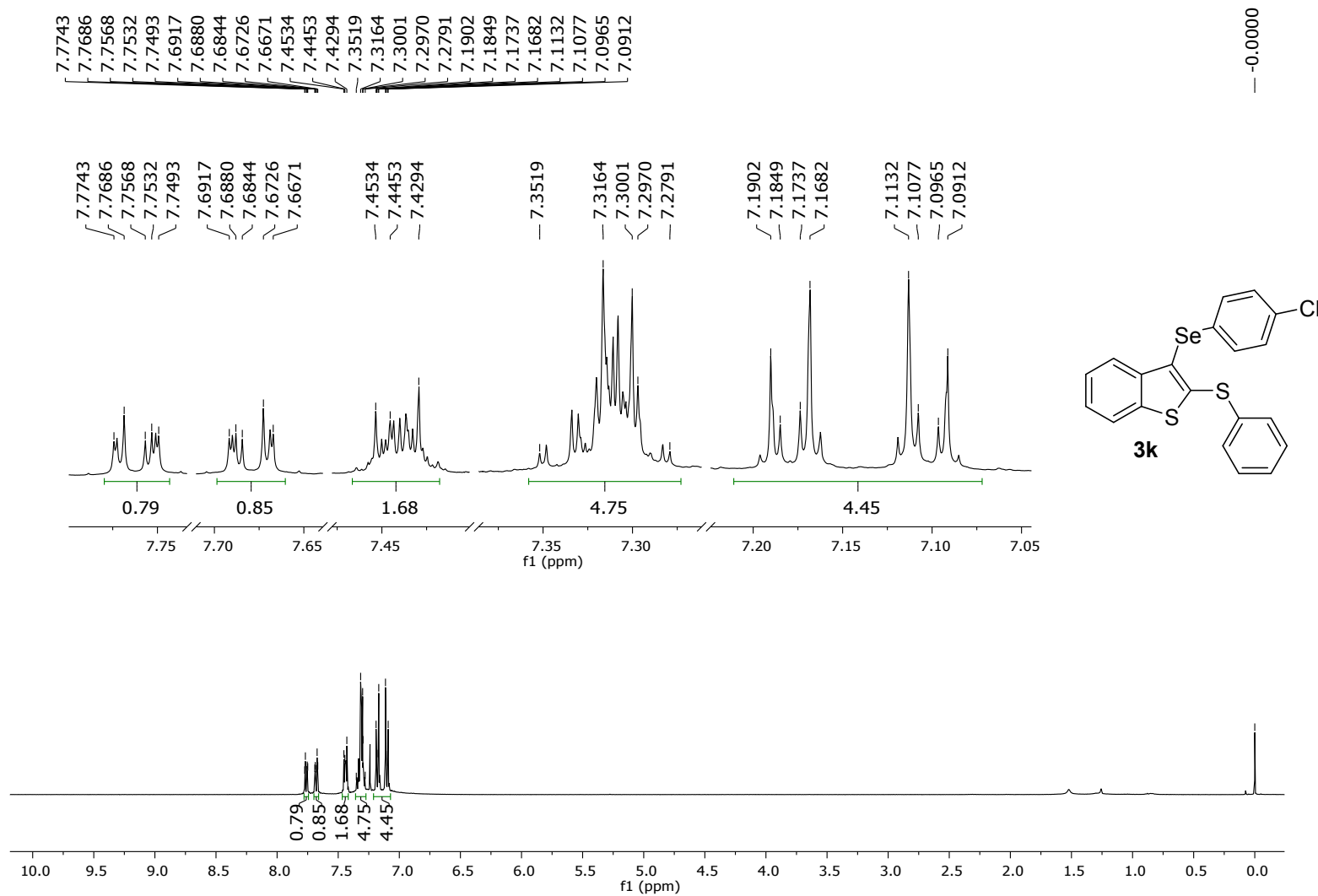


Figure S21: ^1H NMR (400 MHz, CDCl_3) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylsulfanyl)benzo[*b*]thiophene **3k**.

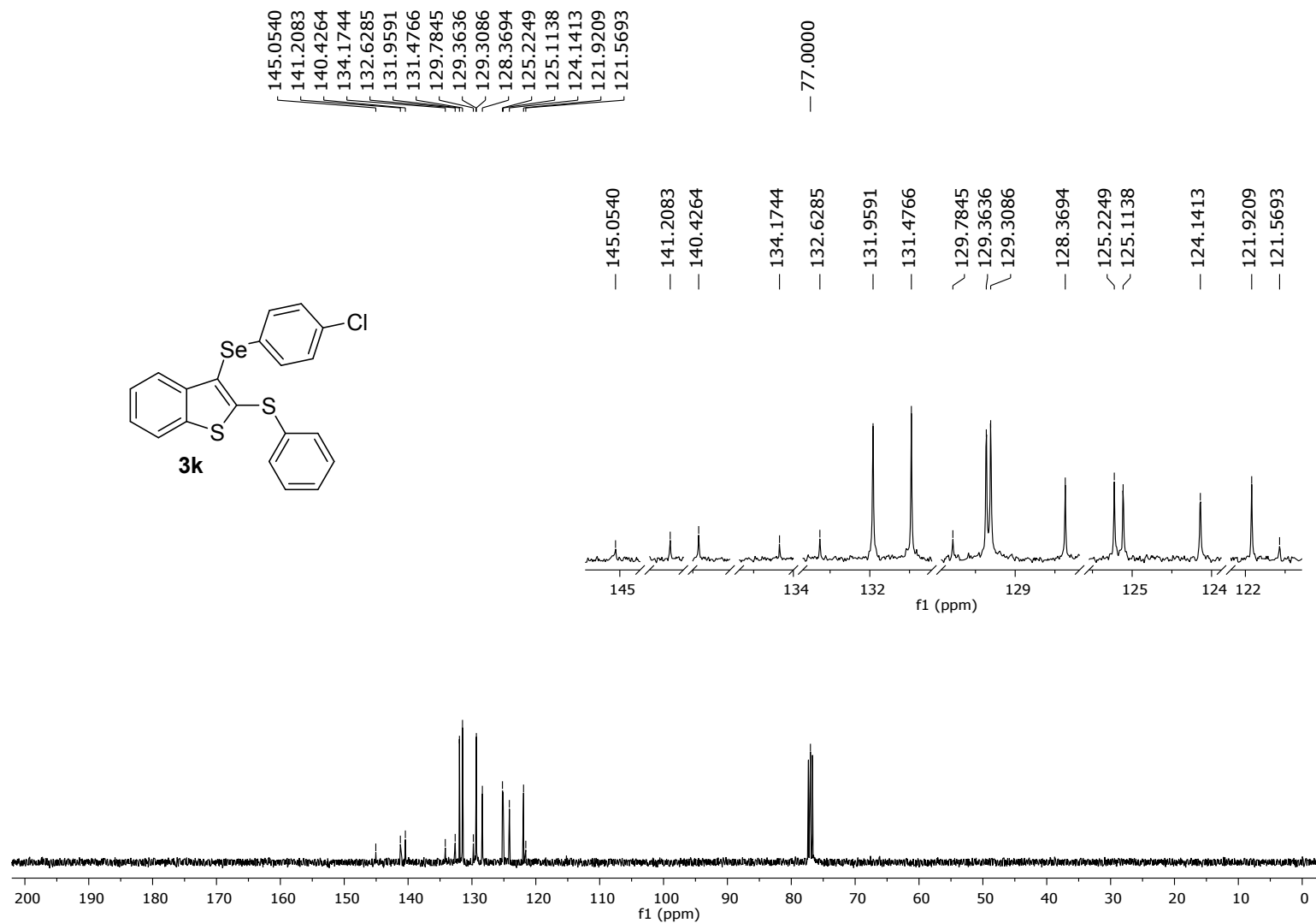


Figure S22: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylsulfanyl)benzo[b]thiophene **3k**.

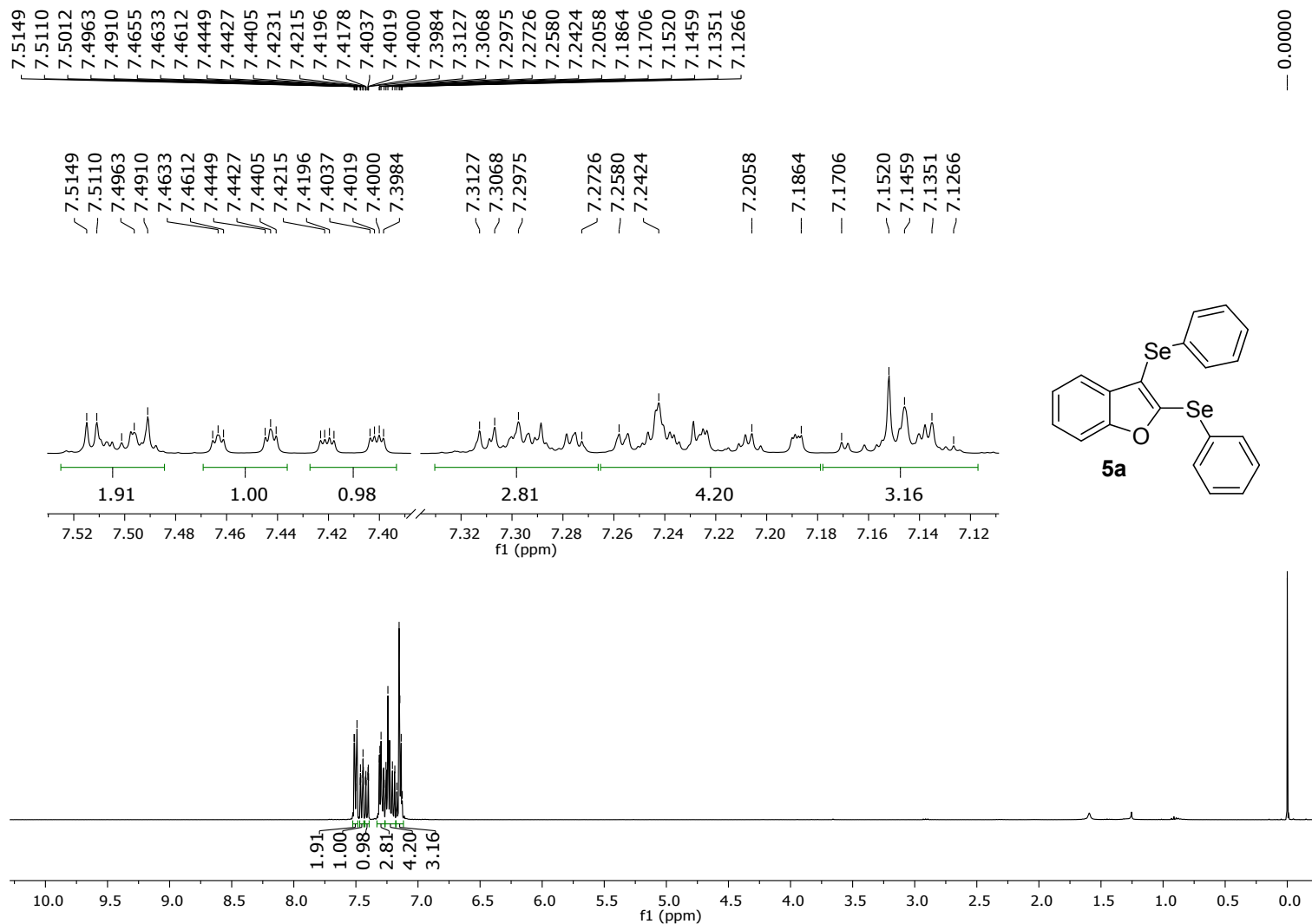


Figure S23: ¹H NMR (400 MHz, CDCl₃) spectrum 2,3-bis(phenylselanyl)benzo[*b*]furan **5a**.

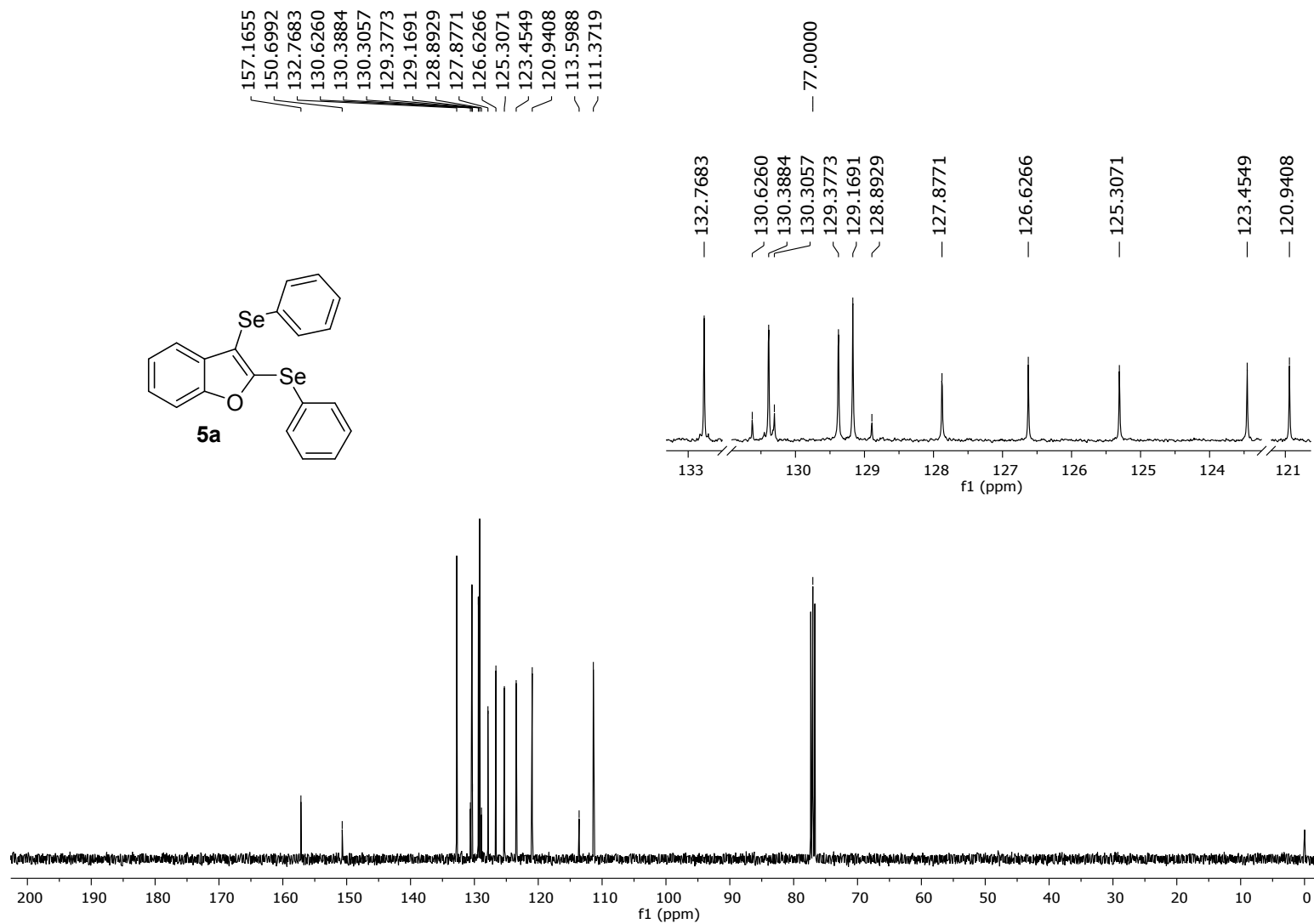


Figure S24: ^{13}C NMR (100 MHz, CDCl_3) spectrum 2,3-bis(phenylselanyl)benzo[*b*]furan **5a**.

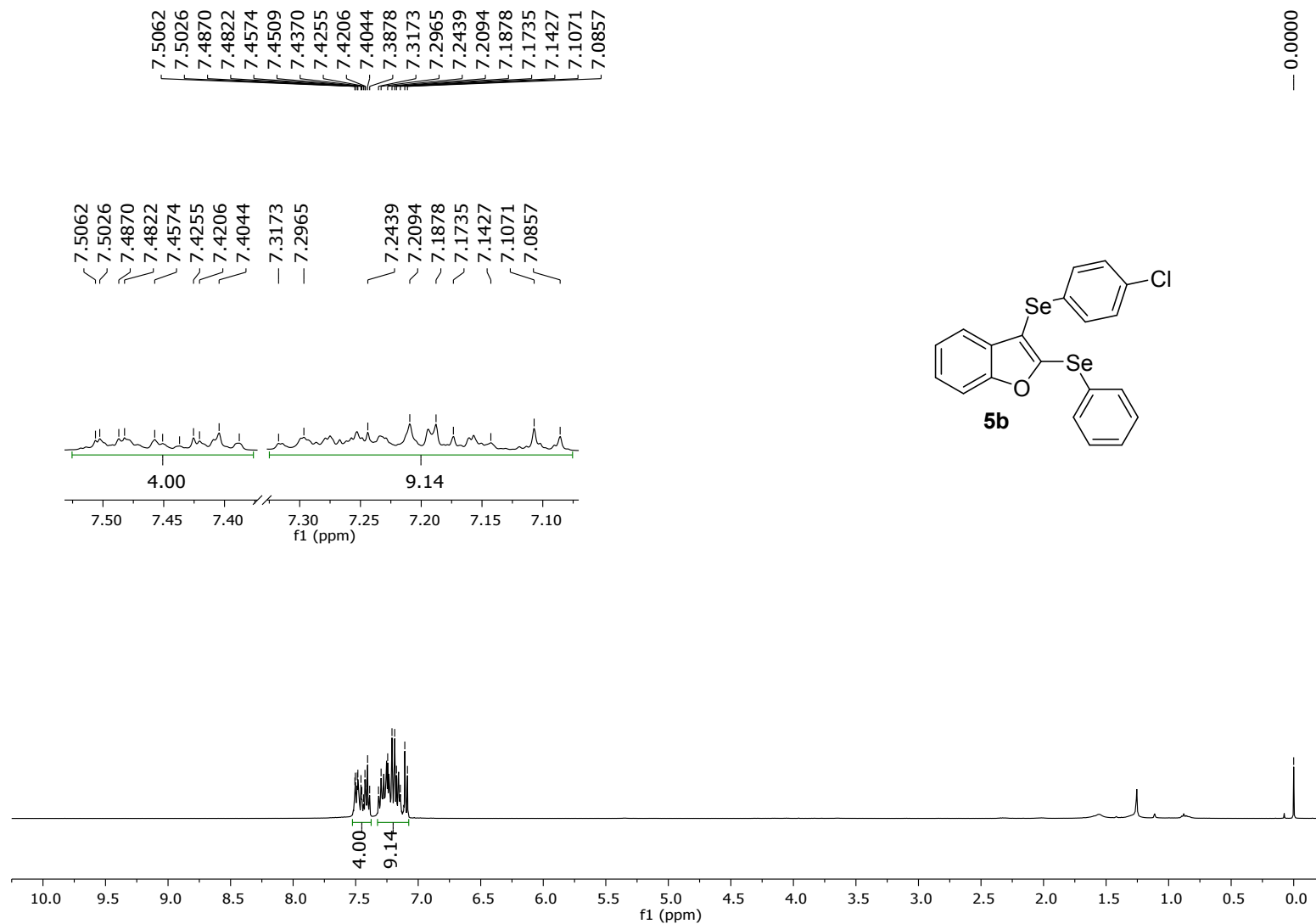


Figure S25: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]furan **5b**.

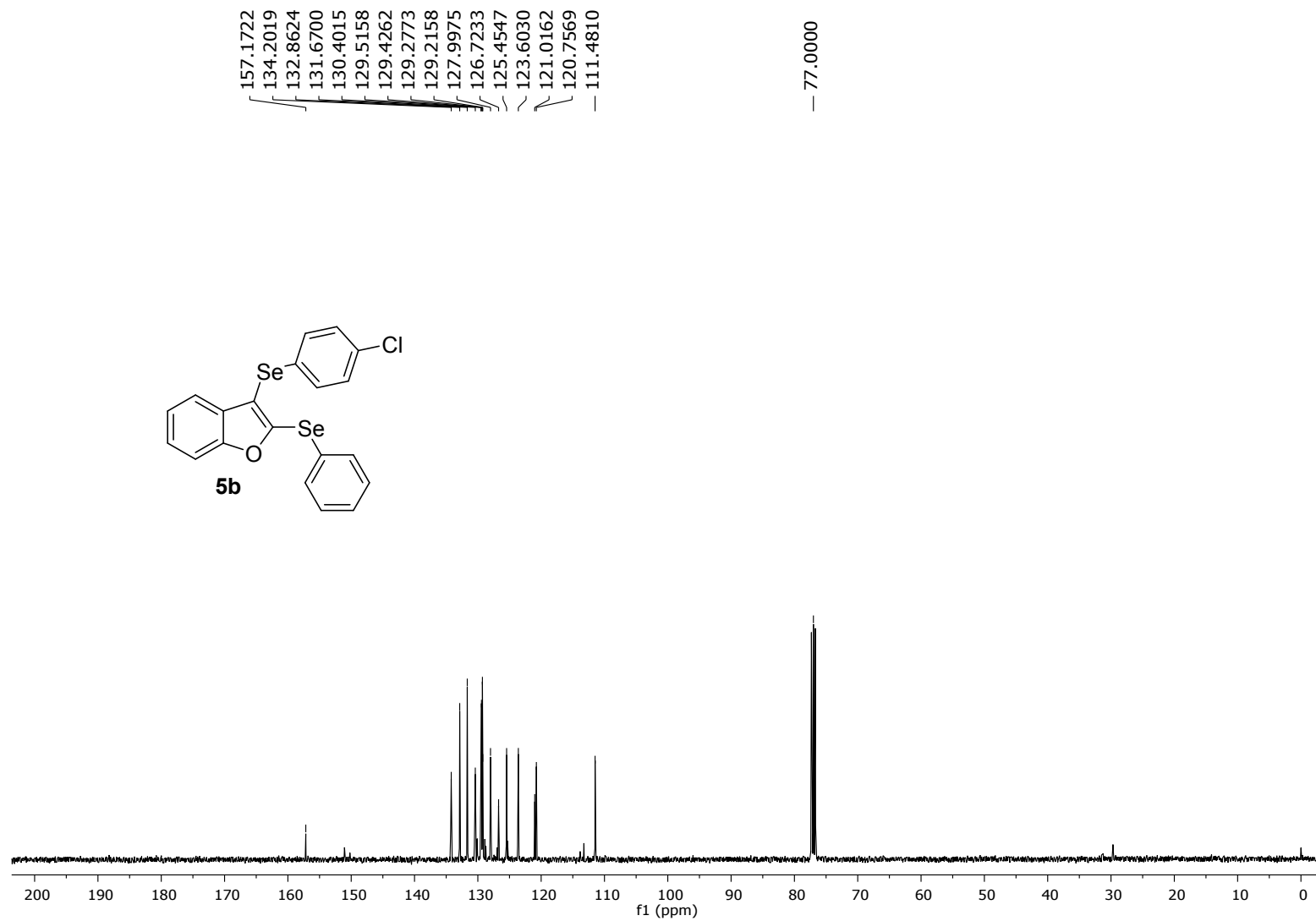


Figure S26: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[4-chlorophenyl]selanyl]-2-(phenylselanyl)benzo[*b*]furan **5b**.

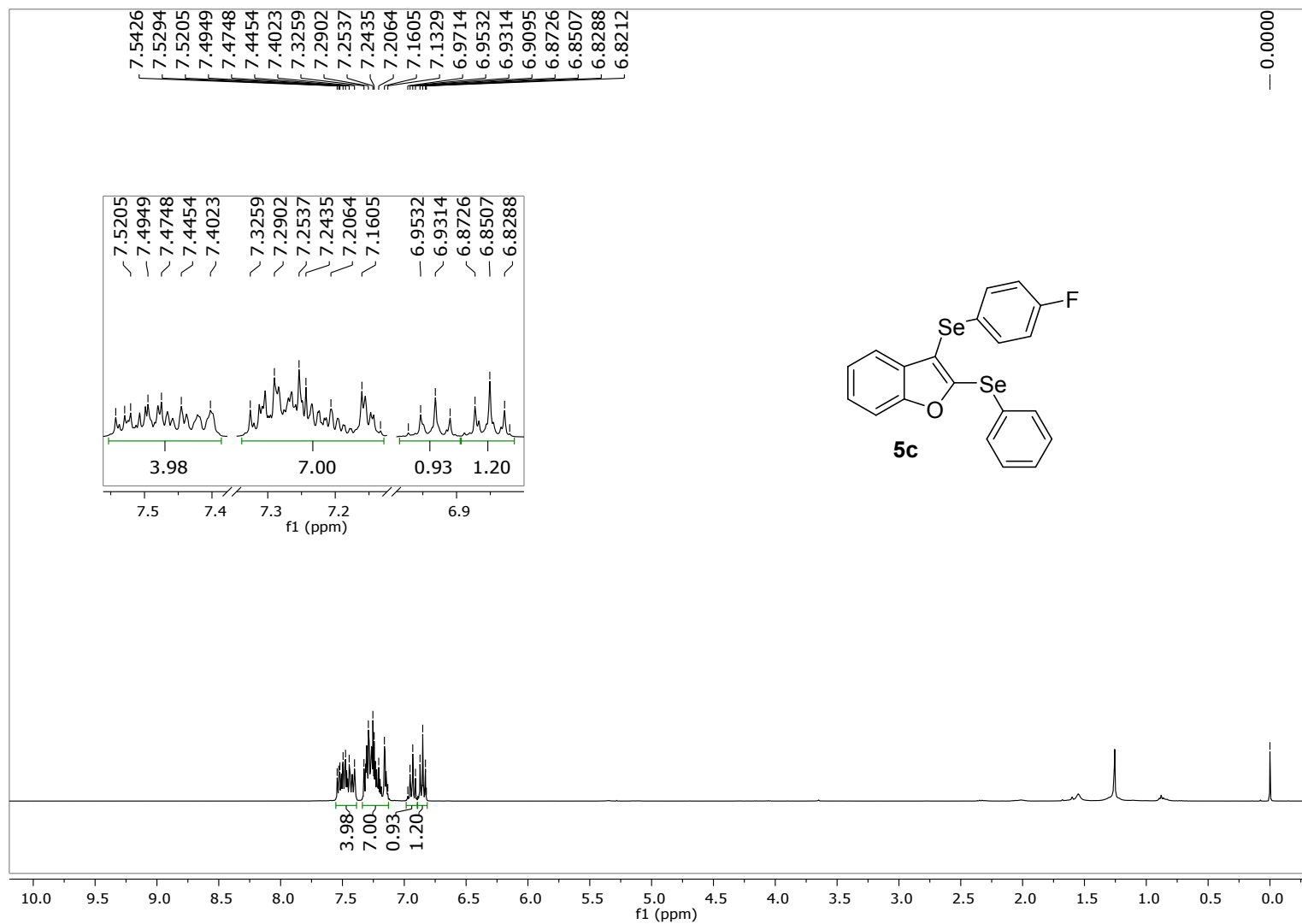


Figure S27: ^1H NMR (400 MHz, CDCl_3) spectrum 3-[(4-fluorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]furan **5c**.

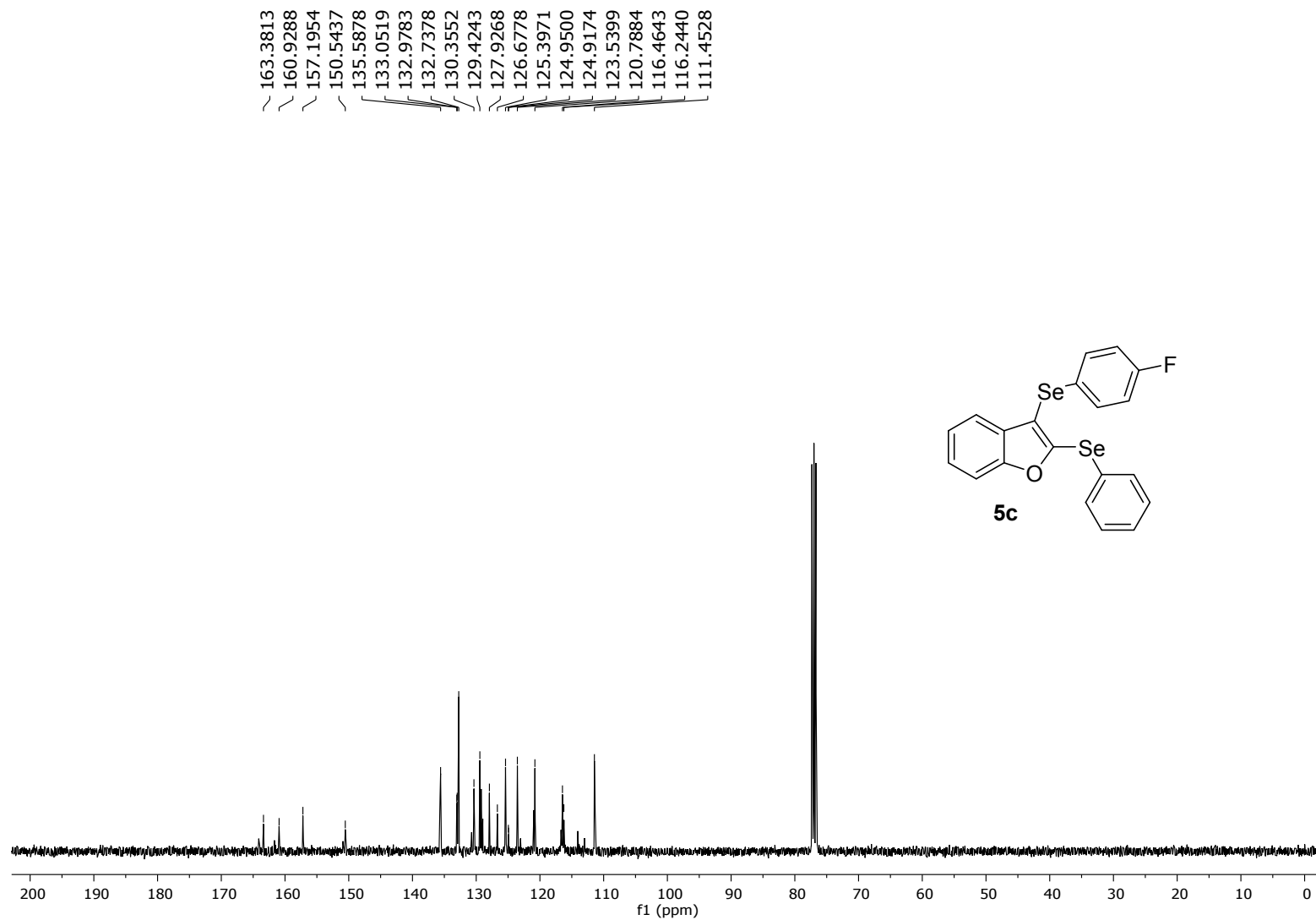


Figure S28: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-fluorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]furan **5c**.

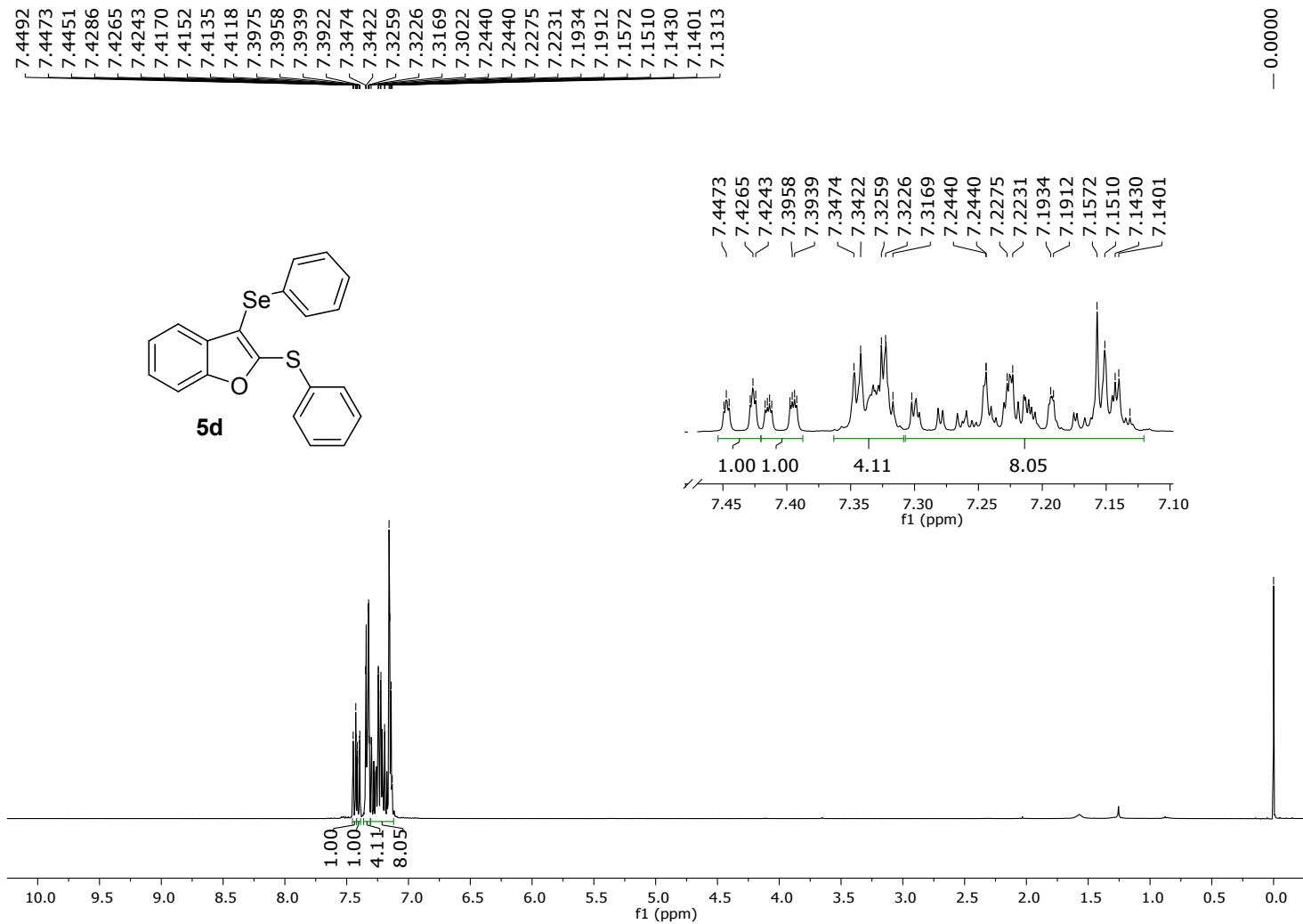


Figure S29: ^1H NMR (400 MHz, CDCl_3) spectrum 3-(phenylselanyl)-2-(phenylsulfanyl)benzo[*b*]furan **5d**.

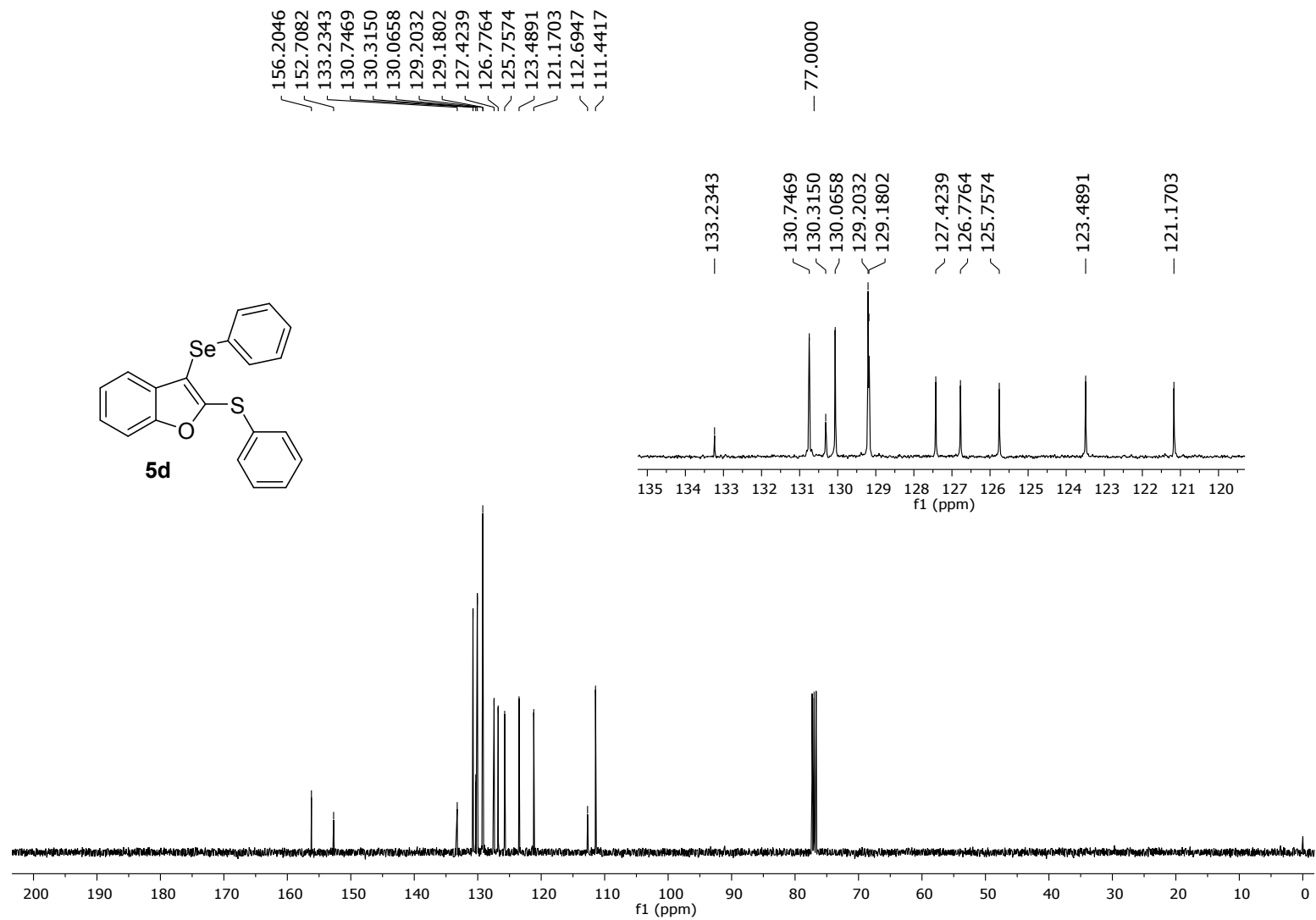


Figure S30: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-(phenylselanyl)-2-(phenylsulfanyl)benzo[*b*]furan **5d**.

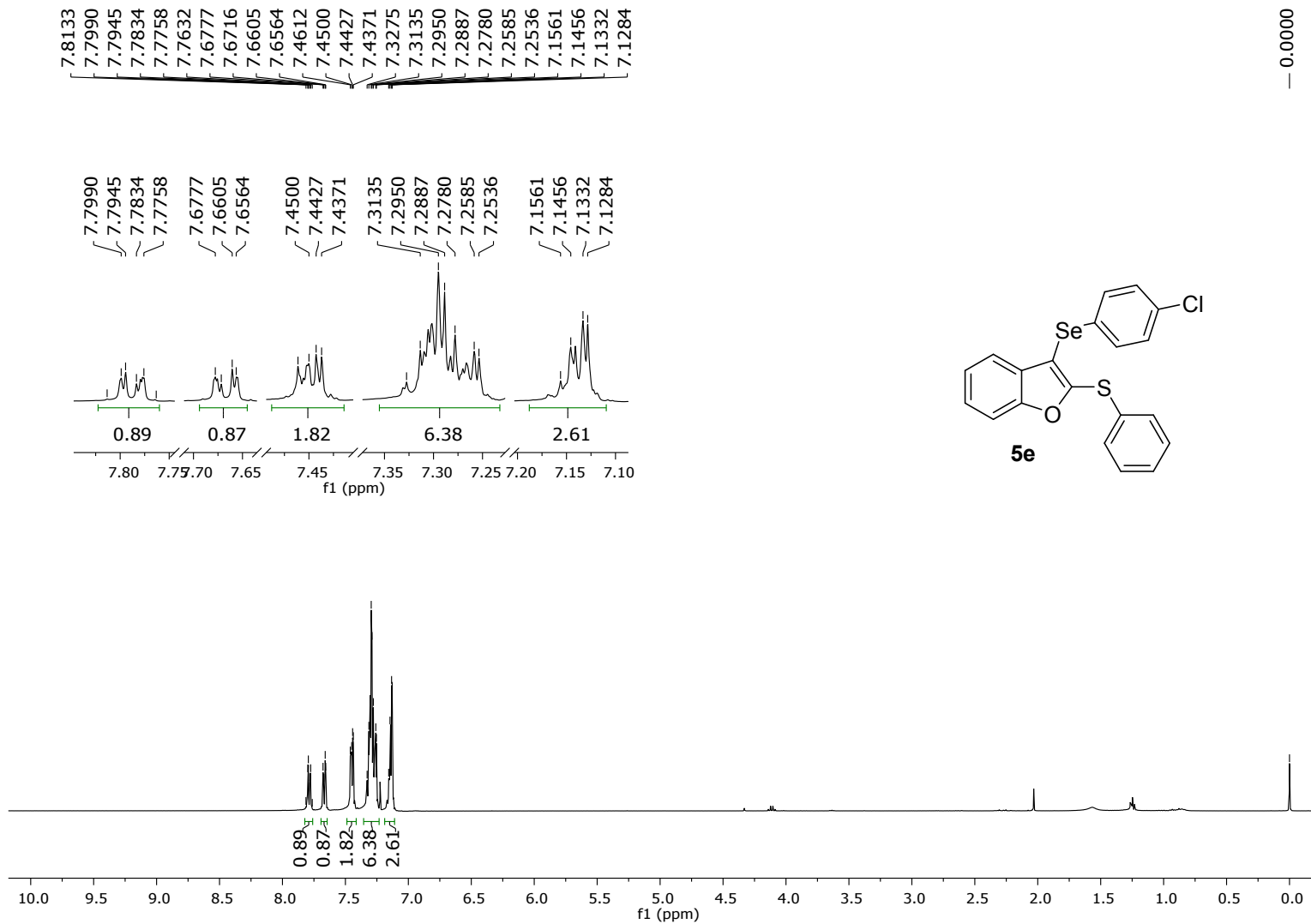


Figure S31: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylsulfanyl)benzo[*b*]furan **5e**.

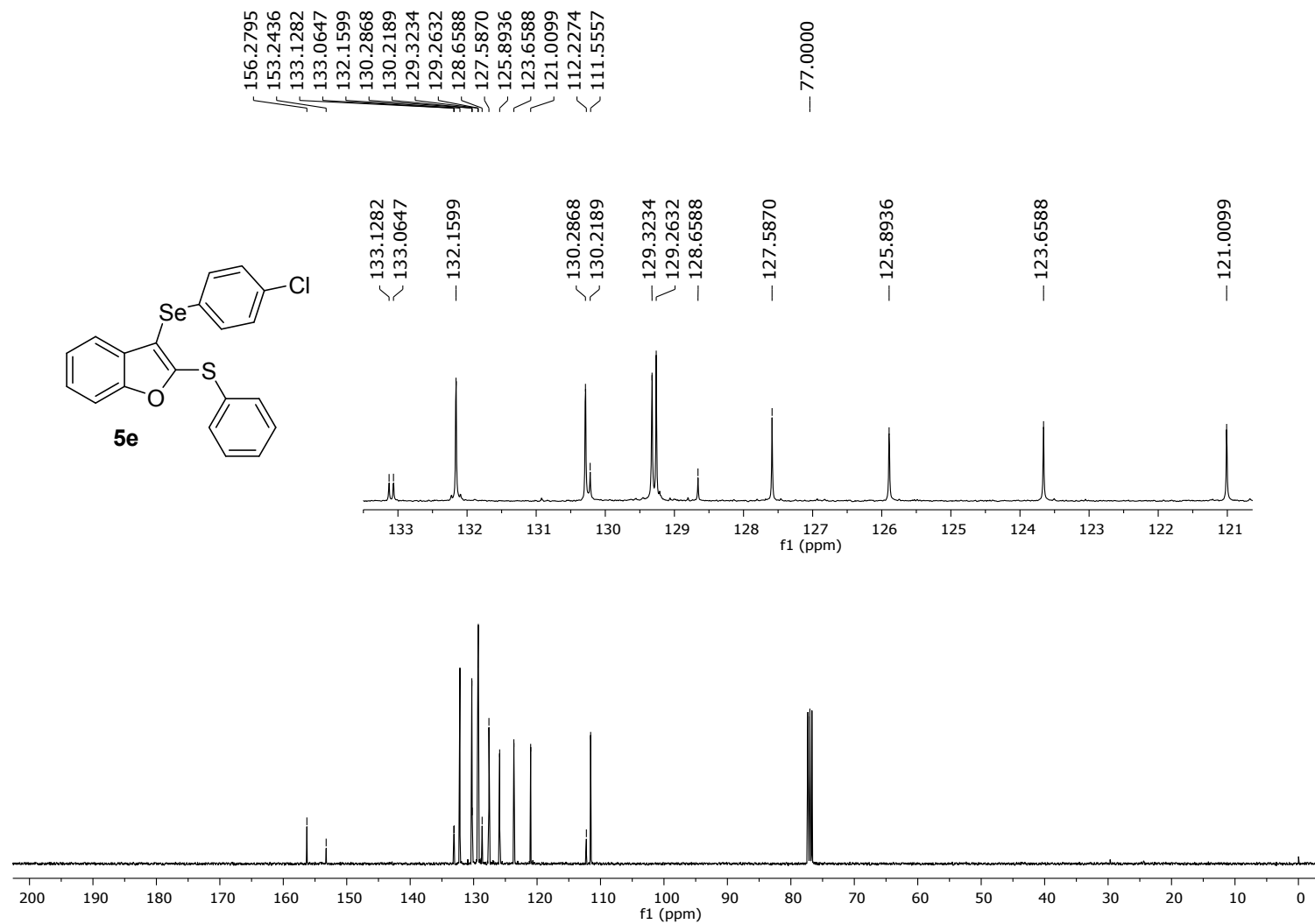


Figure S32: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylsulfanyl)benzo[*b*]furan **5e**.

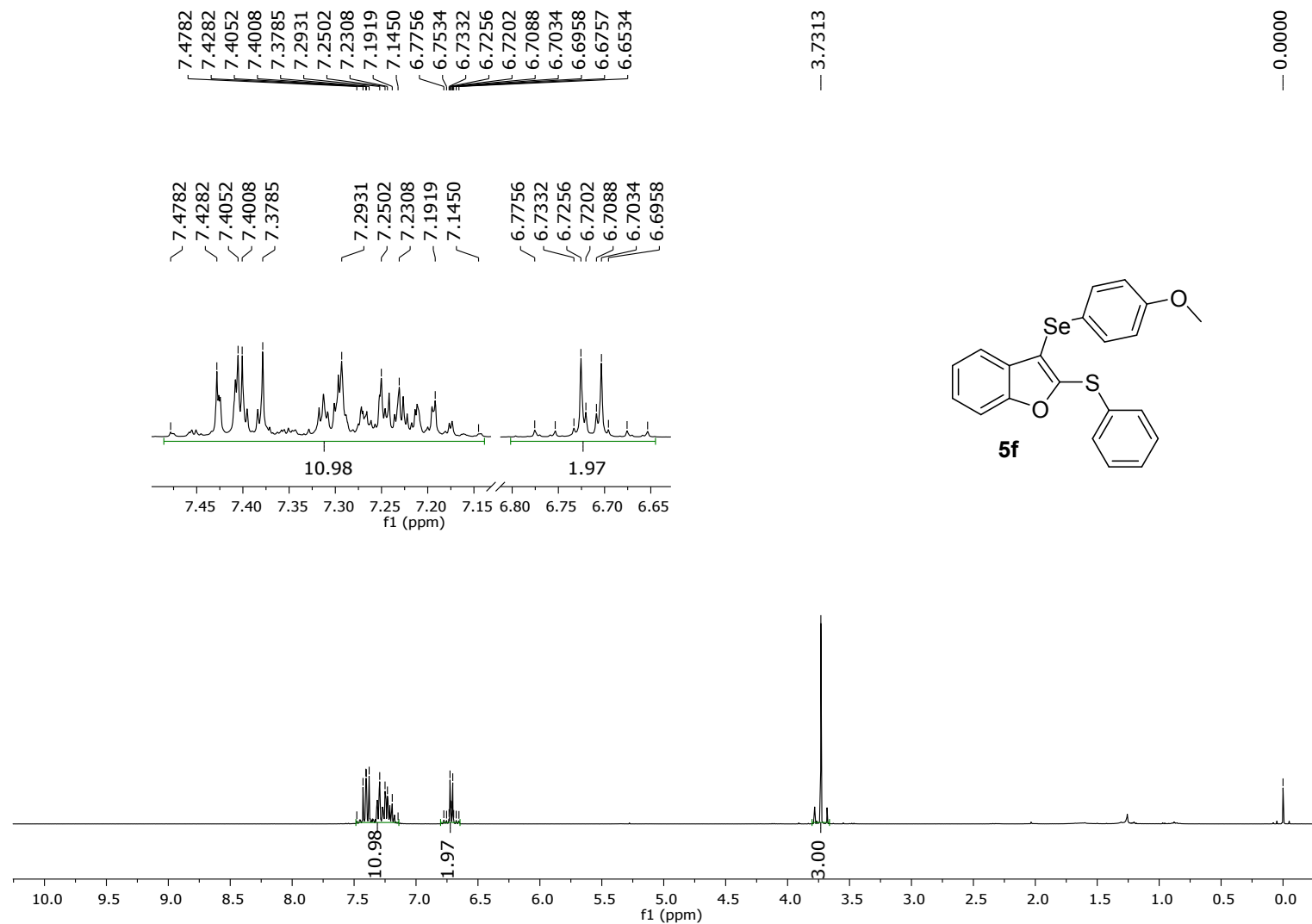


Figure S33: ^1H NMR (400 MHz, CDCl_3) spectrum 3-[(4-methoxyphenyl)selanyl]-2-(phenylsulfanyl)benzo[*b*]furan **5f**.

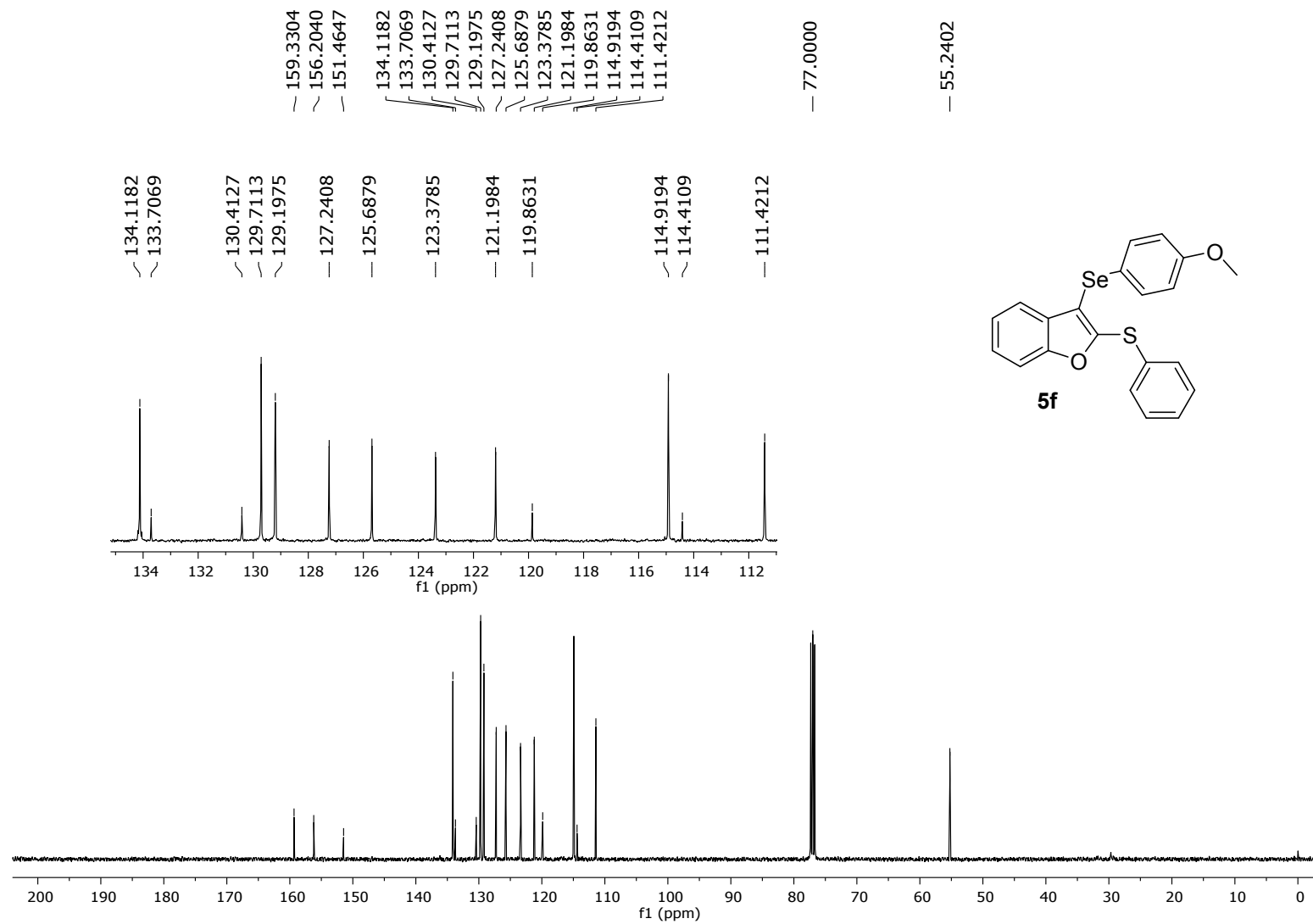


Figure S34: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-methoxyphenyl)selenyl]-2-(phenylsulfanyl)benzo[*b*]furan **5f**.

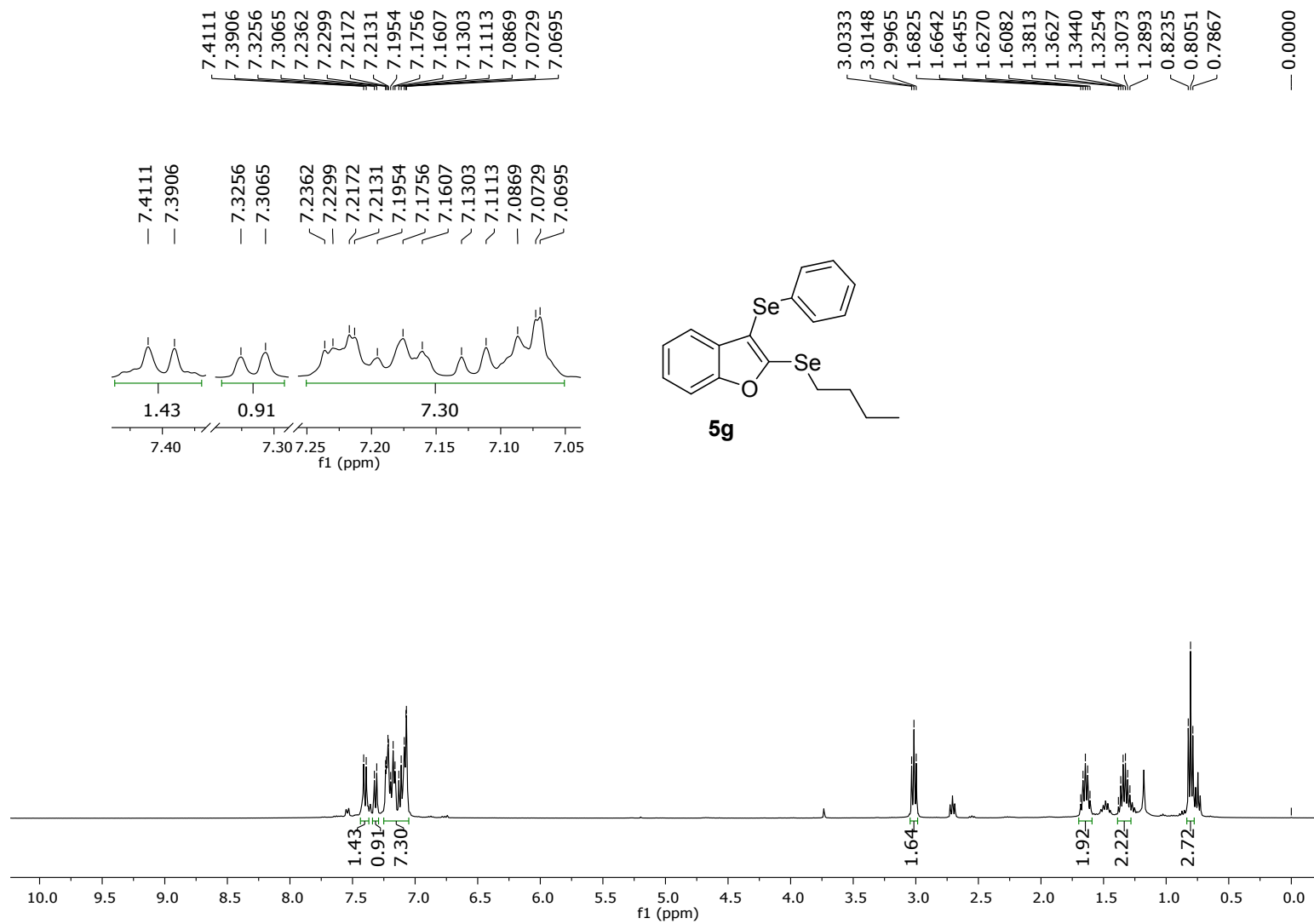


Figure S35: ¹H NMR (400 MHz, CDCl₃) spectrum 2-(butylselanyl)-3-(phenylselanyl)benzo[*b*]furan **5g**.

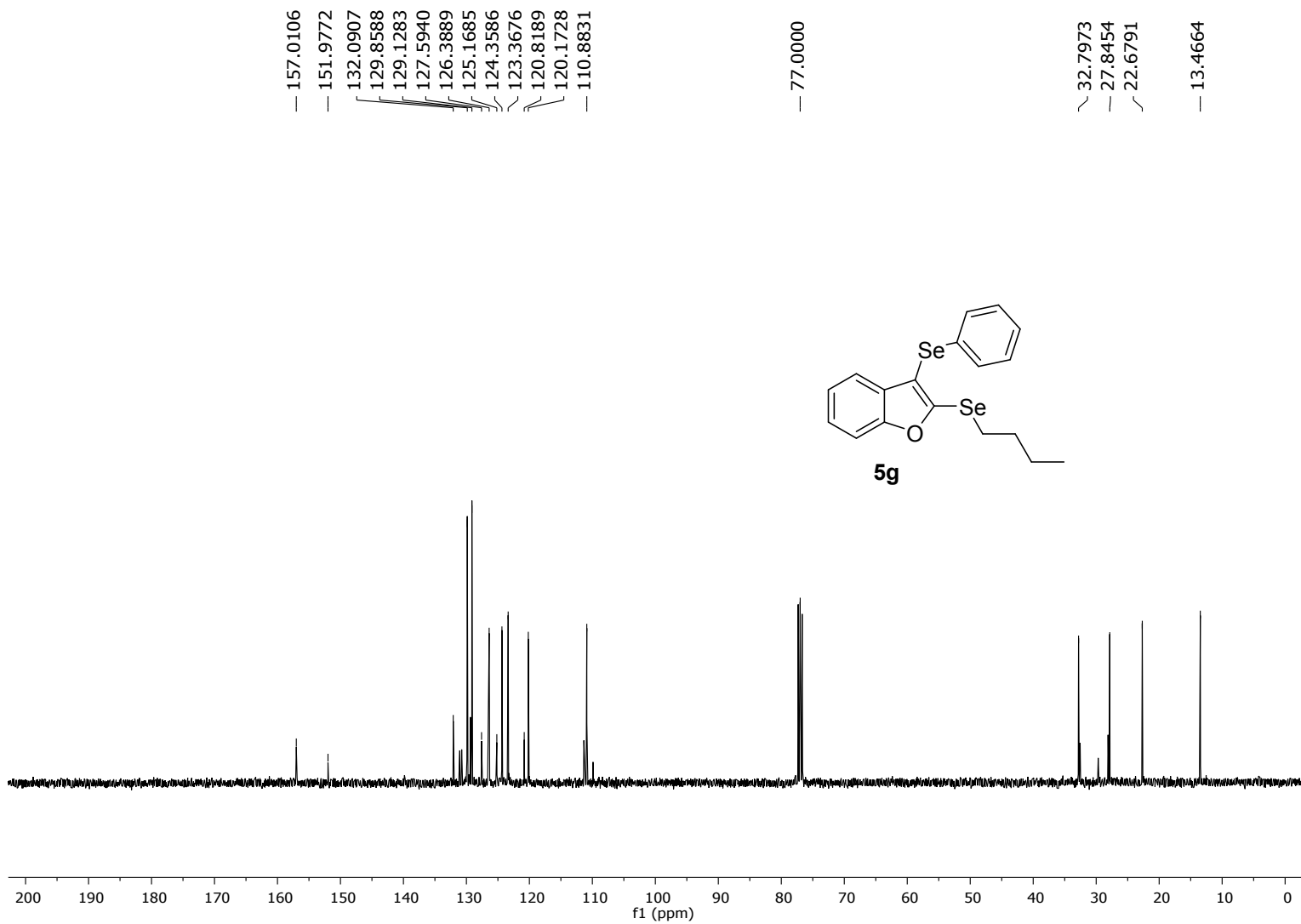


Figure S36: ¹³C NMR (100 MHz, CDCl₃) spectrum 2-(butylselanyl)-3-(phenylselanyl)benzo[*b*]furan **5g**.

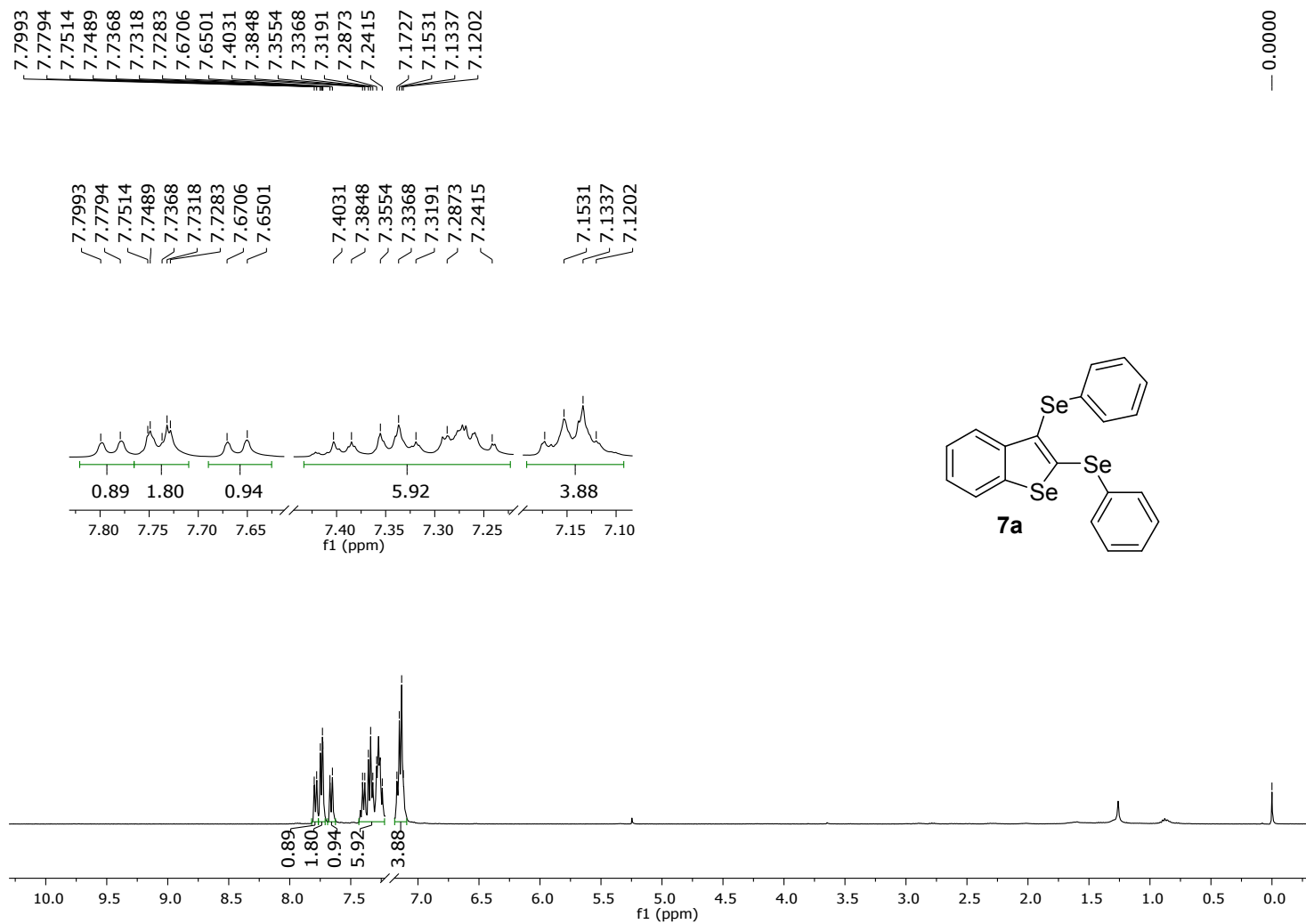


Figure S37: ¹H NMR (400 MHz, CDCl₃) spectrum 2,3-bis(phenylselanyl)benzo[*b*]selenophene **7a**.

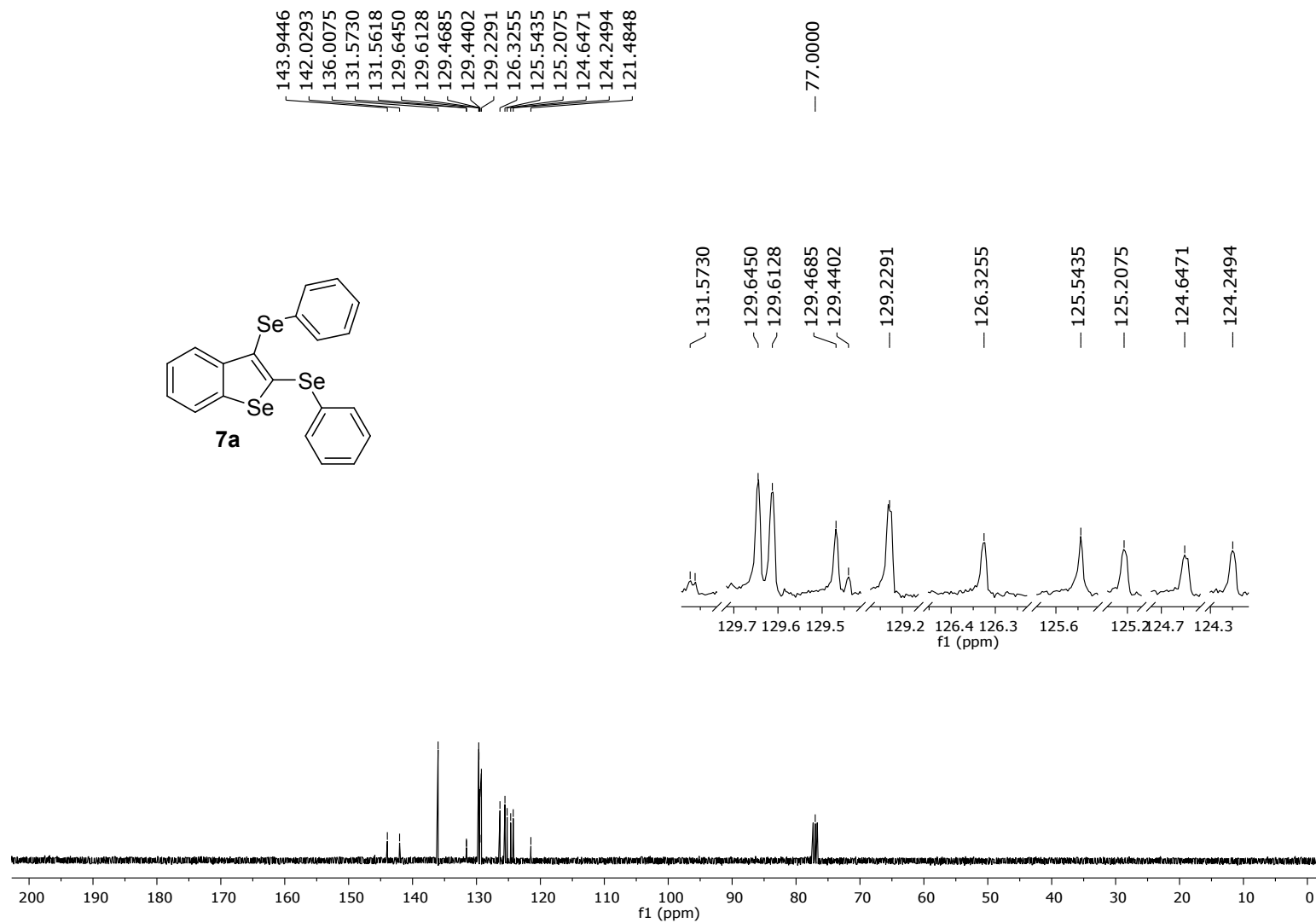


Figure S38: ^{13}C NMR (100 MHz, CDCl_3) spectrum 2,3-bis(phenylselanyl)benzo[*b*]selenophene **7a**.

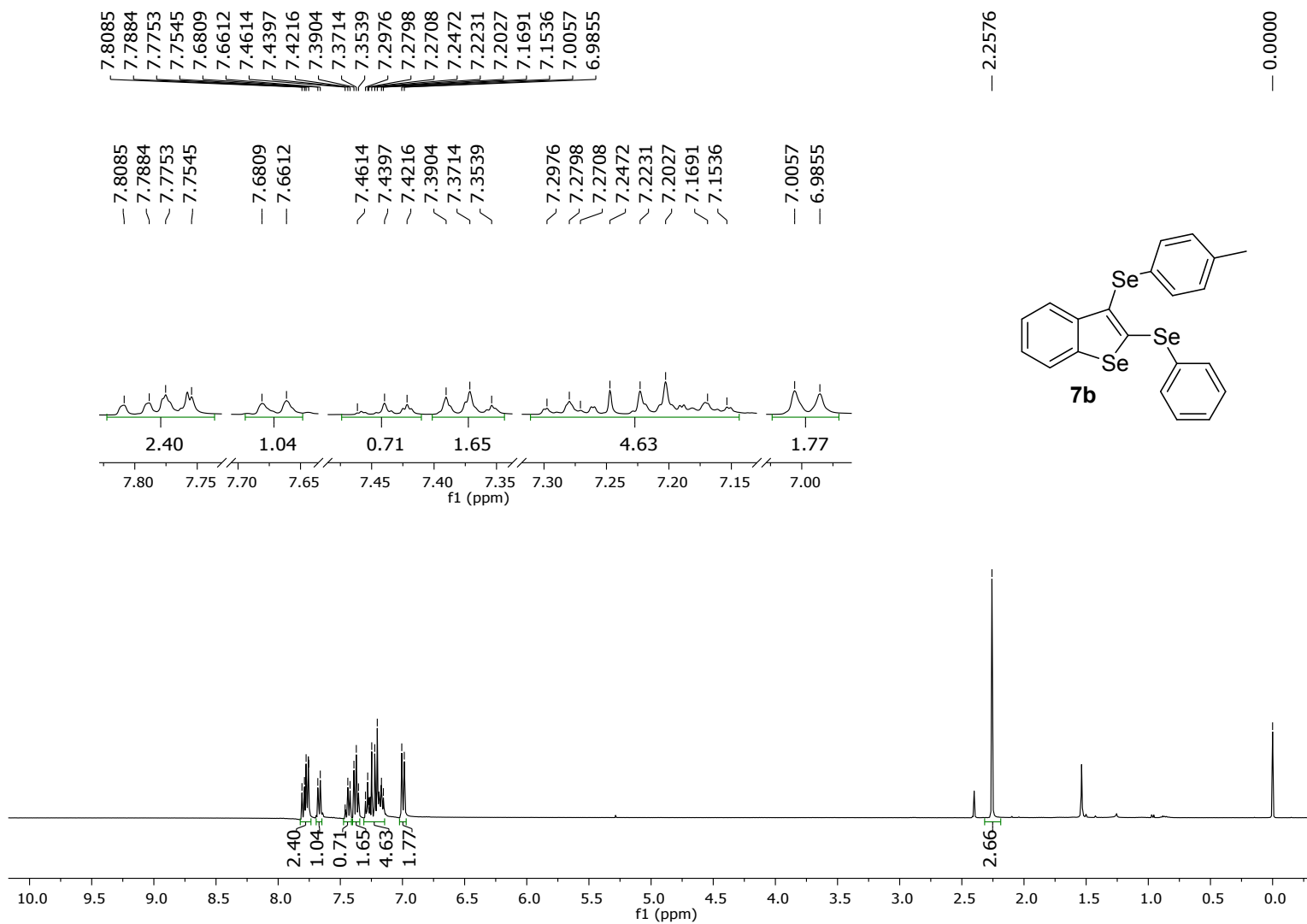


Figure S39: ^1H NMR (400 MHz, CDCl_3) spectrum 2-(phenylselanyl)-3-(4-tolylselanyl)benzo[*b*]selenophene **7b**.

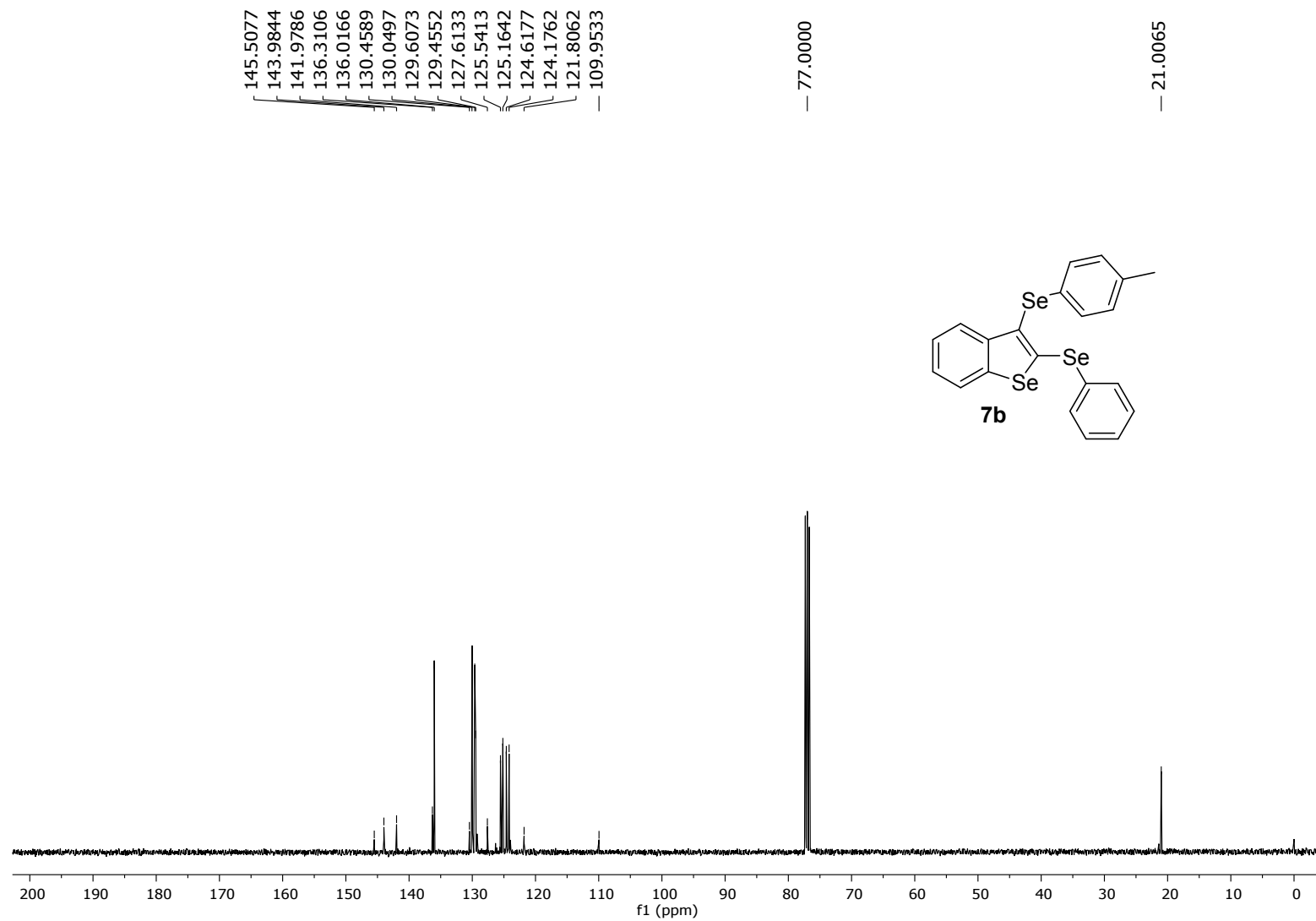


Figure S40: ^{13}C NMR (100 MHz, CDCl_3) spectrum 2-(phenylselanyl)-3-(4-tolylselanyl)benzo[*b*]selenophene **7b**.

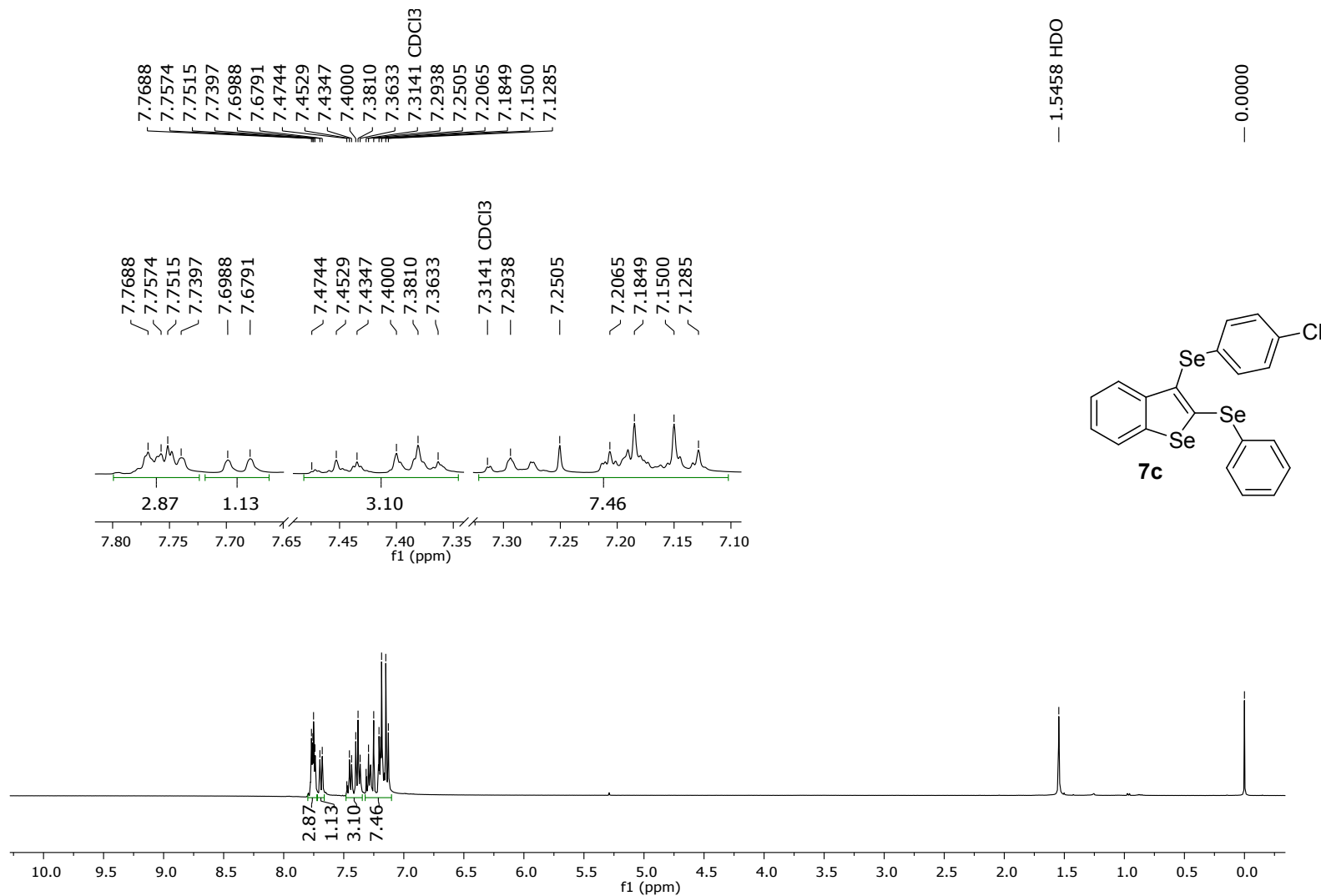


Figure S41: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]selenophene **7c**.

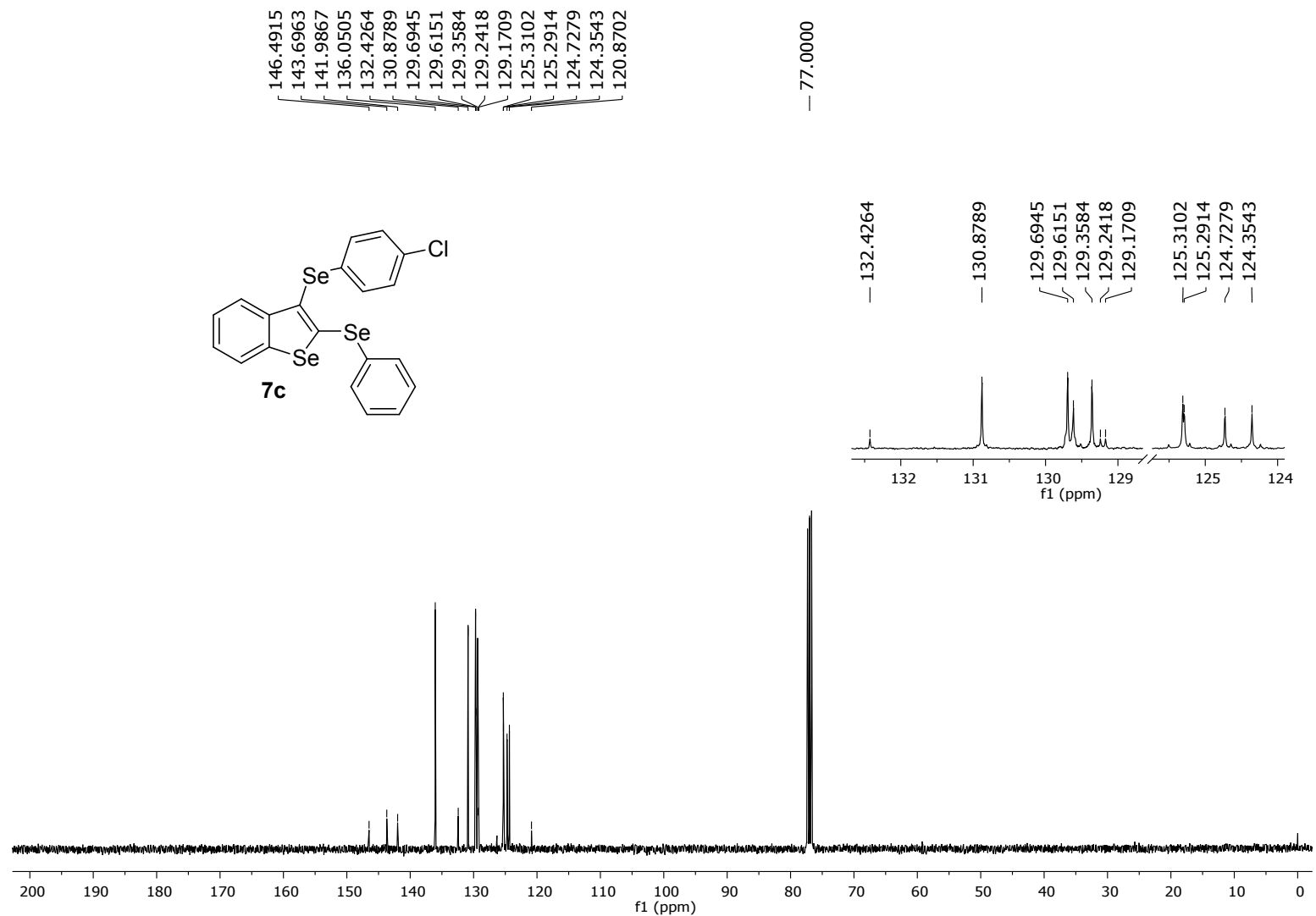


Figure S42: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-chlorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]selenophene **7c**.

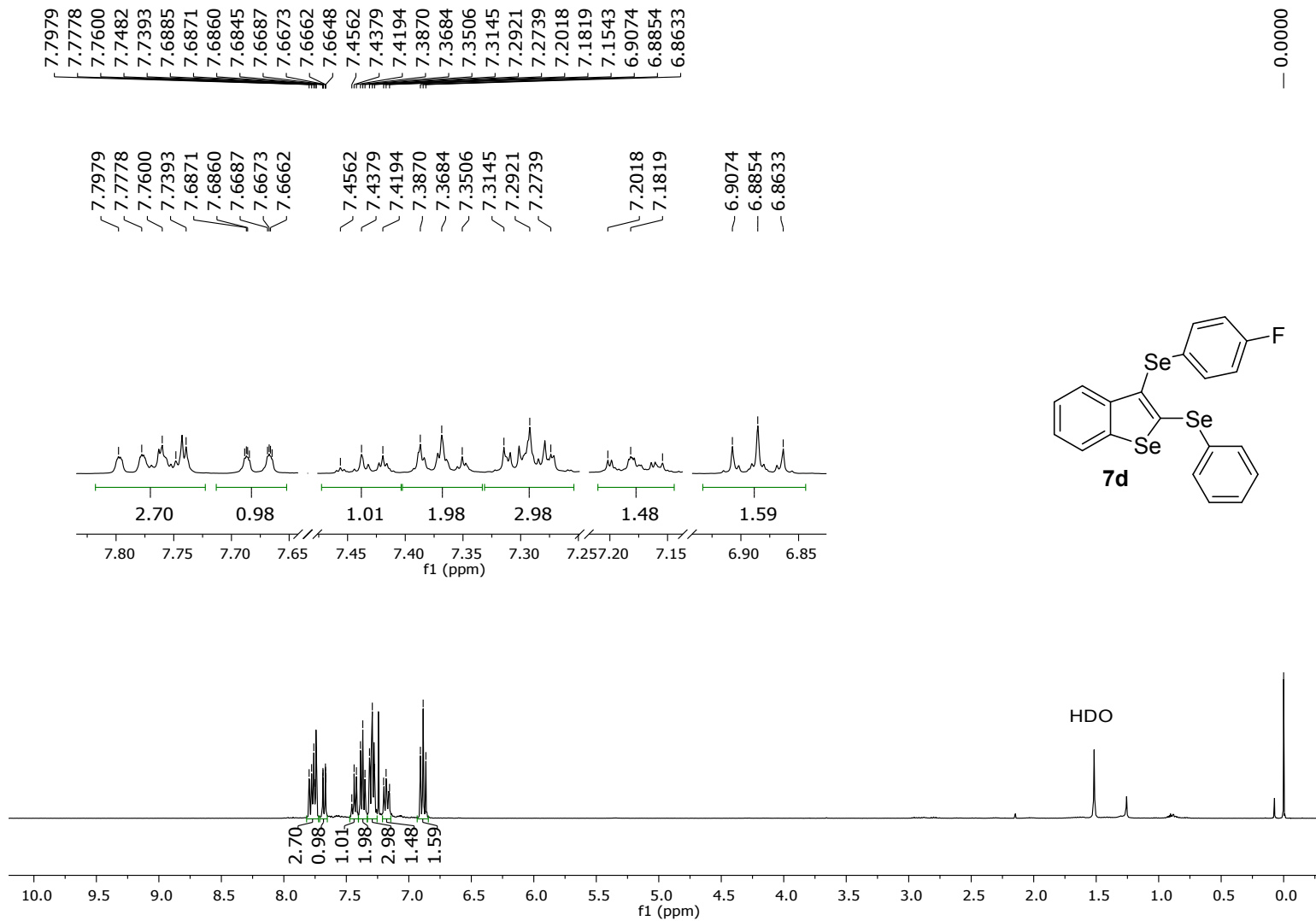


Figure S43: ¹H NMR (400 MHz, CDCl₃) spectrum 3-[(4-fluorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]selenophene **7d**.

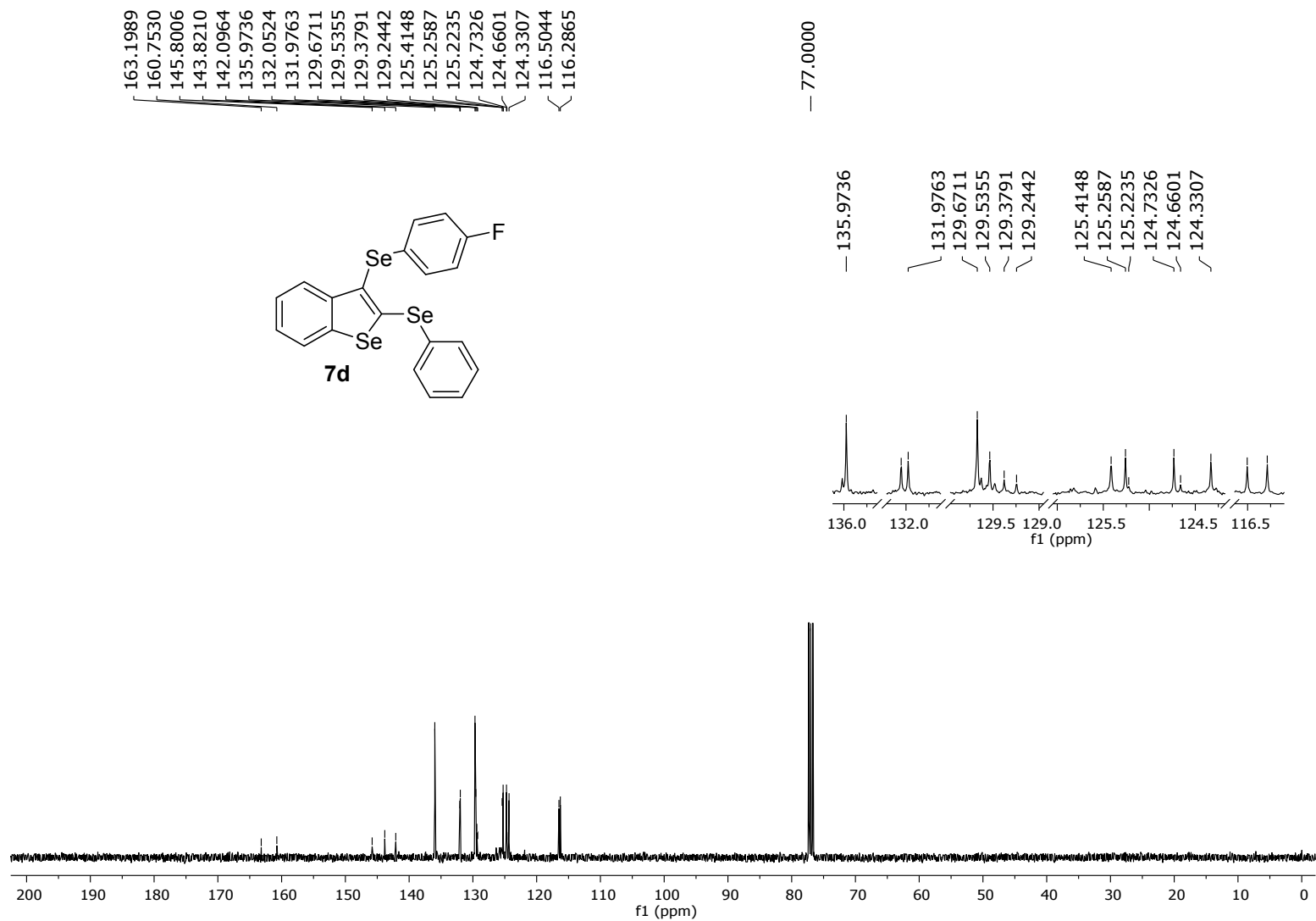


Figure S44: ¹³C NMR (100 MHz, CDCl₃) spectrum 3-[(4-fluorophenyl)selanyl]-2-(phenylselanyl)benzo[*b*]selenophene **7d**.

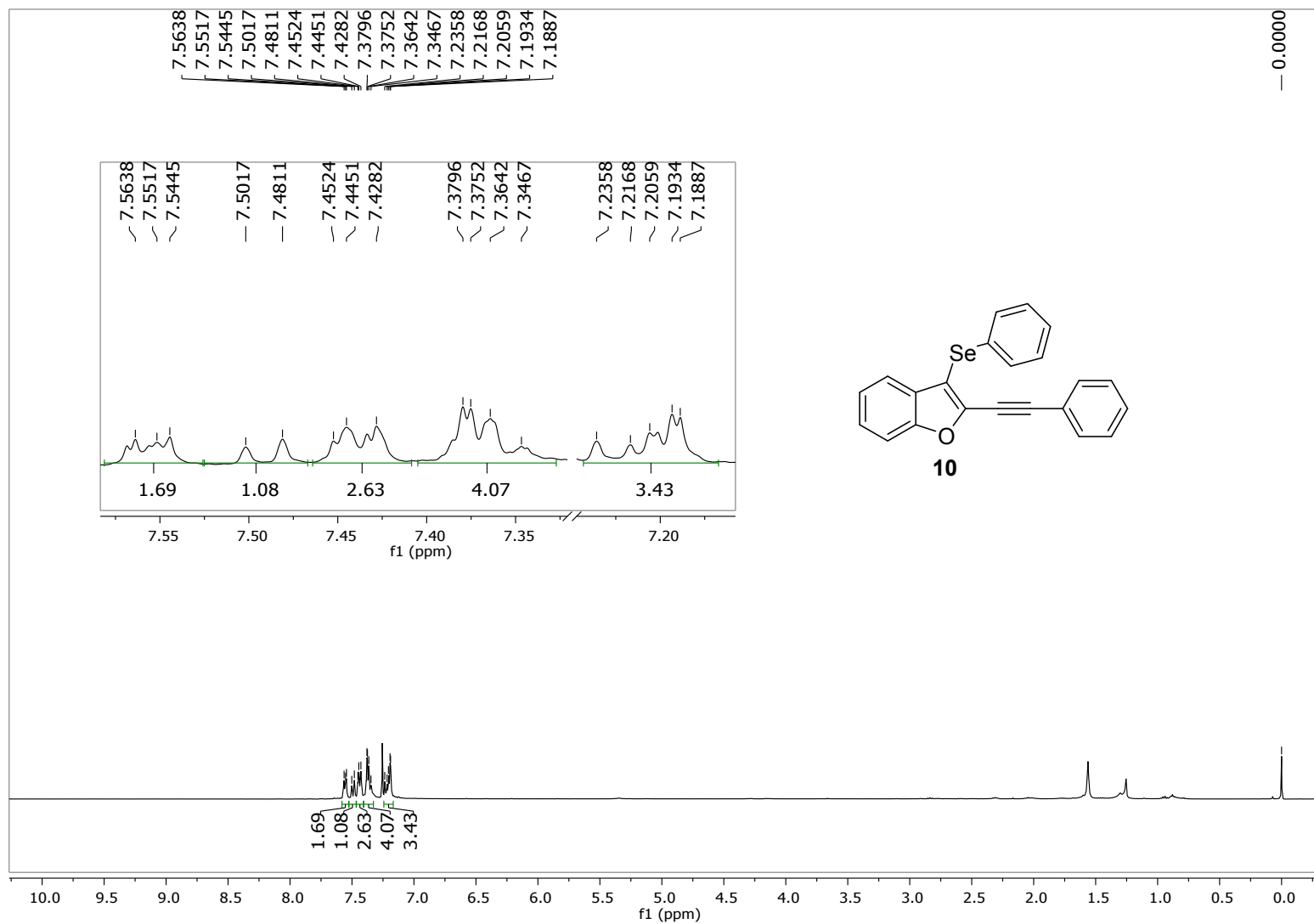


Figure S45: ¹H NMR (400 MHz, CDCl₃) spectrum 2-(phenylethynyl)-3-(phenylselanyl)benzo[*b*]furan **10**.

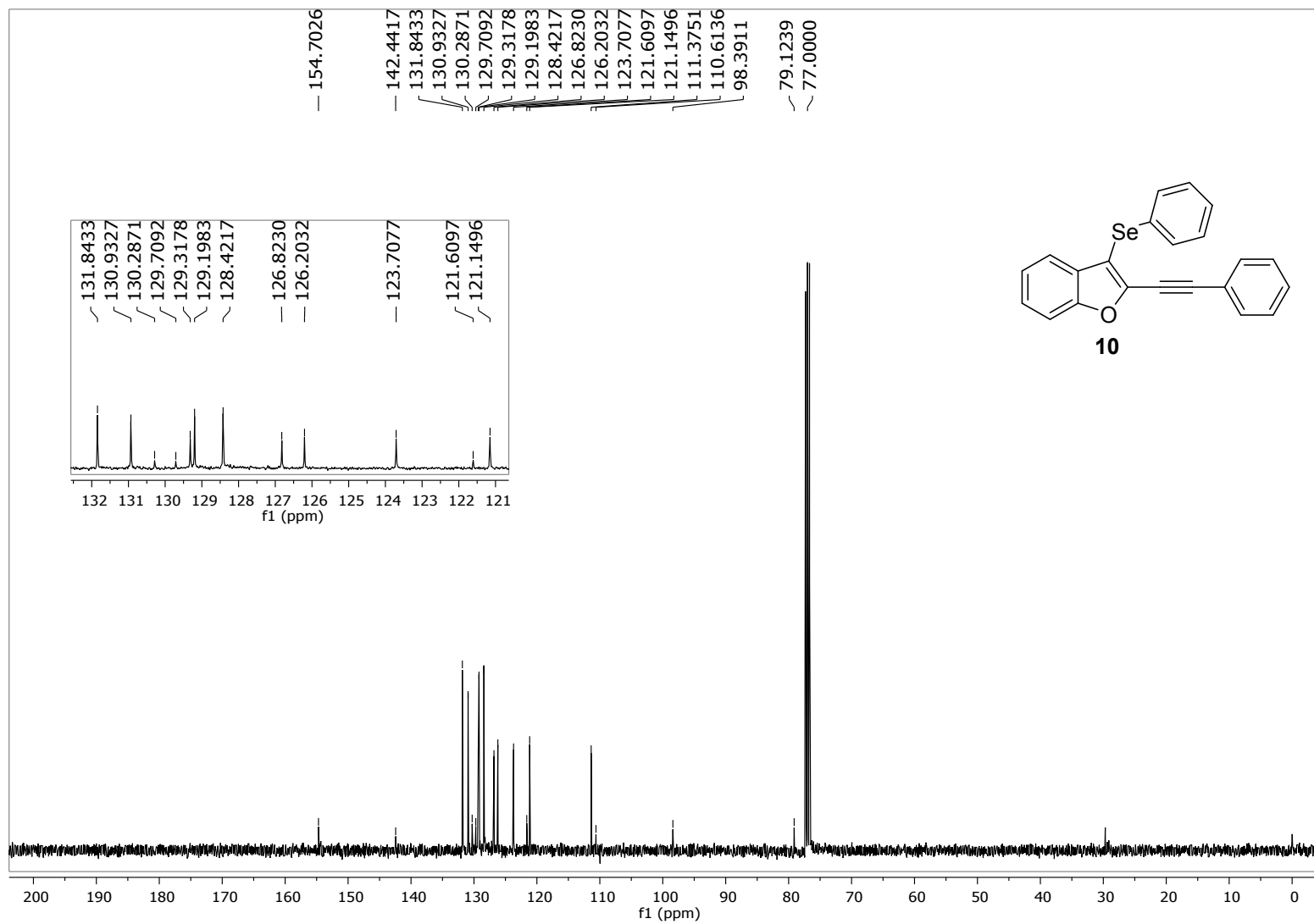
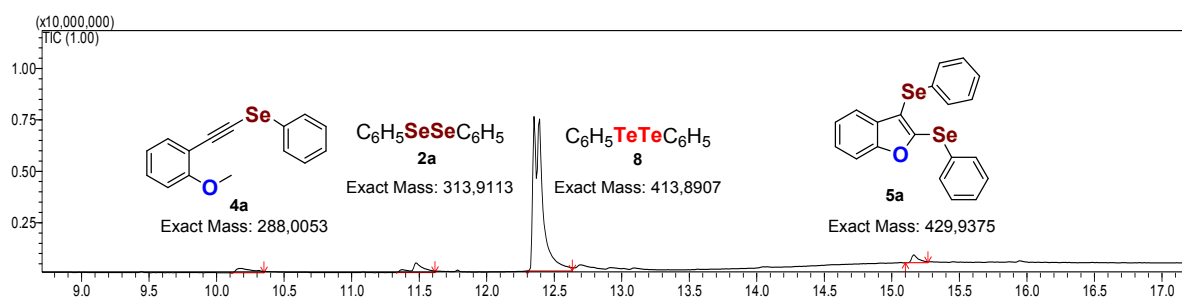


Figure S46: ¹³C NMR (100 MHz, CDCl₃) spectrum 2-(phenylethynyl)-3-(phenylselanyl)benzo[*b*]furan **10**.



Peak Report TIC									
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark
1	10.176	10.108	10.375	1844404	4.26	207375	2.42	8.89	MI
2	11.477	11.317	11.608	2954521	6.83	476790	5.56	6.20	MI
3	12.352	12.292	12.633	37045325	85.64	7516249	87.66	4.93	MI
4	15.162	15.075	15.283	1413785	3.27	374062	4.36	3.78	MI
				43258035	100.00	8574476	100.00		

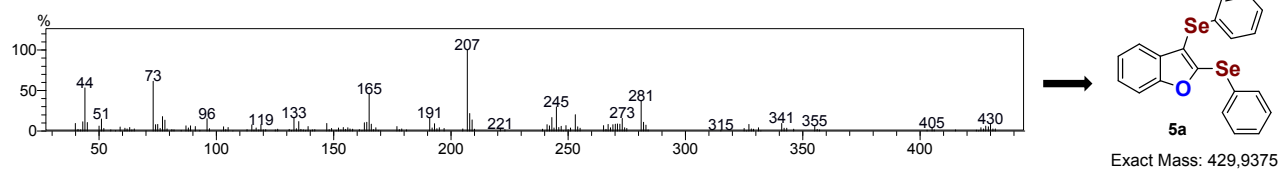
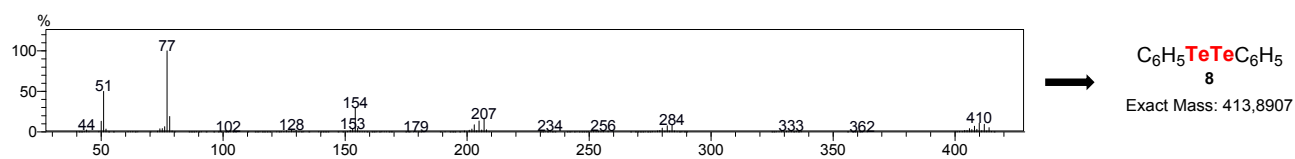
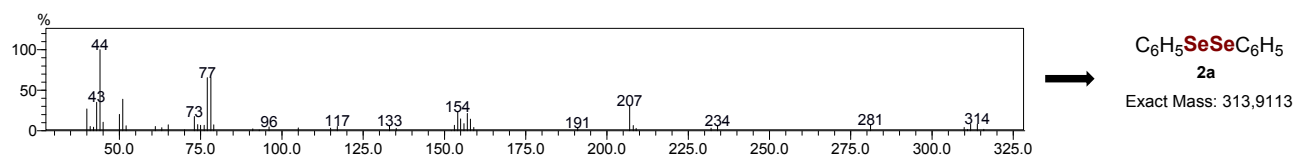
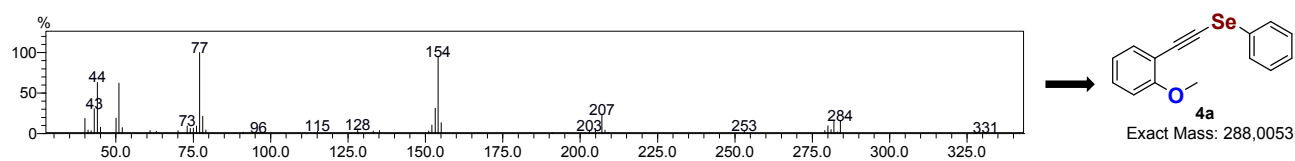
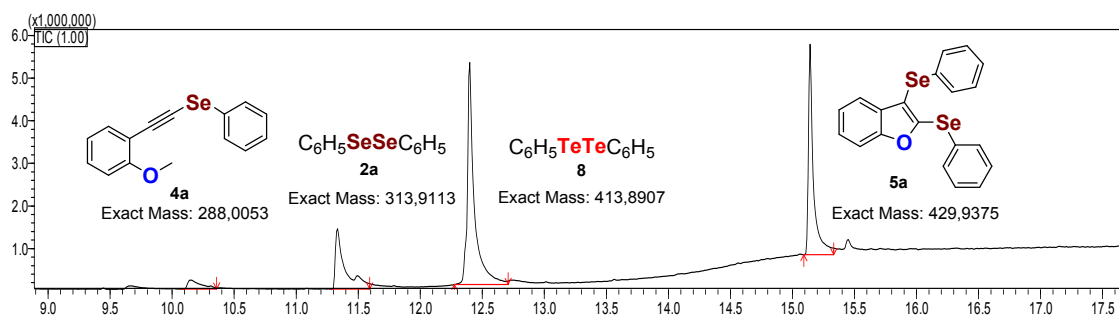


Figure S47: Cyclization reaction of selenoalkyne **4a** with diorganyl ditelluride **8** promoted by Oxone®.



Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark
1	10.148	10.075	10.358	1645446	3.80	210098	1.78	7.83	MI
2	11.332	11.283	11.592	7672895	17.71	1415356	12.02	5.42	MI
3	12.398	12.275	12.708	20154878	46.51	5213155	44.27	3.87	MI
4	15.142	15.092	15.333	13862081	31.99	4936043	41.92	2.81	MI
				43335300	100.00	11774652	100.00		

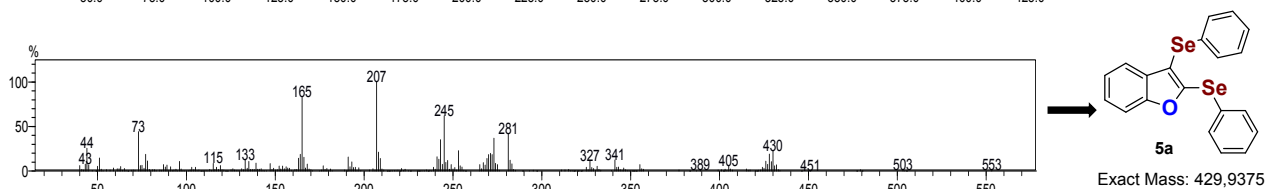
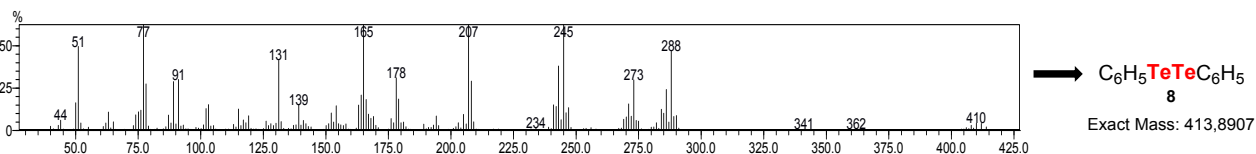
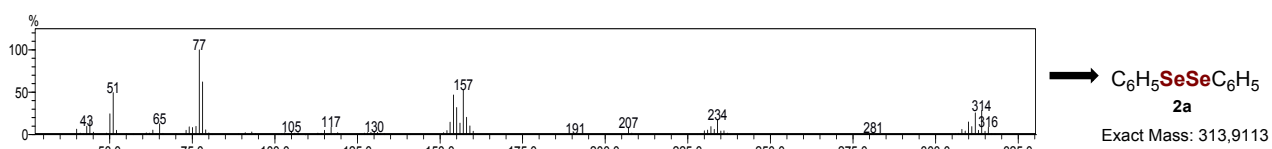
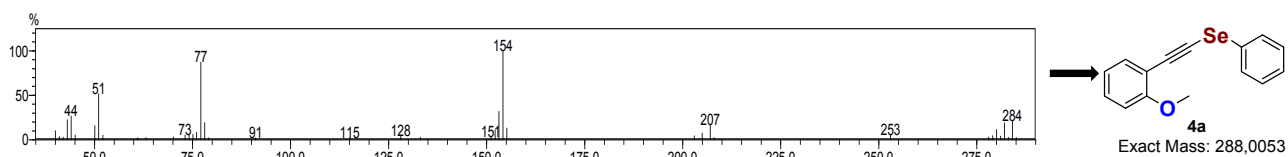


Figure S48: Cyclization reaction of teluroalkyne **4d** with diorganyl diselenide **2a** promoted by Oxone®.