

**Supporting informations  
for  
Novel (+)-neoisopulegol based- *O*-benzyl derivatives  
as antibacterial agents**

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**Table S1: Complete results of antimicrobial activities**

RSD Inhibitory effect (%) $\pm$ (%)							
		Gram positive		Gram negative		Yeast	
Analogue	Conc. ( $\mu\text{g/mL}$ )	<i>B. subtilis</i> SZMC0209	<i>S. aureus</i> SZMC14611	<i>E. coli</i> SZMC6271	<i>P. aeruginosa</i> SZMC23290	<i>C. albicans</i> SZMC1533	<i>C. krusei</i> SZMC1352
Nystatin	100	-	-	-	-	93.38 $\pm$ 2.13	92.01 $\pm$ 3.64
	10	-	-	-	-	92.88 $\pm$ 10.18	58.00 $\pm$ 9.21
Ampicillin	100	95.22 $\pm$ 8.40	81.88 $\pm$ 8.99	94.07 $\pm$ 3.61	29.03 $\pm$ 2.06	-	-
	10	93.00 $\pm$ 3.20	70.37 $\pm$ 6.15	89.37 $\pm$ 0.39	5.36 $\pm$ 8.32	-	-
3	100	97.60 $\pm$ 6.42	57.57 $\pm$ 9.93	26.50 $\pm$ 2.28	49.10 $\pm$ 7.52	9.38 $\pm$ 7.95	-
	10	59.58 $\pm$ 8.06	10.75 $\pm$ 5.41	24.19 $\pm$ 3.99	33.91 $\pm$ 10.35	5.22 $\pm$ 6.73	-
5a	100	92.82 $\pm$ 4.69	80.07 $\pm$ 2.21	38.70 $\pm$ 5.87	54.06 $\pm$ 9.08	91.56 $\pm$ 1.27	94.88 $\pm$ 2.18
	10	48.25 $\pm$ 6.16	-	24.67 $\pm$ 1.84	26.68 $\pm$ 5.56	8.67 $\pm$ 3.99	-
5b	100	86.35 $\pm$ 1.88	71.48 $\pm$ 1.28	29.58 $\pm$ 0.18	46.66 $\pm$ 1.37	92.88 $\pm$ 2.63	93.62 $\pm$ 0.80
	10	23.23 $\pm$ 3.15	-	16.80 $\pm$ 2.82	6.19 $\pm$ 1.77	-	-
6a	100	-	-	13.63 $\pm$ 0.90	4.07 $\pm$ 5.69	-	32.04 $\pm$ 1.45
	10	-	-	14.28 $\pm$ 3.11	-	-	0.16 $\pm$ 28.77
6b	100	-	6.78 $\pm$ 3.84	23.07 $\pm$ 3.03	-	7.32 $\pm$ 1.18	-
	10	-	-	18.66 $\pm$ 2.08	0.52 $\pm$ 8.77	6.35 $\pm$ 1.81	-
7a	100	81.51 $\pm$ 4.73	70.66 $\pm$ 0.91	9.10 $\pm$ 1.86	-	87.90 $\pm$ 10.46	-
	10	-	-	9.82 $\pm$ 8.12	-	2.24 $\pm$ 5.95	-
7b	100	95.34 $\pm$ 4.81	92.34 $\pm$ 1.32	23.19 $\pm$ 0.21	41.59 $\pm$ 3.53	22.68 $\pm$ 8.67	29.02 $\pm$ 4.69
	10	50.00 $\pm$ 7.21	2.69 $\pm$ 2.48	21.21 $\pm$ 6.20	29.09 $\pm$ 1.97	6.60 $\pm$ 1.65	-
8a	100	49.17 $\pm$ 2.41	3.62 $\pm$ 1.47	11.73 $\pm$ 2.01	47.26 $\pm$ 2.69	17.96 $\pm$ 1.27	-
	10	35.67 $\pm$ 4.38	2.45 $\pm$ 1.08	16.13 $\pm$ 3.04	38.18 $\pm$ 2.16	7.64 $\pm$ 0.46	7.56 $\pm$ 38.36
8b	100	29.88 $\pm$ 4.78	-	-	40.81 $\pm$ 2.35	14.63 $\pm$ 0.25	-
	10	18.40 $\pm$ 2.09	-	9.06 $\pm$ 0.85	35.05 $\pm$ 3.94	-	-
9a	100	52.37 $\pm$ 5.19	-	16.94 $\pm$ 4.24	29.26 $\pm$ 1.31	7.58 $\pm$ 1.85	-
	10	-	-	12.39 $\pm$ 4.49	8.37 $\pm$ 6.25	4.81 $\pm$ 2.74	-
9b	100	51.60 $\pm$ 10.30	-	13.92 $\pm$ 0.87	4.13 $\pm$ 1.12	2.33 $\pm$ 1.21	4.90 $\pm$ 49.13
	10	38.16 $\pm$ 3.93	-	12.08 $\pm$ 1.48	-	2.76 $\pm$ 1.08	-
10	100	95.16 $\pm$ 2.81	90.71 $\pm$ 3.27	25.74 $\pm$ 4.75	50.87 $\pm$ 9.72	95.91 $\pm$ 16.31	-
	10	55.43 $\pm$ 15.48	-	16.90 $\pm$ 2.19	44.05 $\pm$ 7.57	6.57 $\pm$ 3.05	-
12a	100	95.16 $\pm$ 6.46	2.81 $\pm$ 6.51	24.95 $\pm$ 4.61	70.85 $\pm$ 6.49	95.83 $\pm$ 11.18	-
	10	73.41 $\pm$ 5.45	-	17.14 $\pm$ 4.41	47.81 $\pm$ 7.92	9.34 $\pm$ 5.24	-
12b	100	91.84 $\pm$ 6.01	83.11 $\pm$ 2.61	50.07 $\pm$ 10.97	75.84 $\pm$ 7.14	94.50 $\pm$ 0.97	67.59 $\pm$ 16.45
	10	32.17 $\pm$ 11.19	-	14.39 $\pm$ 4.75	58.24 $\pm$ 4.20	2.44 $\pm$ 2.28	-
13a	100	6.59 $\pm$ 2.79	-	-	21.30 $\pm$ 6.68	-	-
	10	-	-	10.01 $\pm$ 7.48	-	1.83 $\pm$ 4.80	-
13b	100	51.10 $\pm$ 12.82	-	12.30 $\pm$ 3.93	48.58 $\pm$ 1.33	5.66 $\pm$ 2.32	-
	10	45.85 $\pm$ 4.38	-	11.82 $\pm$ 9.78	47.75 $\pm$ 2.01	5.68 $\pm$ 3.59	-
14a	100	92.67 $\pm$ 3.90	82.35 $\pm$ 3.19	6.48 $\pm$ 0.00	52.97 $\pm$ 7.47	2.69 $\pm$ 2.37	-

RSD Inhibitory effect (%) $\pm$ (%)							
		Gram positive		Gram negative		Yeast	
Analogue	Conc. ( $\mu\text{g/mL}$ )	<i>B. subtilis</i> SZMC0209	<i>S. aureus</i> SZMC14611	<i>E. coli</i> SZMC6271	<i>P. aeruginosa</i> SZMC23290	<i>C. albicans</i> SZMC1533	<i>C. krusei</i> SZMC1352
	10	-	1.87 $\pm$ 6.30	12.92 $\pm$ 5.21	44.00 $\pm$ 1.32	0.09 $\pm$ 5.55	-
15a	100	38.49 $\pm$ 6.18	-	3.57 $\pm$ 2.04	56.86 $\pm$ 11.05	6.66 $\pm$ 5.02	-
	10	7.77 $\pm$ 34.76	-	17.28 $\pm$ 0.91	44.31 $\pm$ 4.75	6.53 $\pm$ 3.65	-
16a	100	-	-	2.34 $\pm$ 5.51	28.43 $\pm$ 2.27	-	-
	10	-	-	8.51 $\pm$ 8.10	24.45 $\pm$ 1.41	-	4.53 $\pm$ 20.51
16b	100	3.09 $\pm$ 24.95	5.55 $\pm$ 5.25	24.29 $\pm$ 0.82	44.60 $\pm$ 6.69	1.14 $\pm$ 2.76	-
	10	-	7.25 $\pm$ 5.79	15.09 $\pm$ 0.78	36.77 $\pm$ 11.02	3.42 $\pm$ 1.50	4.64 $\pm$ 54.48
18a	100	-	-	16.80 $\pm$ 0.79	16.54 $\pm$ 1.30	-	-
	10	-	-	11.94 $\pm$ 0.25	17.34 $\pm$ 3.26	-	0.74 $\pm$ 48.92
20a	100	84.57 $\pm$ 3.18	70.13 $\pm$ 0.90	22.02 $\pm$ 2.97	-	91.35 $\pm$ 1.07	-
	10	89.70 $\pm$ 1.32	65.81 $\pm$ 0.51	2.36 $\pm$ 2.13	-	6.76 $\pm$ 8.04	14.72 $\pm$ 10.68
20b	100	78.34 $\pm$ 2.51	69.49 $\pm$ 0.57	22.78 $\pm$ 3.27	-	90.74 $\pm$ 2.90	79.88 $\pm$ 3.39
	10	78.43 $\pm$ 5.39	61.84 $\pm$ 0.27	17.87 $\pm$ 3.01	-	80.54 $\pm$ 17.23	-
21a	100	53.71 $\pm$ 2.83	8.71 $\pm$ 2.58	15.80 $\pm$ 1.19	35.11 $\pm$ 6.17	5.54 $\pm$ 4.07	-
	10	-	-	14.35 $\pm$ 3.99	25.39 $\pm$ 9.90	1.92 $\pm$ 4.53	-
21b	100	15.01 $\pm$ 3.04	10.23 $\pm$ 2.37	7.27 $\pm$ 2.34	33.25 $\pm$ 1.72	7.85 $\pm$ 4.93	-
	10	-	-	4.58 $\pm$ 8.16	24.48 $\pm$ 10.32	-	-
22a	100	83.44 $\pm$ 20.97	76.39 $\pm$ 1.13	10.96 $\pm$ 0.90	32.16 $\pm$ 8.18	37.72 $\pm$ 8.39	27.69 $\pm$ 8.00
	10	81.63 $\pm$ 1.22	70.02 $\pm$ 1.01	4.10 $\pm$ 2.99	-	5.78 $\pm$ 4.38	-
22b	100	78.43 $\pm$ 10.14	60.32 $\pm$ 1.11	2.91 $\pm$ 1.54	20.72 $\pm$ 4.93	81.97 $\pm$ 4.00	-
	10	81.01 $\pm$ 1.08	62.77 $\pm$ 0.27	4.19 $\pm$ 3.55	-	61.02 $\pm$ 6.51	-
23a	100	73.83 $\pm$ 4.14	73.99 $\pm$ 5.15	16.44 $\pm$ 0.57	47.92 $\pm$ 1.67	9.17 $\pm$ 1.39	-
	10	83.29 $\pm$ 5.94	2.51 $\pm$ 3.47	18.28 $\pm$ 13.03	47.78 $\pm$ 3.40	8.54 $\pm$ 3.44	-
23b	100	75.64 $\pm$ 0.21	71.95 $\pm$ 4.38	3.41 $\pm$ 2.52	46.03 $\pm$ 2.10	6.30 $\pm$ 0.86	-
	10	77.54 $\pm$ 5.94	-	-	42.22 $\pm$ 1.49	4.17 $\pm$ 2.49	-
18b	100	57.36 $\pm$ 4.28	-	8.22 $\pm$ 1.06	-	22.57 $\pm$ 6.29	-
	10	-	-	2.74 $\pm$ 0.40	0.34 $\pm$ 28.88	-	-
25a	100	78.96 $\pm$ 0.88	-	10.51 $\pm$ 1.91	-	-	-
	10	-	-	6.32 $\pm$ 2.1	-	-	-
25b	100	42.11 $\pm$ 10.10	3.04 $\pm$ 2.13	11.20 $\pm$ 2.31	35.40 $\pm$ 10.64	5.25 $\pm$ 0.90	-
	10	-	3.51 $\pm$ 5.19	10.75 $\pm$ 5.28	37.23 $\pm$ 7.38	2.01 $\pm$ 3.69	-
26a	100	-	5.14 $\pm$ 4.72	1.62 $\pm$ 4.90	36.60 $\pm$ 4.48	2.42 $\pm$ 1.77	-
	10	-	-	-	33.48 $\pm$ 4.53	-	-
26b	100	-	-	-	33.56 $\pm$ 4.72	-	-
	10	-	-	4.65 $\pm$ 0.86	33.94 $\pm$ 9.15	-	9.56 $\pm$ 14.00
27a	100	71.13 $\pm$ 4.78	-	13.32 $\pm$ 2.05	43.48 $\pm$ 3.42	27.31 $\pm$ 7.74	-
	10	-	-	9.39 $\pm$ 5.34	38.95 $\pm$ 9.32	2.69 $\pm$ 6.48	-
27b	100	-	-	0.86 $\pm$ 8.18	34.19 $\pm$ 6.00	80.58 $\pm$ 12.34	-
	10	-	-	2.29 $\pm$ 4.70	33.16 $\pm$ 8.01	24.80 $\pm$ 4.83	-
28a	100	58.49 $\pm$ 1.06	-	3.77 $\pm$ 6.14	26.28 $\pm$ 2.93	64.44 $\pm$ 8.94	-

RSD Inhibitory effect (%) $\pm$ (%)							
		Gram positive		Gram negative		Yeast	
Analogue	Conc. ( $\mu\text{g/mL}$ )	<i>B. subtilis</i> SZMC0209	<i>S. aureus</i> SZMC14611	<i>E. coli</i> SZMC6271	<i>P. aeruginosa</i> SZMC23290	<i>C. albicans</i> SZMC1533	<i>C. krusei</i> SZMC1352
	10	-	-	$9.75 \pm 0.64$	$26.51 \pm 0.64$	-	$6.49 \pm 21.22$
28b	100	$67.24 \pm 9.14$	-	$12.63 \pm 9.33$	$27.89 \pm 0.56$	$41.19 \pm 9.83$	$14.84 \pm 6.96$
	10	$0.30 \pm 11.11$	$2.51 \pm 4.71$	$10.13 \pm 6.13$	$26.11 \pm 3.08$	$17.80 \pm 4.06$	-
30b	100	$17.74 \pm 6.94$	-	-	-	$0.96 \pm 1.11$	$27.46 \pm 3.59$
	10	-	-	-	-	-	-
31a	100	$95.13 \pm 9.21$	$82.58 \pm 10.08$	$30.12 \pm 0.97$	$48.38 \pm 1.94$	$17.28 \pm 7.99$	-
	10	$12.76 \pm 9.95$	$13.68 \pm 5.80$	$24.59 \pm 3.59$	$32.10 \pm 3.98$	$1.69 \pm 0.64$	$28.20 \pm 1.39$
31b	100	$93.89 \pm 5.51$	$86.85 \pm 4.00$	$23.33 \pm 2.01$	$53.31 \pm 4.84$	$95.21 \pm 3.59$	$38.27 \pm 2.37$
	10	$47.83 \pm 9.92$	-	$13.89 \pm 2.43$	$47.81 \pm 6.60$	$6.76 \pm 0.58$	-
32a	100	$39.97 \pm 6.05$	-	$9.06 \pm 0.93$	$33.08 \pm 5.20$	$14.04 \pm 4.77$	-
	10	$8.61 \pm 8.01$	-	$12.18 \pm 4.13$	$22.81 \pm 3.94$	-	$5.10 \pm 40.80$
32b	100	$41.93 \pm 6.93$	-	$7.84 \pm 5.50$	$37.43 \pm 2.96$	$14.38 \pm 3.07$	-
	10	$1.19 \pm 15.68$	-	$9.10 \pm 1.81$	$22.01 \pm 4.78$	-	-
34a	100	-	-	$1.05 \pm 1.01$	$23.82 \pm 8.60$	-	-
	10	-	-	$8.56 \pm 0.59$	$27.34 \pm 2.69$	-	-
35a	100	$69.20 \pm 0.76$	$12.92 \pm 7.01$	$13.23 \pm 3.67$	$24.51 \pm 9.67$	-	-
	10	-	-	$10.41 \pm 0.37$	$22.04 \pm 3.36$	-	$11.48 \pm 9.50$
35b	100	-	$7.07 \pm 2.14$	$21.90 \pm 0.11$	$32.59 \pm 4.02$	$3.95 \pm 4.36$	$2.26 \pm 48.23$
	10	-	-	$11.01 \pm 4.49$	$31.38 \pm 7.59$	$14.47 \pm 11.24$	$8.57 \pm 38.32$
36a	100	$51.90 \pm 14.00$	-	$14.16 \pm 1.44$	$36.89 \pm 4.71$	$3.61 \pm 0.15$	-
	10	$0.83 \pm 5.73$	$2.69 \pm 2.36$	$13.04 \pm 1.52$	$38.44 \pm 5.81$	-	$15.49 \pm 9.99$
36b	100	-	-	$6.91 \pm 2.33$	$29.23 \pm 4.53$	$48.67 \pm 1.97$	-
	10	-	-	$5.53 \pm 6.56$	$5.04 \pm 6.13$	$14.42 \pm 6.02$	-
38a	100	-	$2.05 \pm 1.05$	$1.86 \pm 2.39$	-	$4.00 \pm 4.96$	-
	10	-	-	$7.34 \pm 3.49$	-	$1.69 \pm 0.89$	$1.85 \pm 50.46$
38b	100	$40.89 \pm 6.41$	$5.08 \pm 1.72$	$6.53 \pm 1.79$	-	-	$1.76 \pm 48.50$
	10	-	-	$6.24 \pm 3.32$	$1.15 \pm 10.83$	-	$3.57 \pm 46.50$
39a	100	$79.38 \pm 4.19$	$63.47 \pm 4.90$	$15.94 \pm 1.38$	-	$88.22 \pm 3.96$	$20.44 \pm 22.00$
	10	$82.73 \pm 0.52$	$69.84 \pm 0.00$	$10.37 \pm 1.56$	-	-	-
39b	100	$87.80 \pm 7.04$	$79.66 \pm 2.59$	$12.08 \pm 4.28$	$48.09 \pm 1.38$	$90.89 \pm 13.31$	$91.08 \pm 4.90$
	10	$92.94 \pm 1.46$	$83.69 \pm 38.18$	$16.37 \pm 2.25$	$33.59 \pm 6.43$	$85.10 \pm 9.56$	-
40a	100	$72.88 \pm 1.68$	$68.26 \pm 1.66$	$12.75 \pm 0.66$	$37.66 \pm 2.39$	$1.07 \pm 2.07$	$13.12 \pm 35.38$
	10	$55.43 \pm 5.07$	-	$1.14 \pm 14.60$	$38.89 \pm 1.13$	$7.90 \pm 3.78$	-
40b	100	$71.39 \pm 3.84$	$69.37 \pm 1.44$	$3.81 \pm 7.29$	$42.13 \pm 2.25$	$9.22 \pm 1.99$	-
	10	$65.82 \pm 4.56$	$12.39 \pm 1.50$	$5.08 \pm 0.44$	$39.58 \pm 0.73$	$16.79 \pm 6.53$	-
41a	100	$20.92 \pm 4.79$	-	$7.53 \pm 1.10$	-	-	-
	10	-	-	$5.55 \pm 2.23$	-	-	$9.76 \pm 13.24$
41b	100	-	-	$22.59 \pm 1.73$	$29.69 \pm 7.98$	$8.01 \pm 0.15$	$12.17 \pm 13.52$
	10	$6.94 \pm 12.97$	-	$21.97 \pm 1.20$	$24.05 \pm 3.11$	$7.78 \pm 0.59$	$13.86 \pm 12.14$
42a	100	$69.05 \pm 10.02$	$5.79 \pm 6.44$	$11.70 \pm 2.09$	$26.71 \pm 7.59$	$3.20 \pm 0.25$	-

RSD Inhibitory effect (%) ± (%)							
		Gram positive		Gram negative		Yeast	
Analogue	Conc. (µg/mL)	<i>B. subtilis</i> SZMC0209	<i>S. aureus</i> SZMC14611	<i>E. coli</i> SZMC6271	<i>P. aeruginosa</i> SZMC23290	<i>C. albicans</i> SZMC1533	<i>C. krusei</i> SZMC1352
	10	51.75 ± 11.13	-	10.30 ± 10.48	25.65 ± 4.83	1.12 ± 2.51	-
42b	100	86.62 ± 8.48	66.22 ± 4.03	11.13 ± 1.43	26.31 ± 3.55	30.69 ± 3.51	32.51 ± 8.51
	10	43.95 ± 5.65	-	8.70 ± 5.49	12.78 ± 2.95	-	16.64 ± 7.37
43a	100	41.19 ± 1.97	-	2.57 ± 10.50	-	5.02 ± 2.65	-
	10	-	-	8.44 ± 0.73	9.86 ± 4.63	-	-
43b	100	4.63 ± 24.25	-	25.00 ± 4.39	20.61 ± 4.03	80.90 ± 4.76	18.34 ± 20.72
	10	-	-	15.68 ± 1.68	8.48 ± 3.77	20.45 ± 13.47	-

# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of new compounds

Figure S 1: <sup>1</sup>H-NMR of compound 3

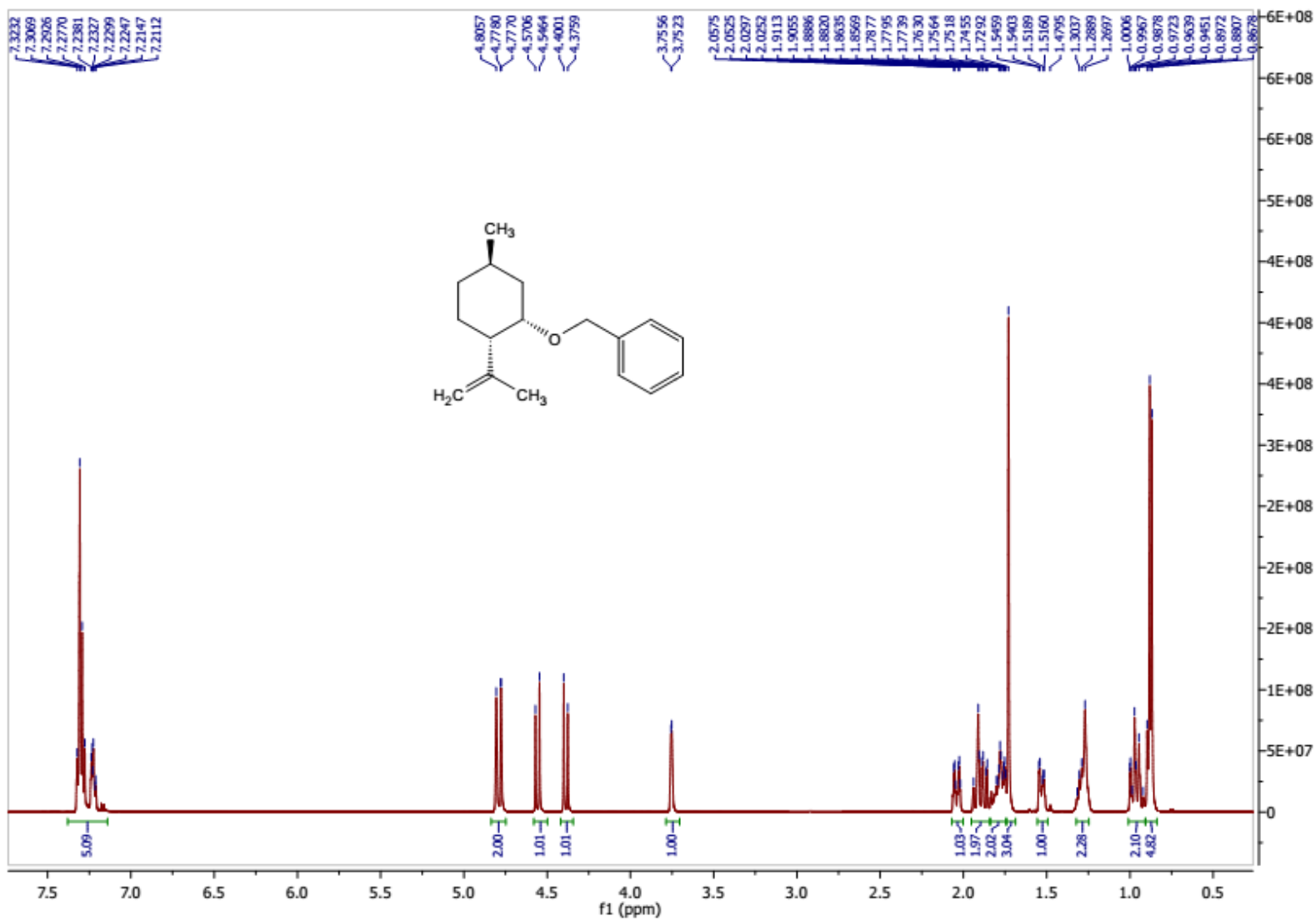


Figure S 2:  $^{13}\text{C}$ -NMR of compound **3**

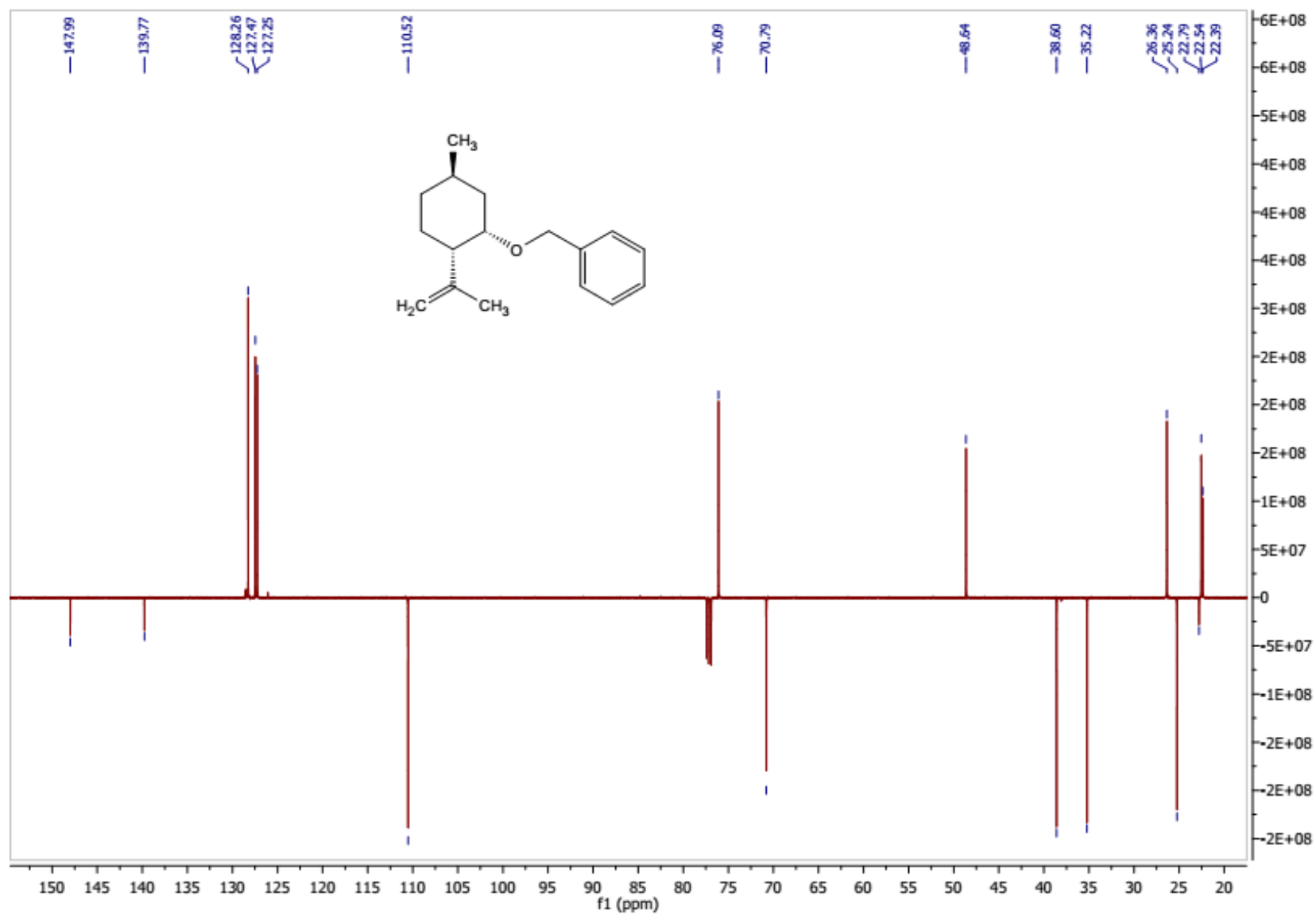




Figure S 3:  $^1\text{H}$ -NMR of compound **4a**

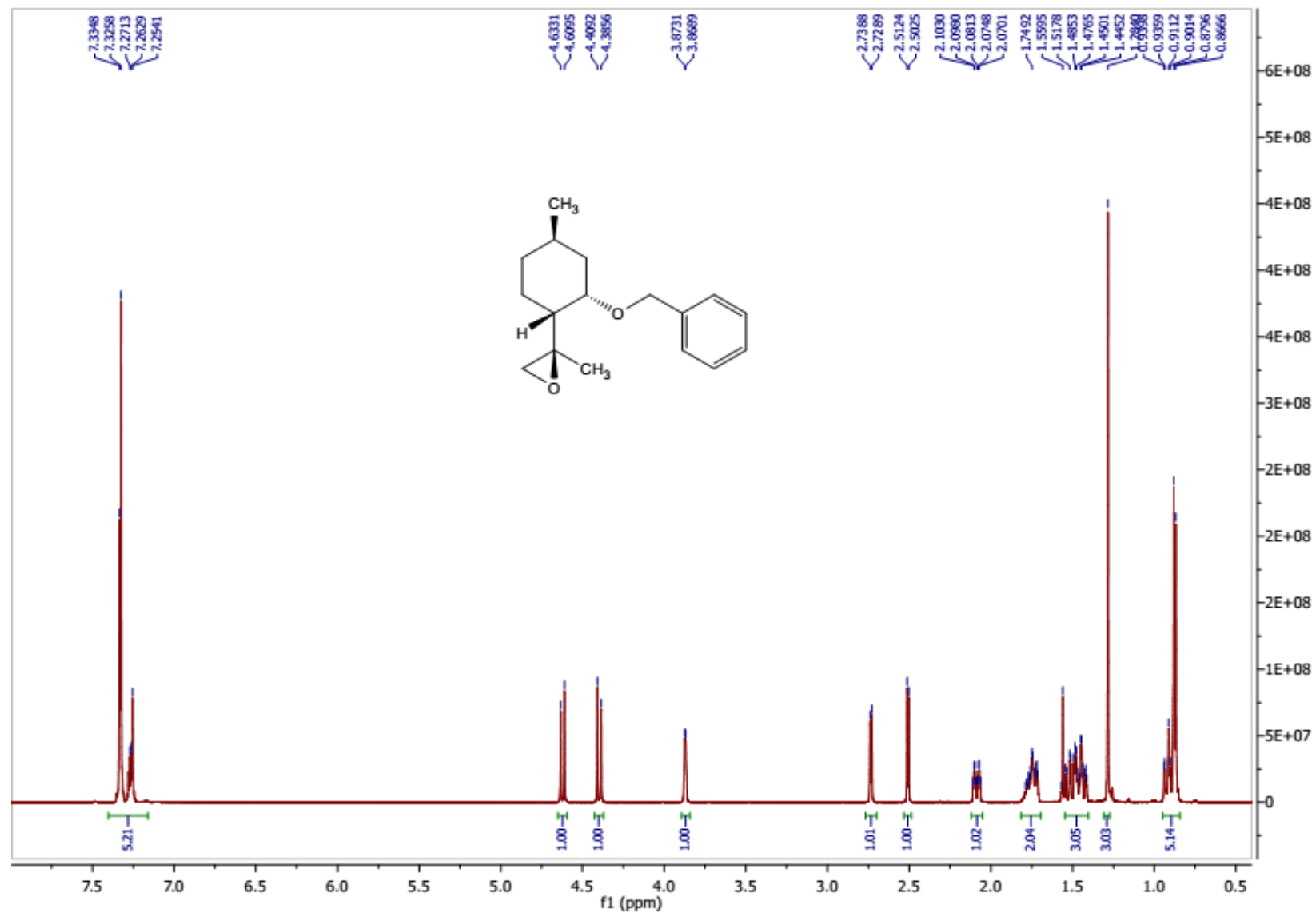


Figure S 4:  $^{13}\text{C}$ -NMR of compound **4a**

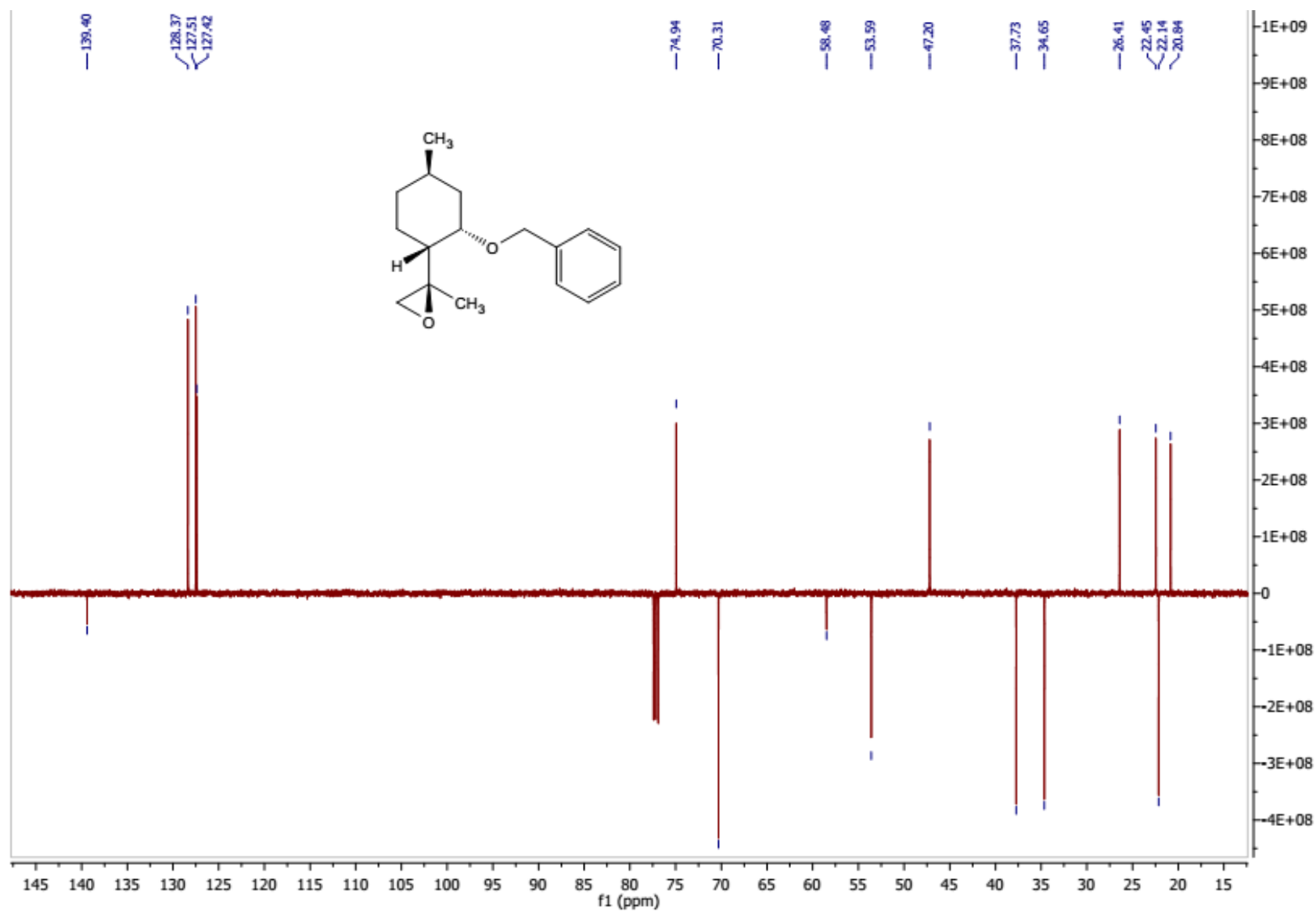


Figure S 5:  $^1\text{H}$ -NMR of compound **4b**

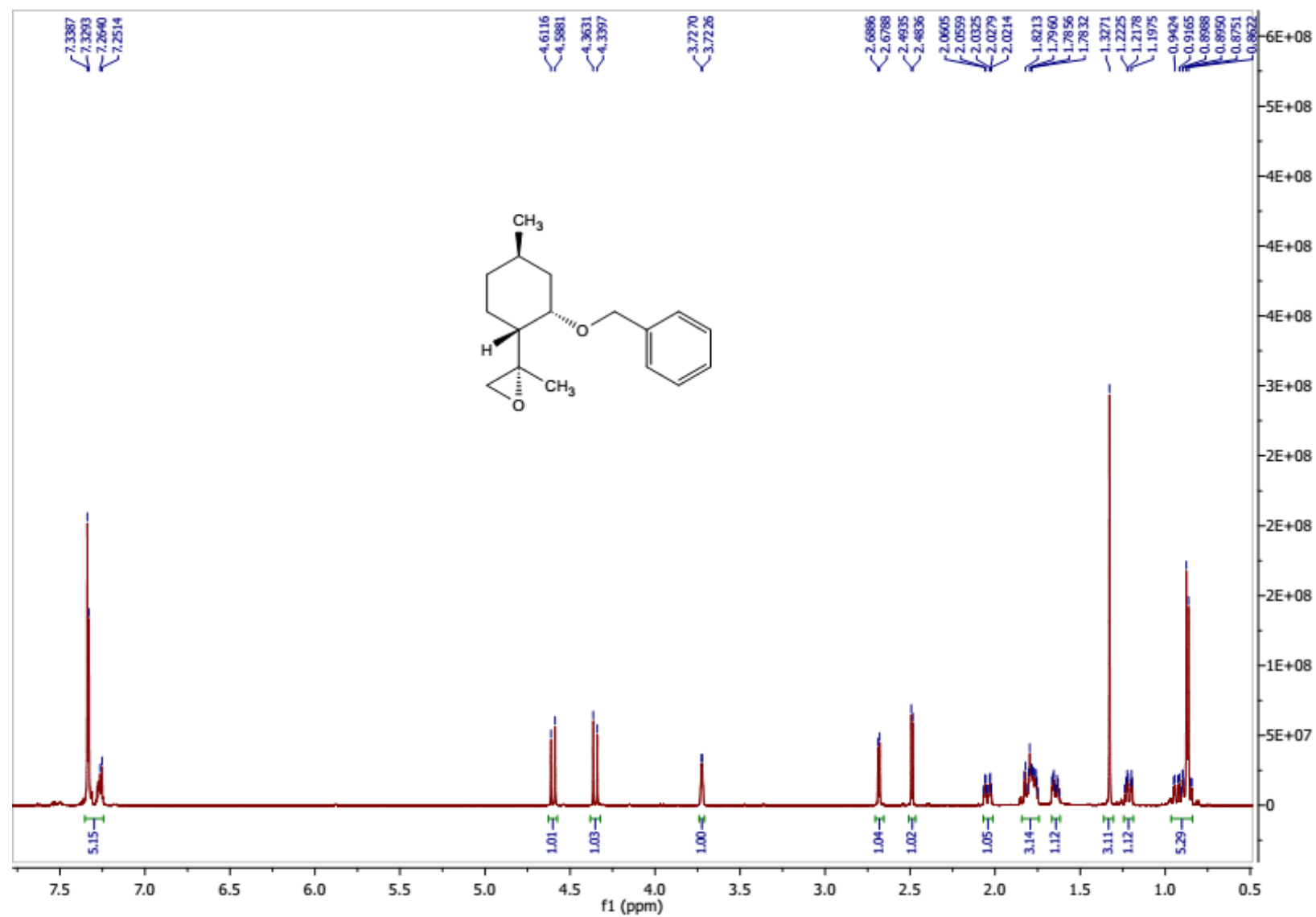


Figure S 6:  $^{13}\text{C}$ -NMR of compound **4b**

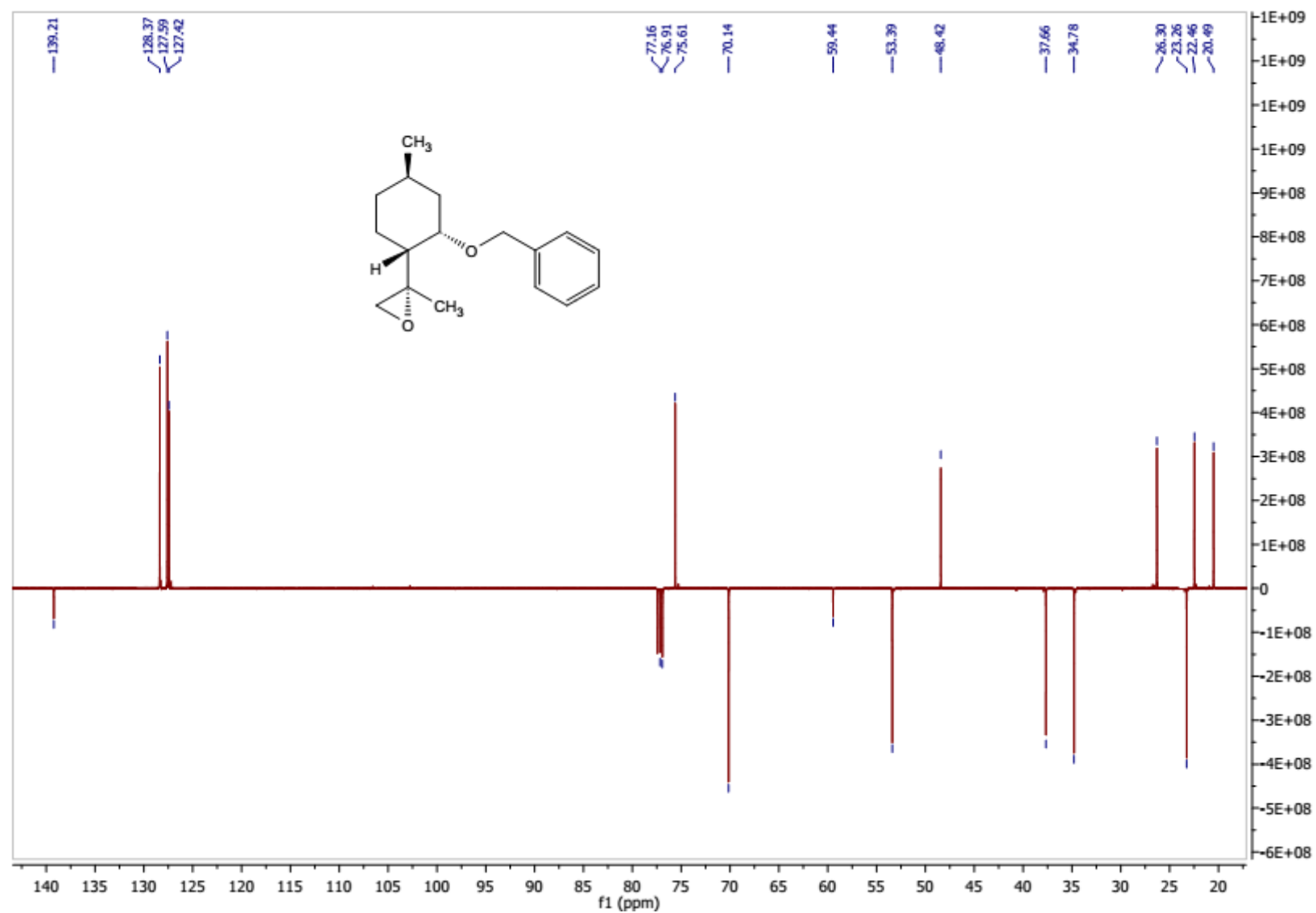


Figure S 7:  $^1\text{H}$ -NMR of compound **5a**

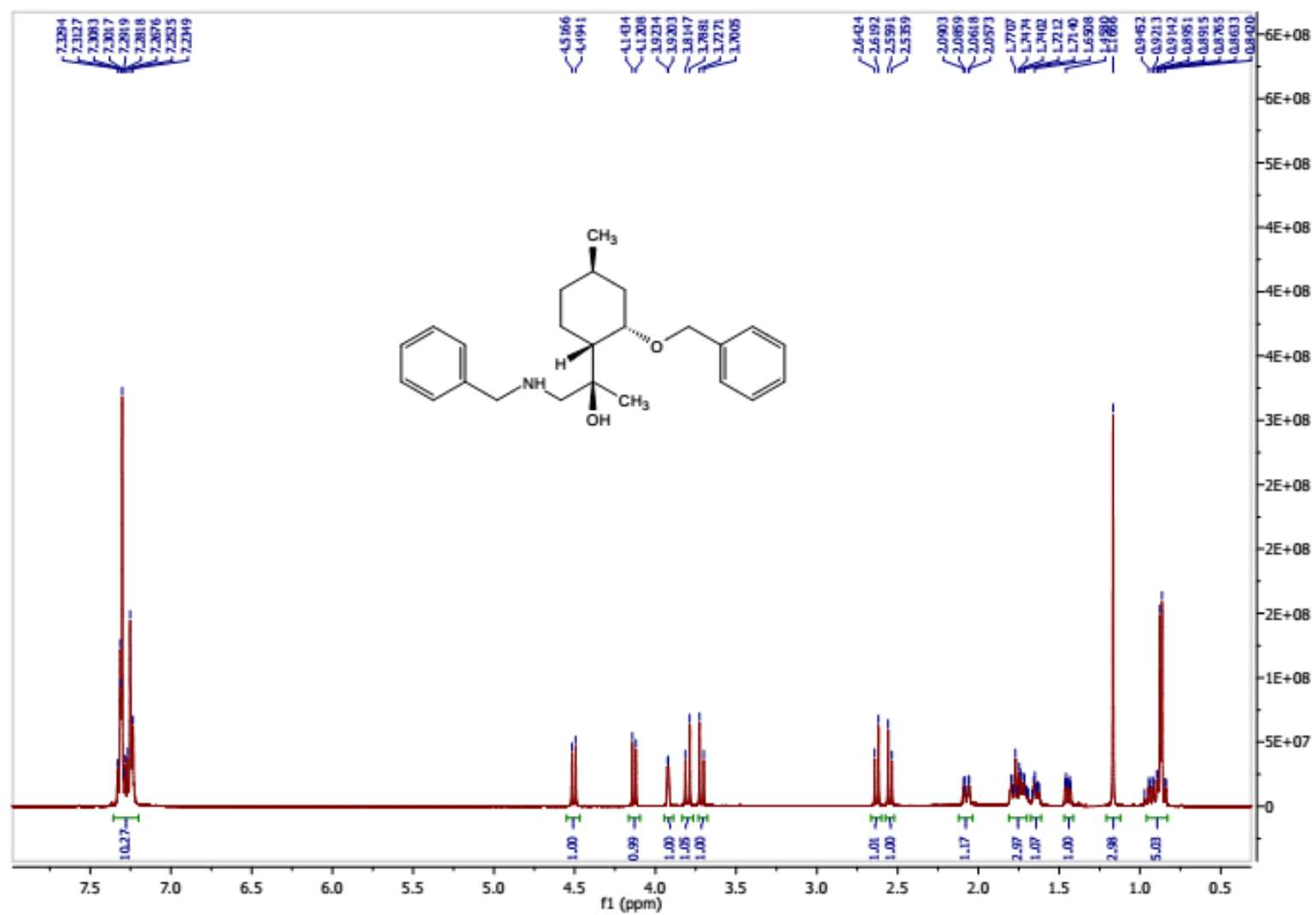


Figure S 8:  $^{13}\text{C}$ -NMR of compound 5a

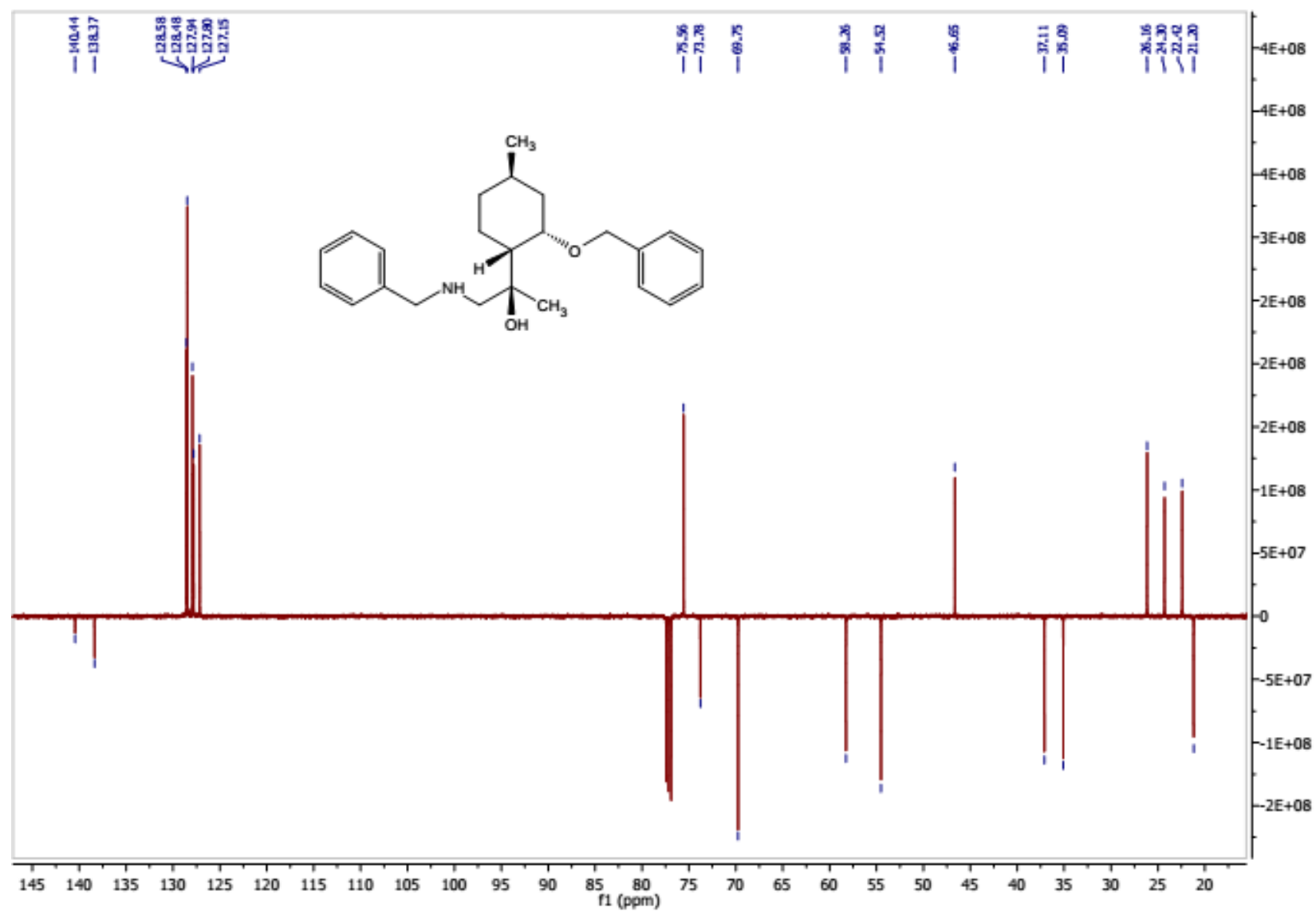


Figure S 9:  $^1\text{H}$ -NMR of compound **5b**

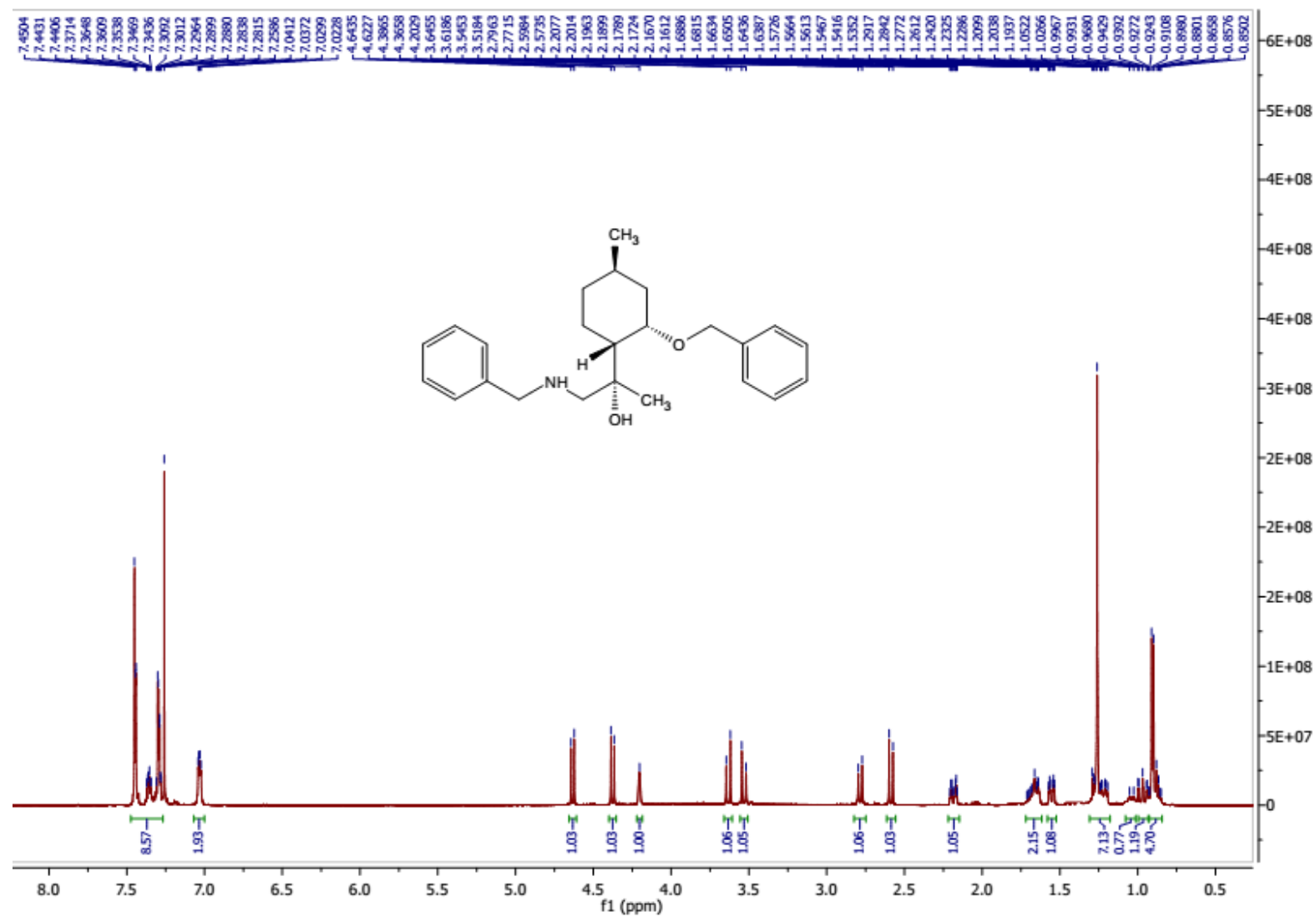


Figure S 10:  $^{13}\text{C}$ -NMR of compound **5b**

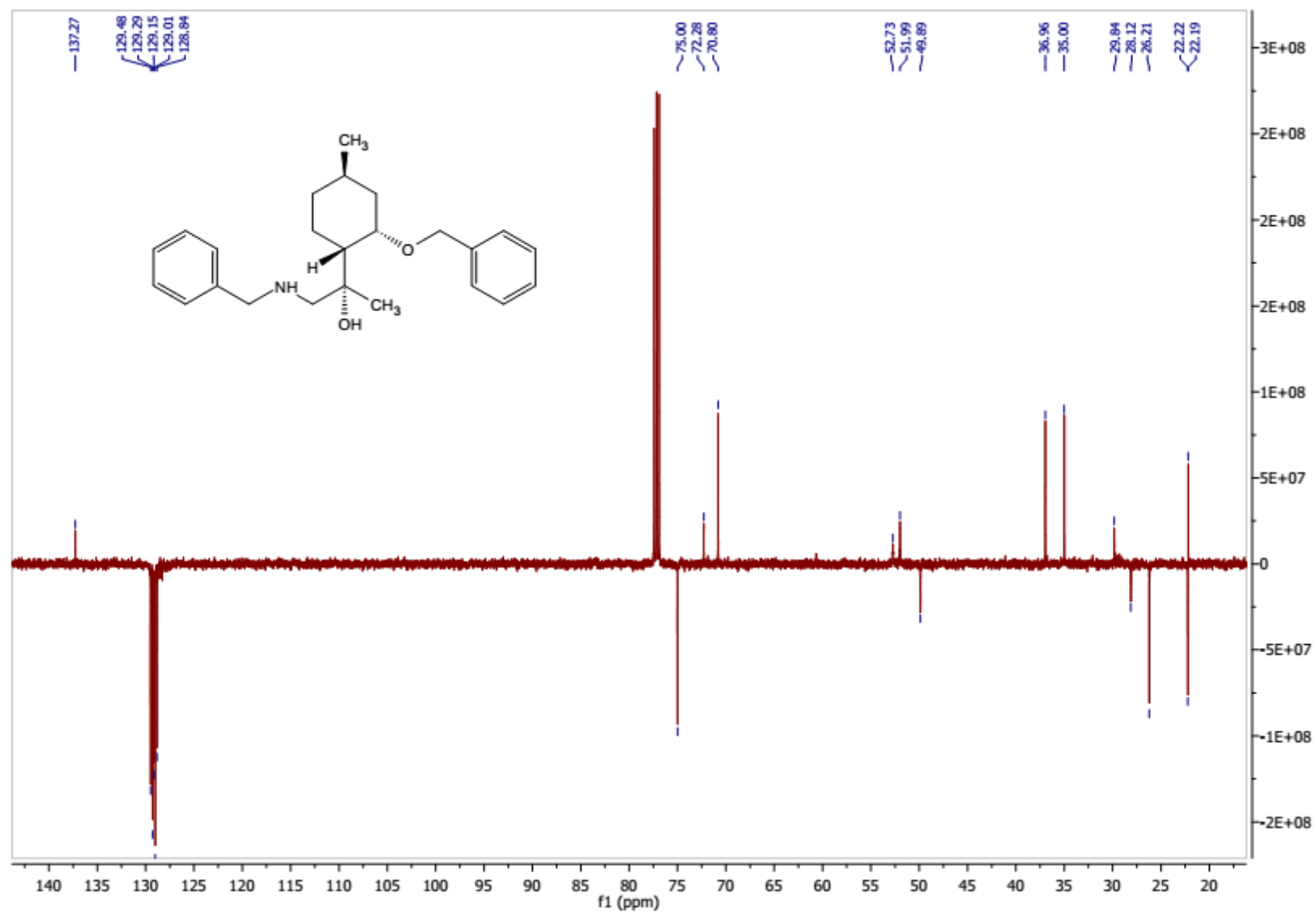




Figure S 11:  $^1\text{H}$ -NMR of compound 6a

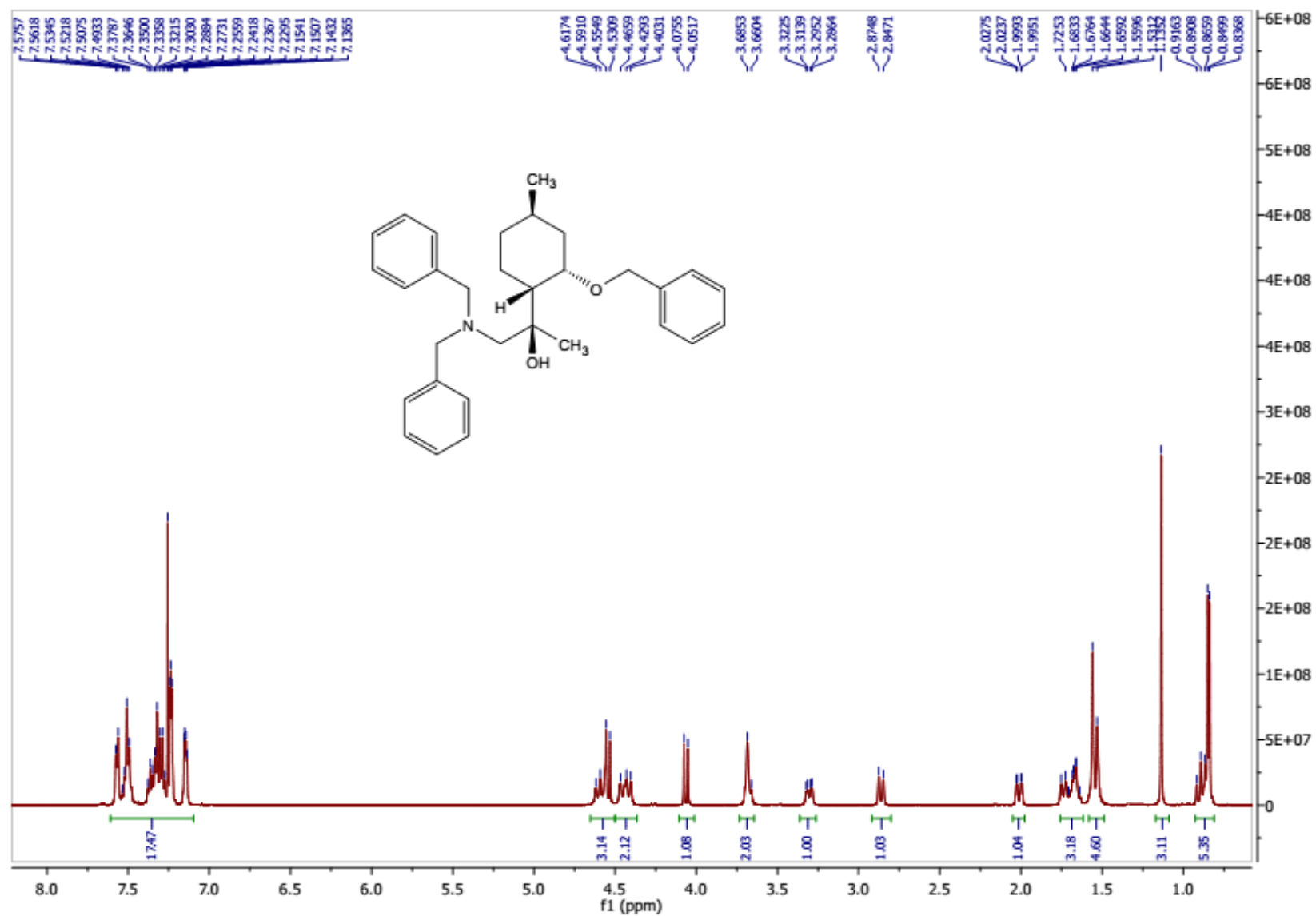


Figure S 12:  $^{13}\text{C}$ -NMR of compound **6a**

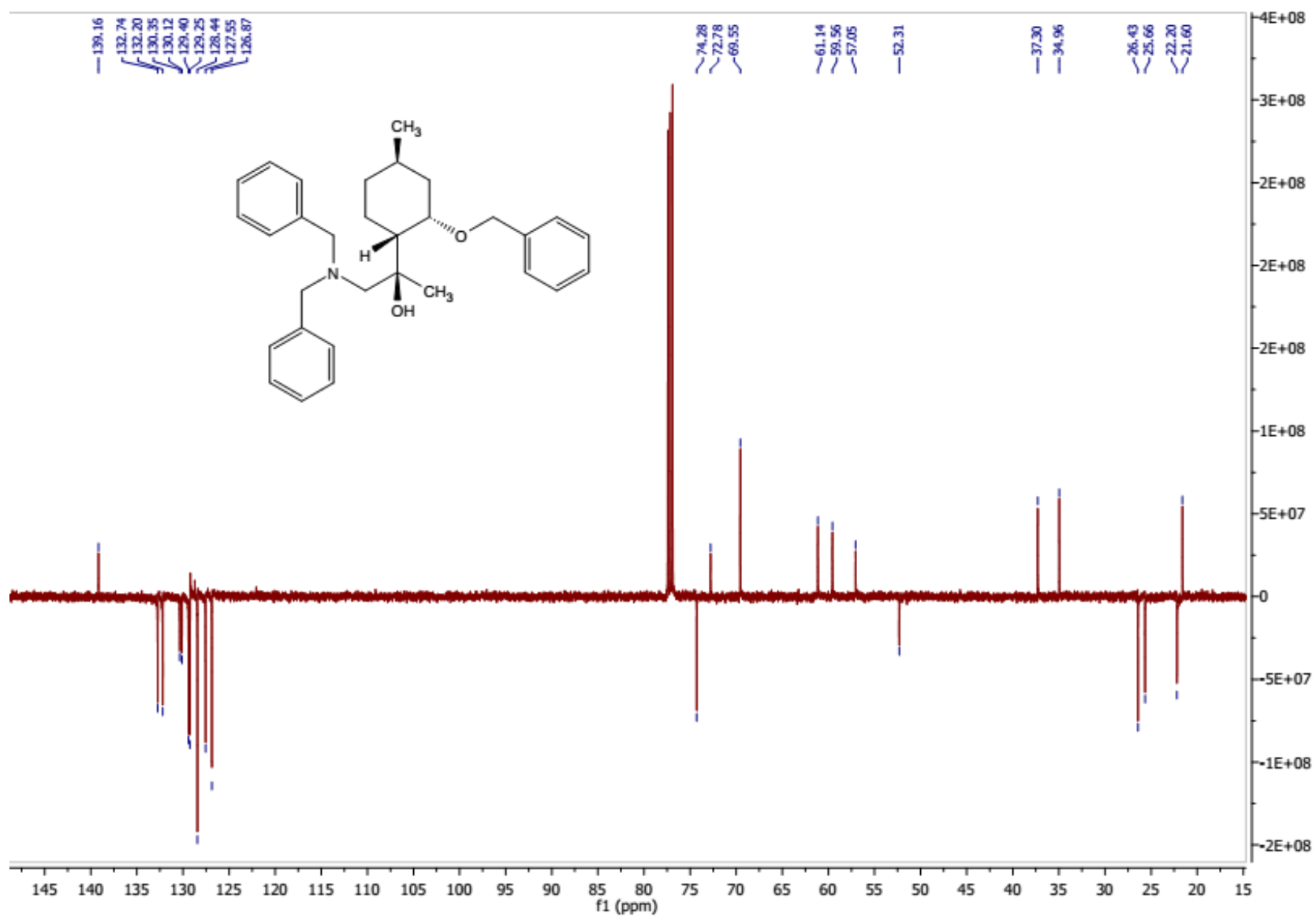
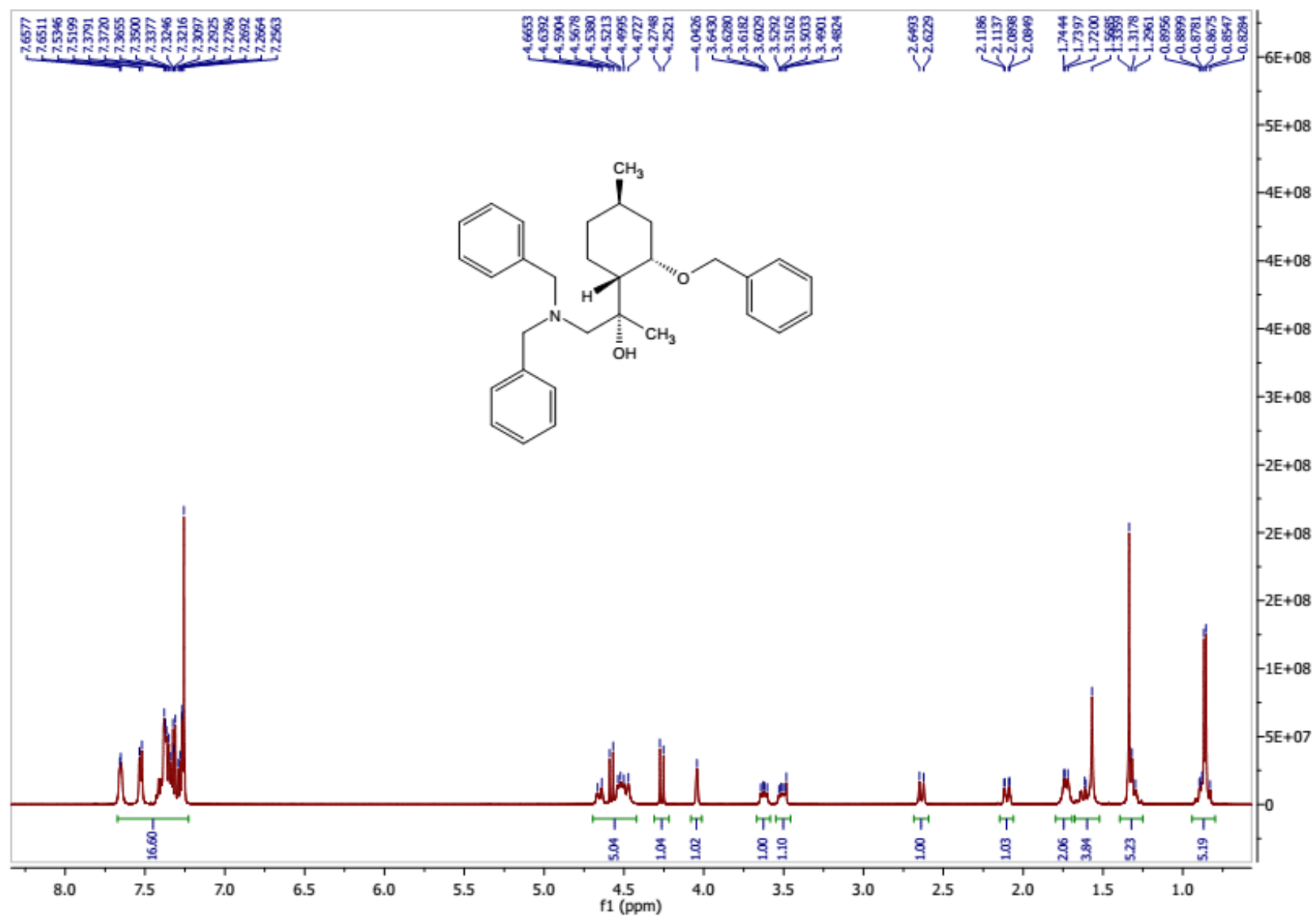


Figure S 13:  $^1\text{H}$ -NMR of compound **6b**



<sup>13</sup>C-NMR of compound **6a**

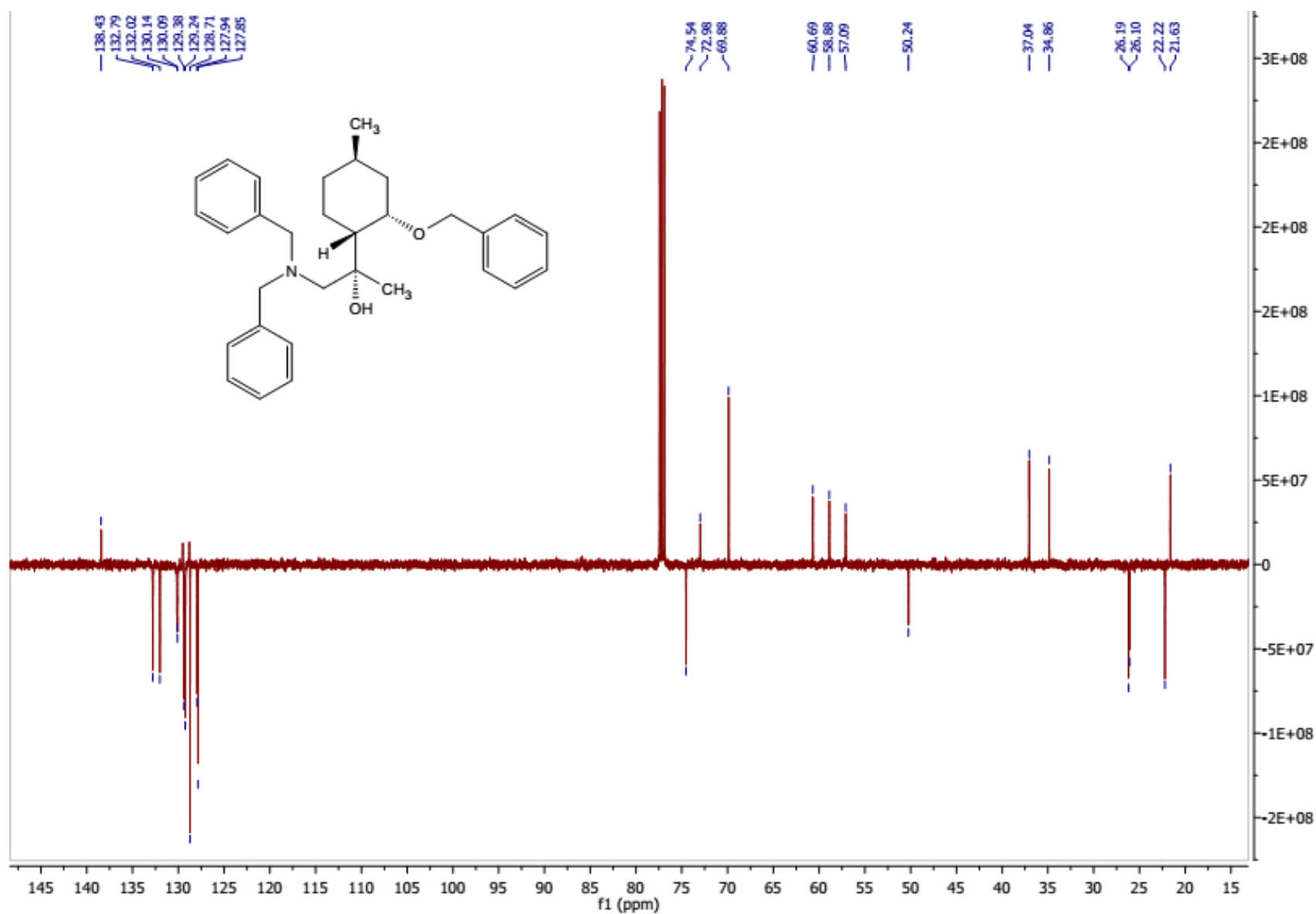


Figure S 14:  $^1\text{H}$ -NMR of compound 7a

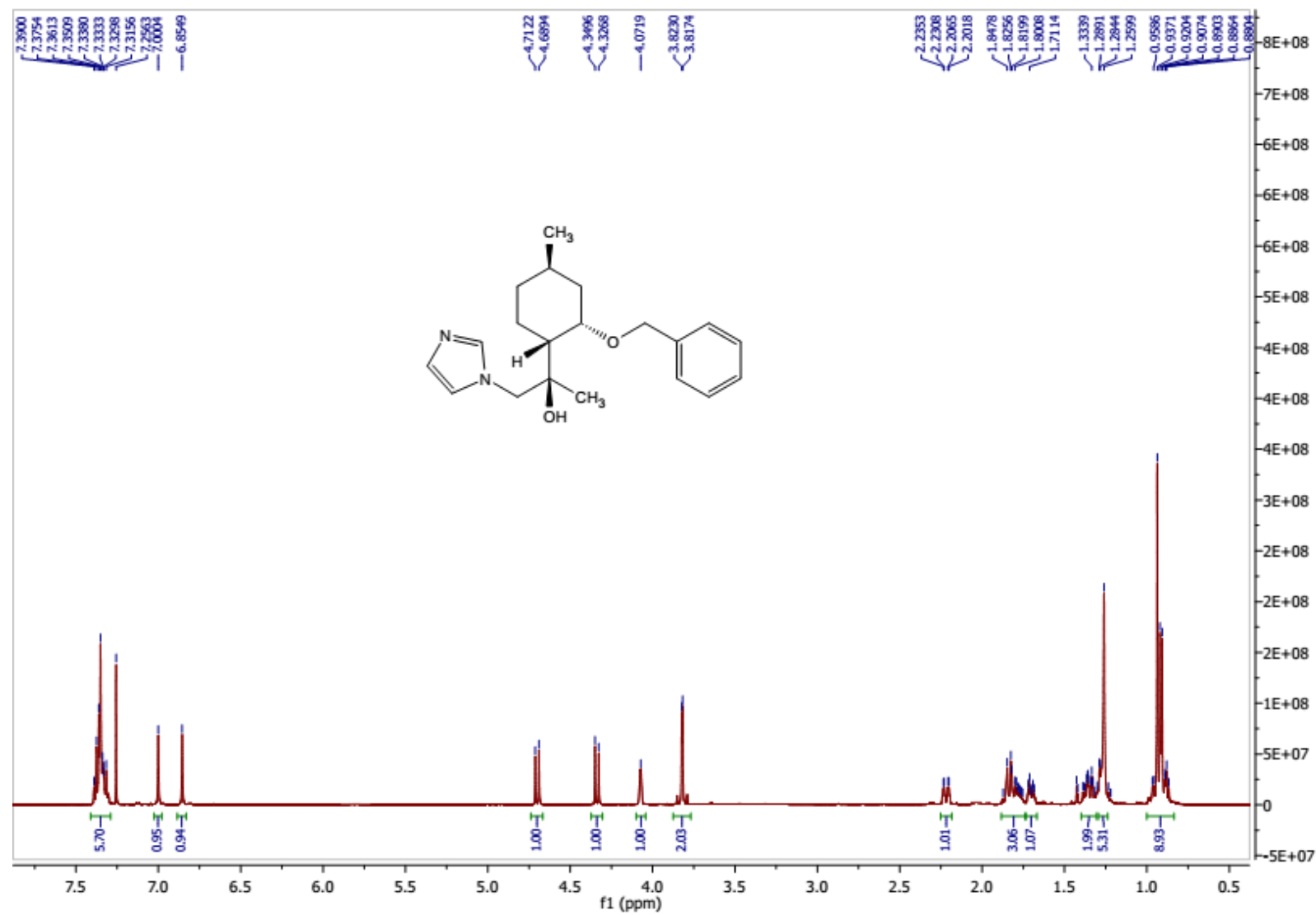


Figure S 15:  $^{13}\text{C}$ -NMR of compound **7a**

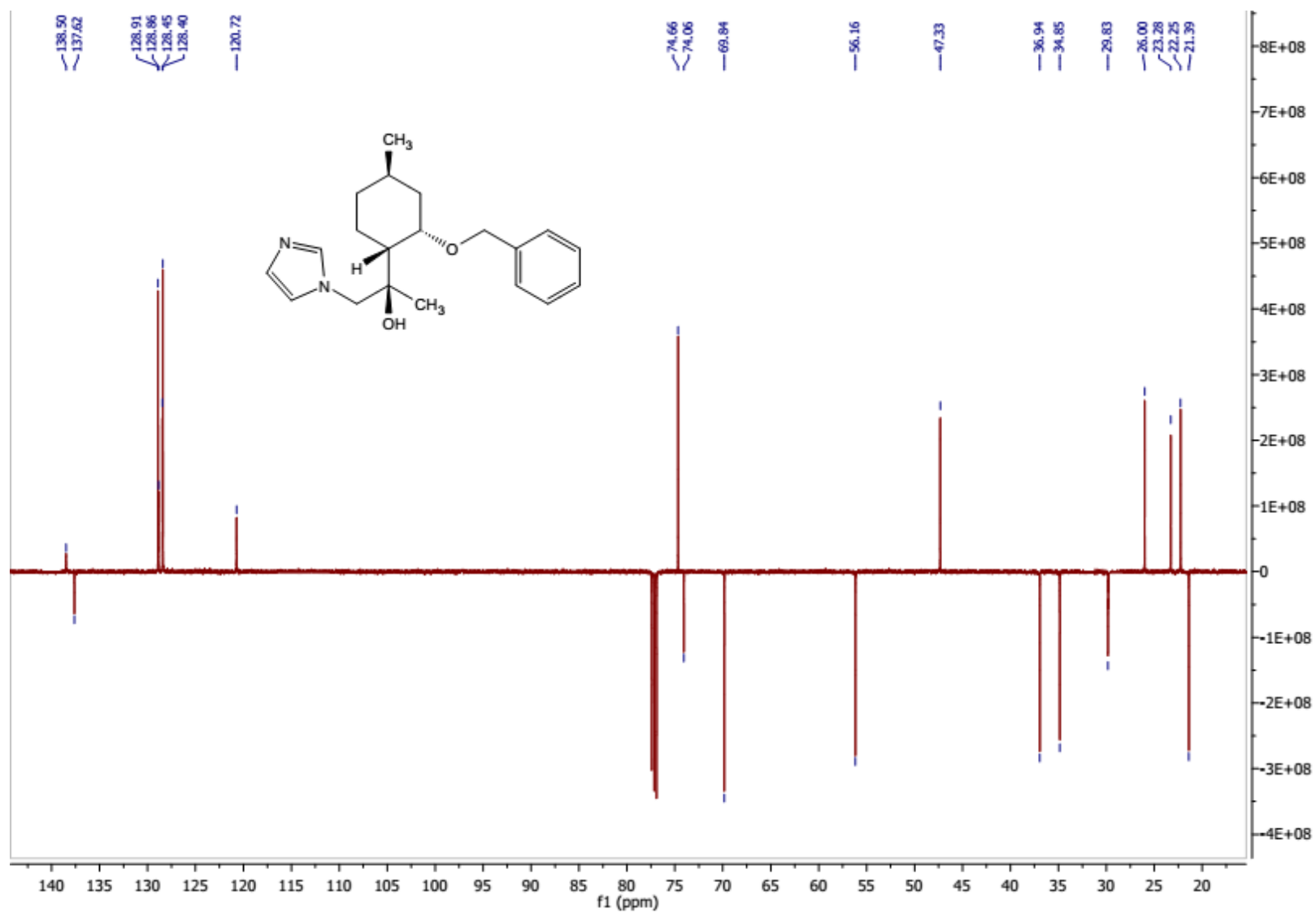


Figure S 16:  $^1\text{H}$ -NMR of compound **7b**

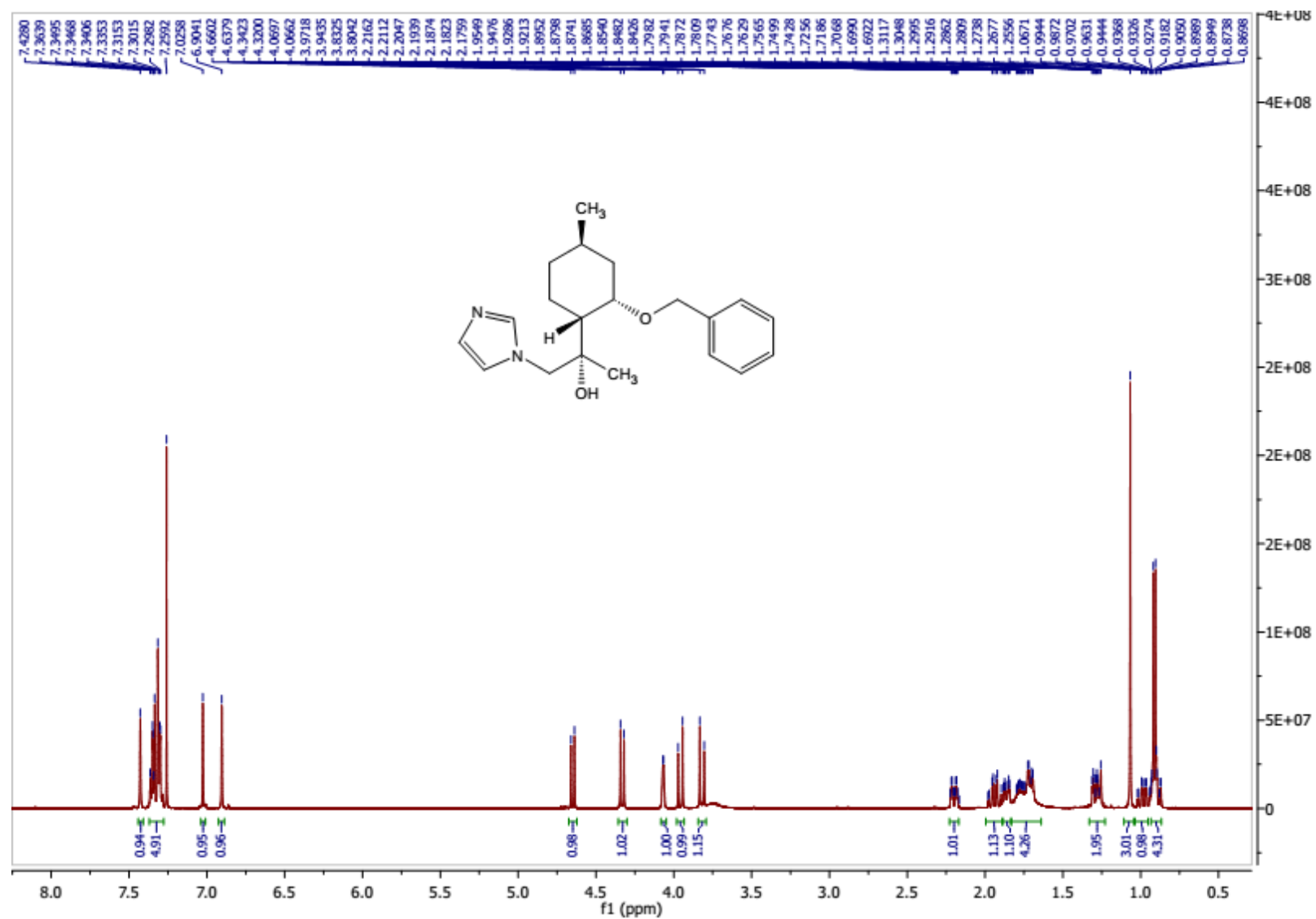


Figure S 17:  $^{13}\text{C}$ -NMR of compound **7b**

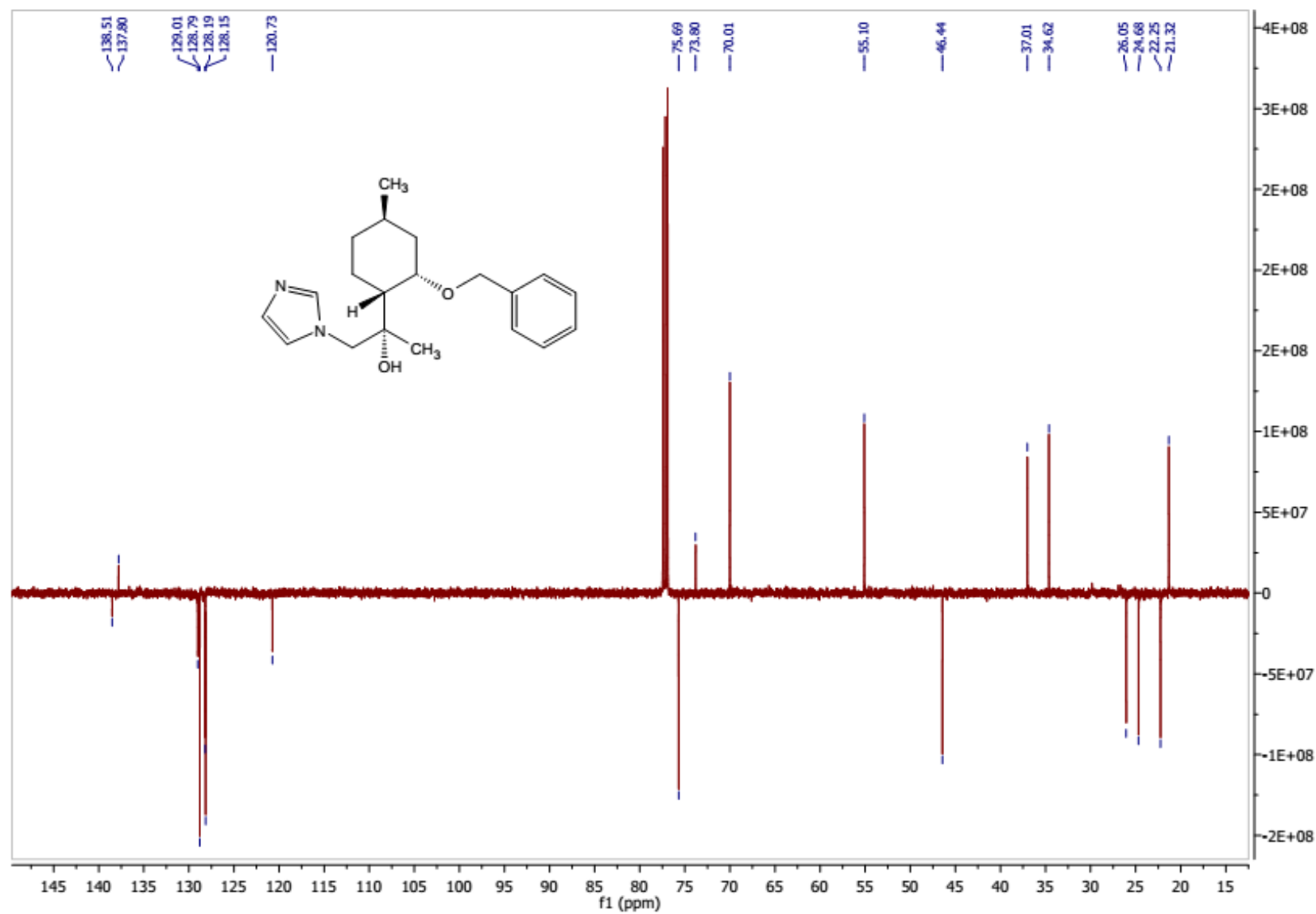




Figure S 18:  $^1\text{H}$ -NMR of compound 8a

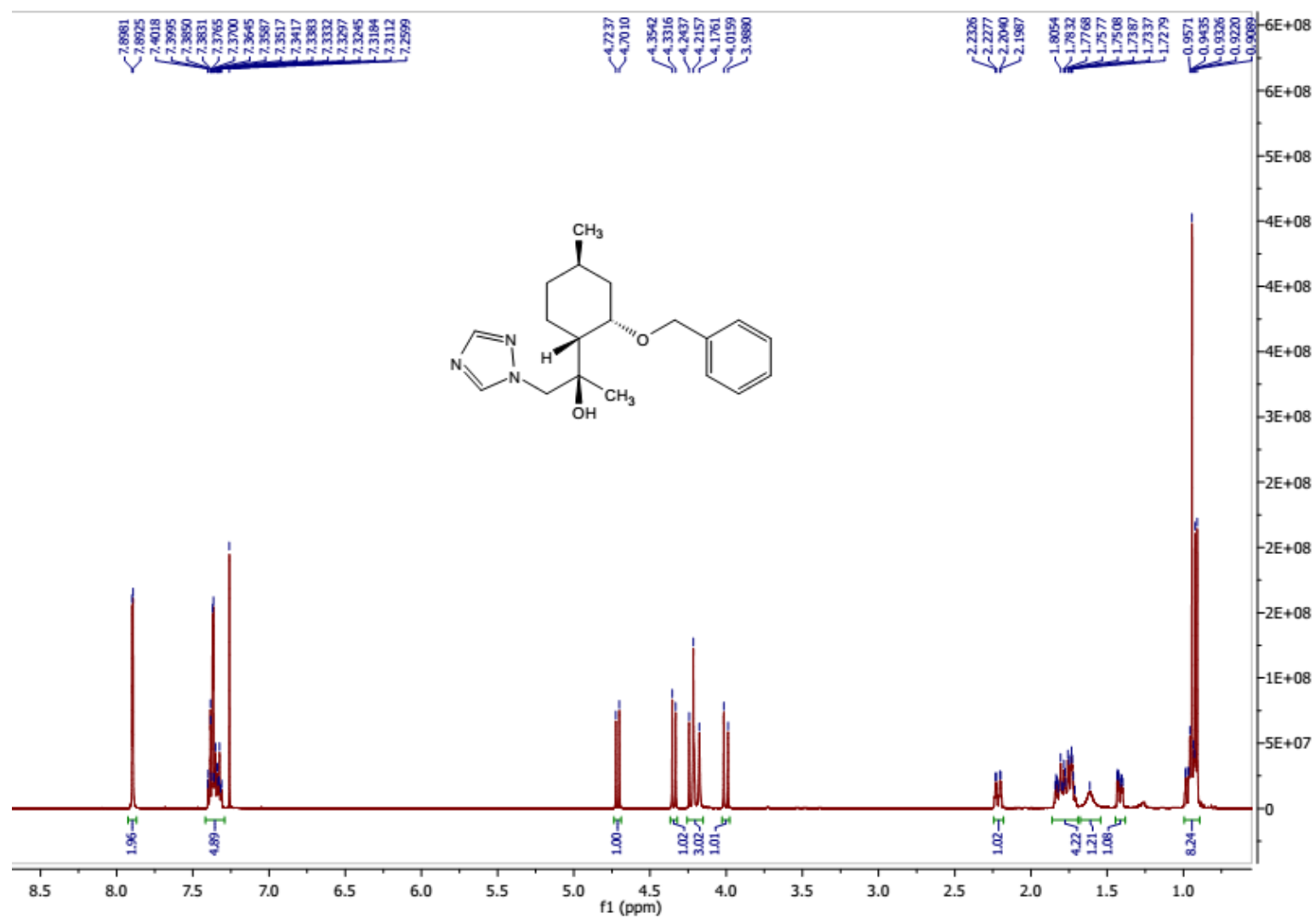


Figure S 19:  $^{13}\text{C}$ -NMR of compound **8a**

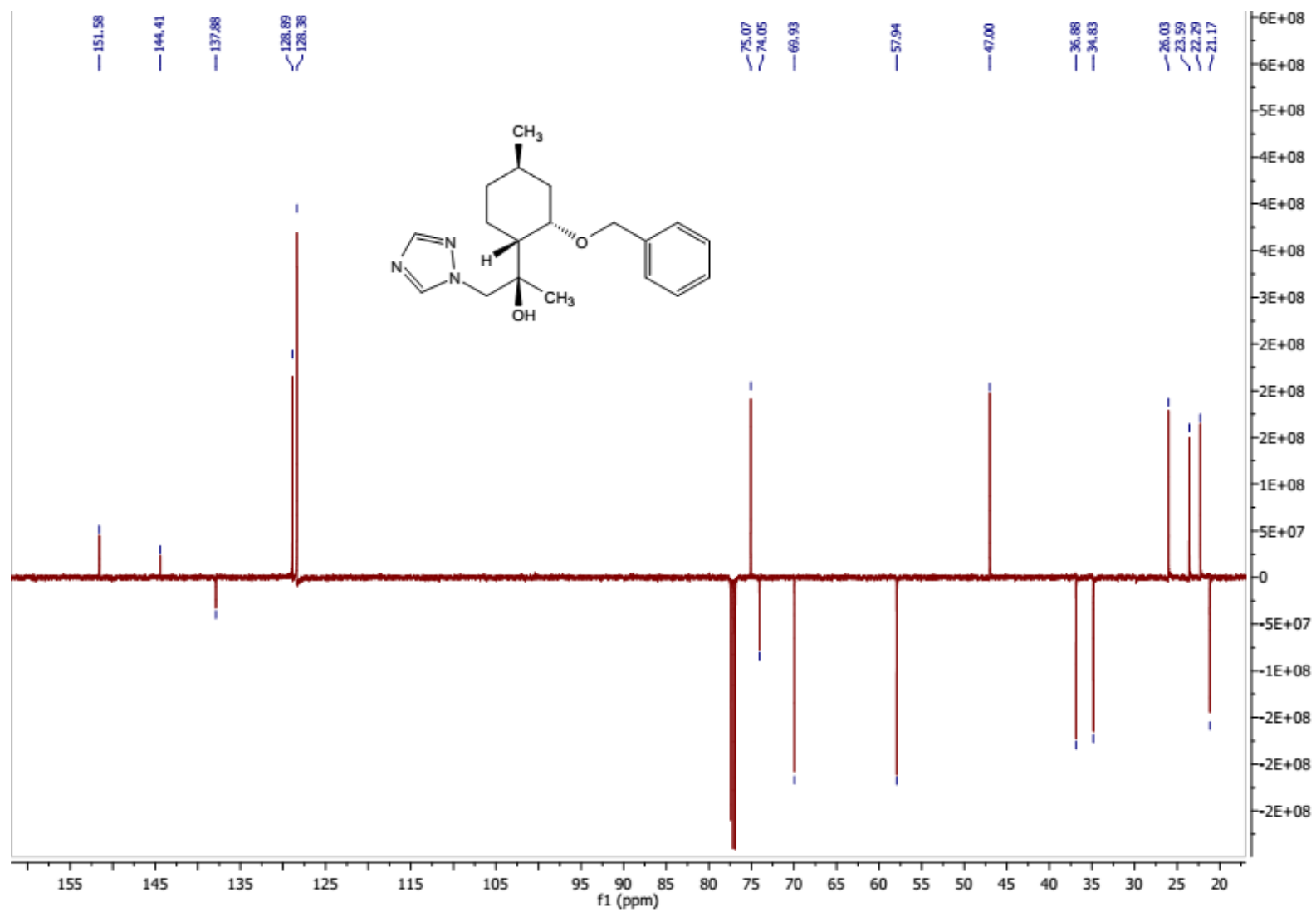


Figure S 20:  $^1\text{H}$ -NMR of compound **8b**

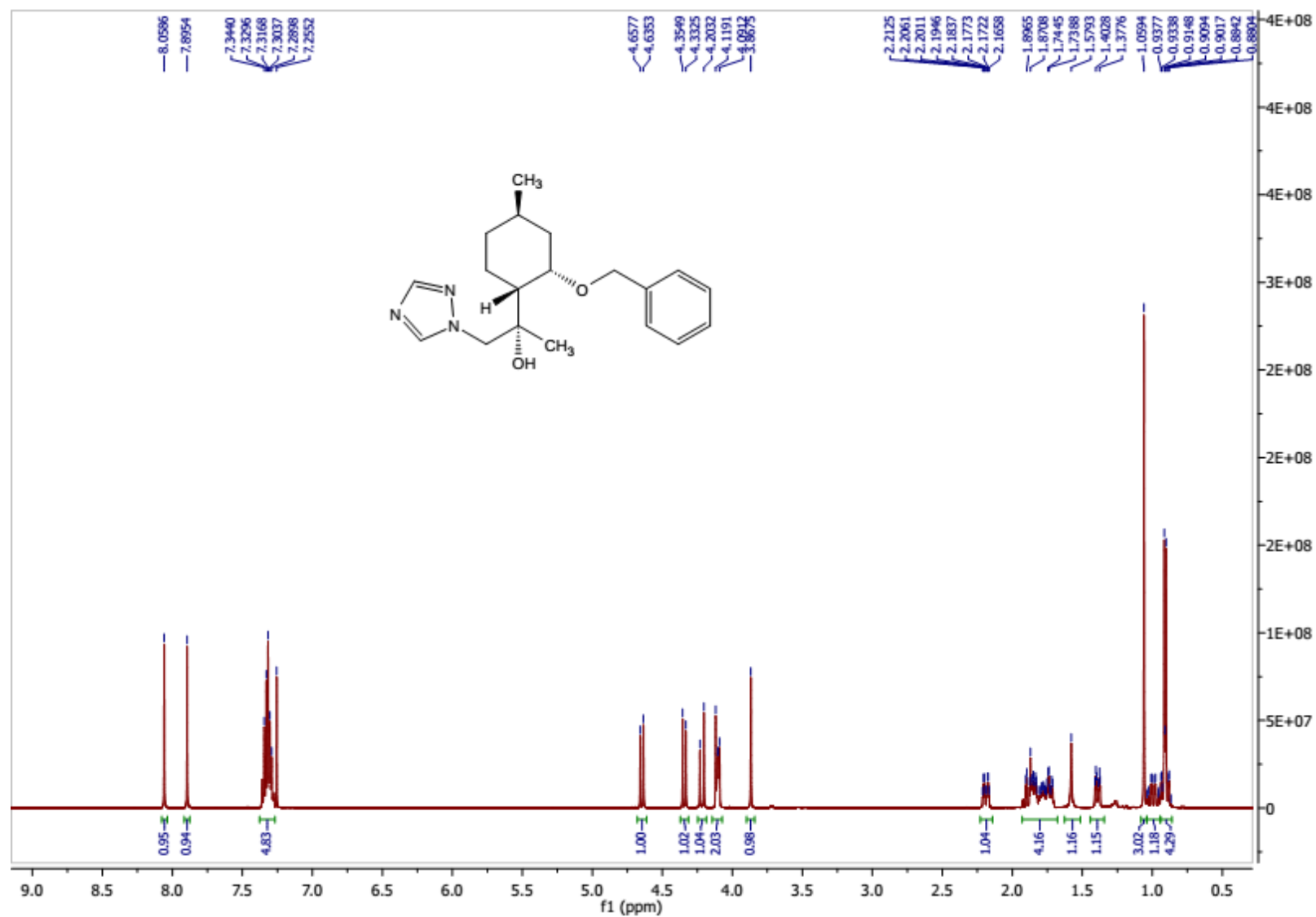


Figure S 21:  $^{13}\text{C}$ -NMR of compound **8b**

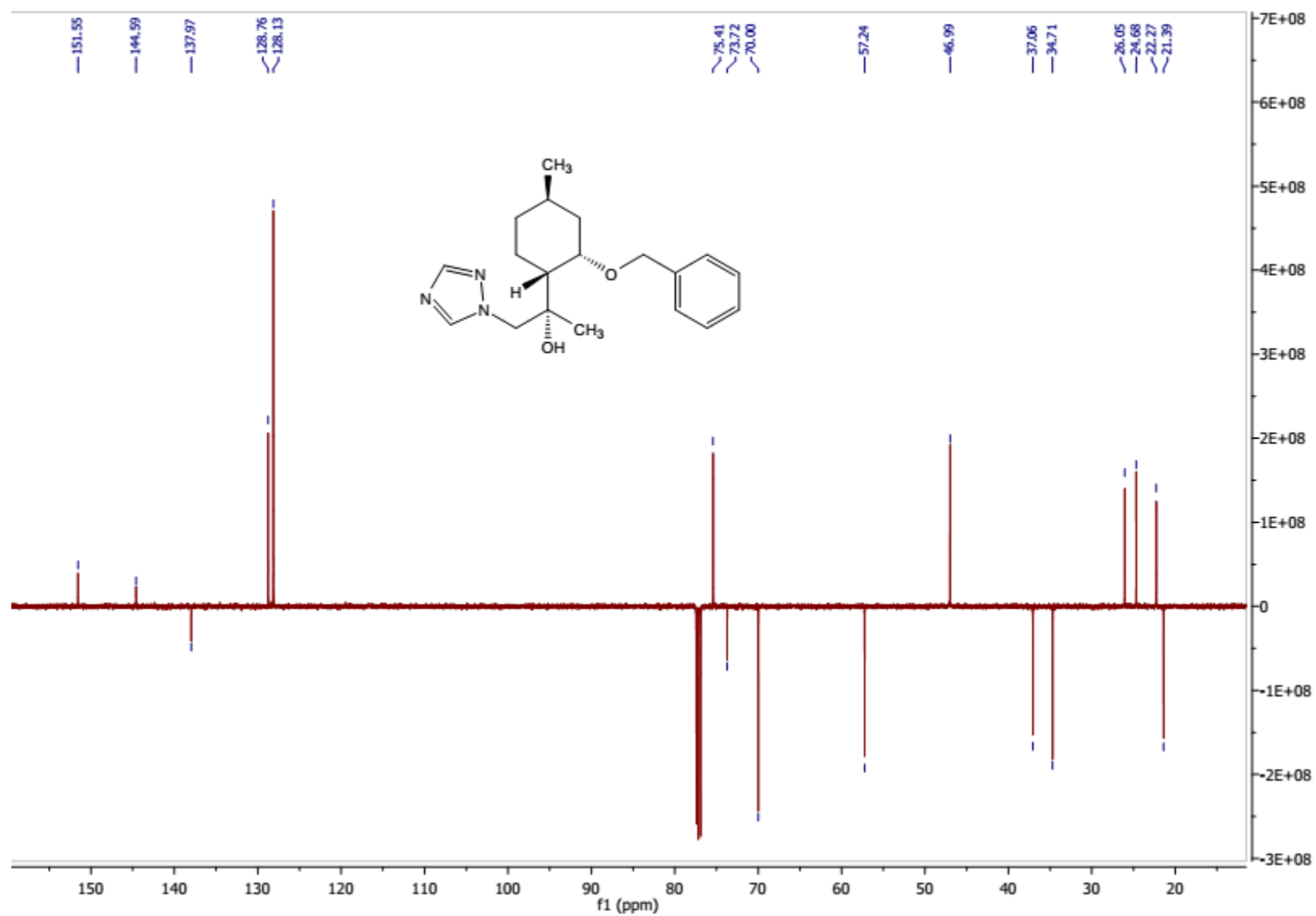


Figure S 22:  $^1\text{H}$ -NMR of compound 9a

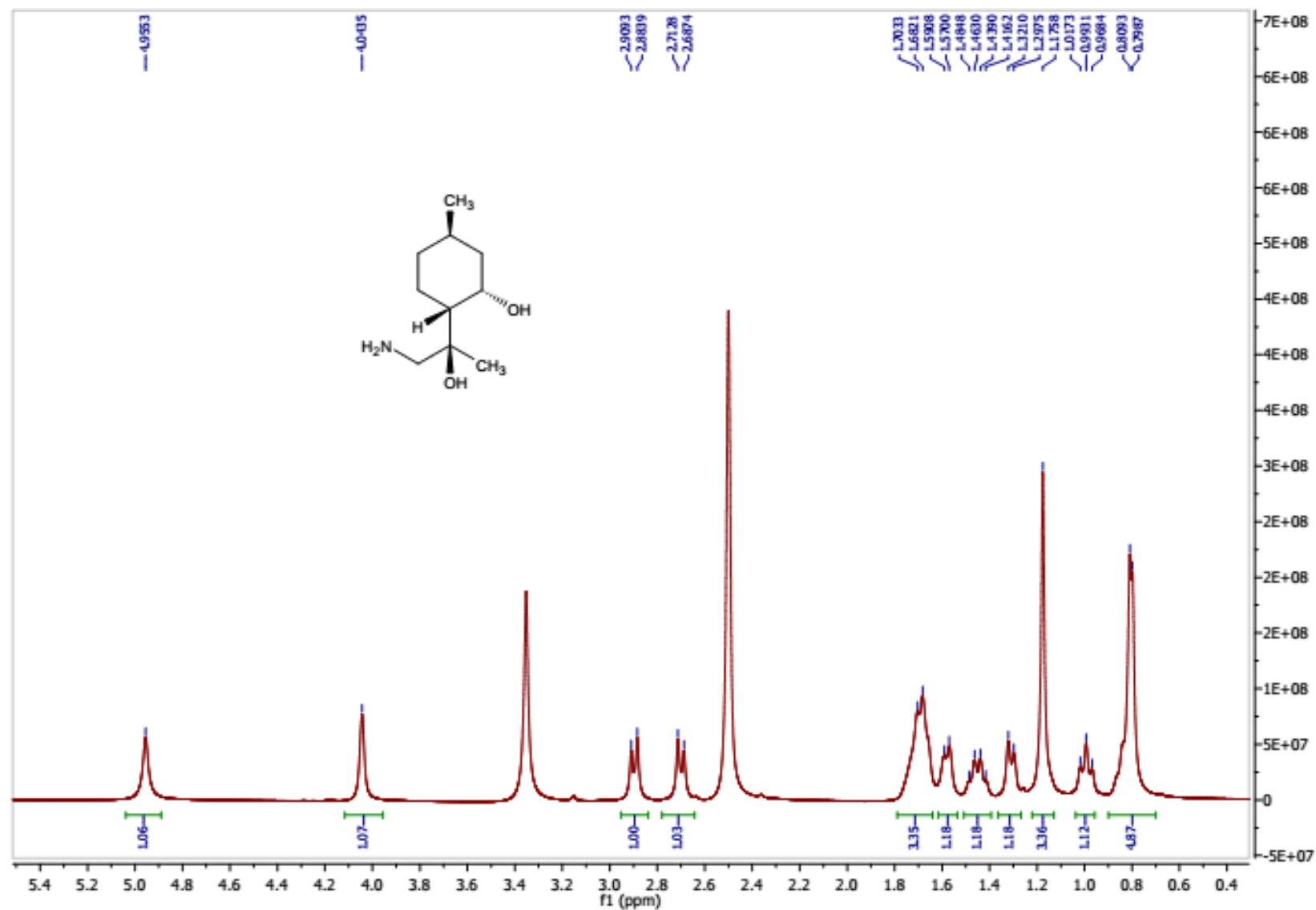


Figure S 23:  $^{13}\text{C}$ -NMR of compound **9a**

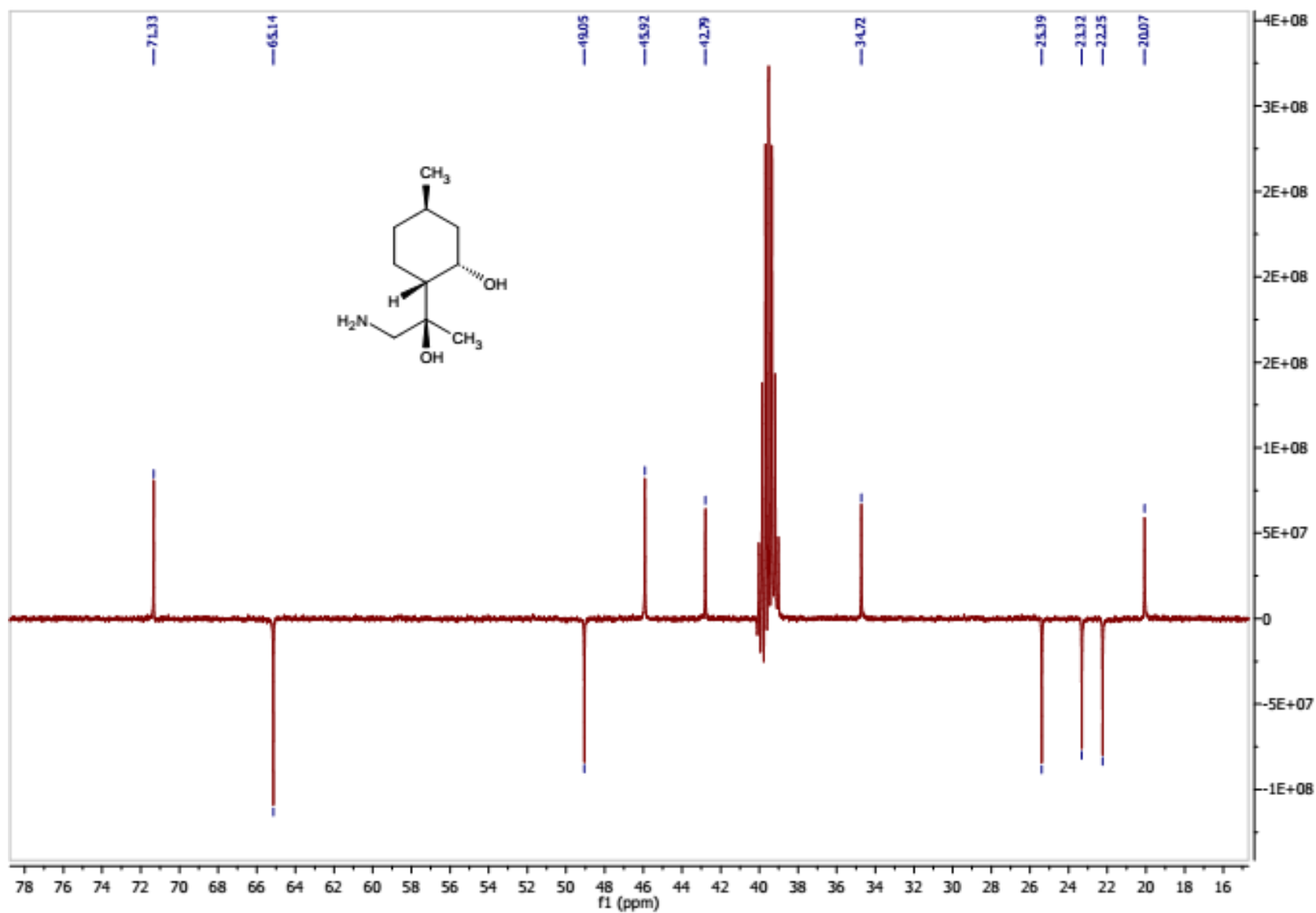


Figure S 24:  $^1\text{H}$ -NMR of compound **9b**

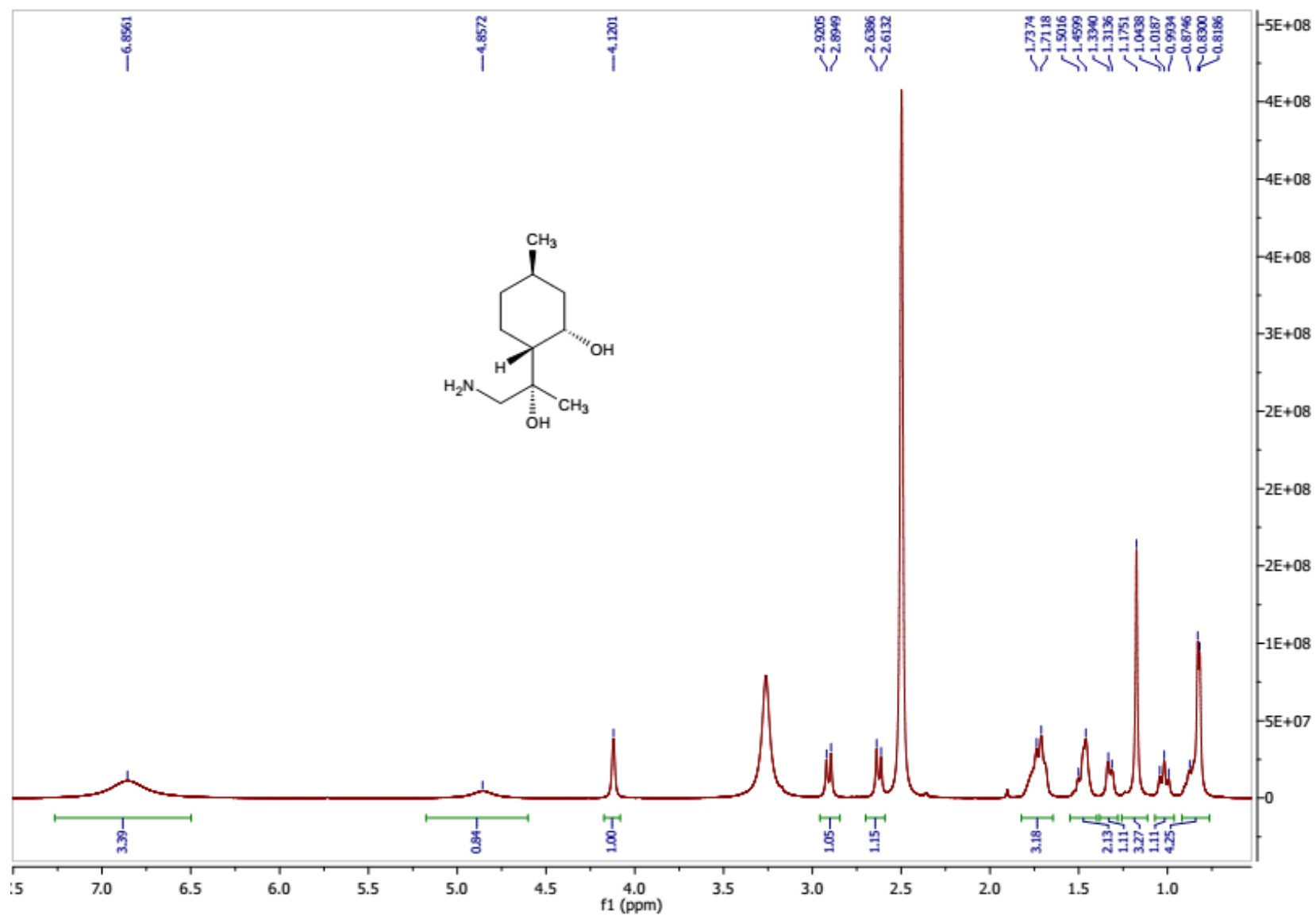


Figure S 25:  $^{13}\text{C}$ -NMR of compound **9b**

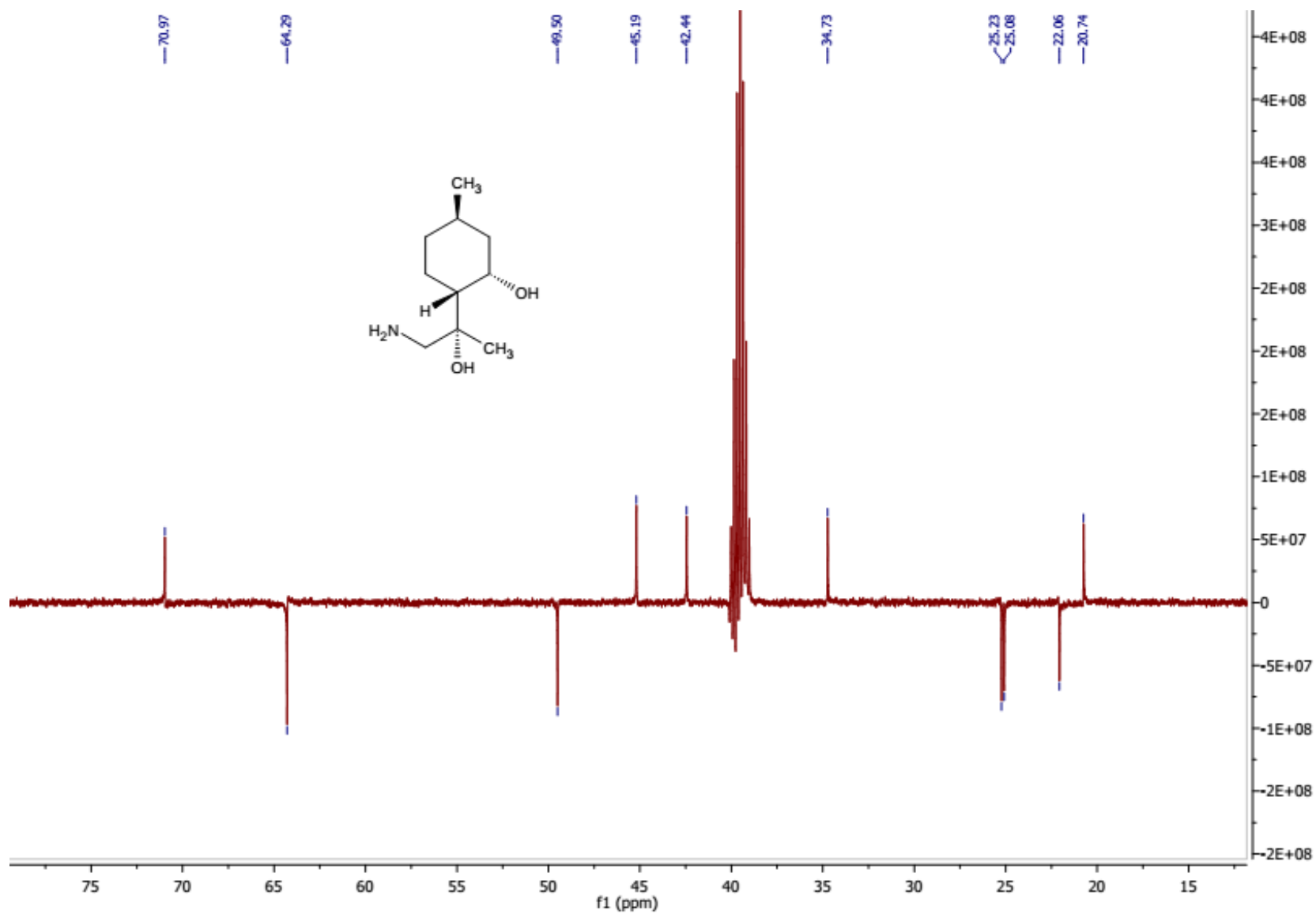




Figure S 26:  $^1\text{H}$ -NMR of compound **10**

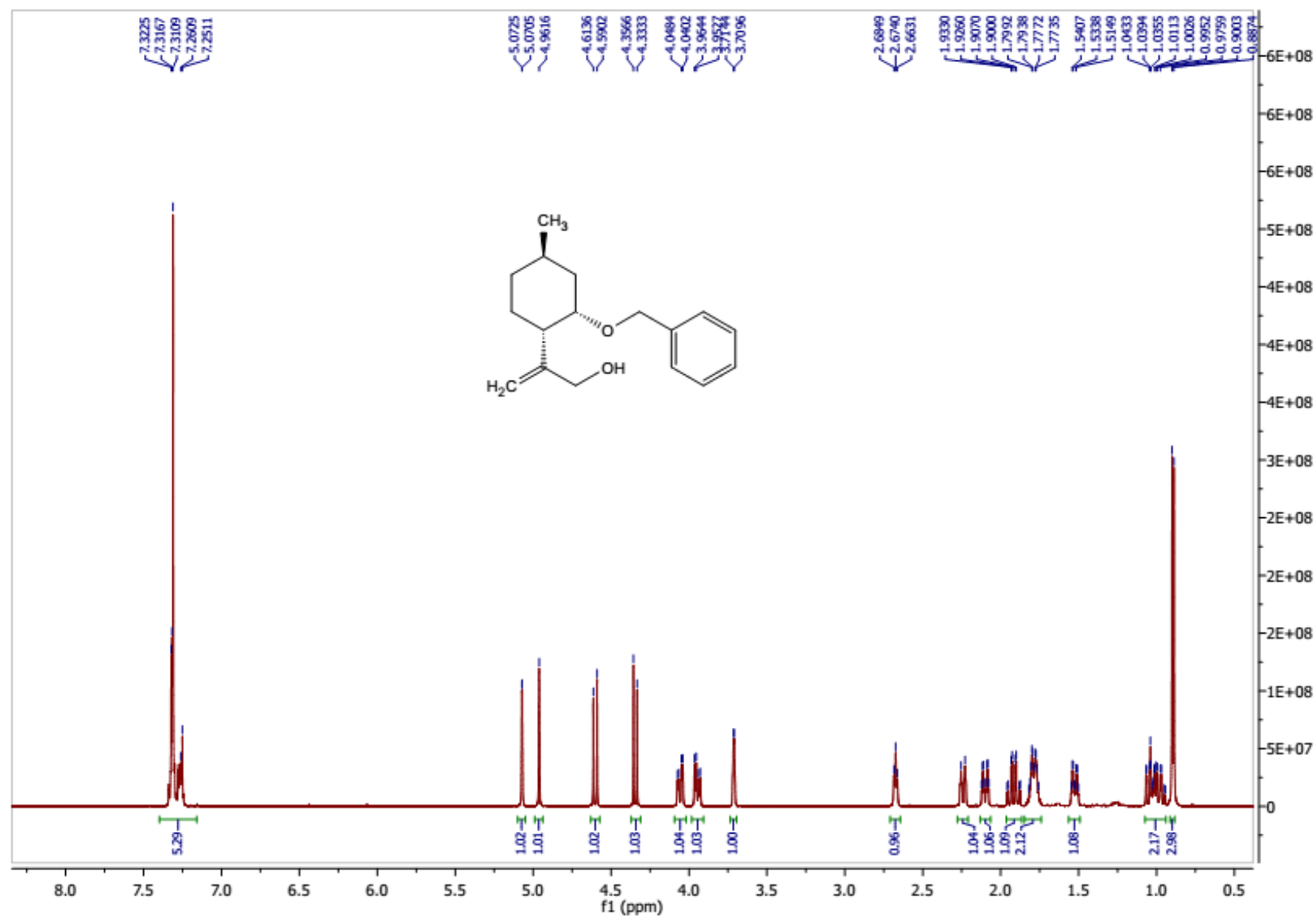


Figure S 27:  $^{13}\text{C}$ -NMR of compound **10**

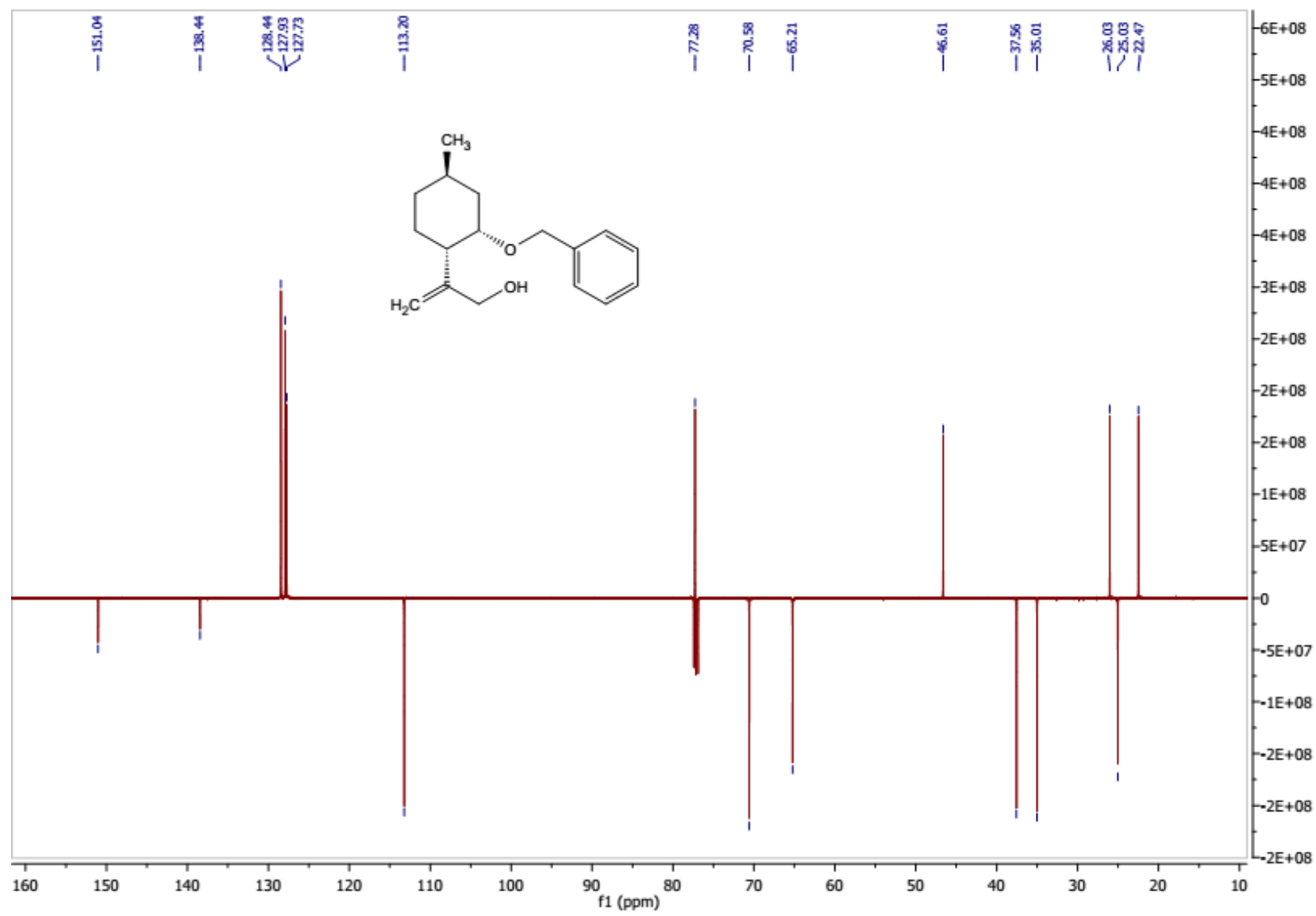


Figure S 28:  $^1\text{H}$ -NMR of compound **12a**

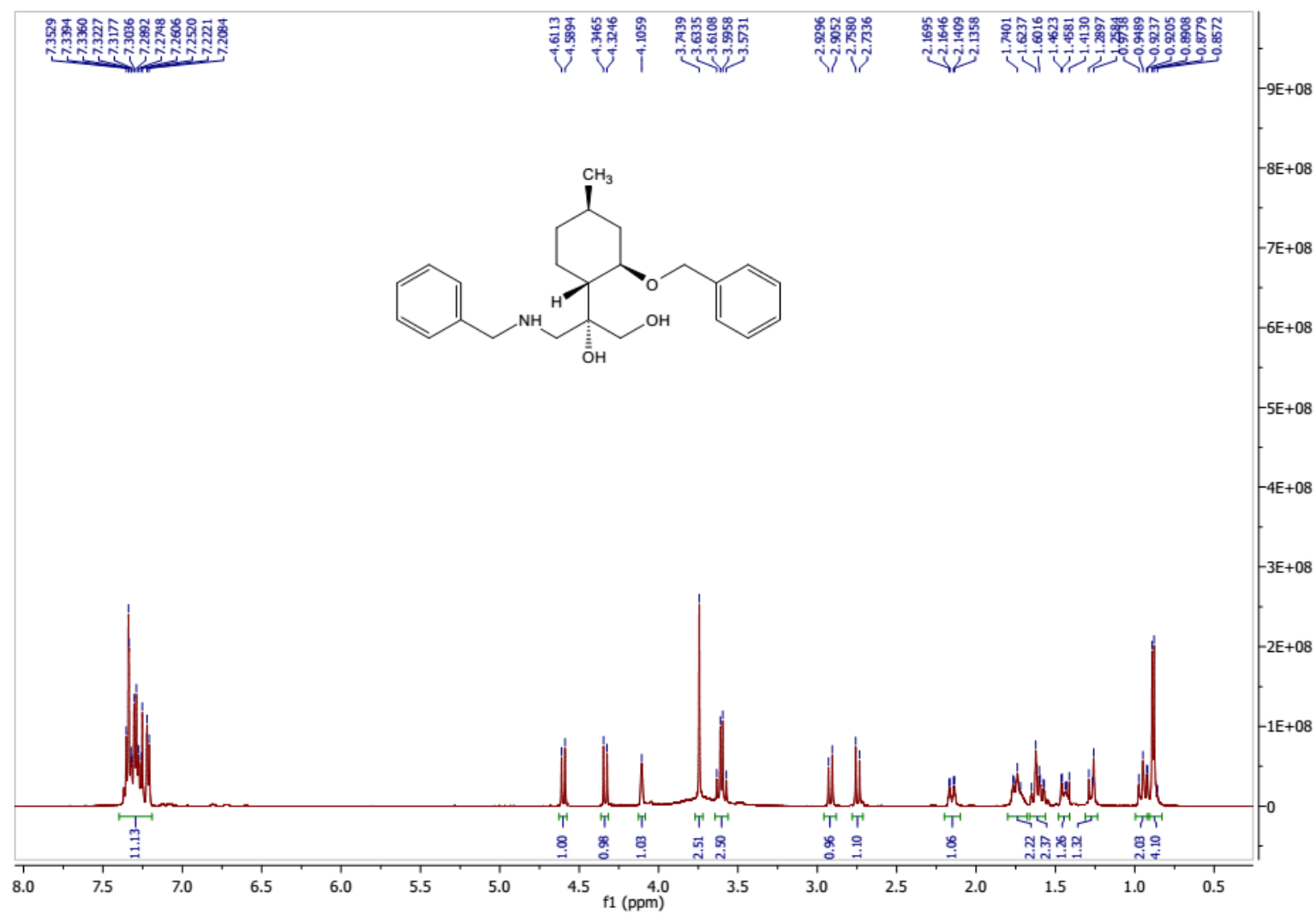


Figure S 29:  $^{13}\text{C}$ -NMR of compound **12a**

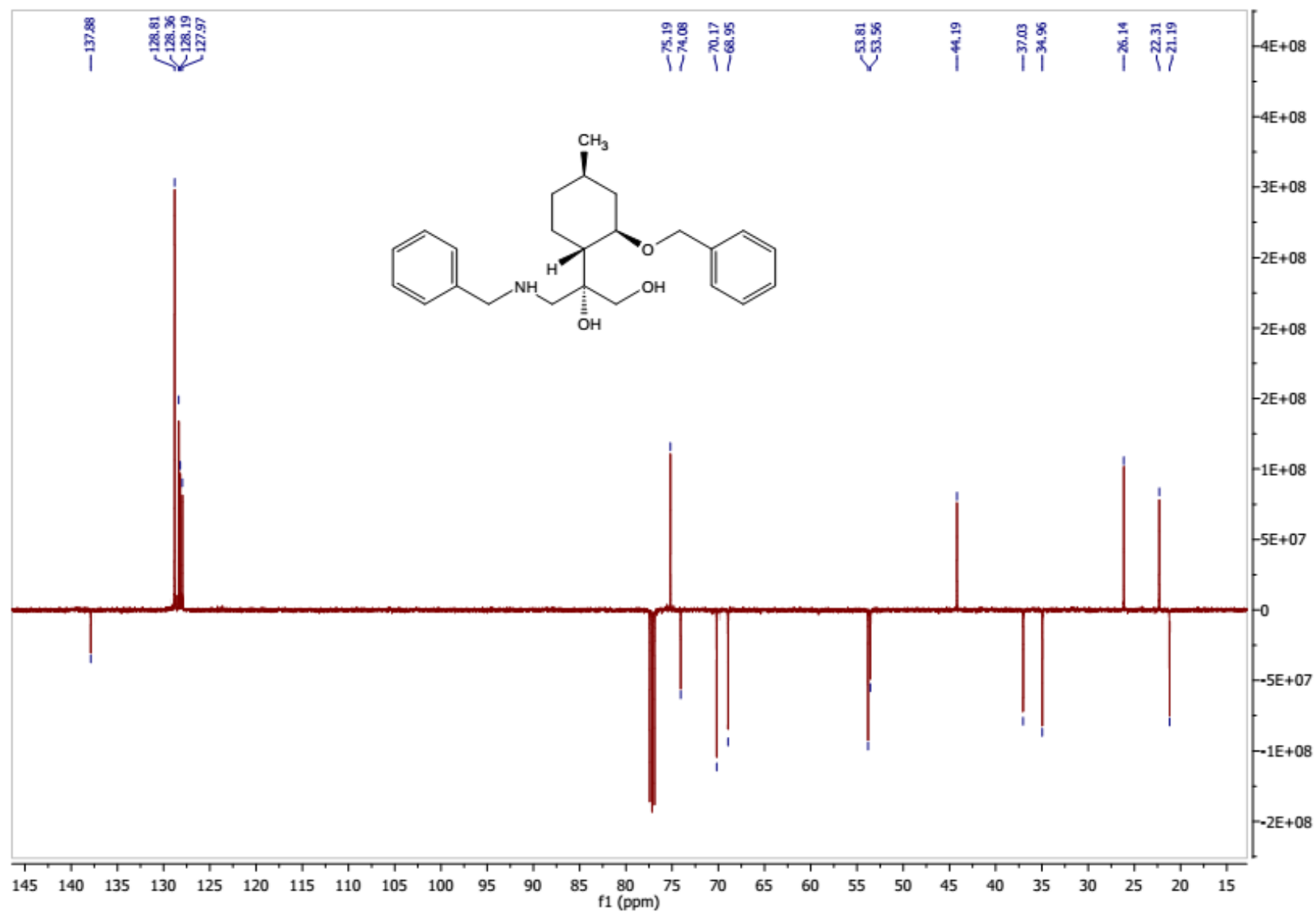


Figure S 30:  $^1\text{H}$ -NMR of compound **12b**

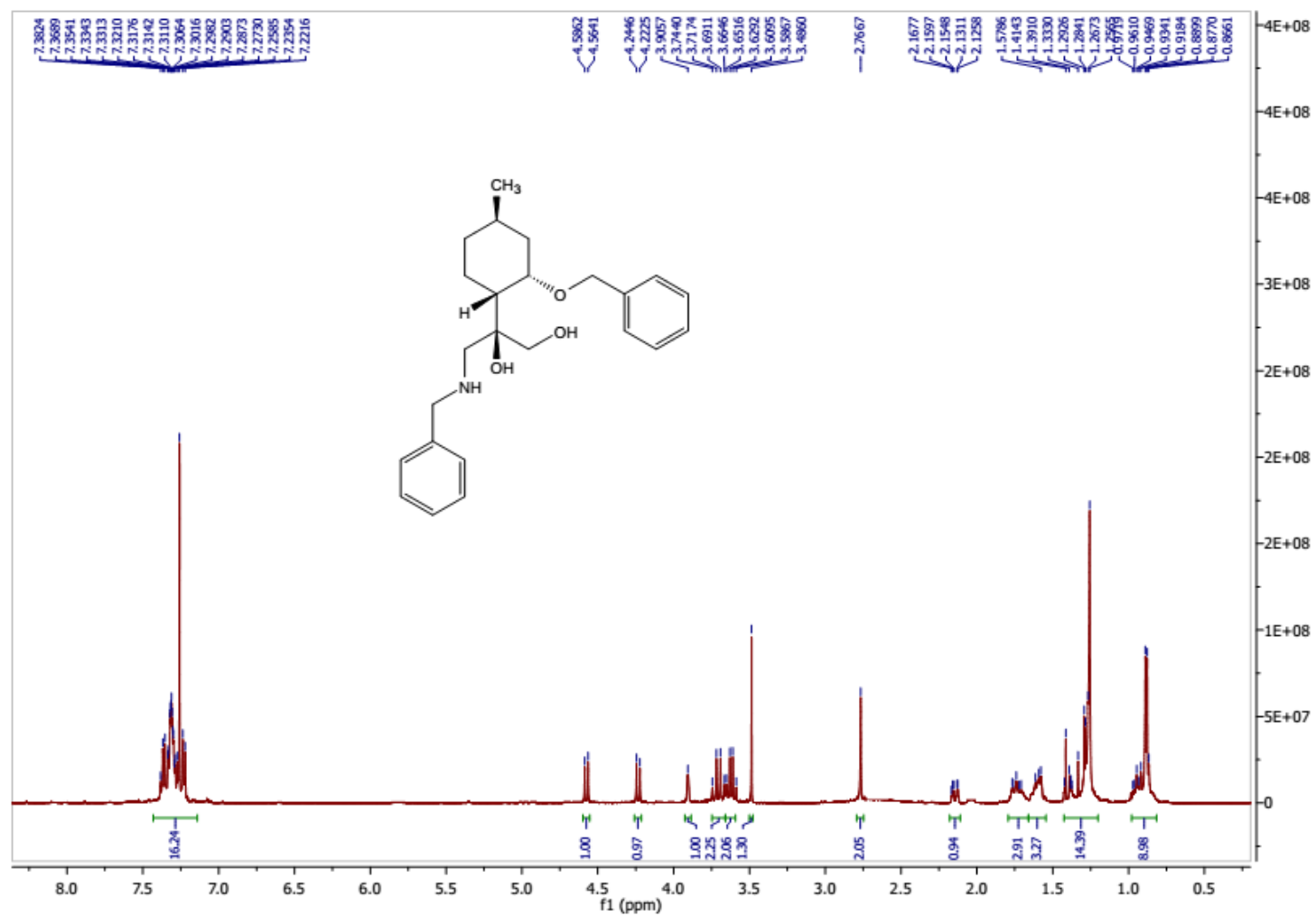


Figure S 31:  $^{13}\text{C}$ -NMR of compound **12b**

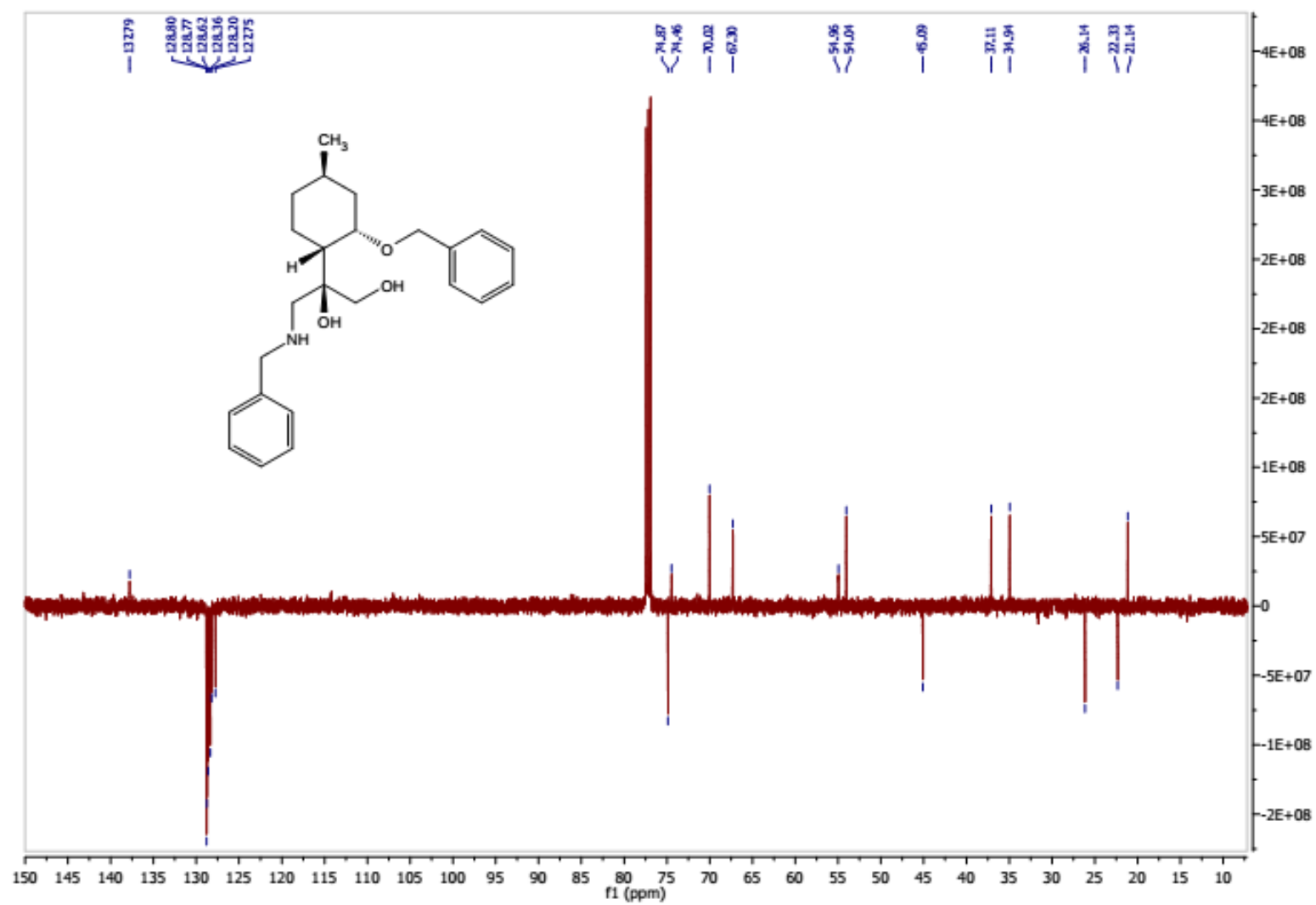


Figure S 32:  $^1\text{H}$ -NMR of compound **13a**

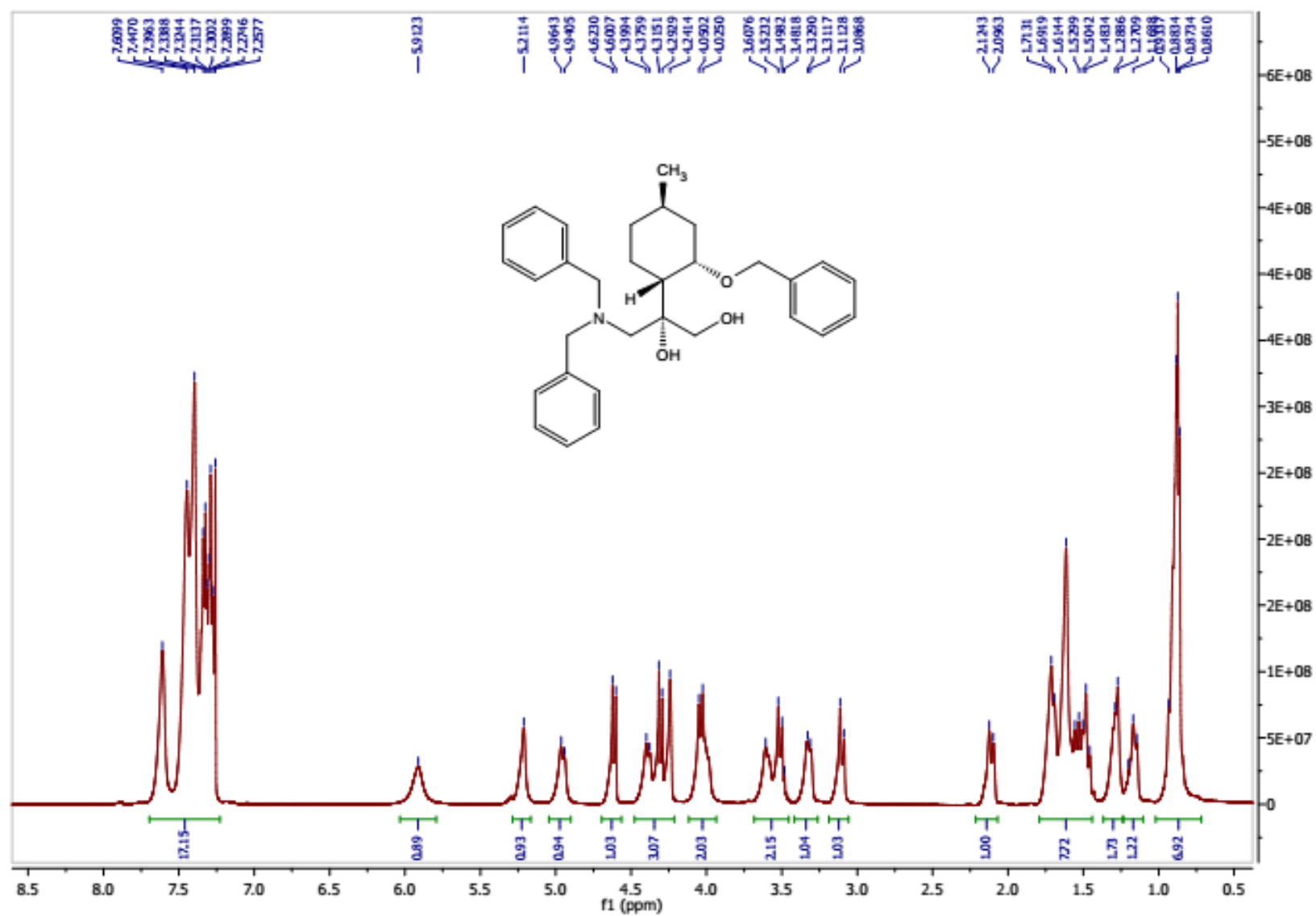


Figure S 33:  $^{13}\text{C}$ -NMR of compound **13a**

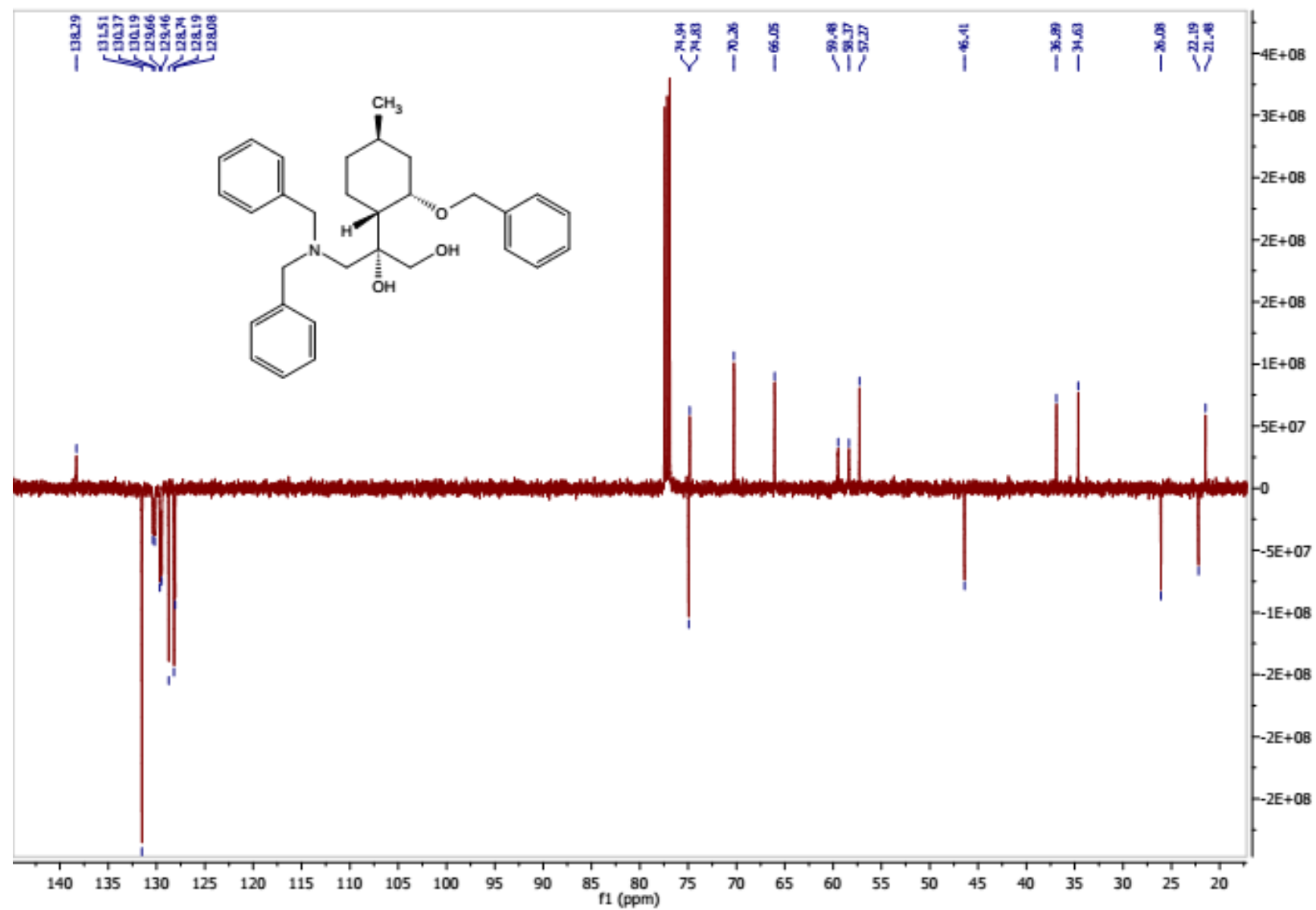




Figure S 34:  $^1\text{H}$ -NMR of compound **13b**

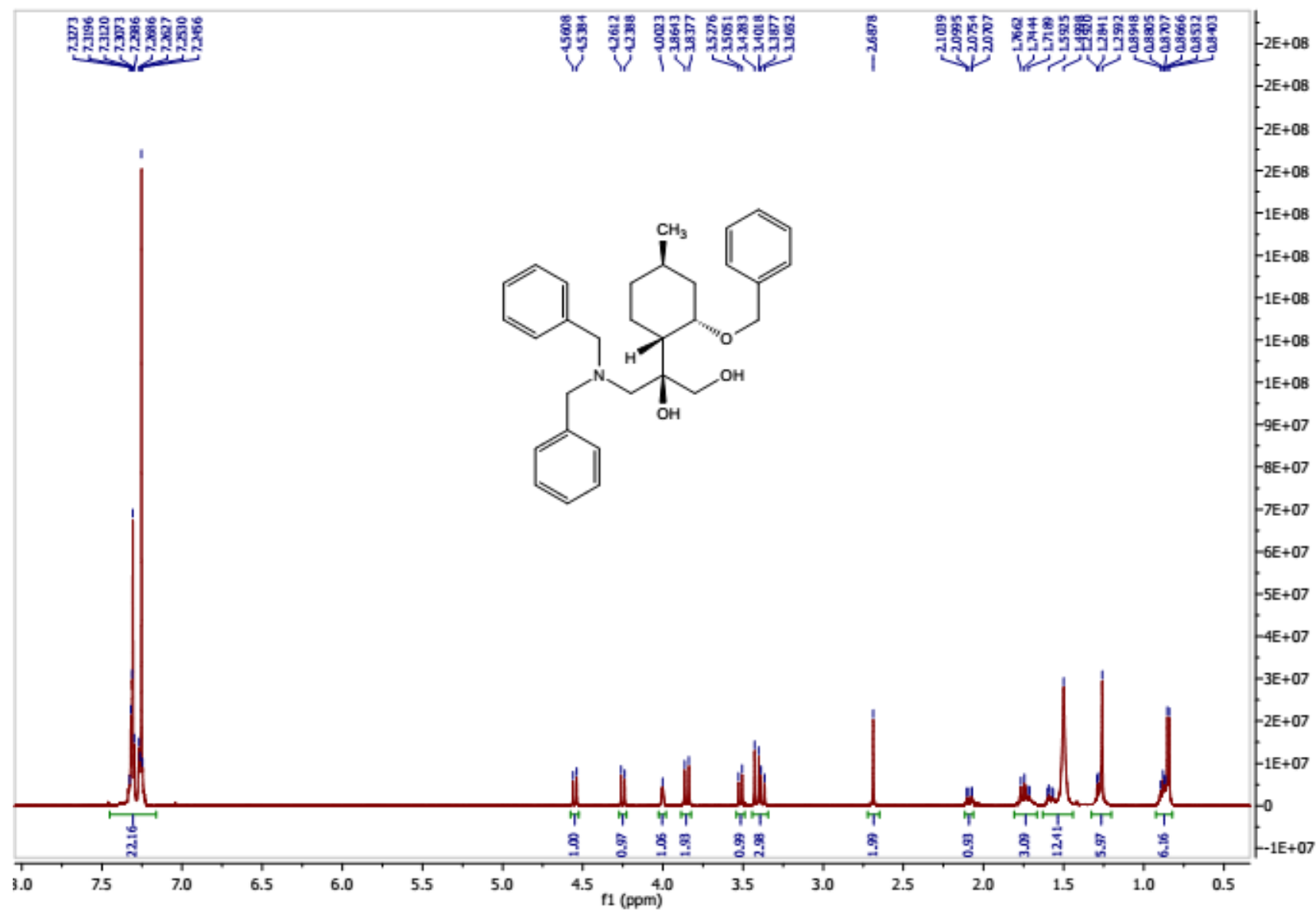


Figure S 35:  $^{13}\text{C}$ -NMR of compound **13b**

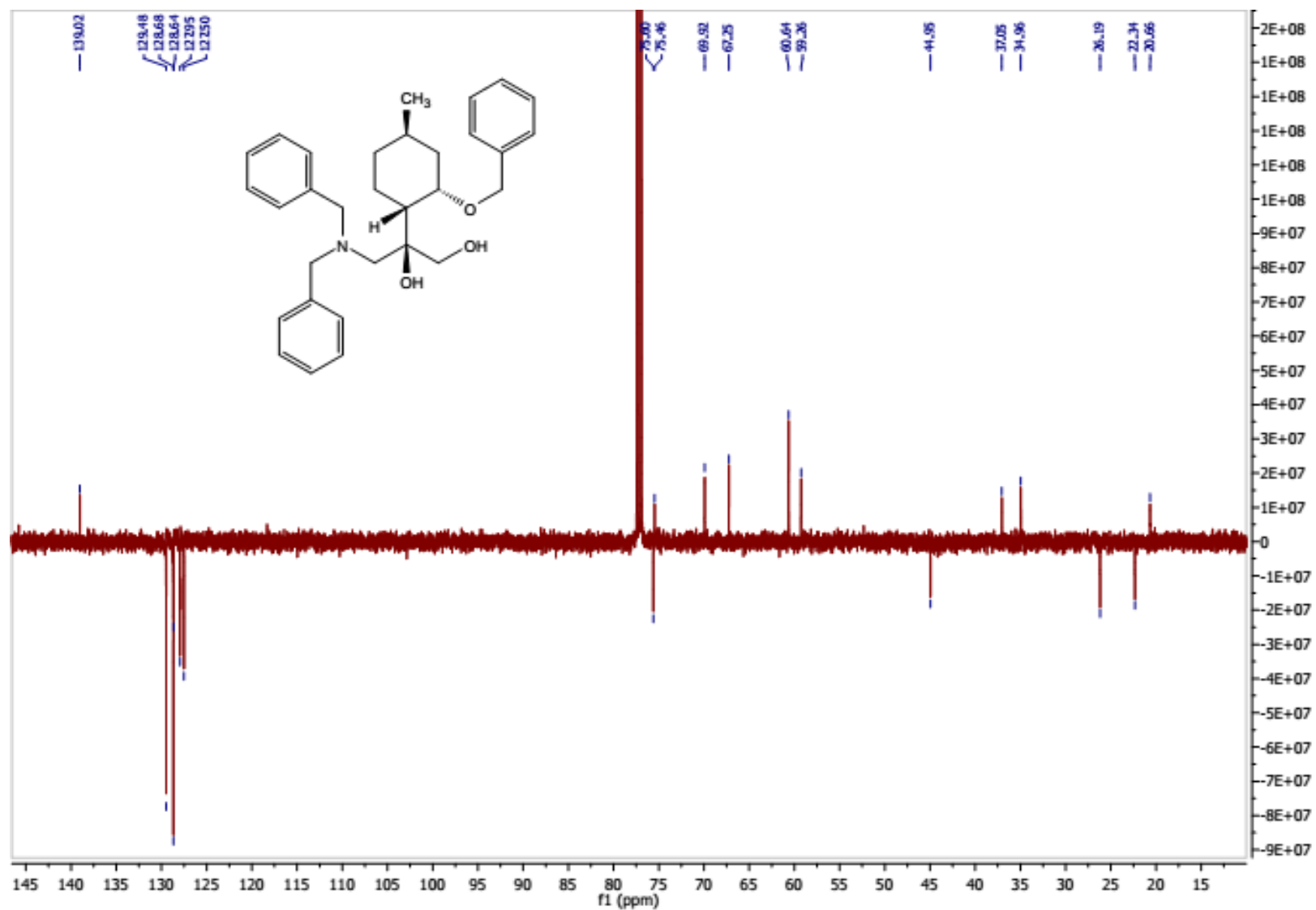


Figure S 36:  $^1\text{H}$ -NMR of compound **14a**

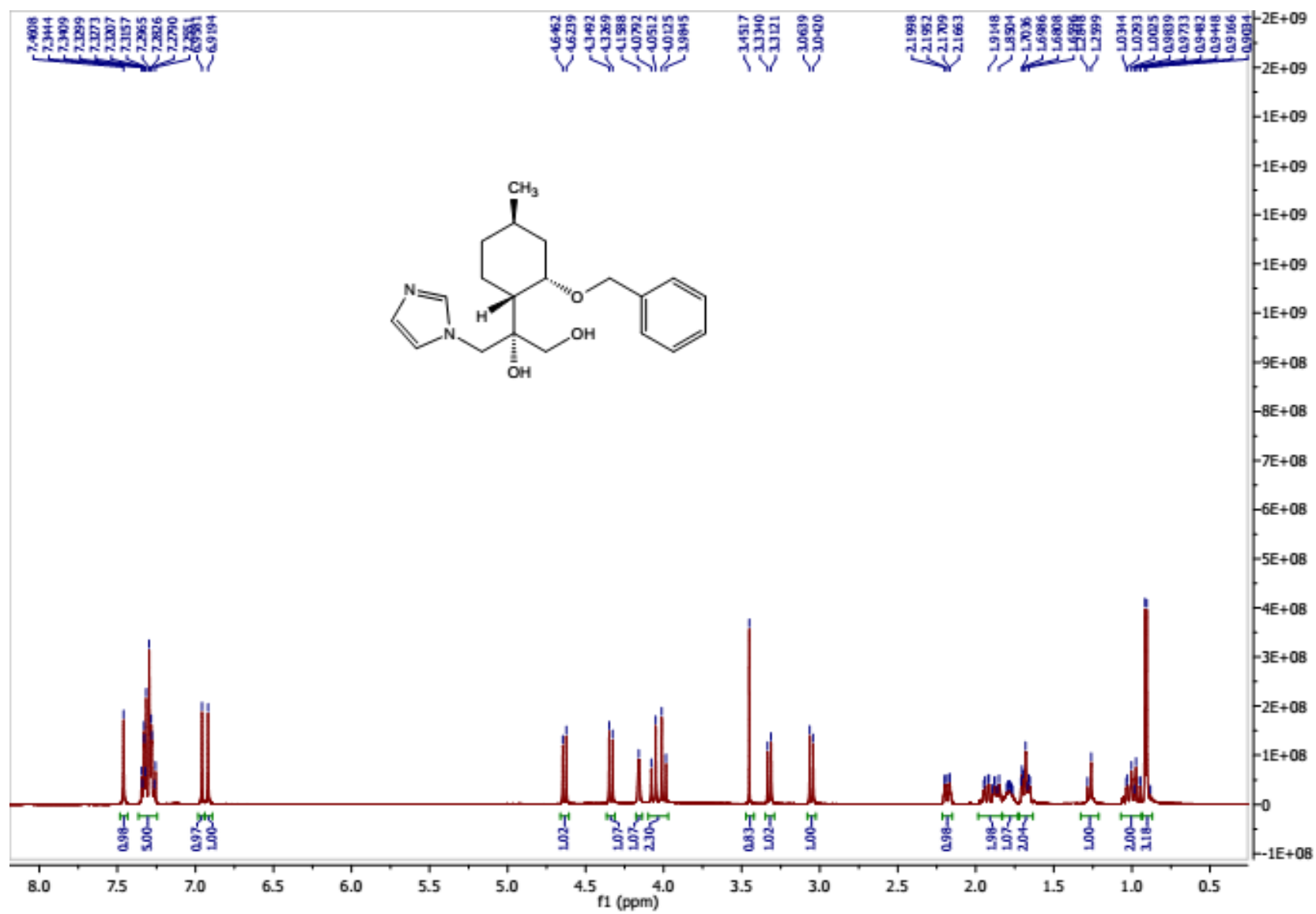


Figure S 37:  $^{13}\text{C}$ -NMR of compound **14a**

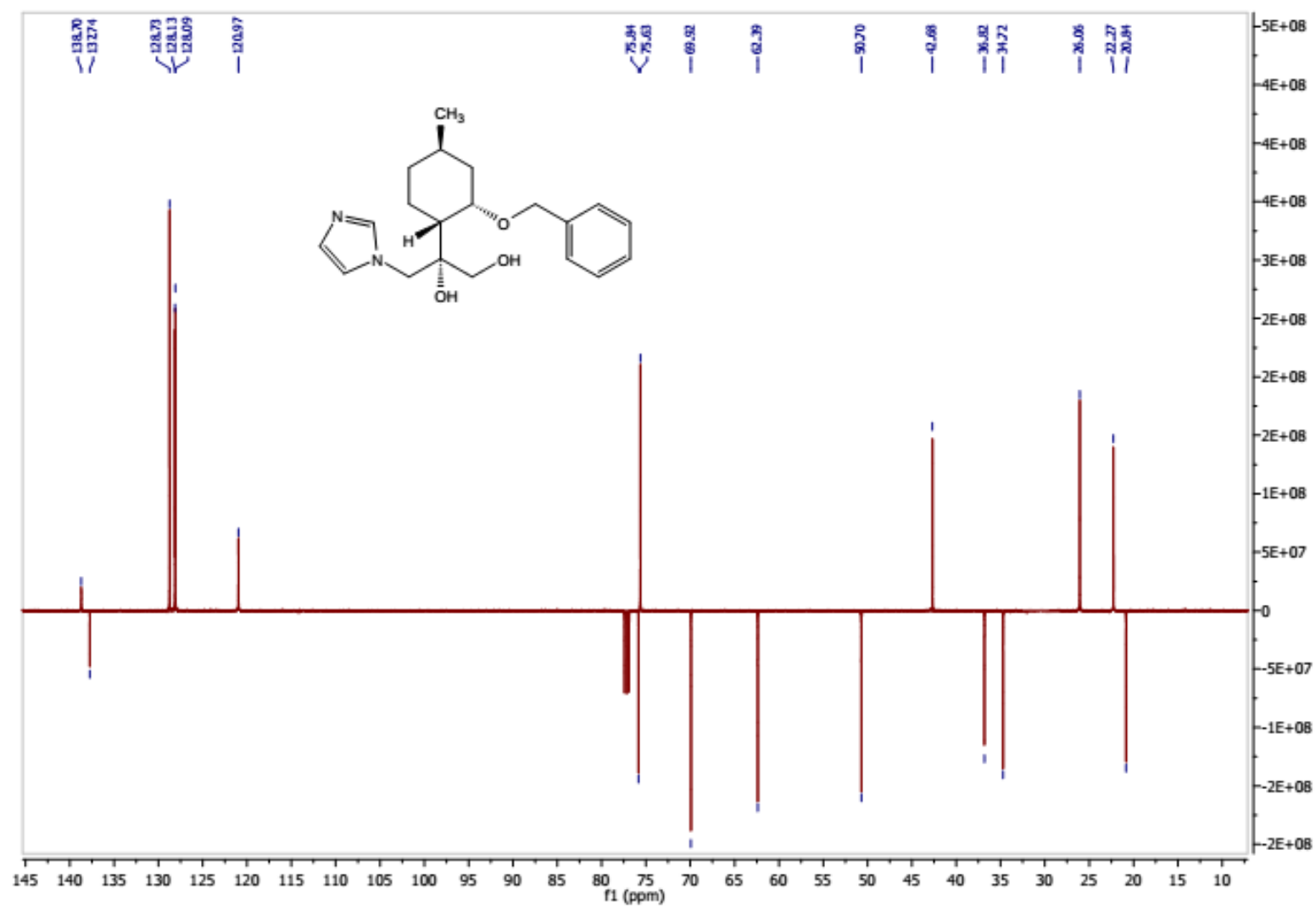


Figure S 38:  $^1\text{H}$ -NMR of compound **15a**

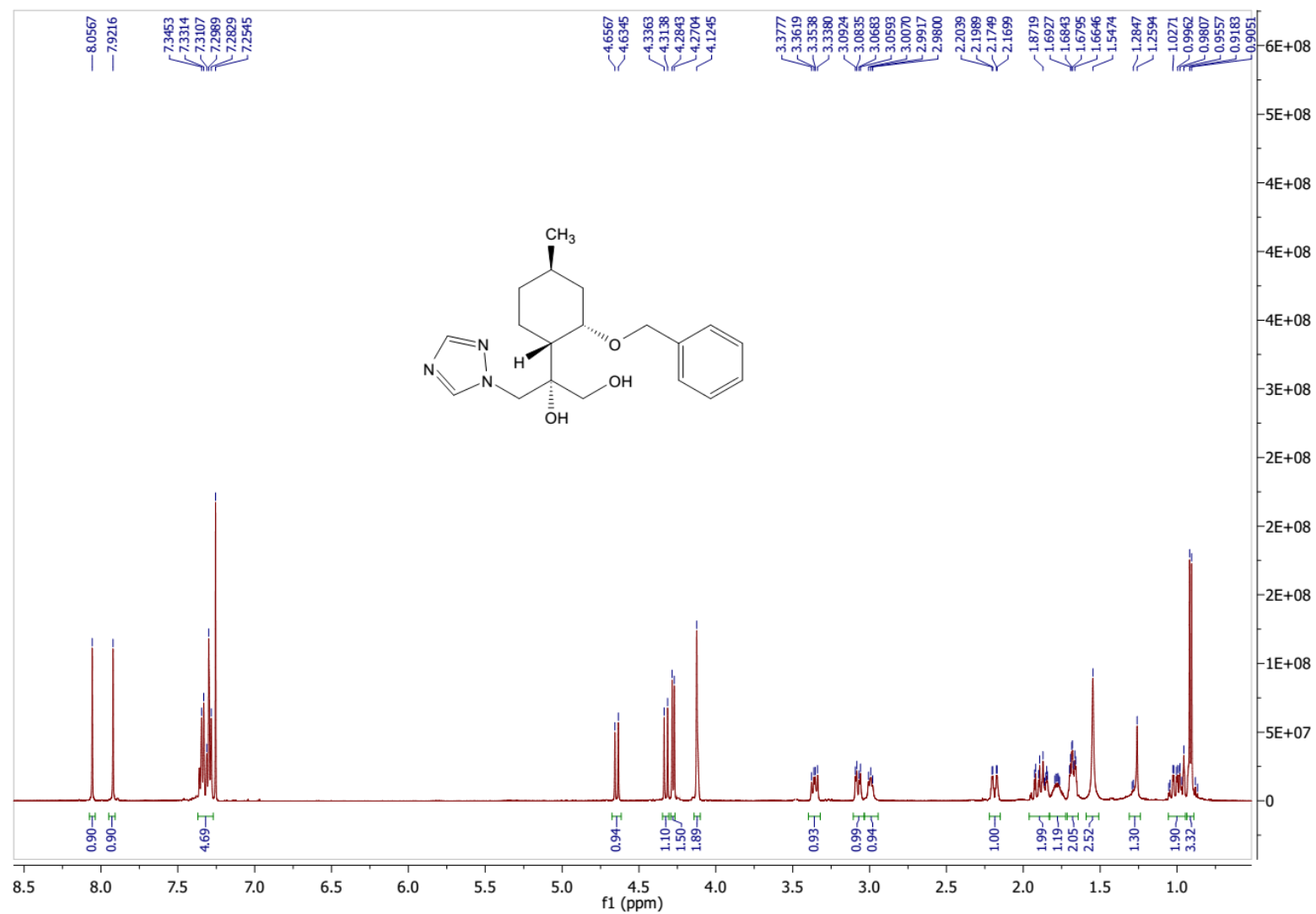


Figure S 39:  $^{13}\text{C}$ -NMR of compound **15a**

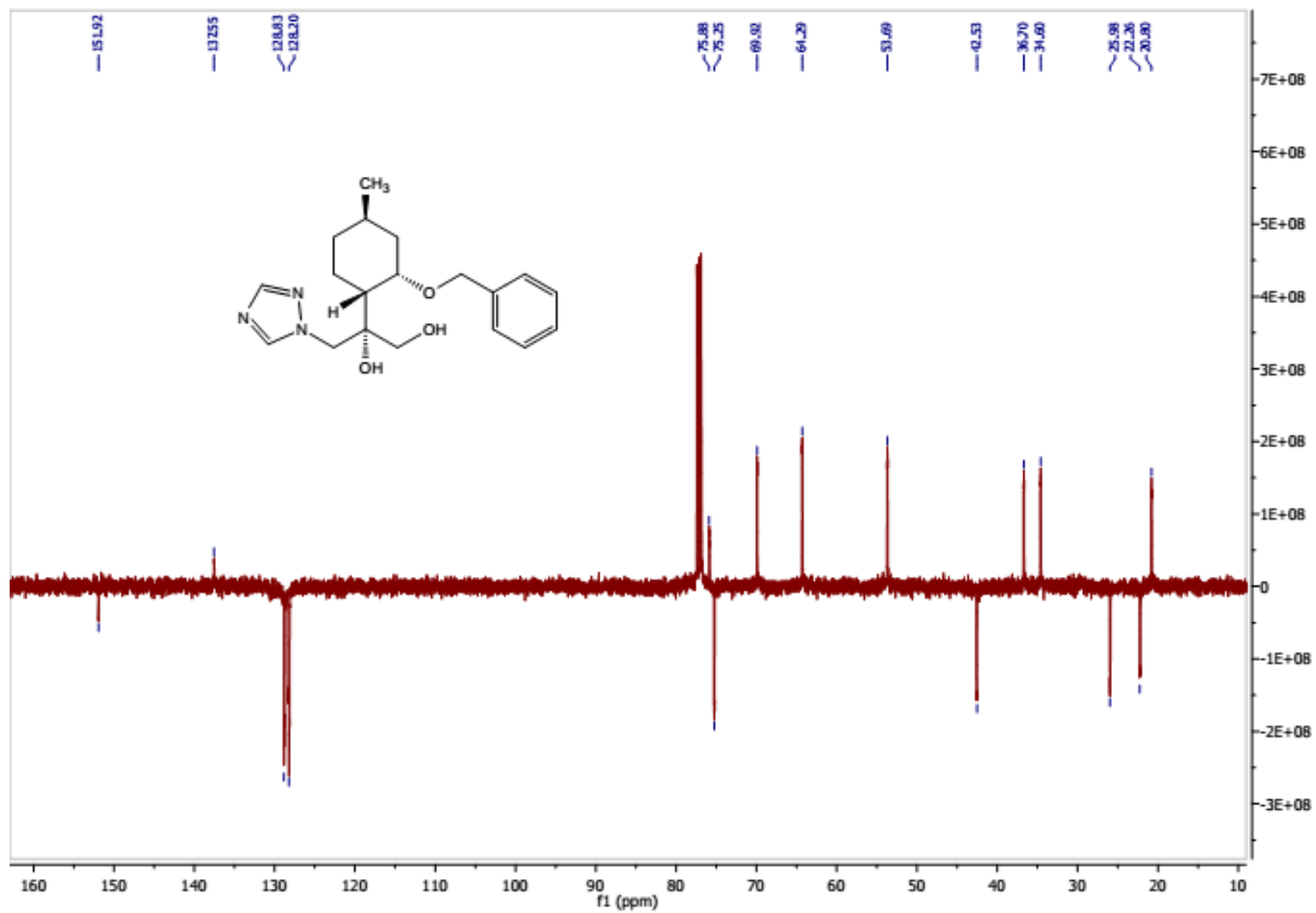


Figure S 40:  $^1\text{H}$ -NMR of compound 16a

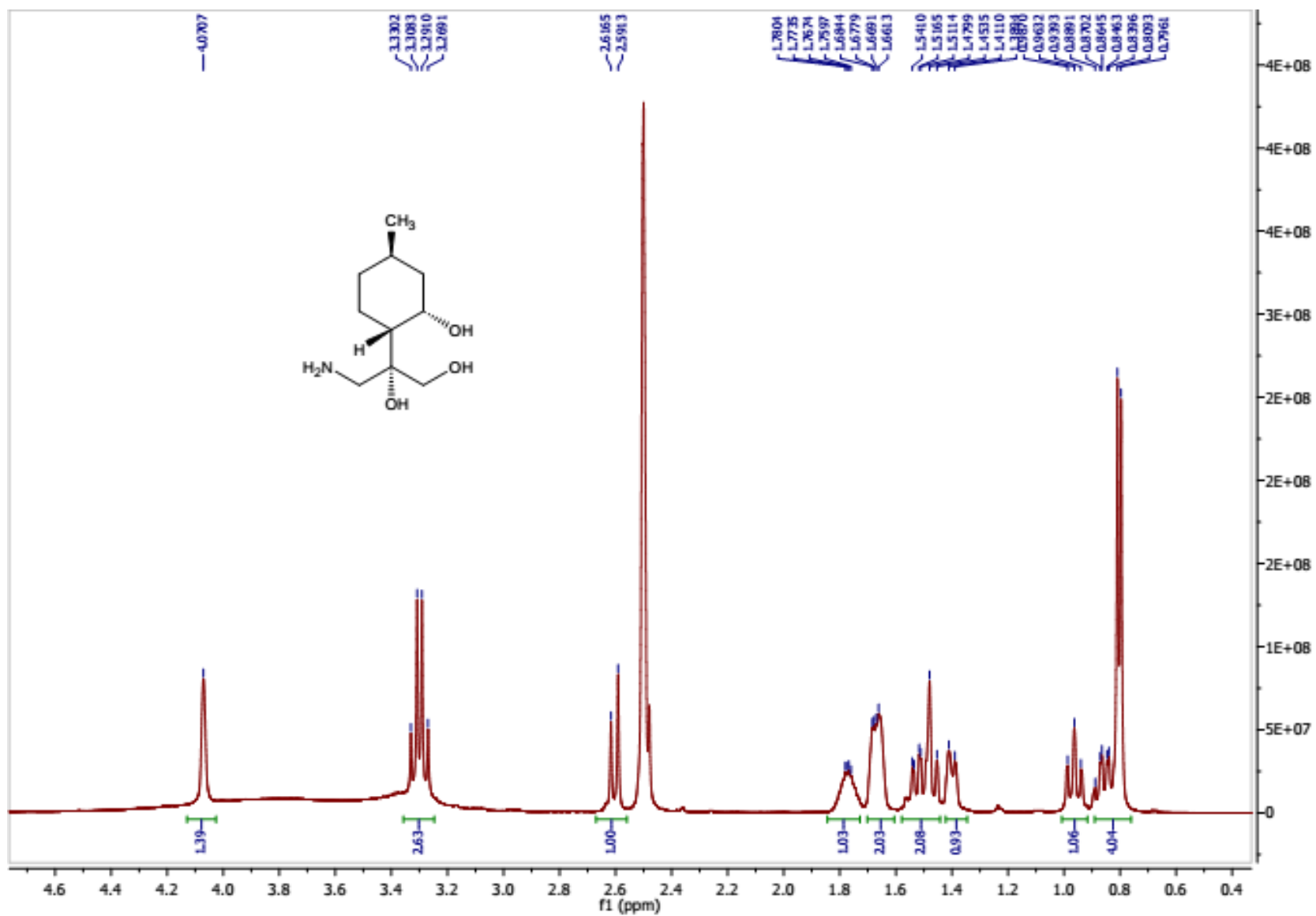


Figure S 41:  $^{13}\text{C}$ -NMR of compound **16a**

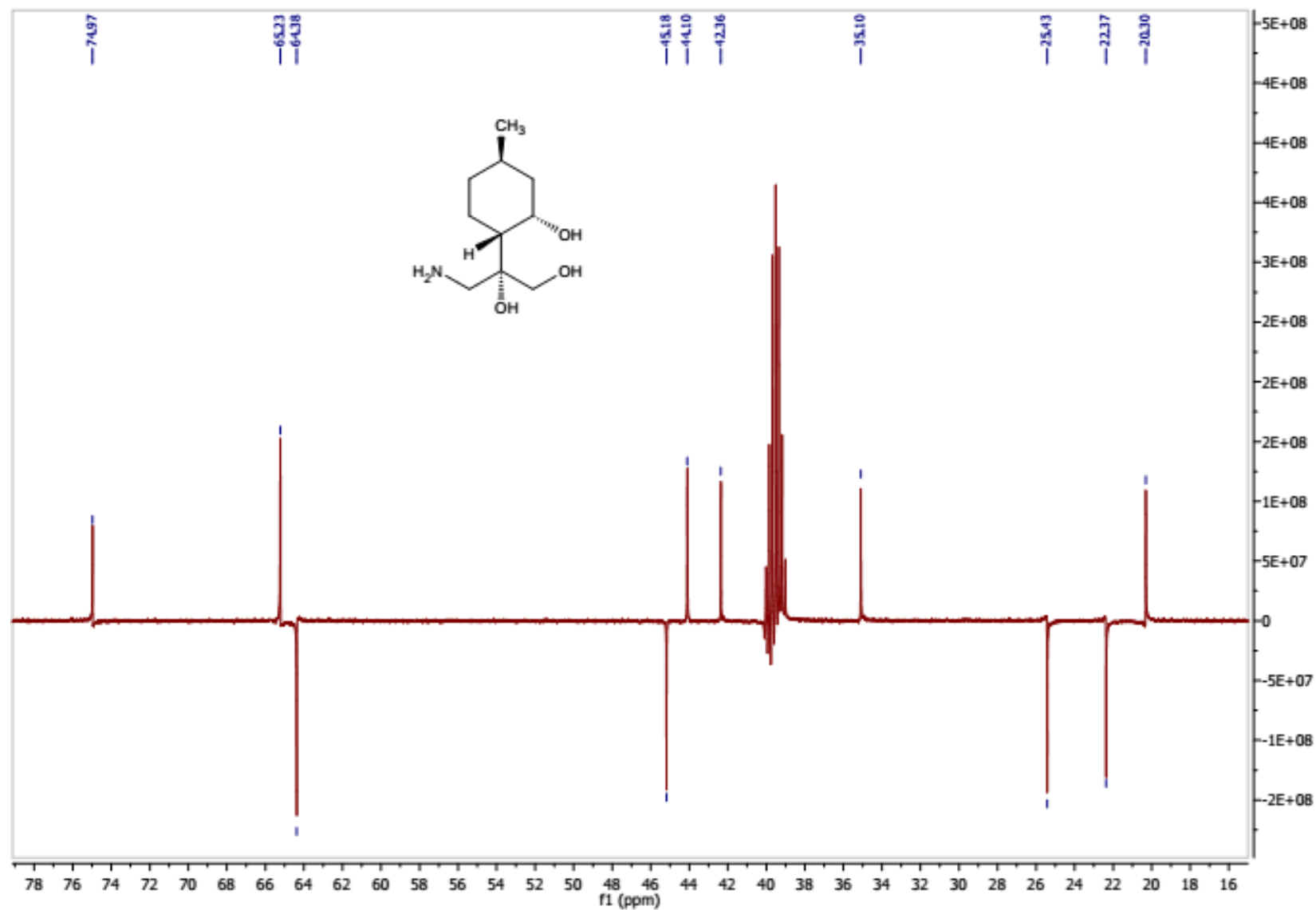




Figure S 42:  $^1\text{H}$ -NMR of compound **16b**

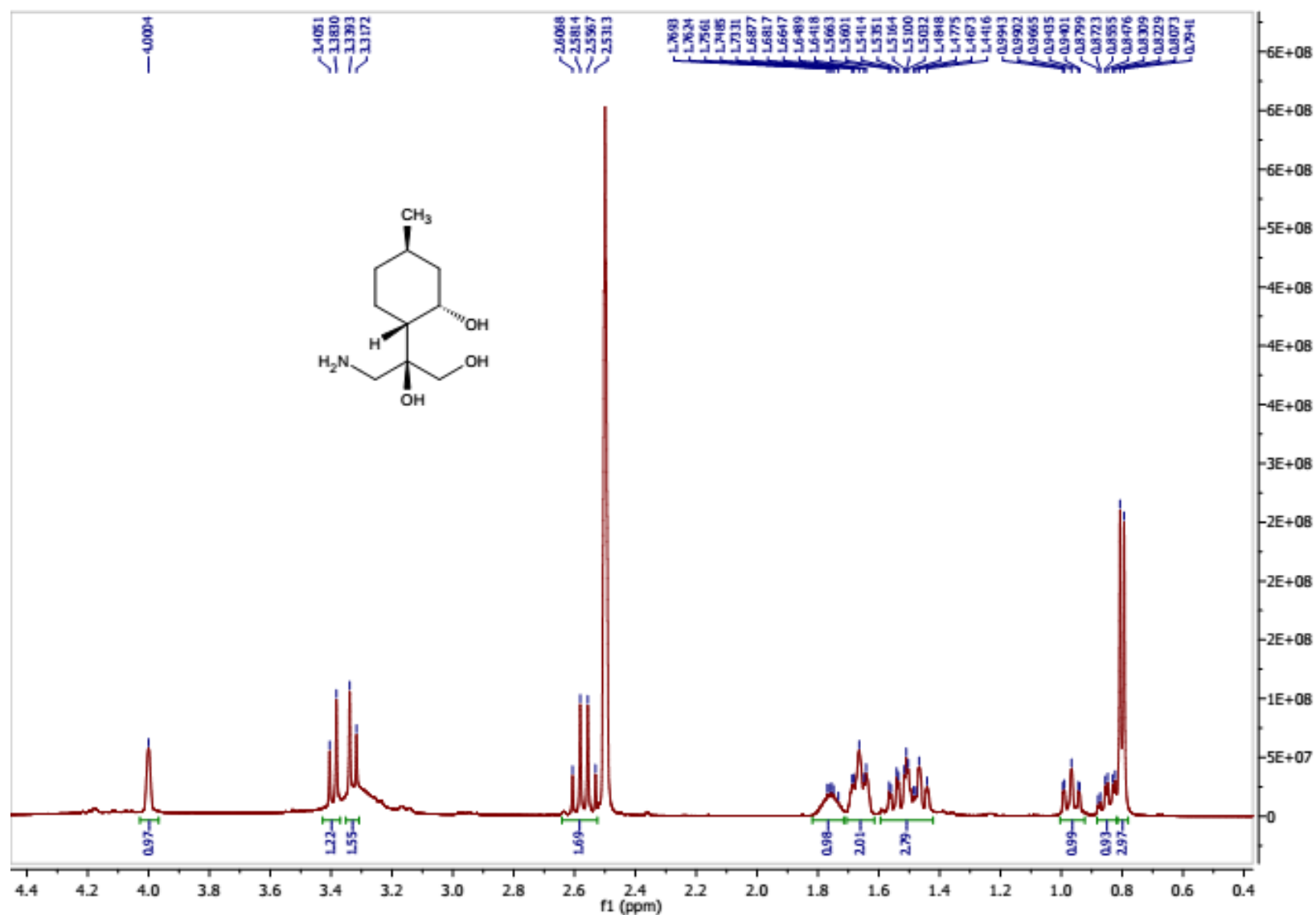


Figure S 43:  $^{13}\text{C}$ -NMR of compound **16b**

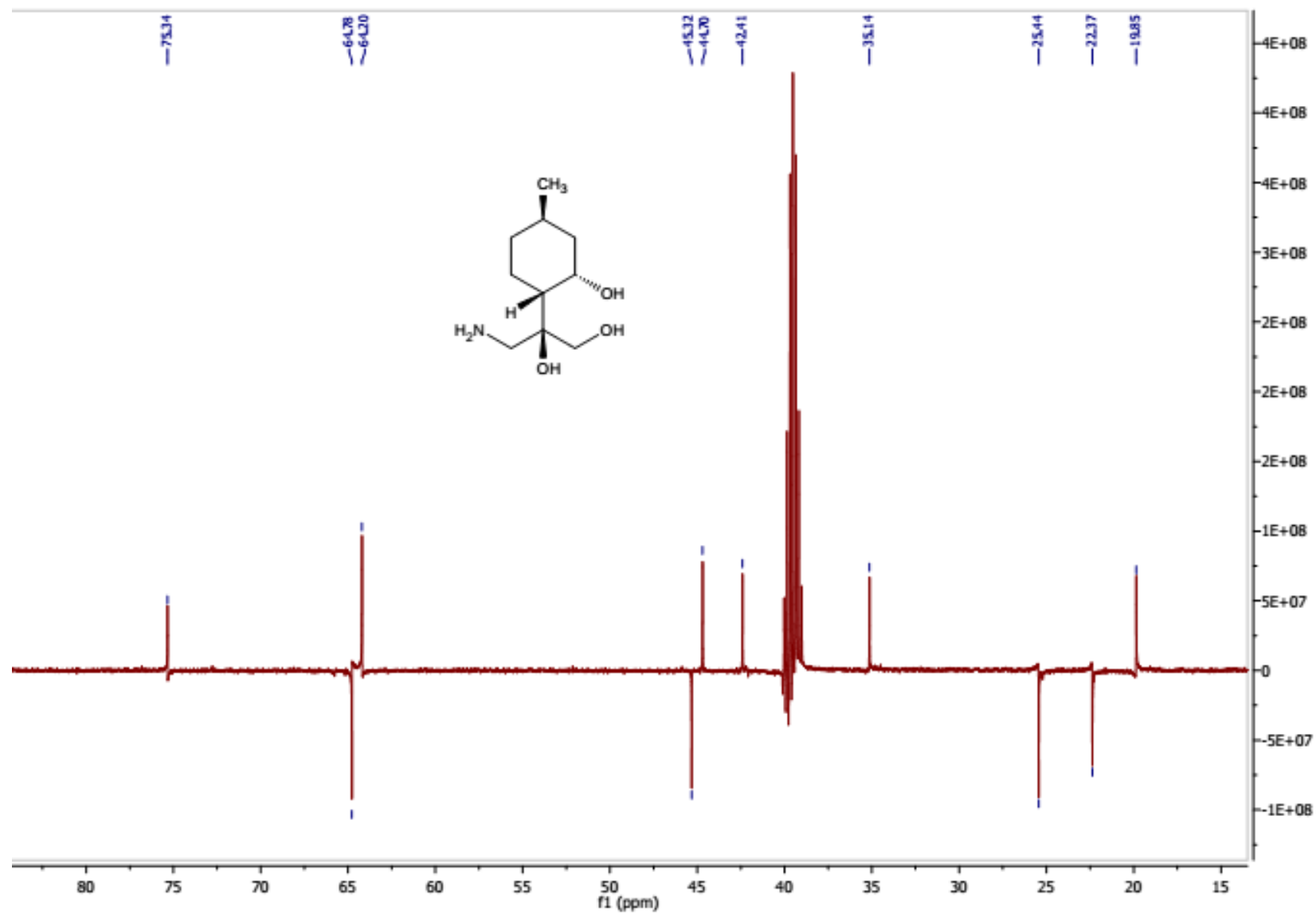


Figure S 44:  $^1\text{H}$ -NMR of compound **18a**

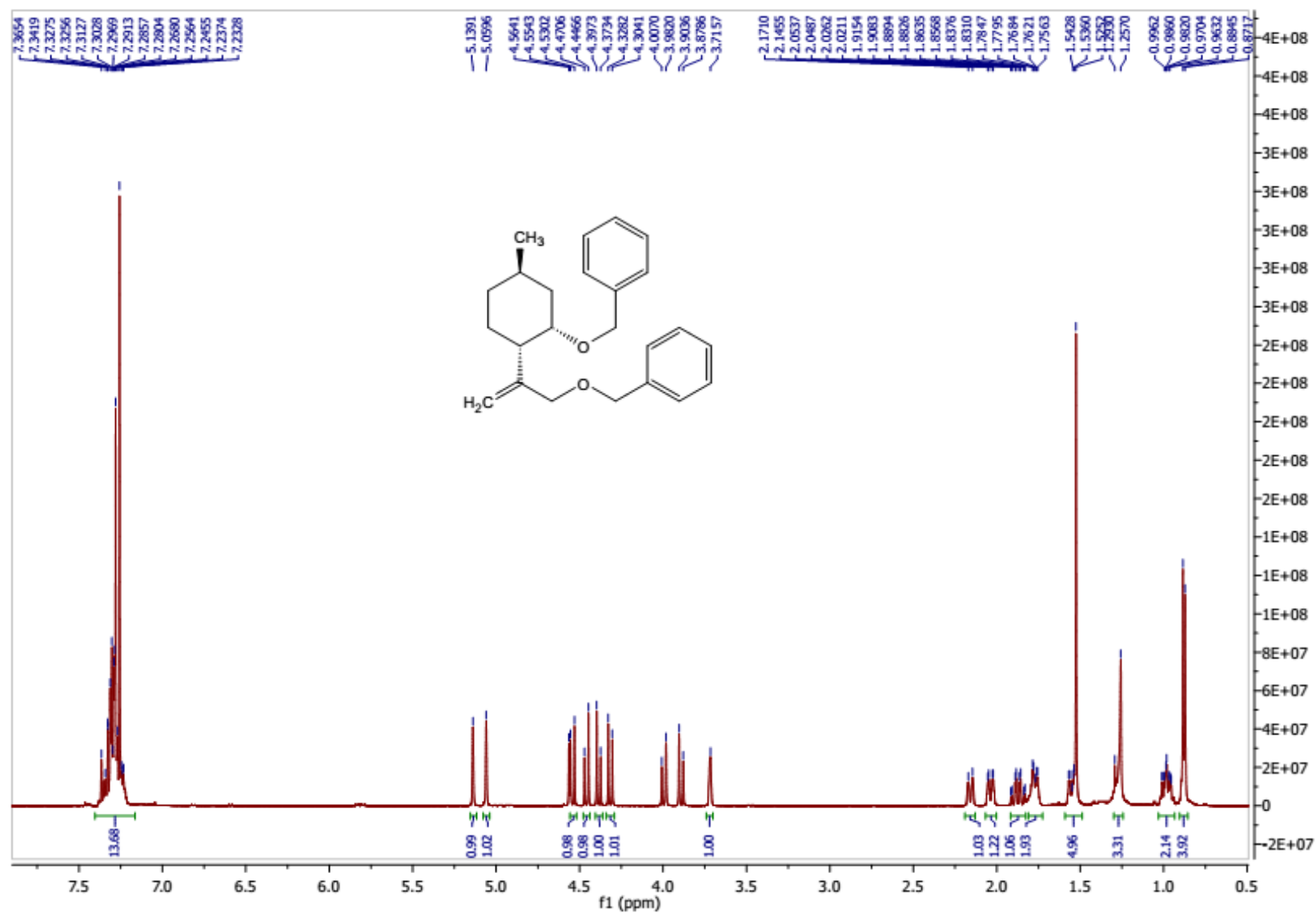


Figure S 45:  $^{13}\text{C}$ -NMR of compound **18a**

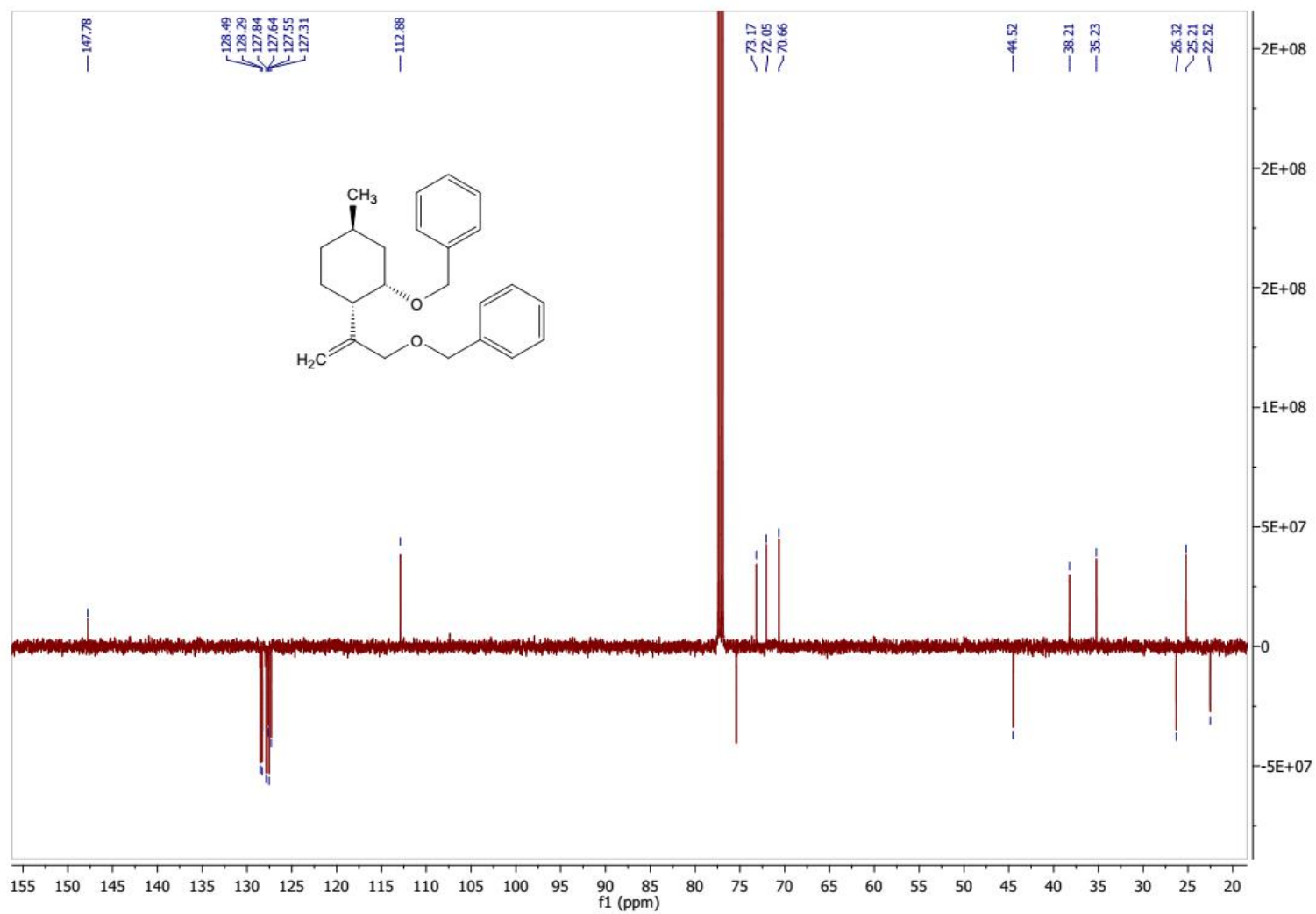


Figure S 46:  $^1\text{H}$ -NMR of compound **19a**

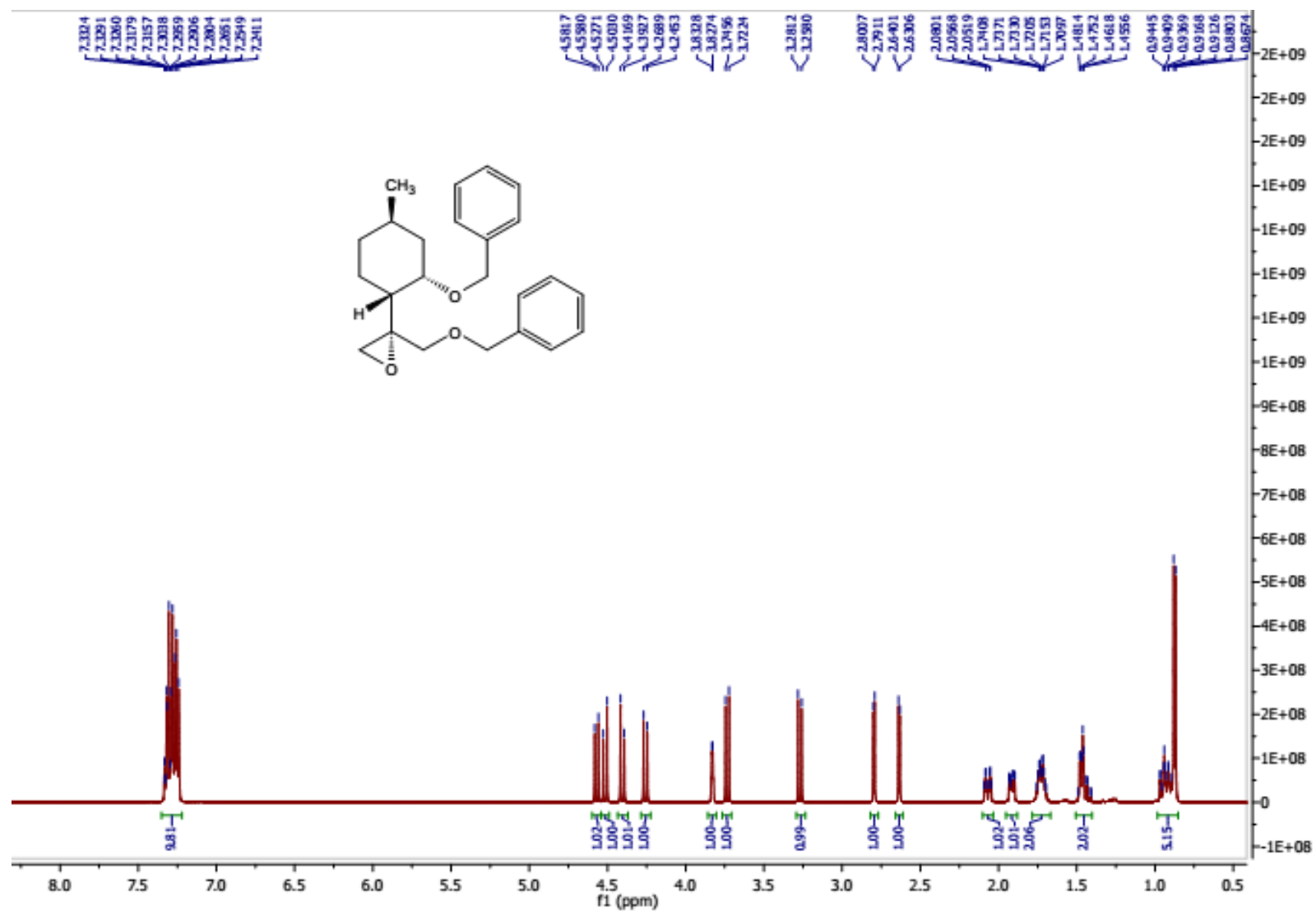


Figure S 47:  $^{13}\text{C}$ -NMR of compound **19**

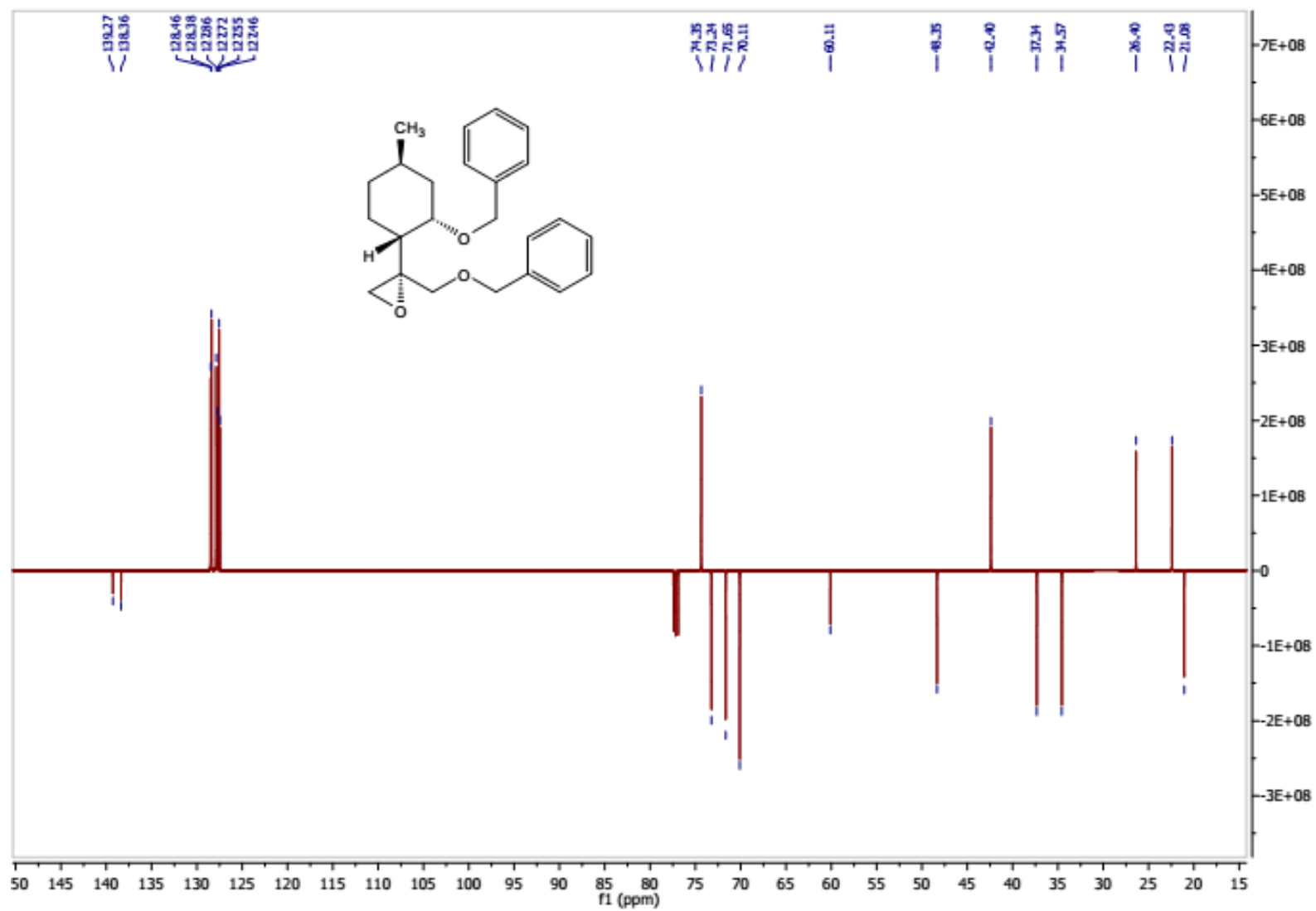


Figure S 48:  $^1\text{H}$ -NMR of compound **19b**

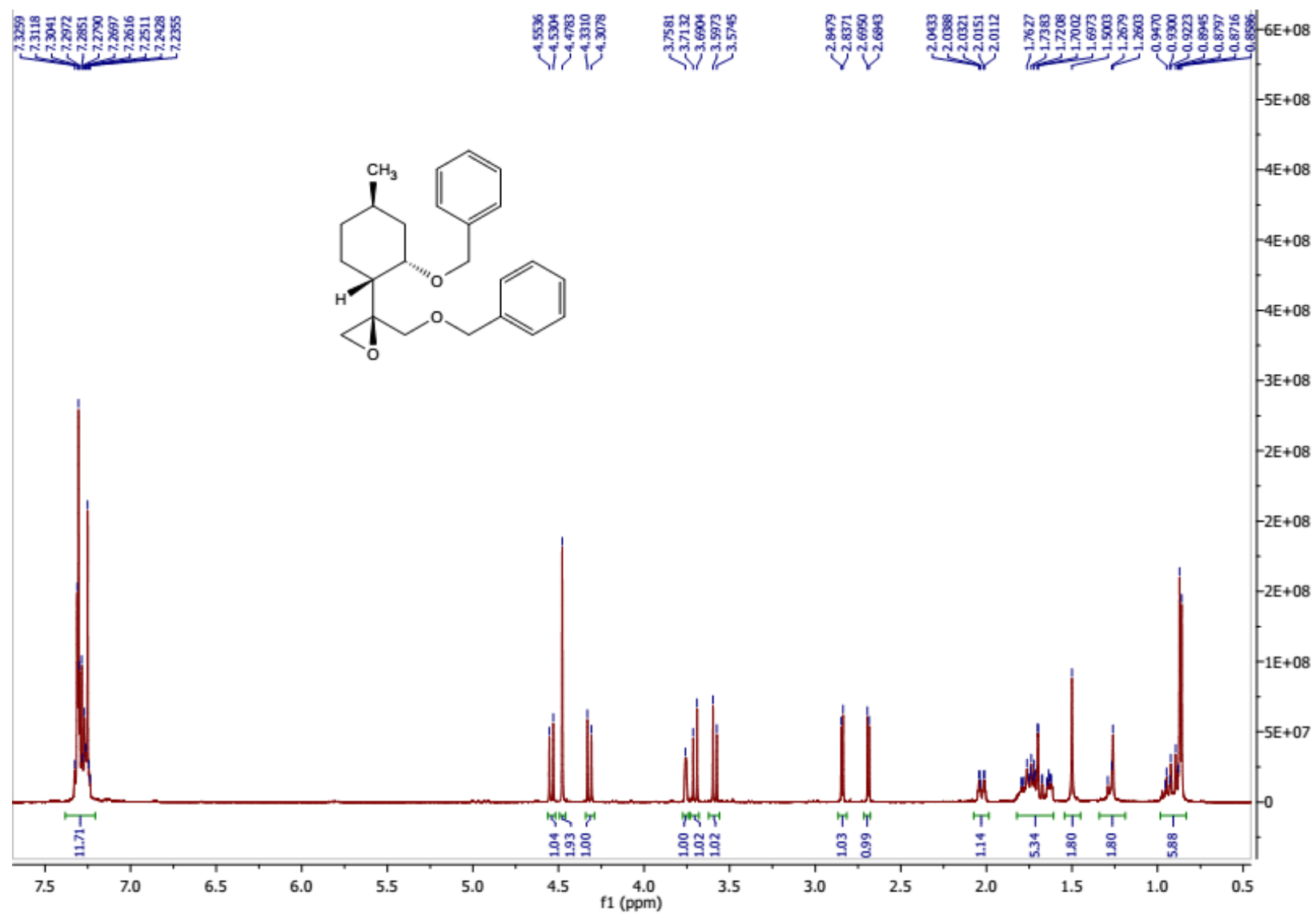


Figure S 49:  $^{13}\text{C}$ -NMR of compound **19b**

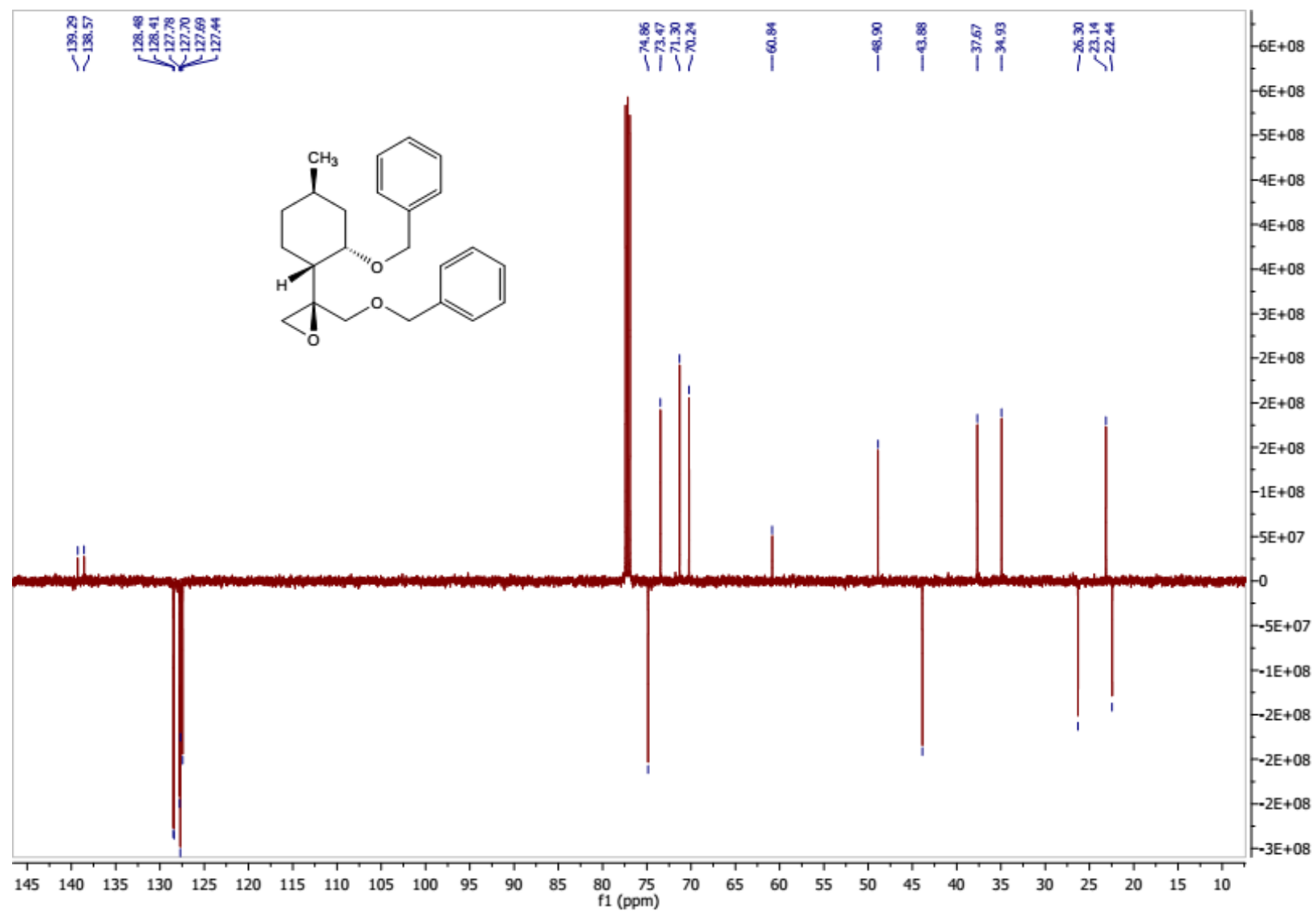




Figure S 50:  $^1\text{H}$ -NMR of compound **20a**

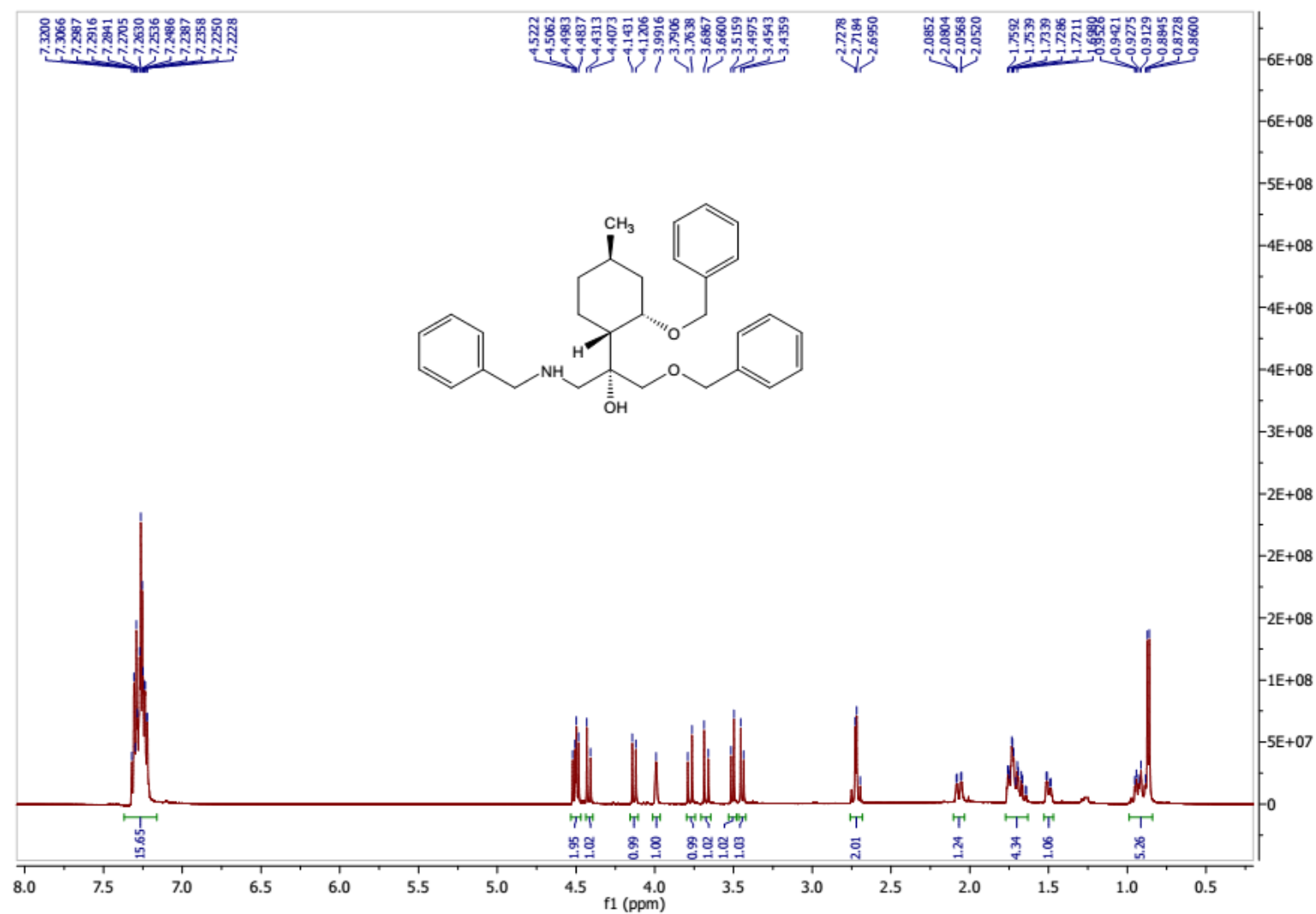


Figure S 51:  $^{13}\text{C}$ -NMR of compound **20a**

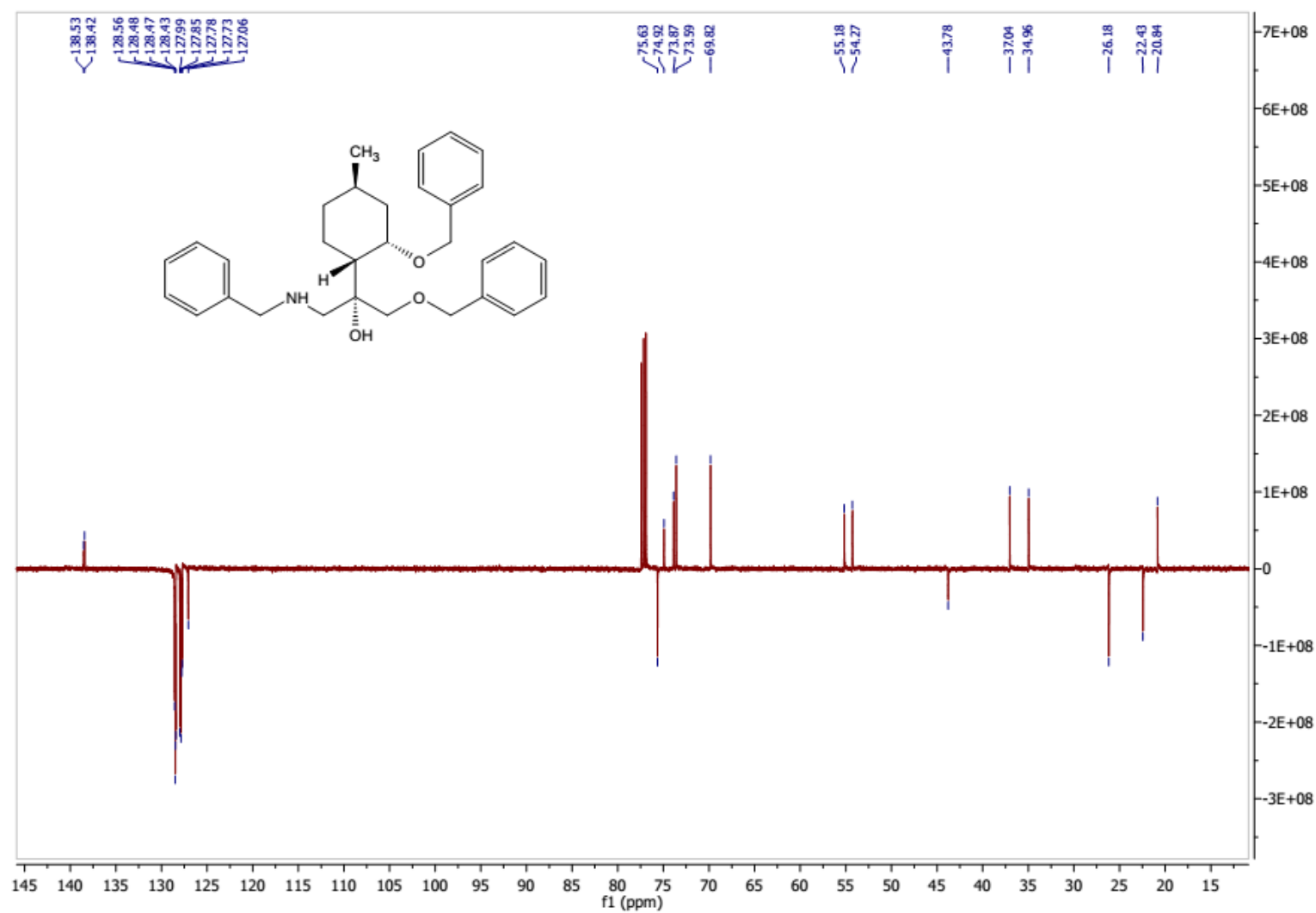


Figure S 52:  $^1\text{H}$ -NMR of compound **20b**

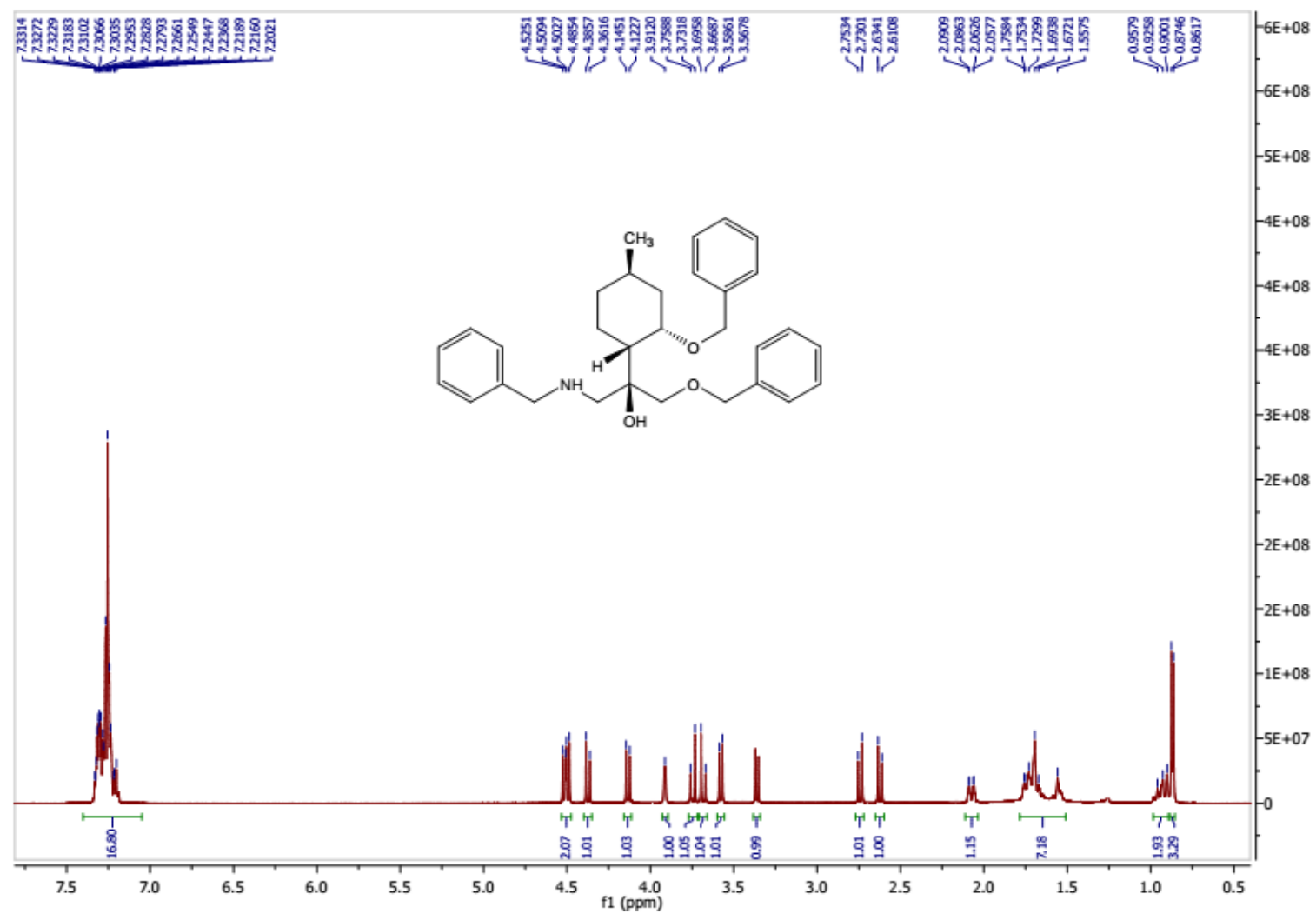


Figure S 53:  $^{13}\text{C}$ -NMR of compound **20b**

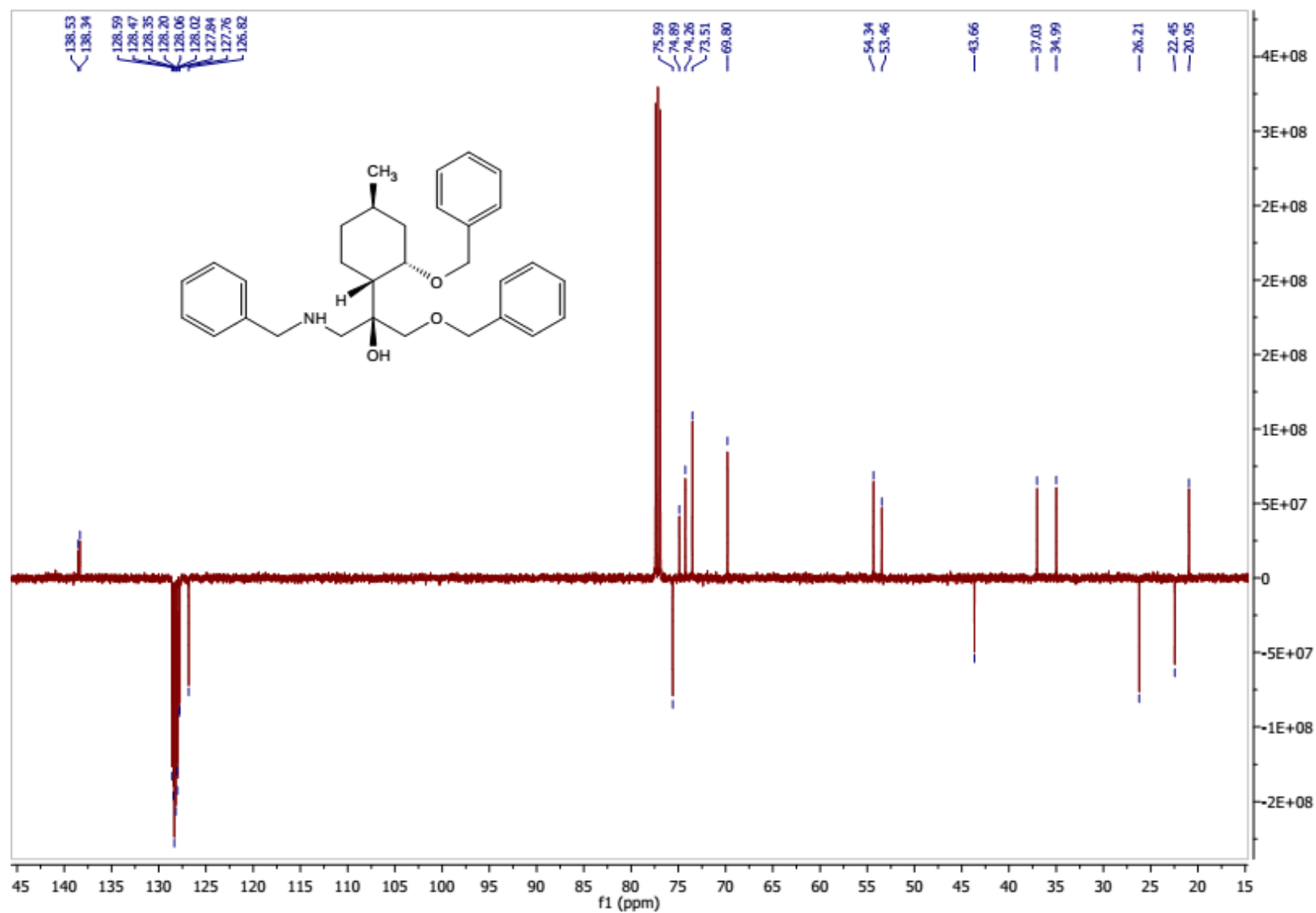


Figure S 54:  $^1\text{H}$ -NMR of compound **21a**

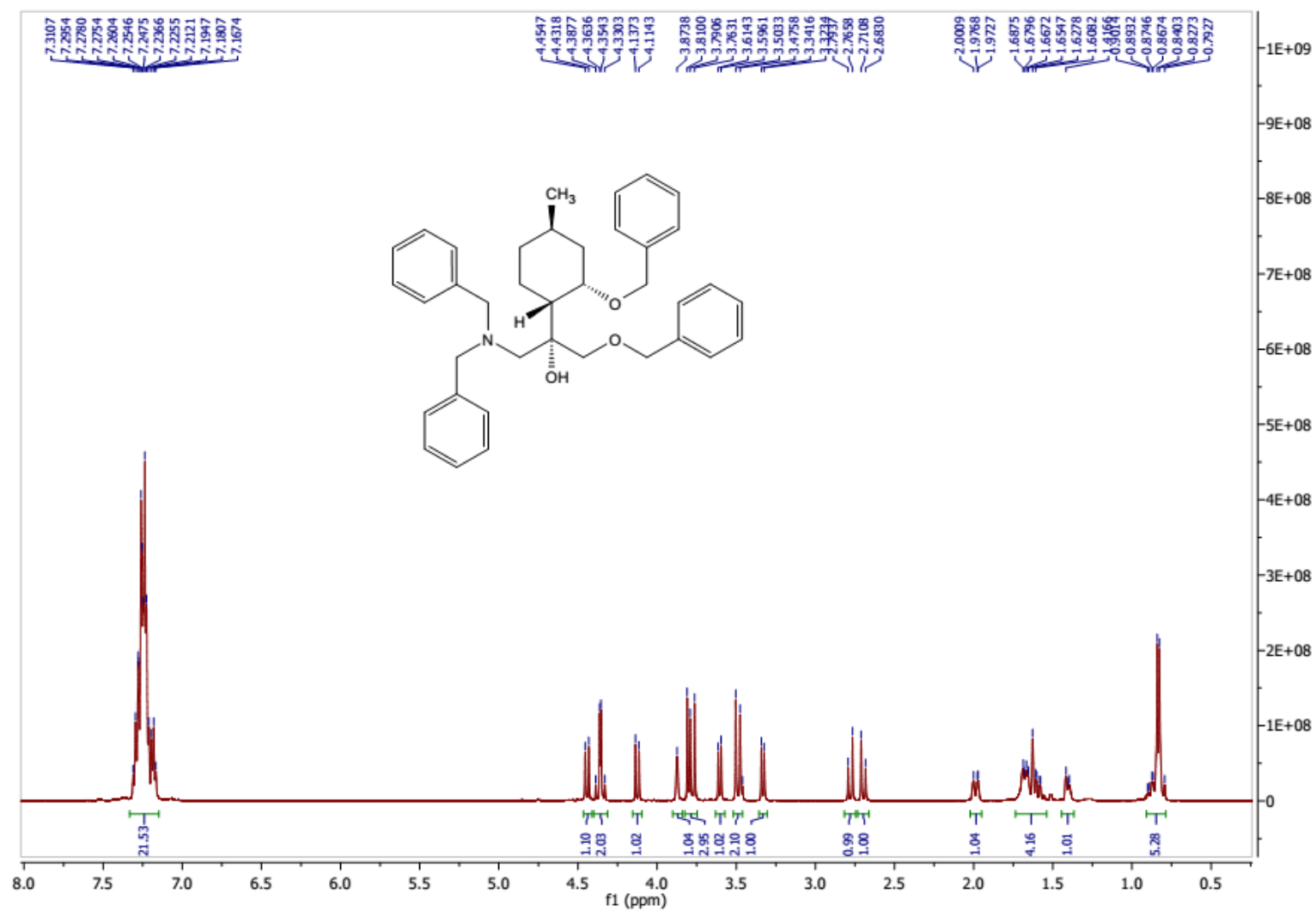


Figure S 55:  $^{13}\text{C}$ -NMR of compound **21a**

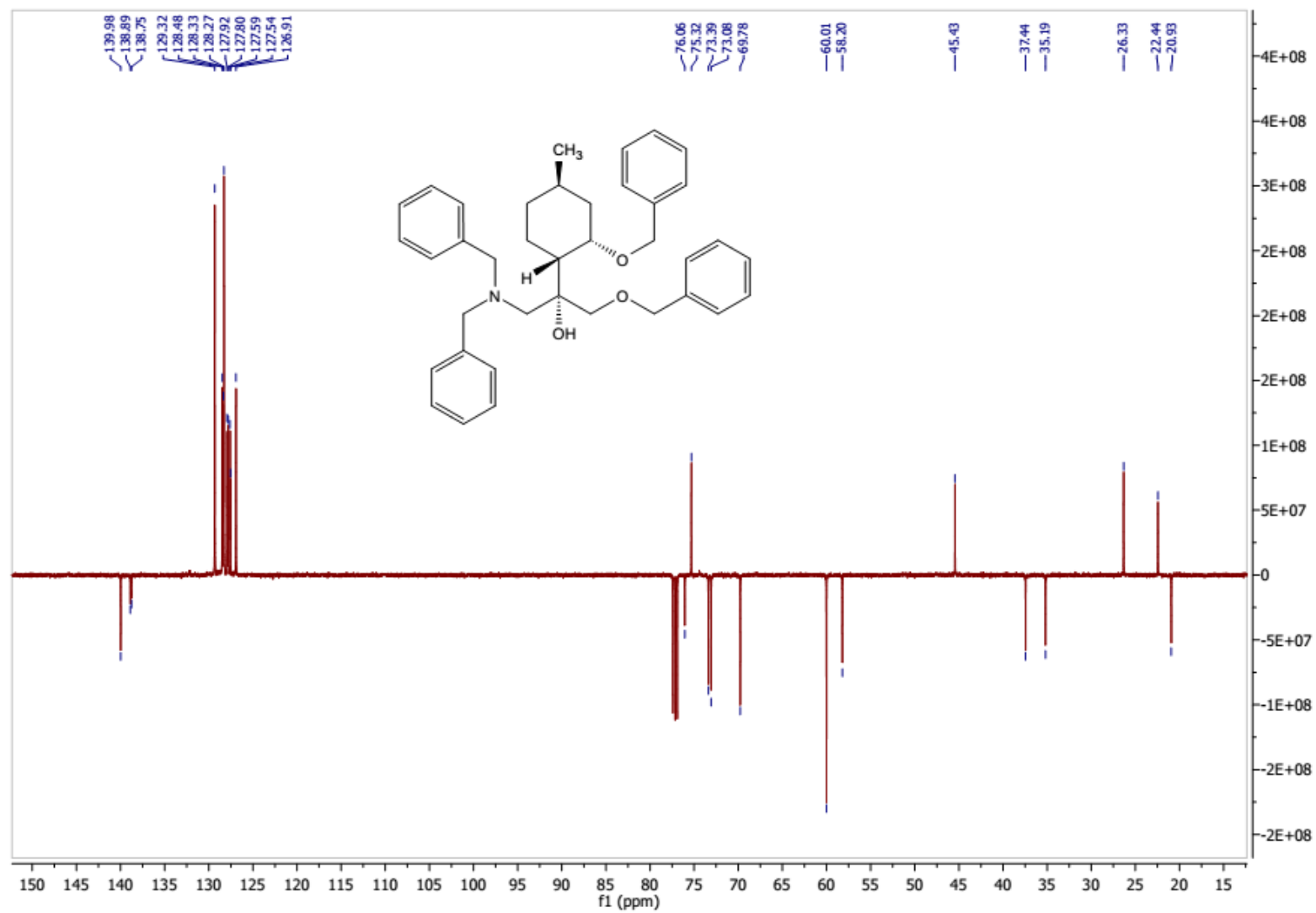


Figure S 56:  $^1\text{H}$ -NMR of compound **21b**

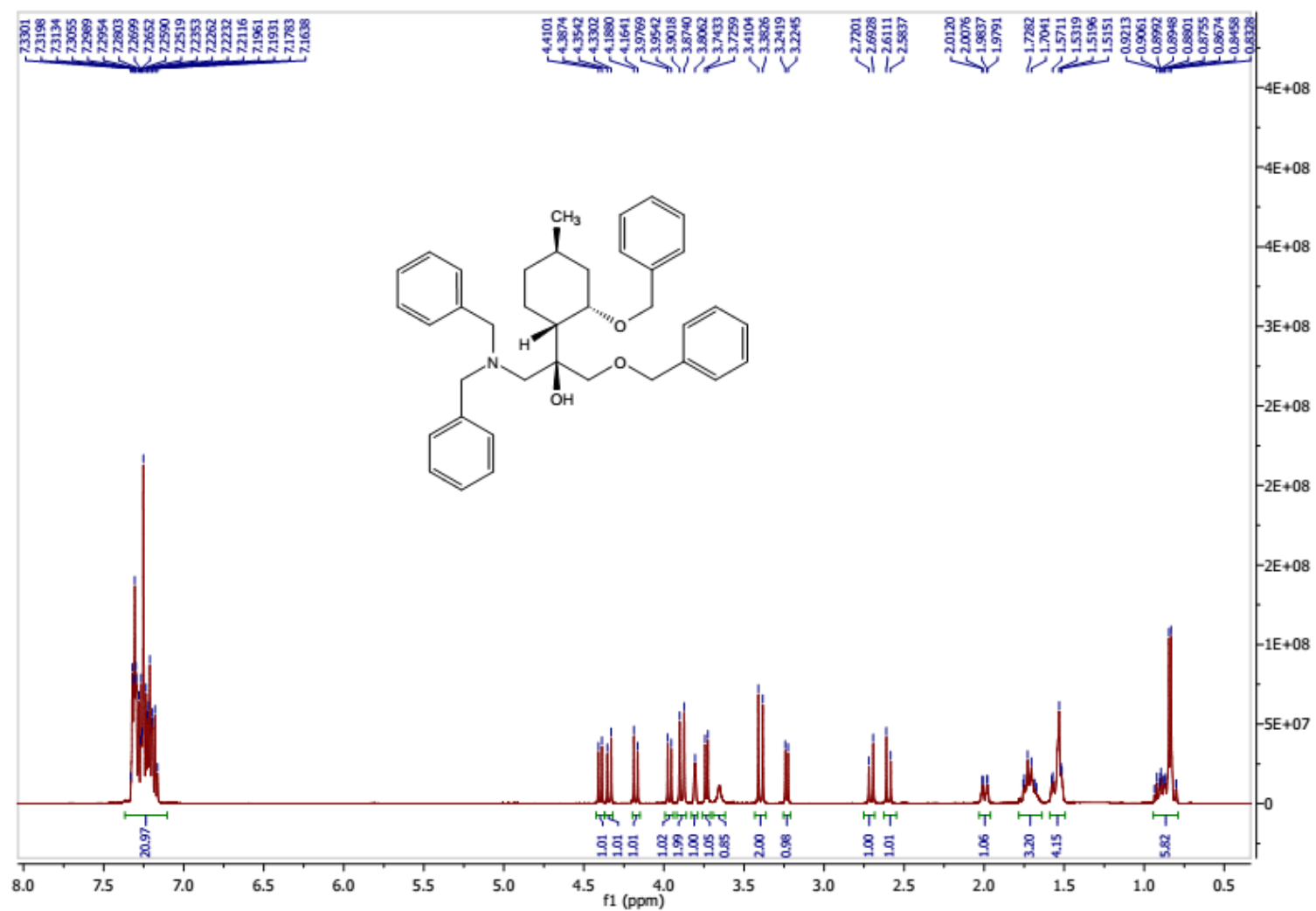


Figure S 57:  $^{13}\text{C}$ -NMR of compound **21b**

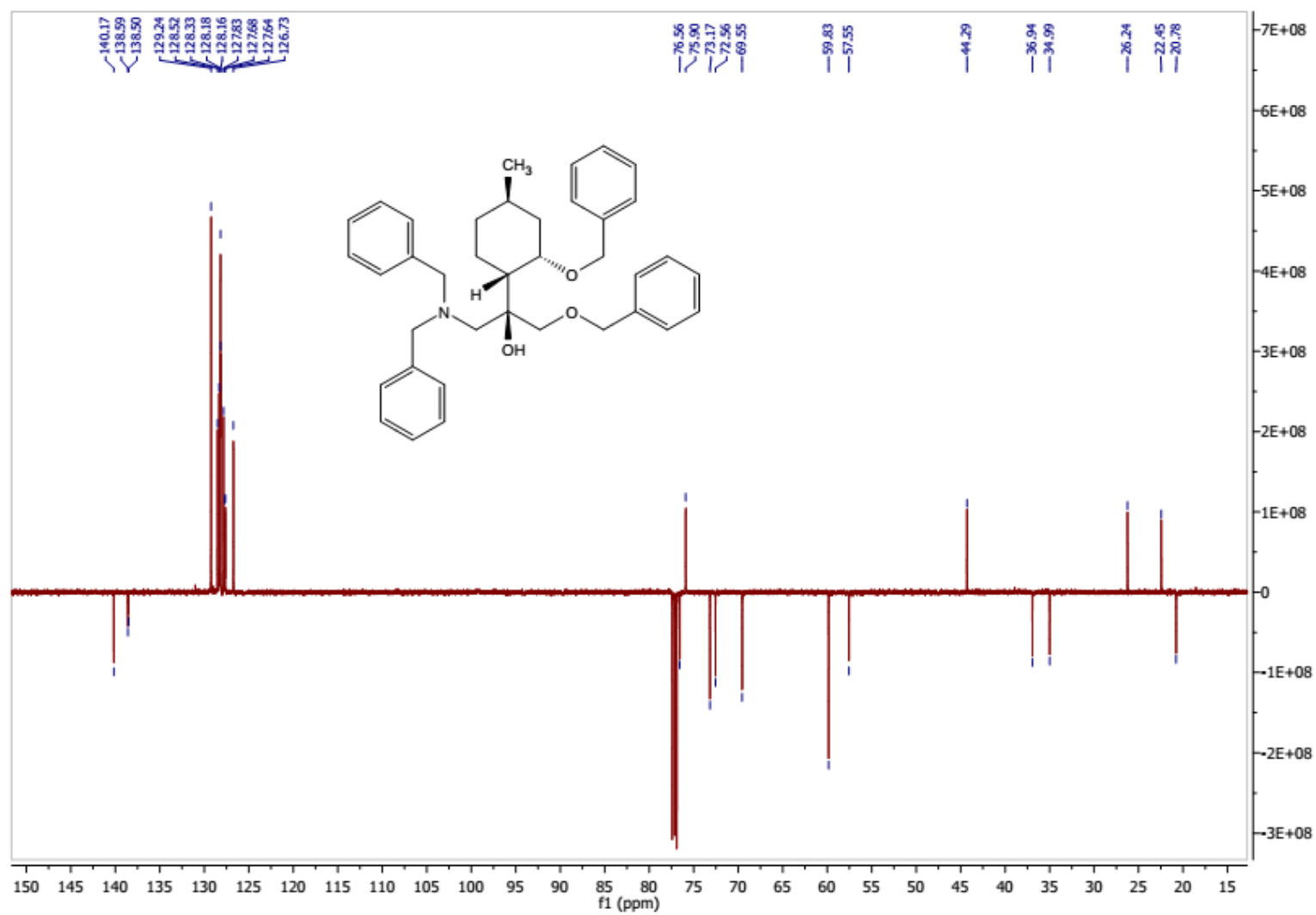




Figure S 58:  $^1\text{H}$ -NMR of compound **22a**

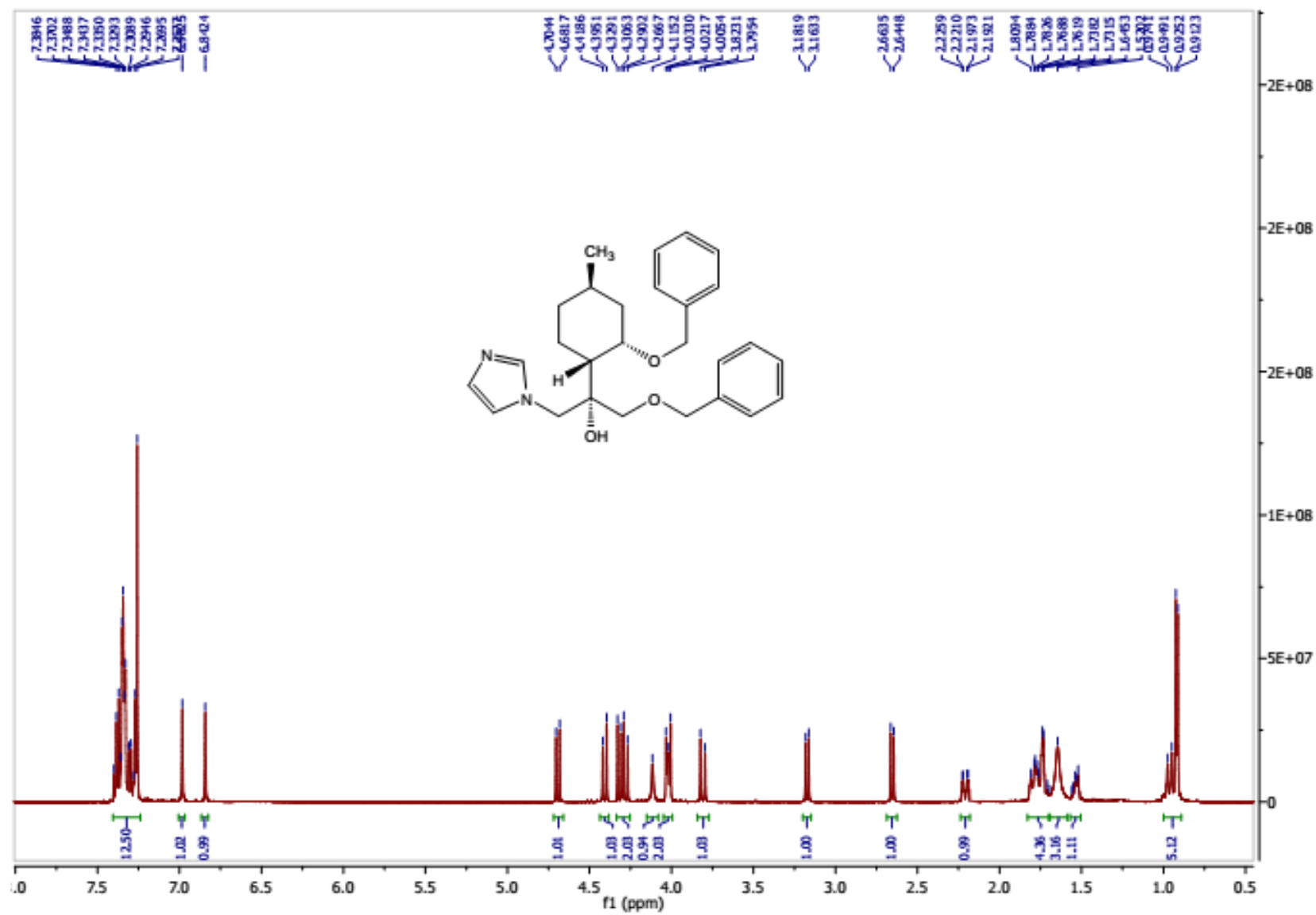


Figure S 59:  $^{13}\text{C}$ -NMR of compound **22a**

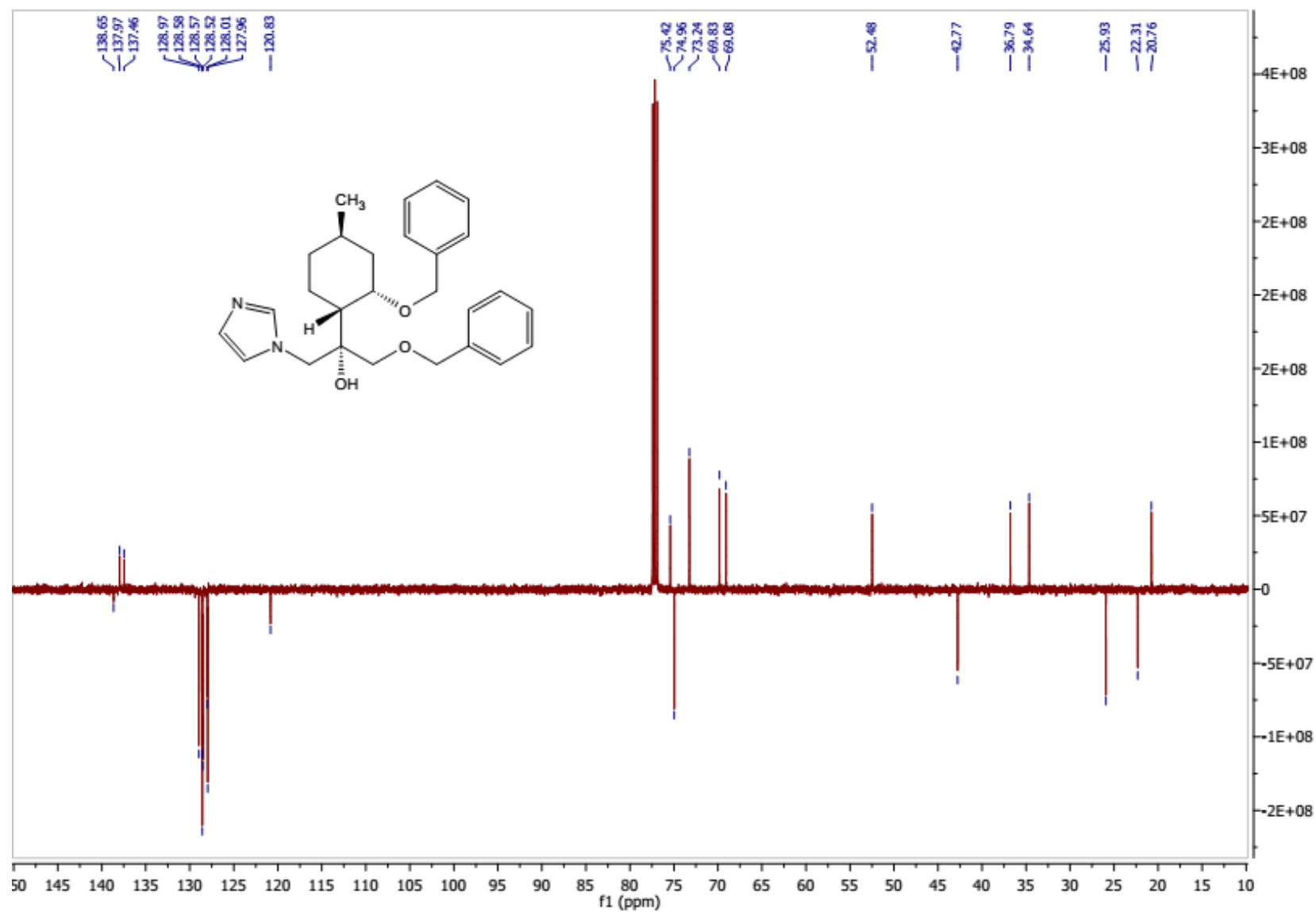


Figure S 60:  $^1\text{H}$ -NMR of compound **22b**

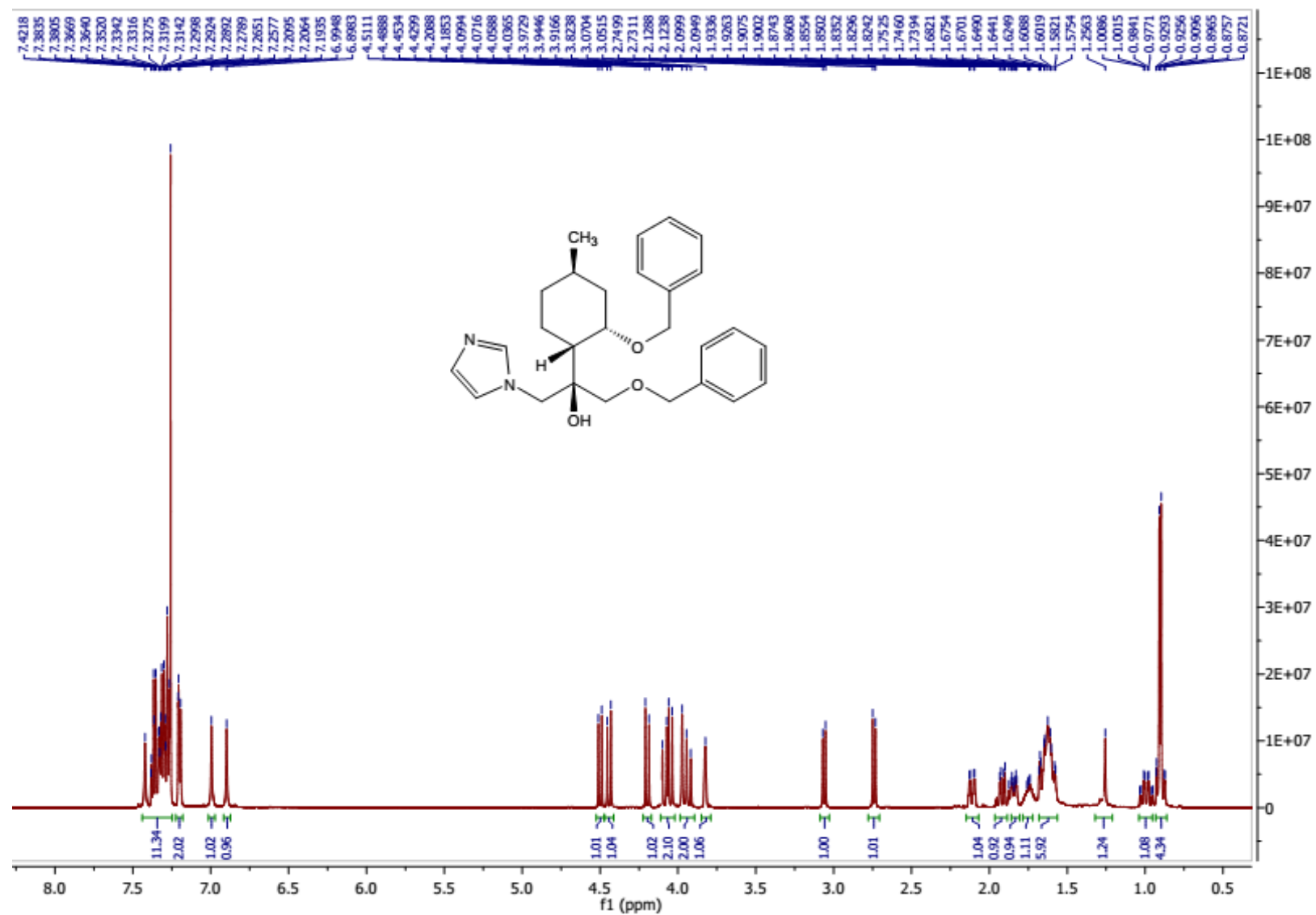


Figure S 61:  $^{13}\text{C}$ -NMR of compound **22b**

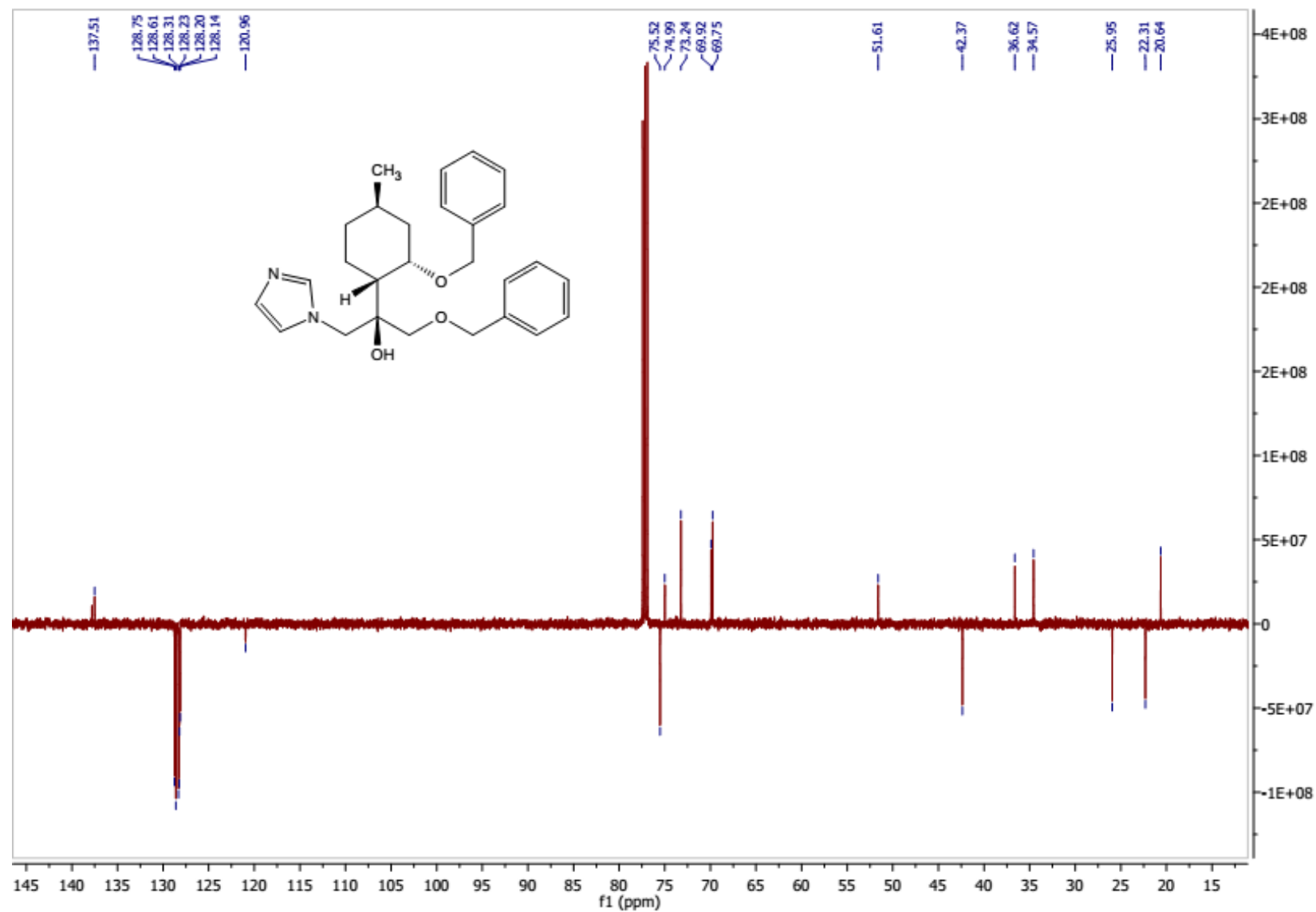


Figure S 62:  $^1\text{H}$ -NMR of compound **23a**

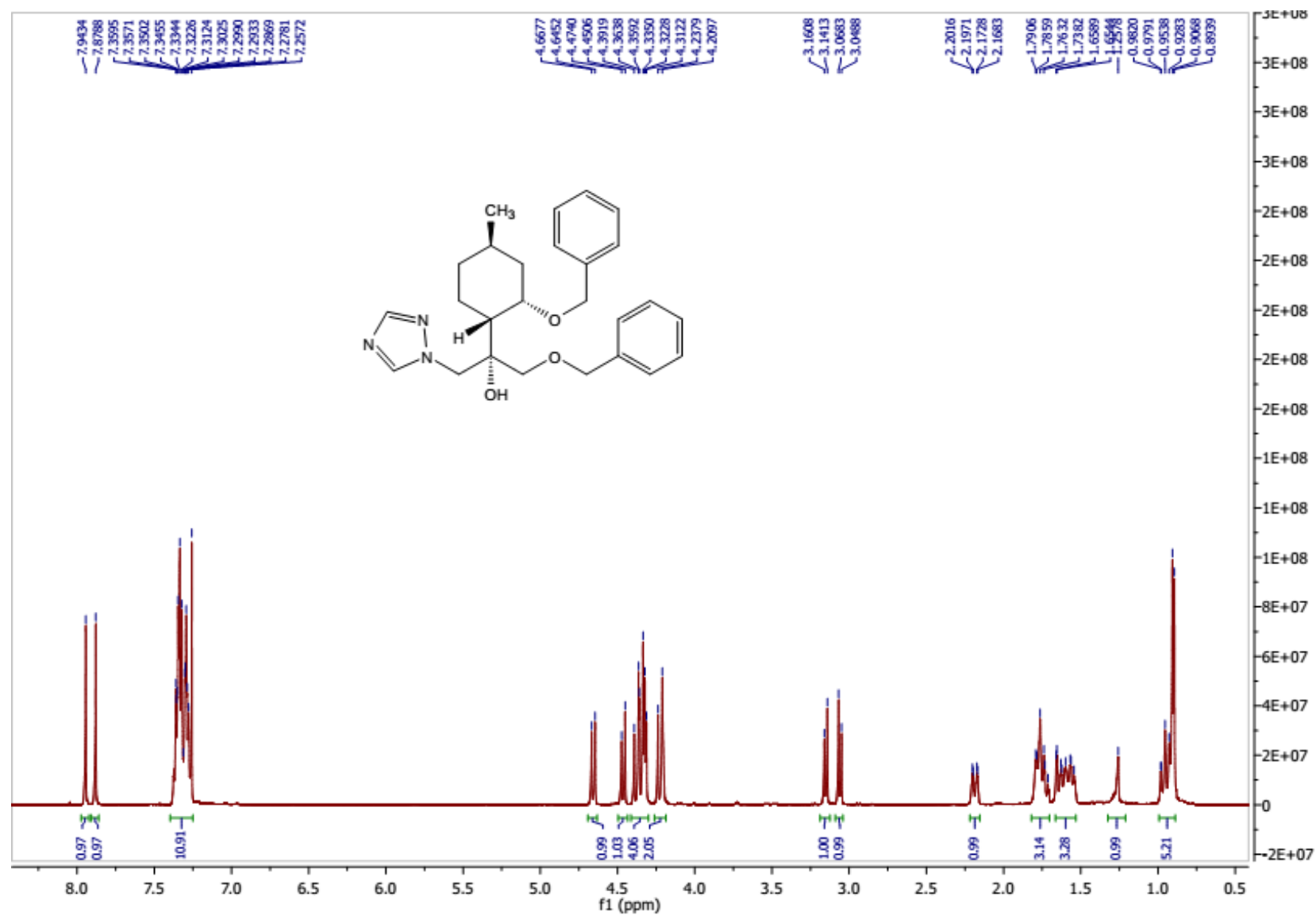


Figure S 63:  $^{13}\text{C}$ -NMR of compound **23a**

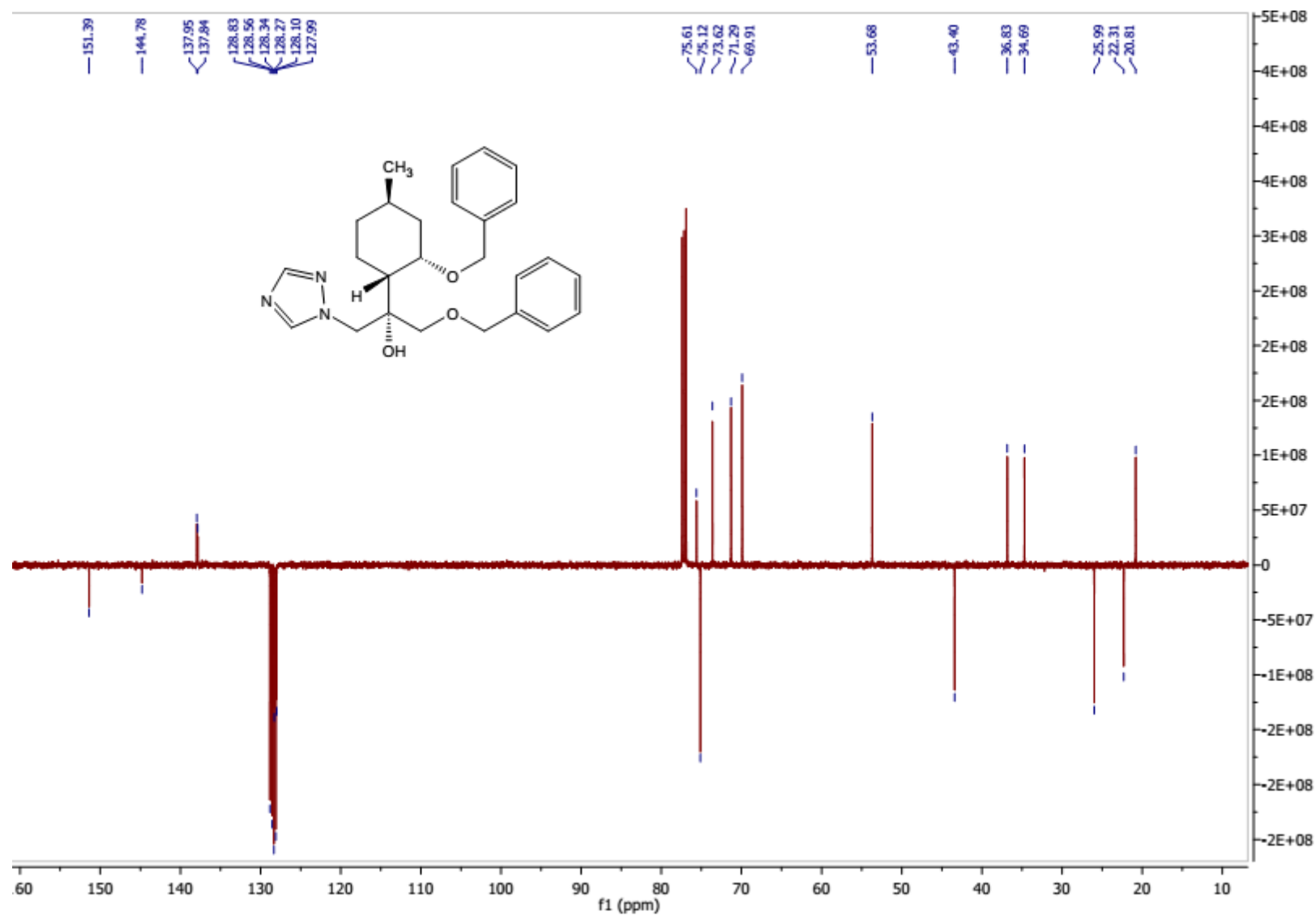


Figure S 64:  $^1\text{H}$ -NMR of compound **23b**

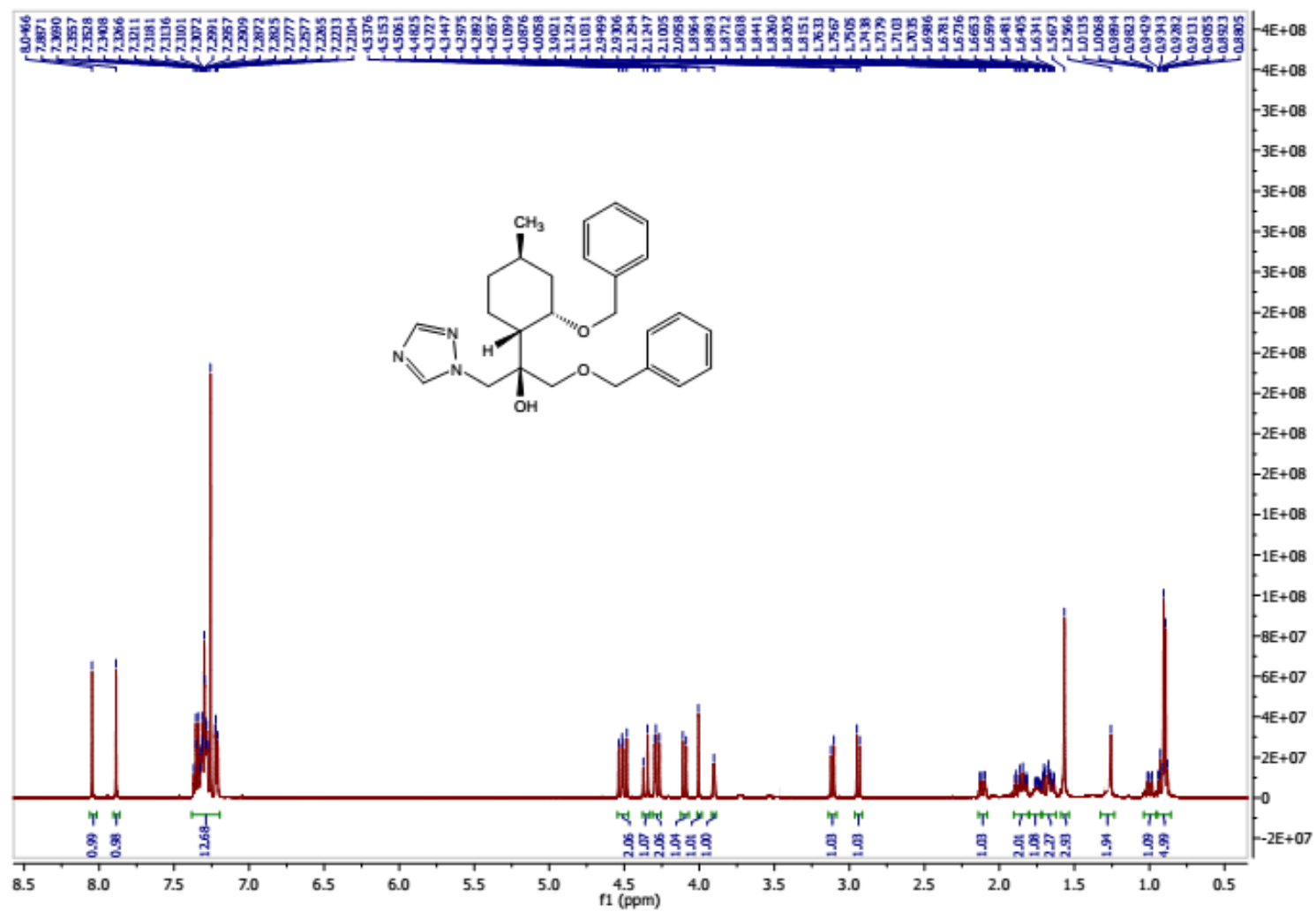


Figure S 65:  $^{13}\text{C}$ -NMR of compound **23b**

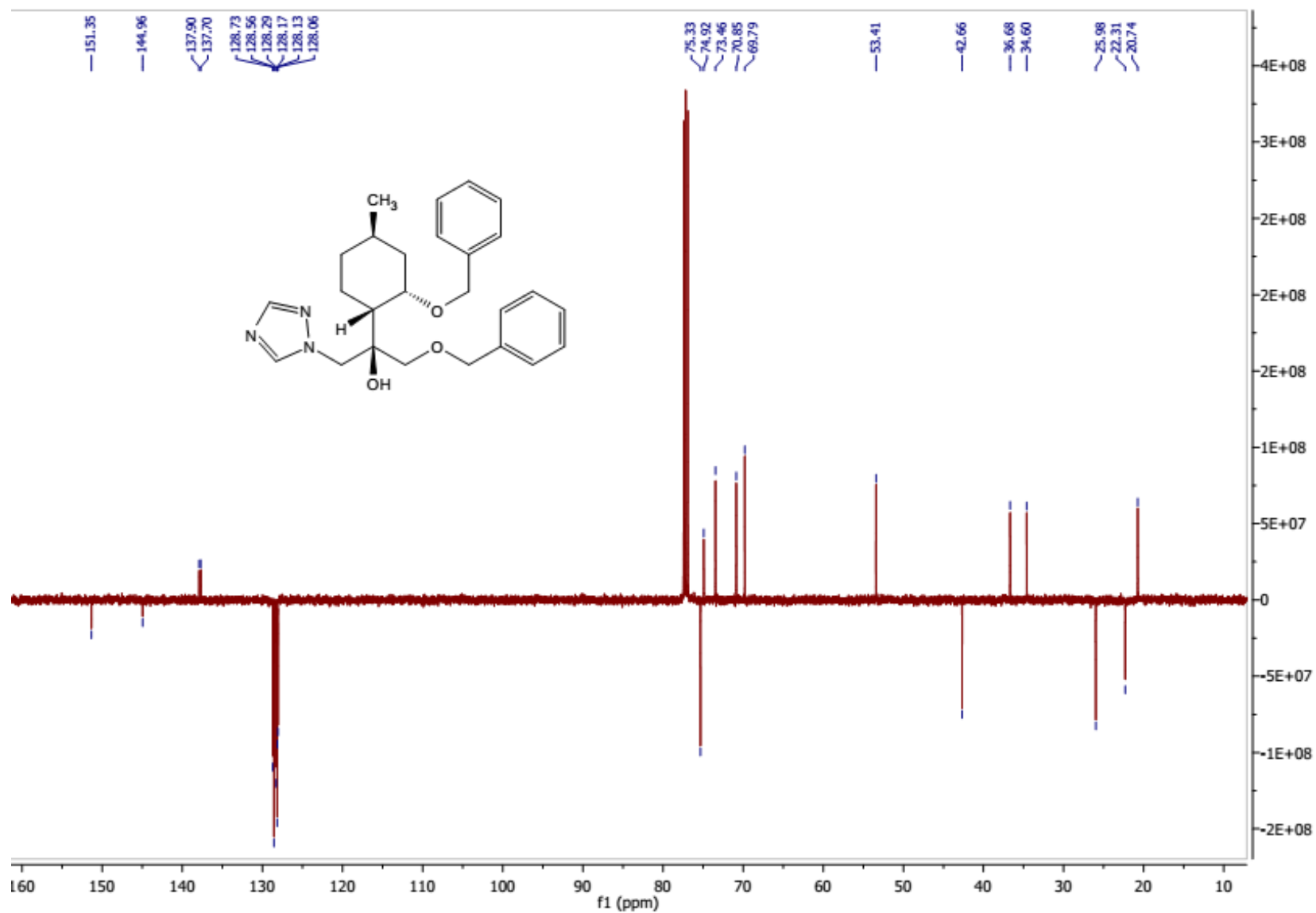




Figure S 66:  $^1\text{H}$ -NMR of compound **24a**

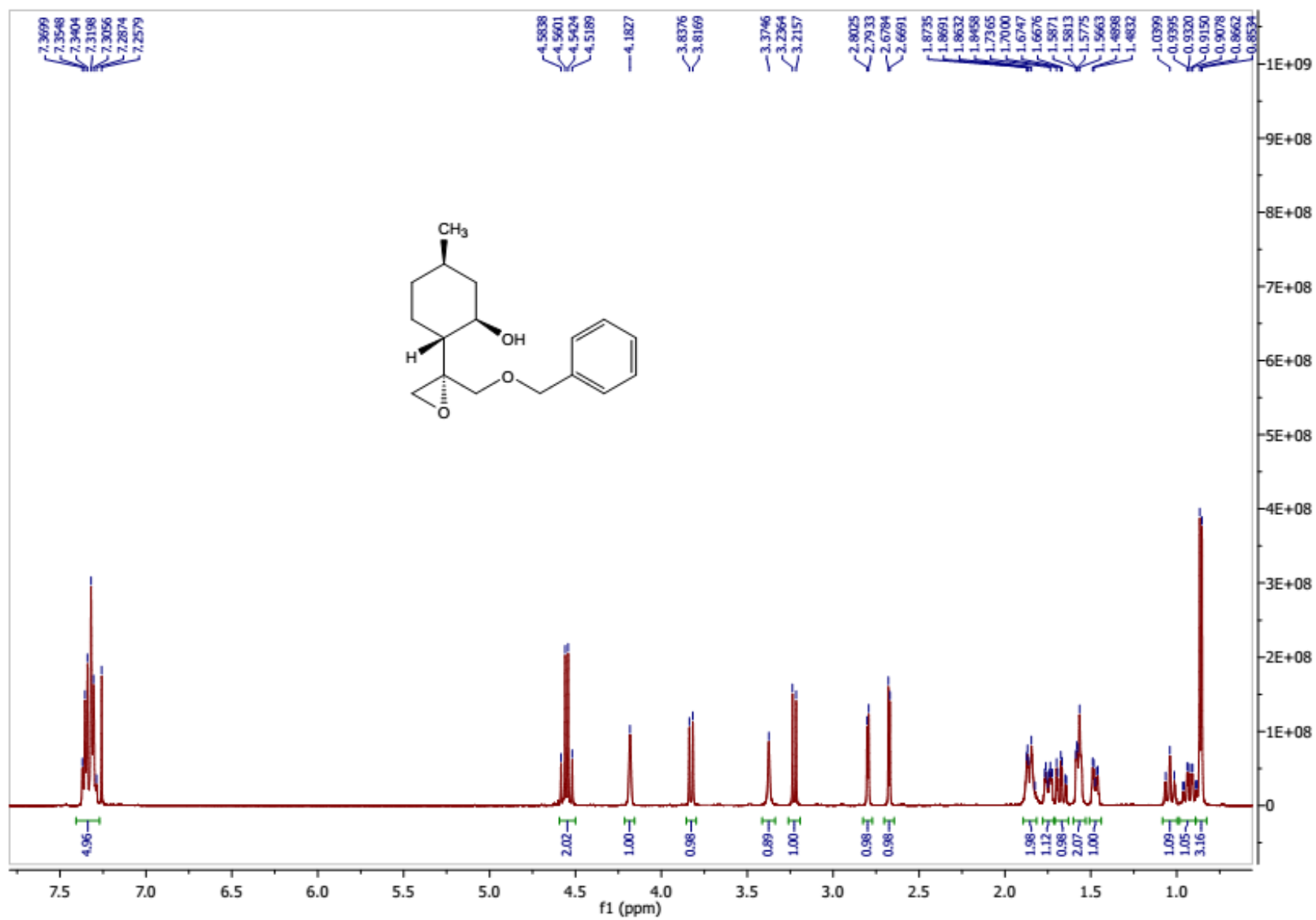


Figure S 67:  $^{13}\text{C}$ -NMR of compound **24a**

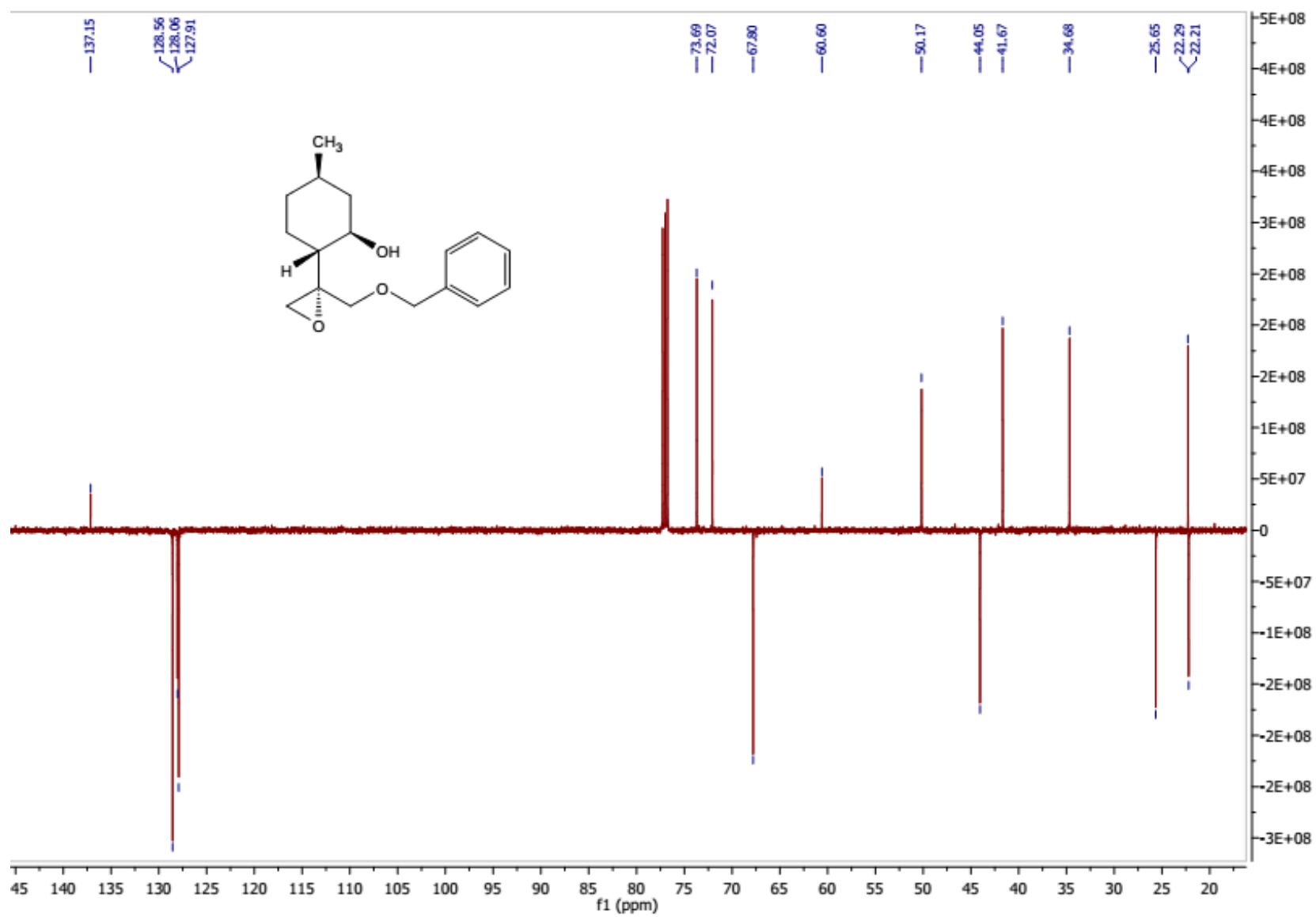


Figure S 68:  $^1\text{H}$ -NMR of compound **24b**

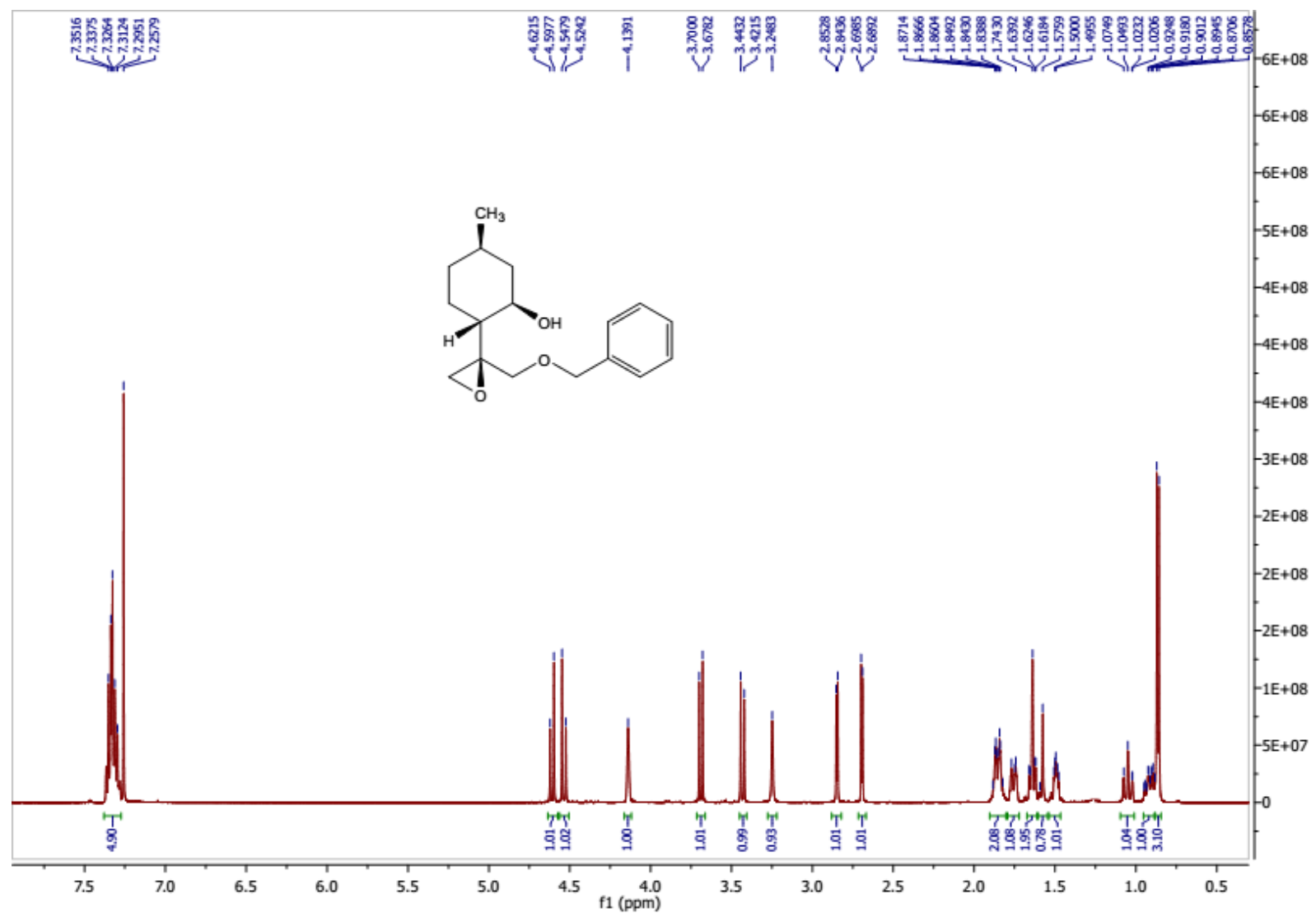


Figure S 69:  $^{13}\text{C}$ -NMR of compound **24b**

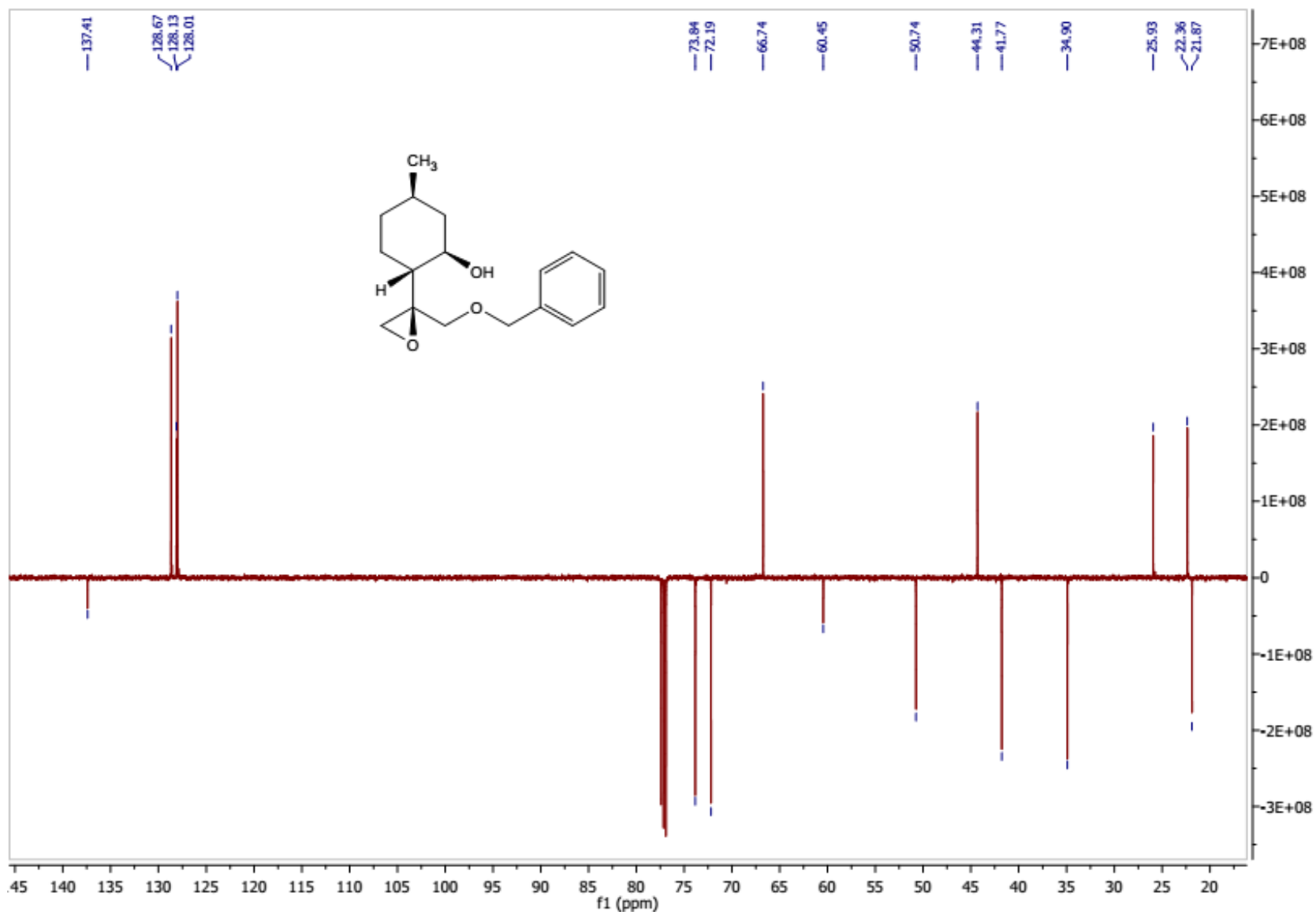


Figure S 70:  $^1\text{H}$ -NMR of compound **25a**

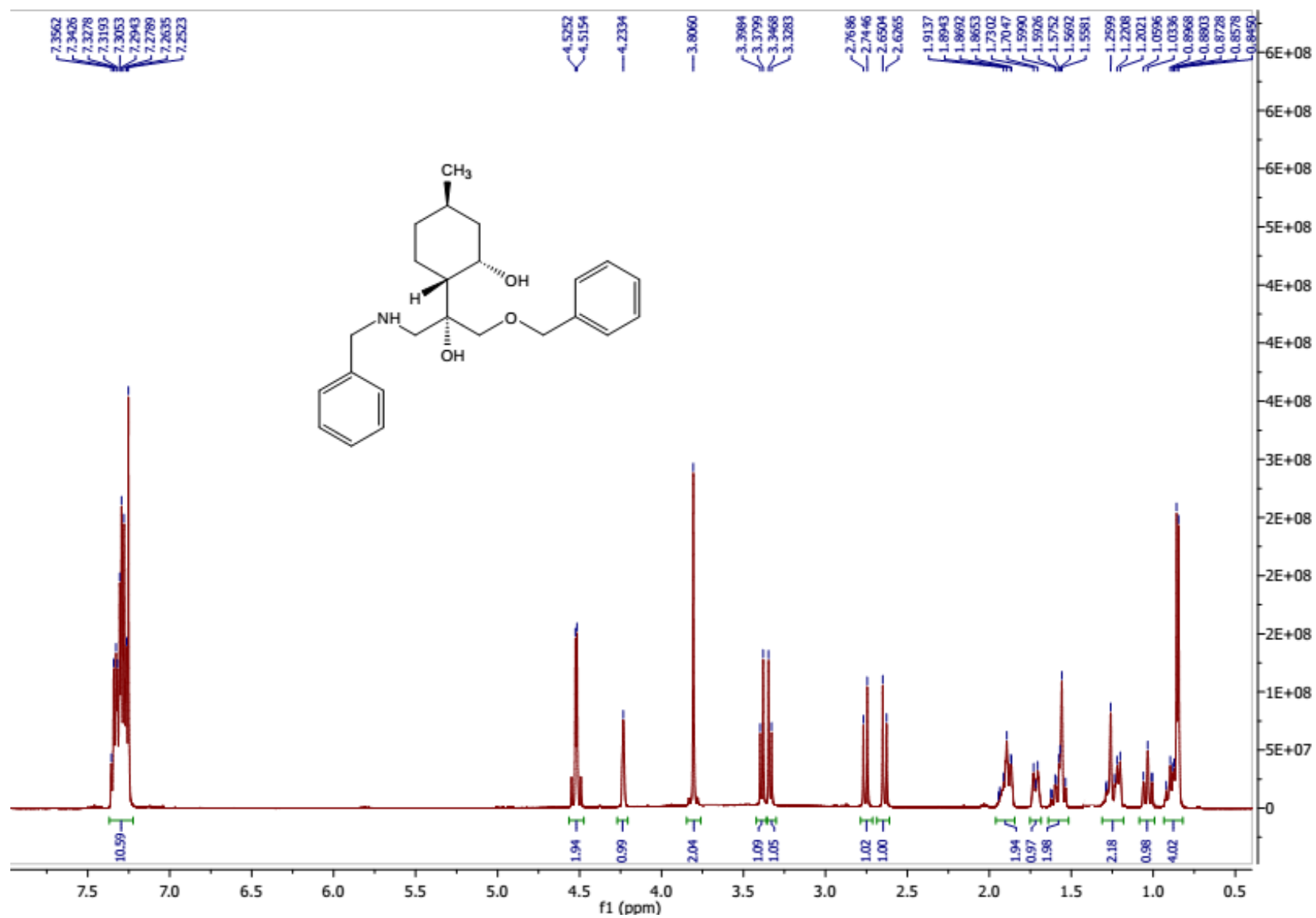


Figure S 71:  $^{13}\text{C}$ -NMR of compound **25a**

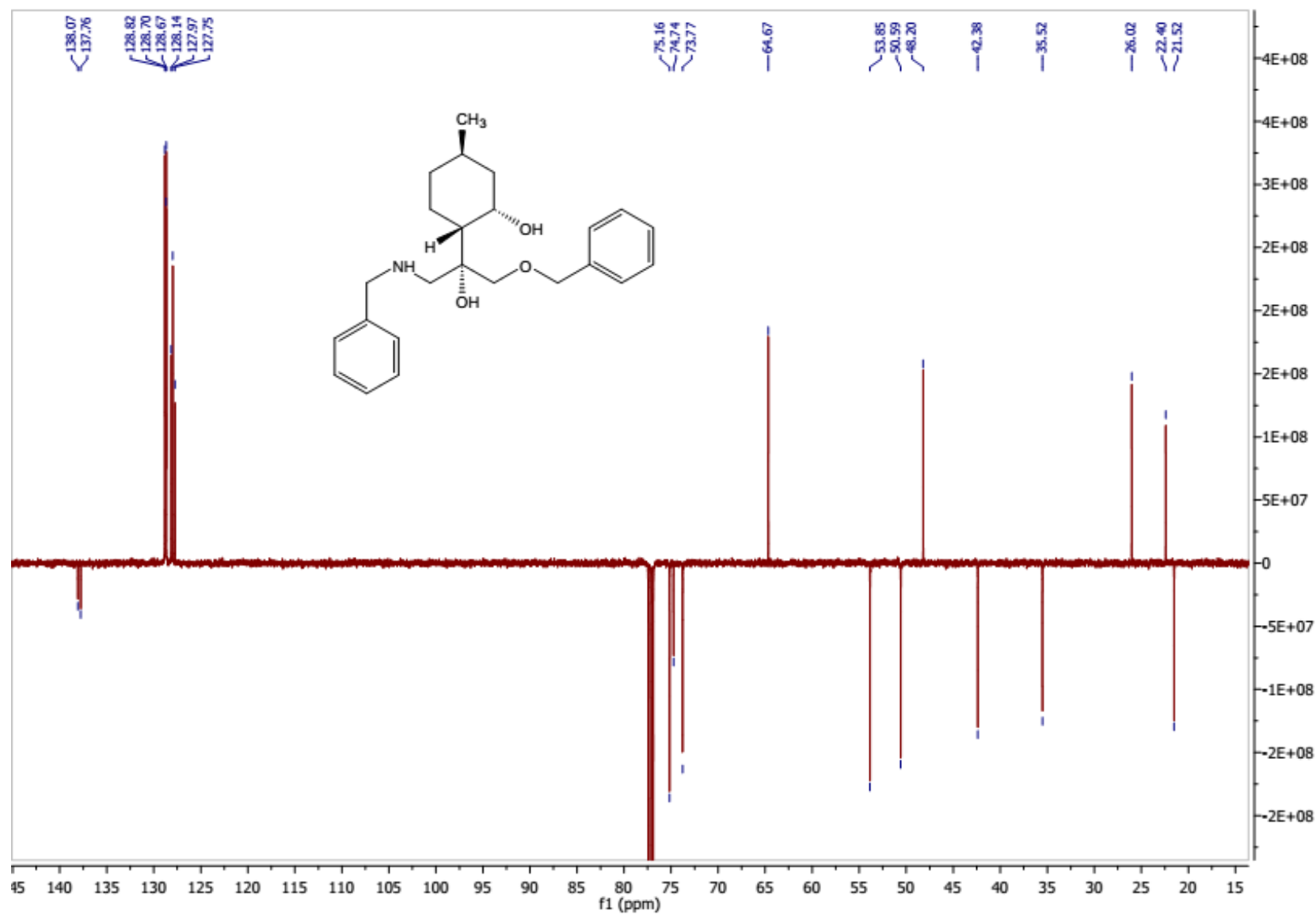


Figure S 72:  $^1\text{H}$ -NMR of compound **25b**

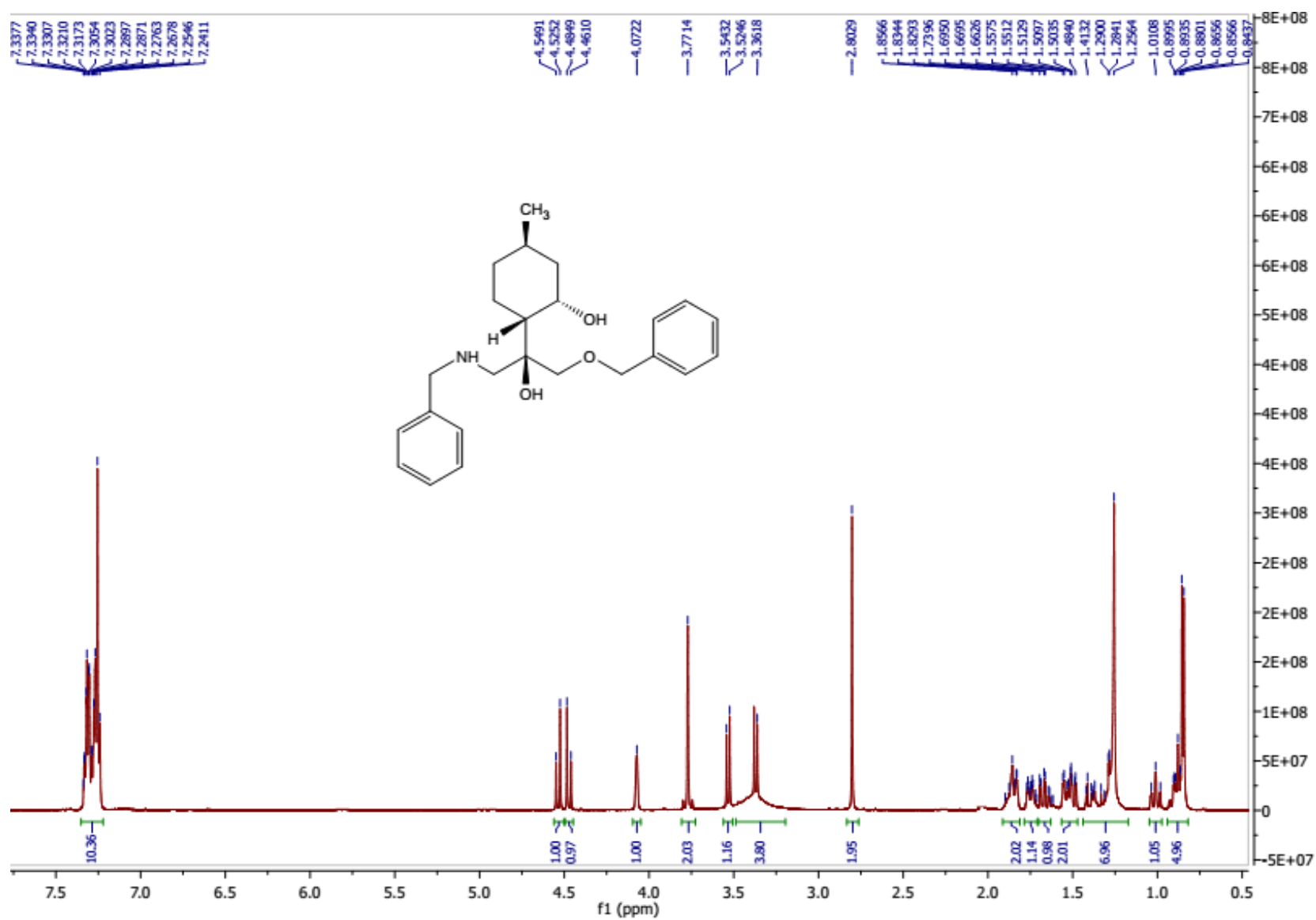


Figure S 73:  $^{13}\text{C}$ -NMR of compound **25b**

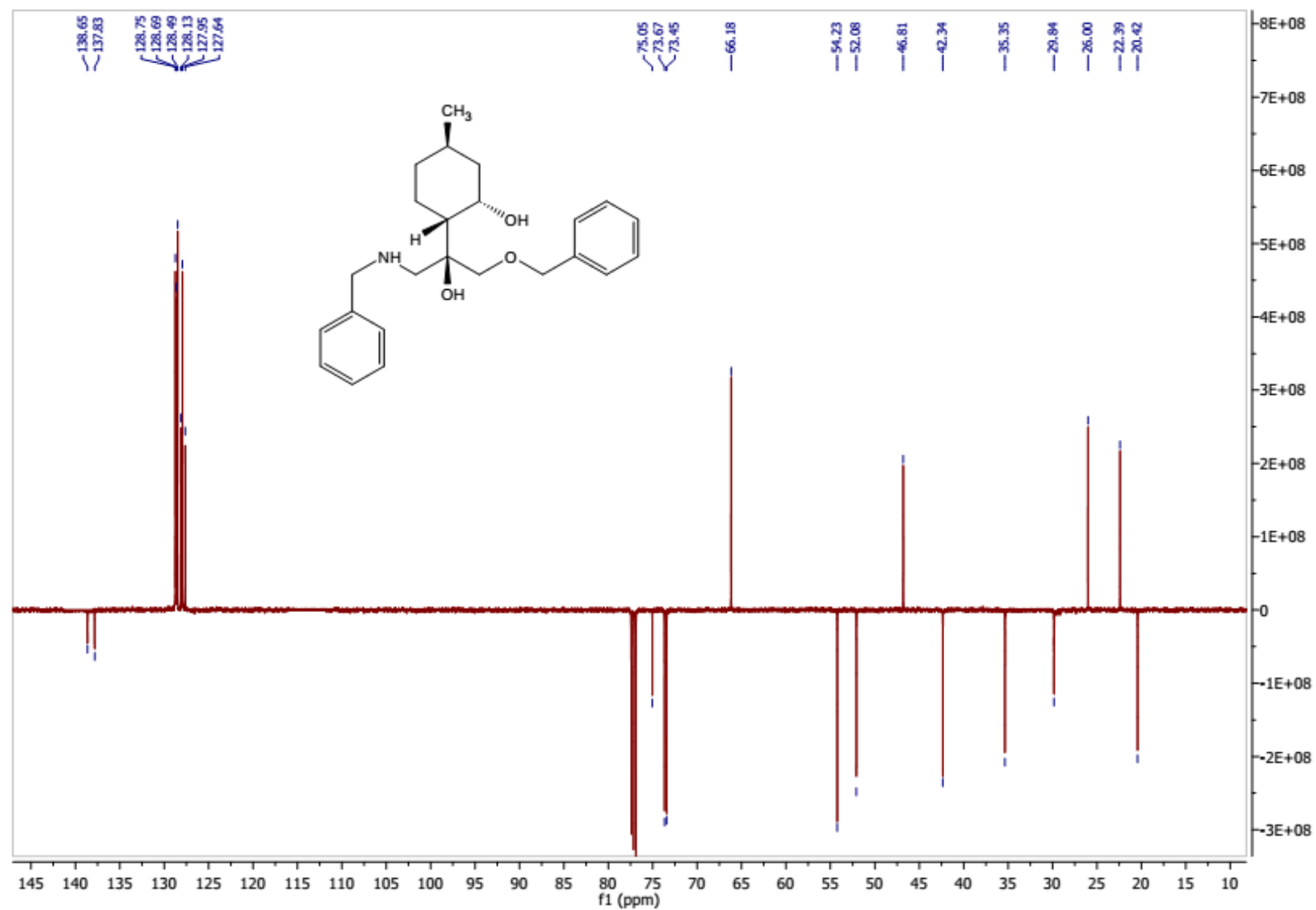




Figure S 74:  $^1\text{H}$ -NMR of compound 26a

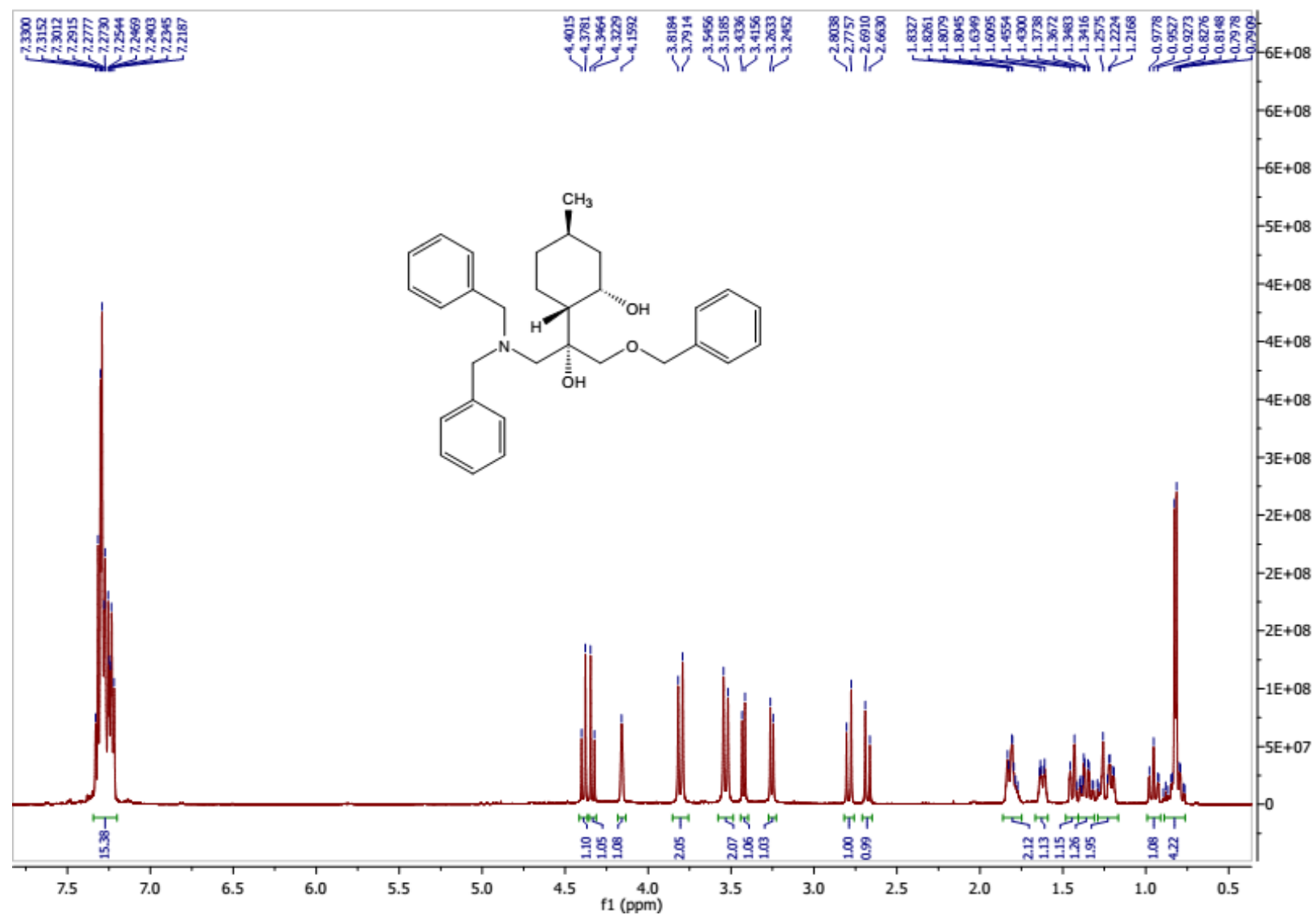


Figure S 75:  $^{13}\text{C}$ -NMR of compound **26a**

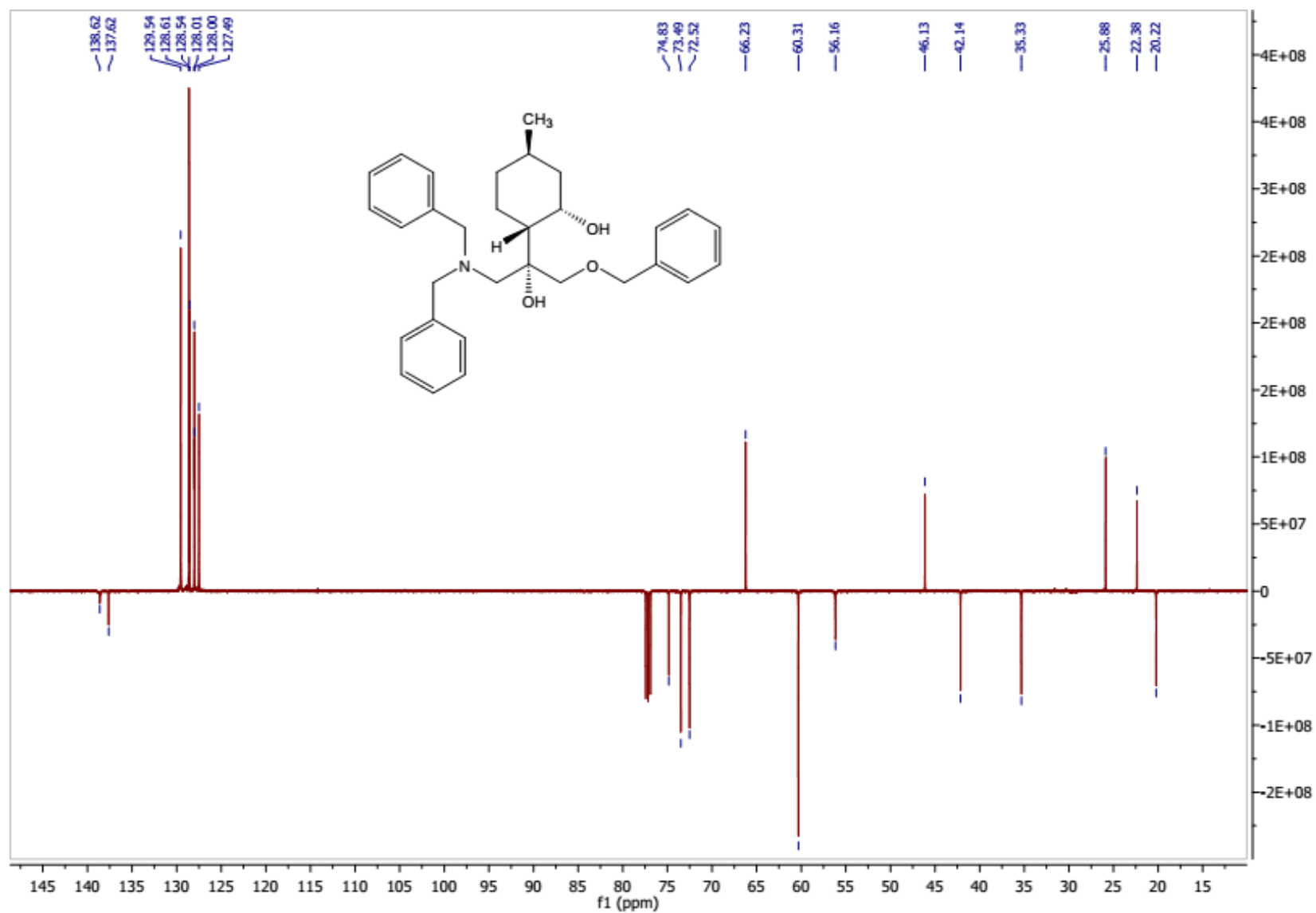


Figure S 76:  $^1\text{H}$ -NMR of compound **26b**

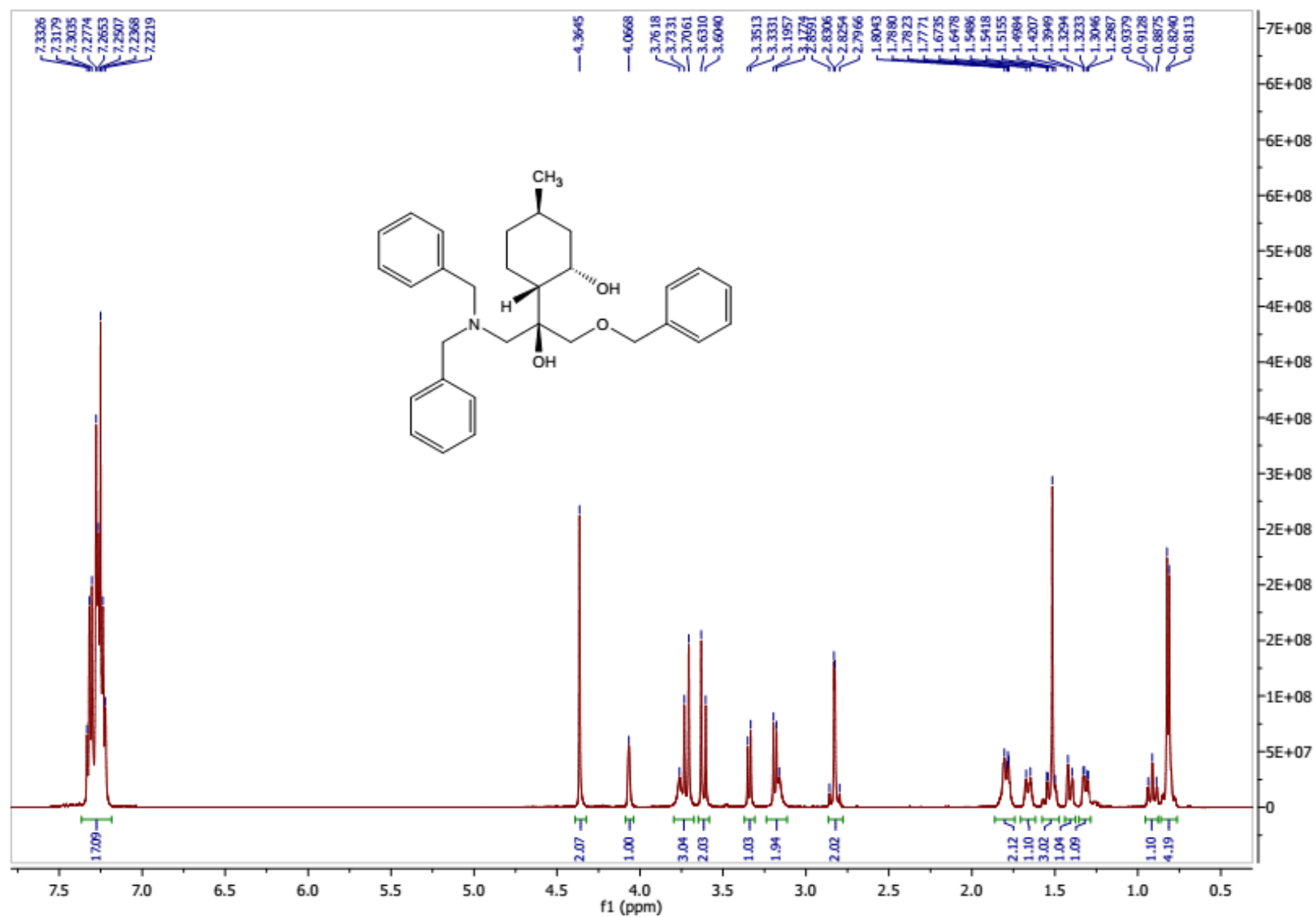


Figure S 77:  $^{13}\text{C}$ -NMR of compound **26b**

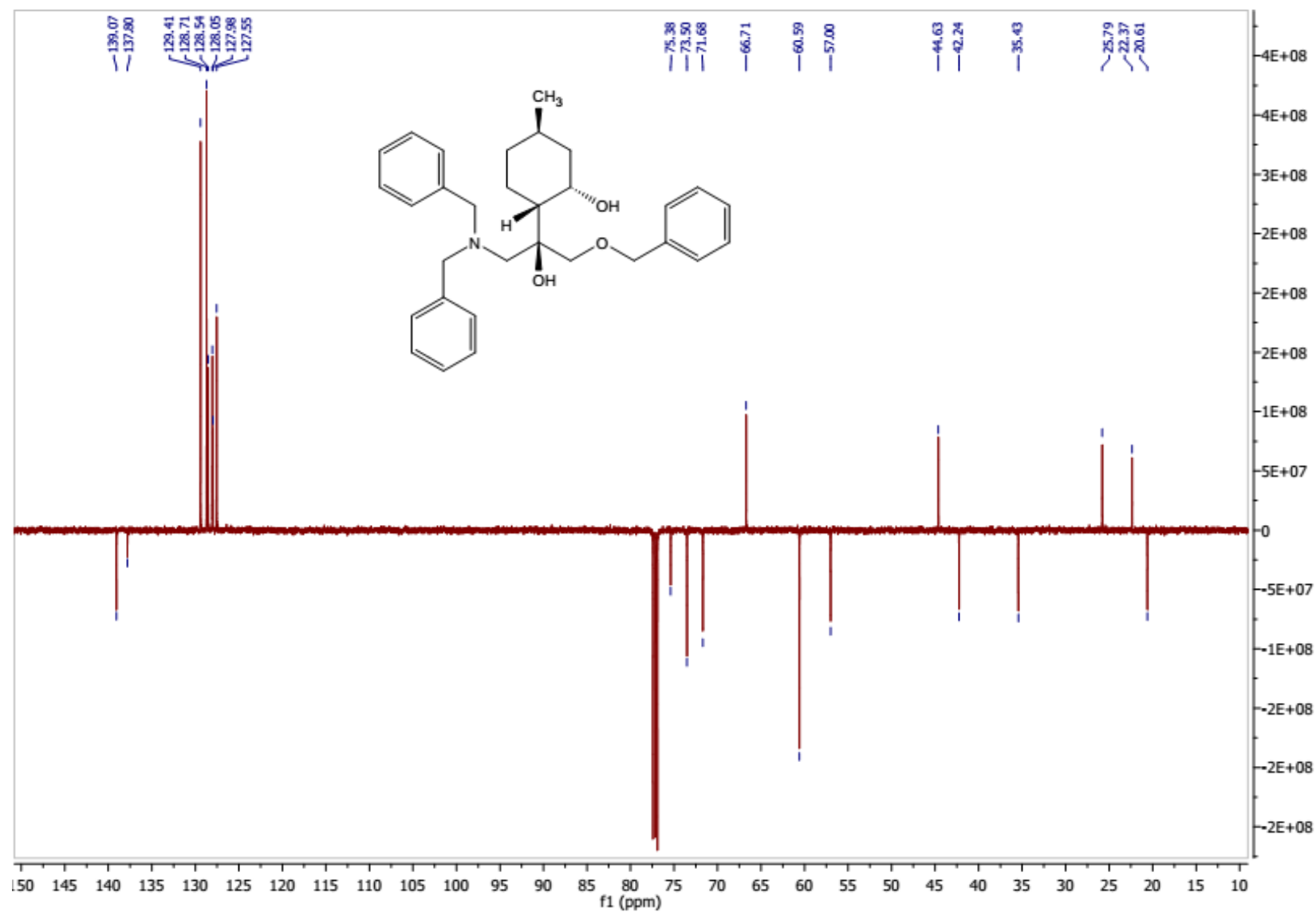


Figure S 78:  $^1\text{H}$ -NMR of compound **27a**

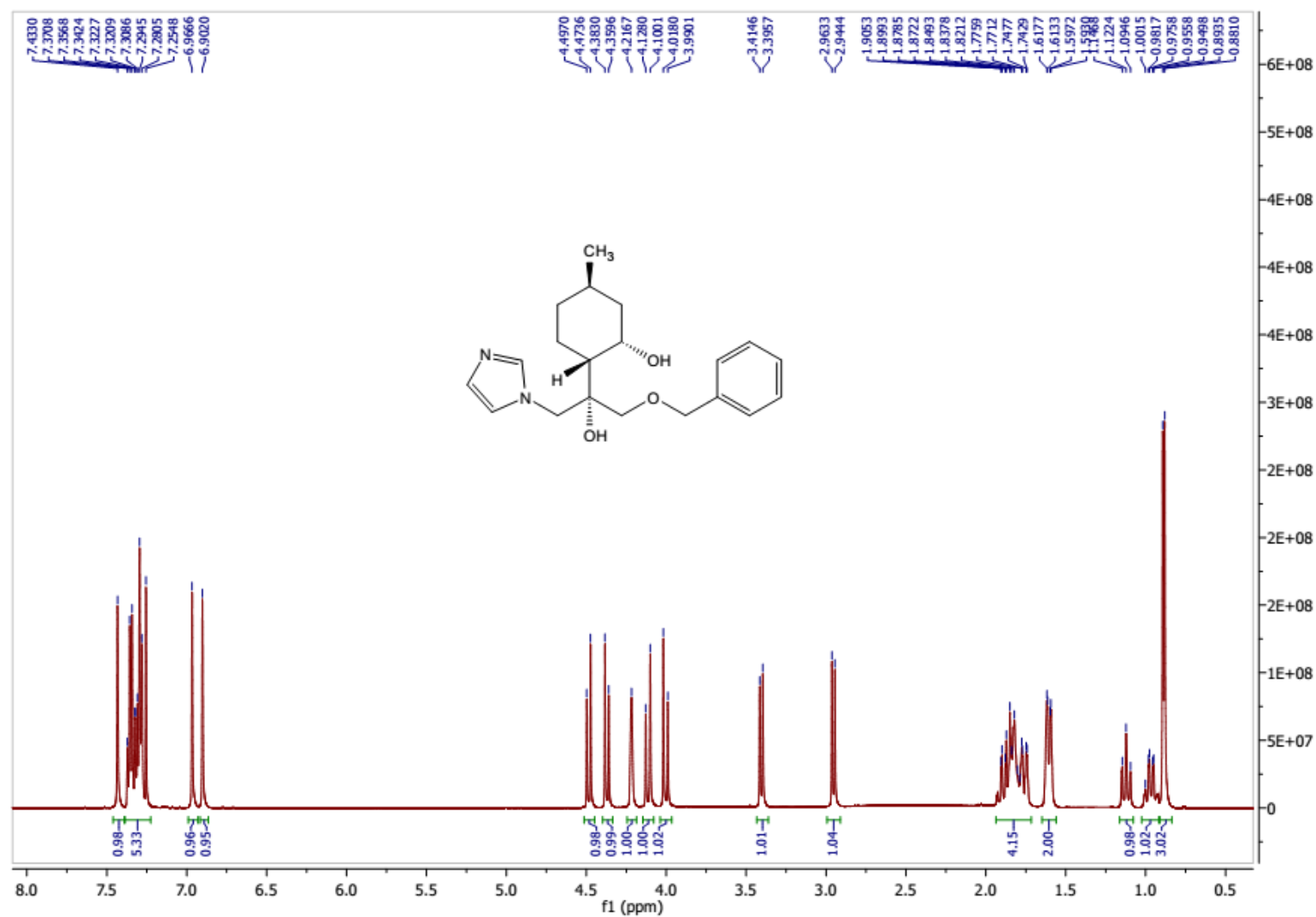


Figure S 79:  $^{13}\text{C}$ -NMR of compound **27a**

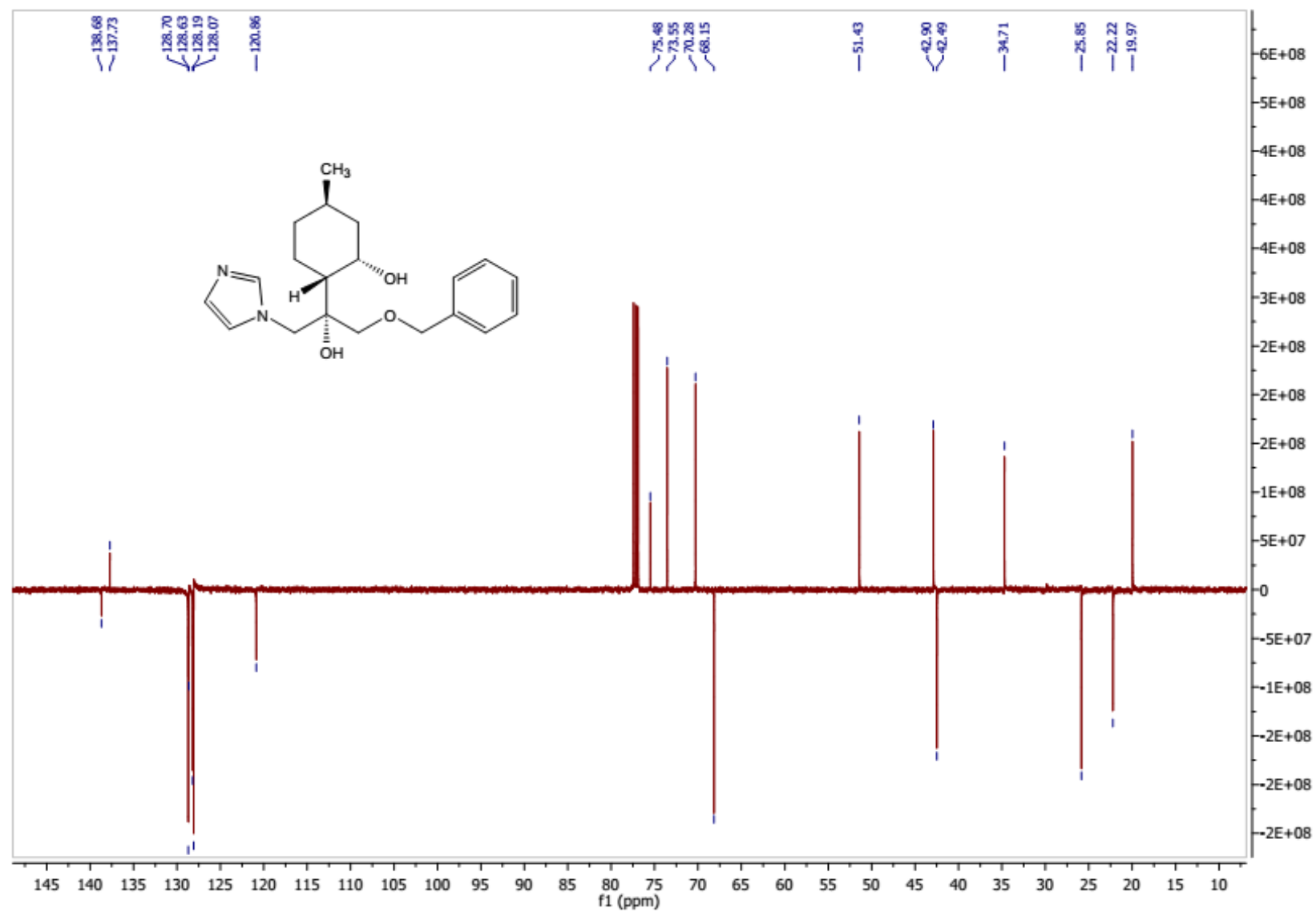


Figure S 80:  $^1\text{H}$ -NMR of compound **27b**

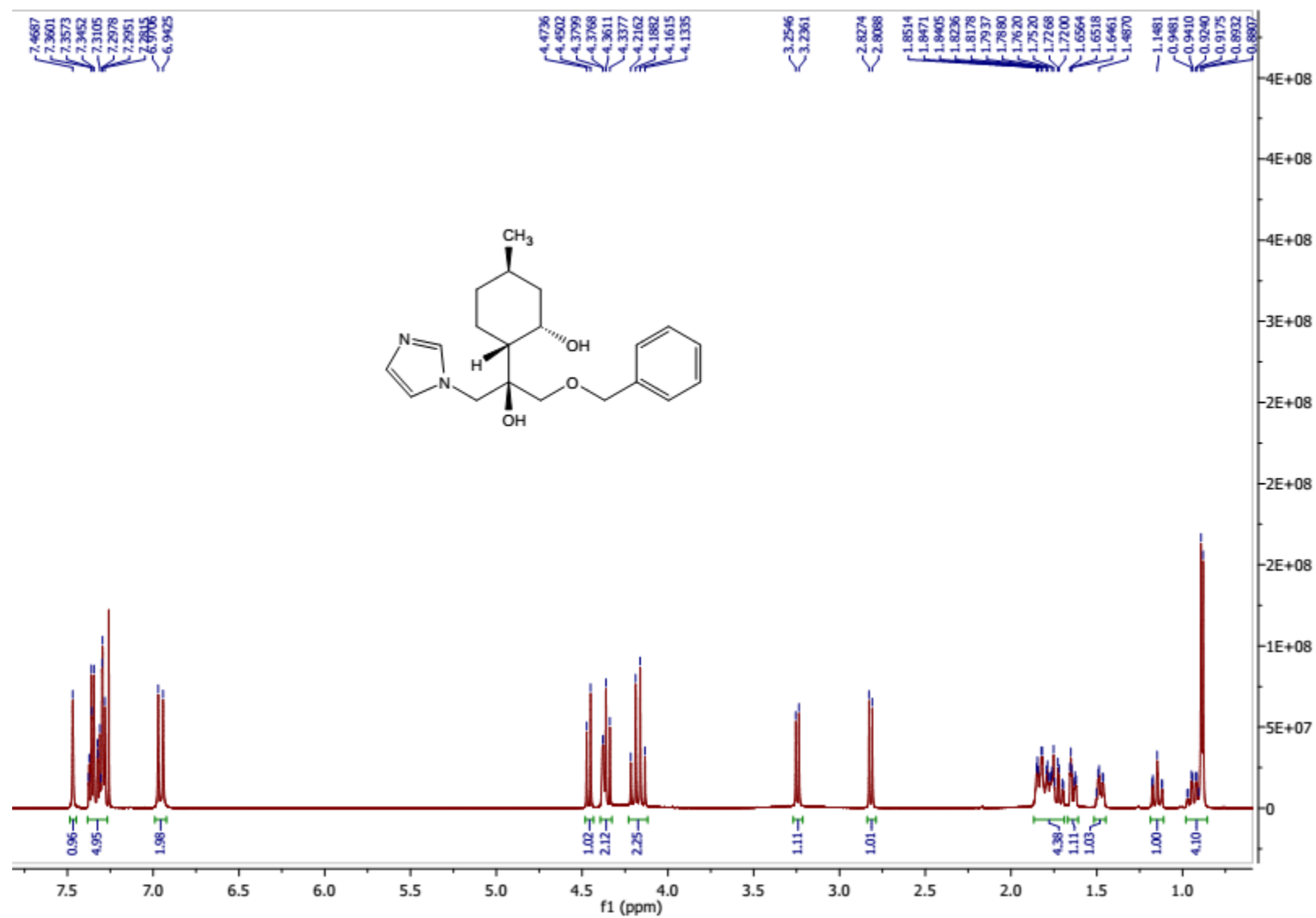


Figure S 81:  $^{13}\text{C}$ -NMR of compound **27b**

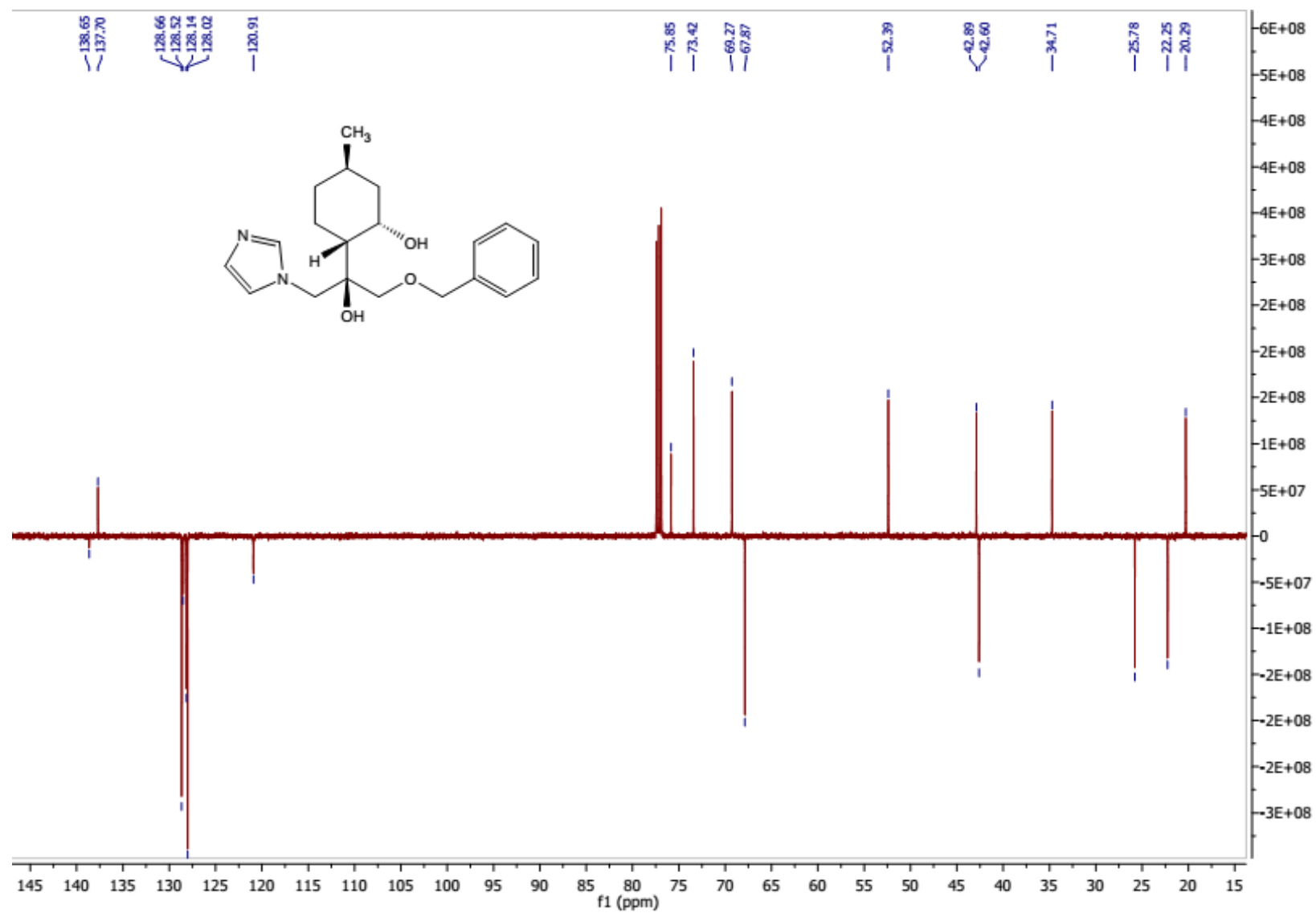




Figure S 82:  $^1\text{H}$ -NMR of compound **28a**

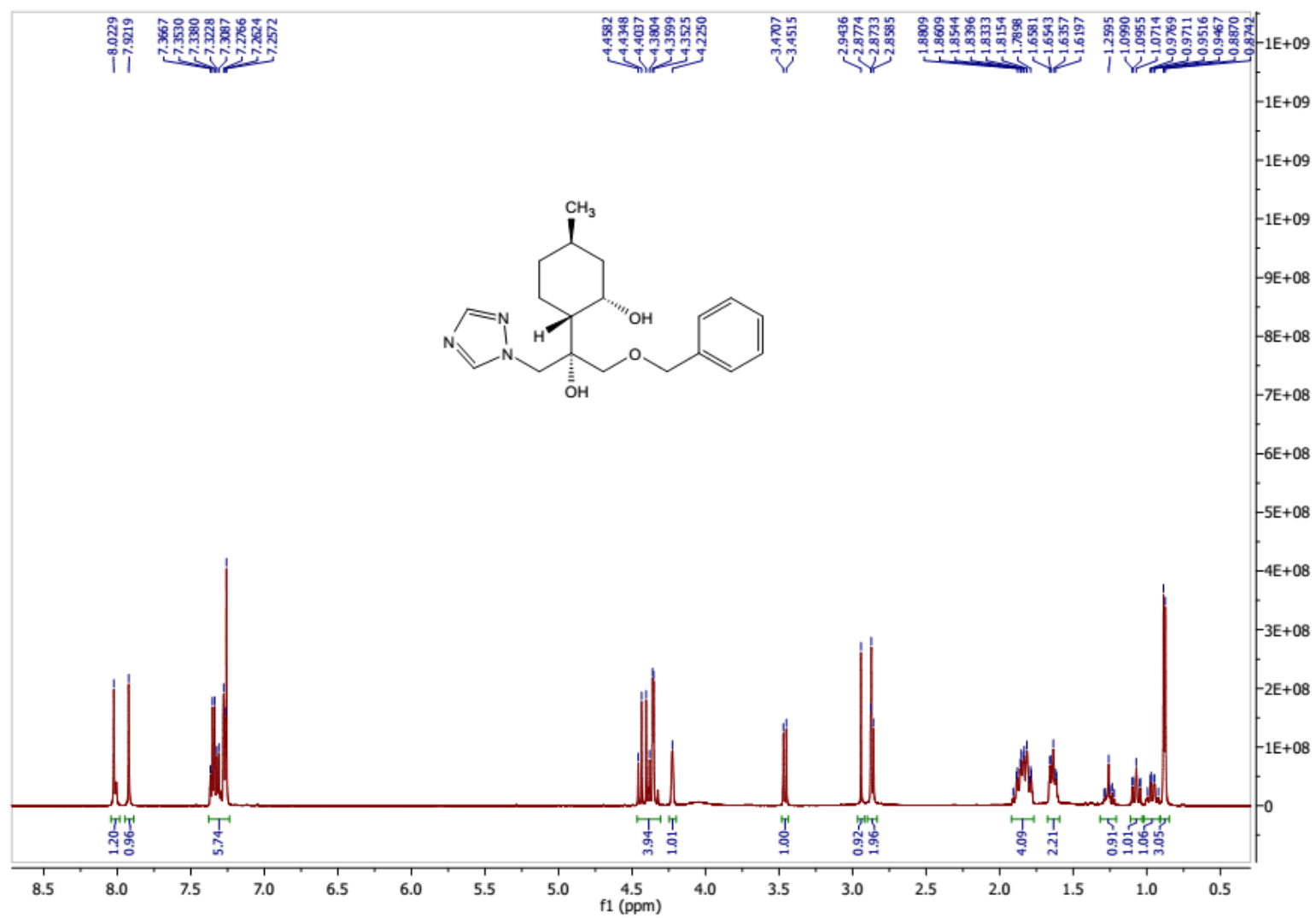


Figure S 83:  $^{13}\text{C}$ -NMR of compound **28a**

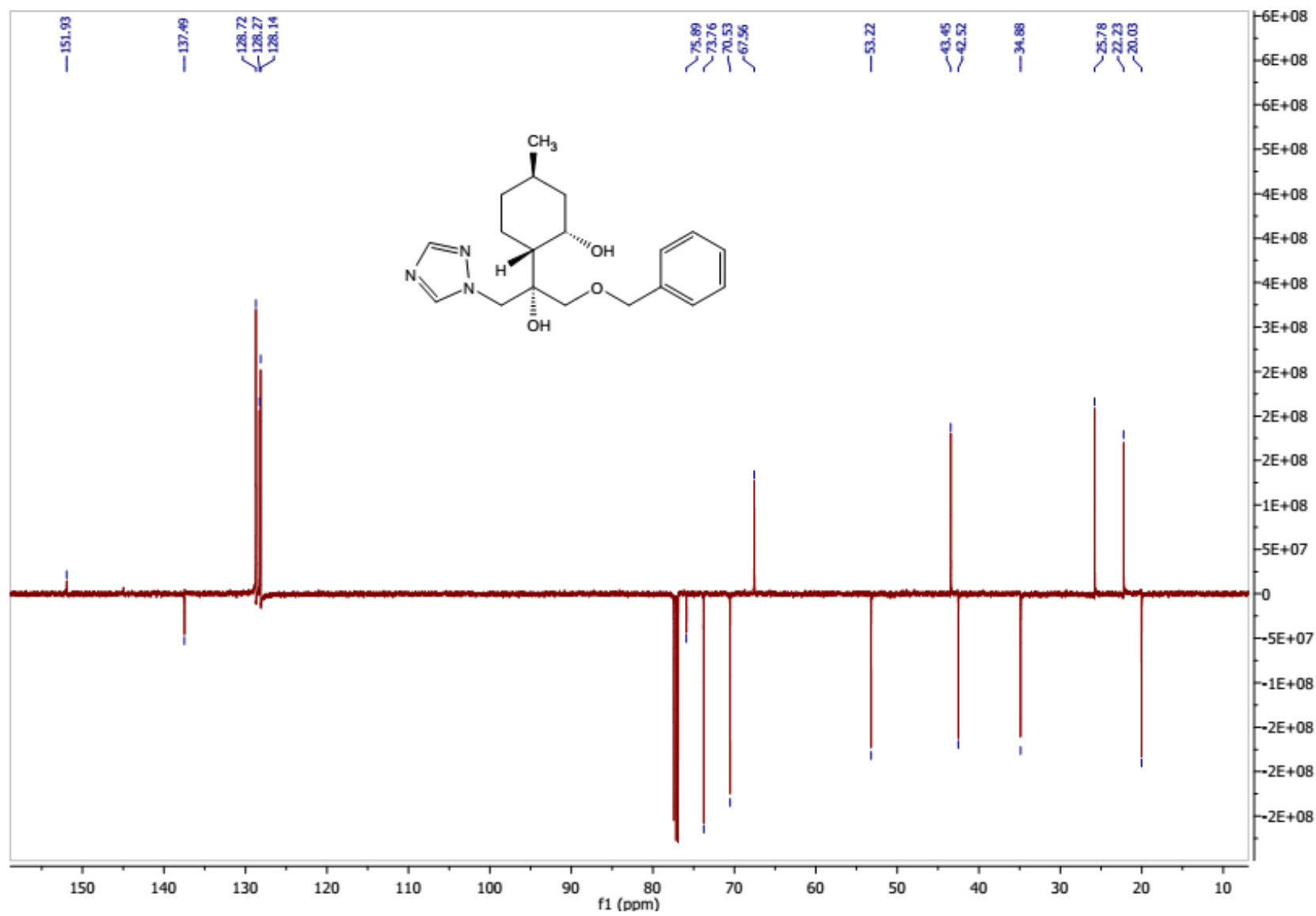


Figure S 84:  $^1\text{H}$ -NMR of compound **28b**

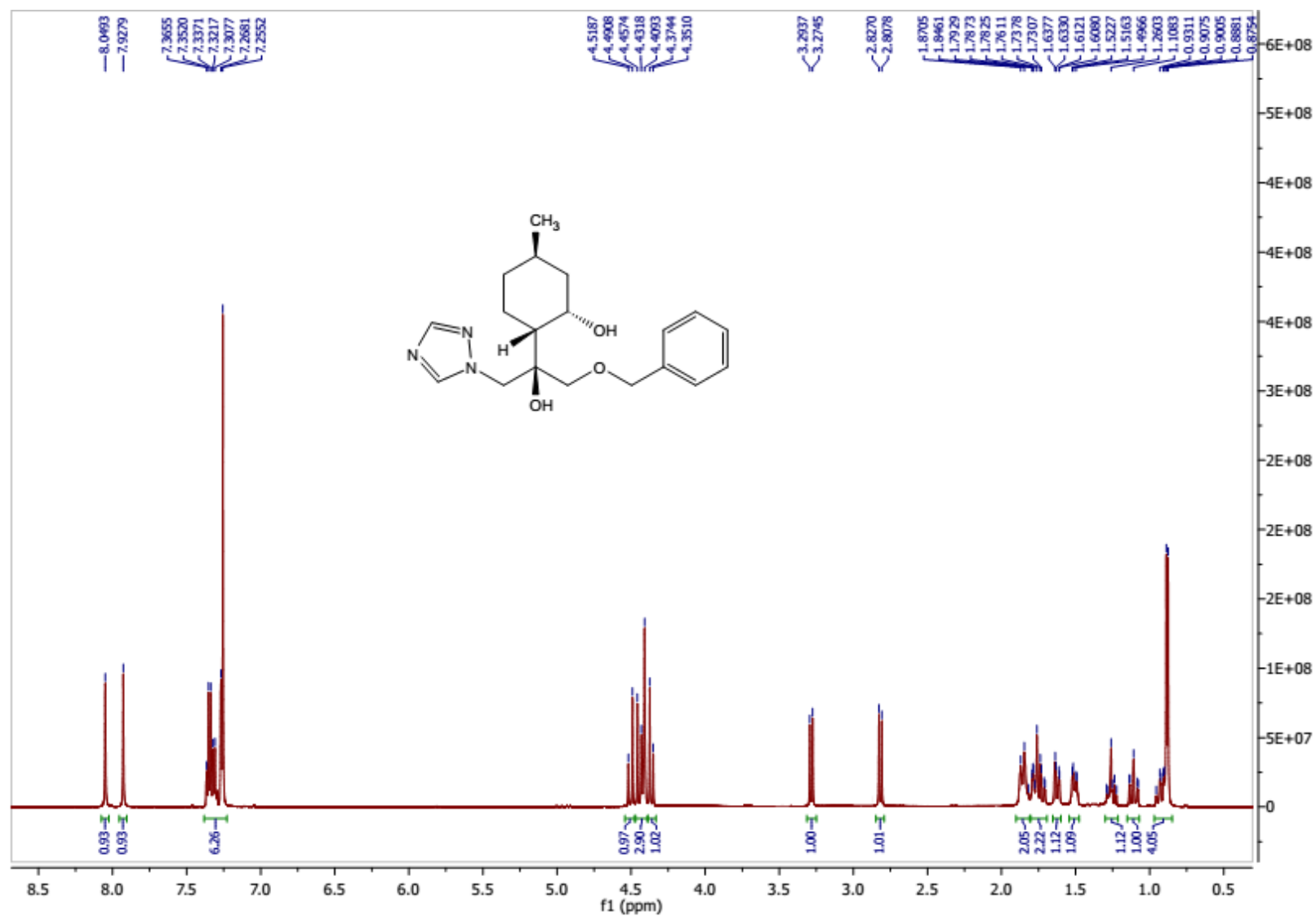


Figure S 85:  $^{13}\text{C}$ -NMR of compound **28b**

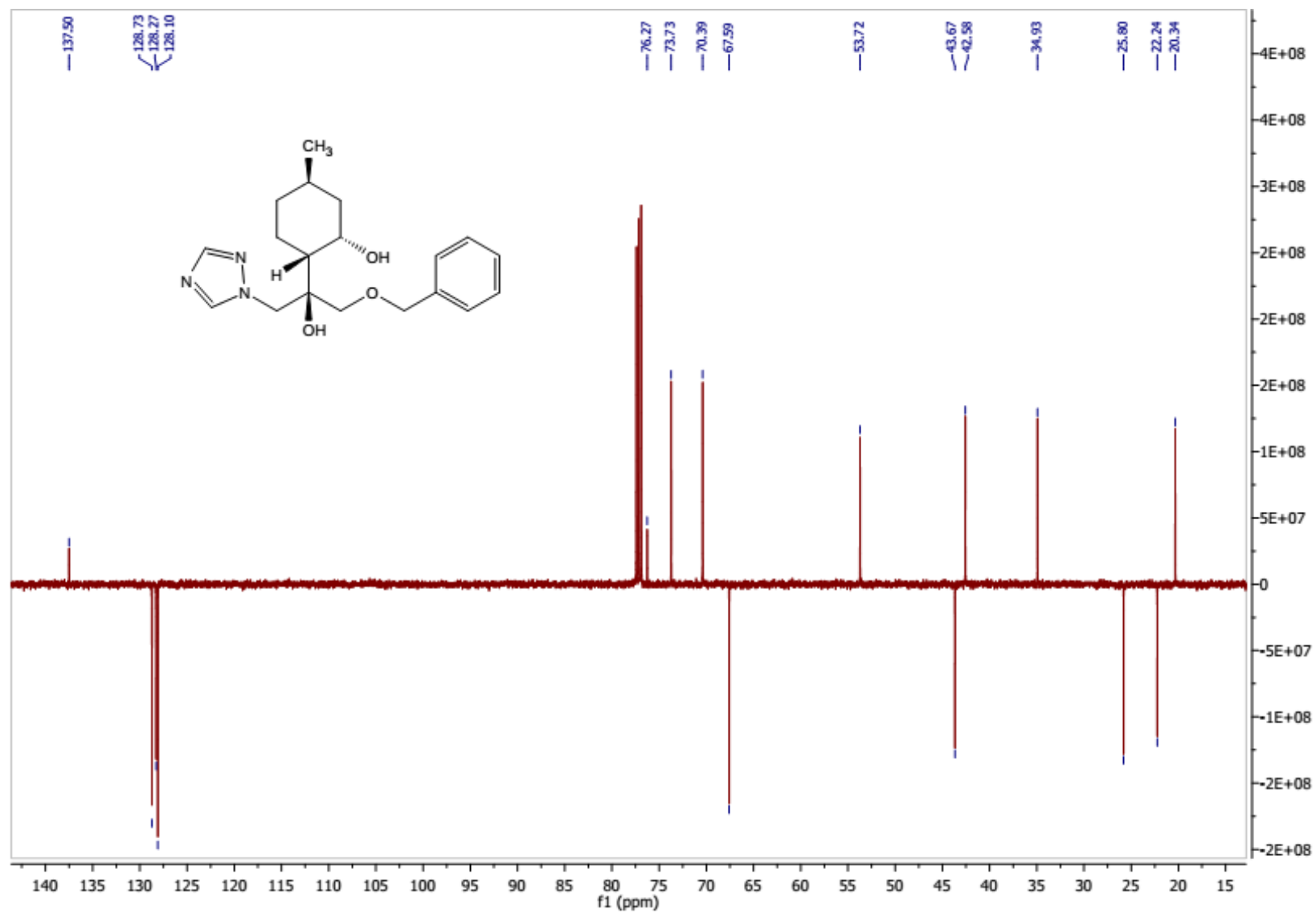


Figure S 86:  $^1\text{H}$ -NMR of compound **30b**

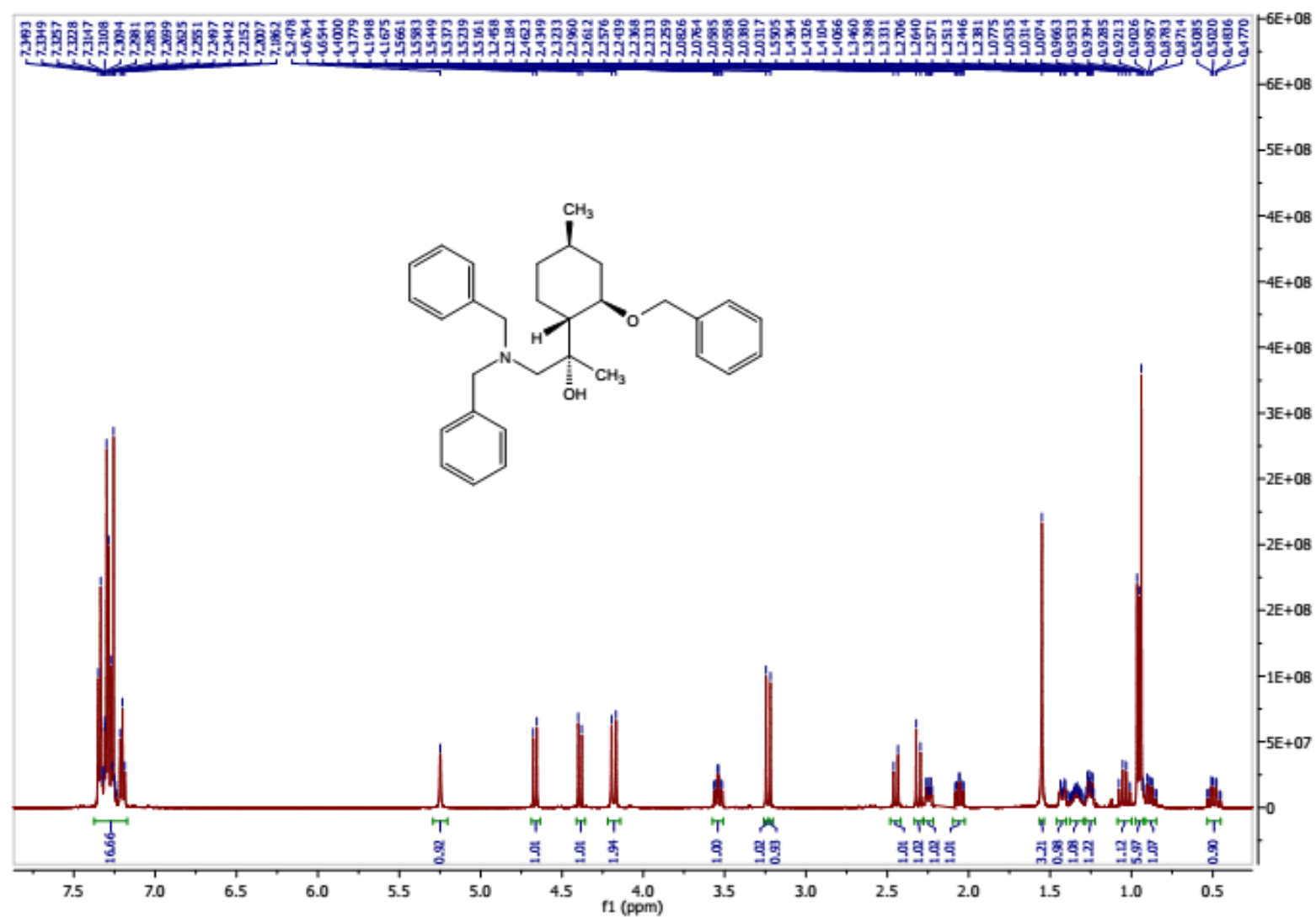


Figure S 87:  $^{13}\text{C}$ -NMR of compound **30b**

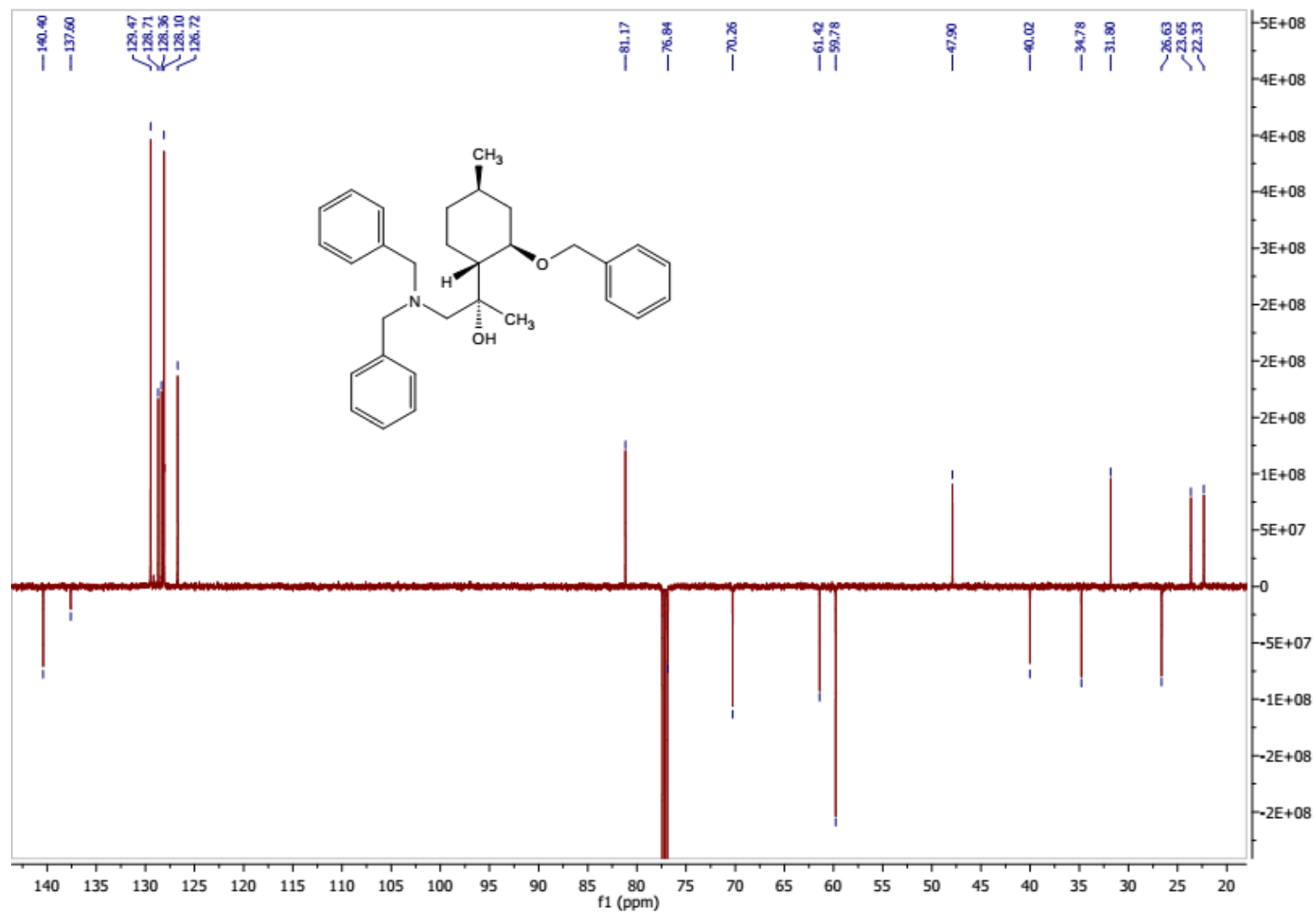


Figure S 88:  $^1\text{H}$ -NMR of compound **31a**

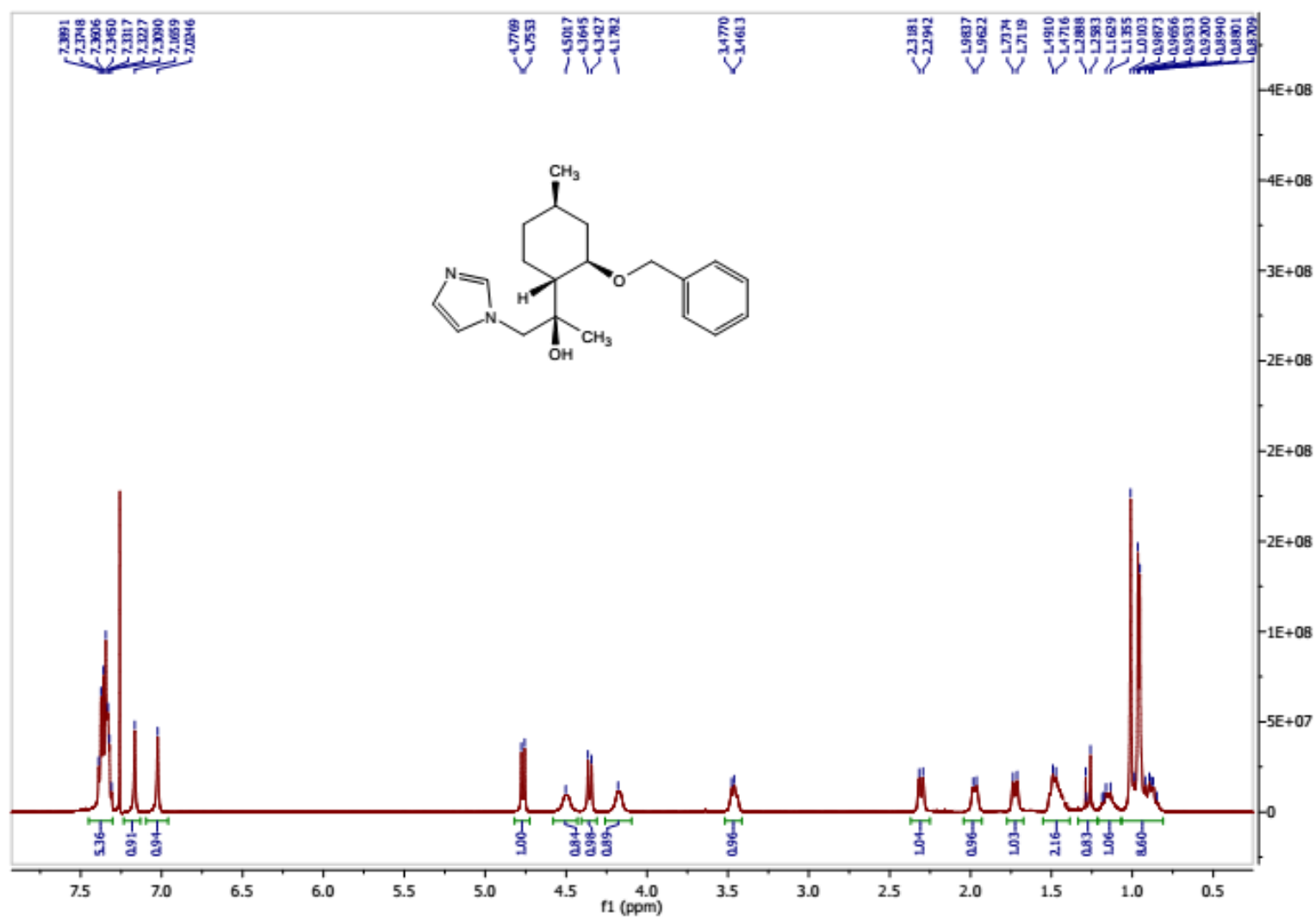


Figure S 89:  $^{13}\text{C}$ -NMR of compound **31a**

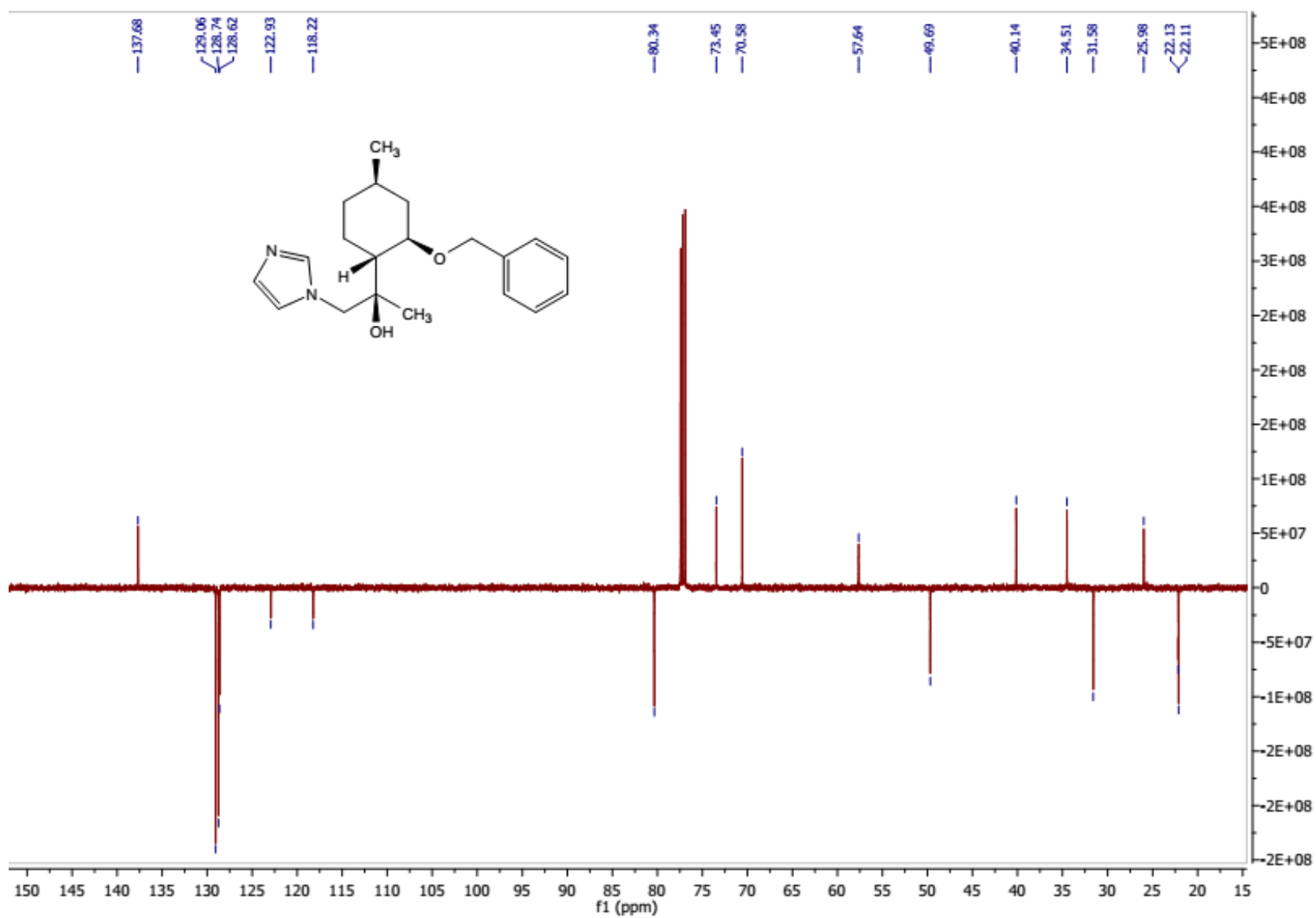




Figure S 90:  $^1\text{H}$ -NMR of compound **31b**

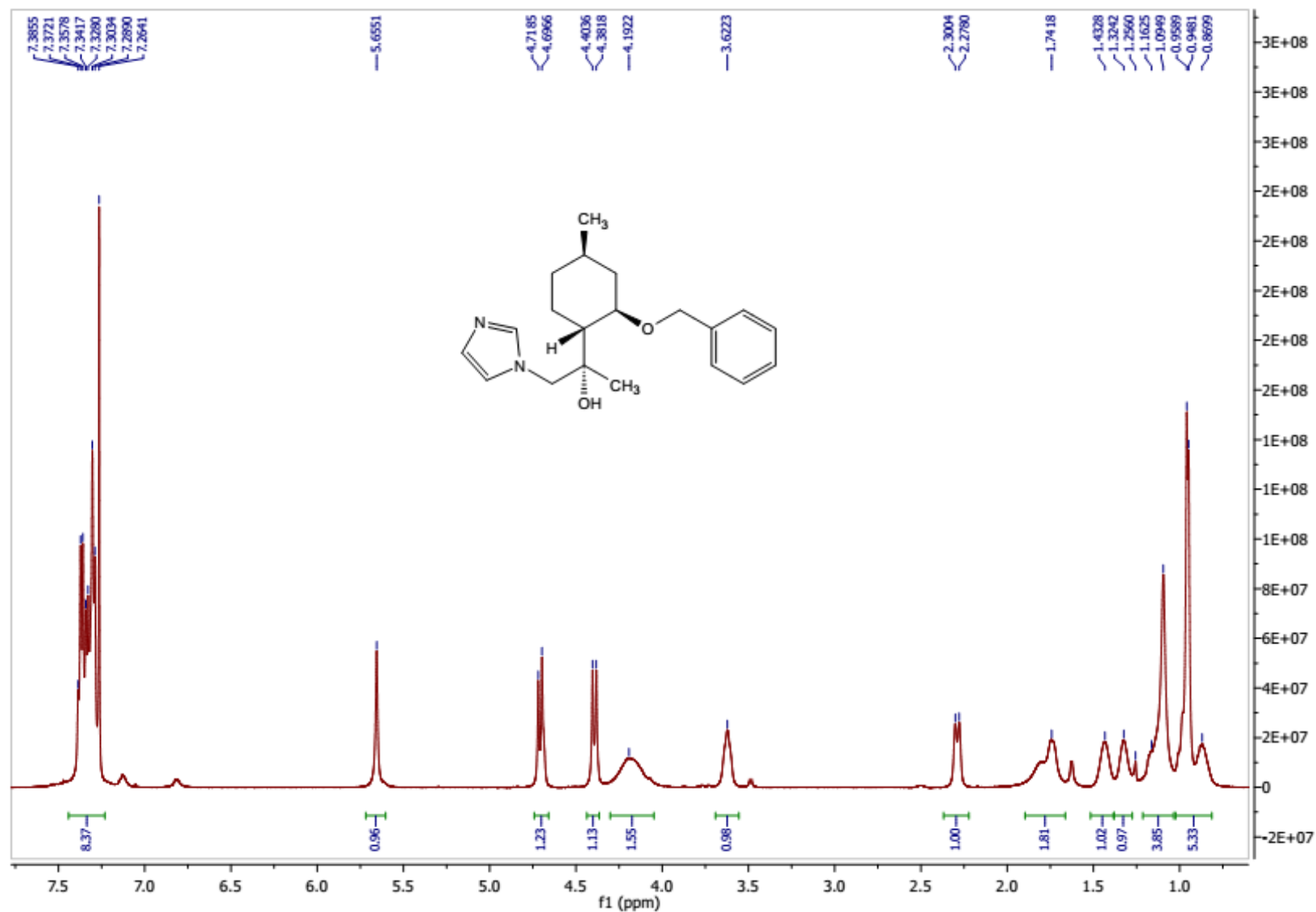


Figure S 91:  $^{13}\text{C}$ -NMR of compound **31b**

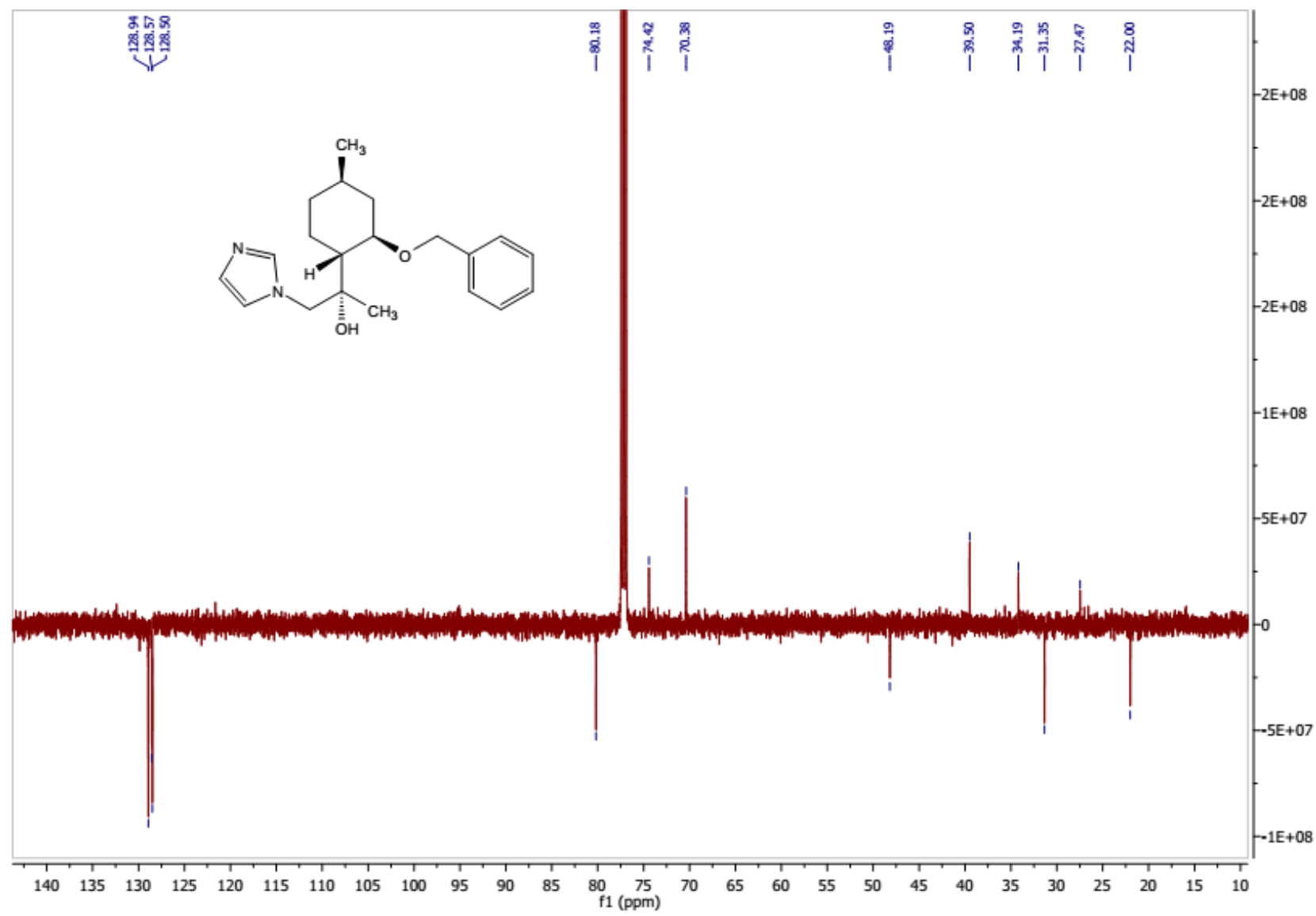


Figure S 92:  $^1\text{H}$ -NMR of compound **32a**

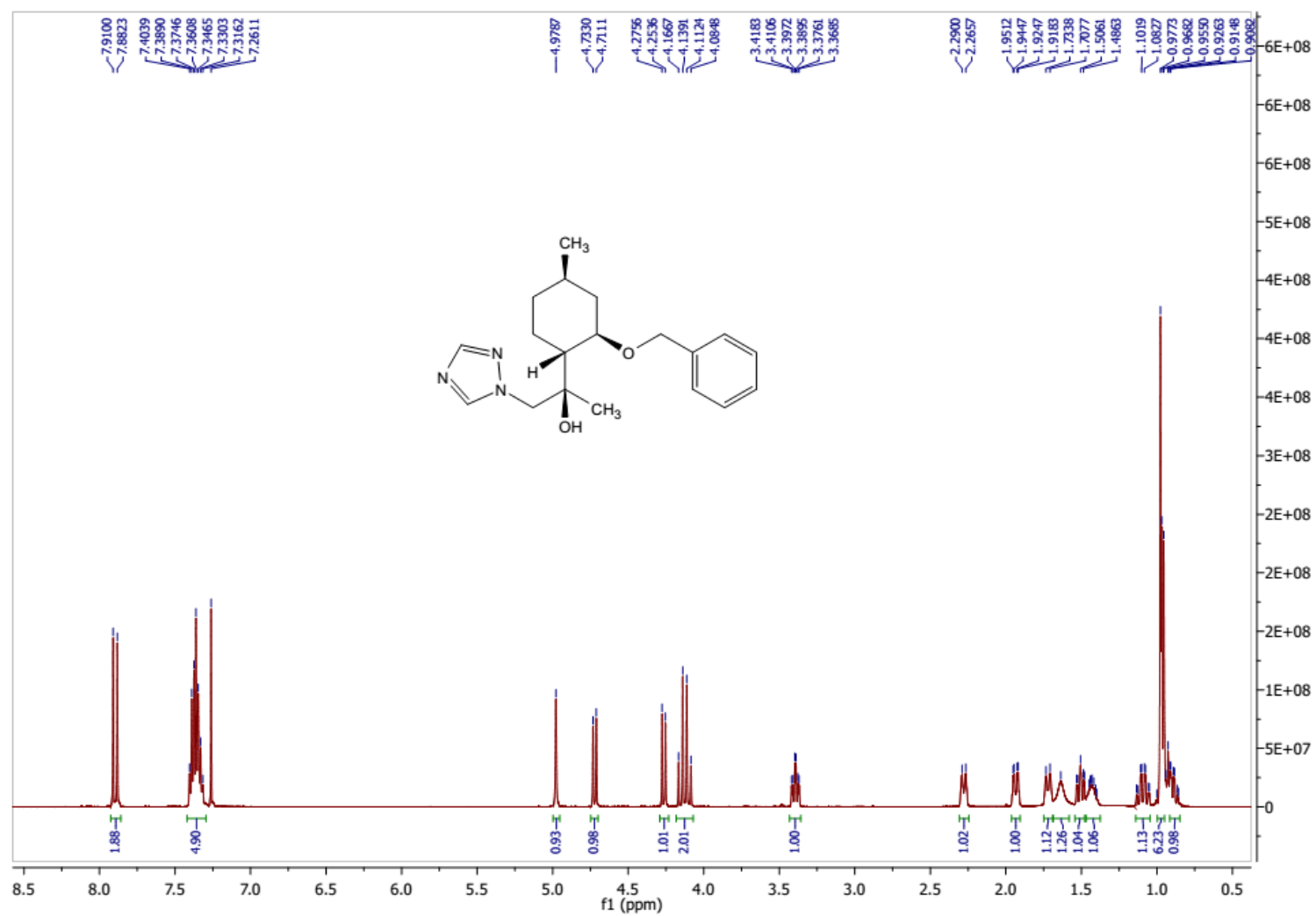


Figure S 93:  $^{13}\text{C}$ -NMR of compound **32a**

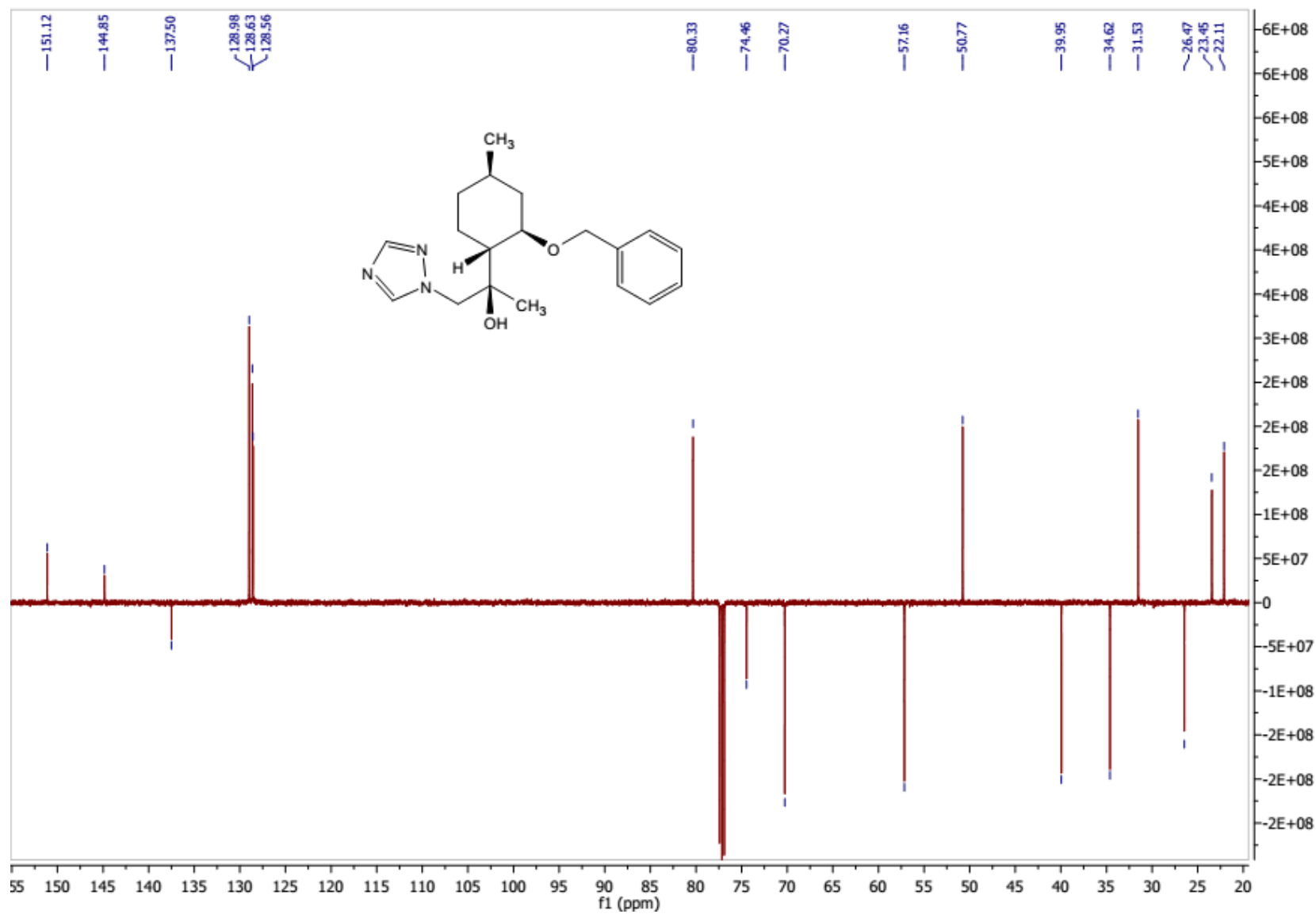


Figure S 94:  $^1\text{H}$ -NMR of compound **32b**

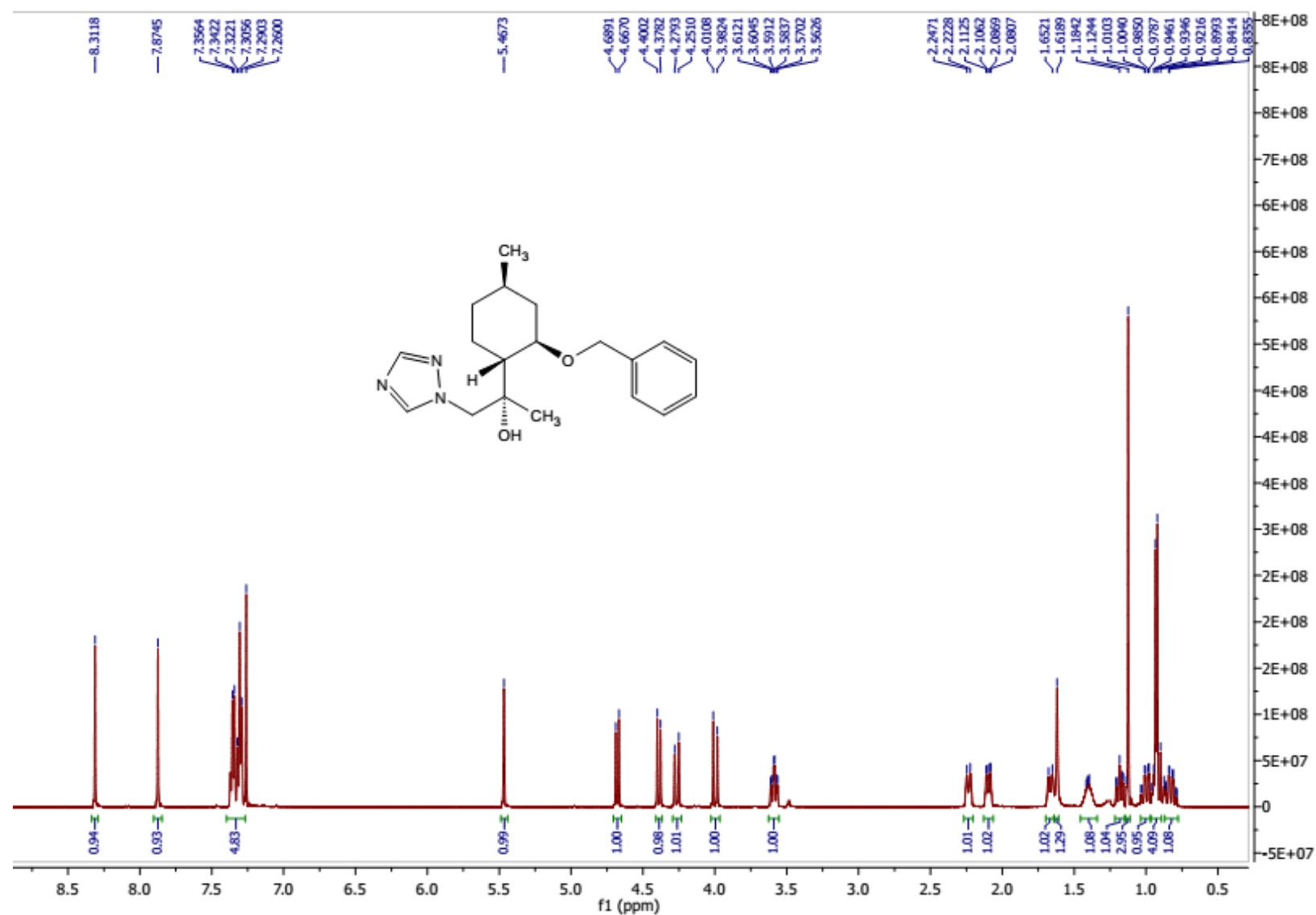


Figure S 95:  $^{13}\text{C}$ -NMR of compound **32b**

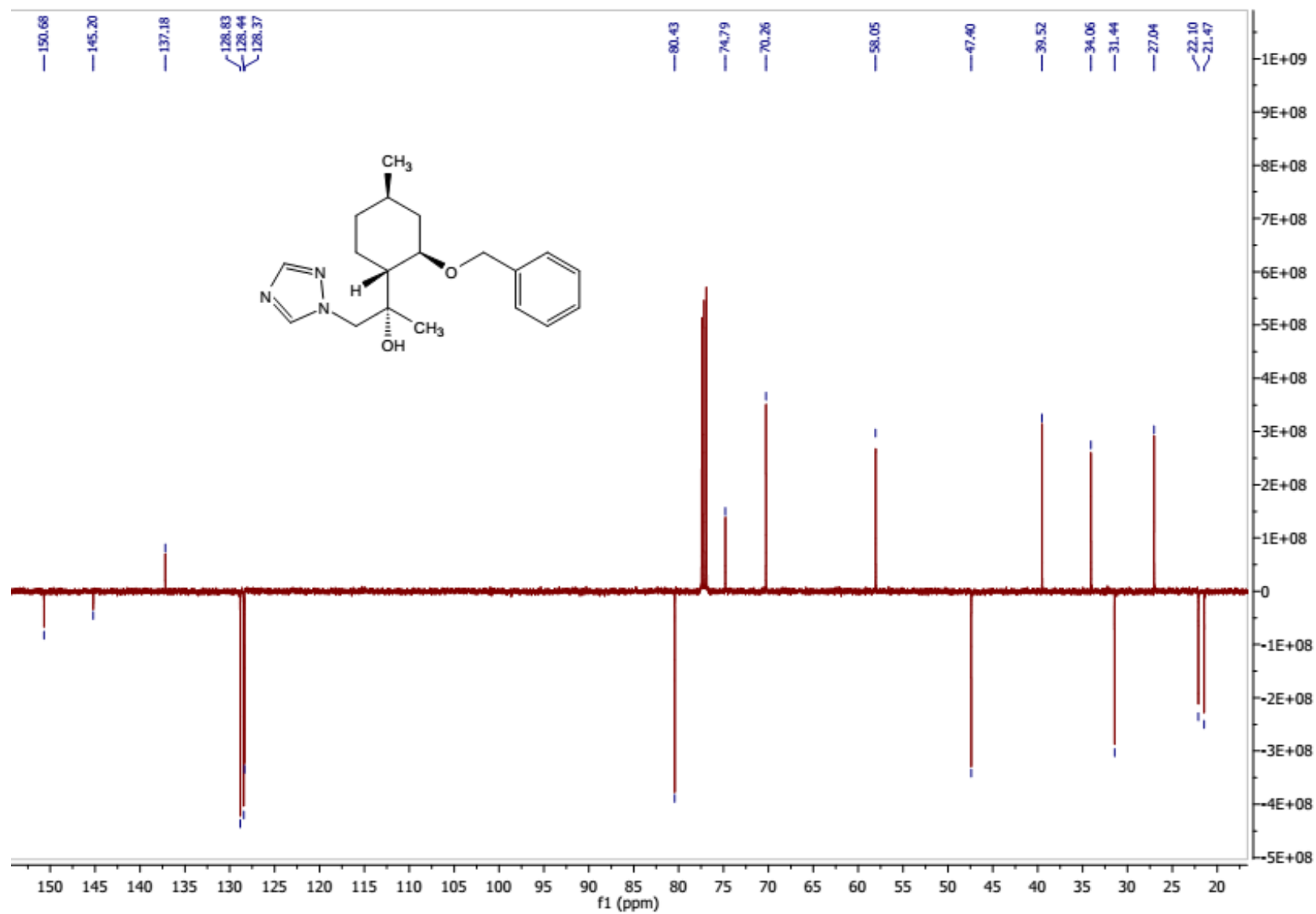


Figure S 96:  $^1\text{H}$ -NMR of compound **34a**

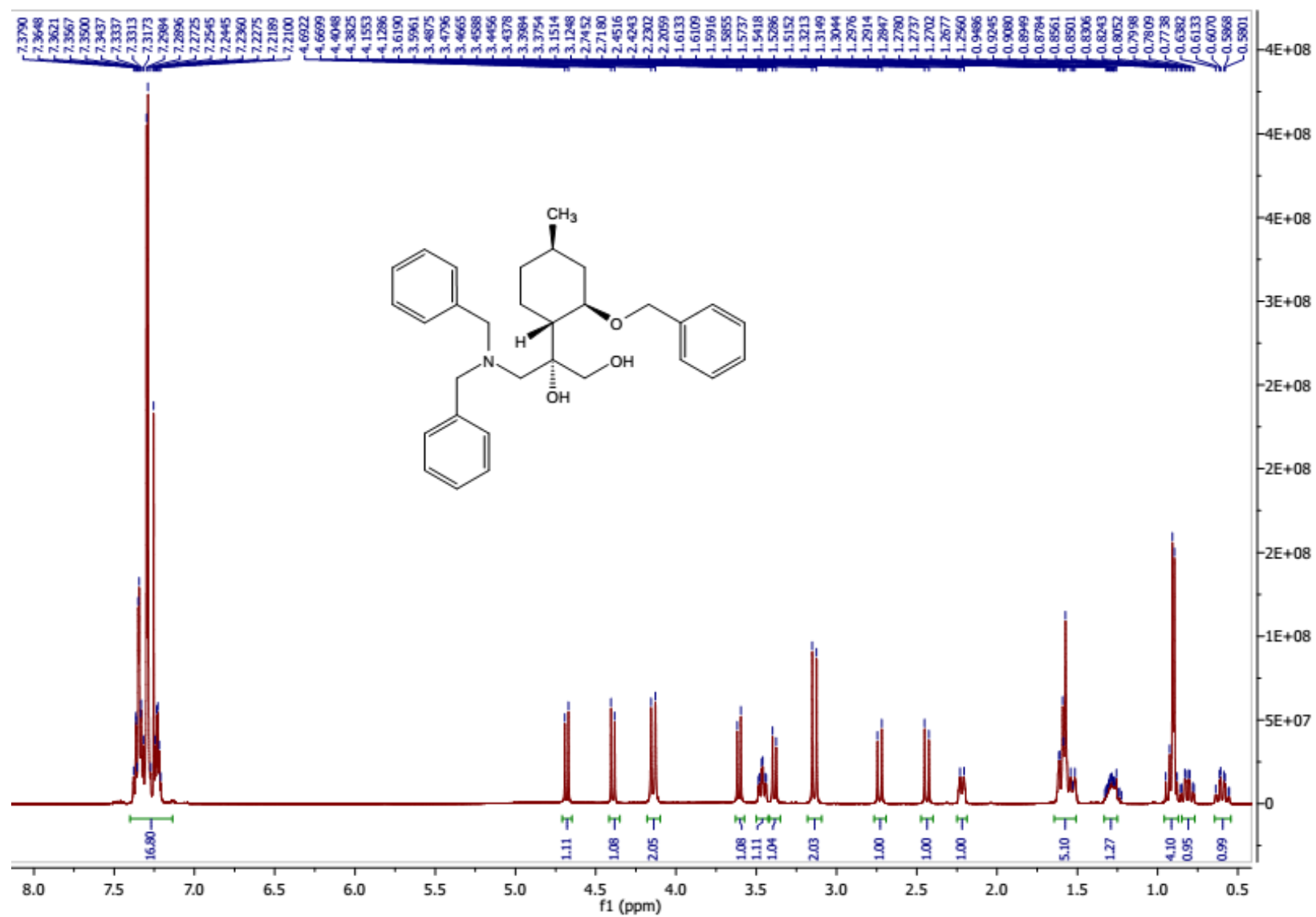


Figure S 97:  $^{13}\text{C}$ -NMR of compound **34a**

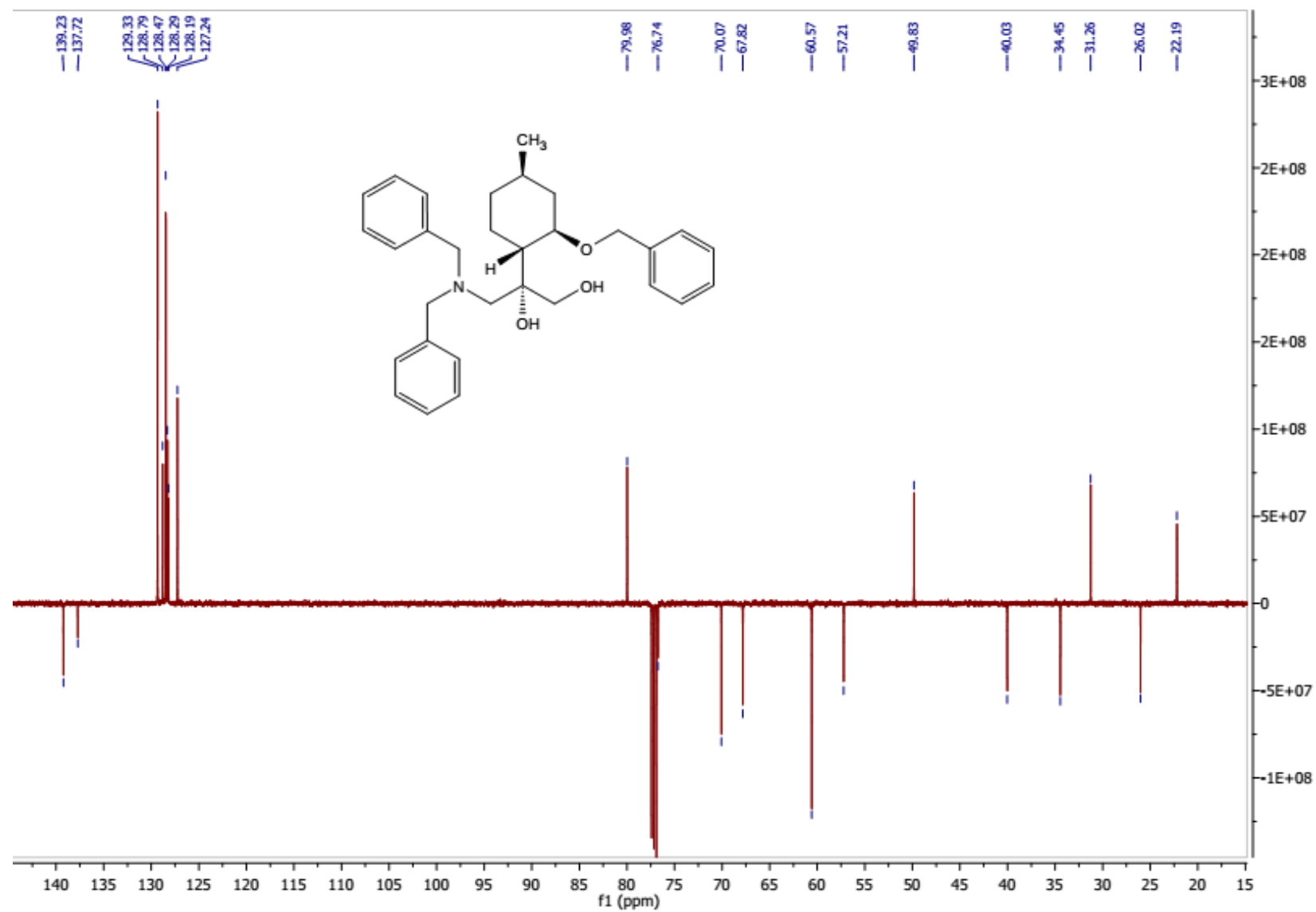




Figure S 98:  $^1\text{H}$ -NMR of compound 35a

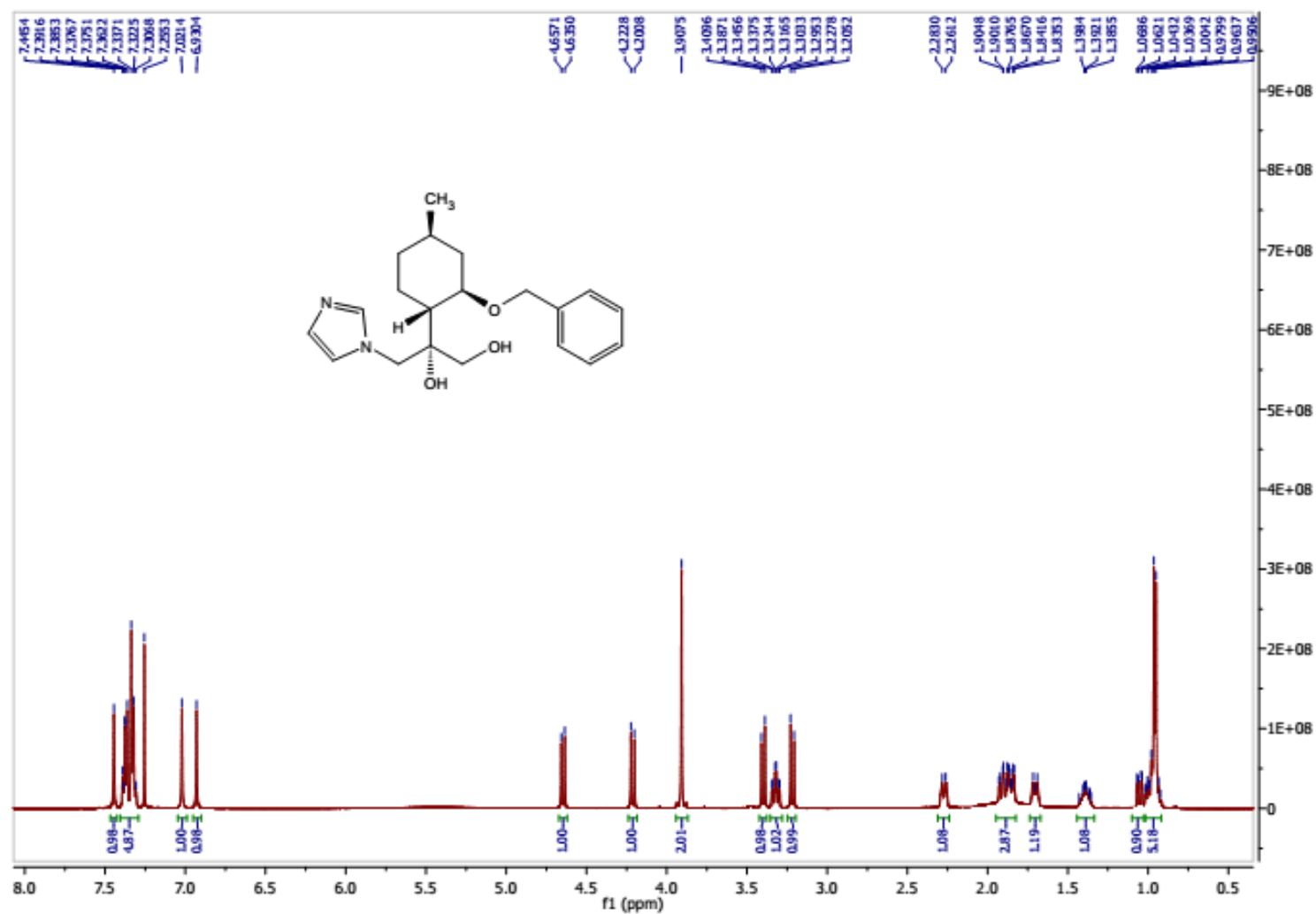


Figure S 99:  $^{13}\text{C}$ -NMR of compound **35a**

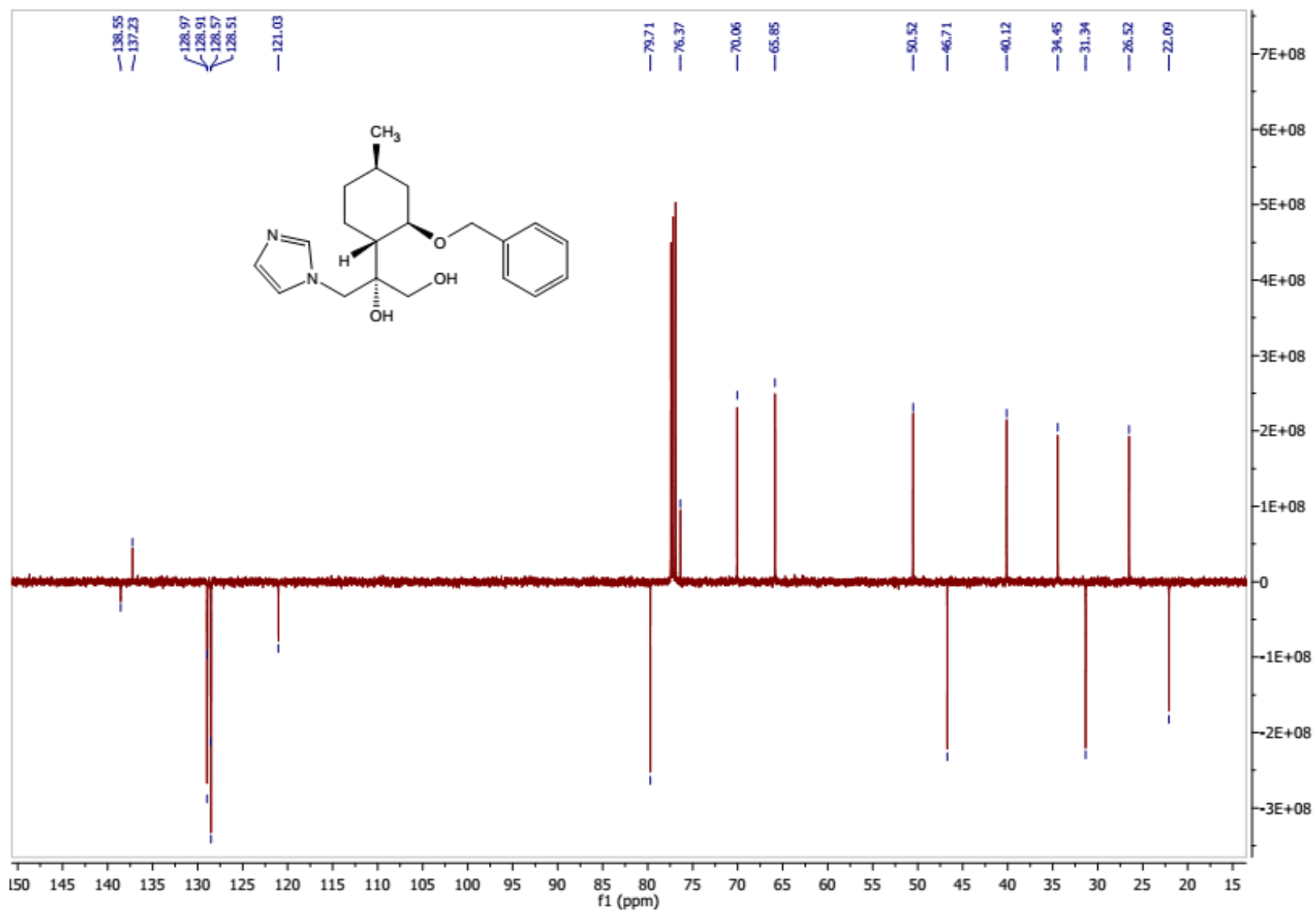


Figure S 100:  $^1\text{H}$ -NMR of compound **35b**

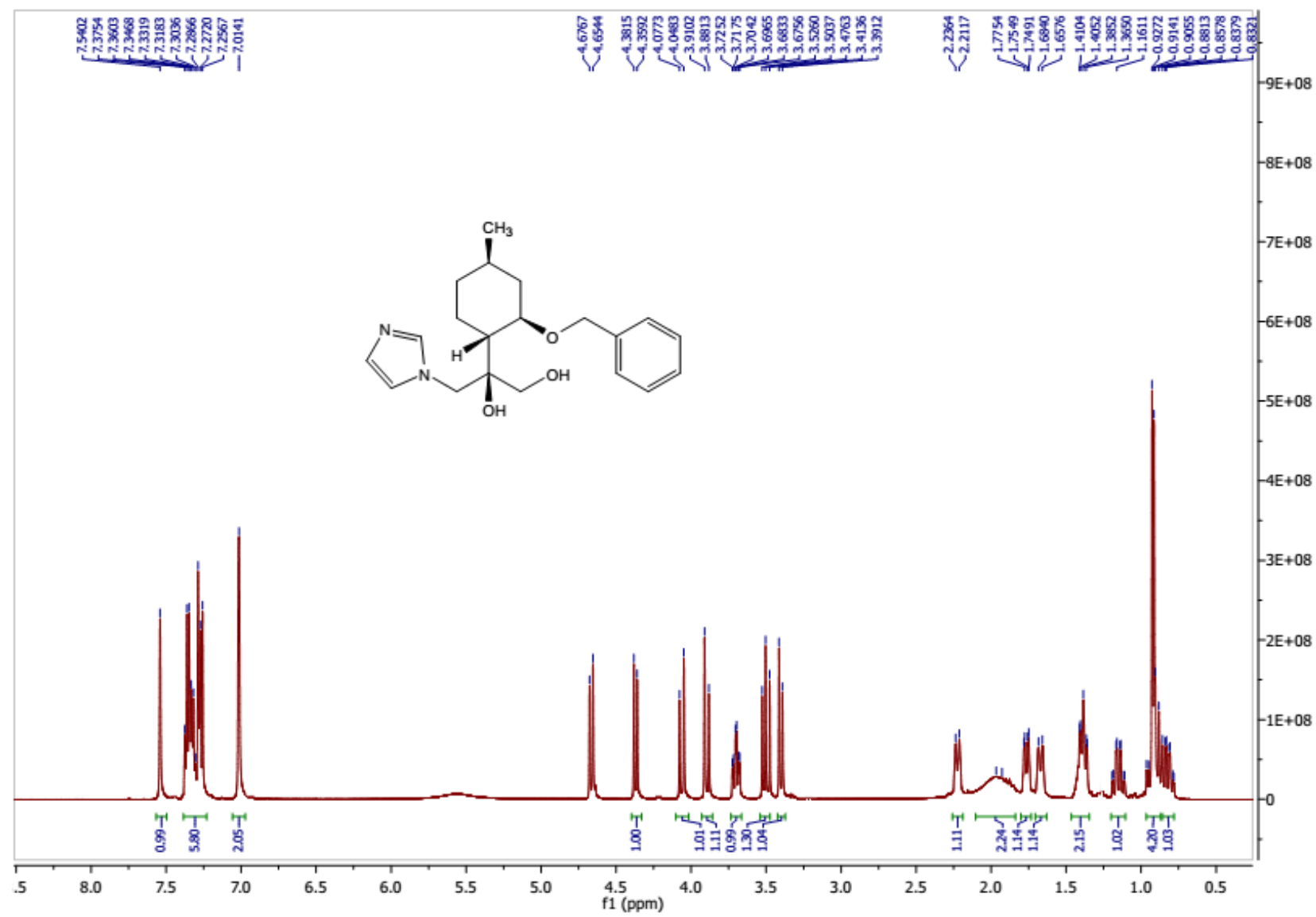
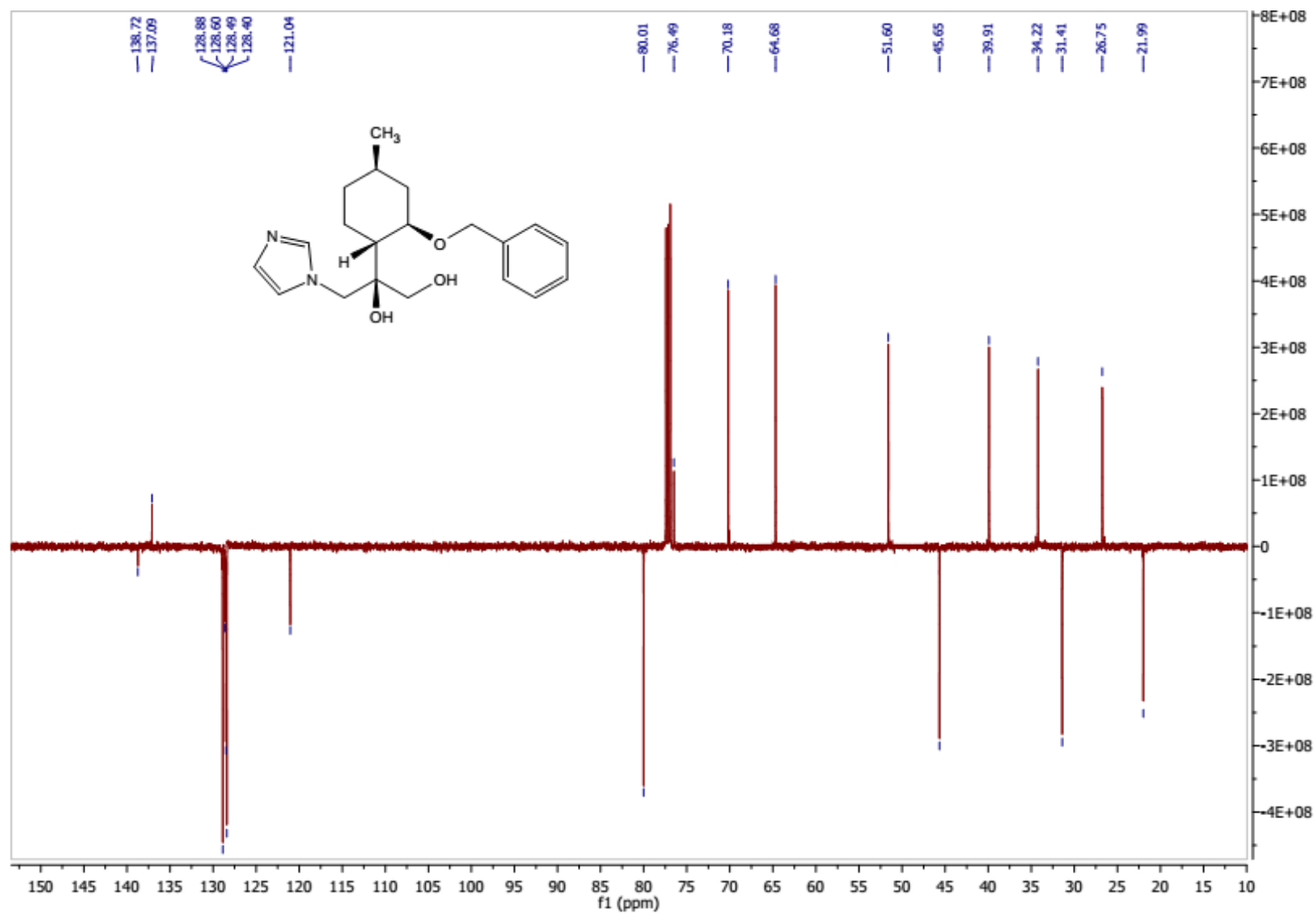


Figure S 101:  $^{13}\text{C}$ -NMR of compound **35b**



Chemical structure of compound 10 is shown above the spectrum. The structure is a cyclohexane ring with a methyl group at C1, a 1H-imidazol-2-ylmethyl group at C2, a hydroxymethyl group at C3, and a (benzyloxy)methyl group at C4.

Integration values (from left to right): 1.80, 4.62, 0.93, 1.84, 0.91, 0.99, 1.84, 1.09, 0.97, 1.93, 1.03, 0.70, 0.98, 4.80.

Peak positions (ppm) listed on the right side of the spectrum (from top to bottom): 7.9253, 7.9135, 7.4205, 7.4040, 7.3915, 7.3619, 7.3503, 7.3470, 7.3371, 7.2610, 7.1759, 7.1637, 7.1503, 7.1370, 7.1237, 7.1104, 7.0971, 7.0838, 7.0705, 7.0572, 7.0439, 7.0306, 7.0173, 7.0040, 6.9907, 6.9774, 6.9641, 6.9508, 6.9375, 6.9242, 6.9109, 6.8976, 6.8843, 6.8710, 6.8577, 6.8444, 6.8311, 6.8178, 6.8045, 6.7912, 6.7779, 6.7646, 6.7513, 6.7380, 6.7247, 6.7114, 6.6981, 6.6848, 6.6715, 6.6582, 6.6449, 6.6316, 6.6183, 6.6050, 6.5917, 6.5784, 6.5651, 6.5518, 6.5385, 6.5252, 6.5119, 6.4986, 6.4853, 6.4720, 6.4587, 6.4454, 6.4321, 6.4188, 6.4055, 6.3922, 6.3789, 6.3656, 6.3523, 6.3390, 6.3257, 6.3124, 6.2991, 6.2858, 6.2725, 6.2592, 6.2459, 6.2326, 6.2193, 6.2060, 6.1927, 6.1794, 6.1661, 6.1528, 6.1395, 6.1262, 6.1129, 6.0996, 6.0863, 6.0730, 6.0597, 6.0464, 6.0331, 6.0198, 6.0065, 5.9932, 5.9799, 5.9666, 5.9533, 5.9400, 5.9267, 5.9134, 5.9001, 5.8868, 5.8735, 5.8602, 5.8469, 5.8336, 5.8203, 5.8070, 5.7937, 5.7804, 5.7671, 5.7538, 5.7405, 5.7272, 5.7139, 5.7006, 5.6873, 5.6740, 5.6607, 5.6474, 5.6341, 5.6208, 5.6075, 5.5942, 5.5809, 5.5676, 5.5543, 5.5410, 5.5277, 5.5144, 5.5011, 5.4878, 5.4745, 5.4612, 5.4479, 5.4346, 5.4213, 5.4080, 5.3947, 5.3814, 5.3681, 5.3548, 5.3415, 5.3282, 5.3149, 5.3016, 5.2883, 5.2750, 5.2617, 5.2484, 5.2351, 5.2218, 5.2085, 5.1952, 5.1819, 5.1686, 5.1553, 5.1420, 5.1287, 5.1154, 5.1021, 5.0888, 5.0755, 5.0622, 5.0489, 5.0356, 5.0223, 5.0090, 4.9957, 4.9824, 4.9691, 4.9558, 4.9425, 4.9292, 4.9159, 4.9026, 4.8893, 4.8760, 4.8627, 4.8494, 4.8361, 4.8228, 4.8095, 4.7962, 4.7829, 4.7696, 4.7563, 4.7430, 4.7297, 4.7164, 4.7031, 4.6898, 4.6765, 4.6632, 4.6499, 4.6366, 4.6233, 4.6100, 4.5967, 4.5834, 4.5701, 4.5568, 4.5435, 4.5302, 4.5169, 4.5036, 4.4903, 4.4770, 4.4637, 4.4504, 4.4371, 4.4238, 4.4105, 4.3972, 4.3839, 4.3706, 4.3573, 4.3440, 4.3307, 4.3174, 4.3041, 4.2908, 4.2775, 4.2642, 4.2509, 4.2376, 4.2243, 4.2110, 4.1977, 4.1844, 4.1711, 4.1578, 4.1445, 4.1312, 4.1179, 4.1046, 4.0913, 4.0780, 4.0647, 4.0514, 4.0381, 4.0248, 4.0115, 3.9982, 3.9849, 3.9716, 3.9583, 3.9450, 3.9317, 3.9184, 3.9051, 3.8918, 3.8785, 3.8652, 3.8519, 3.8386, 3.8253, 3.8120, 3.7987, 3.7854, 3.7721, 3.7588, 3.7455, 3.7322, 3.7189, 3.7056, 3.6923, 3.6790, 3.6657, 3.6524, 3.6391, 3.6258, 3.6125, 3.5992, 3.5859, 3.5726, 3.5593, 3.5460, 3.5327, 3.5194, 3.5061, 3.4928, 3.4795, 3.4662, 3.4529, 3.4396, 3.4263, 3.4130, 3.3997, 3.3864, 3.3731, 3.3598, 3.3465, 3.3332, 3.3199, 3.3066, 3.2933, 3.2800, 3.2667, 3.2534, 3.2401, 3.2268, 3.2135, 3.2002, 3.1869, 3.1736, 3.1603, 3.1470, 3.1337, 3.1204, 3.1071, 3.0938, 3.0805, 3.0672, 3.0539, 3.0406, 3.0273, 3.0140, 3.0007, 2.9874, 2.9741, 2.9608, 2.9475, 2.9342, 2.9209, 2.9076, 2.8943, 2.8810, 2.8677, 2.8544, 2.8411, 2.8278, 2.8145, 2.8012, 2.7879, 2.7746, 2.7613, 2.7480, 2.7347, 2.7214, 2.7081, 2.6948, 2.6815, 2.6682, 2.6549, 2.6416, 2.6283, 2.6150, 2.6017, 2.5884, 2.5751, 2.5618, 2.5485, 2.5352, 2.5219, 2.5086, 2.4953, 2.4820, 2.4687, 2.4554, 2.4421, 2.4288, 2.4155, 2.4022, 2.3889, 2.3756, 2.3623, 2.3490, 2.3357, 2.3224, 2.3091, 2.2958, 2.2825, 2.2692, 2.2559, 2.2426, 2.2293, 2.2160, 2.2027, 2.1894, 2.1761, 2.1628, 2.1495, 2.1362, 2.1229, 2.1096, 2.0963, 2.0830, 2.0697, 2.0564, 2.0431, 2.0298, 2.0165, 2.0032, 1.9899, 1.9766, 1.9633, 1.9500, 1.9367, 1.9234, 1.9101, 1.8968, 1.8835, 1.8702, 1.8569, 1.8436, 1.8303, 1.8170, 1.8037, 1.7904, 1.7771, 1.7638, 1.7505, 1.7372, 1.7239, 1.7106, 1.6973, 1.6840, 1.6707, 1.6574, 1.6441, 1.6308, 1.6175, 1.6042, 1.5909, 1.5776, 1.5643, 1.5510, 1.5377, 1.5244, 1.5111, 1.4978, 1.4845, 1.4712, 1.4579, 1.4446, 1.4313, 1.4180, 1.4047, 1.3914, 1.3781, 1.3648, 1.3515, 1.3382, 1.3249, 1.3116, 1.2983, 1.2850, 1.2717, 1.2584, 1.2451, 1.2318, 1.2185, 1.2052, 1.1919, 1.1786, 1.1653, 1.1520, 1.1387, 1.1254, 1.1121, 1.0988, 1.0855, 1.0722, 1.0589, 1

Figure S 103:  $^{13}\text{C}$ -NMR of compound **36a**

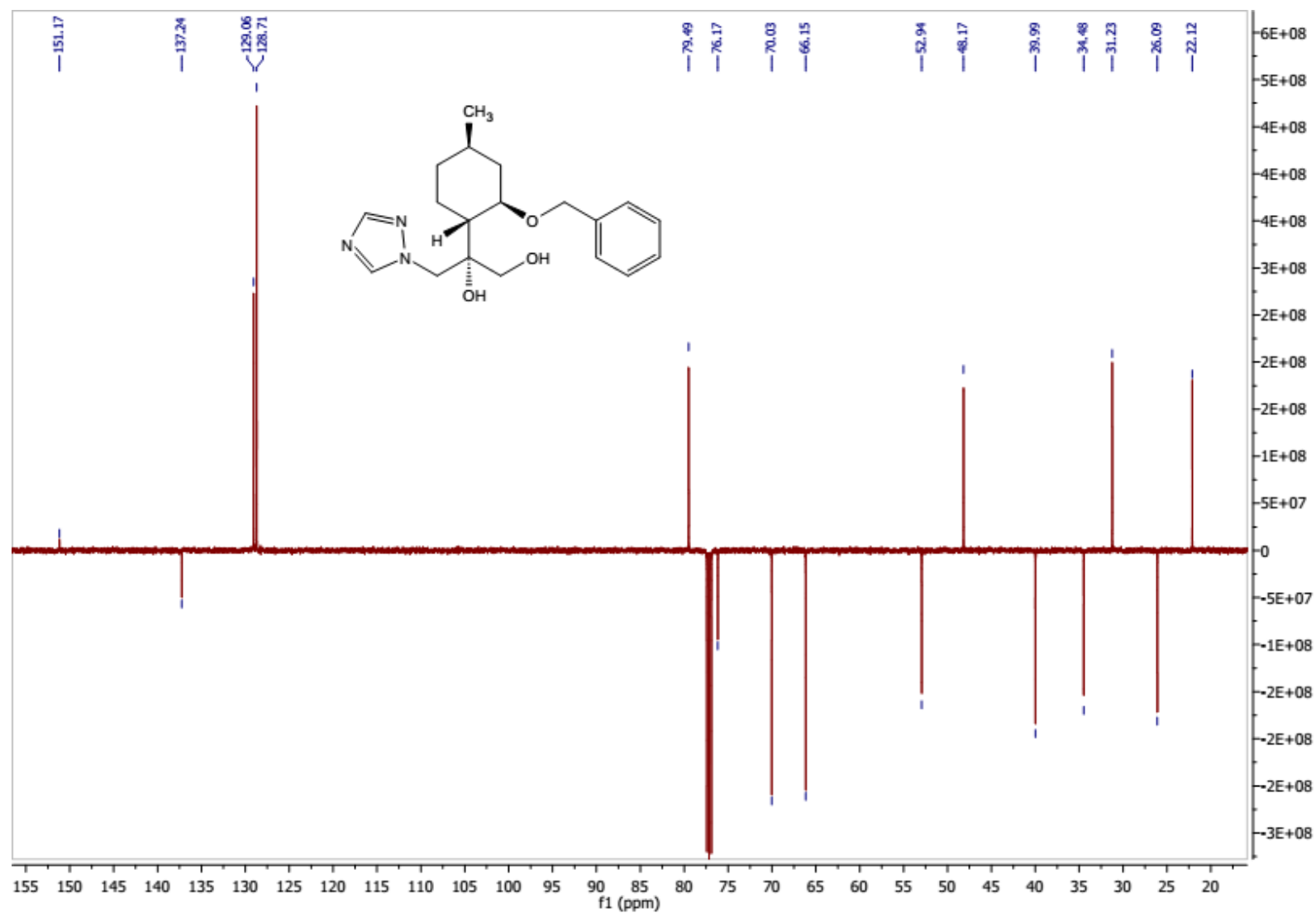


Figure S 104:  $^1\text{H}$ -NMR of compound **36b**

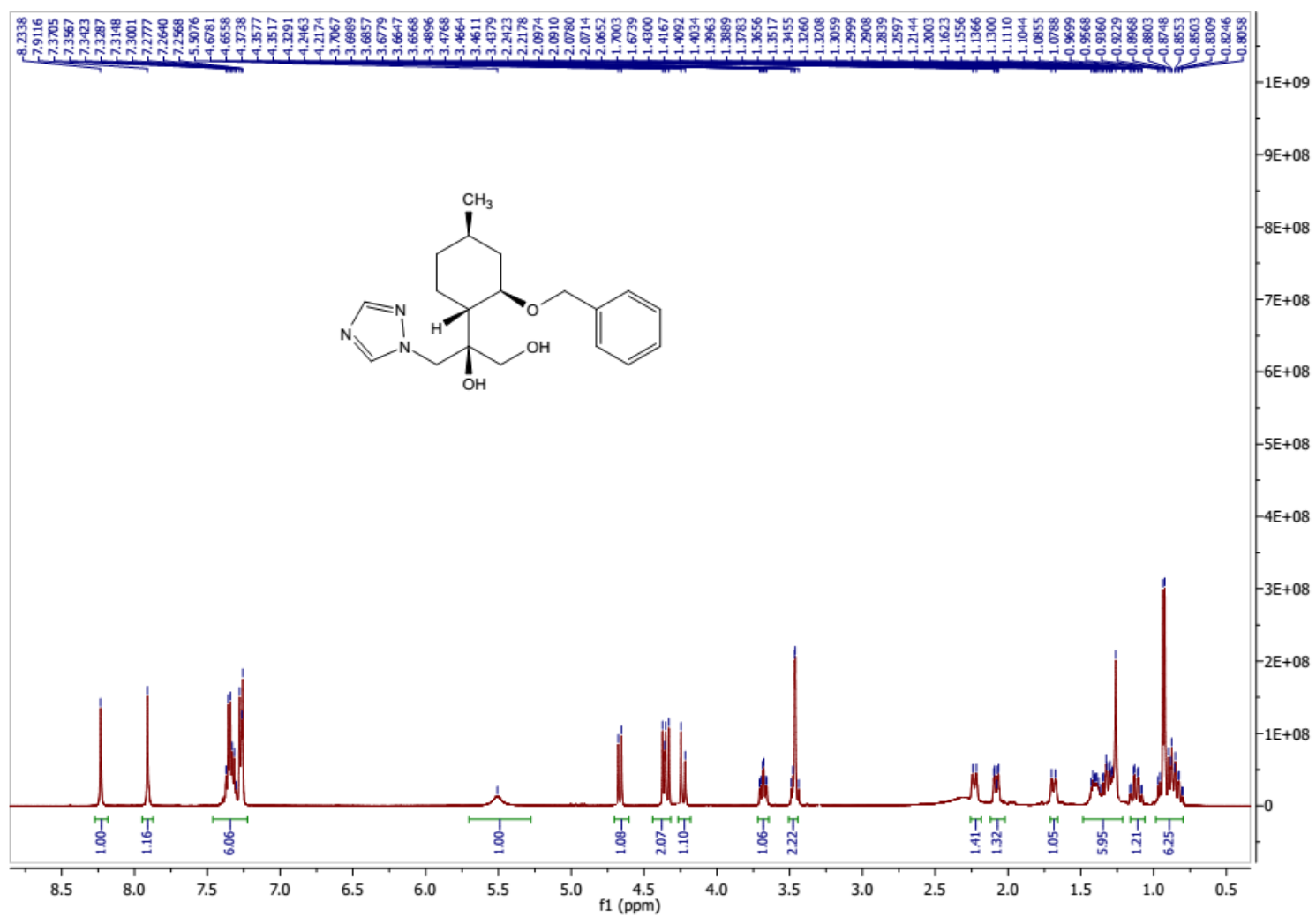


Figure S 105:  $^{13}\text{C}$ -NMR of compound **36b**

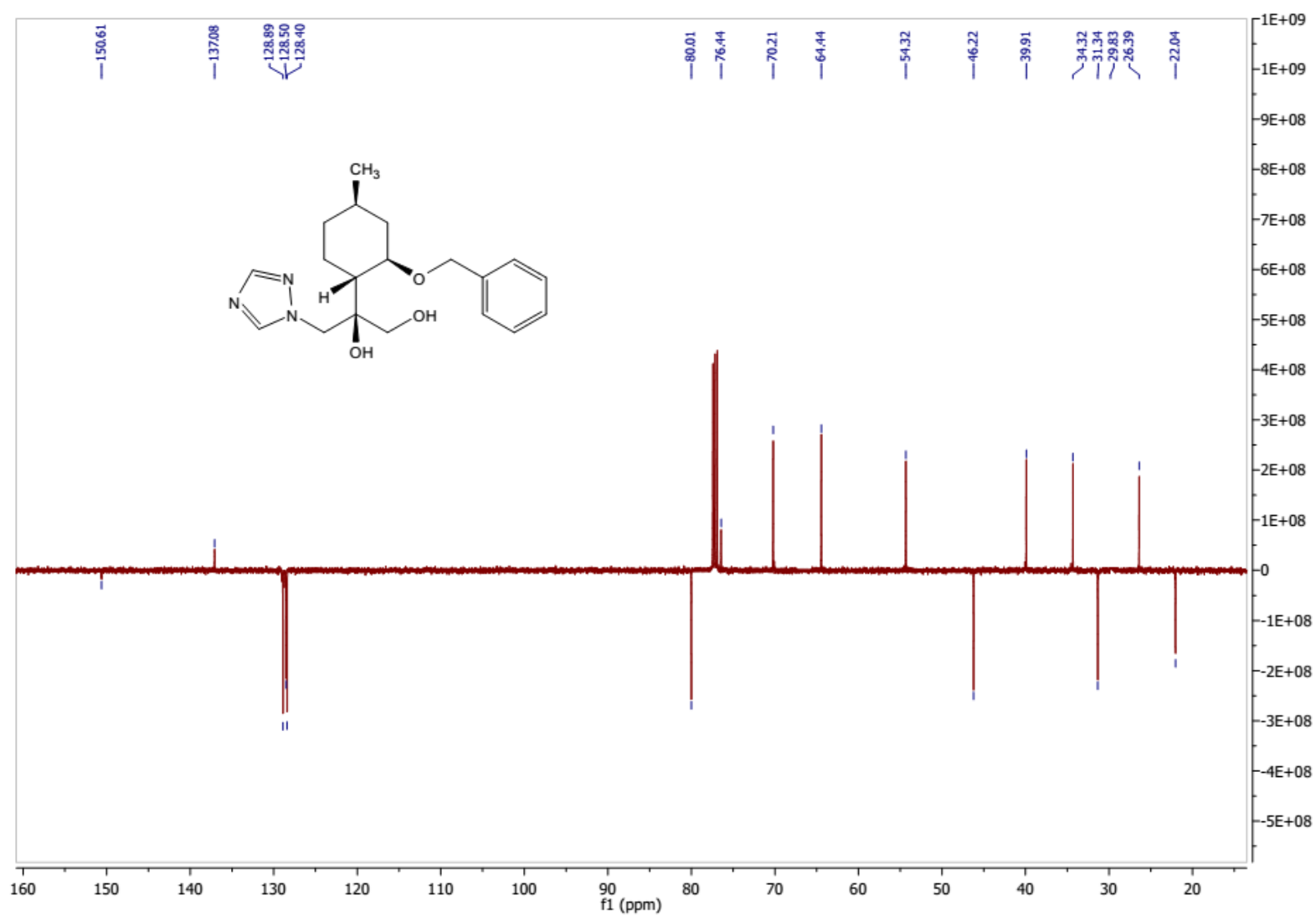




Figure S 106:  $^1\text{H}$ -NMR of compound 38a

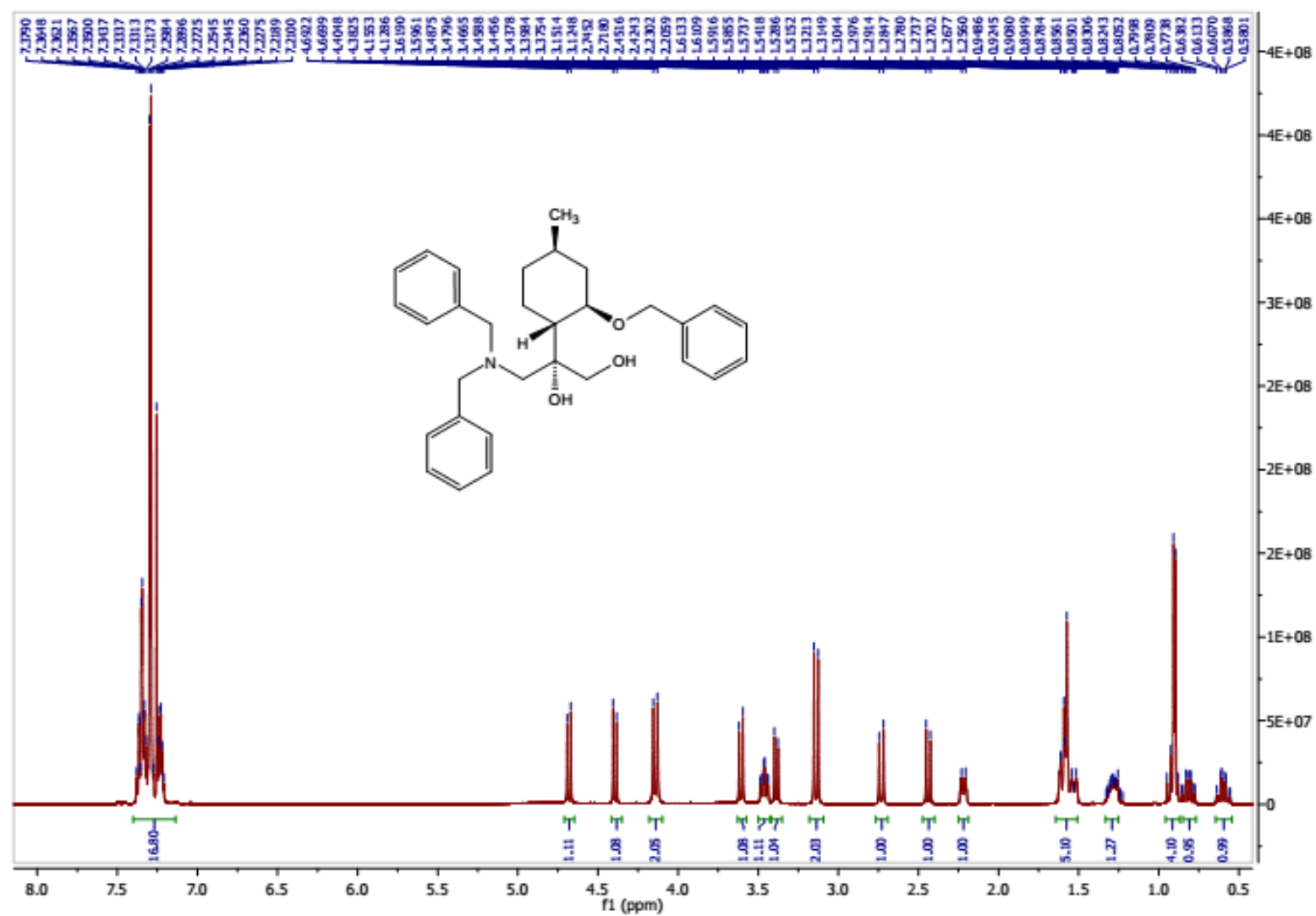


Figure S 107:  $^{13}\text{C}$ -NMR of compound **38b**

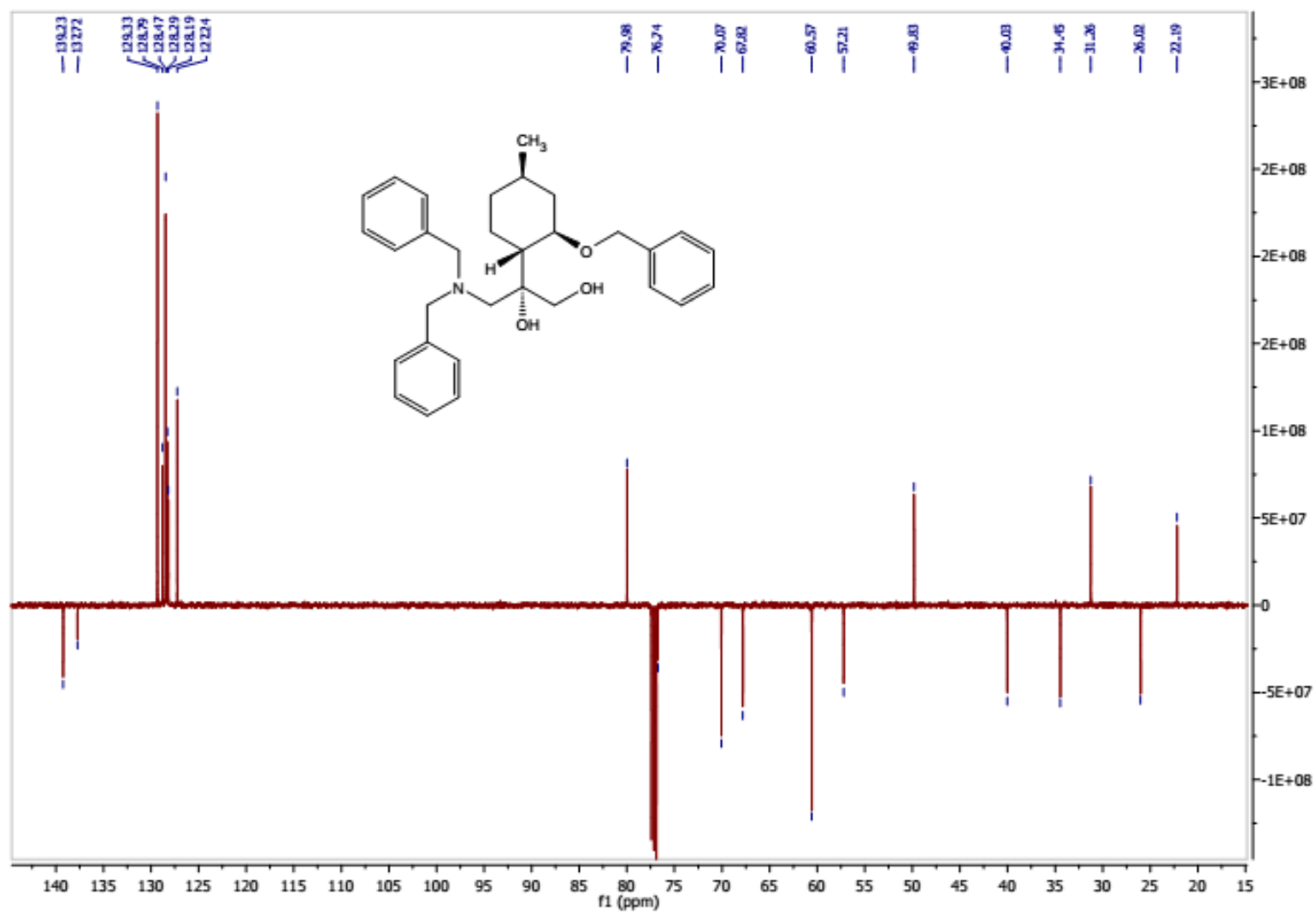


Figure S 108:  $^1\text{H}$ -NMR of compound **38b**

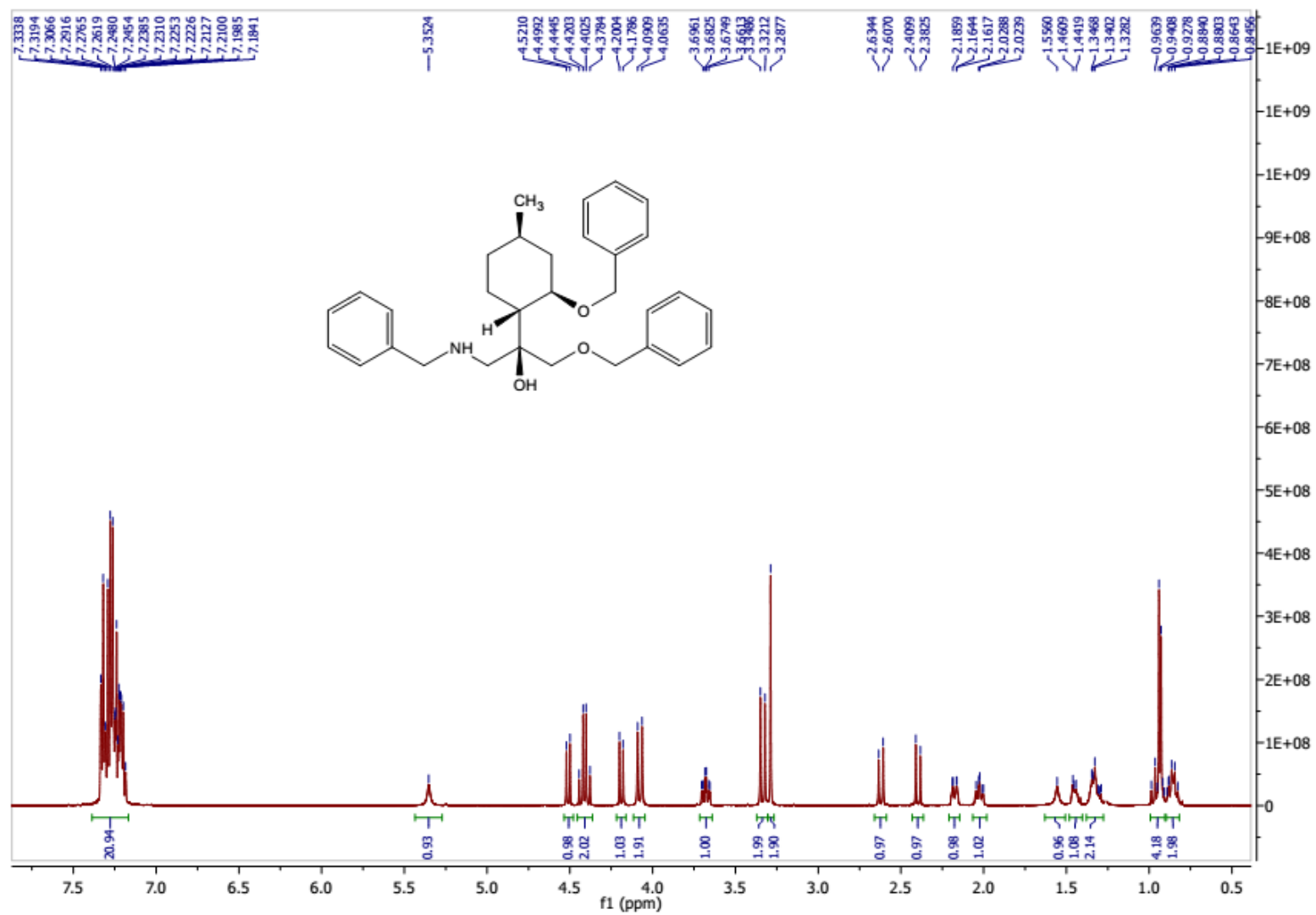


Figure S 109:  $^{13}\text{C}$ -NMR of compound **38b**

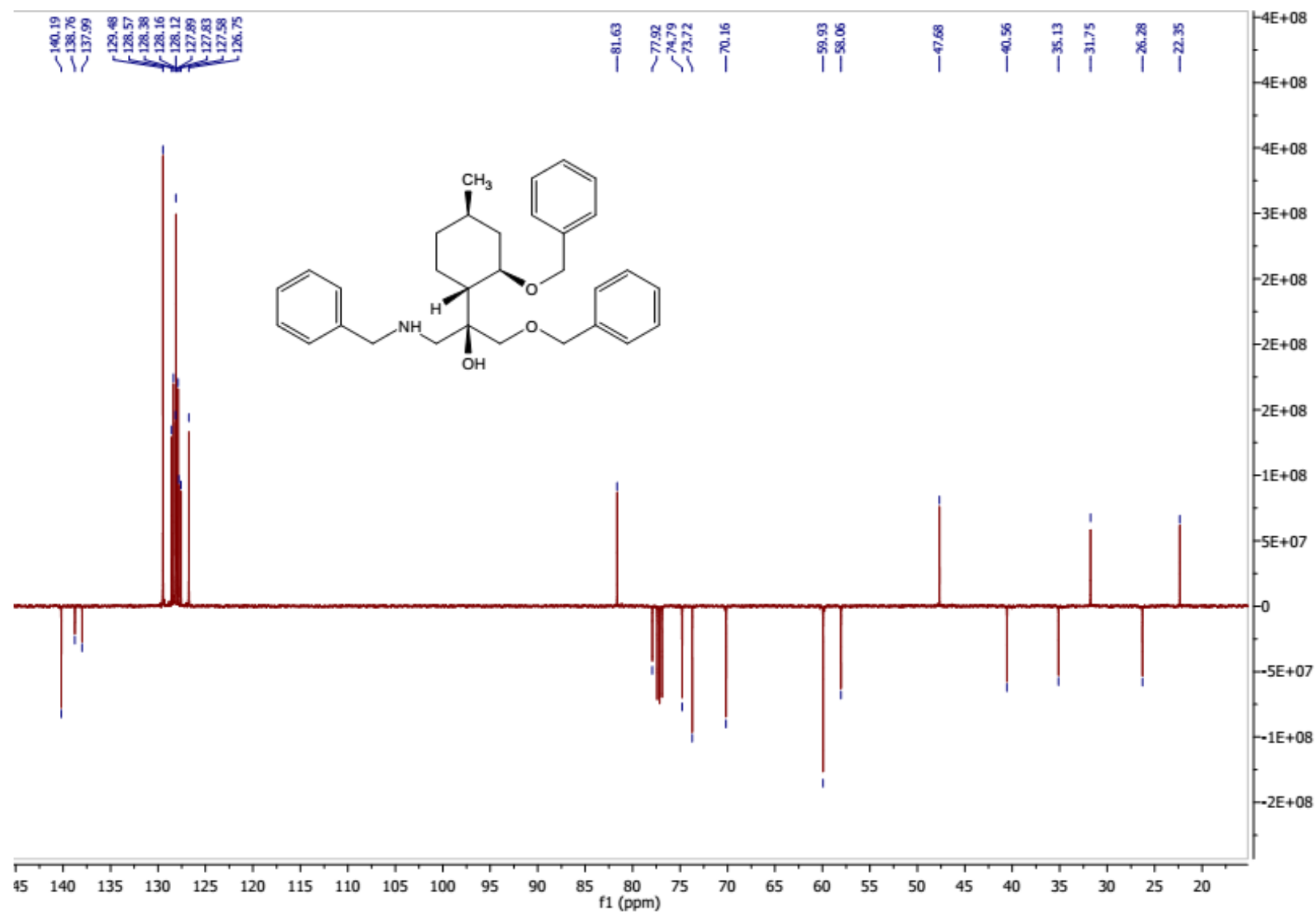
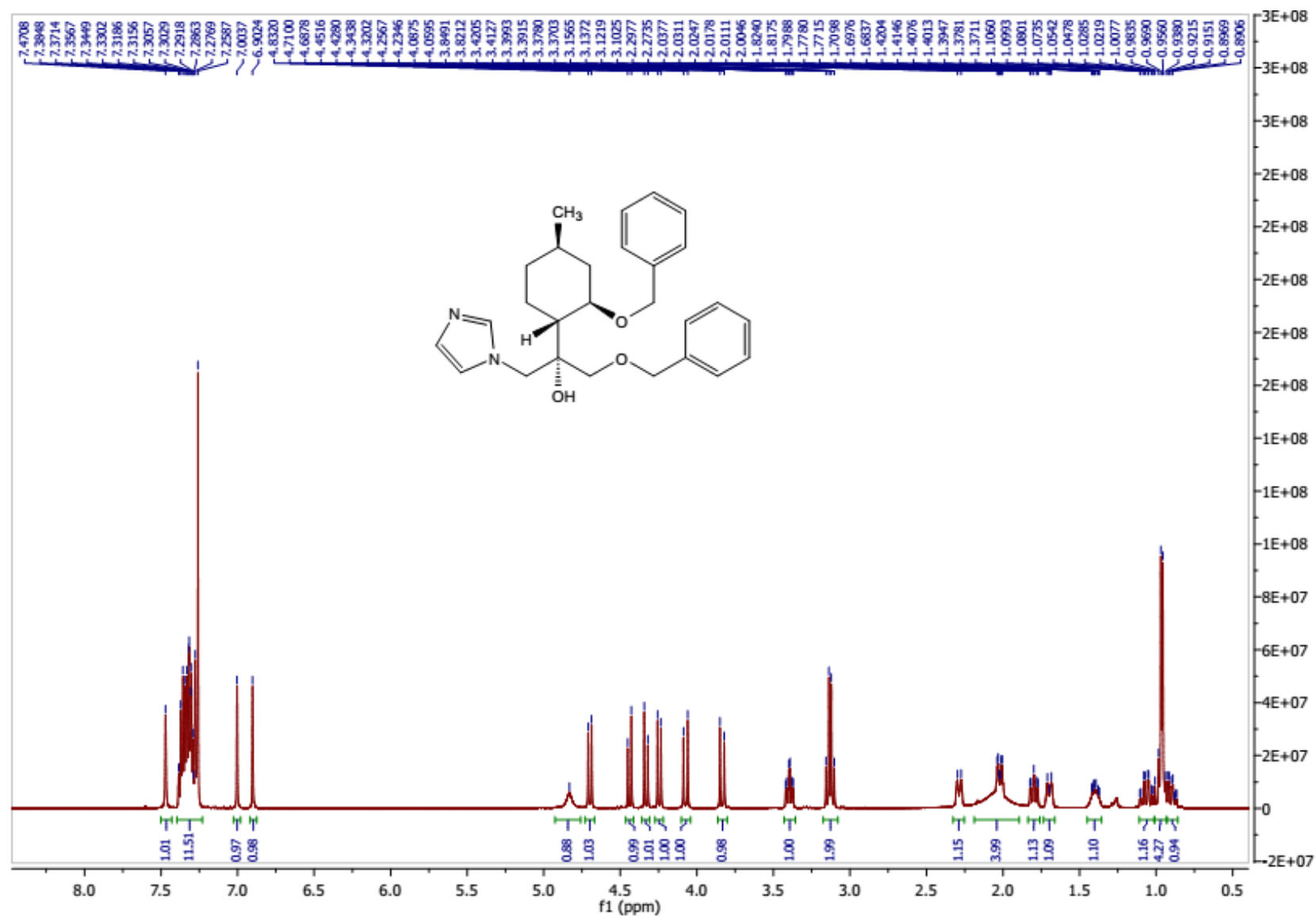


Figure S 110:  $^1\text{H}$ -NMR of compound **39a**



$^{13}\text{C}$ -NMR of compound **39a**

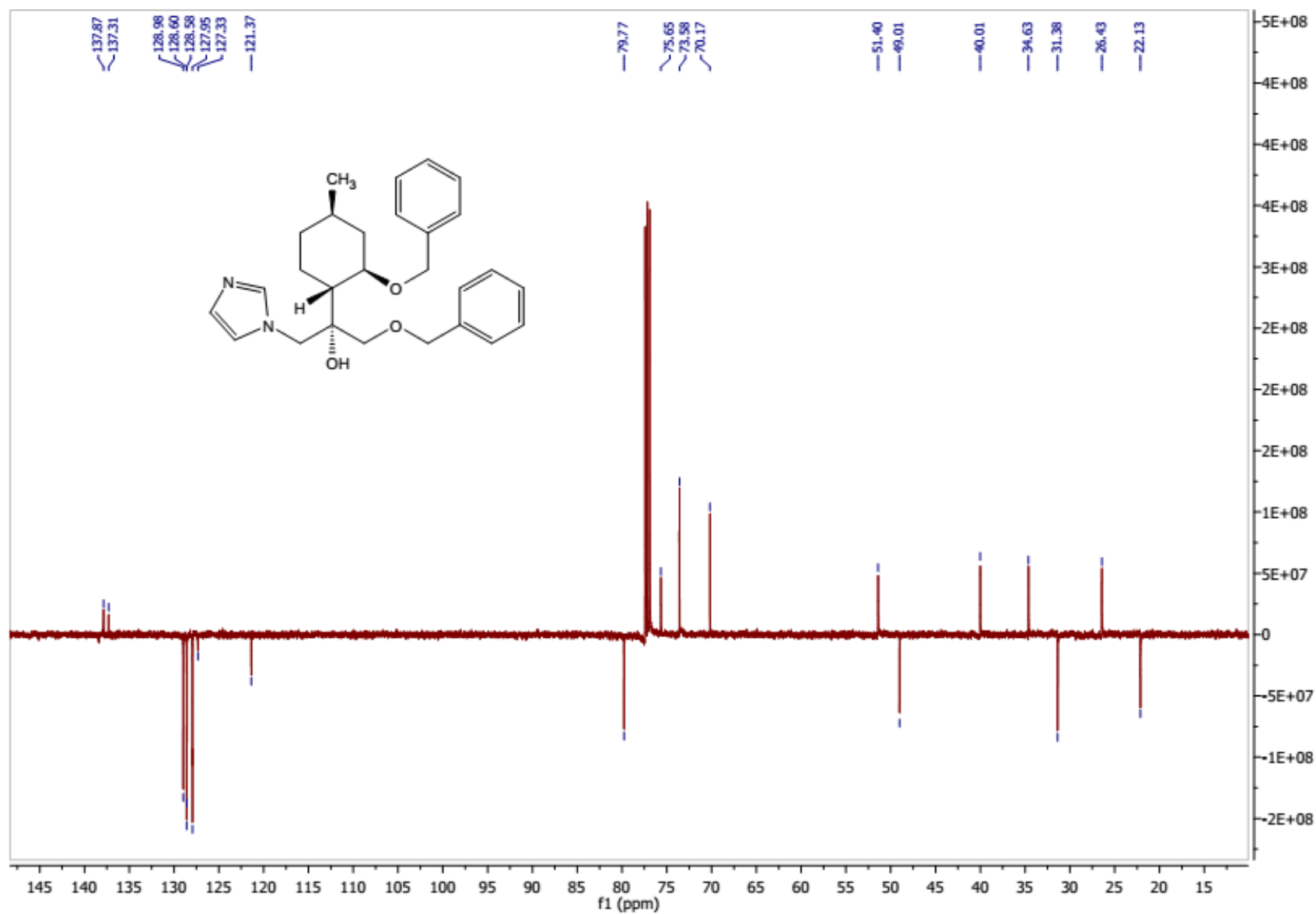


Figure S 111:  $^1\text{H}$ -NMR of compound **39b**

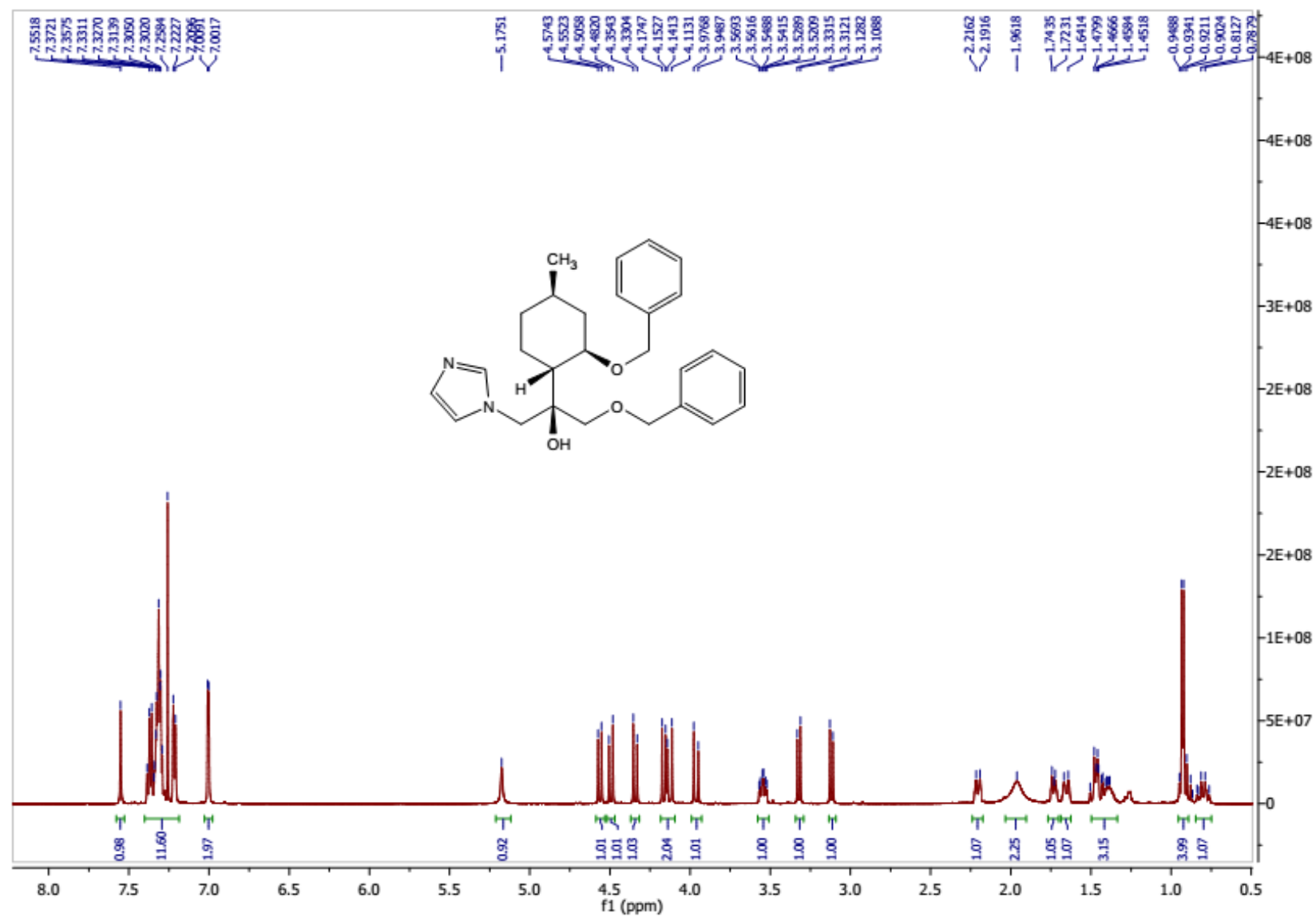


Figure S 112:  $^{13}\text{C}$ -NMR of compound **39b**

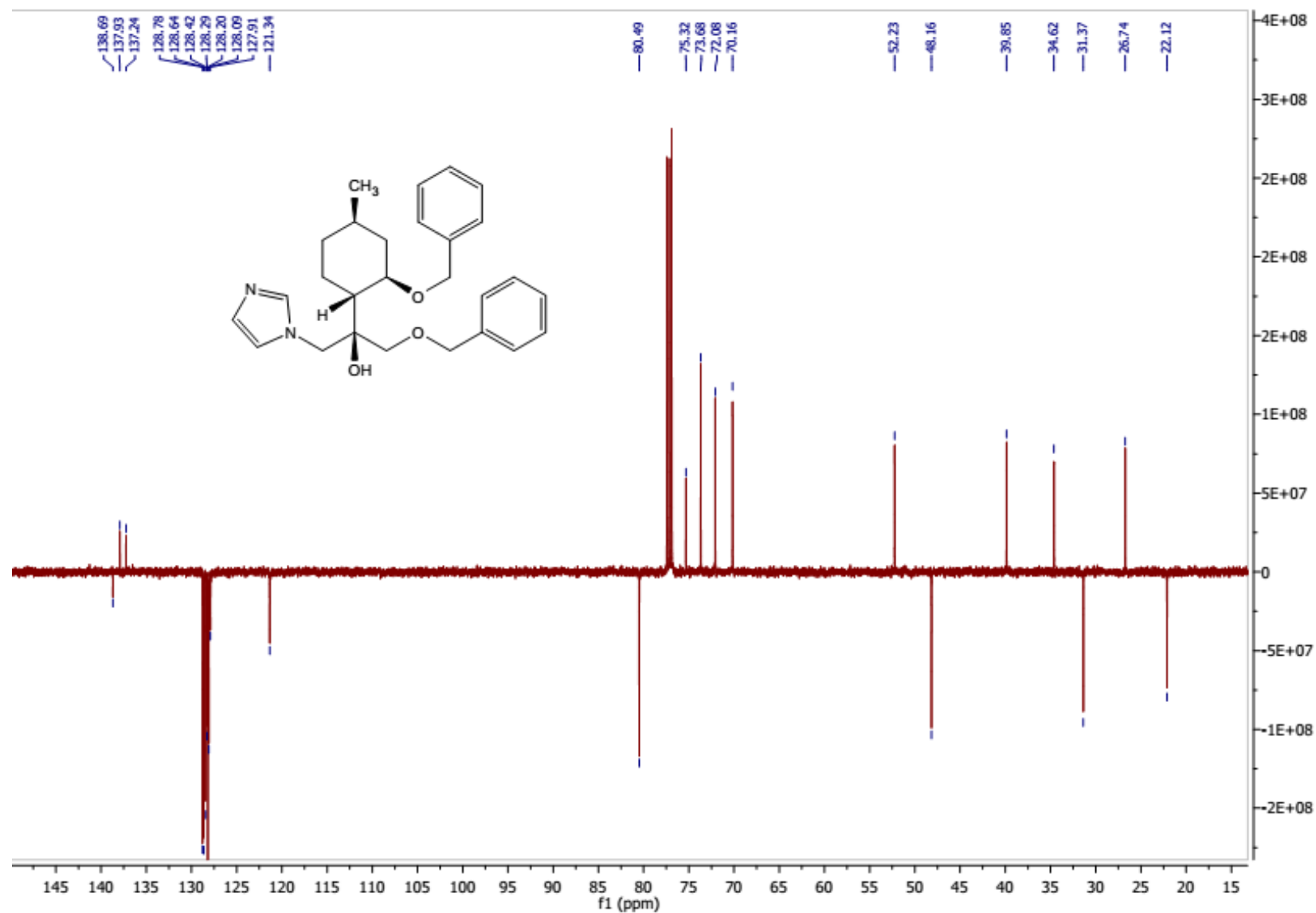




Figure S 113:  $^1\text{H}$ -NMR of compound 40a

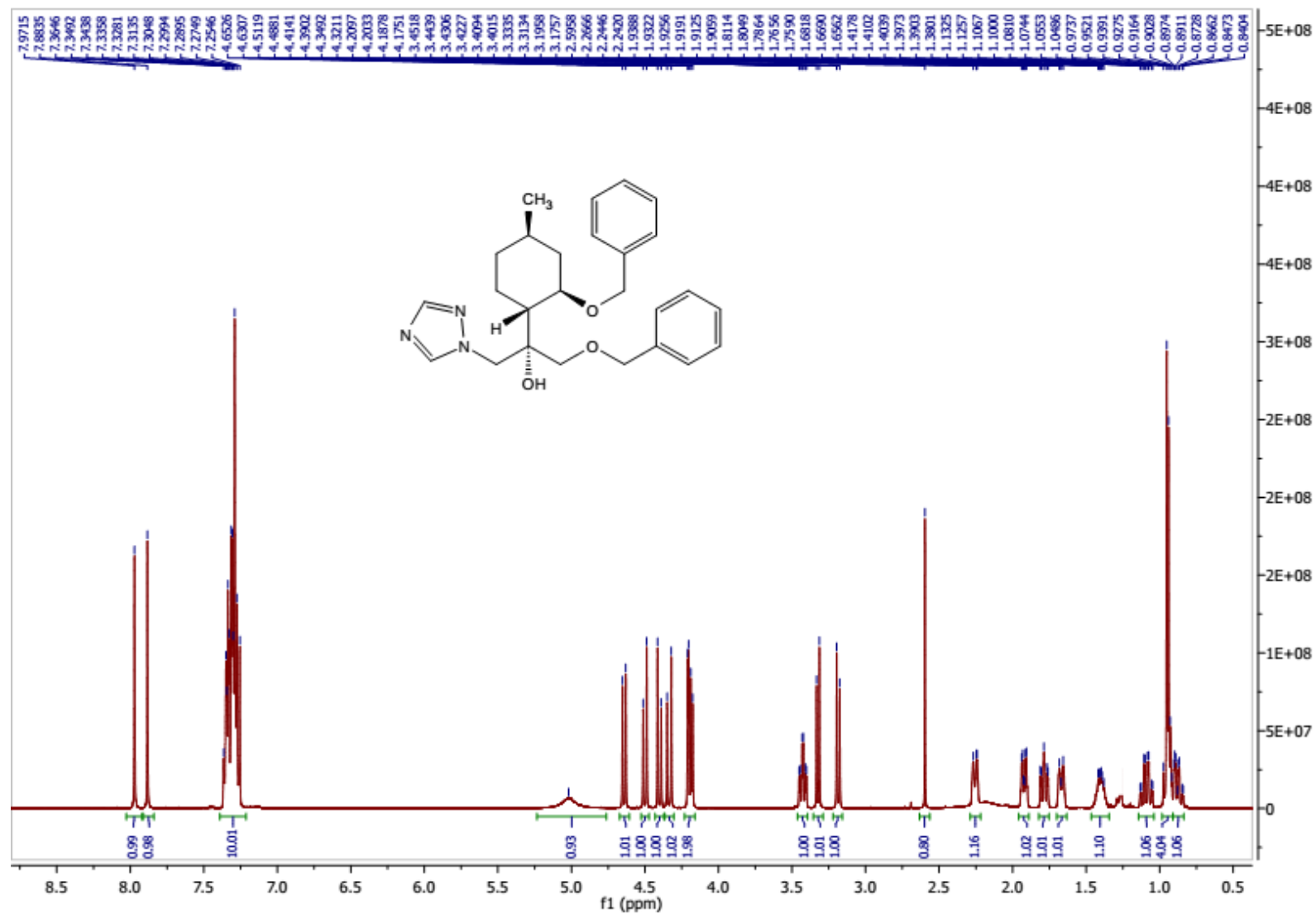


Figure S 114:  $^{13}\text{C}$ -NMR of compound **40a**

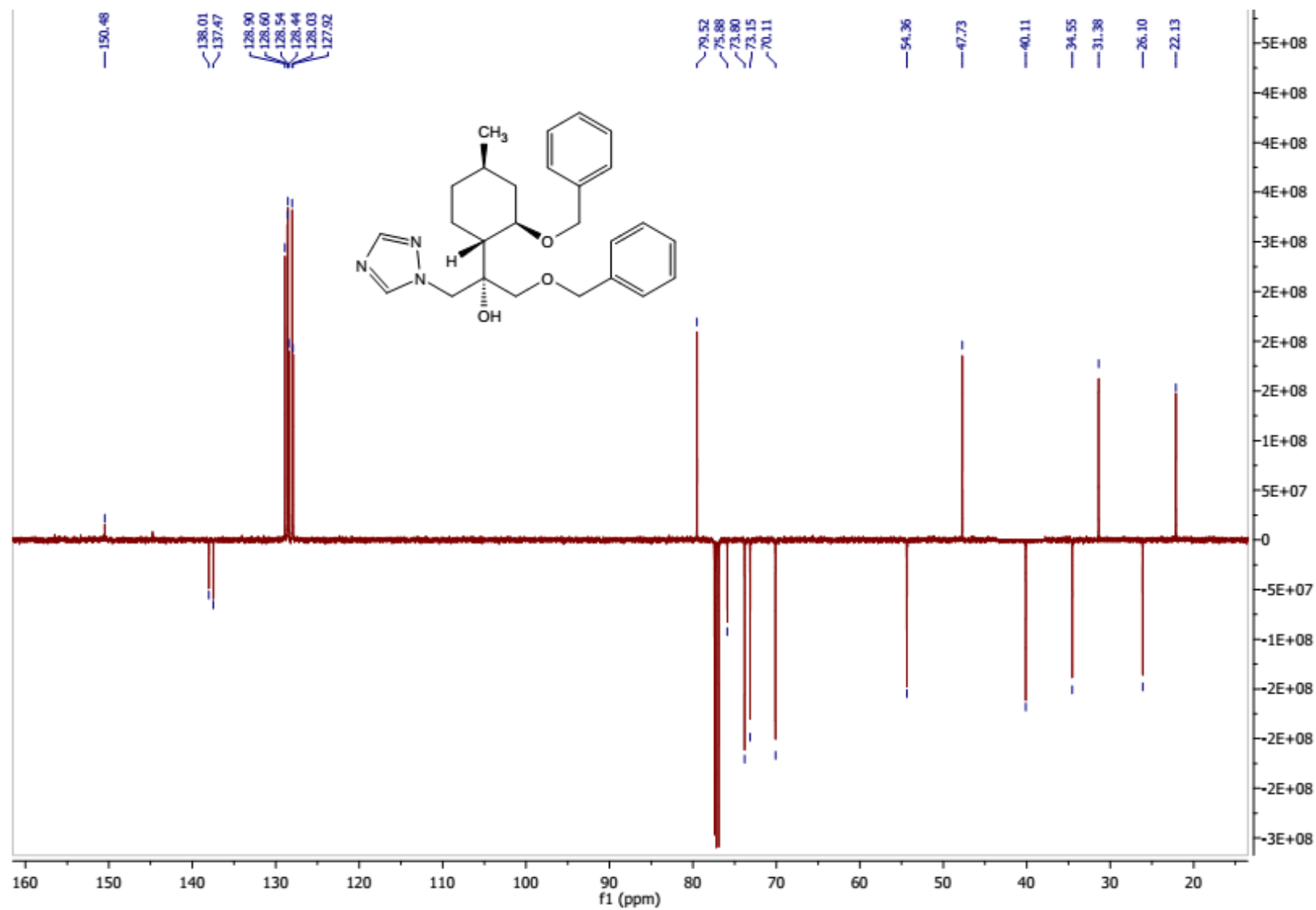


Figure S 115:  $^1\text{H}$ -NMR of compound **40b**

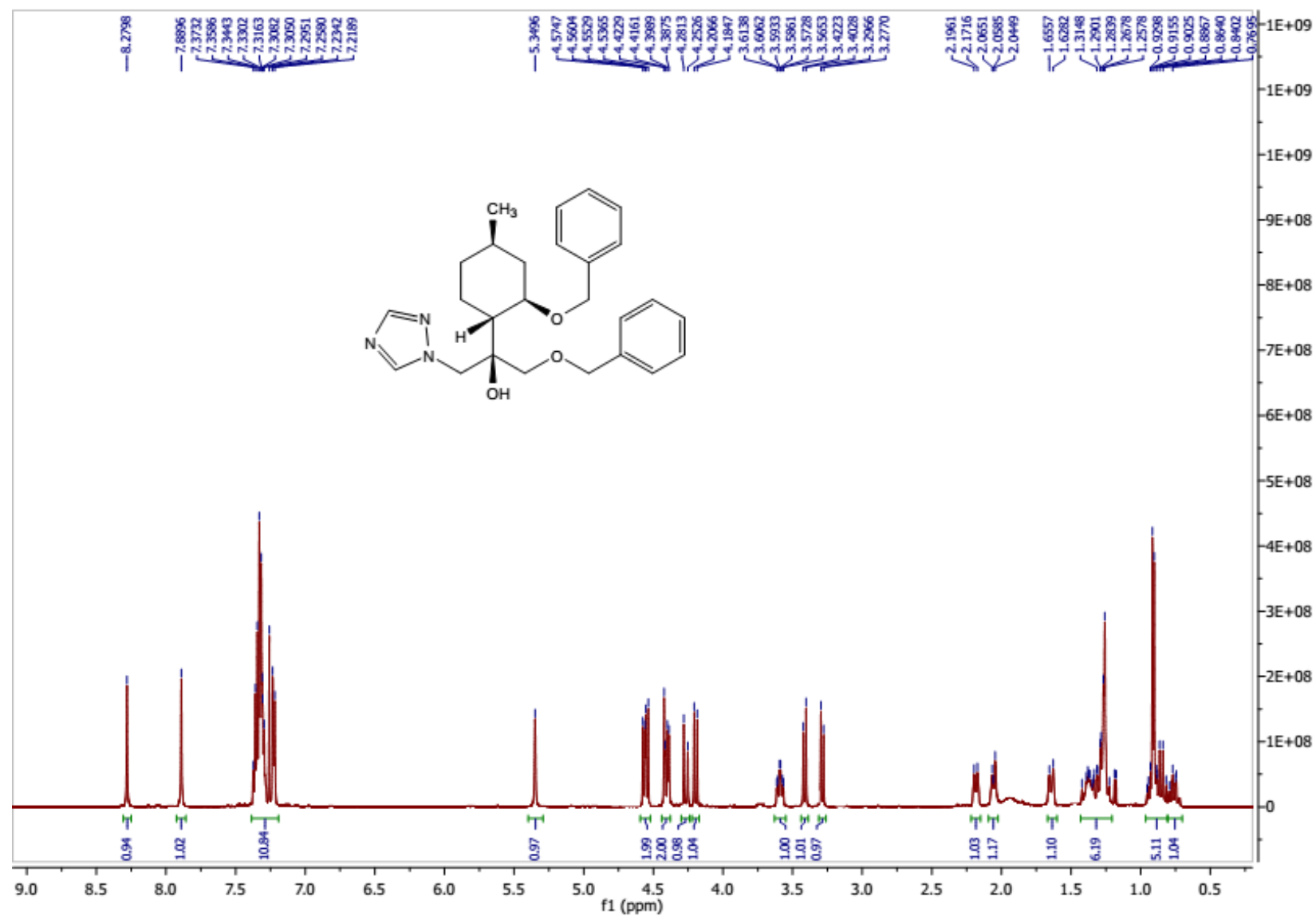


Figure S 116:  $^{13}\text{C}$ -NMR of compound **40b**

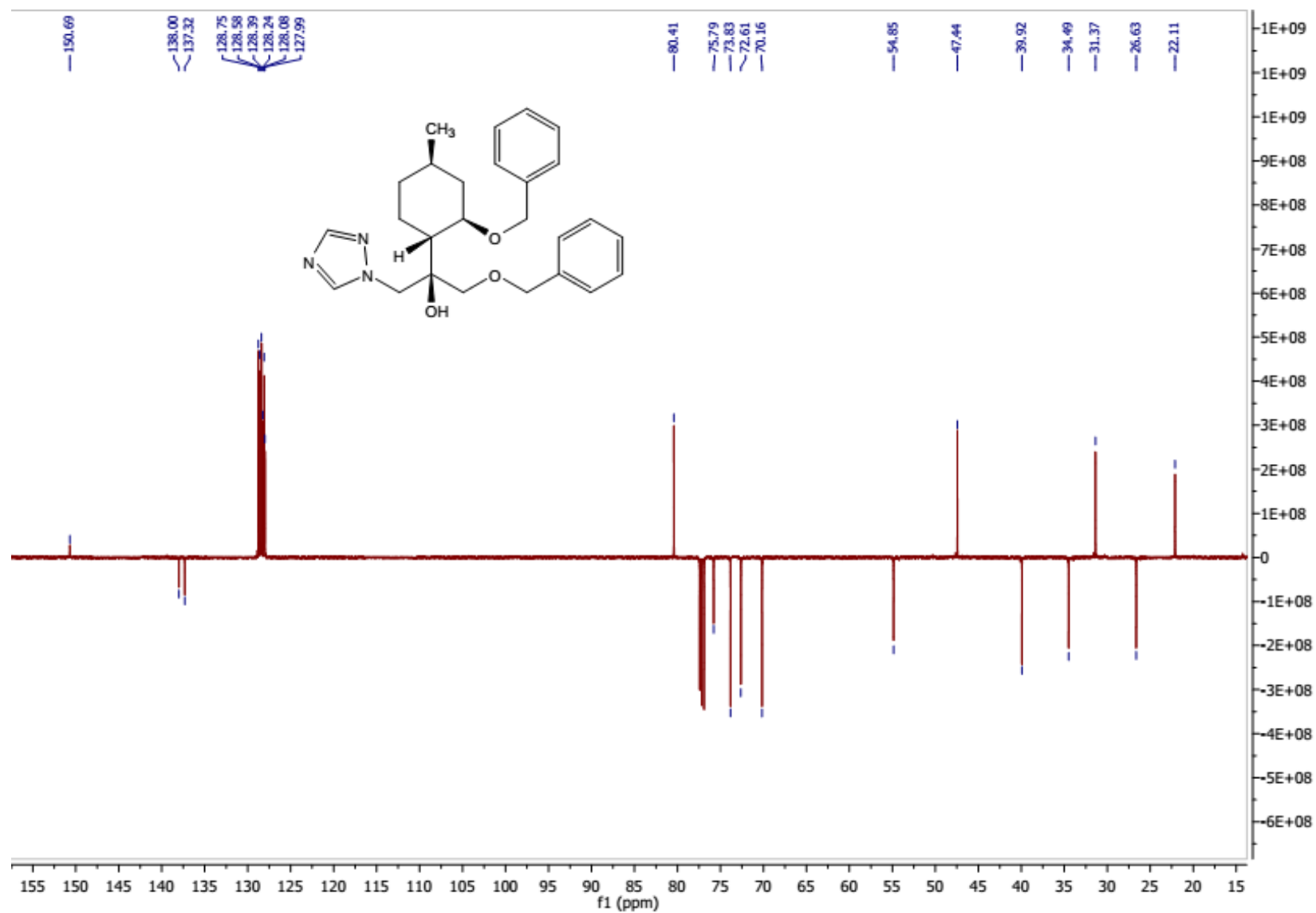


Figure S 117:  $^1\text{H}$ -NMR of compound **41a**

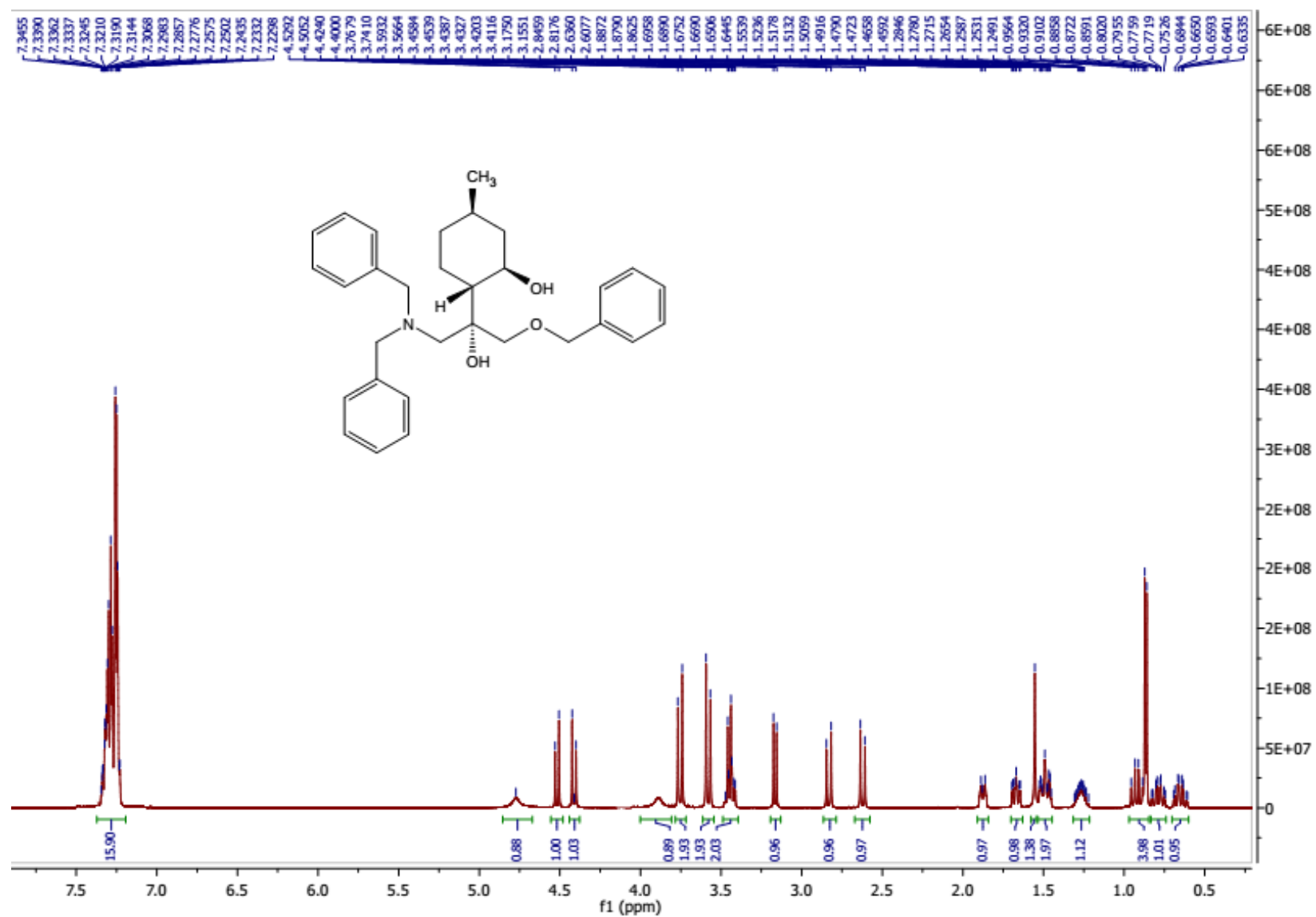


Figure S 118:  $^{13}\text{C}$ -NMR of compound **41a**

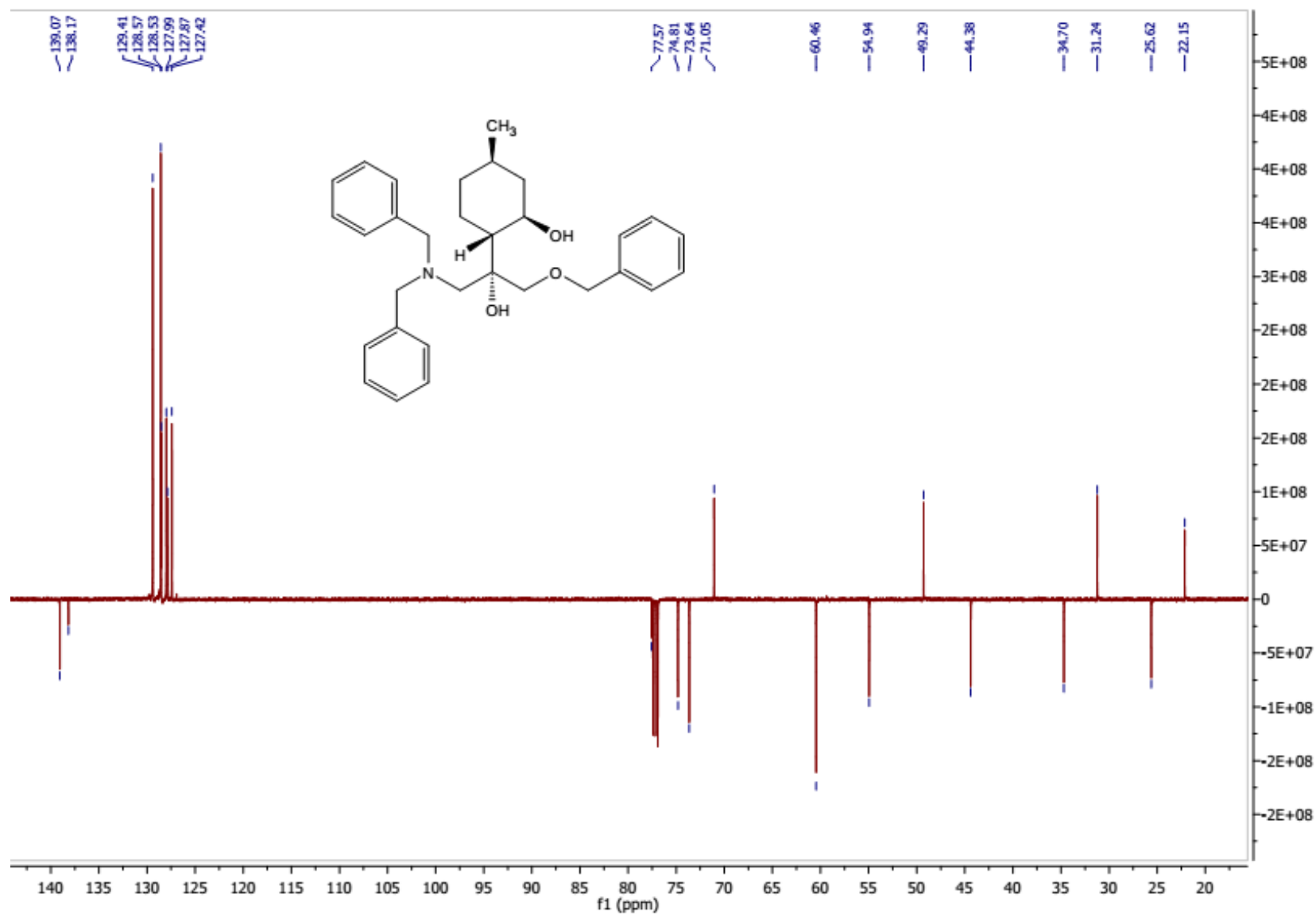


Figure S 119:  $^1\text{H}$ -NMR of compound **41b**

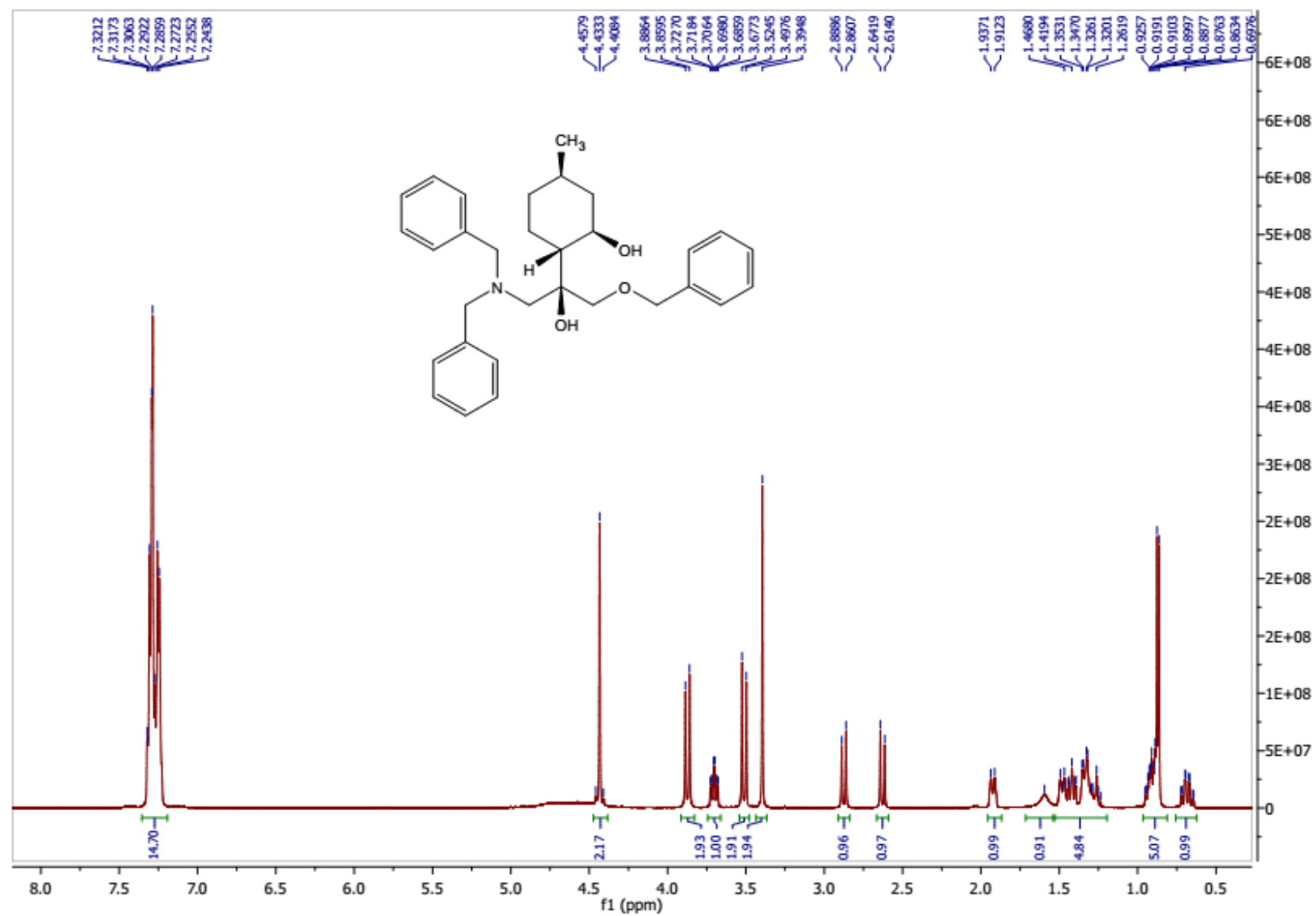


Figure S 120:  $^{13}\text{C}$ -NMR of compound **41b**

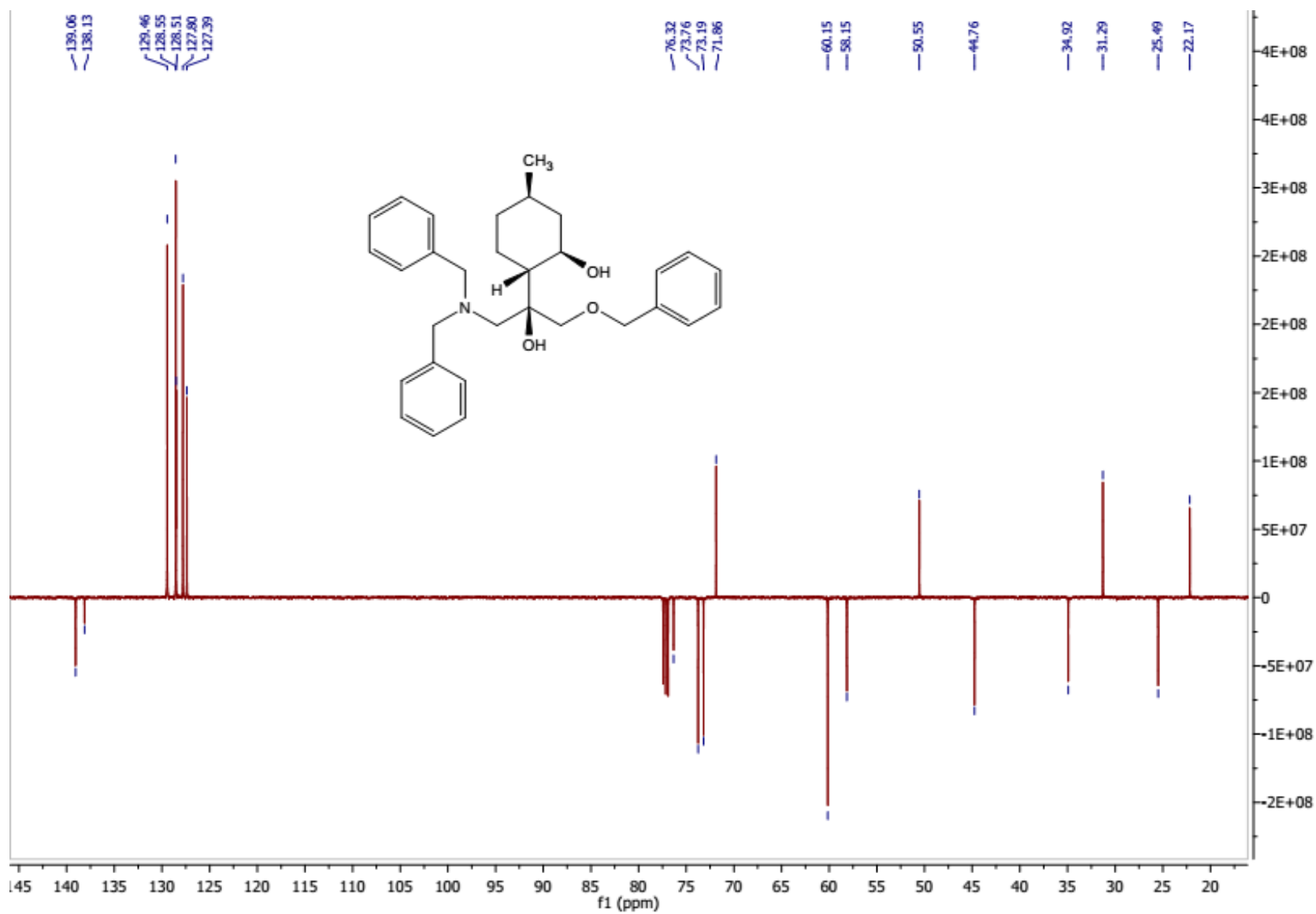




Figure S 121:  $^1\text{H}$ -NMR of compound **42a**

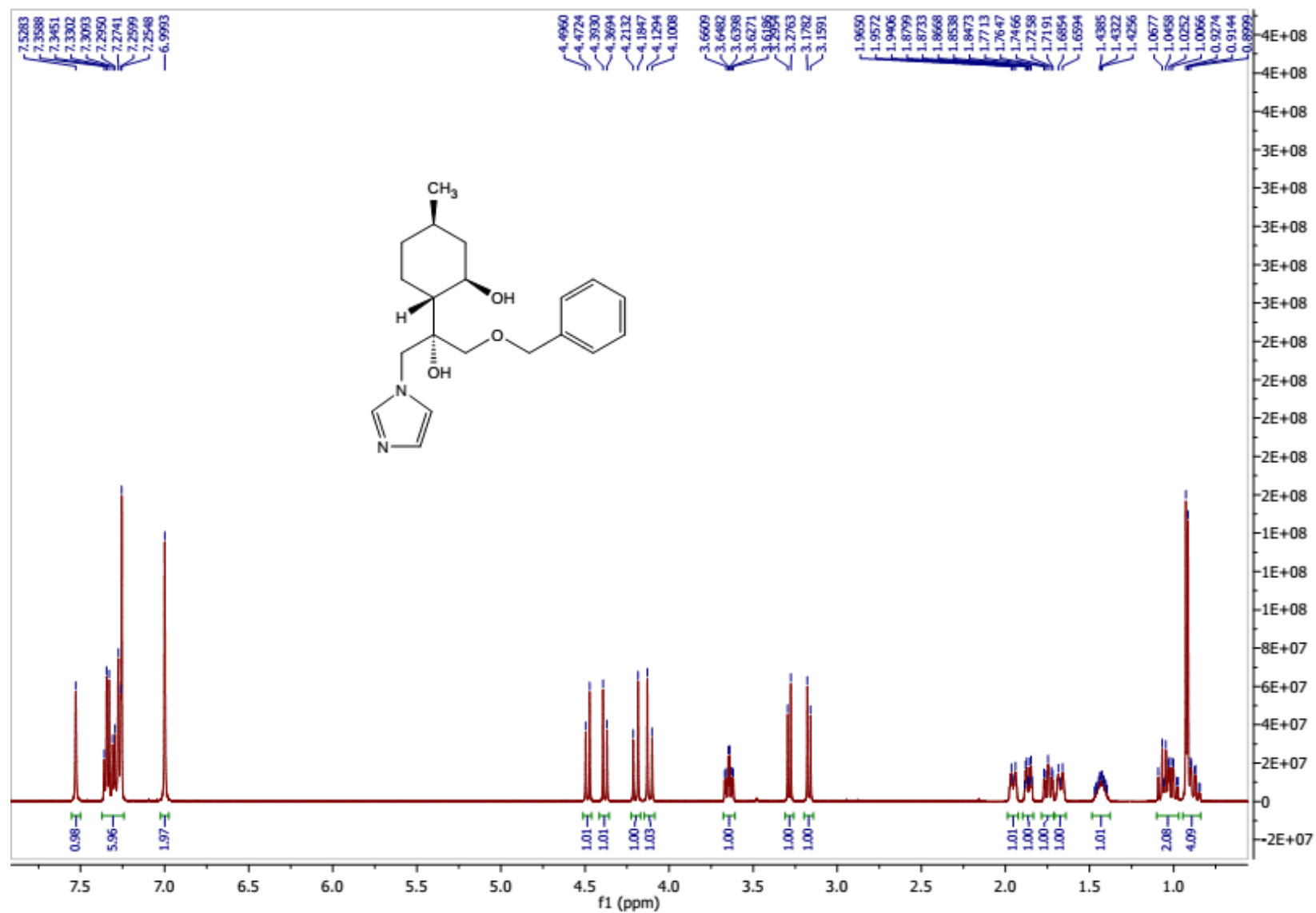


Figure S 122:  $^{13}\text{C}$ -NMR of compound **42a**

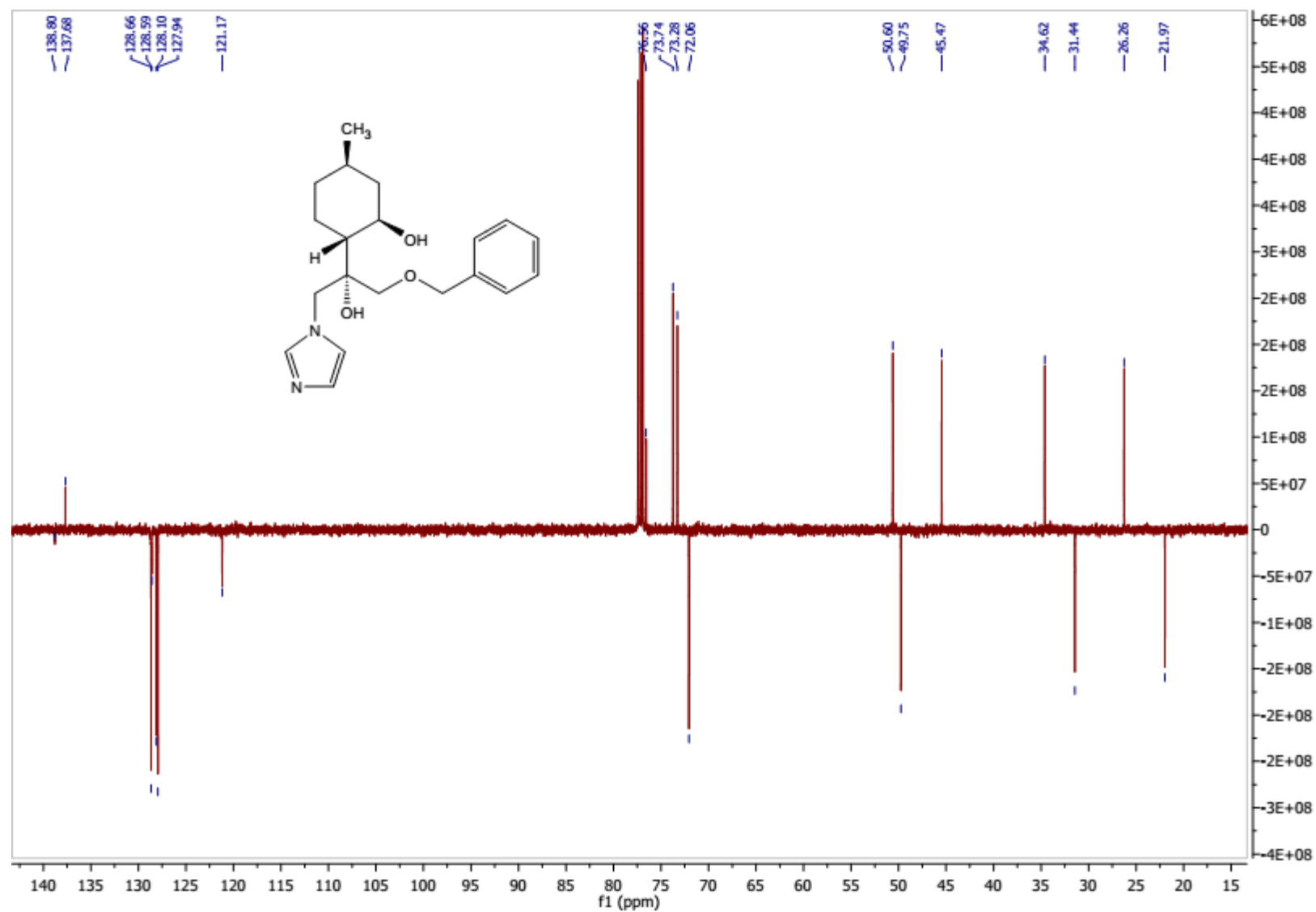


Figure S 123:  $^1\text{H}$ -NMR of compound **42b**

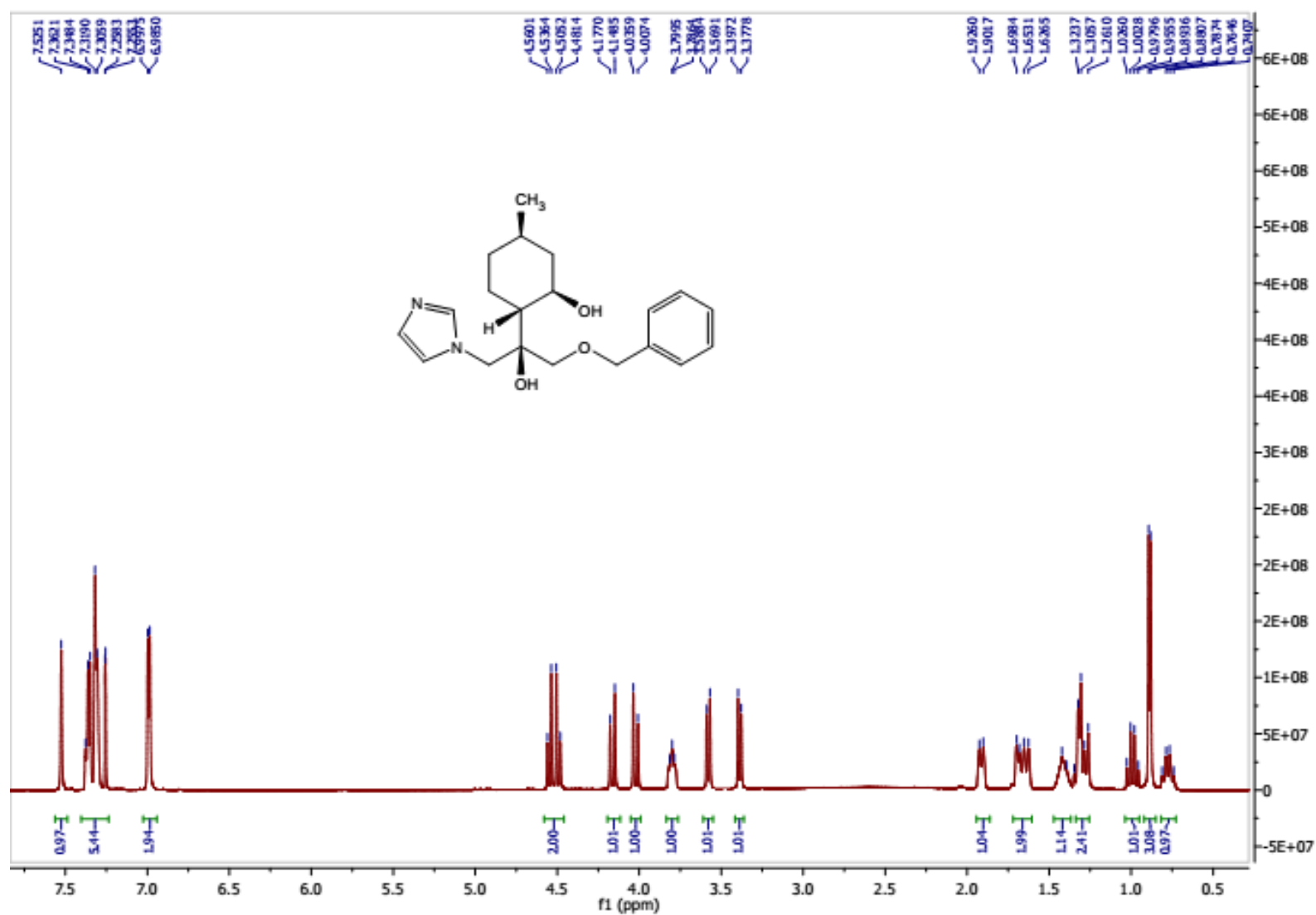


Figure S 124:  $^{13}\text{C}$ -NMR of compound **42b**

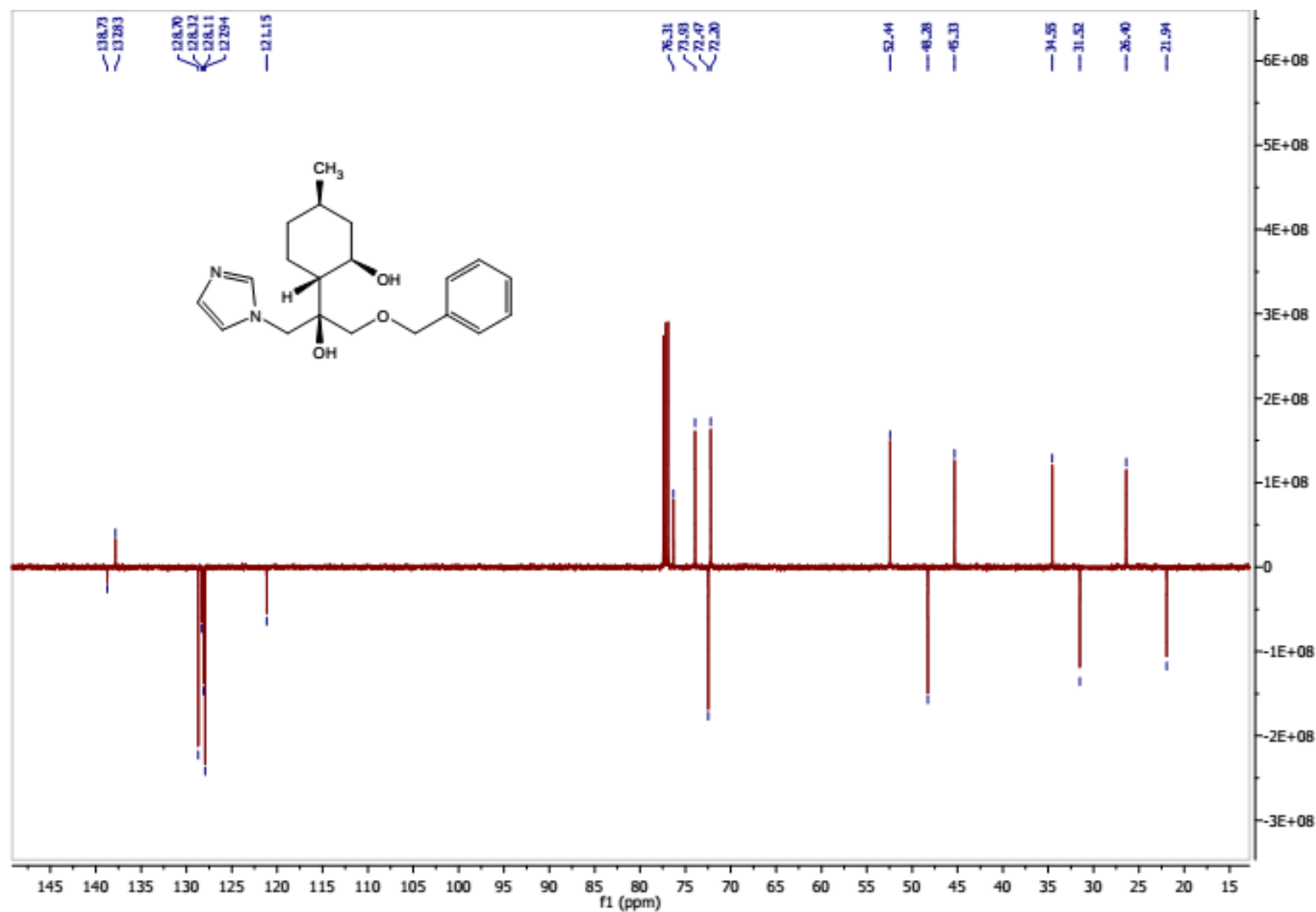


Figure S 125:  $^1\text{H}$ -NMR of compound **43a**

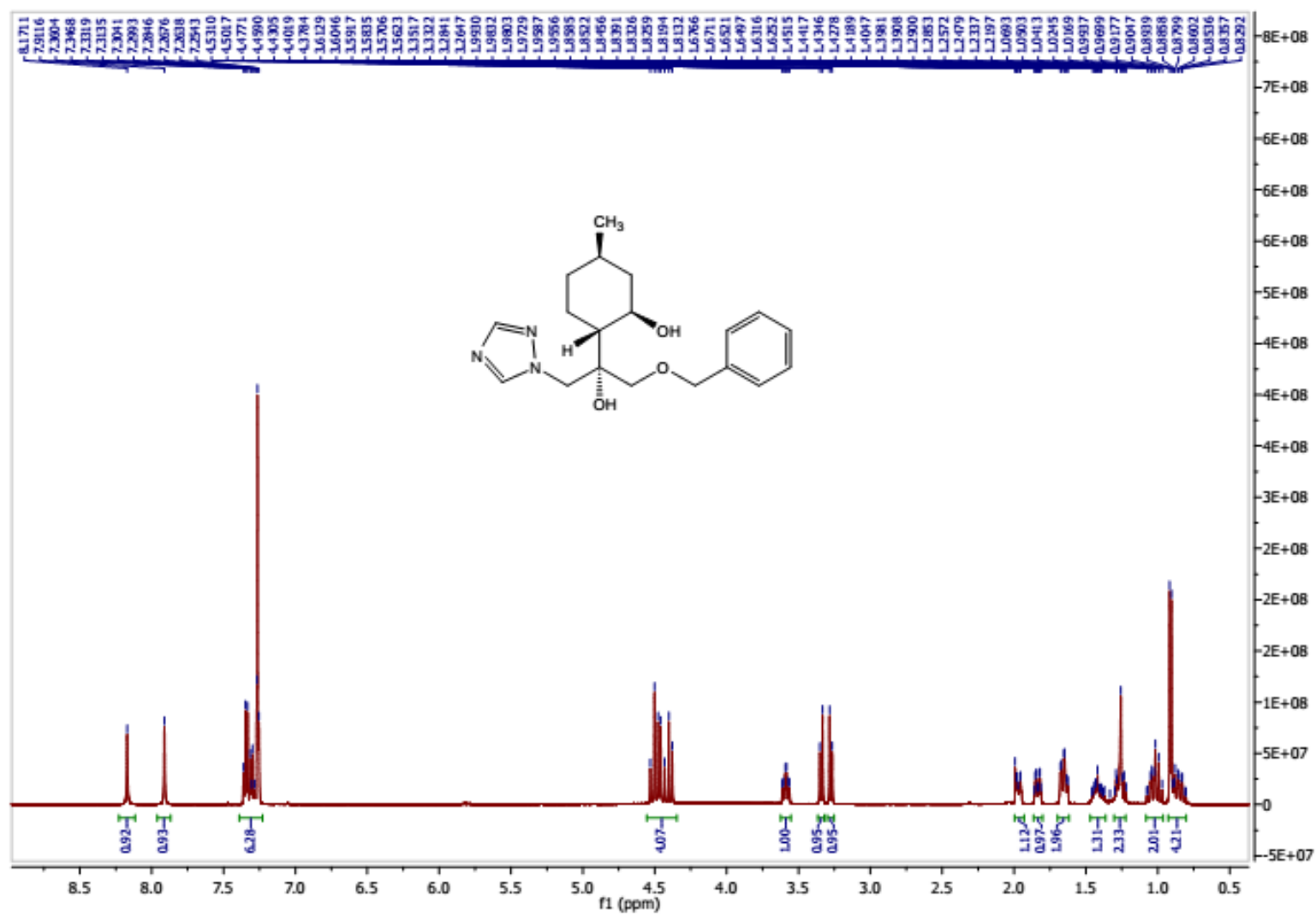


Figure S 126:  $^{13}\text{C}$ -NMR of compound **43a**

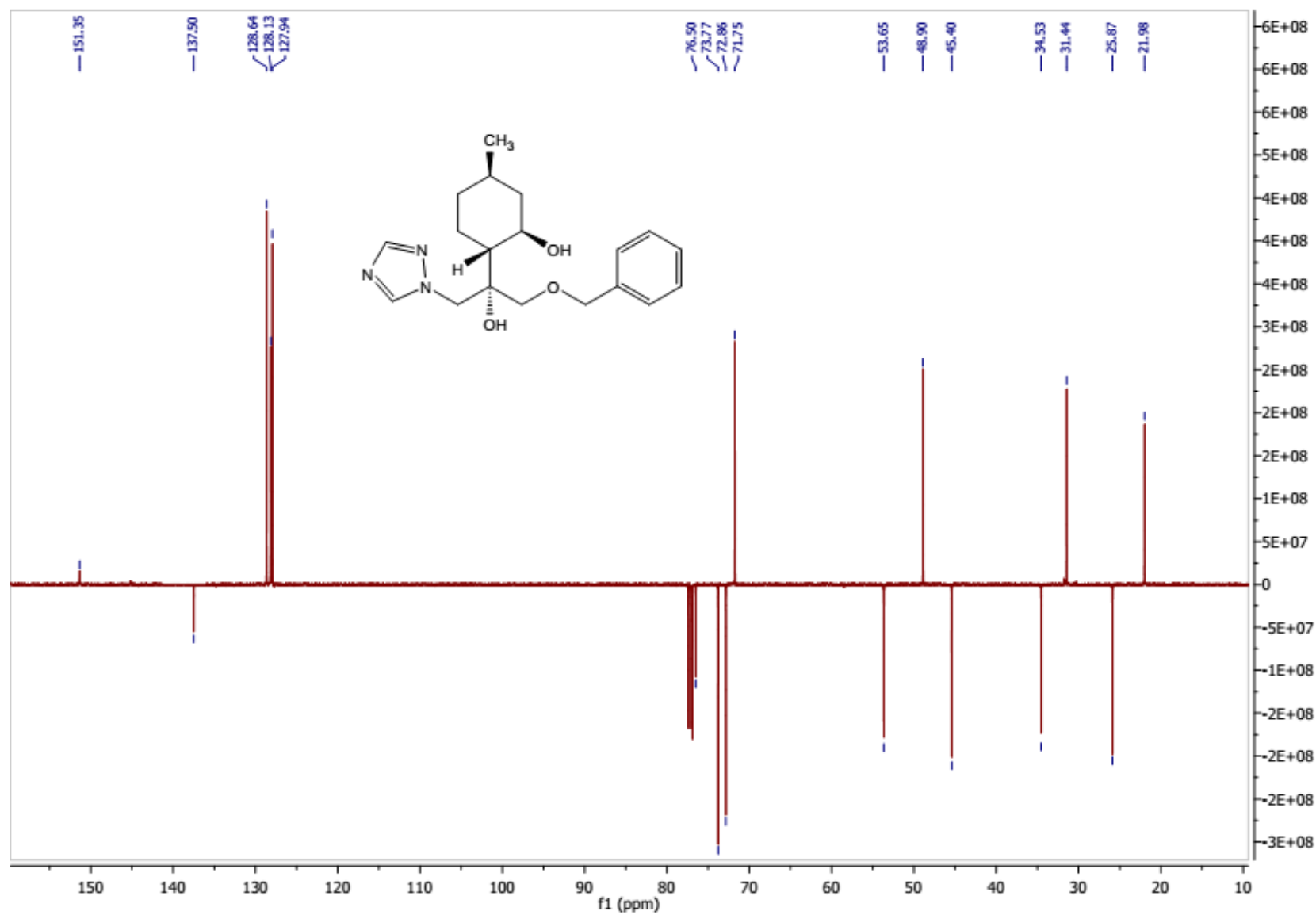
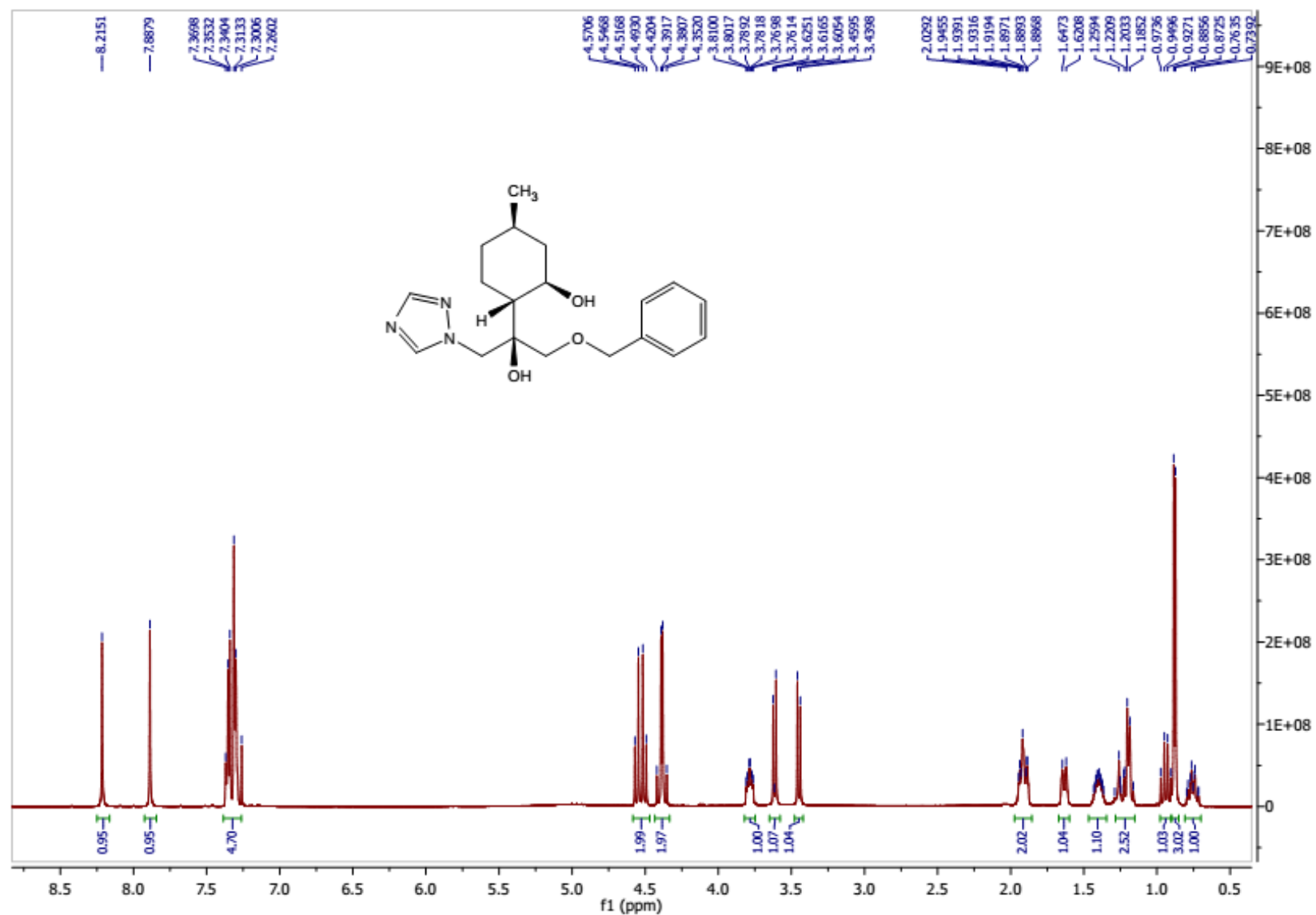


Figure S 127:  $^1\text{H}$ -NMR of compound **43b**



$^{13}\text{C}$ -NMR of compound **43b**

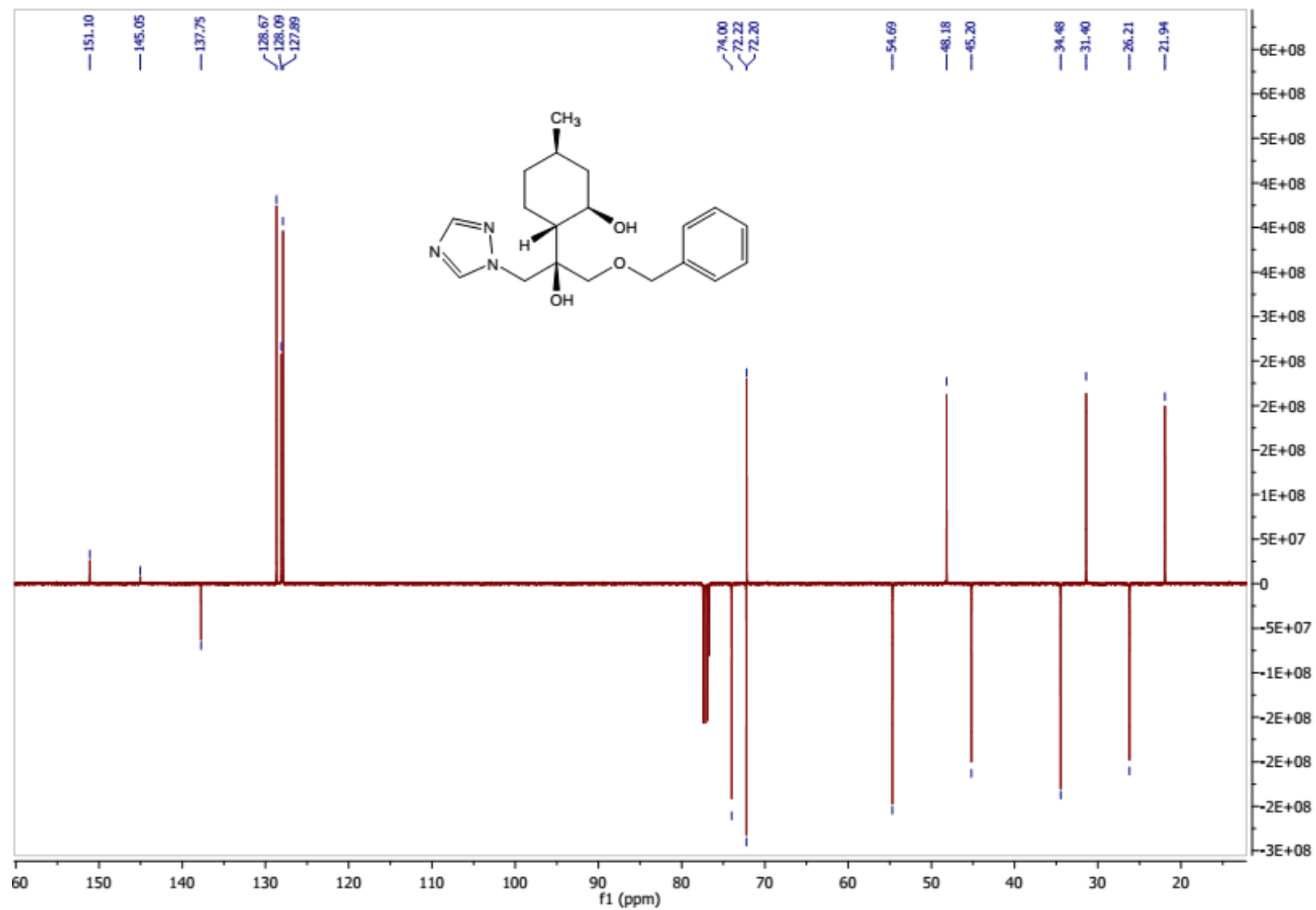




Figure S 128:  $^1\text{H}$ -NMR of compound **44**

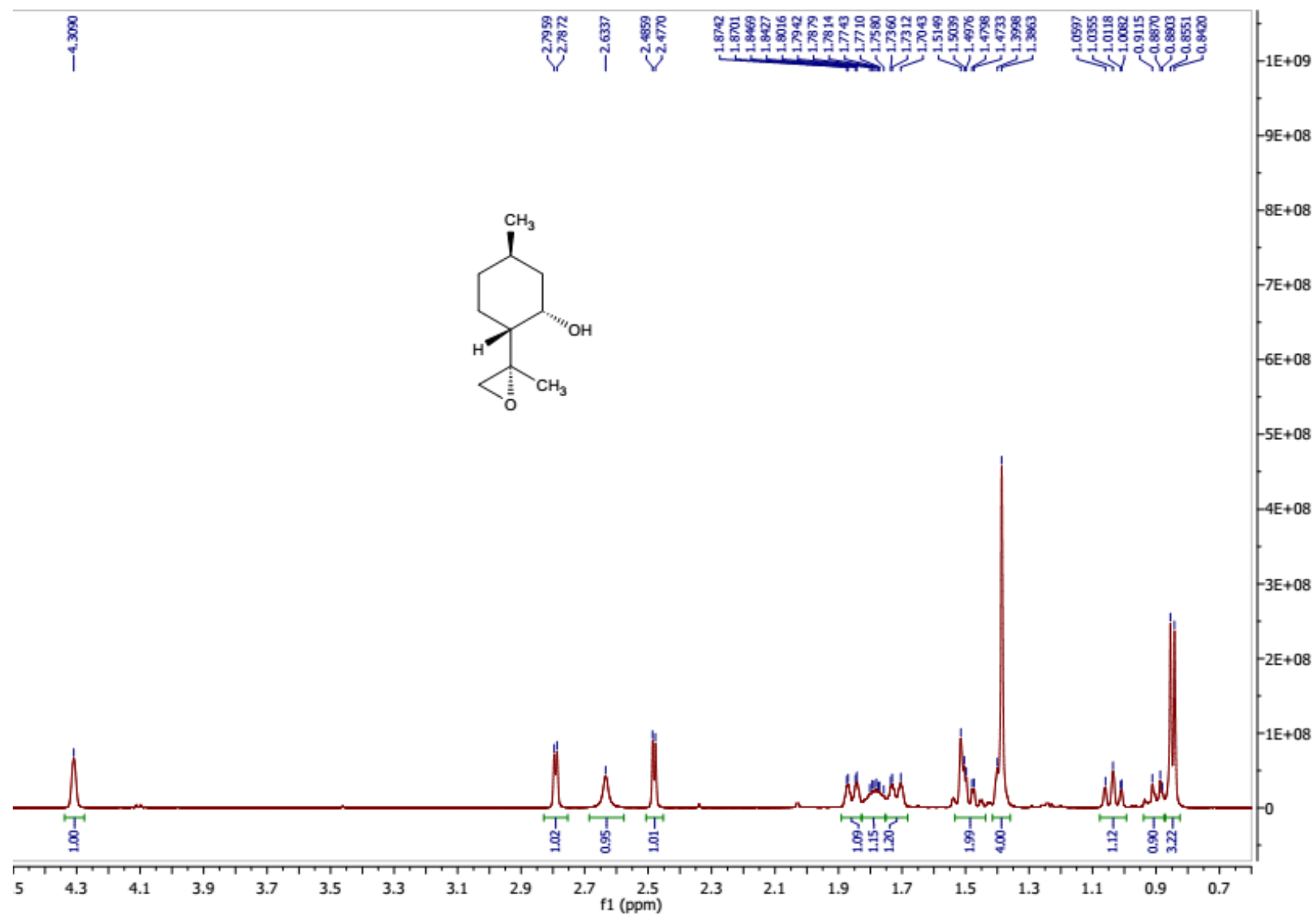


Figure S 129:  $^{13}\text{C}$ -NMR of compound **44**

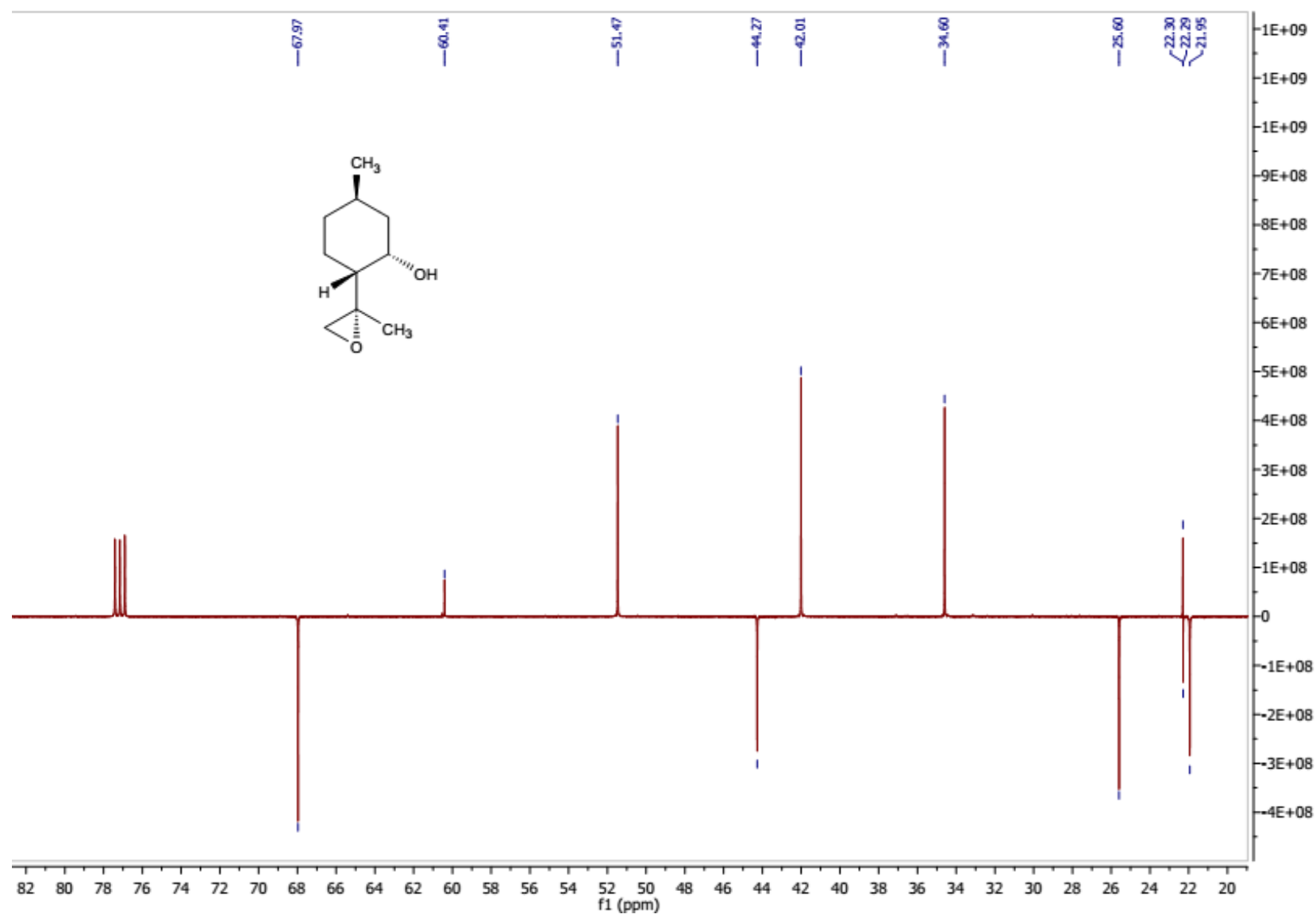


Figure S 130:  $^1\text{H}$ -NMR of compound **45**

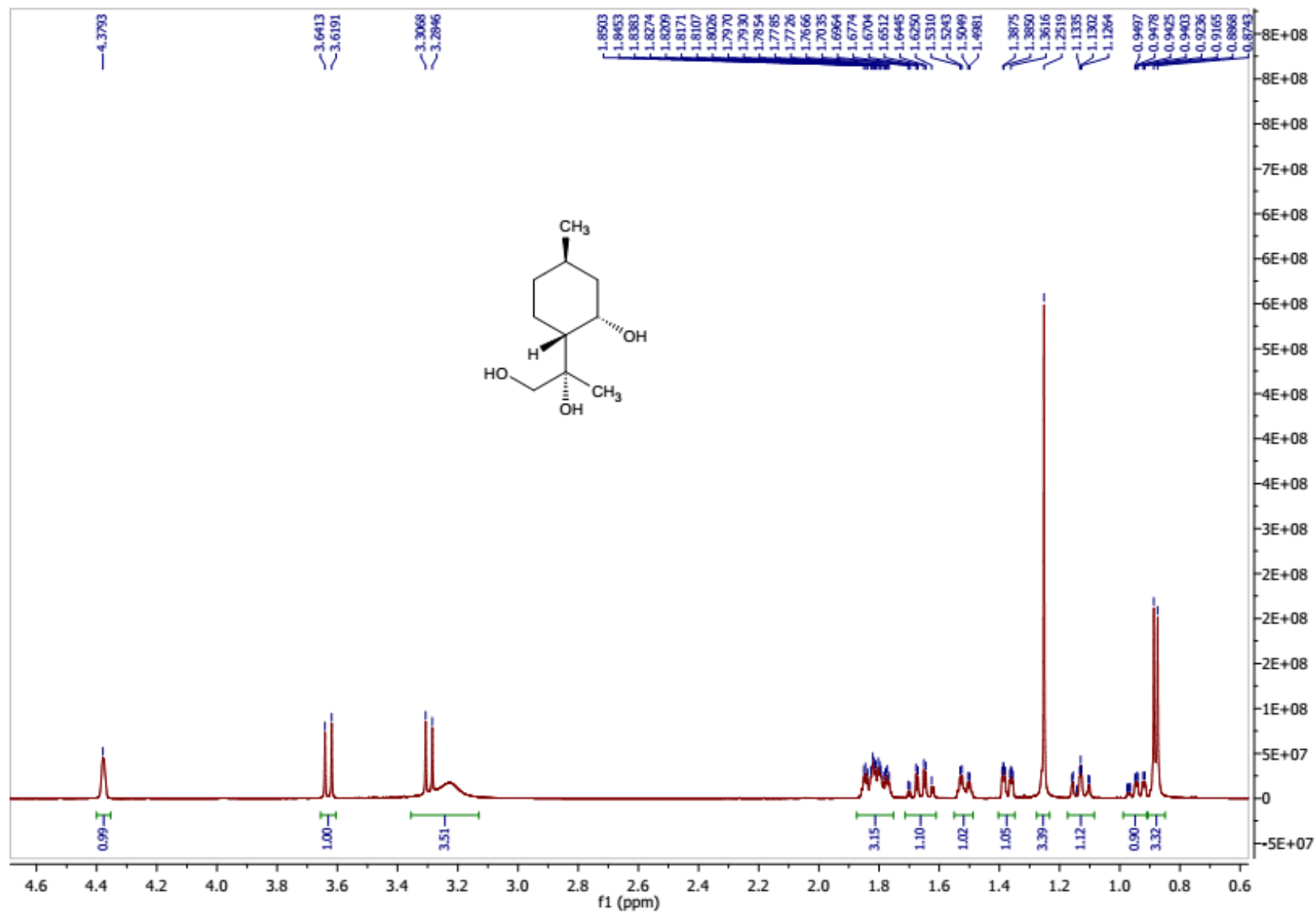
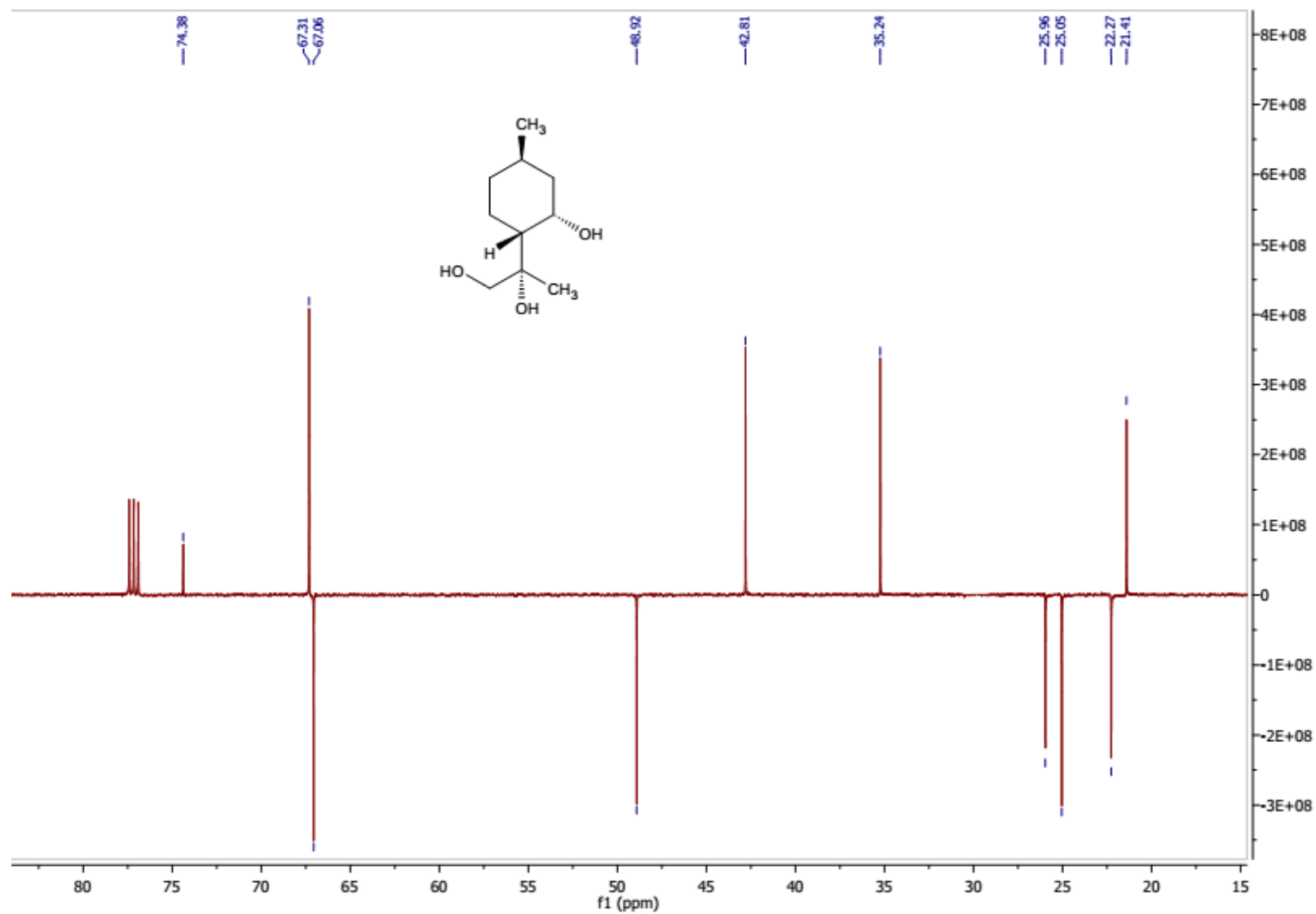
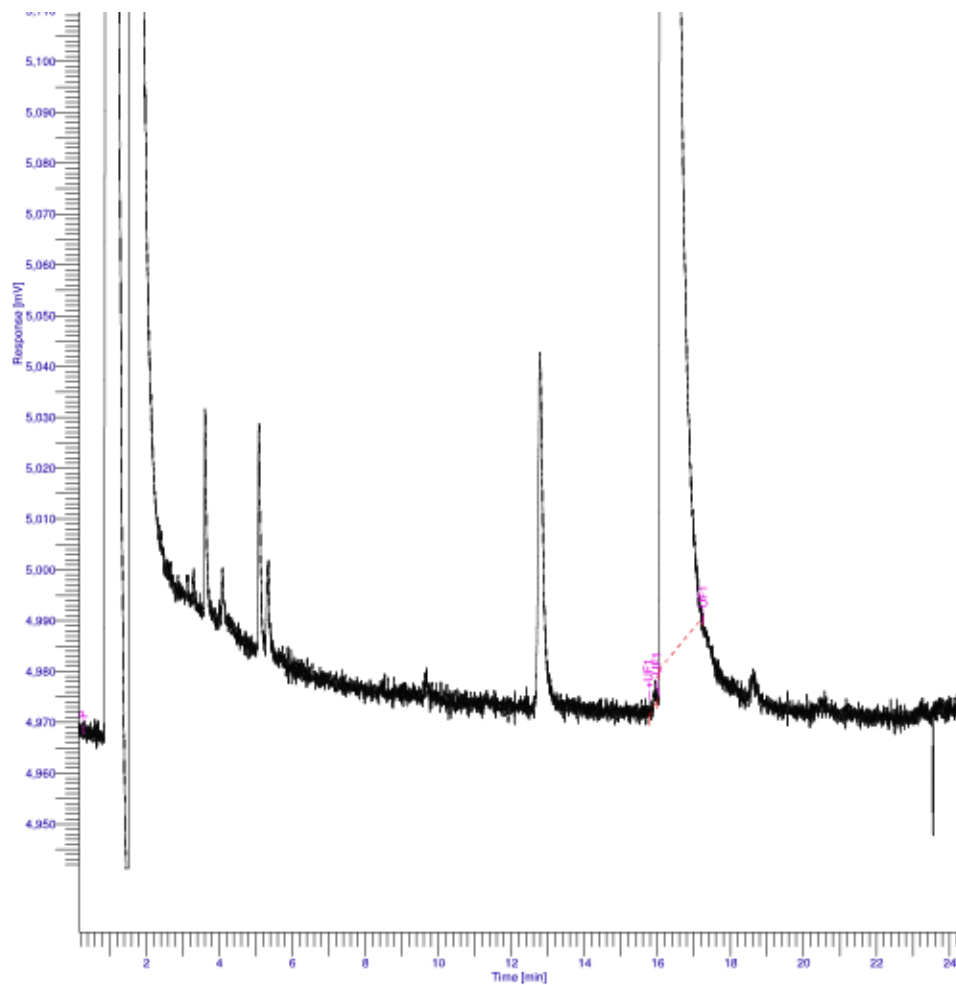


Figure S 131:  $^{13}\text{C}$ -NMR of compound 45



Chiral GC chromatogram of commercially available (-)-isopulegol (1)

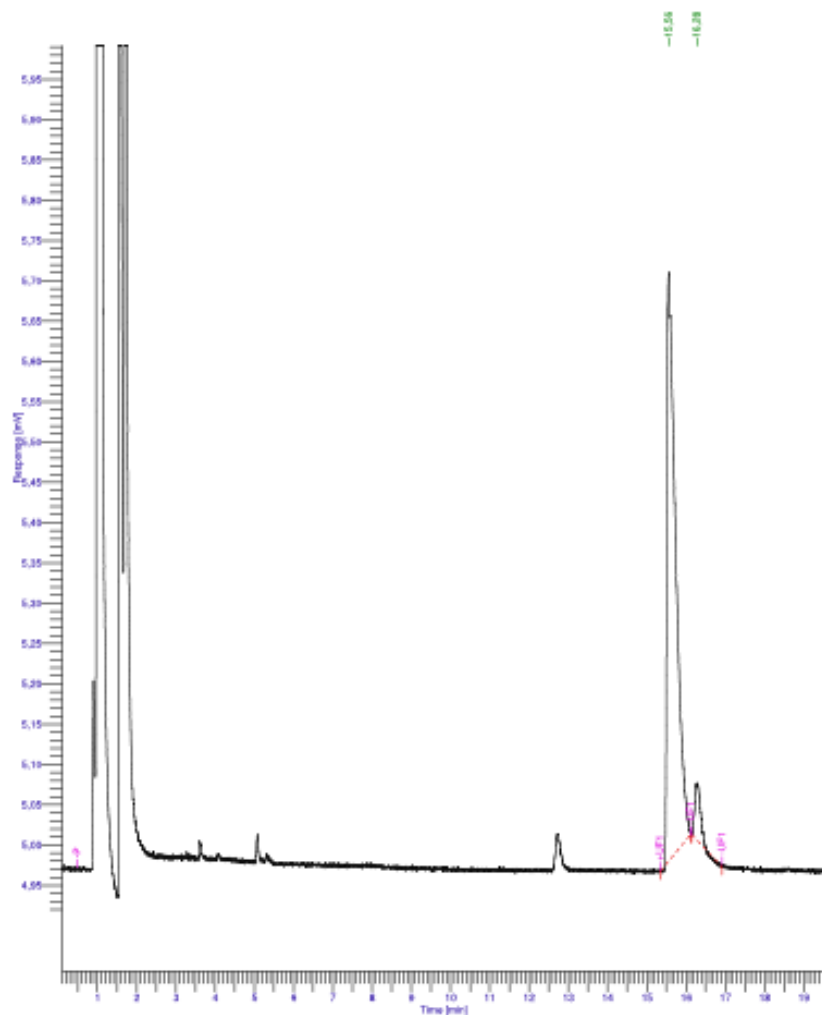


## DEFAULT REPORT

Peak #	Time [min]	Area [μV·s]	Height [μV]	Area [%]	Norm. Area [%]	BL	Area/Height [s]
1	15,943	13,96	4,39	0,07	0,07	*MM	3,1823
2	16,177	19423,27	919,14	99,93	99,93	*MM	21,1319
		19437,23	923,53	100,00	100,00		

# Chiral GC chromatogram of commercially available (+)-isopulegol

Sample Name: E-GC-adamk-2isotipus-isopulegol.nw  
 Plateau: 05.14.14.04.15  
 Date: 2018.03.13.15.54:01  
 Method: 1.1 mV  
 Start Time: 5.10 min End Time: 19.55 min Low Point: 4.91 mV High Point: 5.89 mV  
 Plot Offset: 4.91 mV Plot Scale: 1.1 mV



## DEFAULT REPORT

Peak #	Time [min]	Area [μV·s]	Height [μV]	Area [%]	Norm. Area [%]	BL	Area/Height [s]
1	15,564	11359,73	729,80	93,88	93,88	*MM	15,5655
2	16,277	740,74	70,60	6,12	6,12	*MM	10,4920
		12100,47	800,40	100,00	100,00		