

Supporting Information

Anti-*Acanthamoeba* activity of brominated sesquiterpenes from *Laurencia johnstonii*

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Scheme S1. Isolation process of sesquiterpenes **1-5** from *Laurencia johnstonii*

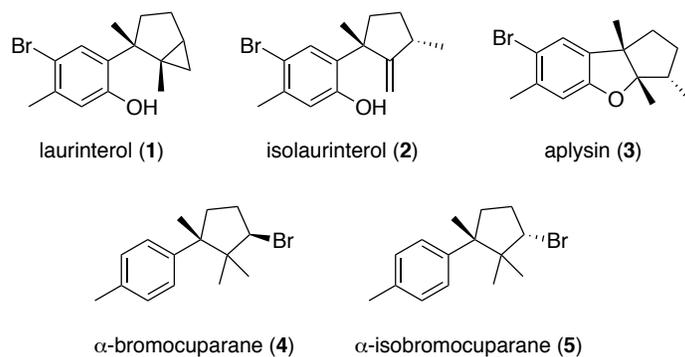
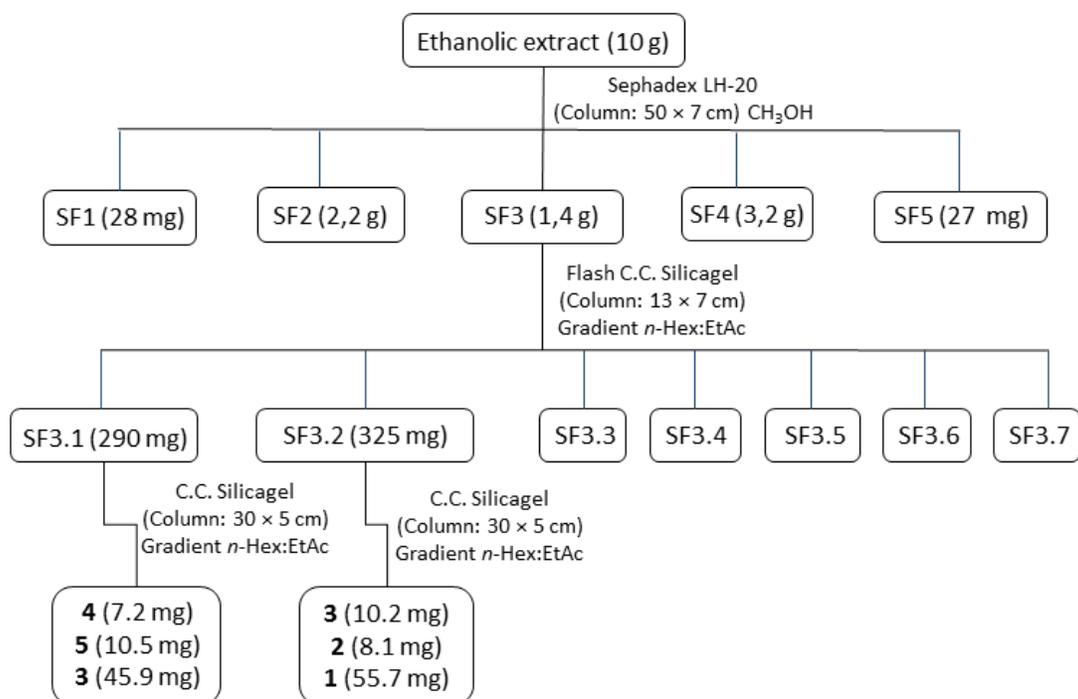


Figure S1. $^1\text{H-NMR}$ spectrum for laurinterol (**1**) (500 MHz, CDCl_3).

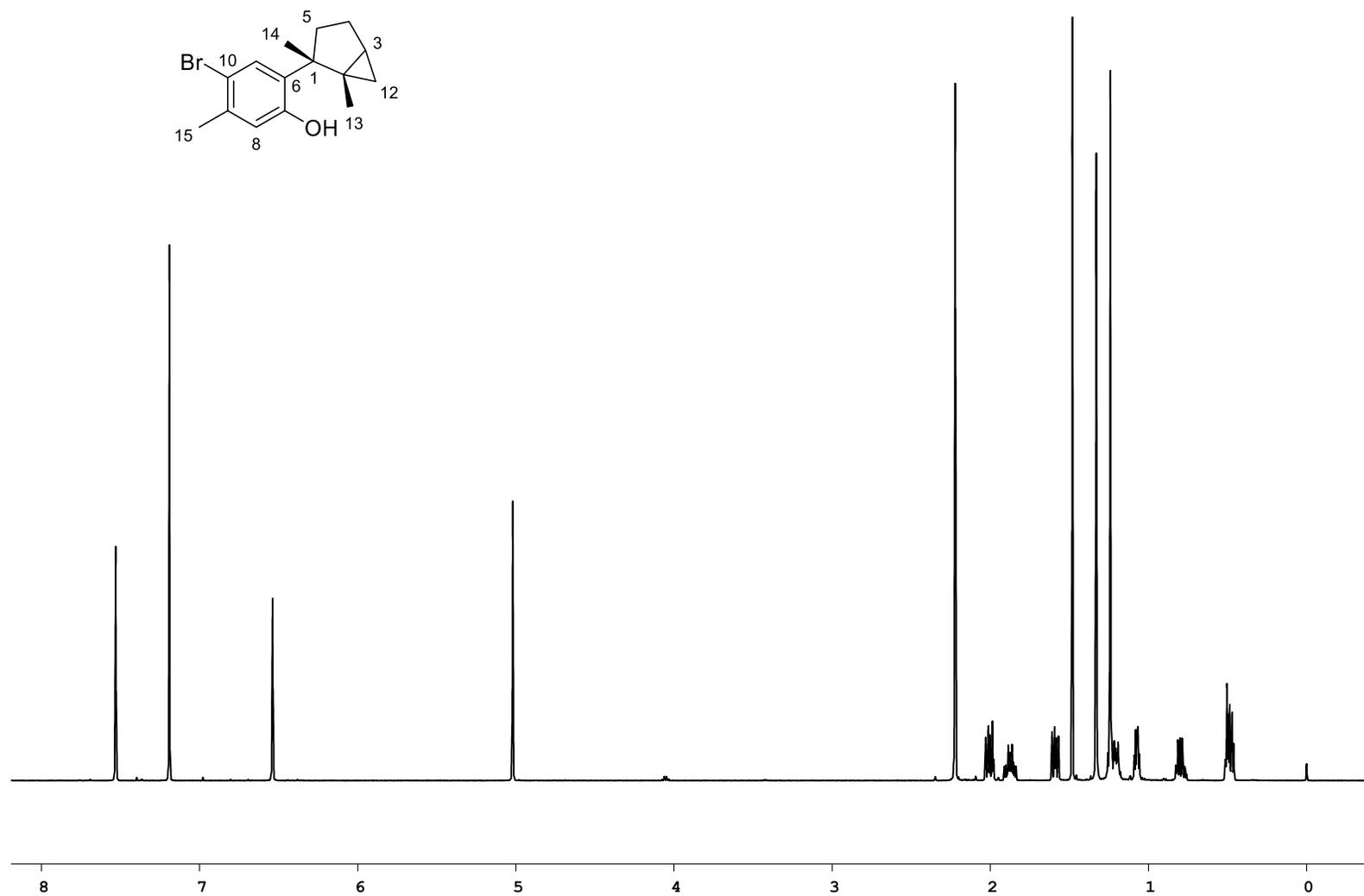


Figure S2. $^1\text{H-NMR}$ spectrum for isolaurinterol (**2**) (500 MHz, CDCl_3).

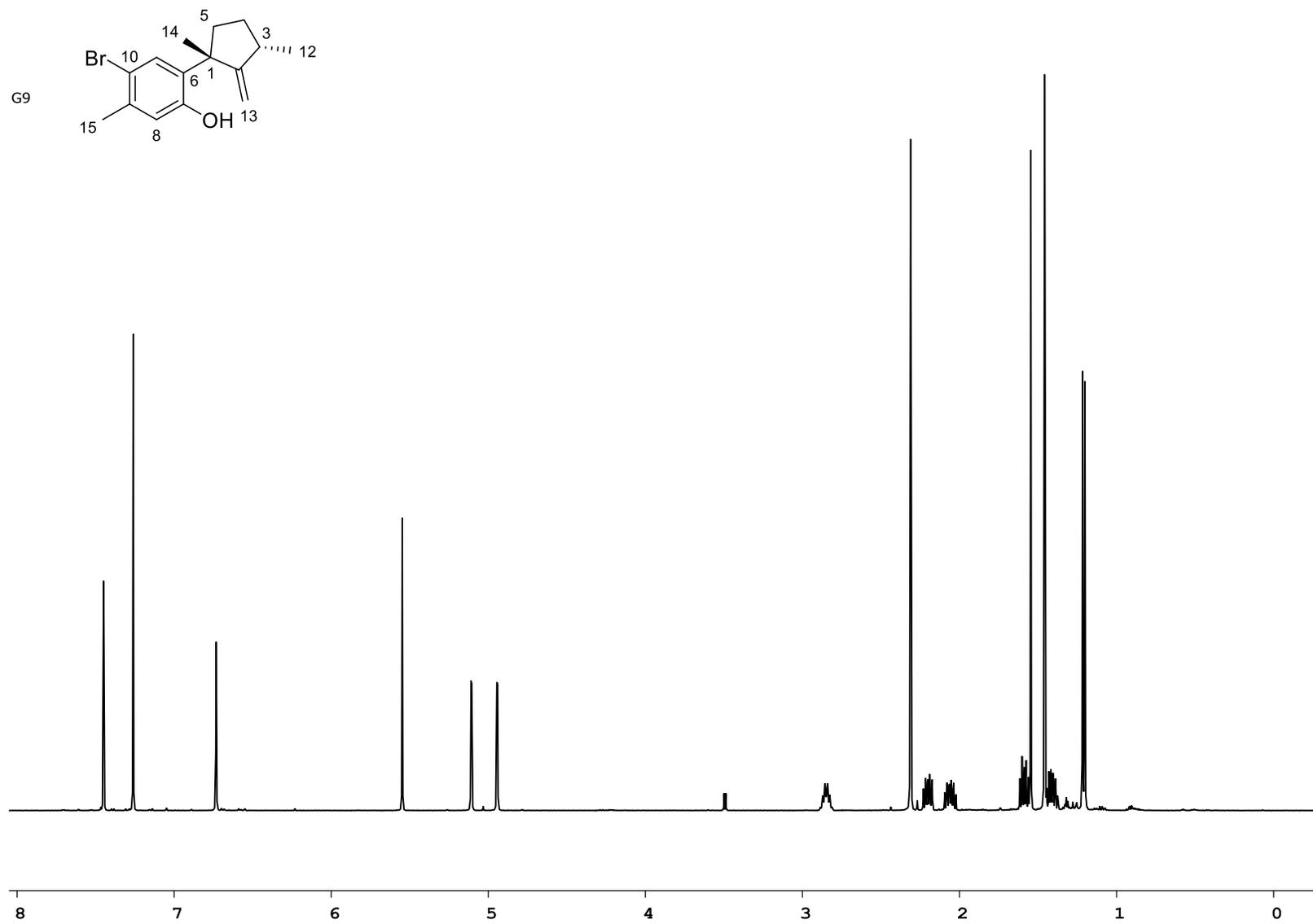


Figure S3. $^1\text{H-NMR}$ spectrum for aplysin (**3**) (500 MHz, CDCl_3).

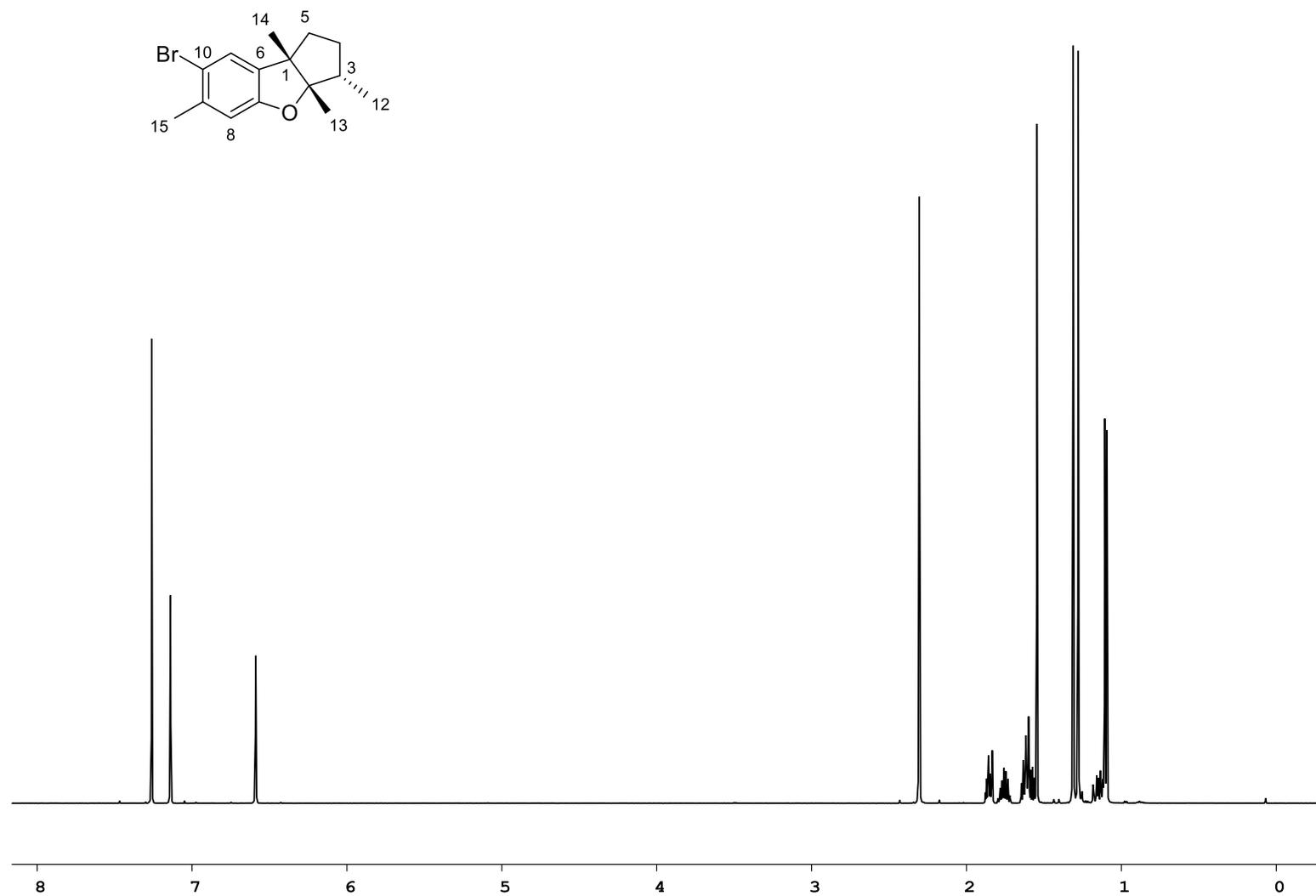


Figure S4. $^1\text{H-NMR}$ spectrum for α -bromocuparane (**4**) (500 MHz, CDCl_3).

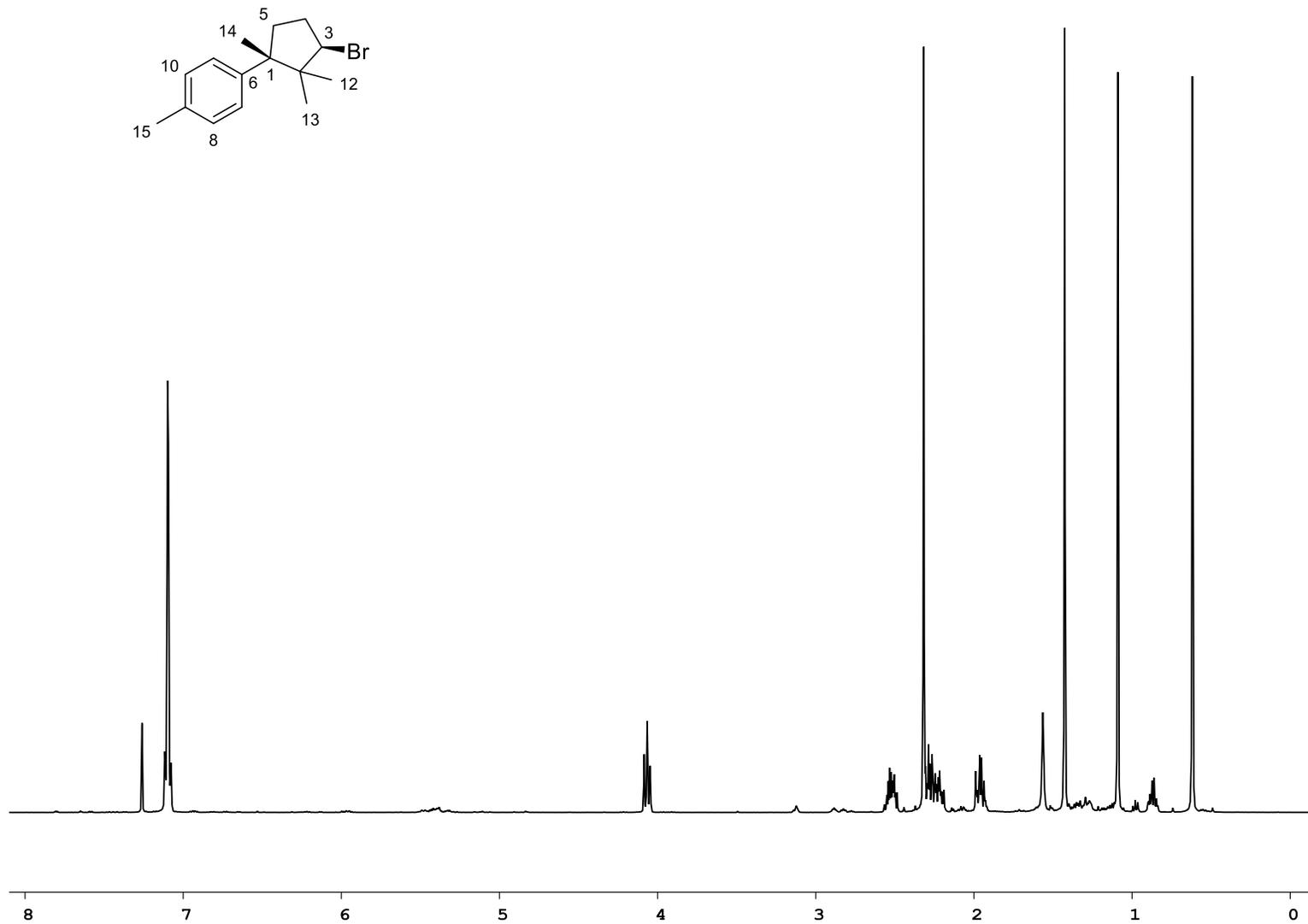


Figure S5. ^1H -NMR spectrum of α -isobromocuparane (**5**) (500 MHz, CDCl_3).

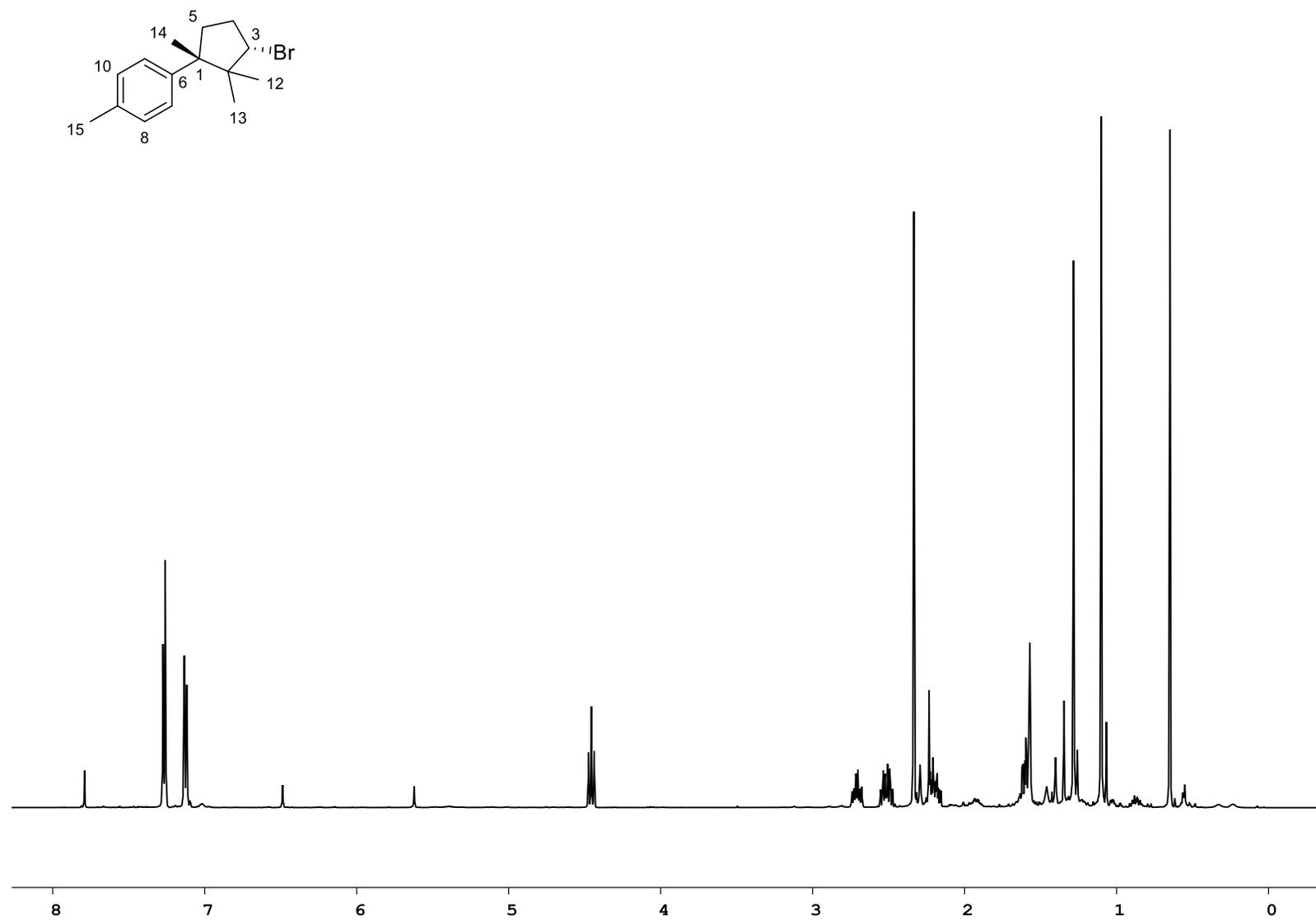
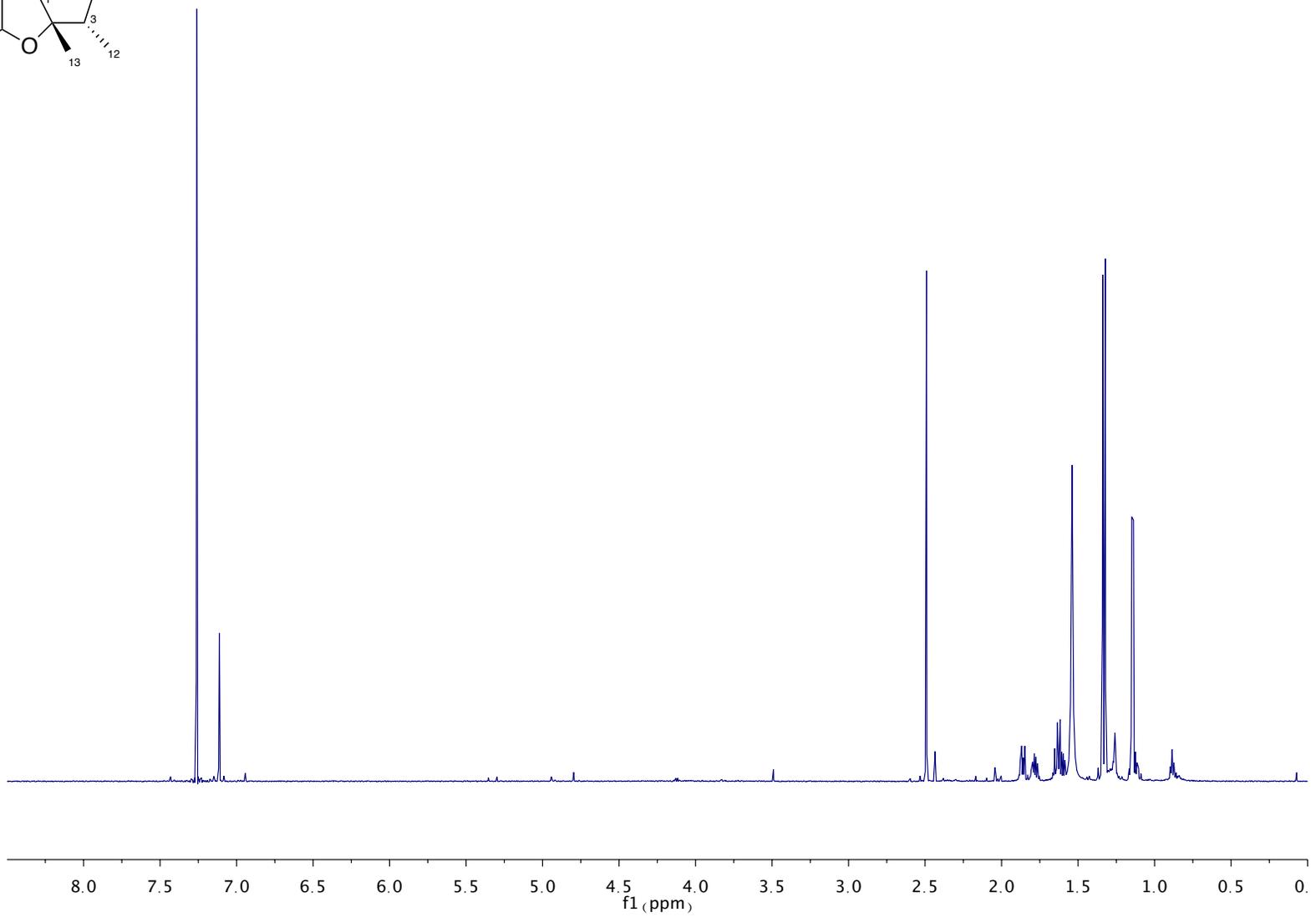
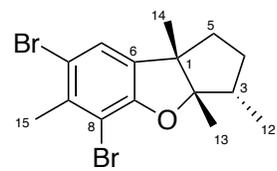


Figure S6. $^1\text{H-NMR}$ spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl_3).



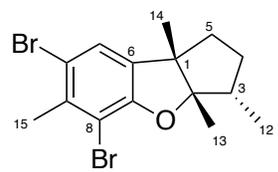
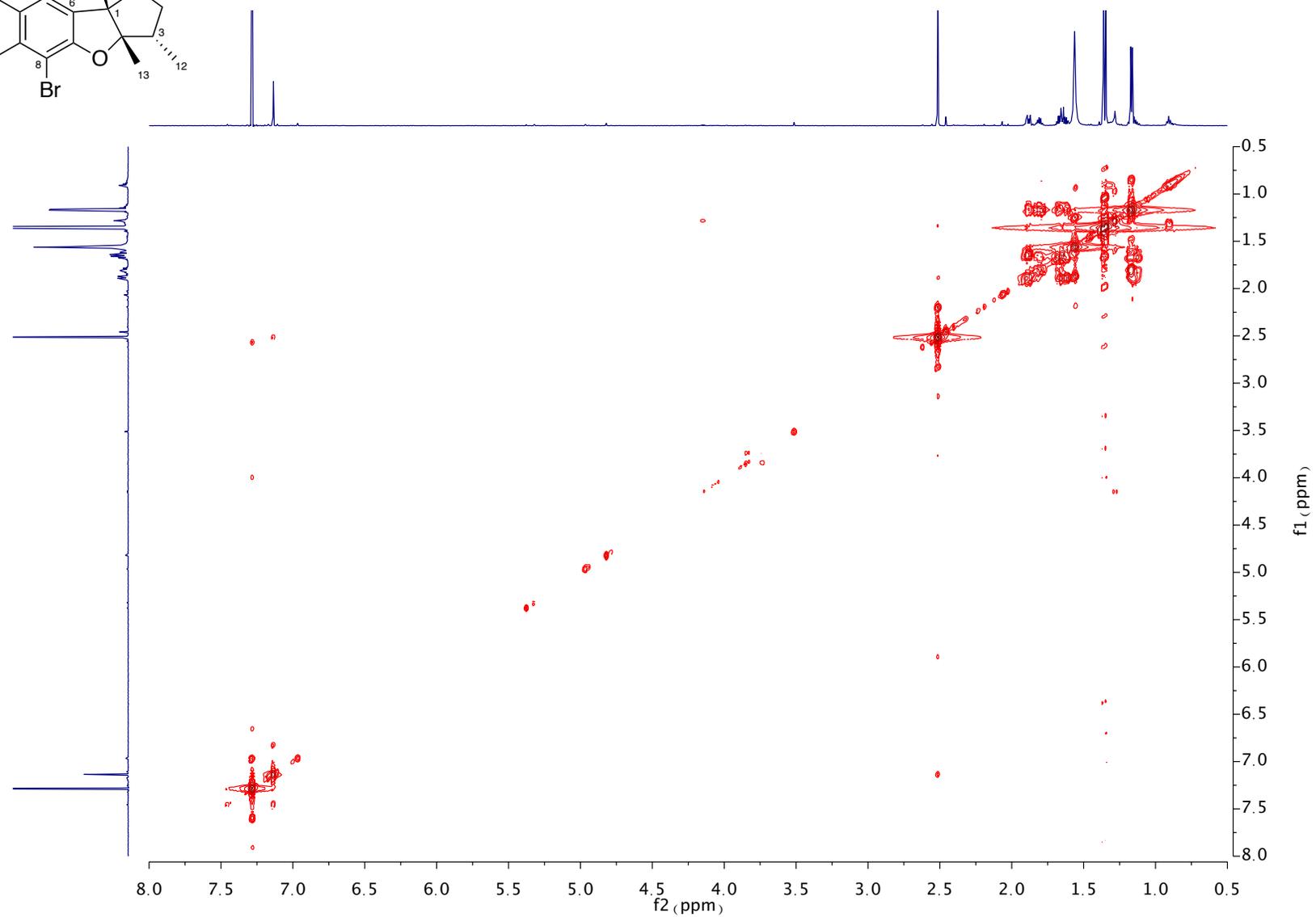


Figure S7. COSY spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl₃).



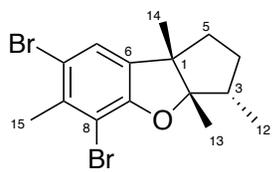
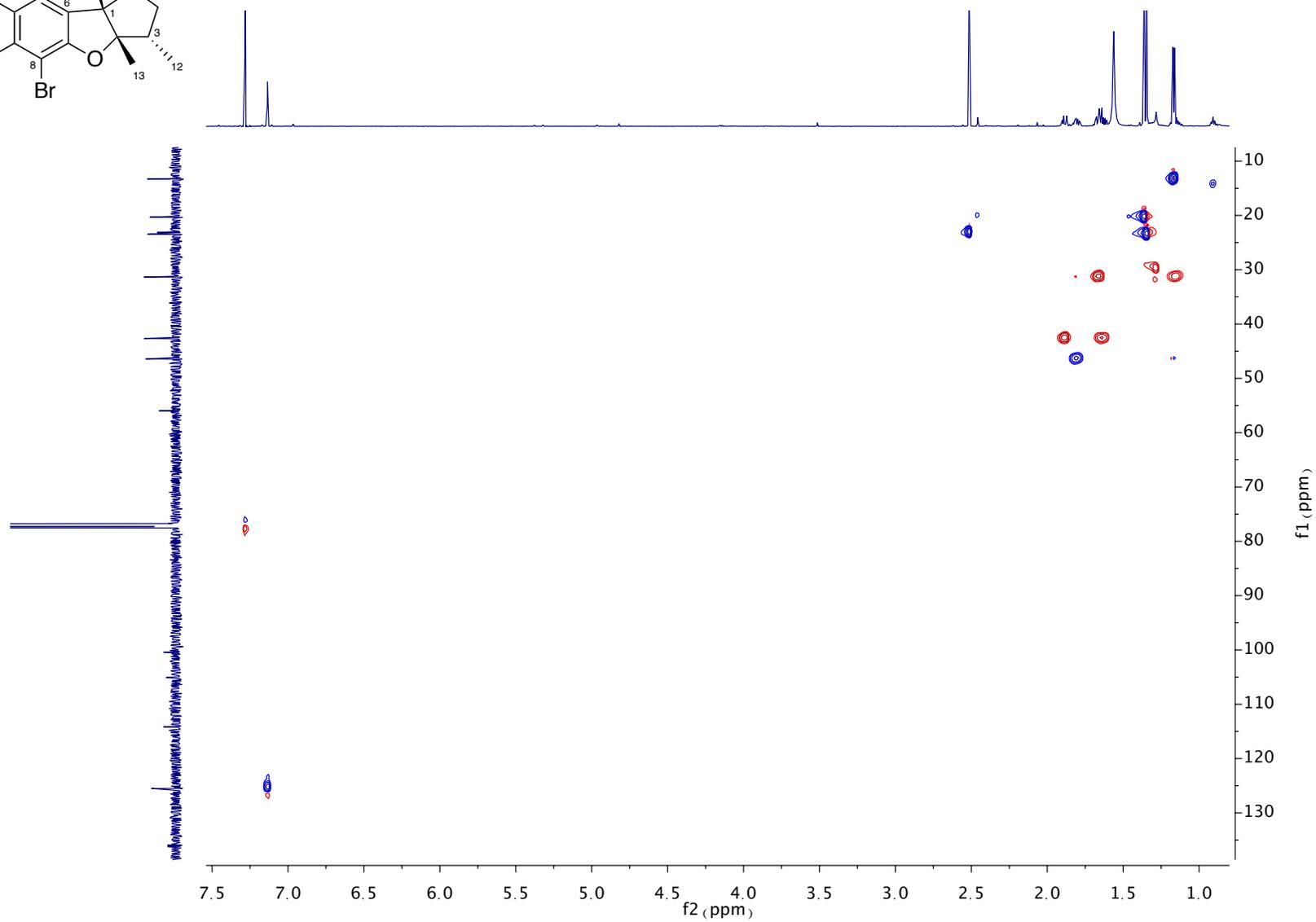


Figure S8. HSQC-ed spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl₃).



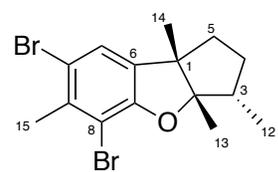


Figure S9. HMBC spectrum of 8-bromoaplysin (6) (600 MHz, CDCl₃).

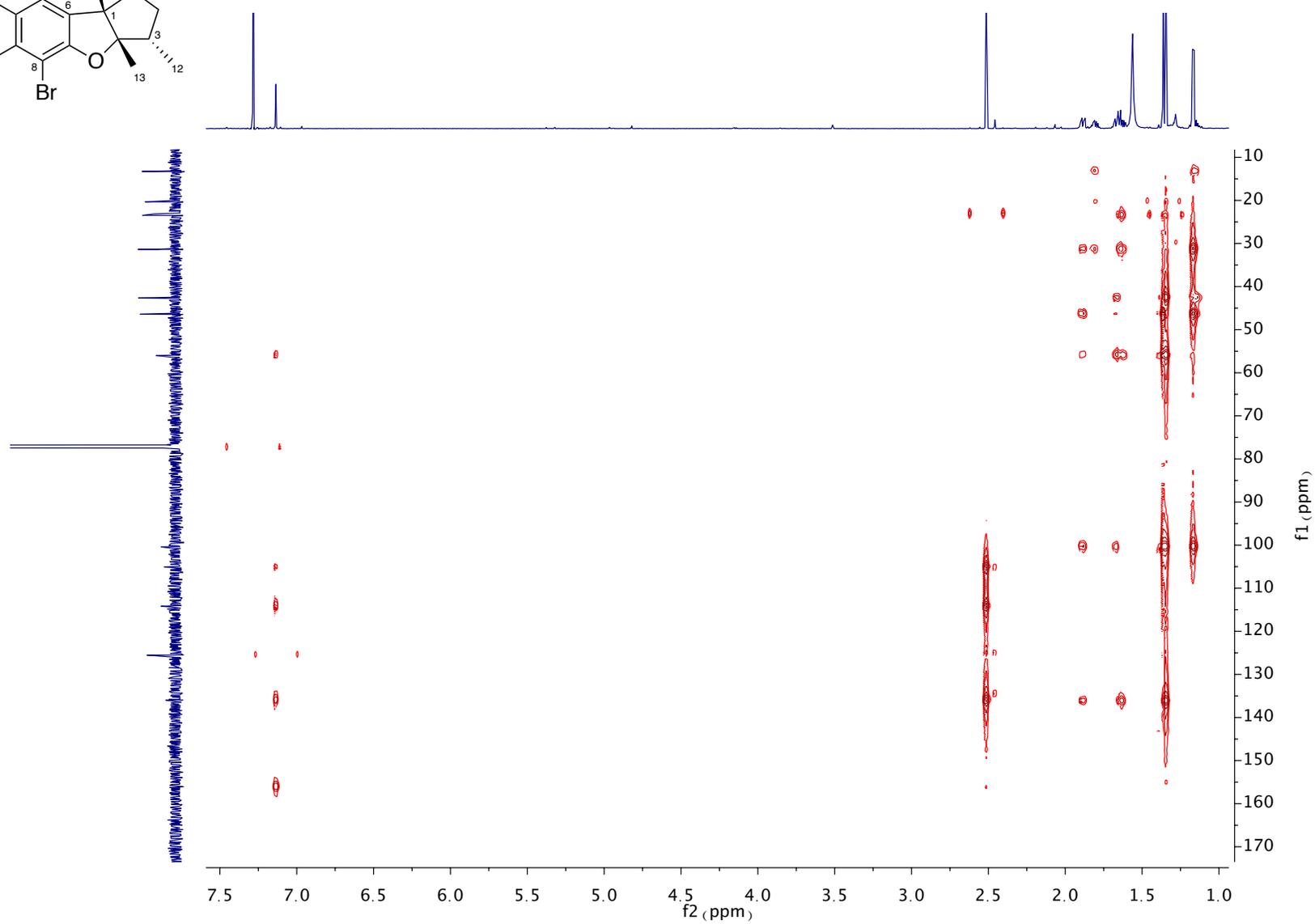


Figure S10. ^{13}C NMR spectrum of 8-bromoaplysin (**6**) (150 MHz, CDCl_3).

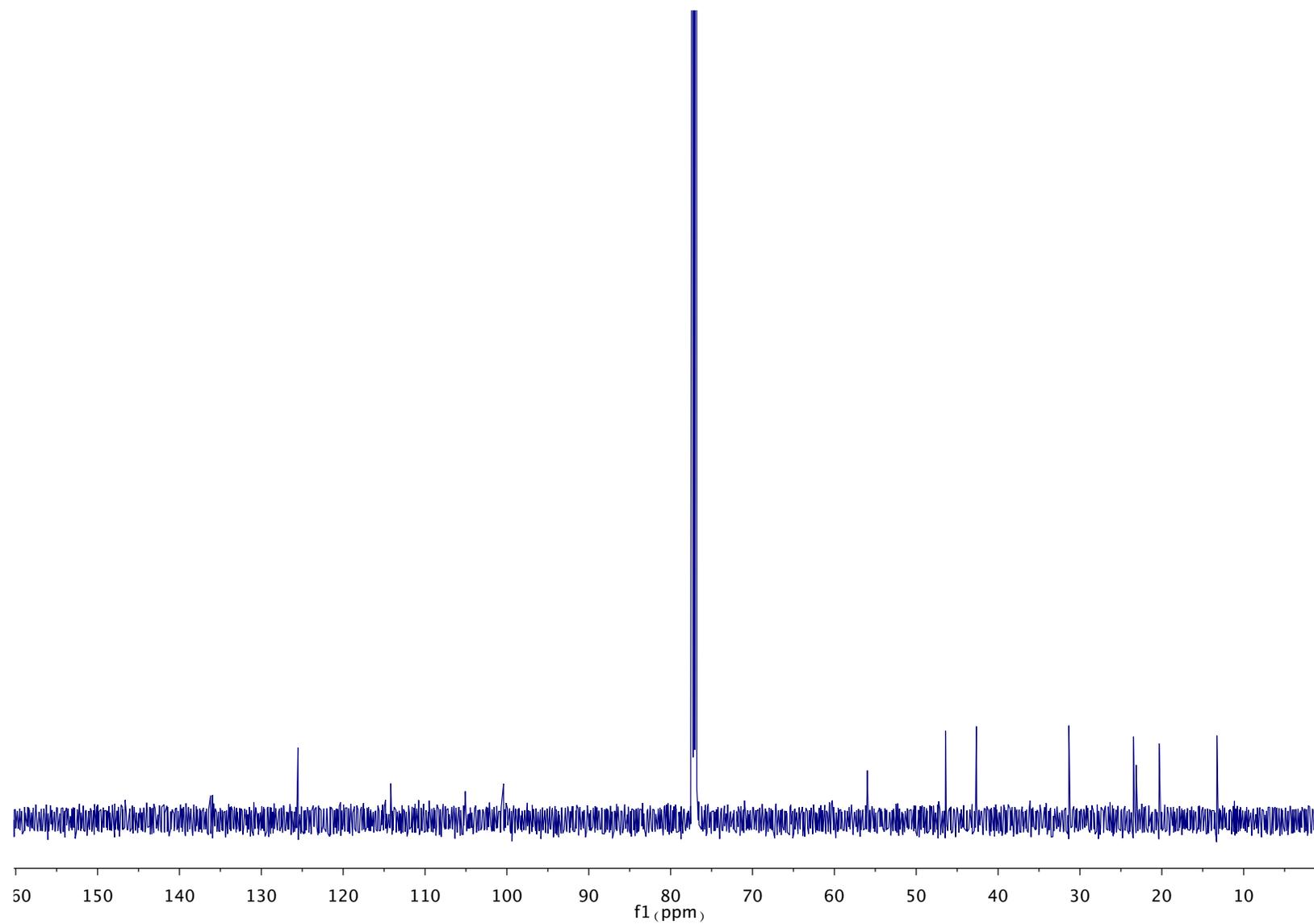


Figure S11. HREIMS spectrum of 8-bromoaplysin (6).

Elemental Composition Report

Multiple Mass Analysis: 1974 mass(es) processed - displaying only valid results

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

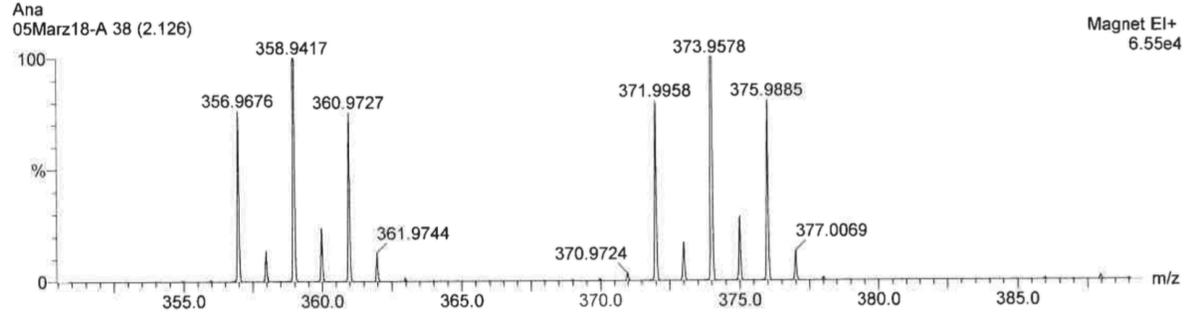
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

24346 formula(e) evaluated with 21 results within limits (all results (up to 1000) for each mass)

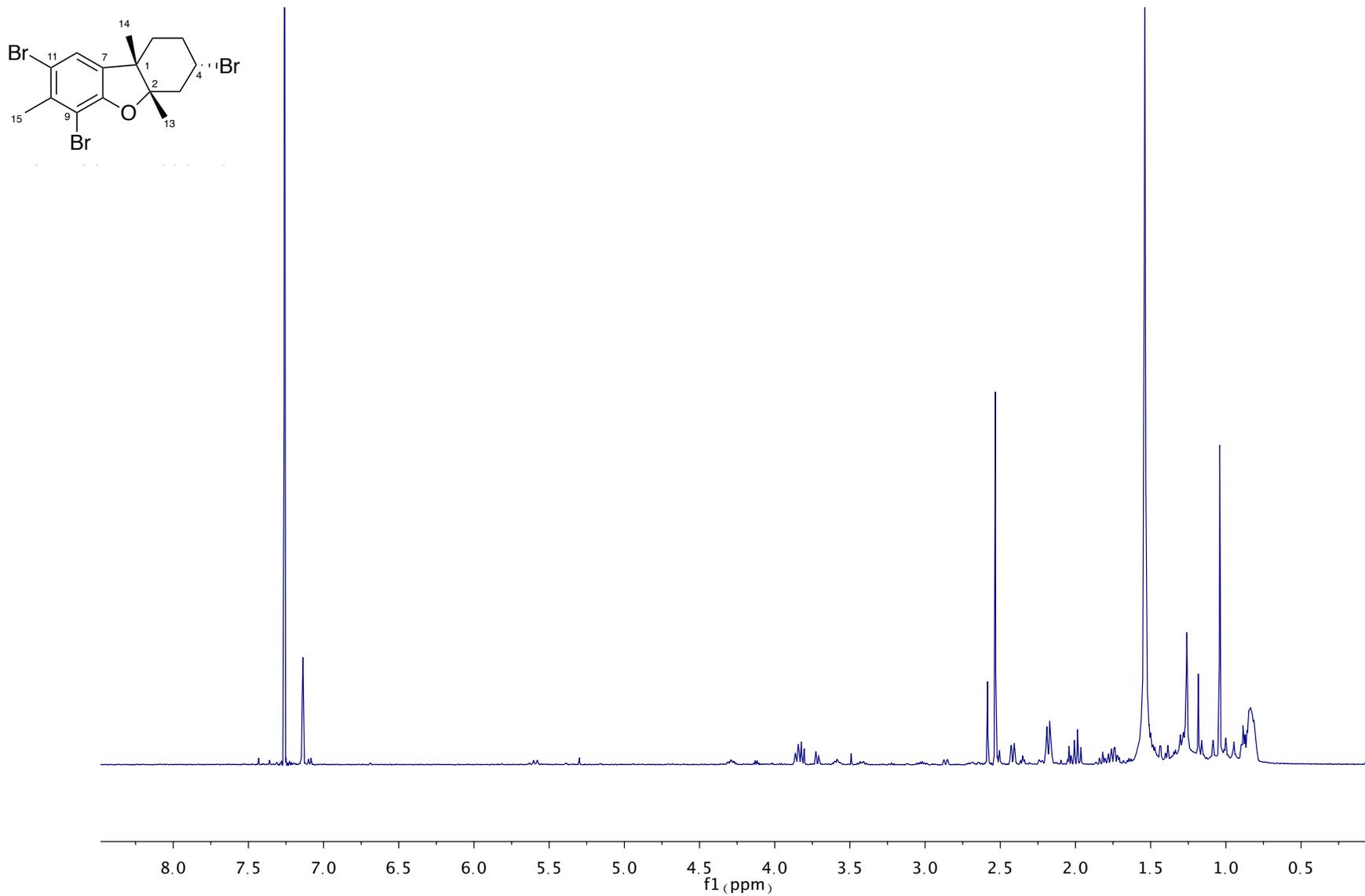
Elements Used:

C: 15-15 H: 18-18 O: 0-1 79Br: 0-2 81Br: 0-2



Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
375.9718	58.99	375.9683	3.5	9.3	6.0	C15 H18 O 81Br2
375.9698	53.56	375.9683	1.5	4.0	6.0	C15 H18 O 81Br2
375.9677	47.91	375.9683	-0.6	-1.6	6.0	C15 H18 O 81Br2
375.9656	42.16	375.9683	-2.7	-7.2	6.0	C15 H18 O 81Br2
373.9723	100.00	373.9704	1.9	5.1	6.0	C15 H18 O 79Br 81Br
373.9702	100.00	373.9704	-0.2	-0.5	6.0	C15 H18 O 79Br 81Br
373.9682	100.00	373.9704	-2.2	-5.9	6.0	C15 H18 O 79Br 81Br
371.9752	57.29	371.9724	2.8	7.5	6.0	C15 H18 O 79Br2
371.9732	54.26	371.9724	0.8	2.2	6.0	C15 H18 O 79Br2
371.9711	49.60	371.9724	-1.3	-3.5	6.0	C15 H18 O 79Br2
371.9690	44.63	371.9724	-3.4	-9.1	6.0	C15 H18 O 79Br2
359.9757	22.43	359.9734	2.3	6.4	6.0	C15 H18 81Br2
359.9737	22.78	359.9734	0.3	0.8	6.0	C15 H18 81Br2
359.9716	23.04	359.9734	-1.8	-5.0	6.0	C15 H18 81Br2
357.9781	13.21	357.9755	2.6	7.3	6.0	C15 H18 79Br 81Br
357.9761	13.42	357.9755	0.6	1.7	6.0	C15 H18 79Br 81Br
357.9742	13.53	357.9755	-1.3	-3.6	6.0	C15 H18 79Br 81Br
357.9721	13.42	357.9755	-3.4	-9.5	6.0	C15 H18 79Br 81Br
355.9798	0.42	355.9775	2.3	6.5	6.0	C15 H18 79Br2
355.9778	0.43	355.9775	0.3	0.8	6.0	C15 H18 79Br2
355.9759	0.50	355.9775	-1.6	-4.5	6.0	C15 H18 79Br2

Figure S12. ^1H NMR spectrum of 3 α -bromojohnstane (**7**) (600 MHz, CDCl_3).



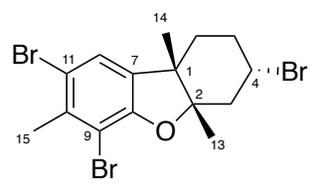
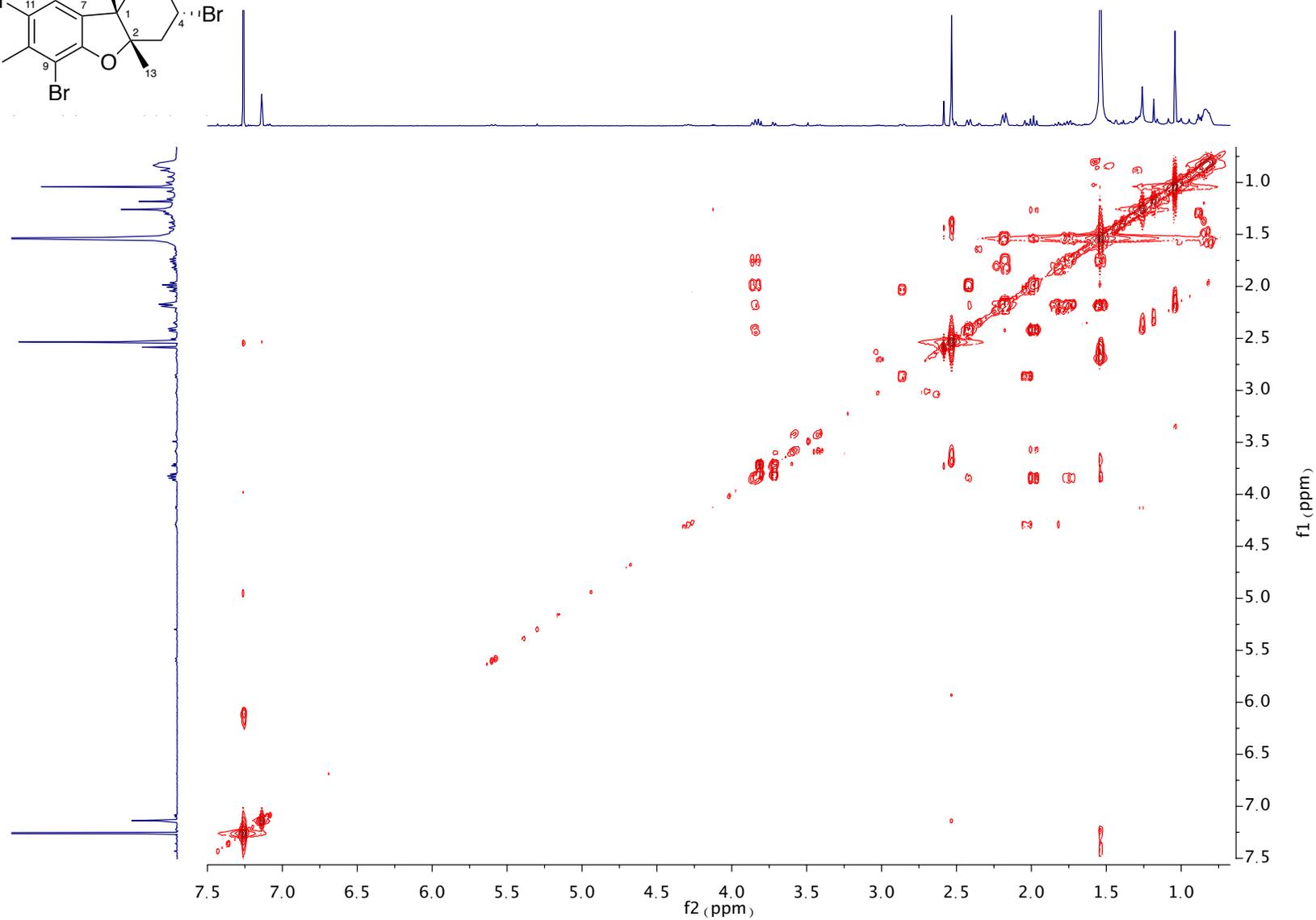


Figure S13. COSY spectrum of 3 α -bromojohnstane (7) (600 MHz, CDCl₃).



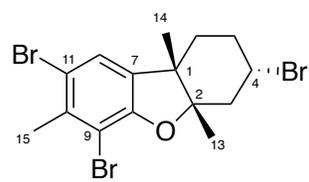
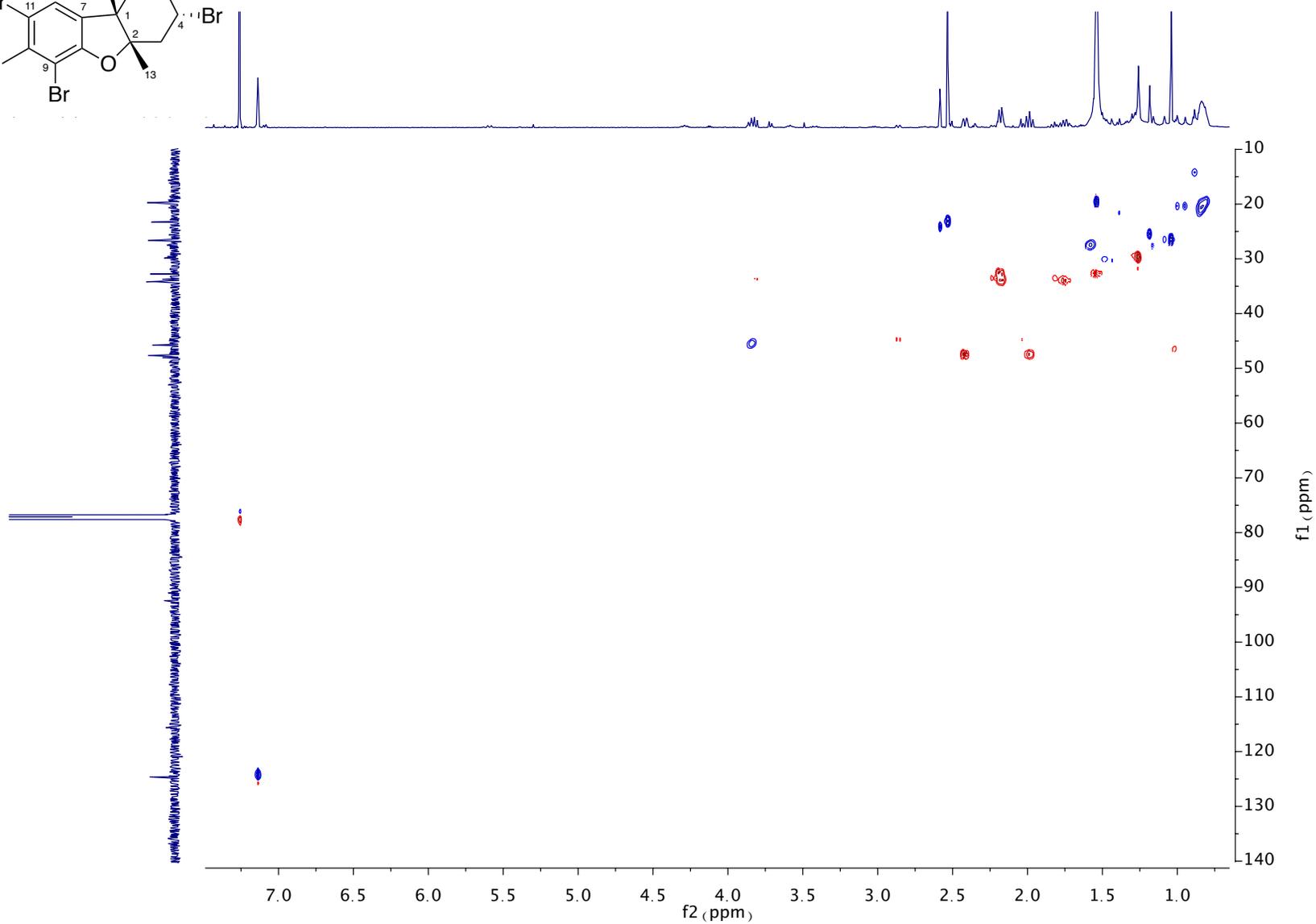


Figure S14. HSQC-ed spectrum of 3 α -bromojohnstane (7) (600 MHz, CDCl₃).



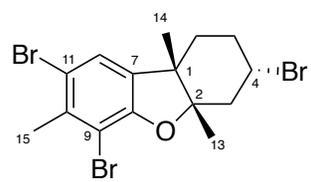
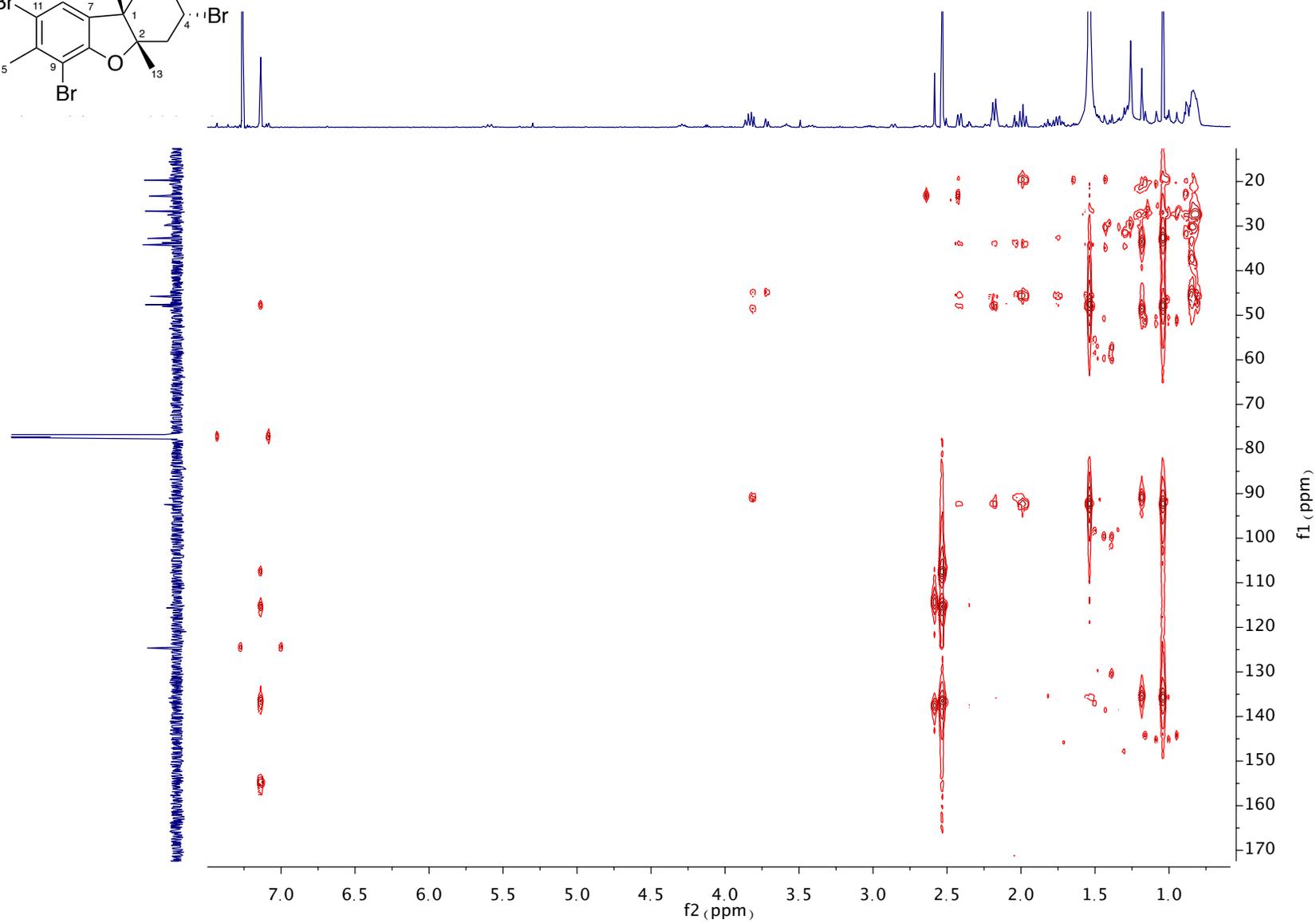


Figure S15. HMBC spectrum of 3 α -bromojohnstane (7) (600 MHz, CDCl₃).



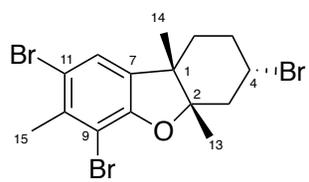


Figure S16. ^{13}C NMR spectrum of 3 α -bromojohnstane (**7**) (150 MHz, CDCl_3).

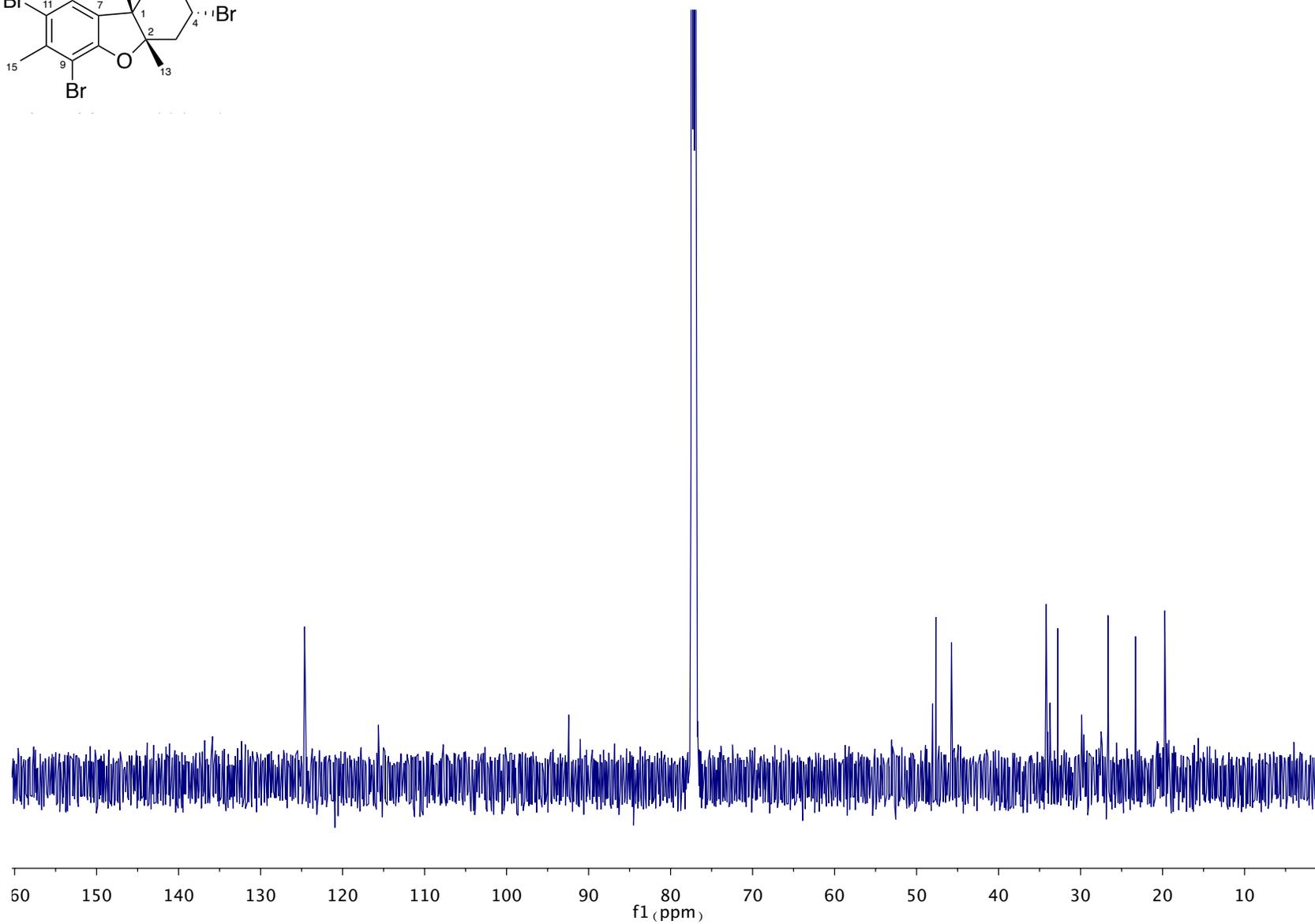


Figure S17. 1D-NOE experiments of 3 α -bromojohnstane (**7**) (600 MHz, CDCl₃).

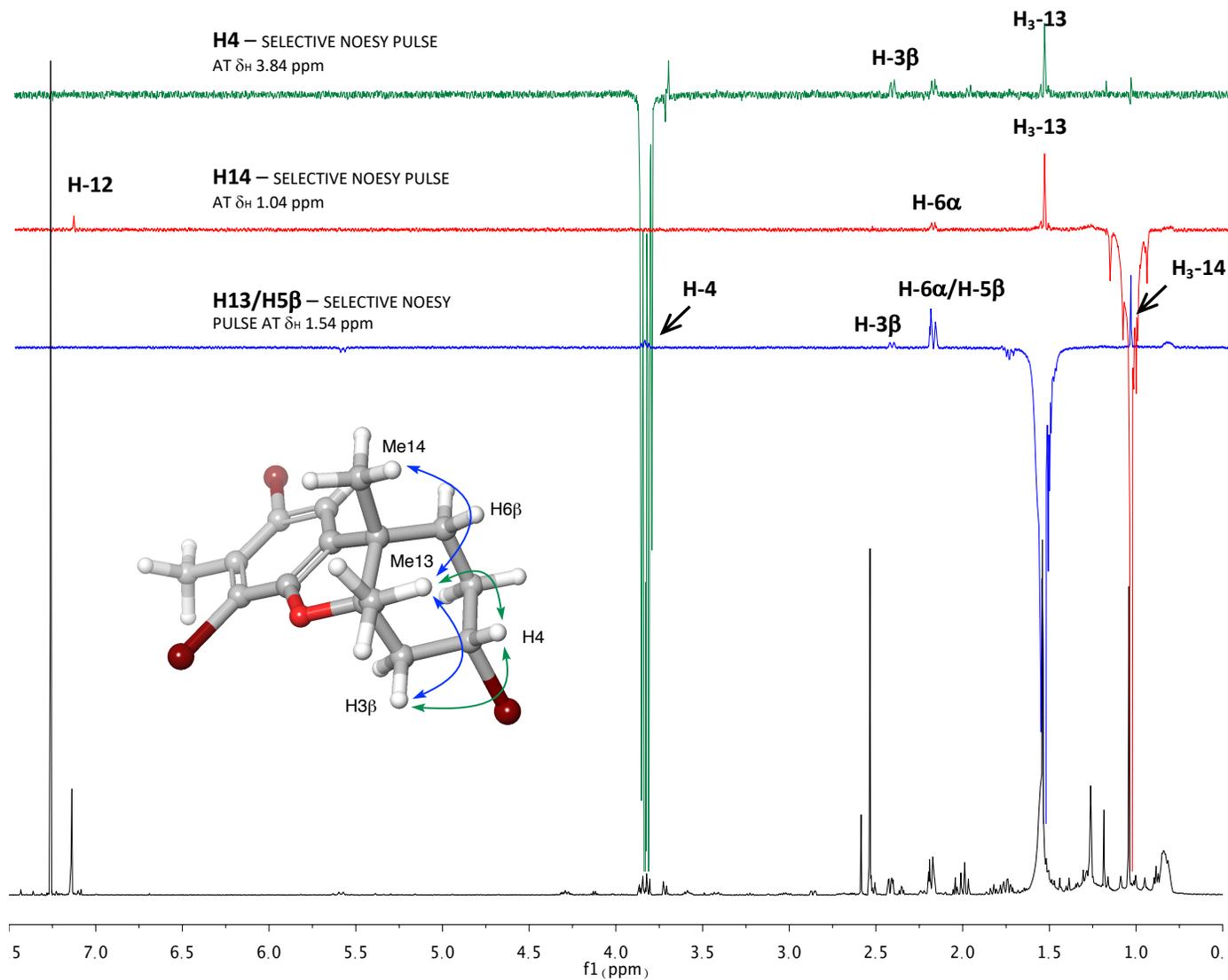


Figure S18. HREIMS spectrum of 3 α -bromojohnstane (7).

Elemental Composition Report

Multiple Mass Analysis: 4297 mass(es) processed - displaying only valid results

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

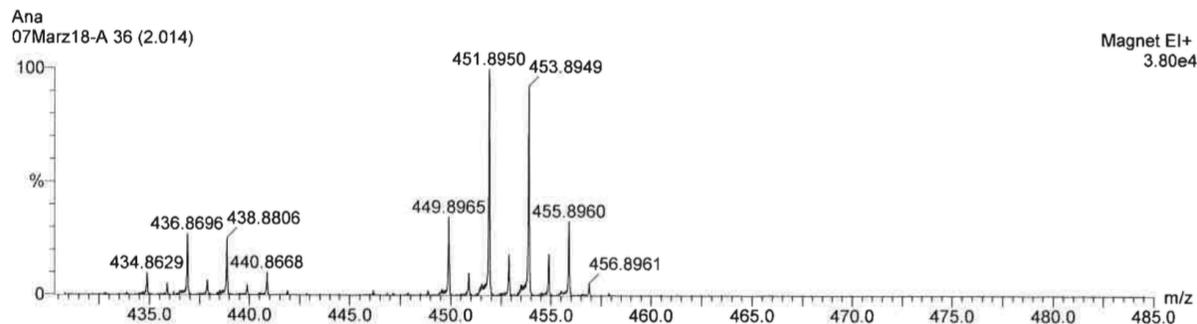
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

48456 formula(e) evaluated with 16 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 15-15 H: 17-17 O: 1-1 79Br: 0-3 81Br: 0-3



Magnet EI+
3.80e4

Minimum: 0.10
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
455.8809	24.09	455.8768	4.1	9.0	6.0	C15 H17 O 81Br3
455.8784	24.88	455.8768	1.6	3.5	6.0	C15 H17 O 81Br3
455.8758	25.80	455.8768	-1.0	-2.2	6.0	C15 H17 O 81Br3
455.8733	24.42	455.8768	-3.5	-7.7	6.0	C15 H17 O 81Br3
453.8823	74.42	453.8789	3.4	7.5	6.0	C15 H17 O 79Br 81Br2
453.8798	67.41	453.8789	0.9	2.0	6.0	C15 H17 O 79Br 81Br2
453.8773	61.33	453.8789	-1.6	-3.5	6.0	C15 H17 O 79Br 81Br2
453.8748	55.32	453.8789	-4.1	-9.0	6.0	C15 H17 O 79Br 81Br2
451.8850	80.74	451.8809	4.1	9.1	6.0	C15 H17 O 79Br2 81Br
451.8824	80.48	451.8809	1.5	3.3	6.0	C15 H17 O 79Br2 81Br
451.8800	78.16	451.8809	-0.9	-2.0	6.0	C15 H17 O 79Br2 81Br
451.8775	72.34	451.8809	-3.4	-7.5	6.0	C15 H17 O 79Br2 81Br
449.8865	28.64	449.8829	3.6	8.0	6.0	C15 H17 O 79Br3
449.8840	26.22	449.8829	1.1	2.4	6.0	C15 H17 O 79Br3
449.8816	23.43	449.8829	-1.3	-2.9	6.0	C15 H17 O 79Br3
449.8791	21.91	449.8829	-3.8	-8.4	6.0	C15 H17 O 79Br3

Figure S19. ^1H NMR spectrum of 8,10-dibromoisoplysin (**8**) (500 MHz, CDCl_3).

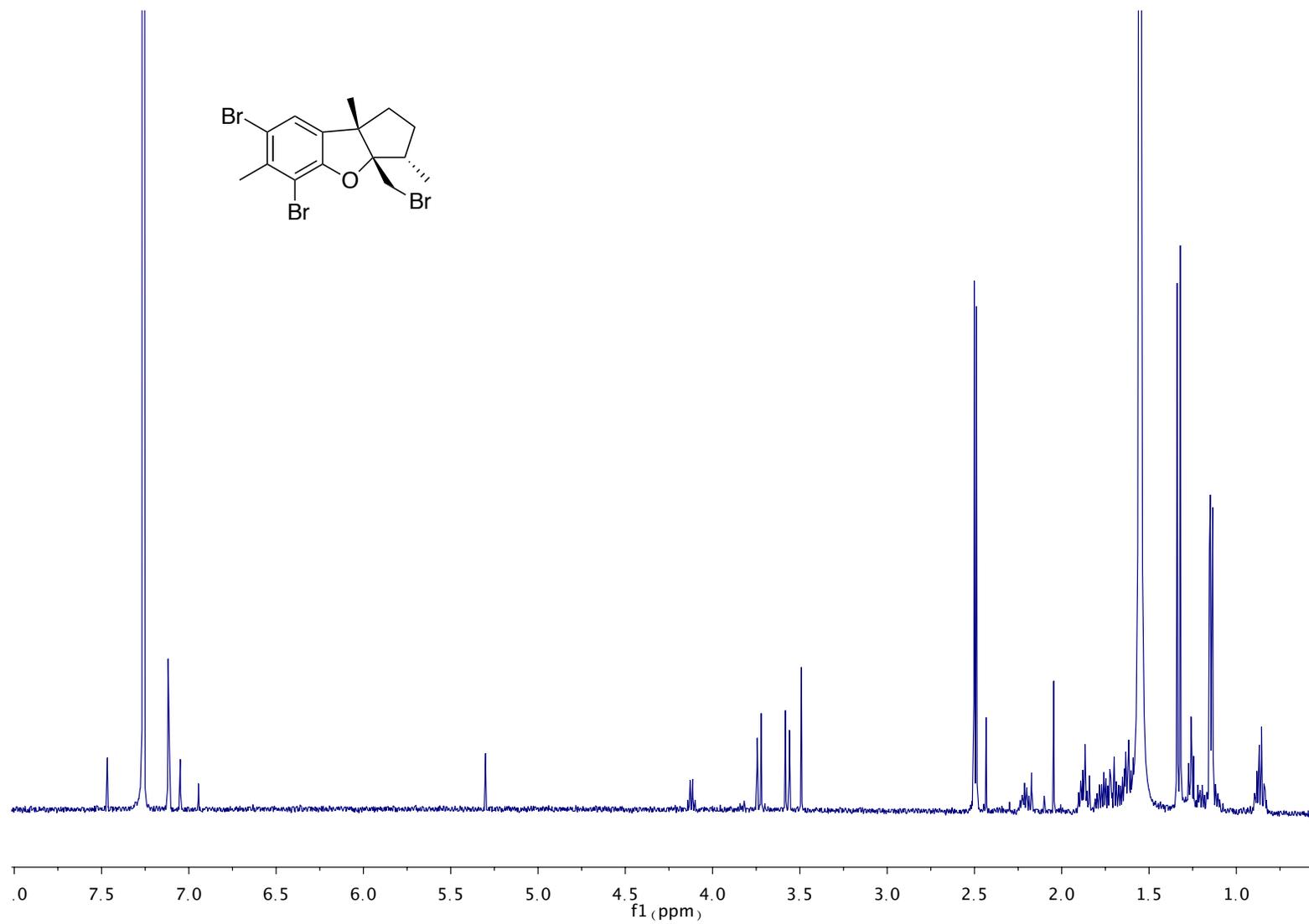


Figure S20. ^1H NMR spectrum of 8,10-dibromoaplysinol (**9**) (500 MHz, CDCl_3).

