

Supporting Information

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

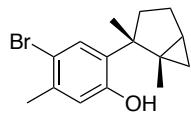
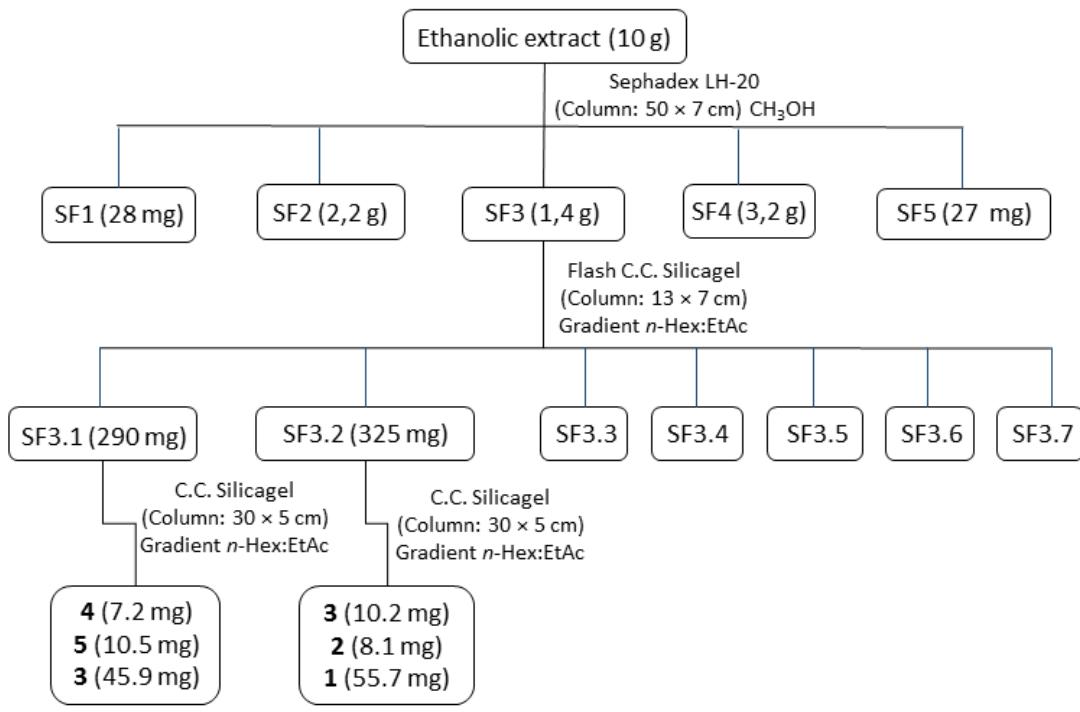
Sara García-Davis^{1,2}, Ines Sifaoui³, María Reyes-Batlle³, Ezequiel Viveros-Valdez², José E. Piñero³, Jacob Lorenzo-Morales³, José J. Fernández^{1,4*} and Ana R. Díaz-Marrero^{1*}

- ¹ Instituto Universitario de Bio-Orgánica Antonio González (IUBO AG), Centro de Investigaciones Biomédicas de Canarias (CIBICAN), Universidad de La Laguna (ULL), Avda. Astrofísico F. Sánchez, 2, 38206 La Laguna, Tenerife, España; sara.garciadv@uanl.edu.mx (S.G.D.); adiazmar@ull.edu.es (A.R.D.M); jifercas@ull.edu.es (J.J.F.)
- ² Universidad Autónoma de Nuevo León (UANL), Facultad de Ciencias Biológicas. Av. Pedro de Alba s/n, 66450 San Nicolás de los Garza, Nuevo León, México; jose.viverosvld@uanl.edu.mx (E.V.V.)
- ³ Instituto Universitario de Enfermedades Tropicales y Salud Pública de Islas Canarias, Universidad de La Laguna. Av. Astrofísico Francisco Sánchez s/n, 38206 La Laguna, Tenerife, España.; ines.sifaoui@hotmail.com (I.S.); jmlorenz@ull.edu.es (J.L.M.)
- ⁴ Departamento de Química Orgánica, Universidad de La Laguna (ULL), Avda. Astrofísico F. Sánchez, 2, 38206 La Laguna, Tenerife, España

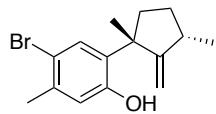
TABLE OF CONTENTS

	Page
Scheme S1. Isolation process of sesquiterpenes 1-5 from <i>Laurencia johnstonii</i>	3
Figure S1. ^1H -NMR spectrum for laurinterol (1) (500 MHz, CDCl_3)	4
Figure S2. ^1H -NMR spectrum for isolaurinterol (2) (500 MHz, CDCl_3)	5
Figure S3. ^1H -NMR spectrum for aplysin (3) (500 MHz, CDCl_3)	6
Figure S4. ^1H -NMR spectrum for α -bromocuparane (4) (500 MHz, CDCl_3)	7
Figure S5. ^1H -NMR spectrum for α -isobromocuparane (5) (500 MHz, CDCl_3)	8
Figure S6. ^1H -NMR spectrum of 8-bromoaplysin (6) (600 MHz, CDCl_3)	9
Figure S7. COSY spectrum of 8-bromoaplysin (6) (600 MHz, CDCl_3)	10
Figure S8. HSQC-ed spectrum of 8-bromoaplysin (6) (600 MHz, CDCl_3)	11
Figure S9. HMBC spectrum of 8-bromoaplysin (6) (600 MHz, CDCl_3)	12
Figure S10. ^{13}C NMR spectrum of 8-bromoaplysin (6) (150 MHz, CDCl_3)	13
Figure S11. HREIMS spectrum of 8-bromoaplysin (6)	14
Figure S12. ^1H NMR spectrum of 3α -bromojohnstane (7) (600 MHz, CDCl_3)	15
Figure S13. COSY spectrum of 3α -bromojohnstane (7) (600 MHz, CDCl_3)	16
Figure S14. HSQC-ed spectrum of 3α -bromojohnstane (7) (600 MHz, CDCl_3)	17
Figure S15. HMBC spectrum of 3α -bromojohnstane (7) (600 MHz, CDCl_3)	18
Figure S16. ^{13}C NMR spectrum of 3α -bromojohnstane (7) (150 MHz, CDCl_3)	19
Figure S17. 1D-NOE experiments of 3α -bromojohnstane (7) (600 MHz, CDCl_3)	20
Figure S18. HREIMS spectrum of 3α -bromojohnstane (7)	21
Figure S19. ^1H NMR spectrum of 8,10-dibromoisoaplysin (8) (500 MHz, CDCl_3)	22
Figure S20. ^1H NMR spectrum of 8,10-dibromoaplysinol (9) (500 MHz, CDCl_3)	23

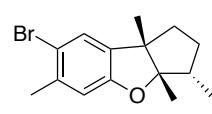
Scheme S1. Isolation process of sesquiterpenes **1-5** from *Laurencia johnstonii*



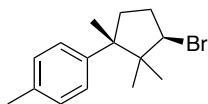
laurinterol (**1**)



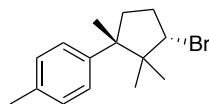
isolaurinterol (**2**)



aplysin (**3**)



α-bromocuparane (**4**)



α-isobromocuparane (**5**)

Figure S1. ^1H -NMR spectrum for laurinterol (**1**) (500 MHz, CDCl_3).

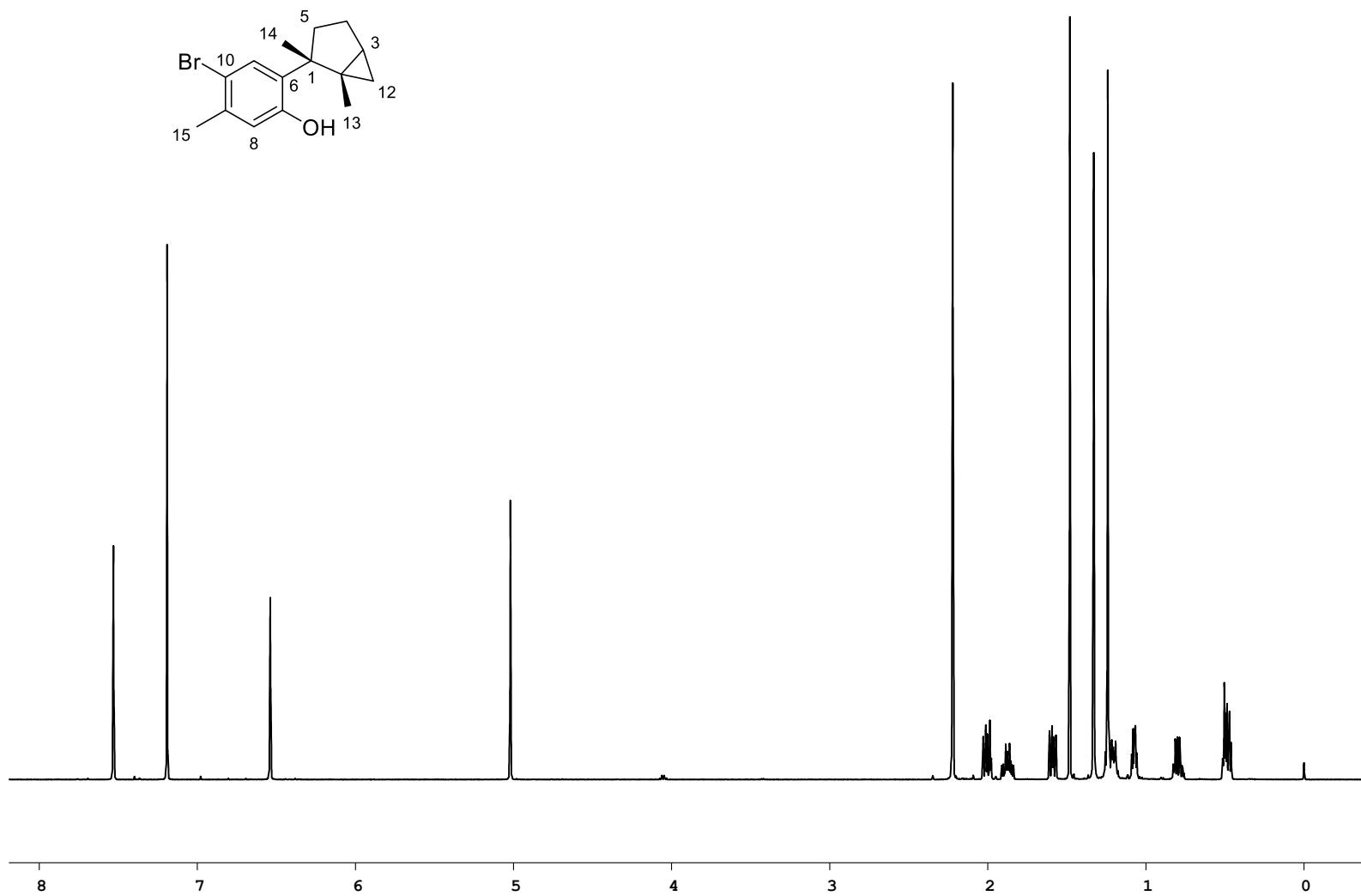


Figure S2. ^1H -NMR spectrum for isolaurinterol (**2**) (500 MHz, CDCl_3).

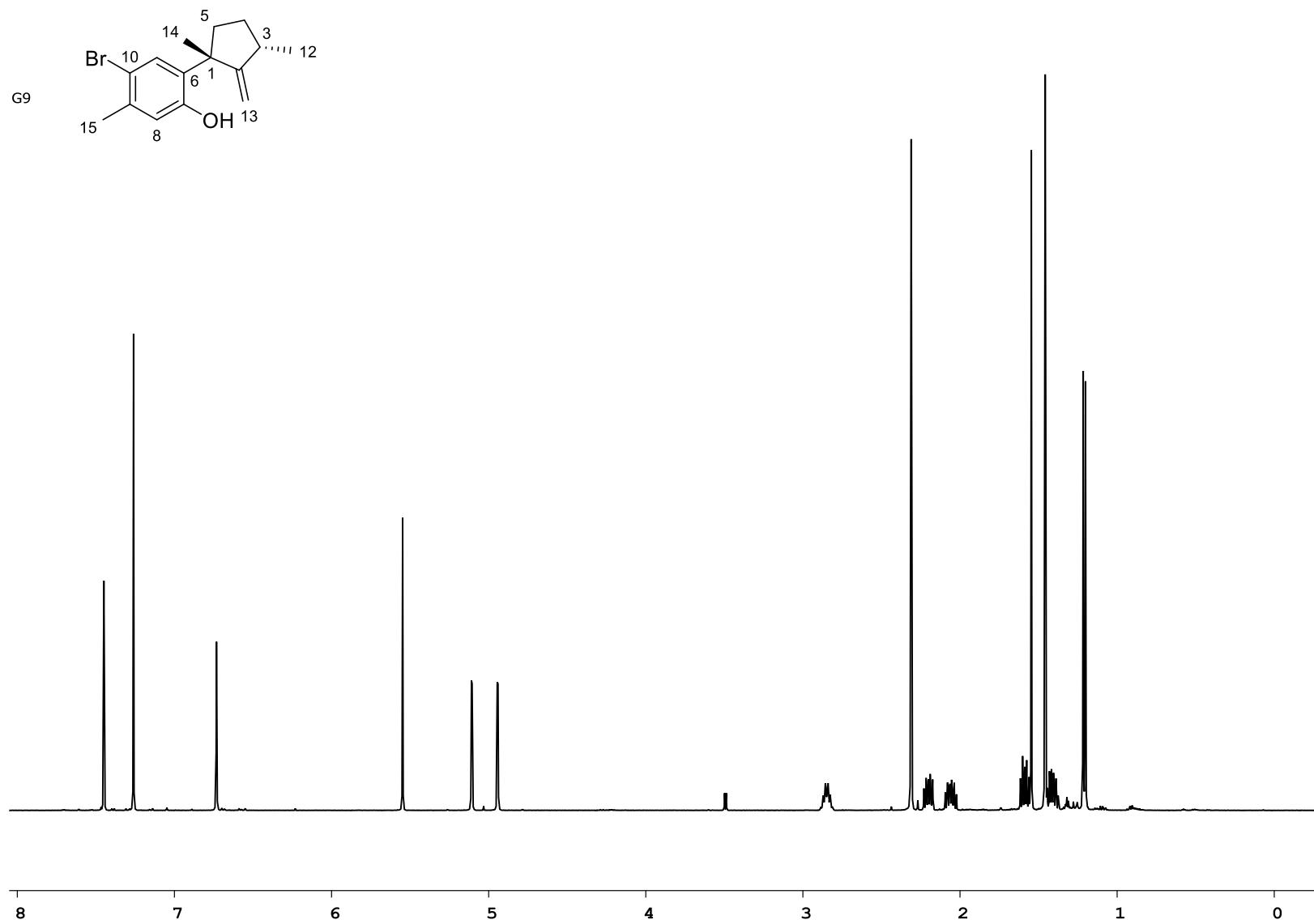


Figure S3. ^1H -NMR spectrum for aplysin (**3**) (500 MHz, CDCl_3).

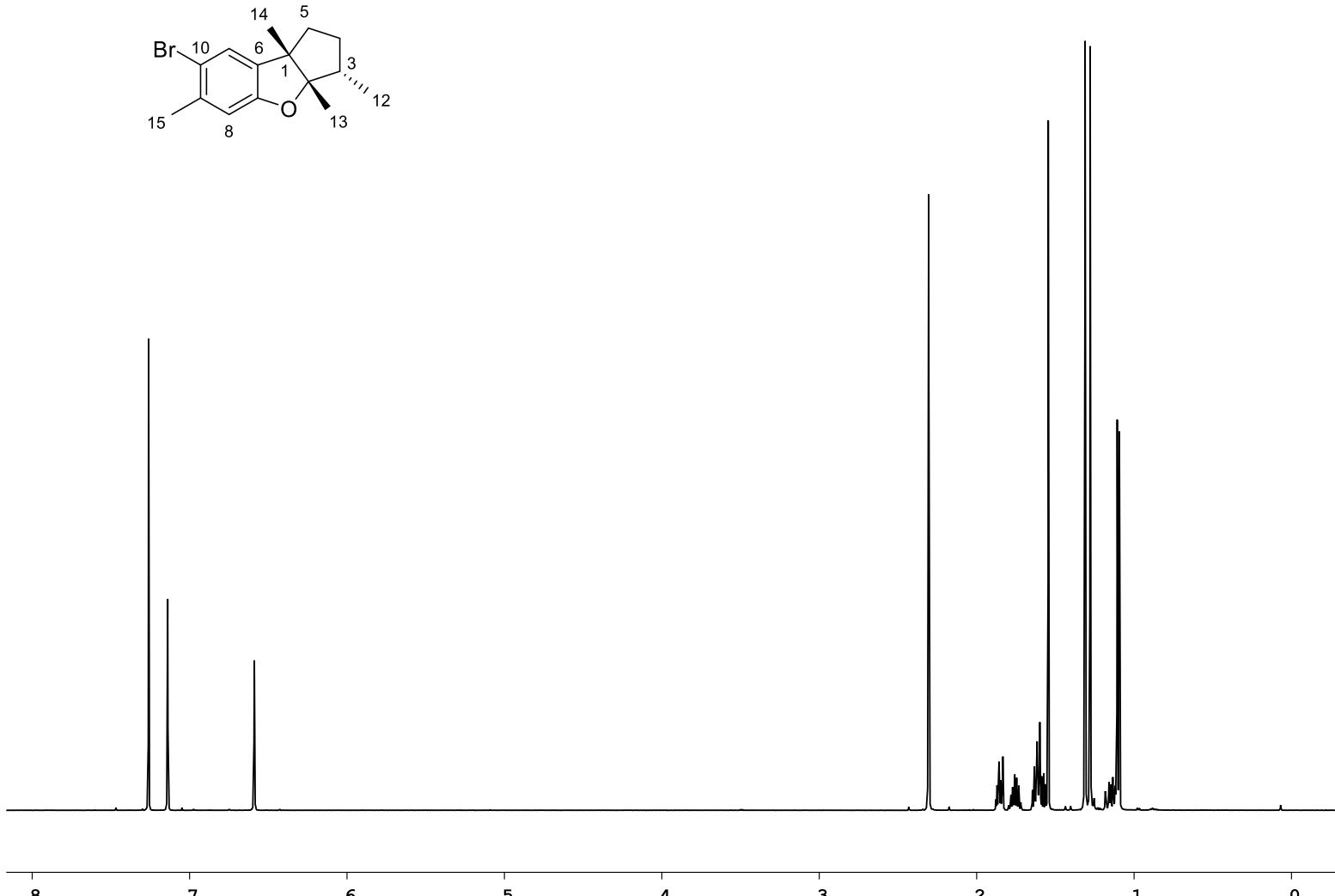


Figure S4. ^1H -NMR spectrum for α -bromocuparane (**4**) (500 MHz, CDCl_3).

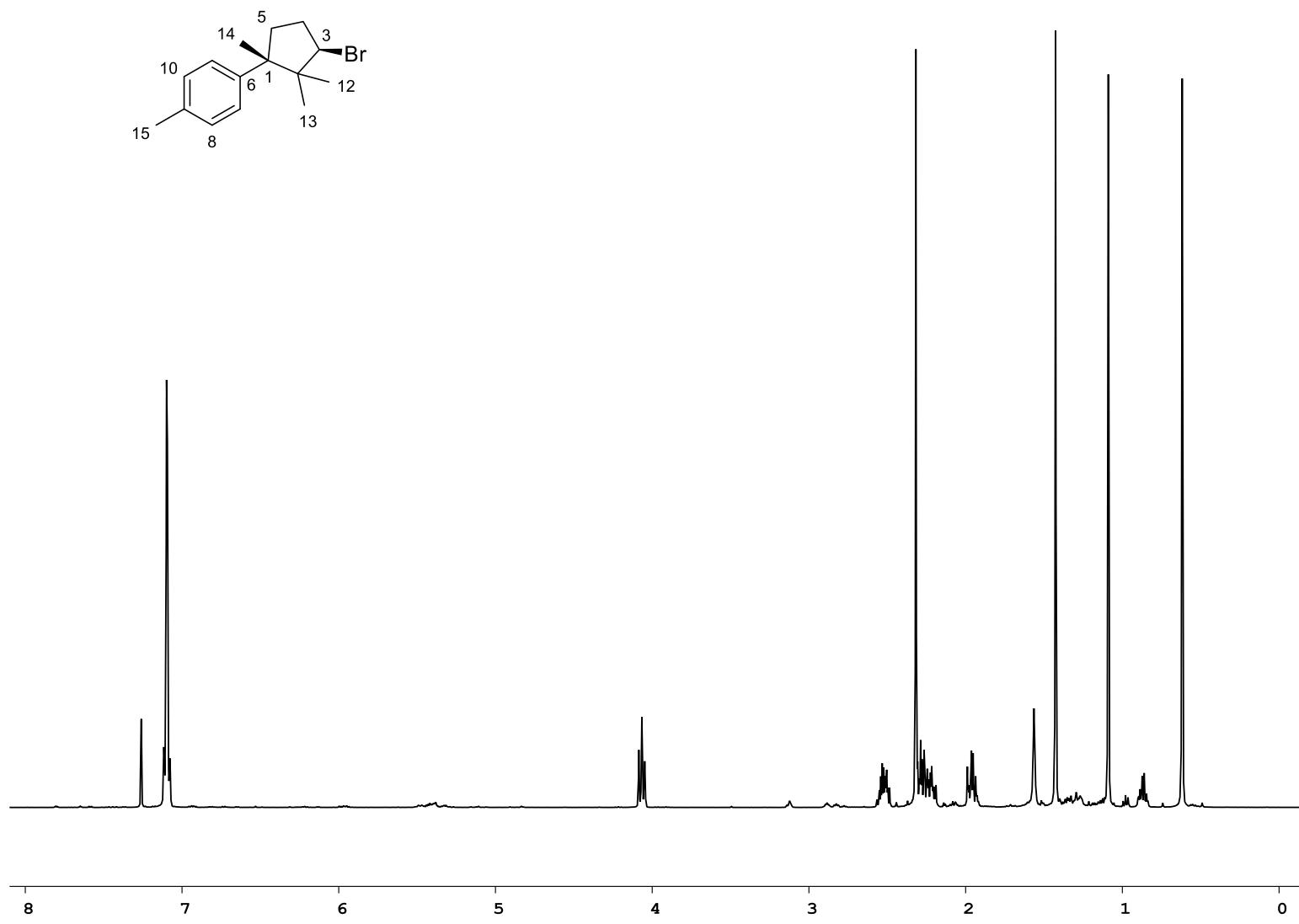


Figure S5. ^1H -NMR spectrum of α -isobromocuparane (**5**) (500 MHz, CDCl_3).

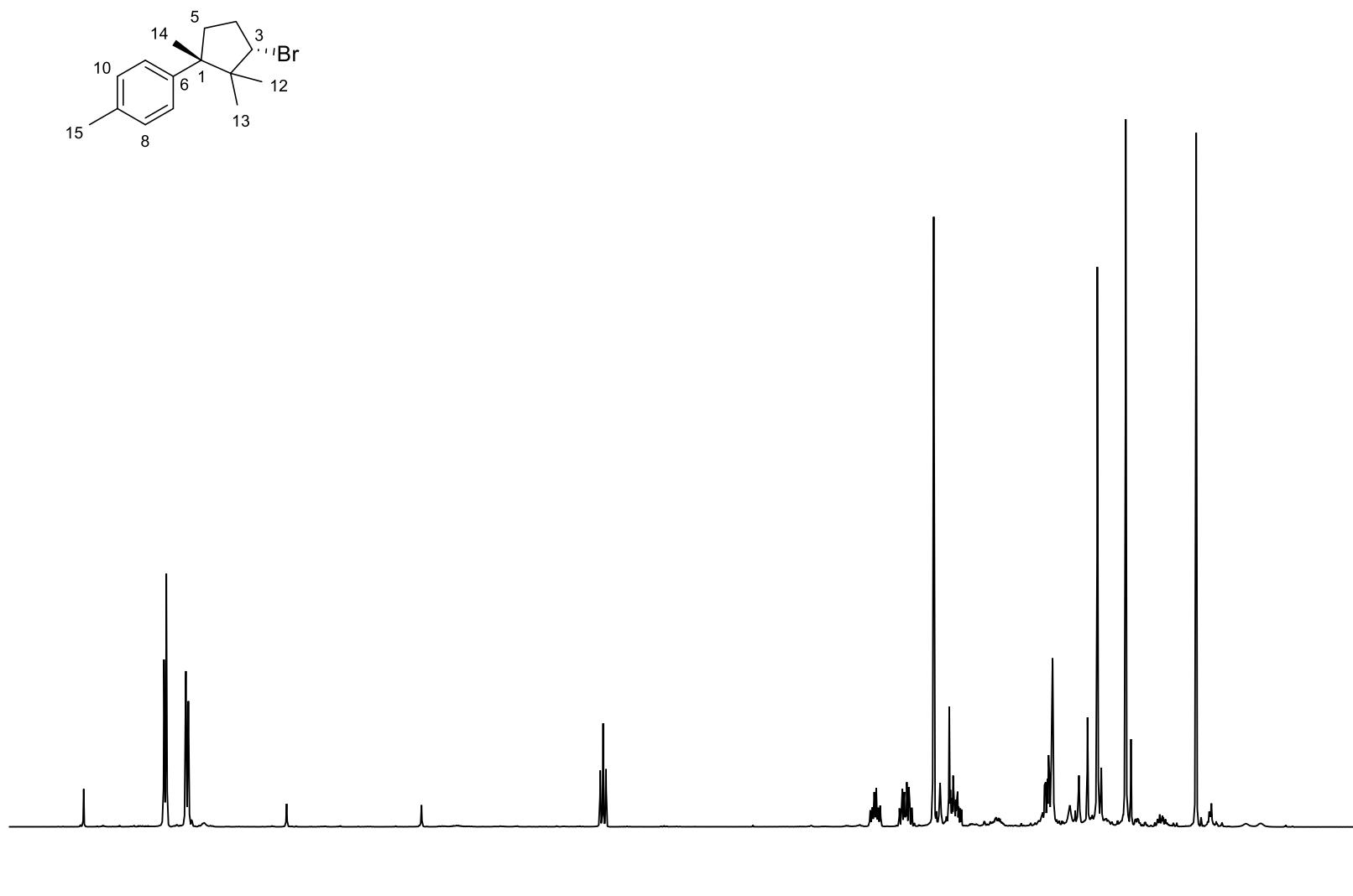


Figure S6. ^1H -NMR spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl_3).

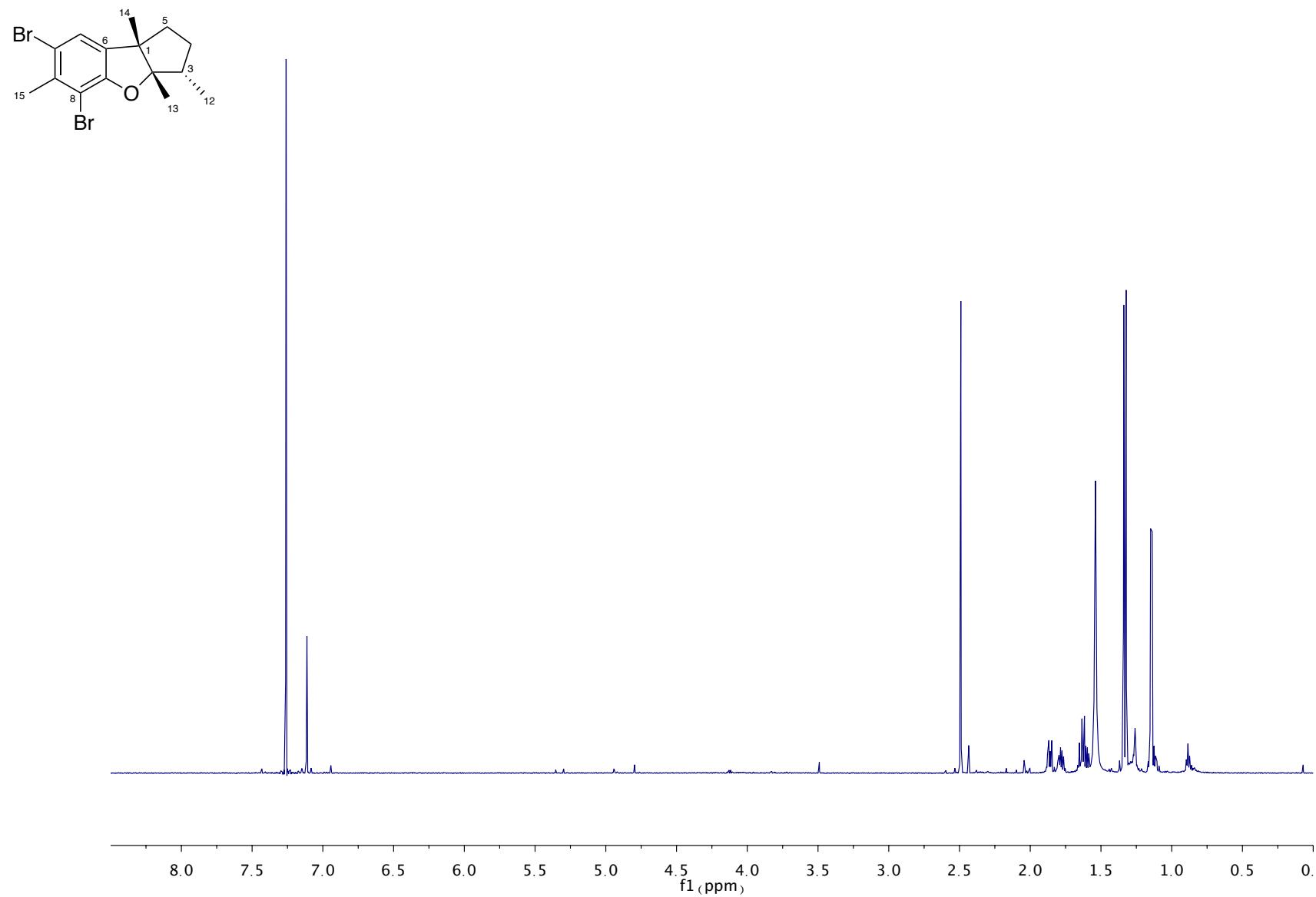
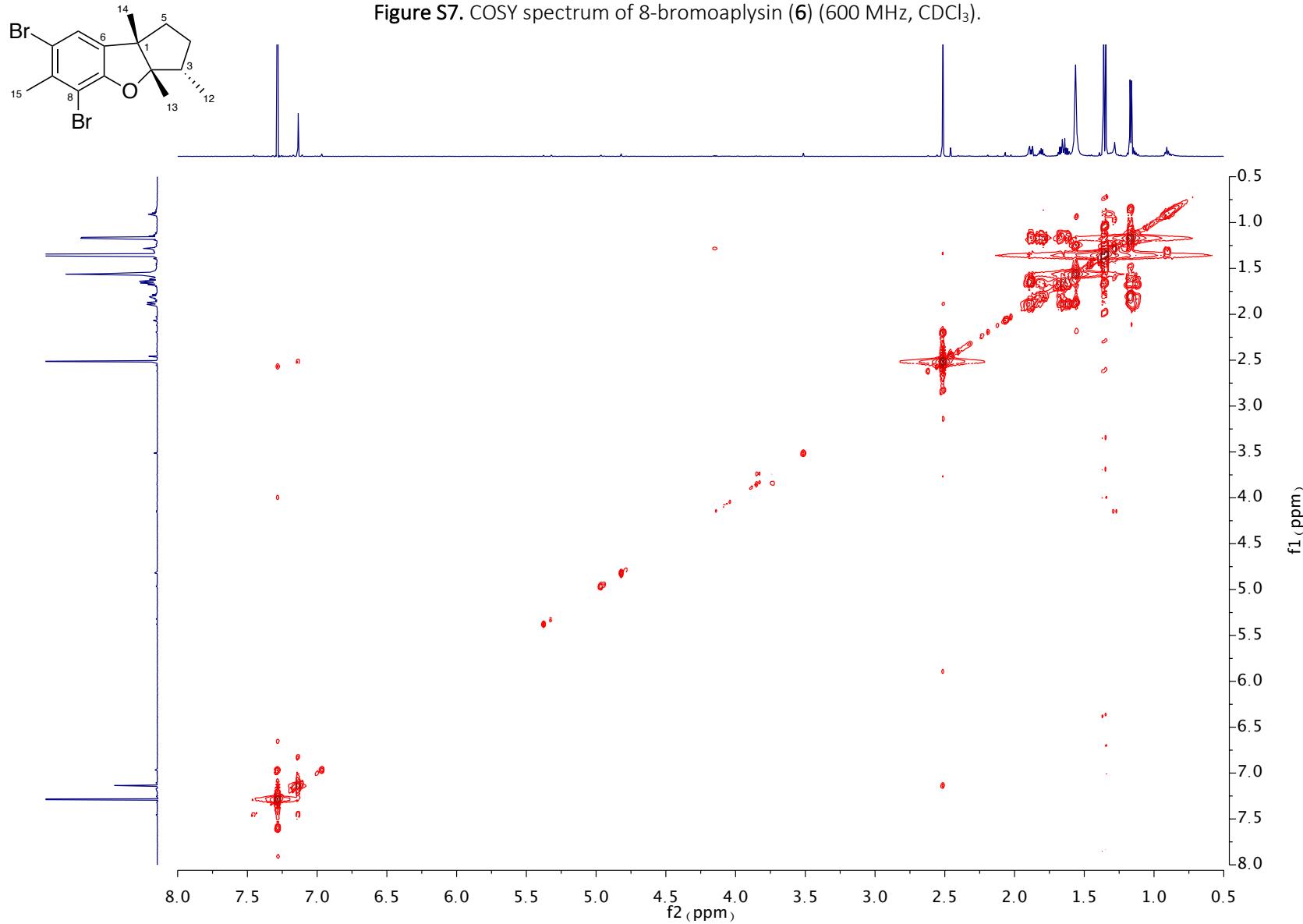


Figure S7. COSY spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl_3).



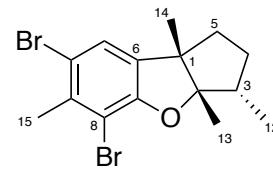
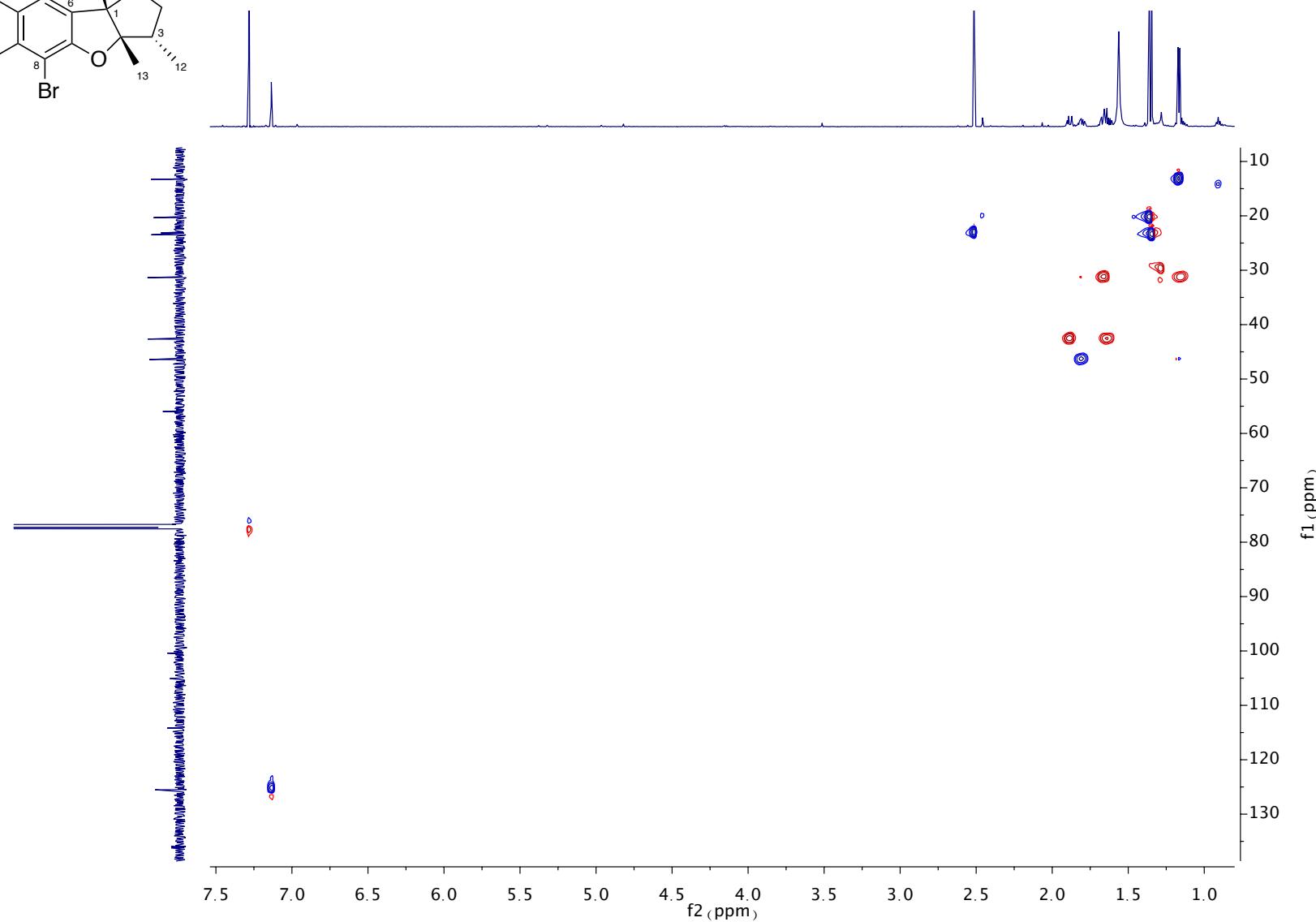


Figure S8. HSQC-ed spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl_3).



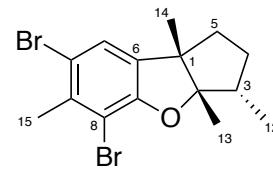


Figure S9. HMBC spectrum of 8-bromoaplysin (**6**) (600 MHz, CDCl_3).

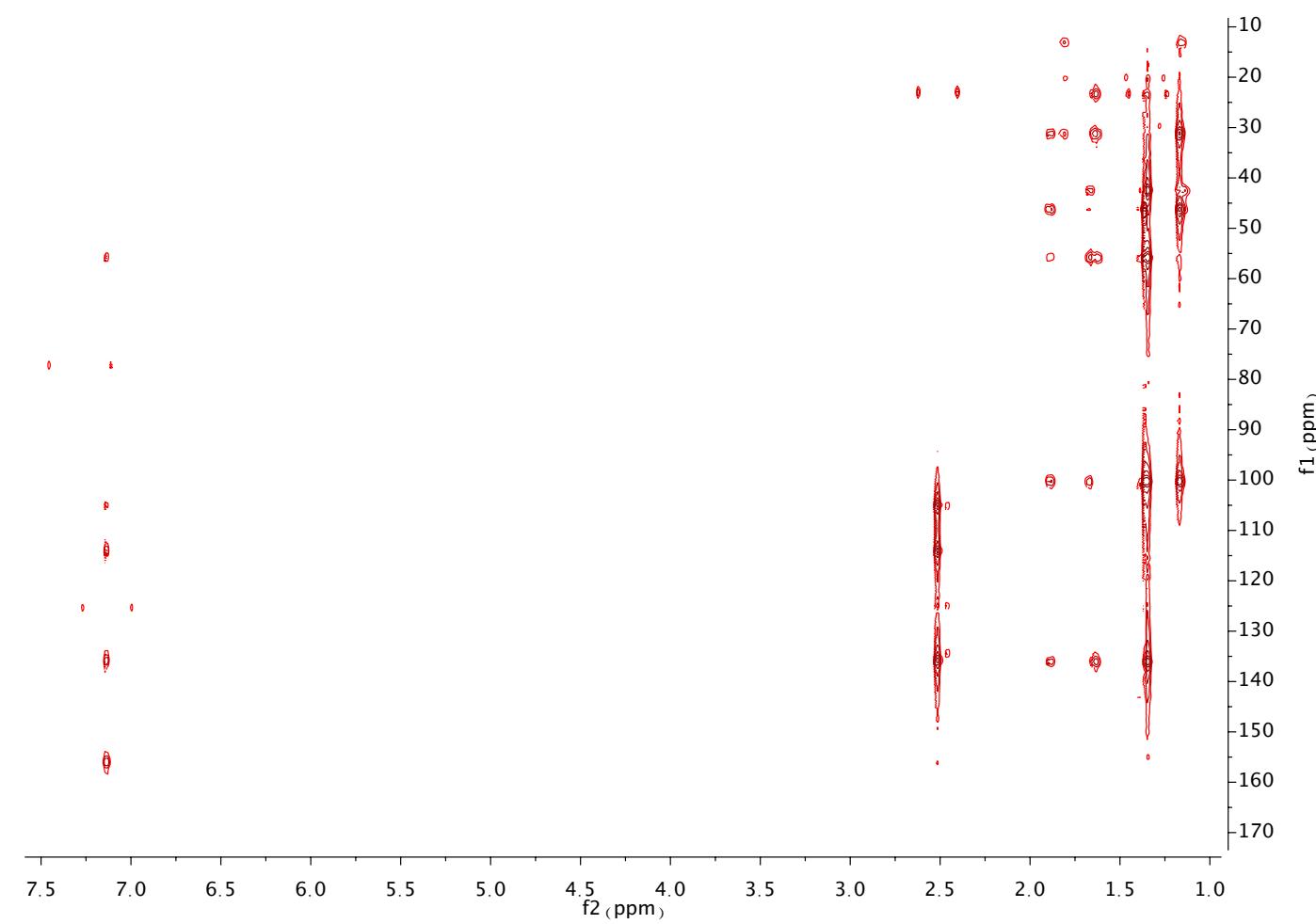


Figure S10. ^{13}C NMR spectrum of 8-bromoaplysin (**6**) (150 MHz, CDCl_3).

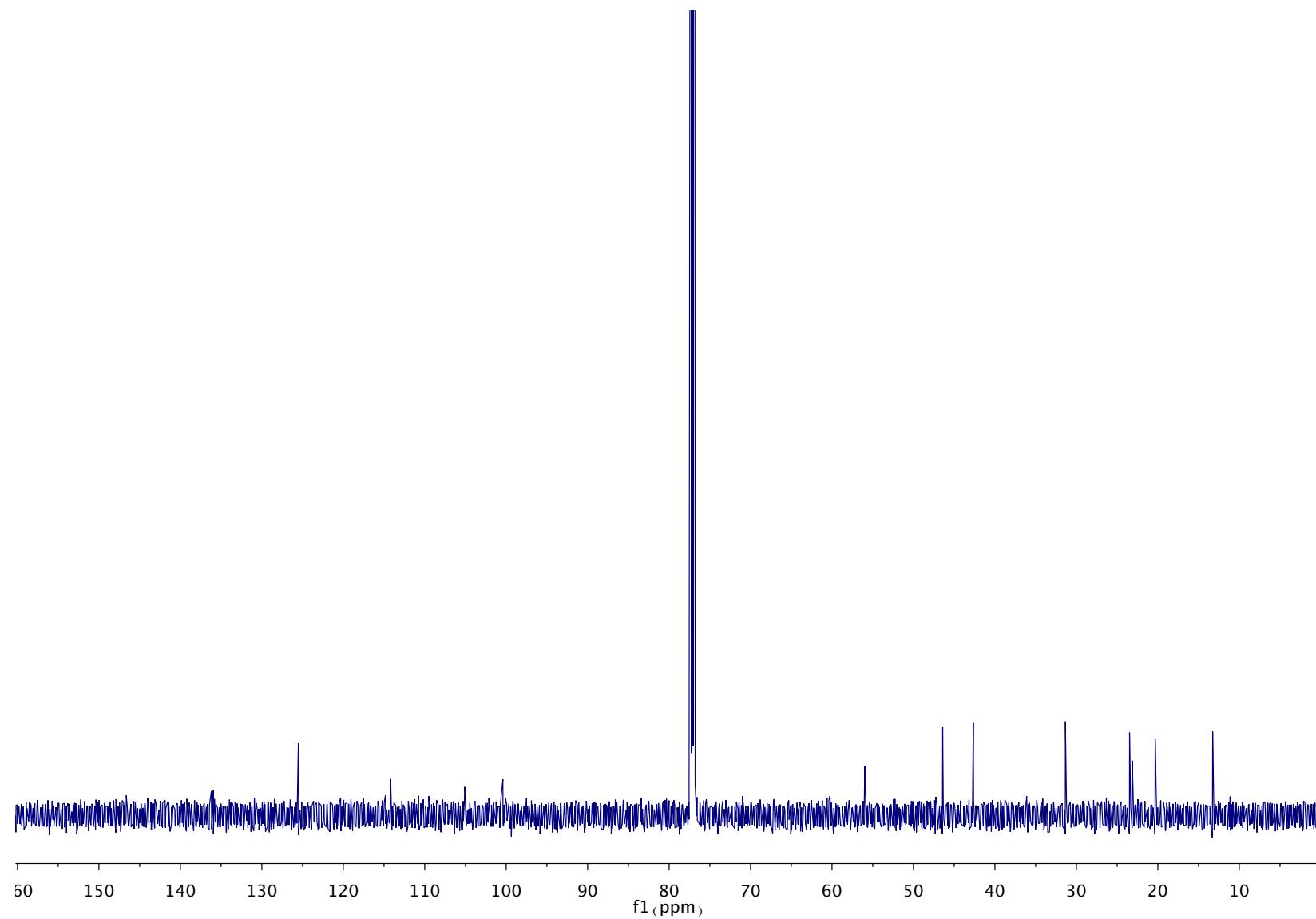


Figure S11. HREIMS spectrum of 8-bromoaplysin (6).

Elemental Composition Report

Page :

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

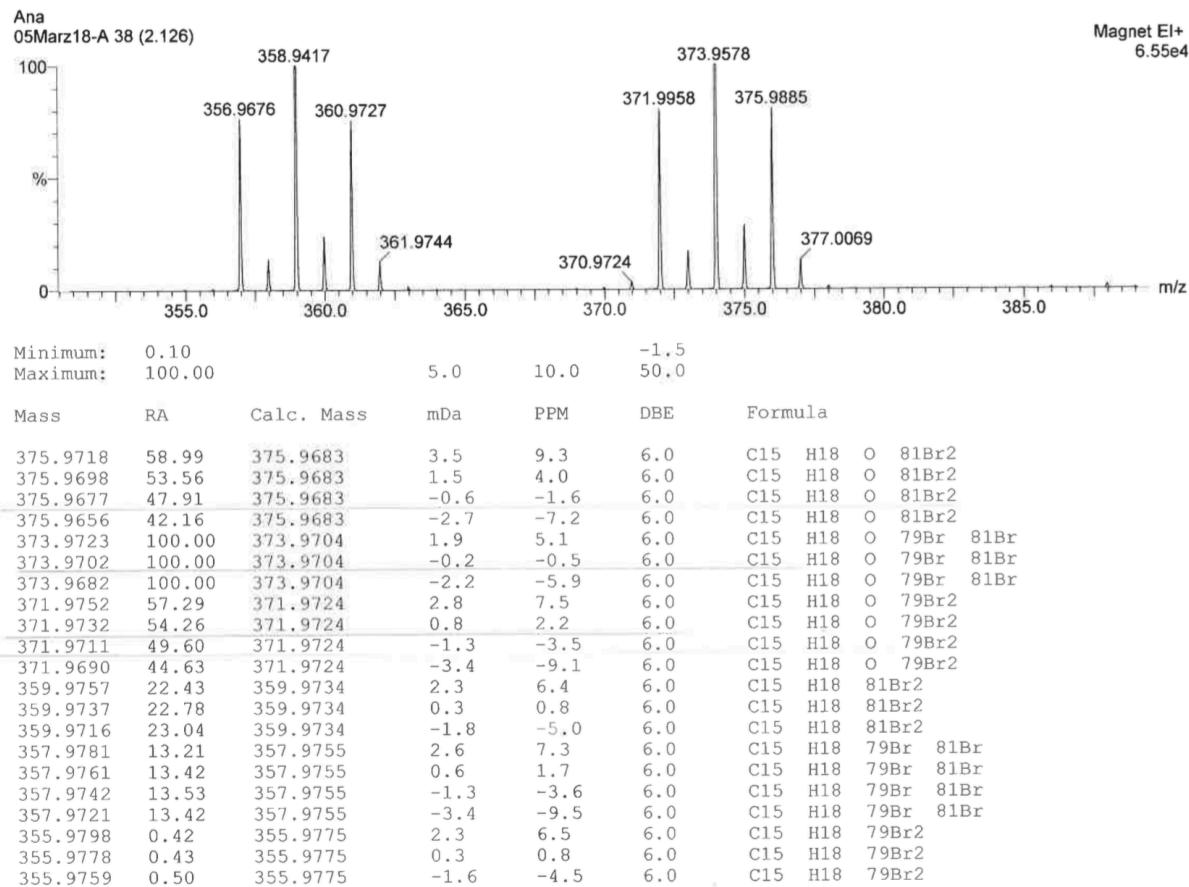
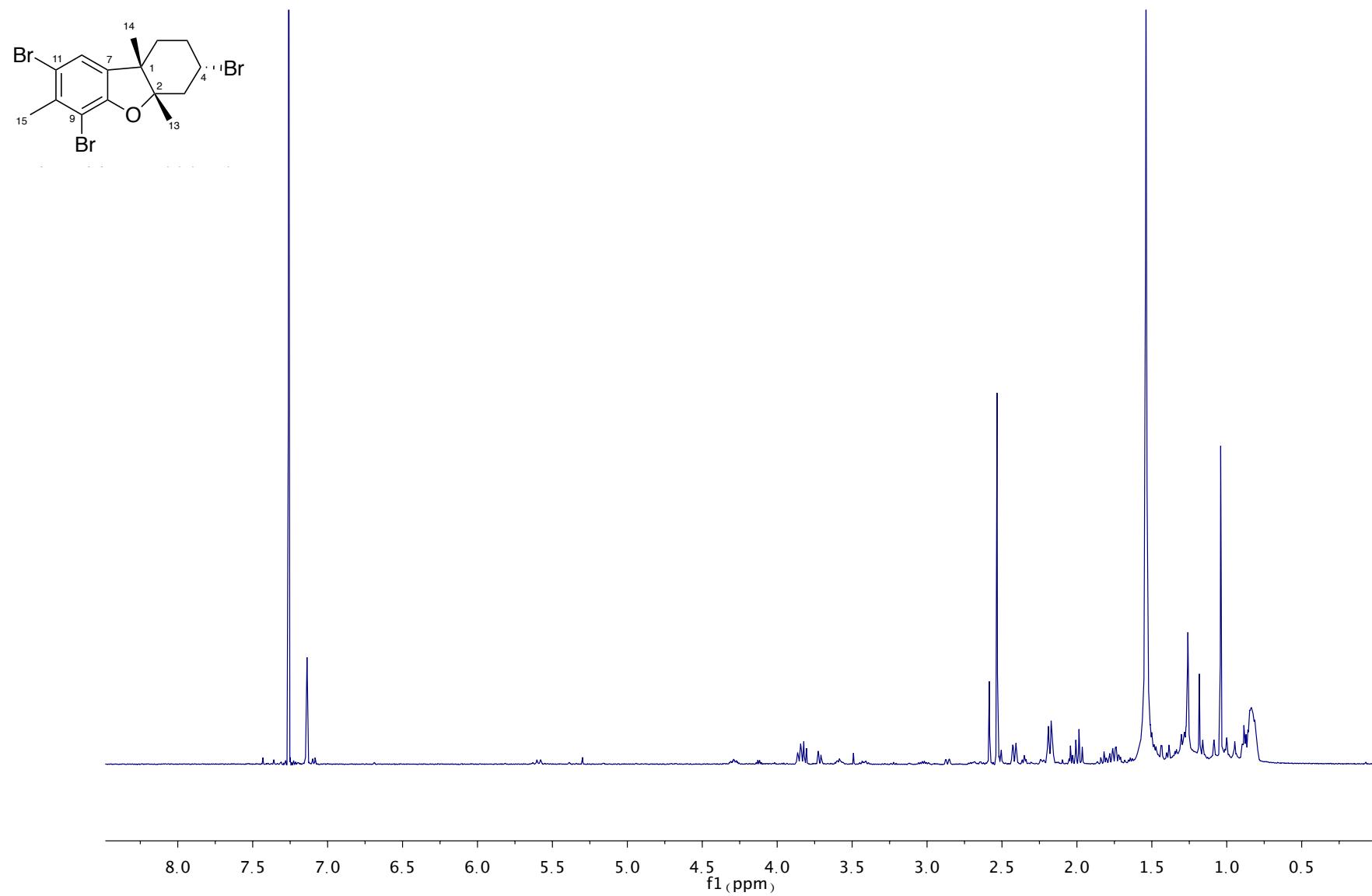
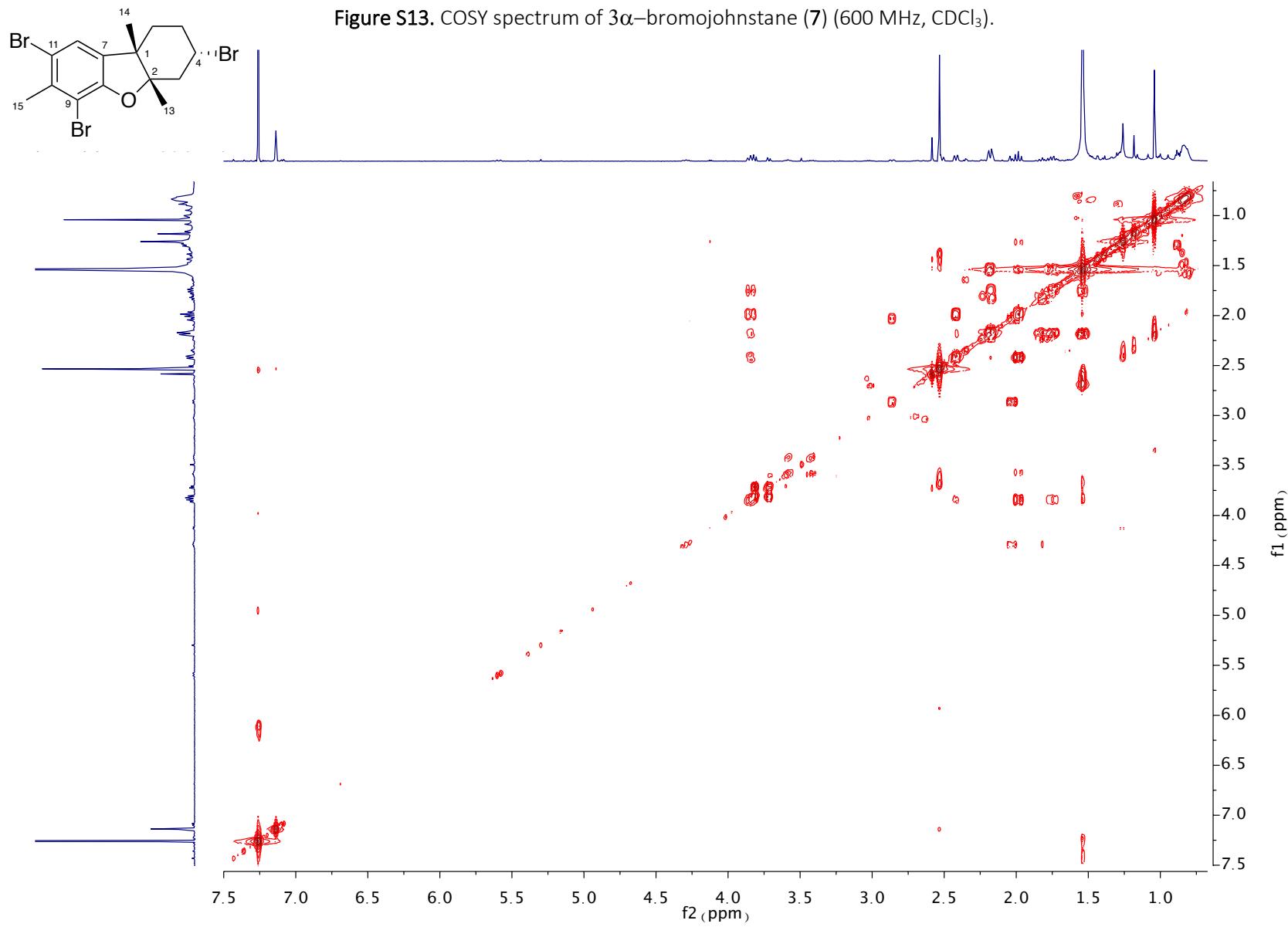
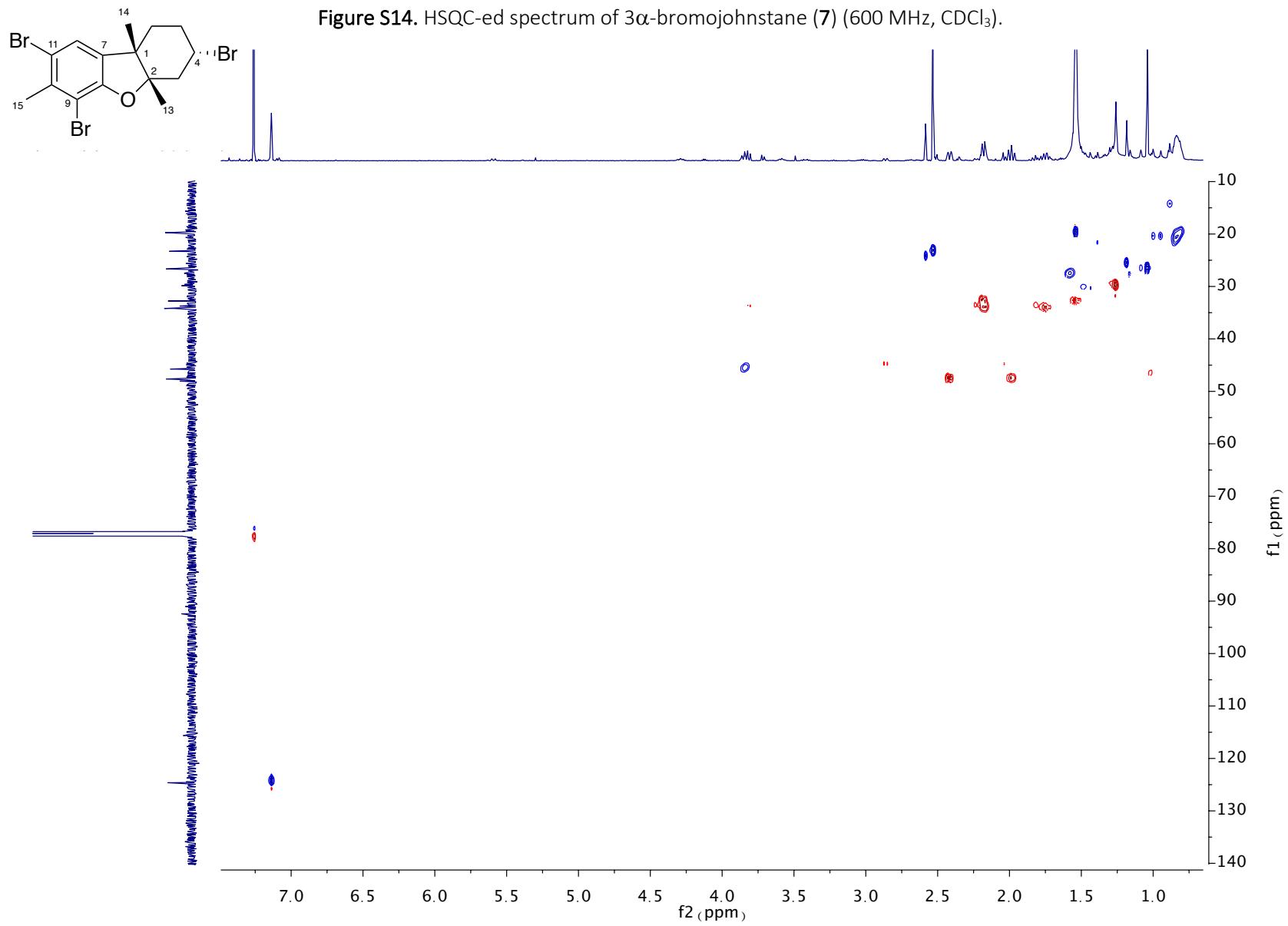
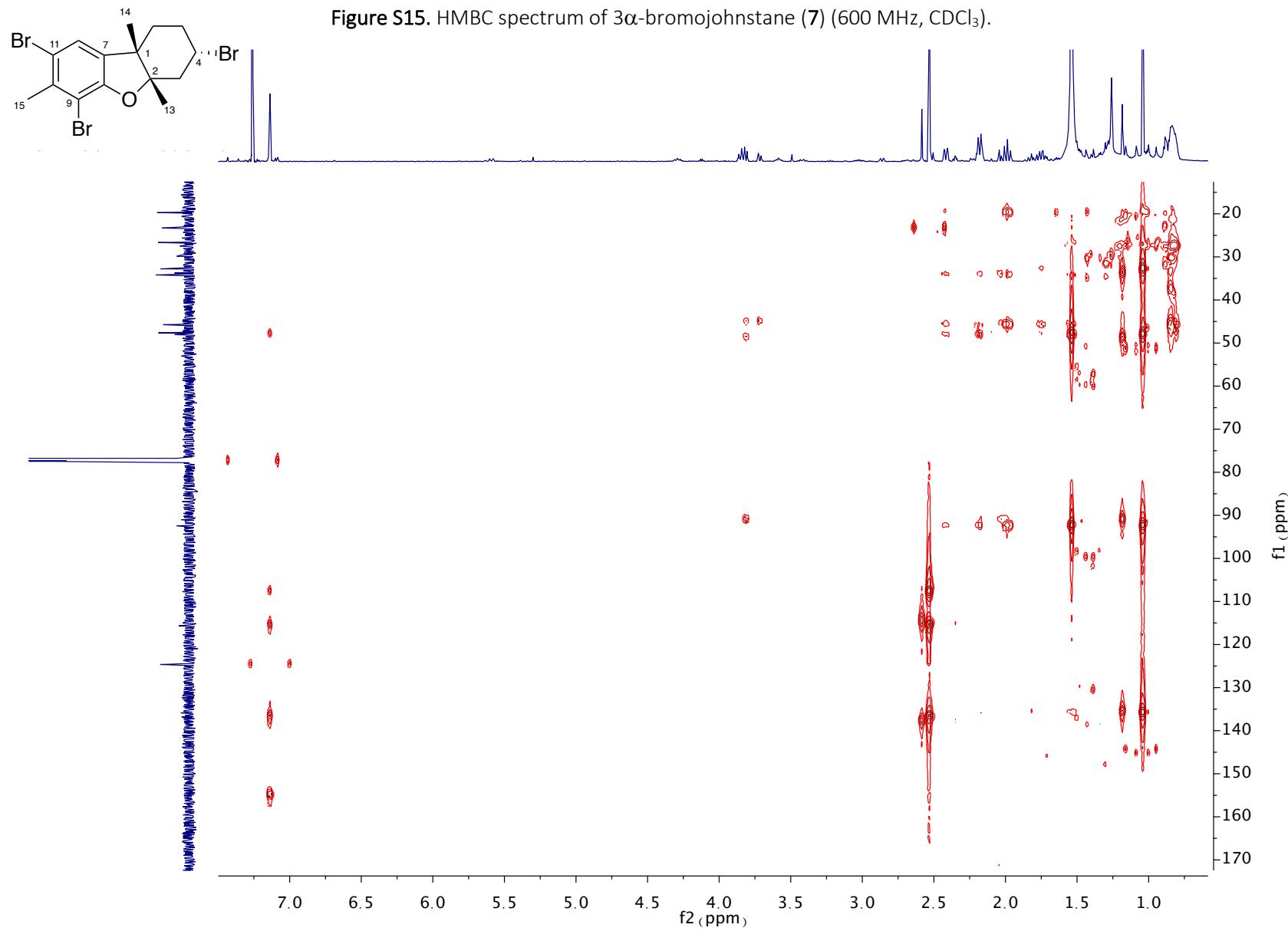


Figure S12. ^1H NMR spectrum of 3α -bromojohnstane (**7**) (600 MHz, CDCl_3).









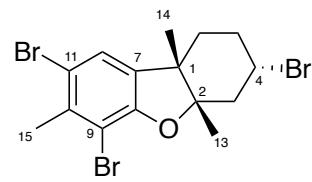


Figure S16. ^{13}C NMR spectrum of 3α -bromojohnstane (**7**) (150 MHz, CDCl_3).

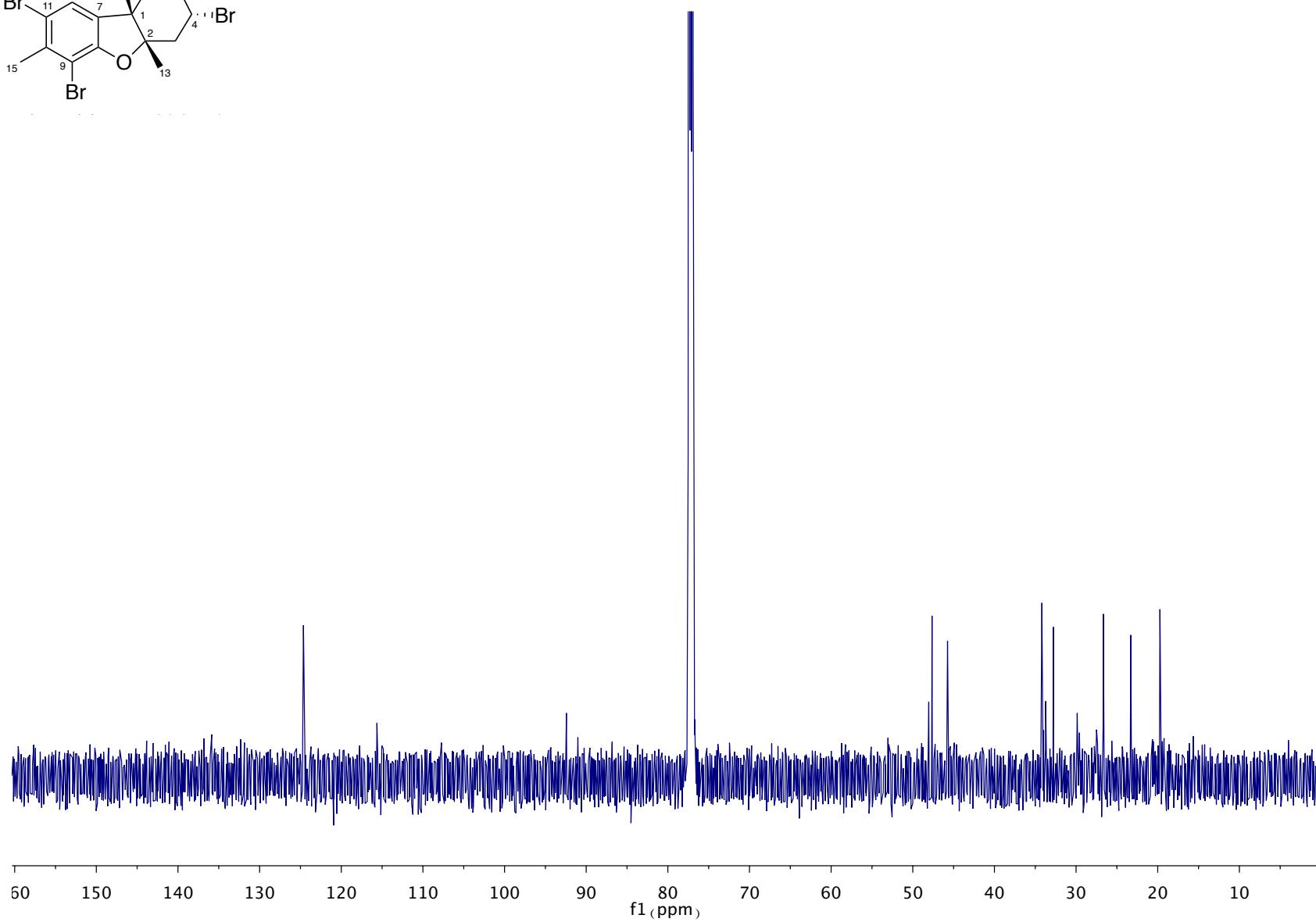


Figure S17. 1D-NOE experiments of 3α -bromojohnstane (**7**) (600 MHz, CDCl_3).

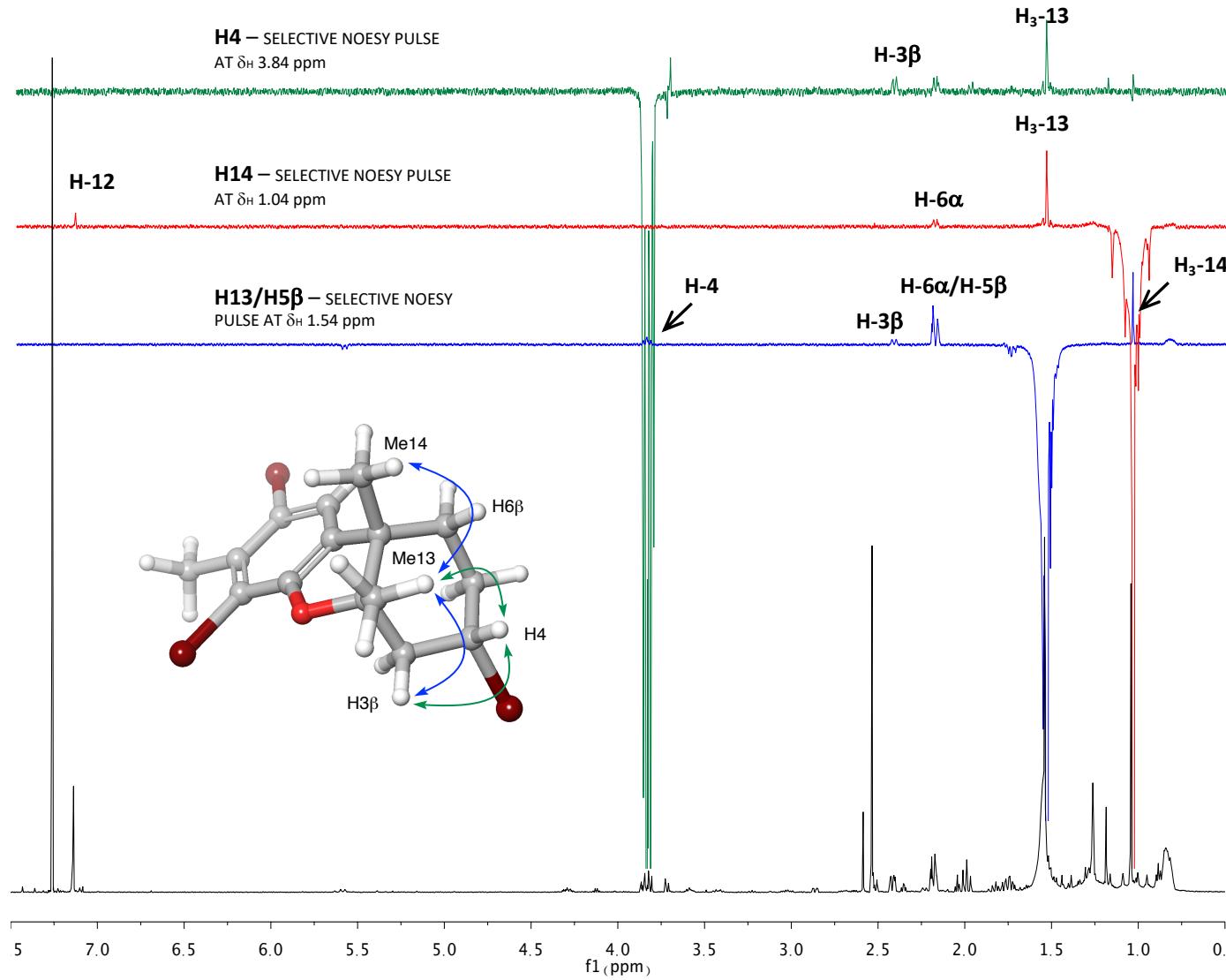


Figure S18. HREIMS spectrum of 3α -bromojohnstane (7).

Elemental Composition Report

Page 1 of

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

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

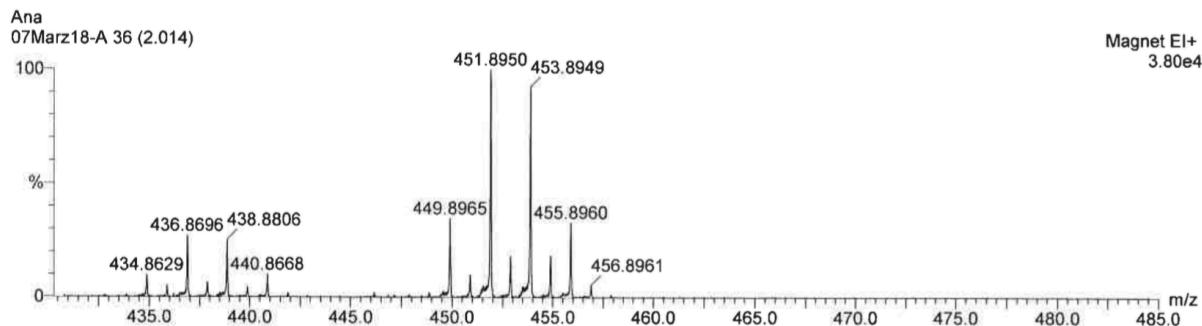
Selected filters: None

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



Minimum: 0.10 Maximum: 100.00

5.0 10.0

-1.5 50.0

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

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-dibromoisoaplysin (**8**) (500 MHz, CDCl_3).

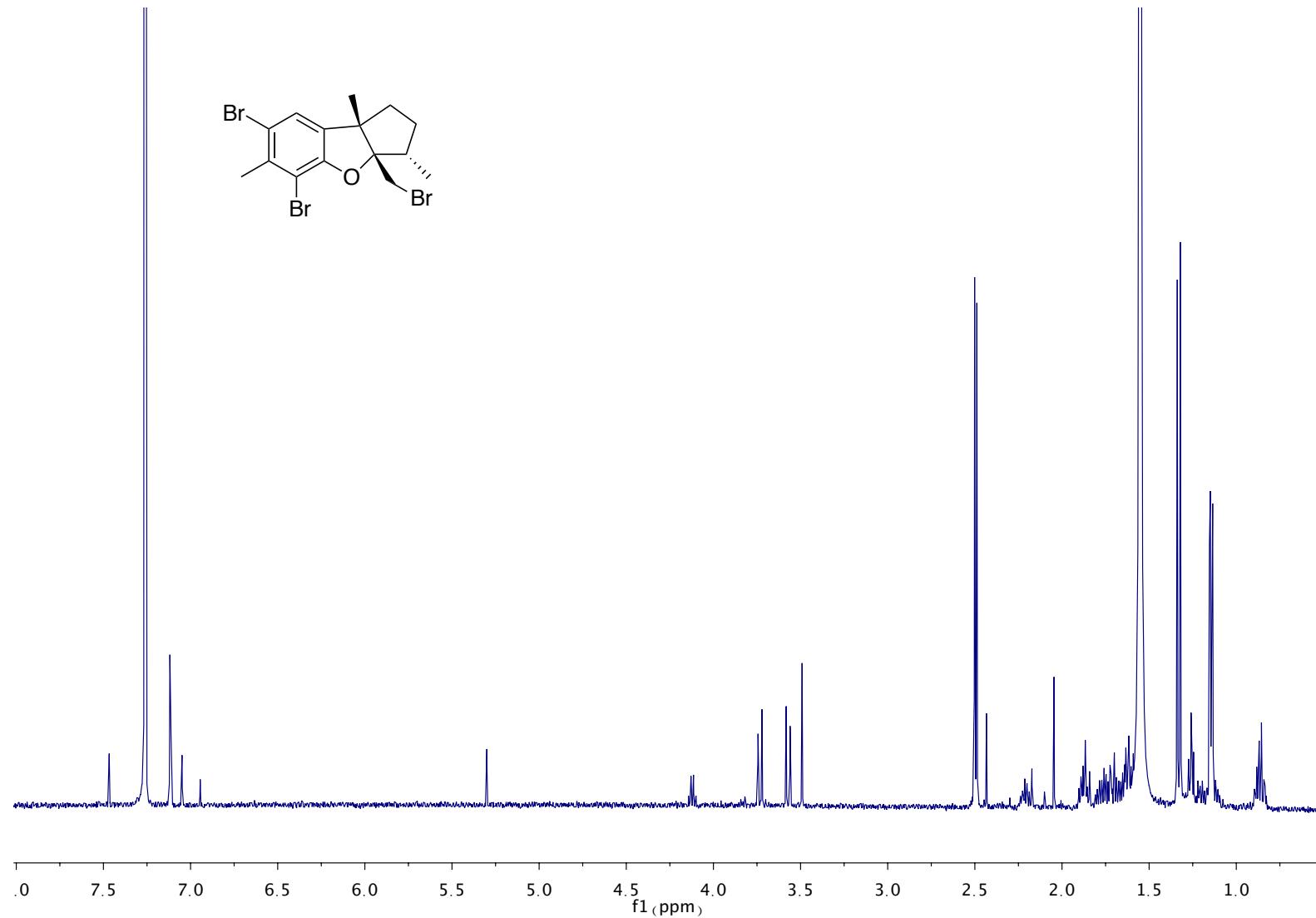


Figure S20. ^1H NMR spectrum of 8,10-dibromoaplysinol (**9**) (500 MHz, CDCl_3).

