Semi-synthesis and evaluation of sargahydroquinoic acid derivatives as potential antimalarial agents

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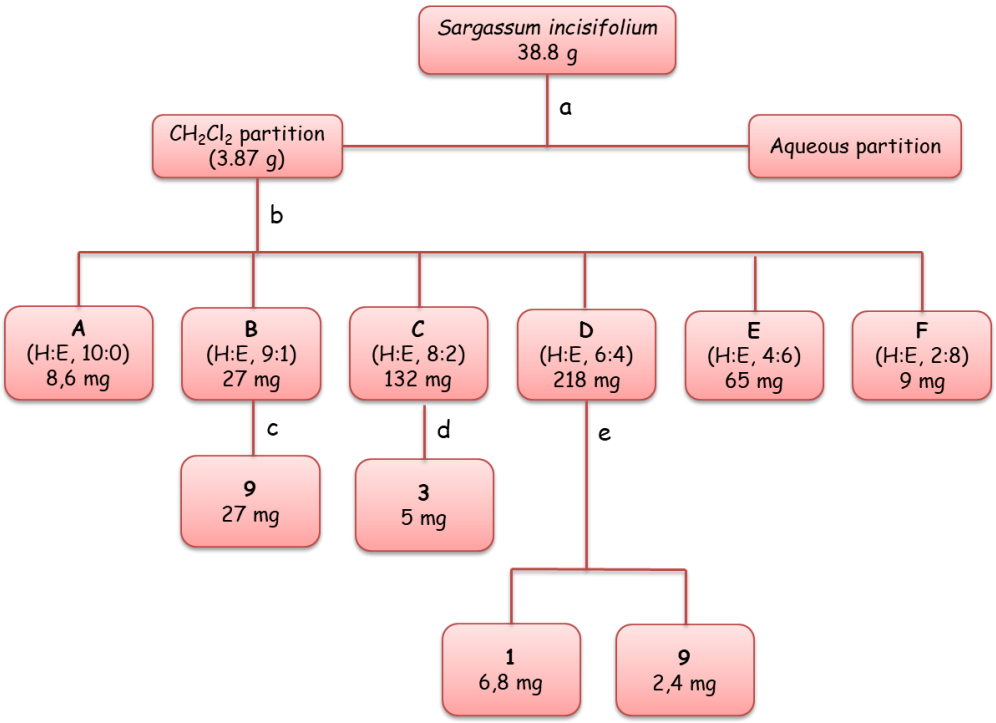
Supplementary data

Contents



Conditions: a) *i) MeOH extraction, ii) MeOH-CH_2Cl_2 (1:2) extraction, iii) combined extracts, collect CH_2Cl_2, concentrate,* b) *1,09 g extract, silica gel column chromatography (hexane-EtOAc gradient),* c) *silica gel column chromatography (hexane-EtOAc, 9:1),* d) *NP (Si) HPLC (hexane-EtOAc, 8:2),* e) *RP (C18) HPLC (MeOH-H2O, 9:1).*

Scheme S1. Isolation of compounds **1**, **3**, **7** and **9**

Table S1. Comparison of ^{13}C NMR data for compounds **1**, **3**-**9**

C #	δ_C							
	1	**3**	**4**	**5**	**6**	**7**	**8**	**9**
1	146.4	188.0	187.96	187.92	188.0	145.6	-	187.96
2	125.5	145.9	145.9	145.81	145.9	121.3	121.3	145.9
3	115.4	133.1	132.27	133.1	133.1	110.3	126.3	132.3
4	148.7	187.9	187.91	187.87	188.0	148.5	117.0	187.91
5	113.9	132.2	132.12	132.11	132.2	117.1	148.6	132.1
6	127.6	148.5	148.4	148.38	148.5	126.3	110.3	148.4
7	16.1	17.7	15.99	16.07	17.7	15.7	15.9	16.0
1′	29.9	27.5	27.33	27.48	27.5	122.9	124.1	27.3
2′	121.7	117.9	118.2	117.97	118.1	130.7	-	118.2
3′	138.2	139.8	139.9	139.78	139.7	77.8	77.8	139.9
4′	39.5	39.6	39.5	39.56	39.8	40.8	40.7	39.5
5′	26.0	26.3	26.4	26.37	26.2	22.6	22.6	26.4
6′	124.2	124.5	125.5	124.39	124.7	124.9	124.7	125.5
7′	134.7	134.6	133.6	134.6	135.0	134.3	134.8	133.6
8′	39.0	39	39.38	39.09	39.5	39.1	39.8	39.4
9′	28.3	28.2	27.54	27.95	26.3	28.1	27.0	27.5
10′	145.5	145.4	145.9	142.06	-	144.9	145.0	154.9
11′	130.5	130.6	132.1	131.36	131.2	130.5	130.6	132.1
12′	34.5	34.5	27.33	34.66	35.2	34.5	35.1	27.3
13′	27.8	27.9	27.45	27.82	27.1	27.9	26.1	25.7
14′	123.4	123.4	123.6	123.46	124.2	123.4	122.9	123.6
15′	132.3	132.2	133.2	133.1	133.7	132.3	131.8	133.2
16′	25.7	25.6	25.15	25.61	25.6	25.7	25.7	25.2
17′	17.7	16.1	17.72	17.59	16.1	17.7	17.7	17.7
18′	172.4	172.7	190.9	168.42	62.8	172.9	60.3	205.4
19′	16.0	16	16.04	15.93	16.1	15.5	15.5	16.0
20′	16.1	16.1	16.1	15.84	16.0	25.9	25.9	16.1
Me				51.03				

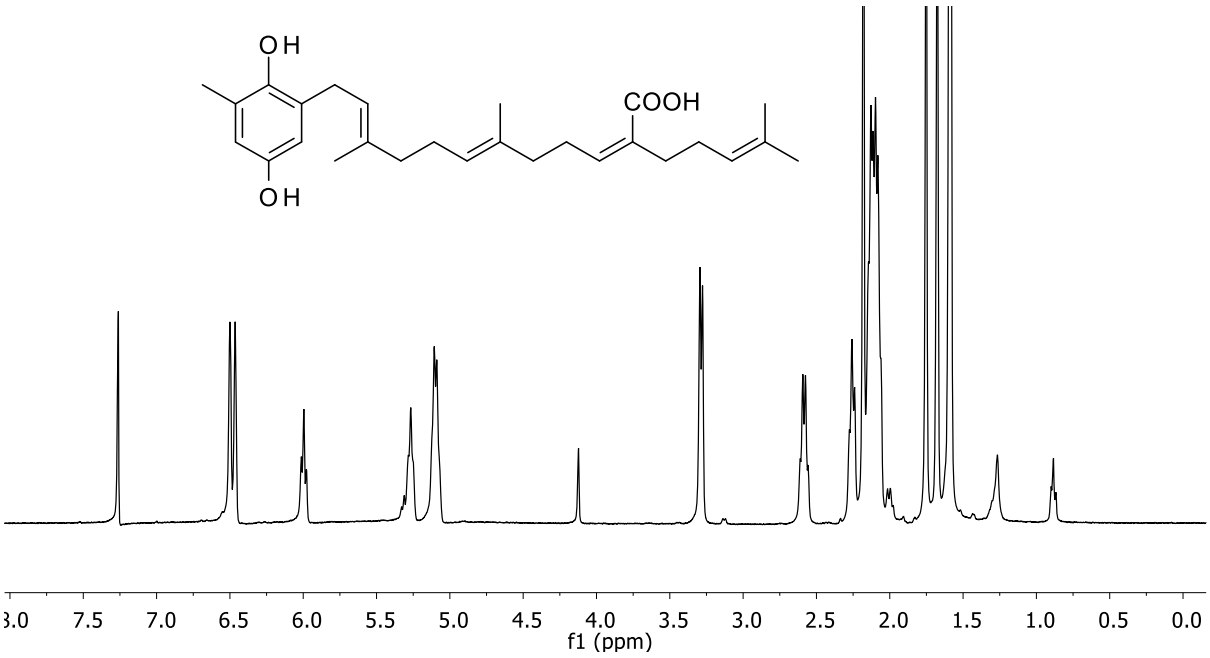


Figure S1. ^{1}H NMR spectrum of sargahydroquinoic acid (**1**) (400 MHz, $CDCl_3$)

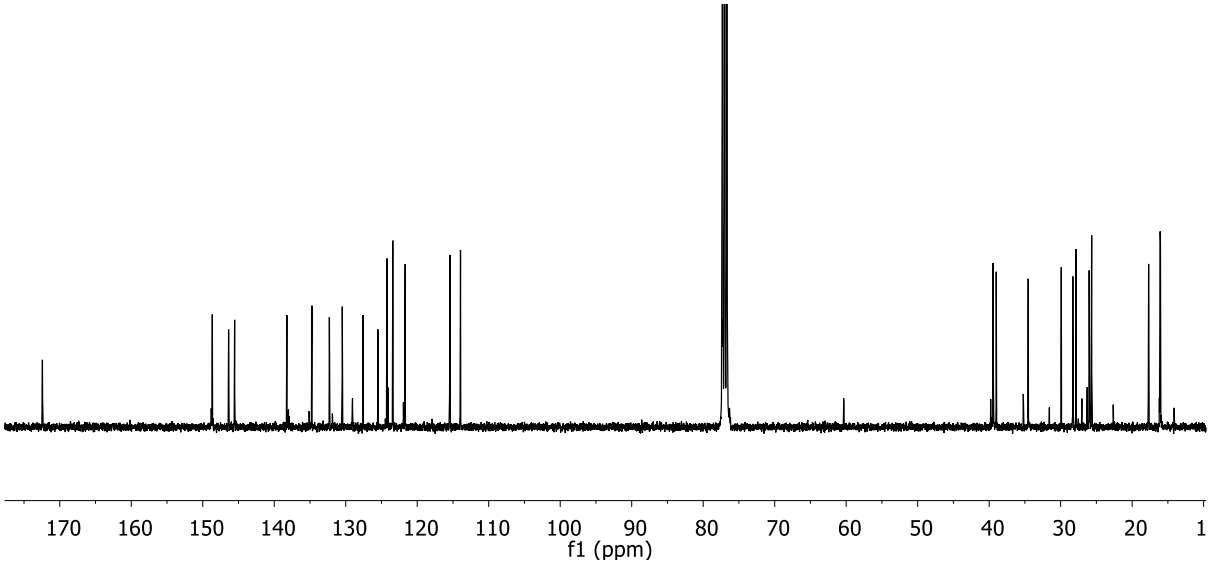


Figure S2. ^{13}C NMR spectrum of sargahydroquinoic acid (**1**) (100 MHz, $CDCl_3$)

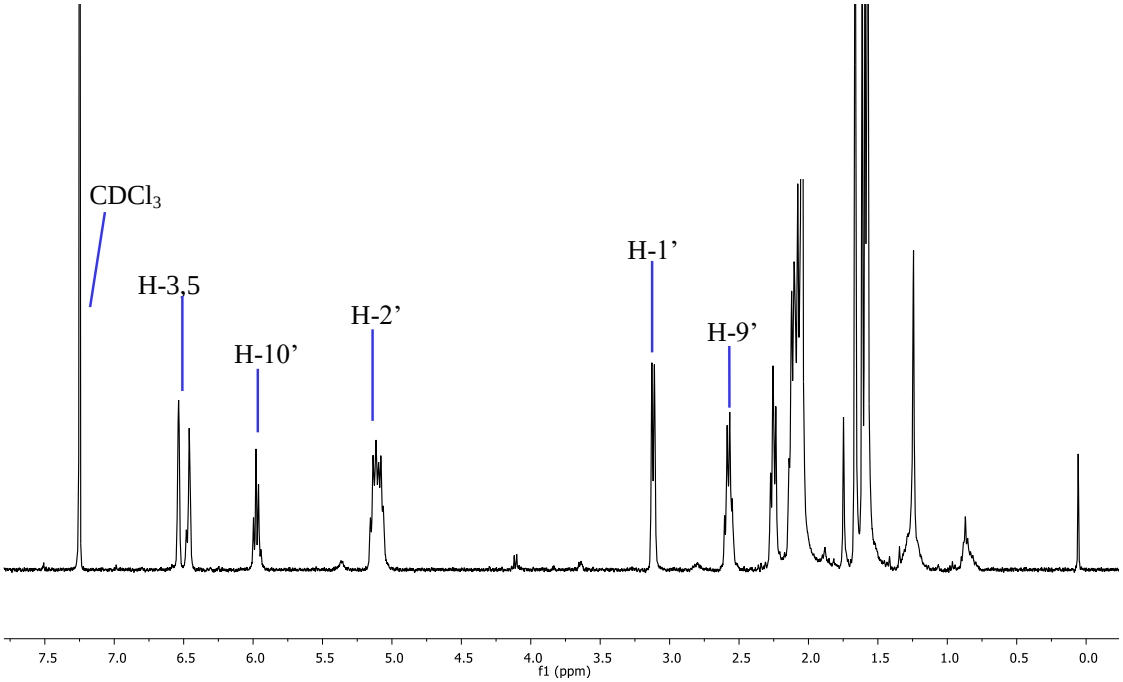


Figure S3. ^{1}H NMR spectrum of sargaquinoic acid **(3)** (400 MHz, $CDCl_3$)

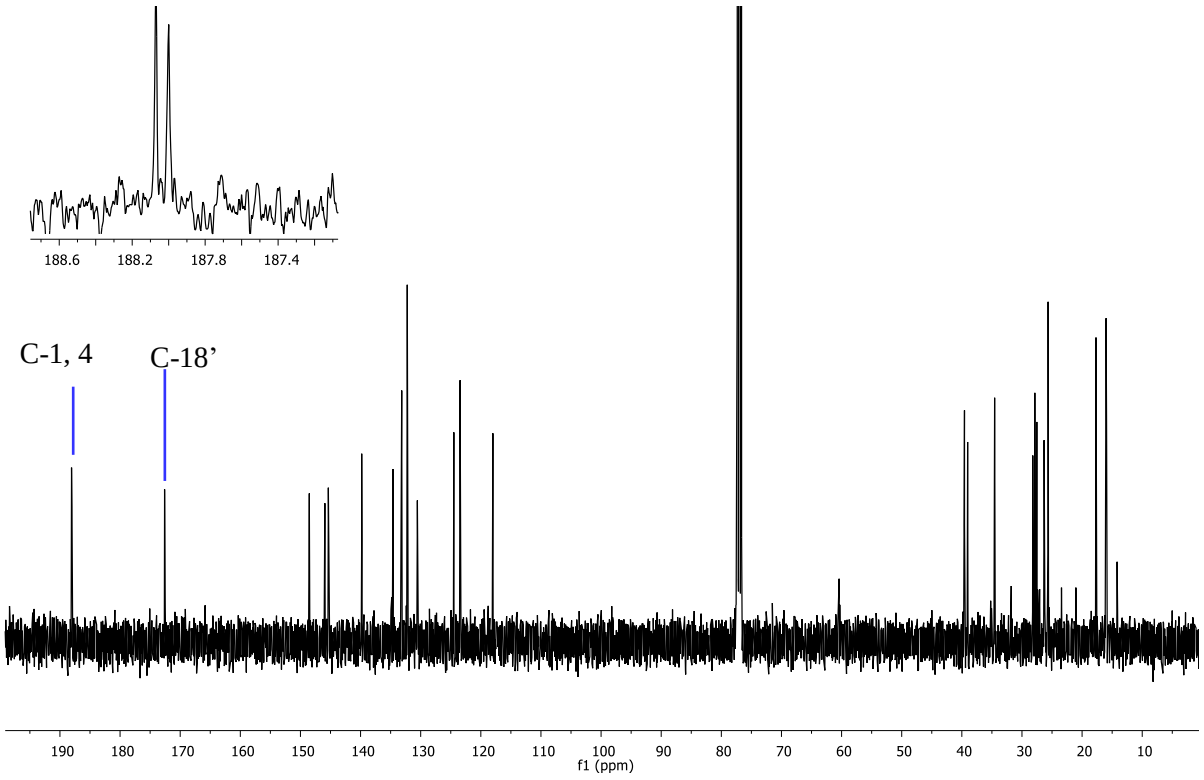


Figure S4. ^{13}C NMR spectrum of compound **3** (400 MHz, $CDCl_3$)

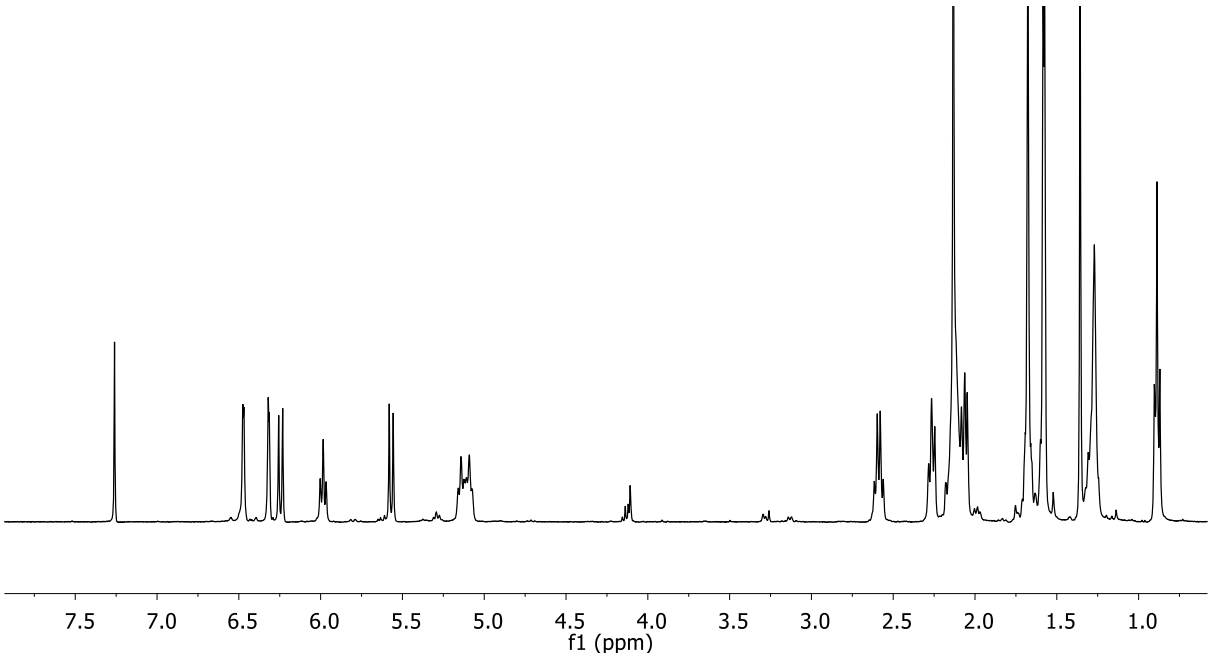


Figure S5. ^{1}H NMR spectrum of sargachromenol (**7**) (400 MHz, $CDCl_3$)

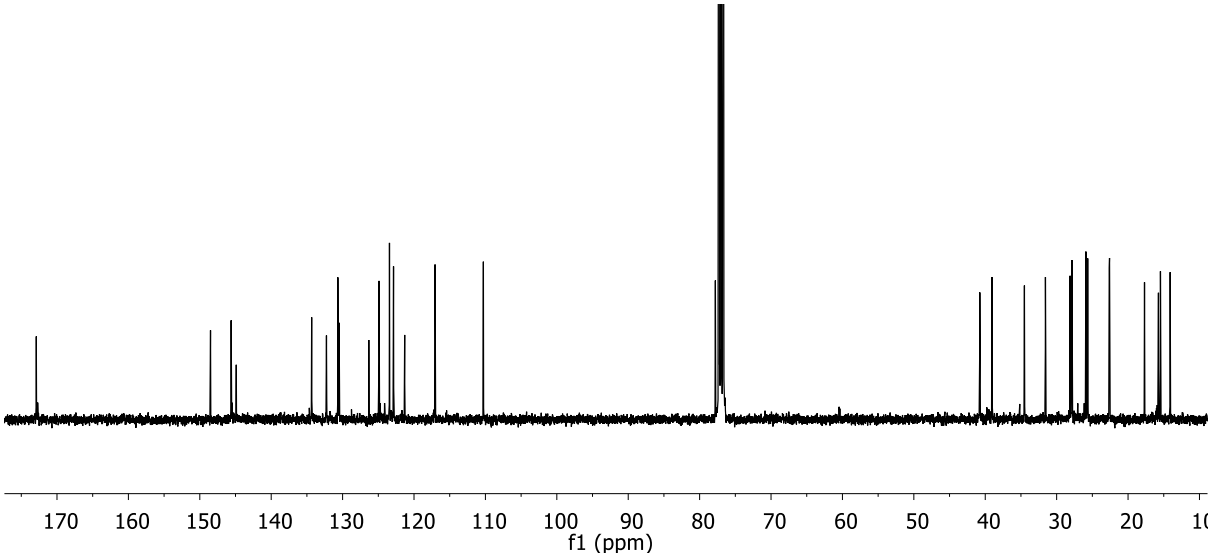


Figure S6. ^{13}C NMR spectrum of sargachromenol (**7**) (100 MHz, $CDCl_3$)

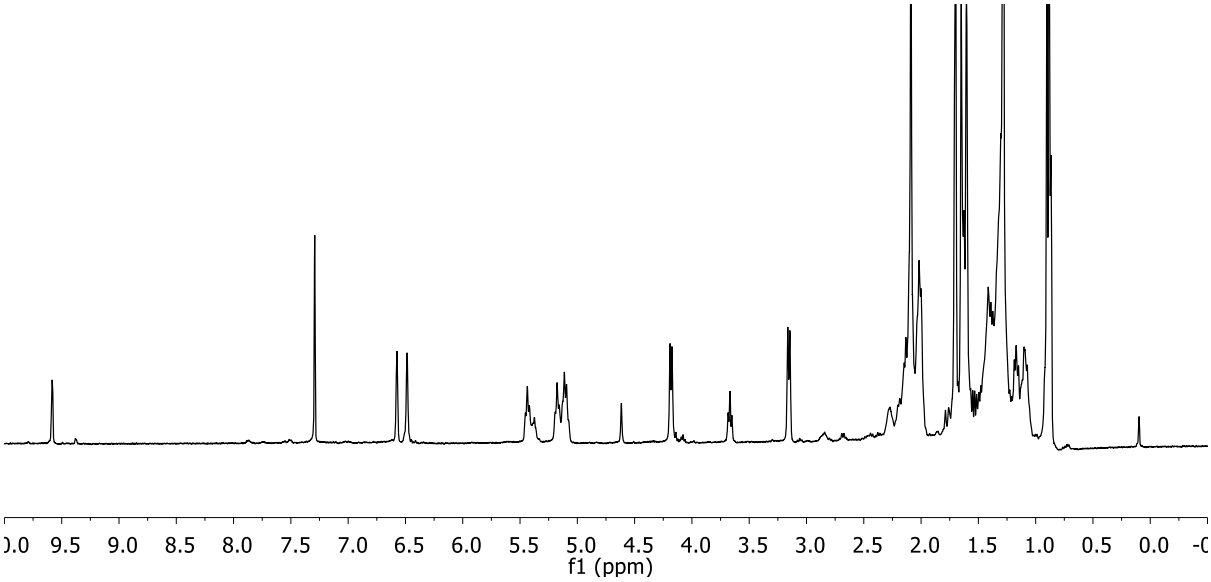


Figure S7. ^{1}H NMR spectrum of 10′*E*-sargaquinal (**9**) (400 MHz, $CDCl_3$)

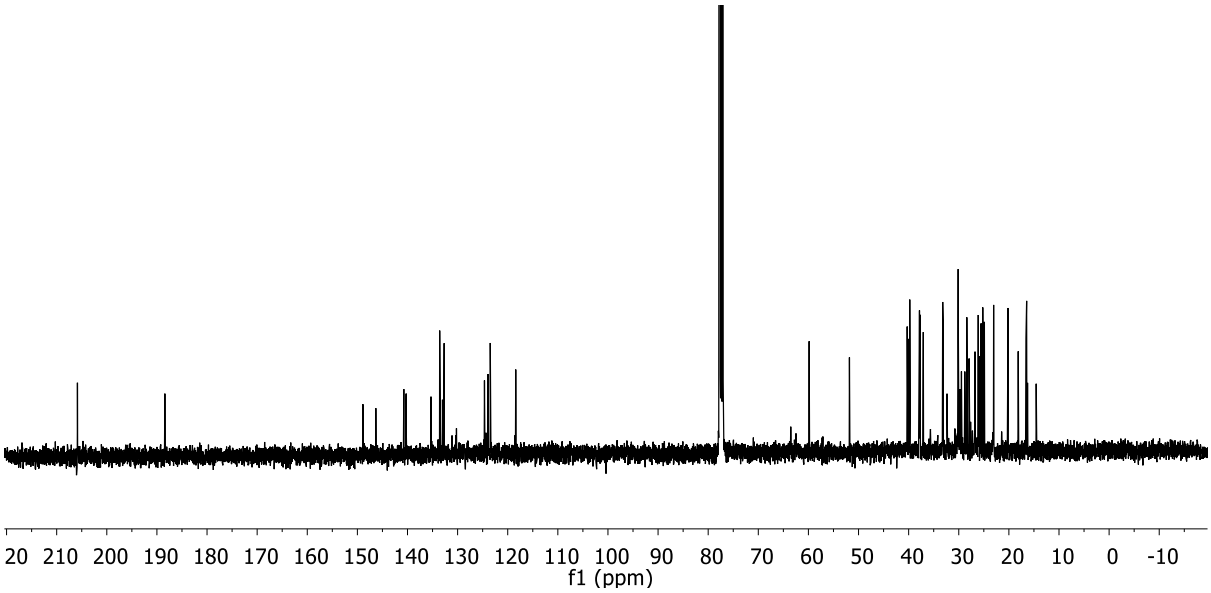


Figure S8. ^{13}C NMR spectrum of 10′*E*-sargaquinal (**9**) (100 MHz, $CDCl_3$)

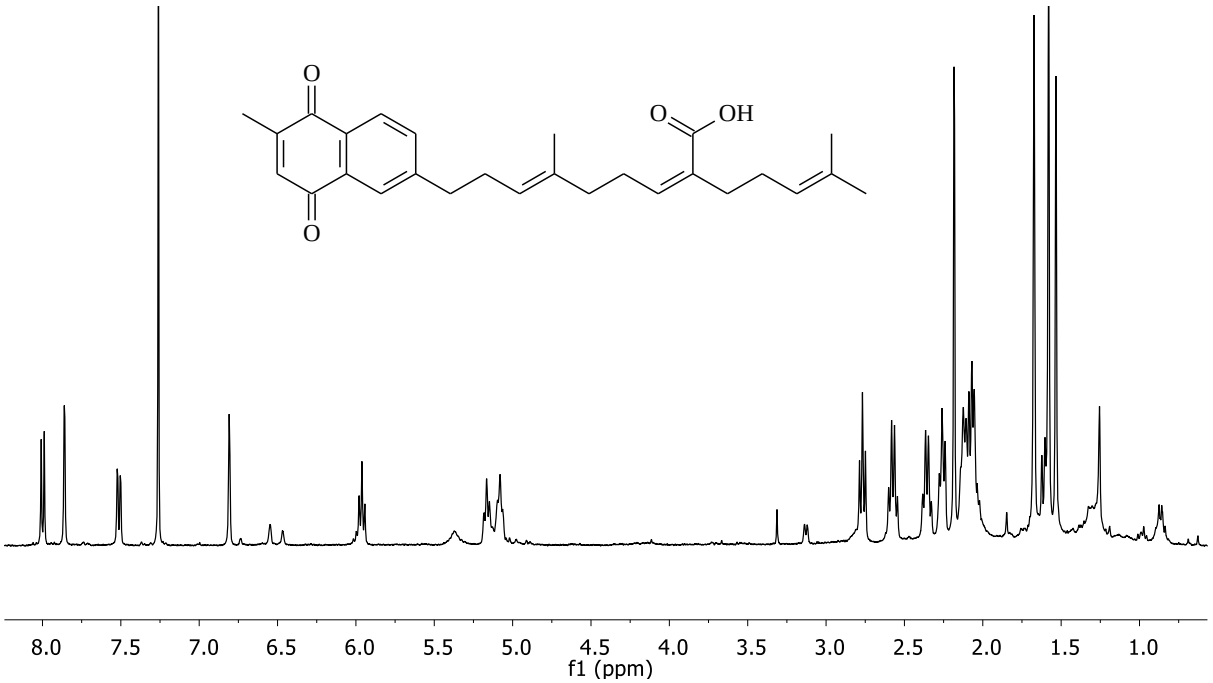


Figure S9. ^{1}H NMR spectrum of sarganaphthoquinoic acid (**10**) (400 MHz, $CDCl_3$)

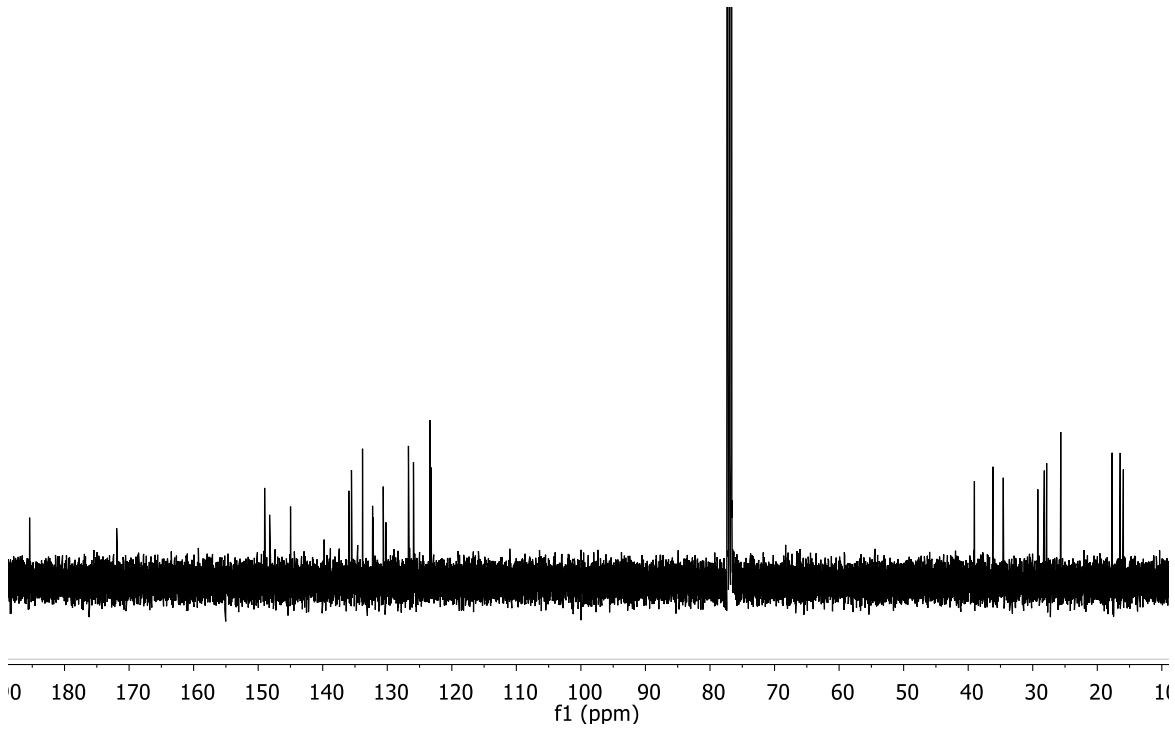


Figure S10. ^{13}C NMR spectrum of sarganaphthoquinoic acid (**10**) (100 MHz, $CDCl_3$)

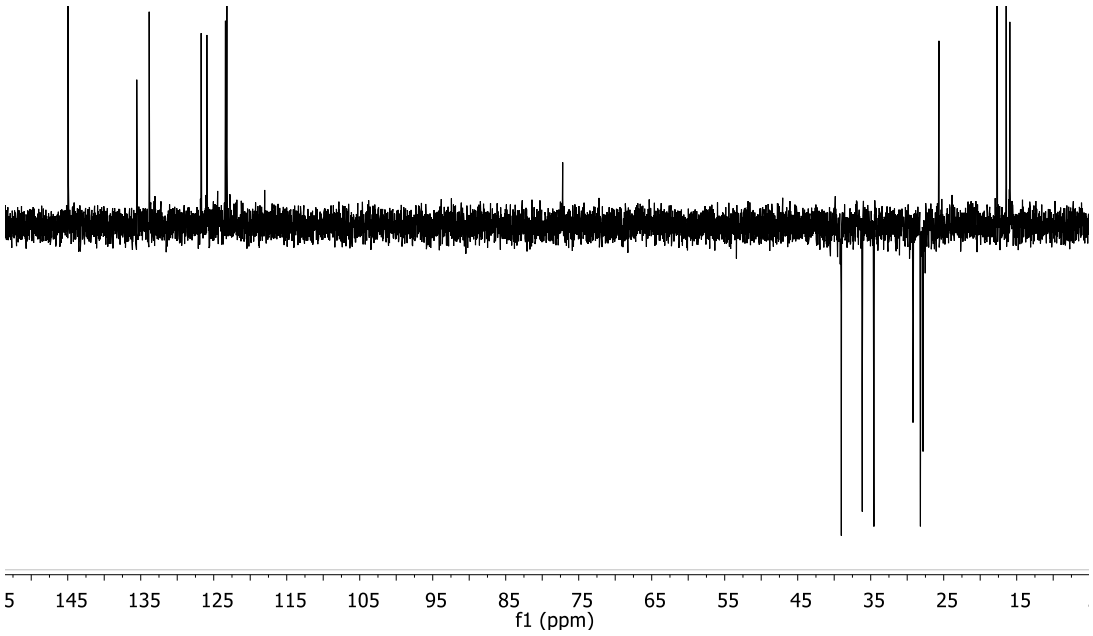


Figure S11. DEPT-135 NMR spectrum of sarganaphthoquinoic acid (**10**) (100 MHz, $CDCl_3$)

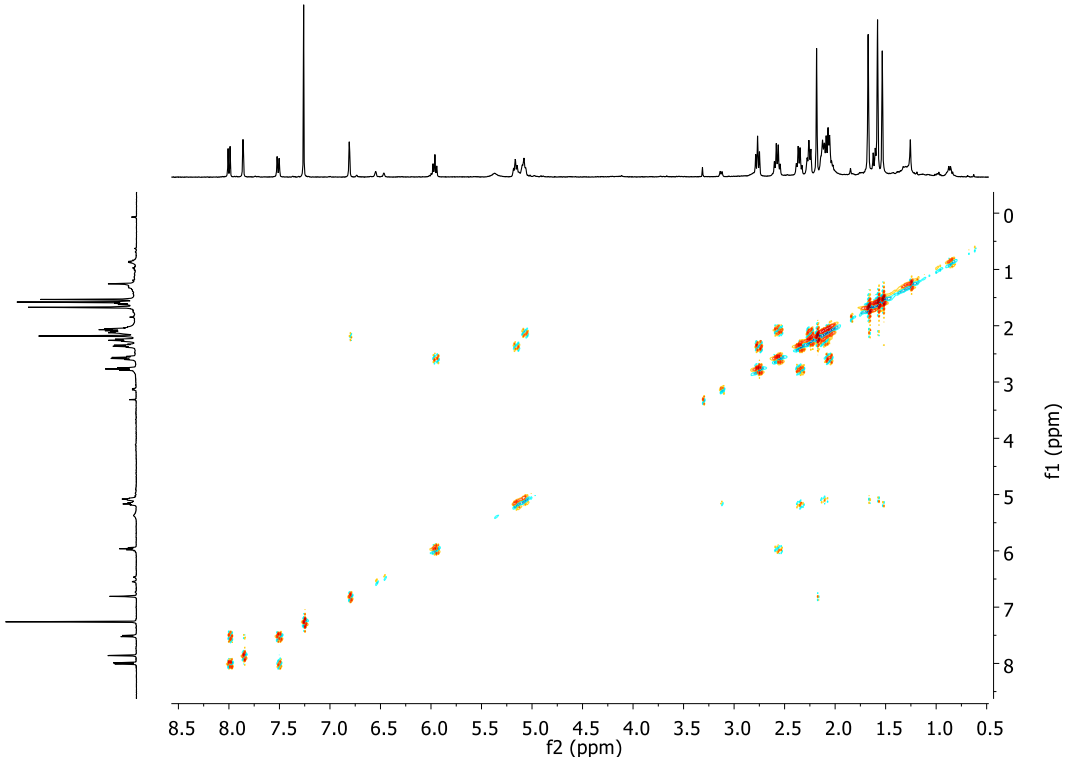


Figure S12. COSY NMR spectrum of sarganaphthoquinoic acid (**10**) ($CDCl_3$)

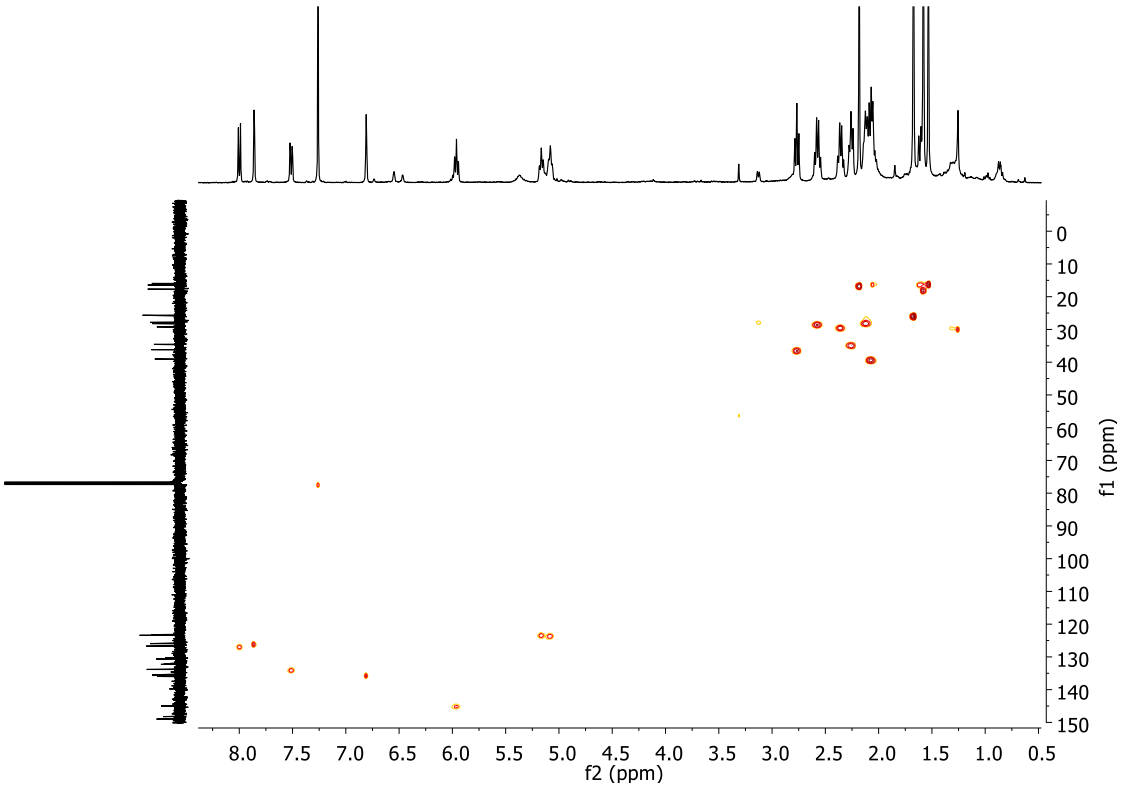


Figure S13. HSQC NMR spectrum of sarganaphthoquinoic acid (**10**) ($CDCl_3$)

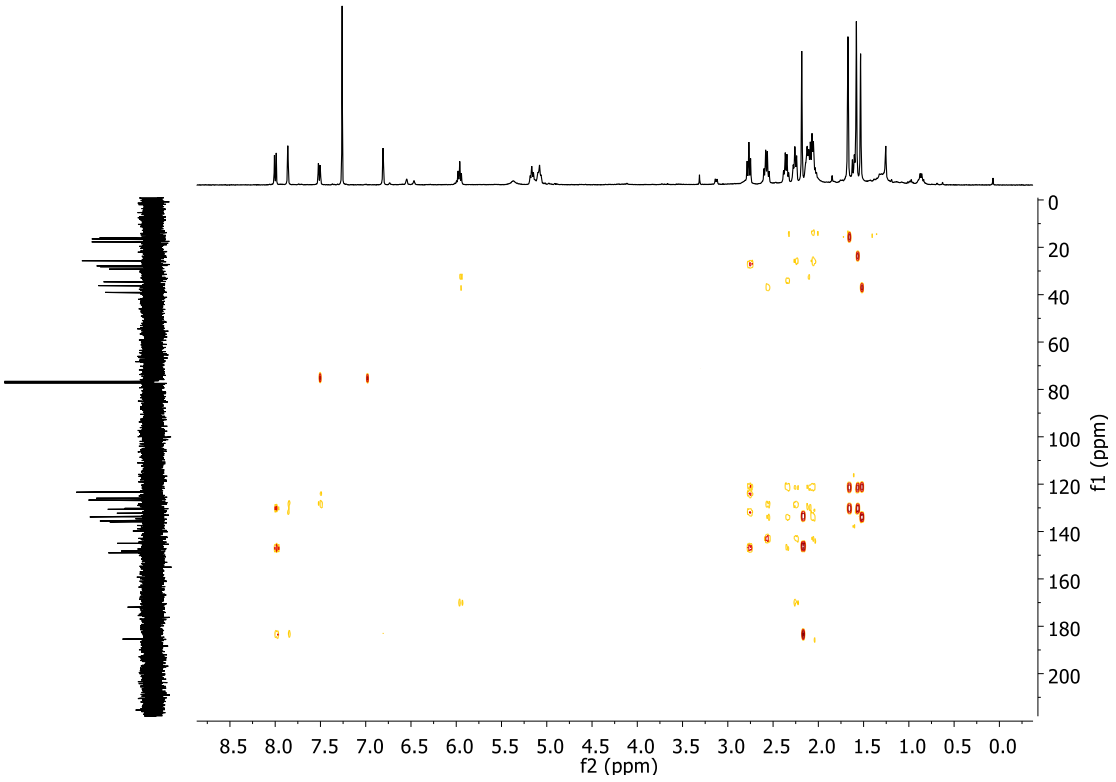


Figure S14. HMBC NMR spectrum of sarganaphthoquinoic acid (**10**) ($CDCl_3$)

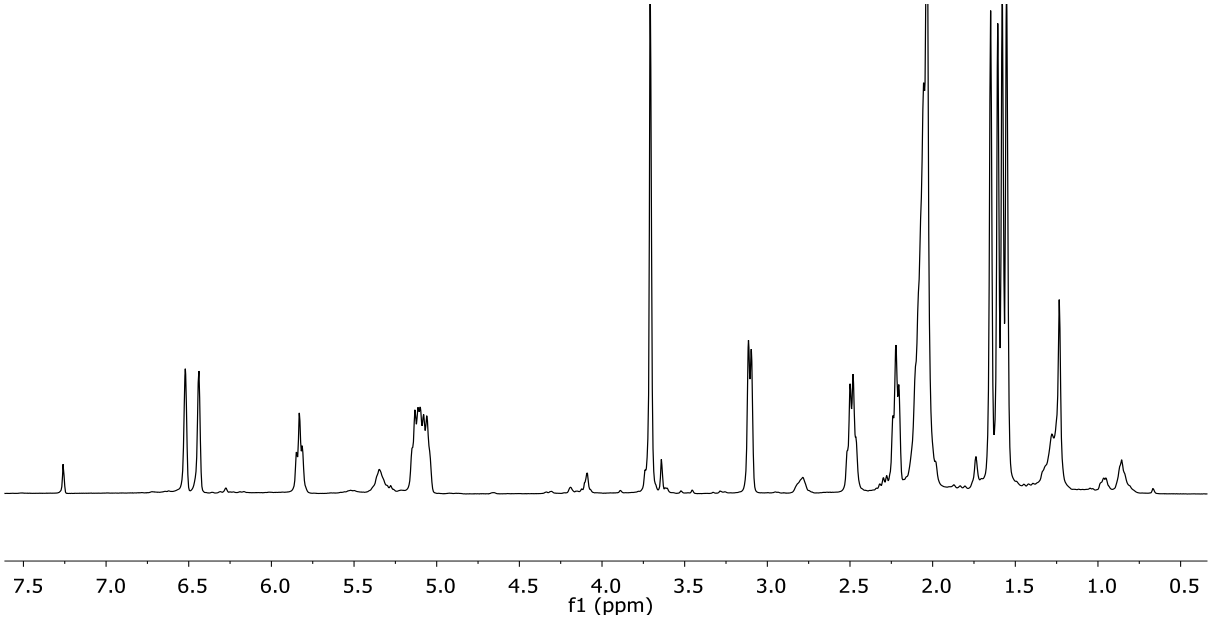


Figure S15. ^{1}H NMR spectrum of sargaquinoic acid methyl ester (**5**) (400 MHz, $CDCl_3$)

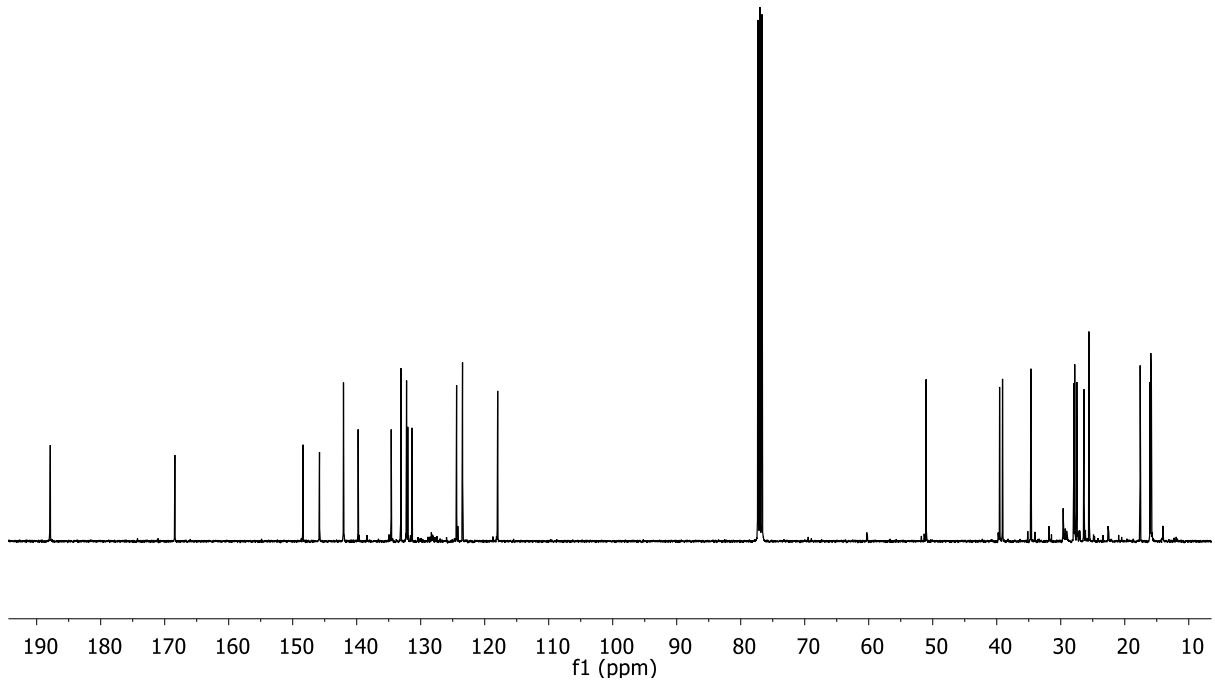


Figure S16. ^{13}C NMR spectrum of sargaquinoic acid methyl ester (**5**) (100 MHz)

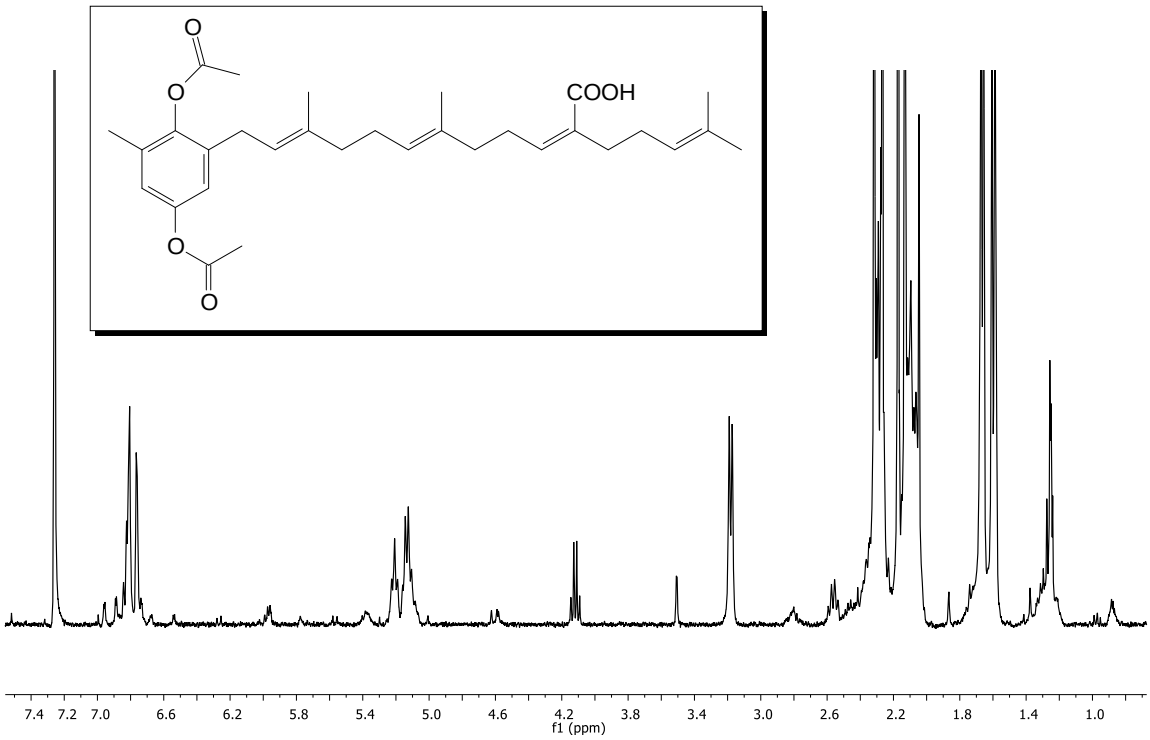


Figure S17. ^{1}H NMR spectrum of sargahydroquinoic acid diacetate (**2**) (400 MHz, $CDCl_3$)

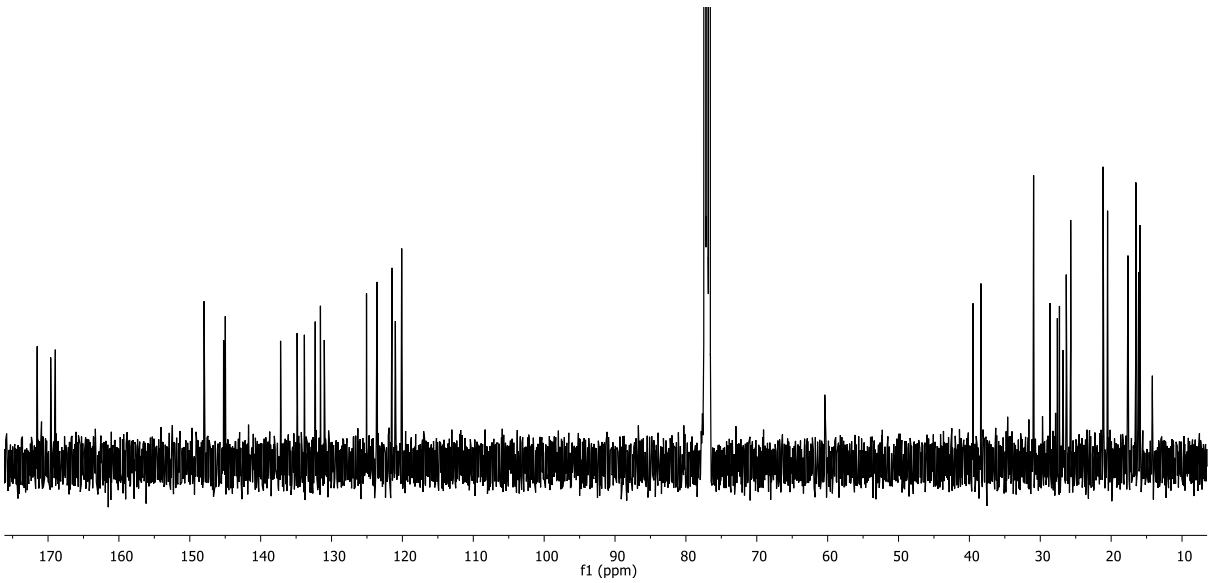


Figure S18. ^{13}C NMR spectrum of sargahydroquinoic acid diacetate (**2**) (100 MHz, $CDCl_3$)

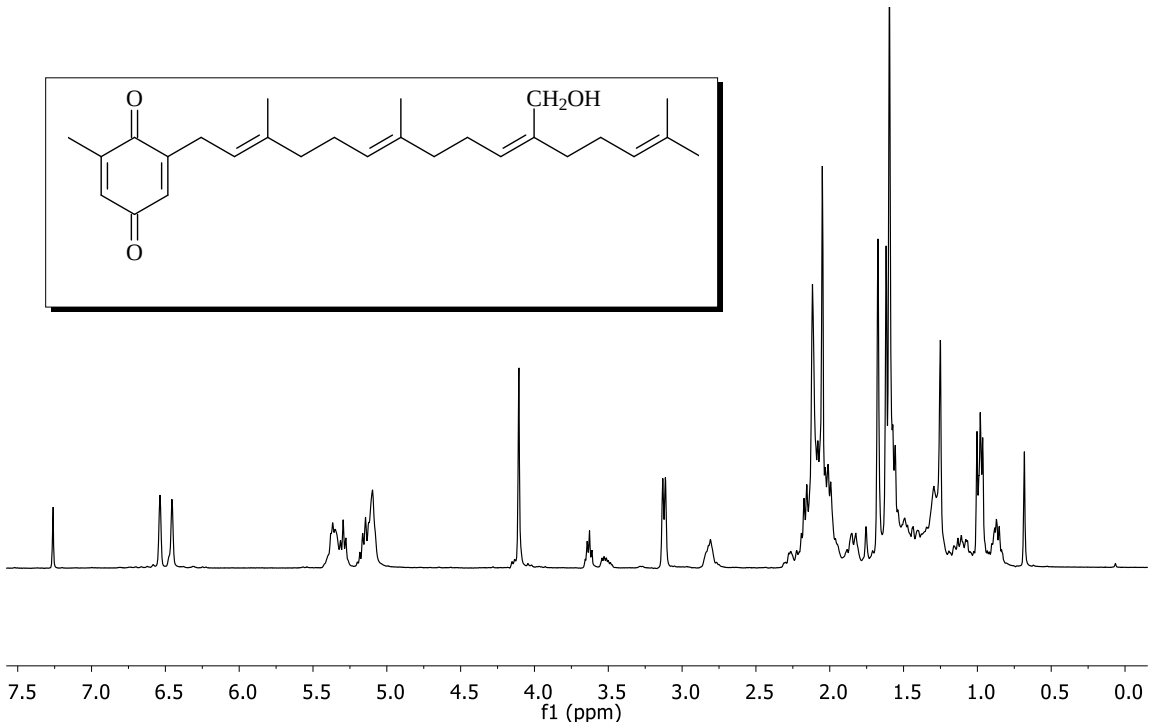


Figure S19. ^{1}H NMR spectrum of sargaquinol (**6**) (400 MHz, $CDCl_3$)

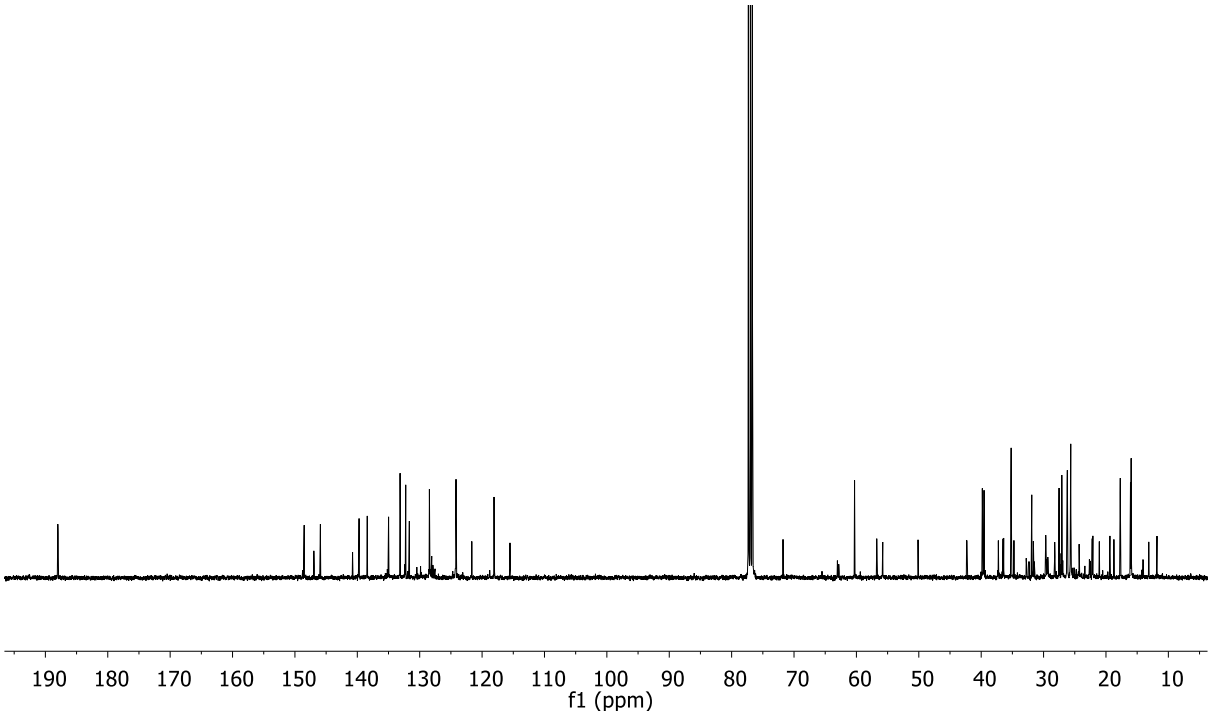


Figure S20. ^{13}C NMR spectrum of sargaquinol (**6**) (100 MHz, $CDCl_3$)

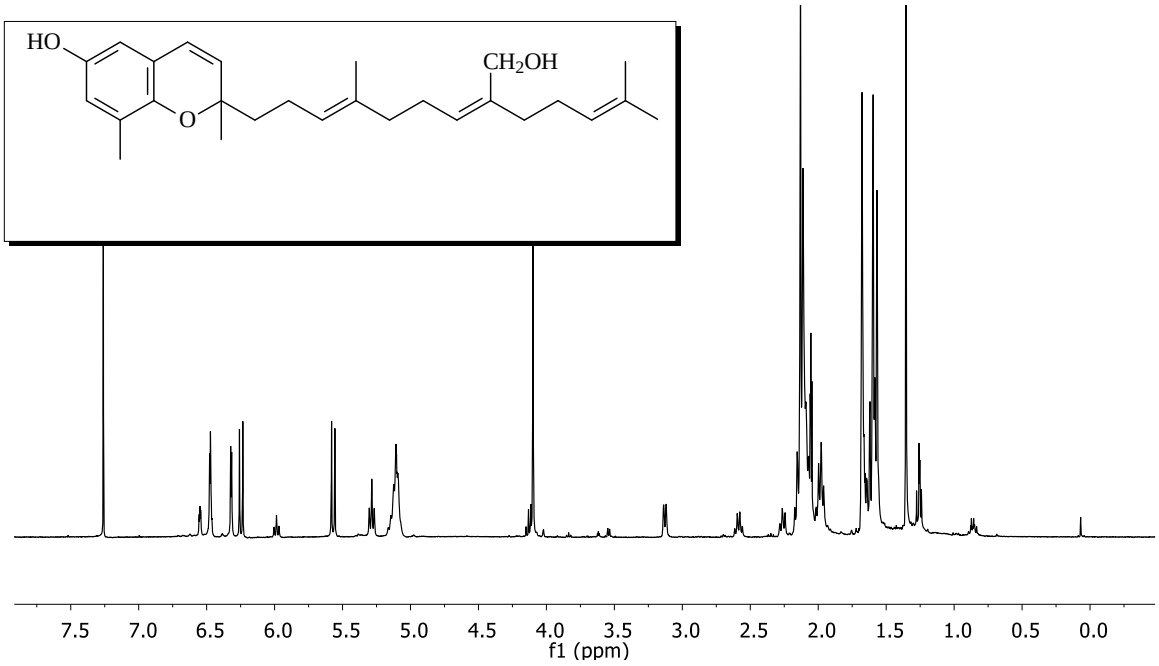


Figure S21. ^{1}H NMR spectrum of sargachromendiol (**8**) (400 MHz, $CDCl_3$)

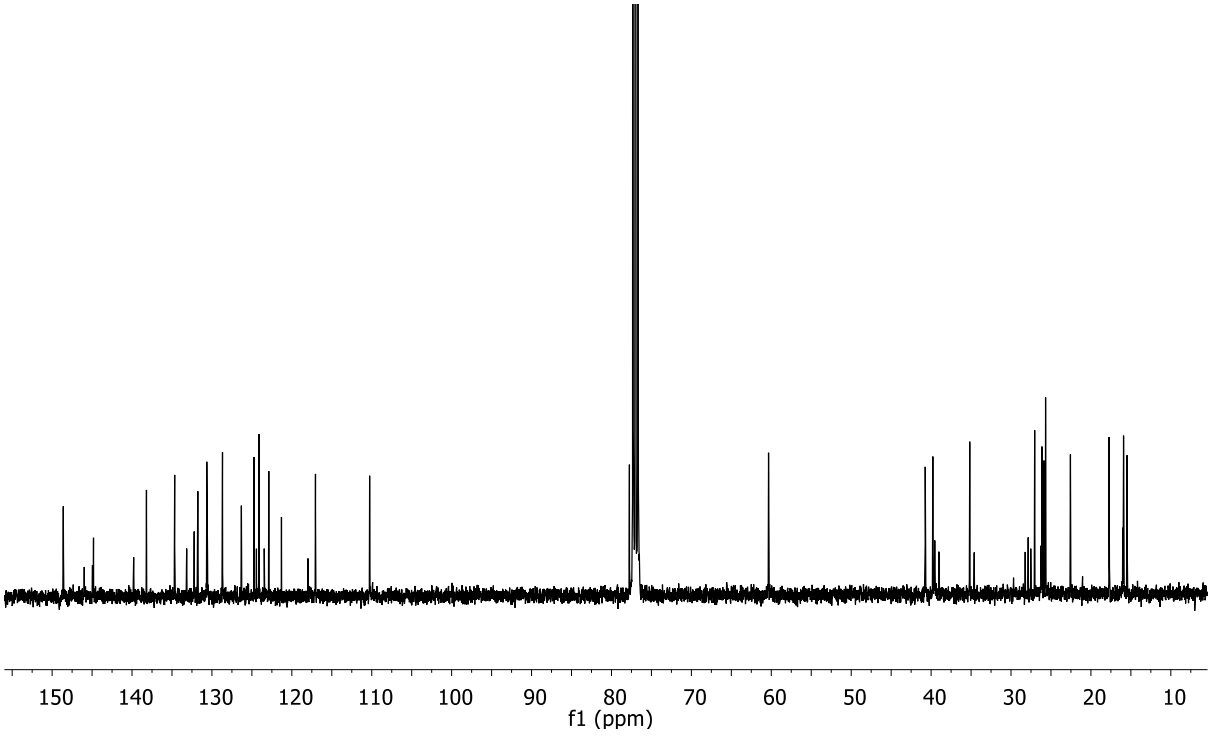


Figure S22. ^{13}C NMR spectrum of sargachromendiol (**8**) (100 MHz, $CDCl_3$)

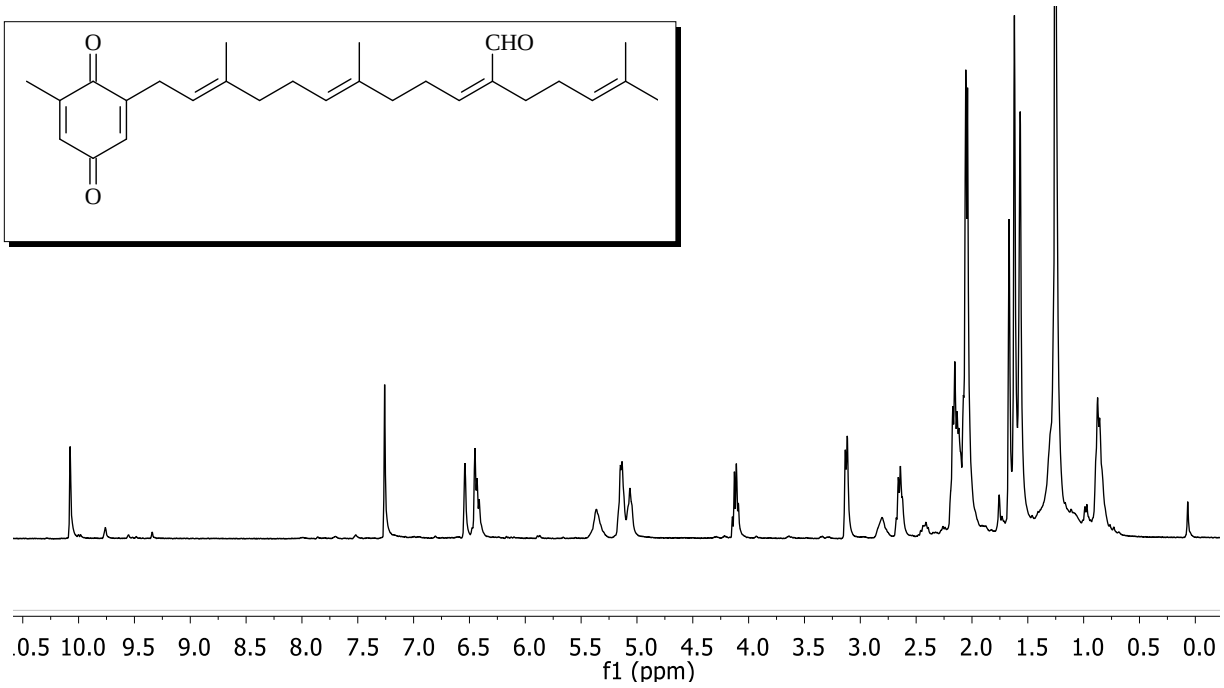


Figure S23. ^{1}H NMR spectrum of 10′*Z*-sargaquinal (**4**) (600 MHz, $CDCl_3$)

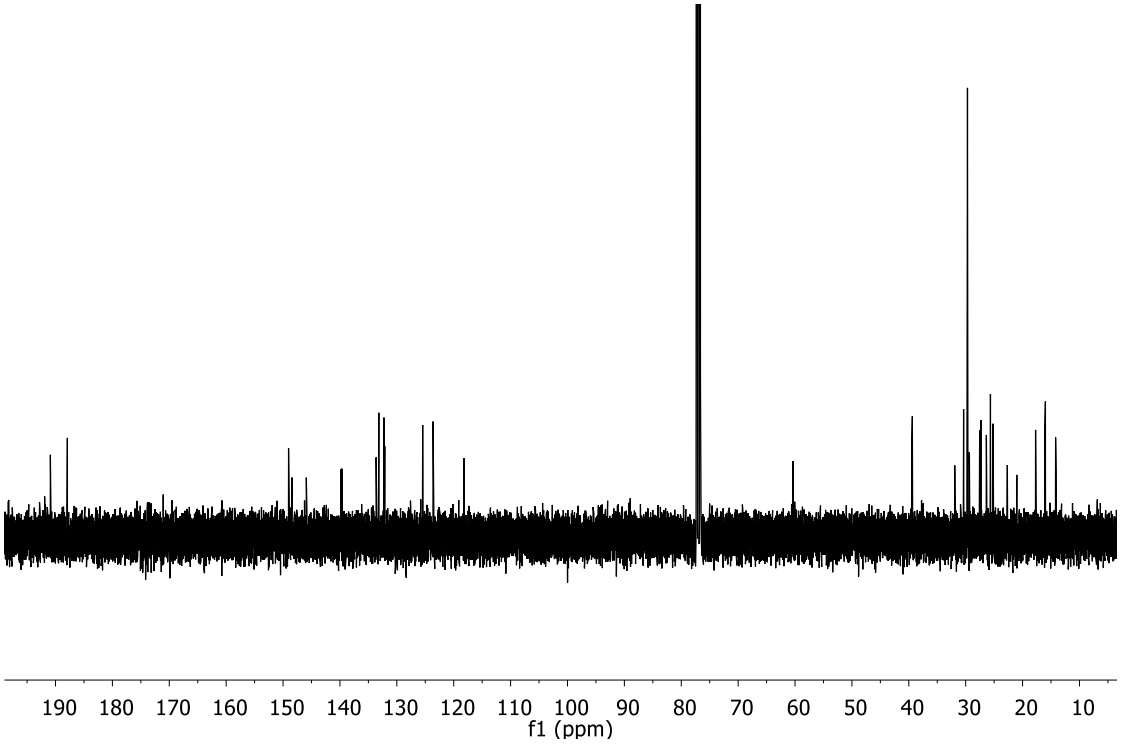


Figure S24. ^{13}C NMR spectrum of 10′*Z*-sargaquinal (**4**) (100 MHz, $CDCl_3$)