

# Supplementary Data

## Aspochalasin H1: A New Cyclic Aspochalasin from Hawaiian Plant-associated Endophytic Fungus *Aspergillus* sp. FT1307

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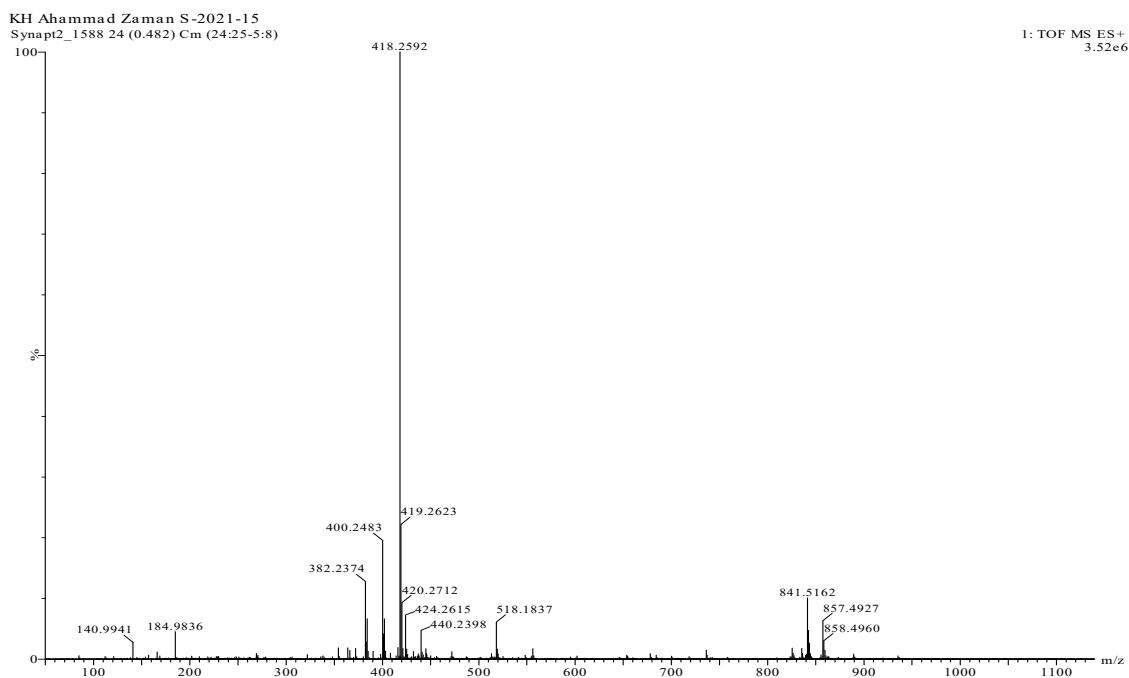


Figure S1: HR-ESI-MS spectrum of **1**

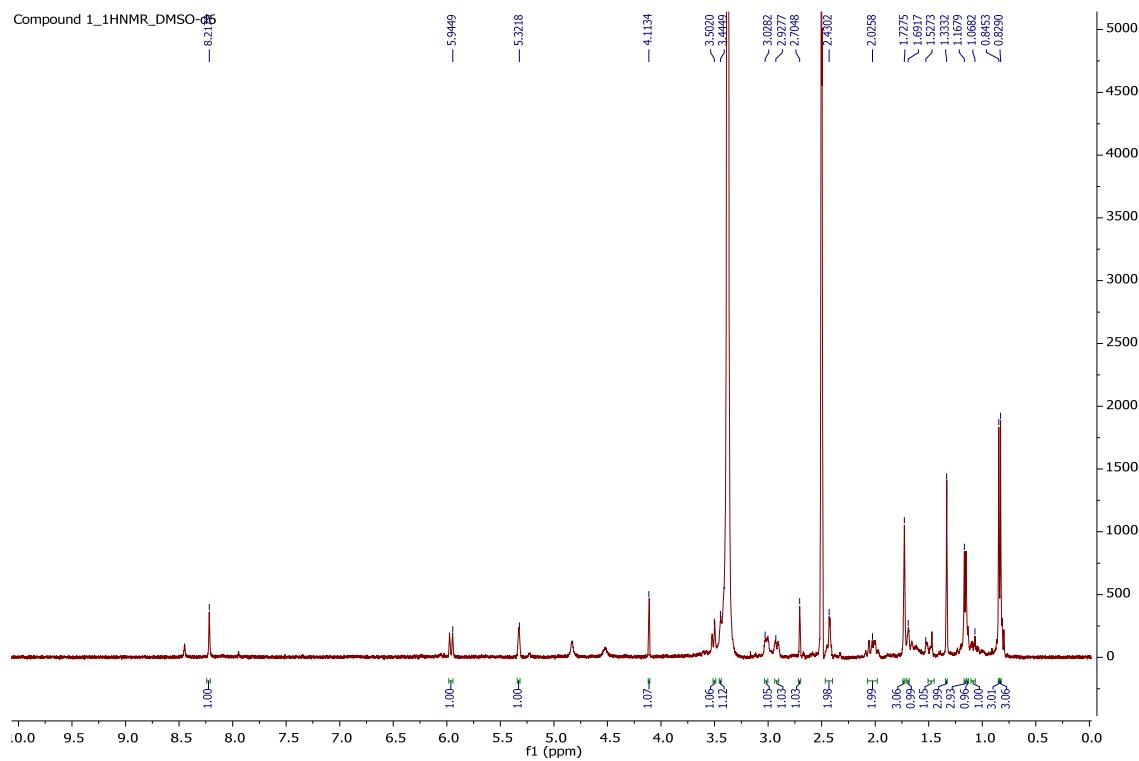


Figure S2:  $^1\text{H}$  NMR spectrum of **1** (400 MHz, DMSO- $d_6$ , 298 K)

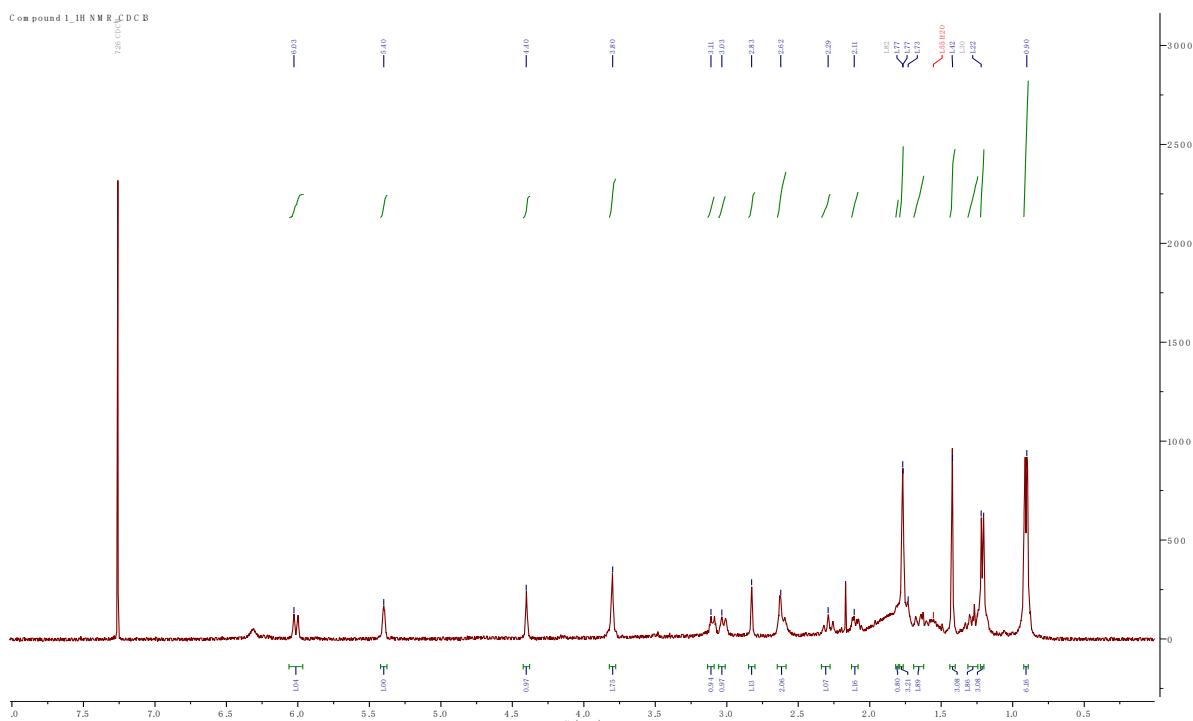
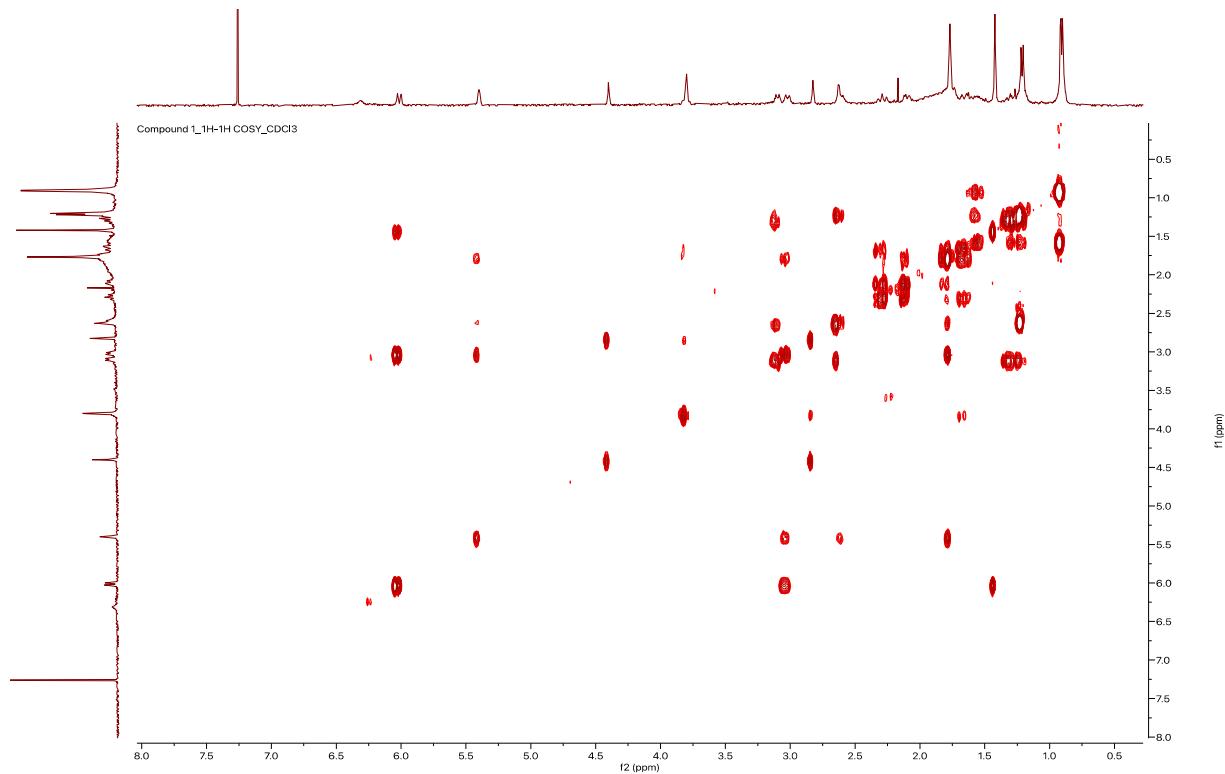


Figure S3:  $^1\text{H}$  NMR spectrum of 1 (400 MHz,  $\text{CDCl}_3$ , 298 K)



**Figure S4:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (400 MHz,  $\text{CDCl}_3$ , 298 K)

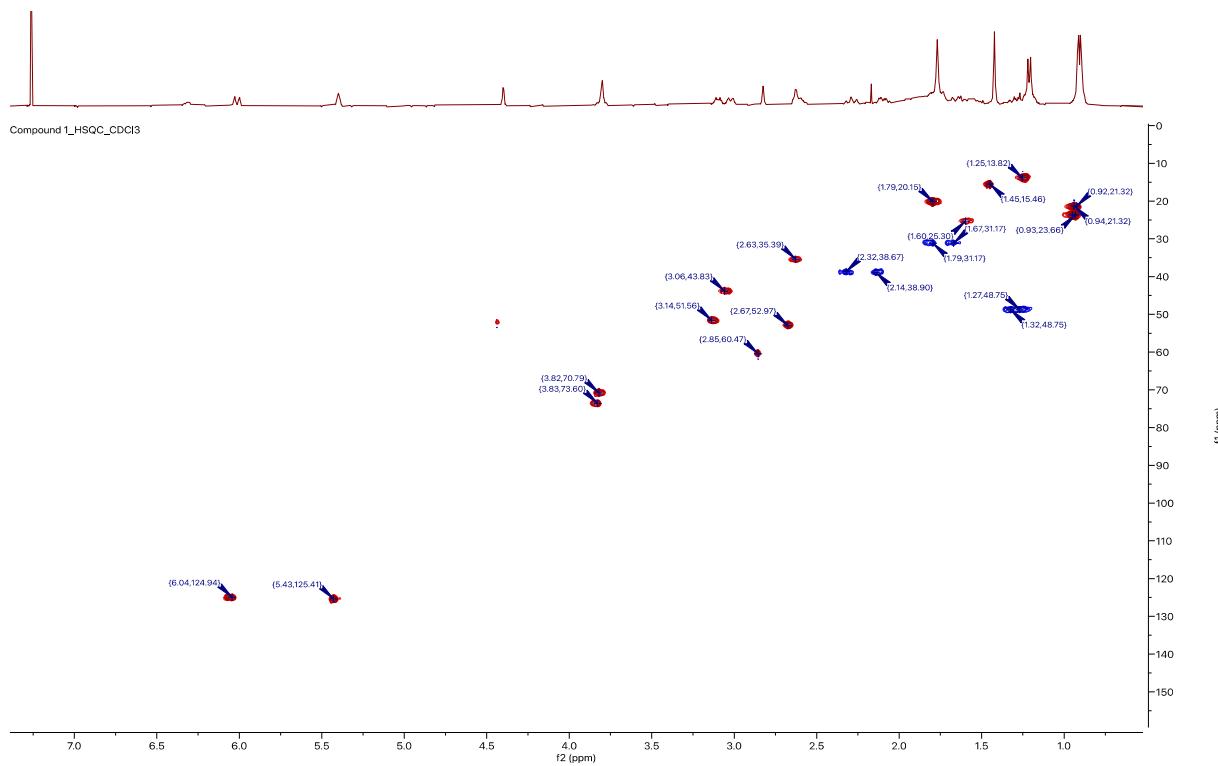


Figure S5: HSQC spectrum of **1** (400 MHz, CDCl<sub>3</sub>, 298 K)

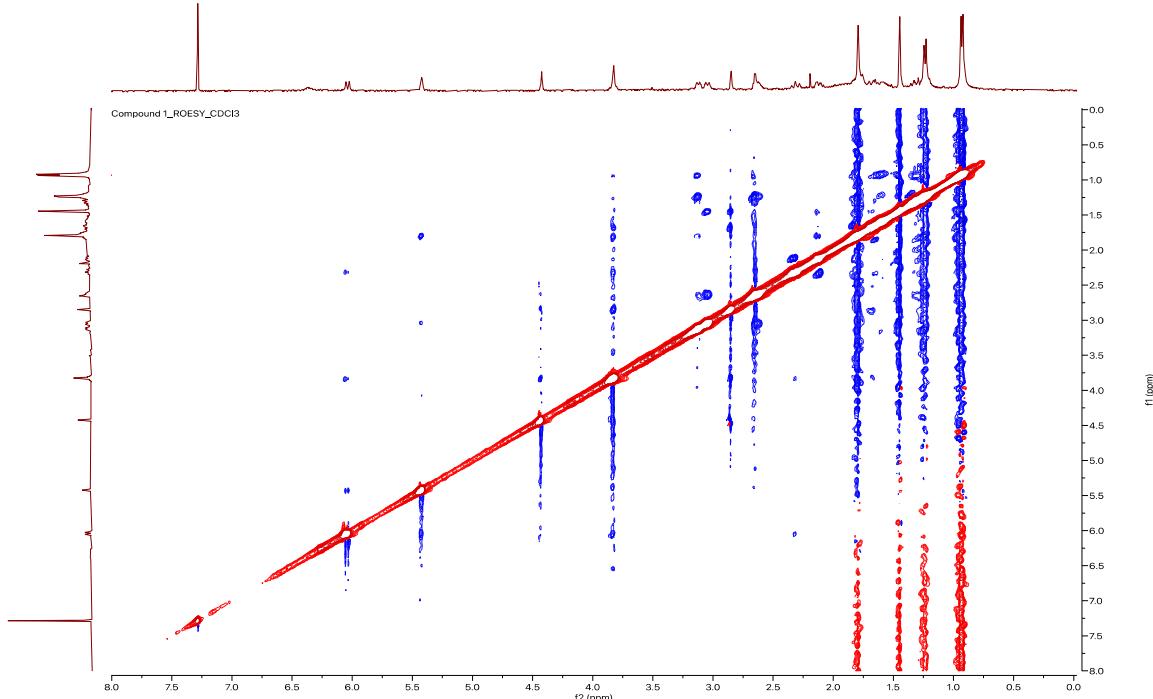


Figure S6: ROESY spectrum of **1** (400 MHz, CDCl<sub>3</sub>, 298 K)

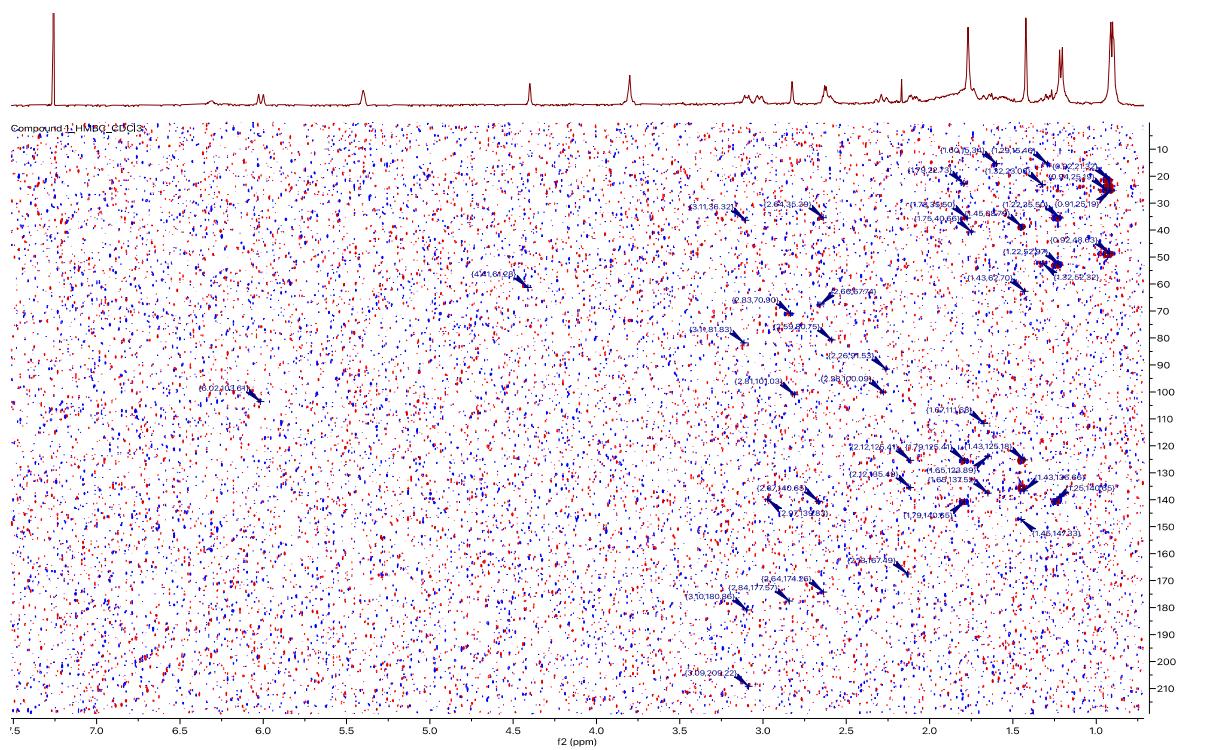


Figure S7: HMBC spectrum of **1** (400 MHz, CDCl<sub>3</sub>, 298 K)

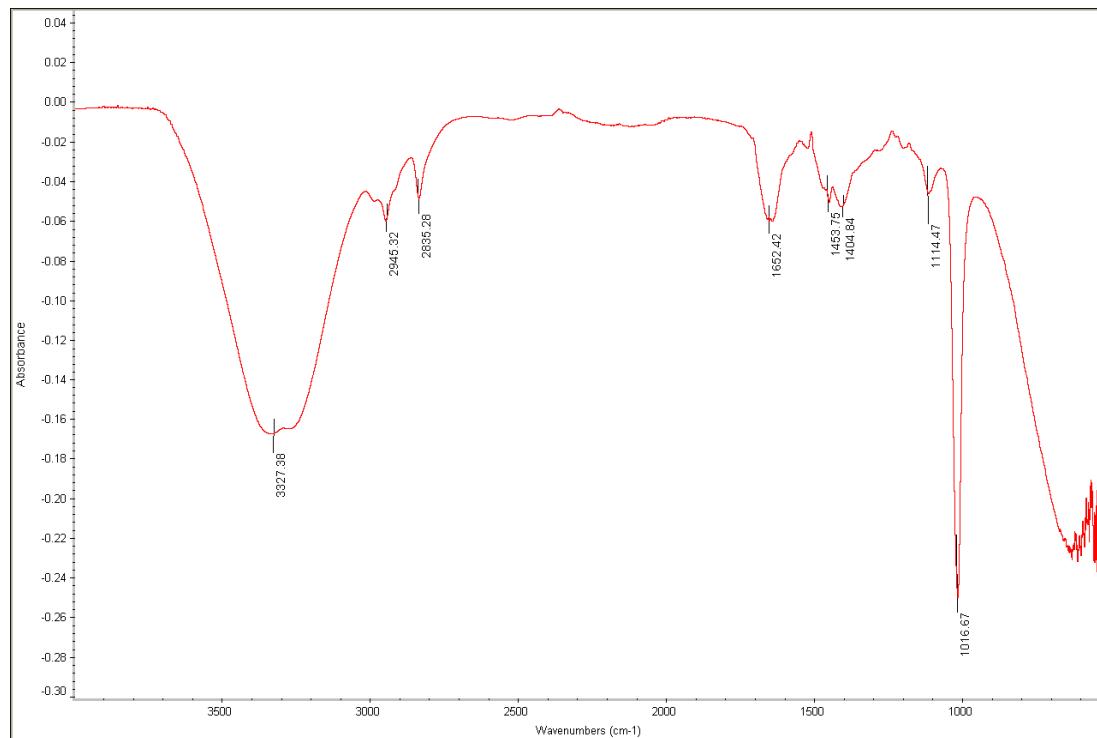


Figure S8: IR spectrum of **1**

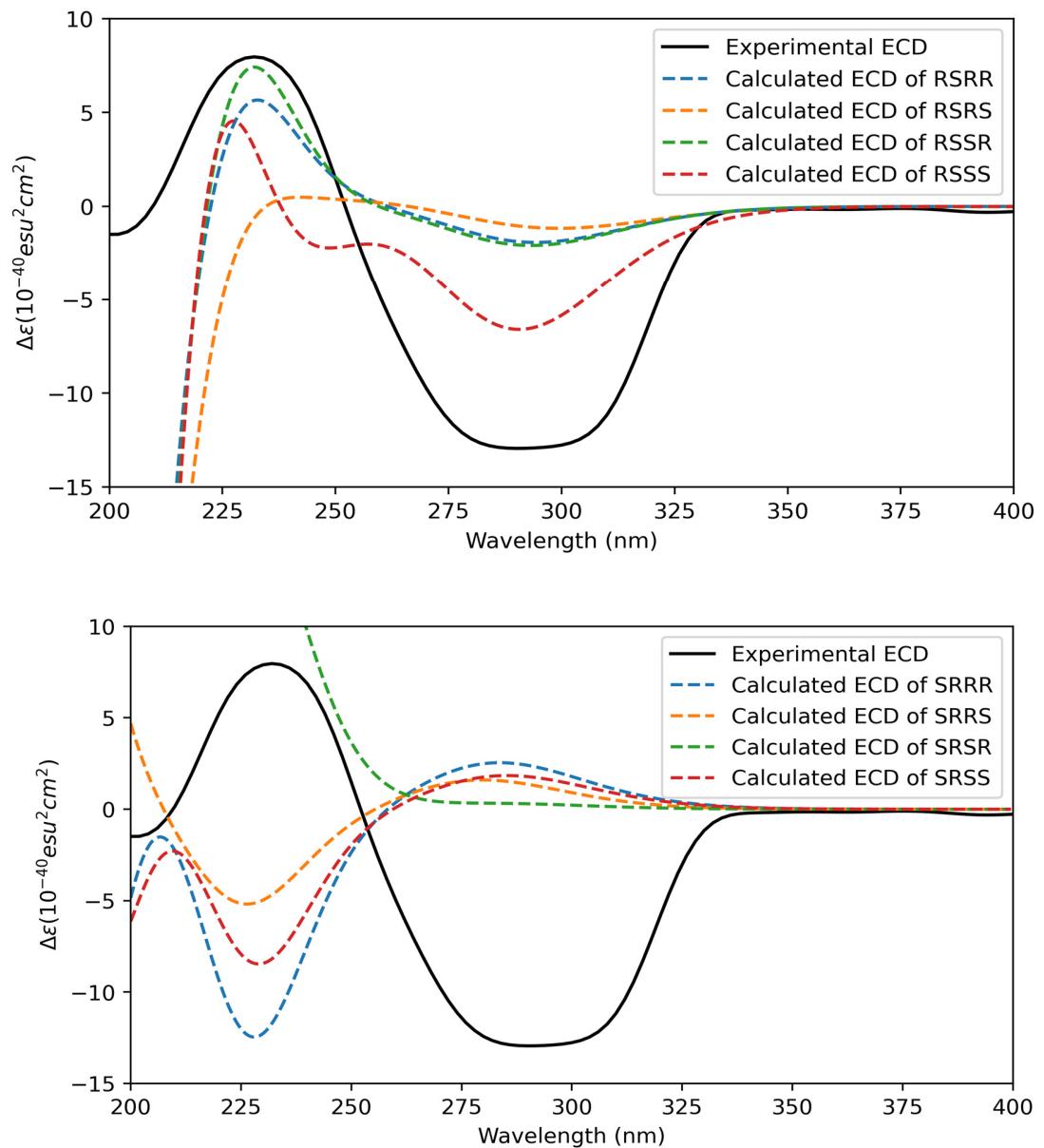


Figure S9: ECD spectra of **1**

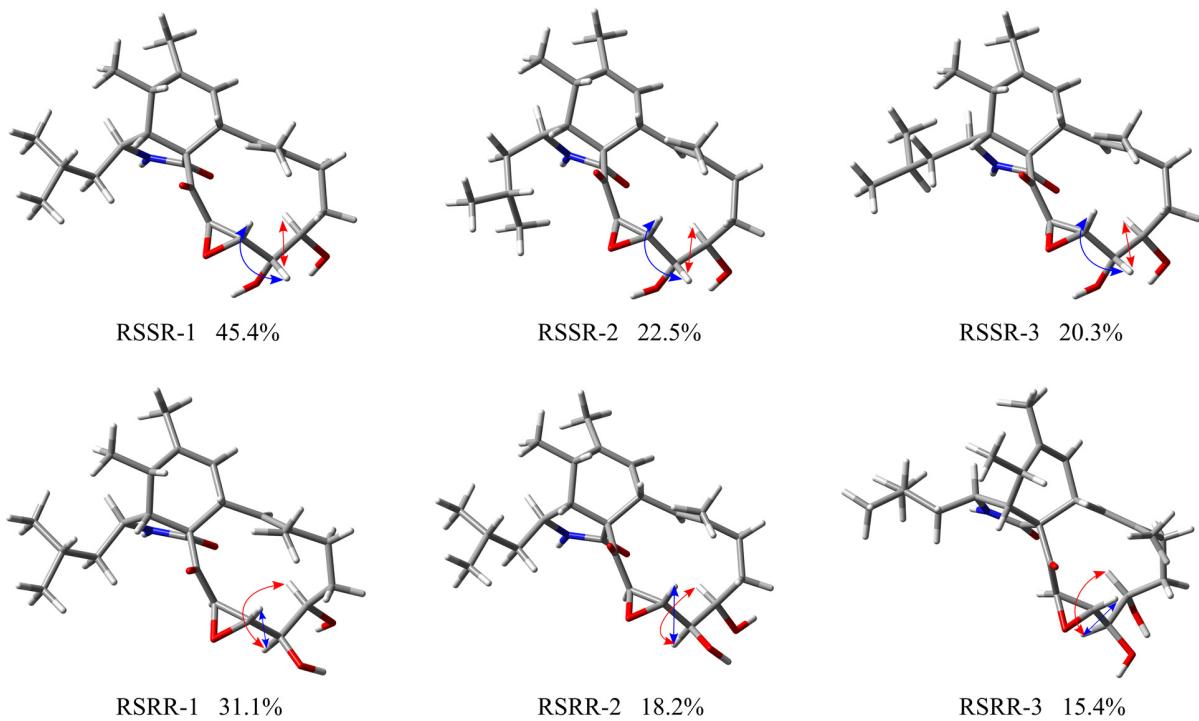


Figure S10: Conformation analysis of **1** (17*R*,18*S*,19*S*,20*R* and 17*R*,18*S*,19*R*,20*R*)

Table S1: NMR calculations of 1

C/H No	Experimental data		RSRR		RSRS		RSSR		RSSS		SRRR		SRRS		SRSR		SRSS	
	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H	$\delta$ C	$\delta$ H
1	174.6		173.5		173.4		173.7		173.1		172.6		172.2		173.5		174.1	
3	51.6	3.10	54.9	3.19	53.9	5.47	52.6	3.15	54.1	5.47	54.2	5.42	52.9	5.34	52.8	5.45	52.8	5.50
4	52.9	2.64	56.2	2.96	55.7	2.97	57.2	2.71	53.8	2.99	59.4	3.45	54.9	3.41	59.3	3.60	59.4	3.68
5	35.4	2.60	38.6	2.52	39.4	4.67	39.3	2.55	39.2	4.88	38.4	3.67	39.0	4.07	39.6	3.46	40.0	3.49
6	140.6		146.5		146.8		146.4		146.7		145.4		147.4		146.1		145.8	
7	125.6	5.39	126.2	5.44	127.3	2.95	126.7	5.44	127.0	2.99	129.1	2.97	126.5	3.23	127.9	2.39	128.0	2.30
8	43.8	3.02	49.0	3.13	48.4	2.48	49.0	3.12	48.5	2.45	39.8	2.45	42.0	2.42	40.6	2.58	41.5	2.60
9	68.4		73.0		72.4		72.7		73.6		71.7		73.3		71.5		71.2	
10	48.8	1.29	47.5	1.26	49.3	1.35	49.2	1.20	46.5	1.30	47.3	1.59	46.4	1.62	46.6	1.63	47.6	1.51
11	13.7	1.21	11.9	1.29	13.3	1.25	12.3	1.28	12.6	1.26	13.7	1.18	14.5	1.28	13.9	1.23	13.4	1.22
12	20.1	1.76	19.2	1.80	20.0	2.24	19.4	1.83	19.6	2.27	19.7	2.17	19.9	2.27	20.0	2.26	19.9	2.31
13	125.2	6.04	127.1	6.27	127.1	2.07	127.9	6.25	126.5	1.96	127.8	2.27	132.2	2.10	129.0	2.30	128.8	1.65
14	135.6		141.1		143.3		140.4		144.0		141.5		142.2		139.7		142.1	
15	38.8	2.10,2.29	40.4	2.17,2.34	36.8	1.97,2.49	40.1	2.13,2.36	37.3	1.63,2.54	42.1	2.28,2.81	35.6	1.91,2.45	40.4	2.06,2.42	31.6	2.19,2.65
16	31.0	1.63,1.76	32.7	1.53,2.29	36.2	1.83,3.67	33.4	1.70,1.79	38.5	2.50,3.61	31.9	1.47,3.94	39.5	1.82,3.03	38.6	1.72,3.51	37.5	1.939,3.96
17	73.7	3.80	74.6	3.74	72.1	3.23	76.7	3.74	75.4	4.31	74.2	4.12	67.8	3.78	72.1	2.74	78.6	2.92
18	70.8	3.78	80.8	3.37	78.3	1.86	74.1	3.71	75.5	1.80	76.9	1.73	72.4	1.86	79.0	1.99	75.0	1.83
19	60.5	2.82	64.6	2.47	65.2	6.48	63.6	2.67	64.1	6.48	63.3	6.32	62.8	6.84	65.2	6.87	62.3	7.25
20	52.2	4.40	56.2	4.17	57.5	2.74	54.6	4.31	51.8	2.99	58.8	3.08	57.8	3.12	59.5	2.81	61.7	3.18
21	208.0		210.6		208.9		211.4		210.1		211.7		209.1		212.7		212.6	
22	25.2	1.56	30.4	1.64	31.5	1.69	29.8	1.62	28.6	1.55	31.8	1.74	31.1	1.71	27.5	1.53	29.1	1.60
23	23.7	0.91	21.9	1.00	21.7	0.96	22.0	0.89	20.5	0.92	21.4	1.00	19.1	1.03	23.2	0.95	19.0	0.95
24	21.4	0.90	23.9	0.96	21.0	0.97	20.9	0.97	23.8	0.92	21.3	1.01	22.3	1.06	20.3	0.96	23.1	0.98
25	15.5	1.42	14.3	1.49	17.0	1.60	14.3	1.47	19.2	1.64	14.4	1.79	17.6	1.82	14.6	1.79	18.2	1.81

