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Stereochemistry of spongosoritins: beyond optical rotation

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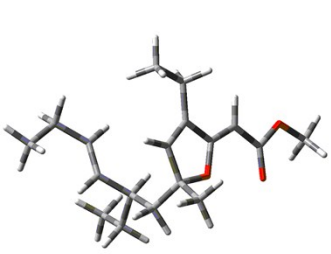
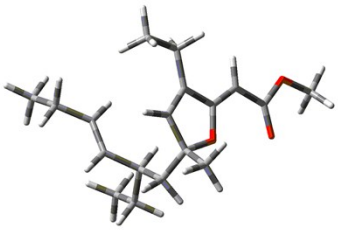
Supplementary Information

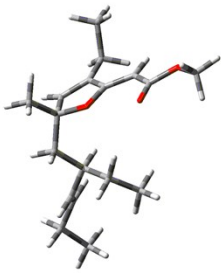
Figure S1. Lowest-energy conformers identified for (6*R*,8*R*)-**1** at the B3PW91/PCM($CHCl_3$)/6-311G(d,p) level.



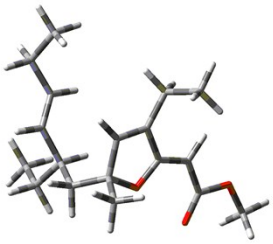
Conf 1. 0.0 kcal/mol (47%)



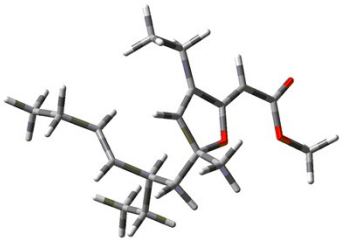
Conf 2. +0.61 kcal/mol (17%)



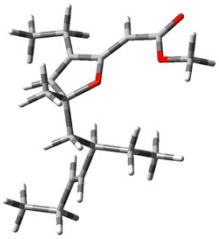
Conf 3. +1.06 kcal/mol (8%)



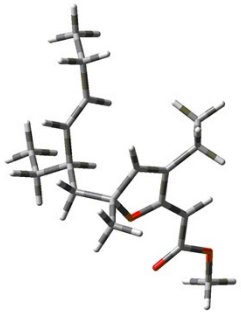
Conf 4. +1.08 kcal/mol (8%)



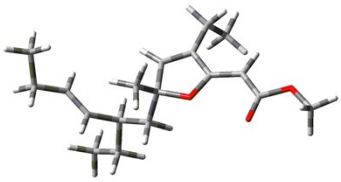
Conf 5. +1.21 kcal/mol (6%)



Conf 6. +1.27 kcal/mol (6%)

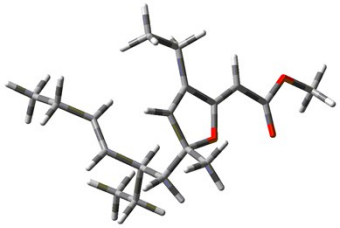


Conf 7. +1.40 kcal/mol (4%)

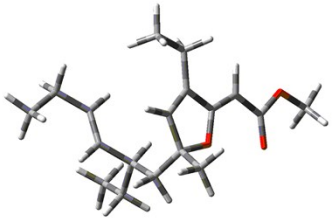


Conf 8. +1.45 kcal/mol (4%)

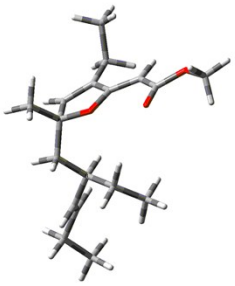
Figure S2. Lowest-energy conformers identified for (6*R*,8*R*)-**1** at the B3PW91/PCM(MeOH)/6-311G(d,p) level.



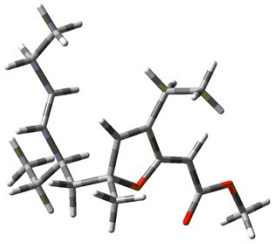
Conf 2. 0.0 kcal/mol (25%)



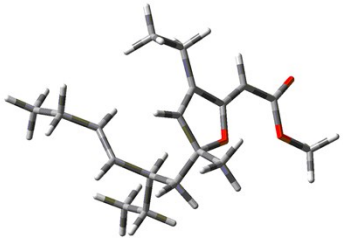
Conf 1. +0.19 kcal/mol (18%)



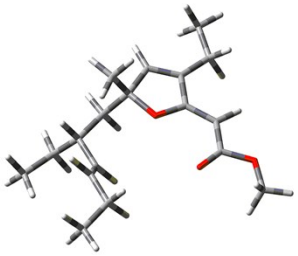
Conf 3. +0.47 kcal/mol (11%)



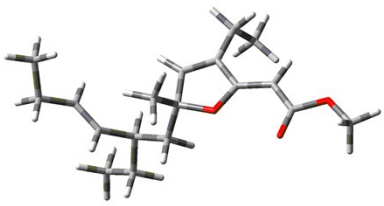
Conf 4. +0.55 kcal/mol (10%)



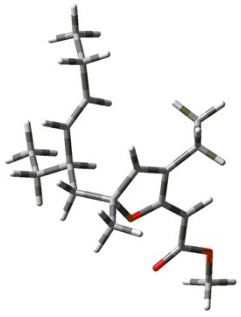
Conf 5. +0.84 kcal/mol (6%)



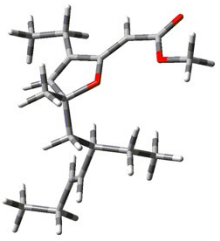
Conf 9. +0.90 kcal/mol (6%)



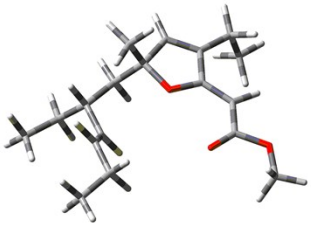
Conf 8. 1.00 kcal/mol (5%)



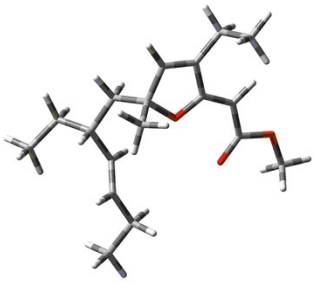
Conf 7. +1.01 kcal/mol (5%)



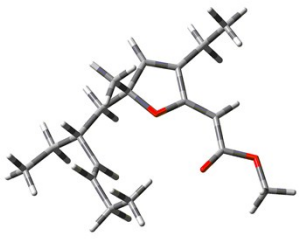
Conf 6. +1.02 kcal/mol (5%)



Conf 10. +1.16 kcal/mol (4%)

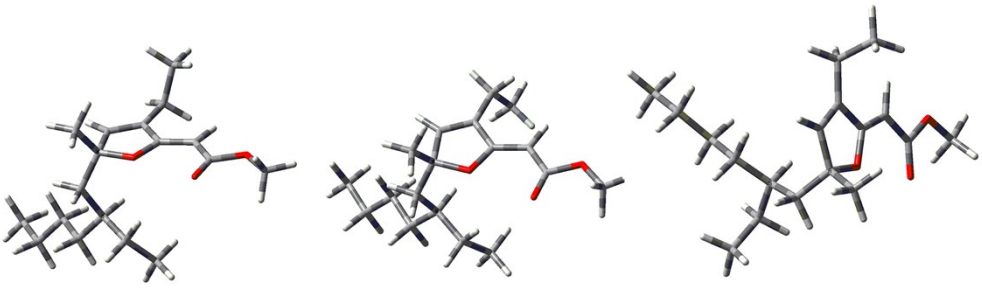


Conf 11. +1.23 kcal/mol (3%)

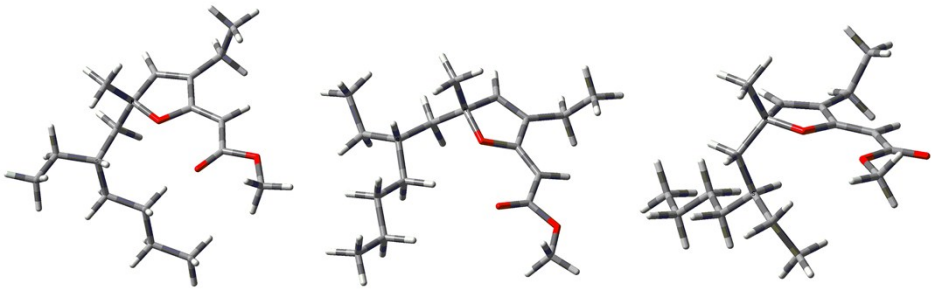


Conf 12. +1.42 kcal/mol (2%)

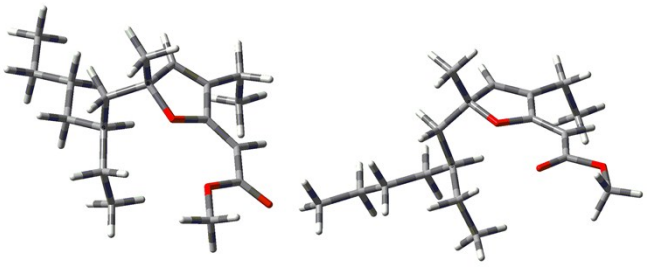
Figure S3. Lowest-energy conformers identified for (6*R*,8*S*)-**2** at the B3PW91/PCM($CHCl_3$)/6-311G(d,p) level.



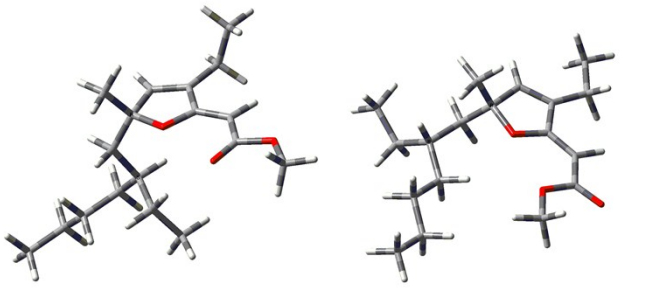
Conf 1. 0.0 kcal/mol (23%) **Conf 2.** +0.19 kcal/mol (17%) **Conf 3.** +0.30 kcal/mol (14%)



Conf 4. +0.30 kcal/mol (14%) **Conf 5.** +0.58 kcal/mol (9%) **Conf 6.** +0.64 kcal/mol (8%)

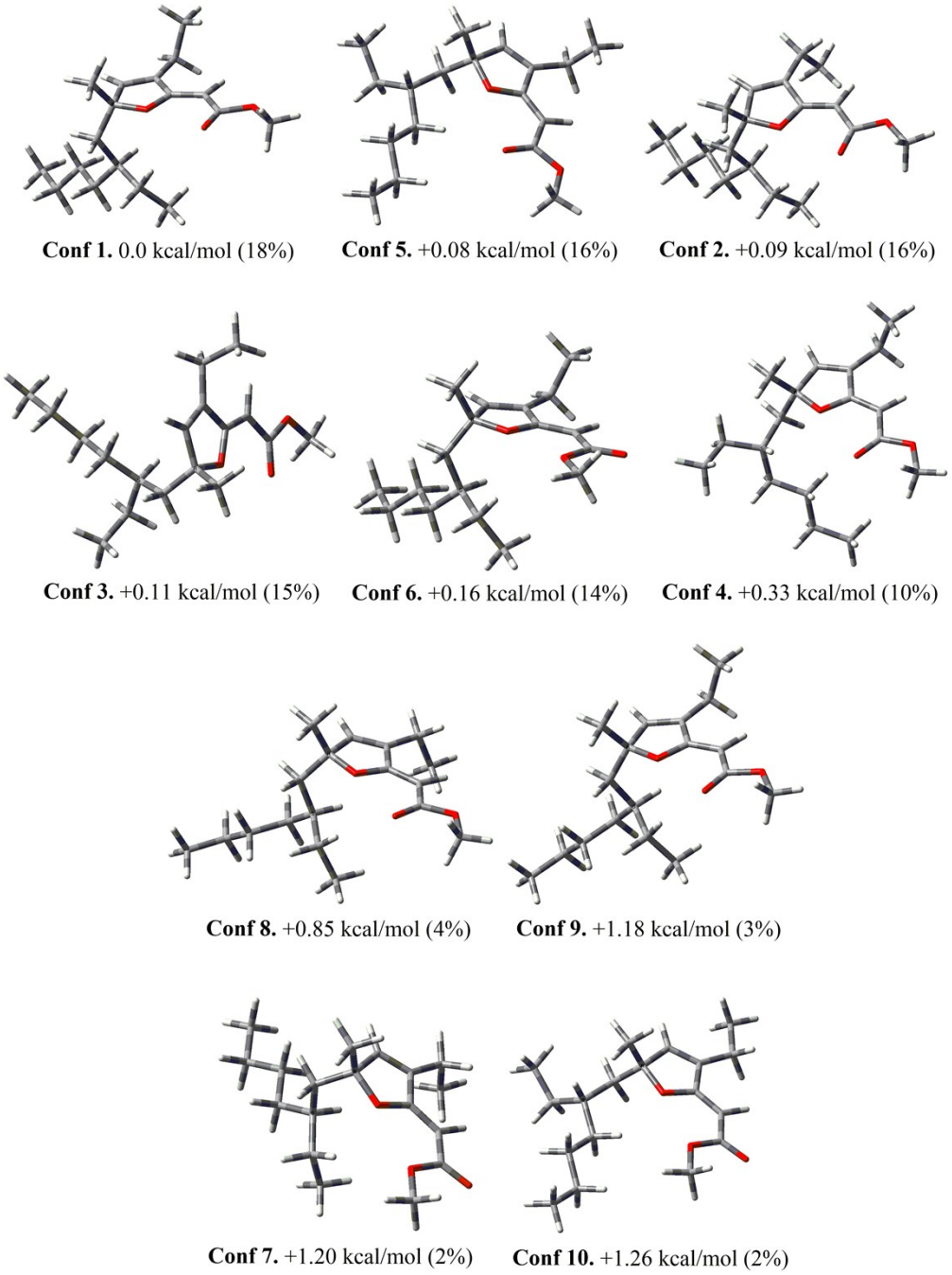


Conf 7. +0.92 kcal/mol (5%) **Conf 8.** +1.03 kcal/mol (4%)



Conf 9. +1.13 kcal/mol (4%) **Conf 10.** +1.38 kcal/mol (2%)

Figure S4. Lowest-energy conformers identified for (6*R*,8*S*)-**2** at the B3PW91/PCM(MeOH)/6-311G(d,p) level.



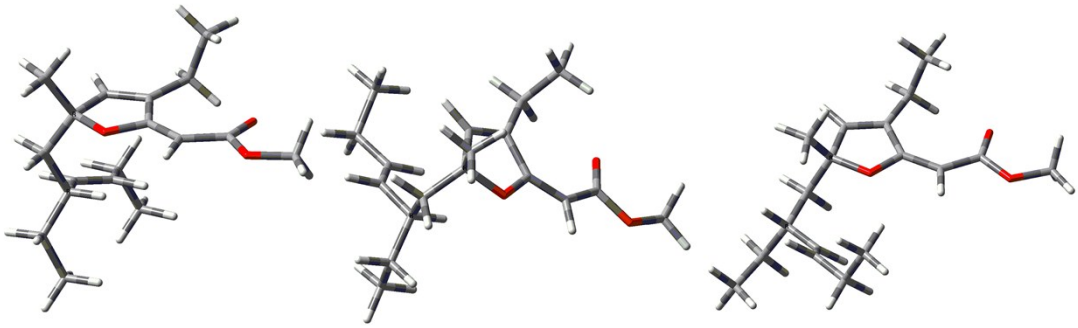
Conf 1. 0.0 kcal/mol (18%) **Conf 5.** +0.08 kcal/mol (16%) **Conf 2.** +0.09 kcal/mol (16%)

Conf 3. +0.11 kcal/mol (15%) **Conf 6.** +0.16 kcal/mol (14%) **Conf 4.** +0.33 kcal/mol (10%)

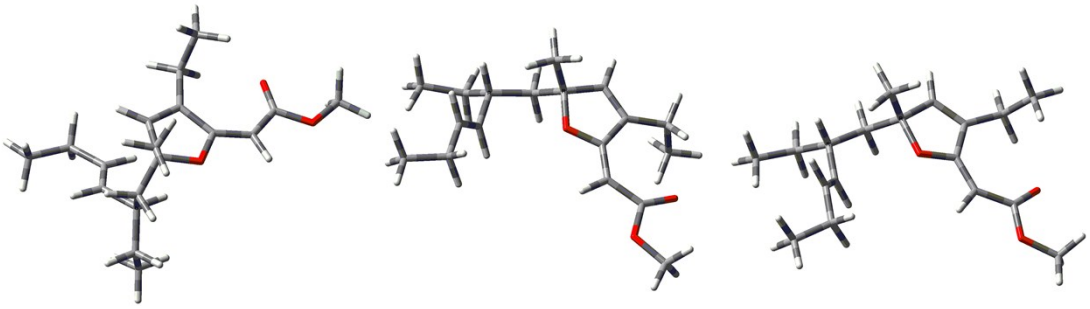
Conf 8. +0.85 kcal/mol (4%) **Conf 9.** +1.18 kcal/mol (3%)

Conf 7. +1.20 kcal/mol (2%) **Conf 10.** +1.26 kcal/mol (2%)

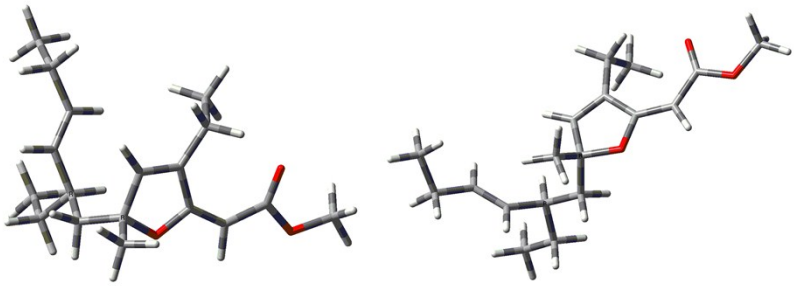
Figure S5. Lowest-energy conformers identified for 2*E*-(6*R*,8*R*)-**1** at the B3PW91/PCM($CHCl_3$)/6-311G(d,p) level.



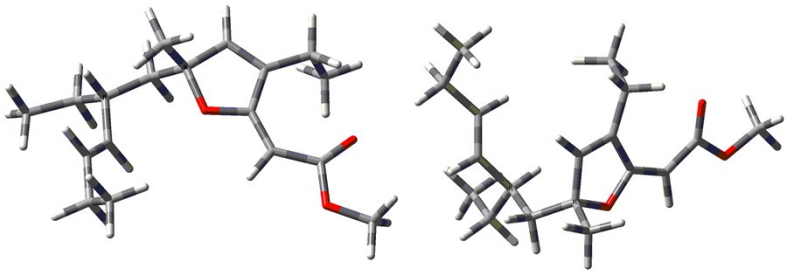
Conf 1. 0.00 kcal/mol (26%) **Conf 2.** +0.22 kcal/mol (18%) **Conf 3.** +0.55 kcal/mol (10%)



Conf 4. +0.60 kcal/mol (10%) **Conf 5.** +0.73 kcal/mol (8%) **Conf 6.** +0.73 kcal/mol (8%)

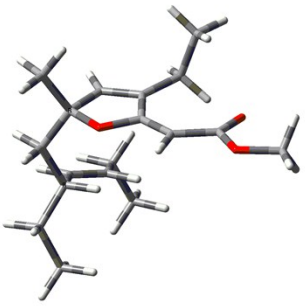


Conf 7. +0.83 kcal/mol (6%) **Conf 8.** +0.83 kcal/mol (6%)

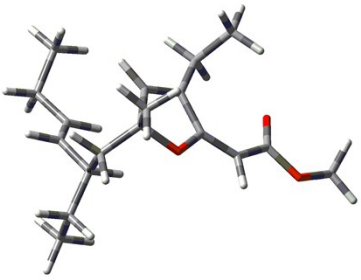


Conf 9. +0.95 kcal/mol (5%) **Conf 10.** +1.39 kcal/mol (3%)

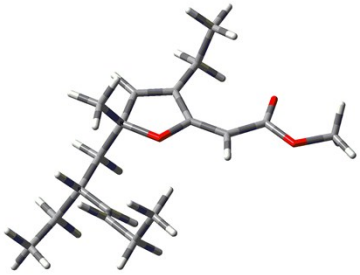
Figure S6. Lowest-energy conformers identified for 2*E*-(6*R*,8*R*)-**1** at the B3PW91/PCM(MeOH)/6-311G(d,p) level.



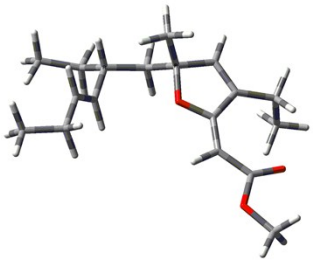
Conf 1. 0.0 kcal/mol (22%)



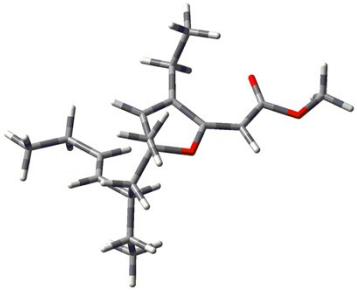
Conf 2. +0.13 kcal/mol (18%)



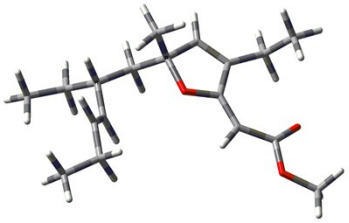
Conf 3. +0.24 kcal/mol (15%)



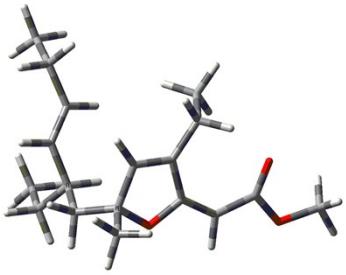
Conf 5. +0.46 kcal/mol (10%)



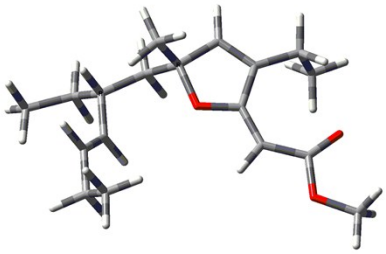
Conf 4. +0.56 kcal/mol (9%)



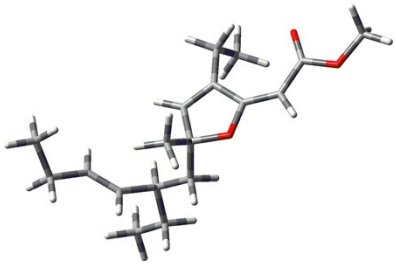
Conf 6. +0.65 kcal/mol (7%)



Conf 7. +0.65 kcal/mol (7%)

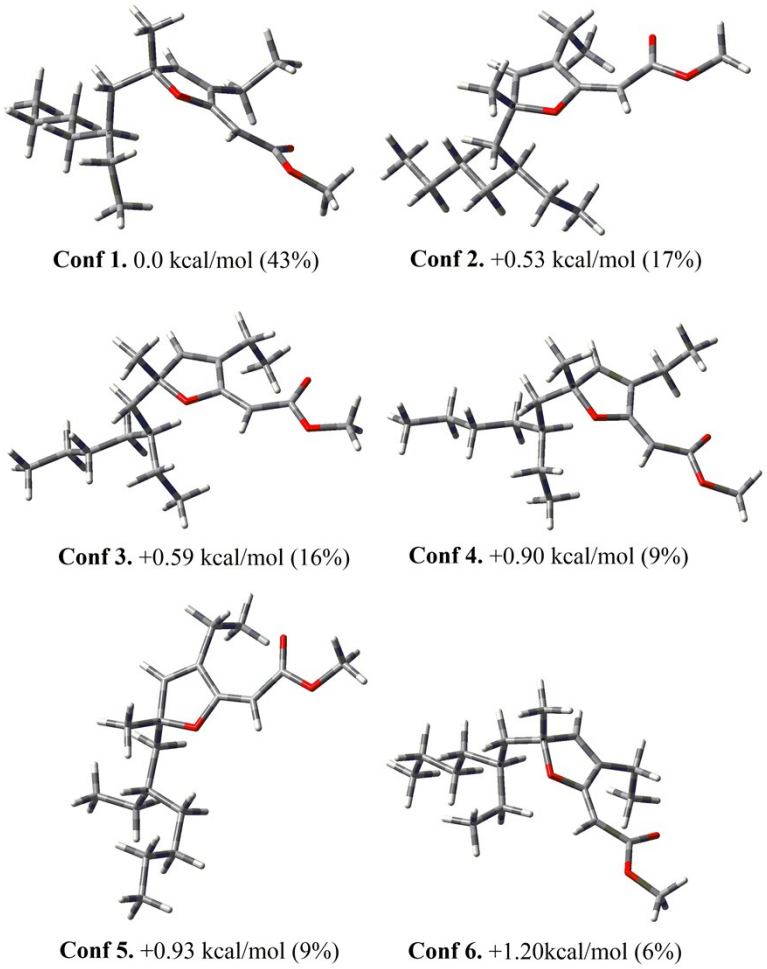


Conf 9. +0.66 kcal/mol (7%)



Conf 8. +0.84 kcal/mol (5%)

Figure S7. Lowest-energy conformers identified for 2*E*-(6*R*,8*S*)-**2** at the B3PW91/PCM($CHCl_3$)/6-311G(d,p) level.



Conf 1. 0.0 kcal/mol (43%)

Conf 2. +0.53 kcal/mol (17%)

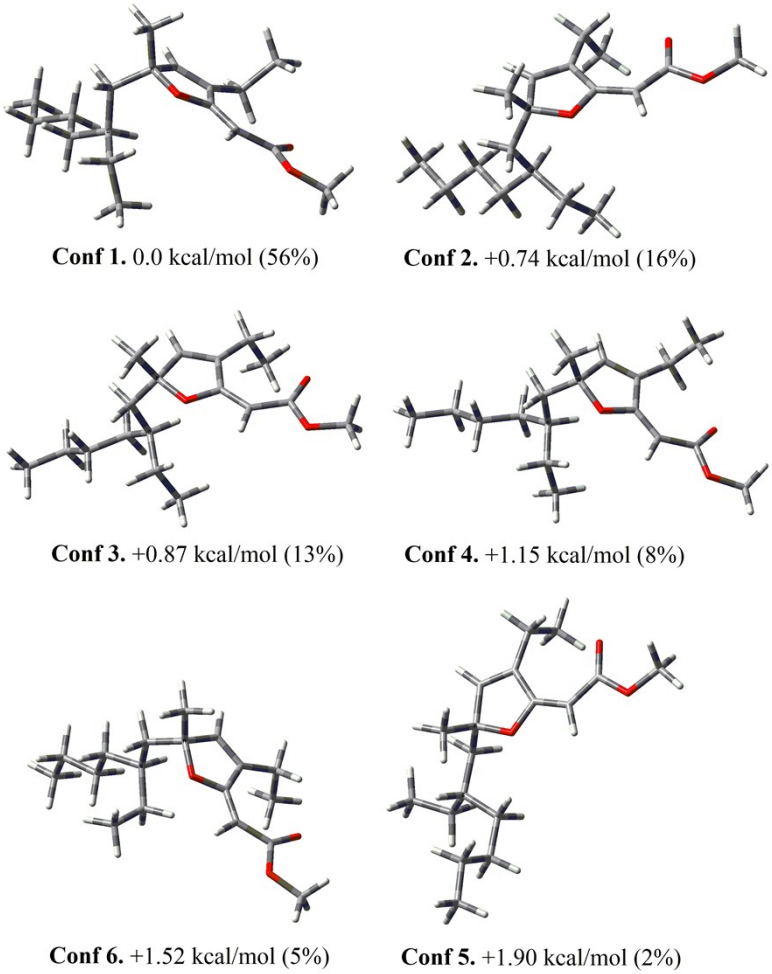
Conf 3. +0.59 kcal/mol (16%)

Conf 4. +0.90 kcal/mol (9%)

Conf 5. +0.93 kcal/mol (9%)

Conf 6. +1.20kcal/mol (6%)

Figure S8. Lowest-energy conformers identified for 2*E*-(6*R*,8*S*)-**2** at the B3PW91/PCM(MeOH)/6-311G(d,p) level.



Conf 1. 0.0 kcal/mol (56%)

Conf 2. +0.74 kcal/mol (16%)

Conf 3. +0.87 kcal/mol (13%)

Conf 4. +1.15 kcal/mol (8%)

Conf 6. +1.52 kcal/mol (5%)

Conf 5. +1.90 kcal/mol (2%)

Figure S9. Calculated ORD in $CHCl_3$ and MeOH using B3LYP/aug-cc-pVDZ level of 2*Z*-(6*R*,8*R*)-**1** and 2*E*-(6*R*,8*R*)-**1**.

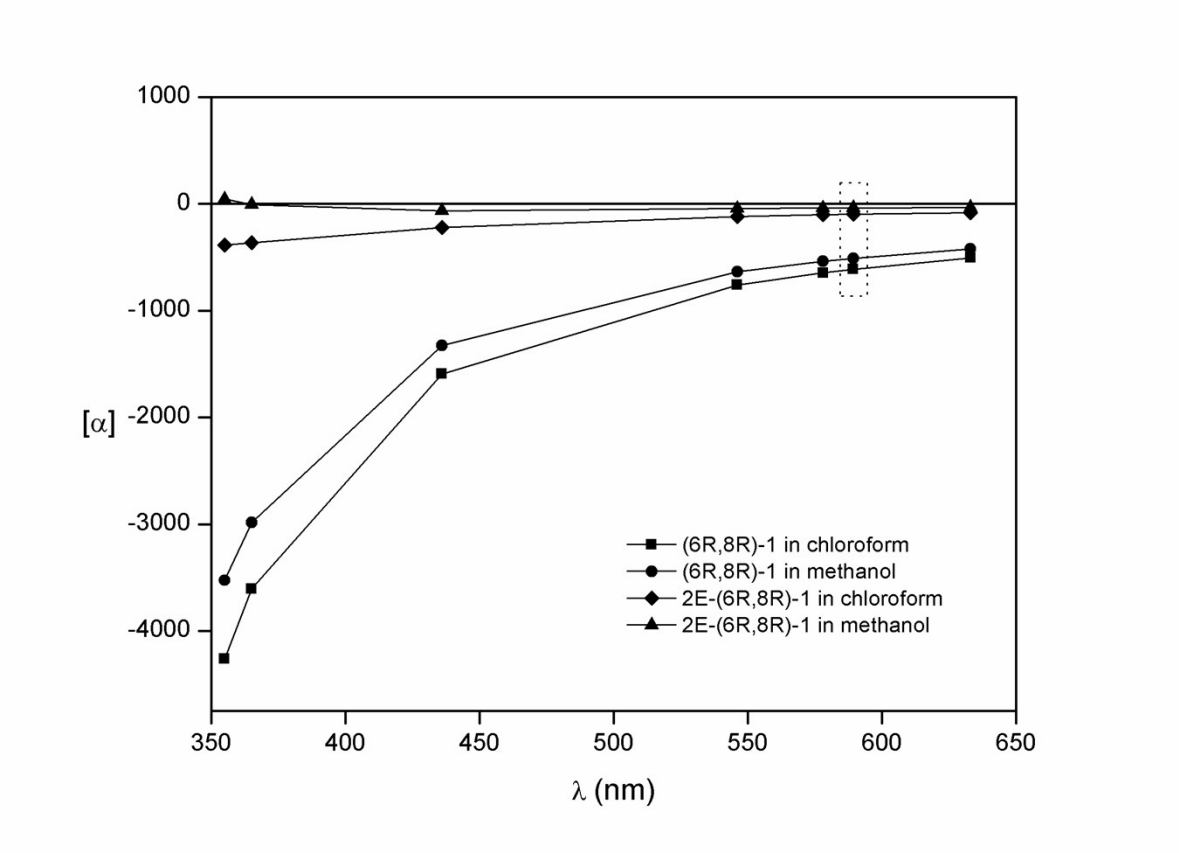


Figure S10. Calculated ORD in $CHCl_3$ and MeOH using B3LYP/aug-cc-pVDZ level of 2*Z*-(6*R*,8*S*)-**2** and 2*E*-(6*R*,8*S*)-**2**.

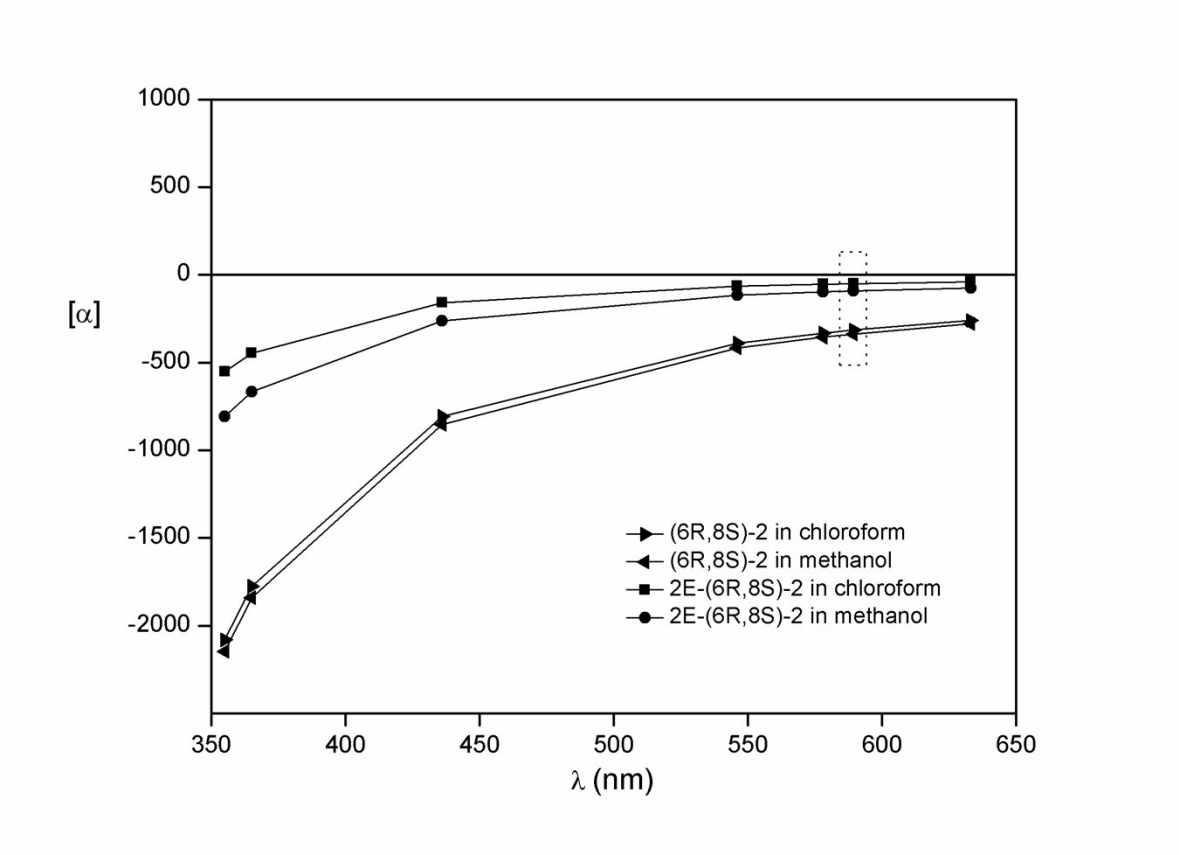


Figure S11. Experimental UV and ECD spectra of (−)-spongosoritin A (A) and (−)-dihydrospongosoritin A (B) in MeOH and calculated [CAM-B3LYP/PCM(MeOH)/TZVP] spectra for (6*R*,8*R*)-**1** (A) and (6*R*,8*S*)-**2** (B).

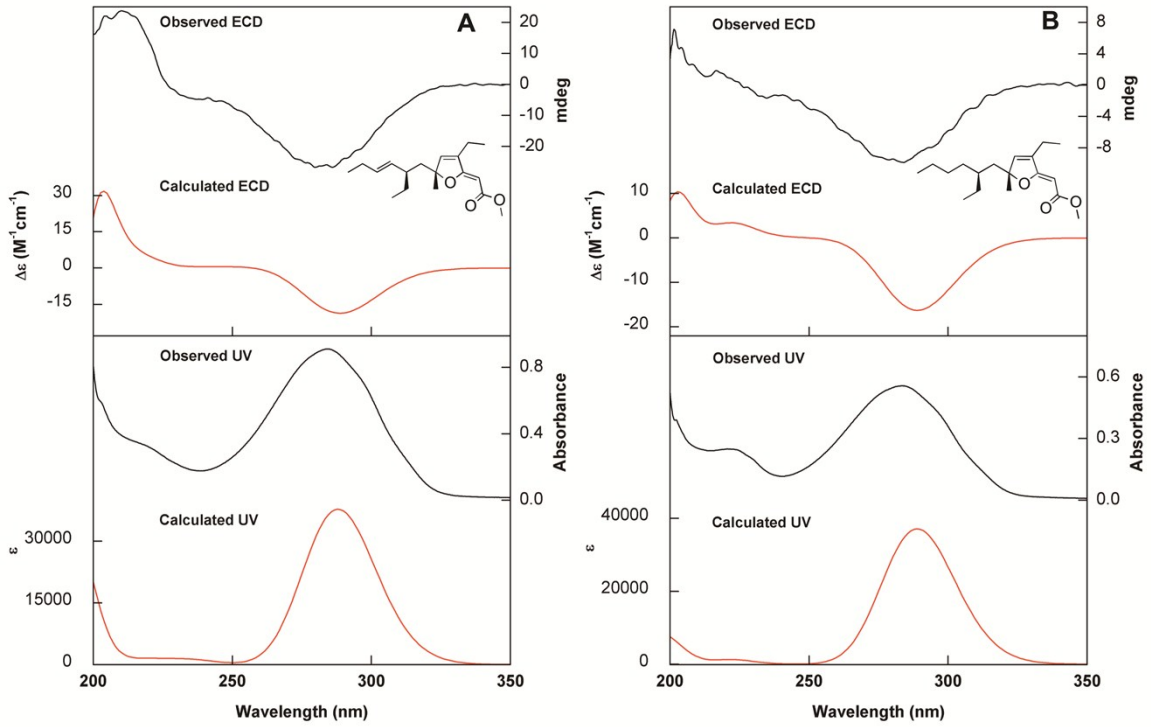


Figure S12. Calculated [CAM-B3LYP/PCM(MeOH)/TZVP] UV and ECD spectra for 2*Z*-(6*R*,8*R*)-**1**/2*E*-(6*R*,8*R*)-**1** (A) and 2*Z*-(6*R*,8*S*)-**2**/2E-(6*R*,8*S*)-**2** (B).

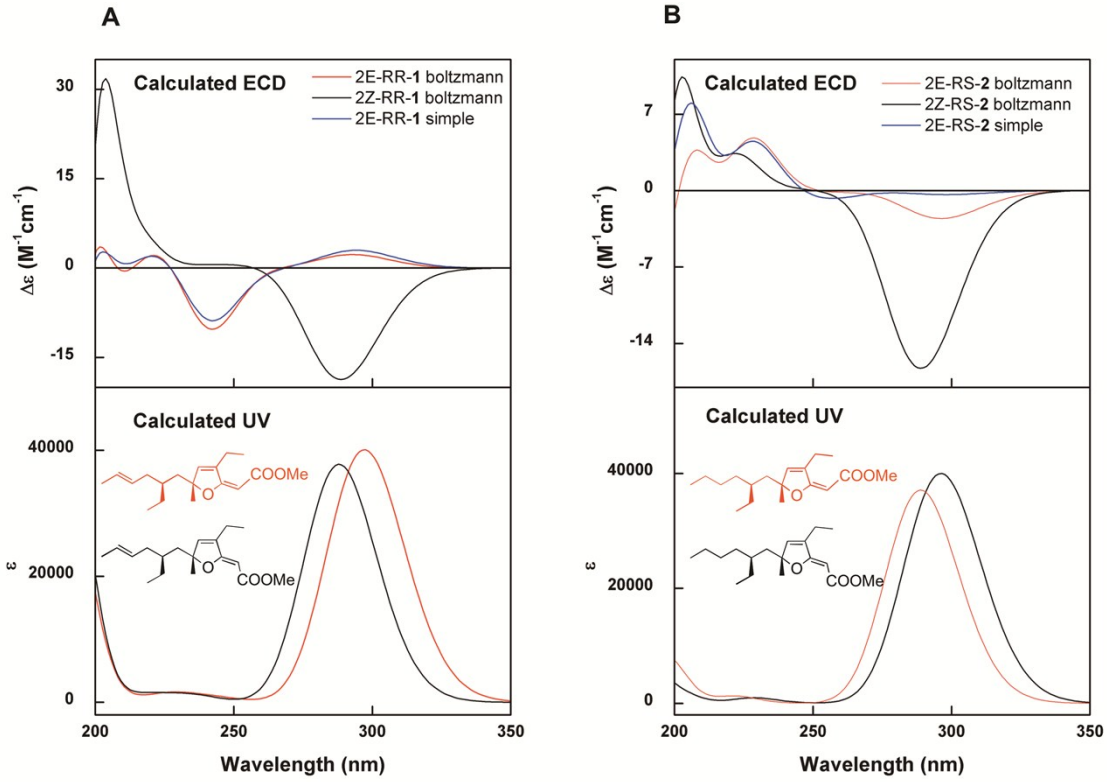


Table S1. Comparison of calculated ^{13}C-NMR chemical shift at the mPW1PW91/6-31G(d)//mPW1PW91/6-31G(d) level for *syn*-(6*R*,8*R*)-**1** and *anti*-(6*R*,8*S*)-**1** with literature data for spongosoritin A (**1**).

Carbon	δ_{exp*}	*syn*-(6*R*,8*R*)-1		*anti*-(6*R*,8*S*)-1	
		δ_{scal**}	$\lvert\delta_{exp} - \delta_{scal}\rvert$	δ_{scal**}	$\lvert\delta_{exp} - \delta_{scal}\rvert$
1	**166.9**	163.08	3.82	162.81	4.09
2	**83.8**	87.13	3.33	87.79	3.99
3	**171.5**	169.65	1.85	167.76	3.74
4	**138.1**	139.75	1.65	139.48	1.38
5	**141.6**	145.65	4.05	146.26	4.66
6	**95.0**	93.63	1.37	93.13	1.87
7	**44.9**	46.03	1.13	47.22	2.32
8	**40**	42.12	2.12	43.30	3.30
9	**133.7**	135.39	1.69	135.41	1.71
10	**132.1**	135.66	3.56	134.65	2.55
11	**25.5**	28.66	3.16	28.92	3.42
12	**13.9**	15.94	2.04	15.95	2.05
13	**18.4**	20.73	2.33	21.72	3.32
14	**11.6**	13.17	1.57	15.39	3.79
15	**26.3**	25.16	1.14	23.91	2.39
17	**29.3**	30.79	1.49	30.70	1.40
18	**11.3**	13.41	2.11	13.32	2.02
OCH_3	**50.3**	50.60	0.30	50.65	0.35
	MAD	**2.15**		**2.69**	
	RMSD	**2.37**		**2.91**	

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Table S2. Comparison of calculated ^{13}C-NMR chemical shift at the B3LYP/PCM($CHCl_3$)/6-31+G(d,p)//B3LYP/6-31G(d) level for *syn*-(6*R*,8*R*)-**1** and *anti*-(6*R*,8*S*)-**1** with literature data for spongosoritin A (**1**).

Carbon	δ_{exp*}	***syn*-(6*R*,8*R*)-1**		***anti*-(6*R*,8*S*)-1**	
		δ_{scal**}	$\lvert\delta_{exp} - \delta_{scal}\rvert$	δ_{scal**}	$\lvert\delta_{exp} - \delta_{scal}\rvert$
1	**166.9**	167.03	0.13	167.04	0.14
2	**83.8**	83.65	0.15	84.40	0.60
3	**171.5**	172.75	1.25	171.27	0.23
4	**138.1**	141.06	2.96	139.93	1.83
5	**141.6**	145.95	4.35	147.47	5.87
6	**95.0**	97.81	2.81	97.17	2.17
7	**44.9**	47.30	2.40	48.80	3.90
8	**40**	45.53	5.53	46.09	6.09
9	**133.7**	135.24	1.54	135.06	1.36
10	**132.1**	135.85	3.75	135.72	3.62
11	**25.5**	29.88	4.38	30.15	4.65
12	**13.9**	15.18	1.28	15.18	1.28
13	**18.4**	21.11	2.71	22.49	4.09
14	**11.6**	12.24	0.64	15.17	3.57
15	**26.3**	23.48	2.82	22.59	3.71
17	**29.3**	31.68	2.38	31.86	2.56
18	**11.3**	12.30	1.00	12.07	0.77
OCH_3	**50.3**	50.27	0.03	50.25	0.05
	MAD	**2.23**		**2.58**	
	RMSD	**2.72**		**3.20**	

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Table S3. Comparison of calculated ^{13}C-NMR chemical shift at the mPW1PW91/6-31G(d)//mPW1PW91/6-31G(d) level for *syn*-(6*R*,8*S*)-**2** and *anti*-(6*R*,8*R*)-**2** with literature data for 9,10-dihydrospongosoritin A (**2**).

Carbon	δ_{exp}*	*syn*-(6*R*,8S)-2		*anti*-(6*R*,8*R*)-2	
		δ_{scal}**	$\lvert\delta_{exp} - \delta_{scal}\rvert$	δ_{scal}**	$\lvert\delta_{exp} - \delta_{scal}\rvert$
1	**141.2**	142.22	1.02	142.43	1.23
2	**138.6**	138.58	0.02	138.33	0.27
3	**95.1**	91.38	3.72	91.36	3.74
4	**171.1**	165.73	5.37	165.76	5.34
5	**18.3**	16.39	1.91	16.34	1.96
6	**11.7**	10.10	1.60	9.94	1.76
7	**83.9**	86.91	3.01	87.01	3.11
8	**166.8**	163.59	3.21	163.28	3.52
9	**50.4**	44.34	6.06	44.26	6.14
10	**42.9**	39.01	3.89	39.44	3.46
11	**34.6**	32.15	2.45	31.89	2.71
12	**34**	31.81	2.19	29.05	4.95
13	**28.8**	26.86	1.94	25.47	3.33
14	**22.8**	18.98	3.82	19.25	3.55
15	**25.4**	21.92	3.48	21.54	3.86
17	**14**	10.41	3.59	10.47	3.53
18	**26.8**	22.17	4.63	24.13	2.67
OCH_3	**10.4**	7.51	2.89	8.04	2.36
	MAD	**3.00**		**3.20**	
	RMSD	**3.30**		**3.50**	

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Table S4. Comparison of calculated ^{13}C-NMR chemical shift at the mPW1PW91/6-31G(d)//mPW1PW91/6-31G(d) level for *2Z*-(6*R*,8*R*)-**1**; *2Z*-(6*R*,8*S*)-**1**; *2E*-(6*R*,8*R*)-**1**; and *2R*-(6*R*,8*S*)-**1** with literature data for spongosoritin A (**1**).

Carbon	δ_{exp}*	2*Z*-(6*R*,8*R*)-1		2*Z*-(6*R*,8*S*)-1		2*E*-(6*R*,8*R*)-1		2*E*-(6*R*,8*S*)-1	
		δ_{scal}**	$\lvert\delta_{exp} - \delta_{scal}\rvert$	δ_{scal}**	$\lvert\delta_{exp} - \delta_{scal}\rvert$	δ_{scal}**	$\lvert\delta_{exp} - \delta_{scal}\rvert$	δ_{scal}**	$\lvert\delta_{exp} - \delta_{scal}\rvert$
1	**166.9**	163.08	3.82	162.81	4.09	165.47	1.43	165.50	1.40
2	**83.8**	87.13	3.33	87.79	3.99	90.59	6.79	90.76	6.96
3	**171.5**	169.65	1.85	167.76	3.74	173.22	1.72	168.45	3.05
4	**138.1**	139.75	1.65	139.48	1.38	141.64	3.54	141.77	3.67
5	**141.6**	145.65	4.05	146.26	4.66	150.84	9.24	149.00	7.40
6	**95.0**	93.63	1.37	93.13	1.87	89.89	5.11	89.84	5.16
7	**44.9**	46.03	1.13	47.22	2.32	46.81	1.91	47.05	2.15
8	**40**	42.12	2.12	43.30	3.30	41.53	1.53	43.11	3.11
9	**133.7**	135.39	1.69	135.41	1.71	135.21	1.51	134.94	1.24
10	**132.1**	135.66	3.56	134.65	2.55	136.53	4.43	134.88	2.78
11	**25.5**	28.66	3.16	28.92	3.42	28.73	3.23	28.84	3.34
12	**13.9**	15.94	2.04	15.95	2.05	15.58	1.68	15.77	1.87
13	**18.4**	20.73	2.33	21.72	3.32	24.53	6.13	24.50	6.10
14	**11.6**	13.17	1.57	15.39	3.79	17.74	6.14	17.99	6.39
15	**26.3**	25.16	1.14	23.91	2.39	26.08	0.22	24.36	1.94
17	**29.3**	30.79	1.49	30.70	1.40	31.14	1.84	30.96	1.66
18	**11.3**	13.41	2.11	13.32	2.02	13.45	2.15	13.25	1.95
OCH_3	**50.3**	50.60	0.30	50.65	0.35	50.93	0.63	50.86	0.56
	MAD	**2.15**		**2.69**		**3.29**		**3.37**	
	RMSD	**2.37**		**2.91**		**4.08**		**3.95**	

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Table S5. Calculated OR values in $CHCl_3$ using either the B3LYP/6-311++(d,p) or B3LYP/aug-cc-pVDZ levels for the optimized conformations of 2*Z*-(6*R*,8*R*)-**1**; 2*E*-(6*R*,8*R*)-**1**; 2*Z*-(6*R*,8*S*)-**2**; and 2*E*-(6*R*,8*S*)-**2**.

Conformer	ΔG kcal/mol	Boltzmann population % in $CHCl_3$	[α] 633 A	633 B	**589.3** A	**589.3** B	578 A	578 B	546 A	546 B	436 A	436 B	365 A	365 B	355 A	355 B
2*Z*-(6*R*,8*R*)-**1**																
1	0	47	-509	-516	**-618**	**-626**	-652	-661	-768	-778	-1618	-1639	-3683	-3732	-4348	-4417
2	0.61	17	-543	-545	**-658**	**-661**	-695	-697	-818	-821	-1725	-1733	-3934	-3963	-4659	-4696
3	1.06	8	-540	-539	**-652**	**-651**	-686	-686	-803	-803	-1639	-1643	-3565	-3590	-4179	-4214
4	1.08	8	-548	-549	**-664**	**-665**	-700	-702	-824	-826	-1730	-1739	-3941	-3974	-4671	-4715
5	1.21	6	-506	-512	**-614**	**-621**	-648	-655	-762	-772	-1605	-1627	-3641	-3700	-4303	-4377
6	1.27	6	-405	-413	**-490**	**-500**	-517	-528	-608	-620	-1264	-1288	-2775	-2826	-3247	-3308
7	1.40	4	-479	-490	**-580**	**-594**	-612	-626	-720	-737	-1509	-1542	-3418	-3486	-4044	-4124
8	1.45	4	-163	-177	**-196**	**-212**	-206	-223	-240	-260	-479	-513	-997	-1057	-1155	-1222
Boltzmann average values			-499	-504	**-605**	**-611**	-638	-645	-750	-759	-1575	-1593	-3561	-3606	-4209	-4264
Simple average			-462	-468	**-559**	**-566**	-589	-597	-693	-702	-1446	-1465	-3244	-3291	-3827	-3884
2*E*-(6*R*,8*R*)-**1**																
1	0	26	-	-299	-	**-360**	-	-379	-	-442	-	-977	-	-1779	-	-2040
2	0.22	18	-	-276	-	**-333**	-	-350	-	-410	-	-831	-	-1739	-	-2010
3	0.55	10	-	271	-	**327**	-	344	-	403	-	837	-	1934	-	2315
4	0.60	10	-	-298	-	**-358**	-	-377	-	-439	-	-871	-	-1754	-	-2004
5	0.73	8	-	369	-	**447**	-	472	-	555	-	1168	-	2699	-	3219
6	0.73	8	-	138	-	**169**	-	179	-	213	-	473	-	1194	-	1454
7	0.83	6	-	-140	-	**-168**	-	-176	-	-204	-	-389	-	-717	-	-795
8	0.83	6	-	-95	-	**-112**	-	-118	-	-136	-	-253	-	-490	-	-562
9	0.95	5	-	511	-	**616**	-	649	-	760	-	1562	-	3503	-	4156
10	1.39	3	-	-123	-	**-148**	-	-156	-	-183	-	-370	-	-764	-	-877
Boltzmann average values			-	-81	-	**-97**	-	-102	-	-118	-	-219	-	-363	-	-383
Simple average			-	6	-	**8**	-	9	-	12	-	45	-	209	-	286
2*Z*-(6*R*,8*S*)-**2**																
1	0	23	-323	-335	**-390**	**-404**	-411	-426	-483	-500	-996	-1029	-2178	-2249	-2550	-2634
2	0.19	17	-213	-238	**-259**	**-289**	-274	-305	-324	-359	-697	-761	-1602	-1721	-1892	-2027
3	0.30	14	-319	-325	**-384**	**-390**	-404	-411	-471	-479	-939	-958	-1966	-2016	-2281	-2342
4	0.30	14	-125	-129	**-154**	**-159**	-163	-169	-194	-201	-433	-450	-1036	-1079	-1233	-1286
5	0.58	9	-239	-228	**-287**	**-273**	-301	-287	-351	-335	-690	-666	-1418	-1392	-1639	-1616
6	0.64	8	-302	-317	**-366**	**-383**	-386	-404	-453	-474	-940	-981	-2064	-2152	-2417	-2520
7	0.92	5	-182	-207	**-223**	**-253**	-236	-267	-280	-316	-615	-681	-1444	-1568	-1711	-1852
8	1.03	4	-196	-207	**-238**	**-251**	-251	-265	-295	-311	-614	-644	-1359	-1421	-1595	-1666
9	1.13	3	-311	-307	**-374**	**-370**	-394	-389	-460	-455	-921	-916	-1940	-1944	-2254	-2263
10	1.38	2	-158	-159	**-192**	**-193**	-202	-203	-238	-239	-499	-504	-1113	-1134	-1306	-1333

Boltzmann average values			-251	-261	**-303**	**-315**	-320	-332	-375	-390	-778	-807	-1711	-1775	-2005	-2081
Simple average			-237	-245	**-287**	**-296**	-302	-313	-355	-367	-734	-759	-1612	-1668	-1888	-1954
2*E*-(6*R*,8*S*)-**2**																
1	0	43	-	-142	-	**-174**	-	-184	-	-219	-	-491	-	1217-	-	-1470
2	0.53	17	-	43	-	**49**	-	51	-	57	-	84	-	61	-	36
3	0.59	16	-	78	-	**94**	-	99	-	115	-	229	-	467	-	538
4	0.90	9	-	-119	-	**-145**	-	-153	-	-180	-	-384	-	-899	-	-1074
5	0.93	9	-	108	-	**131**	-	138	-	162	-	332	-	722	-	846
6	1.20	6	-	52	-	**61**	-	64	-	73	-	128	-	191	-	198
Boltzmann average values			-	-40	**-**	**-50**	-	-53	-	-64	-	-158	-	-446	-	-552
Simple average			-	3	**-**	**3**	-	2	-	1	-	-17	-	-113	-	-154

A: B3LYP/6-311G++(d,p)
B: B3LYP/AUG-cc-pVDZ

Table S6. Calculated OR values in MeOH using either the B3LYP/6-311++(d,p) or B3LYP/aug-cc-pVDZ levels for the optimized conformations of 2*Z*-(6*R*,8*R*)-**1**; 2*E*-(6*R*,8*R*)-**1**; 2*Z*-(6*R*,8*S*)-**2**; and 2*E*-(6*R*,8*S*)-**2**.

Conformer	ΔG kcal/mol	Boltzmann population % in MeOH	[α] 633 A	633 B	**589.3** A	**589.3** B	578 A	578 B	546 A	546 B	436 A	436 B	365 A	365 B	355 A	355 B
2*Z*-(6*R*,8*R*)-**1**																
2	0	25	-564	-566	**-684**	**-686**	-722	-724	-850	-853	-1791	-1799	-4090	-4115	-4848	-4880
1	0.19	18	-528	-535	**-640**	**-649**	-676	-685	-795	-806	-1674	-1695	-3811	-3856	-4512	-4566
3	0.47	11	-556	-557	**-670**	**-671**	-706	-707	-826	-828	-1676	-1684	-3607	-3640	-4214	-4258
4	0.55	10	-579	-581	**-701**	**-704**	-739	-743	-869	-873	-1819	-1831	-4126	-4162	-4888	-4933
5	0.84	6	-526	-533	**-638**	**-646**	-673	-682	-792	-803	-1668	-1691	-3786	-3847	-4478	-4552
9	0.90	6	163	166	**198**	**201**	209	212	246	249	518	524	1183	1192	1401	1411
8	1.00	5	-155	-166	**-186**	**-199**	-195	-209	-228	-243	-450	-478	-923	-974	-1066	-1123
7	1.01	5	-505	-517	**-612**	**-626**	-646	-661	-759	-777	-1591	-1624	-3604	-3672	-4266	-4344
6	1.02	5	-425	-435	**-514**	**-526**	-542	-554	-637	-651	-1317	-1345	-2870	-2930	-3352	-3422
10	1.16	4	238	229	**287**	**277**	302	292	354	342	723	702	1591	1556	1872	1835
11	1.23	3	92	99	**114**	**123**	121	130	145	156	345	363	909	939	1109	1141
12	1.42	2	290	293	**348**	**353**	366	371	427	433	856	868	1817	1846	2118	2153
Boltzmann average values			-418	-422	**-506**	**-511**	-534	-539	-627	-633	-1311	-1324	-2950	-2983	-3484	-3525
Simple average			-255	-258	**-308**	**-313**	-325	-330	-382	-388	-795	-808	-1775	-1805	-2094	-2128
2*E*-(6*R*,8*R*)-**1**																
1	0	22	-	-304	-	**-365**	-	-384	-	-447	-	-878	-	-1727	-	-1958
2	0.13	18	-	-290	-	**-349**	-	-367	-	-429	-	-860	-	-1757	-	-2013
3	0.24	15	-	285	-	**344**	-	362	-	424	-	875	-	1994	-	2377
5	0.46	10	-	385	-	**466**	-	492	-	578	-	1205	-	2741	-	3257
4	0.56	9	-	-309	-	**-371**	-	-390	-	-454	-	-890	-	-1739	-	-1965
6	0.65	7	-	147	-	**179**	-	190	-	225	-	494	-	1218	-	1475
7	0.65	7	-	-148	-	**-177**	-	-186	-	-216	-	-409	-	-735	-	-805
9	0.66	7	-	528	-	**636**	-	670	-	783	-	1598	-	3532	-	4174
8	0.84	5	-	-101	-	**-120**	-	-125	-	-145	-	-269	-	-522	-	-599
Boltzmann average values			-	-31	-	**-36**	-	-37	-	-42	-	-63	-	-5	-	-45
Simple average			-	21	-	**27**	-	29	-	35	-	96	-	334	-	438
2*Z*-(6*R*,8*S*)-**2**																
1	0	18	-342	-355	**-413**	**-428**	-435	-451	-510	-529	-1043	-1079	-2244	-2321	-2615	-2706
5	0.08	16	-229	-217	**-274**	**-261**	-288	-274	-335	-320	-656	-632	-1332	-1302	-1534	-1504
2	0.09	16	-231	-257	**-282**	**-312**	-297	-329	-351	-387	-747	-813	-1690	-1813	-1989	-2129
3	0.11	15	-349	-355	**-419**	**-427**	-441	-449	-514	-524	-1020	-1043	-2114	-2171	-2445	-2514
6	0.16	14	-320	-335	**-387**	**-405**	-408	-427	-479	-501	-990	-1033	-2159	-2251	-2523	-2631
4	0.33	10	-141	-145	**-172**	**-178**	-182	-188	-216	-223	-472	-488	-1094	-1136	-1293	-1344
8	0.85	4	-207	-218	**-250**	**-264**	-264	-278	-310	-327	-641	-674	-1402	-1467	-1639	-1714

9	1.18	3	-326	-323	**-392**	**-388**	-412	-409	-481	-477	-958	-954	-1989	-1998	-2302	-2316
7	1.20	2	-202	-229	**-247**	**-278**	-261	-294	-309	-347	-672	-742	-1553	-1684	-1834	-1984
10	1.26	2	-157	-158	**-190**	**-191**	-201	-202	-236	-238	-492	-498	-1084	-1105	-1269	-1296
Boltzmann average values			-271	-280	**-327**	**-338**	-344	-356	-404	-417	-826	-853	-1780	-1840	-2075	-2147
Simple average			-250	-259	**-303**	**-313**	-319	-330	-374	-387	-769	-795	-1666	-1725	-1944	-2014
2*E*-(6*R*,8*S*)-**2**																
1	0	56	-	-150	-	**-183**	-	-194	-	-229	-	-503	-	-1215	-	-1458
2	0.74	16	-	34	-	**39**	-	41	-	45	-	62	-	26	-	0
3	0.87	13	-	77	-	**93**	-	98	-	114	-	227	-	460	-	529
4	1.15	8	-	-121	-	**-146**	-	-155	-	-182	-	-382	-	-876	-	-1040
6	1.52	5	-	49	-	**58**	-	61	-	70	-	122	-	184	-	192
5	1.90	2	-	122	-	**147**	-	154	-	181	-	368	-	789	-	921
Boltzmann average values			-	-74	**-**	**-91**	-	-96	-	-115	-	-262	-	-666	-	-808
Simple average			-	2	**-**	**1**	-	1	-	0	-	-18	-	-105	-	-143

A: B3LYP/6-311G++(d,p)
B: B3LYP/AUG-cc-pVDZ

Table S7. Relative energies and conformer populations of (6*R*,8*R*)-**1** and (6*R*,8*S*)-**2** at the wB97XD /PCM($CHCl_3$)/6-311G(d,p) level**.**

Conformer	E (kcal/mol)	E_{rel}	Boltzmann Population (%)
spongosoritin A (1)			
6R8R_1_conf1	-582337.5117	0.79	15.6
6R8R_1_conf2	-582338.3048	0	59.7
6R8R_1_conf3	-582335.759	2.55	0.8
6R8R_1_conf4	-582337.41	0.89	13.2
6R8R_1_conf5	-582336.3941	1.91	2.4
6R8R_1_conf6	-582336.7317	1.57	4.2
6R8R_1_conf7	-582336.6959	1.61	3.9
6R8R_1_conf8	-582334.9063	3.40	0.2
dihydropongosoritin A (2)			
6R8S_2_conf1	-583096.8107	0	22.9
6R8S_2_conf2	-583096.3005	0.51	9.7
6R8S_2_conf3	-583096.5609	0.25	15.0
6R8S_2_conf4	-583096.143	0.67	7.4
6R8S_2_conf5	-583095.5626	1.25	2.8
6R8S_2_conf6	-583095.6178	1.19	3.1
6R8S_2_conf7	-583096.4304	0.38	12.1
6R8S_2_conf8	-583096.2692	0.54	9.2
6R8S_2_conf9	-583096.6086	0.20	16.3
6R8S_2_conf10	-583095.2231	1.59	1.6

CARTESIAN COORDINATES

Compound 1: (6*S*,8*S*)-spongosoritin A conf1

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.959683 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.544934	1.340115	1.138253
C	-0.37296	1.723466	0.24124
C	0.10897	0.093178	1.839935
O	-1.15229	-0.22334	1.17788
C	-1.4434	0.721736	0.271657
C	-2.56589	0.723827	-0.49157
C	-3.6108	-0.28219	-0.44949
O	-3.66734	-1.27368	0.248908
O	-4.58937	0.028236	-1.34367
C	-5.68068	-0.89016	-1.40029
C	-0.38614	2.918544	-0.65751
C	0.787581	3.87081	-0.46478
C	-0.20232	0.351055	3.315151
C	1.025745	-1.12879	1.692116
C	1.468606	-1.49204	0.262502
C	2.722187	-0.75943	-0.13239
C	2.876661	-0.00887	-1.22292
C	4.129133	0.694299	-1.66134
C	5.343762	0.530765	-0.75642
C	1.675097	-3.01844	0.161473
C	1.978698	-3.51927	-1.24549
H	1.467938	1.848124	1.381992
H	-2.69445	1.537445	-1.1922
H	-6.35179	-0.50474	-2.16612
H	-5.33517	-1.89076	-1.66948
H	-6.19672	-0.94213	-0.43887
H	-0.41741	2.570965	-1.69805
H	-1.32934	3.457293	-0.50347
H	0.70777	4.717778	-1.15018
H	0.814401	4.267166	0.554308
H	1.741624	3.373311	-0.65896
H	-0.92948	1.159589	3.414805
H	-0.61211	-0.55088	3.775946
H	0.708205	0.63317	3.849761

H	1.904805	-0.97227	2.327908
H	0.474841	-1.96897	2.128655
H	0.664866	-1.22247	-0.43395
H	3.569764	-0.90663	0.538925
H	2.018101	0.121931	-1.88247
H	4.378405	0.349575	-2.67451
H	3.902498	1.762771	-1.78146
H	6.199244	1.079509	-1.15877
H	5.147764	0.911782	0.250451
H	5.635705	-0.51959	-0.66418
H	2.482026	-3.31432	0.845195
H	0.766352	-3.50803	0.530567
H	2.089522	-4.60744	-1.25659
H	1.168926	-3.26087	-1.93592
H	2.900572	-3.08272	-1.63903

Compound 1: **(6*S*,8*S*)-spongosoritin A conf2**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.958712 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.429171	1.299885	1.377676
C	-0.40962	1.708896	0.416907
C	-0.03785	0.008477	1.970884
O	-1.21771	-0.30433	1.171704
C	-1.4486	0.681703	0.291759
C	-2.49354	0.701693	-0.5746
C	-3.51355	-0.32423	-0.68888
O	-3.60661	-1.36135	-0.06467
O	-4.41903	0.027701	-1.64264
C	-5.48001	-0.90386	-1.85294
C	-0.37166	2.950301	-0.41566
C	0.745672	3.921583	-0.05579
C	-0.50083	0.185883	3.418219
C	0.923644	-1.1823	1.860951
C	1.50964	-1.4773	0.468013
C	2.752109	-0.67177	0.205311
C	2.965496	0.13192	-0.83613
C	4.230389	0.891947	-1.1005
C	4.88254	0.518503	-2.43533
C	1.803455	-2.98839	0.349661
C	2.273951	-3.43112	-1.03064
H	1.309615	1.816389	1.735203
H	-2.57748	1.551308	-1.23835
H	-6.0978	-0.47528	-2.64037
H	-5.09007	-1.87502	-2.16579
H	-6.06868	-1.03673	-0.94235
H	-0.2877	2.659616	-1.47059
H	-1.34229	3.454296	-0.33003
H	0.709503	4.801438	-0.70244
H	0.656334	4.263633	0.979269
H	1.729581	3.460105	-0.17514
H	-1.2544	0.973534	3.482477
H	-0.93173	-0.74618	3.791386
H	0.344653	0.459141	4.054588
H	1.734546	-1.03094	2.582856
H	0.359661	-2.05448	2.209153

H	0.757901	-1.22695	-0.29081
H	3.552634	-0.79903	0.939009
H	2.170263	0.254621	-1.57335
H	4.010473	1.968087	-1.1085
H	4.937311	0.724777	-0.28049
H	4.196213	0.687481	-3.27101
H	5.780343	1.116856	-2.61512
H	5.169891	-0.53671	-2.44922
H	2.551475	-3.26473	1.104883
H	0.888408	-3.532	0.612297
H	1.529702	-3.18528	-1.79533
H	3.210412	-2.94251	-1.31171
H	2.435479	-4.51257	-1.05922

Compound 1: **(6*S*,8*S*)-spongosoritin A conf3**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.957990 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.067019	2.174992	0.296165
C	-0.8818	1.84457	-0.58927
C	0.027659	1.266567	1.484526
O	-1.05089	0.347644	1.145423
C	-1.57823	0.672588	-0.04495
C	-2.58959	-0.0126	-0.63579
C	-3.24036	-1.18787	-0.08517
O	-2.99084	-1.76338	0.954724
O	-4.22689	-1.6051	-0.92314
C	-4.94304	-2.76569	-0.49975
C	-1.22274	2.516175	-1.88254
C	-2.45866	3.418627	-1.78673
C	-0.38316	2.001419	2.760246
C	1.326635	0.476063	1.712152
C	1.798427	-0.43197	0.554298
C	3.302218	-0.47638	0.523519
C	4.075093	-0.05083	-0.47526
C	5.573899	-0.09308	-0.4924
C	6.13478	-0.93254	-1.64412
C	1.206445	-1.85013	0.677772
C	1.456899	-2.73106	-0.54122
H	0.775177	2.989905	0.208802
H	-2.94379	0.339438	-1.59489
H	-5.42713	-2.59475	0.464163
H	-5.69092	-2.94797	-1.26962
H	-4.27486	-3.62538	-0.41242
H	-0.36214	3.108774	-2.20516
H	-1.38224	1.754534	-2.65379
H	-2.67524	3.873655	-2.75673
H	-3.34216	2.857875	-1.47223
H	-2.29642	4.22198	-1.06317
H	-1.31843	2.543092	2.604172
H	-0.52148	1.286115	3.574267
H	0.39035	2.716233	3.051504
H	2.096934	1.223282	1.931638
H	1.20691	-0.12001	2.62415

H	1.455881	0.003595	-0.39335
H	3.77916	-0.89206	1.414761
H	3.597962	0.356986	-1.36863
H	5.961787	0.930611	-0.58337
H	5.940189	-0.48046	0.464576
H	5.790091	-0.5553	-2.61207
H	7.228419	-0.91261	-1.64911
H	5.814938	-1.97515	-1.56052
H	1.633114	-2.3244	1.571949
H	0.131366	-1.76779	0.856964
H	1.019152	-3.72385	-0.40255
H	1.007443	-2.29436	-1.43945
H	2.525853	-2.85839	-0.73478

Compound 1: **(6*S*,8*S*)-spongosoritin A conf4**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.957957 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.667162	1.164377	1.242801
C	-0.23863	1.588109	0.351298
C	0.237035	-0.12565	1.863929
O	-1.00798	-0.41793	1.160395
C	-1.295	0.572449	0.301973
C	-2.39772	0.592497	-0.48984
C	-3.42429	-0.43242	-0.52401
O	-3.48359	-1.45409	0.129088
O	-4.38238	-0.09894	-1.43194
C	-5.45628	-1.03076	-1.55812
C	-0.23375	2.853638	-0.44753
C	-1.16337	3.932533	0.121067
C	-0.10425	0.03826	3.345825
C	1.173838	-1.32416	1.658823
C	1.67863	-1.57039	0.225231
C	2.932231	-0.79072	-0.06285
C	3.131537	0.03769	-1.08766
C	4.413875	0.756063	-1.38421
C	4.259594	2.278854	-1.42587
C	1.921596	-3.08143	0.020134
C	2.308792	-3.46731	-1.40249
H	1.579883	1.672287	1.525105
H	-2.52524	1.437057	-1.15283
H	-6.11588	-0.62005	-2.32079
H	-5.08758	-2.01163	-1.86632
H	-5.99344	-1.13692	-0.61284
H	0.789411	3.237137	-0.48564
H	-0.52008	2.629858	-1.4813
H	-1.13327	4.8304	-0.50188
H	-2.19932	3.587774	0.16566
H	-0.85927	4.211318	1.133565
H	-0.84881	0.825711	3.479824
H	-0.50473	-0.89689	3.744483
H	0.791159	0.304418	3.913059
H	2.025816	-1.20963	2.338864
H	0.616798	-2.20087	2.006382

H	0.89897	-1.26351	-0.48297
H	3.759656	-0.97304	0.62823
H	2.308425	0.221421	-1.78028
H	5.170457	0.476901	-0.64276
H	4.793626	0.417071	-2.35761
H	3.512878	2.579574	-2.16734
H	3.941448	2.668647	-0.45456
H	5.204495	2.762179	-1.69025
H	2.698912	-3.41428	0.720995
H	1.005676	-3.61278	0.303865
H	2.445312	-4.54905	-1.48978
H	1.530861	-3.17176	-2.11424
H	3.239463	-2.98349	-1.71017

Compound 1: **(6*S*,8*S*)-spongosoritin A conf5**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.957751 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.343208	1.330094	1.350638
C	-0.35783	1.818272	0.31934
C	-0.27614	0.067986	1.859935
O	-1.3861	-0.14055	0.936302
C	-1.453	0.876351	0.061741
C	-2.3932	1.003961	-0.90934
C	-3.50836	0.133998	-1.24018
O	-4.29662	0.370939	-2.13849
O	-3.60583	-0.96975	-0.47027
C	-4.69759	-1.8385	-0.77973
C	-0.13791	3.06735	-0.47302
C	1.013702	3.935675	0.01809
C	-0.87347	0.254486	3.256129
C	0.60304	-1.18913	1.820716
C	1.298227	-1.51314	0.485551
C	2.612362	-0.79372	0.353405
C	2.98447	-0.00545	-0.65445
C	4.320616	0.662287	-0.78387
C	5.083474	0.230672	-2.04008
C	1.500746	-3.03985	0.375313
C	2.0579	-3.505	-0.9647
H	1.217074	1.771649	1.809823
H	-2.3233	1.87698	-1.54442
H	-4.6251	-2.66277	-0.0724
H	-5.65228	-1.32164	-0.66131
H	-4.62118	-2.21087	-1.80357
H	0.02552	2.789722	-1.52212
H	-1.06808	3.649008	-0.46897
H	1.113387	4.825566	-0.60772
H	0.850401	4.267817	1.047352
H	1.963709	3.395627	-0.016
H	-1.57319	1.092864	3.26141
H	-1.4042	-0.65019	3.56254
H	-0.082	0.456886	3.982063
H	1.349352	-1.10493	2.619367
H	-0.05258	-2.02159	2.098894

H	0.64019	-1.20681	-0.33712
H	3.324979	-0.97779	1.161869
H	2.27822	0.173906	-1.46676
H	4.178937	1.750897	-0.81814
H	4.922411	0.454527	0.107719
H	4.502704	0.436206	-2.94466
H	6.034016	0.765061	-2.12529
H	5.297898	-0.84162	-2.0188
H	2.161492	-3.36938	1.188321
H	0.532972	-3.52357	0.553012
H	1.39679	-3.21202	-1.787
H	3.042145	-3.07262	-1.16216
H	2.156558	-4.5941	-0.98924

Compound 1: **(6*S*,8*S*)-spongosoritin A conf6**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.957660 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.265907	1.845417	0.829073
C	-0.6322	2.006181	-0.15077
C	-0.05855	0.639619	1.654149
O	-1.24418	0.109528	0.994085
C	-1.58971	0.897693	-0.03683
C	-2.6609	0.6928	-0.84416
C	-3.66282	-0.35928	-0.80492
O	-4.5952	-0.42138	-1.58595
O	-3.48093	-1.27178	0.172539
C	-4.45966	-2.3122	0.228926
C	-0.72084	3.075575	-1.1919
C	0.374711	4.13109	-1.10891
C	-0.45671	1.008434	3.083004
C	1.048793	-0.42661	1.658707
C	1.423235	-1.02927	0.285842
C	2.902016	-1.29795	0.223802
C	3.752888	-0.76248	-0.65119
C	5.228313	-1.02342	-0.70341
C	6.064606	0.245427	-0.51214
C	0.612421	-2.31021	0.006139
C	0.773616	-2.84849	-1.41112
H	1.113827	2.481989	1.04633
H	-2.82022	1.410479	-1.63792
H	-4.16779	-2.94334	1.066363
H	-5.45666	-1.8993	0.395827
H	-4.46599	-2.89105	-0.697
H	-0.70651	2.599915	-2.18044
H	-1.70516	3.553811	-1.11398
H	0.246305	4.876486	-1.89709
H	0.351884	4.65394	-0.14855
H	1.366762	3.686539	-1.22873
H	-1.25492	1.75364	3.076625
H	-0.80664	0.119917	3.613811
H	0.400962	1.420005	3.620856
H	1.926032	0.051902	2.107233
H	0.750288	-1.22694	2.345664

H	1.184136	-0.29593	-0.49499
H	3.286862	-1.99753	0.970126
H	3.365148	-0.0655	-1.39684
H	5.497194	-1.76619	0.055463
H	5.480555	-1.46627	-1.67625
H	5.820728	0.996816	-1.26986
H	5.881292	0.691319	0.469914
H	7.133643	0.02802	-0.59119
H	0.917343	-3.07734	0.730841
H	-0.44259	-2.10041	0.202311
H	1.816682	-3.09121	-1.63355
H	0.179205	-3.75535	-1.55539
H	0.439367	-2.11334	-2.15076

Compound 1: **(6*S*,8*S*)-spongosoritin A conf7**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.957448 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.407045	0.745548	1.799511
C	-0.46417	1.458684	1.072791
C	-0.00834	-0.69009	1.866091
O	-1.18282	-0.721	1.000752
C	-1.47634	0.518545	0.579335
C	-2.5625	0.825069	-0.17522
C	-3.56384	-0.12001	-0.63458
O	-3.60974	-1.31759	-0.44115
O	-4.51433	0.531049	-1.35976
C	-5.56249	-0.29078	-1.87316
C	-0.4674	2.931207	0.800554
C	-0.00251	3.303954	-0.61173
C	-0.47167	-1.0733	3.273926
C	0.984577	-1.73047	1.333378
C	1.619882	-1.44906	-0.04171
C	2.894666	-0.66337	0.098858
C	3.173575	0.50241	-0.48313
C	4.461744	1.256622	-0.34331
C	5.169768	1.486293	-1.68186
C	1.875939	-2.78397	-0.77219
C	2.389768	-2.63115	-2.19882
H	1.270358	1.128883	2.327605
H	-2.70075	1.858986	-0.45961
H	-6.11165	-0.77438	-1.06216
H	-6.21996	0.379123	-2.42483
H	-5.16451	-1.06095	-2.53774
H	-1.47913	3.318958	0.965692
H	0.17482	3.422377	1.536879
H	-0.06401	4.385321	-0.7597
H	1.034376	2.999224	-0.77145
H	-0.61512	2.823345	-1.37814
H	-1.25739	-0.39531	3.61353
H	-0.86162	-2.09392	3.275481
H	0.364592	-1.01765	3.975311
H	1.769604	-1.86608	2.085977
H	0.429943	-2.67419	1.294059

H	0.911828	-0.87065	-0.64834
H	3.656721	-1.12613	0.731709
H	2.416903	0.960146	-1.12183
H	4.257689	2.233204	0.116631
H	5.12672	0.72236	0.344078
H	5.442532	0.535936	-2.14945
H	4.525951	2.028622	-2.38134
H	6.083394	2.072353	-1.54714
H	2.58463	-3.38098	-0.18265
H	0.936066	-3.34806	-0.78404
H	2.524038	-3.60837	-2.67152
H	1.683334	-2.0602	-2.81042
H	3.349486	-2.10844	-2.22778

Compound 1: **(6*S*,8*S*)-spongosoritin A conf8**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.957367 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.22747	1.227764	0.047386
C	1.026969	1.595052	0.339516
C	-0.25286	-0.12626	-0.58911
O	1.167928	-0.4739	-0.64731
C	1.904838	0.507109	-0.10748
C	3.259192	0.479186	-0.01793
C	4.110244	-0.60226	-0.47971
O	3.778022	-1.64168	-1.01146
O	5.414635	-0.30246	-0.23187
C	6.358354	-1.293	-0.63944
C	1.495308	2.850402	1.006722
C	1.832983	2.654754	2.489785
C	-0.75631	-0.10479	-2.02792
C	-0.91177	-1.20612	0.290909
C	-2.3186	-0.92545	0.852266
C	-3.378	-0.79051	-0.20486
C	-4.23951	0.221412	-0.31449
C	-5.3304	0.329437	-1.3372
C	-5.23949	1.604527	-2.18024
C	-2.68176	-2.05938	1.837289
C	-3.94653	-1.80277	2.64807
H	-1.12298	1.810266	0.221773
H	3.750632	1.330288	0.432921
H	7.336357	-0.89814	-0.36932
H	6.177869	-2.23922	-0.12428
H	6.304586	-1.46261	-1.71715
H	2.373811	3.235622	0.477416
H	0.715026	3.610145	0.907125
H	2.178991	3.593567	2.930048
H	0.952924	2.322119	3.046658
H	2.618431	1.907696	2.627623
H	-0.18993	0.622248	-2.61438
H	-0.634	-1.09253	-2.47899
H	-1.81316	0.163632	-2.05449
H	-0.92023	-2.14562	-0.27465
H	-0.23959	-1.35922	1.14112

H	-2.2841	0.008824	1.428409
H	-3.45694	-1.62567	-0.90468
H	-4.16228	1.052353	0.389638
H	-5.31288	-0.5524	-1.98675
H	-6.30164	0.317925	-0.82424
H	-5.27304	2.49808	-1.5489
H	-4.30691	1.634712	-2.75103
H	-6.07049	1.66646	-2.88845
H	-2.78367	-2.99595	1.274153
H	-1.83645	-2.20504	2.520131
H	-4.81981	-1.67978	2.002132
H	-4.14671	-2.63396	3.330191
H	-3.84968	-0.89416	3.251687

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Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf1**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.166900 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.45722	1.815814	0.526555
C	0.582237	1.846153	-0.31712
C	-0.29071	0.728925	1.541303
O	0.969549	0.114219	1.141771
C	1.479263	0.753945	0.078557
C	0.842531	2.799991	-1.44075
C	1.84881	3.899127	-1.07871
C	2.643999	0.408766	-0.52665
C	3.507944	-0.68614	-0.12437
O	4.594875	-0.74044	-0.94042
O	3.346383	-1.47122	0.787938
C	5.52761	-1.78289	-0.65398
C	-1.40893	-0.32539	1.516888
C	-1.60813	-1.10379	0.202902
C	-3.09761	-1.4126	-0.02388
C	-3.94711	-0.21466	-0.44533
C	-5.42401	-0.55735	-0.63579
C	-0.10005	1.281849	2.953555
C	-6.26858	0.636302	-1.07146
C	-0.7615	-2.38892	0.194599
C	-0.59284	-3.02893	-1.18099
H	-1.31258	2.480183	0.518506
H	1.20511	2.242751	-2.31161
H	-0.10577	3.256759	-1.73751
H	2.015777	4.56045	-1.93292
H	1.478808	4.504888	-0.24722
H	2.813326	3.478889	-0.78369
H	2.960459	0.994188	-1.37882
H	6.31322	-1.68961	-1.40189
H	5.946063	-1.66695	0.348346
H	5.051054	-2.76293	-0.727
H	-1.22284	-1.03435	2.332376
H	-2.326	0.210059	1.786193
H	-1.2687	-0.47316	-0.63111

H	-3.19231	-2.18623	-0.79443
H	-3.51009	-1.85261	0.89535
H	-3.86515	0.591373	0.295626
H	-3.54758	0.195212	-1.38274
H	-5.51437	-1.36037	-1.3781
H	-5.82245	-0.96587	0.301501
H	-1.01779	1.76477	3.298572
H	0.145146	0.468916	3.641006
H	0.708671	2.01543	2.971934
H	-7.31867	0.358675	-1.20109
H	-6.22778	1.441611	-0.33043
H	-5.91359	1.045328	-2.02317
H	-1.21837	-3.10987	0.886707
H	0.227912	-2.15959	0.598425
H	0.031017	-3.92531	-1.11858
H	-1.54745	-3.32738	-1.62465
H	-0.10581	-2.33687	-1.87592

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf2**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.166593 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.44868	1.723398	0.926691
C	0.581742	1.946591	0.101191
C	-0.23778	0.470995	1.718278
O	1.037072	-0.01643	1.204845
C	1.527582	0.841112	0.297182
C	0.777654	3.077037	-0.86014
C	0.484404	2.693908	-2.31557
C	2.72905	0.693542	-0.31672
C	3.665414	-0.39203	-0.08842
O	4.783972	-0.20374	-0.83938
O	3.536078	-1.35153	0.644481
C	5.788289	-1.20983	-0.70583
C	-1.32174	-0.59781	1.509009
C	-1.52952	-1.11798	0.074214
C	-3.01458	-1.42628	-0.17956
C	-3.91112	-0.19942	-0.33759
C	-5.38209	-0.55054	-0.55665
C	-0.04602	0.760181	3.207467
C	-6.27592	0.673257	-0.73132
C	-0.64686	-2.35037	-0.19261
C	-0.50482	-2.72489	-1.66566
H	-1.32247	2.351091	1.051717
H	0.127483	3.904314	-0.56223
H	1.806342	3.445463	-0.77792
H	0.659214	3.54633	-2.97717
H	1.120777	1.871156	-2.65018
H	-0.5567	2.381663	-2.43209
H	3.025208	1.453087	-1.02703
H	6.144439	-1.27049	0.325017
H	5.402436	-2.18721	-1.00402
H	6.598822	-0.90746	-1.36678
H	-1.09375	-1.44226	2.170191
H	-2.24858	-0.15772	1.892698
H	-1.22794	-0.3306	-0.63103
H	-3.10682	-2.03487	-1.08616
H	-3.38922	-2.05368	0.64192

H	-3.8309	0.449237	0.544853
H	-3.55272	0.399309	-1.18589
H	-5.47019	-1.19708	-1.43891
H	-5.73952	-1.14722	0.292149
H	0.23002	-0.15717	3.732485
H	0.742145	1.501581	3.354941
H	-0.97252	1.145022	3.641012
H	-6.23777	1.321113	0.150857
H	-5.96377	1.271807	-1.59361
H	-7.32033	0.387777	-0.8872
H	-1.05917	-3.20055	0.368374
H	0.347782	-2.16412	0.220778
H	0.152721	-3.59103	-1.78415
H	-1.46338	-2.9793	-2.12748
H	-0.06872	-1.89992	-2.23855

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf3**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.166428 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.13757	1.183201	1.68186
C	0.729827	1.62832	0.763137
C	0.073137	-0.27237	1.952643
O	1.162944	-0.60965	1.042942
C	1.545886	0.478163	0.357722
C	0.901426	3.021424	0.243705
C	2.083839	3.76158	0.88061
C	2.534312	0.481134	-0.57254
C	3.320726	-0.67316	-0.96825
O	4.220479	-0.31342	-1.92398
O	3.241339	-1.81128	-0.55354
C	5.06031	-1.36462	-2.40116
C	-1.1112	-1.19661	1.623938
C	-1.69603	-1.08438	0.203759
C	-2.8413	-0.0619	0.144113
C	-3.37374	0.232993	-1.25702
C	-4.41966	1.346778	-1.27953
C	0.57075	-0.52338	3.376246
C	-4.96848	1.631368	-2.67438
C	-2.09318	-2.47262	-0.33354
C	-3.21912	-3.17435	0.423722
H	-0.87914	1.774098	2.204761
H	1.031933	2.987984	-0.84358
H	-0.02102	3.57892	0.428544
H	2.174184	4.768011	0.463609
H	1.947164	3.852567	1.961477
H	3.026561	3.237706	0.70499
H	2.755399	1.417207	-1.06662
H	5.668745	-1.77511	-1.59202
H	4.466269	-2.16968	-2.83922
H	5.698288	-0.9123	-3.1586
H	-0.74582	-2.21527	1.793656
H	-1.88804	-1.01997	2.376759
H	-0.8975	-0.72332	-0.45712
H	-3.66639	-0.40059	0.784549
H	-2.49075	0.879154	0.584678

H	-2.53639	0.509715	-1.91212
H	-3.81219	-0.67341	-1.69196
H	-5.2463	1.078519	-0.60913
H	-3.97972	2.262949	-0.86528
H	1.457684	0.079171	3.582946
H	-0.20565	-0.26127	4.099398
H	0.823859	-1.57854	3.503647
H	-5.44792	0.743377	-3.09929
H	-5.7123	2.433337	-2.6567
H	-4.16985	1.934254	-3.35954
H	-1.19813	-3.10582	-0.31654
H	-2.3715	-2.38265	-1.38915
H	-2.97569	-3.30932	1.482237
H	-4.15912	-2.61729	0.368671
H	-3.40441	-4.16704	0.00338

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf4**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.166426 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.770699	-2.52173	0.834016
C	1.849367	-1.7377	0.956743
C	-0.21398	-1.92797	-0.12502
O	0.454017	-0.70018	-0.54367
C	1.631867	-0.5772	0.084975
C	3.073667	-1.96327	1.787857
C	4.269472	-2.47581	0.976357
C	2.465651	0.482114	-0.07253
C	2.21464	1.626896	-0.9292
O	3.250557	2.504988	-0.84123
O	1.25305	1.833891	-1.64115
C	3.129113	3.680552	-1.64215
C	-1.52061	-1.53108	0.583753
C	-2.53689	-0.73121	-0.25927
C	-3.16787	0.397041	0.573124
C	-2.23039	1.552504	0.920414
C	-2.92414	2.67085	1.697257
C	-0.40497	-2.78743	-1.37101
C	-1.99172	3.826034	2.04982
C	-3.62116	-1.65257	-0.84694
C	-4.42716	-1.04237	-1.99113
H	0.594748	-3.46083	1.344277
H	3.344691	-1.02889	2.291772
H	2.832546	-2.68189	2.576162
H	5.139429	-2.61377	1.623721
H	4.037378	-3.43683	0.509638
H	4.546291	-1.7765	0.183744
H	3.391931	0.482013	0.485296
H	3.064604	3.425115	-2.70227
H	2.242383	4.253678	-1.3623
H	4.028926	4.262648	-1.45021
H	-1.99014	-2.44783	0.961407
H	-1.22785	-0.95504	1.466858
H	-1.99713	-0.26083	-1.09166
H	-4.02456	0.806197	0.025246
H	-3.58025	-0.03422	1.496939

H	-1.37822	1.18968	1.507946
H	-1.80158	1.961405	-0.00278
H	-3.7686	3.048973	1.107179
H	-3.3587	2.257249	2.61658
H	-1.017	-2.26629	-2.10931
H	0.564219	-3.01157	-1.82203
H	-0.89436	-3.72941	-1.11103
H	-2.51551	4.609906	2.604999
H	-1.15489	3.483488	2.667372
H	-1.56972	4.281689	1.148257
H	-4.29712	-1.95516	-0.03544
H	-3.1561	-2.57702	-1.20464
H	-4.96633	-0.14202	-1.68397
H	-3.77493	-0.76718	-2.82649
H	-5.16868	-1.75227	-2.36933

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf5**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.165978 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-1.31481	-2.55426	-0.10674
C	-2.31527	-1.71702	-0.40739
C	-0.14462	-1.80875	0.458565
O	-0.6182	-0.42943	0.450429
C	-1.85602	-0.3668	-0.06212
C	-3.66648	-2.04292	-0.96264
C	-4.77138	-2.04477	0.100457
C	-2.54803	0.787771	-0.23697
C	-2.06948	2.116534	0.09702
O	-3.01959	3.040714	-0.20905
O	-0.99921	2.428947	0.57891
C	-2.67111	4.396428	0.072438
C	1.083741	-1.94592	-0.45981
C	2.364762	-1.17084	-0.09757
C	2.289933	0.290346	-0.57123
C	3.324642	1.223125	0.057683
C	3.199365	2.666321	-0.42947
C	0.132087	-2.18889	1.91111
C	4.213815	3.60891	0.21107
C	3.592068	-1.8906	-0.6864
C	3.985608	-3.17817	0.033296
H	-1.31007	-3.62909	-0.24063
H	-3.91587	-1.32396	-1.75088
H	-3.61918	-3.02466	-1.44212
H	-5.73839	-2.27604	-0.35377
H	-4.56841	-2.79572	0.868678
H	-4.85438	-1.07393	0.595009
H	-3.54133	0.718238	-0.65872
H	-2.4571	4.53107	1.134887
H	-1.79622	4.702322	-0.50572
H	-3.53755	4.989545	-0.21531
H	1.302882	-3.01901	-0.49218
H	0.775366	-1.669	-1.47534
H	2.482695	-1.16702	0.99426
H	2.397014	0.306662	-1.66584
H	1.294481	0.685168	-0.35321

H	3.20547	1.203715	1.149559
H	4.343147	0.867999	-0.1442
H	3.316473	2.689554	-1.52064
H	2.18367	3.024707	-0.22472
H	-0.78655	-2.12144	2.497615
H	0.508964	-3.21321	1.96789
H	0.872612	-1.52044	2.352988
H	5.240281	3.29147	-0.00161
H	4.099906	4.632208	-0.15894
H	4.095469	3.635422	1.299396
H	4.447999	-1.20817	-0.66603
H	3.400283	-2.0996	-1.7476
H	4.234138	-2.98029	1.081135
H	3.185163	-3.92445	0.019713
H	4.862008	-3.63695	-0.43378

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf6**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.165877 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.38773	1.758511	0.688729
C	0.58113	1.916457	-0.2217
C	-0.12393	0.562394	1.547505
O	1.11341	0.034592	0.984132
C	1.528285	0.80979	-0.03059
C	0.732766	3.006899	-1.23546
C	1.744039	4.081811	-0.81847
C	2.645996	0.587287	-0.76798
C	3.636764	-0.46956	-0.65661
O	3.39739	-1.36296	0.325898
O	4.609799	-0.54991	-1.38485
C	4.368087	-2.40401	0.456732
C	-1.22149	-0.5113	1.473624
C	-1.50101	-1.12844	0.089977
C	-3.00219	-1.41081	-0.08672
C	-3.86329	-0.17076	-0.3208
C	-5.35109	-0.48515	-0.47079
C	0.163463	0.945693	2.998775
C	-6.20481	0.75151	-0.73447
C	-0.6589	-2.39896	-0.12145
C	-0.58074	-2.87523	-1.56957
H	-1.25171	2.396513	0.828926
H	1.033596	2.571499	-2.19463
H	-0.24489	3.469096	-1.39797
H	1.82886	4.84792	-1.59357
H	1.430418	4.569173	0.108528
H	2.737086	3.656586	-0.65436
H	2.857471	1.292355	-1.56052
H	4.028625	-3.01747	1.289397
H	4.423872	-3.00162	-0.45553
H	5.355696	-1.98984	0.670015
H	-0.9641	-1.30812	2.181653
H	-2.12679	-0.03845	1.869689
H	-1.20751	-0.40194	-0.68097
H	-3.14476	-2.09037	-0.9346
H	-3.36643	-1.95318	0.797459

H	-3.73438	0.544559	0.502483
H	-3.51009	0.342919	-1.22506
H	-5.48607	-1.20388	-1.28896
H	-5.70623	-0.98961	0.4367
H	-0.7335	1.358871	3.467028
H	0.474773	0.063118	3.562618
H	0.957825	1.693533	3.046242
H	-7.26277	0.493699	-0.83844
H	-6.11872	1.474291	0.083767
H	-5.89457	1.25679	-1.65506
H	-1.06922	-3.1981	0.511568
H	0.354806	-2.20811	0.241058
H	0.040677	-3.7718	-1.65164
H	-1.56332	-3.12242	-1.98203
H	-0.13556	-2.10657	-2.20971

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf7**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.165434 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.37863	1.612129	1.114132
C	0.582745	2.000614	0.267187
C	-0.06763	0.270136	1.697338
O	1.186465	-0.07747	1.03852
C	1.583611	0.925535	0.238634
C	0.664162	3.266671	-0.52719
C	0.280692	3.084264	-2.00051
C	2.742908	0.94046	-0.46741
C	3.80676	-0.04746	-0.52901
O	3.594405	-1.14974	0.219334
O	4.814672	0.099353	-1.19697
C	4.63392	-2.12989	0.174741
C	-1.12568	-0.80417	1.400181
C	-1.41392	-1.1171	-0.07993
C	-2.90411	-1.43582	-0.28696
C	-3.83613	-0.22722	-0.21532
C	-5.30953	-0.58608	-0.40351
C	0.214774	0.346877	3.198128
C	-6.23545	0.625352	-0.34729
C	-0.51945	-2.26549	-0.57927
C	-0.46181	-2.41444	-2.09743
H	-1.26436	2.17366	1.384666
H	0.004745	4.008391	-0.06793
H	1.680329	3.670736	-0.45911
H	0.369061	4.032181	-2.53762
H	0.925105	2.354526	-2.4964
H	-0.75182	2.737049	-2.09169
H	2.934669	1.815973	-1.07314
H	4.778472	-2.49768	-0.84325
H	5.575828	-1.71398	0.538485
H	4.302373	-2.9377	0.824618
H	-0.82437	-1.7254	1.91293
H	-2.03844	-0.46581	1.902726
H	-1.17847	-0.22511	-0.67753
H	-3.03857	-1.91298	-1.26416
H	-3.21187	-2.18416	0.457303

H	-3.71913	0.288641	0.74671
H	-3.54019	0.498128	-0.9851
H	-5.43519	-1.0995	-1.3651
H	-5.60529	-1.30962	0.366661
H	0.552807	-0.62526	3.564783
H	0.987561	1.090207	3.405088
H	-0.69207	0.626845	3.740043
H	-5.98502	1.350751	-1.12837
H	-7.28171	0.337548	-0.48523
H	-6.15687	1.13835	0.61699
H	-0.8725	-3.2026	-0.12674
H	0.494187	-2.10521	-0.20279
H	0.20671	-3.23192	-2.38292
H	-1.44138	-2.62921	-2.53469
H	-0.08233	-1.50031	-2.56547

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf8**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.165261 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.169121	2.289077	0.52929
C	1.296376	2.084635	-0.16419
C	-0.11669	1.134238	1.436992
O	0.981988	0.222328	1.144439
C	1.808786	0.770018	0.241012
C	1.9433	2.97815	-1.17589
C	1.687018	2.541543	-2.62327
C	2.946645	0.176472	-0.20053
C	3.432863	-1.1233	0.225126
O	4.621113	-1.39375	-0.37912
O	2.909147	-1.90254	0.995353
C	5.205237	-2.65415	-0.0486
C	-1.45371	0.428837	1.156852
C	-1.62545	-0.17709	-0.2501
C	-3.04801	0.06251	-0.78979
C	-4.17734	-0.63209	-0.0287
C	-5.56237	-0.28634	-0.57412
C	-0.00763	1.522648	2.911386
C	-6.6954	-0.9886	0.16809
C	-1.20478	-1.65646	-0.26897
C	-1.19618	-2.29441	-1.65516
H	-0.46518	3.165989	0.484199
H	1.571226	3.996124	-1.0303
H	3.022374	3.012065	-0.9884
H	2.190247	3.216646	-3.32032
H	2.055423	1.529739	-2.80837
H	0.617474	2.555783	-2.84888
H	3.547475	0.712949	-0.92191
H	6.140715	-2.7005	-0.60355
H	5.398549	-2.7249	1.024026
H	4.550088	-3.47663	-0.3445
H	-1.58757	-0.34523	1.920715
H	-2.23187	1.177931	1.344407
H	-0.94937	0.358832	-0.93025
H	-3.23401	1.145055	-0.78949
H	-3.09121	-0.24267	-1.8422

H	-4.04082	-1.71964	-0.07092
H	-4.13603	-0.36253	1.034861
H	-5.709	0.800206	-0.52331
H	-5.60524	-0.54733	-1.63927
H	-0.80529	2.220539	3.178322
H	-0.09885	0.633005	3.53878
H	0.954208	1.999349	3.111959
H	-7.67244	-0.71931	-0.24375
H	-6.59623	-2.0771	0.102392
H	-6.69774	-0.72166	1.230134
H	-1.86654	-2.22734	0.394605
H	-0.20495	-1.73064	0.168063
H	-0.81153	-3.31741	-1.60937
H	-2.19646	-2.34108	-2.09571
H	-0.55613	-1.73269	-2.34399

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf9**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.165102 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.223441	2.261345	0.118248
C	1.33491	1.900967	-0.53599
C	-0.12009	1.262705	1.177966
O	0.926796	0.260596	1.020297
C	1.769212	0.622737	0.040769
C	2.050553	2.632246	-1.62837
C	3.28429	3.397789	-1.13498
C	2.844689	-0.10927	-0.34606
C	3.247033	-1.38039	0.22744
O	4.385087	-1.82151	-0.373
O	2.697959	-2.0105	1.108397
C	4.882495	-3.07296	0.101712
C	-1.49545	0.600588	0.990989
C	-1.70647	-0.18591	-0.31815
C	-3.11868	0.048404	-0.88614
C	-4.27646	-0.46502	-0.02993
C	-5.64618	-0.12702	-0.61743
C	0.013464	1.845357	2.584626
C	-6.80817	-0.6415	0.226928
C	-1.36266	-1.67292	-0.12906
C	-1.39901	-2.49984	-1.41125
H	-0.36679	3.153086	-0.05409
H	2.346673	1.920234	-2.40661
H	1.350998	3.330302	-2.09653
H	3.778685	3.903352	-1.96858
H	3.001352	4.154222	-0.39817
H	4.011053	2.729509	-0.66679
H	3.457177	0.283396	-1.14592
H	5.785048	-3.26954	-0.47449
H	5.118604	-3.01985	1.166834
H	4.151611	-3.86873	-0.05869
H	-1.67252	-0.04997	1.854643
H	-2.22851	1.412325	1.067527
H	-1.00896	0.214224	-1.06675
H	-3.24706	1.127647	-1.04473
H	-3.18597	-0.4058	-1.882

H	-4.19964	-1.55284	0.088239
H	-4.21004	-0.04507	0.982282
H	-5.73061	0.961207	-0.73237
H	-5.71661	-0.54398	-1.63017
H	-0.74808	2.611483	2.75104
H	-0.11824	1.055886	3.328269
H	0.998381	2.297169	2.720424
H	-7.77325	-0.38466	-0.21961
H	-6.76978	-1.73088	0.330517
H	-6.78442	-0.21373	1.234721
H	-2.04652	-2.10986	0.609615
H	-0.36433	-1.73639	0.312485
H	-1.07014	-3.52563	-1.22111
H	-2.4038	-2.55286	-1.84095
H	-0.73448	-2.07691	-2.17244

Compound 2: **(6*R*,8*S*)-dihydrospongosoritin A conf10**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.164705 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-2.12157	-1.8068	0.285132
C	-2.86732	-0.7672	-0.10633
C	-0.73965	-1.36322	0.6578
O	-0.80491	0.080719	0.449553
C	-2.02427	0.429524	0.008705
C	-4.28994	-0.73884	-0.56643
C	-4.9719	-2.10093	-0.59915
C	-2.4186	1.696111	-0.27791
C	-1.69483	2.94959	-0.15616
O	-0.45557	2.83716	0.366092
O	-2.16577	4.024593	-0.48226
C	0.255374	4.068074	0.517168
C	0.292193	-1.99445	-0.29607
C	1.789066	-1.72073	-0.07213
C	2.199996	-0.3208	-0.55902
C	3.540796	0.166283	-0.00983
C	3.973847	1.516065	-0.58054
C	-0.43424	-1.59688	2.134631
C	5.292284	2.019392	-0.00084
C	2.619443	-2.81568	-0.76857
C	2.617592	-4.16974	-0.06366
H	-2.42624	-2.84399	0.337807
H	-4.85139	-0.05714	0.084505
H	-4.32294	-0.2816	-1.5632
H	-6.00442	-2.0019	-0.94181
H	-4.45924	-2.78733	-1.27904
H	-4.99254	-2.56	0.393323
H	-3.42906	1.819118	-0.64439
H	1.204967	3.803612	0.978425
H	0.424353	4.541578	-0.45226
H	-0.29659	4.759155	1.15743
H	0.116229	-3.07433	-0.23495
H	0.021232	-1.70184	-1.31796
H	2.003843	-1.78421	1.003279
H	2.233962	-0.3321	-1.65811
H	1.425896	0.40174	-0.28698

H	3.47124	0.243222	1.083881
H	4.329875	-0.56915	-0.21111
H	4.061055	1.433538	-1.67133
H	3.185014	2.25531	-0.39613
H	-0.33882	-2.66694	2.336275
H	0.497473	-1.10522	2.419119
H	-1.23972	-1.19555	2.753219
H	5.577156	2.984502	-0.43001
H	5.224214	2.145748	1.084795
H	6.106532	1.314641	-0.19983
H	3.655853	-2.47382	-0.85649
H	2.254106	-2.93039	-1.79801
H	3.226382	-4.89629	-0.60964
H	3.029642	-4.08566	0.947297
H	1.612323	-4.59315	0.024028

CARTESIAN COORDINATES

Compound 1: 2*E*-(6*R*,8*R*)-spongosoritin A conf1

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.954133 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.312504	-0.69117	-1.69314
C	-0.77271	-0.02905	-1.2627
C	0.522392	-1.95669	-0.93643
O	-0.55345	-1.91078	0.037029
C	-1.31942	-0.80644	-0.13916
C	-2.3644	-0.66967	0.722696
C	-1.3122	1.225974	-1.87875
C	-2.50677	0.965019	-2.80126
C	0.300131	-3.18864	-1.81704
C	1.846176	-2.08157	-0.16743
C	2.235181	-0.8974	0.736486
C	2.964578	0.169816	-0.03271
C	2.604374	1.448241	-0.13994
C	3.360291	2.504127	-0.88864
C	3.79868	3.66909	0.004006
C	3.095097	-1.41041	1.910734
C	3.43506	-0.34932	2.950422
H	0.949795	-0.38924	-2.51436
C	-3.32251	0.409056	0.845813
H	-1.61465	1.924144	-1.09856
H	-0.50207	1.687698	-2.45173
H	-2.85417	1.901066	-3.2473
H	-2.23695	0.280613	-3.6112
H	-3.34047	0.5326	-2.24495
H	1.061835	-3.23878	-2.5991
H	0.36068	-4.09773	-1.21361
H	-0.68292	-3.14399	-2.29036
H	1.756579	-2.98926	0.439667
H	2.64365	-2.27419	-0.89449
H	1.320594	-0.46439	1.160614
H	3.88464	-0.15789	-0.52402
H	1.687209	1.775262	0.352344
H	4.234316	2.05664	-1.37462
H	2.723921	2.899185	-1.69205

H	4.309764	4.440269	-0.57947
H	2.938479	4.136196	0.493539
H	4.482087	3.327258	0.78656
H	2.553764	-2.23154	2.395537
H	4.018767	-1.84861	1.509503
H	2.525786	0.08418	3.379926
H	4.01808	-0.77889	3.770201
H	4.016455	0.468007	2.515909
O	-4.21672	0.102617	1.823566
O	-3.39181	1.457261	0.231617
H	-2.4841	-1.47454	1.438216
C	-5.2181	1.089074	2.073065
H	-5.83058	0.688628	2.879077
H	-4.7656	2.035439	2.377183
H	-5.82915	1.258694	1.183752

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf2**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.953787 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.48376	0.553352	1.593407
C	0.653729	0.784282	0.919433
C	-0.68955	-0.89997	1.846084
O	0.456166	-1.48994	1.177825
C	1.248797	-0.53244	0.637991
C	2.356973	-0.98153	-0.01272
C	1.202853	2.140506	0.596795
C	2.320779	2.567375	1.553016
C	-0.58822	-1.24087	3.334485
C	-1.95542	-1.52397	1.24015
C	-2.22041	-1.22854	-0.24893
C	-3.06574	0.002652	-0.42777
C	-2.749	1.082445	-1.14177
C	-3.63455	2.275308	-1.34423
C	-3.01812	3.580675	-0.8337
C	-2.89547	-2.45103	-0.90567
C	-3.09271	-2.32515	-2.41165
H	-1.16427	1.311504	1.959167
C	3.356054	-0.23966	-0.75364
H	1.586129	2.153238	-0.42329
H	0.377168	2.855904	0.658538
H	2.679145	3.567865	1.295442
H	1.967227	2.587644	2.588294
H	3.169988	1.884287	1.490748
H	-1.40936	-0.77663	3.886181
H	-0.64252	-2.32315	3.475714
H	0.356572	-0.87861	3.745015
H	-1.85711	-2.60501	1.388611
H	-2.81273	-1.20658	1.844729
H	-1.2594	-1.07227	-0.75458
H	-4.04526	-0.03369	0.056746
H	-1.77153	1.12199	-1.62508
H	-3.84434	2.383874	-2.41689
H	-4.59979	2.101734	-0.85591
H	-3.67548	4.430937	-1.03695
H	-2.84585	3.537538	0.245668

H	-2.05681	3.779531	-1.31738
H	-2.27931	-3.33265	-0.69318
H	-3.86252	-2.62838	-0.41627
H	-3.73813	-1.47952	-2.66359
H	-2.1351	-2.17313	-2.92059
H	-3.54788	-3.23083	-2.82275
O	4.309465	-1.09966	-1.20147
O	3.412825	0.950602	-0.99989
H	2.498179	-2.05579	-0.00055
C	5.355772	-0.51013	-1.97352
H	6.01499	-1.33102	-2.25043
H	4.955711	-0.02852	-2.86848
H	5.902523	0.231765	-1.3873

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf3**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.953253 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.47142	-2.38496	0.364056
C	-1.61803	-1.74195	0.098636
C	0.663621	-1.437	0.568573
O	0.01256	-0.15069	0.402738
C	-1.29819	-0.30387	0.100697
C	-1.98951	0.845231	-0.13265
C	-2.94894	-2.40121	-0.09987
C	-3.82966	-2.34257	1.151857
C	1.229752	-1.50057	1.984553
C	1.727758	-1.61758	-0.52918
C	3.037327	-0.81655	-0.42039
C	2.817934	0.669642	-0.41985
C	3.331901	1.527701	0.460594
C	3.134934	3.013836	0.440812
C	2.471578	3.543299	1.715522
C	3.960048	-1.23562	-1.58651
C	5.387098	-0.71284	-1.47275
H	-0.35155	-3.45961	0.432369
C	-3.37529	1.030896	-0.51106
H	-3.47753	-1.92786	-0.92691
H	-2.7649	-3.44619	-0.36846
H	-4.78026	-2.85171	0.970721
H	-3.33926	-2.82691	2.001586
H	-4.05268	-1.30891	1.422253
H	1.751464	-2.44843	2.141646
H	1.931374	-0.68153	2.149185
H	0.422677	-1.42176	2.715981
H	1.985824	-2.68306	-0.54786
H	1.244829	-1.40174	-1.48976
H	3.544533	-1.09339	0.513055
H	2.204598	1.057133	-1.23517
H	3.939908	1.138023	1.279712
H	4.110166	3.505122	0.321281
H	2.537397	3.291712	-0.43414
H	2.368614	4.631796	1.682724
H	1.475489	3.111201	1.845155

H	3.062625	3.291205	2.601811
H	3.979139	-2.33125	-1.63584
H	3.512658	-0.89571	-2.52935
H	5.869317	-1.08089	-0.56104
H	5.991714	-1.04047	-2.32334
H	5.411848	0.379587	-1.44281
O	-3.633	2.361974	-0.61651
O	-4.23802	0.20093	-0.72894
H	-1.41446	1.758734	-0.03929
C	-4.96559	2.702417	-0.99936
H	-4.98831	3.789656	-1.04931
H	-5.21288	2.273982	-1.97304
H	-5.68661	2.34367	-0.26154

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf4**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.953172 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.40135	0.769699	1.4837
C	0.734791	0.930594	0.787469
C	-0.59036	-0.64497	1.910781
O	0.561125	-1.29841	1.315013
C	1.34534	-0.40305	0.66737
C	2.459453	-0.91518	0.075566
C	1.259213	2.244151	0.292185
C	2.357658	2.821371	1.190099
C	-0.47977	-0.80138	3.429001
C	-1.85023	-1.35211	1.389196
C	-2.14001	-1.21899	-0.11728
C	-2.92109	0.031484	-0.4194
C	-2.55439	0.994073	-1.26499
C	-3.32631	2.234945	-1.60885
C	-4.6755	2.401983	-0.92142
C	-2.90037	-2.4686	-0.60842
C	-3.12074	-2.51394	-2.11596
H	-1.09252	1.558449	1.751556
C	3.461155	-0.25348	-0.73397
H	1.652888	2.129693	-0.71745
H	0.417155	2.942017	0.250796
H	2.691534	3.789755	0.807122
H	1.995846	2.965455	2.212628
H	3.224942	2.159166	1.21888
H	-1.30246	-0.28003	3.924562
H	-0.52307	-1.85869	3.702039
H	0.463666	-0.38286	3.785648
H	-1.72999	-2.41	1.648148
H	-2.70772	-0.98849	1.967119
H	-1.18551	-1.18009	-0.65719
H	-3.87865	0.108642	0.098411
H	-1.59303	0.894959	-1.77005
H	-2.69284	3.106008	-1.39077
H	-3.46477	2.260461	-2.69858
H	-5.15456	3.332196	-1.23771
H	-5.3538	1.578811	-1.16507

H	-4.57012	2.436065	0.167261
H	-2.33529	-3.35558	-0.29816
H	-3.8663	-2.52407	-0.08875
H	-2.16605	-2.48735	-2.65175
H	-3.64051	-3.43111	-2.4077
H	-3.71637	-1.6646	-2.4609
O	4.413092	-1.15607	-1.09307
O	3.523002	0.907248	-1.09413
H	2.607069	-1.98025	0.209427
C	5.465228	-0.64689	-1.91278
H	6.123088	-1.49259	-2.10555
H	5.0716	-0.25289	-2.85237
H	6.011567	0.146532	-1.39794

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf5**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.952975 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.71044	-2.28719	0.771743
C	-1.82906	-1.61576	0.461208
C	0.474671	-1.38398	0.859264
O	-0.1152	-0.0881	0.578321
C	-1.4453	-0.19756	0.351403
C	-2.0998	0.969135	0.099778
C	-3.17182	-2.2405	0.233085
C	-3.49239	-2.41953	-1.25409
C	1.077145	-1.33125	2.260812
C	1.496869	-1.73212	-0.23772
C	2.854074	-1.00639	-0.23212
C	2.721878	0.485532	-0.35108
C	3.285007	1.378661	0.461877
C	3.172381	2.867554	0.32893
C	4.530032	3.559488	0.175598
C	3.713998	-1.57814	-1.38085
C	5.171608	-1.13414	-1.35028
H	-0.6407	-3.35636	0.932791
C	-3.5098	1.208089	-0.12944
H	-3.17184	-3.21712	0.727133
H	-3.94933	-1.62977	0.690982
H	-4.46881	-2.89609	-1.37734
H	-3.52689	-1.45461	-1.76316
H	-2.7421	-3.04594	-1.74583
H	1.550131	-2.28609	2.505465
H	1.827499	-0.54158	2.320859
H	0.297239	-1.13023	2.9983
H	1.691998	-2.80848	-0.16119
H	1.002374	-1.57731	-1.20412
H	3.371719	-1.23416	0.708794
H	2.123284	0.842504	-1.19098
H	3.883101	1.018638	1.301599
H	2.529673	3.111411	-0.52376
H	2.671924	3.269467	1.220245
H	4.414118	4.645783	0.120934
H	5.184622	3.336625	1.024172

H	5.039045	3.226815	-0.73367
H	3.667859	-2.67322	-1.33603
H	3.258109	-1.29286	-2.33766
H	5.72924	-1.56649	-2.18602
H	5.258581	-0.04646	-1.41348
H	5.661058	-1.45272	-0.4239
O	-3.70569	2.535245	-0.3522
O	-4.43925	0.422707	-0.13384
H	-1.47784	1.856317	0.093864
C	-5.05919	2.928087	-0.5799
H	-5.03159	4.006561	-0.72559
H	-5.46347	2.437816	-1.46828
H	-5.6871	2.678831	0.278346

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf6**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.952967 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.73377	-2.38762	0.213632
C	-1.83325	-1.65105	-0.00363
C	0.455281	-1.53653	0.514441
O	-0.10973	-0.2015	0.456565
C	-1.42279	-0.24241	0.129635
C	-2.03733	0.964934	-0.0023
C	-3.20243	-2.20191	-0.26277
C	-4.09058	-2.18277	0.985092
C	0.989286	-1.76138	1.926642
C	1.5271	-1.68875	-0.58028
C	2.883072	-0.98738	-0.38088
C	2.755288	0.505805	-0.27391
C	3.263331	1.261464	0.69897
C	3.150596	2.753741	0.786549
C	4.510204	3.458072	0.809432
C	3.809255	-1.37941	-1.55303
C	5.259903	-0.94787	-1.37456
H	-0.68414	-3.46973	0.190351
C	-3.39979	1.271862	-0.38606
H	-3.68986	-1.62986	-1.05187
H	-3.08554	-3.2324	-0.61248
H	-5.07074	-2.61174	0.759417
H	-3.64258	-2.76362	1.796872
H	-4.24793	-1.16094	1.3352
H	1.446998	-2.75108	2.005353
H	1.738045	-1.00719	2.173269
H	0.174724	-1.69519	2.650987
H	1.716407	-2.7633	-0.68944
H	1.079584	-1.35761	-1.52487
H	3.343688	-1.36476	0.541097
H	2.208101	0.990813	-1.08434
H	3.810731	0.776204	1.509673
H	2.551415	3.125152	-0.0517
H	2.602224	3.017588	1.700964
H	4.390825	4.540281	0.914715
H	5.123014	3.107669	1.646056

H	5.066338	3.267095	-0.11301
H	3.768632	-2.46857	-1.67642
H	3.404656	-0.95236	-2.47973
H	5.697746	-1.39999	-0.47837
H	5.866625	-1.25484	-2.23134
H	5.344834	0.137073	-1.2728
O	-3.58036	2.619145	-0.34789
O	-4.30036	0.522543	-0.71489
H	-1.40918	1.82709	0.187683
C	-4.8797	3.076936	-0.7225
H	-4.84497	4.161634	-0.63699
H	-5.11442	2.786529	-1.74899
H	-5.64376	2.670052	-0.05646

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf7**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.952807 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.232837	-0.4906	-1.74615
C	-0.85668	0.157624	-1.30351
C	0.358104	-1.84155	-1.12799
O	-0.73625	-1.83958	-0.17379
C	-1.49478	-0.72515	-0.31222
C	-2.62304	-0.68372	0.447918
C	-1.29587	1.518752	-1.75353
C	-0.96984	2.628142	-0.75017
C	0.078135	-2.95061	-2.14797
C	1.650133	-2.14886	-0.36035
C	2.142066	-1.08515	0.638577
C	3.03459	-0.07842	-0.0341
C	2.89233	1.246204	-0.01031
C	3.818091	2.229898	-0.66069
C	4.458729	3.197201	0.339099
C	2.880022	-1.77768	1.803922
C	3.295754	-0.83964	2.930622
H	0.9203	-0.12497	-2.49807
C	-3.66475	0.3207	0.504576
H	-0.79656	1.729161	-2.70453
H	-2.37119	1.514261	-1.93376
H	-1.31488	3.593712	-1.13027
H	-1.46865	2.450266	0.203926
H	0.106894	2.69692	-0.5751
H	0.844988	-2.95072	-2.92651
H	0.083267	-3.92537	-1.65392
H	-0.89546	-2.79761	-2.61819
H	1.461073	-3.089	0.169796
H	2.436495	-2.36366	-1.09293
H	1.271697	-0.5654	1.0587
H	3.891312	-0.50122	-0.56549
H	2.043839	1.669838	0.528645
H	4.597393	1.691544	-1.21119
H	3.258208	2.814106	-1.4035
H	5.09465	3.925783	-0.17189
H	3.696781	3.751712	0.895696

H	5.075105	2.658826	1.064663
H	2.221661	-2.55686	2.205921
H	3.76179	-2.29764	1.406311
H	2.425066	-0.33342	3.360421
H	3.789964	-1.39172	3.735239
H	3.985462	-0.06845	2.578061
O	-4.58476	-0.04323	1.437516
O	-3.79037	1.343681	-0.14195
H	-2.78006	-1.54299	1.089121
C	-5.69048	0.846765	1.591168
H	-6.31808	0.405095	2.363269
H	-5.35287	1.8383	1.900723
H	-6.24934	0.939082	0.657241

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf8**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.952804 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.13528	-0.6466	0.481913
C	1.185461	-0.60554	0.715855
C	-0.46875	-0.18808	-0.89699
O	0.848327	0.112763	-1.44073
C	1.817015	-0.12704	-0.5262
C	3.092732	0.104803	-0.94059
C	1.838429	-0.94539	2.02094
C	2.185246	0.297724	2.846233
C	-1.06546	-1.28709	-1.77125
C	-1.26021	1.134798	-0.9312
C	-2.53156	1.243406	-0.06747
C	-3.61742	0.282153	-0.46111
C	-4.23989	-0.56396	0.360155
C	-5.35472	-1.48967	-0.02459
C	-5.03644	-2.96109	0.256216
C	-3.04423	2.698691	-0.14324
C	-4.16888	3.018851	0.834365
H	-0.88688	-0.97562	1.188363
C	4.344623	-0.09906	-0.24085
H	1.145171	-1.57703	2.585151
H	2.749335	-1.51629	1.843196
H	2.64139	0.007259	3.796605
H	2.898553	0.930766	2.31516
H	1.290303	0.888483	3.063277
H	-2.05294	-1.56921	-1.40406
H	-1.1633	-0.93076	-2.79977
H	-0.41795	-2.16684	-1.76296
H	-0.56767	1.91503	-0.59968
H	-1.50567	1.356539	-1.97702
H	-2.2591	1.047335	0.97791
H	-3.93385	0.328357	-1.50591
H	-3.92597	-0.60454	1.405183
H	-6.25724	-1.21363	0.537179
H	-5.59564	-1.35366	-1.08443
H	-5.88443	-3.60185	-0.00142
H	-4.17208	-3.29551	-0.32472

H	-4.80843	-3.1206	1.314787
H	-2.19834	3.370357	0.044621
H	-3.37411	2.903312	-1.16997
H	-3.84989	2.855085	1.869084
H	-4.47655	4.064474	0.743845
H	-5.04716	2.393112	0.655531
O	5.369817	0.310733	-1.03452
O	4.547753	-0.56167	0.866085
H	3.189275	0.476873	-1.95368
C	6.676802	0.154712	-0.48153
H	7.363739	0.517843	-1.24397
H	6.785411	0.740594	0.433906
H	6.881975	-0.89419	-0.25683

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf9**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.952617 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.43965	-2.24877	0.917505
C	-1.60401	-1.67824	0.575303
C	0.686494	-1.26929	0.900723
O	0.00996	-0.0417	0.524745
C	-1.31384	-0.25398	0.334847
C	-2.04577	0.841957	-0.00586
C	-2.90764	-2.40352	0.432411
C	-3.24689	-2.72531	-1.02605
C	1.308337	-1.06211	2.279016
C	1.708936	-1.64684	-0.18652
C	3.016085	-0.83918	-0.27689
C	2.7856	0.621565	-0.54221
C	3.315065	1.626979	0.153782
C	3.103823	3.084278	-0.12791
C	2.448875	3.826992	1.040552
C	3.897543	-1.46679	-1.37954
C	5.31632	-0.91328	-1.4365
H	-0.29854	-3.29321	1.168733
C	-3.47147	0.96817	-0.22793
H	-2.83356	-3.33424	1.003744
H	-3.71366	-1.80808	0.860379
H	-4.18885	-3.27773	-1.08323
H	-3.3626	-1.81005	-1.60941
H	-2.46449	-3.336	-1.48651
H	1.836167	-1.96627	2.593958
H	2.015687	-0.23199	2.256577
H	0.530846	-0.83987	3.012949
H	1.974731	-2.69793	-0.02224
H	1.187967	-1.60788	-1.1505
H	3.559403	-0.93857	0.671587
H	2.148194	0.851904	-1.39765
H	3.947702	1.394283	1.012903
H	4.072745	3.55404	-0.34476
H	2.494016	3.197776	-1.03067
H	2.335233	4.891498	0.81595
H	1.458485	3.417115	1.256641

H	3.051487	3.740903	1.950368
H	3.937695	-2.55054	-1.21489
H	3.403548	-1.32385	-2.34926
H	5.844634	-1.08446	-0.49258
H	5.891913	-1.39638	-2.23126
H	5.317293	0.163208	-1.6259
O	-3.75694	2.251651	-0.57496
O	-4.34755	0.128766	-0.13591
H	-1.48322	1.762578	-0.10507
C	-5.1363	2.531624	-0.81444
H	-5.18288	3.591335	-1.05926
H	-5.51621	1.935221	-1.64692
H	-5.73653	2.321873	0.073546

Compound 1: **2*E*-(6*R*,8*R*)-spongosoritin A conf10**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -927.951924 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.40717	0.132836	1.666541
C	0.72614	0.593505	1.112883
C	-0.51289	-1.34975	1.551747
O	0.65986	-1.67586	0.759946
C	1.426088	-0.57705	0.556187
C	2.611938	-0.79492	-0.07506
C	1.149282	2.030822	1.072627
C	0.9364	2.685623	-0.29484
C	-0.35681	-2.03528	2.9124
C	-1.74126	-1.90339	0.81755
C	-2.10402	-1.23658	-0.52517
C	-3.172	-0.19385	-0.33899
C	-3.10319	1.087465	-0.69832
C	-4.20306	2.092896	-0.53173
C	-3.80404	3.285873	0.341935
C	-2.56052	-2.31006	-1.53545
C	-2.82861	-1.777	-2.9378
H	-1.14712	0.734228	2.17903
C	3.676024	0.134985	-0.39316
H	0.570011	2.568439	1.829761
H	2.203751	2.109306	1.338796
H	1.258624	3.730207	-0.26774
H	1.519937	2.178476	-1.06492
H	-0.11804	2.662377	-0.58249
H	-1.18953	-1.76861	3.567821
H	-0.34608	-3.1208	2.787024
H	0.575206	-1.72511	3.389328
H	-1.53567	-2.96801	0.660085
H	-2.59453	-1.85514	1.502961
H	-1.20866	-0.7548	-0.93728
H	-4.09858	-0.5586	0.112477
H	-2.18153	1.454578	-1.15178
H	-4.49614	2.467223	-1.52182
H	-5.08766	1.601914	-0.1116
H	-4.61715	4.014609	0.405695
H	-3.55845	2.963935	1.358185

H	-2.92814	3.799185	-0.06643
H	-1.78371	-3.08235	-1.5823
H	-3.46043	-2.80391	-1.14526
H	-3.62621	-1.02934	-2.93758
H	-1.93311	-1.30462	-3.35518
H	-3.12397	-2.5849	-3.61341
O	4.657654	-0.52405	-1.06459
O	3.772779	1.319551	-0.13335
H	2.802205	-1.82328	-0.35871
C	5.790864	0.26492	-1.42746
H	6.470935	-0.41479	-1.93791
H	5.500993	1.079944	-2.09435
H	6.271698	0.686347	-0.54198

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Compound 2: 2*E*-(6*R*,8*S*)-dihydrospongosoritin A conf1

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.162712 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.292102	-1.63241	0.55004
C	-0.87101	-1.37351	-0.06657
C	0.520364	-0.7235	1.709073
O	-0.65497	0.125957	1.662464
C	-1.47389	-0.23168	0.643906
C	-1.42973	-2.15931	-1.21362
C	-2.50117	-3.16294	-0.77723
C	-2.60691	0.509698	0.508141
C	1.79049	0.136451	1.595339
C	1.900723	1.066402	0.373012
C	3.361002	1.17278	-0.09744
C	3.904656	-0.06887	-0.80242
C	5.367036	0.067735	-1.22388
C	0.497008	-1.47372	3.041767
C	5.907785	-1.16877	-1.93538
C	1.313062	2.454106	0.686061
C	1.021565	3.313346	-0.54151
H	0.989008	-2.41602	0.277997
H	-1.85824	-1.48364	-1.95354
H	-0.59841	-2.69399	-1.68369
H	-2.86225	-3.73041	-1.63937
H	-2.10265	-3.87161	-0.04499
H	-3.35744	-2.65068	-0.33491
C	-3.65014	0.426102	-0.49366
H	1.879053	0.730728	2.51273
H	2.627666	-0.56959	1.61269
H	1.316049	0.631785	-0.4501
H	3.458731	2.02381	-0.78105
H	3.993189	1.410674	0.770169
H	3.805411	-0.94976	-0.15461
H	3.290607	-0.27543	-1.6893
H	5.473444	0.942469	-1.87775
H	5.978766	0.276774	-0.33709
H	0.544311	-0.76291	3.870342

H	-0.41835	-2.0622	3.132984
H	1.353992	-2.14806	3.113098
H	5.846342	-2.05347	-1.29285
H	5.338227	-1.38244	-2.84592
H	6.955431	-1.0401	-2.22251
H	0.386571	2.321306	1.251505
H	2.007636	2.982633	1.353708
H	1.92097	3.520252	-1.12858
H	0.300457	2.819819	-1.20105
H	0.595356	4.277768	-0.24995
O	-4.60903	1.348999	-0.21693
C	-5.70326	1.392842	-1.13326
O	-3.73724	-0.30656	-1.46099
H	-2.74114	1.292131	1.245568
H	-6.35426	2.188626	-0.77558
H	-5.35609	1.613928	-2.14482
H	-6.24064	0.441954	-1.14366

Compound 2: **2*E*-(6*R*,8*S*)-dihydrospongosoritin A conf2**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.161869 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.26507	0.973317	1.52066
C	0.896889	1.171361	0.879713
C	-0.4647	-0.46022	1.878818
O	0.723189	-1.07818	1.320366
C	1.541572	-0.14918	0.769496
C	1.384415	2.492692	0.36762
C	1.153271	2.670842	-1.13583
C	2.71998	-0.61848	0.276552
C	-1.72462	-1.09313	1.264749
C	-1.83396	-1.09423	-0.27096
C	-3.30086	-0.94924	-0.70877
C	-3.89237	0.448427	-0.53072
C	-5.3619	0.538953	-0.93871
C	-0.43382	-0.68671	3.391811
C	-5.9487	1.937429	-0.77147
C	-1.19953	-2.36473	-0.86509
C	-0.91014	-2.29006	-2.36199
H	-0.98229	1.743885	1.777056
H	0.851538	3.27699	0.914352
H	2.448717	2.600635	0.575966
H	1.511672	3.651679	-1.46027
H	1.696125	1.914271	-1.70507
H	0.090078	2.597922	-1.38316
C	3.819413	0.10128	-0.33388
H	-1.79807	-2.12371	1.632694
H	-2.57112	-0.55551	1.705572
H	-1.28121	-0.22798	-0.66085
H	-3.3907	-1.22677	-1.76509
H	-3.90698	-1.67967	-0.15393
H	-3.79524	0.773195	0.513563
H	-3.30759	1.163311	-1.12496
H	-5.46598	0.220666	-1.98371
H	-5.94485	-0.17659	-0.3451
H	-0.46083	-1.75703	3.609923
H	0.474263	-0.26098	3.823935
H	-1.29887	-0.2141	3.863753

H	-5.40556	2.669362	-1.37834
H	-6.99933	1.97024	-1.07421
H	-5.89379	2.267598	0.271197
H	-0.2655	-2.57009	-0.33519
H	-1.86448	-3.21453	-0.65686
H	-1.81536	-2.12931	-2.95512
H	-0.21722	-1.47242	-2.58555
H	-0.45071	-3.21739	-2.71662
O	4.786202	-0.7844	-0.69272
C	5.947062	-0.21676	-1.30005
O	3.950609	1.295012	-0.52847
H	2.869637	-1.68735	0.371878
H	6.610958	-1.05481	-1.50485
H	5.689473	0.296003	-2.22941
H	6.431628	0.493558	-0.62665

Compound 2: **2*E*-(6*R*,8*S*)-dihydrospongosoritin A conf3**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.161776 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.188716	-2.04303	0.319996
C	1.360017	-1.45382	0.60449
C	-0.35872	-1.58745	-0.98967
O	0.636478	-0.62025	-1.41258
C	1.656368	-0.55186	-0.52278
C	2.155487	-1.67488	1.8551
C	1.956162	-0.56357	2.890081
C	2.677253	0.283013	-0.85787
C	-1.7364	-0.90917	-0.89101
C	-1.80739	0.367974	-0.03091
C	-3.09029	0.399526	0.820345
C	-4.4067	0.475637	0.046494
C	-5.63318	0.42657	0.957176
C	-0.38415	-2.70994	-2.02833
C	-6.95312	0.516206	0.197286
C	-1.61688	1.624563	-0.89647
C	-1.49644	2.926156	-0.10933
H	-0.31465	-2.7764	0.93863
H	1.841918	-2.6324	2.282554
H	3.215223	-1.74453	1.610886
H	2.543718	-0.77269	3.788229
H	2.284087	0.399838	2.495601
H	0.904999	-0.48062	3.181849
C	3.917025	0.555197	-0.15878
H	-2.07821	-0.69783	-1.91056
H	-2.41769	-1.67157	-0.49565
H	-0.97199	0.339088	0.681447
H	-3.10204	-0.50026	1.450124
H	-3.03971	1.245298	1.516508
H	-4.44132	1.399492	-0.54391
H	-4.46634	-0.34855	-0.67639
H	-5.60985	-0.50078	1.543686
H	-5.57331	1.245786	1.684919
H	-0.66764	-2.30855	-3.00427
H	0.598791	-3.17859	-2.1106
H	-1.11177	-3.47345	-1.74205

H	-7.02078	1.451029	-0.36887
H	-7.05633	-0.3088	-0.51539
H	-7.8101	0.477047	0.876067
H	-0.71419	1.48385	-1.49815
H	-2.44639	1.700884	-1.61075
H	-2.41332	3.16435	0.437683
H	-0.67993	2.872394	0.61857
H	-1.28749	3.767056	-0.7771
O	4.621021	1.49029	-0.84991
C	5.880338	1.855575	-0.28446
O	4.347051	0.073304	0.87213
H	2.555127	0.811587	-1.79579
H	6.300592	2.599343	-0.95914
H	5.750726	2.281043	0.713094
H	6.542837	0.989935	-0.21647

Compound 2: **2*E*-(6*R*,8*S*)-dihydrospongosoritin A conf4**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.161274 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	0.209022	1.988175	-0.25093
C	1.364281	1.378497	-0.55658
C	-0.37371	1.468959	1.019188
O	0.584111	0.446046	1.394765
C	1.597686	0.375905	0.498067
C	2.24175	1.727641	-1.71971
C	3.428377	2.609334	-1.31831
C	2.551036	-0.56012	0.75601
C	-1.76934	0.840095	0.861489
C	-1.871	-0.369	-0.08888
C	-3.15842	-0.31044	-0.93228
C	-4.47186	-0.41398	-0.15664
C	-5.70257	-0.27756	-1.05261
C	-0.38064	2.527595	2.122778
C	-7.0193	-0.39477	-0.29094
C	-1.70704	-1.69006	0.680947
C	-1.62956	-2.93415	-0.19903
H	-0.25461	2.783131	-0.82285
H	2.618551	0.818128	-2.18678
H	1.625756	2.256482	-2.45375
H	4.031658	2.856078	-2.19624
H	3.087795	3.544685	-0.86422
H	4.073971	2.092718	-0.60584
C	3.718857	-0.92888	-0.0188
H	-2.12815	0.567593	1.860422
H	-2.42329	1.648589	0.514776
H	-1.0383	-0.30528	-0.80254
H	-3.1535	0.632285	-1.4958
H	-3.12891	-1.10503	-1.68734
H	-4.52165	-1.37568	0.368872
H	-4.51071	0.359165	0.621963
H	-5.66446	0.687973	-1.57297
H	-5.66329	-1.0448	-1.83625
H	-0.68997	2.077068	3.069014
H	0.614819	2.959431	2.245961
H	-1.0805	3.329627	1.874934

H	-7.10245	-1.36608	0.207705
H	-7.10105	0.37906	0.479643
H	-7.87967	-0.29011	-0.9584
H	-0.79615	-1.61827	1.282262
H	-2.53234	-1.79532	1.396594
H	-2.55833	-3.10897	-0.74993
H	-0.81985	-2.8494	-0.9316
H	-1.43572	-3.82586	0.404295
O	4.407971	-1.89285	0.647258
C	5.583952	-2.37182	-0.00589
O	4.096805	-0.51142	-1.09716
H	2.407085	-1.1305	1.665912
H	5.996208	-3.134	0.652985
H	5.340493	-2.80445	-0.97869
H	6.306332	-1.56509	-0.14833

Compound 2: **2*E*-(6*R*,8*S*)-dihydrospongosoritin A conf5**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.161222 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.6672	-2.05619	0.850446
C	-1.84754	-1.48955	0.560702
C	0.449099	-1.06545	0.828802
O	-0.25355	0.164787	0.506185
C	-1.58153	-0.05568	0.353945
C	-3.14681	-2.22578	0.43524
C	-3.52754	-2.50482	-1.02176
C	-2.33528	1.042062	0.073276
C	1.451387	-1.41529	-0.28983
C	2.754374	-0.60628	-0.4089
C	2.49121	0.830933	-0.89178
C	3.676155	1.799848	-0.82136
C	4.144914	2.134441	0.595061
C	1.096311	-0.88447	2.199753
C	5.259393	3.176629	0.621014
C	3.729292	-1.34282	-1.3463
C	4.345554	-2.61504	-0.76892
H	-0.50766	-3.10585	1.066416
H	-3.04448	-3.17317	0.97381
H	-3.94563	-1.65401	0.906702
H	-4.46626	-3.06369	-1.06815
H	-3.668	-1.5728	-1.57222
H	-2.75443	-3.09342	-1.52466
C	-3.7696	1.1597	-0.0938
H	1.707452	-2.46919	-0.13711
H	0.907475	-1.36849	-1.24122
H	3.224738	-0.56691	0.581884
H	2.133159	0.777501	-1.92913
H	1.664477	1.256013	-0.31566
H	4.526114	1.41939	-1.40146
H	3.378756	2.732959	-1.31686
H	3.289105	2.498174	1.178006
H	4.492737	1.225364	1.0994
H	1.650413	-1.7849	2.477599
H	1.787493	-0.03992	2.19277
H	0.32977	-0.70012	2.95535

H	5.575574	3.401242	1.64391
H	6.139638	2.827846	0.070672
H	4.933554	4.11499	0.160195
H	3.20792	-1.57368	-2.28506
H	4.542255	-0.66174	-1.61661
H	4.89805	-2.40031	0.151813
H	3.595399	-3.37604	-0.53473
H	5.047559	-3.06373	-1.47775
O	-4.07953	2.450374	-0.38771
C	-5.46956	2.723748	-0.56637
O	-4.6333	0.308156	0.002084
H	-1.78626	1.971891	-0.01648
H	-5.53436	3.789175	-0.78013
H	-5.87626	2.14616	-1.39939
H	-6.03298	2.484765	0.338236

Compound 2: **2*E*-(6*R*,8*S*)-dihydrospongosoritin A conf6**

B3PW91/PCM($CHCl_3$)/6-311G(d,p) opt

Total energy = -929.160801 Hartree

Imaginary frequencies = 0

Symbol	X	Y	Z
C	-0.30171	1.718332	1.199982
C	-1.3783	0.917586	1.221187
C	0.108813	2.056194	-0.19203
O	-0.83141	1.281194	-0.98202
C	-1.73719	0.664248	-0.18549
C	-2.0286	0.37992	2.459363
C	-1.63588	-1.07079	2.755213
C	-2.72584	-0.01313	-0.83022
C	1.551765	1.675516	-0.55844
C	2.091712	0.299887	-0.13504
C	3.624413	0.314362	-0.27957
C	4.342058	-0.94461	0.203496
C	5.86371	-0.80263	0.200155
C	-0.14201	3.53187	-0.52025
C	6.587333	-2.06221	0.666543
C	1.43429	-0.89199	-0.85515
C	1.620374	-0.93529	-2.37026
H	0.209707	2.109117	2.07153
H	-1.7274	1.017846	3.296199
H	-3.11246	0.439173	2.362926
H	-2.12339	-1.41561	3.671208
H	-1.94682	-1.73211	1.944438
H	-0.5542	-1.16779	2.887079
C	-3.86314	-0.72866	-0.28744
H	1.659012	1.812268	-1.64053
H	2.186857	2.441767	-0.09833
H	1.875049	0.17615	0.935534
H	3.894083	0.506561	-1.32664
H	4.009997	1.172177	0.287139
H	4.004767	-1.18869	1.220418
H	4.066752	-1.80197	-0.42228
H	6.198793	-0.54205	-0.81188
H	6.148506	0.042114	0.840124
H	0.094328	3.727348	-1.56917
H	-1.18856	3.787318	-0.34109
H	0.485388	4.173233	0.103361

H	6.351981	-2.91526	0.021663
H	7.672946	-1.92809	0.655769
H	6.296258	-2.33077	1.687491
H	1.834437	-1.81422	-0.4196
H	0.365573	-0.90309	-0.62821
H	2.676284	-0.98064	-2.65374
H	1.132644	-1.8205	-2.78845
H	1.179111	-0.0621	-2.85834
O	-4.56968	-1.28148	-1.30855
C	-5.74029	-2.00453	-0.92683
O	-4.21614	-0.85825	0.869516
H	-2.67175	0.007464	-1.91224
H	-6.17569	-2.36969	-1.85532
H	-5.48566	-2.84226	-0.27395
H	-6.44782	-1.35394	-0.40808