Supporting information

Medermycin-type Naphthoquinones from the Marine-derived *Streptomyces* sp. XMA39

Yong-Jun Jiang, [†] Da-Shan Zhang, [†] Hao-Jian Zhang, [†] Jia-Qi Li, [†] Wan-Jing Ding, [†] Cheng-Dong Xu, [†] Zhong-Jun Ma[*, †, ‡]

[†]Institute of Marine Biology, Ocean College, Zhejiang University, Zhoushan 316021, People's Republic of China;

[‡]Ocean Academy, Zhejiang University, Zhoushan 316021, People's Republic of China

[*]Corresponding author *E*-mail: mazj@zju.edu.cn

Table of contents

Strain Isolation and Identification. Strain XMA39 was isolated from marine sediments collected in Xiamen Island, Fujian province of China (118° 08′ 12.91″N and 24°47′99.06″E), by using standard dilution plating method. The sample of sediment were diluted and then spread on the surface of Gause's solid medium consisting of (per liter) 20 g of soluble starch, 1 g of KNO_3, 0.5 g of K_2HPO_4, 0.5 g of $MgSO_4 \cdot 7H_2O$, 0.5 g of NaCl, 0.01 g of $FeSO_4 \cdot 7H_2O$, 20 g of agar, 25 g of sea salt, pH = 7.2-7.4). After about 5-7 days of incubation at room temperature, the single colony was picked with sterile needles and transferred to a Gause's solid medium. Title strain was maintained in Gause's solid medium and subcultured monthly. The strain XMA39 was identified using 16S rDNA sequence analysis by TaKaRa (Dalian, China), and its DNA sequence using BLAST (nucleotide sequence comparison) was compared to the GenBank database. A BLAST search result showed the sequence of the strain to be identical with *Streptomyces* sp. DUT11 chromosome (accession number CP025511.1), confirming that the strain is a member of the genus *Streptomyces* sp. The sequence of strain is deposited in GenBank under accession no. MH725564. A voucher strain (*Streptomyces sp.* XMA39) was preserved at the Laboratory of Institute of Marine Biology, Ocean College, Zhejiang University, China.

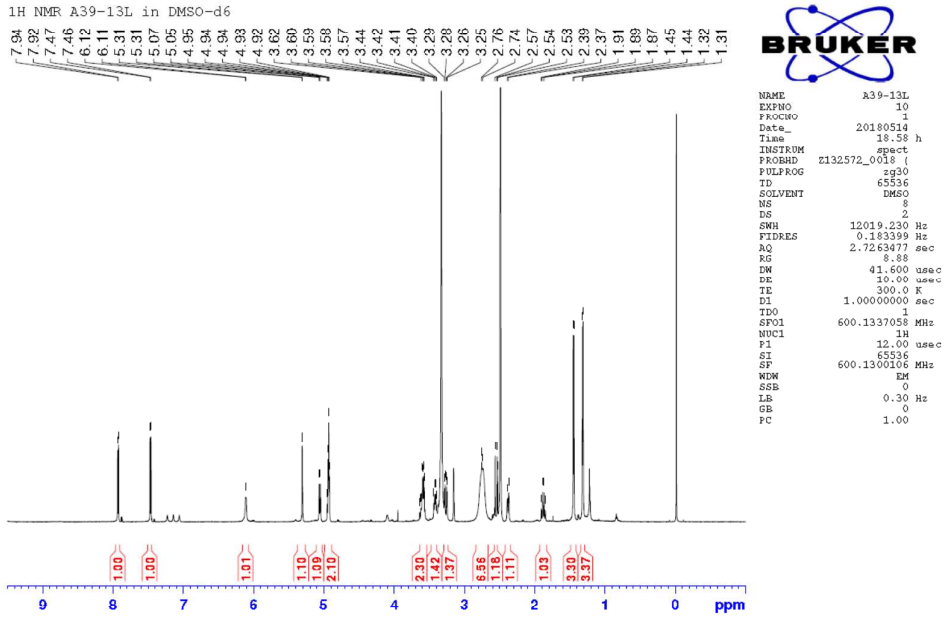


Figure S1. ^{1}H NMR spectrum of **1**

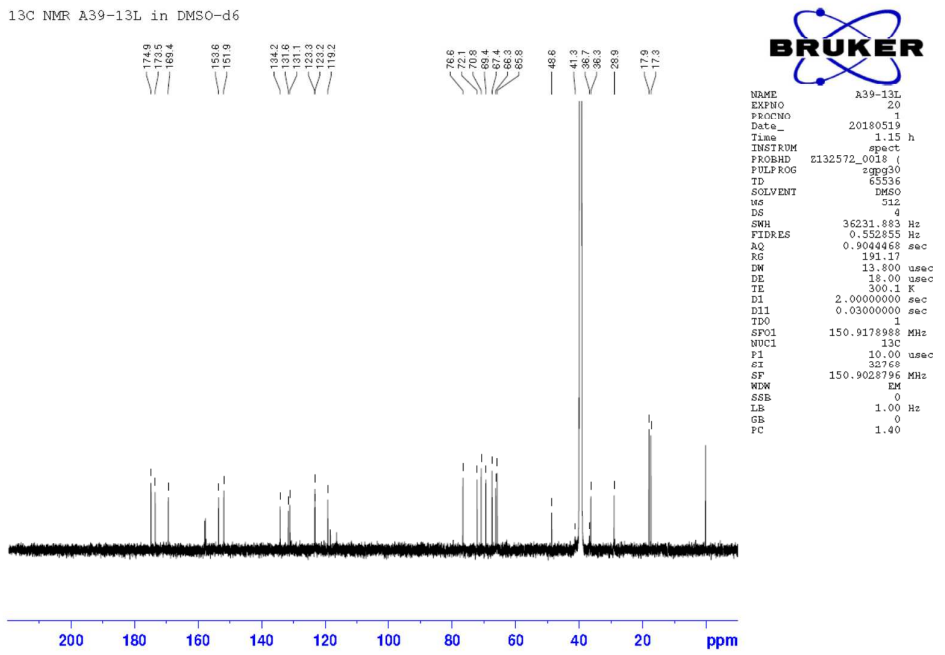


Figure S2. ^{13}C NMR spectrum of **1**

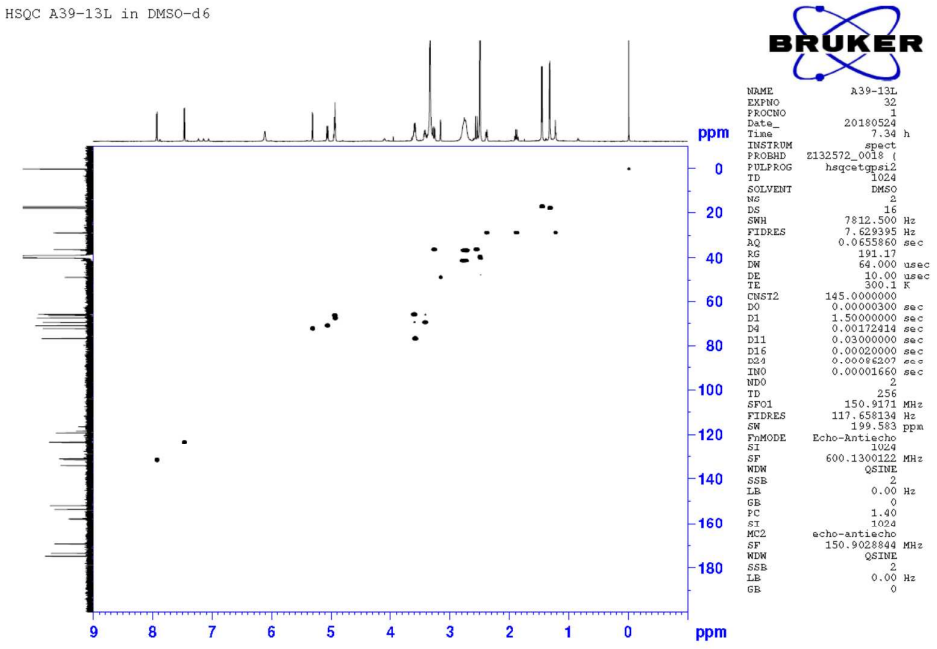


Figure S3. HSQC spectrum of **1**

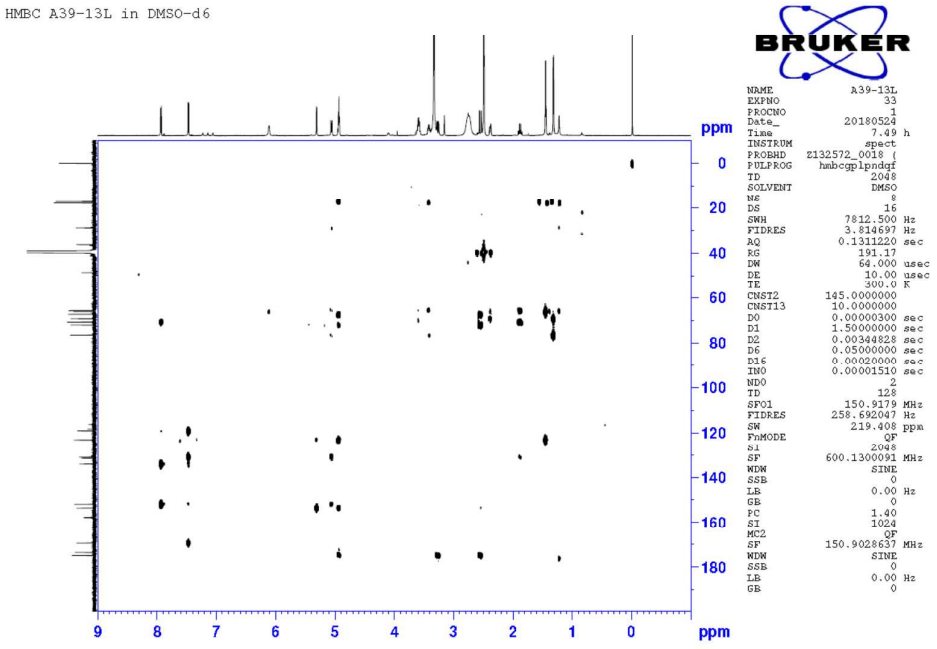


Figure S4. HMBC spectrum of **1**

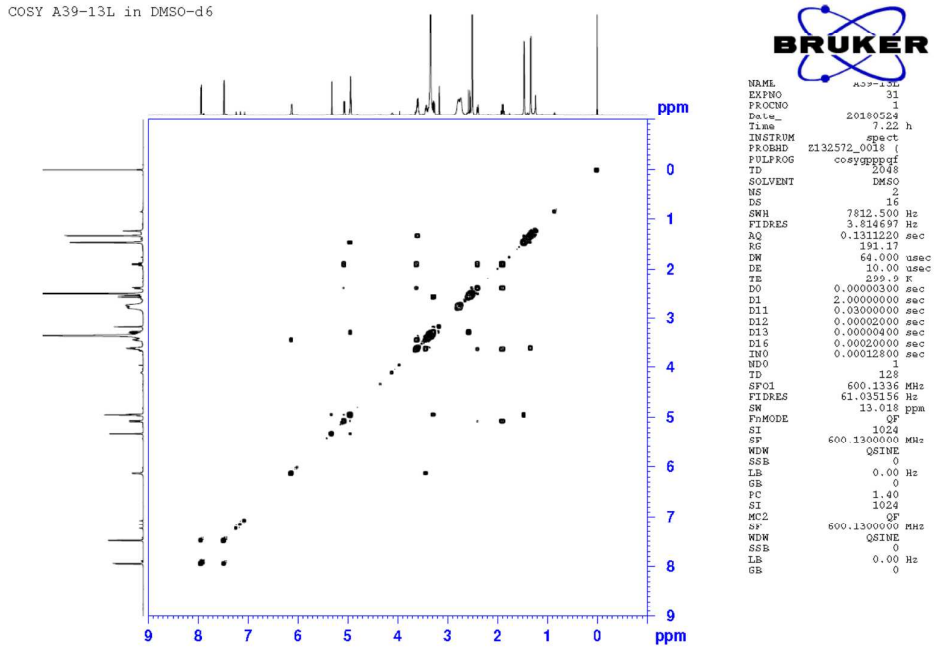


Figure S5. COSY spectrum of **1**

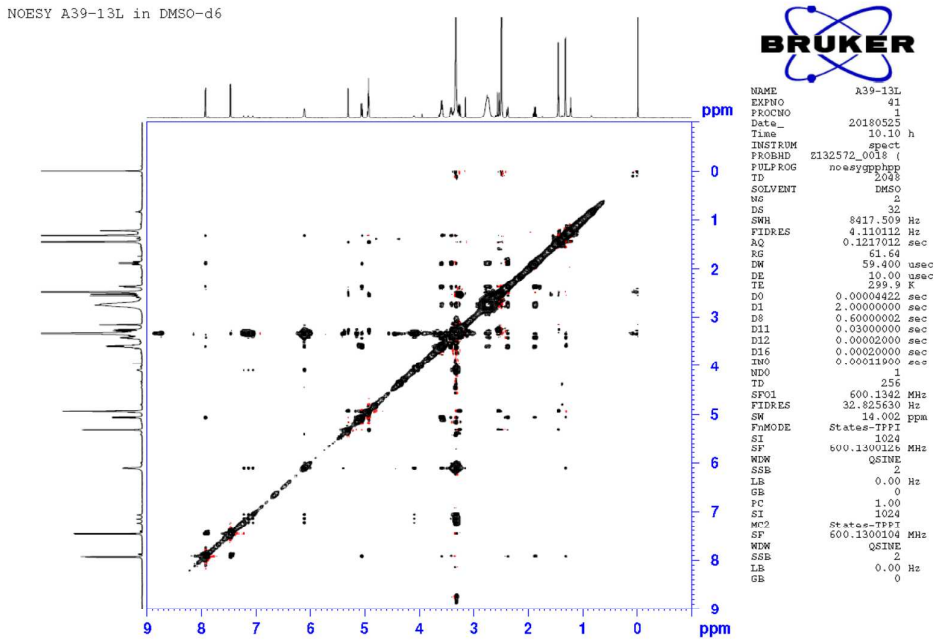


Figure S6. NOESY spectrum of **1**

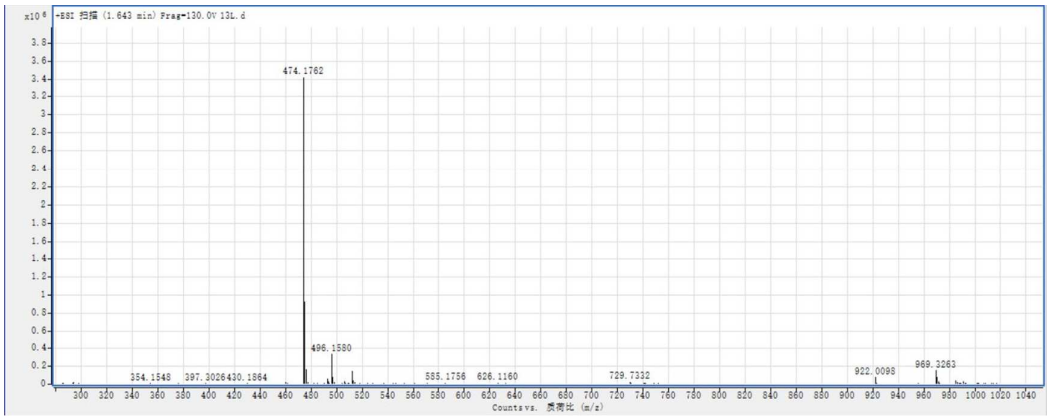


Figure S7. HRESIMS spectrum of **1**

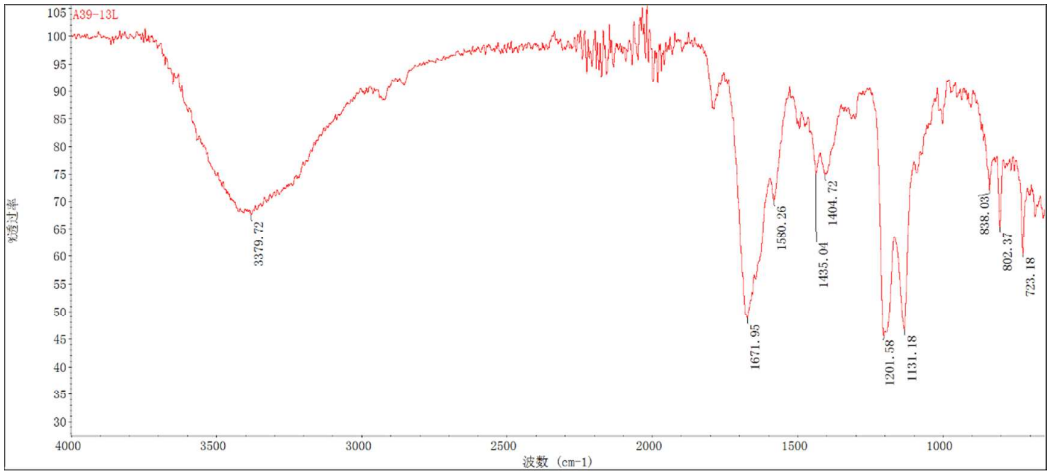


Figure S8. IR spectrum of **1**.

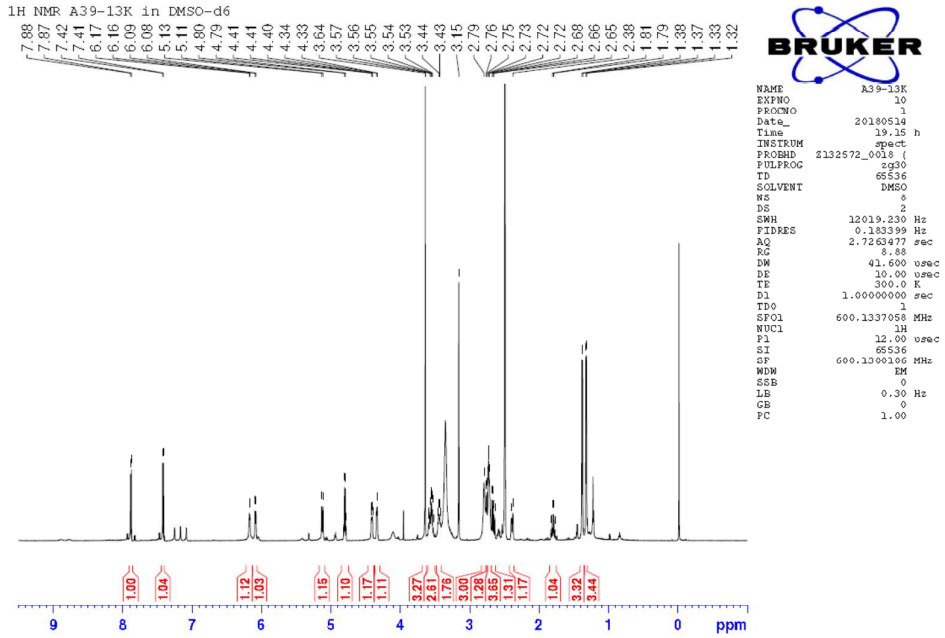


Figure S9. ^{1}H NMR spectrum of **2**

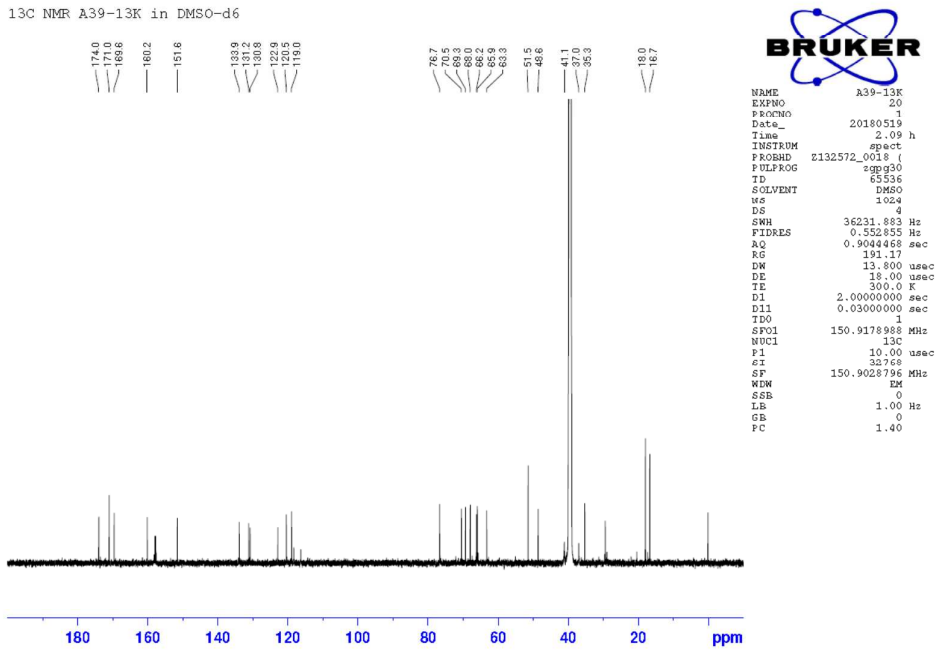


Figure S10. ^{13}C NMR spectrum of **2**

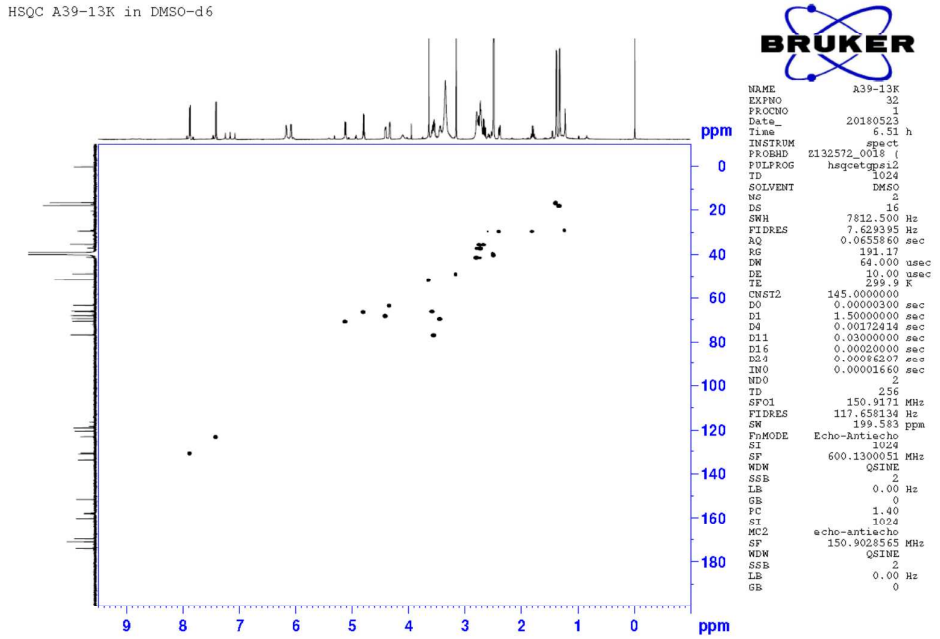


Figure S11. HSQC spectrum of **2**

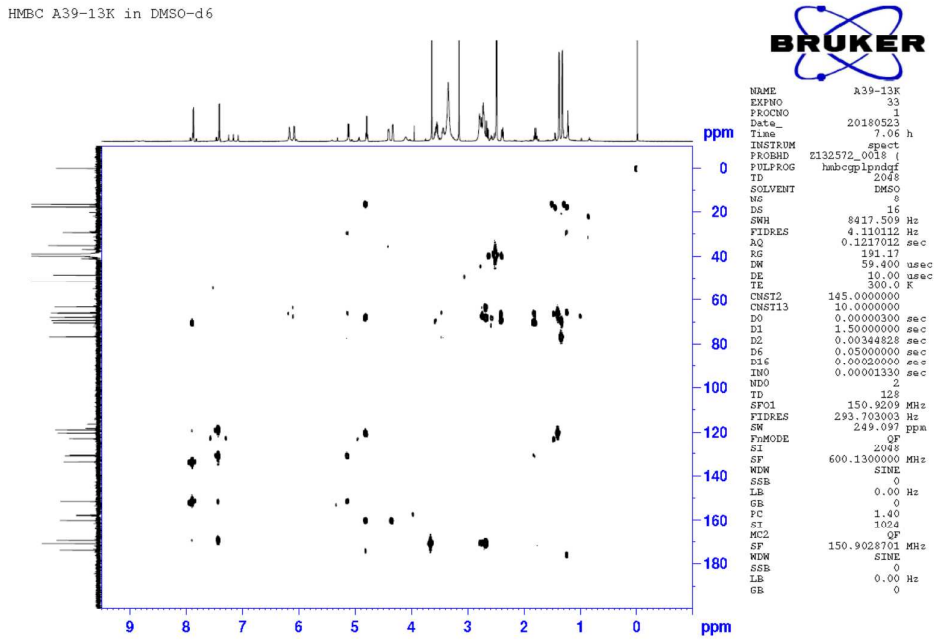


Figure S12. HMBC spectrum of **2**

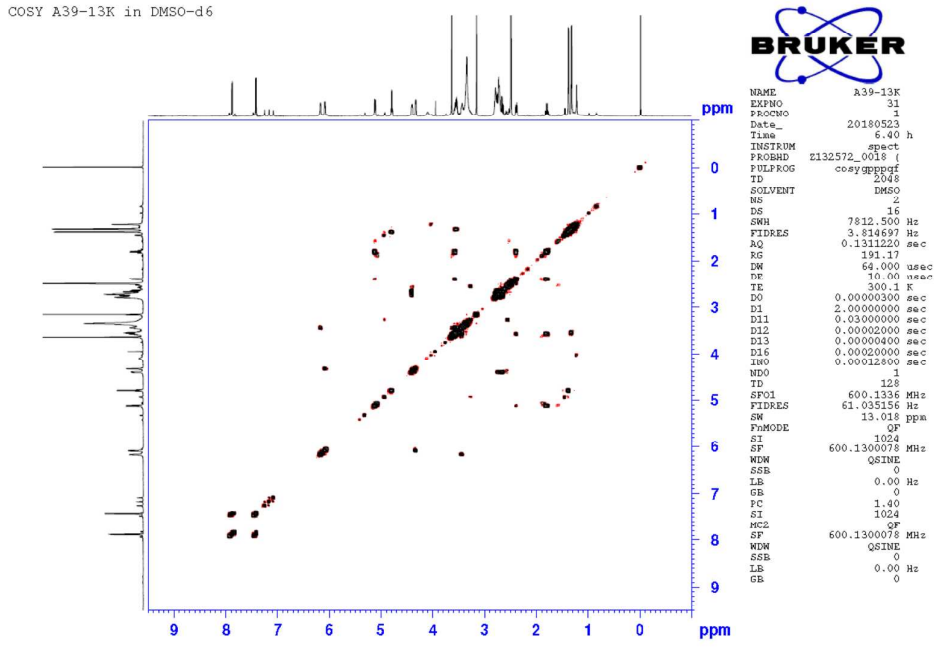


Figure S13. COSY spectrum of **2**

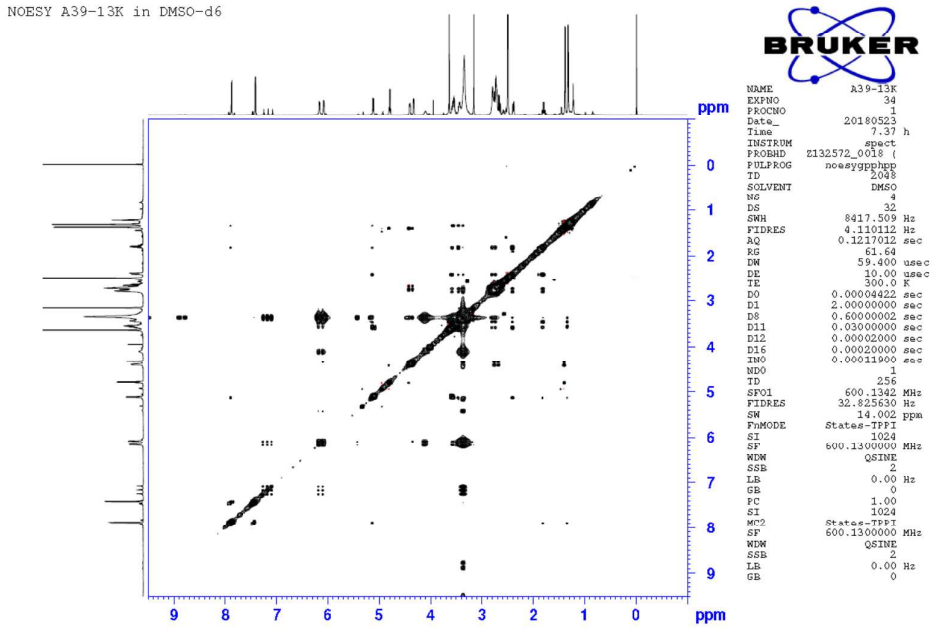


Figure S14. NOESY spectrum of **2**

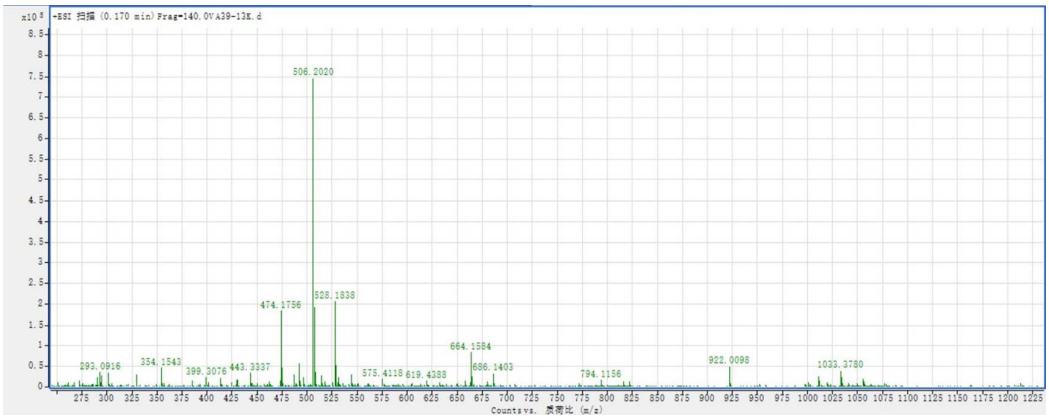


Figure S15. HRESIMS data of **2**

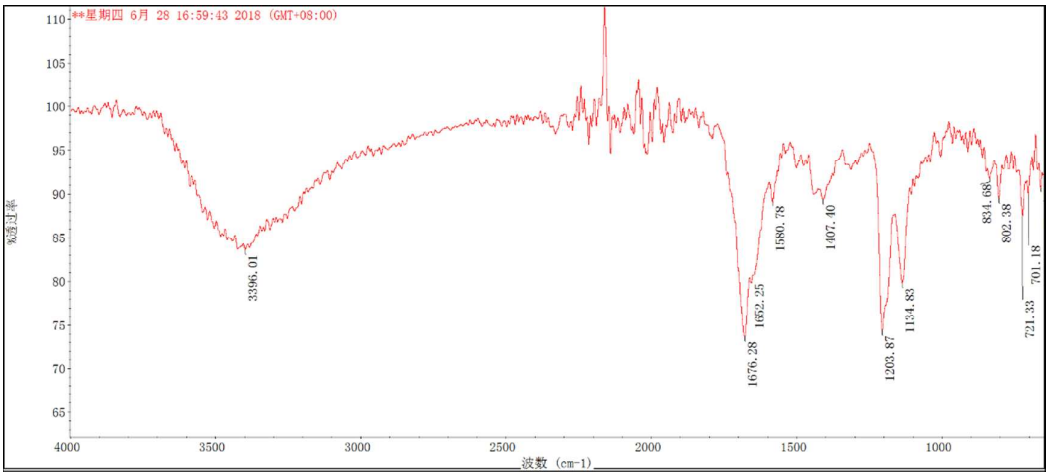


Figure S16. IR spectrum of **2**

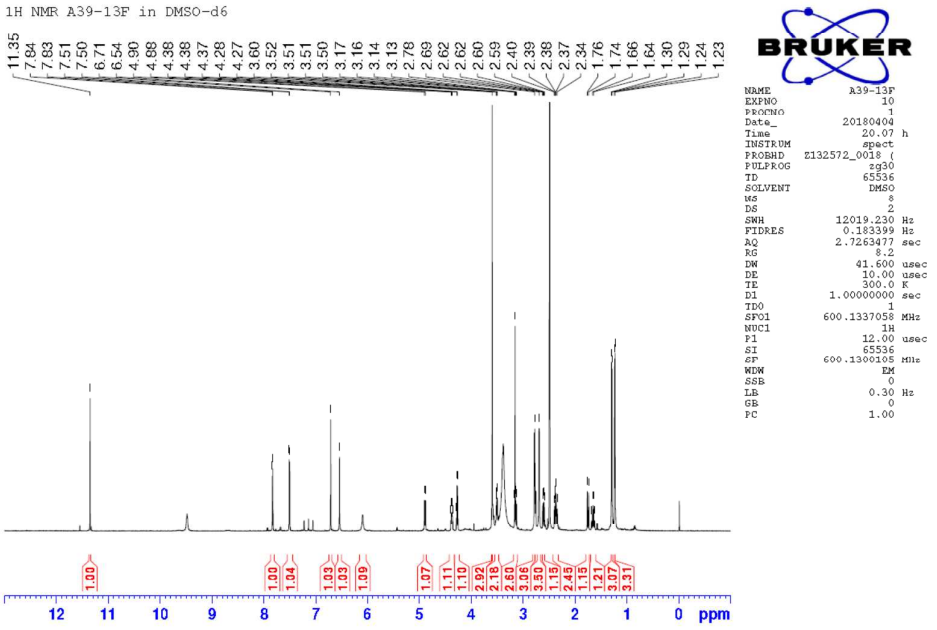


Figure S17. ^{1}H NMR spectrum of **3**

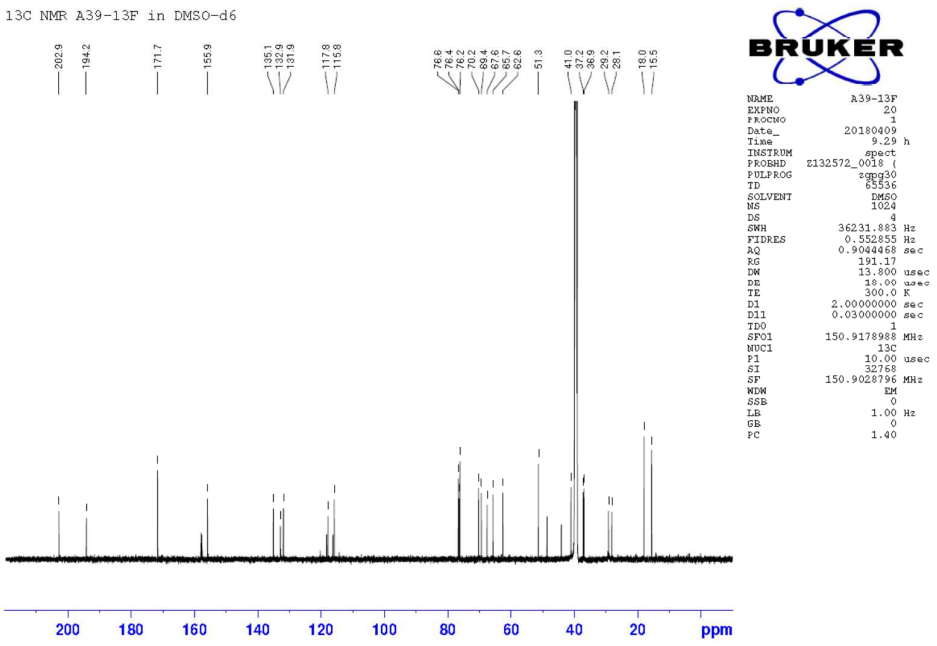


Figure S18. ^{13}C NMR spectrum of **3**

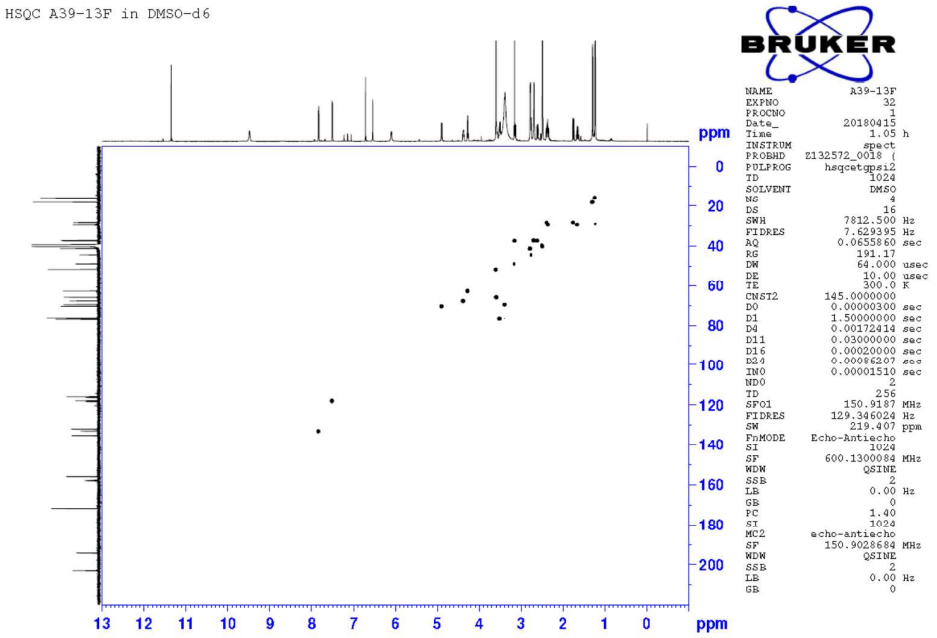


Figure S19. HSQC spectrum of **3**

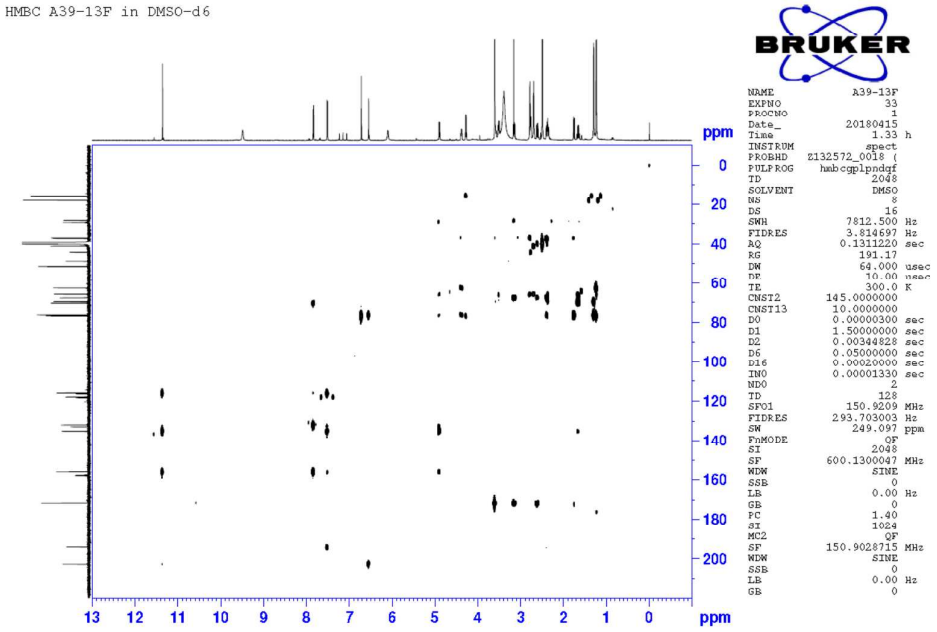


Figure S20. HMBC spectrum of **3**

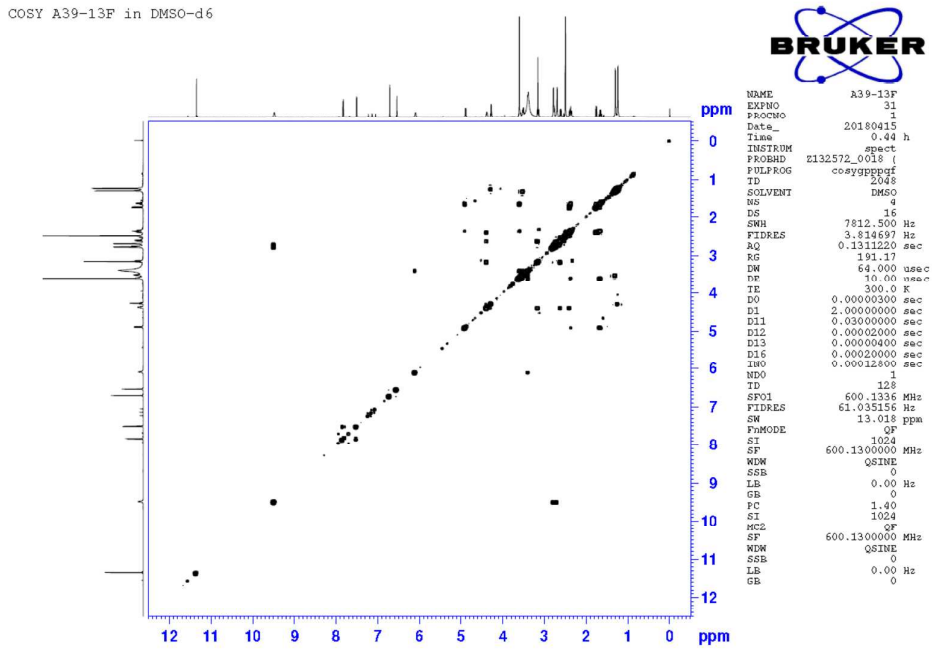


Figure S21. COSY spectrum of **3**

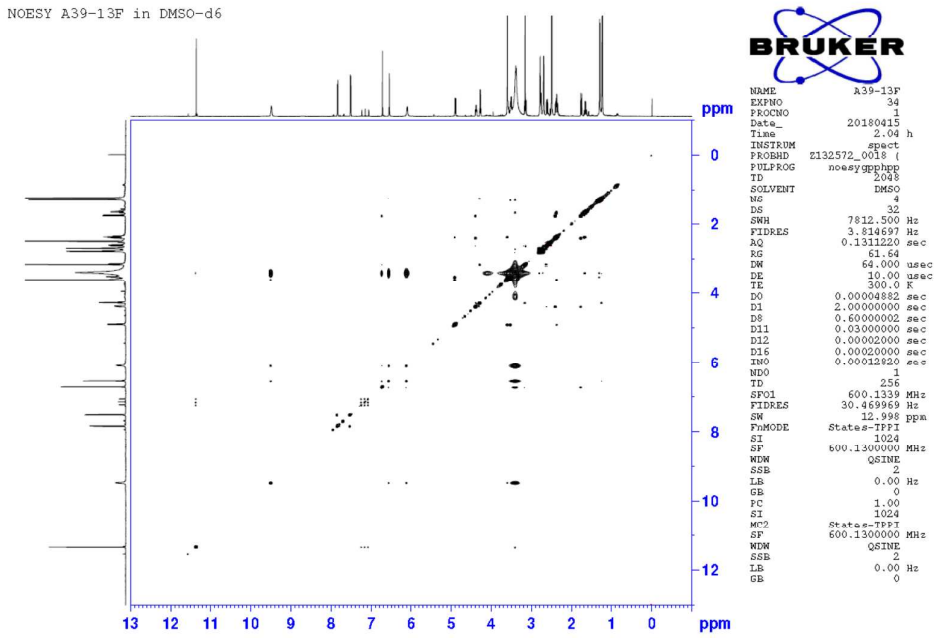


Figure S22. NOESY spectrum of **3**

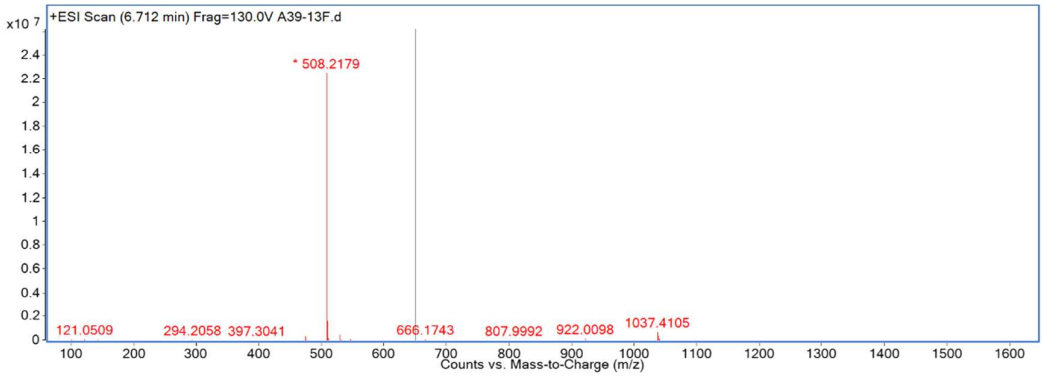


Figure S23. HRESIMS data of **3**

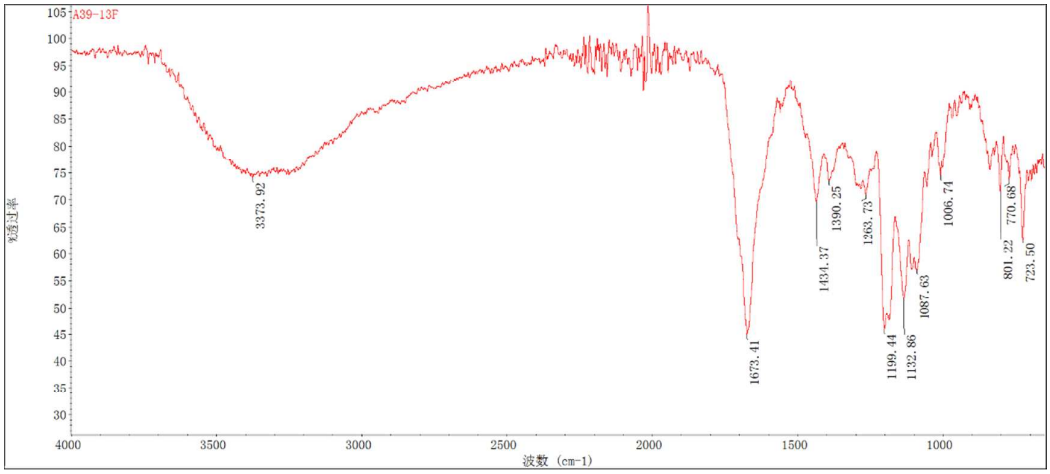


Figure S24. IR spectrum of **3**

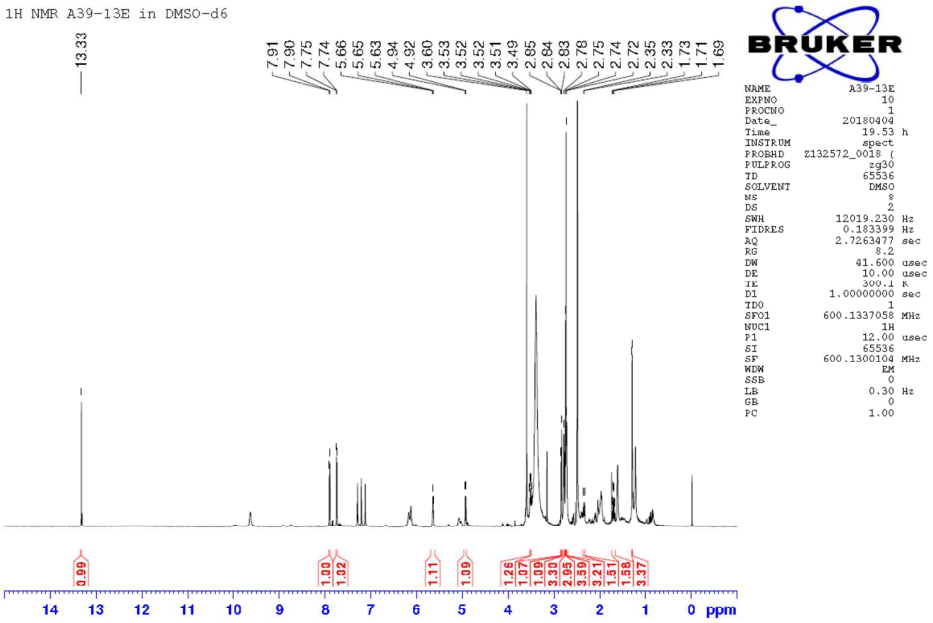


Figure S25. [1]HNMR spectrum of **4**

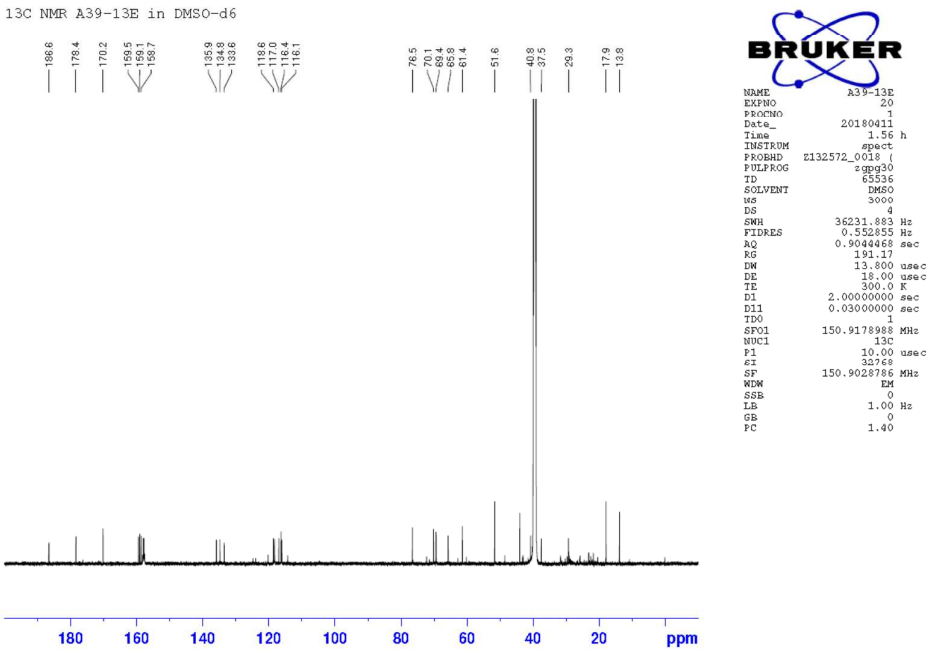


Figure S26. [13]C NMR spectrum of **4**

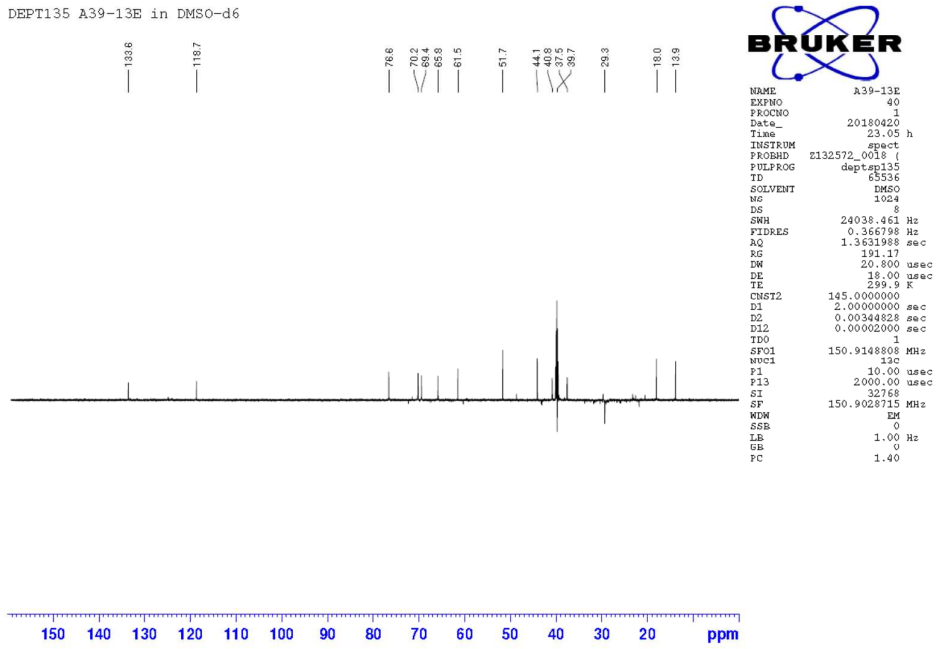


Figure S27. DEPT 135 spectrum of **4**

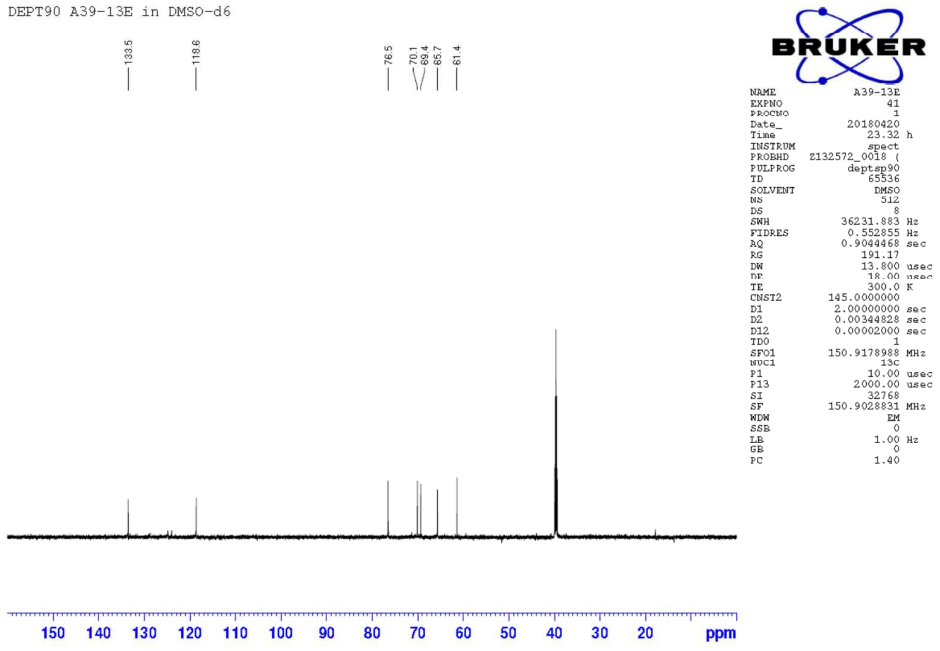


Figure S28. DEPT 90 spectrum of **4**

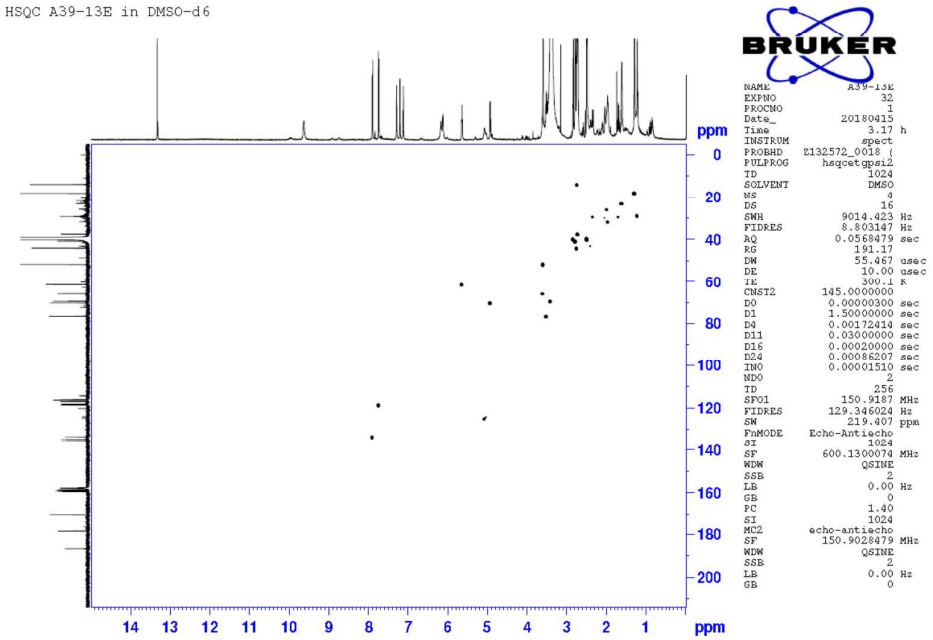


Figure S29. HSQC spectrum of **4**

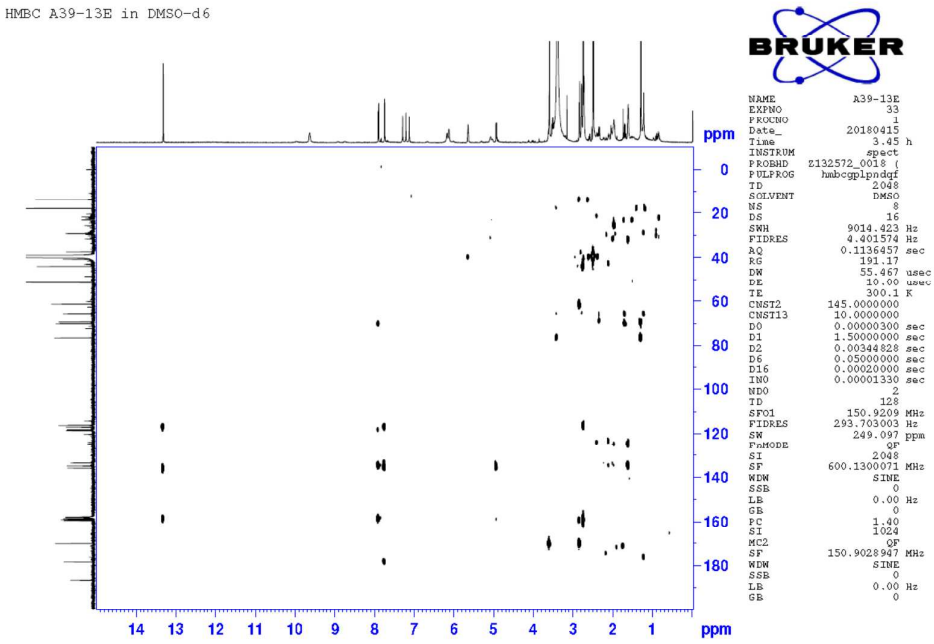


Figure S30. HMBC spectrum of **4**

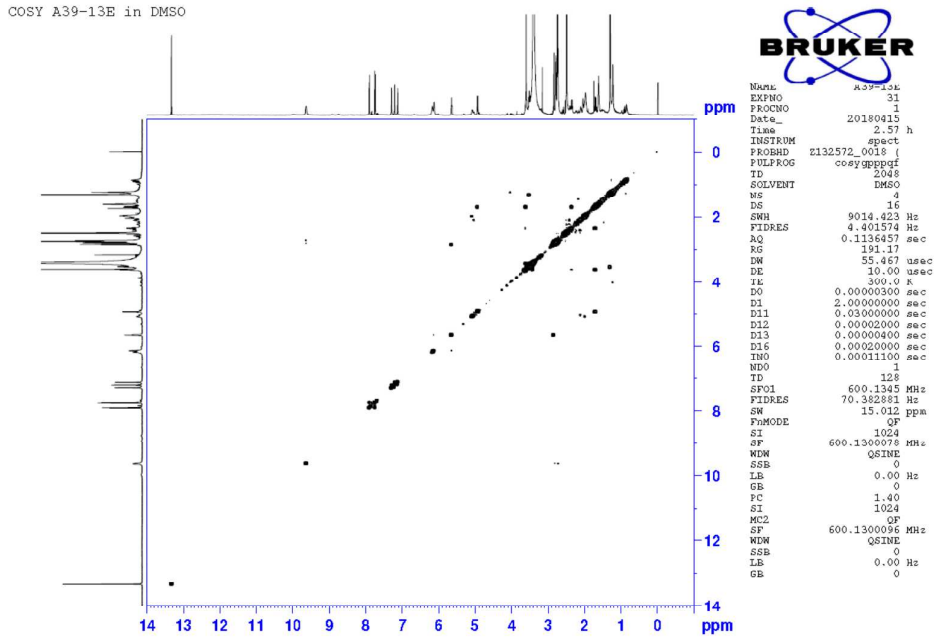


Figure S31. COSY spectrum of **4**

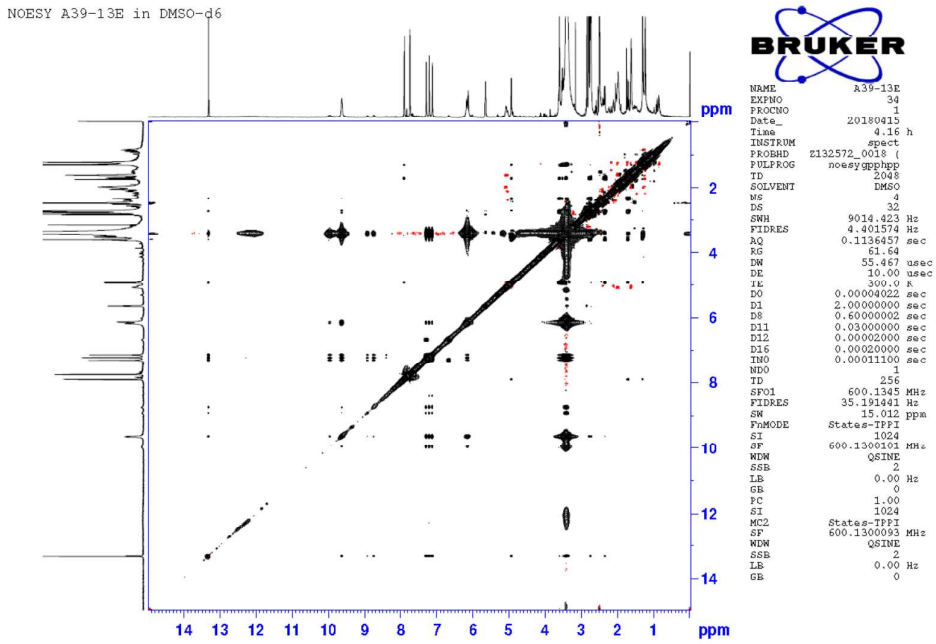


Figure S32. NOESY spectrum of **4**

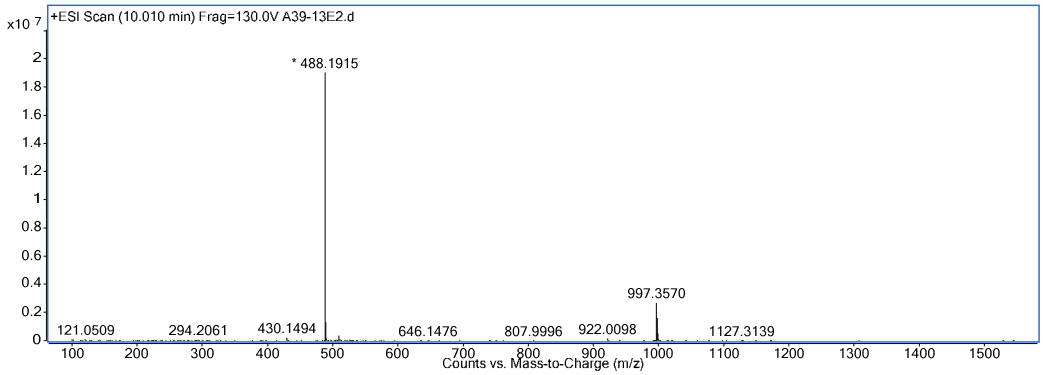


Figure S33. HRESIMS data of **4**

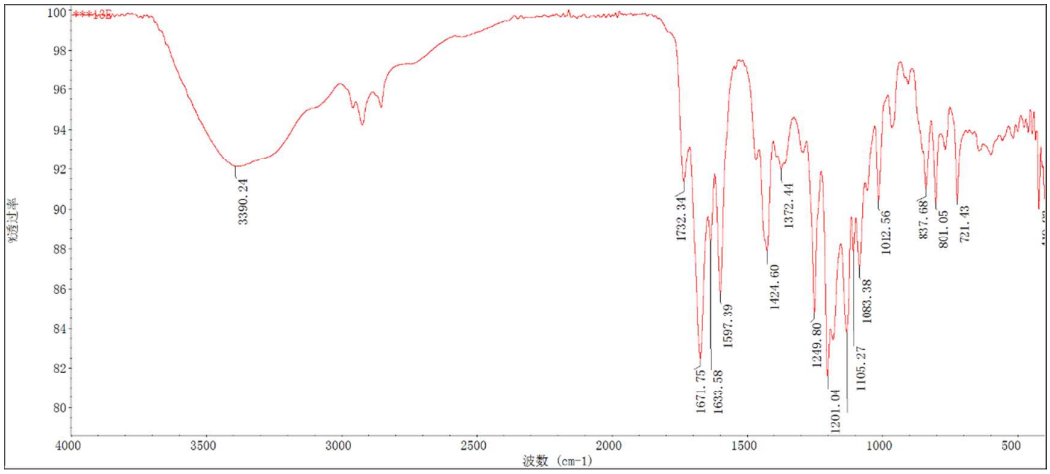


Figure S34. IR spectrum of **4**

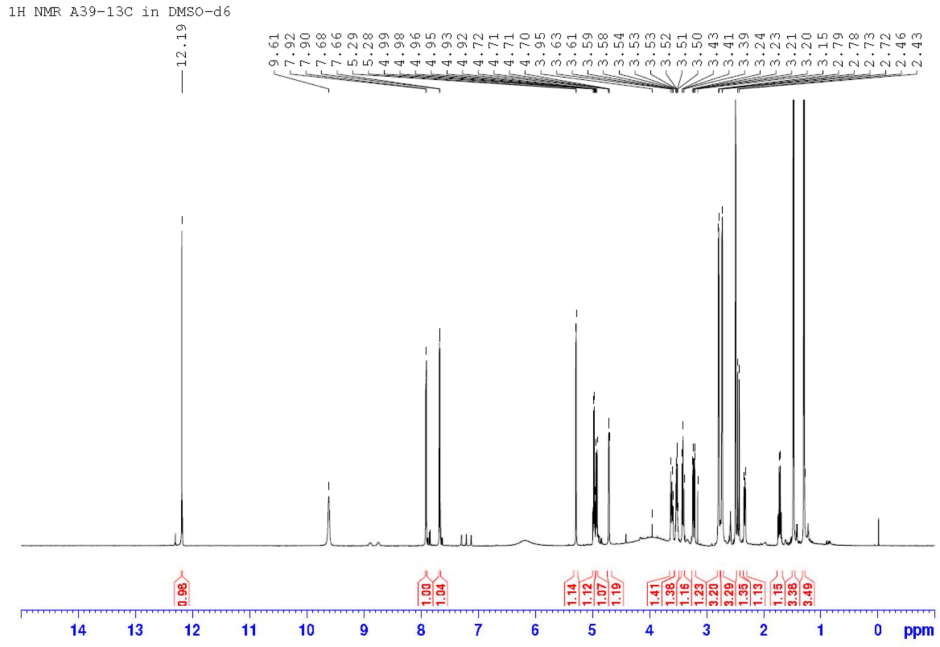


Figure S35. ^{1}H NMR spectrum of **5**

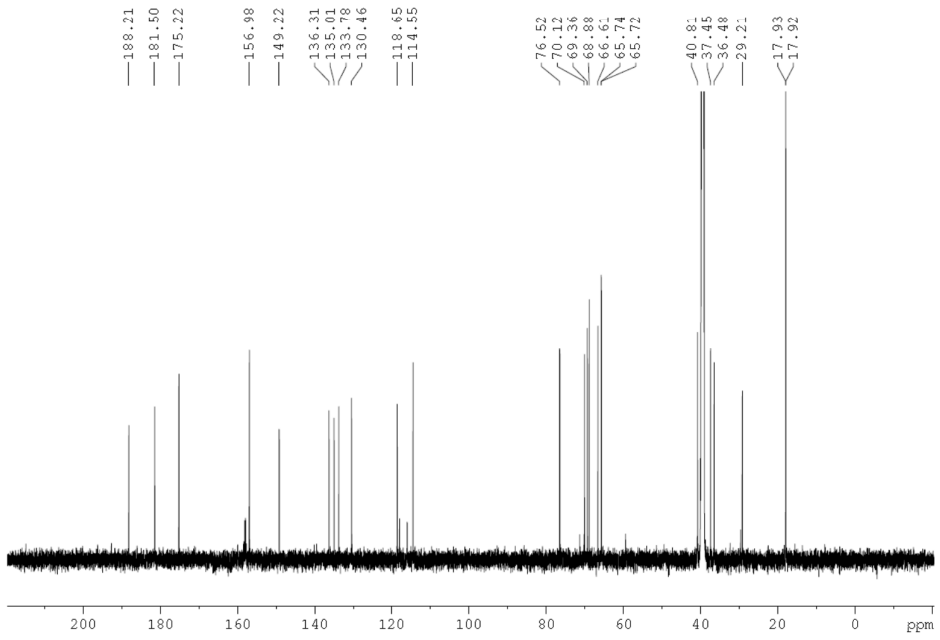


Figure S36. ^{13}C NMR spectrum of **5**

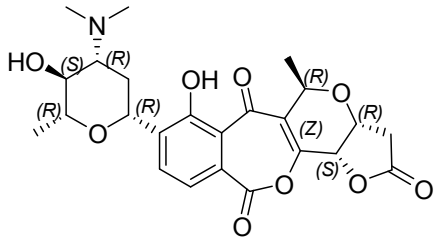
Quantum chemical calculations

ECD Calculation: The theoretical calculations of compounds **1-4** were performed using Gaussian 09 and figured using GaussView 5.0.[1-2] Conformational analysis of all of compounds were carried out via Monte Carlo searching using molecular mechanism with MMFF94 force field by means of the Spartan's 10 software.[3] The conformers with Boltzmann-population of over 5% were chosen for ECD calculations, and then the conformers were initially reoptimized using DFT at B3LYP/6-31+g (d, p) level in methanol in the Gaussian 09 program.[1] The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-311+g (d, p) level for all conformers of compounds in the Gaussian 09 program.[1] Rotatory strengths for a total of 50 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.[4]

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E) = \frac{1}{2.297\times10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2} \qquad (1)$$

The σ represented the width of the band at $1/e$ height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i, respectively. R_{vel} had been used in this work.



Strepoxepinmycin A (**1**)

Table S1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **1**.

Conformers	In MeOH	
	ΔG	P (%)
1-a	0	27.52
1-b	0.36	17.40
1-c	0	27.52

1-d	0	27.52
1-e	3.11	0.05

[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Table S2. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **1** at B3LYP/6-311+G(d,p) level of theory in CH_3OH.

1-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.493701	1.921537	0.210329
2.	6.	0.	1.782096	0.564396	0.262411
3.	6.	0.	0.749581	-0.359342	-0.017943
4.	6.	0.	-0.590265	0.074787	-0.262606
5.	6.	0.	-0.821268	1.476728	-0.372344
6.	6.	0.	0.221596	2.374326	-0.146721
7.	8.	0.	1.087913	-1.659655	-0.003177
8.	6.	0.	3.172102	0.052812	0.572973
9.	6.	0.	3.964925	-0.301224	-0.702833
10.	6.	0.	5.387718	-0.735835	-0.304935
11.	6.	0.	6.042074	0.355006	0.558828
12.	6.	0.	5.159801	0.665697	1.776572
13.	8.	0.	3.855469	1.063922	1.321100
14.	6.	0.	5.699254	1.793021	2.642128
15.	8.	0.	7.326769	-0.083902	0.997414
16.	7.	0.	6.310552	-1.130875	-1.385569
17.	6.	0.	6.403510	-0.189395	-2.505610
18.	6.	0.	6.088834	-2.496603	-1.864344
19.	6.	0.	-2.057672	2.119118	-0.890027
20.	8.	0.	-3.307392	1.593868	-0.668633

21.	6.	0.	-3.708270	0.438757	-0.061814
22.	6.	0.	-3.039057	-0.721763	0.064079
23.	6.	0.	-1.628547	-0.970349	-0.307734
24.	8.	0.	-1.301271	-2.162452	-0.505859
25.	8.	0.	-2.043643	3.167336	-1.500171
26.	6.	0.	-5.125300	0.612879	0.408968
27.	6.	0.	-5.718194	-0.624511	1.099558
28.	8.	0.	-5.193316	-1.806605	0.507244
29.	6.	0.	-3.773242	-1.949489	0.611985
30.	6.	0.	-3.334691	-2.324549	2.034416
31.	8.	0.	-5.990826	0.870735	-0.737325
32.	6.	0.	-7.185094	0.234851	-0.584088
33.	6.	0.	-7.190688	-0.534215	0.721986
34.	8.	0.	-8.063616	0.338020	-1.410938
35.	1.	0.	3.083115	-0.850727	1.194368
36.	1.	0.	2.280219	2.635263	0.425127
37.	1.	0.	0.036403	3.434702	-0.262979
38.	1.	0.	0.271468	-2.171540	-0.259286
39.	1.	0.	3.990982	0.581567	-1.351145
40.	1.	0.	3.449974	-1.101956	-1.242236
41.	1.	0.	5.299571	-1.622284	0.337946
42.	1.	0.	6.145369	1.284872	-0.022473
43.	1.	0.	5.063164	-0.252945	2.378194
44.	1.	0.	5.032806	1.972686	3.490890
45.	1.	0.	6.689015	1.531607	3.025273
46.	1.	0.	5.783344	2.717490	2.060601

47.	1.	0.	7.665130	-0.615104	0.251468
48.	1.	0.	7.253714	-0.470553	-3.134455
49.	1.	0.	5.501942	-0.180470	-3.140933
50.	1.	0.	6.577809	0.826287	-2.142540
51.	1.	0.	6.898369	-2.774655	-2.546412
52.	1.	0.	5.134894	-2.617486	-2.406723
53.	1.	0.	6.097757	-3.192870	-1.020866
54.	1.	0.	-5.174662	1.492226	1.060223
55.	1.	0.	-5.544435	-0.605198	2.179300
56.	1.	0.	-3.541670	-2.780467	-0.056723
57.	1.	0.	-3.883310	-3.213024	2.359414
58.	1.	0.	-2.266749	-2.557017	2.049223
59.	1.	0.	-3.513867	-1.515143	2.747787
60.	1.	0.	-7.759230	0.042131	1.460219
61.	1.	0.	-7.663097	-1.511248	0.609084

1-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-1.462662	2.081371	0.451680
2.	6.	0.	-1.778714	0.993693	-0.350489
3.	6.	0.	-0.734750	0.328920	-1.034136
4.	6.	0.	0.633991	0.707873	-0.860023
5.	6.	0.	0.900584	1.865377	-0.070618
6.	6.	0.	-0.146956	2.534945	0.562056
7.	8.	0.	-1.097684	-0.689184	-1.831904
8.	6.	0.	-3.201402	0.505748	-0.518211

9.	6.	0.	-3.495546	-0.746677	0.334028
10.	6.	0.	-4.975740	-1.133919	0.159296
11.	6.	0.	-5.870592	0.071485	0.489400
12.	6.	0.	-5.472700	1.277862	-0.373906
13.	8.	0.	-4.082630	1.573598	-0.155228
14.	6.	0.	-6.259125	2.538091	-0.050833
15.	8.	0.	-7.236460	-0.261657	0.247119
16.	7.	0.	-5.463231	-2.324059	0.880594
17.	6.	0.	-5.141683	-2.367049	2.310389
18.	6.	0.	-5.107448	-3.583305	0.223724
19.	6.	0.	2.201250	2.573191	0.045939
20.	8.	0.	3.407342	1.914865	0.006049
21.	6.	0.	3.732395	0.623344	-0.280900
22.	6.	0.	3.031822	-0.295090	-0.973085
23.	6.	0.	1.649265	-0.169752	-1.473723
24.	8.	0.	1.304358	-0.987953	-2.359032
25.	8.	0.	2.282720	3.768323	0.236533
26.	6.	0.	5.126964	0.375297	0.229858
27.	6.	0.	5.719663	-0.990894	-0.152691
28.	8.	0.	4.683698	-1.956605	-0.284698
29.	6.	0.	3.703437	-1.641198	-1.281366
30.	6.	0.	4.278265	-1.720954	-2.702754
31.	8.	0.	5.078402	0.387461	1.689452
32.	6.	0.	5.878613	-0.586306	2.204761
33.	6.	0.	6.540943	-1.352888	1.078228
34.	8.	0.	5.998479	-0.734072	3.400473

35.	1.	0.	-3.362306	0.256162	-1.577531
36.	1.	0.	-2.259289	2.606558	0.964921
37.	1.	0.	0.071413	3.427675	1.134084
38.	1.	0.	-0.263038	-1.009432	-2.279066
39.	1.	0.	-3.270833	-0.514145	1.380859
40.	1.	0.	-2.840028	-1.564455	0.020346
41.	1.	0.	-5.140660	-1.354202	-0.904427
42.	1.	0.	-5.739958	0.360416	1.544180
43.	1.	0.	-5.618122	1.009384	-1.433074
44.	1.	0.	-6.107537	2.828439	0.994447
45.	1.	0.	-5.936863	3.362754	-0.693449
46.	1.	0.	-7.326292	2.366047	-0.213357
47.	1.	0.	-7.297904	-1.206522	0.485397
48.	1.	0.	-5.721142	-3.168324	2.778965
49.	1.	0.	-4.074375	-2.561361	2.509319
50.	1.	0.	-5.416653	-1.427694	2.796177
51.	1.	0.	-5.625009	-4.408402	0.722869
52.	1.	0.	-4.024963	-3.798101	0.252598
53.	1.	0.	-5.427480	-3.561190	-0.821962
54.	1.	0.	5.779225	1.196731	-0.081508
55.	1.	0.	6.319874	-0.923948	-1.064167
56.	1.	0.	2.949384	-2.422536	-1.164831
57.	1.	0.	4.769857	-2.689094	-2.838299
58.	1.	0.	3.469008	-1.633595	-3.429527
59.	1.	0.	5.000667	-0.924670	-2.903004
60.	1.	0.	7.575987	-1.005906	0.986756

61.	1.	0.	6.554610	-2.425368	1.279269

1-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.493871	1.921622	0.209248
2.	6.	0.	1.782187	0.564487	0.262021
3.	6.	0.	0.749635	-0.359324	-0.017934
4.	6.	0.	-0.590198	0.074708	-0.262649
5.	6.	0.	-0.821203	1.476605	-0.372877
6.	6.	0.	0.221744	2.374284	-0.147876
7.	8.	0.	1.088024	-1.659646	-0.002706
8.	6.	0.	3.172172	0.053027	0.572862
9.	6.	0.	3.965129	-0.301358	-0.702767
10.	6.	0.	5.387902	-0.735793	-0.304573
11.	6.	0.	6.042100	0.355366	0.558933
12.	6.	0.	5.159701	0.666322	1.776497
13.	8.	0.	3.855423	1.064390	1.320737
14.	6.	0.	5.699020	1.793857	2.641866
15.	8.	0.	7.326801	-0.083318	0.997731
16.	7.	0.	6.310889	-1.131127	-1.384962
17.	6.	0.	6.403920	-0.190038	-2.505311
18.	6.	0.	6.089384	-2.497042	-1.863291
19.	6.	0.	-2.057852	2.118936	-0.890013
20.	8.	0.	-3.307551	1.594403	-0.666753
21.	6.	0.	-3.708285	0.438724	-0.061048
22.	6.	0.	-3.039073	-0.721938	0.063847

23.	6.	0.	-1.628521	-0.970424	-0.307802
24.	8.	0.	-1.301182	-2.162511	-0.505976
25.	8.	0.	-2.044112	3.166731	-1.500879
26.	6.	0.	-5.125302	0.612522	0.409964
27.	6.	0.	-5.718361	-0.625475	1.099309
28.	8.	0.	-5.193514	-1.807016	0.505850
29.	6.	0.	-3.773450	-1.950088	0.610659
30.	6.	0.	-3.335194	-2.326334	2.032859
31.	8.	0.	-5.990788	0.871679	-0.736058
32.	6.	0.	-7.185192	0.235889	-0.583420
33.	6.	0.	-7.190830	-0.534701	0.721754
34.	8.	0.	-8.063768	0.340208	-1.410062
35.	1.	0.	3.083149	-0.850334	1.194500
36.	1.	0.	2.280411	2.635452	0.423620
37.	1.	0.	0.036565	3.434618	-0.264513
38.	1.	0.	0.271722	-2.171668	-0.258728
39.	1.	0.	3.991231	0.581249	-1.351325
40.	1.	0.	3.450285	-1.102270	-1.242006
41.	1.	0.	5.299713	-1.622033	0.338580
42.	1.	0.	6.145366	1.285073	-0.022634
43.	1.	0.	5.063014	-0.252178	2.378336
44.	1.	0.	5.783171	2.718212	2.060165
45.	1.	0.	5.032458	1.973678	3.490503
46.	1.	0.	6.688739	1.532537	3.025181
47.	1.	0.	7.665288	-0.614591	0.251885
48.	1.	0.	7.254213	-0.471369	-3.133960

49.	1.	0.	5.502428	-0.181388	-3.140747
50.	1.	0.	6.578117	0.825780	-2.142574
51.	1.	0.	6.899099	-2.775293	-2.545065
52.	1.	0.	5.135571	-2.618198	-2.405838
53.	1.	0.	6.098151	-3.192994	-1.019554
54.	1.	0.	-5.174483	1.491246	1.062077
55.	1.	0.	-5.544683	-0.607250	2.179082
56.	1.	0.	-3.541883	-2.780531	-0.058707
57.	1.	0.	-3.884045	-3.214951	2.357073
58.	1.	0.	-2.267303	-2.558990	2.047658
59.	1.	0.	-3.514342	-1.517441	2.746823
60.	1.	0.	-7.759429	0.040738	1.460651
61.	1.	0.	-7.663245	-1.511591	0.607646

1-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.493931	1.921664	0.209427
2.	6.	0.	1.782218	0.564522	0.262162
3.	6.	0.	0.749617	-0.359241	-0.017740
4.	6.	0.	-0.590226	0.074849	-0.262388
5.	6.	0.	-0.821189	1.476759	-0.372629
6.	6.	0.	0.221806	2.374382	-0.147632
7.	8.	0.	1.087887	-1.659576	-0.002632
8.	6.	0.	3.172197	0.052991	0.572878
9.	6.	0.	3.965040	-0.301426	-0.702794
10.	6.	0.	5.387808	-0.735940	-0.304724

11.	6.	0.	6.042149	0.355166	0.558754
12.	6.	0.	5.159862	0.666133	1.776408
13.	8.	0.	3.855577	1.064316	1.320733
14.	6.	0.	5.699314	1.793601	2.641781
15.	8.	0.	7.326876	-0.083594	0.997359
16.	7.	0.	6.310690	-1.131274	-1.385196
17.	6.	0.	6.403807	-0.190038	-2.505429
18.	6.	0.	6.088986	-2.497104	-1.863701
19.	6.	0.	-2.057779	2.119115	-0.889869
20.	8.	0.	-3.307516	1.594475	-0.666970
21.	6.	0.	-3.708328	0.438892	-0.061132
22.	6.	0.	-3.039127	-0.721737	0.064102
23.	6.	0.	-1.628545	-0.970283	-0.307375
24.	8.	0.	-1.301190	-2.162437	-0.505200
25.	8.	0.	-2.043985	3.166976	-1.500612
26.	6.	0.	-5.125418	0.612749	0.409642
27.	6.	0.	-5.718445	-0.625021	1.099386
28.	8.	0.	-5.193583	-1.806729	0.506296
29.	6.	0.	-3.773515	-1.949768	0.611161
30.	6.	0.	-3.335258	-2.325663	2.033457
31.	8.	0.	-5.990793	0.871307	-0.736631
32.	6.	0.	-7.185007	0.235222	-0.584058
33.	6.	0.	-7.190916	-0.534357	0.721722
34.	8.	0.	-8.063267	0.338629	-1.411163
35.	1.	0.	3.083181	-0.850374	1.194509
36.	1.	0.	2.280499	2.635468	0.423788

37.	1.	0.	0.036674	3.434724	-0.264263
38.	1.	0.	0.271303	-2.171415	-0.258519
39.	1.	0.	3.991139	0.581167	-1.351374
40.	1.	0.	3.450096	-1.102308	-1.241991
41.	1.	0.	5.299648	-1.622194	0.338418
42.	1.	0.	6.145370	1.284909	-0.022769
43.	1.	0.	5.063133	-0.252376	2.378225
44.	1.	0.	5.032818	1.973441	3.490465
45.	1.	0.	6.689039	1.532185	3.025020
46.	1.	0.	5.783503	2.717963	2.060099
47.	1.	0.	7.665079	-0.615150	0.251578
48.	1.	0.	7.254052	-0.471391	-3.134131
49.	1.	0.	5.502297	-0.181200	-3.140836
50.	1.	0.	6.578129	0.825702	-2.142540
51.	1.	0.	6.898678	-2.775383	-2.545489
52.	1.	0.	5.135170	-2.618033	-2.406289
53.	1.	0.	6.097623	-3.193153	-1.020044
54.	1.	0.	-5.174782	1.491752	1.061358
55.	1.	0.	-5.544815	-0.606460	2.179161
56.	1.	0.	-3.541929	-2.780367	-0.058003
57.	1.	0.	-3.884128	-3.214184	2.357900
58.	1.	0.	-2.267374	-2.558365	2.048276
59.	1.	0.	-3.514355	-1.516582	2.747218
60.	1.	0.	-7.759246	0.041993	1.460130
61.	1.	0.	-7.663599	-1.511214	0.608562

1-e		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.453777	2.009704	0.106241
2.	6.	0.	1.722392	0.659833	0.285989
3.	6.	0.	0.656174	-0.263003	0.172118
4.	6.	0.	-0.684305	0.174836	-0.050378
5.	6.	0.	-0.898966	1.561501	-0.309907
6.	6.	0.	0.170517	2.451853	-0.227208
7.	8.	0.	0.967228	-1.561012	0.325415
8.	6.	0.	3.118127	0.146792	0.565835
9.	6.	0.	3.795401	-0.424566	-0.697513
10.	6.	0.	5.227267	-0.861796	-0.339932
11.	6.	0.	5.985682	0.314701	0.294228
12.	6.	0.	5.213880	0.847306	1.511549
13.	8.	0.	3.889029	1.227741	1.099804
14.	6.	0.	5.856934	2.068104	2.149129
15.	8.	0.	7.284618	-0.112794	0.701053
16.	7.	0.	6.047937	-1.462486	-1.407951
17.	6.	0.	6.084166	-0.712185	-2.667065
18.	6.	0.	5.743026	-2.874613	-1.645840
19.	6.	0.	-2.138114	2.161618	-0.873378
20.	8.	0.	-3.356155	1.522871	-0.825144
21.	6.	0.	-3.810713	0.557779	0.033280
22.	6.	0.	-3.120623	-0.484180	0.528220
23.	6.	0.	-1.742072	-0.833621	0.121336
24.	8.	0.	-1.469365	-2.053329	0.064830

25.	8.	0.	-2.142575	3.224319	-1.459218
26.	6.	0.	-5.293408	0.750563	0.245625
27.	6.	0.	-5.939093	-0.452413	0.962921
28.	8.	0.	-5.072914	-1.012122	1.924468
29.	6.	0.	-3.801445	-1.485656	1.468261
30.	6.	0.	-2.999474	-1.752712	2.742971
31.	8.	0.	-5.957016	0.812840	-1.048155
32.	6.	0.	-6.579851	-0.366173	-1.340328
33.	6.	0.	-6.397783	-1.346173	-0.200728
34.	8.	0.	-7.170918	-0.514768	-2.385325
35.	1.	0.	3.052862	-0.651490	1.320732
36.	1.	0.	2.263717	2.723635	0.196972
37.	1.	0.	-0.000327	3.497046	-0.451370
38.	1.	0.	0.126901	-2.079100	0.188870
39.	1.	0.	3.801933	0.353453	-1.468909
40.	1.	0.	3.212288	-1.270328	-1.073232
41.	1.	0.	5.156543	-1.634171	0.438209
42.	1.	0.	6.076499	1.139490	-0.429951
43.	1.	0.	5.136824	0.036335	2.254130
44.	1.	0.	5.264659	2.406379	3.004498
45.	1.	0.	6.863389	1.822745	2.497966
46.	1.	0.	5.928172	2.887638	1.425864
47.	1.	0.	7.541959	-0.769748	0.026207
48.	1.	0.	6.867485	-1.130965	-3.306021
49.	1.	0.	5.133560	-0.756239	-3.224439
50.	1.	0.	6.327719	0.337303	-2.484383

51.	1.	0.	6.487959	-3.293359	-2.329663
52.	1.	0.	4.746794	-3.035545	-2.093613
53.	1.	0.	5.792773	-3.429531	-0.704632
54.	1.	0.	-5.484869	1.704991	0.740375
55.	1.	0.	-6.807044	-0.110366	1.529697
56.	1.	0.	-3.936364	-2.430216	0.924438
57.	1.	0.	-3.573827	-2.427314	3.383531
58.	1.	0.	-2.043073	-2.224941	2.515993
59.	1.	0.	-2.823087	-0.819207	3.285382
60.	1.	0.	-7.321565	-1.892913	-0.007621
61.	1.	0.	-5.631858	-2.071107	-0.497736

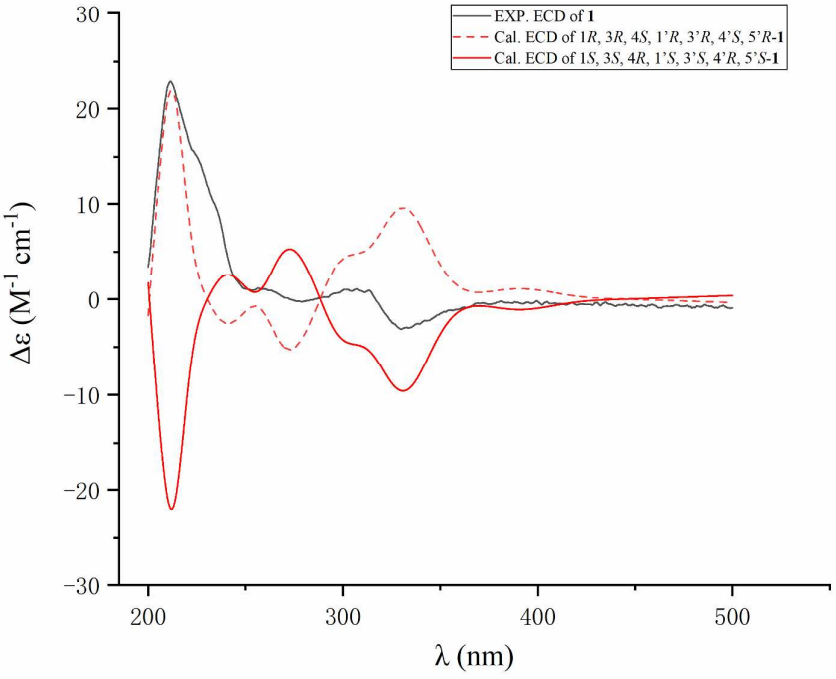
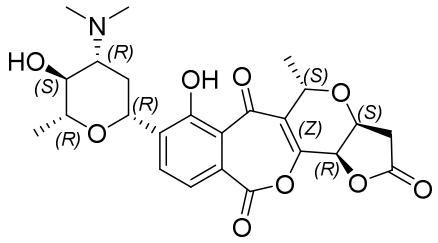


Figure S37. Comparison of the calculated ECD spectra for 1*R*, 3*R*, 4*S*, 1′*R*, 3′*R*, 4′*S*, 5′*R* and its enantiomer with the experimental spectrum of **1**.



E-1

Table S3. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **E-1**.

Conformers	In MeOH	
	ΔG	P (%)
E-1-a	0	49.96
E-1-b	0.02	49.94
E-1-c	1.13	0.09
E-1-d	1.87	0.00
E-1-e	1.91	0.00

[a] B3LYP/6-31+G(d,p), in kcal/mol. [b] From ΔG values at 298.15K.

Table S4. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **E-1** at B3LYP/6-311+G(d,p) level of theory in CH_3OH.

E-1-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.544860	-2.091123	0.466523
2.	6.	0.	1.839454	-0.971150	-0.294864
3.	6.	0.	0.773392	-0.216790	-0.836671
4.	6.	0.	-0.590062	-0.544496	-0.553215
5.	6.	0.	-0.841983	-1.732930	0.192343
6.	6.	0.	0.224035	-2.488233	0.678054

7.	8.	0.	1.114562	0.827553	-1.603096
8.	6.	0.	3.264262	-0.542779	-0.571597
9.	6.	0.	3.686551	0.671026	0.284357
10.	6.	0.	5.166780	0.985872	0.007149
11.	6.	0.	6.022490	-0.270997	0.232745
12.	6.	0.	5.493881	-1.421775	-0.634593
13.	8.	0.	4.115843	-1.659268	-0.315748
14.	6.	0.	6.238900	-2.728653	-0.418443
15.	8.	0.	7.373640	0.003986	-0.103776
16.	7.	0.	5.775665	2.124706	0.718325
17.	6.	0.	5.559184	2.141690	2.166846
18.	6.	0.	5.446097	3.419202	0.122903
19.	6.	0.	-2.158442	-2.390377	0.402981
20.	8.	0.	-3.334913	-1.679637	0.494412
21.	6.	0.	-3.627737	-0.367608	0.285918
22.	6.	0.	-2.943534	0.562024	-0.406305
23.	6.	0.	-1.607070	0.415447	-1.018491
24.	8.	0.	-1.301174	1.269031	-1.883332
25.	8.	0.	-2.275216	-3.583186	0.567632
26.	6.	0.	-4.964870	-0.085721	0.918354
27.	6.	0.	-5.439012	1.367782	0.772498
28.	8.	0.	-5.010166	1.885810	-0.477865
29.	6.	0.	-3.593408	1.929342	-0.648257
30.	6.	0.	-2.947742	3.049886	0.177702
31.	8.	0.	-5.980606	-0.894100	0.262868
32.	6.	0.	-7.135038	-0.181077	0.112900

33.	6.	0.	-6.950722	1.206315	0.700242
34.	8.	0.	-8.111943	-0.667059	-0.401623
35.	1.	0.	3.343095	-0.260998	-1.633287
36.	1.	0.	2.360324	-2.682684	0.864371
37.	1.	0.	0.011082	-3.404771	1.212581
38.	1.	0.	0.256469	1.206116	-1.950805
39.	1.	0.	3.531466	0.420472	1.339281
40.	1.	0.	3.049427	1.526632	0.042541
41.	1.	0.	5.264839	1.227380	-1.060198
42.	1.	0.	5.941817	-0.592080	1.285502
43.	1.	0.	5.575151	-1.117237	-1.691425
44.	1.	0.	5.831306	-3.512791	-1.062470
45.	1.	0.	7.298187	-2.597449	-0.651412
46.	1.	0.	6.148264	-3.052112	0.623725
47.	1.	0.	7.481804	0.938516	0.157682
48.	1.	0.	6.207874	2.901020	2.614027
49.	1.	0.	4.520415	2.377016	2.451125
50.	1.	0.	5.823143	1.176810	2.606359
51.	1.	0.	4.383562	3.695611	0.233399
52.	1.	0.	5.689068	3.410718	-0.943420
53.	1.	0.	6.043616	4.200416	0.603057
54.	1.	0.	-4.924155	-0.388000	1.970534
55.	1.	0.	-5.103014	1.987835	1.609329
56.	1.	0.	-3.457470	2.156974	-1.707283
57.	1.	0.	-1.894432	3.154223	-0.091871
58.	1.	0.	-3.454151	3.995042	-0.035601

59.	1.	0.	-3.004445	2.852546	1.251620
60.	1.	0.	-7.431167	1.969294	0.086740
61.	1.	0.	-7.403535	1.224276	1.697376

E-1-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.544857	-2.091339	0.466472
2.	6.	0.	1.839427	-0.971255	-0.294783
3.	6.	0.	0.773353	-0.216869	-0.836512
4.	6.	0.	-0.590114	-0.544609	-0.553087
5.	6.	0.	-0.842000	-1.733096	0.192371
6.	6.	0.	0.224049	-2.488457	0.677978
7.	8.	0.	1.114548	0.827546	-1.602833
8.	6.	0.	3.264229	-0.542827	-0.571503
9.	6.	0.	3.686549	0.671029	0.284351
10.	6.	0.	5.166737	0.985932	0.006954
11.	6.	0.	6.022518	-0.270868	0.232615
12.	6.	0.	5.493901	-1.421766	-0.634555
13.	8.	0.	4.115882	-1.659263	-0.315607
14.	6.	0.	6.238959	-2.728596	-0.418271
15.	8.	0.	7.373641	0.004146	-0.104042
16.	7.	0.	5.775651	2.124839	0.717989
17.	6.	0.	5.559500	2.141781	2.166549
18.	6.	0.	5.445861	3.419310	0.122627
19.	6.	0.	-2.158435	-2.390512	0.403191
20.	8.	0.	-3.334937	-1.679739	0.494368

21.	6.	0.	-3.627799	-0.367744	0.285933
22.	6.	0.	-2.943558	0.561979	-0.406142
23.	6.	0.	-1.607127	0.415358	-1.018373
24.	8.	0.	-1.301230	1.268924	-1.883218
25.	8.	0.	-2.275261	-3.583267	0.568147
26.	6.	0.	-4.965024	-0.085925	0.918208
27.	6.	0.	-5.438993	1.367658	0.772757
28.	8.	0.	-5.010087	1.885966	-0.477468
29.	6.	0.	-3.593334	1.929371	-0.647901
30.	6.	0.	-2.947527	3.049674	0.178281
31.	8.	0.	-5.980721	-0.893952	0.262199
32.	6.	0.	-7.135070	-0.180755	0.112357
33.	6.	0.	-6.950713	1.206337	0.700400
34.	8.	0.	-8.111919	-0.666384	-0.402606
35.	1.	0.	3.343040	-0.261122	-1.633222
36.	1.	0.	2.360357	-2.682904	0.864231
37.	1.	0.	0.011064	-3.405014	1.212456
38.	1.	0.	0.256507	1.206060	-1.950646
39.	1.	0.	3.531615	0.420470	1.339297
40.	1.	0.	3.049367	1.526610	0.042617
41.	1.	0.	5.264666	1.227344	-1.060426
42.	1.	0.	5.941952	-0.591811	1.285420
43.	1.	0.	5.575113	-1.117353	-1.691424
44.	1.	0.	5.831362	-3.512829	-1.062180
45.	1.	0.	7.298236	-2.597408	-0.651297
46.	1.	0.	6.148370	-3.051916	0.623943

47.	1.	0.	7.481799	0.938698	0.157342
48.	1.	0.	6.207837	2.901536	2.613516
49.	1.	0.	4.520666	2.376503	2.451080
50.	1.	0.	5.824162	1.177088	2.606061
51.	1.	0.	4.383360	3.695718	0.233461
52.	1.	0.	5.688449	3.410772	-0.943783
53.	1.	0.	6.043538	4.200552	0.602538
54.	1.	0.	-4.924576	-0.388597	1.970282
55.	1.	0.	-5.102962	1.987466	1.609761
56.	1.	0.	-3.457397	2.157182	-1.706887
57.	1.	0.	-3.004309	2.852107	1.252152
58.	1.	0.	-1.894190	3.153888	-0.091236
59.	1.	0.	-3.453767	3.994959	-0.034845
60.	1.	0.	-7.431131	1.969651	0.087296
61.	1.	0.	-7.403503	1.223792	1.697554

E-1-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.450682	-2.050558	0.621520
2.	6.	0.	1.725701	-0.975481	-0.208673
3.	6.	0.	0.645435	-0.219585	-0.721480
4.	6.	0.	-0.703099	-0.506115	-0.347726
5.	6.	0.	-0.942287	-1.659950	0.456122
6.	6.	0.	0.135350	-2.408958	0.923889
7.	8.	0.	0.959771	0.790840	-1.543096
8.	6.	0.	3.140937	-0.592686	-0.582467

9.	6.	0.	3.634309	0.644680	0.198667
10.	6.	0.	5.102795	0.915455	-0.171733
11.	6.	0.	5.943451	-0.350501	0.060020
12.	6.	0.	5.345487	-1.522680	-0.730196
13.	8.	0.	3.982195	-1.717116	-0.328516
14.	6.	0.	6.074807	-2.836228	-0.501189
15.	8.	0.	7.280087	-0.120074	-0.357778
16.	7.	0.	5.772649	2.068308	0.456424
17.	6.	0.	5.645663	2.144710	1.913439
18.	6.	0.	5.431280	3.345496	-0.168658
19.	6.	0.	-2.260417	-2.300168	0.714144
20.	8.	0.	-3.455474	-1.648427	0.489590
21.	6.	0.	-3.740284	-0.312245	0.476740
22.	6.	0.	-2.979283	0.686074	-0.003717
23.	6.	0.	-1.711473	0.491826	-0.737671
24.	8.	0.	-1.463918	1.322879	-1.639862
25.	8.	0.	-2.370545	-3.448174	1.081214
26.	6.	0.	-5.152815	-0.113707	0.974174
27.	6.	0.	-5.666727	1.312739	0.695624
28.	8.	0.	-4.652081	2.274170	0.857316
29.	6.	0.	-3.481892	2.133054	0.050570
30.	6.	0.	-2.463466	3.091924	0.669900
31.	8.	0.	-6.043579	-0.985878	0.233790
32.	6.	0.	-6.712877	-0.292013	-0.737880
33.	6.	0.	-6.323313	1.172705	-0.686459
34.	8.	0.	-7.483605	-0.848077	-1.479281

35.	1.	0.	3.165564	-0.355343	-1.657635
36.	1.	0.	2.275184	-2.641541	1.001279
37.	1.	0.	-0.065364	-3.298819	1.505939
38.	1.	0.	0.093267	1.187563	-1.843043
39.	1.	0.	3.532614	0.439328	1.269836
40.	1.	0.	3.001796	1.503828	-0.042784
41.	1.	0.	5.145768	1.110720	-1.252134
42.	1.	0.	5.911952	-0.627435	1.127825
43.	1.	0.	5.374857	-1.262144	-1.801314
44.	1.	0.	7.122411	-2.737838	-0.795109
45.	1.	0.	6.033898	-3.116530	0.556485
46.	1.	0.	5.617602	-3.635872	-1.090505
47.	1.	0.	7.419899	0.822768	-0.145724
48.	1.	0.	6.332424	2.908777	2.290064
49.	1.	0.	4.630128	2.409481	2.250867
50.	1.	0.	5.921020	1.192656	2.373325
51.	1.	0.	4.383702	3.649627	-0.002300
52.	1.	0.	5.605158	3.289815	-1.246998
53.	1.	0.	6.073730	4.131273	0.240876
54.	1.	0.	-5.225992	-0.403183	2.024825
55.	1.	0.	-6.426335	1.570731	1.436654
56.	1.	0.	-3.696929	2.453609	-0.977968
57.	1.	0.	-1.558696	3.149717	0.064803
58.	1.	0.	-2.908325	4.088555	0.727412
59.	1.	0.	-2.203977	2.766421	1.681000
60.	1.	0.	-5.618910	1.368446	-1.502302

61.	1.	0.	-7.195580	1.809377	-0.837116

E-1-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.544840	-2.091323	0.466565
2.	6.	0.	1.839401	-0.971255	-0.294728
3.	6.	0.	0.773325	-0.216915	-0.836502
4.	6.	0.	-0.590136	-0.544702	-0.553129
5.	6.	0.	-0.842008	-1.733177	0.192339
6.	6.	0.	0.224045	-2.488491	0.678020
7.	8.	0.	1.114485	0.827497	-1.602851
8.	6.	0.	3.264204	-0.542821	-0.571442
9.	6.	0.	3.686533	0.671081	0.284347
10.	6.	0.	5.166721	0.985959	0.006936
11.	6.	0.	6.022488	-0.270834	0.232709
12.	6.	0.	5.493888	-1.421770	-0.634424
13.	8.	0.	4.115852	-1.659247	-0.315499
14.	6.	0.	6.238926	-2.728593	-0.418040
15.	8.	0.	7.373633	0.004154	-0.103882
16.	7.	0.	5.775632	2.124920	0.717876
17.	6.	0.	5.559424	2.142009	2.166426
18.	6.	0.	5.445899	3.419341	0.122377
19.	6.	0.	-2.158405	-2.390658	0.402987
20.	8.	0.	-3.334904	-1.679844	0.494374
21.	6.	0.	-3.627773	-0.367877	0.285950
22.	6.	0.	-2.943587	0.561858	-0.406187

23.	6.	0.	-1.607171	0.415253	-1.018439
24.	8.	0.	-1.301266	1.268803	-1.883286
25.	8.	0.	-2.275248	-3.583434	0.567684
26.	6.	0.	-4.964963	-0.086017	0.918259
27.	6.	0.	-5.438808	1.367593	0.773026
28.	8.	0.	-5.010114	1.885891	-0.477310
29.	6.	0.	-3.593373	1.929234	-0.647976
30.	6.	0.	-2.947471	3.049653	0.177969
31.	8.	0.	-5.980760	-0.893827	0.262070
32.	6.	0.	-7.135033	-0.180481	0.112426
33.	6.	0.	-6.950549	1.206396	0.700951
34.	8.	0.	-8.111917	-0.665849	-0.402722
35.	1.	0.	3.343014	-0.261160	-1.633177
36.	1.	0.	2.360348	-2.682836	0.864385
37.	1.	0.	0.011070	-3.405048	1.212510
38.	1.	0.	0.256392	1.205933	-1.950664
39.	1.	0.	3.531612	0.420585	1.339311
40.	1.	0.	3.049346	1.526643	0.042567
41.	1.	0.	5.264664	1.227281	-1.060462
42.	1.	0.	5.941861	-0.591731	1.285525
43.	1.	0.	5.575128	-1.117419	-1.691307
44.	1.	0.	7.298221	-2.597399	-0.650982
45.	1.	0.	6.148249	-3.051874	0.624178
46.	1.	0.	5.831390	-3.512851	-1.061957
47.	1.	0.	7.481757	0.938752	0.157367
48.	1.	0.	6.207818	2.901731	2.613365

49.	1.	0.	4.520598	2.376863	2.450884
50.	1.	0.	5.823957	1.177322	2.606028
51.	1.	0.	4.383406	3.695794	0.233170
52.	1.	0.	5.688505	3.410681	-0.944027
53.	1.	0.	6.043598	4.200607	0.602220
54.	1.	0.	-4.924586	-0.388895	1.970276
55.	1.	0.	-5.102543	1.987370	1.609953
56.	1.	0.	-3.457600	2.156922	-1.707013
57.	1.	0.	-1.894160	3.153843	-0.091649
58.	1.	0.	-3.453751	3.994893	-0.035258
59.	1.	0.	-3.004161	2.852252	1.251875
60.	1.	0.	-7.431143	1.969987	0.088342
61.	1.	0.	-7.403007	1.223381	1.698269

E-1-e		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.378040	-1.798366	0.653462
2.	6.	0.	1.687173	-0.600740	0.028436
3.	6.	0.	0.702463	0.412224	-0.028698
4.	6.	0.	-0.619758	0.194779	0.472625
5.	6.	0.	-0.871940	-1.031609	1.155074
6.	6.	0.	0.129562	-1.997187	1.244038
7.	8.	0.	1.070018	1.564085	-0.604166
8.	6.	0.	3.055541	-0.336042	-0.560678
9.	6.	0.	3.939126	0.515633	0.375983
10.	6.	0.	5.335345	0.663136	-0.253223

11.	6.	0.	5.914963	-0.723360	-0.575616
12.	6.	0.	4.942163	-1.496080	-1.477380
13.	8.	0.	3.670028	-1.598001	-0.822701
14.	6.	0.	5.405916	-2.909504	-1.788431
15.	8.	0.	7.165971	-0.578437	-1.230149
16.	7.	0.	6.342097	1.456648	0.474646
17.	6.	0.	6.516398	1.100980	1.884693
18.	6.	0.	6.162978	2.899342	0.316417
19.	6.	0.	-2.076832	-1.375451	1.954312
20.	8.	0.	-3.329545	-0.884184	1.657088
21.	6.	0.	-3.758492	0.022423	0.737895
22.	6.	0.	-3.068888	0.993552	0.111275
23.	6.	0.	-1.616307	1.239069	0.170524
24.	8.	0.	-1.232990	2.365595	-0.223599
25.	8.	0.	-2.046828	-2.145933	2.886647
26.	6.	0.	-5.244170	-0.165550	0.567213
27.	6.	0.	-5.926742	0.891324	-0.318113
28.	8.	0.	-5.022271	1.354480	-1.309774
29.	6.	0.	-3.842509	1.969187	-0.787144
30.	6.	0.	-4.141740	3.309381	-0.101466
31.	8.	0.	-5.454403	-1.438252	-0.107472
32.	6.	0.	-6.446894	-1.332069	-1.038530
33.	6.	0.	-7.003593	0.078938	-1.023257
34.	8.	0.	-6.781077	-2.276009	-1.711219
35.	1.	0.	2.928607	0.210460	-1.508125
36.	1.	0.	2.130520	-2.576545	0.696441

37.	1.	0.	-0.073869	-2.907899	1.792027
38.	1.	0.	0.276249	2.170944	-0.537437
39.	1.	0.	3.998047	0.011537	1.346770
40.	1.	0.	3.470908	1.492228	0.529605
41.	1.	0.	5.215410	1.170127	-1.220684
42.	1.	0.	6.028212	-1.305531	0.355045
43.	1.	0.	4.823504	-0.928668	-2.415639
44.	1.	0.	5.504829	-3.491504	-0.866205
45.	1.	0.	4.688433	-3.413383	-2.441939
46.	1.	0.	6.377227	-2.881156	-2.287771
47.	1.	0.	7.541261	0.223449	-0.818401
48.	1.	0.	7.408122	1.604635	2.270045
49.	1.	0.	5.664014	1.395098	2.518945
50.	1.	0.	6.668074	0.024518	1.994057
51.	1.	0.	5.256251	3.285149	0.812949
52.	1.	0.	6.106798	3.153176	-0.745888
53.	1.	0.	7.024186	3.420042	0.746741
54.	1.	0.	-5.715440	-0.228387	1.553036
55.	1.	0.	-6.327487	1.714762	0.280241
56.	1.	0.	-3.227555	2.161011	-1.669586
57.	1.	0.	-3.205061	3.814951	0.136079
58.	1.	0.	-4.723124	3.940637	-0.779673
59.	1.	0.	-4.702252	3.179381	0.828146
60.	1.	0.	-7.213564	0.438402	-2.031335
61.	1.	0.	-7.939020	0.075218	-0.453674

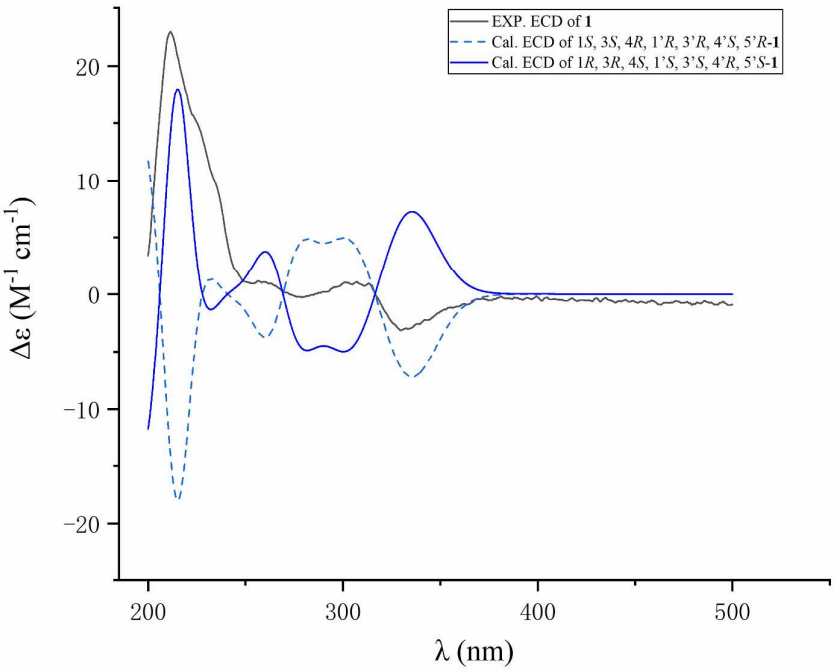
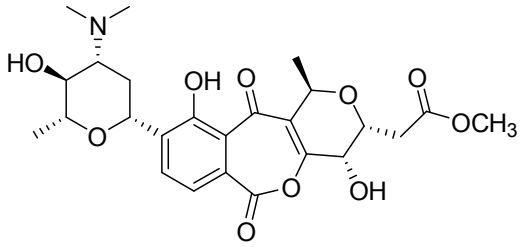


Figure S38. Comparison of the calculated ECD spectra for 1*S*, 3*S*, 4*R*, 1′*R*, 3′*R*, 4′*S*, 5′*R* and its enantiomer with the experimental spectrum of **1**.



Strepoxepinmycin B (**2**)

Table S5. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**.

Conformers	In MeOH	
	Δ*G*	*P* (%)
2-a	1.12	6.25

2-b	0.09	38.12
2-c	1.12	6.25
2-d	0	43.97
2-e	1.57	5.41

[a] B3LYP/6-31+G (d, p), in kcal/mol. [b] From Δ*G* values at 298.15K.

Table S6. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **2** at B3LYP/6-311+G (d, p) level of theory in CH_3OH.

2-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.093528	-1.939190	-0.211321
2.	6.	0.	-2.406504	-0.633050	0.132211
3.	6.	0.	-1.421990	0.368484	-0.028403
4.	6.	0.	-0.095900	0.046534	-0.456256
5.	6.	0.	0.160845	-1.298814	-0.848011
6.	6.	0.	-0.840411	-2.262322	-0.732062
7.	8.	0.	-1.793801	1.620494	0.271116
8.	6.	0.	-3.779969	-0.246570	0.637105
9.	6.	0.	-4.647183	0.401162	-0.464358
10.	6.	0.	-6.051087	0.677430	0.101718
11.	6.	0.	-6.642184	-0.614050	0.689970
12.	6.	0.	-5.686464	-1.189184	1.744203
13.	8.	0.	-4.406306	-1.425761	1.142780
14.	6.	0.	-6.161402	-2.509102	2.329264
15.	8.	0.	-7.902363	-0.337981	1.281574
16.	7.	0.	-7.044445	1.305920	-0.788214

17.	6.	0.	-7.186306	0.679955	-2.104565
18.	6.	0.	-6.878327	2.753632	-0.910526
19.	6.	0.	1.374293	-1.803995	-1.540588
20.	8.	0.	2.621834	-1.265748	-1.323928
21.	6.	0.	3.049721	-0.171248	-0.629942
22.	6.	0.	2.350035	0.917776	-0.258530
23.	6.	0.	0.898729	1.135764	-0.395038
24.	8.	0.	0.504163	2.322710	-0.304330
25.	8.	0.	1.353913	-2.753981	-2.290259
26.	6.	0.	4.549197	-0.317178	-0.456355
27.	6.	0.	5.109112	0.804948	0.420398
28.	8.	0.	4.510808	2.046197	0.055880
29.	6.	0.	3.112066	2.116016	0.323524
30.	6.	0.	2.828007	2.339694	1.816162
31.	6.	0.	6.615446	0.999374	0.279697
32.	8.	0.	5.191181	-0.297398	-1.729408
33.	6.	0.	7.419146	-0.193374	0.745909
34.	8.	0.	8.718719	-0.046108	0.437881
35.	6.	0.	9.594580	-1.110726	0.864012
36.	8.	0.	6.973194	-1.159711	1.337267
37.	1.	0.	-2.847259	-2.707642	-0.089807
38.	1.	0.	-0.632766	-3.271030	-1.064842
39.	1.	0.	-1.005030	2.198587	0.056252
40.	1.	0.	-3.660205	0.481029	1.455244
41.	1.	0.	-4.697905	-0.289216	-1.313282
42.	1.	0.	-4.170479	1.324168	-0.806277

43.	1.	0.	-5.942407	1.370459	0.947129
44.	1.	0.	-6.743820	-1.371805	-0.105956
45.	1.	0.	-5.577242	-0.443164	2.549164
46.	1.	0.	-5.453820	-2.872548	3.079610
47.	1.	0.	-7.138109	-2.378314	2.800915
48.	1.	0.	-6.252608	-3.264885	1.542256
49.	1.	0.	-8.269233	0.360137	0.705743
50.	1.	0.	-7.325450	-0.399058	-2.004000
51.	1.	0.	-6.323305	0.856042	-2.767492
52.	1.	0.	-8.074191	1.087216	-2.597659
53.	1.	0.	-7.732602	3.170411	-1.453244
54.	1.	0.	-6.849732	3.210199	0.082889
55.	1.	0.	-5.962816	3.046914	-1.452372
56.	1.	0.	4.731296	-1.273628	0.050359
57.	1.	0.	4.876100	0.554374	1.462925
58.	1.	0.	2.772870	2.997547	-0.225563
59.	1.	0.	3.391271	3.209887	2.164035
60.	1.	0.	1.764481	2.531930	1.972759
61.	1.	0.	3.108872	1.473892	2.421930
62.	1.	0.	6.874142	1.222347	-0.757637
63.	1.	0.	6.912948	1.867731	0.877985
64.	1.	0.	4.889672	-1.076493	-2.217736
65.	1.	0.	9.298812	-2.055542	0.403437
66.	1.	0.	9.569352	-1.214184	1.950785
67.	1.	0.	10.590010	-0.820300	0.532083

2-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	2.055286	-1.903961	0.385323
2.	6.	0.	2.371806	-0.633338	-0.069841
3.	6.	0.	1.398918	0.387340	0.030005
4.	6.	0.	0.081676	0.113975	0.514706
5.	6.	0.	-0.176943	-1.190964	1.025050
6.	6.	0.	0.812715	-2.170736	0.961198
7.	8.	0.	1.770934	1.606653	-0.382661
8.	6.	0.	3.737473	-0.302365	-0.631743
9.	6.	0.	4.631526	0.422042	0.397896
10.	6.	0.	6.026835	0.637537	-0.213845
11.	6.	0.	6.594625	-0.702423	-0.708309
12.	6.	0.	5.613603	-1.347954	-1.696903
13.	8.	0.	4.343366	-1.524354	-1.054612
14.	6.	0.	6.066640	-2.713425	-2.186705
15.	8.	0.	7.845951	-0.487735	-1.342494
16.	7.	0.	7.041757	1.325282	0.605042
17.	6.	0.	7.207072	0.801031	1.962422
18.	6.	0.	6.883875	2.779036	0.619652
19.	6.	0.	-1.369733	-1.617910	1.804187
20.	8.	0.	-2.610670	-1.053039	1.633207
21.	6.	0.	-3.058618	-0.051236	0.825004
22.	6.	0.	-2.363229	0.967860	0.281099
23.	6.	0.	-0.909163	1.196637	0.369940
24.	8.	0.	-0.517282	2.369285	0.161783

25.	8.	0.	-1.329502	-2.517656	2.613988
26.	6.	0.	-4.572865	-0.141138	0.753058
27.	6.	0.	-5.085519	0.710884	-0.408109
28.	8.	0.	-4.534309	2.019921	-0.235630
29.	6.	0.	-3.123009	2.077716	-0.460563
30.	6.	0.	-2.805036	2.117989	-1.962378
31.	6.	0.	-6.600751	0.872550	-0.440446
32.	8.	0.	-5.134867	0.255874	2.002188
33.	6.	0.	-7.323720	-0.399647	-0.825322
34.	8.	0.	-8.652836	-0.207826	-0.844722
35.	6.	0.	-9.452705	-1.354402	-1.203329
36.	8.	0.	-6.791617	-1.462445	-1.088863
37.	1.	0.	2.799429	-2.687500	0.309242
38.	1.	0.	0.606346	-3.146019	1.382466
39.	1.	0.	0.989617	2.206699	-0.205145
40.	1.	0.	3.607848	0.359128	-1.502706
41.	1.	0.	4.691318	-0.197662	1.299154
42.	1.	0.	4.169896	1.374828	0.672380
43.	1.	0.	5.908174	1.262294	-1.109789
44.	1.	0.	6.703696	-1.396134	0.142858
45.	1.	0.	5.494766	-0.664885	-2.554560
46.	1.	0.	7.034309	-2.627953	-2.686650
47.	1.	0.	6.168759	-3.406313	-1.345058
48.	1.	0.	5.341085	-3.127906	-2.892068
49.	1.	0.	8.229513	0.251757	-0.833058
50.	1.	0.	7.338183	-0.283451	1.942436

51.	1.	0.	6.359206	1.033722	2.627420
52.	1.	0.	8.107454	1.238142	2.404787
53.	1.	0.	7.748870	3.231250	1.114846
54.	1.	0.	6.840092	3.158905	-0.404961
55.	1.	0.	5.978799	3.117067	1.152898
56.	1.	0.	-4.853687	-1.186263	0.605464
57.	1.	0.	-4.750439	0.263561	-1.351965
58.	1.	0.	-2.812574	3.026051	-0.016012
59.	1.	0.	-3.366765	2.933269	-2.425857
60.	1.	0.	-1.740033	2.298907	-2.120578
61.	1.	0.	-3.069348	1.181596	-2.461060
62.	1.	0.	-6.971108	1.205318	0.533754
63.	1.	0.	-6.860917	1.653834	-1.161859
64.	1.	0.	-4.964152	1.207798	2.085978
65.	1.	0.	-9.291231	-2.168796	-0.494164
66.	1.	0.	-9.201483	-1.694923	-2.209883
67.	1.	0.	-10.485830	-1.013307	-1.163356

2-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.093183	-1.939100	-0.210099
2.	6.	0.	-2.406400	-0.632902	0.132918
3.	6.	0.	-1.421981	0.368707	-0.027917
4.	6.	0.	-0.095877	0.046799	-0.455743
5.	6.	0.	0.161051	-1.298621	-0.847226
6.	6.	0.	-0.840015	-2.262223	-0.730787

7.	8.	0.	-1.793830	1.620747	0.271331
8.	6.	0.	-3.779992	-0.246402	0.637436
9.	6.	0.	-4.646932	0.400922	-0.464491
10.	6.	0.	-6.051004	0.677262	0.101074
11.	6.	0.	-6.642173	-0.614071	0.689544
12.	6.	0.	-5.686739	-1.188840	1.744242
13.	8.	0.	-4.406346	-1.425474	1.143319
14.	6.	0.	-6.161761	-2.508635	2.329500
15.	8.	0.	-7.902527	-0.337897	1.280722
16.	7.	0.	-7.044174	1.305347	-0.789382
17.	6.	0.	-7.185432	0.678989	-2.105626
18.	6.	0.	-6.878142	2.753037	-0.912059
19.	6.	0.	1.374253	-1.803589	-1.540436
20.	8.	0.	2.621629	-1.264426	-1.325469
21.	6.	0.	3.049677	-0.170634	-0.630264
22.	6.	0.	2.349984	0.918009	-0.257826
23.	6.	0.	0.898652	1.136049	-0.394323
24.	8.	0.	0.504081	2.322989	-0.303371
25.	8.	0.	1.353580	-2.753839	-2.289786
26.	6.	0.	4.549133	-0.316692	-0.456997
27.	6.	0.	5.109040	0.804640	0.420792
28.	8.	0.	4.510694	2.046237	0.057515
29.	6.	0.	3.111947	2.115785	0.325185
30.	6.	0.	2.827868	2.338263	1.817990
31.	6.	0.	6.615356	0.999254	0.280197
32.	8.	0.	5.191085	-0.295721	-1.730038

33.	6.	0.	7.419105	-0.193913	0.745268
34.	8.	0.	8.718602	-0.046496	0.437039
35.	6.	0.	9.594520	-1.111542	0.862052
36.	8.	0.	6.973215	-1.160671	1.335985
37.	1.	0.	-2.846772	-2.707650	-0.088334
38.	1.	0.	-0.632290	-3.271005	-1.063289
39.	1.	0.	-1.004865	2.198776	0.056546
40.	1.	0.	-3.660481	0.481480	1.455358
41.	1.	0.	-4.697358	-0.289746	-1.313197
42.	1.	0.	-4.170162	1.323834	-0.806570
43.	1.	0.	-5.942684	1.370591	0.946283
44.	1.	0.	-6.743533	-1.372068	-0.106191
45.	1.	0.	-5.577847	-0.442574	2.549020
46.	1.	0.	-7.138754	-2.377837	2.800546
47.	1.	0.	-6.252389	-3.264690	1.542686
48.	1.	0.	-5.454551	-2.871723	3.080371
49.	1.	0.	-8.269365	0.359893	0.704478
50.	1.	0.	-7.324069	-0.400064	-2.004820
51.	1.	0.	-6.322347	0.855330	-2.768376
52.	1.	0.	-8.073402	1.085692	-2.599032
53.	1.	0.	-7.732093	3.169525	-1.455509
54.	1.	0.	-6.850307	3.209946	0.081224
55.	1.	0.	-5.962295	3.046252	-1.453373
56.	1.	0.	4.731286	-1.273603	0.048859
57.	1.	0.	4.876103	0.553054	1.463090
58.	1.	0.	2.772719	2.997719	-0.223240

59.	1.	0.	3.390963	3.208300	2.166526
60.	1.	0.	1.764310	2.530169	1.974797
61.	1.	0.	3.108941	1.472045	2.423072
62.	1.	0.	6.874024	1.223246	-0.756920
63.	1.	0.	6.912838	1.867045	0.879321
64.	1.	0.	4.888411	-1.073551	-2.219670
65.	1.	0.	9.297828	-2.056178	0.401726
66.	1.	0.	9.570499	-1.215066	1.948847
67.	1.	0.	10.589680	-0.821462	0.529024

2-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	2.281015	1.897360	0.762402
2.	6.	0.	2.419019	0.566282	0.399794
3.	6.	0.	1.336584	-0.080915	-0.238543
4.	6.	0.	0.085948	0.583382	-0.435489
5.	6.	0.	0.010736	1.964958	-0.097130
6.	6.	0.	1.108595	2.599831	0.481636
7.	8.	0.	1.538220	-1.351844	-0.612402
8.	6.	0.	3.701924	-0.199915	0.640050
9.	6.	0.	4.556663	-0.336055	-0.638534
10.	6.	0.	5.870297	-1.052816	-0.281472
11.	6.	0.	6.575745	-0.314370	0.867166
12.	6.	0.	5.627750	-0.197457	2.068869
13.	8.	0.	4.430755	0.479862	1.662411
14.	6.	0.	6.220778	0.587672	3.227107

15.	8.	0.	7.745957	-1.023242	1.244641
16.	7.	0.	6.837150	-1.305682	-1.365489
17.	6.	0.	7.154862	-0.143570	-2.198813
18.	6.	0.	6.489401	-2.462535	-2.189893
19.	6.	0.	-1.089556	2.902245	-0.446521
20.	8.	0.	-2.398971	2.499185	-0.560832
21.	6.	0.	-2.994366	1.278005	-0.455242
22.	6.	0.	-2.451697	0.056451	-0.633532
23.	6.	0.	-1.035017	-0.252497	-0.904073
24.	8.	0.	-0.798181	-1.365596	-1.429548
25.	8.	0.	-0.907307	4.088210	-0.609864
26.	6.	0.	-4.487672	1.493361	-0.268529
27.	6.	0.	-5.134731	0.197014	0.210581
28.	8.	0.	-4.751952	-0.824581	-0.716679
29.	6.	0.	-3.367937	-1.176337	-0.635061
30.	6.	0.	-3.105995	-2.119662	0.547832
31.	6.	0.	-6.655436	0.246502	0.230826
32.	8.	0.	-5.061316	1.966993	-1.484477
33.	6.	0.	-7.243607	-1.000929	0.861367
34.	8.	0.	-8.423476	-1.319244	0.302757
35.	6.	0.	-9.101684	-2.460504	0.868578
36.	8.	0.	-6.739391	-1.624548	1.775422
37.	1.	0.	3.109796	2.395061	1.251033
38.	1.	0.	1.041617	3.657415	0.701433
39.	1.	0.	0.700911	-1.636411	-1.080519
40.	1.	0.	3.442990	-1.211931	0.989713

41.	1.	0.	4.753305	0.666954	-1.032377
42.	1.	0.	3.995601	-0.893060	-1.394257
43.	1.	0.	5.614167	-2.045887	0.112762
44.	1.	0.	6.828076	0.712105	0.550042
45.	1.	0.	5.372916	-1.217285	2.402549
46.	1.	0.	7.139580	0.107182	3.571395
47.	1.	0.	6.457805	1.609868	2.914319
48.	1.	0.	5.514184	0.634345	4.060358
49.	1.	0.	8.061139	-1.397746	0.399685
50.	1.	0.	7.430832	0.711161	-1.576699
51.	1.	0.	6.325213	0.162743	-2.856840
52.	1.	0.	8.012511	-0.385876	-2.833668
53.	1.	0.	7.315820	-2.680159	-2.873674
54.	1.	0.	6.332451	-3.338778	-1.554484
55.	1.	0.	5.582211	-2.310281	-2.799320
56.	1.	0.	-4.627932	2.290514	0.467801
57.	1.	0.	-4.775734	-0.039394	1.219392
58.	1.	0.	-3.166458	-1.719377	-1.561390
59.	1.	0.	-3.787327	-2.971844	0.483469
60.	1.	0.	-2.080474	-2.492666	0.515029
61.	1.	0.	-3.258236	-1.622106	1.509263
62.	1.	0.	-6.983707	1.103853	0.831299
63.	1.	0.	-7.054584	0.385527	-0.774895
64.	1.	0.	-5.029396	1.221931	-2.105931
65.	1.	0.	-9.312932	-2.292985	1.926703
66.	1.	0.	-8.490616	-3.358780	0.759220

67.	1.	0.	-10.028210	-2.558893	0.305324

2-e		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-1.956949	1.823770	0.604569
2.	6.	0.	-2.291150	0.611138	0.021596
3.	6.	0.	-1.332606	-0.427770	0.014476
4.	6.	0.	-0.011090	-0.222680	0.520013
5.	6.	0.	0.265678	1.018493	1.162509
6.	6.	0.	-0.710765	2.012552	1.203407
7.	8.	0.	-1.721317	-1.593251	-0.520200
8.	6.	0.	-3.660339	0.358020	-0.570854
9.	6.	0.	-4.569631	-0.446225	0.382898
10.	6.	0.	-5.962604	-0.584911	-0.255280
11.	6.	0.	-6.511121	0.802640	-0.623638
12.	6.	0.	-5.514792	1.528080	-1.539068
13.	8.	0.	-4.246177	1.623762	-0.876678
14.	6.	0.	-5.946805	2.940612	-1.896320
15.	8.	0.	-7.759240	0.663687	-1.285018
16.	7.	0.	-6.991336	-1.337038	0.485664
17.	6.	0.	-7.171716	-0.936276	1.882816
18.	6.	0.	-6.838674	-2.786897	0.371681
19.	6.	0.	1.466108	1.345051	1.977732
20.	8.	0.	2.699279	0.786577	1.740553
21.	6.	0.	3.131120	-0.121423	0.819984
22.	6.	0.	2.421772	-1.069160	0.175356

23.	6.	0.	0.966347	-1.294477	0.255508
24.	8.	0.	0.561063	-2.434986	-0.070563
25.	8.	0.	1.439703	2.152233	2.880242
26.	6.	0.	4.645424	-0.031524	0.738178
27.	6.	0.	5.138478	-0.757133	-0.514164
28.	8.	0.	4.576308	-2.072895	-0.479259
29.	6.	0.	3.162669	-2.094939	-0.694401
30.	6.	0.	2.828131	-1.964511	-2.187255
31.	6.	0.	6.653573	-0.939019	-0.575604
32.	8.	0.	5.225374	-0.556423	1.929829
33.	6.	0.	7.477357	0.329465	-0.675936
34.	8.	0.	6.797018	1.339689	-1.250336
35.	6.	0.	7.525491	2.573737	-1.426638
36.	8.	0.	8.632971	0.419422	-0.313082
37.	1.	0.	-2.690038	2.621393	0.610294
38.	1.	0.	-0.490929	2.935843	1.723407
39.	1.	0.	-0.947512	-2.218177	-0.409770
40.	1.	0.	-3.537771	-0.219712	-1.500373
41.	1.	0.	-4.627182	0.088679	1.337129
42.	1.	0.	-4.122870	-1.426796	0.570753
43.	1.	0.	-5.843779	-1.122799	-1.206106
44.	1.	0.	-6.620473	1.414150	0.288509
45.	1.	0.	-5.400117	0.930320	-2.458786
46.	1.	0.	-6.913780	2.916958	-2.404258
47.	1.	0.	-6.042395	3.551619	-0.992699
48.	1.	0.	-5.213157	3.410354	-2.557266

49.	1.	0.	-8.153613	-0.118846	-0.854250
50.	1.	0.	-7.304369	0.145583	1.958735
51.	1.	0.	-6.330835	-1.226880	2.533858
52.	1.	0.	-8.076190	-1.411699	2.274321
53.	1.	0.	-7.712858	-3.278216	0.810244
54.	1.	0.	-6.779512	-3.073096	-0.682207
55.	1.	0.	-5.943157	-3.174954	0.886495
56.	1.	0.	4.923130	1.025262	0.701993
57.	1.	0.	4.799898	-0.209079	-1.400678
58.	1.	0.	2.848474	-3.084487	-0.354581
59.	1.	0.	3.375395	-2.728542	-2.745629
60.	1.	0.	1.759452	-2.116070	-2.351462
61.	1.	0.	3.097245	-0.980686	-2.581373
62.	1.	0.	7.007302	-1.488915	0.298209
63.	1.	0.	6.885962	-1.547886	-1.457127
64.	1.	0.	5.056406	-1.512173	1.916074
65.	1.	0.	8.384458	2.415645	-2.081698
66.	1.	0.	7.868865	2.953761	-0.462651
67.	1.	0.	6.820013	3.266502	-1.882064

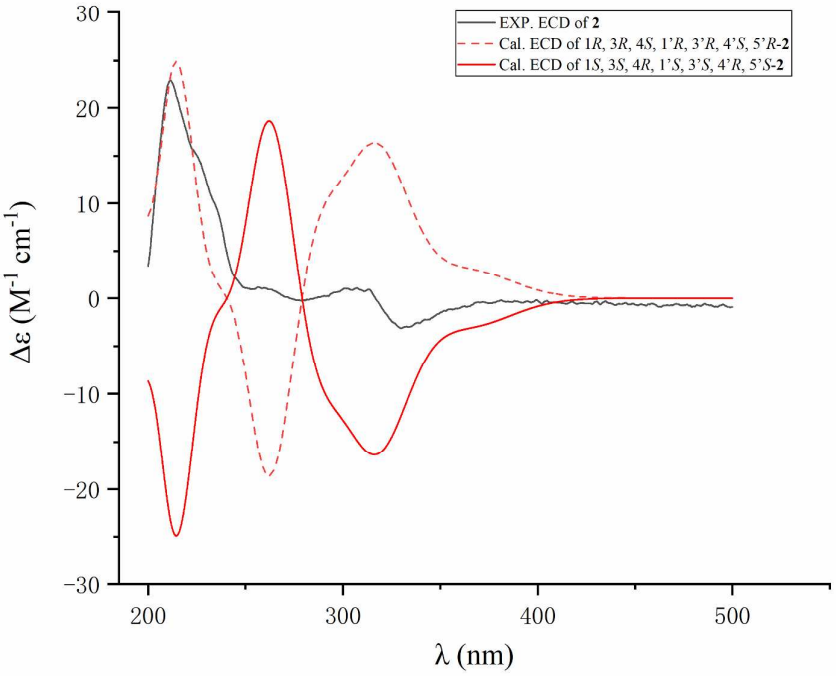
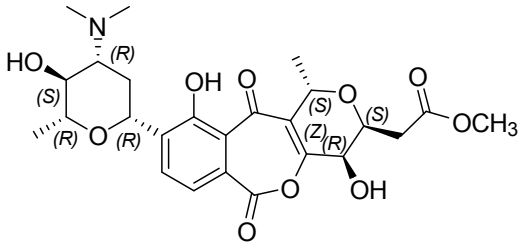


Figure S39. Comparison of the calculated ECD spectra for 1*R*, 3*R*, 4*S*, 1′*R*, 3′*R*, 4′*S*, 5′*R* and its enantiomer with the experimental spectrum of **2**.



E-2

Table S7. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **E-2**.

Conformers	In MeOH	
	Δ*G*	*P* (%)
E-2-a	0	46.15

E-2-b	0.09	40.55
E-2-c	1.53	6.65
E-2-d	1.53	6.65

[a] B3LYP/6-31+G (d, p), in kcal/mol. [b] From Δ*G* values at 298.15K.

Table S8. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **E-2** at B3LYP/6-311+G (d, p) level of theory in CH_3OH.

E-2-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.427978	-2.094278	-0.728922
2.	6.	0.	-2.561104	-1.066685	0.192427
3.	6.	0.	-1.415058	-0.630797	0.895878
4.	6.	0.	-0.121935	-1.174509	0.619133
5.	6.	0.	-0.044332	-2.263748	-0.295691
6.	6.	0.	-1.194972	-2.710774	-0.943461
7.	8.	0.	-1.605919	0.332583	1.808118
8.	6.	0.	-3.894821	-0.407812	0.469881
9.	6.	0.	-4.009886	0.977142	-0.203218
10.	6.	0.	-5.420223	1.539773	0.046849
11.	6.	0.	-6.477896	0.525434	-0.417300
12.	6.	0.	-6.249949	-0.819864	0.285726
13.	8.	0.	-4.922184	-1.282034	0.003030
14.	6.	0.	-7.212327	-1.904960	-0.168340
15.	8.	0.	-7.775363	1.013850	-0.113733
16.	7.	0.	-5.743503	2.868530	-0.502221
17.	6.	0.	-5.423899	3.055808	-1.918992

18.	6.	0.	-5.220689	3.970204	0.304779
19.	6.	0.	1.136694	-3.134057	-0.538323
20.	8.	0.	2.429032	-2.680389	-0.422873
21.	6.	0.	2.948682	-1.475814	-0.055067
22.	6.	0.	2.390989	-0.513733	0.707546
23.	6.	0.	1.024058	-0.504383	1.261787
24.	8.	0.	0.828367	0.244158	2.247889
25.	8.	0.	1.033841	-4.287169	-0.893798
26.	6.	0.	4.400807	-1.431182	-0.501509
27.	6.	0.	4.913408	0.004839	-0.437098
28.	8.	0.	4.637139	0.485560	0.882938
29.	6.	0.	3.243873	0.690348	1.133943
30.	6.	0.	2.759348	2.013187	0.523140
31.	8.	0.	5.176706	-2.319414	0.299360
32.	6.	0.	6.413744	0.123098	-0.660494
33.	1.	0.	-3.998216	-0.273155	1.557906
34.	6.	0.	6.853027	1.572204	-0.743509
35.	8.	0.	8.089994	1.734937	-0.244578
36.	6.	0.	8.633327	3.069261	-0.328303
37.	8.	0.	6.195191	2.474695	-1.224583
38.	1.	0.	-3.308822	-2.443460	-1.253754
39.	1.	0.	-1.119932	-3.561701	-1.607934
40.	1.	0.	-0.718611	0.474097	2.247724
41.	1.	0.	-3.821867	0.856271	-1.275644
42.	1.	0.	-3.242752	1.643408	0.201854
43.	1.	0.	-5.554773	1.637642	1.132938

44.	1.	0.	-6.372375	0.348647	-1.501547
45.	1.	0.	-6.355760	-0.659615	1.371770
46.	1.	0.	-7.018121	-2.838366	0.367195
47.	1.	0.	-8.241661	-1.594989	0.026277
48.	1.	0.	-7.100674	-2.089774	-1.241810
49.	1.	0.	-7.680912	1.979350	-0.225209
50.	1.	0.	-5.889627	3.982329	-2.268450
51.	1.	0.	-4.342078	3.128343	-2.118432
52.	1.	0.	-5.826854	2.234326	-2.516011
53.	1.	0.	-5.625895	4.915873	-0.068745
54.	1.	0.	-4.120005	4.046088	0.283780
55.	1.	0.	-5.536106	3.851309	1.345233
56.	1.	0.	4.455550	-1.815002	-1.524647
57.	1.	0.	4.395152	0.613011	-1.188196
58.	1.	0.	3.167585	0.763338	2.221260
59.	1.	0.	1.736793	2.225116	0.841686
60.	1.	0.	3.405480	2.824525	0.867944
61.	1.	0.	2.779213	1.990610	-0.569650
62.	1.	0.	5.211600	-1.924355	1.185301
63.	1.	0.	6.966814	-0.394611	0.124474
64.	1.	0.	6.677598	-0.354981	-1.611860
65.	1.	0.	9.625409	3.009516	0.116188
66.	1.	0.	8.006957	3.770504	0.226727
67.	1.	0.	8.699638	3.389564	-1.370160

E-2-b	Standard Orientation (Ångstroms)

No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.169541	2.051900	0.724783
2.	6.	0.	-2.493120	1.057490	-0.185455
3.	6.	0.	-1.467183	0.512301	-0.990979
4.	6.	0.	-0.103538	0.910700	-0.829096
5.	6.	0.	0.171444	1.971384	0.081244
6.	6.	0.	-0.862860	2.529177	0.831559
7.	8.	0.	-1.840942	-0.411727	-1.887047
8.	6.	0.	-3.908539	0.548030	-0.349074
9.	6.	0.	-4.114415	-0.831411	0.313286
10.	6.	0.	-5.591464	-1.236650	0.165769
11.	6.	0.	-6.498033	-0.128933	0.726226
12.	6.	0.	-6.181624	1.203509	0.033053
13.	8.	0.	-4.793785	1.514572	0.216560
14.	6.	0.	-6.984090	2.370851	0.583538
15.	8.	0.	-7.859123	-0.469693	0.512473
16.	7.	0.	-6.012474	-2.536902	0.717242
17.	6.	0.	-5.615223	-2.785867	2.104618
18.	6.	0.	-5.663037	-3.669144	-0.139589
19.	6.	0.	1.456824	2.705242	0.225487
20.	8.	0.	2.677654	2.118024	-0.007048
21.	6.	0.	3.031976	0.875502	-0.439378
22.	6.	0.	2.307053	-0.007703	-1.155903
23.	6.	0.	0.901527	0.133174	-1.578304
24.	8.	0.	0.537868	-0.575771	-2.546162
25.	8.	0.	1.511078	3.855704	0.599897

26.	6.	0.	4.506470	0.671238	-0.136726
27.	6.	0.	4.855422	-0.811756	-0.259062
28.	8.	0.	4.411755	-1.232851	-1.552288
29.	6.	0.	2.987527	-1.283673	-1.675438
30.	6.	0.	2.424479	-2.563256	-1.040000
31.	8.	0.	5.289879	1.480682	-1.011316
32.	6.	0.	6.348601	-1.108571	-0.186983
33.	1.	0.	-4.119619	0.447870	-1.425331
34.	6.	0.	6.925419	-0.907455	1.197182
35.	8.	0.	8.239532	-1.184068	1.212829
36.	6.	0.	8.904001	-1.029949	2.484648
37.	8.	0.	6.300030	-0.547157	2.177624
38.	1.	0.	-2.957732	2.486040	1.327811
39.	1.	0.	-0.638019	3.356709	1.491700
40.	1.	0.	-1.016130	-0.641155	-2.404805
41.	1.	0.	-3.832439	-0.754657	1.369072
42.	1.	0.	-3.455668	-1.564269	-0.161287
43.	1.	0.	-5.817198	-1.294261	-0.907998
44.	1.	0.	-6.295470	0.007485	1.802351
45.	1.	0.	-6.387933	1.084595	-1.043800
46.	1.	0.	-6.735061	3.292835	0.050920
47.	1.	0.	-8.052733	2.175125	0.468387
48.	1.	0.	-6.768531	2.514568	1.647433
49.	1.	0.	-7.861856	-1.442319	0.598456
50.	1.	0.	-6.143571	-3.670903	2.471987
51.	1.	0.	-4.534208	-2.966064	2.224844

52.	1.	0.	-5.893838	-1.942972	2.741514
53.	1.	0.	-6.144387	-4.574572	0.243310
54.	1.	0.	-4.577845	-3.863203	-0.189296
55.	1.	0.	-6.026883	-3.492869	-1.155792
56.	1.	0.	4.707269	1.024696	0.876961
57.	1.	0.	4.338619	-1.365126	0.534413
58.	1.	0.	2.805859	-1.323937	-2.751927
59.	1.	0.	1.358744	-2.658151	-1.257057
60.	1.	0.	2.940978	-3.429855	-1.461095
61.	1.	0.	2.553026	-2.571221	0.045759
62.	1.	0.	5.186569	1.098085	-1.897623
63.	1.	0.	6.521574	-2.146227	-0.490104
64.	1.	0.	6.898709	-0.477201	-0.891019
65.	1.	0.	9.945229	-1.291192	2.303297
66.	1.	0.	8.465881	-1.699485	3.227606
67.	1.	0.	8.823959	0.001444	2.834000

E-2-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.204774	2.081712	0.575287
2.	6.	0.	-2.520281	1.030243	-0.271454
3.	6.	0.	-1.484575	0.418929	-1.014371
4.	6.	0.	-0.118882	0.808768	-0.846948
5.	6.	0.	0.148959	1.922341	-0.000239
6.	6.	0.	-0.894350	2.547256	0.682269
7.	8.	0.	-1.852353	-0.557207	-1.856266

8.	6.	0.	-3.937573	0.522344	-0.423541
9.	6.	0.	-4.167089	-0.789485	0.357504
10.	6.	0.	-5.646133	-1.195141	0.233634
11.	6.	0.	-6.547763	-0.031010	0.675261
12.	6.	0.	-6.211068	1.225519	-0.139574
13.	8.	0.	-4.823645	1.543458	0.035251
14.	6.	0.	-7.011766	2.446574	0.282122
15.	8.	0.	-7.909664	-0.379995	0.481506
16.	7.	0.	-6.082146	-2.432724	0.905260
17.	6.	0.	-5.697850	-2.548319	2.313722
18.	6.	0.	-5.733132	-3.645129	0.165808
19.	6.	0.	1.445462	2.632433	0.147487
20.	8.	0.	2.653833	1.981033	0.049478
21.	6.	0.	2.997297	0.721542	-0.347346
22.	6.	0.	2.288818	-0.153067	-1.087037
23.	6.	0.	0.892050	-0.017638	-1.536787
24.	8.	0.	0.533051	-0.771496	-2.472177
25.	8.	0.	1.522701	3.807116	0.428118
26.	6.	0.	4.435290	0.501695	0.082267
27.	6.	0.	4.883258	-0.930862	-0.216891
28.	8.	0.	4.406976	-1.328379	-1.499969
29.	6.	0.	2.987248	-1.425416	-1.586103
30.	6.	0.	2.460454	-2.701890	-0.913792
31.	8.	0.	5.291441	1.422616	-0.590114
32.	6.	0.	6.398507	-1.102601	-0.252683
33.	1.	0.	-4.127783	0.328650	-1.490513

34.	6.	0.	7.063727	-0.820988	1.075513
35.	8.	0.	8.400052	-0.775893	0.943177
36.	6.	0.	9.148406	-0.546122	2.155310
37.	8.	0.	6.487121	-0.669672	2.137134
38.	1.	0.	-3.001054	2.565533	1.127776
39.	1.	0.	-0.671899	3.412538	1.293064
40.	1.	0.	-1.021148	-0.823120	-2.345800
41.	1.	0.	-3.894693	-0.618416	1.404671
42.	1.	0.	-3.510115	-1.568458	-0.040181
43.	1.	0.	-5.862398	-1.355011	-0.831755
44.	1.	0.	-6.354184	0.207674	1.735050
45.	1.	0.	-6.401962	1.004257	-1.202984
46.	1.	0.	-8.080124	2.251016	0.163929
47.	1.	0.	-6.815433	2.688376	1.331869
48.	1.	0.	-6.742104	3.311628	-0.330021
49.	1.	0.	-7.921912	-1.339410	0.662402
50.	1.	0.	-6.235942	-3.390158	2.760035
51.	1.	0.	-4.619415	-2.723818	2.460454
52.	1.	0.	-5.975338	-1.646115	2.863773
53.	1.	0.	-6.217308	-4.506904	0.635791
54.	1.	0.	-4.648293	-3.845318	0.138055
55.	1.	0.	-6.094434	-3.570503	-0.863733
56.	1.	0.	4.482147	0.657920	1.167789
57.	1.	0.	4.467774	-1.576123	0.567250
58.	1.	0.	2.782998	-1.493155	-2.657251
59.	1.	0.	1.395463	-2.825258	-1.121347

60.	1.	0.	2.993264	-3.567794	-1.316103
61.	1.	0.	2.593736	-2.679864	0.171189
62.	1.	0.	5.042843	2.312186	-0.301481
63.	1.	0.	6.626428	-2.135968	-0.537076
64.	1.	0.	6.835002	-0.456409	-1.017061
65.	1.	0.	8.963884	-1.345830	2.875617
66.	1.	0.	8.870519	0.412084	2.598962
67.	1.	0.	10.194950	-0.537945	1.855205

E-2-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.204566	2.081506	0.575630
2.	6.	0.	-2.520148	1.030203	-0.271299
3.	6.	0.	-1.484512	0.418999	-1.014392
4.	6.	0.	-0.118791	0.808795	-0.846992
5.	6.	0.	0.149106	1.922257	-0.000167
6.	6.	0.	-0.894139	2.547036	0.682568
7.	8.	0.	-1.852361	-0.556988	-1.856424
8.	6.	0.	-3.937476	0.522395	-0.423430
9.	6.	0.	-4.167130	-0.789495	0.357469
10.	6.	0.	-5.646210	-1.194990	0.233479
11.	6.	0.	-6.547729	-0.030841	0.675325
12.	6.	0.	-6.210953	1.225746	-0.139384
13.	8.	0.	-4.823484	1.543542	0.035436
14.	6.	0.	-7.011504	2.446838	0.282472
15.	8.	0.	-7.909672	-0.379700	0.481665

16.	7.	0.	-6.082398	-2.432685	0.904778
17.	6.	0.	-5.698354	-2.548599	2.313282
18.	6.	0.	-5.733369	-3.644970	0.165134
19.	6.	0.	1.445552	2.632497	0.147269
20.	8.	0.	2.654037	1.981330	0.048489
21.	6.	0.	2.997360	0.721581	-0.347619
22.	6.	0.	2.288751	-0.153334	-1.086833
23.	6.	0.	0.892068	-0.017733	-1.536788
24.	8.	0.	0.533050	-0.771547	-2.472203
25.	8.	0.	1.522743	3.807134	0.428063
26.	6.	0.	4.435423	0.501819	0.081778
27.	6.	0.	4.883129	-0.930997	-0.216482
28.	8.	0.	4.406639	-1.329271	-1.499268
29.	6.	0.	2.986905	-1.426104	-1.585162
30.	6.	0.	2.459822	-2.701972	-0.911901
31.	8.	0.	5.291482	1.422168	-0.591598
32.	6.	0.	6.398338	-1.102989	-0.252369
33.	1.	0.	-4.127690	0.328831	-1.490425
34.	6.	0.	7.063818	-0.820664	1.075532
35.	8.	0.	8.400172	-0.776392	0.943007
36.	6.	0.	9.148777	-0.546055	2.154841
37.	8.	0.	6.487430	-0.668156	2.137092
38.	1.	0.	-3.000816	2.565204	1.128265
39.	1.	0.	-0.671620	3.412246	1.293441
40.	1.	0.	-1.021185	-0.822924	-2.345987
41.	1.	0.	-3.894767	-0.618548	1.404663

42.	1.	0.	-3.510209	-1.568489	-0.040261
43.	1.	0.	-5.862447	-1.354604	-0.831953
44.	1.	0.	-6.354023	0.207719	1.735118
45.	1.	0.	-6.401898	1.004632	-1.202811
46.	1.	0.	-6.741693	3.311952	-0.329522
47.	1.	0.	-8.079884	2.251448	0.164184
48.	1.	0.	-6.815206	2.688454	1.332268
49.	1.	0.	-7.921890	-1.339216	0.662086
50.	1.	0.	-6.236231	-3.390794	2.759178
51.	1.	0.	-4.619892	-2.723764	2.460197
52.	1.	0.	-5.976317	-1.646694	2.863585
53.	1.	0.	-6.217950	-4.506759	0.634672
54.	1.	0.	-4.648564	-3.845402	0.137752
55.	1.	0.	-6.094221	-3.569955	-0.864536
56.	1.	0.	4.482679	0.658862	1.167153
57.	1.	0.	4.467609	-1.575694	0.568103
58.	1.	0.	2.782503	-1.494545	-2.656234
59.	1.	0.	1.394836	-2.825274	-1.119561
60.	1.	0.	2.992503	-3.568309	-1.313449
61.	1.	0.	2.592892	-2.679121	0.173088
62.	1.	0.	5.043395	2.311941	-0.303153
63.	1.	0.	6.626095	-2.136549	-0.536187
64.	1.	0.	6.834793	-0.457307	-1.017203
65.	1.	0.	10.195340	-0.539403	1.854737
66.	1.	0.	8.963367	-1.344677	2.876125
67.	1.	0.	8.872002	0.412998	2.597374

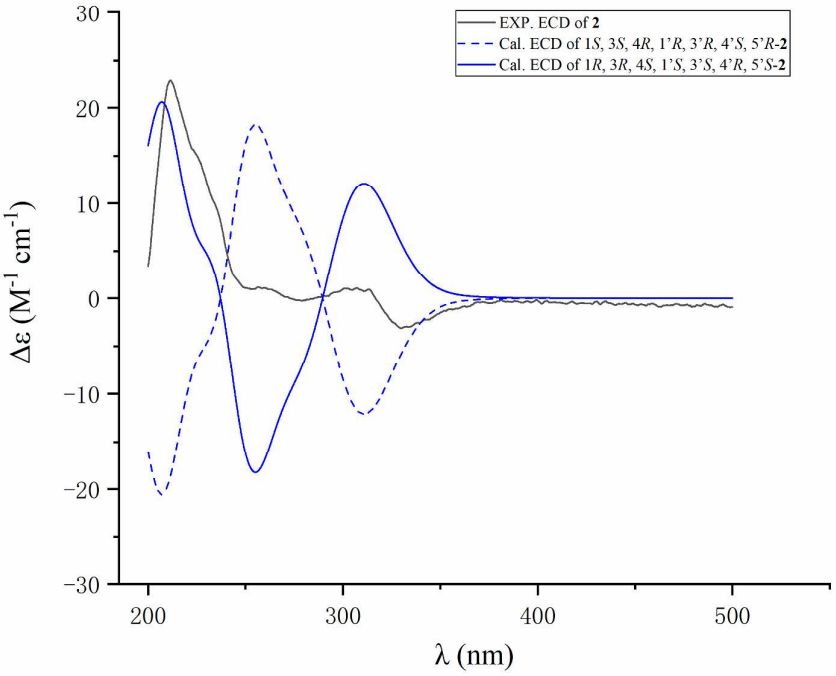
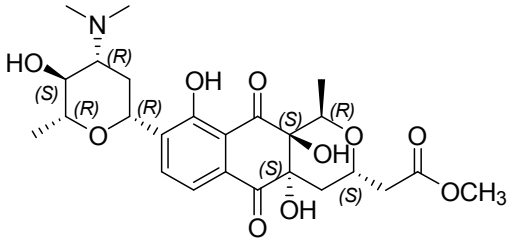


Figure S40. Comparison of the calculated ECD spectra for 1*S*, 3*S*, 4*R*, 1′*R*, 3′*R*, 4′*S*, 5′*R* and its enantiomer with the experimental spectrum of **2**.



Strepoxepinmycin C (3)

Table S9. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **3**.

Conformers	In MeOH	
	Δ*G*	P (%)
3-a	0	74.61

3-b	1.65	8.99
3-c	1.72	7.58
3-d	1.89	6.27
3-e	1.99	2.55

[a] B3LYP/6-31+G (d, p), in kcal/mol. [b] From Δ*G* values at 298.15K.

Table S10. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **3** at B3LYP/6-311+G (d, p) level of theory in CH_3OH.

3-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-1.796735	-0.390925	-1.955615
2.	6.	0.	-2.197303	-0.612173	-0.640318
3.	6.	0.	-1.203147	-0.838377	0.340211
4.	6.	0.	0.167868	-0.855414	-0.014220
5.	6.	0.	0.536935	-0.598420	-1.361872
6.	6.	0.	-0.443403	-0.374358	-2.319817
7.	6.	0.	1.180161	-1.154337	1.003534
8.	6.	0.	2.613949	-1.453805	0.504904
9.	6.	0.	2.968378	-0.383944	-0.563051
10.	6.	0.	1.974573	-0.513937	-1.740017
11.	8.	0.	2.345514	-0.463573	-2.905054
12.	8.	0.	0.888856	-1.237119	2.206876
13.	8.	0.	-1.608241	-1.047046	1.608665
14.	6.	0.	-3.653235	-0.590901	-0.227014
15.	6.	0.	-4.045264	0.731564	0.464623
16.	6.	0.	-5.548211	0.696990	0.794085

17.	6.	0.	-6.349963	0.405361	-0.483489
18.	6.	0.	-5.862340	-0.902139	-1.126906
19.	8.	0.	-4.453067	-0.799492	-1.395531
20.	6.	0.	-6.550853	-1.220250	-2.444249
21.	8.	0.	-7.737071	0.295353	-0.168185
22.	7.	0.	-6.126497	1.864373	1.486023
23.	6.	0.	-5.798352	3.166226	0.896920
24.	6.	0.	-5.876765	1.862933	2.928733
25.	6.	0.	3.668780	-1.468763	1.644947
26.	8.	0.	5.003105	-1.546815	1.113906
27.	6.	0.	5.396519	-0.545154	0.167915
28.	6.	0.	4.417593	-0.535838	-1.011789
29.	6.	0.	5.655819	0.800973	0.910469
30.	6.	0.	5.815908	1.989013	-0.006004
31.	8.	0.	7.078494	2.398312	-0.125775
32.	6.	0.	7.326141	3.534278	-0.993549
33.	8.	0.	4.879464	2.528601	-0.592297
34.	6.	0.	3.562931	-2.650400	2.605309
35.	8.	0.	2.699066	0.889545	0.037187
36.	8.	0.	2.570418	-2.688758	-0.219560
37.	1.	0.	-3.828921	-1.419580	0.476325
38.	1.	0.	-2.559205	-0.221832	-2.707127
39.	1.	0.	-0.150153	-0.170654	-3.343428
40.	1.	0.	-0.792783	-1.147046	2.162933
41.	1.	0.	-3.810528	1.559563	-0.213500
42.	1.	0.	-3.449567	0.858273	1.373365

43.	1.	0.	-5.724966	-0.153290	1.466972
44.	1.	0.	-6.198473	1.213541	-1.216345
45.	1.	0.	-6.030104	-1.723471	-0.410983
46.	1.	0.	-6.167202	-2.157736	-2.857588
47.	1.	0.	-7.627973	-1.322822	-2.289172
48.	1.	0.	-6.377865	-0.419829	-3.171806
49.	1.	0.	-7.868626	0.938652	0.554485
50.	1.	0.	-6.432842	3.931743	1.353730
51.	1.	0.	-4.747089	3.459776	1.055031
52.	1.	0.	-5.996868	3.164611	-0.177625
53.	1.	0.	-6.460480	2.662335	3.395849
54.	1.	0.	-4.815724	2.025530	3.186956
55.	1.	0.	-6.195268	0.909922	3.360756
56.	1.	0.	3.541683	-0.535548	2.206944
57.	1.	0.	6.361134	-0.898688	-0.206017
58.	1.	0.	4.516401	-1.493501	-1.529053
59.	1.	0.	4.665930	0.240868	-1.738558
60.	1.	0.	4.811960	1.030240	1.564724
61.	1.	0.	6.549552	0.682799	1.525132
62.	1.	0.	8.400903	3.697864	-0.947397
63.	1.	0.	6.785124	4.407882	-0.626364
64.	1.	0.	7.012694	3.300579	-2.012282
65.	1.	0.	3.742516	-3.597751	2.086137
66.	1.	0.	4.333487	-2.548512	3.374211
67.	1.	0.	2.586860	-2.679043	3.089876
68.	1.	0.	3.339923	1.553677	-0.297702

69.	1.	0.	2.379733	-3.420434	0.385068

3-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-1.924974	-1.107010	-1.629022
2.	6.	0.	-2.306807	-0.746523	-0.338770
3.	6.	0.	-1.297915	-0.512694	0.624129
4.	6.	0.	0.068036	-0.677676	0.288965
5.	6.	0.	0.418341	-1.018135	-1.044295
6.	6.	0.	-0.576948	-1.230553	-1.990573
7.	6.	0.	1.095325	-0.519480	1.319707
8.	6.	0.	2.512803	-1.028978	0.979800
9.	6.	0.	2.879187	-0.516705	-0.445032
10.	6.	0.	1.847666	-1.089154	-1.448735
11.	8.	0.	2.195762	-1.503588	-2.546585
12.	8.	0.	0.831010	-0.049438	2.435182
13.	8.	0.	-1.683046	-0.148543	1.862793
14.	6.	0.	-3.758483	-0.574285	0.052183
15.	6.	0.	-4.186685	0.908288	0.078588
16.	6.	0.	-5.686374	0.990257	0.417022
17.	6.	0.	-6.489032	0.124824	-0.567605
18.	6.	0.	-5.961981	-1.317864	-0.552401
19.	8.	0.	-4.561081	-1.309229	-0.877203
20.	6.	0.	-6.653637	-2.225491	-1.556620
21.	8.	0.	-7.868662	0.134933	-0.204495
22.	7.	0.	-6.297410	2.328936	0.511769

23.	6.	0.	-6.023480	3.224686	-0.615939
24.	6.	0.	-6.035066	2.995350	1.788792
25.	6.	0.	3.604013	-0.613600	1.997912
26.	8.	0.	4.859119	-1.141752	1.525927
27.	6.	0.	5.337607	-0.619277	0.272273
28.	6.	0.	4.309167	-0.899694	-0.833181
29.	6.	0.	5.786199	0.843893	0.421469
30.	6.	0.	6.679299	1.306128	-0.710038
31.	8.	0.	6.826727	2.642076	-0.697433
32.	6.	0.	7.701932	3.210472	-1.700085
33.	8.	0.	7.223169	0.579717	-1.525637
34.	6.	0.	3.439608	-1.166882	3.409658
35.	8.	0.	2.682890	0.907707	-0.389150
36.	8.	0.	2.385314	-2.455306	0.924219
37.	1.	0.	-3.901618	-0.998845	1.057716
38.	1.	0.	-2.698951	-1.287083	-2.366118
39.	1.	0.	-0.299320	-1.478186	-3.008713
40.	1.	0.	-0.860263	0.012390	2.390145
41.	1.	0.	-3.978908	1.345468	-0.904409
42.	1.	0.	-3.590535	1.447146	0.821133
43.	1.	0.	-5.830633	0.537377	1.407654
44.	1.	0.	-6.371659	0.511159	-1.592283
45.	1.	0.	-6.089386	-1.722282	0.465094
46.	1.	0.	-6.240228	-3.236971	-1.502970
47.	1.	0.	-7.724319	-2.274707	-1.342036
48.	1.	0.	-6.518876	-1.845283	-2.575038

49.	1.	0.	-8.016363	1.033685	0.147231
50.	1.	0.	-6.677221	4.098817	-0.539918
51.	1.	0.	-4.980821	3.583332	-0.640807
52.	1.	0.	-6.239017	2.727796	-1.565056
53.	1.	0.	-6.643427	3.902924	1.852607
54.	1.	0.	-4.978504	3.288196	1.918286
55.	1.	0.	-6.315157	2.337171	2.616221
56.	1.	0.	3.640619	0.480924	2.032553
57.	1.	0.	6.227702	-1.216716	0.063005
58.	1.	0.	4.328587	-1.970152	-1.057942
59.	1.	0.	4.586042	-0.392488	-1.762289
60.	1.	0.	4.945851	1.536201	0.505236
61.	1.	0.	6.369990	0.935004	1.346326
62.	1.	0.	7.691906	4.283172	-1.514935
63.	1.	0.	7.322896	2.989561	-2.699794
64.	1.	0.	8.711808	2.810603	-1.589631
65.	1.	0.	3.369578	-2.258384	3.401584
66.	1.	0.	4.317861	-0.883784	3.996415
67.	1.	0.	2.547748	-0.760276	3.884524
68.	1.	0.	2.908241	1.302207	-1.244943
69.	1.	0.	3.271838	-2.832545	1.048600

3-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.752515	0.082048	1.951306
2.	6.	0.	2.153807	-0.431042	0.720047

3.	6.	0.	1.159209	-0.837224	-0.199236
4.	6.	0.	-0.213147	-0.756645	0.142804
5.	6.	0.	-0.583105	-0.202089	1.397420
6.	6.	0.	0.398790	0.210856	2.289542
7.	6.	0.	-1.223892	-1.266331	-0.785123
8.	6.	0.	-2.654181	-1.448106	-0.232025
9.	6.	0.	-3.022698	-0.164669	0.569345
10.	6.	0.	-2.018830	-0.006806	1.736384
11.	8.	0.	-2.387347	0.337433	2.851559
12.	8.	0.	-0.939628	-1.587272	-1.947714
13.	8.	0.	1.563562	-1.315553	-1.391903
14.	6.	0.	3.611610	-0.544685	0.330642
15.	6.	0.	4.065428	0.602831	-0.595941
16.	6.	0.	5.567782	0.440341	-0.891047
17.	6.	0.	6.350300	0.358977	0.429727
18.	6.	0.	5.797265	-0.778606	1.300992
19.	8.	0.	4.394585	-0.557356	1.528611
20.	6.	0.	6.466294	-0.877525	2.662495
21.	8.	0.	7.731423	0.126734	0.158020
22.	7.	0.	6.203341	1.426973	-1.783811
23.	6.	0.	5.945734	2.831058	-1.450399
24.	6.	0.	5.950256	1.168094	-3.202576
25.	6.	0.	-3.715131	-1.732433	-1.325488
26.	8.	0.	-5.017130	-1.783815	-0.704432
27.	6.	0.	-5.461306	-0.595634	-0.031549
28.	6.	0.	-4.462569	-0.231079	1.073634

29.	6.	0.	-5.806326	0.513665	-1.063833
30.	6.	0.	-6.279916	1.789272	-0.406802
31.	8.	0.	-5.252822	2.633958	-0.153332
32.	6.	0.	-5.579015	3.884915	0.504356
33.	8.	0.	-7.433351	2.043040	-0.111899
34.	6.	0.	-3.570055	-3.065507	-2.052211
35.	8.	0.	-2.792245	0.940321	-0.319383
36.	8.	0.	-2.548251	-2.539676	0.691312
37.	1.	0.	3.757031	-1.499069	-0.198379
38.	1.	0.	2.515468	0.392640	2.655792
39.	1.	0.	0.106581	0.643575	3.239515
40.	1.	0.	0.749379	-1.512593	-1.920577
41.	1.	0.	3.862958	1.555426	-0.093876
42.	1.	0.	3.482459	0.577622	-1.521527
43.	1.	0.	5.707488	-0.529500	-1.388171
44.	1.	0.	6.235108	1.297500	0.994513
45.	1.	0.	5.924070	-1.726920	0.753539
46.	1.	0.	7.537683	-1.057335	2.541579
47.	1.	0.	6.329717	0.051655	3.226258
48.	1.	0.	6.036801	-1.702587	3.238367
49.	1.	0.	7.896200	0.611246	-0.673543
50.	1.	0.	6.616037	3.463176	-2.040594
51.	1.	0.	4.909984	3.144472	-1.663955
52.	1.	0.	6.151532	3.020267	-0.394053
53.	1.	0.	6.571800	1.836114	-3.806982
54.	1.	0.	4.897897	1.331702	-3.493844

55.	1.	0.	6.219419	0.136349	-3.446313
56.	1.	0.	-3.674341	-0.914050	-2.052209
57.	1.	0.	-6.397210	-0.897004	0.446468
58.	1.	0.	-4.522633	-1.000352	1.849053
59.	1.	0.	-4.725353	0.708363	1.567073
60.	1.	0.	-4.944252	0.741731	-1.691311
61.	1.	0.	-6.616873	0.141690	-1.694077
62.	1.	0.	-4.631422	4.409887	0.608705
63.	1.	0.	-6.023032	3.688516	1.481689
64.	1.	0.	-6.272233	4.457777	-0.113448
65.	1.	0.	-3.593164	-3.904327	-1.350846
66.	1.	0.	-4.407835	-3.175951	-2.746121
67.	1.	0.	-2.637020	-3.100391	-2.613392
68.	1.	0.	-3.371931	1.683136	-0.079133
69.	1.	0.	-3.436987	-2.906132	0.824987

3-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.737056	0.044736	1.938445
2.	6.	0.	2.134082	-0.452588	0.699670
3.	6.	0.	1.136571	-0.851514	-0.220329
4.	6.	0.	-0.234110	-0.777191	0.126908
5.	6.	0.	-0.599513	-0.240902	1.390796
6.	6.	0.	0.384248	0.164079	2.284094
7.	6.	0.	-1.249770	-1.278112	-0.804412
8.	6.	0.	-2.679338	-1.473339	-0.244154

9.	6.	0.	-3.037491	-0.203288	0.571735
10.	6.	0.	-2.035154	-0.065669	1.742341
11.	8.	0.	-2.403725	0.247425	2.866289
12.	8.	0.	-0.964514	-1.604280	-1.966718
13.	8.	0.	1.538466	-1.316358	-1.419826
14.	6.	0.	3.590880	-0.557288	0.304266
15.	6.	0.	4.044864	0.619287	-0.584751
16.	6.	0.	5.547079	0.467603	-0.885603
17.	6.	0.	6.330055	0.341712	0.431447
18.	6.	0.	5.777666	-0.824562	1.264370
19.	8.	0.	4.375357	-0.610439	1.500650
20.	6.	0.	6.447898	-0.969478	2.621106
21.	8.	0.	7.711143	0.119437	0.151019
22.	7.	0.	6.181933	1.485496	-1.743244
23.	6.	0.	5.920545	2.876691	-1.361824
24.	6.	0.	5.931456	1.275093	-3.170419
25.	6.	0.	-3.741034	-1.739236	-1.345874
26.	8.	0.	-5.068804	-1.721577	-0.793842
27.	6.	0.	-5.473712	-0.549688	-0.079181
28.	6.	0.	-4.482082	-0.261891	1.055576
29.	6.	0.	-5.769264	0.609513	-1.075097
30.	6.	0.	-6.188146	1.882496	-0.378354
31.	8.	0.	-5.125448	2.673485	-0.094419
32.	6.	0.	-5.395794	3.912079	0.610357
33.	8.	0.	-7.329437	2.177493	-0.074977
34.	6.	0.	-3.626057	-3.095145	-2.037654

35.	8.	0.	-2.783455	0.906269	-0.303777
36.	8.	0.	-2.622209	-2.522369	0.728321
37.	1.	0.	3.734011	-1.494175	-0.255349
38.	1.	0.	2.501961	0.348262	2.643938
39.	1.	0.	0.094457	0.581113	3.241848
40.	1.	0.	0.722688	-1.516723	-1.944989
41.	1.	0.	3.842738	1.555145	-0.052032
42.	1.	0.	3.461031	0.624289	-1.510297
43.	1.	0.	5.687772	-0.484291	-1.415823
44.	1.	0.	6.215202	1.260628	1.027617
45.	1.	0.	5.903658	-1.753925	0.685059
46.	1.	0.	6.019727	-1.814336	3.168583
47.	1.	0.	7.519387	-1.143831	2.493310
48.	1.	0.	6.310572	-0.060312	3.216390
49.	1.	0.	7.875290	0.634254	-0.662279
50.	1.	0.	6.591706	3.530466	-1.926945
51.	1.	0.	4.884884	3.195213	-1.568067
52.	1.	0.	6.122039	3.028877	-0.298673
53.	1.	0.	6.552050	1.965229	-3.750467
54.	1.	0.	4.879077	1.445795	-3.457521
55.	1.	0.	6.203715	0.253087	-3.449375
56.	1.	0.	-3.632627	-0.943124	-2.092338
57.	1.	0.	-6.426632	-0.832564	0.376561
58.	1.	0.	-4.563172	-1.073395	1.783192
59.	1.	0.	-4.732588	0.658749	1.589383
60.	1.	0.	-4.897561	0.814458	-1.697659

61.	1.	0.	-6.595454	0.292618	-1.715010
62.	1.	0.	-4.425204	4.387706	0.737502
63.	1.	0.	-5.852944	3.699055	1.578060
64.	1.	0.	-6.058480	4.540155	0.013083
65.	1.	0.	-3.800130	-3.914274	-1.331852
66.	1.	0.	-4.396809	-3.161893	-2.810193
67.	1.	0.	-2.649762	-3.218230	-2.506560
68.	1.	0.	-3.356937	1.653573	-0.059992
69.	1.	0.	-2.451803	-3.369149	0.291096

3-e		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-1.904541	-0.729967	-1.796119
2.	6.	0.	-2.278335	-0.664524	-0.455924
3.	6.	0.	-1.264592	-0.664691	0.530655
4.	6.	0.	0.098180	-0.763207	0.160770
5.	6.	0.	0.440126	-0.801056	-1.216927
6.	6.	0.	-0.558894	-0.785074	-2.182483
7.	6.	0.	1.132389	-0.850922	1.197001
8.	6.	0.	2.546287	-1.287643	0.741276
9.	6.	0.	2.900133	-0.467168	-0.527525
10.	6.	0.	1.868615	-0.806626	-1.631887
11.	8.	0.	2.215989	-0.989759	-2.790737
12.	8.	0.	0.871358	-0.660764	2.394327
13.	8.	0.	-1.643317	-0.583623	1.821645
14.	6.	0.	-3.727011	-0.562822	-0.031996

15.	6.	0.	-4.152659	0.894982	0.241701
16.	6.	0.	-5.650454	0.922870	0.596927
17.	6.	0.	-6.460337	0.228124	-0.509622
18.	6.	0.	-5.934566	-1.197200	-0.735886
19.	8.	0.	-4.536267	-1.134507	-1.065631
20.	6.	0.	-6.634904	-1.927264	-1.870513
21.	8.	0.	-7.837265	0.178401	-0.139165
22.	7.	0.	-6.257869	2.231183	0.905447
23.	6.	0.	-5.994184	3.290594	-0.073220
24.	6.	0.	-5.977145	2.691711	2.266611
25.	6.	0.	3.637951	-1.106762	1.830316
26.	8.	0.	4.932613	-1.394423	1.283358
27.	6.	0.	5.358996	-0.612320	0.157981
28.	6.	0.	4.335196	-0.724362	-0.981558
29.	6.	0.	5.740008	0.813999	0.594583
30.	6.	0.	6.563365	1.550162	-0.440041
31.	8.	0.	6.558670	2.875991	-0.216419
32.	6.	0.	7.361063	3.689015	-1.104891
33.	8.	0.	7.182012	1.028184	-1.353344
34.	6.	0.	3.506680	-2.029668	3.039515
35.	8.	0.	2.678723	0.902766	-0.147127
36.	8.	0.	2.453361	-2.639947	0.282243
37.	1.	0.	-3.865398	-1.147021	0.890000
38.	1.	0.	-2.682044	-0.732349	-2.551500
39.	1.	0.	-0.286391	-0.804062	-3.231562
40.	1.	0.	-0.817573	-0.562306	2.368322

41.	1.	0.	-3.950365	1.490609	-0.655323
42.	1.	0.	-3.551215	1.302840	1.060192
43.	1.	0.	-5.791144	0.318528	1.503597
44.	1.	0.	-6.350438	0.776036	-1.458646
45.	1.	0.	-6.054586	-1.763711	0.202003
46.	1.	0.	-7.703794	-2.012823	-1.658453
47.	1.	0.	-6.508756	-1.384236	-2.813458
48.	1.	0.	-6.221077	-2.933159	-1.988052
49.	1.	0.	-7.981978	1.008594	0.353836
50.	1.	0.	-6.647575	4.141533	0.141911
51.	1.	0.	-4.951887	3.650502	-0.051910
52.	1.	0.	-6.217921	2.945048	-1.085446
53.	1.	0.	-6.579178	3.581156	2.477112
54.	1.	0.	-4.917320	2.956871	2.426146
55.	1.	0.	-6.251240	1.914920	2.986219
56.	1.	0.	3.589717	-0.062961	2.165411
57.	1.	0.	6.276459	-1.105926	-0.171300
58.	1.	0.	4.384983	-1.737399	-1.389078
59.	1.	0.	4.588995	-0.045972	-1.801653
60.	1.	0.	4.872577	1.422713	0.854834
61.	1.	0.	6.361889	0.738078	1.496099
62.	1.	0.	7.227410	4.711949	-0.757243
63.	1.	0.	7.009041	3.583401	-2.132874
64.	1.	0.	8.410663	3.395267	-1.040560
65.	1.	0.	3.613720	-3.080740	2.749902
66.	1.	0.	4.314289	-1.803424	3.740885

67.	1.	0.	2.551851	-1.887249	3.545133
68.	1.	0.	2.891605	1.483215	-0.892958
69.	1.	0.	2.326537	-3.235865	1.034627

w

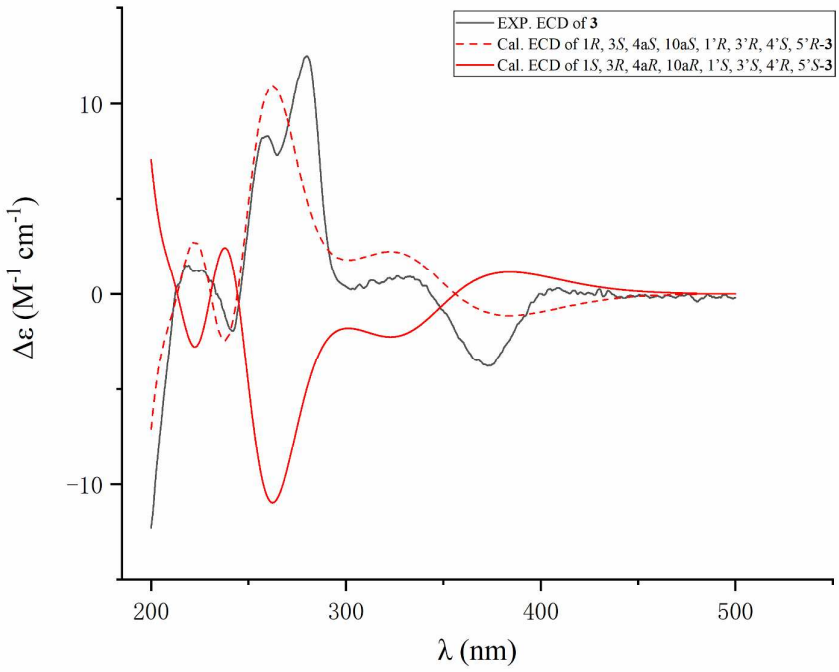
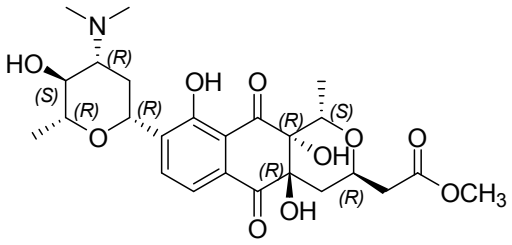


Figure S41. Comparison of the calculated ECD spectra for 1*R*, 3*R*, 4a*S*, 10a*S*, 1′*R*, 3′*R*, 4′*S*, 5′*R* and its enantiomer with the experimental spectrum of **3**.



E-3

Table S11. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **E-3**.

Conformers	In MeOH	
	ΔG	P (%)
E-3-a	0	93.42
E-3-b	0.97	2.00
E-3-c	1.16	3.02
E-3-d	1.08	1.29
E-3-e	1.56	0.26

[a] B3LYP/6-31+G (d, p), in kcal/mol. [b] From ΔG values at 298.15K.

Table S12. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **E-3** at B3LYP/6-311+G(d,p) level of theory in CH_3OH.

E-3-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.721279	-1.666387	0.927684
2.	6.	0.	2.126671	-0.716192	-0.004753
3.	6.	0.	1.175399	0.212401	-0.485841
4.	6.	0.	-0.155643	0.187883	-0.002154
5.	6.	0.	-0.537689	-0.814304	0.926946
6.	6.	0.	0.400078	-1.728277	1.387309
7.	6.	0.	-1.106055	1.208300	-0.445758
8.	6.	0.	-2.427380	1.323500	0.341876
9.	6.	0.	-2.984908	-0.112946	0.552465
10.	6.	0.	-1.956211	-0.929247	1.365287
11.	8.	0.	-2.302226	-1.693014	2.254432
12.	8.	0.	-0.843111	1.983176	-1.375991
13.	8.	0.	1.580233	1.112745	-1.398060
14.	6.	0.	3.551015	-0.645052	-0.511532

15.	6.	0.	4.346939	0.501679	0.148265
16.	6.	0.	5.800041	0.455802	-0.353773
17.	6.	0.	6.393517	-0.941604	-0.111620
18.	6.	0.	5.508242	-2.004278	-0.777365
19.	8.	0.	4.175296	-1.903372	-0.257549
20.	6.	0.	5.984586	-3.425520	-0.526423
21.	8.	0.	7.706065	-1.002907	-0.648202
22.	7.	0.	6.737494	1.477378	0.147219
23.	6.	0.	6.747098	1.653122	1.601179
24.	6.	0.	6.610287	2.763503	-0.536821
25.	6.	0.	-3.481241	2.222633	-0.348038
26.	8.	0.	-4.703650	2.174801	0.414633
27.	6.	0.	-5.316024	0.885759	0.566983
28.	6.	0.	-4.336538	-0.065311	1.261223
29.	6.	0.	-5.912978	0.414463	-0.790741
30.	6.	0.	-6.351139	-1.030191	-0.793173
31.	8.	0.	-7.675314	-1.175630	-0.762124
32.	6.	0.	-8.174938	-2.533663	-0.756776
33.	8.	0.	-5.574131	-1.979974	-0.815196
34.	6.	0.	-3.121531	3.702632	-0.423540
35.	8.	0.	-3.056712	-0.719567	-0.741241
36.	8.	0.	-2.052321	1.853955	1.618090
37.	1.	0.	3.525142	-0.465555	-1.598163
38.	1.	0.	2.452318	-2.385507	1.278011
39.	1.	0.	0.089302	-2.494242	2.088355
40.	1.	0.	0.779050	1.637945	-1.653521

41.	1.	0.	4.304526	0.369695	1.234911
42.	1.	0.	3.875459	1.458603	-0.094564
43.	1.	0.	5.783663	0.589592	-1.444144
44.	1.	0.	6.405646	-1.158134	0.970393
45.	1.	0.	5.491516	-1.803454	-1.861682
46.	1.	0.	5.329317	-4.143462	-1.027353
47.	1.	0.	7.000770	-3.550996	-0.907592
48.	1.	0.	5.985095	-3.644458	0.546424
49.	1.	0.	8.047110	-0.099472	-0.502882
50.	1.	0.	7.604540	2.273690	1.878706
51.	1.	0.	5.838262	2.142574	1.987990
52.	1.	0.	6.855954	0.689042	2.103500
53.	1.	0.	7.428712	3.420570	-0.226219
54.	1.	0.	5.662111	3.284883	-0.319815
55.	1.	0.	6.681544	2.618171	-1.618472
56.	1.	0.	-3.643091	1.834522	-1.359722
57.	1.	0.	-6.153499	1.066431	1.246684
58.	1.	0.	-4.739561	-1.075467	1.352915
59.	1.	0.	-4.183242	0.293940	2.282748
60.	1.	0.	-6.753443	1.061510	-1.045282
61.	1.	0.	-5.156784	0.496510	-1.573422
62.	1.	0.	-7.808372	-3.066425	0.122279
63.	1.	0.	-7.856487	-3.055427	-1.660847
64.	1.	0.	-9.258878	-2.442275	-0.727316
65.	1.	0.	-2.255833	3.853384	-1.066540
66.	1.	0.	-3.974041	4.251115	-0.832068

67.	1.	0.	-2.898520	4.103498	0.568681
68.	1.	0.	-3.812957	-1.343482	-0.758101
69.	1.	0.	-2.858085	2.227100	2.009774

E-3-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.848994	-1.722586	0.849064
2.	6.	0.	2.234712	-0.744021	-0.062204
3.	6.	0.	1.263364	0.171413	-0.528693
4.	6.	0.	-0.067312	0.106508	-0.048908
5.	6.	0.	-0.427871	-0.921395	0.859640
6.	6.	0.	0.528746	-1.824602	1.303181
7.	6.	0.	-1.041989	1.111455	-0.474520
8.	6.	0.	-2.359843	1.190110	0.323135
9.	6.	0.	-2.897795	-0.254739	0.520344
10.	6.	0.	-1.841530	-1.076131	1.295891
11.	8.	0.	-2.171545	-1.873721	2.161105
12.	8.	0.	-0.797818	1.905319	-1.393073
13.	8.	0.	1.649666	1.098352	-1.421944
14.	6.	0.	3.660198	-0.629770	-0.557753
15.	6.	0.	4.427808	0.511967	0.143554
16.	6.	0.	5.888487	0.506178	-0.339146
17.	6.	0.	6.503125	-0.887507	-0.130890
18.	6.	0.	5.646394	-1.944285	-0.841498
19.	8.	0.	4.305561	-1.883299	-0.335942
20.	6.	0.	6.144278	-3.364240	-0.628084

21.	8.	0.	7.824211	-0.909257	-0.649278
22.	7.	0.	6.800347	1.527609	0.207478
23.	6.	0.	6.788070	1.655510	1.666517
24.	6.	0.	6.658578	2.833251	-0.435403
25.	6.	0.	-3.448319	2.079906	-0.323989
26.	8.	0.	-4.594842	2.044908	0.546262
27.	6.	0.	-5.236860	0.766282	0.689168
28.	6.	0.	-4.241765	-0.256635	1.253403
29.	6.	0.	-5.949004	0.350141	-0.607763
30.	6.	0.	-7.000164	-0.714149	-0.373403
31.	8.	0.	-7.551167	-1.109033	-1.534831
32.	6.	0.	-8.584196	-2.111476	-1.436327
33.	8.	0.	-7.325025	-1.161668	0.710933
34.	6.	0.	-3.094330	3.556819	-0.459002
35.	8.	0.	-2.983020	-0.804586	-0.803780
36.	8.	0.	-1.991256	1.708343	1.604511
37.	1.	0.	3.638587	-0.418258	-1.638569
38.	1.	0.	2.595854	-2.431140	1.187081
39.	1.	0.	0.234170	-2.611446	1.987784
40.	1.	0.	0.837016	1.607825	-1.672002
41.	1.	0.	4.374051	0.349469	1.225497
42.	1.	0.	3.942297	1.466961	-0.078812
43.	1.	0.	5.885562	0.673480	-1.424960
44.	1.	0.	6.503302	-1.137241	0.943999
45.	1.	0.	5.639940	-1.710078	-1.919206
46.	1.	0.	7.166754	-3.461326	-1.000499

47.	1.	0.	6.135792	-3.615686	0.437595
48.	1.	0.	5.507083	-4.077268	-1.158494
49.	1.	0.	8.146872	-0.005032	-0.470889
50.	1.	0.	7.631136	2.280760	1.975800
51.	1.	0.	5.866164	2.116988	2.056721
52.	1.	0.	6.906760	0.677497	2.138848
53.	1.	0.	7.461172	3.493801	-0.092569
54.	1.	0.	5.698641	3.330439	-0.213550
55.	1.	0.	6.745928	2.725379	-1.520244
56.	1.	0.	-3.697975	1.664802	-1.306823
57.	1.	0.	-6.008430	0.939273	1.443527
58.	1.	0.	-4.669296	-1.262967	1.242580
59.	1.	0.	-4.056145	-0.018465	2.304634
60.	1.	0.	-6.451323	1.226365	-1.034228
61.	1.	0.	-5.252968	-0.018070	-1.365379
62.	1.	0.	-9.420071	-1.741482	-0.838932
63.	1.	0.	-8.189742	-3.022599	-0.981762
64.	1.	0.	-8.903359	-2.303648	-2.459428
65.	1.	0.	-3.986273	4.100913	-0.779969
66.	1.	0.	-2.765868	3.968470	0.499100
67.	1.	0.	-2.301781	3.698482	-1.191597
68.	1.	0.	-3.338140	-1.703894	-0.743875
69.	1.	0.	-2.806917	2.073534	1.986669

E-3-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z

1.	6.	0.	1.671329	-1.652244	0.913329
2.	6.	0.	2.082437	-0.698985	-0.013372
3.	6.	0.	1.132718	0.227483	-0.501962
4.	6.	0.	-0.202389	0.198681	-0.029897
5.	6.	0.	-0.589719	-0.806034	0.894396
6.	6.	0.	0.346225	-1.718879	1.360849
7.	6.	0.	-1.150985	1.217827	-0.479523
8.	6.	0.	-2.477953	1.331304	0.299458
9.	6.	0.	-3.037096	-0.104257	0.509914
10.	6.	0.	-2.010264	-0.925263	1.321864
11.	8.	0.	-2.363081	-1.693785	2.204035
12.	8.	0.	-0.882385	1.994465	-1.406381
13.	8.	0.	1.543150	1.130025	-1.409095
14.	6.	0.	3.511623	-0.621748	-0.505340
15.	6.	0.	4.295511	0.527573	0.164503
16.	6.	0.	5.754677	0.487635	-0.320245
17.	6.	0.	6.350477	-0.907806	-0.072626
18.	6.	0.	5.477283	-1.972876	-0.750336
19.	8.	0.	4.137912	-1.877827	-0.246000
20.	6.	0.	5.955982	-3.392685	-0.495910
21.	8.	0.	7.669598	-0.963491	-0.593418
22.	7.	0.	6.682071	1.512061	0.193567
23.	6.	0.	6.671821	1.686917	1.647639
24.	6.	0.	6.559629	2.798216	-0.491336
25.	6.	0.	-3.533108	2.228030	-0.391770
26.	8.	0.	-4.741742	2.192130	0.393701

27.	6.	0.	-5.367617	0.910823	0.544757
28.	6.	0.	-4.390572	-0.060696	1.216247
29.	6.	0.	-5.988789	0.444504	-0.800278
30.	6.	0.	-6.670601	-0.899026	-0.681818
31.	8.	0.	-5.810029	-1.915265	-0.947895
32.	6.	0.	-6.349563	-3.252685	-0.833269
33.	8.	0.	-7.827778	-1.080234	-0.366937
34.	6.	0.	-3.168568	3.705446	-0.488453
35.	8.	0.	-3.105763	-0.698858	-0.792887
36.	8.	0.	-2.113383	1.862092	1.577647
37.	1.	0.	3.496557	-0.441021	-1.591975
38.	1.	0.	2.401275	-2.369701	1.269210
39.	1.	0.	0.031576	-2.487068	2.057686
40.	1.	0.	0.743128	1.653831	-1.670901
41.	1.	0.	4.240936	0.394747	1.250481
42.	1.	0.	3.823391	1.482925	-0.083179
43.	1.	0.	5.751068	0.622792	-1.410550
44.	1.	0.	6.350388	-1.125682	1.009175
45.	1.	0.	5.472505	-1.770459	-1.834477
46.	1.	0.	5.309041	-4.112318	-1.005171
47.	1.	0.	6.976838	-3.513924	-0.865773
48.	1.	0.	5.945214	-3.613097	0.576582
49.	1.	0.	8.005596	-0.059107	-0.442420
50.	1.	0.	7.523681	2.309741	1.937026
51.	1.	0.	5.756479	2.173532	2.022484
52.	1.	0.	6.776627	0.722845	2.150849

53.	1.	0.	7.371644	3.457811	-0.169477
54.	1.	0.	5.606931	3.316321	-0.286655
55.	1.	0.	6.645809	2.653872	-1.572030
56.	1.	0.	-3.714736	1.827828	-1.395012
57.	1.	0.	-6.194719	1.095206	1.236475
58.	1.	0.	-4.799685	-1.071297	1.289422
59.	1.	0.	-4.232006	0.271960	2.245840
60.	1.	0.	-6.741688	1.177775	-1.095933
61.	1.	0.	-5.225315	0.382149	-1.575530
62.	1.	0.	-7.187672	-3.377514	-1.520639
63.	1.	0.	-6.682956	-3.439483	0.189075
64.	1.	0.	-5.532368	-3.920518	-1.098765
65.	1.	0.	-2.318733	3.847270	-1.154040
66.	1.	0.	-4.029220	4.253755	-0.879698
67.	1.	0.	-2.918724	4.113380	0.494479
68.	1.	0.	-3.791200	-1.388356	-0.790484
69.	1.	0.	-2.921088	2.245833	1.955868

E-3-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.645521	-1.612803	0.959944
2.	6.	0.	2.054878	-0.676804	0.015647
3.	6.	0.	1.108601	0.253003	-0.474926
4.	6.	0.	-0.223427	0.238089	0.003873
5.	6.	0.	-0.608670	-0.748291	0.948857
6.	6.	0.	0.324350	-1.659846	1.422473

7.	6.	0.	-1.173857	1.251725	-0.462815
8.	6.	0.	-2.501635	1.381287	0.319034
9.	6.	0.	-3.047903	-0.048923	0.554050
10.	6.	0.	-2.025829	-0.844797	1.395402
11.	8.	0.	-2.377640	-1.578644	2.306448
12.	8.	0.	-0.895188	2.030052	-1.387119
13.	8.	0.	1.521048	1.143223	-1.394037
14.	6.	0.	3.479361	-0.618598	-0.492185
15.	6.	0.	4.283362	0.525971	0.161479
16.	6.	0.	5.735796	0.467988	-0.341089
17.	6.	0.	6.320139	-0.932296	-0.093179
18.	6.	0.	5.426908	-1.992070	-0.752896
19.	8.	0.	4.095333	-1.879850	-0.231860
20.	6.	0.	5.894356	-3.415279	-0.496298
21.	8.	0.	7.631557	-1.004996	-0.631034
22.	7.	0.	6.680481	1.485418	0.154651
23.	6.	0.	6.693183	1.666983	1.607845
24.	6.	0.	6.560802	2.769546	-0.534477
25.	6.	0.	-3.556024	2.261470	-0.404230
26.	8.	0.	-4.826616	2.193283	0.260134
27.	6.	0.	-5.399260	0.899226	0.451483
28.	6.	0.	-4.419031	0.003432	1.218670
29.	6.	0.	-5.944612	0.346883	-0.896470
30.	6.	0.	-6.573951	-1.018775	-0.753809
31.	8.	0.	-5.656073	-2.008388	-0.914310
32.	6.	0.	-6.142898	-3.361865	-0.760049

33.	8.	0.	-7.739463	-1.239467	-0.501048
34.	6.	0.	-3.222214	3.750015	-0.439265
35.	8.	0.	-3.073559	-0.671027	-0.737162
36.	8.	0.	-2.190460	1.865082	1.626812
37.	1.	0.	3.454383	-0.444671	-1.579690
38.	1.	0.	2.372690	-2.331344	1.319460
39.	1.	0.	0.010922	-2.412212	2.137025
40.	1.	0.	0.724386	1.674095	-1.652412
41.	1.	0.	4.240572	0.399561	1.248791
42.	1.	0.	3.818187	1.484846	-0.085809
43.	1.	0.	5.719598	0.596986	-1.432055
44.	1.	0.	6.332159	-1.143916	0.989816
45.	1.	0.	5.409987	-1.796051	-1.838091
46.	1.	0.	5.233840	-4.131168	-0.993264
47.	1.	0.	6.909226	-3.548921	-0.878209
48.	1.	0.	5.894887	-3.629604	0.577478
49.	1.	0.	7.979151	-0.103352	-0.490257
50.	1.	0.	7.555217	2.282770	1.881769
51.	1.	0.	5.788230	2.164194	1.993901
52.	1.	0.	6.796137	0.704223	2.113920
53.	1.	0.	7.383803	3.422584	-0.227492
54.	1.	0.	5.616265	3.297931	-0.318522
55.	1.	0.	6.629872	2.619339	-1.615602
56.	1.	0.	-3.640275	1.883839	-1.430802
57.	1.	0.	-6.264640	1.079170	1.096688
58.	1.	0.	-4.806211	-1.010118	1.349463

59.	1.	0.	-4.293619	0.423364	2.219638
60.	1.	0.	-6.716270	1.033738	-1.249502
61.	1.	0.	-5.146005	0.295319	-1.636539
62.	1.	0.	-6.922188	-3.564465	-1.496357
63.	1.	0.	-6.541290	-3.507745	0.245489
64.	1.	0.	-5.279959	-4.003169	-0.928312
65.	1.	0.	-2.281130	3.930229	-0.957966
66.	1.	0.	-4.022944	4.280568	-0.960302
67.	1.	0.	-3.166962	4.157055	0.575494
68.	1.	0.	-3.748151	-1.372225	-0.734035
69.	1.	0.	-1.842430	2.765447	1.556738

E-3-e		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.805177	-1.671154	0.959647
2.	6.	0.	2.192924	-0.736323	0.004978
3.	6.	0.	1.229723	0.177888	-0.482501
4.	6.	0.	-0.095392	0.151137	0.012724
5.	6.	0.	-0.458711	-0.833309	0.967398
6.	6.	0.	0.489598	-1.732025	1.435889
7.	6.	0.	-1.064628	1.150390	-0.446802
8.	6.	0.	-2.377195	1.275940	0.361960
9.	6.	0.	-2.915307	-0.156177	0.606370
10.	6.	0.	-1.869132	-0.943544	1.429561
11.	8.	0.	-2.203120	-1.681300	2.344141
12.	8.	0.	-0.810198	1.920351	-1.384443

13.	8.	0.	1.620253	1.065229	-1.414207
14.	6.	0.	3.611448	-0.664602	-0.517718
15.	6.	0.	4.405115	0.500779	0.111666
16.	6.	0.	5.853857	0.455310	-0.402980
17.	6.	0.	6.459758	-0.932521	-0.138241
18.	6.	0.	5.576514	-2.014647	-0.774690
19.	8.	0.	4.247450	-1.913089	-0.245173
20.	6.	0.	6.065742	-3.426978	-0.499501
21.	8.	0.	7.767819	-0.995458	-0.685402
22.	7.	0.	6.788381	1.493560	0.068174
23.	6.	0.	6.810433	1.699719	1.517964
24.	6.	0.	6.645890	2.764325	-0.641156
25.	6.	0.	-3.454263	2.151609	-0.330522
26.	8.	0.	-4.681061	2.101854	0.405712
27.	6.	0.	-5.274054	0.813171	0.597949
28.	6.	0.	-4.279863	-0.129898	1.290398
29.	6.	0.	-5.898260	0.289960	-0.706903
30.	6.	0.	-6.889917	-0.829413	-0.473783
31.	8.	0.	-7.292980	-1.367716	-1.639226
32.	6.	0.	-8.267564	-2.426952	-1.542701
33.	8.	0.	-7.295126	-1.201913	0.612095
34.	6.	0.	-3.113116	3.636944	-0.413980
35.	8.	0.	-2.958264	-0.755979	-0.698490
36.	8.	0.	-2.040960	1.757865	1.663640
37.	1.	0.	3.573523	-0.506647	-1.607336
38.	1.	0.	2.545097	-2.377895	1.316337

39.	1.	0.	0.192847	-2.484159	2.157727
40.	1.	0.	0.813902	1.582658	-1.668823
41.	1.	0.	4.373623	0.390077	1.201093
42.	1.	0.	3.924355	1.449217	-0.145723
43.	1.	0.	5.826266	0.566859	-1.495637
44.	1.	0.	6.483046	-1.127090	0.947771
45.	1.	0.	5.548777	-1.835711	-1.862600
46.	1.	0.	5.412120	-4.159792	-0.980653
47.	1.	0.	7.079816	-3.552190	-0.886317
48.	1.	0.	6.076516	-3.624415	0.577444
49.	1.	0.	8.103580	-0.086798	-0.562064
50.	1.	0.	7.665407	2.332836	1.773939
51.	1.	0.	5.901450	2.190051	1.903341
52.	1.	0.	6.932026	0.747344	2.039313
53.	1.	0.	7.462557	3.433173	-0.351831
54.	1.	0.	5.696174	3.283639	-0.425962
55.	1.	0.	6.708122	2.597057	-1.720175
56.	1.	0.	-3.594192	1.752057	-1.343470
57.	1.	0.	-6.095866	0.998308	1.295009
58.	1.	0.	-4.685140	-1.143766	1.353323
59.	1.	0.	-4.134084	0.215235	2.317101
60.	1.	0.	-6.439752	1.114253	-1.186876
61.	1.	0.	-5.146394	-0.053377	-1.420433
62.	1.	0.	-9.180072	-2.064920	-1.064359
63.	1.	0.	-7.865959	-3.264185	-0.968050
64.	1.	0.	-8.470703	-2.731811	-2.568084

65.	1.	0.	-3.938774	4.160943	-0.901777
66.	1.	0.	-3.003829	4.065548	0.587718
67.	1.	0.	-2.199811	3.802441	-0.984037
68.	1.	0.	-3.316744	-1.651738	-0.613193
69.	1.	0.	-1.729714	2.671357	1.590722

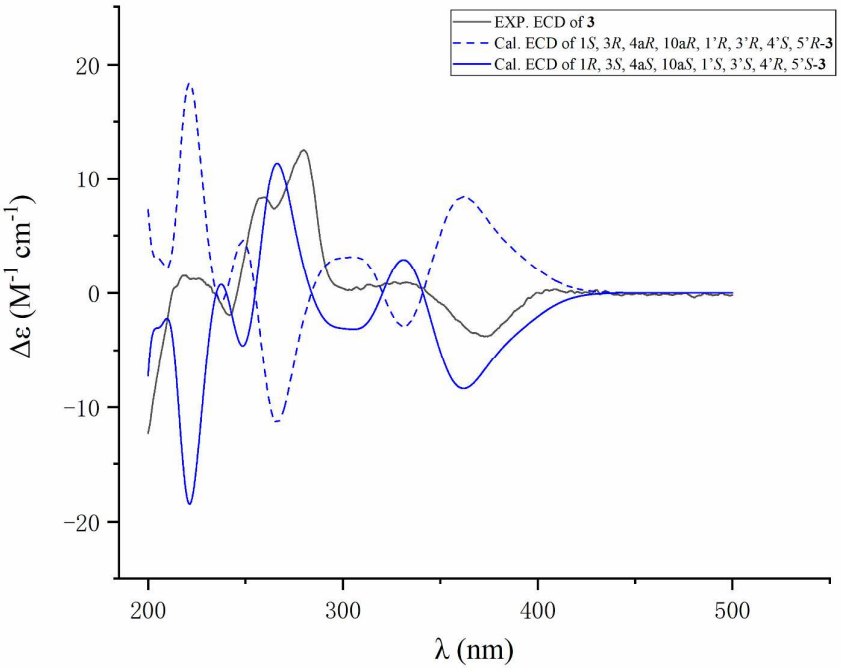
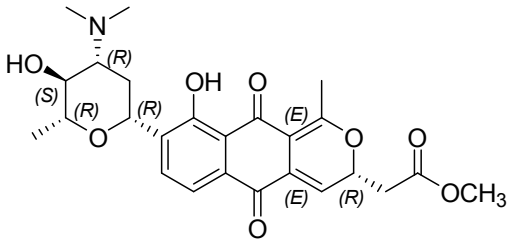


Figure S42. Comparison of the calculated ECD spectra for 1*S*, 3*S*, 4a*R*, 10a*R*, 1′*R*, 3′*R*, 4′*S*, 5′*R* and its enantiomer with the experimental spectrum of **3**.



Strepoxepinmycin D (4)

Table S13. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **4.**

Conformers	In MeOH	
	ΔG	P (%)
4.-a	0.97	22.00
4-b	0	49.94
4.-c	1.05	18.55
4-d	2.56	5.99
13E.-e	2.75	3.51

[a] B3LYP/6-31+G (d, p), in kcal/mol. [b]From ΔG values at 298.15K.

Table S14. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **4** at B3LYP/6-311+G (d, p) level of theory in CH_3OH.

4-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.774498	-1.876958	0.463590
2.	6.	0.	2.176775	-0.781096	-0.301037
3.	6.	0.	1.188392	0.025694	-0.906236
4.	6.	0.	-0.192370	-0.267236	-0.740934
5.	6.	0.	-0.558106	-1.393977	0.045662
6.	6.	0.	0.424711	-2.187483	0.638697
7.	6.	0.	-1.196632	0.599741	-1.386147
8.	6.	0.	-2.600455	0.298883	-1.167734
9.	6.	0.	-2.963373	-0.895956	-0.395509
10.	6.	0.	-1.977111	-1.736628	0.226077
11.	8.	0.	-2.322749	-2.754769	0.903544
12.	8.	0.	-0.815202	1.571633	-2.100363

13.	8.	0.	1.593380	1.078928	-1.642040
14.	6.	0.	3.634950	-0.421598	-0.483128
15.	6.	0.	4.081261	0.706872	0.469972
16.	6.	0.	5.584576	0.969632	0.269400
17.	6.	0.	6.368478	-0.341156	0.442102
18.	6.	0.	5.824343	-1.412557	-0.514774
19.	8.	0.	4.421421	-1.598963	-0.263655
20.	6.	0.	6.497000	-2.766257	-0.351786
21.	8.	0.	7.751329	-0.113808	0.172562
22.	7.	0.	6.211646	2.031179	1.079541
23.	6.	0.	5.937142	1.966586	2.518149
24.	6.	0.	5.965470	3.376706	0.557467
25.	6.	0.	-3.603761	1.136255	-1.600409
26.	8.	0.	-4.903682	0.842482	-1.392487
27.	6.	0.	-5.361891	-0.467896	-0.979024
28.	6.	0.	-4.289712	-1.235560	-0.255271
29.	6.	0.	-3.465296	2.461031	-2.277888
30.	8.	0.	-4.696302	-2.291051	0.418226
31.	6.	0.	-6.660959	-0.272134	-0.203076
32.	6.	0.	-6.490618	0.466966	1.109897
33.	8.	0.	-7.677178	0.863577	1.591208
34.	6.	0.	-7.667586	1.546187	2.868719
35.	8.	0.	-5.428181	0.662731	1.673108
36.	1.	0.	3.785331	-0.084076	-1.519719
37.	1.	0.	2.536033	-2.500136	0.918400
38.	1.	0.	0.125490	-3.044103	1.230986

39.	1.	0.	0.747986	1.502924	-1.988800
40.	1.	0.	3.869949	0.394601	1.498768
41.	1.	0.	3.496944	1.608953	0.263536
42.	1.	0.	5.734331	1.278452	-0.774283
43.	1.	0.	6.248182	-0.720942	1.468962
44.	1.	0.	5.957764	-1.052626	-1.548278
45.	1.	0.	6.357726	-3.144737	0.666713
46.	1.	0.	6.071824	-3.488975	-1.054554
47.	1.	0.	7.568909	-2.679386	-0.547475
48.	1.	0.	7.910935	0.793020	0.497395
49.	1.	0.	6.605138	2.660552	3.037333
50.	1.	0.	4.899879	2.240433	2.774122
51.	1.	0.	6.132980	0.962974	2.903539
52.	1.	0.	4.912158	3.693503	0.651897
53.	1.	0.	6.247061	3.423713	-0.498416
54.	1.	0.	6.581056	4.095174	1.107809
55.	1.	0.	-5.604199	-1.024700	-1.896451
56.	1.	0.	-3.170536	2.322064	-3.323860
57.	1.	0.	-2.687257	3.066473	-1.810985
58.	1.	0.	-4.425879	2.978638	-2.247695
59.	1.	0.	-3.823791	-2.714648	0.775905
60.	1.	0.	-7.378567	0.261492	-0.831552
61.	1.	0.	-7.099480	-1.252663	0.010373
62.	1.	0.	-7.077296	2.461738	2.800106
63.	1.	0.	-7.254625	0.893363	3.639952
64.	1.	0.	-8.710604	1.776243	3.077996

4-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.038212	-1.931691	-0.449451
2.	6.	0.	-2.310577	-0.764077	0.263885
3.	6.	0.	-1.229439	0.012272	0.736805
4.	6.	0.	0.112909	-0.389651	0.502022
5.	6.	0.	0.345239	-1.583863	-0.234284
6.	6.	0.	-0.727873	-2.341476	-0.703842
7.	6.	0.	1.216516	0.433817	1.032655
8.	6.	0.	2.578070	-0.027976	0.820706
9.	6.	0.	2.807616	-1.217670	-0.009411
10.	6.	0.	1.721809	-2.020583	-0.517464
11.	8.	0.	1.951081	-3.061684	-1.201101
12.	8.	0.	0.954320	1.500315	1.657949
13.	8.	0.	-1.510887	1.138405	1.419848
14.	6.	0.	-3.725644	-0.296924	0.525910
15.	6.	0.	-4.176161	0.790260	-0.472744
16.	6.	0.	-5.643951	1.159434	-0.188528
17.	6.	0.	-6.511706	-0.109217	-0.205572
18.	6.	0.	-5.960046	-1.140401	0.789799
19.	8.	0.	-4.594172	-1.433520	0.451537
20.	6.	0.	-6.721584	-2.456170	0.781598
21.	8.	0.	-7.855770	0.222118	0.140557
22.	7.	0.	-6.267522	2.196035	-1.032937
23.	6.	0.	-6.107453	2.006267	-2.477948

24.	6.	0.	-5.902511	3.558151	-0.639385
25.	6.	0.	3.656929	0.555032	1.445680
26.	8.	0.	4.911947	0.096489	1.244044
27.	6.	0.	5.260273	-0.748746	0.119743
28.	6.	0.	4.094322	-1.587499	-0.315585
29.	6.	0.	3.654072	1.663714	2.446608
30.	8.	0.	4.399991	-2.655047	-1.030933
31.	6.	0.	5.805314	0.113983	-1.025917
32.	6.	0.	7.135089	0.755438	-0.673689
33.	8.	0.	7.313310	1.901661	-1.343574
34.	6.	0.	8.577491	2.581831	-1.146585
35.	8.	0.	7.953557	0.278914	0.092748
36.	1.	0.	-3.774400	0.119952	1.543164
37.	1.	0.	-2.870033	-2.529595	-0.803886
38.	1.	0.	-0.530001	-3.247468	-1.264380
39.	1.	0.	-0.618282	1.531741	1.667445
40.	1.	0.	-4.058851	0.397146	-1.488768
41.	1.	0.	-3.527732	1.666145	-0.372368
42.	1.	0.	-5.698189	1.552045	0.836160
43.	1.	0.	-6.488277	-0.568840	-1.206140
44.	1.	0.	-5.990609	-0.698638	1.799402
45.	1.	0.	-6.686408	-2.914839	-0.212541
46.	1.	0.	-6.285042	-3.152541	1.503701
47.	1.	0.	-7.767660	-2.286490	1.049639
48.	1.	0.	-7.987516	1.111643	-0.239882
49.	1.	0.	-6.771532	2.700593	-3.001650

50.	1.	0.	-5.078345	2.193866	-2.827236
51.	1.	0.	-6.389341	0.991045	-2.767599
52.	1.	0.	-4.843020	3.798465	-0.836220
53.	1.	0.	-6.096990	3.702632	0.427212
54.	1.	0.	-6.515844	4.271519	-1.198748
55.	1.	0.	6.057584	-1.396044	0.493780
56.	1.	0.	2.814133	1.576996	3.136077
57.	1.	0.	3.551162	2.629585	1.938595
58.	1.	0.	4.602341	1.655444	2.987893
59.	1.	0.	3.495462	-3.075167	-1.263397
60.	1.	0.	5.976609	-0.530070	-1.897272
61.	1.	0.	5.081929	0.877243	-1.322974
62.	1.	0.	9.401716	1.939736	-1.462561
63.	1.	0.	8.696939	2.852339	-0.095996
64.	1.	0.	8.522891	3.472584	-1.769532

4-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.020334	1.958349	0.299386
2.	6.	0.	-2.299966	0.741196	-0.322447
3.	6.	0.	-1.223958	-0.087118	-0.711869
4.	6.	0.	0.120609	0.311223	-0.483871
5.	6.	0.	0.360183	1.557589	0.157634
6.	6.	0.	-0.707872	2.367452	0.543824
7.	6.	0.	1.219345	-0.570397	-0.923250
8.	6.	0.	2.585262	-0.118144	-0.715466

9.	6.	0.	2.819639	1.132296	0.018366
10.	6.	0.	1.738609	1.994761	0.431002
11.	8.	0.	1.973587	3.086747	1.027119
12.	8.	0.	0.950708	-1.677822	-1.468857
13.	8.	0.	-1.512613	-1.259253	-1.308908
14.	6.	0.	-3.718153	0.276589	-0.572438
15.	6.	0.	-4.202889	-0.723210	0.498895
16.	6.	0.	-5.672492	-1.088584	0.219682
17.	6.	0.	-6.516898	0.192990	0.131492
18.	6.	0.	-5.935127	1.134941	-0.932560
19.	8.	0.	-4.567977	1.429314	-0.600618
20.	6.	0.	-6.671884	2.460958	-1.034858
21.	8.	0.	-7.863148	-0.139486	-0.204175
22.	7.	0.	-6.326847	-2.049657	1.127419
23.	6.	0.	-6.173380	-1.764763	2.557358
24.	6.	0.	-5.991768	-3.443914	0.831701
25.	6.	0.	3.665845	-0.771916	-1.261990
26.	8.	0.	4.925745	-0.322241	-1.062546
27.	6.	0.	5.259524	0.596865	0.005964
28.	6.	0.	4.105897	1.501921	0.326128
29.	6.	0.	3.664626	-1.956593	-2.171472
30.	8.	0.	4.418590	2.621243	0.954182
31.	6.	0.	5.716236	-0.192038	1.246261
32.	6.	0.	6.927404	-1.073106	1.001210
33.	8.	0.	7.895890	-0.424711	0.339431
34.	6.	0.	9.114850	-1.160862	0.075481

35.	8.	0.	7.020599	-2.224903	1.386757
36.	1.	0.	-3.757125	-0.216821	-1.555324
37.	1.	0.	-2.847924	2.595902	0.588456
38.	1.	0.	-0.504405	3.313014	1.032375
39.	1.	0.	-0.623018	-1.685005	-1.508211
40.	1.	0.	-4.095252	-0.254492	1.483520
41.	1.	0.	-3.568085	-1.614483	0.477971
42.	1.	0.	-5.719584	-1.553214	-0.774789
43.	1.	0.	-6.494712	0.725825	1.095228
44.	1.	0.	-5.963392	0.617528	-1.905641
45.	1.	0.	-6.217514	3.089906	-1.806149
46.	1.	0.	-7.719044	2.289222	-1.297217
47.	1.	0.	-6.634841	2.996161	-0.079831
48.	1.	0.	-8.014603	-0.995435	0.240847
49.	1.	0.	-6.860161	-2.403194	3.121326
50.	1.	0.	-5.152479	-1.955207	2.928336
51.	1.	0.	-6.429743	-0.724706	2.773174
52.	1.	0.	-4.939573	-3.694577	1.053168
53.	1.	0.	-6.182597	-3.657160	-0.223955
54.	1.	0.	-6.625705	-4.102275	1.433918
55.	1.	0.	6.091868	1.187637	-0.382262
56.	1.	0.	2.851211	-1.903233	-2.895419
57.	1.	0.	3.516720	-2.875832	-1.593091
58.	1.	0.	4.630152	-2.015987	-2.677863
59.	1.	0.	3.519166	3.078396	1.126159
60.	1.	0.	5.977207	0.529489	2.029359

61.	1.	0.	4.907846	-0.821994	1.622899
62.	1.	0.	8.896828	-2.039358	-0.534490
63.	1.	0.	9.578607	-1.465193	1.015487
64.	1.	0.	9.757161	-0.467339	-0.463969

4-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.020334	1.958349	0.299386
2.	6.	0.	-2.299966	0.741196	-0.322447
3.	6.	0.	-1.223958	-0.087118	-0.711869
4.	6.	0.	0.120609	0.311223	-0.483871
5.	6.	0.	0.360183	1.557589	0.157634
6.	6.	0.	-0.707872	2.367452	0.543824
7.	6.	0.	1.219345	-0.570397	-0.923250
8.	6.	0.	2.585262	-0.118144	-0.715466
9.	6.	0.	2.819639	1.132296	0.018366
10.	6.	0.	1.738609	1.994761	0.431002
11.	8.	0.	1.973587	3.086747	1.027119
12.	8.	0.	0.950708	-1.677822	-1.468857
13.	8.	0.	-1.512613	-1.259253	-1.308908
14.	6.	0.	-3.718153	0.276589	-0.572438
15.	6.	0.	-4.202889	-0.723210	0.498895
16.	6.	0.	-5.672492	-1.088584	0.219682
17.	6.	0.	-6.516898	0.192990	0.131492
18.	6.	0.	-5.935127	1.134941	-0.932560
19.	8.	0.	-4.567977	1.429314	-0.600618

20.	6.	0.	-6.671884	2.460958	-1.034858
21.	8.	0.	-7.863148	-0.139486	-0.204175
22.	7.	0.	-6.326847	-2.049657	1.127419
23.	6.	0.	-6.173380	-1.764763	2.557358
24.	6.	0.	-5.991768	-3.443914	0.831701
25.	6.	0.	3.665845	-0.771916	-1.261990
26.	8.	0.	4.925745	-0.322241	-1.062546
27.	6.	0.	5.259524	0.596865	0.005964
28.	6.	0.	4.105897	1.501921	0.326128
29.	6.	0.	3.664626	-1.956593	-2.171472
30.	8.	0.	4.418590	2.621243	0.954182
31.	6.	0.	5.716236	-0.192038	1.246261
32.	6.	0.	6.927404	-1.073106	1.001210
33.	8.	0.	7.895890	-0.424711	0.339431
34.	6.	0.	9.114850	-1.160862	0.075481
35.	8.	0.	7.020599	-2.224903	1.386757
36.	1.	0.	-3.757125	-0.216821	-1.555324
37.	1.	0.	-2.847924	2.595902	0.588456
38.	1.	0.	-0.504405	3.313014	1.032375
39.	1.	0.	-0.623018	-1.685005	-1.508211
40.	1.	0.	-4.095252	-0.254492	1.483520
41.	1.	0.	-3.568085	-1.614483	0.477971
42.	1.	0.	-5.719584	-1.553214	-0.774789
43.	1.	0.	-6.494712	0.725825	1.095228
44.	1.	0.	-5.963392	0.617528	-1.905641
45.	1.	0.	-6.217514	3.089906	-1.806149

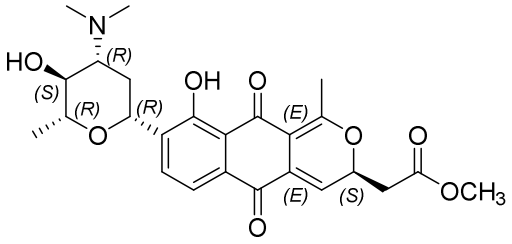
46.	1.	0.	-7.719044	2.289222	-1.297217
47.	1.	0.	-6.634841	2.996161	-0.079831
48.	1.	0.	-8.014603	-0.995435	0.240847
49.	1.	0.	-6.860161	-2.403194	3.121326
50.	1.	0.	-5.152479	-1.955207	2.928336
51.	1.	0.	-6.429743	-0.724706	2.773174
52.	1.	0.	-4.939573	-3.694577	1.053168
53.	1.	0.	-6.182597	-3.657160	-0.223955
54.	1.	0.	-6.625705	-4.102275	1.433918
55.	1.	0.	6.091868	1.187637	-0.382262
56.	1.	0.	2.851211	-1.903233	-2.895419
57.	1.	0.	3.516720	-2.875832	-1.593091
58.	1.	0.	4.630152	-2.015987	-2.677863
59.	1.	0.	3.519166	3.078396	1.126159
60.	1.	0.	5.977207	0.529489	2.029359
61.	1.	0.	4.907846	-0.821994	1.622899
62.	1.	0.	8.896828	-2.039358	-0.534490
63.	1.	0.	9.578607	-1.465193	1.015487
64.	1.	0.	9.757161	-0.467339	-0.463969

4-e		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.730618	-1.832972	-0.382545
2.	6.	0.	2.188465	-0.528461	-0.569014
3.	6.	0.	1.242624	0.511499	-0.708164
4.	6.	0.	-0.150856	0.237681	-0.670572

5.	6.	0.	-0.573880	-1.105614	-0.473095
6.	6.	0.	0.366360	-2.126043	-0.329421
7.	6.	0.	-1.109266	1.345790	-0.846154
8.	6.	0.	-2.527829	1.028971	-0.854428
9.	6.	0.	-2.953894	-0.346774	-0.569536
10.	6.	0.	-2.008790	-1.424892	-0.404831
11.	8.	0.	-2.407506	-2.607748	-0.191681
12.	8.	0.	-0.680218	2.525200	-0.991621
13.	8.	0.	1.702606	1.764823	-0.884440
14.	6.	0.	3.663393	-0.194311	-0.608148
15.	6.	0.	4.179376	0.339952	0.744451
16.	6.	0.	5.694954	0.591925	0.641285
17.	6.	0.	6.403421	-0.684292	0.158332
18.	6.	0.	5.791102	-1.158943	-1.167879
19.	8.	0.	4.382230	-1.375029	-0.983517
20.	6.	0.	6.385305	-2.462422	-1.677083
21.	8.	0.	7.794956	-0.423988	-0.021330
22.	7.	0.	6.385754	1.121519	1.832316
23.	6.	0.	6.115256	0.405488	3.082604
24.	6.	0.	6.211387	2.564819	2.006127
25.	6.	0.	-3.485051	1.952535	-1.206392
26.	8.	0.	-4.797796	1.628109	-1.213358
27.	6.	0.	-5.317468	0.468865	-0.521730
28.	6.	0.	-4.293162	-0.626690	-0.451656
29.	6.	0.	-3.285652	3.352963	-1.685667
30.	8.	0.	-4.771176	-1.836164	-0.218559

31.	6.	0.	-5.816458	0.914672	0.873135
32.	6.	0.	-6.660538	-0.123948	1.587958
33.	8.	0.	-7.704092	-0.511734	0.839993
34.	6.	0.	-8.595755	-1.494065	1.420386
35.	8.	0.	-6.439332	-0.535352	2.712974
36.	1.	0.	3.826890	0.578036	-1.374809
37.	1.	0.	2.458747	-2.630052	-0.284906
38.	1.	0.	0.023733	-3.142869	-0.178184
39.	1.	0.	0.882718	2.342202	-0.967195
40.	1.	0.	3.954506	-0.402514	1.518290
41.	1.	0.	3.648310	1.262838	0.997271
42.	1.	0.	5.855885	1.344124	-0.143195
43.	1.	0.	6.269061	-1.492549	0.894390
44.	1.	0.	5.935308	-0.364970	-1.918996
45.	1.	0.	7.457899	-2.344839	-1.851646
46.	1.	0.	6.236396	-3.264306	-0.945780
47.	1.	0.	5.909242	-2.754319	-2.617857
48.	1.	0.	8.011048	0.217296	0.682311
49.	1.	0.	6.823522	0.744063	3.844873
50.	1.	0.	5.096088	0.577295	3.467437
51.	1.	0.	6.255876	-0.669887	2.949310
52.	1.	0.	5.178536	2.848703	2.273730
53.	1.	0.	6.485577	3.086613	1.084779
54.	1.	0.	6.871709	2.913486	2.806359
55.	1.	0.	-6.167023	0.137097	-1.122715
56.	1.	0.	-2.414413	3.432858	-2.335784

57.	1.	0.	-3.111239	4.020587	-0.833812
58.	1.	0.	-4.188269	3.682200	-2.204581
59.	1.	0.	-3.939713	-2.432280	-0.157652
60.	1.	0.	-4.976547	1.178087	1.518413
61.	1.	0.	-6.433735	1.806532	0.720133
62.	1.	0.	-9.046284	-1.097757	2.332200
63.	1.	0.	-8.047590	-2.411257	1.643375
64.	1.	0.	-9.355851	-1.674389	0.662559



E-4

Table S13. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **E-4**.

Conformers	In MeOH	
	ΔG	P (%)
E-4-a	0	40.90
E-4-b	0.09	34.60
E-4-c	0.53	16.59
E-4-d	0.97	7.91

[a] B3LYP/6-31+G (d, p), in kcal/mol. [b] From ΔG values at 298.15K.

Table S14. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **E-4** at B3LYP/6-311+G (d, p) level of theory in CH_3OH.

E-4-a		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-2.043392	1.938507	0.093190
2.	6.	0.	-2.364759	0.660448	-0.359686
3.	6.	0.	-1.328699	-0.282738	-0.539141
4.	6.	0.	0.020776	0.066350	-0.269078
5.	6.	0.	0.304549	1.378672	0.195988
6.	6.	0.	-0.725429	2.300940	0.373862
7.	6.	0.	1.077952	-0.939221	-0.484679
8.	6.	0.	2.453898	-0.544347	-0.235251
9.	6.	0.	2.729690	0.792486	0.303452
10.	6.	0.	1.689139	1.768591	0.506855
11.	8.	0.	1.954895	2.922348	0.954010
12.	8.	0.	0.770389	-2.097117	-0.880420
13.	8.	0.	-1.660428	-1.509474	-0.973676
14.	6.	0.	-3.791919	0.247237	-0.644683
15.	6.	0.	-4.394405	-0.594615	0.500673
16.	6.	0.	-5.863508	-0.909418	0.170364
17.	6.	0.	-6.625838	0.393310	-0.118612
18.	6.	0.	-5.922459	1.168810	-1.241660
19.	8.	0.	-4.565136	1.428844	-0.860193
20.	6.	0.	-6.572578	2.508908	-1.544133
21.	8.	0.	-7.959169	0.092831	-0.502201
22.	7.	0.	-6.631329	-1.722446	1.131187
23.	6.	0.	-6.570058	-1.267372	2.521857
24.	6.	0.	-6.344926	-3.153120	1.034106

25.	6.	0.	3.517306	-1.345919	-0.573583
26.	8.	0.	4.788579	-0.957971	-0.344846
27.	6.	0.	5.125851	0.125543	0.556072
28.	6.	0.	4.015385	1.136435	0.647525
29.	6.	0.	3.484711	-2.671176	-1.264075
30.	8.	0.	4.344711	2.316225	1.129993
31.	6.	0.	6.446392	0.710193	0.069142
32.	6.	0.	7.598857	-0.253265	0.283574
33.	8.	0.	8.598494	-0.002828	-0.573820
34.	6.	0.	9.780269	-0.819610	-0.423879
35.	8.	0.	7.631509	-1.117939	1.137330
36.	1.	0.	-3.801585	-0.363670	-1.561273
37.	1.	0.	-2.844684	2.657454	0.218136
38.	1.	0.	-0.483790	3.295093	0.730340
39.	1.	0.	-0.788548	-2.009041	-1.036426
40.	1.	0.	-4.315719	-0.019294	1.429696
41.	1.	0.	-3.811530	-1.512553	0.621008
42.	1.	0.	-5.880697	-1.481514	-0.767698
43.	1.	0.	-6.615026	1.037025	0.777735
44.	1.	0.	-5.931687	0.539160	-2.147328
45.	1.	0.	-7.611770	2.359952	-1.846671
46.	1.	0.	-6.556097	3.151171	-0.657410
47.	1.	0.	-6.040435	3.018746	-2.352098
48.	1.	0.	-8.168053	-0.703005	0.023598
49.	1.	0.	-5.588744	-1.435348	2.995302
50.	1.	0.	-6.802959	-0.201987	2.588398

51.	1.	0.	-7.319429	-1.809915	3.106271
52.	1.	0.	-7.051457	-3.706658	1.660530
53.	1.	0.	-5.325986	-3.419871	1.363151
54.	1.	0.	-6.470232	-3.488255	0.000611
55.	1.	0.	5.284449	-0.318123	1.549532
56.	1.	0.	2.738313	-2.686867	-2.057967
57.	1.	0.	3.207199	-3.459284	-0.555536
58.	1.	0.	4.478334	-2.890437	-1.659042
59.	1.	0.	3.450639	2.830329	1.159340
60.	1.	0.	6.379201	0.993403	-0.983775
61.	1.	0.	6.659813	1.620159	0.639941
62.	1.	0.	9.534748	-1.872545	-0.575155
63.	1.	0.	10.211480	-0.685615	0.570137
64.	1.	0.	10.471980	-0.474521	-1.190278

E-4-b		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.699215	-1.788610	0.492804
2.	6.	0.	2.092097	-0.627063	-0.169676
3.	6.	0.	1.132755	0.381160	-0.409368
4.	6.	0.	-0.213993	0.211711	0.008688
5.	6.	0.	-0.572109	-0.987578	0.681313
6.	6.	0.	0.383862	-1.973861	0.919241
7.	6.	0.	-1.191508	1.280016	-0.272002
8.	6.	0.	-2.567545	1.069400	0.144146
9.	6.	0.	-2.915290	-0.155806	0.871553

10.	6.	0.	-1.956516	-1.193647	1.135569
11.	8.	0.	-2.289029	-2.252541	1.748453
12.	8.	0.	-0.817033	2.332846	-0.859312
13.	8.	0.	1.532510	1.495129	-1.044556
14.	6.	0.	3.518826	-0.409281	-0.623996
15.	6.	0.	4.299518	0.522938	0.327629
16.	6.	0.	5.756872	0.625799	-0.154392
17.	6.	0.	6.362270	-0.780177	-0.293414
18.	6.	0.	5.492273	-1.629105	-1.230666
19.	8.	0.	4.156099	-1.685099	-0.714830
20.	6.	0.	5.983745	-3.060550	-1.371610
21.	8.	0.	7.679927	-0.684863	-0.812467
22.	7.	0.	6.682213	1.481452	0.610831
23.	6.	0.	6.692901	1.250941	2.057136
24.	6.	0.	6.536080	2.904498	0.307988
25.	6.	0.	-3.571765	1.947550	-0.185959
26.	8.	0.	-4.846751	1.748028	0.205132
27.	6.	0.	-5.229113	0.754468	1.184518
28.	6.	0.	-4.202507	-0.337148	1.320781
29.	6.	0.	-3.465252	3.186755	-1.016143
30.	8.	0.	-4.595450	-1.408745	1.972067
31.	6.	0.	-6.629613	0.271906	0.818660
32.	6.	0.	-6.681009	-0.451945	-0.513039
33.	8.	0.	-7.944162	-0.551879	-0.951167
34.	6.	0.	-8.129072	-1.266996	-2.192463
35.	8.	0.	-5.717152	-0.902530	-1.100993

36.	1.	0.	3.499845	0.057264	-1.621875
37.	1.	0.	2.440964	-2.559896	0.664387
38.	1.	0.	0.086358	-2.879193	1.434583
39.	1.	0.	0.705345	2.065763	-1.114604
40.	1.	0.	4.250415	0.103578	1.338453
41.	1.	0.	3.818753	1.505599	0.345468
42.	1.	0.	5.746055	1.049230	-1.168266
43.	1.	0.	6.366819	-1.281004	0.689929
44.	1.	0.	5.480388	-1.140765	-2.219570
45.	1.	0.	5.977897	-3.563456	-0.398986
46.	1.	0.	5.341081	-3.621009	-2.056202
47.	1.	0.	7.004483	-3.067905	-1.761030
48.	1.	0.	8.009404	0.150742	-0.429141
49.	1.	0.	5.778459	1.602180	2.562698
50.	1.	0.	6.817835	0.187827	2.276151
51.	1.	0.	7.541952	1.784267	2.495460
52.	1.	0.	5.580916	3.331841	0.658366
53.	1.	0.	6.607333	3.064390	-0.771572
54.	1.	0.	7.345660	3.461553	0.789917
55.	1.	0.	-5.294666	1.267919	2.155117
56.	1.	0.	-2.865050	3.012658	-1.909772
57.	1.	0.	-2.961484	3.979251	-0.452932
58.	1.	0.	-4.468037	3.523557	-1.284054
59.	1.	0.	-3.743784	-1.995518	2.016661
60.	1.	0.	-6.984212	-0.410784	1.597668
61.	1.	0.	-7.317168	1.120770	0.802651

62.	1.	0.	-7.772530	-2.294342	-2.095744
63.	1.	0.	-7.589946	-0.769263	-3.000824
64.	1.	0.	-9.200991	-1.250435	-2.381169

E-4-c		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	-1.975247	-1.944391	-0.163771
2.	6.	0.	-2.256899	-0.664224	0.308871
3.	6.	0.	-1.207402	0.276338	0.405706
4.	6.	0.	0.115428	-0.075908	0.028711
5.	6.	0.	0.359060	-1.391723	-0.449157
6.	6.	0.	-0.683229	-2.312532	-0.540772
7.	6.	0.	1.186586	0.931603	0.146903
8.	6.	0.	2.524369	0.557068	-0.280717
9.	6.	0.	2.775221	-0.819974	-0.721937
10.	6.	0.	1.719357	-1.796190	-0.840067
11.	8.	0.	1.957643	-2.967328	-1.250976
12.	8.	0.	0.920933	2.077656	0.602099
13.	8.	0.	-1.501682	1.504669	0.862156
14.	6.	0.	-3.656565	-0.247747	0.703672
15.	6.	0.	-4.346547	0.589278	-0.395235
16.	6.	0.	-5.787910	0.902265	0.042271
17.	6.	0.	-6.523054	-0.399663	0.399037
18.	6.	0.	-5.733643	-1.164657	1.470255
19.	8.	0.	-4.410718	-1.427762	0.984652
20.	6.	0.	-6.356502	-2.502556	1.834456

21.	8.	0.	-7.823625	-0.097763	0.881156
22.	7.	0.	-6.628021	1.704633	-0.865806
23.	6.	0.	-6.665800	1.238605	-2.253822
24.	6.	0.	-6.340932	3.137113	-0.801585
25.	6.	0.	3.547665	1.470333	-0.365277
26.	8.	0.	4.781038	1.110573	-0.780505
27.	6.	0.	5.210994	-0.269328	-0.845025
28.	6.	0.	4.055144	-1.208793	-1.029998
29.	6.	0.	3.489949	2.939521	-0.095662
30.	8.	0.	4.373814	-2.416100	-1.453156
31.	6.	0.	6.026876	-0.610607	0.407644
32.	6.	0.	7.337949	0.154590	0.443151
33.	8.	0.	7.751859	0.345663	1.703335
34.	6.	0.	9.023376	1.014632	1.856456
35.	8.	0.	7.948748	0.522465	-0.541061
36.	1.	0.	-3.593416	0.367370	1.615289
37.	1.	0.	-2.785739	-2.661362	-0.223767
38.	1.	0.	-0.470647	-3.310802	-0.904203
39.	1.	0.	-0.624968	1.999255	0.864952
40.	1.	0.	-4.336226	0.012171	-1.326398
41.	1.	0.	-3.776947	1.508464	-0.561409
42.	1.	0.	-5.737129	1.482636	0.973994
43.	1.	0.	-6.579202	-1.050219	-0.490594
44.	1.	0.	-5.671546	-0.526955	2.368147
45.	1.	0.	-7.368758	-2.351984	2.216975
46.	1.	0.	-6.409315	-3.151962	0.954370

47.	1.	0.	-5.761370	-3.005359	2.601798
48.	1.	0.	-8.074795	0.691668	0.364334
49.	1.	0.	-5.721436	1.405281	-2.797680
50.	1.	0.	-6.899515	0.172113	-2.295127
51.	1.	0.	-7.456872	1.774577	-2.787064
52.	1.	0.	-5.350473	3.404386	-1.208114
53.	1.	0.	-6.389967	3.480150	0.235713
54.	1.	0.	-7.094505	3.683092	-1.377792
55.	1.	0.	5.869954	-0.320570	-1.716092
56.	1.	0.	3.482714	3.126916	0.983537
57.	1.	0.	2.576573	3.379967	-0.495544
58.	1.	0.	4.371897	3.414904	-0.528512
59.	1.	0.	3.478076	-2.914840	-1.477080
60.	1.	0.	5.449655	-0.423357	1.315961
61.	1.	0.	6.266981	-1.680241	0.386284
62.	1.	0.	8.981306	2.012646	1.416101
63.	1.	0.	9.816261	0.437838	1.376306
64.	1.	0.	9.191999	1.076890	2.930012

E-4-d		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1.	6.	0.	1.770898	-1.812477	-0.202456
2.	6.	0.	2.260543	-0.536300	-0.473204
3.	6.	0.	1.349497	0.537999	-0.579365
4.	6.	0.	-0.044962	0.320813	-0.422617
5.	6.	0.	-0.501750	-0.996059	-0.144824

6.	6.	0.	0.405804	-2.047995	-0.035028
7.	6.	0.	-0.968403	1.462844	-0.561510
8.	6.	0.	-2.393830	1.203866	-0.438805
9.	6.	0.	-2.847045	-0.143858	-0.077445
10.	6.	0.	-1.938354	-1.255563	0.042430
11.	8.	0.	-2.360925	-2.416121	0.316647
12.	8.	0.	-0.510703	2.615815	-0.788729
13.	8.	0.	1.843183	1.760328	-0.836058
14.	6.	0.	3.740517	-0.266541	-0.636302
15.	6.	0.	4.365552	0.339813	0.638435
16.	6.	0.	5.880248	0.502930	0.427104
17.	6.	0.	6.496732	-0.840068	0.003673
18.	6.	0.	5.782450	-1.366552	-1.248829
19.	8.	0.	4.381401	-1.497910	-0.975290
20.	6.	0.	6.285514	-2.728811	-1.697536
21.	8.	0.	7.879704	-0.667986	-0.265865
22.	7.	0.	6.674823	1.078612	1.527880
23.	6.	0.	6.443281	0.475729	2.842505
24.	6.	0.	6.591216	2.536923	1.597538
25.	6.	0.	-3.341557	2.145310	-0.759560
26.	8.	0.	-4.660517	1.875460	-0.653342
27.	6.	0.	-5.156874	0.776924	0.147162
28.	6.	0.	-4.181440	-0.368808	0.159288
29.	6.	0.	-3.126310	3.517422	-1.311192
30.	8.	0.	-4.677762	-1.552595	0.453491
31.	6.	0.	-6.531972	0.410068	-0.411840

32.	6.	0.	-7.383456	-0.314400	0.613327
33.	8.	0.	-8.266160	-1.128954	0.018639
34.	6.	0.	-9.176646	-1.822594	0.899384
35.	8.	0.	-7.308228	-0.150068	1.815550
36.	1.	0.	3.876184	0.451455	-1.460679
37.	1.	0.	2.477310	-2.631186	-0.131255
38.	1.	0.	0.033227	-3.042458	0.179493
39.	1.	0.	1.039496	2.364292	-0.877126
40.	1.	0.	4.159532	-0.333441	1.477700
41.	1.	0.	3.890481	1.301910	0.852633
42.	1.	0.	6.030375	1.183070	-0.422646
43.	1.	0.	6.346503	-1.586189	0.802906
44.	1.	0.	5.928038	-0.631470	-2.058188
45.	1.	0.	6.127251	-3.472855	-0.909930
46.	1.	0.	5.755382	-3.056106	-2.596180
47.	1.	0.	7.354293	-2.677467	-1.917963
48.	1.	0.	8.147690	0.014409	0.379303
49.	1.	0.	5.461886	0.732574	3.273781
50.	1.	0.	6.516137	-0.612869	2.783642
51.	1.	0.	7.214649	0.825708	3.535250
52.	1.	0.	5.593028	2.905858	1.889550
53.	1.	0.	6.846349	2.971073	0.626650
54.	1.	0.	7.310504	2.905423	2.335660
55.	1.	0.	-5.284048	1.141971	1.176222
56.	1.	0.	-2.297109	3.538074	-2.017471
57.	1.	0.	-2.873012	4.212978	-0.503213

58.	1.	0.	-4.049794	3.858155	-1.783405
59.	1.	0.	-3.855371	-2.173773	0.452698
60.	1.	0.	-7.048373	1.343574	-0.662577
61.	1.	0.	-6.452678	-0.178682	-1.327385
62.	1.	0.	-9.769969	-1.107849	1.472930
63.	1.	0.	-8.623132	-2.468333	1.583880
64.	1.	0.	-9.816443	-2.415566	0.248223

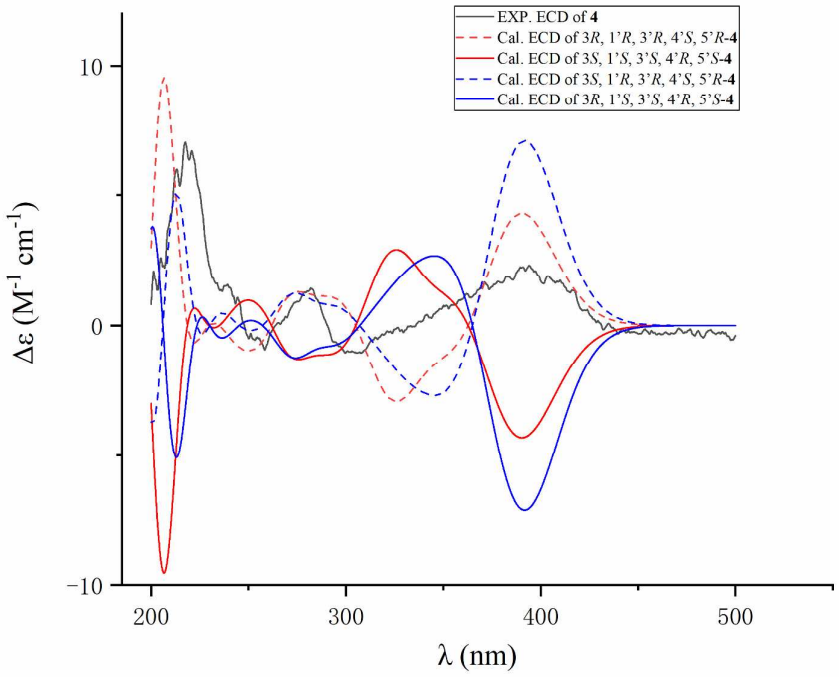


Figure S43. Comparison of the calculated ECD spectra with the experimental spectrum of **4**.

References

(1) Gaussian 09, Revision C.01,M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J.

Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

(2) GaussView, Version 5, Dennington, R.; Keith, T.; Millam, J. *Semichem Inc.*, Shawnee Mission, KS, **2009**.

(3) *Spartan 10*; Wavefuction Inc.: Irvine, CA.

(4) Stephens, P. J.; Harada, N. *Chirality* **2010**, *22*, 229–233.