Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Trimeric and Dimeric Sesquiterpenoids from *Artemisia atrovirens* and Their Cytotoxicities

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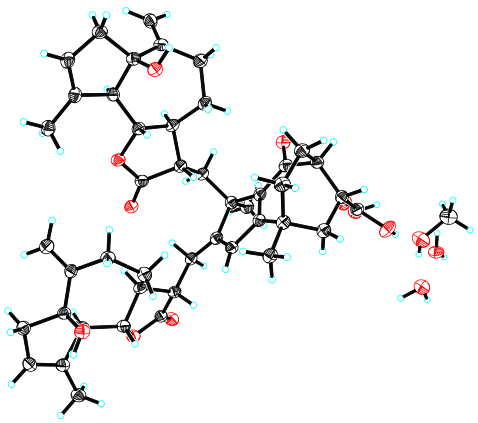
Contents

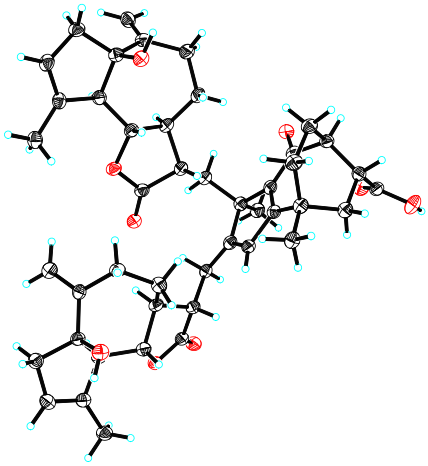
1. Crystal data of compounds 1, 3, and 4.

The crystal data of compound **1** had been deposited in CCDC with number 2039193. Crystal data for artematrotrimer A (**1**): $C_{45}H_{54}O_9$•CH_3OH•3(H_2O), M = 824.97, a = 12.8191(8) Å, b = 13.7773(9) Å, c = 23.8597(14) Å, α = 90°, β = 90°, γ = 90°, V = 4213.9(5) Å^3, T = 100.(2) K, space group $P2_12_12_1$, Z = 4, μ(Cu Kα) = 0.772 mm^{-1}, 79788 reflections measured, 8329 independent reflections (R_{int} = 0.3014). The final R_1 values were 0.0749 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1864 ($I > 2\sigma(I)$). The final R_1 values were 0.1183 (all data). The final $wR(F^2)$ values were 0.2231 (all data). The goodness of fit on F^2 was 1.030. Flack parameter = 0.2(3).



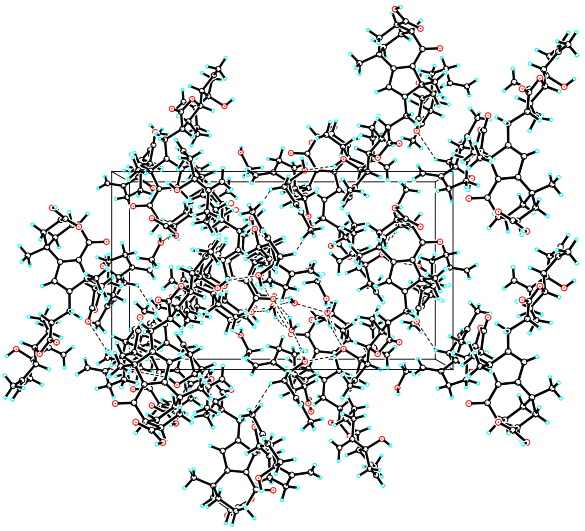
View of the molecules in an asymmetric unit.

Displacement ellipsoids are drawn at the 30% probability level.



View of a molecule of compound **1** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of compound **1**.

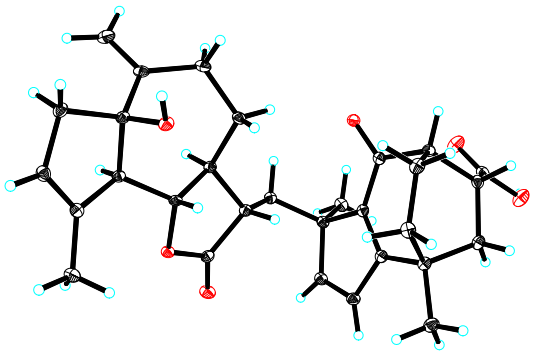
Hydrogen-bonds are shown as dashed lines.

Crystal data and structure refinement for compound **1**.

Identification code	global	
Empirical formula	$C_{46}H_{64}O_{13}$	
Formula weight	824.97	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 12.8191(8) Å	α= 90°.
	b = 13.7773(9) Å	β= 90°.
	c = 23.8597(14) Å	γ = 90°.
Volume	4213.9(5) $Å^3$	
Z	4	
Density (calculated)	1.300 Mg/m^3	
Absorption coefficient	0.772 mm^{-1}	
F(000)	1776	
Crystal size	0.200 x 0.080 x 0.060 mm^3	
Theta range for data collection	3.71 to 72.74°.	
Index ranges	-15<=h<=15, -16<=k<=17, -29<=l<=28	

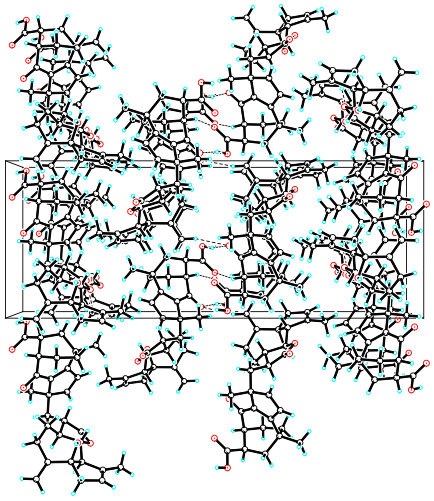
Reflections collected	79788
Independent reflections	8329 [R(int) = 0.3014]
Completeness to theta = 72.74°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.95 and 0.65
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8329 / 0 / 542
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0749, wR2 = 0.1864
R indices (all data)	R1 = 0.1183, wR2 = 0.2231
Absolute structure parameter	0.2(3)
Largest diff. peak and hole	0.301 and -0.321 e.Å^{-3}

The crystal data of compound **3** had been deposited in CCDC with number 1999131. Crystal data for artematrodimer A (**3**): $C_{30}H_{36}O_6$, M = 492.59, a = 8.9468(3) Å, b = 10.4309(3) Å, c = 27.7390(8) Å, α = 90°, β = 90°, γ = 90°, V = 2588.69(14) Å^3, T = 100.(2) K, space group $P2_12_12_1$, Z = 4, μ(Cu Kα) = 0.702 mm^{-1}, 26058 reflections measured, 5100 independent reflections (R_{int} = 0.0445). The final R_1 values were 0.0281 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0699 ($I > 2\sigma(I)$). The final R_1 values were 0.0288 (all data). The final $wR(F^2)$ values were 0.0704 (all data). The goodness of fit on F^2 was 1.048. Flack parameter = 0.01(4).



View of a molecule of compound **3** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of compound **3**.

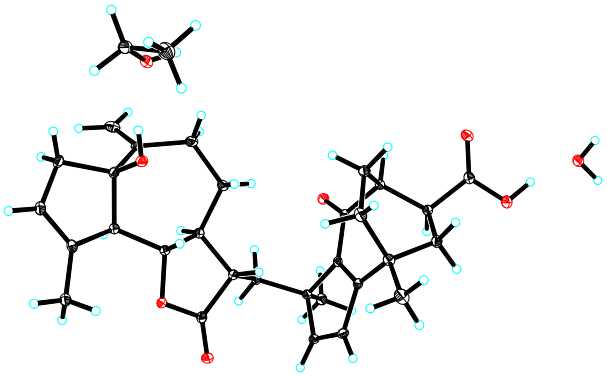
Hydrogen-bonds are shown as dashed lines.

Crystal data and structure refinement for compound **3**.

Identification code	global	
Empirical formula	$C_{30}H_{36}O_6$	
Formula weight	492.59	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 8.9468(3) Å	α= 90°.
	b = 10.4309(3) Å	β= 90°.
	c = 27.7390(8) Å	γ = 90°.
Volume	2588.69(14) $Å^3$	
Z	4	
Density (calculated)	1.264 Mg/m^3	
Absorption coefficient	0.702 mm^{-1}	
F(000)	1056	
Crystal size	0.330 x 0.330 x 0.090 mm^3	
Theta range for data collection	3.19 to 72.39°.	
Index ranges	-9<=h<=11, -12<=k<=12, -34<=l<=33	
Reflections collected	26058	
Independent reflections	5100 [R(int) = 0.0445]	
Completeness to theta = 72.39°	100.0 %	
Absorption correction	Semi-empirical from equivalents	

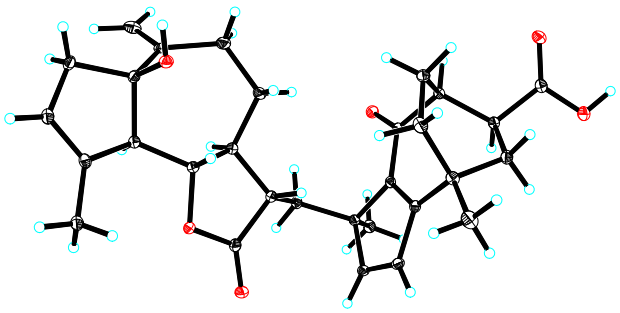
Max. and min. transmission	0.94 and 0.76
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5100 / 0 / 332
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0281, wR2 = 0.0699
R indices (all data)	R1 = 0.0288, wR2 = 0.0704
Absolute structure parameter	0.01(4)
Largest diff. peak and hole	0.185 and -0.211 e.Å^{-3}

The crystal data of compound **4** had been deposited in CCDC with number 2016459. Crystal data for artematrodimer B (**4**): $C_{30}H_{36}O_6$•C_2H_6O•H_2O, M = 556.67, a = 6.81670(10) Å, b = 11.7590(2) Å, c = 18.1156(4) Å, α = 90°, β = 96.5470(10)°, γ = 90°, V = 1442.63(5) Å^3, T = 101.(2) K, space group $P1211$, Z = 2, μ(Cu Kα) = 0.740 mm^{-1}, 23251 reflections measured, 5682 independent reflections (R_{int} = 0.0460). The final R_1 values were 0.0315 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0745 ($I > 2\sigma(I)$). The final R_1 values were 0.0337 (all data). The final $wR(F^2)$ values were 0.0763 (all data). The goodness of fit on F^2 was 1.058. Flack parameter = 0.11(7).



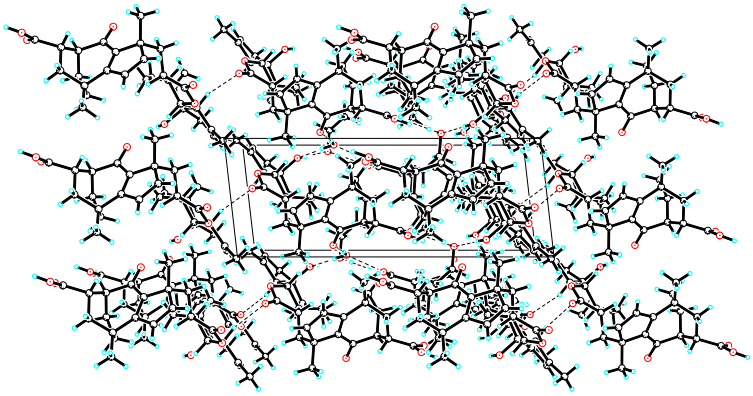
View of the molecules in an asymmetric unit.

Displacement ellipsoids are drawn at the 30% probability level.



View of a molecule of compound **4** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of compound **4**.

Hydrogen-bonds are shown as dashed lines.

Crystal data and structure refinement for compound **4**.

Identification code	global	
Empirical formula	$C_{32}H_{44}O_8$	
Formula weight	556.67	
Temperature	101(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P1211	
Unit cell dimensions	a = 6.81670(10) Å	α= 90°.
	b = 11.7590(2) Å	β= 96.5470(10)°.
	c = 18.1156(4) Å	γ = 90°.
Volume	1442.63(5) $Å^3$	
Z	2	
Density (calculated)	1.282 Mg/m^3	

Absorption coefficient	0.740 mm^{-1}
F(000)	600
Crystal size	0.450 x 0.060 x 0.040 mm^3
Theta range for data collection	2.46 to 72.38°.
Index ranges	-8<=h<=6, -14<=k<=14, -22<=l<=22
Reflections collected	23251
Independent reflections	5682 [R(int) = 0.0460]
Completeness to theta = 72.38°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.88
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5682 / 1 / 371
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0745
R indices (all data)	R1 = 0.0337, wR2 = 0.0763
Absolute structure parameter	0.11(7)
Largest diff. peak and hole	0.216 and -0.189 e.$Å^{-3}$

2. Cytotoxicity assays

2.1 Cell lines and cell culture

Human hepatocellular carcinoma HepG2 cells were obtained as a gift from Service Center for Bioactivity Screening (Kunming Institute of Botany, Chinese Academy of Sciences, Kunming, China). Huh7 cell line was purchased from the Shanghai Jining Biotechnology Co., Ltd. (Shanghai, China) and maintained at 37 °C with 5% CO_2 at a humidified atmosphere. Both two cell lines were cultured in Dulbecco's modified Eagle medium (DMEM) (Gibco, Thermo Fisher Scientific Co., Ltd., Suzhou, China) supplemented with 10% fetal bovine serum (FBS) (Gibco, Life Technologies, NY, USA) and maintained at 37 °C with 5% CO_2 at a humidified atmosphere. Sorafenib (purity > 99%, Aladdin Biotechnology Co., Ltd., Shanghai, China) was used as a positive control.

2.2 MTT assay

The cytotoxicity of the compounds **1**–**4** were assessed by MTT method.[1–3] Briefly, cells in a density of 3×10^4 cells/well were seeded into 96-well plates and grown for 24

h and were treated with increasing concentrations of compounds and incubated for another 48 h. At the end of exposure time and removal of all the remaining liquid in the wells, 100 μL of MTT reagent (1mg/mL) was added into each well and the plates were kept in the incubator for 4 h at 37 °C in the dark. After the formazan crystals were dissolved with dimethyl sulfoxide, then measured at 490 nm using microplate reader (BIO-RAD, USA). The inhibitory ratio was calculated as (1–A490 treated/A490 control) ×100%. The cytotoxicity of **1**–**4** was expressed as IC_{50} values, determined by GraphPad Prism 5 (GraphPad Software, CA, USA). The results are as follows:

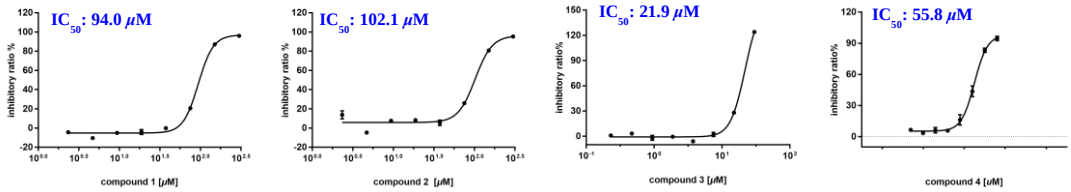


Figure S1. IC_{50} curve of compounds **1–4** inhibit HepG2 proliferation, sorafenib was used as positive control. IC_{50}: 12.8 μM.

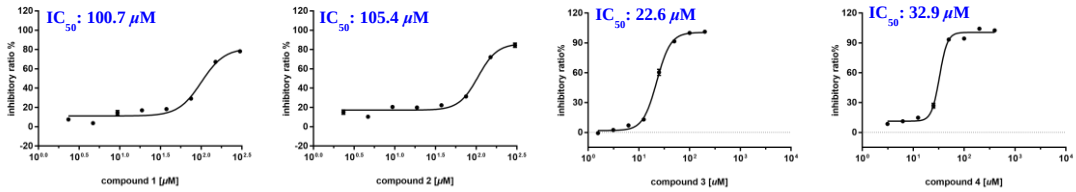


Figure S2. IC_{50} curve of compounds **1–4** inhibit Huh7 proliferation, sorafenib was used as positive control. IC_{50}: 11.2 μM.

References

(1) L. H. Su, C. A. Geng, T. Z. Li, Y. B. Ma, X. Y. Huang, X. M. Zhang, J. J. Chen, *J. Org. Chem.*, 2020, **85**, 13466–13471.

(2) L. H. Su, X. T. Zhang, Y. B. Ma, C. A. Geng, X. Y. Huang, J. Hu, T. Z. Li, S. Tang, C. Shen, Z. Gao, X. M. Zhang, J. J. Chen, *Acta Pharm. Sin. B*, 2020, doi.org/10.1016/j.apsb.2020.12.006.

(3) S. Tang, X. T. Zhang, Y. B. Ma, X. Y. Huang, C. A. Geng, T. Z. Li, X. M. Zhang, C. Shen, L. H. Su, Z. Gao, J. J. Chen, *J. Nat. Prod.*, 2020, **83**, 2618–2630.

3. Computational data of compounds 1 and 2

The ECD calculations for compounds **1** and **2** were performed using the Gaussian 09 program. The 3D structure of **1** was yielded from the X-ray crystallographic data and optimized by the DFT calculation at the b3lyp/6-31G(d,p) level in the gas phase. Conformers of **2** were obtained by MMFF94s force field, and the appropriate low-energy conformers were selected and optimized using the DFT calculation at b3lyp/6-31G(d,p) level in the gas phase. In order to exclude imaginary frequencies, frequency calculations were performed at the same level. ECD calculations were performed by means of the TDDFT methodology at b3lyp/6-311+g(d,p) level with the consideration of solvent effects. The overall calculated ECD curves were generated by Boltzmann weighting of all the conformers calculated using SpecDis 1.62 with σ = ~0.3 eV.[4–5]

References

(4) 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, D. J. Fox, **Gaussian 09**, Revision C.01; Gaussian, Inc., Wallingford CT: 2010.

(5) P. H.Willoughby, M. J. Jansma, T. R. Hoye, *Nat. Protoc.* 2014, **9**, 643–660.

Cartesian coordinates of the lowest-energy formers optimized at the b3lyp/6-311+g(d,p) level

Standard orientation of **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	8	0	-4.844312	-2.291823	-1.225423
2	8	0	-3.561030	-3.381328	-2.730337
3	8	0	4.219924	-4.826386	-1.005859
4	8	0	4.528616	-6.203457	0.751197
5	1	0	4.606217	-6.787046	0.151375
6	8	0	4.306590	-1.638270	-1.530053
7	8	0	-0.160901	2.735879	-0.549116
8	8	0	3.144883	4.209941	1.473205
9	1	0	3.998938	4.381872	1.758923
10	6	0	-7.751485	0.359287	0.685993
11	1	0	-8.824392	0.369708	0.927838
12	8	0	-5.284811	0.132773	2.326920
13	1	0	-6.039303	-0.120821	2.596773
14	6	0	-7.090882	-0.654997	0.147438
15	6	0	-5.620655	-0.330080	-0.064574
16	1	0	-5.549687	0.127336	-0.951330
17	6	0	-4.602572	-1.448645	-0.072597
18	1	0	-4.697489	-1.989109	0.763568
19	6	0	-3.148176	-0.986162	-0.222248
20	1	0	-3.133110	-0.246158	-0.895955
21	6	0	-4.144185	2.637382	-0.048774
22	1	0	-3.209820	3.184375	-0.242766
23	1	0	-5.078304	3.000488	-0.502309
24	6	0	-2.525276	-2.227596	-0.882722
25	1	0	-2.359202	-2.911632	-0.172272
26	8	0	-1.165689	0.977836	-1.551196
27	6	0	-1.241940	-2.056621	-1.700443
28	1	0	-1.193714	-2.793053	-2.360517
29	1	0	-1.304530	-1.209397	-2.205119
30	1	0	-0.675973	-2.745028	1.023370
31	1	0	5.078751	4.722927	-2.573652
32	6	0	0.056751	-2.054943	-0.904568
33	6	0	1.367863	-1.709923	-1.543695
34	6	0	1.435136	-0.236810	-1.989471
35	1	0	2.337240	-0.065028	-2.359714
36	1	0	0.784346	-0.105845	-2.724130
37	6	0	1.152377	0.811260	-0.903669
38	1	0	1.192797	0.361308	-0.011348
39	1	0	3.951789	6.124160	-1.974400
40	1	0	0.936734	7.523695	1.199729
41	6	0	2.070865	2.047777	-0.869114
42	1	0	2.176759	2.395955	-1.800827
43	6	0	1.194667	3.022548	-0.073472
44	1	0	1.260000	2.810685	0.900987
45	6	0	1.495441	4.483226	-0.292573
46	1	0	1.470262	4.645243	-1.279031
47	6	0	2.923020	4.846809	0.194888
48	6	0	2.830357	6.363217	0.442618
49	1	0	3.399027	6.638204	1.205068
50	1	0	3.098764	6.874493	-0.362097

51	6	0	-6.757606	1.487416	0.983265
52	1	0	-6.969034	1.899962	1.858928
53	1	0	-6.773144	2.185736	0.281544
54	6	0	4.345611	5.105019	-1.847943
55	6	0	-5.423445	0.763948	1.017838
56	6	0	-4.145333	1.547995	0.726235
57	6	0	-2.863027	1.007266	1.380184
58	1	0	-2.904458	1.106886	2.364125
59	1	0	-2.116593	1.571471	1.059397
60	6	0	-2.521461	-0.451635	1.066714
61	1	0	-1.536834	-0.538979	1.000237
62	1	0	-2.820753	-1.017542	1.822007
63	6	0	-3.691190	-2.720352	-1.727729
64	6	0	2.250813	-2.024152	-0.393406
65	6	0	1.585647	-2.333753	0.713852
66	6	0	0.144869	-2.420692	0.366788
67	6	0	2.172502	-2.668725	2.082526
68	6	0	1.031818	-2.817833	3.106524
69	1	0	1.408210	-3.022434	3.986940
70	1	0	0.436269	-3.543613	2.827416
71	1	0	0.525346	-1.980055	3.154443
72	6	0	3.136887	-1.580299	2.560080
73	1	0	3.330240	-1.734054	3.519720
74	1	0	2.681457	-0.704734	2.486661
75	6	0	4.487095	-1.495169	1.798215
76	1	0	4.591108	-0.582053	1.429666
77	1	0	5.227634	-1.650423	2.435914
78	6	0	4.589816	-2.516792	0.649680
79	1	0	5.545020	-2.539516	0.351817
80	6	0	4.247682	-3.915308	1.227942
81	1	0	4.957362	-4.119003	1.901182
82	6	0	2.912093	-4.019095	1.971471
83	1	0	3.078505	-4.369911	2.882343
84	1	0	2.329972	-4.666186	1.500674
85	6	0	4.319550	-5.023581	0.181808
86	6	0	3.750253	-2.022988	-0.529225
87	6	0	-0.205604	1.493863	-1.030202
88	6	0	0.640289	5.560669	0.356651
89	6	0	-0.871679	5.469513	0.383990
90	1	0	-1.225278	6.281765	0.801341
91	1	0	-1.154448	4.686157	0.900385
92	1	0	-1.211750	5.397231	-0.532266
93	6	0	1.349918	6.606551	0.754816
94	6	0	3.940143	4.341646	-0.827891
95	6	0	4.479002	2.915515	-0.633732
96	1	0	5.175531	2.922911	0.070506
97	1	0	4.920379	2.652556	-1.479370
98	6	0	3.450225	1.821930	-0.272618
99	1	0	3.793277	0.946494	-0.586967
100	1	0	3.367726	1.775009	0.711690
101	6	0	1.611071	-2.602425	-2.774218
102	1	0	2.517453	-2.449679	-3.113993
103	1	0	0.957718	-2.381148	-3.470507
104	1	0	1.511239	-3.543864	-2.519623
105	6	0	-7.683416	-1.986258	-0.260039
106	1	0	-8.651291	-1.965454	-0.111357
107	1	0	-7.284977	-2.699576	0.280751

108	1	0	-7.501099	-2.154635	-1.208025

Rotational constants (GHZ): 0.0582425 0.0436304 0.0287913

Standard orientation of **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) *X*	*Y*	*Z*
1	8	0	5.183300	-1.730231	1.532984
2	8	0	3.891697	-2.835159	3.004353
3	8	0	-5.857272	-5.212816	-1.027826
4	8	0	-4.351730	-6.783645	-0.620883
5	1	0	-3.472345	-6.961228	-0.306101
6	8	0	-4.034653	-1.637296	1.630226
7	8	0	-0.361681	2.923909	0.044198
8	8	0	-4.084442	4.033403	-1.249466
9	1	0	-4.936286	4.286991	-1.589332
10	6	0	8.153911	0.657650	-0.578508
11	1	0	9.221034	0.703886	-0.684433
12	8	0	5.779867	-0.046184	-2.255869
13	1	0	6.601471	-0.507840	-2.392581
14	6	0	7.507382	-0.195332	0.211058
15	6	0	6.009503	0.105960	0.173821
16	1	0	5.777087	0.774607	0.999619
17	6	0	5.035306	-1.049355	0.245483
18	1	0	5.243742	-1.783653	-0.519379
19	6	0	3.545413	-0.649947	0.226867
20	1	0	3.415238	0.247822	0.822439
21	6	0	4.520568	2.968399	-0.796639
22	1	0	3.586458	3.497349	-0.787069
23	1	0	5.370260	3.514461	-0.435838
24	6	0	2.898547	-1.821701	1.002642
25	1	0	2.784940	-2.678478	0.340090
26	8	0	1.061470	1.393527	0.846512
27	6	0	1.583474	-1.551417	1.748723
28	1	0	1.575677	-2.190161	2.627404
29	1	0	1.587567	-0.529826	2.102579
30	1	0	0.922685	-2.705182	-0.858757
31	1	0	-5.352548	4.384474	3.027380
32	6	0	0.309975	-1.813657	0.997481
33	6	0	-1.058603	-1.554684	1.632913
34	6	0	-1.337490	-0.050390	1.939353
35	1	0	-2.307910	-0.017350	2.414918
36	1	0	-0.611753	0.287713	2.671084
37	6	0	-1.349380	0.920328	0.747003
38	1	0	-1.504852	0.369239	-0.179303
39	1	0	-4.616330	5.885793	2.320121
40	1	0	-2.355378	7.473008	-1.523020
41	6	0	-2.396710	2.059246	0.817649
42	1	0	-2.346818	2.481558	1.820866
43	6	0	-1.805894	3.087468	-0.163618
44	1	0	-2.013944	2.818043	-1.187039
45	6	0	-2.190282	4.523991	0.110017
46	1	0	-1.911972	4.739122	1.139822
47	6	0	-3.723882	4.735814	-0.034141
48	6	0	-3.843857	6.250886	-0.318047

49	1	0	-4.705499	6.455779	-0.946624
50	1	0	-3.972206	6.831182	0.588091
51	6	0	7.221257	1.623066	-1.279281
52	1	0	7.459142	1.801685	-2.321352
53	1	0	7.220818	2.584706	-0.779048
54	6	0	-4.839979	4.843969	2.203065
55	6	0	5.863260	0.899291	-1.160741
56	6	0	4.588119	1.713031	-1.221006
57	6	0	3.347993	1.017870	-1.755628
58	1	0	3.447308	0.927590	-2.831502
59	1	0	2.510179	1.672716	-1.557871
60	6	0	3.017622	-0.386565	-1.187201
61	1	0	1.940539	-0.482598	-1.179471
62	1	0	3.406436	-1.146977	-1.854763
63	6	0	3.999055	-2.201233	1.983722
64	6	0	-1.993563	-2.127509	0.574403
65	6	0	-1.282637	-2.604267	-0.472937
66	6	0	0.142177	-2.398918	-0.198085
67	6	0	-1.839381	-3.238756	-1.741502
68	6	0	-0.729375	-3.484156	-2.779390
69	1	0	-1.152494	-3.928998	-3.672419
70	1	0	0.031340	-4.158699	-2.403846
71	1	0	-0.249087	-2.555529	-3.067073
72	6	0	-2.911690	-2.305508	-2.370225
73	1	0	-3.036492	-2.591271	-3.409662
74	1	0	-2.527937	-1.291495	-2.374513
75	6	0	-4.281180	-2.373013	-1.662756
76	1	0	-4.704318	-1.380504	-1.558430
77	1	0	-4.982376	-2.942139	-2.260979
78	6	0	-4.223202	-3.040855	-0.275500
79	1	0	-5.227833	-3.091825	0.118679
80	6	0	-3.650248	-4.472188	-0.365060
81	1	0	-3.257096	-4.743865	0.611573
82	6	0	-2.507827	-4.594917	-1.412591
83	1	0	-2.899211	-4.992467	-2.344860
84	1	0	-1.753707	-5.294038	-1.065354
85	6	0	-4.733400	-5.480662	-0.688046
86	6	0	-3.435354	-2.207863	0.716106
87	6	0	-0.070482	1.715531	0.569436
88	6	0	-1.612236	5.620533	-0.778879
89	6	0	-0.191677	5.629624	-1.255488
90	1	0	0.022919	6.543938	-1.795804
91	1	0	0.010130	4.789901	-1.910680
92	1	0	0.500731	5.545399	-0.425145
93	6	0	-2.522830	6.563762	-0.978512
94	6	0	-4.511648	4.144263	1.123829
95	6	0	-4.903618	2.674821	1.020564
96	1	0	-5.774673	2.591355	0.376737
97	1	0	-5.227547	2.360622	2.006413
98	6	0	-3.841551	1.670843	0.505161
99	1	0	-4.061265	0.712407	0.956914
100	1	0	-3.943411	1.552763	-0.566394
101	6	0	-1.190070	-2.344411	2.958396
102	1	0	-2.200426	-2.265525	3.335755
103	1	0	-0.514221	-1.954206	3.710238
104	1	0	-0.956440	-3.392259	2.805796
105	6	0	8.119887	-1.238915	1.094895

106	1	0	9.199887	-1.229255	1.007078
107	1	0	7.762741	-2.231657	0.846115
108	1	0	7.853178	-1.071921	2.132262

Rotational constants (GHZ): 0.0556079 0.0382099 0.0259206

Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **1**.

State	*XX*	*YY*	*ZZ*	*R* (velocity)	E-M Angle
1	0.6191	31.5184	25.7367	19.2914	29.95
2	-95.6667	3.6235	-39.8323	-43.9585	94.04
3	-0.3675	0.0640	-0.1661	-0.1565	130.10
4	0.0237	0.1162	0.0142	0.0514	90.00
5	3.3344	0.3413	0.5014	1.3924	60.85
6	-7.7518	2.0283	-5.4258	-3.7164	121.24
7	-18.4962	6.9694	-7.0264	-6.1844	109.35
8	-3.4365	1.6542	-5.3726	-2.3850	102.44
9	5.2488	2.5351	11.6294	6.4711	64.58
10	3.1675	-0.1689	0.8261	1.2749	76.25
11	-38.9732	-9.9809	-30.1461	-26.3667	114.43
12	0.9604	-2.8264	-3.3131	-1.7264	100.79
13	3.1814	0.6128	10.1393	4.6445	41.75
14	37.3088	64.3440	-15.3954	28.7525	65.49
15	0.9334	10.0021	-3.6256	2.4366	17.64
16	1.2258	1.8362	3.5310	2.1977	43.95
17	-3.1860	-36.3152	-3.3775	-14.2929	112.83
18	0.2487	-2.6991	-4.0934	-2.1813	105.32
19	-15.2694	21.4888	1.0179	2.4125	61.23
20	-7.5567	-3.2038	0.2972	-3.4878	104.54
21	0.0816	0.2267	-2.0223	-0.5713	94.21
22	0.6966	-0.9195	-1.2025	-0.4751	97.75
23	6.4598	16.8101	3.9158	9.0619	55.11
24	-0.2240	0.8222	-1.2366	-0.2128	92.98
25	5.8942	6.0599	1.3518	4.4353	27.39
26	0.0980	0.0946	-0.2059	-0.0044	90.00
27	-1.0154	-13.2296	3.9808	-3.4214	91.87
28	74.6931	66.9254	0.3381	47.3189	40.18
29	2.2484	-11.6413	6.9361	-0.8190	92.49
30	-42.7408	43.8082	-8.9025	-2.6117	92.05

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

State	*XX*	*YY*	*ZZ*	*R* (length)
1	56.2607	-5.9740	6.6950	18.9939
2	-67.4221	-123.0492	54.6145	-45.2856
3	0.0040	-0.3569	-0.1275	-0.1601
4	0.1352	0.0351	-0.0278	0.0475
5	1.9874	4.2629	-2.0510	1.3998
6	-0.0087	-4.3538	-6.9753	-3.7793
7	1.0347	-24.1507	5.4132	-5.9009
8	4.1184	-5.6724	-5.6887	-2.4143
9	6.8988	13.9744	-1.3997	6.4911
10	-1.8413	3.0932	3.0589	1.4369
11	-0.1170	-1.7526	-79.4872	-27.1189
12	-6.8521	-1.4313	3.0856	-1.7326
13	1.3525	12.4192	-0.5087	4.4210
14	-39.8479	6.7270	119.3524	28.7438
15	5.9842	0.9539	0.3543	2.4308
16	4.2442	2.4952	-0.2347	2.1682

17	-24.4878	3.8759	-23.2889	-14.6336
18	-8.2072	-4.2407	5.6129	-2.2783
19	8.4920	1.6876	-2.5879	2.5306
20	1.8831	-6.0027	-7.1002	-3.7399
21	-1.6394	-2.4908	2.3276	-0.6009
22	-3.1536	0.0171	1.4635	-0.5577
23	14.5201	-5.8205	17.9635	8.8877
24	-0.5028	-2.3475	2.2512	-0.1997
25	0.5935	0.2047	12.2468	4.3484
26	-0.2987	0.0766	0.2640	0.0140
27	-1.5678	80.0071	-88.3081	-3.2896
28	27.5265	10.0530	107.1565	48.2454
29	1.5889	19.6689	-23.1255	-0.6226
30	96.8843	-33.5673	-70.0961	-2.2597

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	-0.0022	-0.0001	-0.0002	0.0025	0.0017
2	-0.3570	-0.0272	-0.0004	0.3845	0.2563
3	0.0000	-0.0002	0.0000	0.0003	0.0002
4	-0.0001	0.0000	0.0000	0.0001	0.0001
5	-0.0005	-0.0006	-0.0003	0.0014	0.0009
6	0.0000	-0.0053	-0.0009	0.0061	0.0041
7	-0.0068	-0.0134	-0.0002	0.0205	0.0136
8	-0.0005	-0.0060	-0.0003	0.0067	0.0045
9	-0.0094	-0.0149	0.0000	0.0243	0.0162
10	-0.0017	-0.0002	-0.0001	0.0020	0.0014
11	0.0000	-0.0304	-0.0124	0.0427	0.0285
12	-0.0018	0.0000	0.0000	0.0019	0.0012
13	-0.0001	-0.0056	-0.0007	0.0063	0.0042
14	-0.0062	-0.0238	-0.0577	0.0877	0.0585
15	-0.0013	-0.0005	-0.0001	0.0019	0.0013
16	-0.0007	-0.0019	0.0000	0.0026	0.0017
17	-0.0095	-0.0070	-0.0008	0.0173	0.0115
18	-0.0013	-0.0005	-0.0001	0.0019	0.0012
19	-0.0022	-0.0002	-0.0025	0.0049	0.0033
20	0.0000	-0.0006	-0.0007	0.0013	0.0009
21	0.0000	-0.0010	-0.0001	0.0011	0.0008
22	-0.0012	0.0000	0.0000	0.0012	0.0008
23	-0.0009	-0.0002	-0.0003	0.0014	0.0009
24	0.0000	-0.0004	-0.0001	0.0004	0.0003
25	0.0000	0.0000	-0.0004	0.0004	0.0002
26	-0.0001	-0.0001	0.0000	0.0001	0.0001
27	-0.0051	-0.0208	-0.0024	0.0283	0.0189
28	-0.0010	-0.0040	-0.0229	0.0278	0.0185
29	-0.0002	-0.0007	-0.0030	0.0039	0.0026
30	-0.0238	-0.0218	-0.0119	0.0575	0.0383

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.5501 eV 349.24 nm *f*=0.0017 <S**2>=0.000
193 -> 199 -0.13307
195 -> 199 0.67375
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2424.82468533
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited State 2: Singlet-A 3.8569 eV 321.46 nm *f*=0.2580 <S**2>=0.000
198 -> 199 0.69720

Excited State 3:	Singlet-A	4.2169 eV	294.02 nm	*f*=0.0002	<S**2>=0.000
197 -> 199	0.70661				
Excited State 4:	Singlet-A	4.3894 eV	282.46 nm	*f*=0.0001	<S**2>=0.000
196 -> 199	0.70273				
Excited State 5:	Singlet-A	4.5223 eV	274.16 nm	*f*=0.0009	<S**2>=0.000
194 -> 199	0.70084				
Excited State 6:	Singlet-A	4.5498 eV	272.50 nm	*f*=0.0041	<S**2>=0.000
193 -> 199	0.69011				
195 -> 199	0.13997				
Excited State 7:	Singlet-A	4.8201 eV	257.22 nm	*f*=0.0135	<S**2>=0.000
198 -> 200	0.70375				
Excited State 8:	Singlet-A	4.9978 eV	248.08 nm	*f*=0.0045	<S**2>=0.000
192 -> 199	0.69538				
Excited State 9:	Singlet-A	5.0658 eV	244.75 nm	*f*=0.0164	<S**2>=0.000
198 -> 202	0.68708				
Excited State 10:	Singlet-A	5.1055 eV	242.84 nm	*f*=0.0014	<S**2>=0.000
198 -> 201	0.70071				
Excited State 11:	Singlet-A	5.1680 eV	239.91 nm	*f*=0.0286	<S**2>=0.000
187 -> 199	0.12633				
188 -> 199	-0.38308				
189 -> 199	0.51694				
190 -> 199	0.15601				
Excited State 12:	Singlet-A	5.2918 eV	234.29 nm	*f*=0.0013	<S**2>=0.000
185 -> 199	-0.10735				
188 -> 199	0.23332				
189 -> 199	0.22357				
191 -> 199	0.60430				
Excited State 13:	Singlet-A	5.3209 eV	233.01 nm	*f*=0.0042	<S**2>=0.000
188 -> 200	0.10637				
189 -> 200	-0.12710				
193 -> 200	-0.10825				
195 -> 200	0.64161				
Excited State 14:	Singlet-A	5.3533 eV	231.60 nm	*f*=0.0591	<S**2>=0.000
186 -> 199	-0.12977				
187 -> 199	0.57380				
195 -> 200	-0.12321				
198 -> 206	0.22786				
198 -> 209	-0.15868				
Excited State 15:	Singlet-A	5.4393 eV	227.94 nm	*f*=0.0013	<S**2>=0.000
197 -> 203	-0.12511				
198 -> 202	0.10489				
198 -> 203	0.64902				
198 -> 204	-0.16174				
198 -> 205	-0.10191				

Excited State 16:	Singlet-A	5.4544 eV	227.31 nm	*f*=0.0017	<S**2>=0.000
189 -> 199	-0.17234				
190 -> 199	0.64458				
192 -> 202	0.10947				
197 -> 203	-0.12503				
Excited State 17:	Singlet-A	5.4572 eV	227.19 nm	*f*=0.0116	<S**2>=0.000
190 -> 199	0.17851				
197 -> 202	0.16671				
197 -> 203	0.57731				
197 -> 204	0.19256				
198 -> 204	-0.20738				
Excited State 18:	Singlet-A	5.4660 eV	226.83 nm	*f*=0.0013	<S**2>=0.000
185 -> 199	-0.23182				
188 -> 199	0.39942				
189 -> 199	0.25168				
191 -> 199	-0.30693				
198 -> 203	-0.10909				
198 -> 204	-0.26946				
Excited State 19:	Singlet-A	5.4683 eV	226.73 nm	*f*=0.0034	<S**2>=0.000
185 -> 199	-0.11570				
188 -> 199	0.18417				
191 -> 199	-0.14174				
197 -> 203	0.17766				
198 -> 203	0.20308				
198 -> 204	0.55701				
Excited State 20:	Singlet-A	5.4781 eV	226.33 nm	*f*=0.0009	<S**2>=0.000
190 -> 199	0.12030				
192 -> 202	-0.50571				
195 -> 202	-0.13034				
197 -> 202	0.33543				
197 -> 203	-0.17149				
198 -> 204	0.10352				
Excited State 21:	Singlet-A	5.5017 eV	225.35 nm	*f*=0.0008	<S**2>=0.000
181 -> 199	-0.10221				
185 -> 199	0.56186				
186 -> 199	0.15484				
188 -> 199	0.26191				
189 -> 199	0.16596				
Excited State 22:	Singlet-A	5.5422 eV	223.71 nm	*f*=0.0008	<S**2>=0.000
198 -> 204	-0.11224				
198 -> 205	0.64196				
198 -> 206	0.16716				
Excited State 23:	Singlet-A	5.5480 eV	223.48 nm	*f*=0.0008	<S**2>=0.000
187 -> 200	-0.28283				
188 -> 200	0.34016				
189 -> 200	-0.43625				
190 -> 200	-0.11591				
195 -> 200	-0.20142				
Excited State 24:	Singlet-A	5.5633 eV	222.86 nm	*f*=0.0003	<S**2>=0.000

192 -> 202 0.33047
195 -> 202 0.11702
197 -> 200 0.14669
197 -> 202 0.55500
197 -> 203 -0.13468

Excited State 25: Singlet-A 5.5755 eV 222.37 nm *f*=0.0003 <S**2>=0.000
188 -> 201 -0.30076
189 -> 201 -0.22327
191 -> 201 -0.27018
196 -> 201 0.50782

Excited State 26: Singlet-A 5.6073 eV 221.11 nm *f*=0.0001 <S**2>=0.000
197 -> 200 0.68777
197 -> 202 -0.14531

Excited State 27: Singlet-A 5.6337 eV 220.08 nm *f*=0.0191 <S**2>=0.000
196 -> 202 -0.17340
196 -> 203 -0.19433
196 -> 204 0.62314
196 -> 208 -0.13553

Excited State 28: Singlet-A 5.6404 eV 219.82 nm *f*=0.0187 <S**2>=0.000
183 -> 199 0.12331
185 -> 199 0.10900
188 -> 201 -0.16610
189 -> 201 -0.12148
191 -> 201 -0.14910
192 -> 202 -0.11025
195 -> 202 0.28664
195 -> 206 -0.18039
195 -> 209 0.17457
196 -> 201 -0.27704
198 -> 206 -0.22693
198 -> 209 0.11985

Excited State 29: Singlet-A 5.6437 eV 219.69 nm *f*=0.0024 <S**2>=0.000
188 -> 201 0.26991
189 -> 201 0.19872
191 -> 201 0.24033
195 -> 202 0.20881
195 -> 206 -0.12602
195 -> 209 0.12284
196 -> 201 0.40075

Excited State 30: Singlet-A 5.6829 eV 218.17 nm *f*=0.0388 <S**2>=0.000
181 -> 199 0.10324
183 -> 199 -0.11496
185 -> 199 -0.12838
186 -> 199 0.47341
187 -> 199 0.28131
198 -> 206 -0.29467
198 -> 209 0.12368
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 30 LETran= 550.
****

Rotatory strengths (R) in cgs (10**−40 erg−esu−cm/Gauss) of **2**.

State	*XX*	*YY*	*ZZ*	*R* (velocity)	E-M Angle
1	1.2298	28.6075	23.9991	17.9454	36.03
2	-68.1484	-34.7558	16.7547	-28.7165	92.45
3	-0.4214	-0.1460	-0.1108	-0.2261	90.00
4	0.0526	0.1336	0.0170	0.0678	90.00
5	3.8417	0.7290	-0.0497	1.5070	67.28
6	-5.5829	0.3375	-3.9587	-3.0680	139.84
7	-2.7237	-0.8339	-5.6224	-3.0600	112.91
8	2.1470	3.1970	7.1416	4.1619	45.49
9	-5.6417	-1.2882	-2.9653	-3.2984	106.08
10	7.0611	-3.8472	5.3299	2.8480	77.80
11	12.7705	-3.1653	4.3336	4.6463	70.83
12	-12.6493	73.6507	-73.5562	-4.1849	91.77
13	4.1527	-8.2433	-0.7746	-1.6217	103.69
14	1.0212	0.2352	0.1478	0.4681	38.95
15	4.7738	9.3268	-1.5809	4.1732	67.90
16	3.6334	-8.6968	-9.0102	-4.6912	125.54
17	4.0072	11.9883	12.9129	9.6361	73.73
18	2.0910	-17.7413	-13.0170	-9.5558	133.18
19	-5.9649	-4.1918	-2.7973	-4.3180	125.77
20	-10.7558	6.8774	3.8829	0.0015	90.00
21	-2.0243	4.5675	4.3025	2.2819	64.19
22	-22.6071	2.3211	8.3060	-3.9934	106.76
23	6.6401	4.7531	3.0519	4.8150	45.75
24	2.9631	1.4709	-2.7433	0.5636	84.45
25	-6.8779	9.5227	17.6721	6.7723	75.47
26	5.5677	-9.0587	-11.2514	-4.9141	121.49
27	-11.4194	-22.7936	-1.6950	-11.9694	96.51
28	9.9666	-6.8376	-8.1888	-1.6866	102.33
29	10.7816	24.6619	4.0774	13.1736	33.66
30	65.6167	49.3414	2.9063	39.2881	64.87

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

State	*XX*	*YY*	*ZZ*	*R* (length)
1	52.3403	-6.2919	7.5612	17.8699
2	-20.3309	-33.7024	-34.1476	-29.3936
3	-0.2441	-0.4199	-0.0228	-0.2289
4	0.1752	0.0520	-0.0428	0.0615
5	2.8631	4.5176	-2.8706	1.5034
6	-3.5822	-4.4089	-1.3222	-3.1044
7	-1.4722	-6.1159	-1.8225	-3.1369
8	2.3574	8.9076	1.3405	4.2018
9	-1.5574	-7.2865	-0.7062	-3.1834
10	-12.0495	13.2321	7.0344	2.7390
11	-13.3571	17.7740	9.8090	4.7420
12	-87.1315	48.7693	24.3839	-4.6595
13	-7.3740	0.4690	1.6407	-1.7548
14	-0.0201	0.0839	1.3486	0.4708
15	-7.7979	3.0067	16.9143	4.0410
16	-16.4499	1.4062	3.2502	-3.9311
17	20.6193	15.3551	-8.3453	9.2097
18	-26.5690	0.1273	-3.2124	-9.8847
19	-0.4188	-8.0780	-4.6247	-4.3738
20	17.5903	0.9377	-18.1501	0.1260
21	10.5699	-2.4186	-1.3457	2.2685
22	13.7920	-1.1761	-23.9306	-3.7716

23	-1.9511	6.1064	9.8954	4.6836
24	0.0481	-4.2519	6.8498	0.8820
25	31.1794	-28.7329	17.5386	6.6617
26	-19.4665	-0.5324	4.3362	-5.2209
27	0.0693	79.2422	-113.2828	-11.3238
28	-10.5774	-2.5239	6.6768	-2.1415
29	6.9043	1.1287	31.2699	13.1010
30	36.5253	76.6937	8.6978	40.6389

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

State	*X*	*Y*	*Z*	Dip. S.	Osc.(frdel)
1	-0.0027	-0.0001	-0.0002	0.0030	0.0020
2	-0.4024	-0.0091	-0.0001	0.4116	0.2744
3	-0.0001	-0.0003	0.0000	0.0004	0.0003
4	-0.0002	0.0000	0.0000	0.0002	0.0001
5	-0.0009	-0.0007	-0.0002	0.0019	0.0012
6	-0.0005	-0.0034	-0.0003	0.0043	0.0029
7	-0.0001	-0.0053	0.0000	0.0054	0.0036
8	-0.0135	-0.0154	-0.0003	0.0292	0.0195
9	-0.0013	-0.0041	0.0000	0.0055	0.0036
10	-0.0047	-0.0015	-0.0005	0.0066	0.0044
11	-0.0059	-0.0038	-0.0019	0.0115	0.0077
12	-0.0067	-0.0601	-0.0769	0.1436	0.0957
13	-0.0010	0.0000	-0.0061	0.0071	0.0047
14	0.0000	-0.0001	-0.0001	0.0002	0.0002
15	-0.0005	-0.0011	-0.0045	0.0061	0.0041
16	-0.0007	0.0000	-0.0003	0.0011	0.0007
17	-0.0111	-0.0083	-0.0001	0.0195	0.0130
18	-0.0008	0.0000	-0.0012	0.0020	0.0013
19	0.0000	-0.0004	-0.0002	0.0006	0.0004
20	-0.0014	-0.0003	-0.0024	0.0041	0.0028
21	-0.0002	-0.0001	0.0000	0.0003	0.0002
22	-0.0020	0.0000	-0.0016	0.0036	0.0024
23	0.0000	-0.0005	-0.0003	0.0008	0.0005
24	0.0000	-0.0016	-0.0003	0.0019	0.0013
25	-0.0096	-0.0050	-0.0026	0.0172	0.0114
26	-0.0014	-0.0001	-0.0010	0.0025	0.0017
27	-0.0067	-0.0168	-0.0039	0.0273	0.0182
28	-0.0011	-0.0001	-0.0014	0.0027	0.0018
29	-0.0002	0.0000	-0.0027	0.0029	0.0019
30	-0.0010	-0.0265	-0.0269	0.0544	0.0362

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.4883 eV 355.43 nm *f*=0.0021 <S**2>=0.000
193 -> 199 0.20366
195 -> 199 0.65452
198 -> 199 0.10166
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2424.82600882
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.8397 eV 322.90 nm *f*=0.2765 <S**2>=0.000
198 -> 199 0.69612

Excited State 3: Singlet-A 4.0840 eV 303.58 nm *f*=0.0003 <S**2>=0.000
197 -> 199 0.70670

Excited State 4:	Singlet-A	4.2550 eV	291.38 nm	*f*=0.0001	<S**2>=0.000
196 -> 199	0.70314				
Excited State 5:	Singlet-A	4.3913 eV	282.34 nm	*f*=0.0012	<S**2>=0.000
194 -> 199	0.69919				
Excited State 6:	Singlet-A	4.4157 eV	280.78 nm	*f*=0.0029	<S**2>=0.000
193 -> 199	0.66989				
195 -> 199	-0.21355				
Excited State 7:	Singlet-A	4.8944 eV	253.32 nm	*f*=0.0037	<S**2>=0.000
192 -> 199	0.69895				
Excited State 8:	Singlet-A	5.0185 eV	247.05 nm	*f*=0.0197	<S**2>=0.000
198 -> 200	0.68769				
198 -> 202	0.13808				
Excited State 9:	Singlet-A	5.1643 eV	240.08 nm	*f*=0.0036	<S**2>=0.000
189 -> 199	-0.14665				
191 -> 199	-0.25279				
198 -> 200	-0.11068				
198 -> 201	-0.36223				
198 -> 202	0.50406				
Excited State 10:	Singlet-A	5.1668 eV	239.96 nm	*f*=0.0045	<S**2>=0.000
189 -> 199	0.27477				
191 -> 199	0.56288				
198 -> 201	-0.10385				
198 -> 202	0.27049				
Excited State 11:	Singlet-A	5.1975 eV	238.55 nm	*f*=0.0079	<S**2>=0.000
188 -> 199	-0.12135				
198 -> 201	0.58633				
198 -> 202	0.33825				
Excited State 12:	Singlet-A	5.2543 eV	235.97 nm	*f*=0.0965	<S**2>=0.000
186 -> 199	0.10085				
187 -> 199	0.19954				
188 -> 199	0.57386				
189 -> 199	0.13684				
198 -> 202	0.16101				
198 -> 206	0.15236				
198 -> 207	-0.11612				
Excited State 13:	Singlet-A	5.3061 eV	233.66 nm	*f*=0.0048	<S**2>=0.000
184 -> 199	0.14098				
187 -> 199	0.55666				
188 -> 199	-0.30274				
189 -> 199	0.16389				
191 -> 199	-0.13942				
Excited State 14:	Singlet-A	5.3217 eV	232.98 nm	*f*=0.0002	<S**2>=0.000
190 -> 199	0.69913				
Excited State 15:	Singlet-A	5.3454 eV	231.95 nm	*f*=0.0041	<S**2>=0.000
187 -> 199	-0.24232				
189 -> 199	0.58129				

191 -> 199	-0.29492				
Excited State 16:	Singlet-A	5.4485 eV	227.55 nm	*f*=0.0007	<S**2>=0.000
184 -> 199	-0.25093				
186 -> 199	0.12799				
187 -> 200	-0.10745				
188 -> 200	0.13778				
192 -> 202	0.13736				
193 -> 200	0.14927				
195 -> 200	0.51800				
197 -> 202	-0.10551				
Excited State 17:	Singlet-A	5.4607 eV	227.05 nm	*f*=0.0131	<S**2>=0.000
184 -> 199	0.11410				
192 -> 202	0.11099				
197 -> 202	-0.19429				
197 -> 203	0.57960				
197 -> 204	0.24757				
Excited State 18:	Singlet-A	5.4679 eV	226.75 nm	*f*=0.0013	<S**2>=0.000
181 -> 199	-0.14724				
183 -> 199	0.12561				
184 -> 199	0.47957				
186 -> 199	-0.18862				
192 -> 202	0.17440				
195 -> 200	0.22075				
197 -> 202	-0.12859				
197 -> 203	-0.19015				
Excited State 19:	Singlet-A	5.4771 eV	226.37 nm	*f*=0.0004	<S**2>=0.000
184 -> 199	0.16236				
192 -> 202	-0.36330				
195 -> 200	0.25832				
197 -> 200	0.17572				
197 -> 202	0.34386				
197 -> 203	0.19670				
Excited State 20:	Singlet-A	5.5179 eV	224.69 nm	*f*=0.0028	<S**2>=0.000
198 -> 203	0.56548				
198 -> 204	-0.21526				
198 -> 205	-0.31388				
Excited State 21:	Singlet-A	5.5447 eV	223.61 nm	*f*=0.0002	<S**2>=0.000
192 -> 201	-0.10275				
192 -> 202	0.42249				
195 -> 202	0.10143				
197 -> 200	0.33878				
197 -> 201	-0.10036				
197 -> 202	0.35234				
Excited State 22:	Singlet-A	5.5563 eV	223.14 nm	*f*=0.0025	<S**2>=0.000
198 -> 203	0.32964				
198 -> 204	0.58612				
198 -> 205	0.17077				
Excited State 23:	Singlet-A	5.5737 eV	222.45 nm	*f*=0.0005	<S**2>=0.000
189 -> 201	-0.35061				

191 -> 201 -0.24806
196 -> 201 0.50666
198 -> 205 -0.12425

Excited State 24: Singlet-A 5.5792 eV 222.23 nm *f*=0.0013 <S**2>=0.000
186 -> 199 -0.12376
196 -> 201 0.12573
198 -> 203 0.20963
198 -> 204 -0.27244
198 -> 205 0.55323

Excited State 25: Singlet-A 5.5858 eV 221.96 nm *f*=0.0115 <S**2>=0.000
184 -> 199 0.23522
186 -> 199 0.60003
187 -> 199 -0.14088
198 -> 204 -0.10262

Excited State 26: Singlet-A 5.6329 eV 220.11 nm *f*=0.0016 <S**2>=0.000
187 -> 200 -0.25399
188 -> 200 0.30153
195 -> 200 -0.10057
197 -> 200 0.44059
197 -> 201 0.10333
197 -> 202 -0.28292

Excited State 27: Singlet-A 5.6363 eV 219.97 nm *f*=0.0184 <S**2>=0.000
196 -> 202 0.13127
196 -> 203 -0.25152
196 -> 204 0.60134
196 -> 209 -0.15685

Excited State 28: Singlet-A 5.6380 eV 219.91 nm *f*=0.0016 <S**2>=0.000
187 -> 200 0.28798
188 -> 200 -0.34087
195 -> 200 0.14601
197 -> 200 0.36641
197 -> 202 -0.24071

Excited State 29: Singlet-A 5.6410 eV 219.79 nm *f*=0.0020 <S**2>=0.000
189 -> 201 0.39863
191 -> 201 0.28122
196 -> 201 0.45209
196 -> 204 -0.10697

Excited State 30: Singlet-A 5.6824 eV 218.19 nm *f*=0.0368 <S**2>=0.000
181 -> 199 -0.31026
183 -> 199 0.14581
184 -> 199 -0.15183
195 -> 202 -0.12165
198 -> 206 0.37293
198 -> 207 -0.26117
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 30 LETran= 550.
****

4. HRESIMS, IR, $[\alpha]_D$, ECD and NMR spectra of compound 1

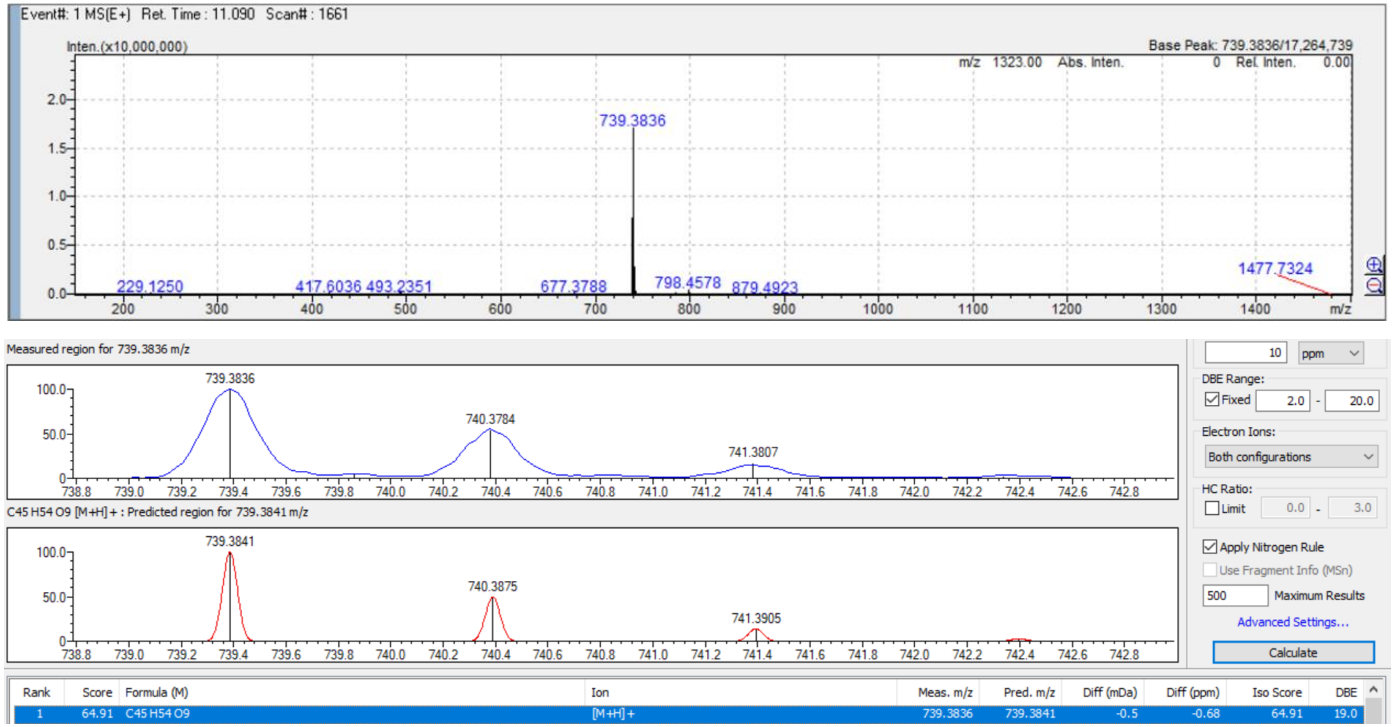


Figure S3. HRESIMS spectrum of artematrotrimer A (**1**).

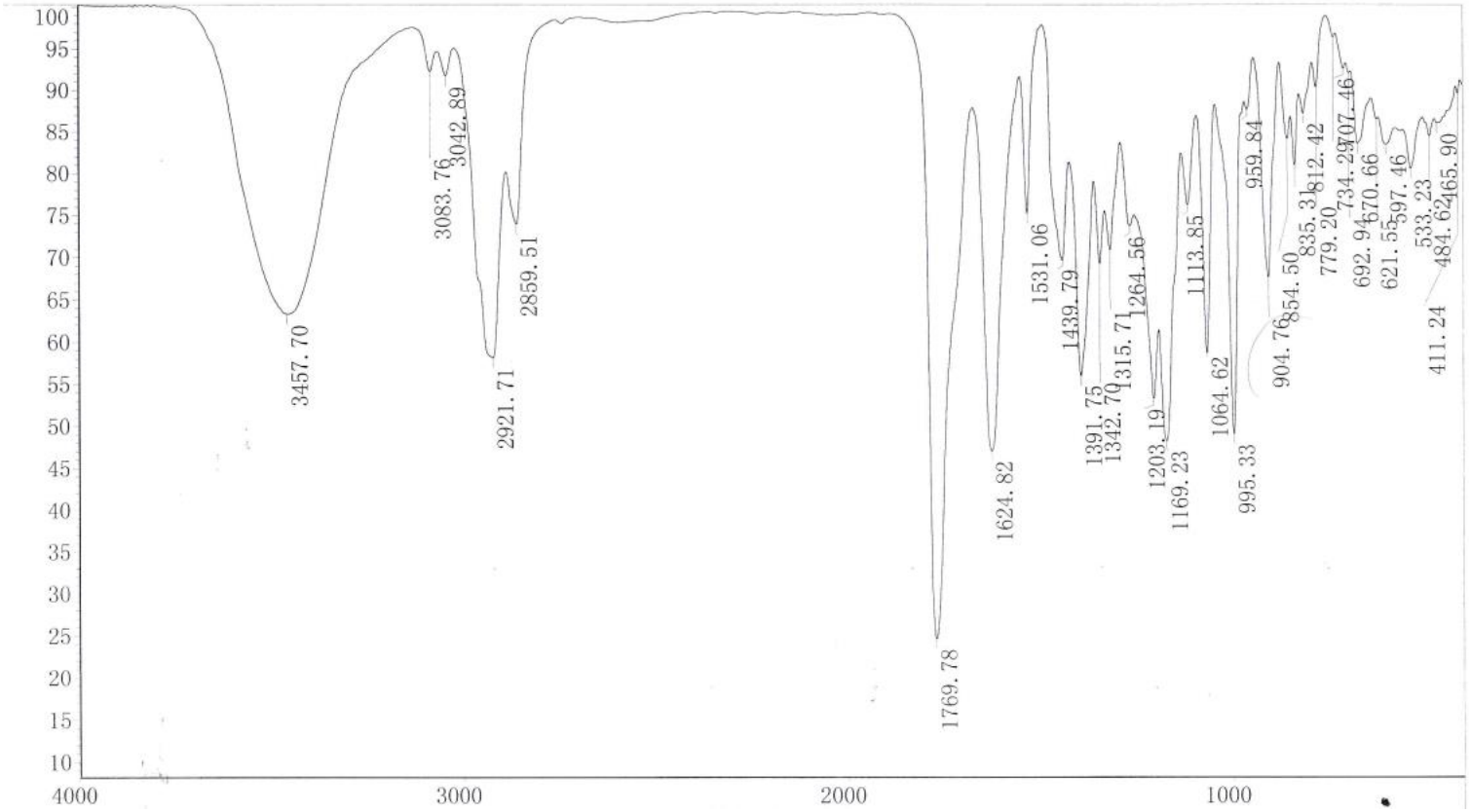


Figure S4. IR spectrum of artematrotrimer A (**1**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 30-SEP-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-38.27	0.85	-2.22	-37.27	-39.55

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JAR129A	10:20:34 AM	-37.27	SR	-0.0328	589	100.00	0.088	23.1
2	JAR129A	10:20:42 AM	-38.18	SR	-0.0336	589	100.00	0.088	23.1
3	JAR129A	10:20:51 AM	-37.84	SR	-0.0333	589	100.00	0.088	23.1
4	JAR129A	10:20:58 AM	-38.52	SR	-0.0339	589	100.00	0.088	23.1
5	JAR129A	10:21:07 AM	-39.55	SR	-0.0348	589	100.00	0.088	23.1

Figure S5. Optical rotation spectrum of artematrotrimer A (**1**).

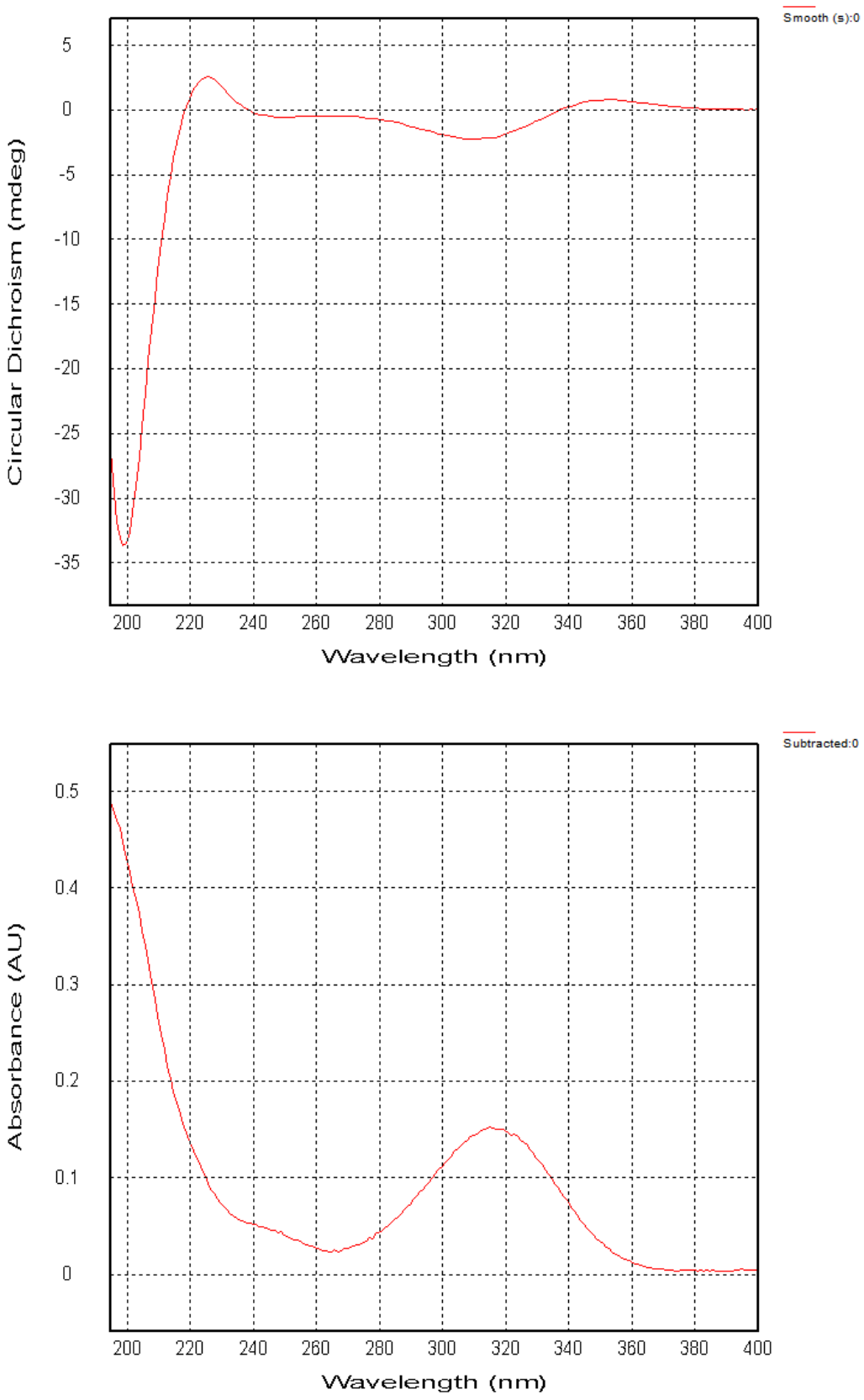


Figure S6. ECD (top) and UV (bottom) spectra of artematrotrimer A (**1**).

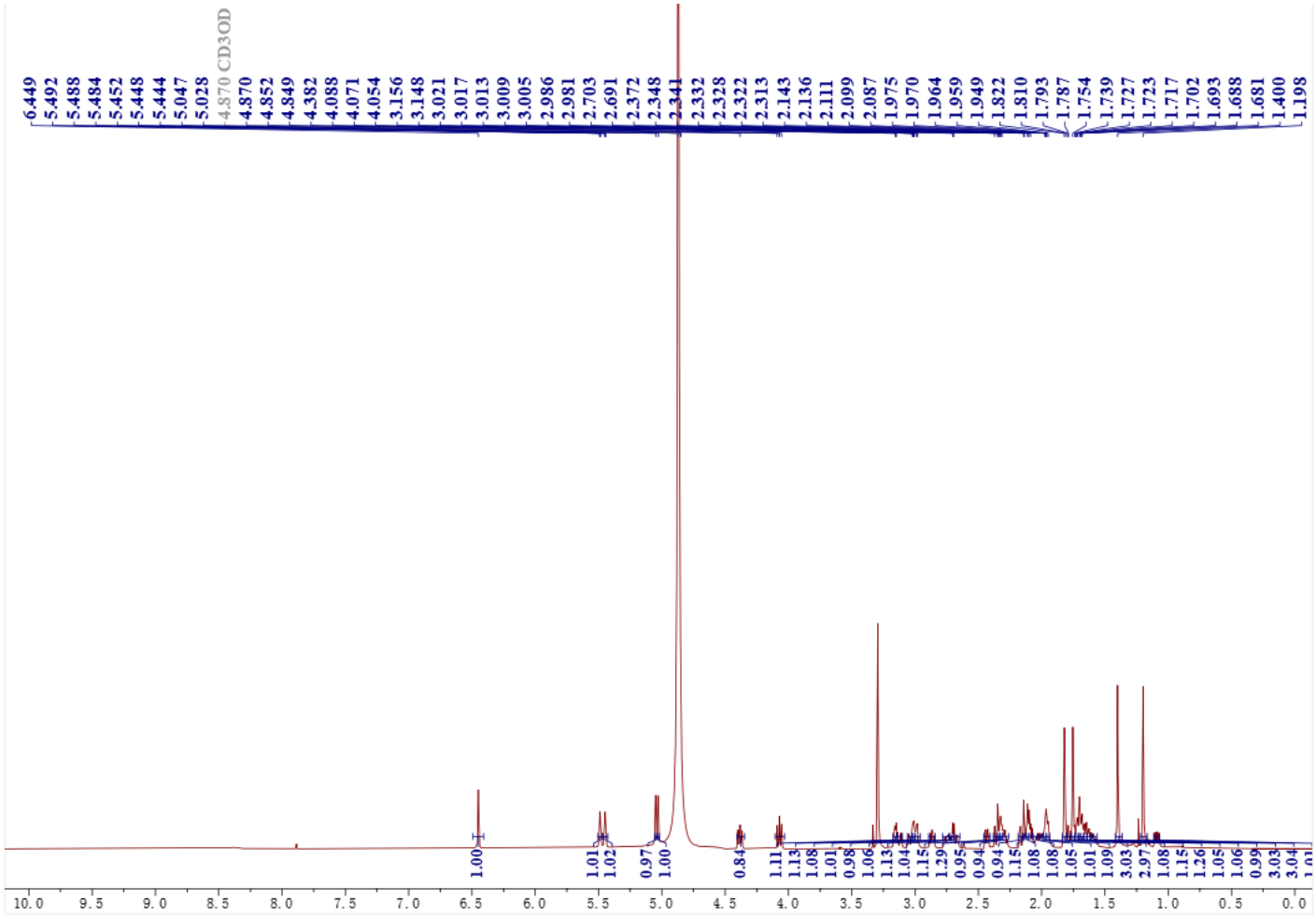


Figure S7. ^{1}H spectrum (600 MHz) of artematrotrimer A (**1**) in CD_3OD.

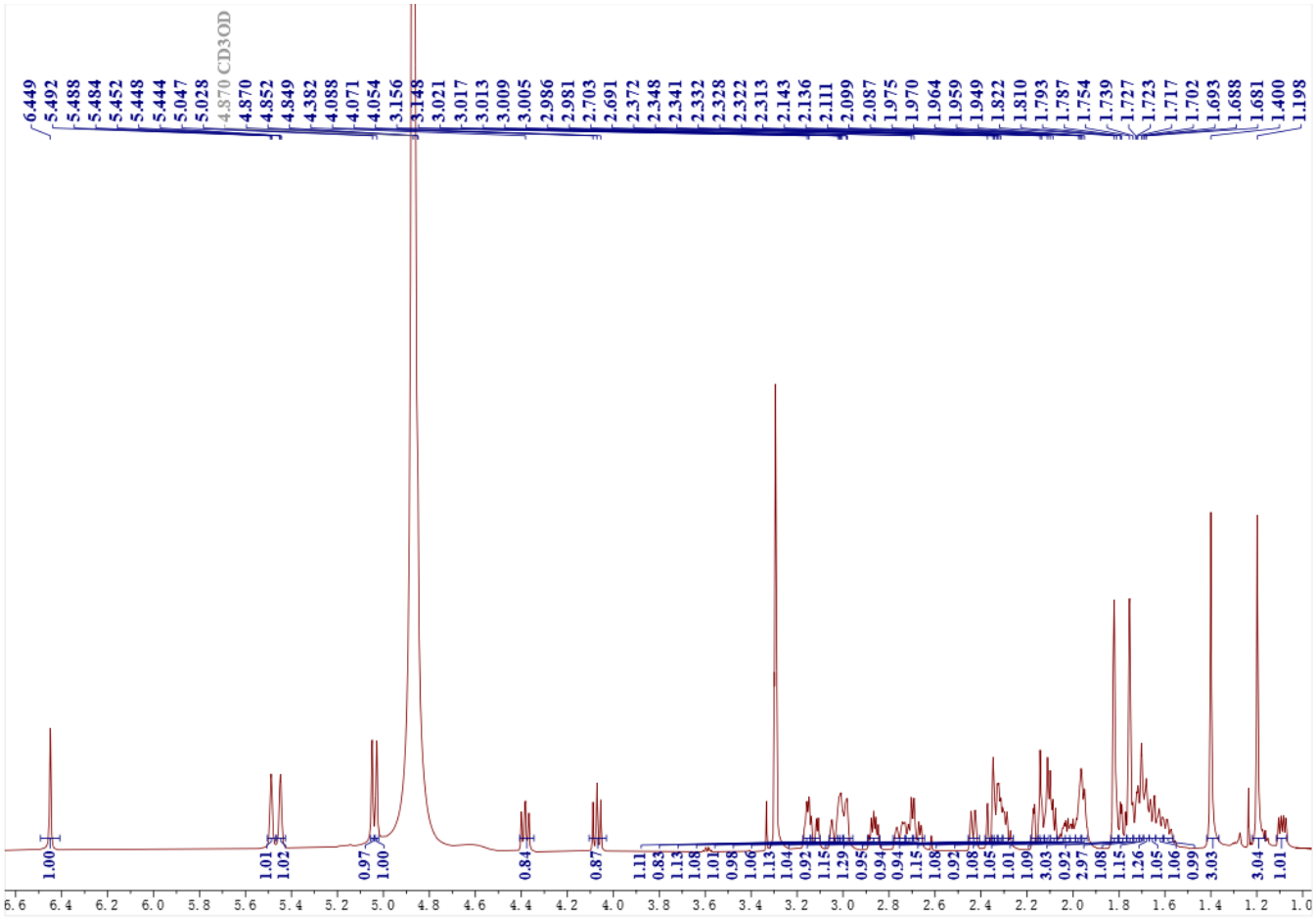


Figure S8. enlarged ^{1}H spectrum (600 MHz) of artematrotrimer A (**1**) in CD_3OD.

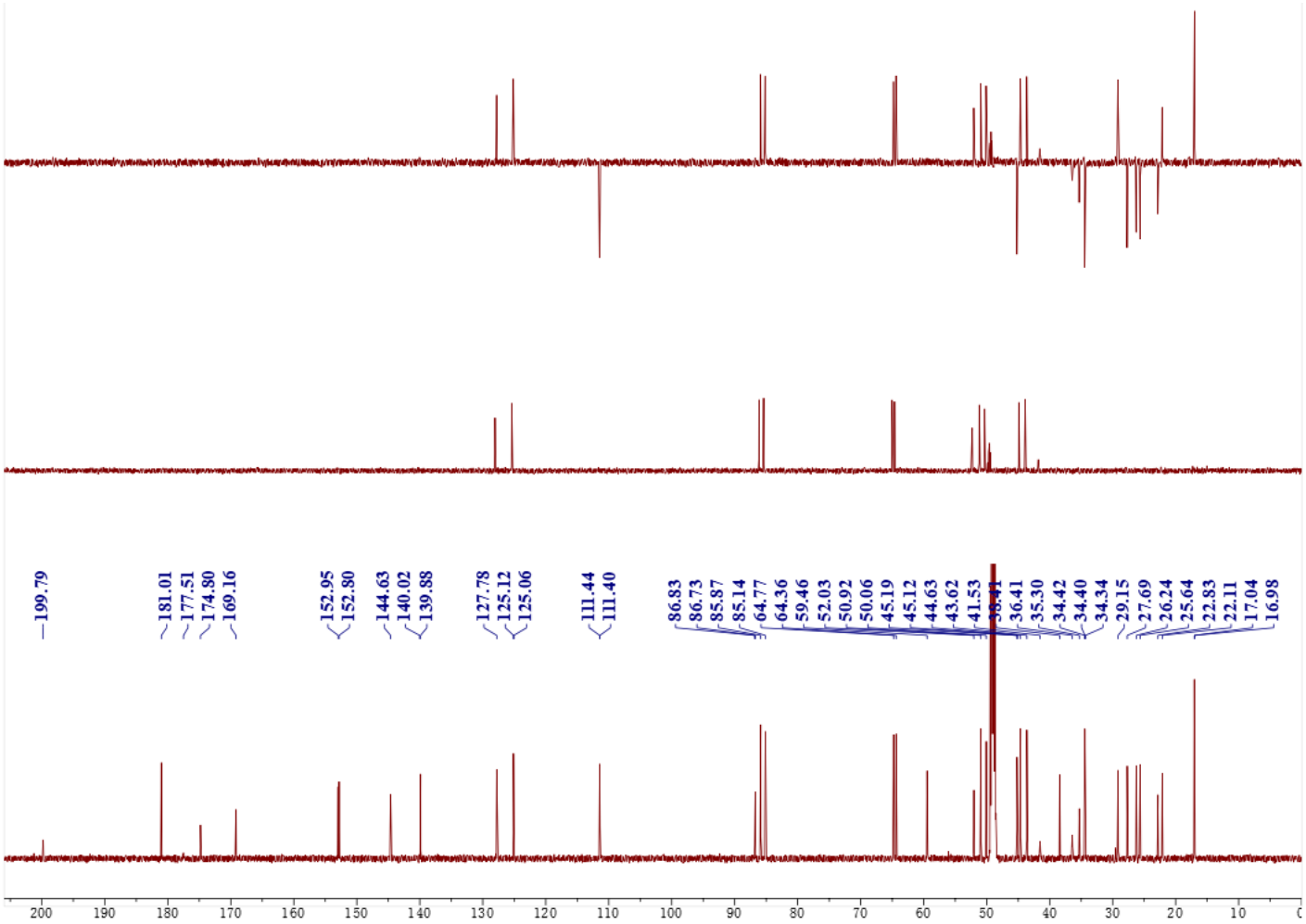


Figure S9. ^{13}C and DEPT spectra (150 MHz) of artematrotrimer A (**1**) in CD_3OD.

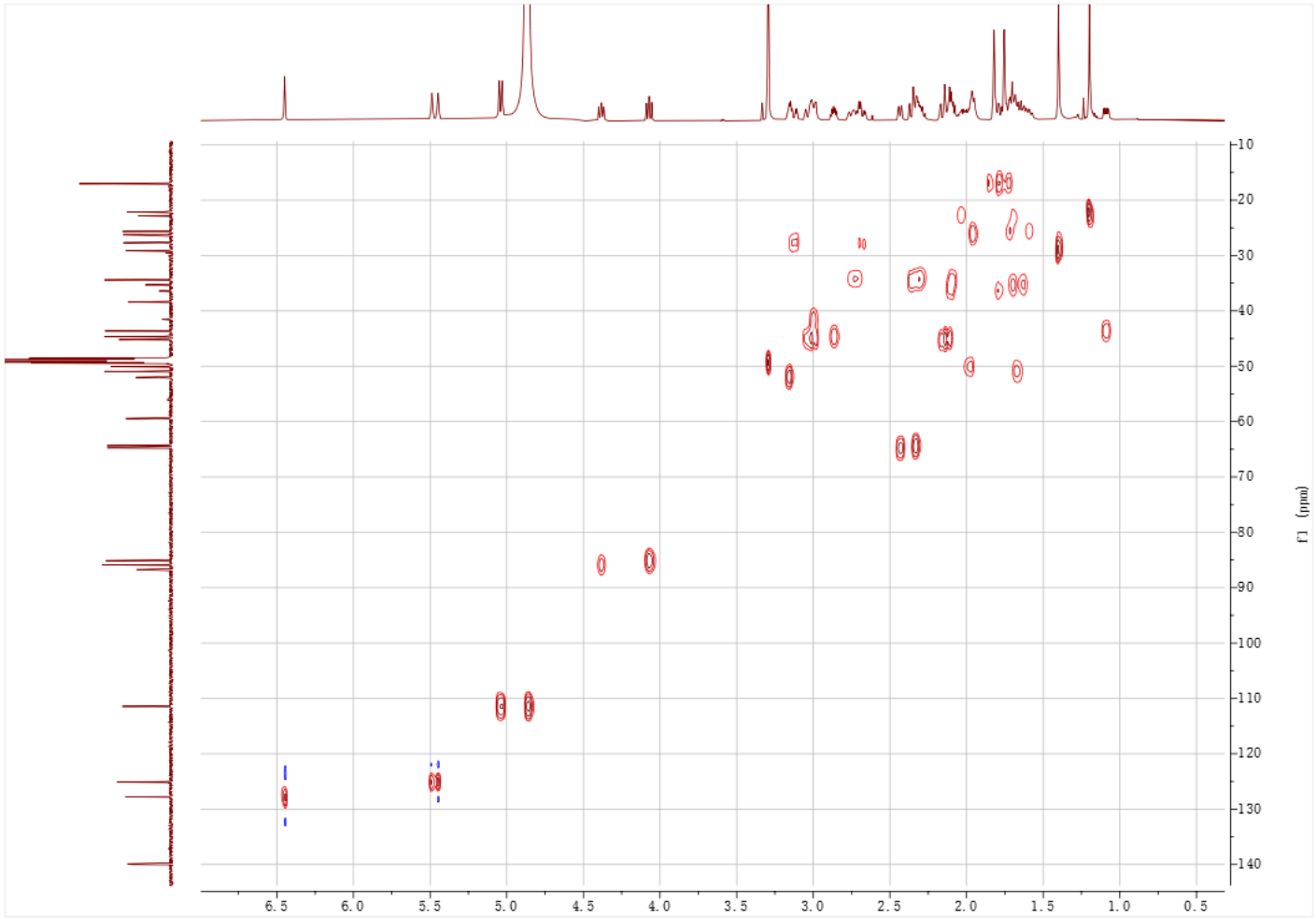


Figure S10. HSQC spectrum (600 MHz) of artematrotrimer A (**1**) in CD_3OD.

Figure S11. ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrotrimer A (**1**) in CD_3OD.

Figure S12. HMBC spectrum (600 MHz) of artematrotrimer A (**1**) in CD_3OD.

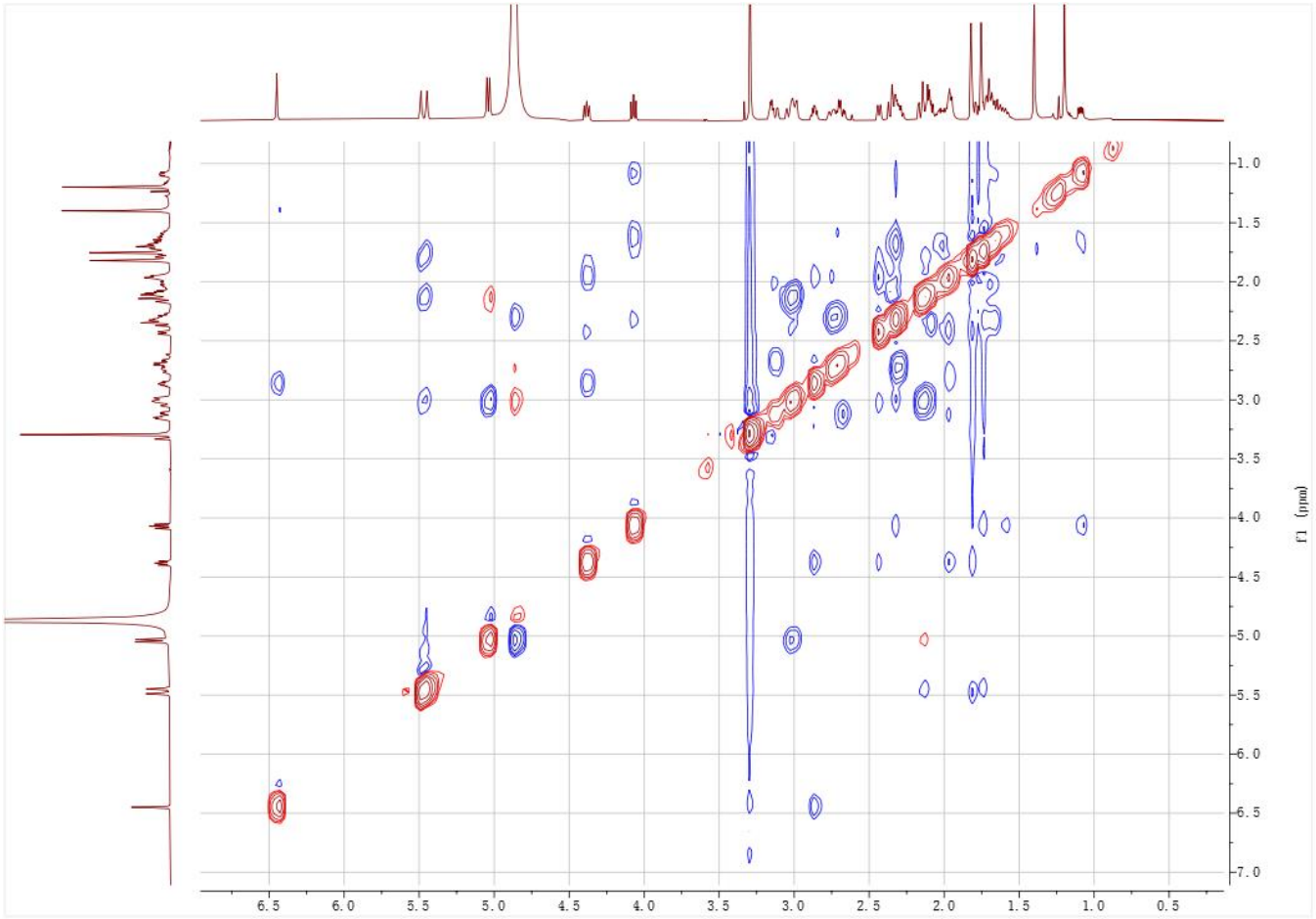


Figure S13. ROESY spectrum (600 MHz) of artematrotrimer A (**1**) in CD_3OD.

5. HRESIMS, IR, $[\alpha]_D$, ECD and NMR spectra of compound 2

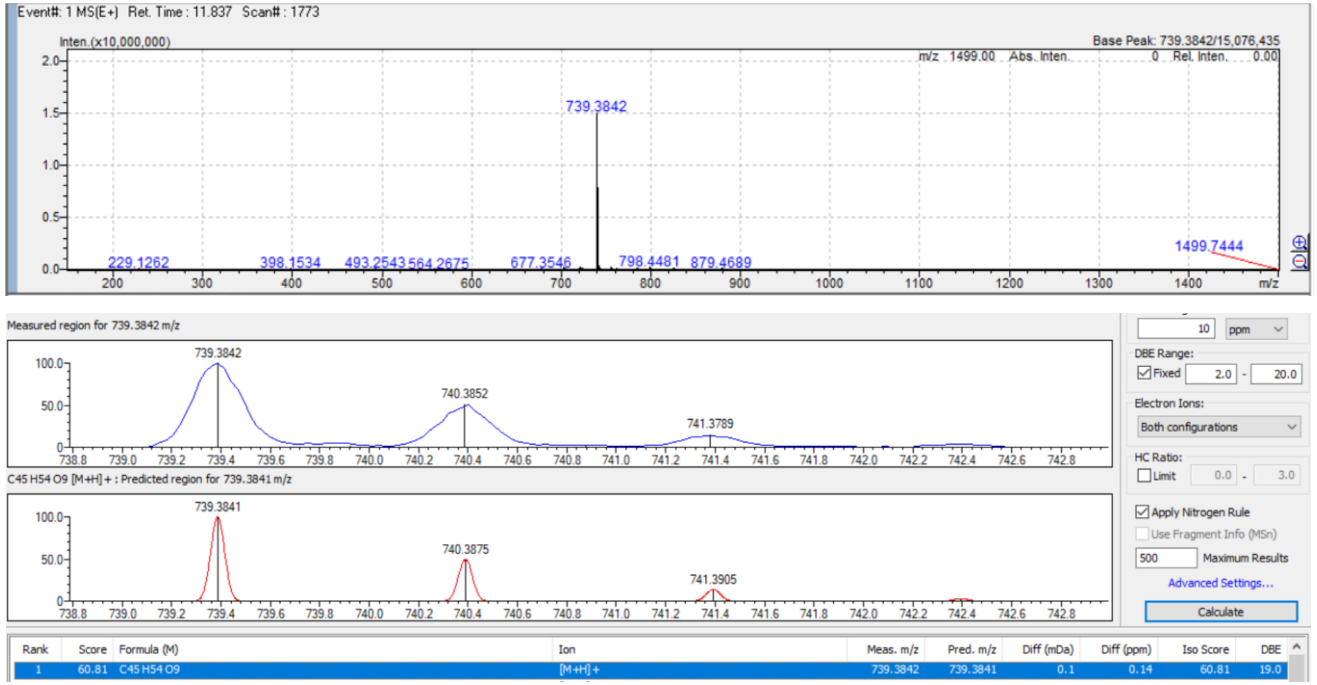


Figure S14. HRESIMS spectrum of artematrotrimer B (**2**).

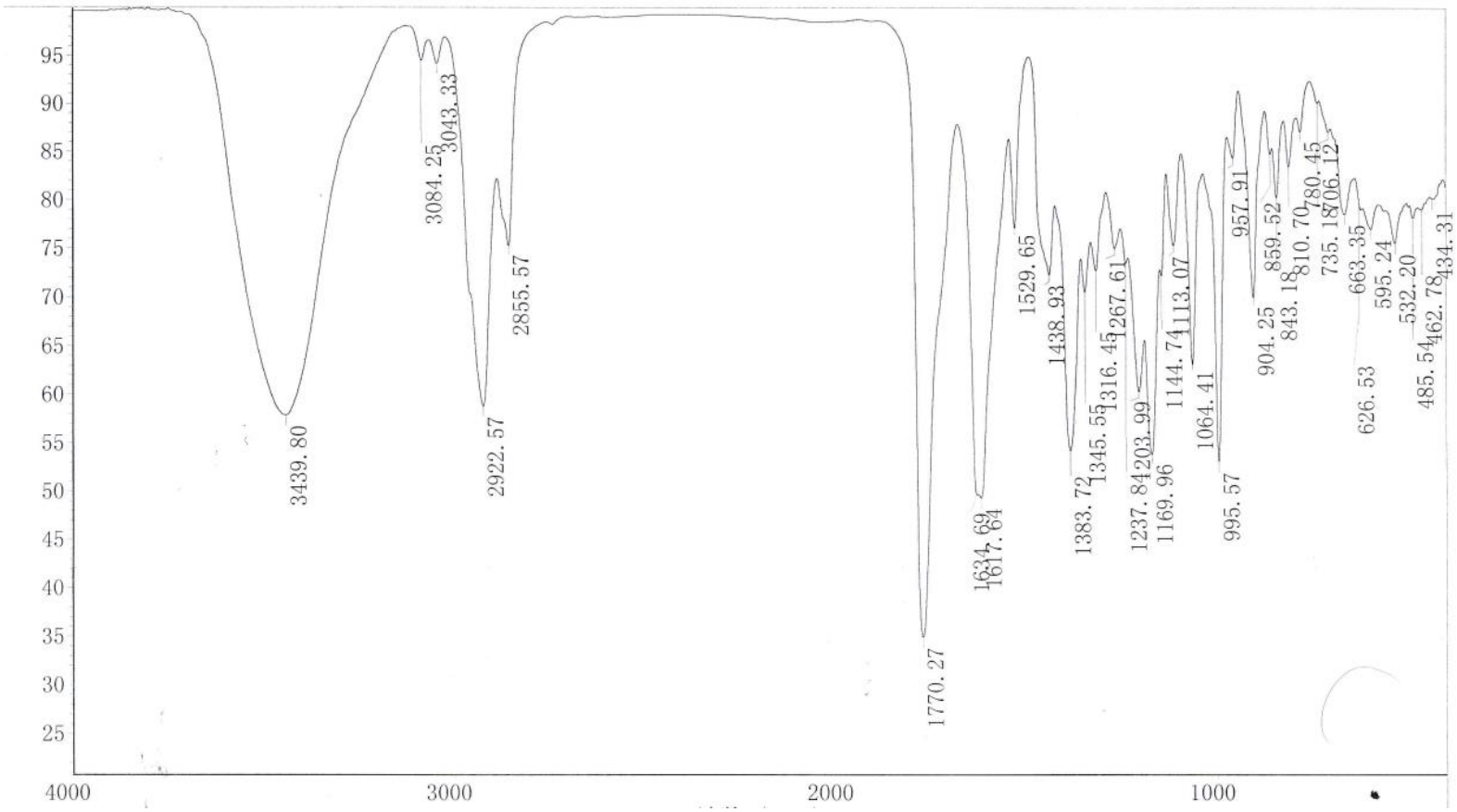


Figure S15. IR spectrum of artematrotrimer B (**2**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 30-SEP-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-4.91	0.29	-5.90	-4.41	-5.08

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JAR129B	10:35:33 AM	-4.41	SR	-0.0026	589	100.00	0.059	23.2
2	JAR129B	10:35:41 AM	-5.08	SR	-0.0030	589	100.00	0.059	23.2
3	JAR129B	10:35:49 AM	-5.08	SR	-0.0030	589	100.00	0.059	23.2
4	JAR129B	10:35:57 AM	-5.08	SR	-0.0030	589	100.00	0.059	23.2
5	JAR129B	10:36:05 AM	-4.92	SR	-0.0029	589	100.00	0.059	23.2

Figure S16. Optical rotation spectrum of artematrotrimer B (**2**).

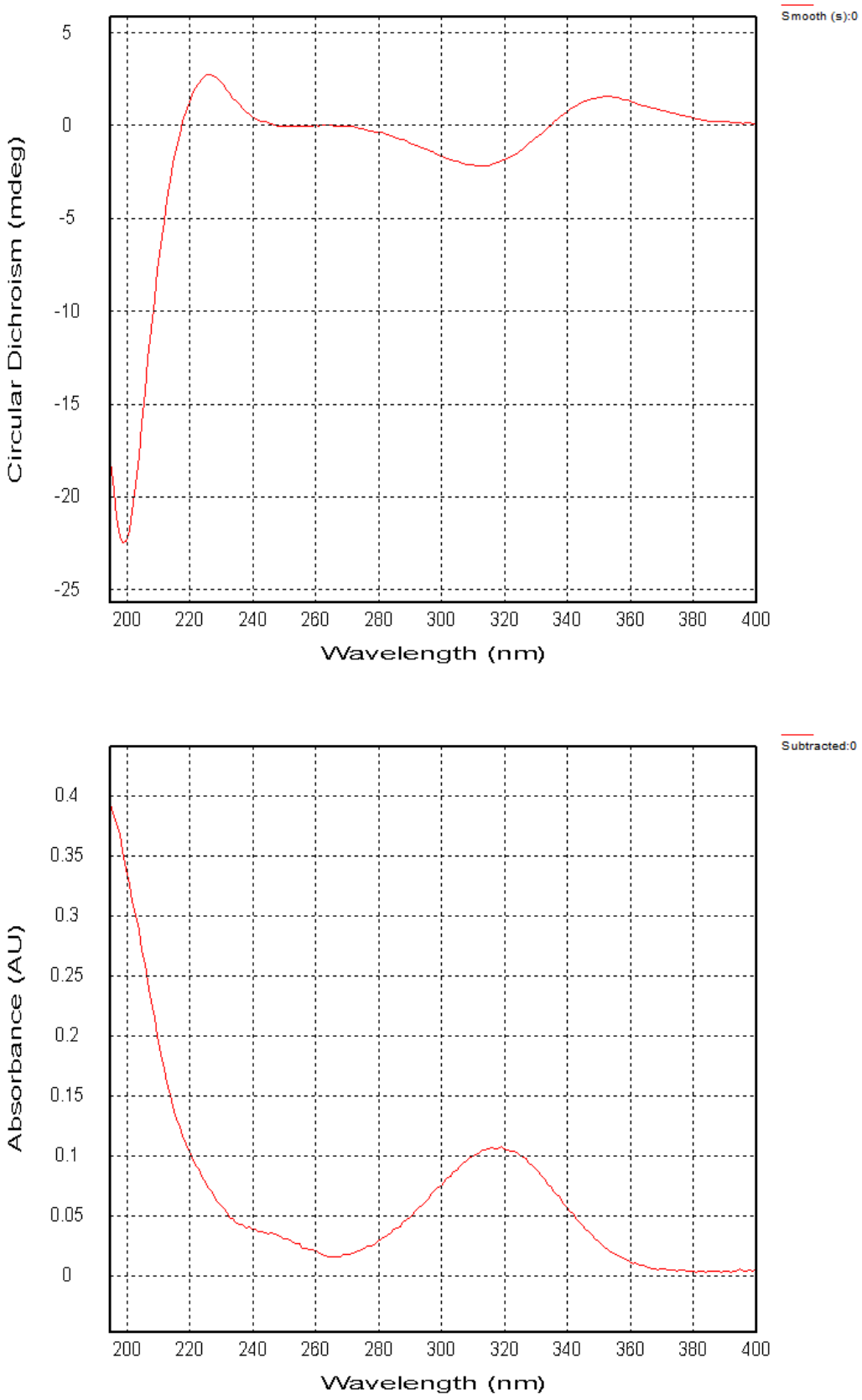


Figure S17. ECD (top) and UV (bottom) spectra of artematrotrimer B (**2**).

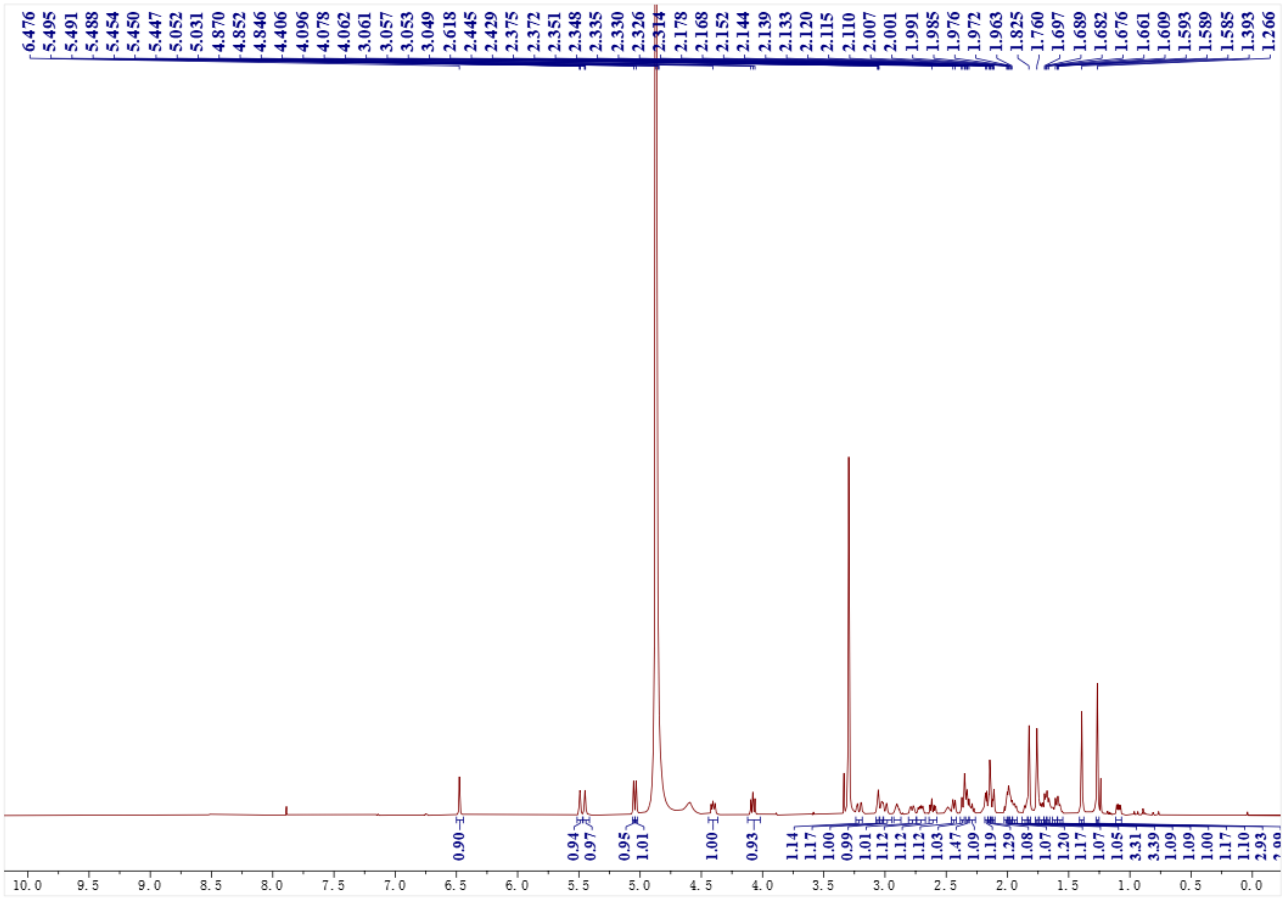


Figure S18. ^{1}H spectrum (600 MHz) of artematrotrimer B (**2**) in CD_3OD.

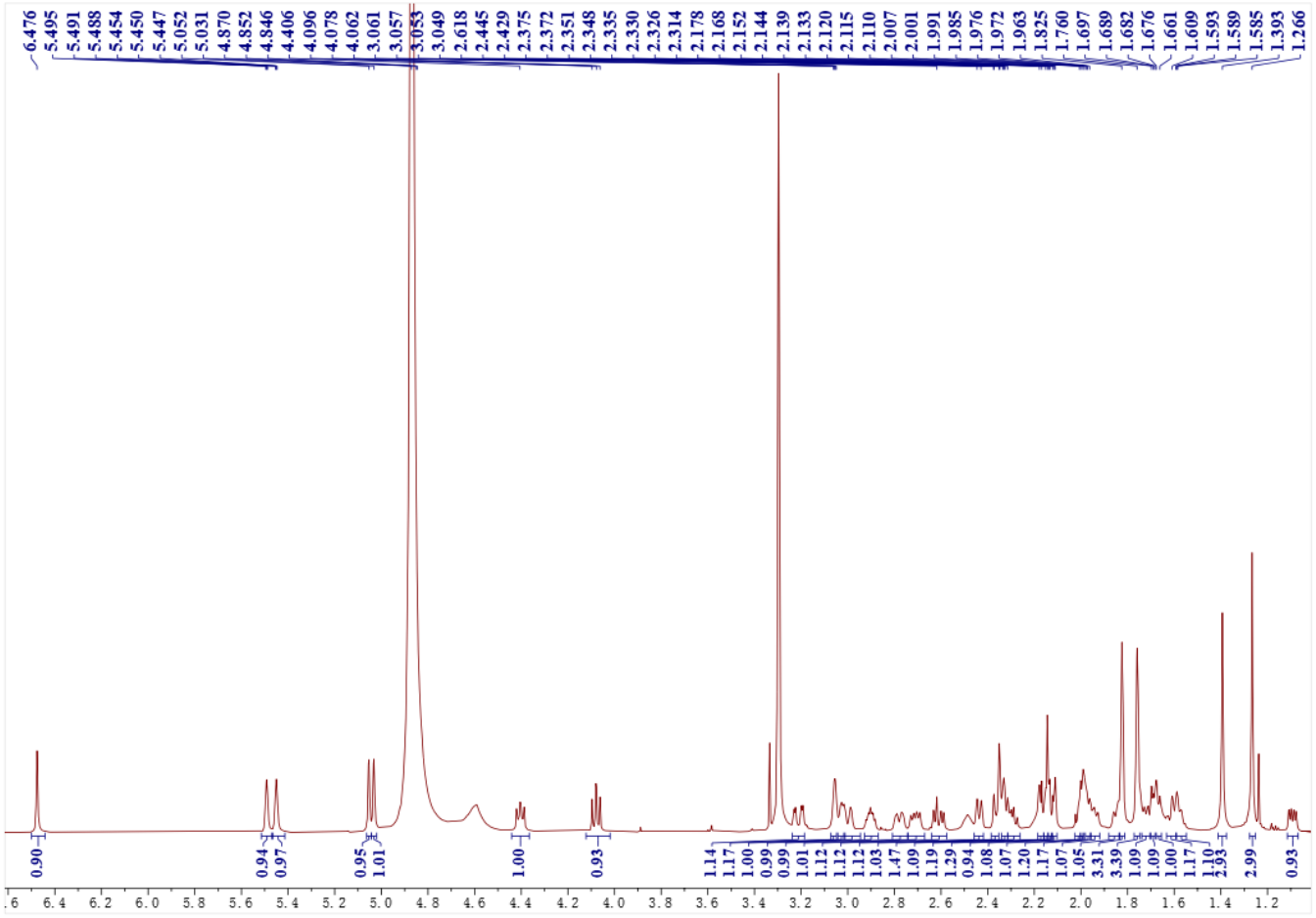


Figure S19. enlarged ^{1}H spectrum (600 MHz) of artematrotrimer B (**2**) in CD_3OD.

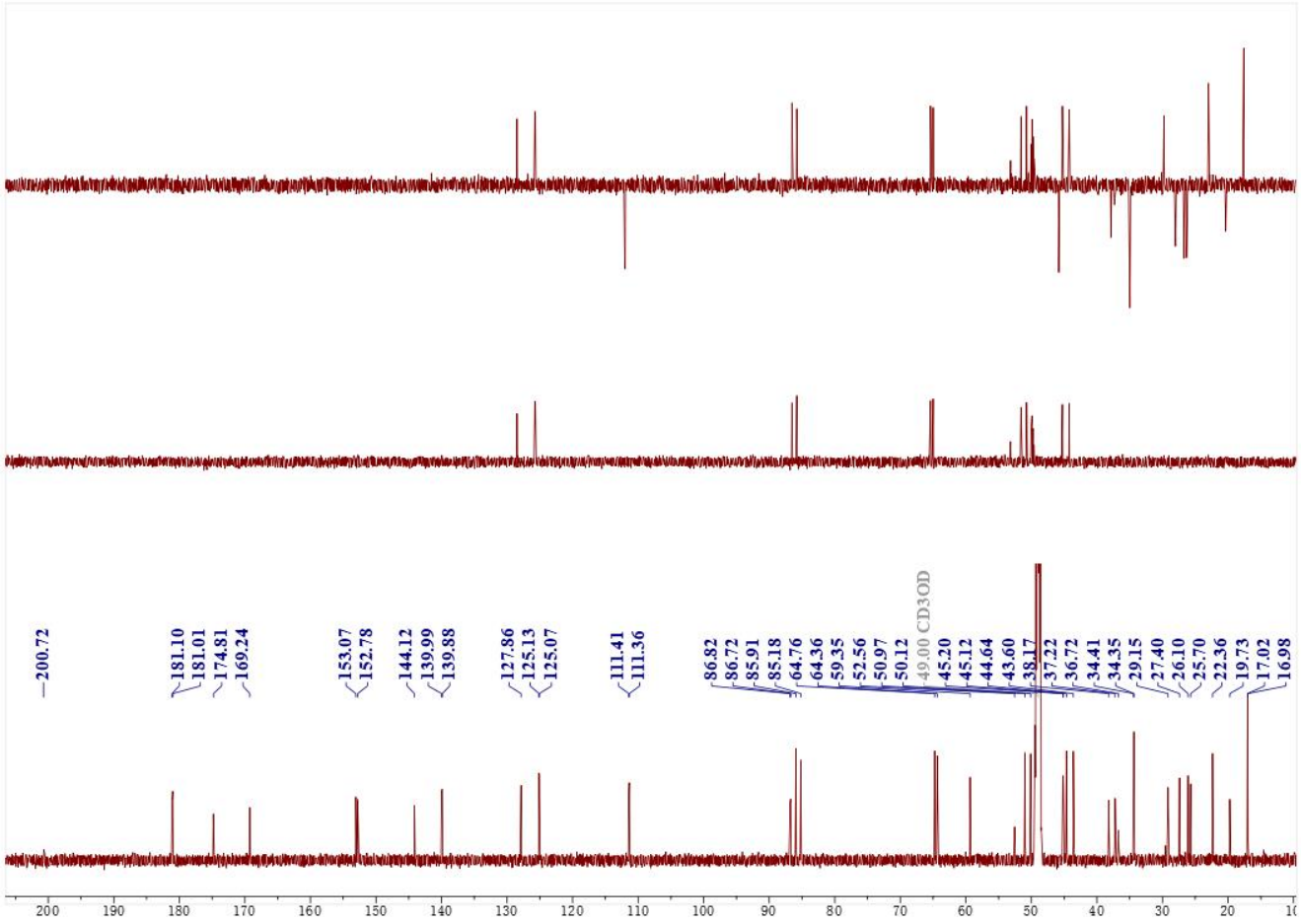


Figure S20. ^{13}C and DEPT spectra (150 MHz) of artematrotrimer B (**2**) in CD_3OD.

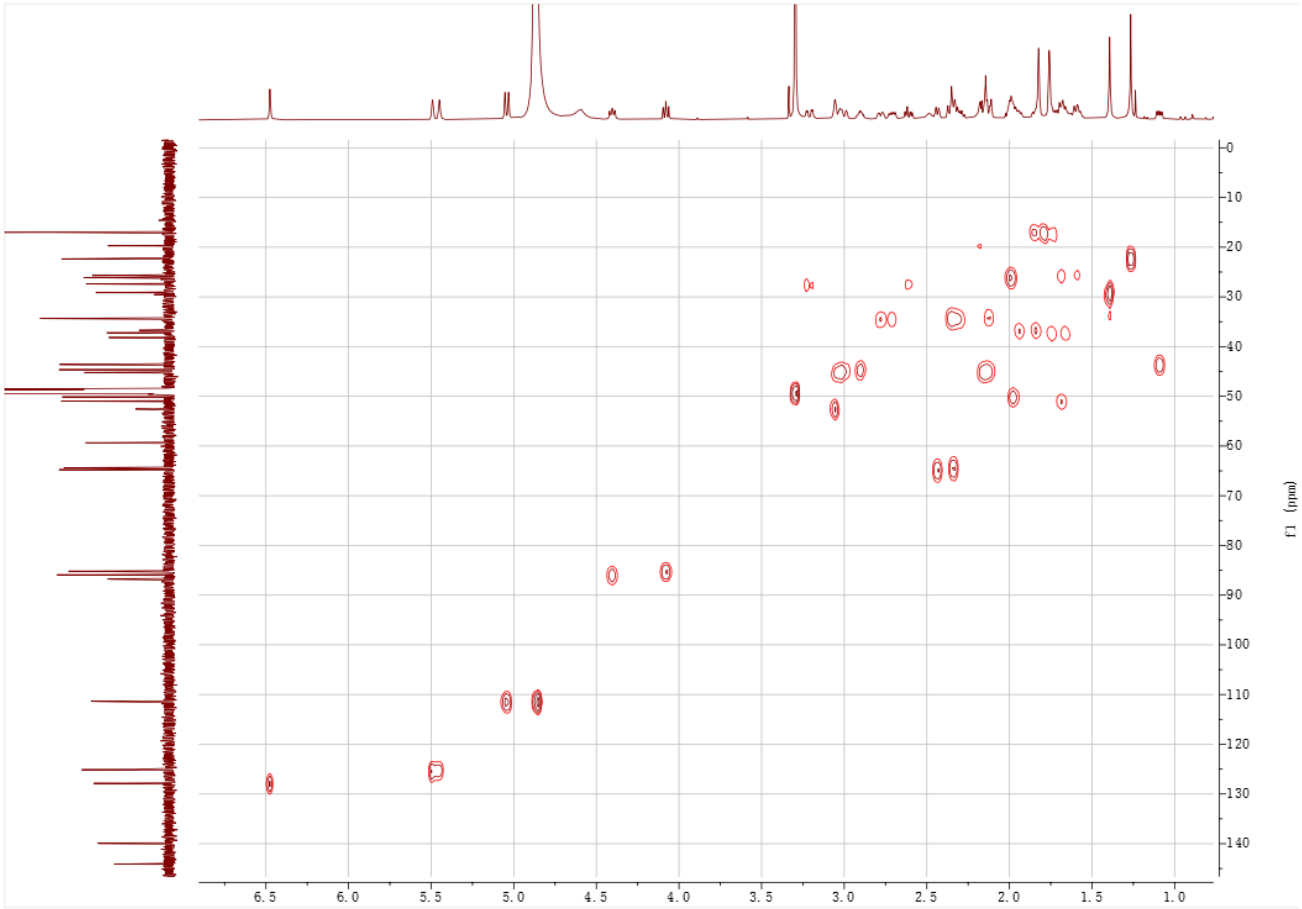


Figure S21. HSQC spectrum (600 MHz) of artematrotrimer B (**2**) in CD_3OD.

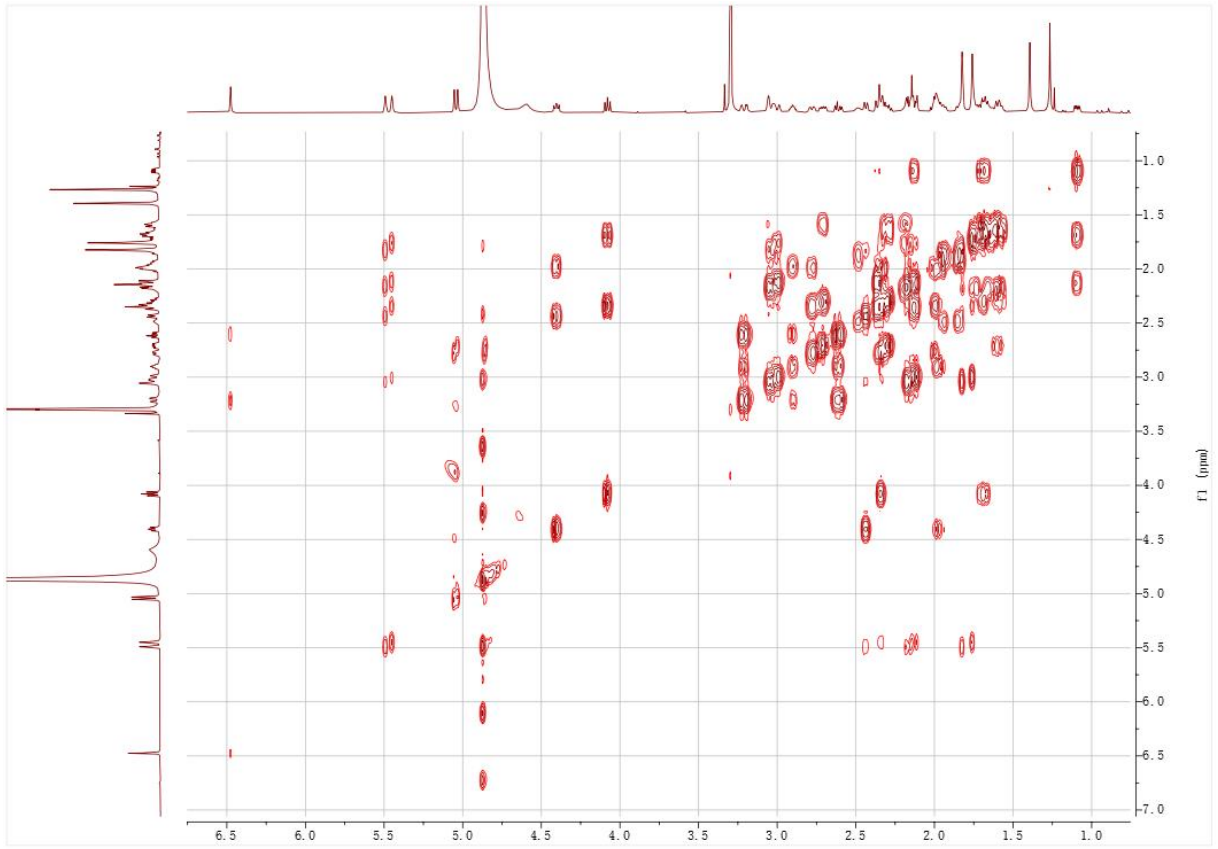


Figure S22. ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrotrimer B (**2**) in CD_3OD.

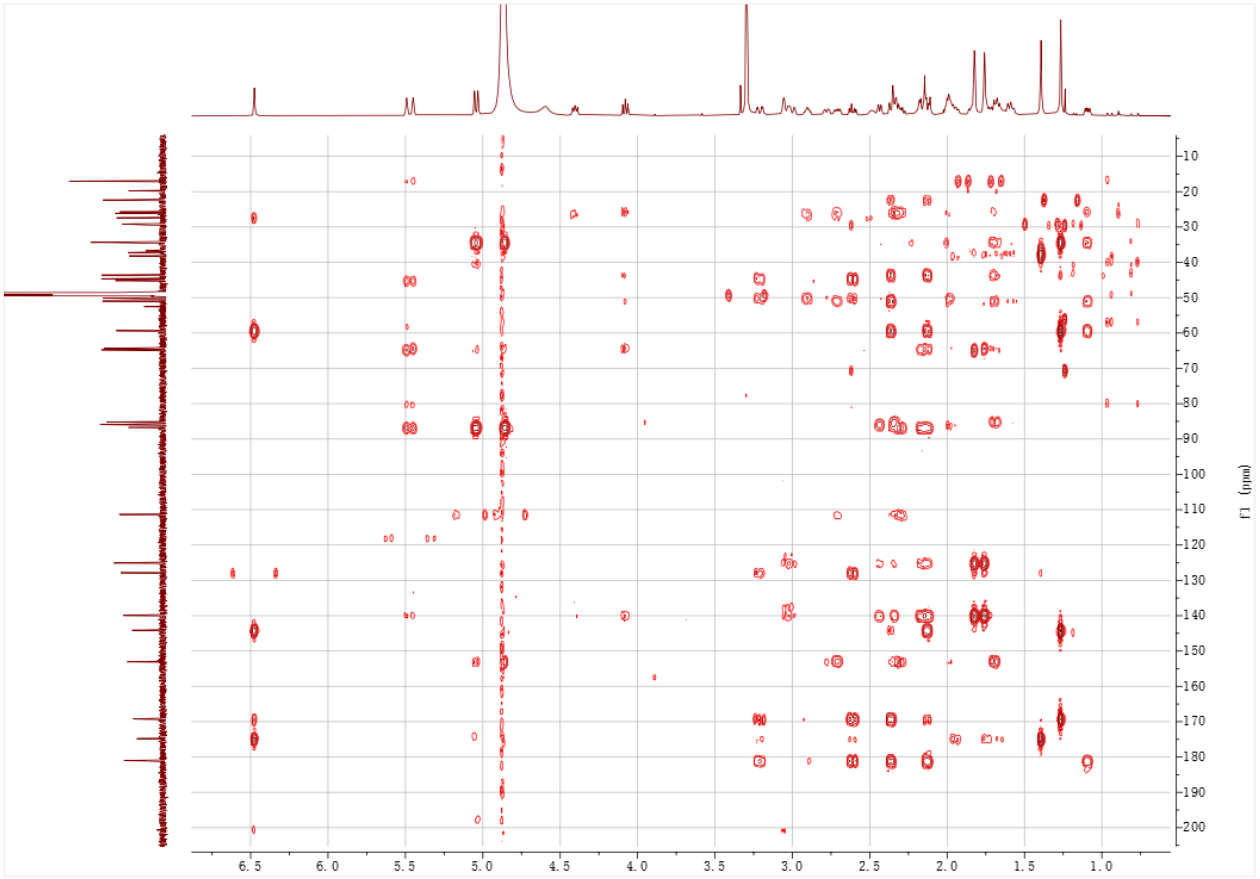


Figure S23. HMBC spectrum (600 MHz) of artematrotrimer B (**2**) in CD_3OD.

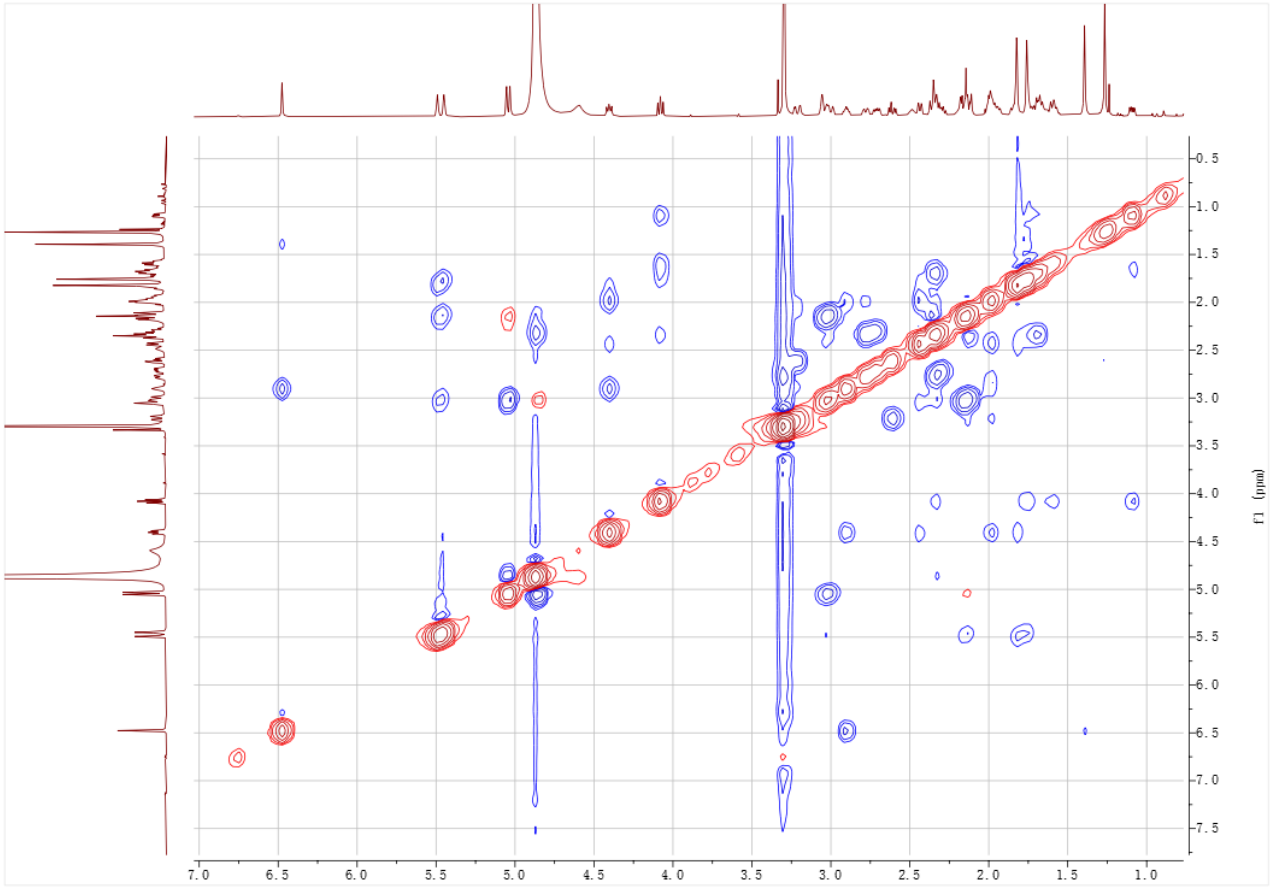


Figure S24. ROESY spectrum (600 MHz) of artematrotrimer B (**2**) in CD_3OD.

6. HRESIMS, IR, $[\alpha]_D$, ECD and NMR spectra of compound 3

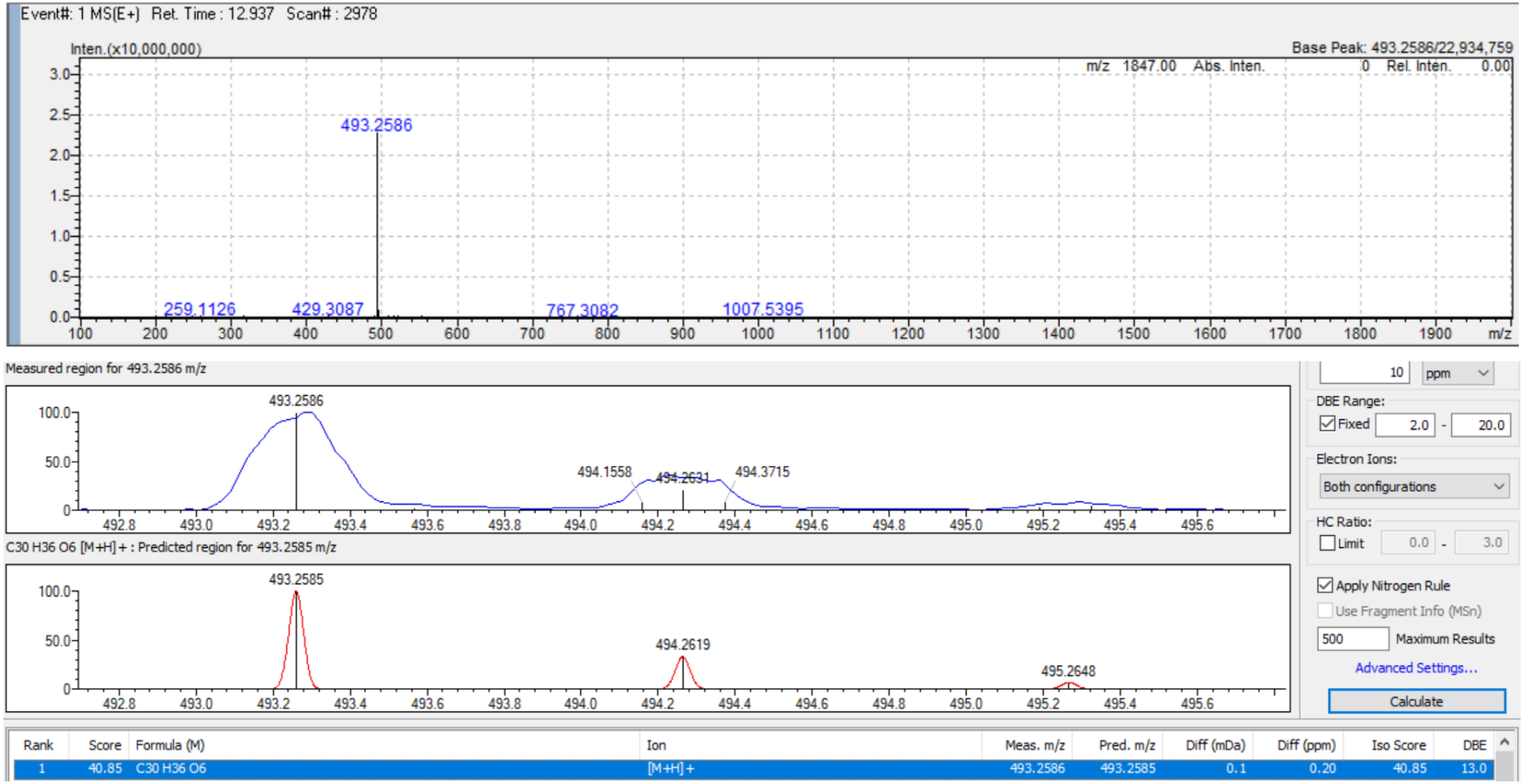


Figure S25. HRESIMS spectrum of artematrodimer A (**3**).

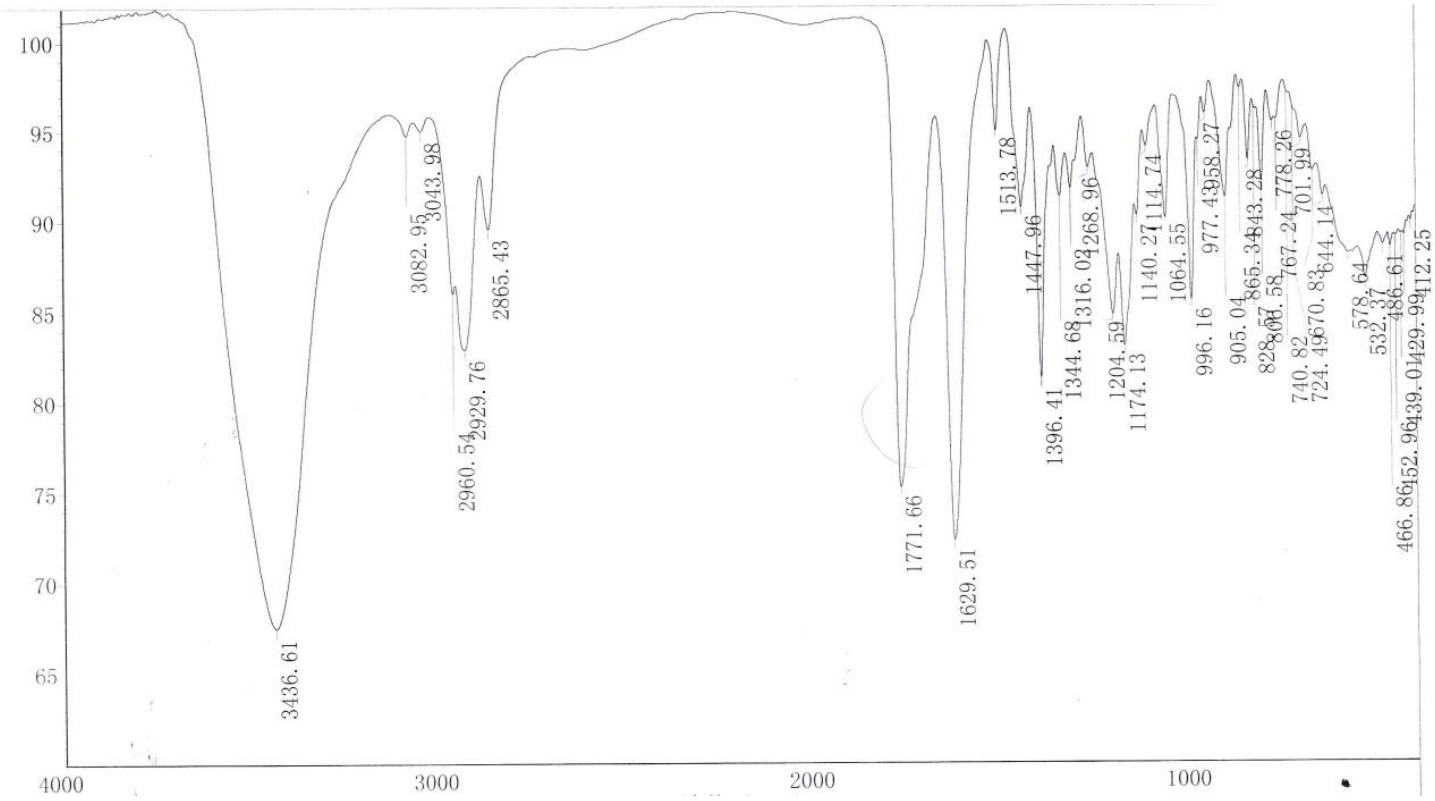


Figure S26. IR spectrum of artematrodimer A (**3**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 13-DEC-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-129.62	0.34	-0.26	-129.12	-130.00

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JAR109C	02:19:59 PM	-130.00	SR	-0.0884	589	100.00	0.068	21.7
2	JAR109C	02:20:08 PM	-129.56	SR	-0.0881	589	100.00	0.068	21.7
3	JAR109C	02:20:16 PM	-129.85	SR	-0.0883	589	100.00	0.068	21.7
4	JAR109C	02:20:24 PM	-129.56	SR	-0.0881	589	100.00	0.068	21.7
5	JAR109C	02:20:32 PM	-129.12	SR	-0.0878	589	100.00	0.068	21.8

Figure S27. Optical rotation spectrum of artematrodimer A (**3**).

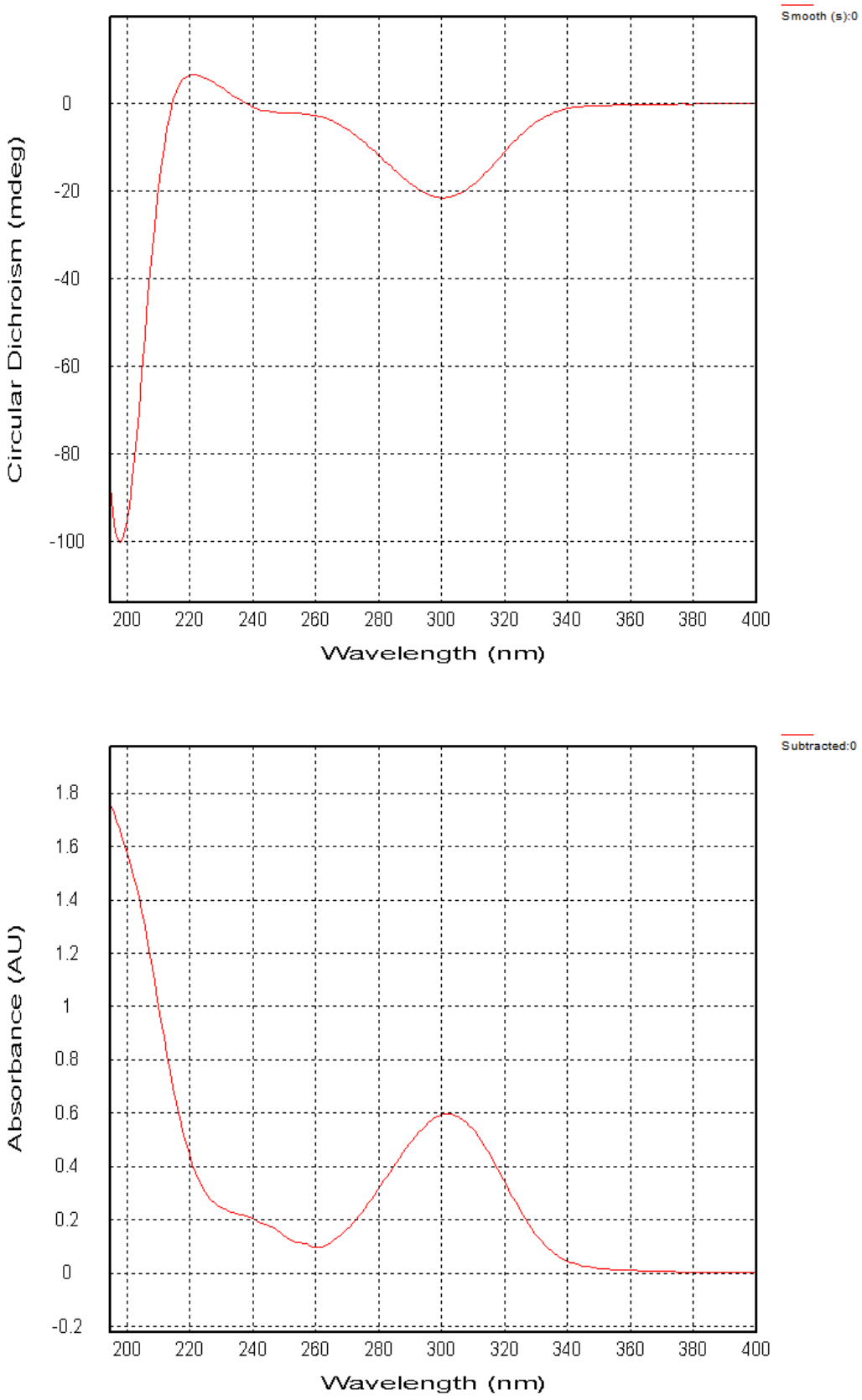


Figure S28. ECD (top) and UV (bottom) spectra of artematrodimer A (**3**).

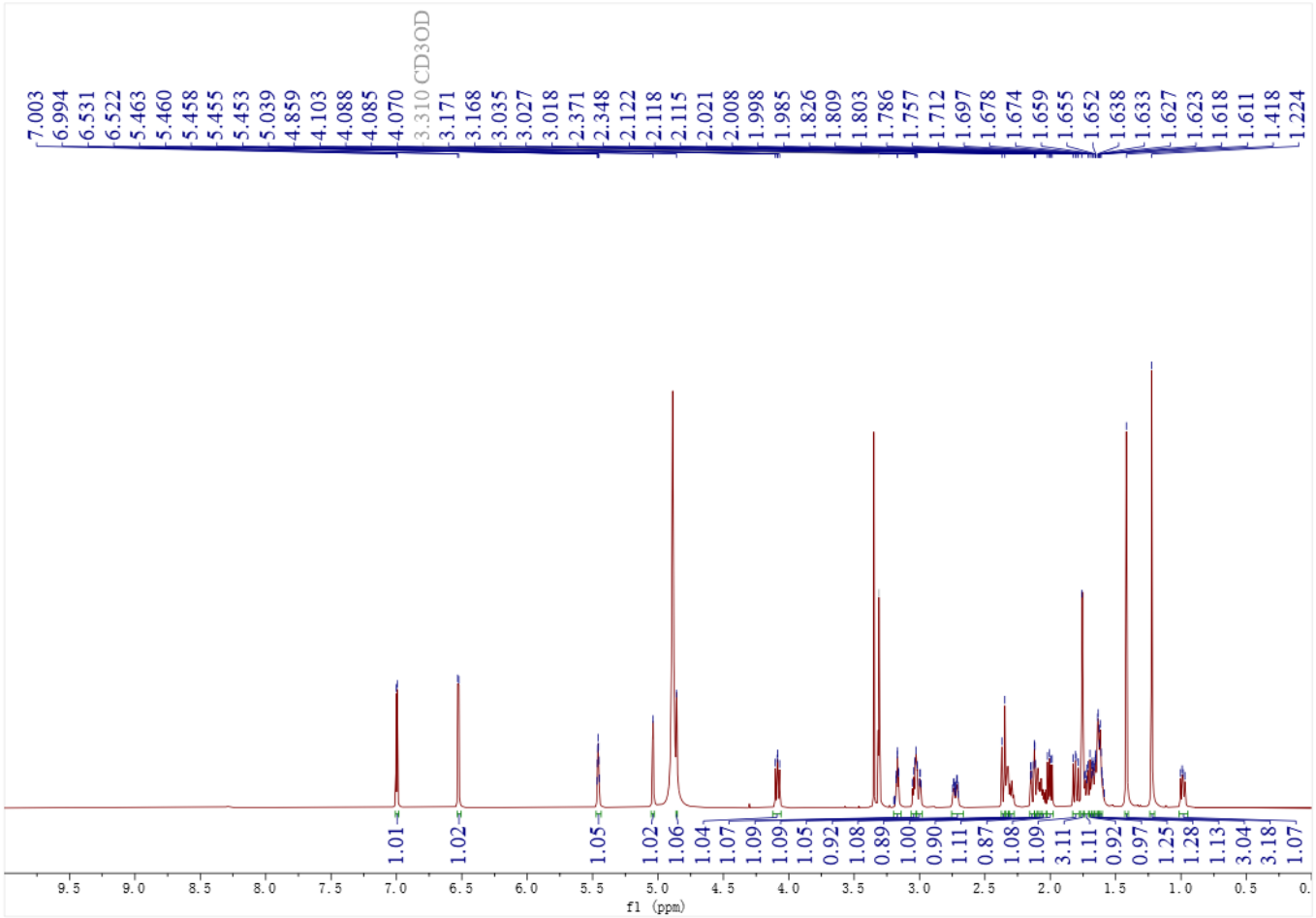


Figure S29. ^{1}H spectrum (600 MHz) of artematrodimer A (**3**) in CD_3OD.

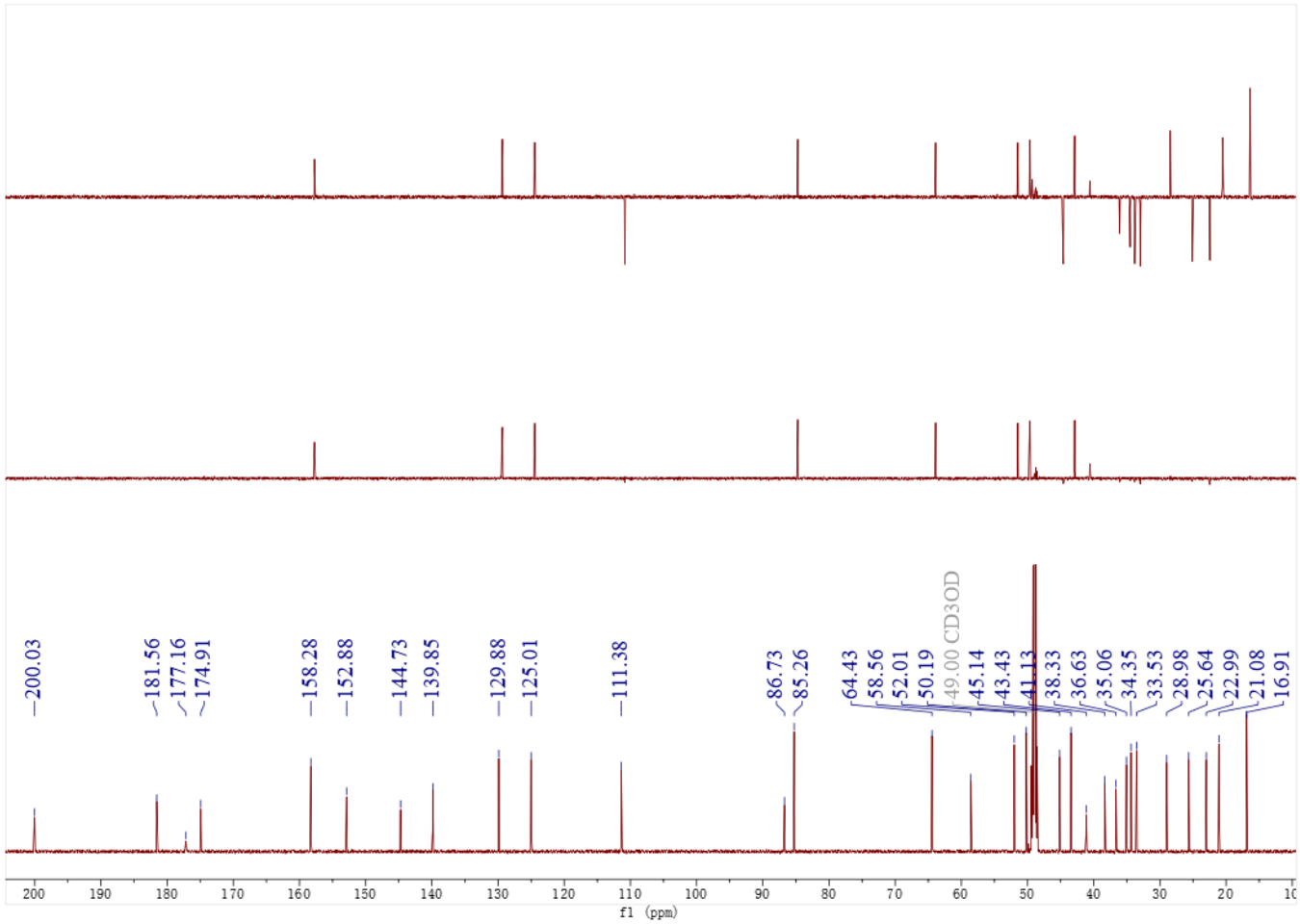


Figure S30. ^{13}C and DEPT spectra (150 MHz) of artematrodimer A (**3**) in CD_3OD.

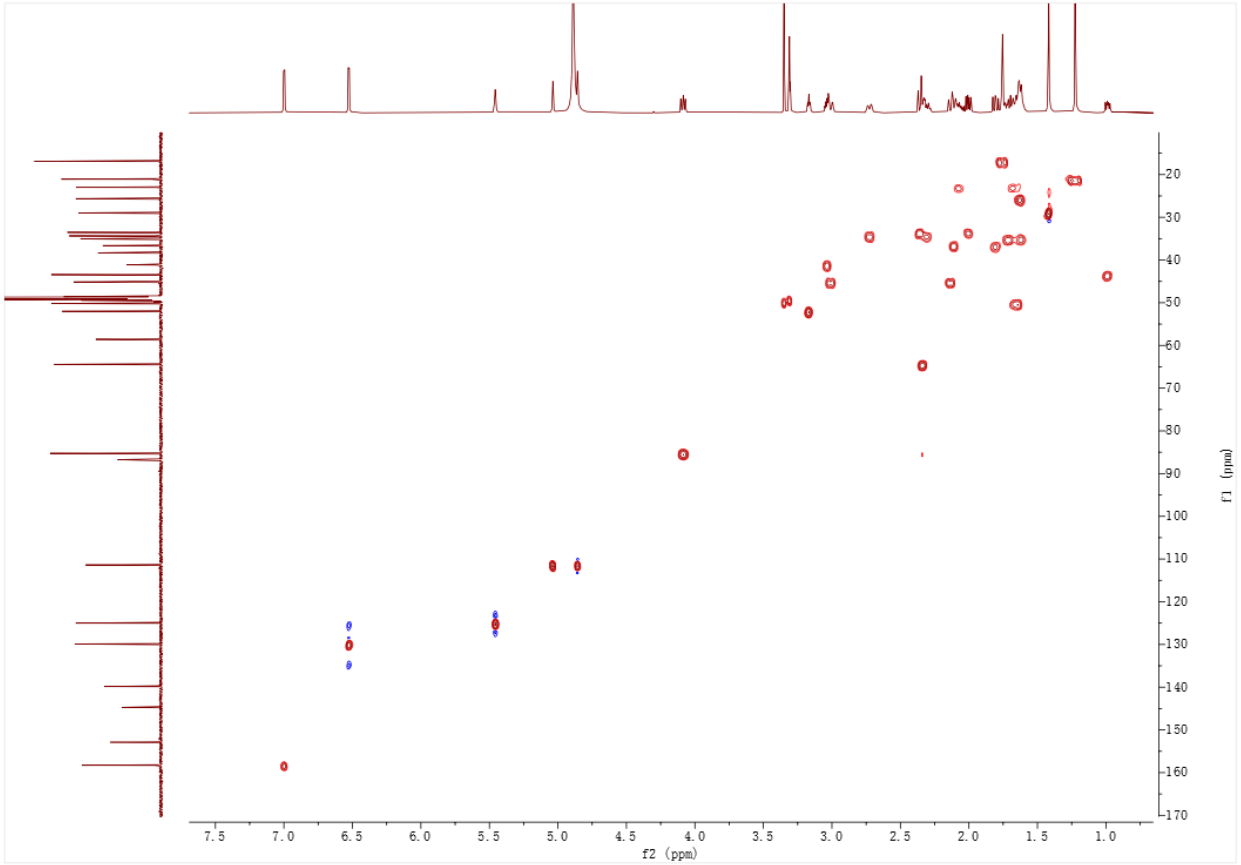


Figure S31. HSQC spectrum (600 MHz) of artematrodimer A (**3**) in CD_3OD.

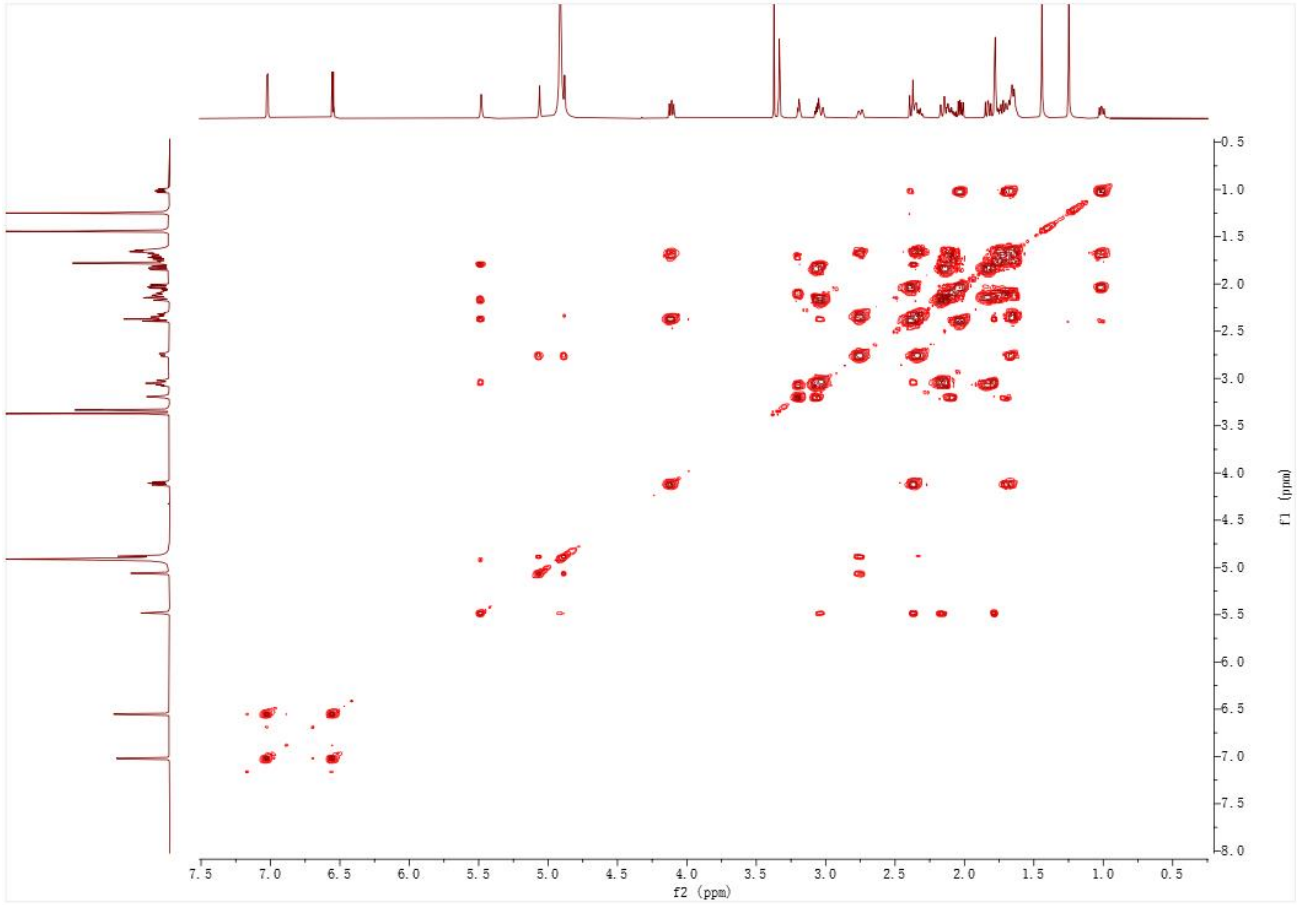


Figure S32. ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrodimer A (**3**) in CD_3OD.

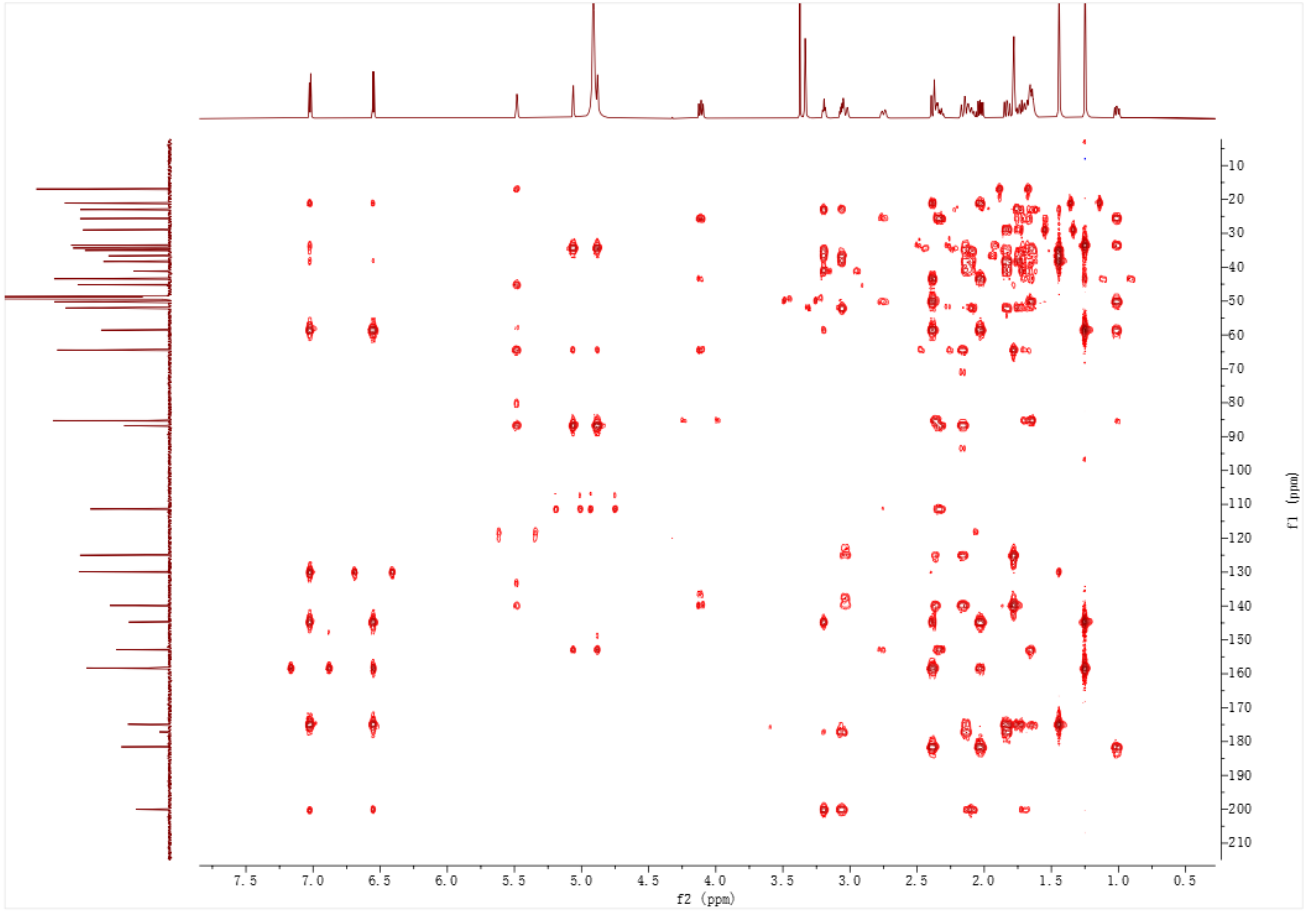


Figure S33. HMBC spectrum (600 MHz) of artematrodimer A (**3**) in CD_3OD.

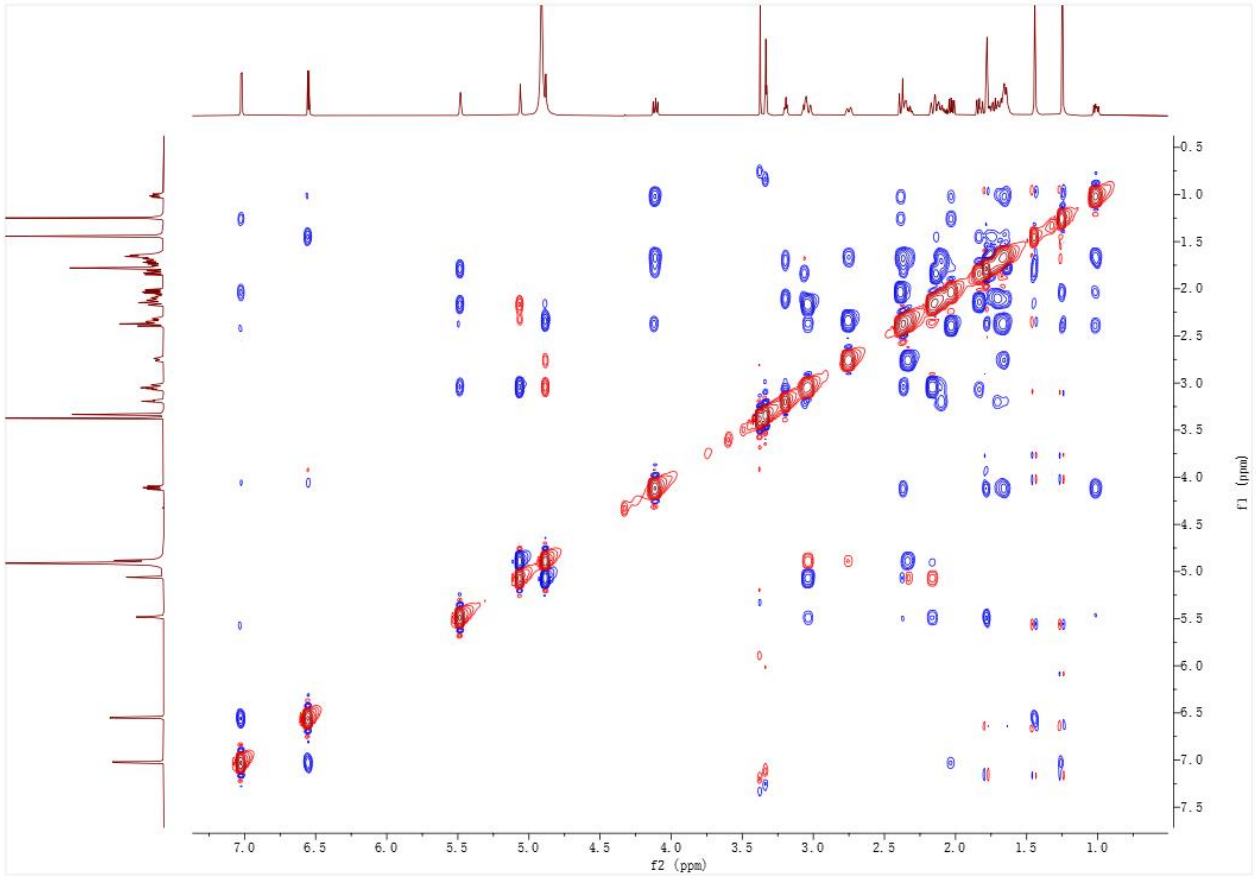


Figure S34. ROESY spectrum (600 MHz) of artematrodimer A (**3**) in CD_3OD.

7. HRESIMS, IR, $[\alpha]_D$, ECD and NMR spectra of compound 4

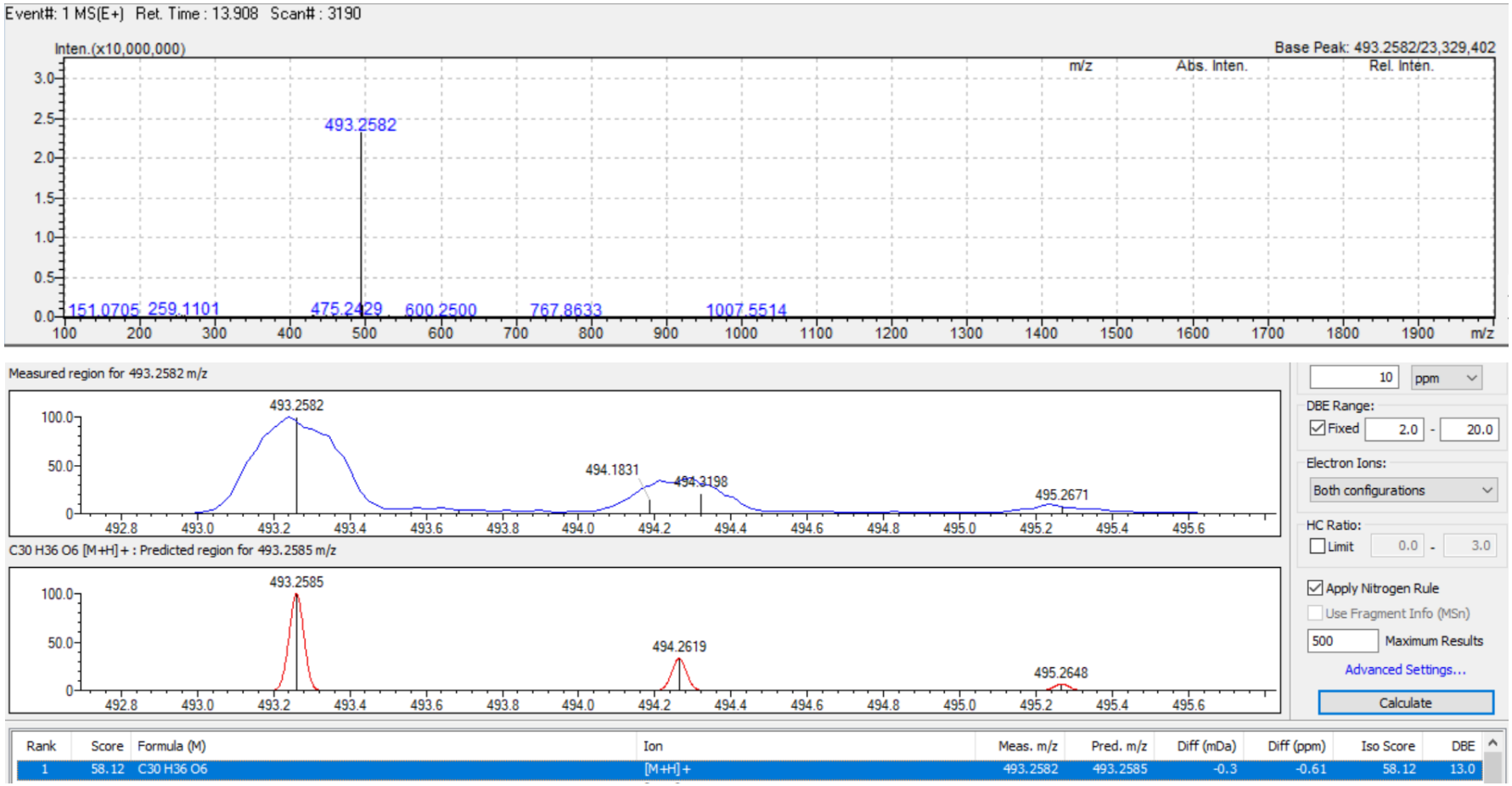


Figure S35. HRESIMS spectrum of artematrodimer B (**4**).

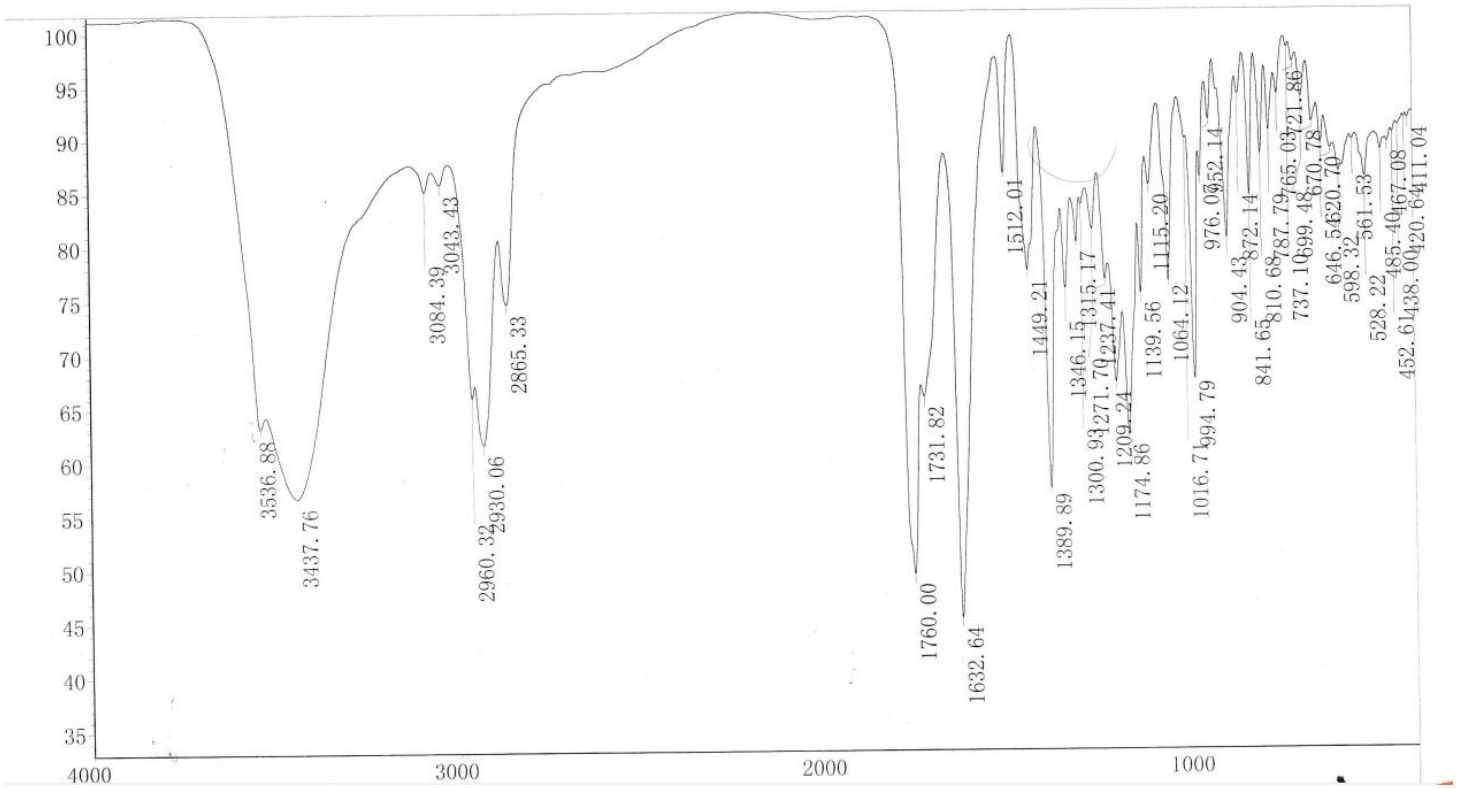


Figure S36. IR spectrum of artematrodimer B (**4**).

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 14-MAY-2020

Set Temperature : OFF

Time Delay: Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-88.37	1.30	-1.47	-86.57	-89.76

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JAR109D	05:49:05 PM	-86.57	SR	-0.1818	589	100.00	0.210	25.2
2	JAR109D	05:49:13 PM	-87.67	SR	-0.1841	589	100.00	0.210	25.2
3	JAR109D	05:49:21 PM	-88.43	SR	-0.1857	589	100.00	0.210	25.2
4	JAR109D	05:49:29 PM	-89.76	SR	-0.1885	589	100.00	0.210	25.2
5	JAR109D	05:49:37 PM	-89.43	SR	-0.1878	589	100.00	0.210	25.2

Figure S37. Optical rotation spectrum of artematrodimer B (**4**).

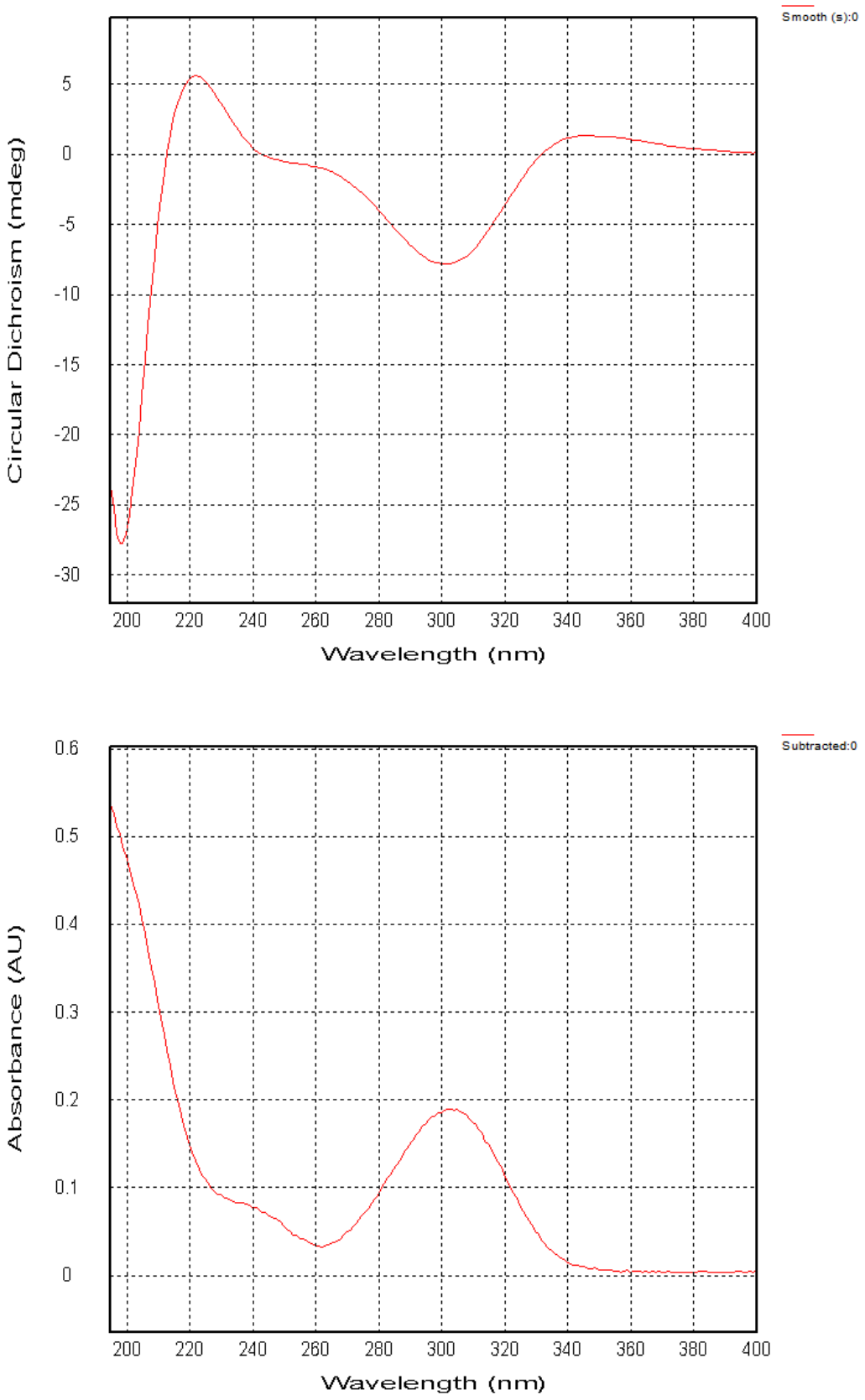


Figure S38. ECD (top) and UV (bottom) spectra of artematrodimer B (**4**).

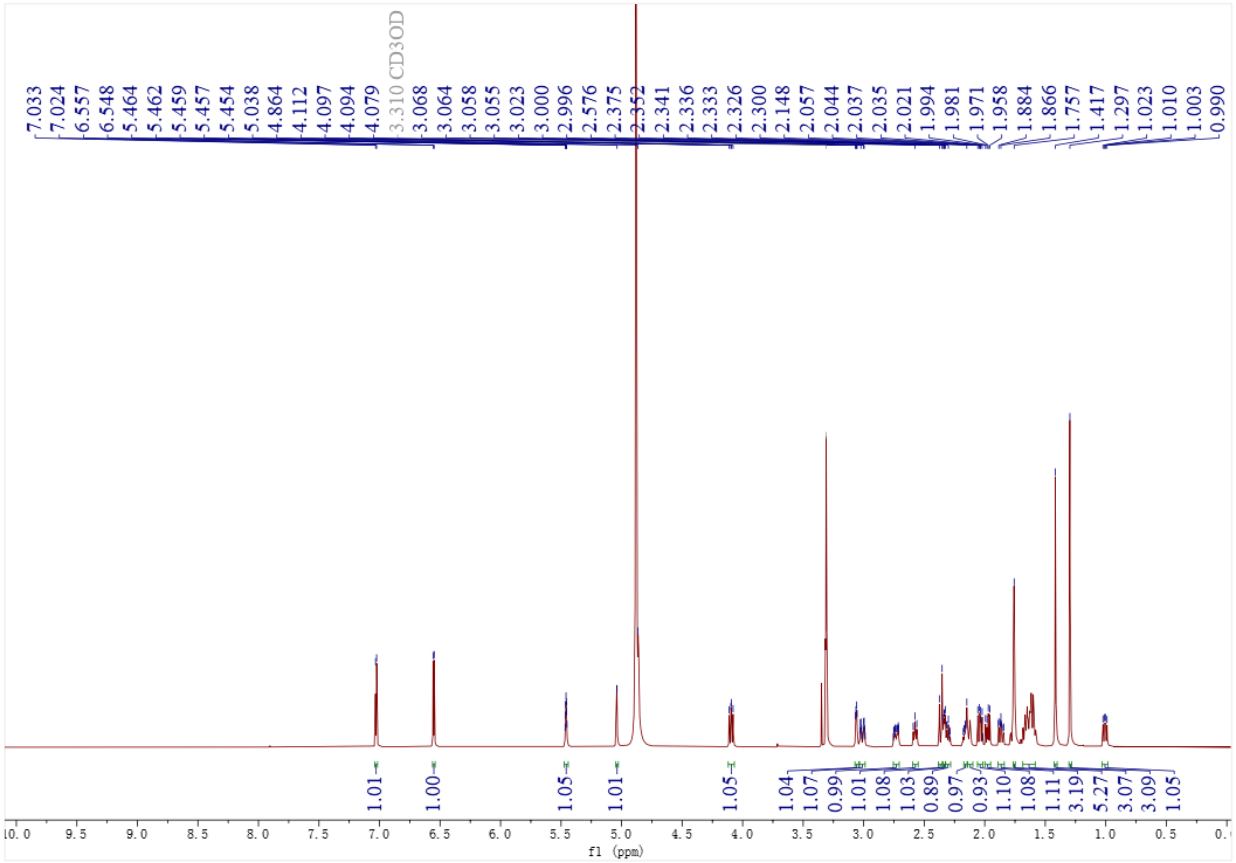


Figure S39. ^{1}H spectrum (600 MHz) of artematrodimer B (**4**) in CD_3OD.

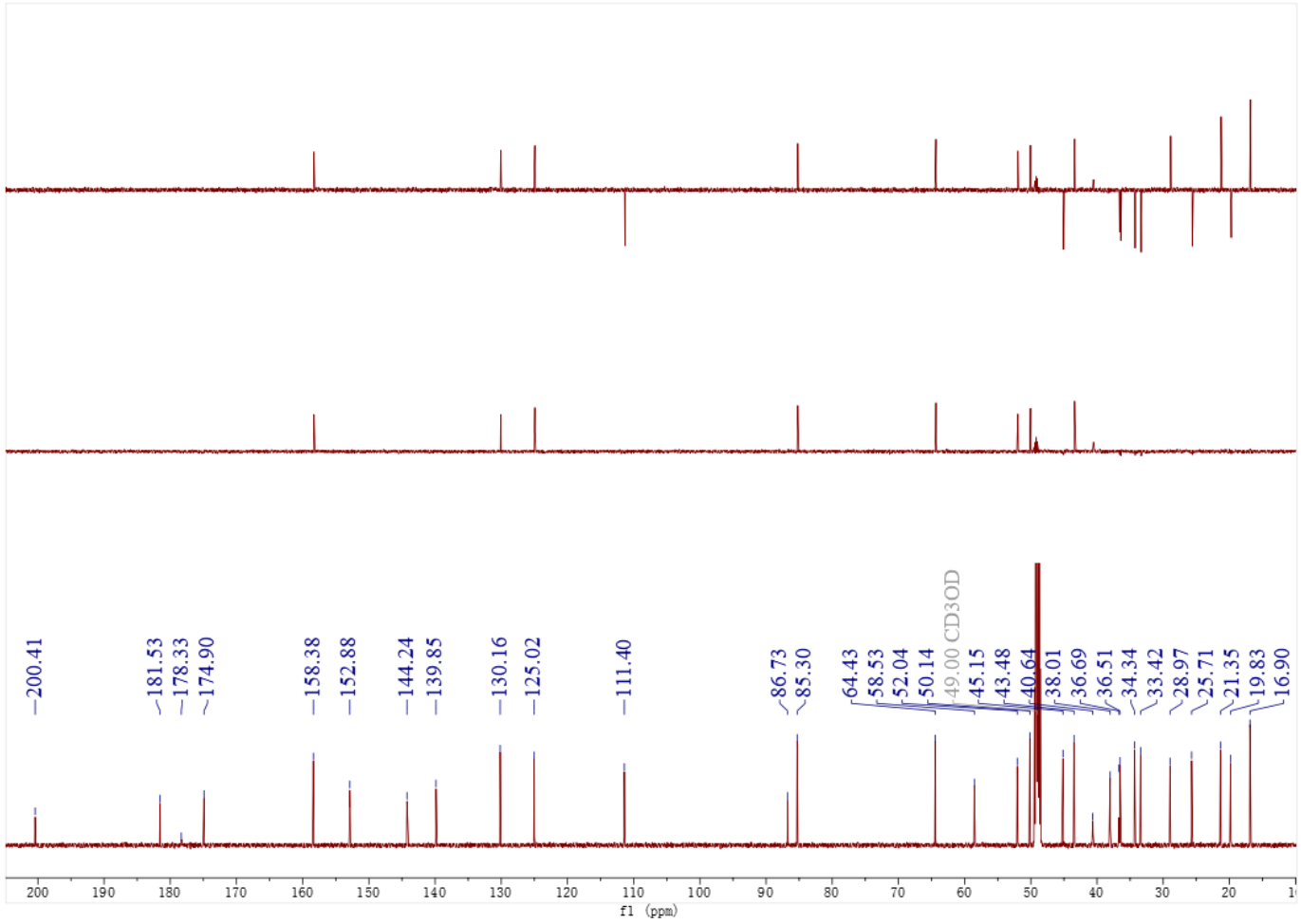


Figure S40. ^{13}C and DEPT spectra (150 MHz) of artematrodimer B (**4**) in CD_3OD.

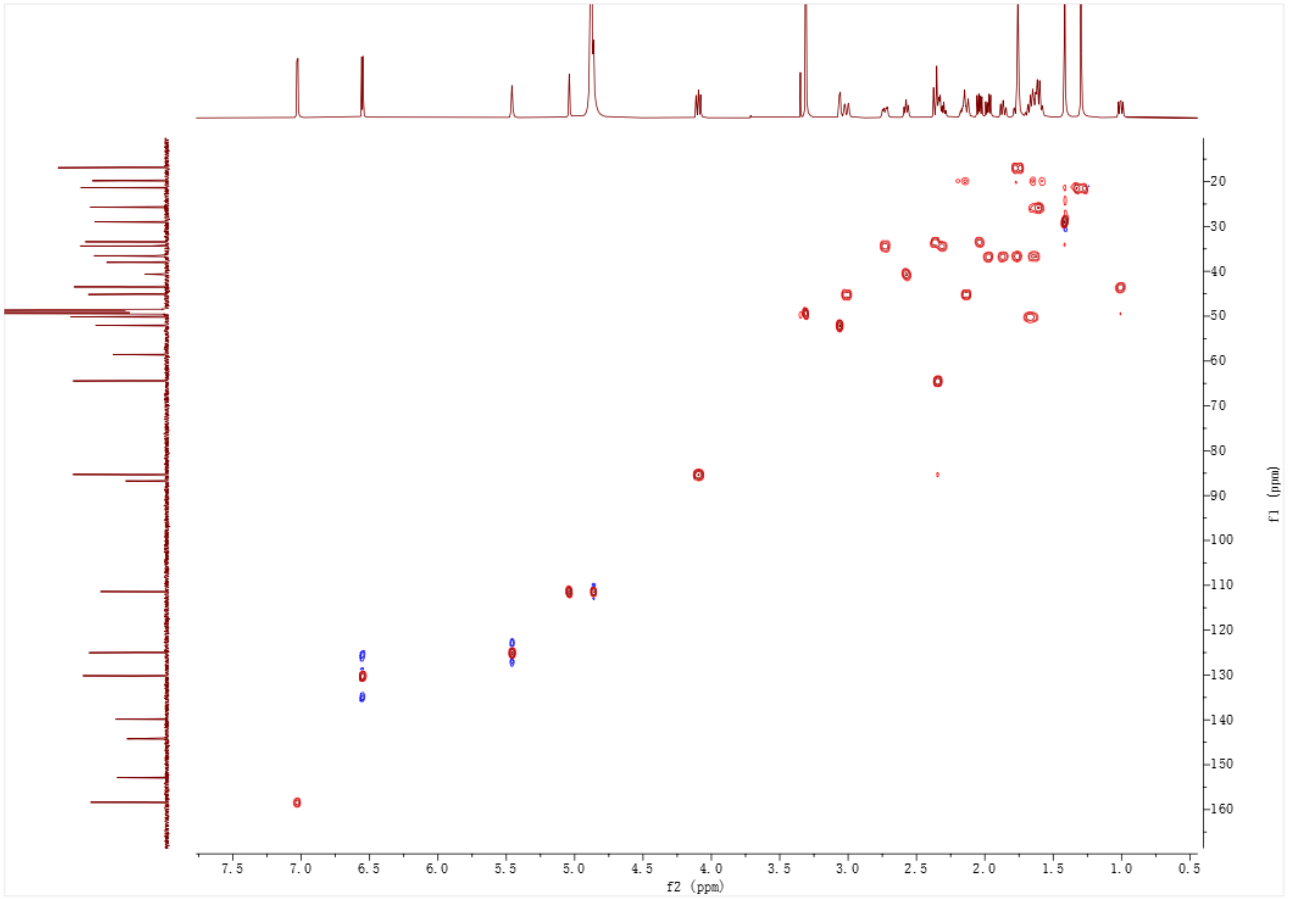


Figure S41. HSQC spectrum (600 MHz) of artematrodimer B (**4**) in CD_3OD.

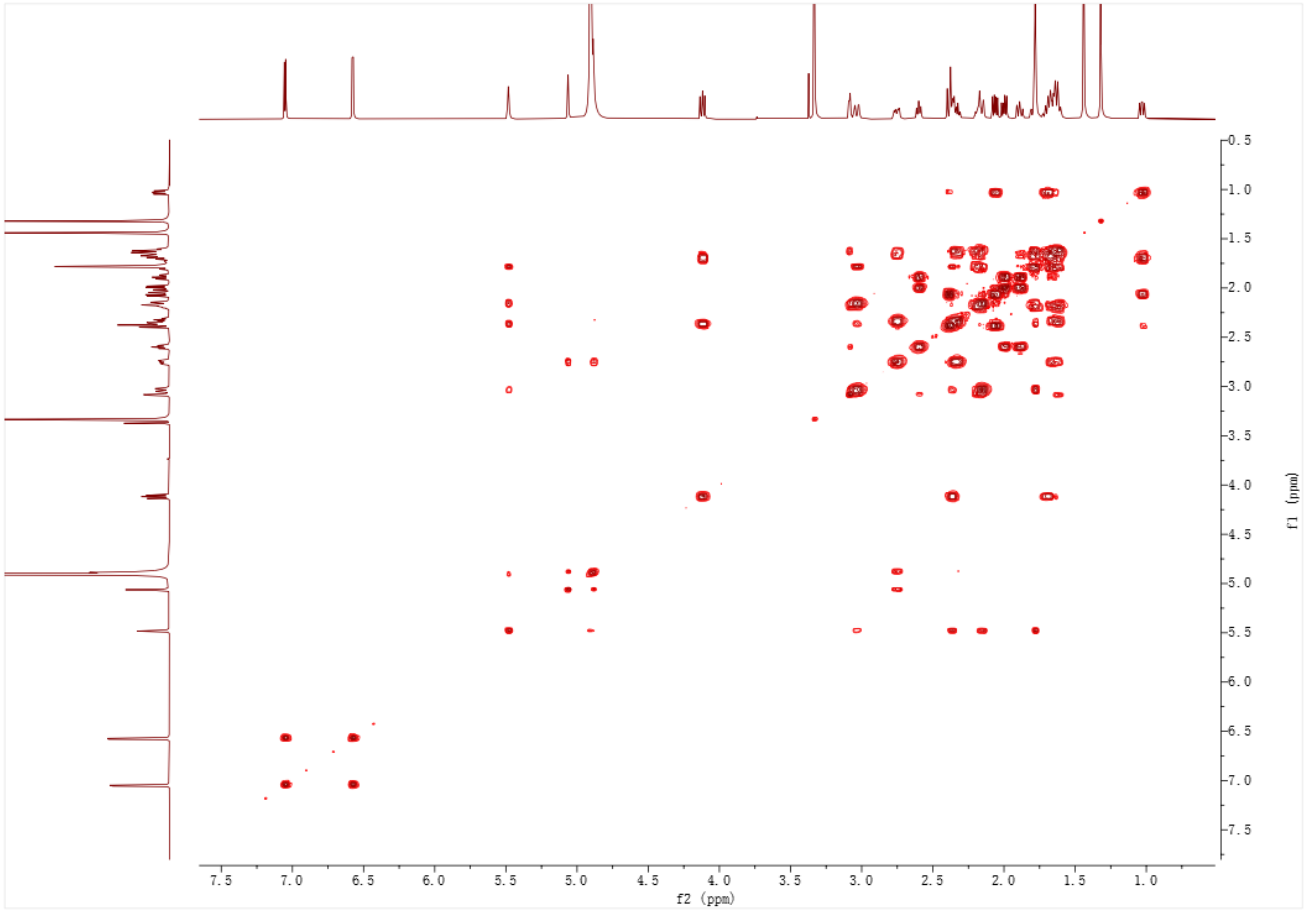


Figure S42. ^{1}H–^{1}H COSY spectrum (600 MHz) of artematrodimer B (**4**) in CD_3OD.

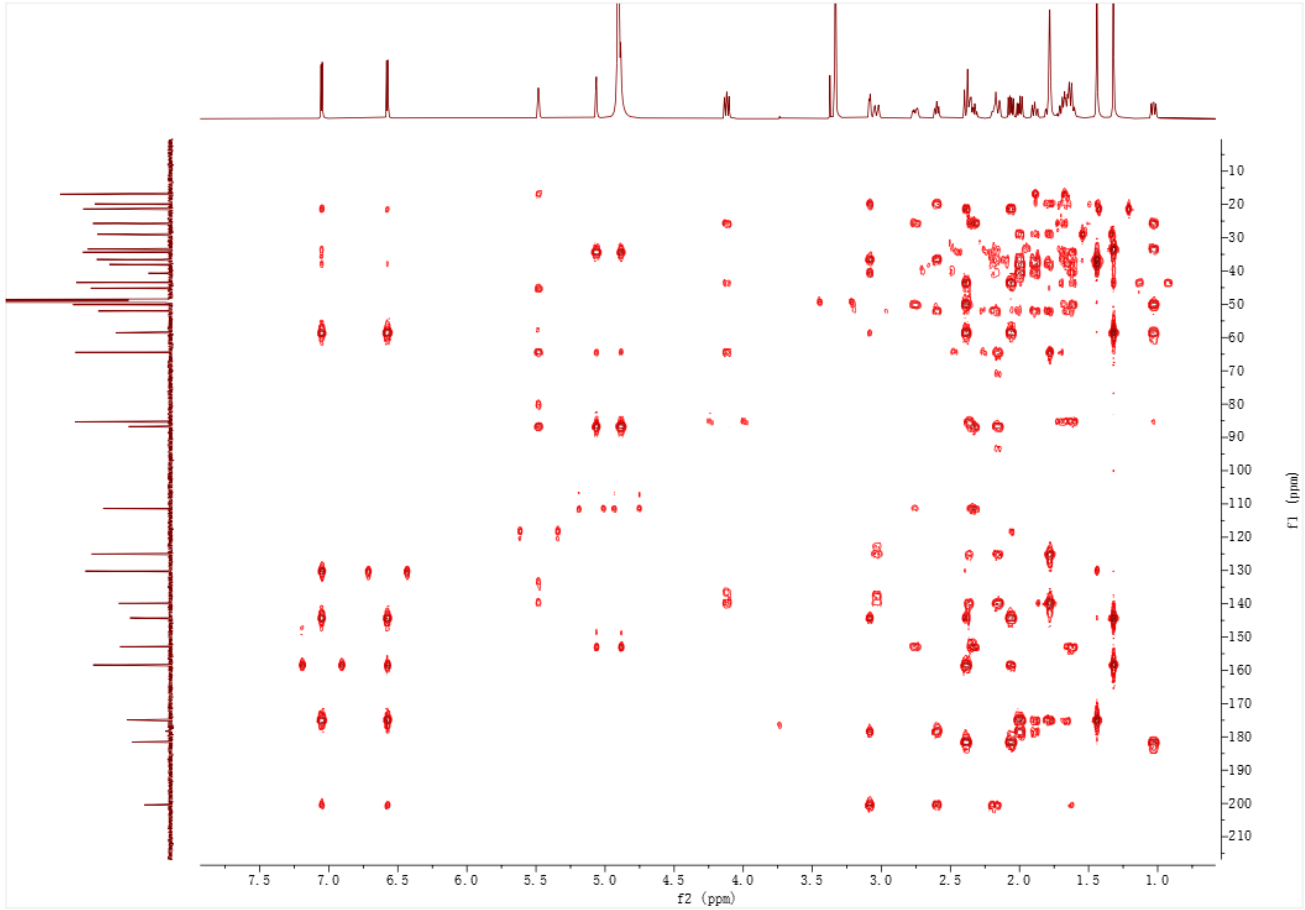


Figure S43. HMBC spectrum (600 MHz) of artematrodimer B (**4**) in CD_3OD.

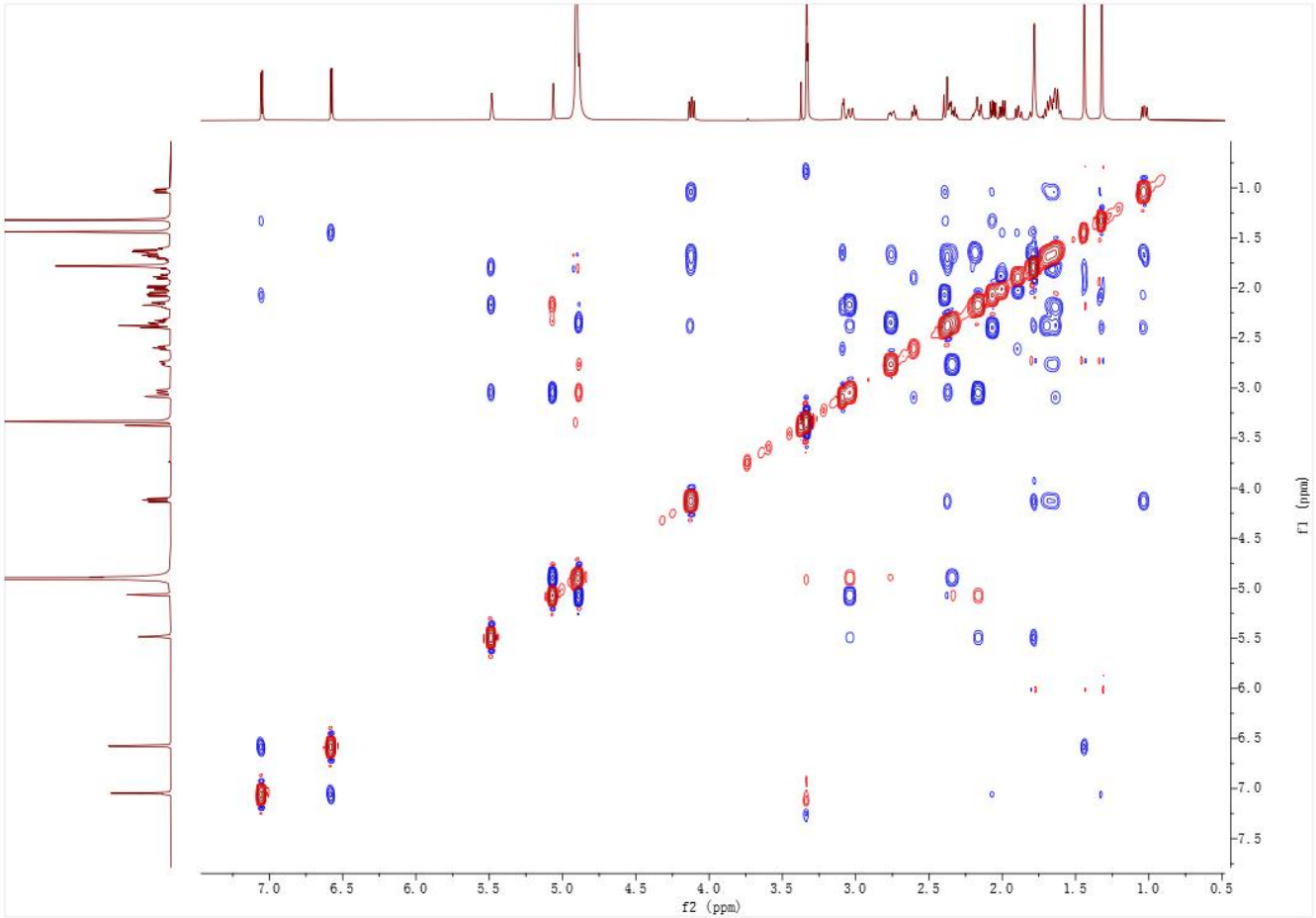


Figure S44. ROESY spectrum (600 MHz) of artematrodimer B (**4**) in CD_3OD.

8. Chiral HPLC analyses of compounds 1 and 2

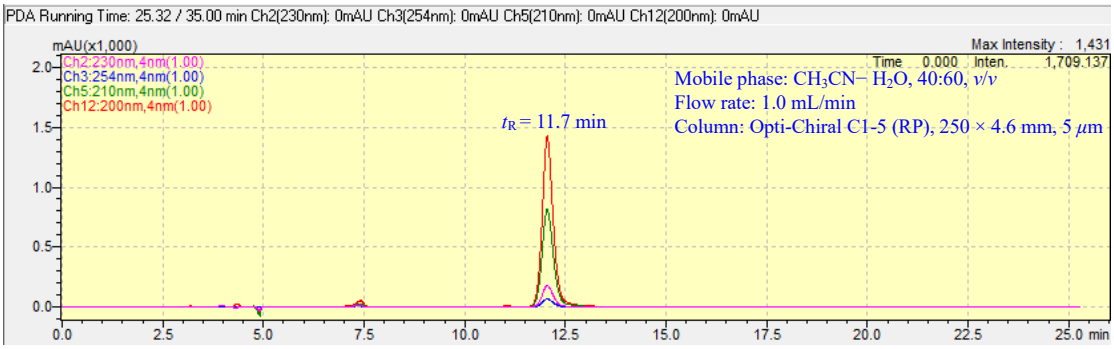


Figure S45. HPLC chart of compound **1** by using a chiral column.

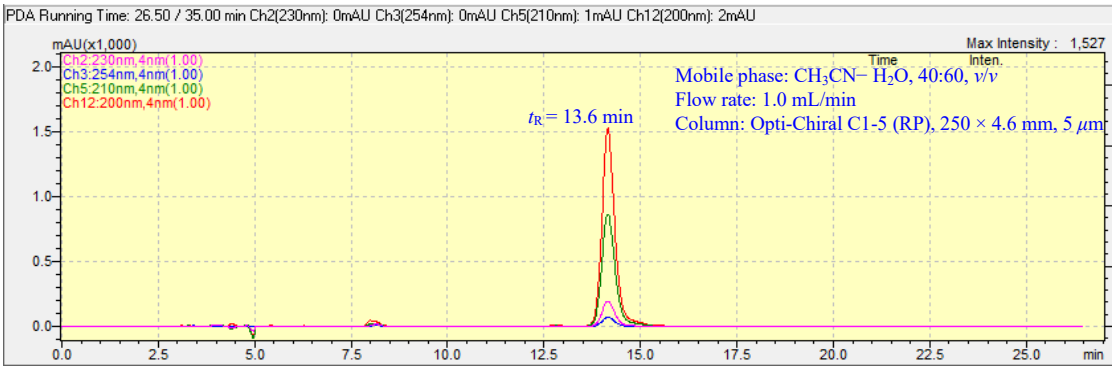


Figure S46. HPLC chart of compound **2** by using a chiral column.