Supporting Information

Three Rare Nor-sesquiterpenoids with Lipid-Lowering Activity from *Belamcanda chinensis*

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CONTENT

1. Spectra of physico-chemical properties of **1**

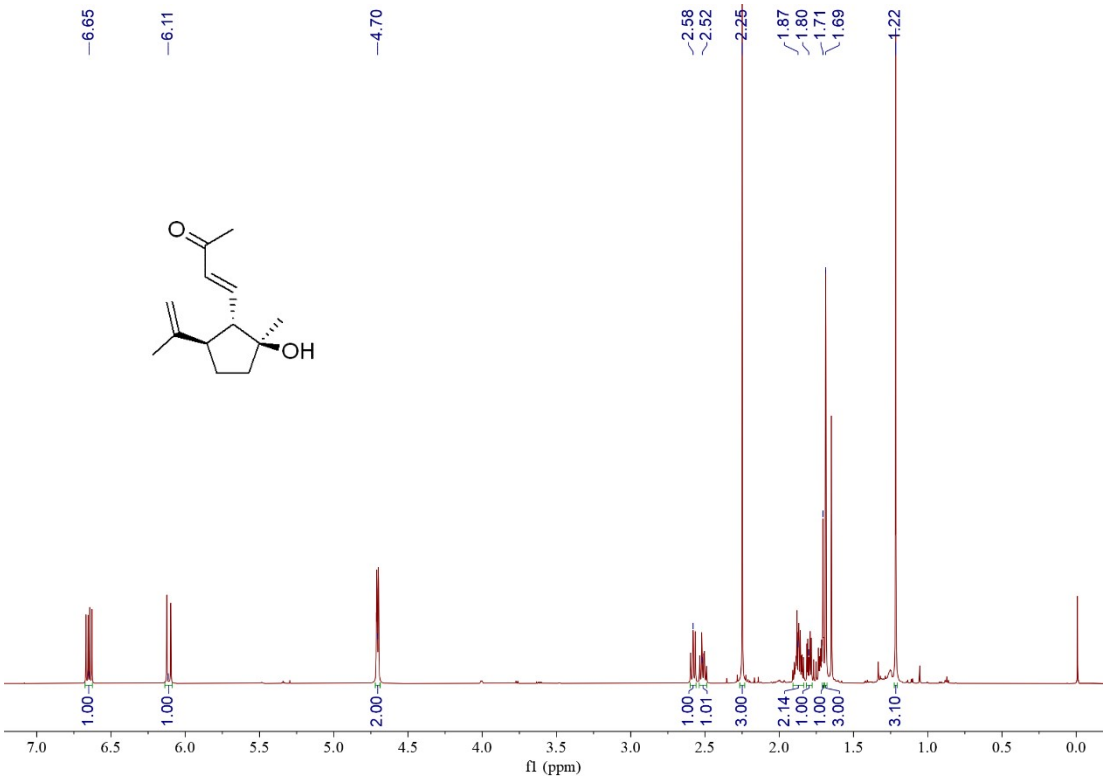


Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **1**

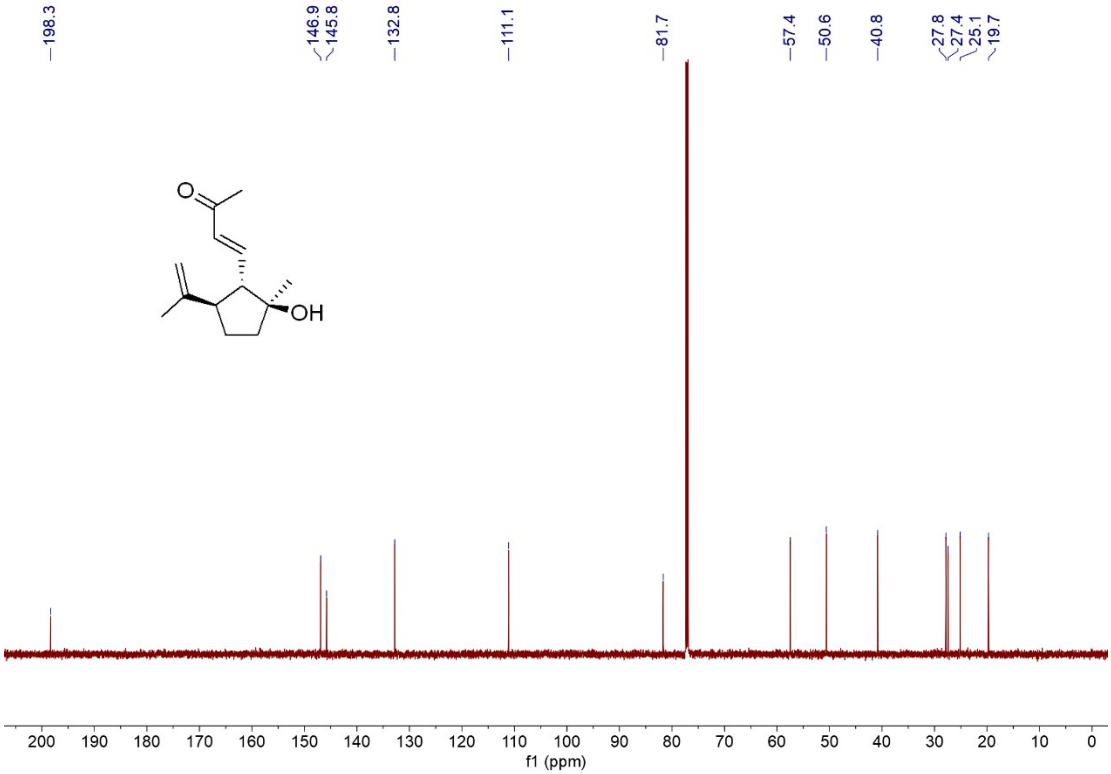


Figure S2. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **1**

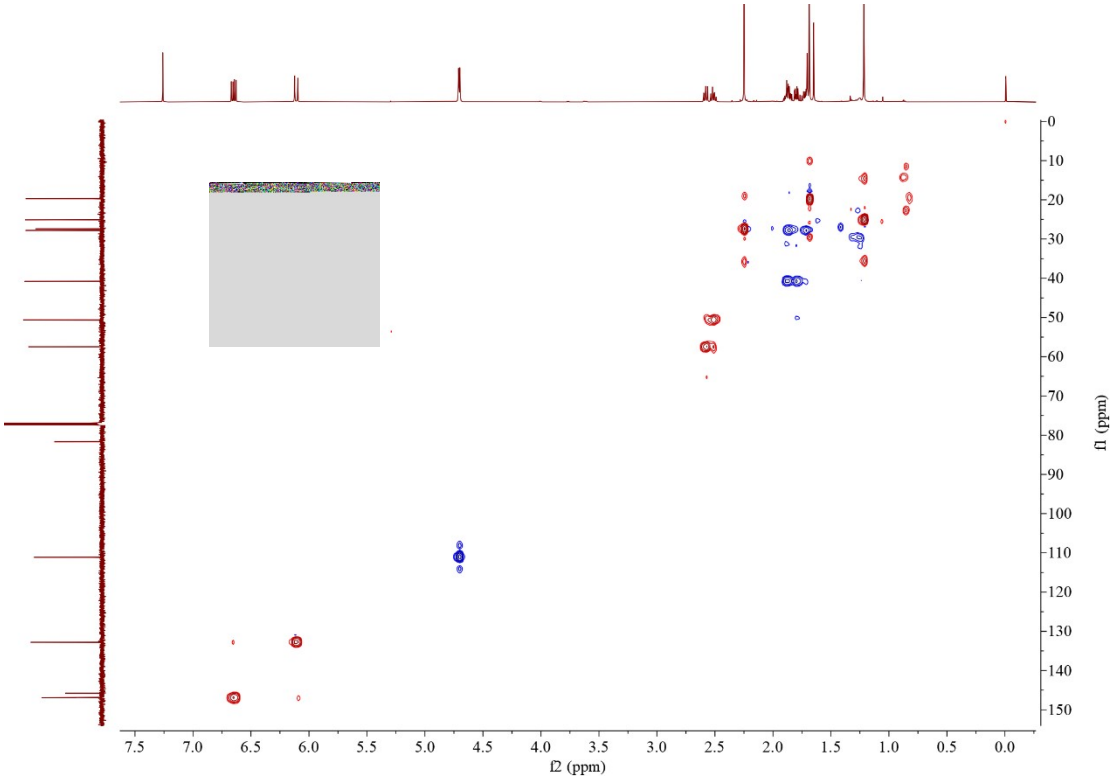


Figure S3. HSQC spectrum of **1** ($CDCl_3$)

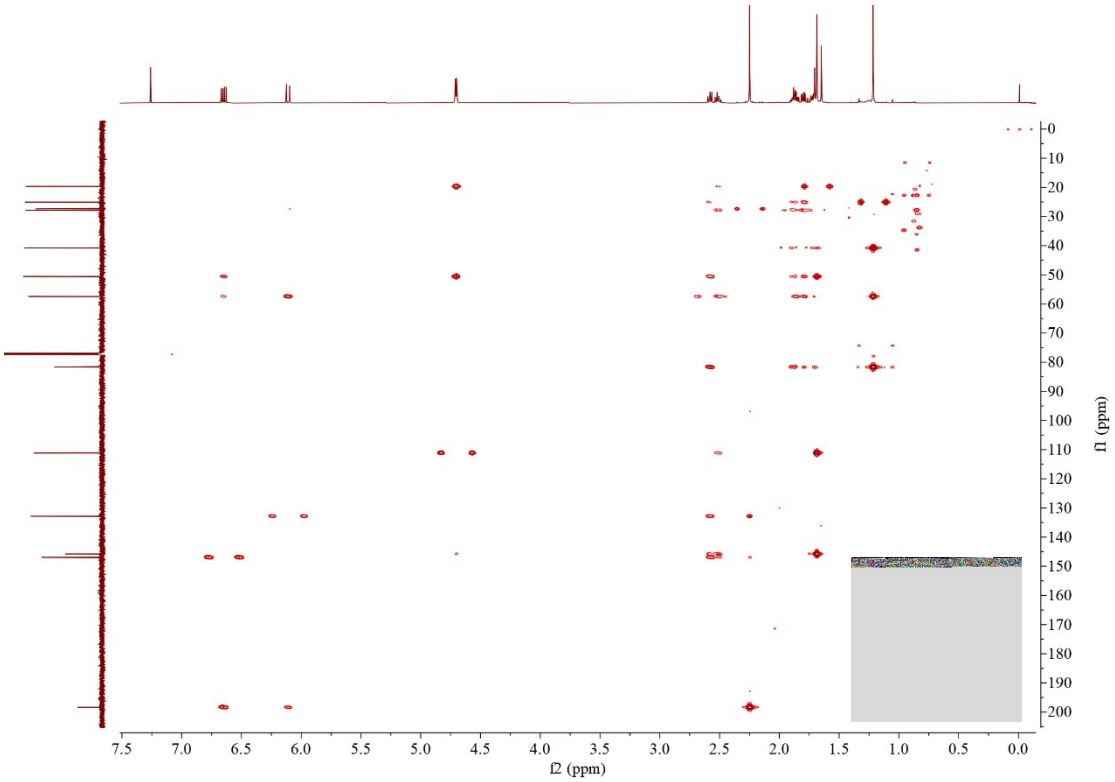


Figure S4. HMBC spectrum of **1** ($CDCl_3$)

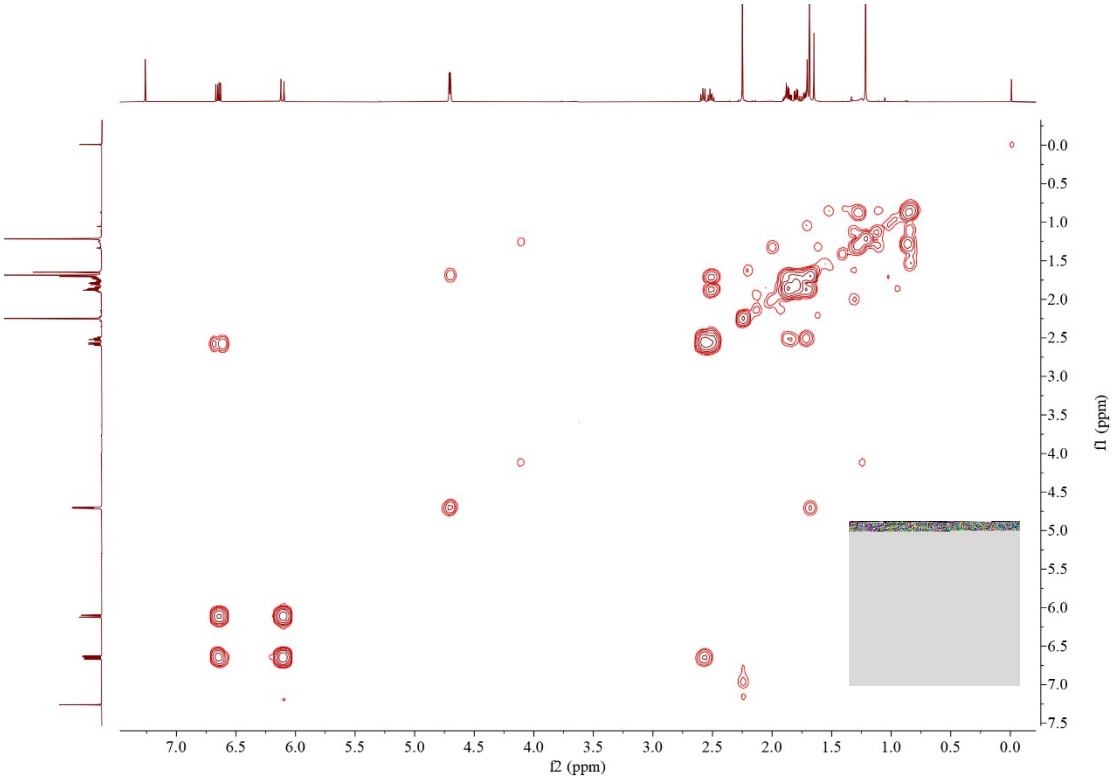


Figure S5. ^{1}H-^{1}H COSY spectrum of **1** ($CDCl_3$)

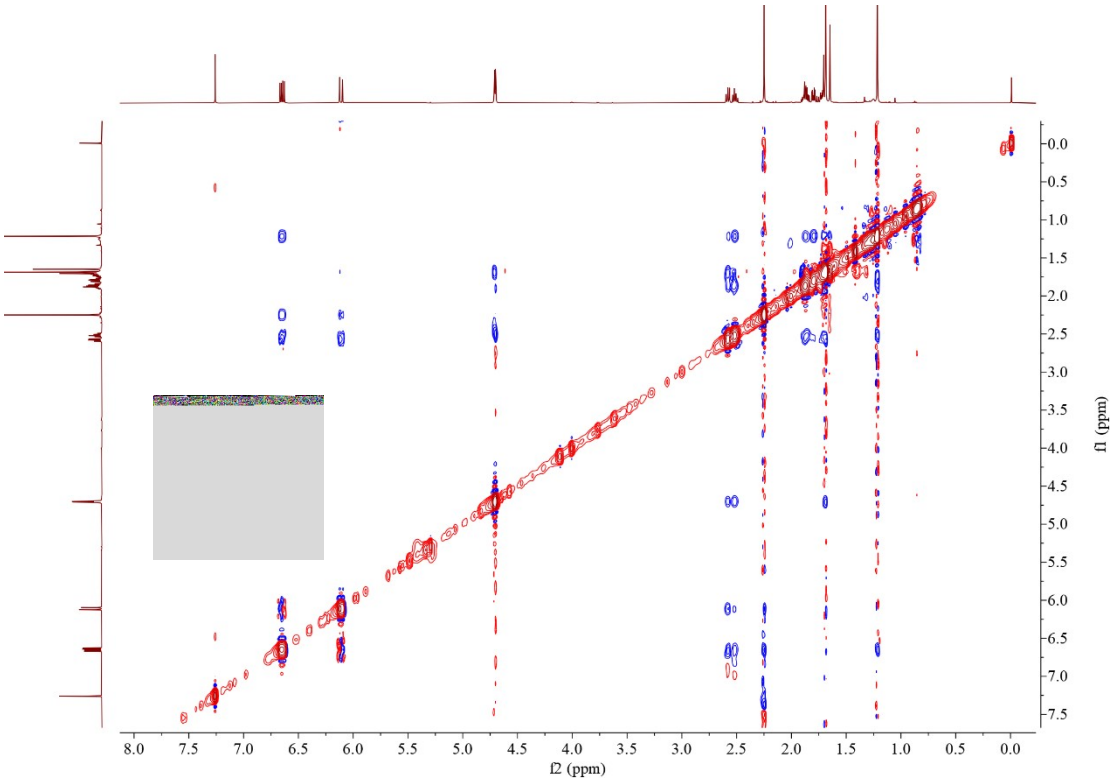


Figure S6. NOESY spectrum of **1** ($CDCl_3$)

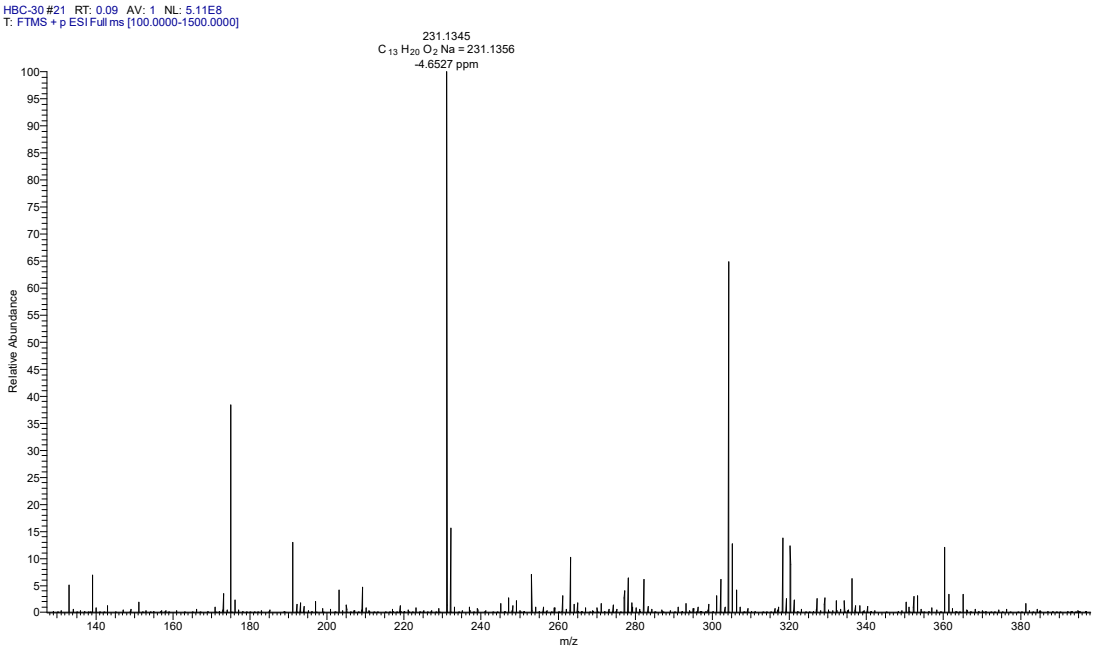


Figure S7. HR-ESI-MS spectrum of **1**

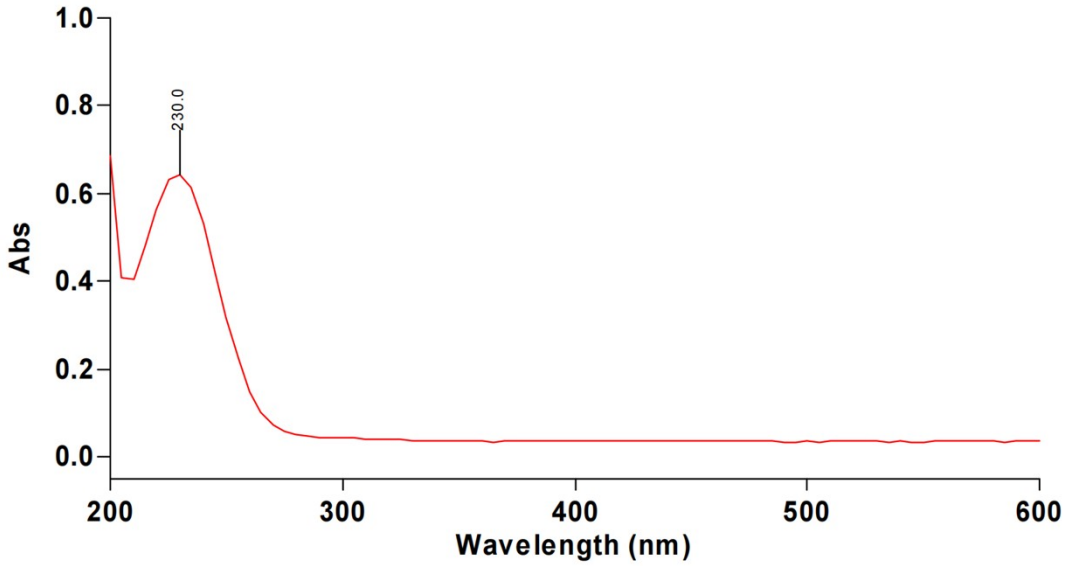


Figure S8. UV spectrum of **1**

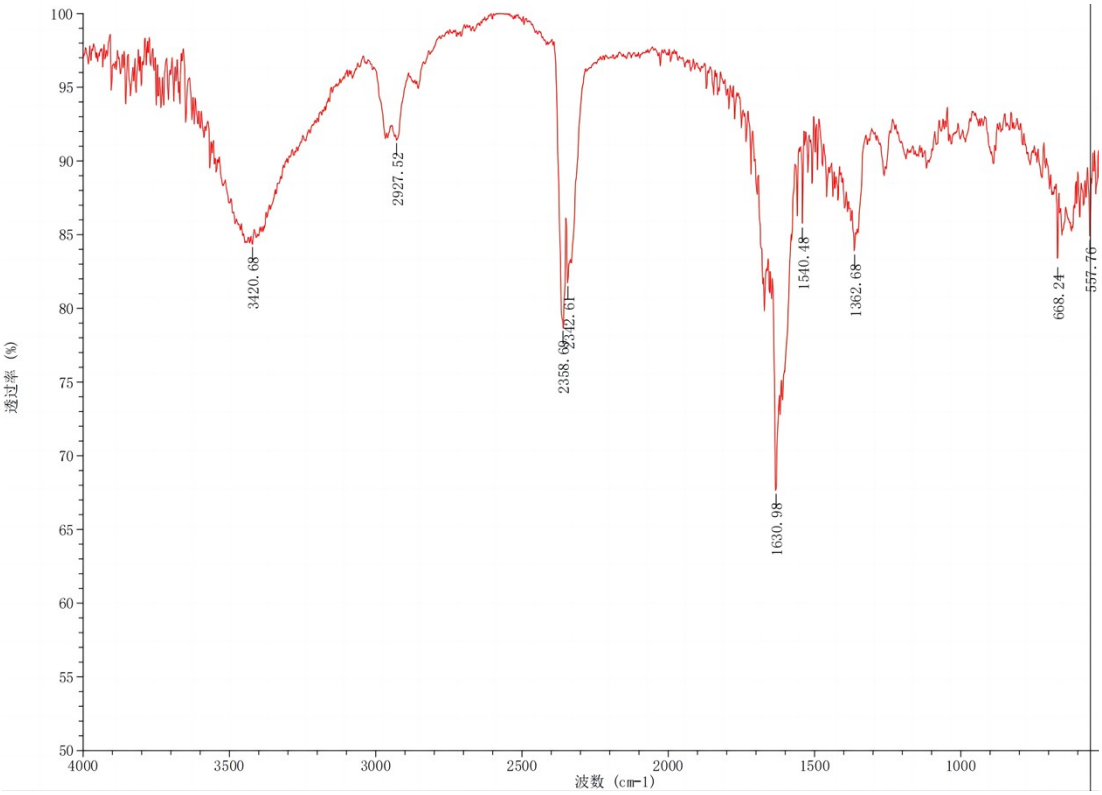


Figure S9. IR spectrum of **1**

2. Spectra of physico-chemical properties of **2**

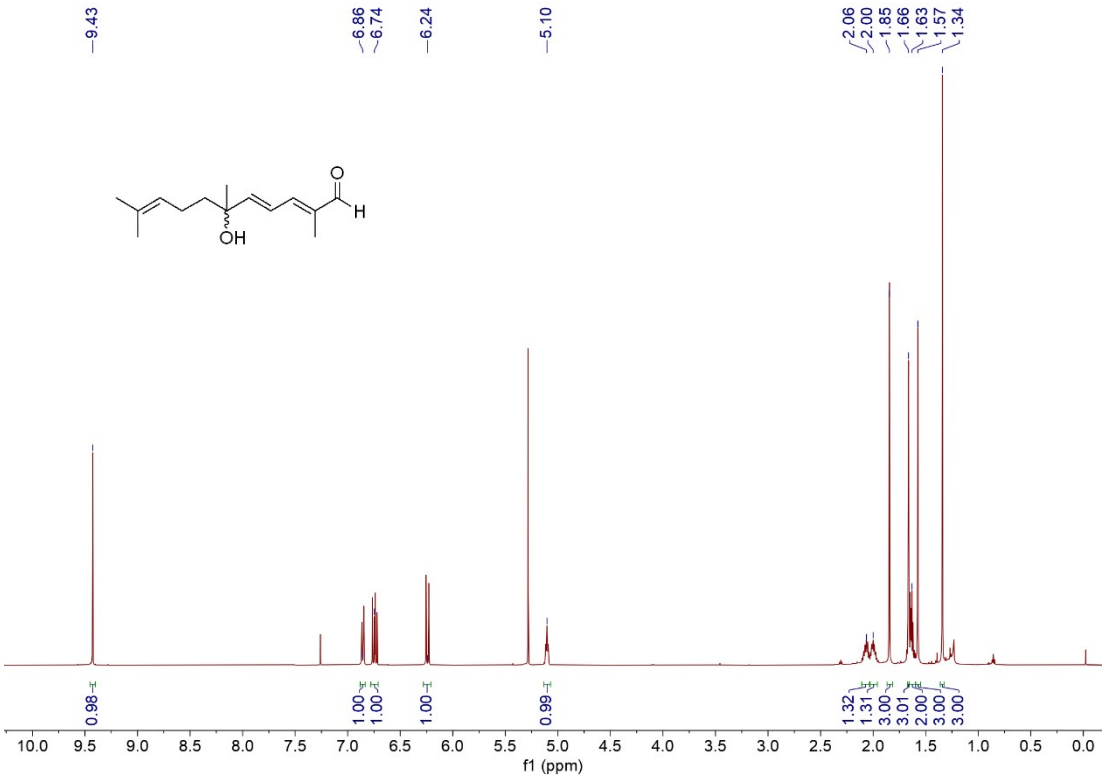


Figure S10. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2**

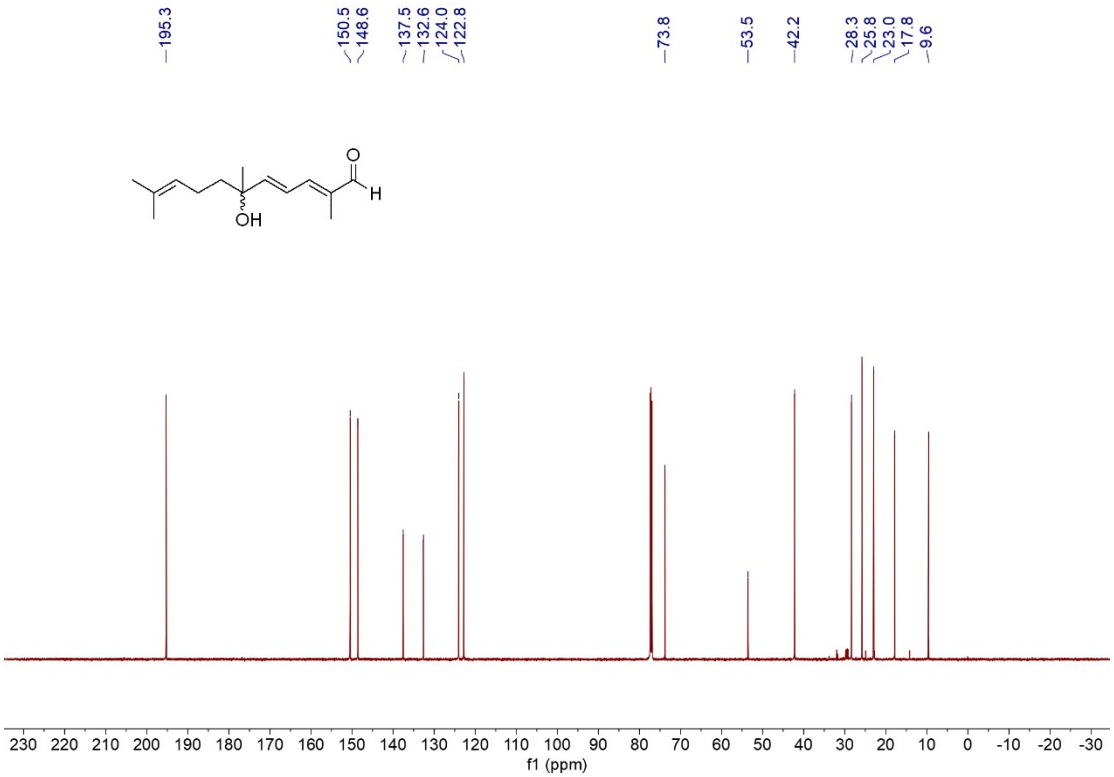


Figure S11. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **2**

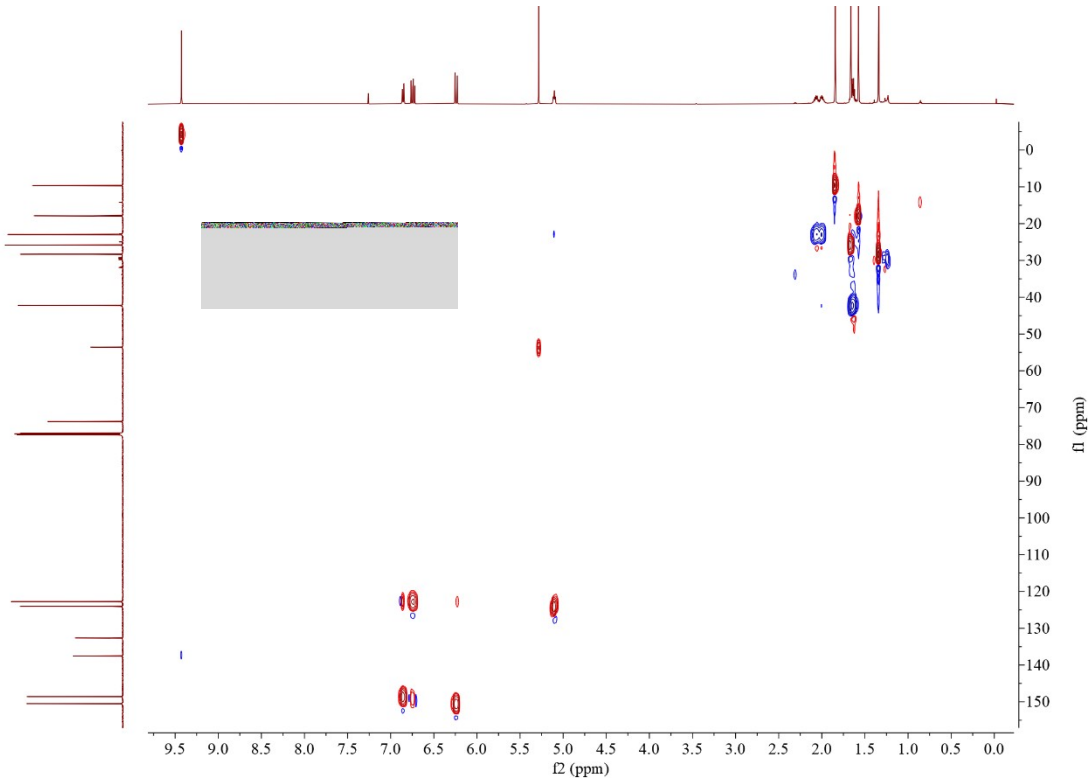


Figure S12. HSQC spectrum of **2** ($CDCl_3$)

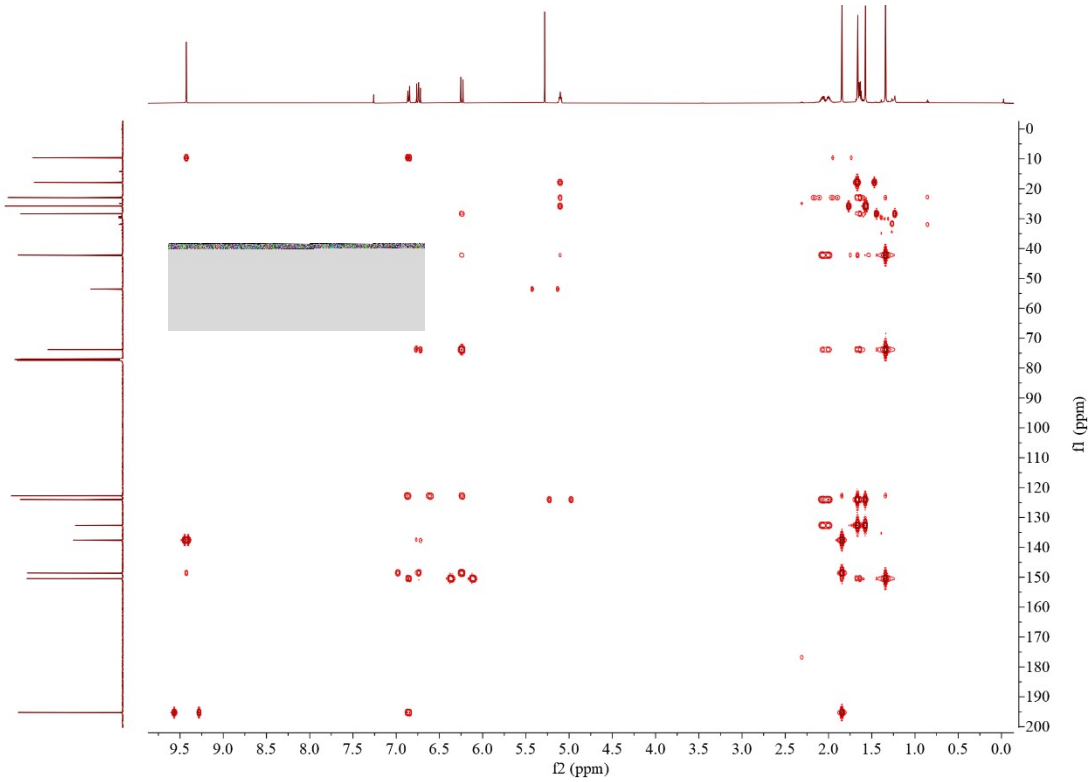


Figure S13. HMBC spectrum of **2** ($CDCl_3$)

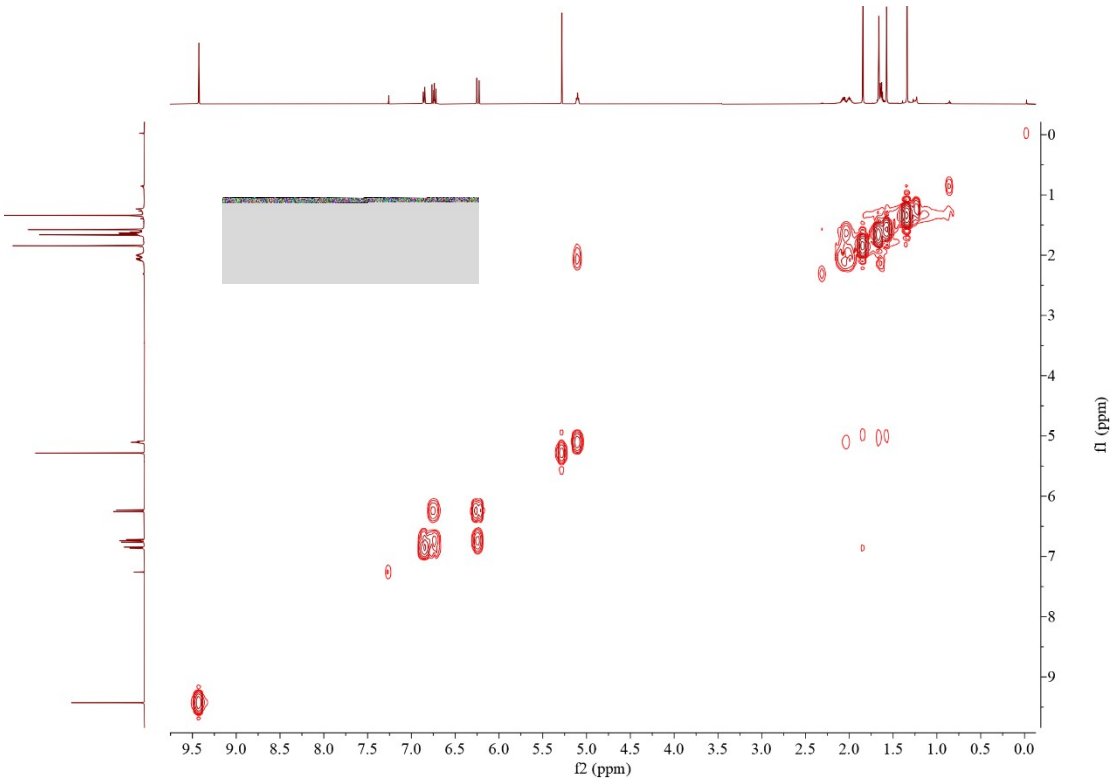


Figure S14. ^{1}H-^{1}H COSY spectrum of **2** ($CDCl_3$)

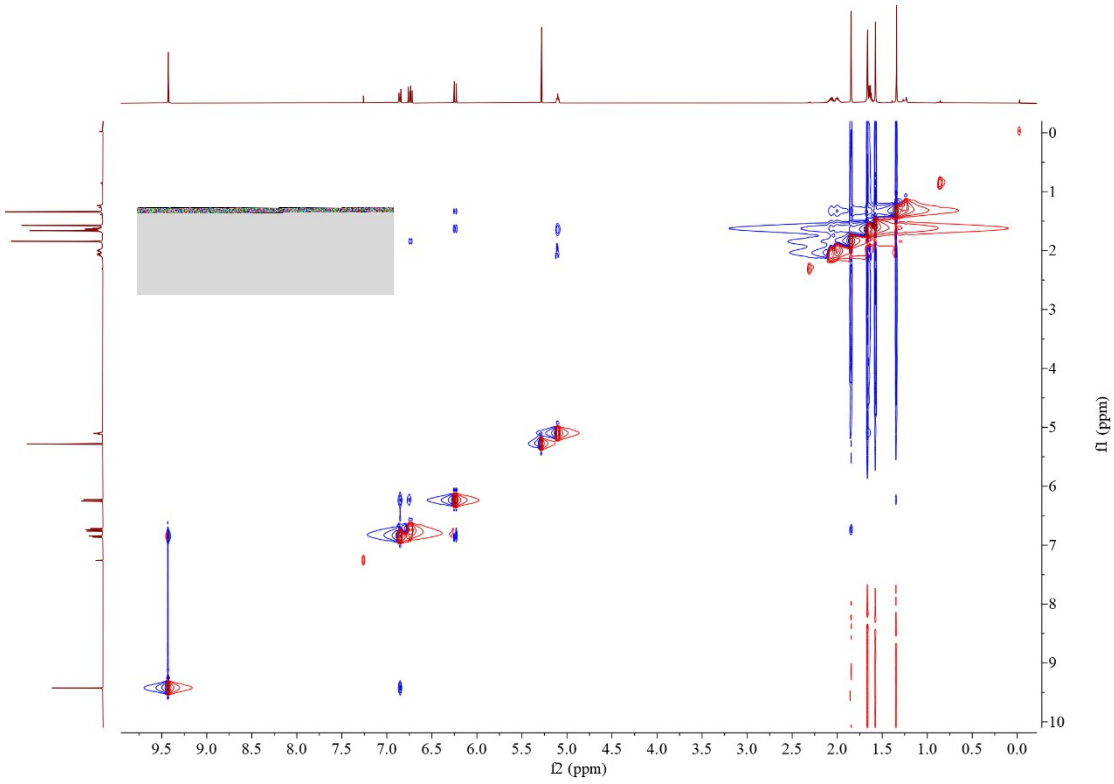


Figure S15. NOESY spectrum of **2** ($CDCl_3$)

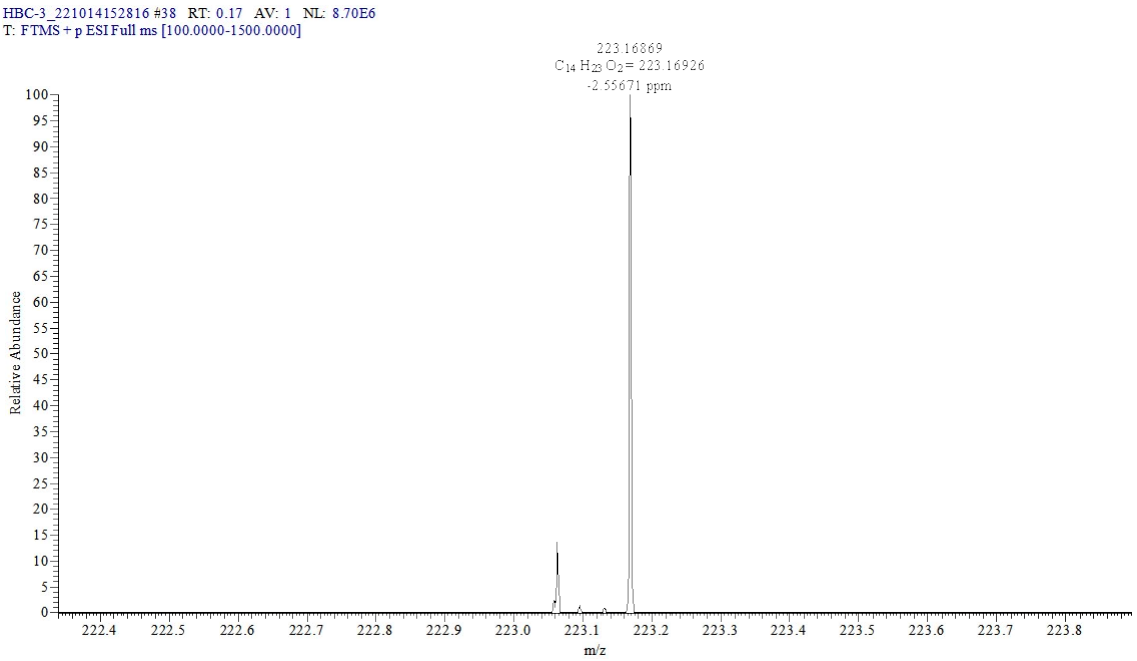


Figure S16. HR-ESI-MS spectrum of **2**

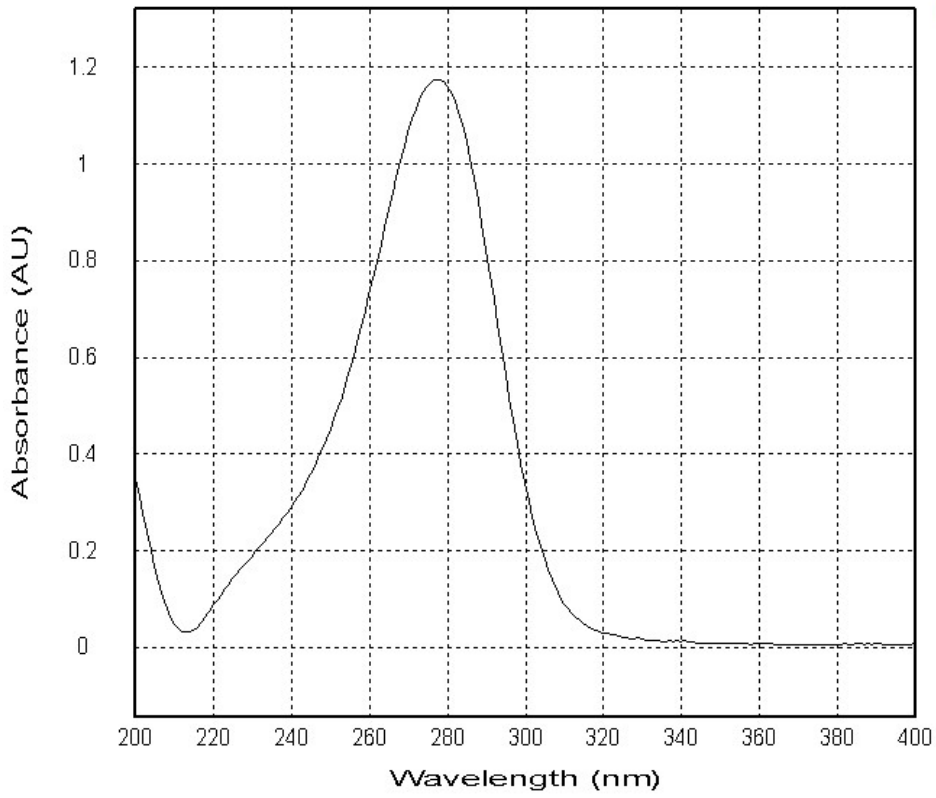


Figure S17. UV spectrum of **2**

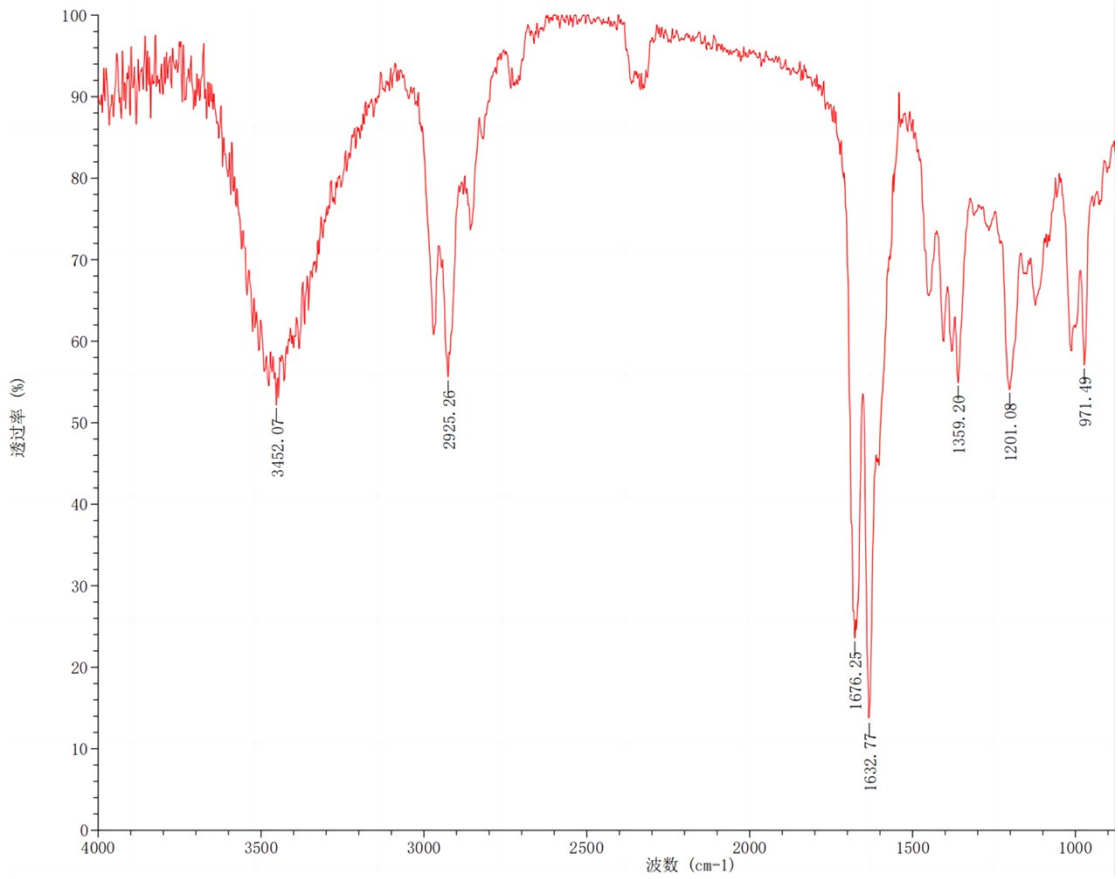


Figure S18. IR spectrum of **2**

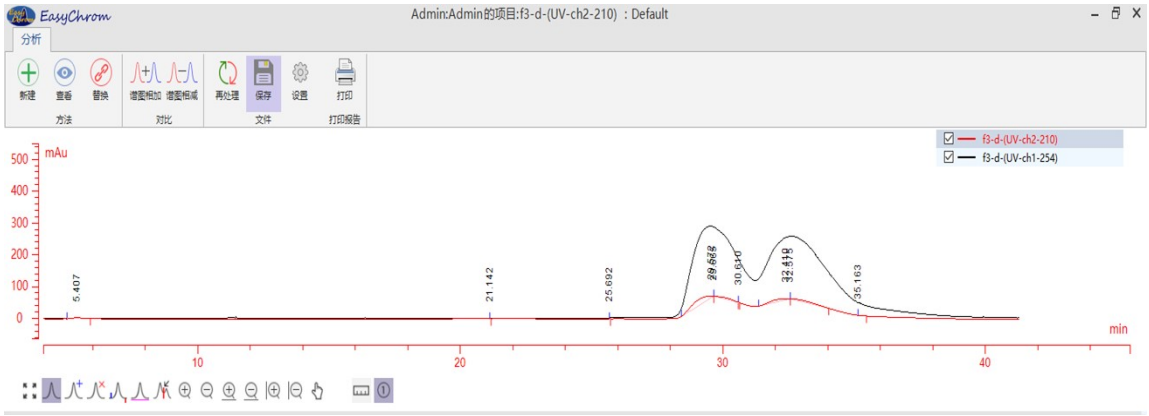
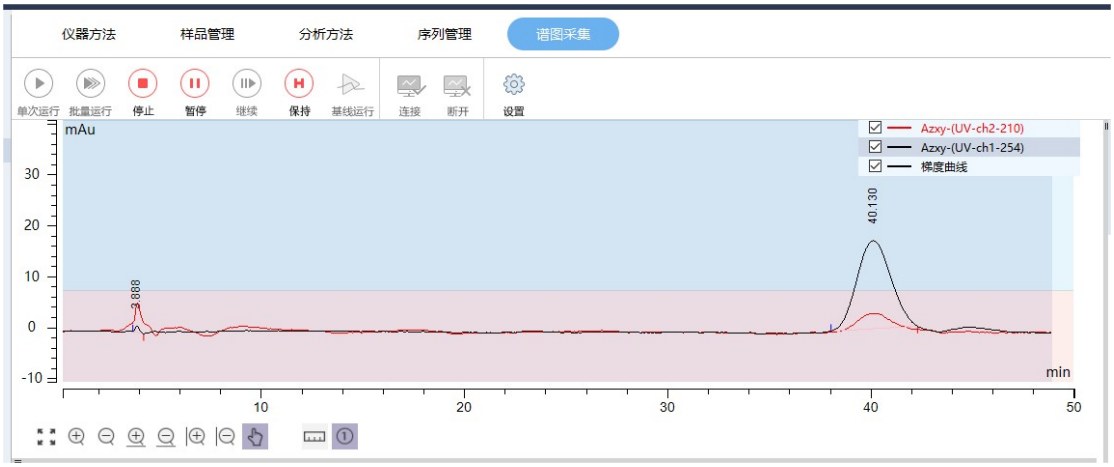


Figure S19. Chiral analysis of **2**

(A)



(B)

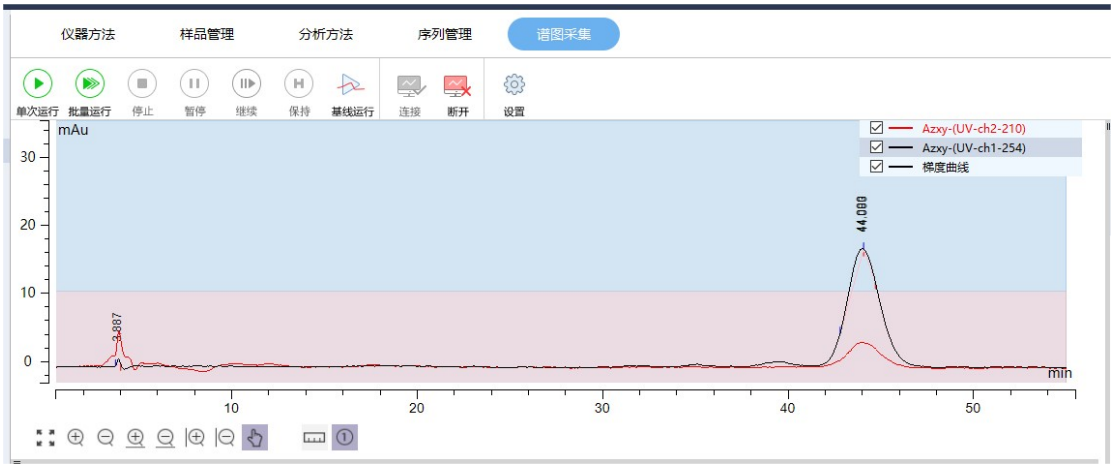


Figure S20. Optical purity analysis of (+)-**2** and (−)-**2**. (A) The levoisomer of **2** using chiral column analysis; (B) The dextroisomer of **2** using chiral column analysis.

3. Spectra of physico-chemical properties of **3**

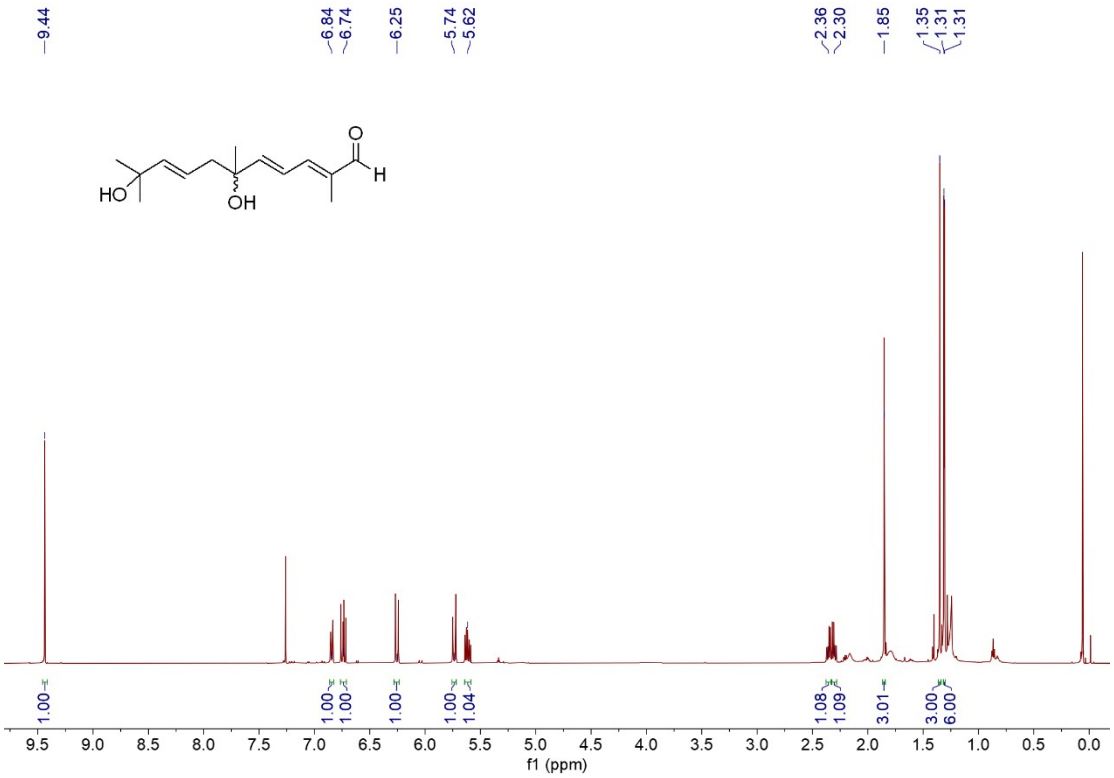


Figure S21. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3**

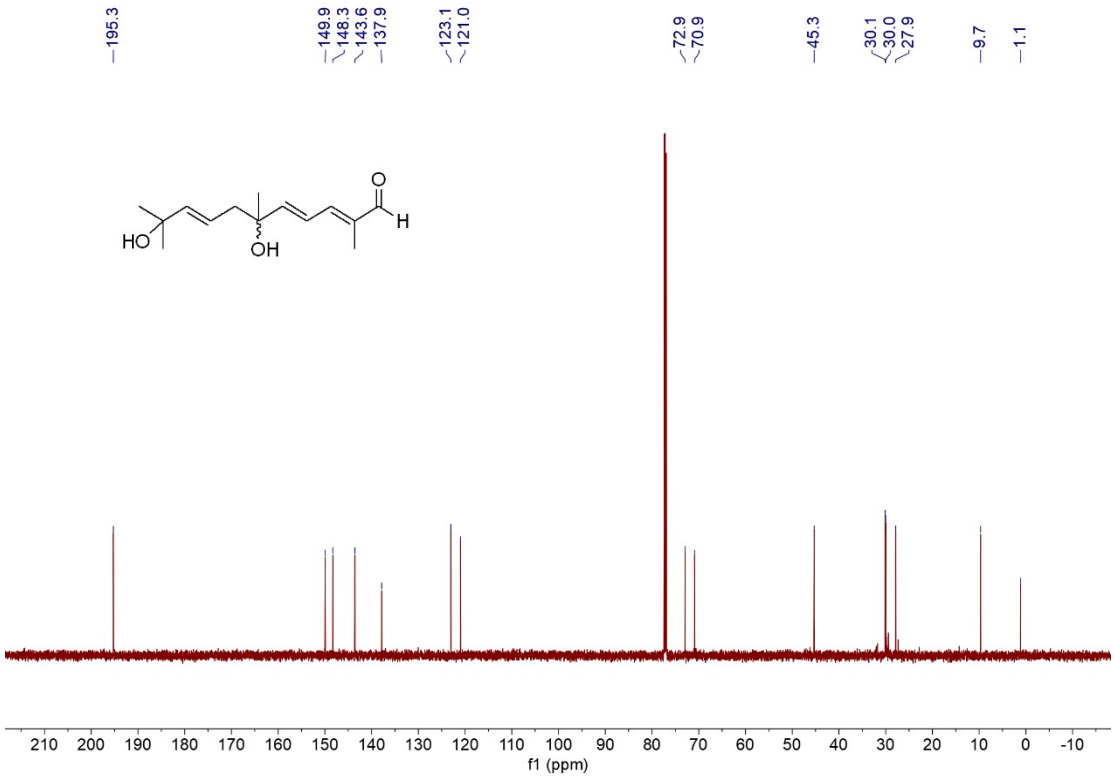


Figure S22. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **3**

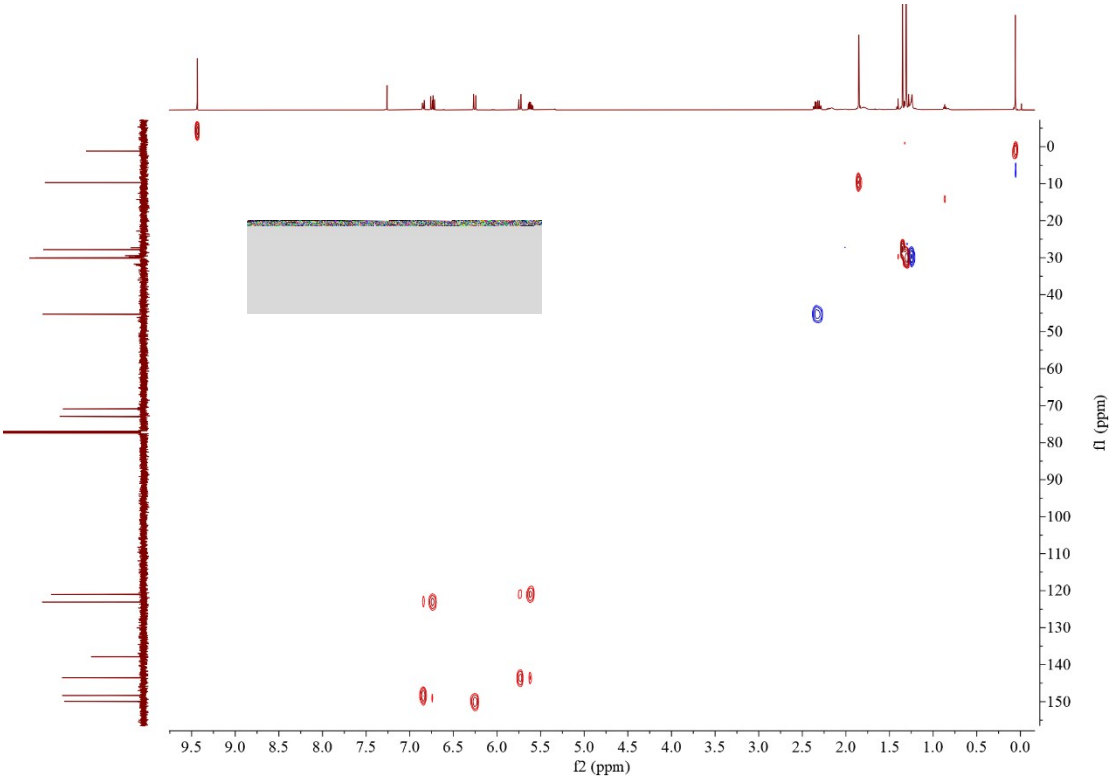


Figure S23. HSQC spectrum of **3** ($CDCl_3$)

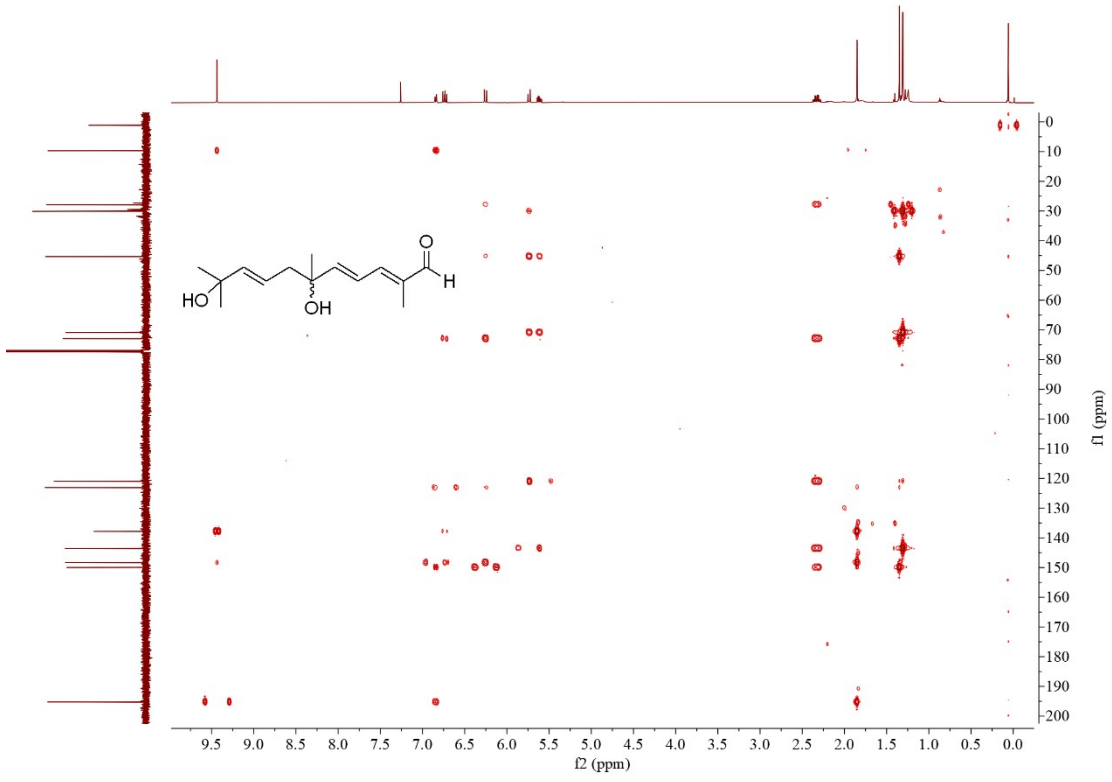


Figure S24. HMBC spectrum of **3** ($CDCl_3$)

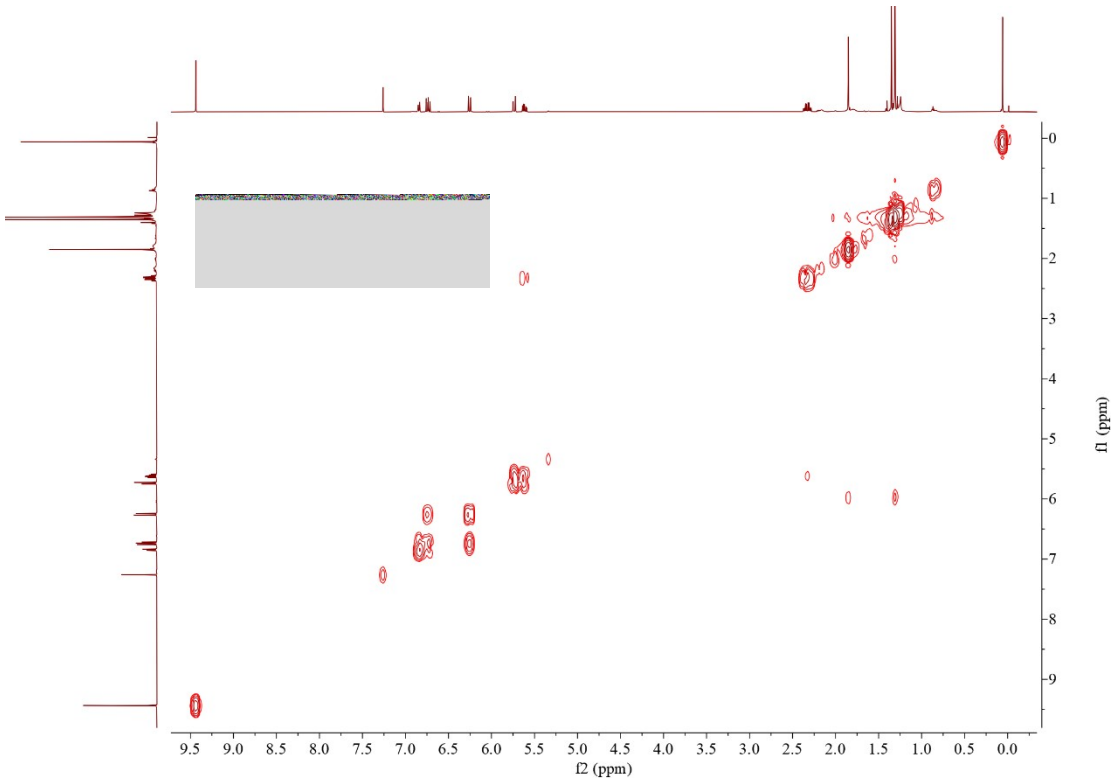


Figure S25. ^{1}H-^{1}H COSY spectrum of **3** ($CDCl_3$)

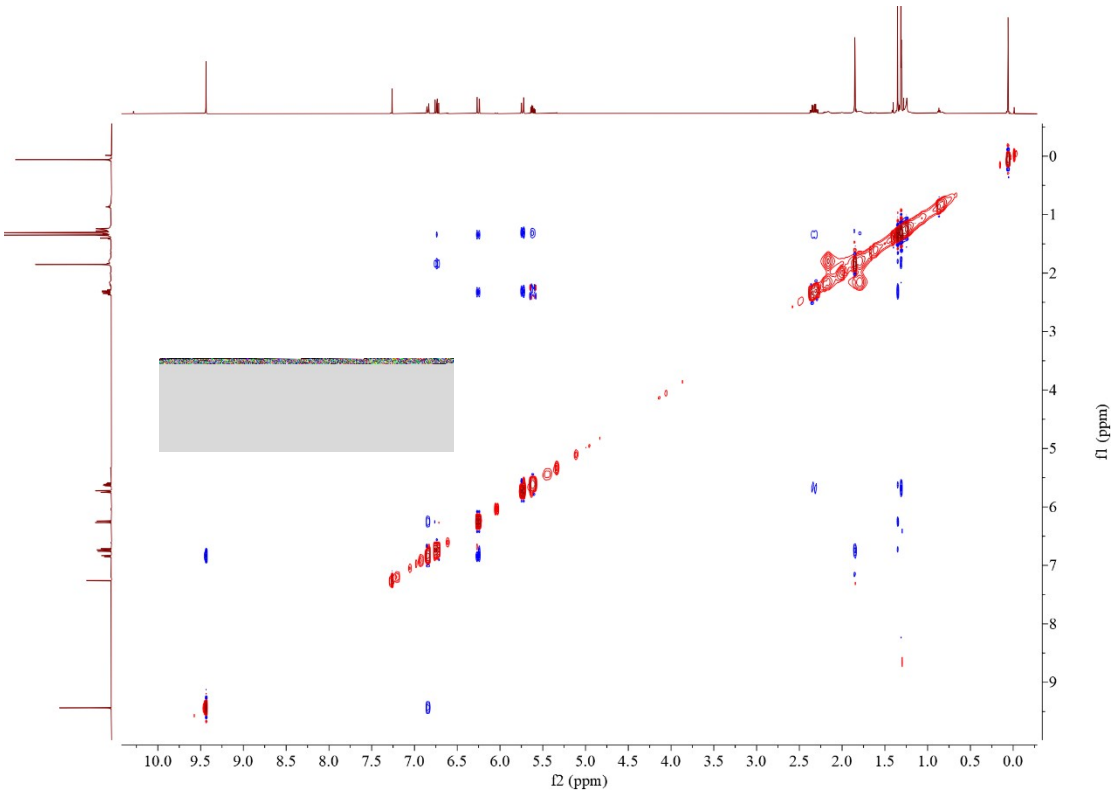


Figure S26. NOESY spectrum of **3** ($CDCl_3$)

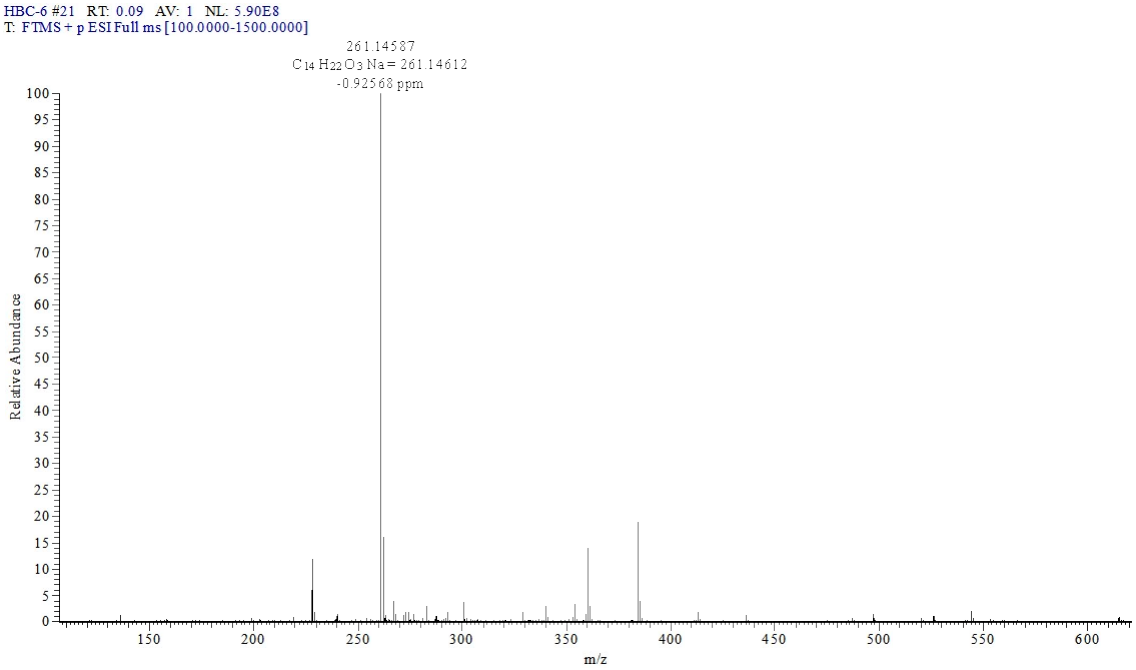


Figure S27. HR-ESI-MS spectrum of **3**

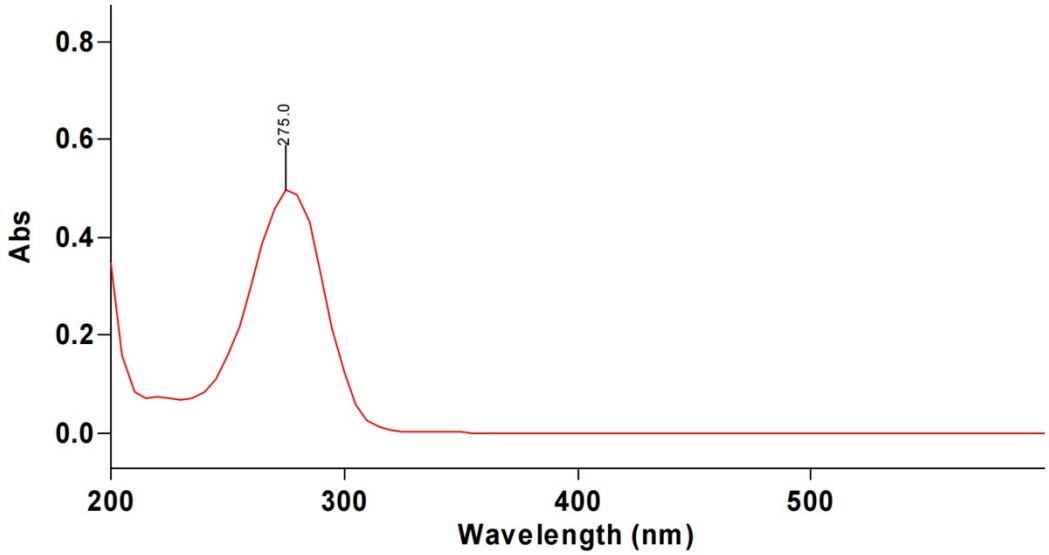


Figure S28. UV spectrum of **3**

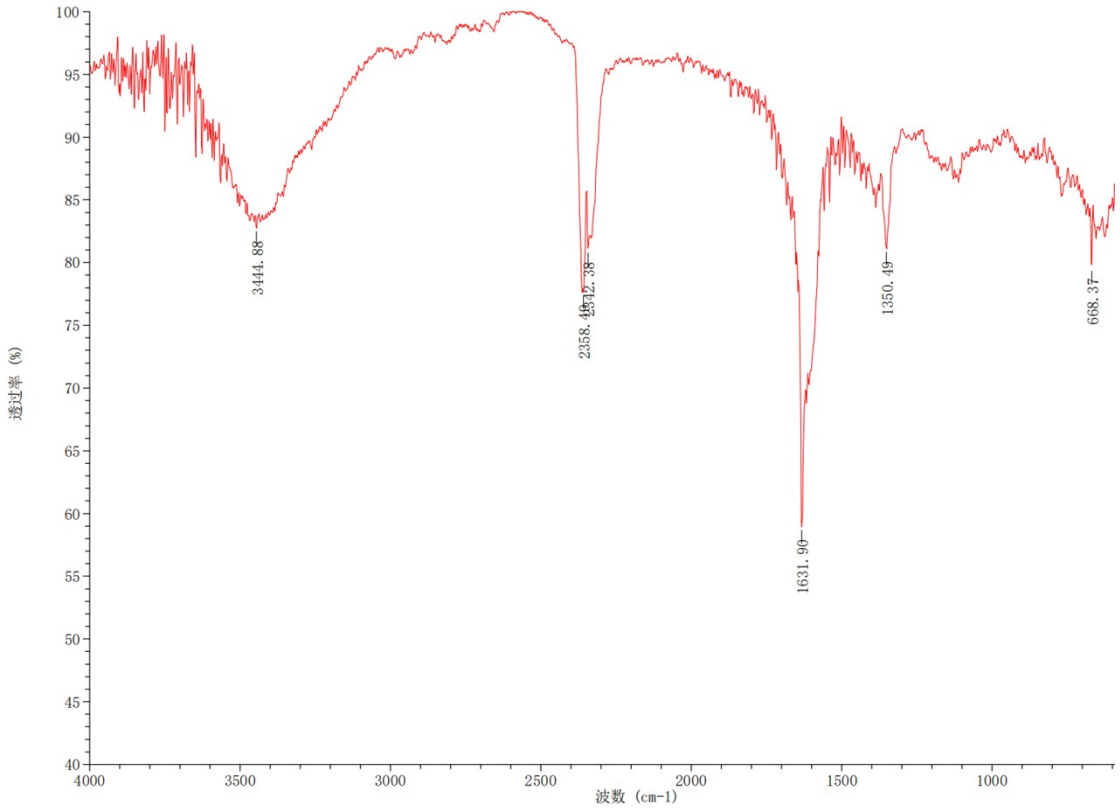


Figure S29. IR spectrum of **3**

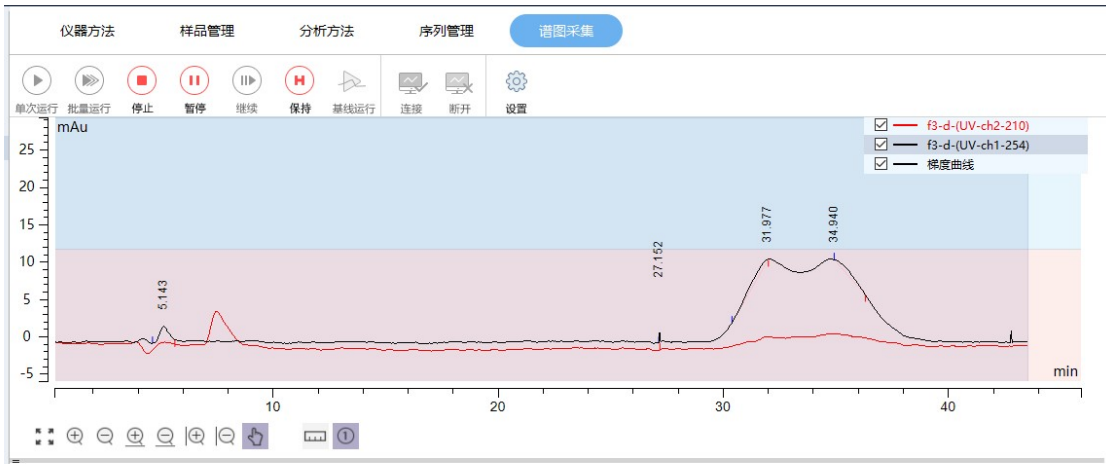


Figure S30. Chiral analysis of **3**

4. Spectra of physico-chemical properties of **4**

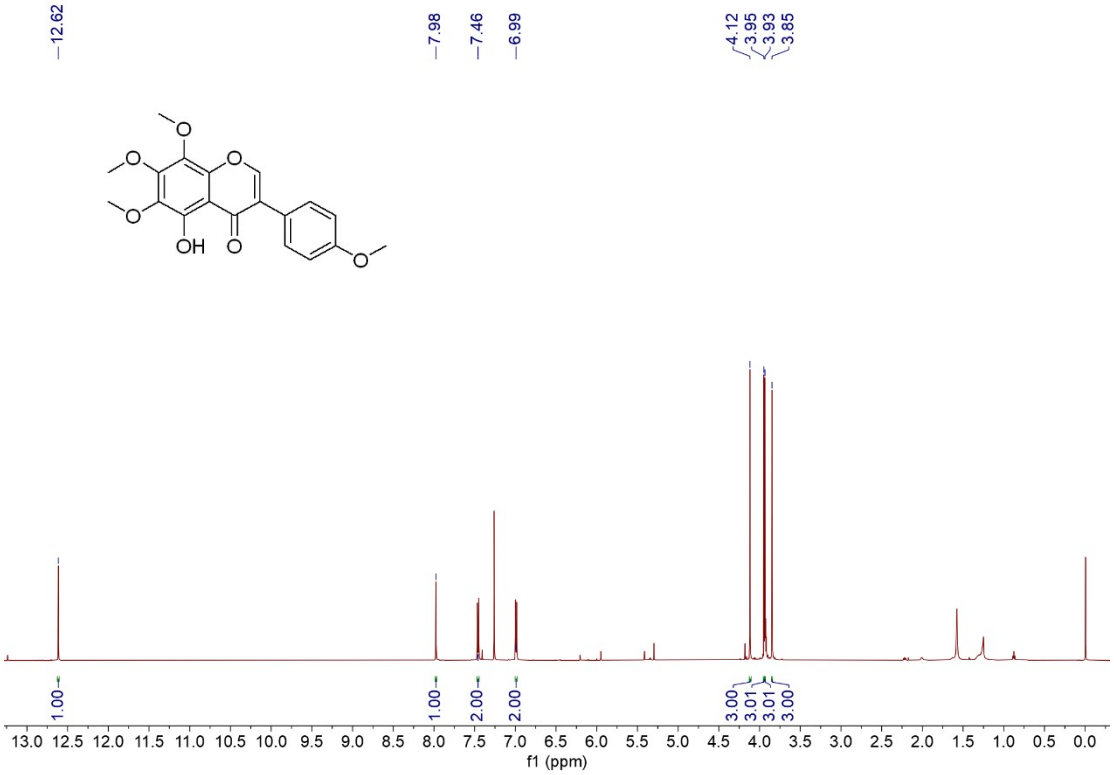


Figure S31. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **4**

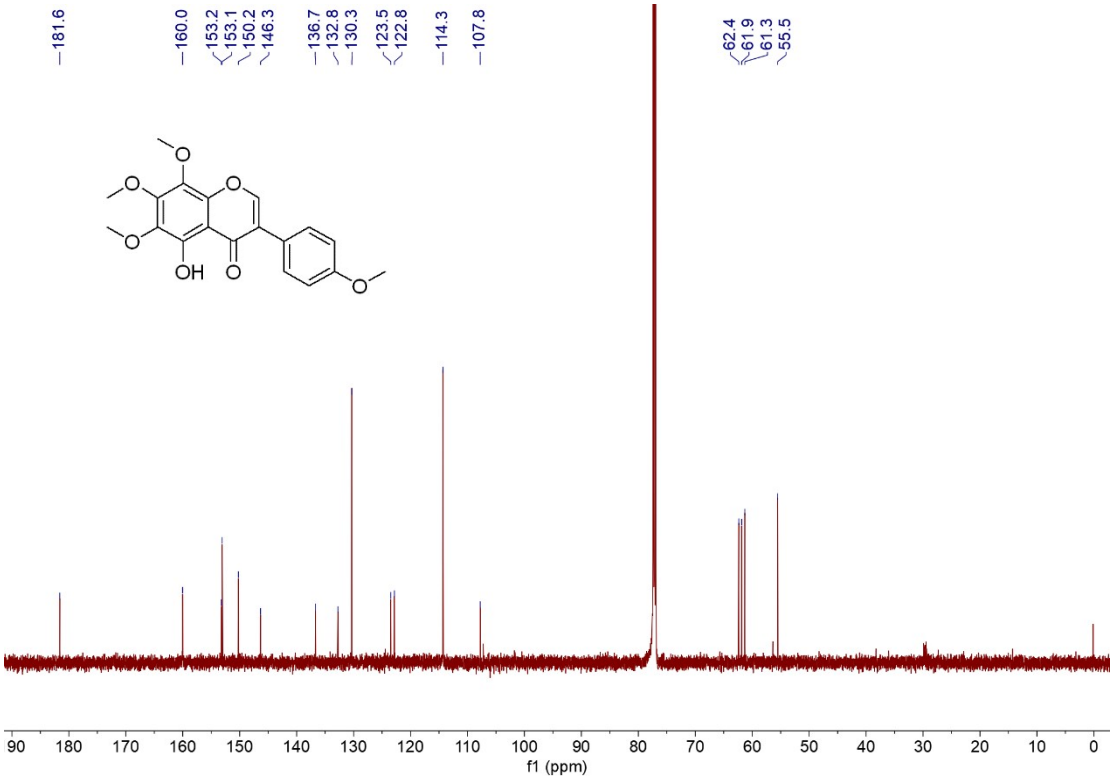


Figure S32. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **4**

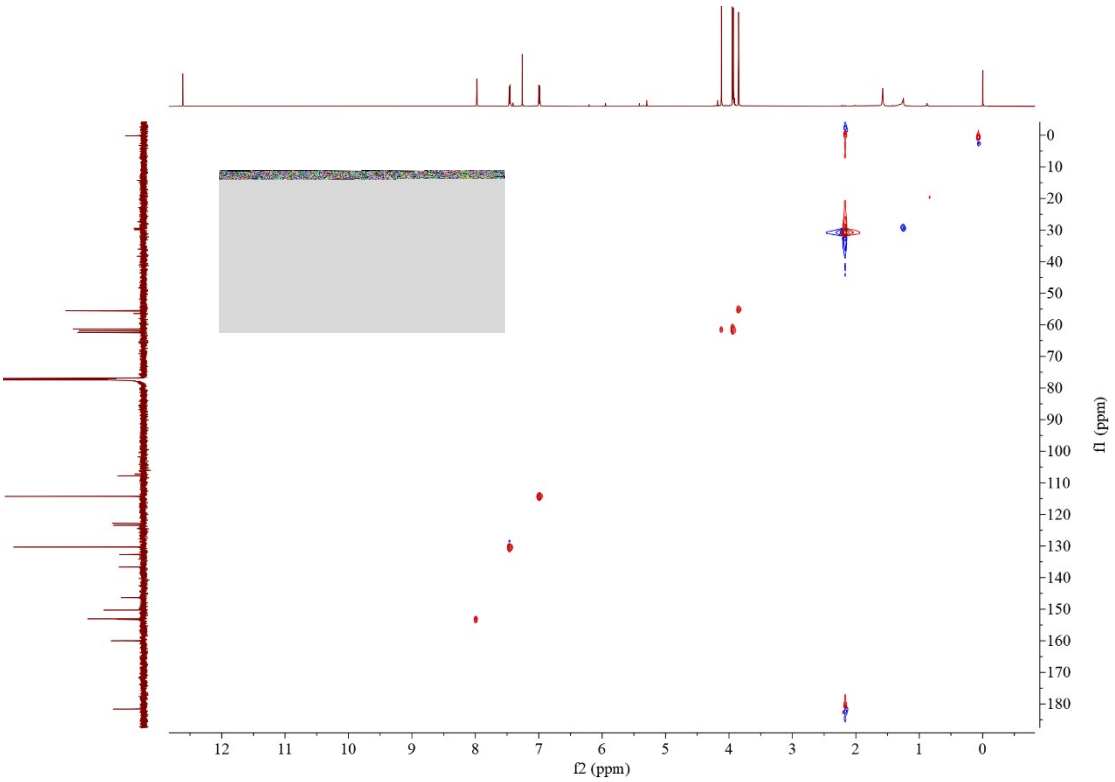


Figure S33. HSQC spectrum of **4** ($CDCl_3$)

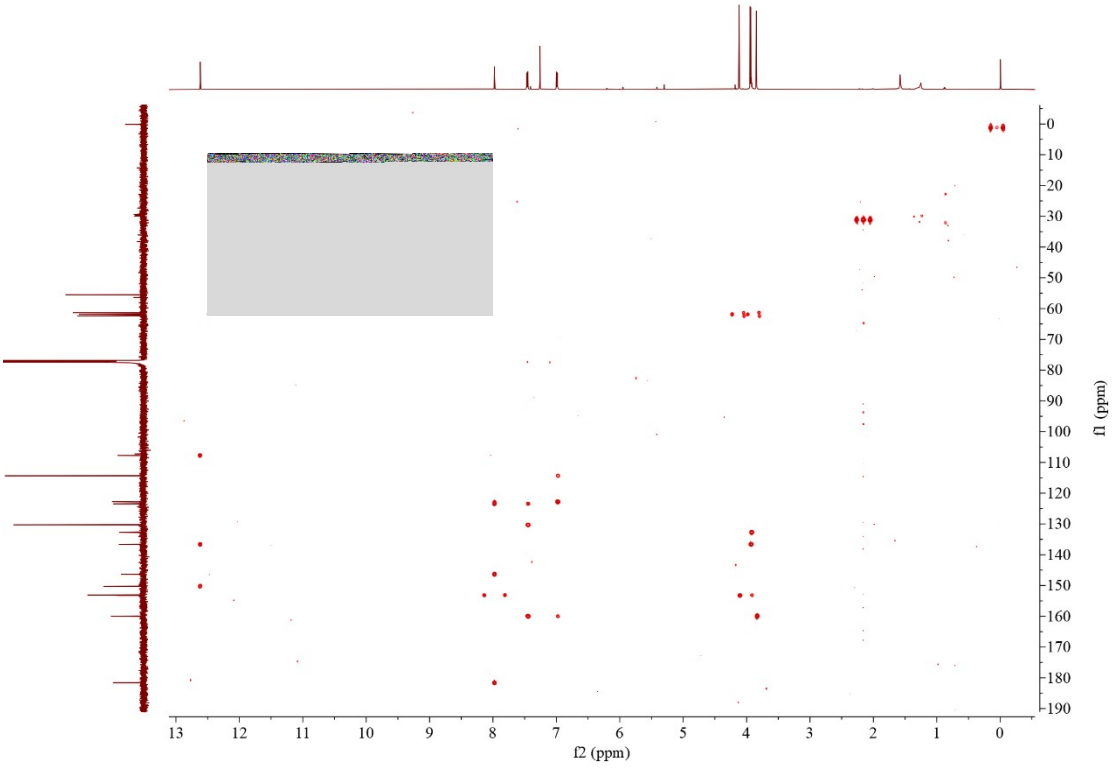


Figure S34. HMBC spectrum of **4** ($CDCl_3$)

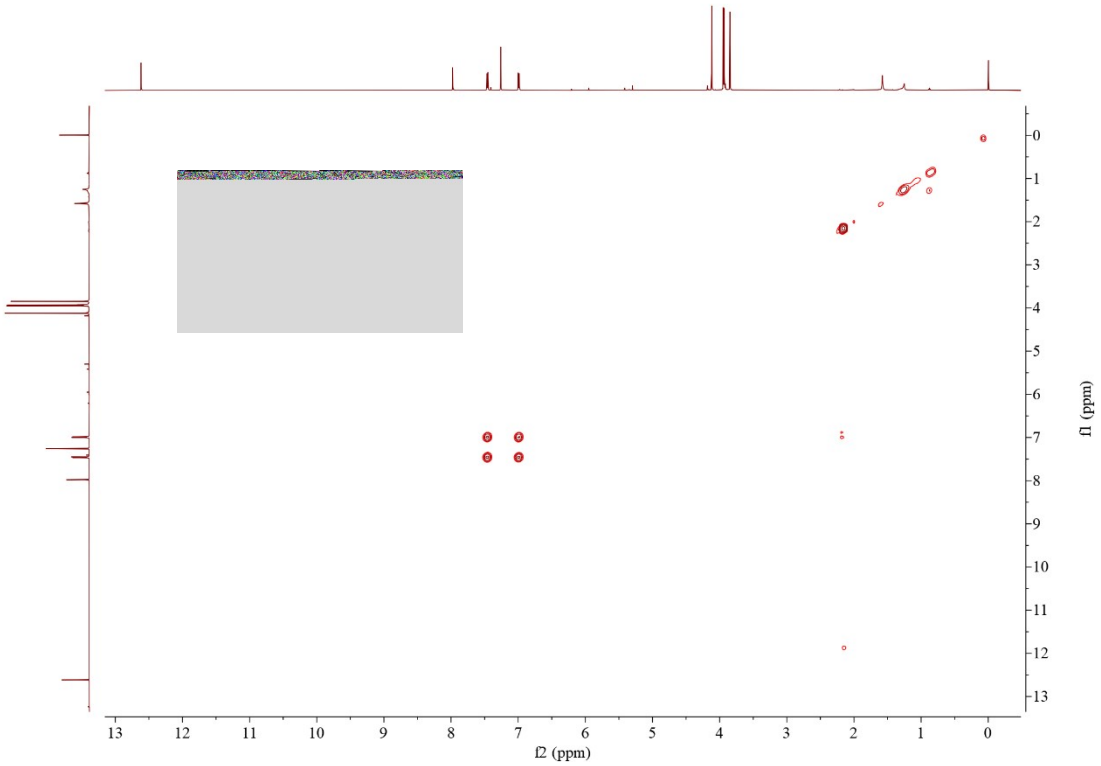


Figure S35. ^{1}H-^{1}H COSY spectrum of **4** ($CDCl_3$)

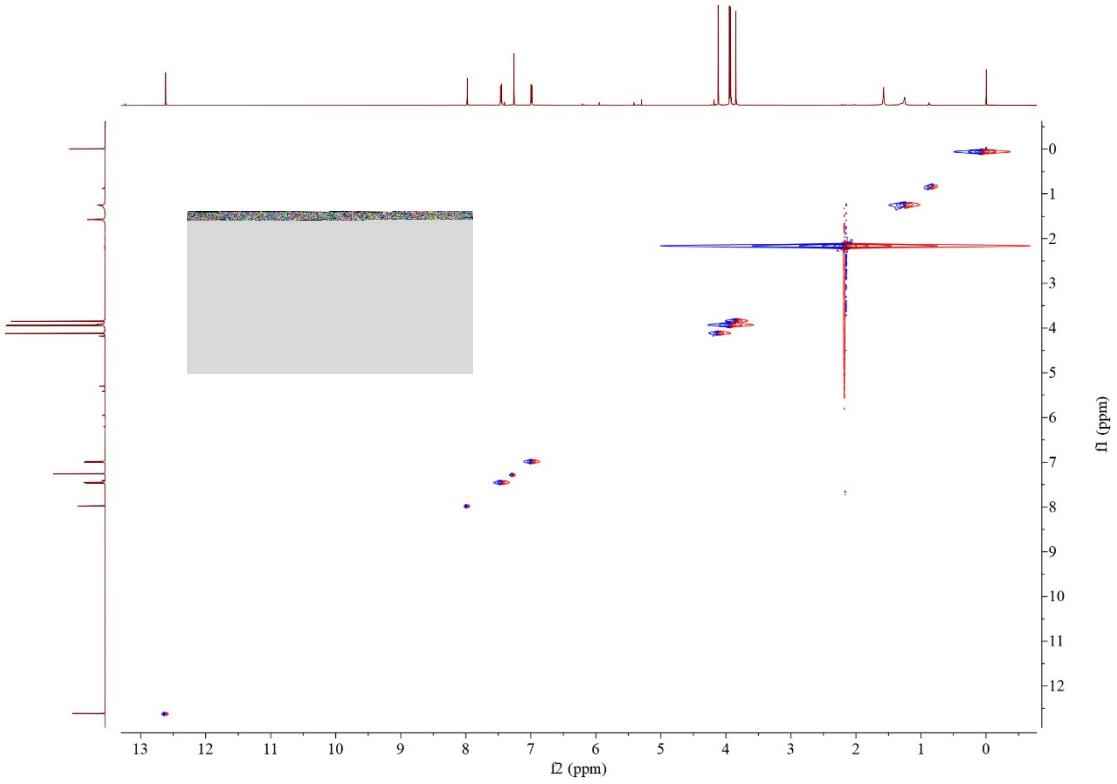


Figure S36. NOESY spectrum of **4** ($CDCl_3$)

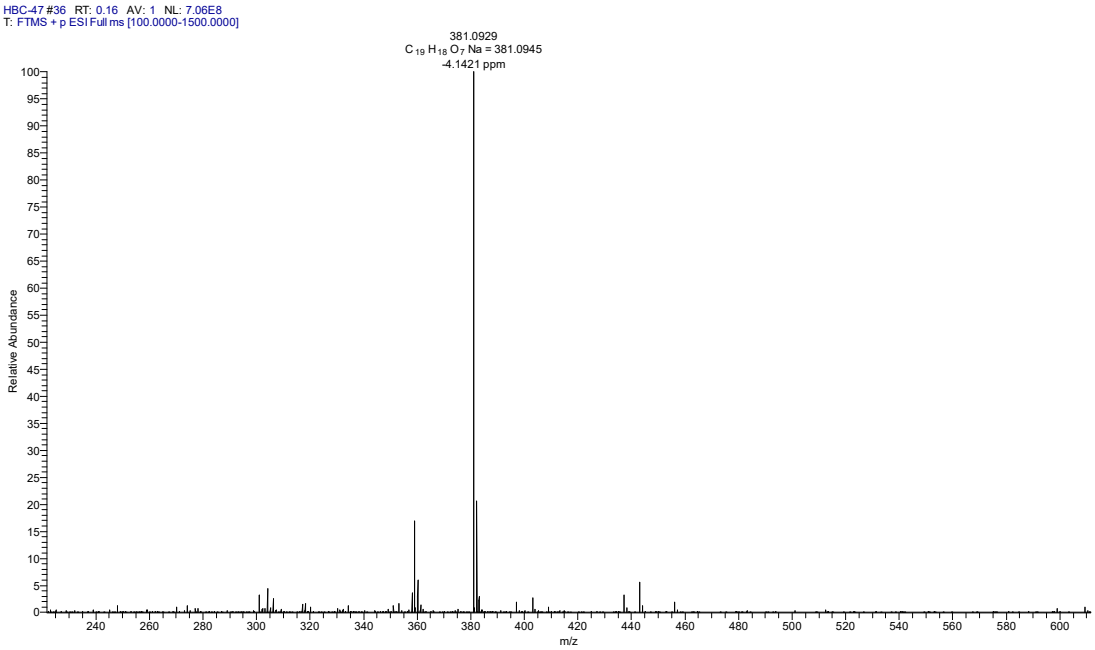


Figure S37. HR-ESI-MS spectrum of **4**

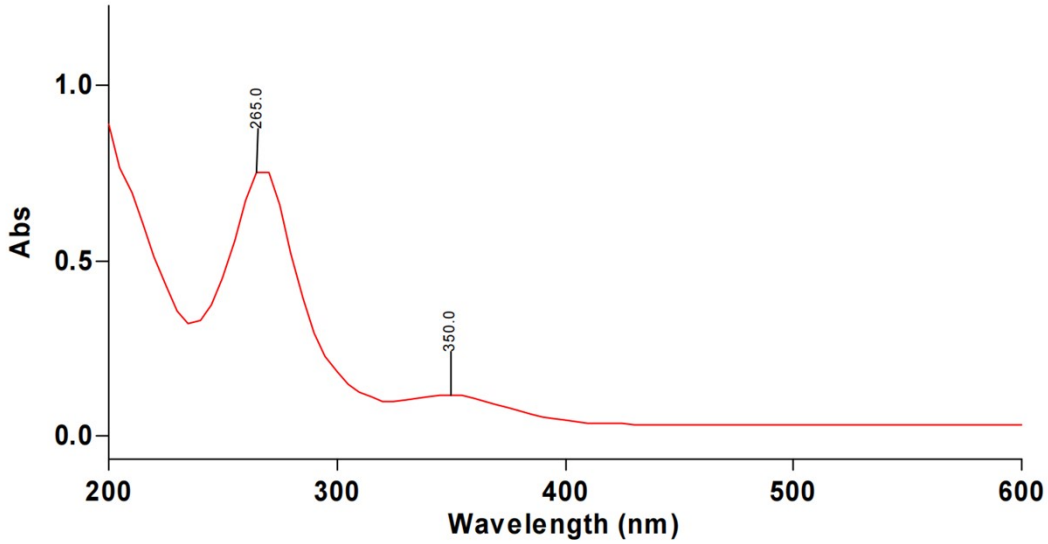


Figure S38. UV spectrum of **4**

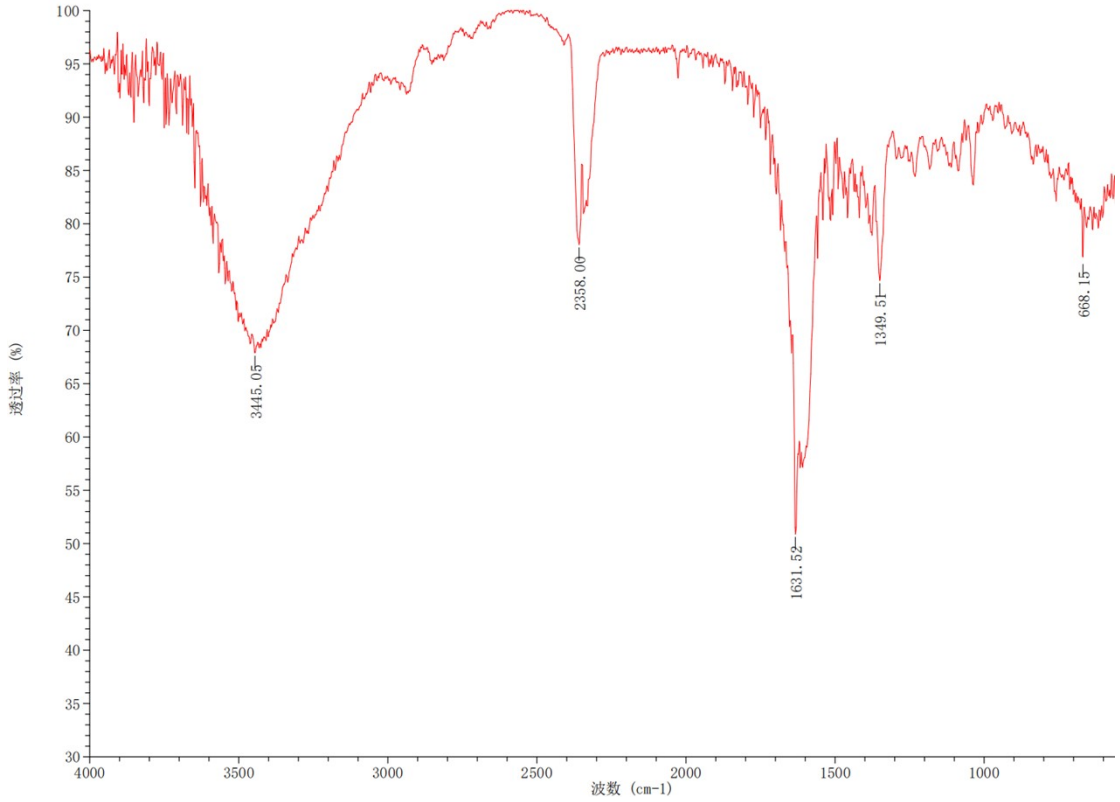
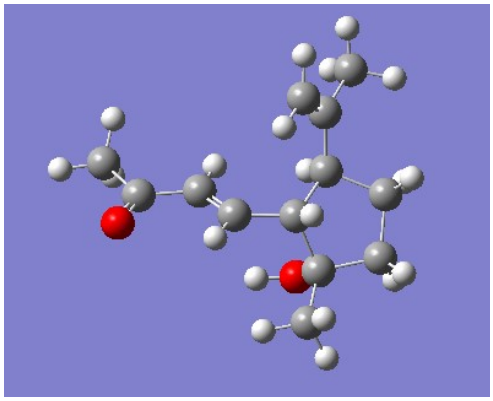


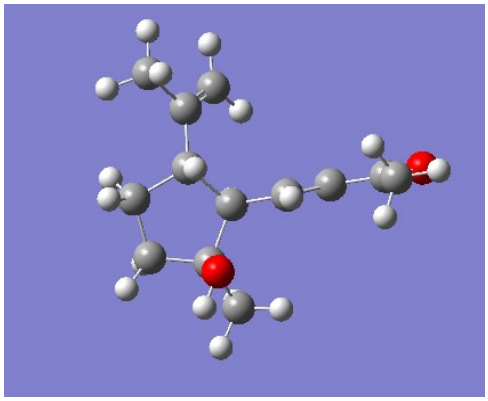
Figure S39. IR spectrum of **4**

5. ECD spectra calculation of **1**

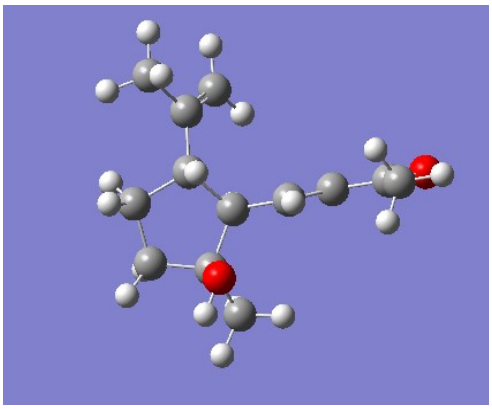
(1) DFT-optimized structures for low-energy conformers for **1** (**1a**–**1d**)



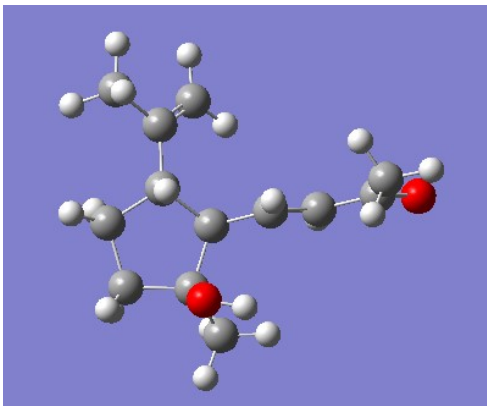
Conf. **1a**



Conf. **1b**



Conf. **1c**



Conf. **1d**

(2) Four stable conformers of optimized geometries of **1** at the B3LYP/6-311+G (d, p) level in the gas phase.

Table S1. Important imaginary frequencies, energy (a. u.), and Boltzmann distributions of the optimized **1** at the B3LYP/6-311+G (d, p) level in MeOH.

Conformers	Imaginary frequencies	Energy (a. u.)	Ratio
1a	0	-657.920919	16.21%
1b	0	-657.919746	14.75%
1c	0	-657.920354	52.35%
1d	0	-657.920756	16.70%

Table S2. The Cartesian coordinates for the lowest-energy conformer of 1a in the ECD calculations.

Atoms	X	Y	Z
C	1.28585	0.67856	-0.22623
C	2.72865	0.10972	-0.37988
C	2.59914	-1.42905	-0.26733
C	1.1059	-1.73763	-0.06359
C	0.56367	-0.41217	0.58669
C	-0.93097	-0.38716	0.65064
C	-1.77289	0.19453	-0.21262
C	-3.25207	0.08516	-0.0396
O	-3.75461	-0.58491	0.8412
C	-4.09757	0.86572	-1.02737
C	1.25913	2.09541	0.30718
C	1.88213	3.12592	-0.60436
C	0.74097	2.4414	1.48621
C	0.8382	-2.99431	0.76098
O	0.56213	-1.88925	-1.38065
H	0.84358	0.68626	-1.22925
H	3.18085	0.41714	-1.3244
H	3.36356	0.50214	0.41987
H	3.17818	-1.81006	0.57769
H	2.94542	-1.95074	-1.16114
H	0.94879	-0.40153	1.61482
H	-1.39432	-0.94657	1.46238
H	-1.40834	0.7961	-1.04006
H	-5.1547	0.7111	-0.81674
H	-3.86574	1.93445	-0.96719
H	-3.87967	0.55284	-2.05415
H	2.94291	2.91879	-0.78133
H	1.39759	3.12513	-1.58782
H	1.80284	4.13276	-0.1901
H	0.75952	3.47162	1.82863
H	0.27147	1.72808	2.15382
H	1.30668	-3.85749	0.28205
H	1.23519	-2.9051	1.77641
H	-0.23388	-3.20012	0.83614
H	-0.40087	-1.92805	-1.30838

Table S3. The Cartesian coordinates for the lowest-energy conformer of **1b** in the ECD calculations.

Atoms	X	Y	Z
C	-1.49137	0.56472	0.29855
C	-2.83321	-0.20007	0.04314
C	-2.43709	-1.63129	-0.38555
C	-0.93571	-1.76785	-0.0717
C	-0.40541	-0.33359	-0.3484
C	0.97715	-0.10116	0.17288
C	2.05475	0.14925	-0.58002
C	3.43262	0.36157	-0.07493
O	4.33916	0.56472	-0.86165
C	3.69137	0.32259	1.42303
C	-1.54871	2.0182	-0.12343
C	-2.47524	2.87355	0.70747
C	-0.8591	2.53539	-1.14062
C	-0.22927	-2.8626	-0.86304
O	-0.74514	-1.97987	1.34011
H	-1.30989	0.54294	1.37934
H	-3.45336	-0.20314	0.94134
H	-3.41209	0.2928	-0.74175
H	-2.60219	-1.77463	-1.45782
H	-3.0137	-2.40735	0.12768
H	-0.41692	-0.20016	-1.43581
H	1.07713	-0.17268	1.25249
H	1.97755	0.21473	-1.66329
H	4.75208	0.49597	1.5981
H	3.11145	1.08939	1.94476
H	3.40979	-0.64405	1.85059
H	-3.50395	2.49766	0.68035
H	-2.1709	2.87044	1.76066
H	-2.48804	3.90938	0.36331
H	-0.95103	3.58436	-1.40513
H	-0.1701	1.95479	-1.74176
H	-0.66932	-3.84176	-0.64231
H	-0.31409	-2.70057	-1.94101
H	0.83025	-2.90249	-0.60288
H	-1.07948	-2.85669	1.56113

Table S4. The Cartesian coordinates for the lowest-energy conformer of **1c** in the ECD calculations.

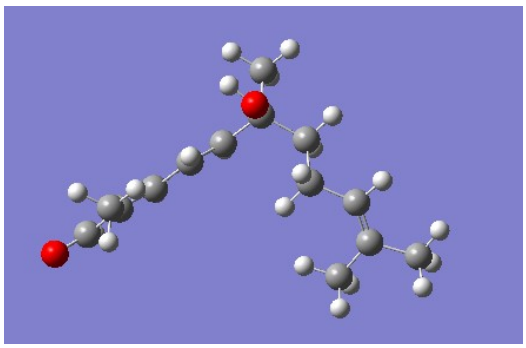
Atoms	X	Y	Z
C	-1.42592	0.70903	0.4483
C	-2.86071	0.18198	0.14297
C	-2.69814	-1.29506	-0.29147
C	-1.2145	-1.65322	-0.0597
C	-0.49841	-0.29683	-0.29497
C	0.92216	-0.26101	0.16619
C	1.9772	-0.00761	-0.61762
C	3.39222	0.04119	-0.17623
O	4.26997	0.26633	-0.98913
C	3.72334	-0.18878	1.28976
C	-1.21027	2.17191	0.12337
C	-1.17789	2.58323	-1.32838
C	-1.06033	3.0683	1.10043
C	-0.70424	-2.79141	-0.93691
O	-0.99135	-1.96637	1.32813
H	-1.2436	0.57017	1.51641
H	-3.49358	0.28936	1.02573
H	-3.33448	0.76664	-0.64907
H	-2.94773	-1.41995	-1.34962
H	-3.34747	-1.9774	0.26566
H	-0.53747	-0.10007	-1.37228
H	1.0672	-0.4626	1.22393
H	1.84975	0.18712	-1.68052
H	4.8024	-0.11931	1.41865
H	3.23691	0.55649	1.92571
H	3.38384	-1.17296	1.62528
H	-0.27601	2.21143	-1.8263
H	-2.03238	2.18928	-1.88875
H	-1.18448	3.66957	-1.43294
H	-0.92818	4.12611	0.89381
H	-1.06335	2.77705	2.14654
H	-1.26956	-3.71032	-0.74394
H	-0.80829	-2.55976	-2.00041
H	0.34862	-2.99336	-0.72979
H	-1.43814	-2.79751	1.52553

Table S5. The Cartesian coordinates for the lowest-energy conformer of **1d** in the ECD calculations.

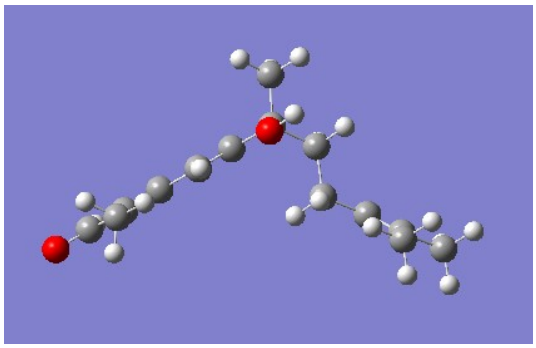
Atoms	X	Y	Z
C	-1.56161	0.53185	0.23372
C	-2.83069	-0.26753	-0.15826
C	-2.41046	-1.75308	-0.10805
C	-0.86922	-1.79081	0.01849
C	-0.42342	-0.33163	-0.35206
C	0.94188	0.01304	0.15366
C	2.05815	0.05125	-0.58527
C	3.41879	0.37484	-0.08904
O	4.36104	0.34841	-0.85851
C	3.61333	0.74162	1.37382
C	-1.6209	1.99468	-0.15153
C	-2.63913	2.81152	0.60778
C	-0.85413	2.54877	-1.09196
C	-0.20646	-2.86171	-0.84154
O	-0.59788	-2.04849	1.40854
H	-1.46743	0.47349	1.32695
H	-3.67485	-0.05226	0.49966
H	-3.13321	0.01741	-1.17101
H	-2.74072	-2.29087	-0.99975
H	-2.8281	-2.27247	0.7559
H	-0.43795	-0.25858	-1.4463
H	1.00183	0.23386	1.21772
H	2.02648	-0.15711	-1.65265
H	3.01912	1.61896	1.6448
H	3.30826	-0.07483	2.03522
H	4.6673	0.9576	1.54131
H	-3.65755	2.44699	0.43571
H	-2.46545	2.75158	1.68841
H	-2.60872	3.86376	0.31896
H	-0.9452	3.60134	-1.34258
H	-0.1055	1.99261	-1.64292
H	-0.56127	-3.85157	-0.5436
H	-0.42996	-2.72091	-1.90249
H	0.88263	-2.8427	-0.72807
H	0.34818	-2.21252	1.5059

6. ECD spectra calculation of **2**

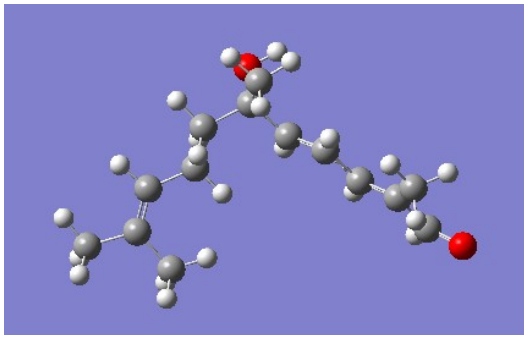
(1) DFT-optimized structures for low-energy conformers for **2** (**2a**–**2d**)



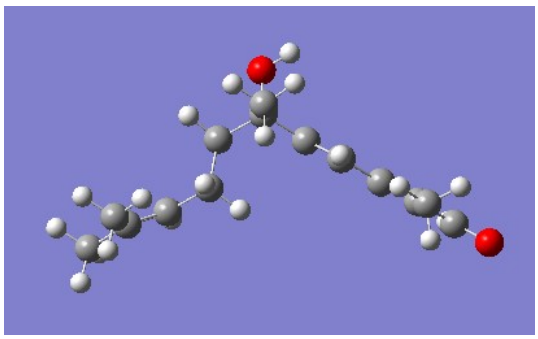
Conf. **2a**



Conf. **2b**



Conf. **2c**



Conf. **2d**

(2) Four stable conformers of optimized geometries of **2** at the B3LYP/6-311+G (d, p) level in the gas phase.

Table S6. Important imaginary frequencies, energy (a. u.), and Boltzmann distributions of the optimized **2** at the B3LYP/6-311+G (d, p) level in MeOH.

Conformers	Imaginary frequencies	Energy (a. u.)	Ratio
2a	0	-697.270223	89.51%
2b	0	-697.270727	0.00%
2c	0	-697.269360	5.25%
2d	0	-697.269634	5.24%

Table S7. The Cartesian coordinates for the lowest-energy conformer of **2a** in the ECD calculations.

Atoms	X	Y	Z
C	-0.54061	1.26852	-0.7088
C	-1.52921	0.72819	0.02082
C	-2.59185	-0.06718	-0.55452
C	-3.62133	-0.66448	0.09026
C	-4.5784	-1.42023	-0.739
H	-4.35309	-1.42491	-1.82887
O	-5.54904	-2.00564	-0.30985
C	-3.89478	-0.63834	1.56599
C	0.58453	2.12456	-0.16984
O	0.40331	2.42073	1.21924
C	1.93699	1.38478	-0.26988
C	0.65056	3.43752	-0.97135
C	2.04408	0.1104	0.58483
C	3.42758	-0.47756	0.53711
C	3.82062	-1.65816	0.04415
C	5.27119	-2.07283	0.09185
C	2.90572	-2.67952	-0.58389
H	-0.5212	1.10104	-1.78563
H	-1.52084	0.88732	1.09446
H	-2.54976	-0.19383	-1.63698
H	-3.13989	-0.09044	2.12903
H	-4.87142	-0.18757	1.76527
H	-3.94763	-1.65692	1.96033
H	-0.36653	2.99572	1.30956
H	2.71461	2.09324	0.03588
H	2.12948	1.14313	-1.32066
H	-0.29486	3.98533	-0.89893
H	1.44728	4.07137	-0.57607
H	0.84557	3.25521	-2.03147
H	1.28978	-0.61189	0.26673
H	1.79898	0.37471	1.6188
H	4.20046	0.16421	0.96271
H	5.66169	-2.26828	-0.91427
H	5.90058	-1.30986	0.5546
H	5.39884	-3.00349	0.65797
H	1.86522	-2.35965	-0.63395
H	2.93635	-3.62323	-0.02631
H	3.23155	-2.916	-1.60382

Table S8. The Cartesian coordinates for the lowest-energy conformer of **2b** in the ECD calculations.

Atoms	X	Y	Z
C	-0.73437	1.17382	-0.5934
C	-1.71927	0.5808	0.09814
C	-2.85654	-0.0418	-0.54221
C	-3.90157	-0.66639	0.05016
C	-4.93875	-1.21894	-0.83941
H	-4.75456	-1.06477	-1.92632
O	-5.93184	-1.80329	-0.4622
C	-4.11655	-0.85599	1.52365
C	0.46699	1.85833	0.00127
O	0.39388	1.69292	1.42306
C	1.77902	1.23871	-0.54333
C	0.41529	3.35955	-0.34245
C	1.97529	-0.24894	-0.20776
C	3.2799	-0.77837	-0.73564
C	4.30239	-1.3142	-0.05813
C	5.5412	-1.79139	-0.77627
C	4.33989	-1.50917	1.43674
H	-0.77832	1.1957	-1.68161
H	-1.65187	0.57346	1.17993
H	-2.86464	0.00237	-1.6322
H	-3.31429	-0.43373	2.1277
H	-5.06075	-0.39828	1.83273
H	-4.20591	-1.91993	1.76107
H	1.12322	2.18378	1.81915
H	2.62009	1.81444	-0.13511
H	1.81705	1.38625	-1.62939
H	-0.48253	3.80996	0.08448
H	1.29109	3.87463	0.06759
H	0.40956	3.52858	-1.42246
H	1.14912	-0.82092	-0.64873
H	1.88689	-0.38049	0.87127
H	3.38913	-0.70332	-1.81882
H	5.71239	-2.86062	-0.60265
H	5.47705	-1.63266	-1.85472
H	6.436	-1.27287	-0.41119
H	3.44183	-1.15778	1.94393
H	5.19904	-0.98744	1.87502
H	4.46658	-2.56949	1.68528

Table S9. The Cartesian coordinates for the lowest-energy conformer of **2c** in the ECD calculations.

Atoms	X	Y	Z
C	0.50873	1.13719	-0.67809
C	1.57869	0.72558	0.02305
C	2.57955	-0.16364	-0.52714
C	3.68615	-0.64726	0.08394
C	4.5483	-1.54284	-0.71083
H	4.19639	-1.73369	-1.74896
O	5.56957	-2.05281	-0.30402
C	4.13401	-0.37119	1.48978
C	-0.58592	2.08099	-0.2369
O	-0.67435	3.12416	-1.2334
C	-1.96075	1.38751	-0.32745
C	-0.34748	2.71859	1.13454
C	-2.19298	0.21933	0.64569
C	-3.55896	-0.38744	0.47071
C	-3.88111	-1.63185	0.09908
C	-5.32561	-2.052	-0.02344
C	-2.89049	-2.72178	-0.22474
H	0.38739	0.79412	-1.70546
H	1.71036	1.06407	1.0459
H	2.41046	-0.47374	-1.5588
H	3.46468	0.29924	2.02821
H	4.21378	-1.30499	2.05365
H	5.1362	0.06671	1.49047
H	0.17755	3.57723	-1.26575
H	-2.08816	1.03878	-1.35686
H	-2.71866	2.16372	-0.17621
H	0.58662	3.28861	1.14206
H	-1.16212	3.41055	1.35609
H	-0.294	1.9827	1.93972
H	-2.10537	0.58376	1.67721
H	-1.40572	-0.52764	0.5211
H	-4.38135	0.30055	0.67114
H	-5.55093	-2.89405	0.64209
H	-6.01161	-1.23825	0.22034
H	-5.55405	-2.39288	-1.04039
H	-3.0186	-3.57566	0.4511
H	-3.05624	-3.10573	-1.23817
H	-1.85113	-2.40124	-0.15827

Table S10. The Cartesian coordinates for the lowest-energy conformer of **2d** in the ECD calculations.

Atoms	X	Y	Z
C	0.74601	1.09002	-0.64177
C	1.75641	0.57502	0.07916
C	2.88661	-0.09665	-0.52617
C	3.9498	-0.65681	0.09651
C	4.97265	-1.28156	-0.76398
H	4.76344	-1.22932	-1.85551
O	5.97821	-1.82061	-0.3555
C	4.20286	-0.71299	1.57503
C	-0.46748	1.83826	-0.14105
O	-0.51966	3.09131	-0.85939
C	-1.76106	1.12292	-0.58181
C	-0.45029	2.12335	1.36322
C	-2.01406	-0.25846	0.04501
C	-3.20298	-0.9418	-0.57453
C	-4.3567	-1.30245	-0.00071
C	-5.439	-1.983	-0.80294
C	-4.70514	-1.08937	1.45094
H	0.77696	1.00544	-1.72797
H	1.73716	0.65656	1.16132
H	2.86755	-0.15135	-1.61504
H	3.41986	-0.23324	2.16167
H	4.29424	-1.75153	1.90572
H	5.15704	-0.23588	1.81594
H	0.29083	3.57879	-0.66575
H	-1.72989	1.03727	-1.67317
H	-2.59553	1.79467	-0.35719
H	0.42586	2.71861	1.63792
H	-1.34006	2.69639	1.63053
H	-0.43485	1.21208	1.96519
H	-2.13708	-0.16212	1.12583
H	-1.12664	-0.88726	-0.10527
H	-3.08913	-1.15448	-1.63828
H	-6.3697	-1.40332	-0.78438
H	-5.15009	-2.12163	-1.84672
H	-5.68066	-2.96826	-0.38624
H	-3.92893	-0.57301	2.01534
H	-4.89628	-2.04747	1.94878
H	-5.62816	-0.50538	1.54489