Supporting information

Garcimultiflins A–C, unusual polycyclic polyprenylated acylphloroglucinols from the pericarps of *Garcinia multiflora* as interleukin-1*β* and pyroptosis inhibitors

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Table S1. Crystal data and structure refinement for garcimultiflin A.

Empirical formula	$C_{34}H_{48}O_{10}$
Formula weight	616.72
Temperature/K	150.00
Crystal system	monoclinic
Space group	$P2_1$
a/Å	8.3050(2)
b/Å	18.9835(5)
c/Å	10.5728(2)
α/°	90
β/°	102.7180(10)
γ/°	90
Volume/Å^3	1625.99(7)
Z	2
ρ_{calc}g/cm^3	1.260
μ/mm^{-1}	0.754
F(000)	664.0
Crystal size/mm^3	$0.2 \times 0.15 \times 0.1$
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	8.574 to 149.642
Index ranges	$-10 \leq h \leq 10, -22 \leq k \leq 23, -13 \leq l \leq 11$
Reflections collected	15933
Independent reflections	6226 [R_{int} = 0.0365, R_{sigma} = 0.0366]
Data/restraints/parameters	6226/1/410
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0666, wR_2 = 0.1554
Final R indexes [all data]	R_1 = 0.0686, wR_2 = 0.1582
Largest diff. peak/hole / e Å^{-3}	0.42/-0.19
Flack parameter	0.06(9)
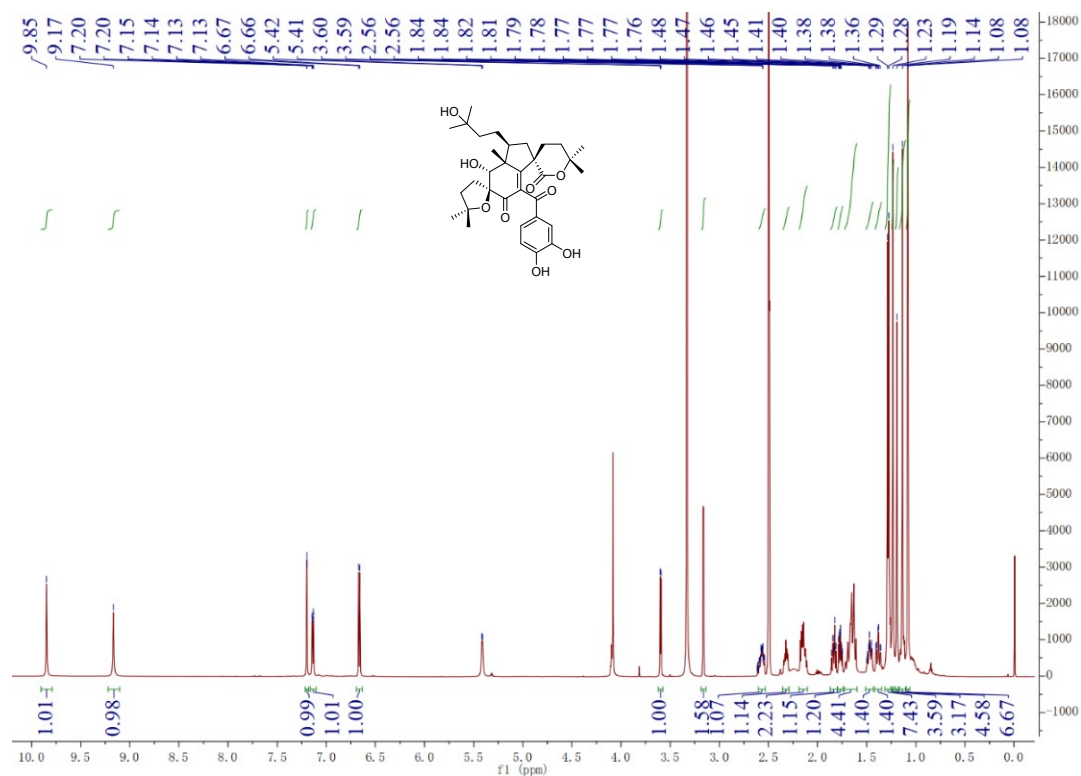
Fig. S1. The ^{1}H NMR spectrum of **1** (600 MHz, DMSO-*d*$_6$).
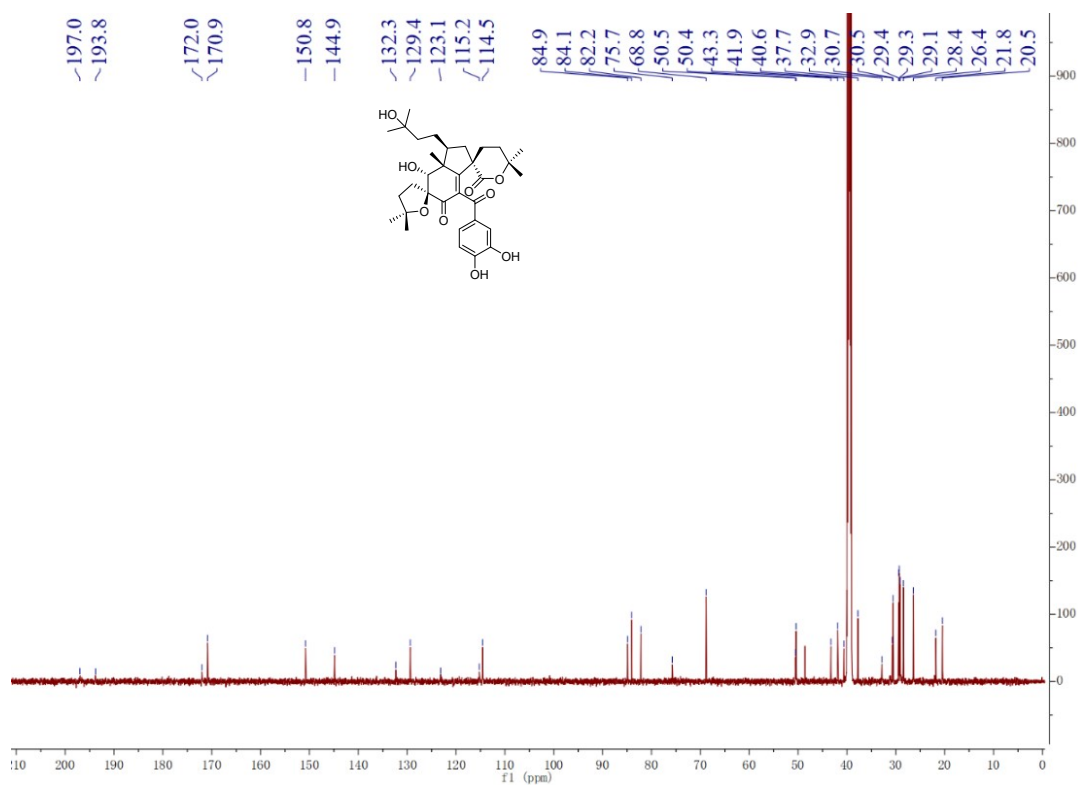
Fig. S2. The ^{13}C NMR spectrum of **1** (150 MHz, DMSO-*d*$_6$).
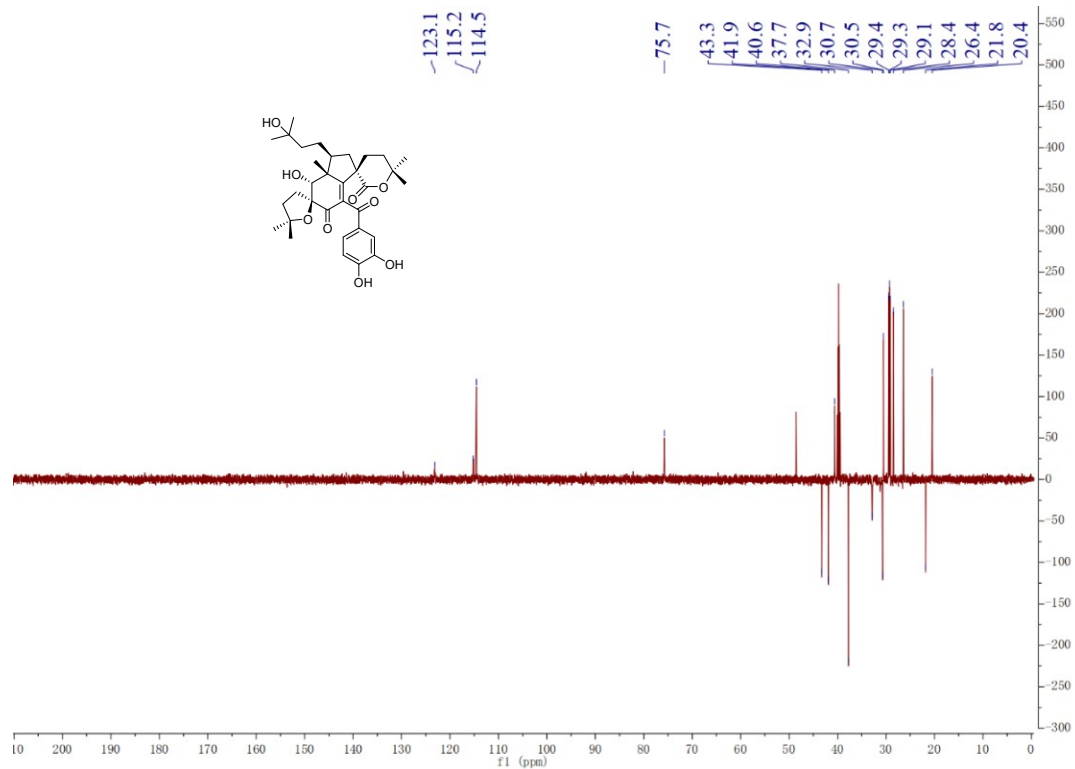
Fig. S3. The DEPT135 spectrum of 1 (600 MHz, DMSO-*d*₆).

Fig. S4. The HSQC spectrum of 1 (600 MHz, DMSO-*d*₆).

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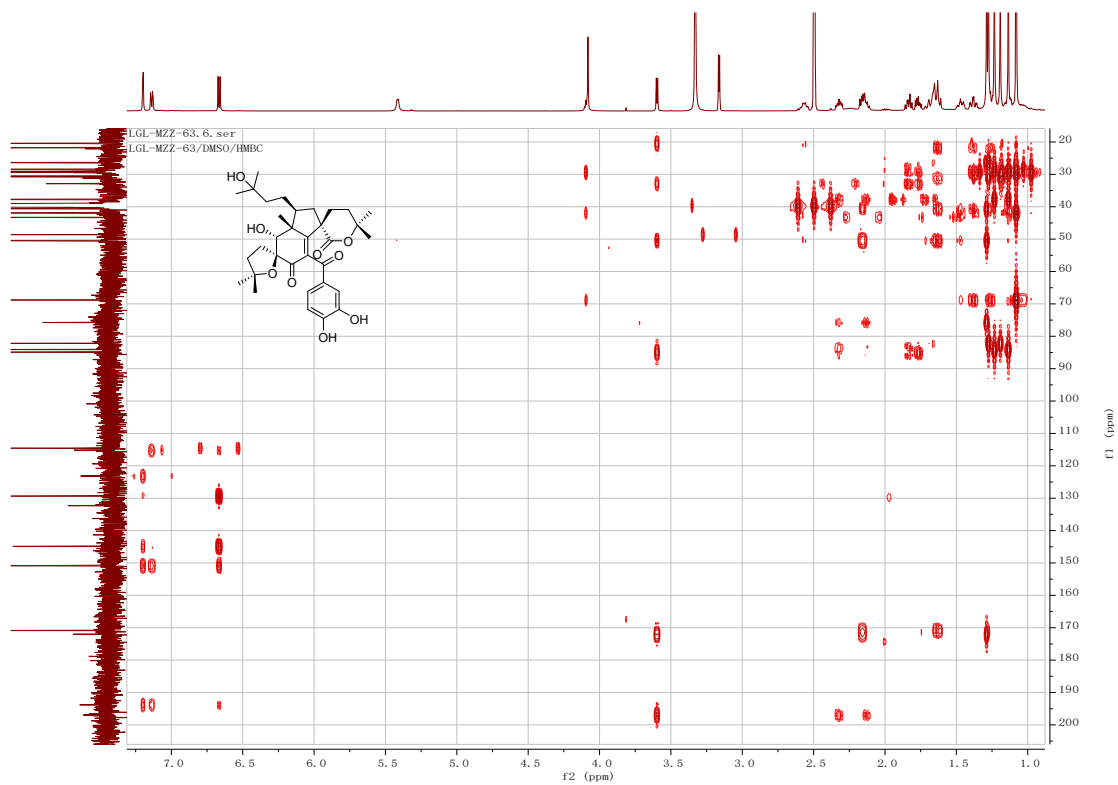
Fig. S5. The HMBC spectrum of 1 (600 MHz, DMSO-d_6).
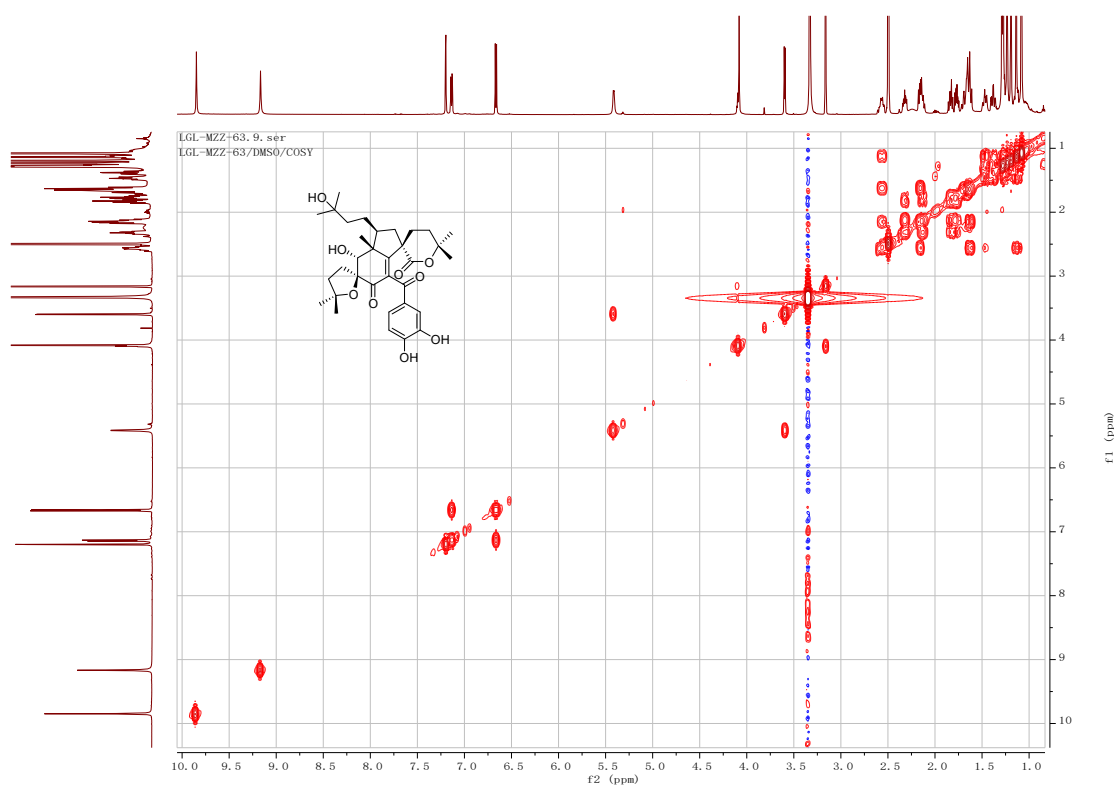
Fig. S6. The ^{1}H-^{1}H COSY spectrum of 1 (600 MHz, DMSO-d_6).
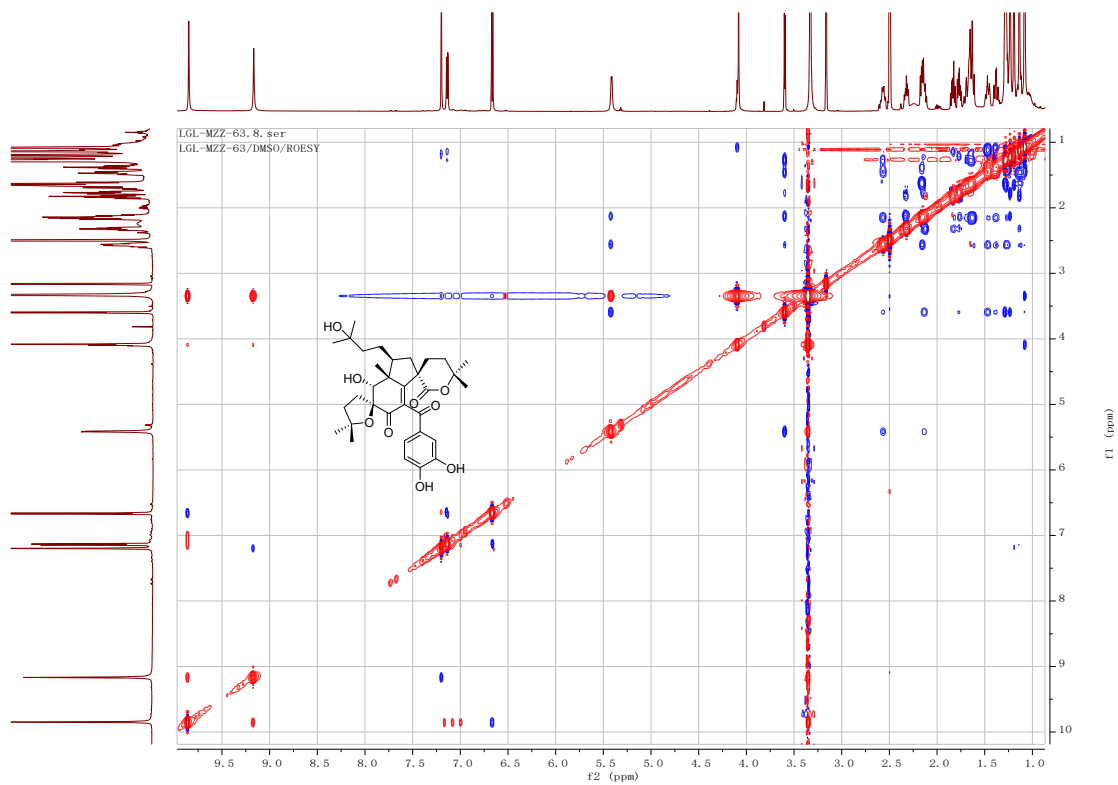
Fig. S7. The ROESY spectrum of 1 (600 MHz, DMSO-d_6).

Thermo Qexactive Focus Report

compound NO. : MII-63
Method :   LCMS(compound)-low

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NL: 2.11E9
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585.30669 F: FTMS
+ p ESI Full ms
[100.0000-
1500.0000] MS
MII-63

MII-63 #665 RT: 6.54 AV: 1 NL: 1.83E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]
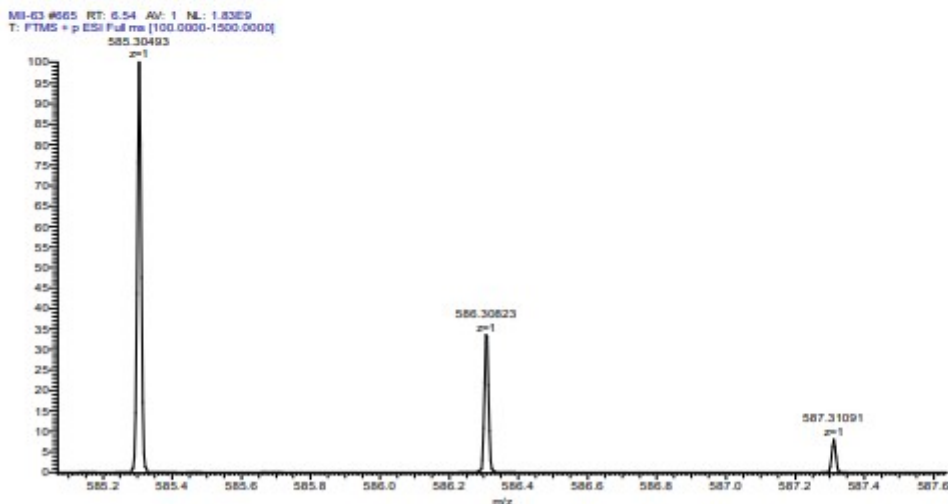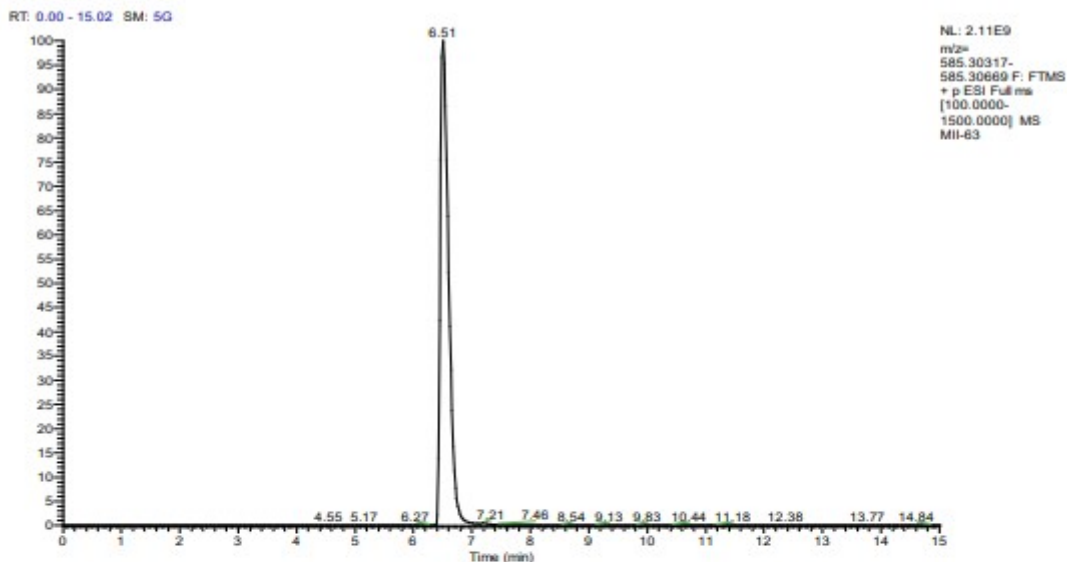
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
585.30493	585.30581	-1.5	11.5	C33 H45 O9	M+H

Fig. S8. The HR-ESI-MS spectrum of 1.
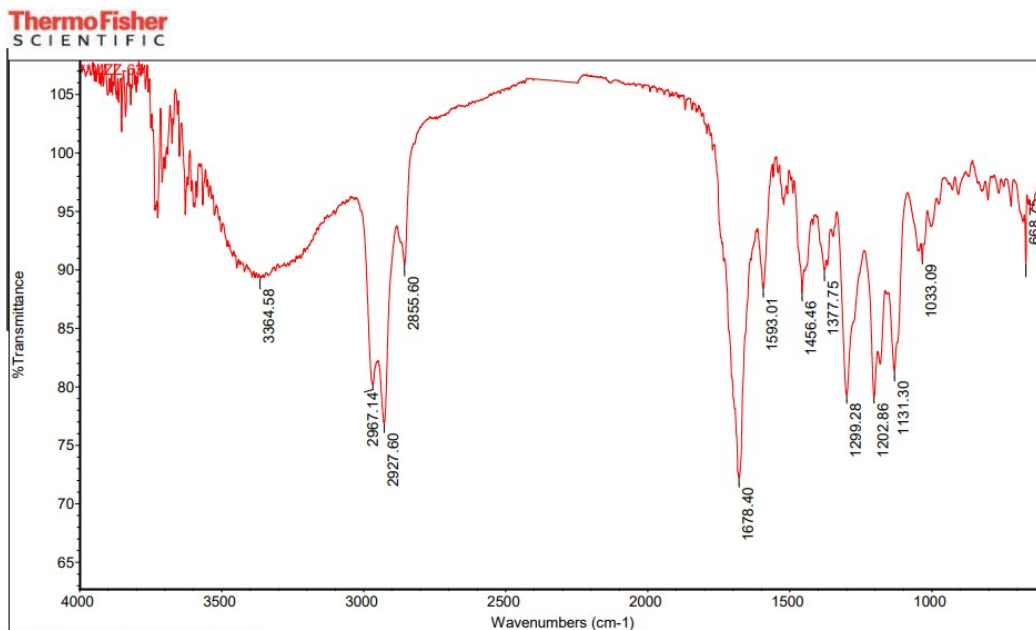
Fig. S9. The IR spectrum of 1.
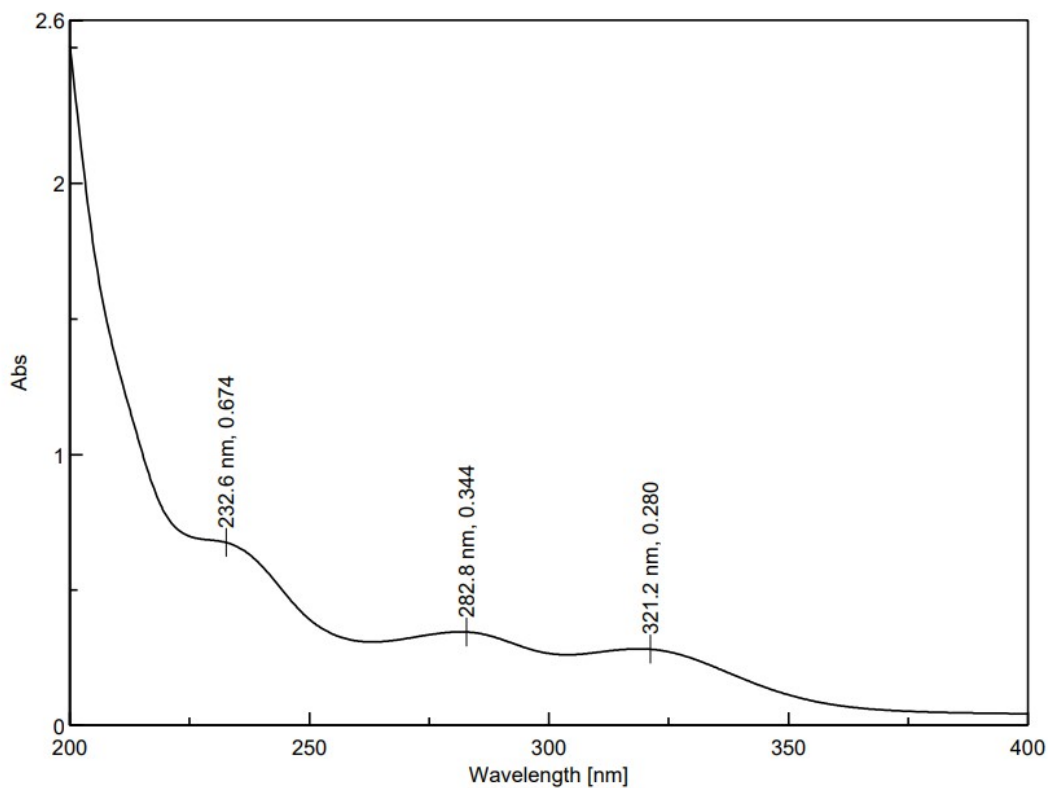
Fig. S10. The UV spectrum of 1.

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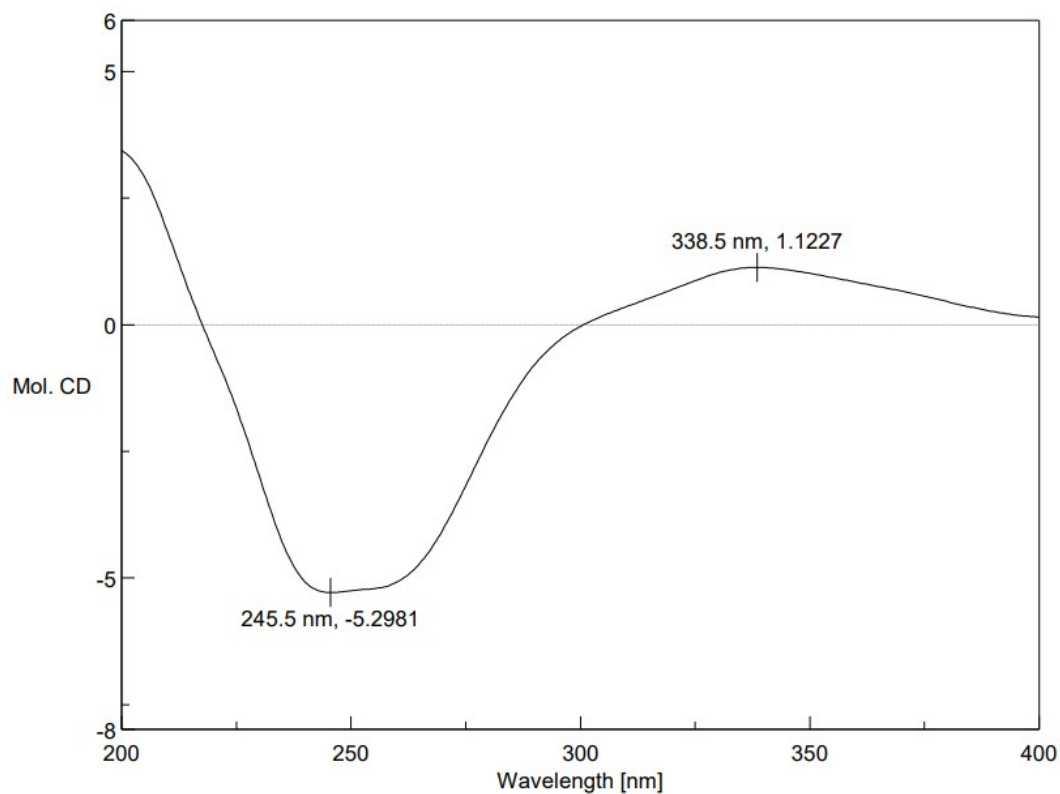
Fig. S11. The experimental ECD spectrum of 1 in CH₃OH.
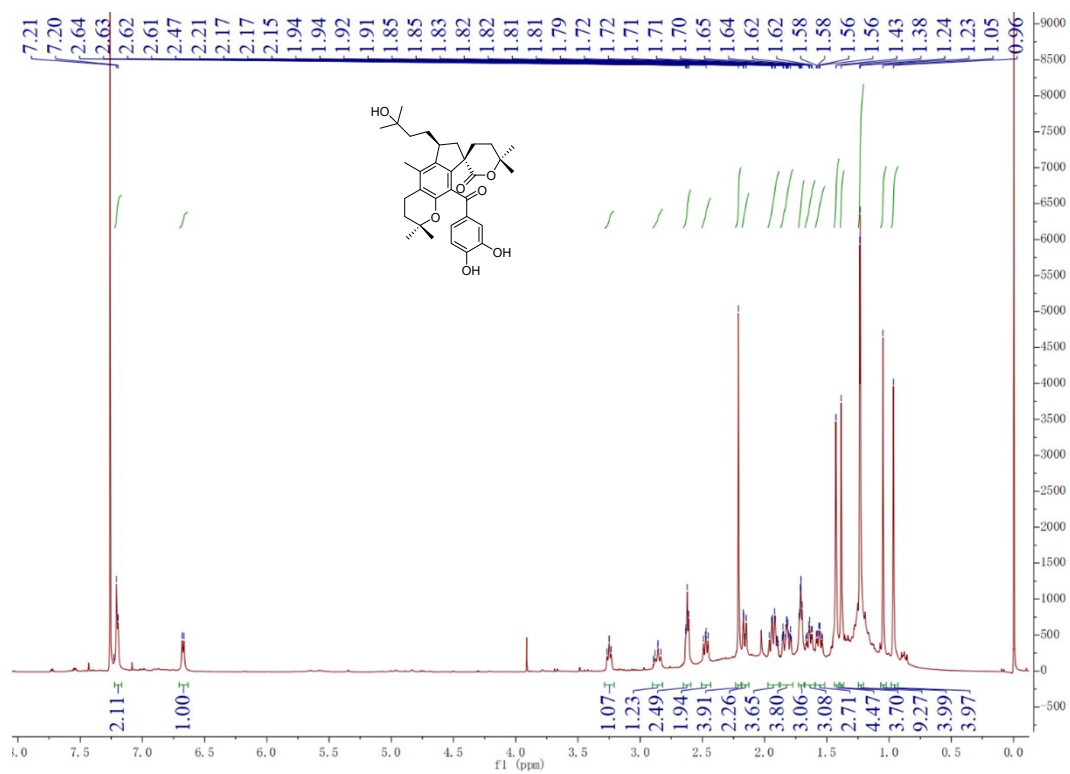
Fig. S12. The ¹H NMR spectrum of 2 (600 MHz, CDCl₃).

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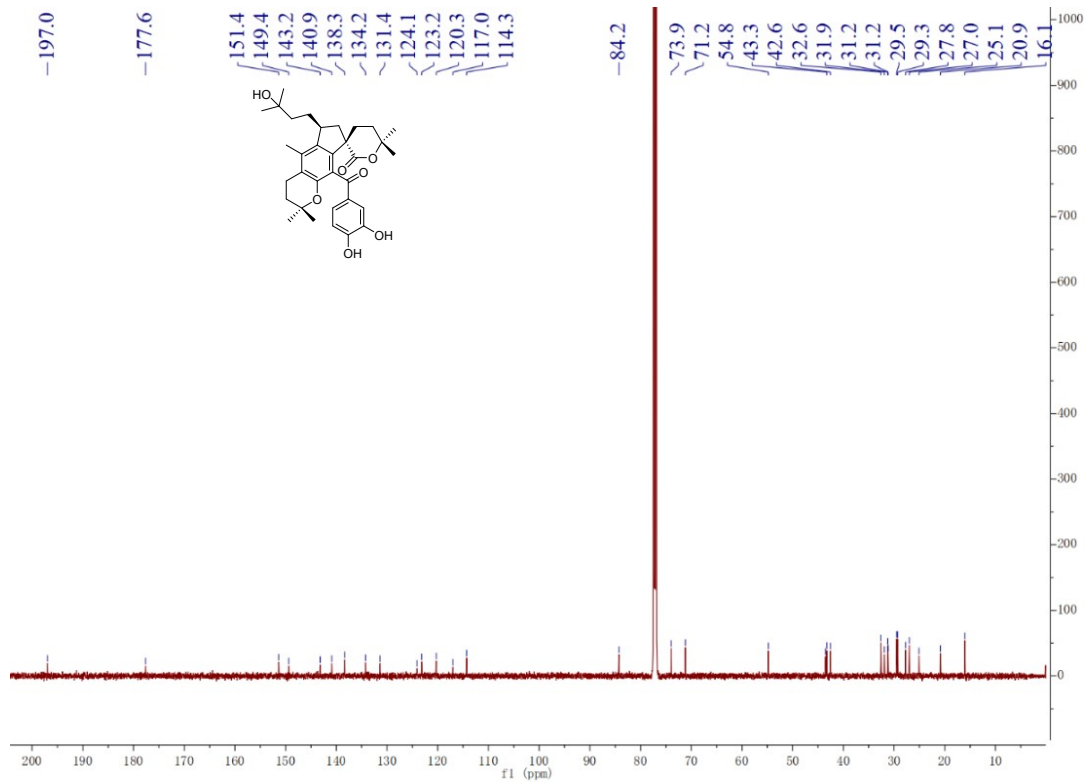
Fig. S13. The ^{13}C NMR spectrum of 2 (150 MHz, CDCl$_3$).
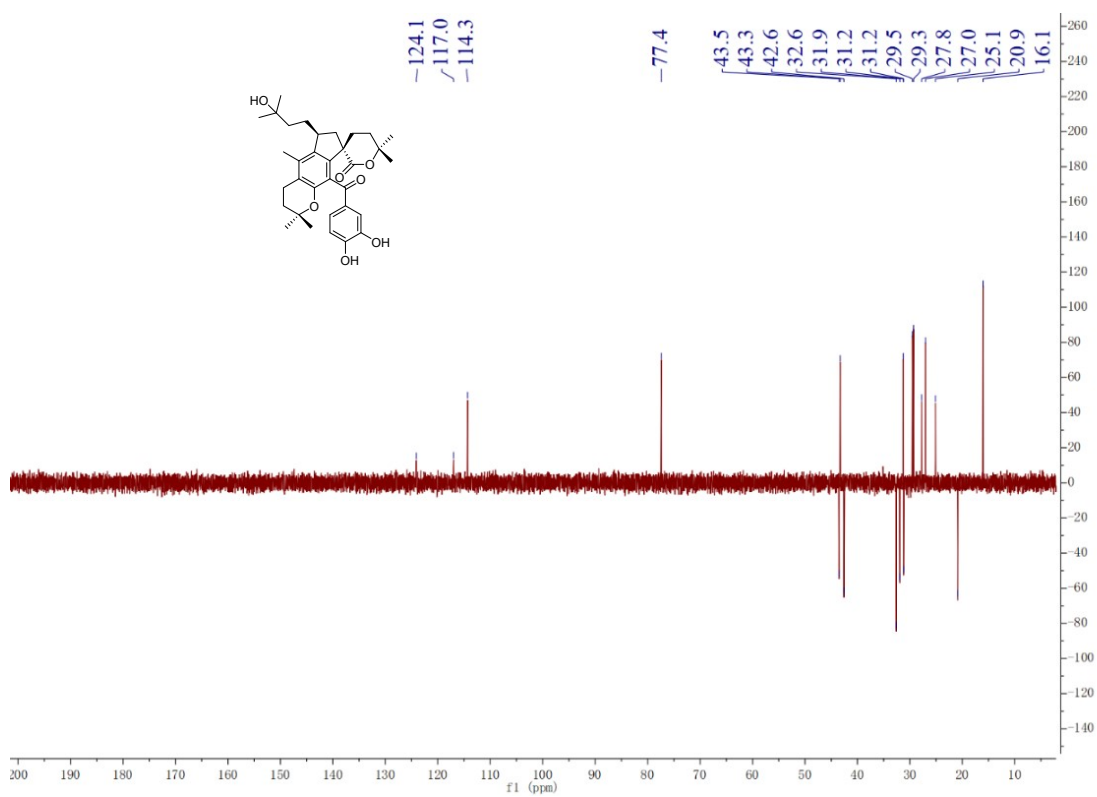
Fig. S14. The DEPT135 spectrum of 2 (600 MHz, CDCl$_3$).
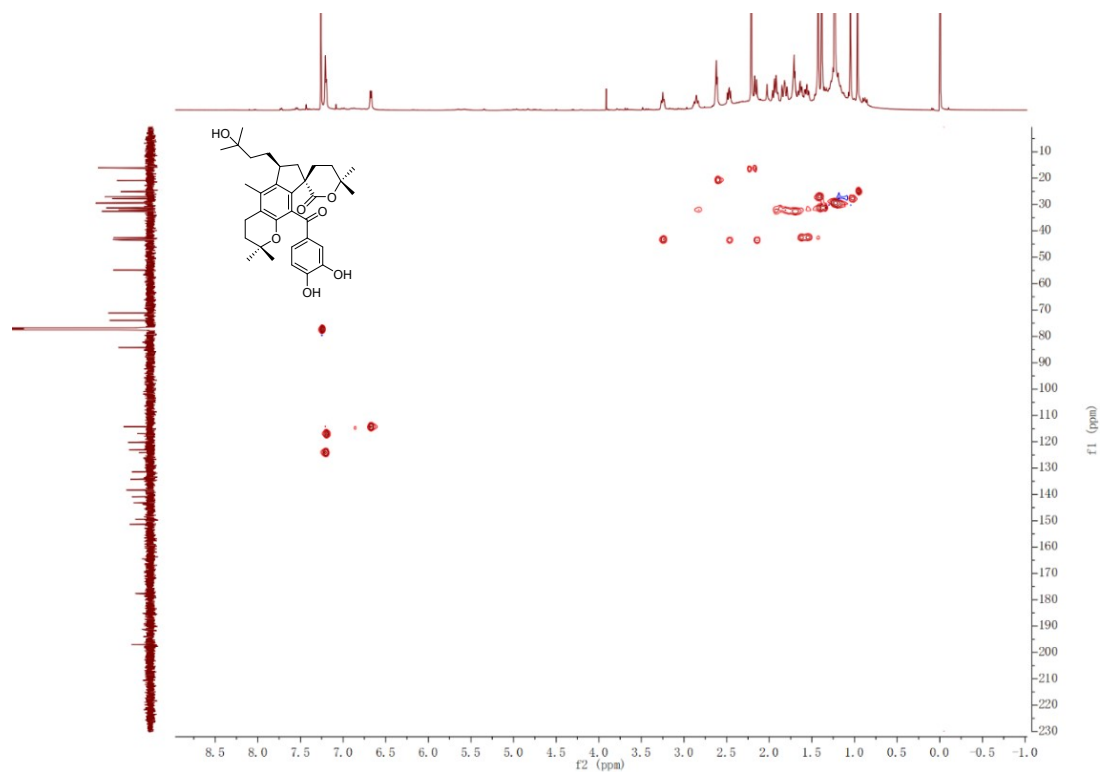
Fig. S15. The HSQC spectrum of 2 (600 MHz, CDCl₃).
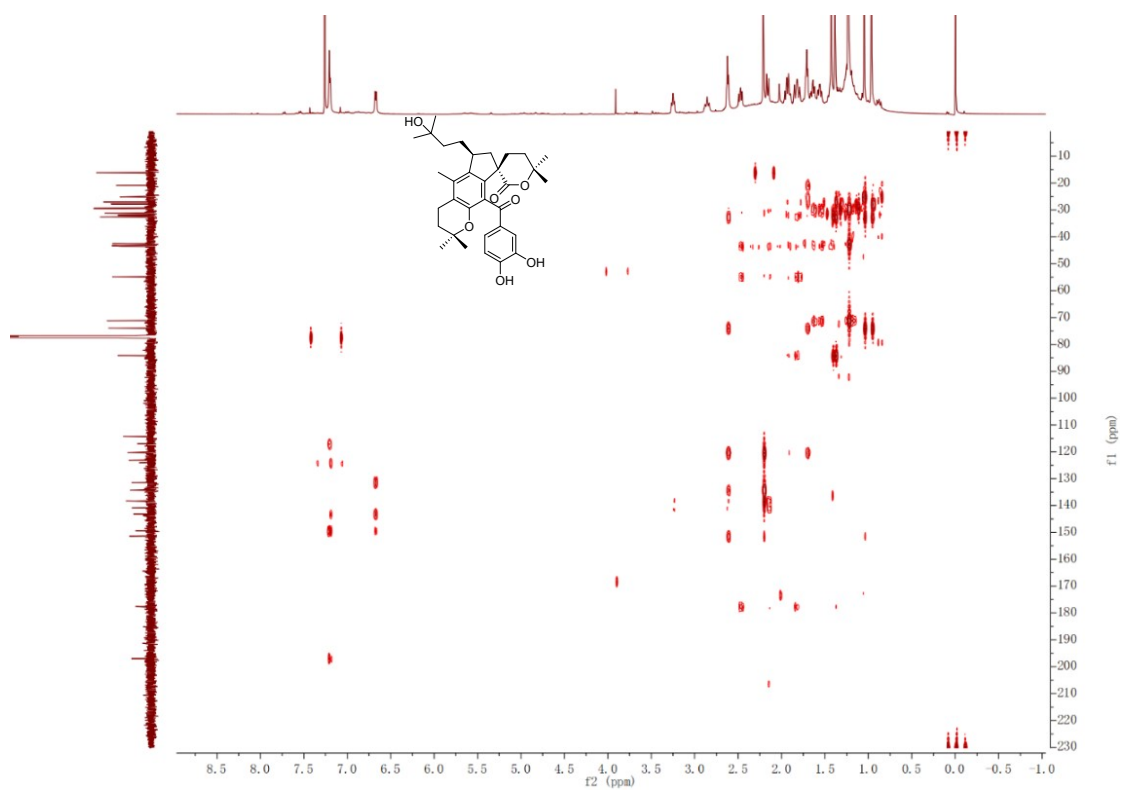
Fig. S16. The HMBC spectrum of 2 (600 MHz, CDCl₃).

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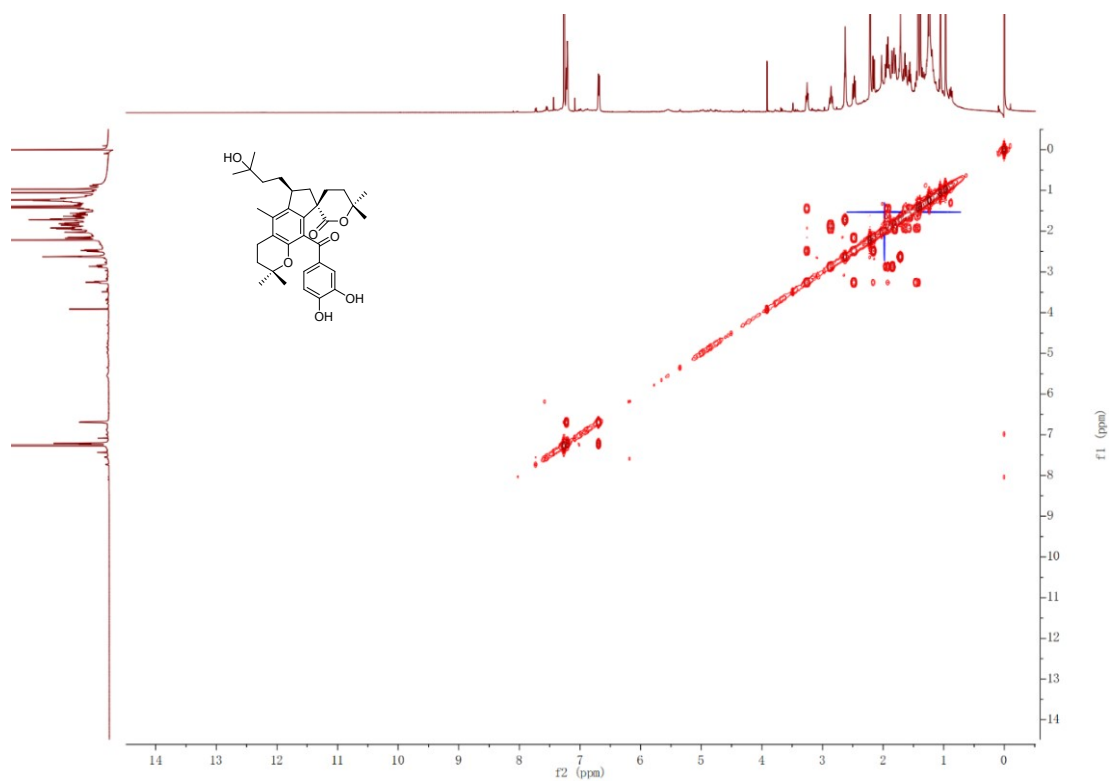
Fig. S17. The ¹H–¹H COSY spectrum of 2 (600 MHz, CDCl₃).
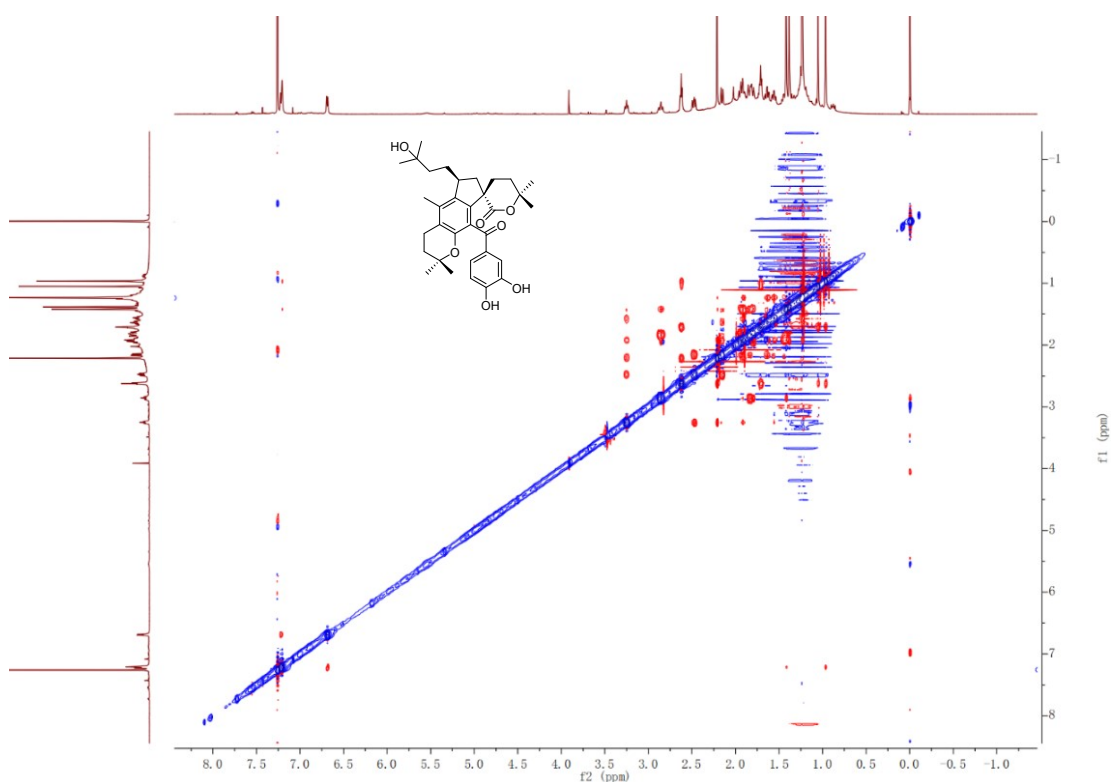
Fig. S18. The ROESY spectrum of 2 (600 MHz, CDCl₃).

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compound NO. : MZZ-64

Method : LCMS(compound)-low

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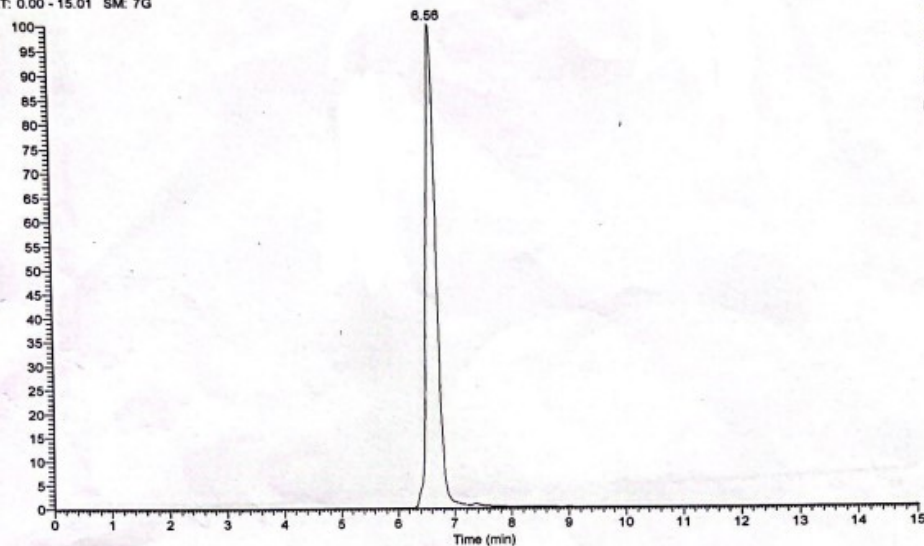
NL: 2.41E9
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551.30177 F: FTMS
+ p ESI Full ms
[100.0000-
1500.0000] MS
MZZ-64

MZZ-64 #661 RT: 6.58 AV: 1 NL: 2.52E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]
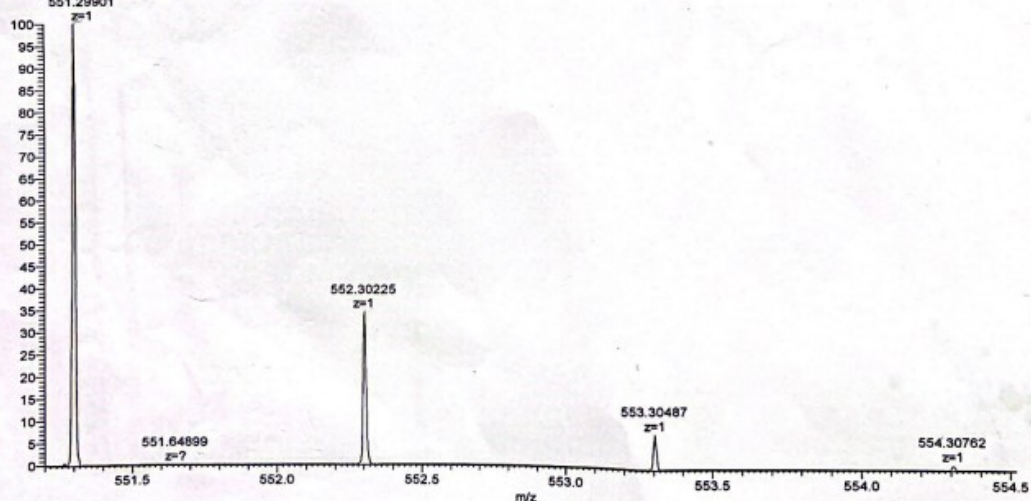
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
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Fig. S19. The HR-ESI-MS spectrum of 2.

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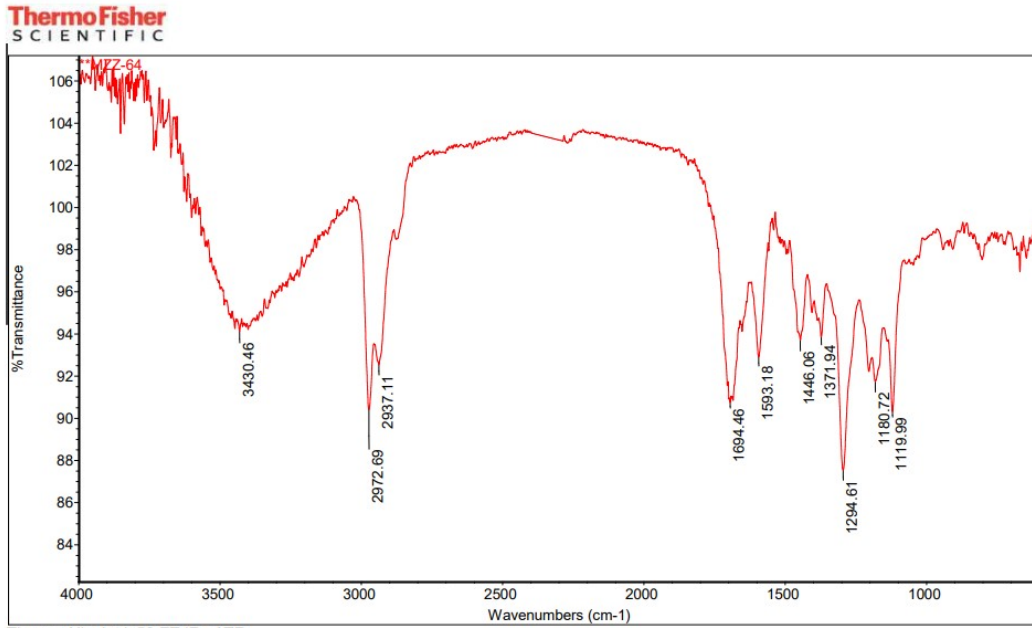
Fig. S20. The IR spectrum of 2.
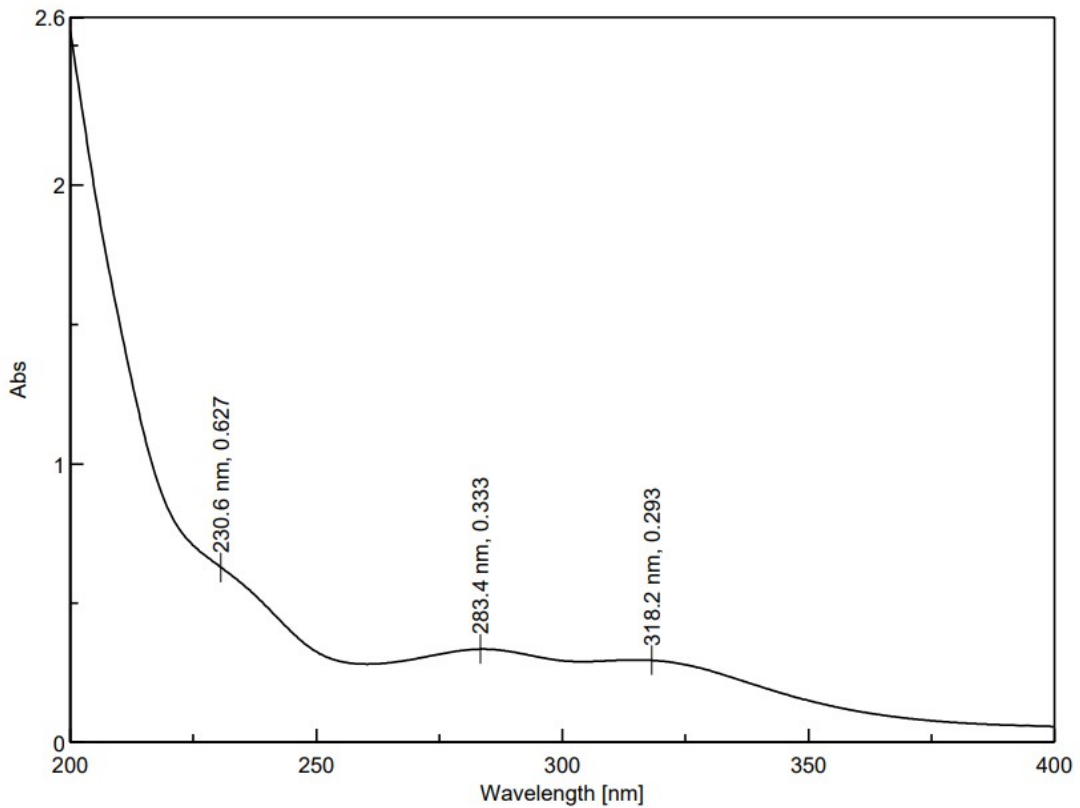
Fig. S21. The UV spectrum of 2.
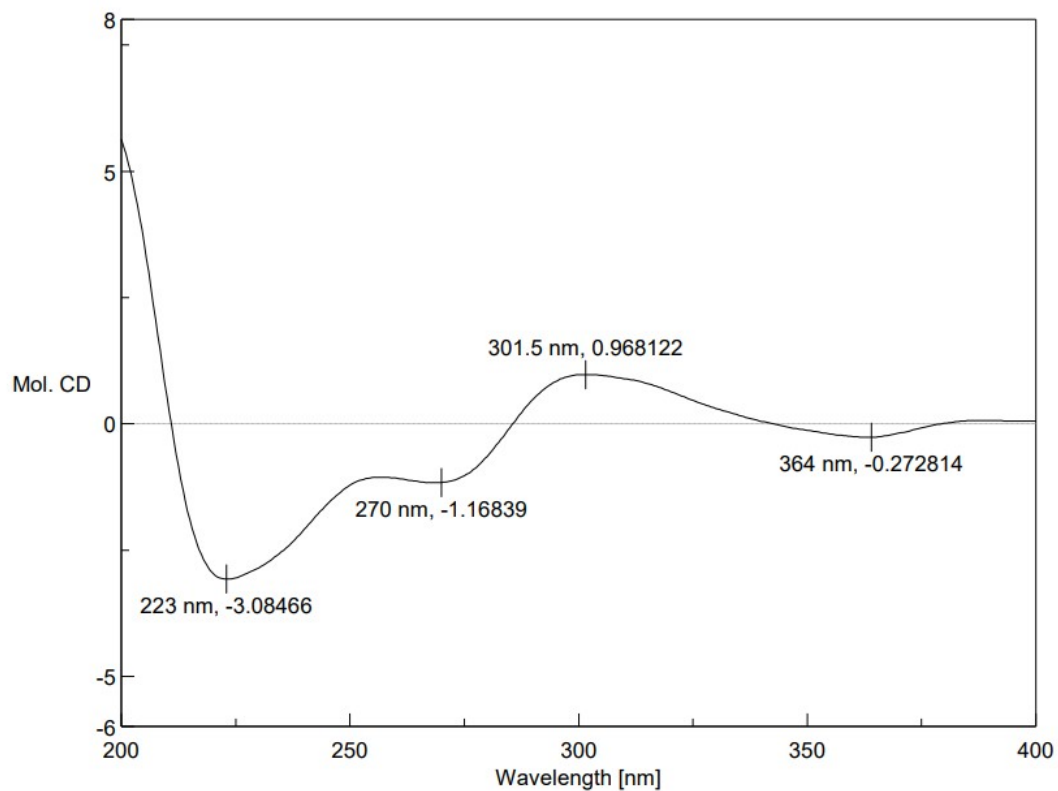
Fig. S22. The experimental ECD spectrum of 2 in CH$_3$OH.
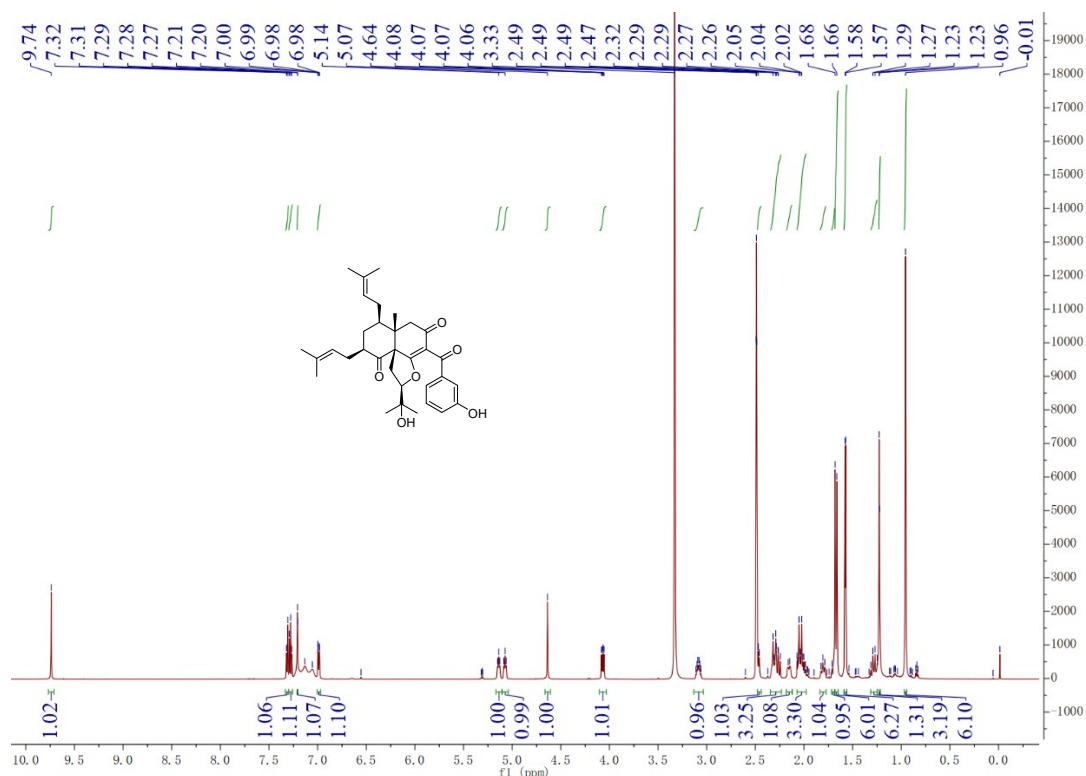
Fig. S23. The ^{1}H NMR spectrum of 3 (600 MHz, DMSO-d_6).
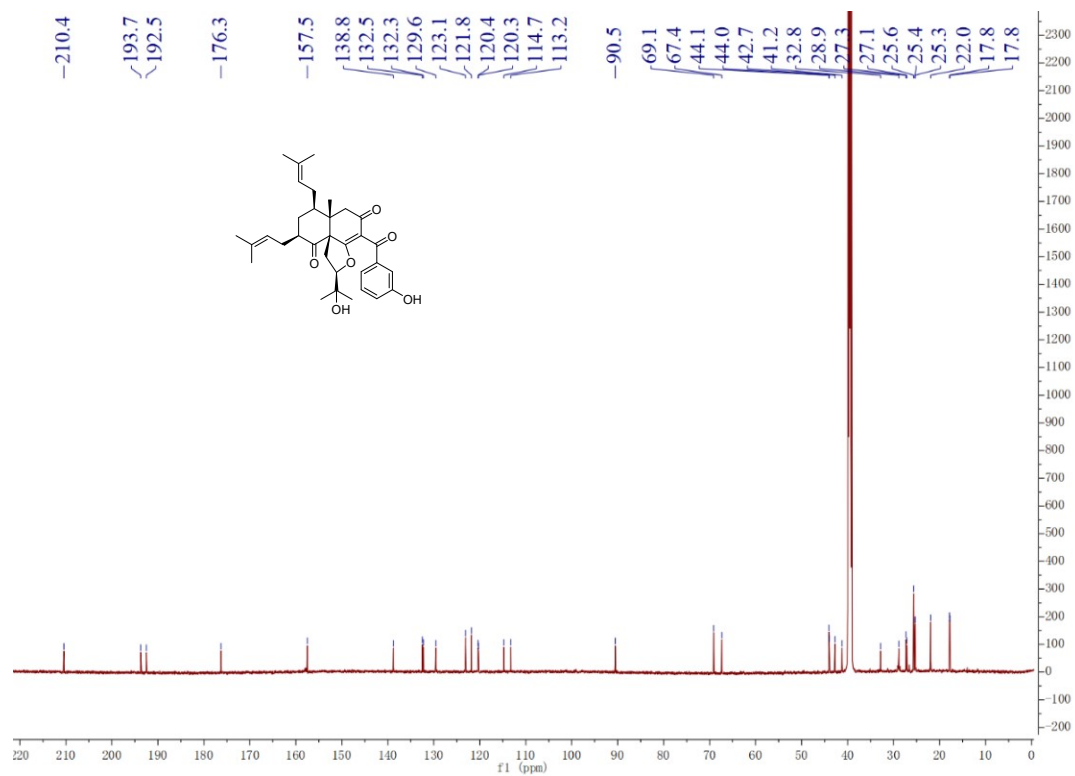
Fig. S24. The ¹³C NMR spectrum of 3 (150 MHz, DMSO-d_6).
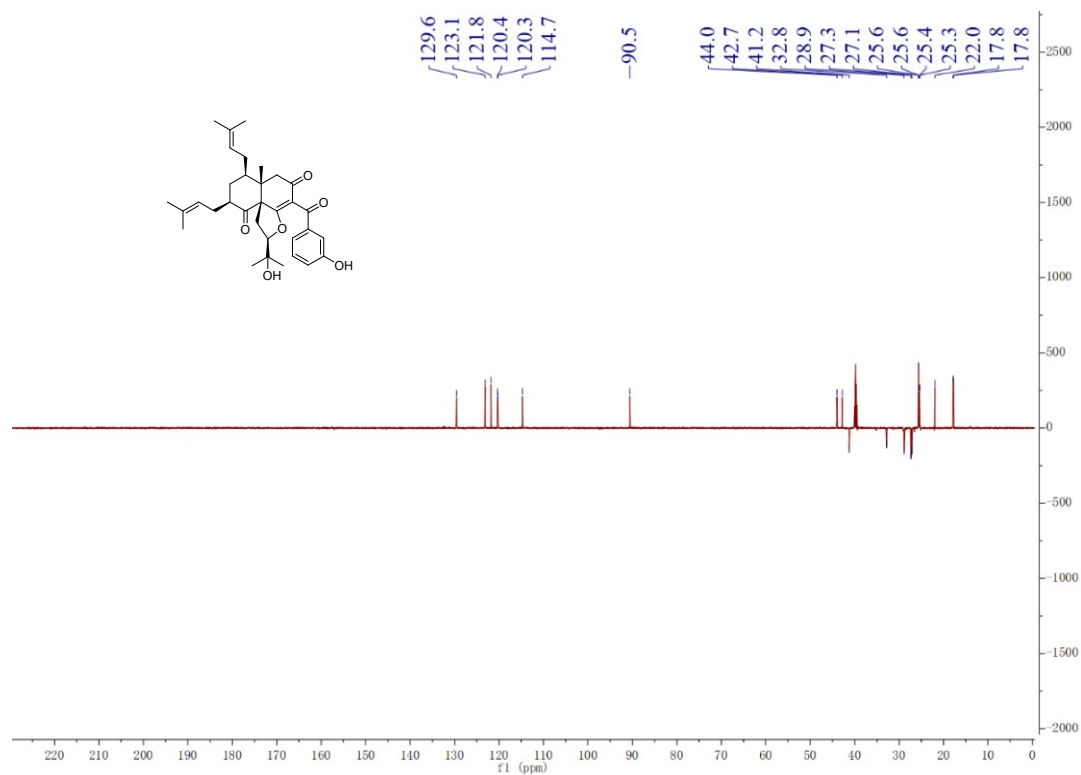
Fig. S25. The DEPT135 spectrum of 3 (600 MHz, DMSO-d_6).
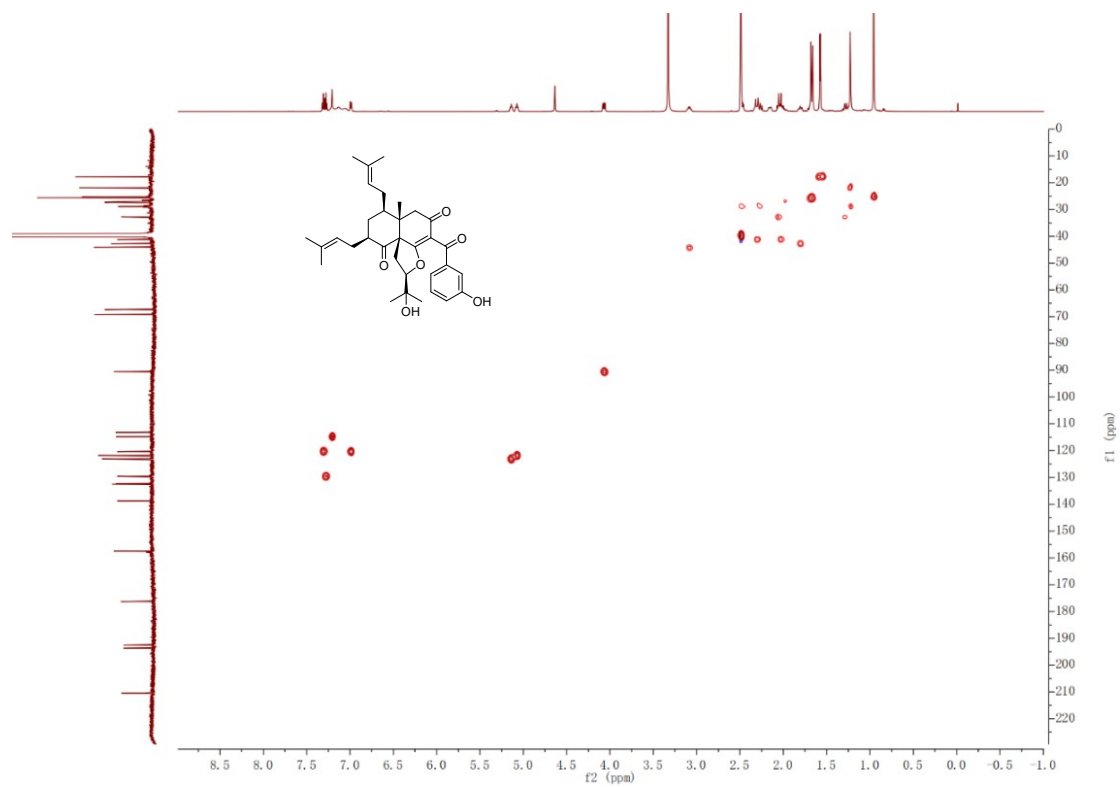
Fig. S26. The HSQC spectrum of 3 (600 MHz, DMSO-*d*₆).
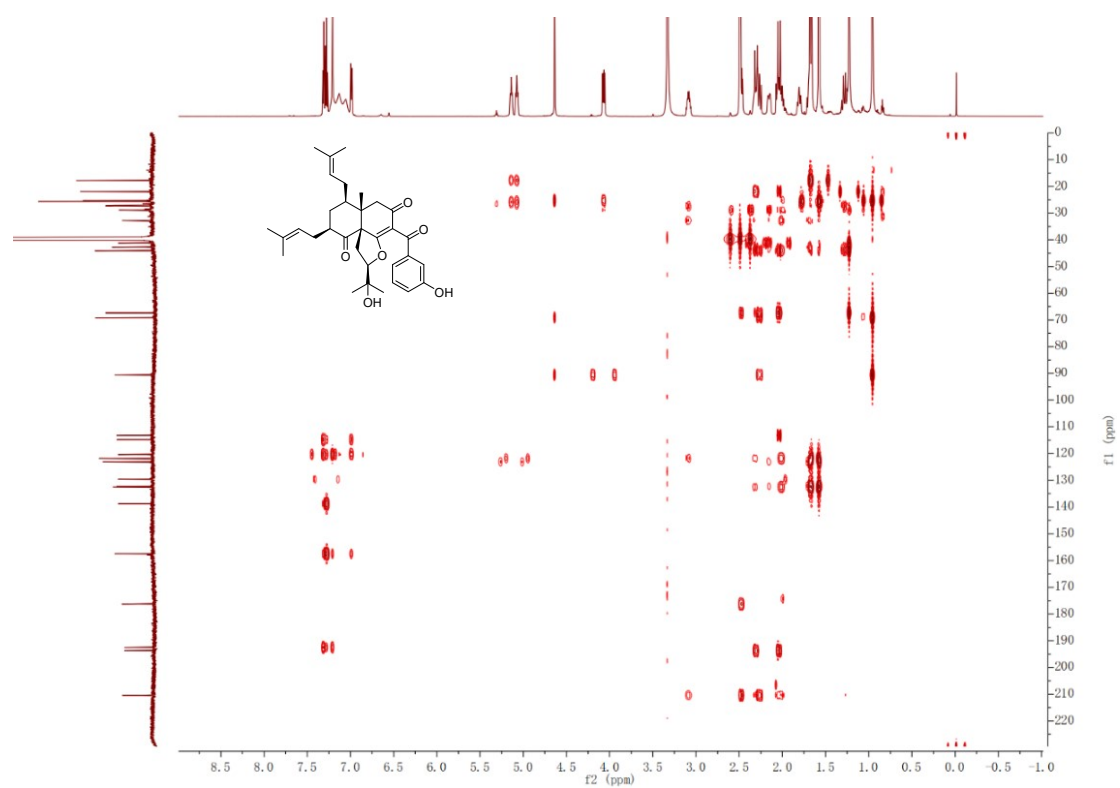
Fig. S27. The HMBC spectrum of 3 (600 MHz, DMSO-*d*₆).
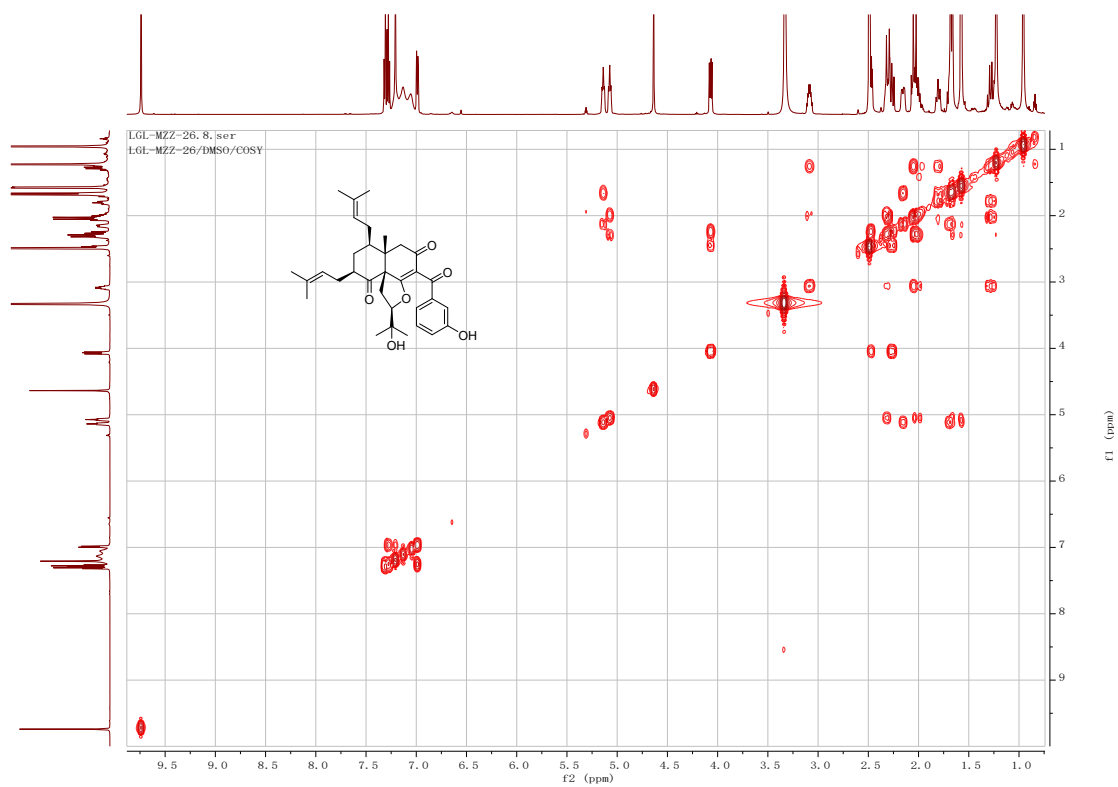
Fig. S28. The ^{1}H-^{1}H COSY spectrum of 3 (600 MHz, DMSO-d_6).
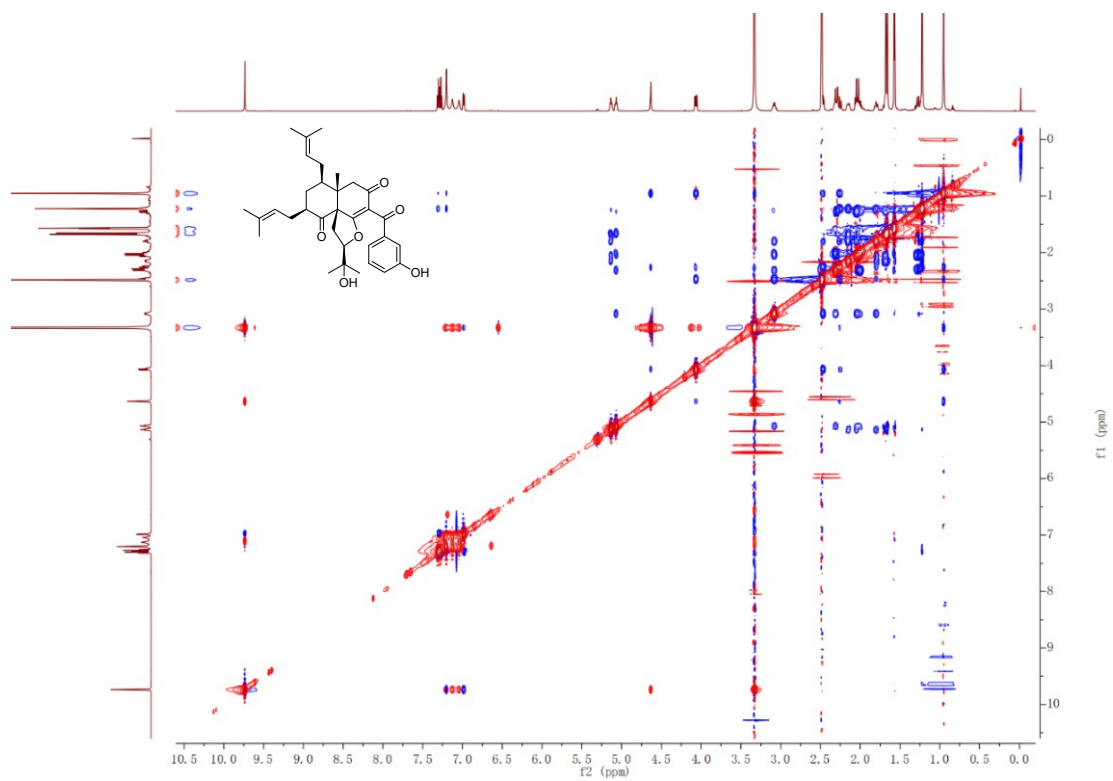
Fig. S29. The ROESY spectrum of 3 (600 MHz, DMSO-d_6).

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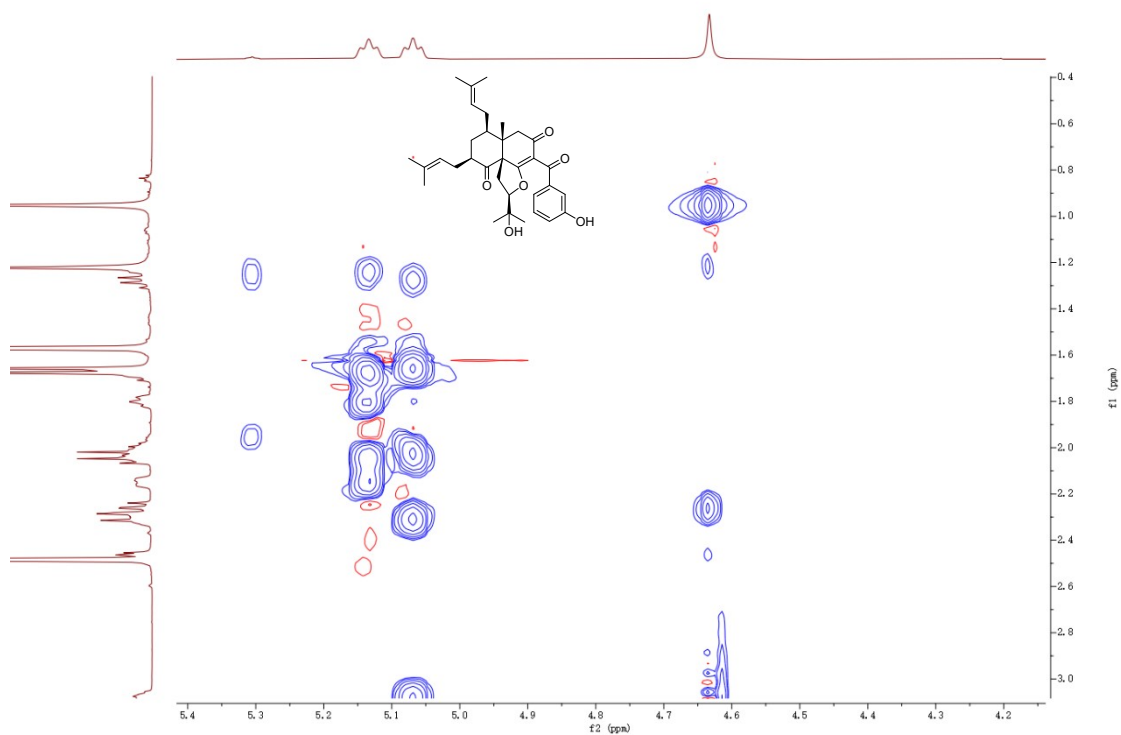
Fig. S30. The ROESY spectrum (OH-18/H$_2$-16) of 3 (600 MHz, DMSO-d_6).

compound NO. : MII-26
Method : LCMS(compound)-low

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NL: 3.19E9
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535.30611 F: FTMS
+ p ESI Full ms
[100.0000-
1500.0000] MS
MII-26

7.43

6.04 7.26 7.95 8.63 9.23 10.43 11.82 12.29 13.00 13.45 14.50

Time (min)

MII-26 #761 RT: 7.43 AV: 1 NL: 3.29E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

535.30450
z=1

536.30780
z=1

537.31067
z=1

m/z
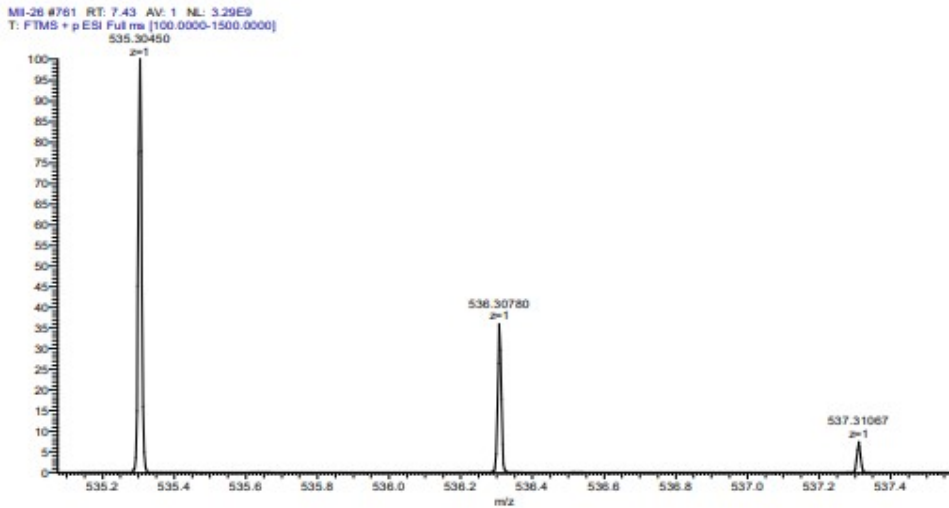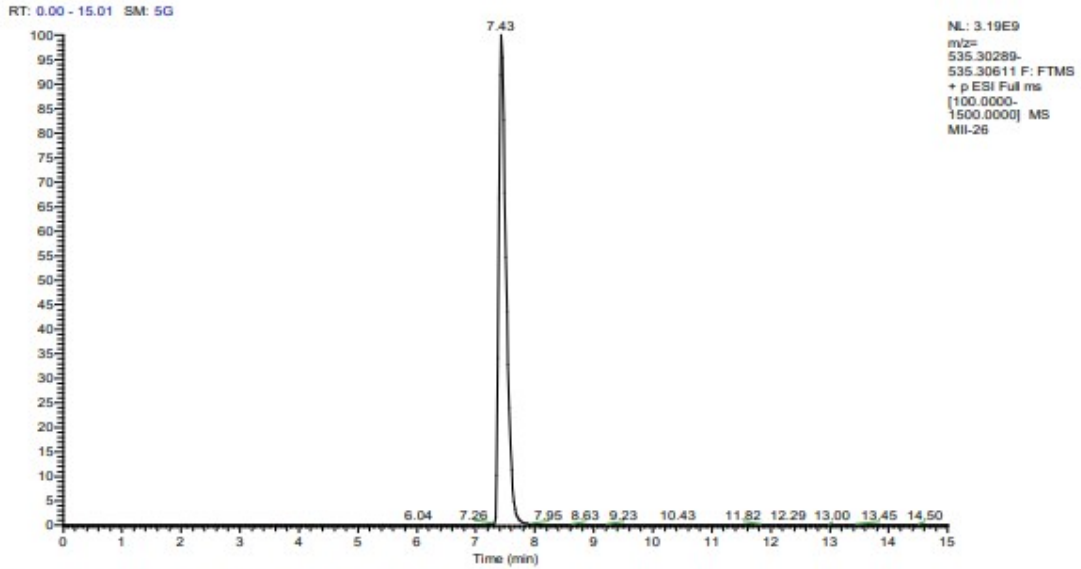
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
535.30450	535.30542	-1.71	12.5	C33 H43 O6	M+H

Fig. S31. The HR-ESI-MS spectrum of 3.

23
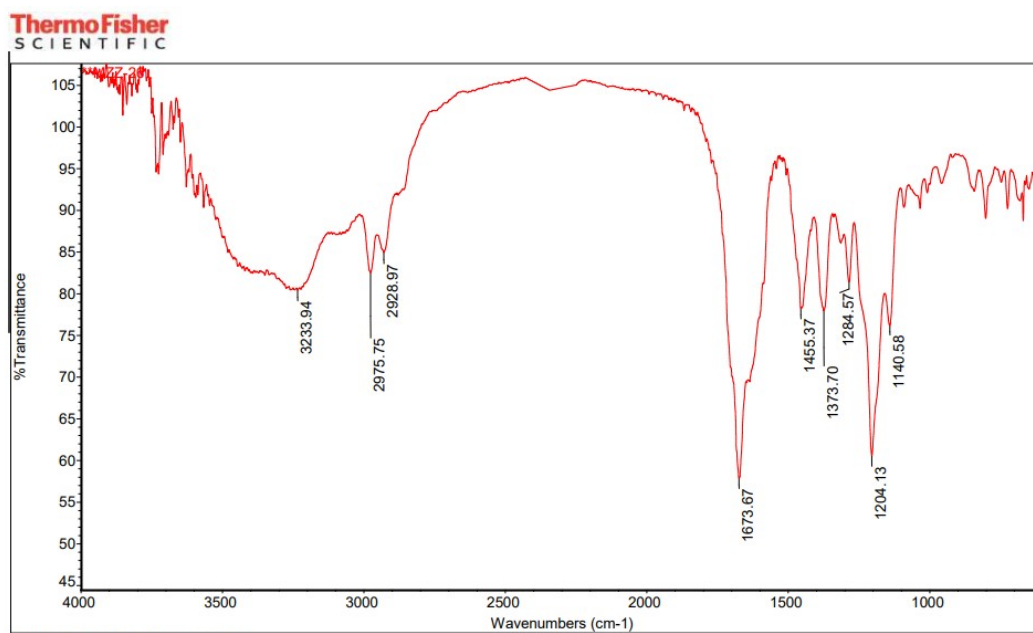
Fig. S32. The IR spectrum of 3.
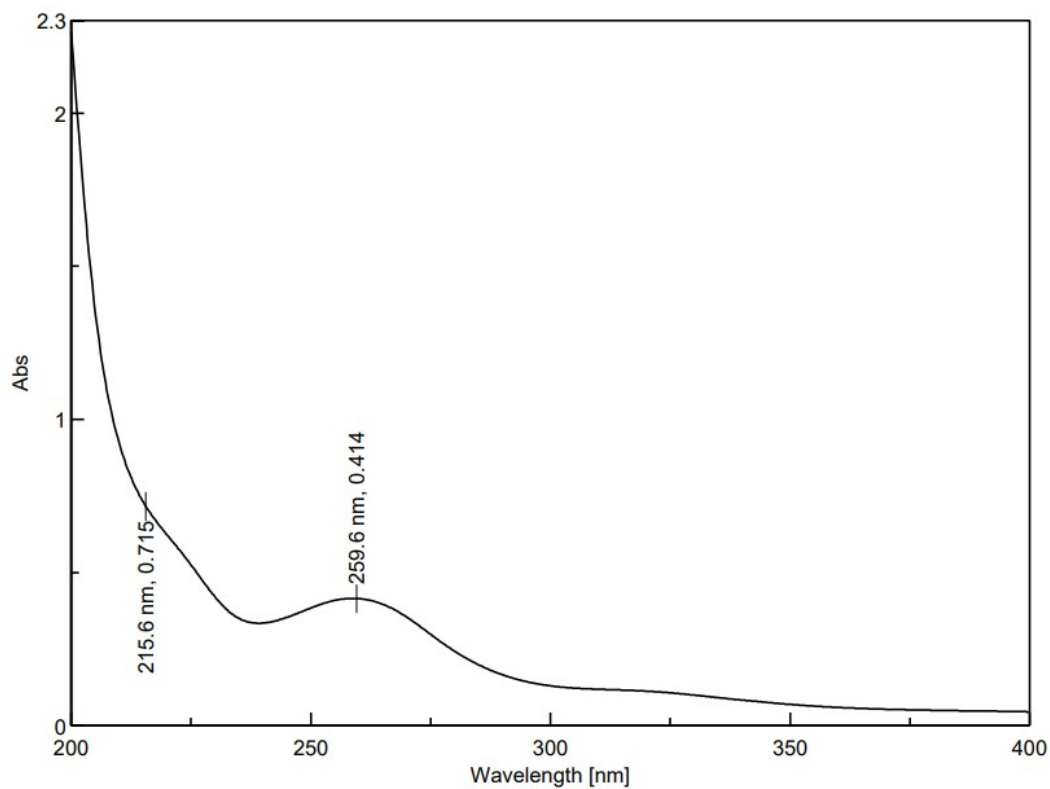
Fig. S33. The UV spectrum of 3.
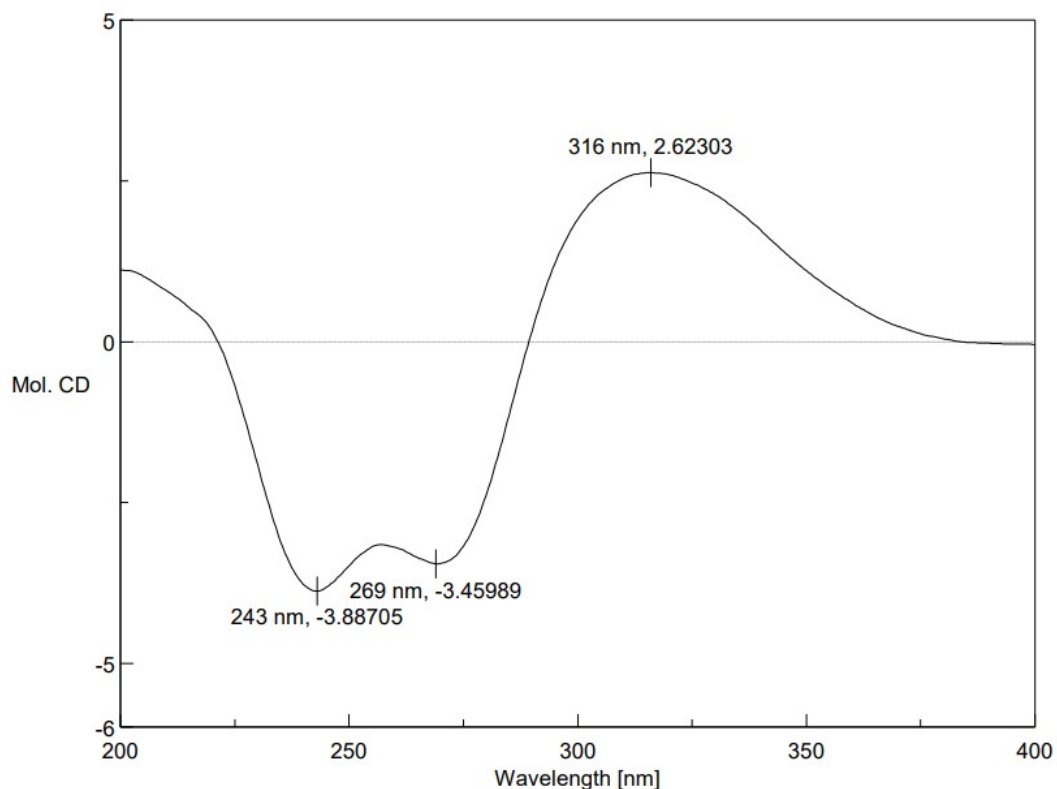
Fig. S34. The experimental ECD spectrum of 3 in CH₃OH.

(**1***R*,3*S*,5*S*,6*R*,10*R*)-**1**   (1*S*,3*S*,5*S*,6*R*,10*R*)-1
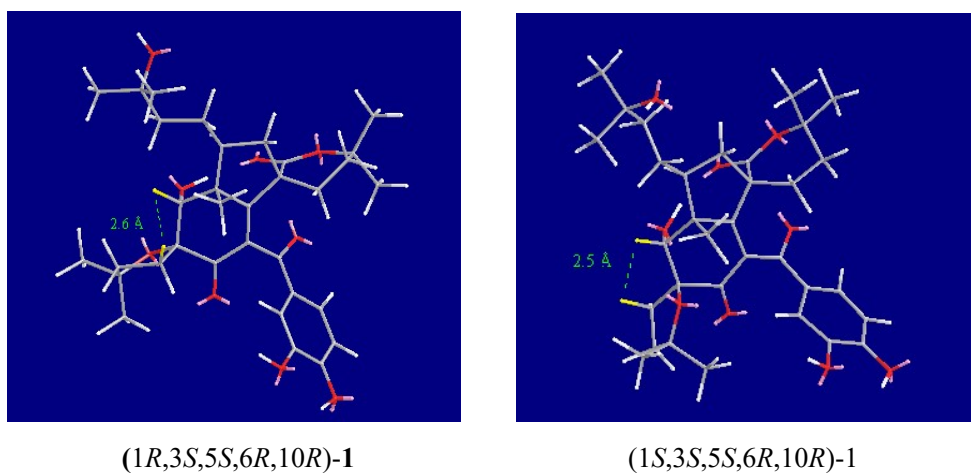
Fig. S35. Space distance measurement in ChemBio 3D.

ECD calculation method

In consideration of the nature of the structure, the structures of compounds **1** and **3** were simplified (**Fig. S36**). The CONFLEX searches based on molecular mechanics with MMFF94S force fields were performed for compounds **1a** and **3a**, which gave a series of stable conformers.[1] The conformers with Boltzmann-population of over 1% were further optimized by the DFT (density

functional theory) method at the B3LYP/6-31g (d) level in Gaussian 16 program package.[2] The ECD of the conformer of selected conformers was then calculated by the TD-DFT (time-dependent density functional theory) method at the M062X/6-31+g(d,p) level for compound **1a** and the PBE1PBE/6-31+g(d,p) level for compound **3a** with the SMD model in methanol solution, respectively. The calculated ECD curve was generated using SpecDis 1.71.[3]

(3*S*, 5*S*)-**2** was chosen for theoretical study. Conformational analyses were firstly carried out via Monte Carlo searching using molecular mechanism with MMFF force field in the *Spartan 18* program.[4] Within an energy window of 2 Kcal/mol, the result showed 17 lowest energy conformers for (3*S*, 5*S*)-**2**, those conformers were then reoptimized using DFT at the B3LYP/6-31G(d) level in the *Gaussian 09* program.[5] The B3LYP/6-31G(d) harmonic vibrational frequencies were further calculated to confirm their stability, 10 conformers for (3*S*, 5*S*)-**2**, whose relative Gibbs free energies ranged within 0-2 Kcal/mol, were harvested and subjected to next steps.

The electronic excitation energies and rotatory strengths (velocity) of the first 60 excited states of these conformers were calculated using the TDDFT methodology at the M062X/TZVP level in methanol. The ECD spectra were simulated by the overlapping Gaussian function ($\sigma = 0.3$ eV, $-$ 15 nm shifted in wavelength),[6] in which velocity rotatory strengths of the first 8 exited states was adopted. To get the final ECD spectra, the simulated spectra of the lowest energy conformers were averaged according to the Boltzmann distribution theory and their relative Gibbs free energy (ΔG). The theoretical ECD curves of (3*R*, 5*R*)-**2** obtained by directly reversing that of (3*S*, 5*S*)-**2**. Compared to the experimental ECD curve of **2** in the 200–400 nm region, the calculated ECD curve for (3*S*, 5*S*)-**2** showed similar trends.
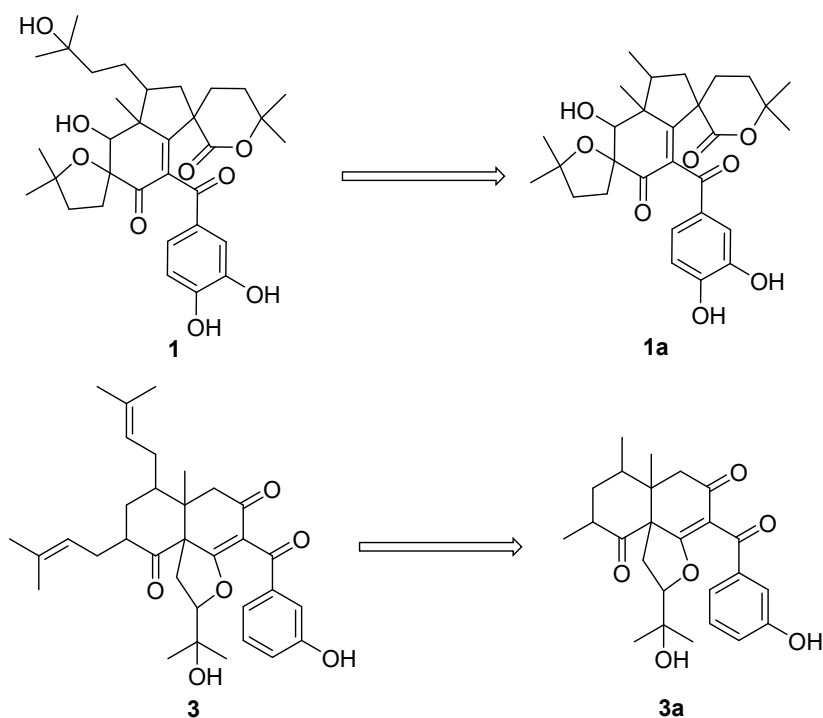
Fig. S36. Simplification of calculation structures.
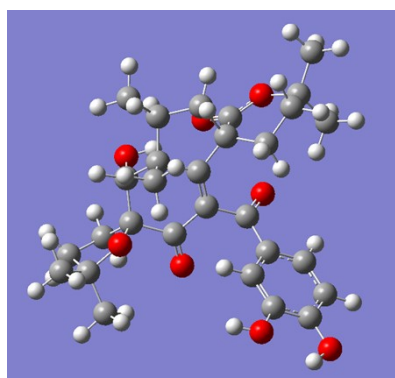
Conf (1*S*,2*S*,5*S*,6*R*,10*R*)-1a1 (50.02%)   Conf (1*S*,2*S*,5*S*,6*R*,10*R*)-1a2 (49.98%)
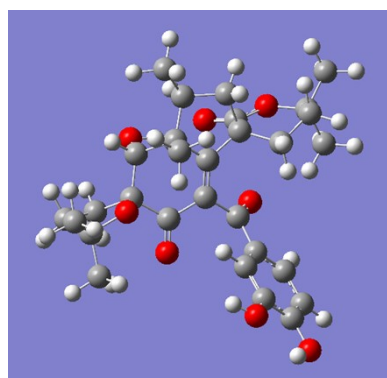
Fig. S37. DFT-optimized structures for low-energy conformers and Boltzmann distributions of compound (1*S*,2*S*,5*S*,6*R*,10*R*)-1a [(1*S*,2*S*,5*S*,6*R*,10*R*)-1a1–(1*S*,2*S*,5*S*,6*R*,10*R*)-1a2].

Table S2. The Cartesian coordinates for the lowest-energy conformer of (1*S*,2*S*,5*S*,6*R*,10*R*)-1a1 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	1.38180000	-2.51662200	-0.30582800
2	C	2.30706500	-1.33260300	-0.70657000
3	C	1.50969500	-0.02050100	-0.93351000
4	C	0.11492900	0.08687400	-0.42397600
5	C	-0.46309400	-0.92864900	0.26137500
6	C	0.34304700	-2.11907500	0.77541900
7	C	-0.67233000	1.29028800	-0.90373700
8	C	-0.26965800	2.64962900	-0.46954000
9	O	2.01671700	0.90805700	-1.54931600

10	O	3.21102400	-1.04768500	0.38632800
11	C	4.60531400	-1.16108100	-0.02218900
12	C	4.54228000	-2.05159800	-1.27510400
13	C	3.20154500	-1.67325900	-1.91771700
14	C	5.35268700	-1.80376200	1.14594200
15	C	5.15255200	0.24106000	-0.32229600
16	O	-1.66661200	1.11395700	-1.60451400
17	C	-0.96107800	3.75432200	-0.99167200
18	C	-0.64682000	5.04755300	-0.59039400
19	C	0.36615400	5.25720700	0.34661000
20	C	1.06098900	4.15279900	0.87815500
21	C	0.74725200	2.86559800	0.47977700
22	C	-1.95683500	-1.11812000	0.55757400
23	C	-1.98240600	-2.42974000	1.41653700
24	C	-0.73677900	-3.22545000	1.00227000
25	C	-2.63235900	-1.49511500	-0.77695600
26	O	-3.94918500	-1.29214800	-0.92246000
27	C	-4.77933200	-0.39730800	-0.09516900
28	C	-4.18185500	-0.22568400	1.30944500
29	C	-2.67518000	0.04054300	1.27596000
30	C	1.00524200	-1.72530200	2.12124600
31	C	-0.37034600	-4.35346800	1.96939500
32	O	-2.04022400	-2.11311900	-1.64335500
33	O	0.68234600	6.51528200	0.74074800
34	O	0.75056100	-3.05633200	-1.45788100
35	O	2.03296800	4.47658100	1.80057500
36	C	-6.13412800	-1.10387500	-0.03139700
37	C	-4.89042500	0.92485900	-0.86176800
38	H	2.02950900	-3.30999800	0.08805400
39	H	4.54749200	-3.10829600	-0.98097100
40	H	5.39265700	-1.88926500	-1.94511600
41	H	2.75979300	-2.47275800	-2.51348400
42	H	3.30788500	-0.78821700	-2.54916700
43	H	5.28963900	-1.17432600	2.04045000
44	H	4.92651900	-2.78368300	1.38435700
45	H	6.41197500	-1.93642900	0.89775300
46	H	4.58598500	0.72223500	-1.12390500
47	H	5.07429300	0.87102700	0.57119200
48	H	6.20875300	0.19177800	-0.61264500
49	H	-1.74131400	3.57681400	-1.72347800
50	H	-1.16624300	5.91033400	-0.99498400
51	H	1.29509300	2.02706200	0.89965000
52	H	-1.93551800	-2.15502900	2.47905500
53	H	-2.90327900	-3.00495900	1.27670900
54	H	-0.93679300	-3.68029300	0.02948300
55	H	-4.70239200	0.60175700	1.80537200
56	H	-4.38656200	-1.12553000	1.90257000
57	H	-2.47943900	0.99400400	0.78261700
58	H	-2.28375800	0.12457800	2.29657000
59	H	1.63660100	-2.54069400	2.48811400
60	H	1.63727000	-0.84513600	2.01376900
61	H	0.24473500	-1.51816700	2.88292100
62	H	-1.16762700	-5.10563500	1.98759000
63	H	0.54872200	-4.86250900	1.65681500
64	H	-0.22892900	-3.99759600	2.99590900
65	H	1.42806600	6.44825900	1.36338500
66	H	-0.09908600	-2.59858800	-1.62677800
67	H	2.58167500	3.69885500	1.98268800
68	H	-6.53521800	-1.25397700	-1.03821900
69	H	-6.04072200	-2.08175700	0.45221800

Number	Atom	X	Y	Z
70	H	-6.84742800	-0.50010200	0.54045700
71	H	-5.56509200	1.60902400	-0.33424600
72	H	-3.91725700	1.40483100	-0.98705300
73	H	-5.29831500	0.73850500	-1.85992200

Table S3. The Cartesian coordinates for the lowest-energy conformer of (1*S*,2*S*,5*S*,6*R*,10*R*)-1a2 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	1.37942900	-2.51808900	-0.30511200
2	C	2.30562700	-1.33499700	-0.70661200
3	C	1.50935700	-0.02245800	-0.93443800
4	C	0.11498200	0.08660300	-0.42432300
5	C	-0.46397300	-0.92807900	0.26147900
6	C	0.34096000	-2.11916600	0.77593800
7	C	-0.67091200	1.29084600	-0.90439400
8	C	-0.26702600	2.64967500	-0.46965200
9	O	2.01679000	0.90512800	-1.55138300
10	O	3.20971700	-1.05006000	0.38622900
11	C	4.60396800	-1.16412800	-0.02233600
12	C	4.54050600	-2.05568000	-1.27448900
13	C	3.19995500	-1.67725500	-1.91744100
14	C	5.35123900	-1.80599600	1.14631600
15	C	5.15161400	0.23758500	-0.32367600
16	O	-1.66500700	1.11564000	-1.60568500
17	C	-0.95787000	3.75515200	-0.99086700
18	C	-0.64236400	5.04797000	-0.58920200
19	C	0.37139600	5.25643500	0.34721200
20	C	1.06573700	4.15123800	0.87777800
21	C	0.75069900	2.86444200	0.47910400
22	C	-1.95788400	-1.11600900	0.55766100
23	C	-1.98480000	-2.42723200	1.41711500
24	C	-0.74003900	-3.22435800	1.00301300
25	C	-2.63367600	-1.49298700	-0.77674600
26	O	-3.95072900	-1.29016900	-0.92160100
27	C	-4.77979800	-0.39336200	-0.09534700
28	C	-4.18216700	-0.22111000	1.30910800
29	C	-2.67524400	0.04367300	1.27538500
30	C	1.00349100	-1.72565200	2.12168700
31	C	-0.37479400	-4.35258200	1.97035400
32	O	-2.04194800	-2.11106500	-1.64332100
33	O	0.68879600	6.51407200	0.74173100
34	O	0.74766300	-3.05814100	-1.45669300
35	O	2.03864400	4.47390100	1.79960000
36	C	-6.13548800	-1.09815800	-0.03100600
37	C	-4.88923900	0.92818100	-0.86330100
38	H	2.02664600	-3.31168800	0.08909900
39	H	4.54516900	-3.11212000	-0.97942300
40	H	5.39096100	-1.89432600	-1.94463000
41	H	2.75781000	-2.47712600	-2.51242300
42	H	3.30671500	-0.79289400	-2.54977100
43	H	6.41044400	-1.93925100	0.89813700
44	H	5.28847800	-1.17571000	2.04024300
45	H	4.92474000	-2.78553600	1.38568300
46	H	5.07349400	0.86837400	0.56924300
47	H	6.20781300	0.18765800	-0.61389200
48	H	4.58530300	0.71826600	-1.12575600
49	H	-1.73867900	3.57856900	-1.72228500
50	H	-1.16145700	5.91131600	-0.99300500

51	H	1.29817400	2.02531100	0.89824000
52	H	-1.93752700	-2.15214800	2.47952100
53	H	-2.90629000	-3.00150000	1.27751900
54	H	-0.94049000	-3.67917400	0.03029100
55	H	-4.70184800	0.60729400	1.80433200
56	H	-4.38775100	-1.12024500	1.90300700
57	H	-2.47867700	0.99665500	0.78145400
58	H	-2.28368500	0.12800900	2.29592000
59	H	1.63408100	-2.54153600	2.48876700
60	H	1.63634400	-0.84611300	2.01398700
61	H	0.24319700	-1.51756600	2.88330900
62	H	0.54366400	-4.86272000	1.65778700
63	H	-0.23287700	-3.99662700	2.99676400
64	H	-1.17291400	-5.10384500	1.98881600
65	H	1.43467800	6.44622600	1.36408300
66	H	-0.10090100	-2.59877800	-1.62659400
67	H	2.58584600	3.69525400	1.98227000
68	H	-6.04341800	-2.07563100	0.45368500
69	H	-6.84813600	-0.49285900	0.54002500
70	H	-6.53653800	-1.24886300	-1.03775500
71	H	-5.29717700	0.74125300	-1.86132500
72	H	-5.56317800	1.61367000	-0.33658300
73	H	-3.91551900	1.40693500	-0.98898800
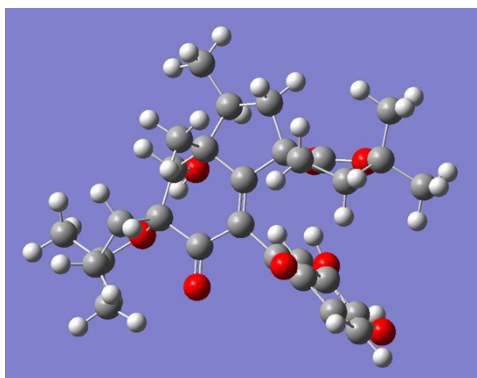
Conf (1*R*,2*S*,5*S*,6*R*,10*R*)-1a1 (99.90%)

Fig. S38. DFT-optimized structures for low-energy conformers and Boltzmann distributions of compound (1*R*,2*S*,5*S*,6*R*,10*R*)-1a [(1*R*,2*S*,5*S*,6*R*,10*R*)-1a1].

Table S4. The Cartesian coordinates for the lowest-energy conformer of (1*R*,2*S*,5*S*,6*R*,10*R*)-1a1 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-2.35575700	-1.33340600	0.80127400
2	C	-2.87255200	-0.32662000	-0.25415400
3	C	-1.70636400	0.44497900	-0.91725300
4	C	-0.32909000	-0.10469200	-0.85691900
5	C	-0.06036300	-1.28918100	-0.26737600
6	C	-1.15677900	-2.17419500	0.31505400
7	C	0.70053300	0.79007700	-1.52714400
8	C	1.17926000	1.98357600	-0.80053500
9	O	-1.92876500	1.50196300	-1.49353600
10	O	-3.67689100	0.61314500	0.47613000
11	C	-4.93099800	0.93701200	-0.19508300
12	C	-4.80156500	0.26869200	-1.57792300
13	C	-3.81999400	-0.88757600	-1.34241800

30

14	C	-6.07068100	0.34090300	0.64035600
15	C	-5.02959400	2.45985800	-0.27354400
16	O	1.09997600	0.49452800	-2.65013500
17	C	1.99687800	2.91291700	-1.46508200
18	C	2.49203500	4.02498100	-0.79548200
19	C	2.19550700	4.20926200	0.55805500
20	C	1.38202800	3.27573100	1.22754700
21	C	0.85935600	2.18659600	0.55435000
22	C	1.32252100	-1.93985200	-0.03905700
23	C	0.97139100	-3.18103200	0.86570000
24	C	-0.40408300	-2.88409400	1.48054000
25	C	2.17462100	-1.02899900	0.87402700
26	O	3.49836700	-0.90122000	0.66901300
27	C	4.23686200	-1.52225200	-0.43880400
28	C	3.32323700	-1.60681200	-1.65978500
29	C	2.02478900	-2.36357900	-1.37320900
30	C	-1.61682200	-3.19652300	-0.75750400
31	C	-1.08975000	-4.10354000	2.09811100
32	O	1.68783100	-0.47430100	1.83816800
33	O	2.69902000	5.27514500	1.22875000
34	C	4.74529100	-2.88392600	0.04848100
35	O	-1.95646900	-0.60582900	1.95376900
36	O	1.16518100	3.54227100	2.56264300
37	H	-3.18724500	-2.01237000	1.05791800
38	H	-5.76696600	-0.07552800	-1.96294100
39	H	-4.37663000	0.97642900	-2.29424100
40	H	-4.33428600	-1.77640600	-0.95847000
41	H	-3.29931700	-1.17394100	-2.25967500
42	H	-6.01730600	0.70885600	1.67057500
43	H	-6.01507300	-0.75329000	0.66747300
44	H	-7.04529100	0.62423900	0.22643700
45	H	-5.07188600	2.89738900	0.73012100
46	H	-4.15444100	2.85832000	-0.79267000
47	H	-5.93552700	2.75921600	-0.81374700
48	H	2.22808000	2.74510000	-2.51153100
49	H	3.12177900	4.75589300	-1.29282600
50	H	0.24358300	1.46811800	1.08699300
51	H	0.93357000	-4.08358800	0.24426100
52	H	1.73049800	-3.35947200	1.63440600
53	H	-0.26509000	-2.12937600	2.25849400
54	C	5.40392500	-0.56543700	-0.68442000
55	H	3.09603200	-0.59318800	-2.00193900
56	H	3.86235900	-2.10198300	-2.47655700
57	H	1.33984100	-2.20773000	-2.21057900
58	H	2.23201000	-3.43835900	-1.32916400
59	H	-1.91120800	-2.70401700	-1.68615700
60	H	-0.81795800	-3.89944800	-1.01016600
61	H	-2.46914800	-3.78187500	-0.39505600
62	H	-0.49028700	-4.49428700	2.92862200
63	H	-2.07408300	-3.84245900	2.50352700
64	H	-1.22303600	-4.91870700	1.37717200
65	H	2.41330500	5.19034500	2.15638100
66	H	5.33859100	-2.75826300	0.95958000
67	H	3.92571100	-3.57389900	0.27085200
68	H	5.38031000	-3.34629400	-0.71554600
69	H	-2.64724400	0.07212700	2.06748100
70	H	0.88172700	2.72660900	3.00486300
71	H	5.03261600	0.42371500	-0.96869300
72	H	6.04152600	-0.94501500	-1.49036800
73	H	6.01145100	-0.45969000	0.21995000

Conformers and energy analysis of (3*S*, 5*S*)-2
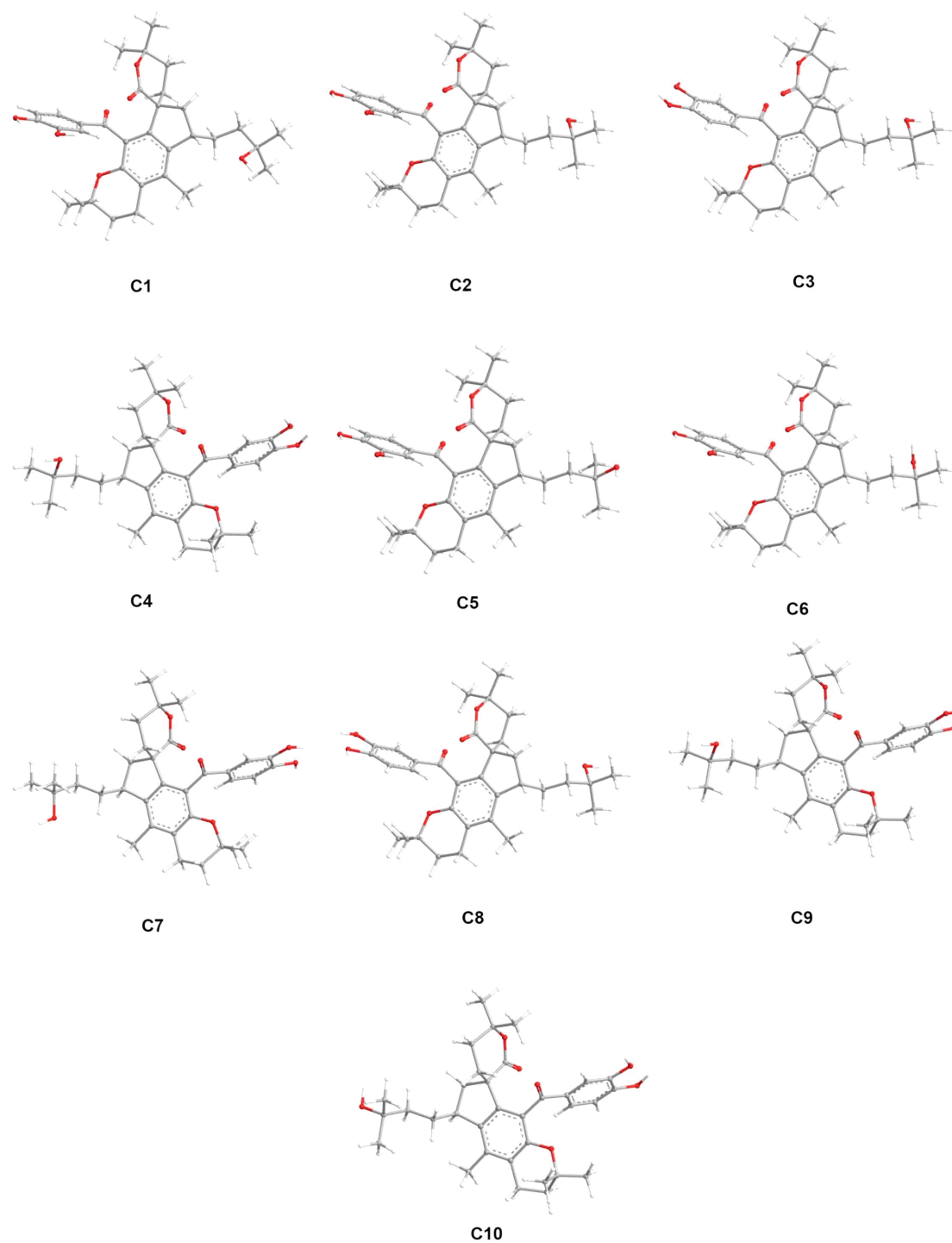
Figure S39. B3LYP/6-31G(d) optimized lowest energy conformers for (3*S*, 5*S*)-2.

Table S5. Energy (298.15 K) analysis for (3*S*, 5*S*)-2.

Conf.	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
C1	-1808.782395	1.39809228	0.027674862

C2	-1808.784623	0	0.29337097
C3	-1808.783907	0.44929716	0.137376355
C4	-1808.784	0.39093873	0.151604063
C5	-1808.783405	0.76430718	0.080703101
C6	-1808.784128	0.31061745	0.173626811
C7	-1808.782525	1.31651598	0.031762291
C8	-1808.782244	1.49284629	0.023582772
C9	-1808.782489	1.33910634	0.030573456
C10	-1808.782948	1.05107925	0.049725319

ECD simulation

ECD spectrum of each conformation is simulated according to the overlapping Gaussian functions expressed as:

$$\Delta\varepsilon(E) = \frac{1}{2.296 \times 10^{-39}\sqrt{\pi}\sigma} \sum_i^A \Delta E_i R_i e^{[-(E-\Delta Ei)^2/\sigma^2]}$$

Where σ is half the bandwidth at 1/e peak height and expressed in energy units. The parameters ΔE_i and R_i are the excitation energies and rotational strengths for the transition i, respectively.

The above function is converted to Δε, λ (wavelength) correlations as:

$$\Delta\varepsilon(\lambda) = \frac{1}{2.296 \times 10^{-39}\sqrt{\pi}\sigma} \sum_i^A \Delta E_i R_i e^{[-(1240/\lambda-\Delta Ei)^2/\sigma^2]}$$

and then simulation were accomplished by using the Excel 2003 and the Origin 7.0 software.

To get the final spectra, all the simulated spectra of conformations of each compound were averaged according to their energy and the Boltzmann distribution theory expressed as:

$$\frac{N_i^*}{N} = \frac{g_i e^{-\varepsilon_i/k_B T}}{\sum g_i e^{-\varepsilon_i/k_B T}}$$

Table S6. Calculated ECD Data for (3*S*, 5*S*)-2 in methanol.

State	C1		C2	
	Excitation energies(eV)	Rotatory Strengths*	Excitation energies(eV)	Rotatory Strengths*
1	3.7969	34.6698	3.7975	32.6194
2	4.2368	5.9546	4.2602	9.4797
3	4.5694	-36.3022	4.5672	-36.1223
4	4.8256	15.4115	4.8417	20.7841
5	4.931	-19.2027	4.9292	-26.2577
6	5.1205	-19.3757	5.1263	-19.3929

7	5.4528	5.741	5.4516	4.7105
8	5.7816	57.4481	5.7843	66.4423
9	5.8141	-77.5999	5.814	-90.3352
10	6.1317	53.6999	6.1463	61.7638
11	6.2223	-6.4113	6.2209	-14.8961
12	6.245	1.8595	6.2574	-2.4996
13	6.3182	-56.0615	6.3361	-56.4547
14	6.455	-8.8872	6.4592	-7.4255
15	6.477	-53.902	6.4777	-45.1981
16	6.5022	8.7803	6.5165	15.9448
17	6.6052	29.6862	6.6074	2.5428
18	6.6118	-0.6286	6.6115	17.9747
19	6.6359	5.5731	6.6501	4.8969
20	6.7365	4.5537	6.7526	2.332
21	6.8938	2.9713	6.8884	7.5489
22	6.904	-6.8494	6.9242	-19.5283
23	6.9597	62.3066	6.9658	117.2837
24	6.9792	-21.4435	6.9817	-68.9156
25	7.0276	1.7434	7.019	-1.478
26	7.0501	4.6636	7.0681	1.2669
27	7.144	-1.6597	7.1293	1.6268
28	7.2255	8.7167	7.2301	11.7992
29	7.2405	-1.9204	7.2596	-2.4337
30	7.2511	-0.7103	7.2656	-3.4282
31	7.329	8.3755	7.3346	8.4978
32	7.3506	6.1418	7.3514	9.4945
33	7.3876	-41.3357	7.3779	-28.1675
34	7.4072	-6.356	7.4011	-16.3305
35	7.4259	-17.1763	7.4315	12.5532
36	7.4457	2.6465	7.457	-21.1089
37	7.4542	14.3646	7.4663	-7.2766
38	7.4904	-24.2796	7.4947	-6.5993
39	7.5095	-1.8434	7.5137	-6.3005
40	7.5218	-15.8978	7.5214	-6.9781
41	7.5612	-20.6637	7.5764	-28.0264
42	7.5818	9.6083	7.5989	-4.1183
43	7.6123	12.2855	7.6336	41.4776
44	7.6194	36.1739	7.6357	2.2747
45	7.6291	9.4535	7.6685	62.7345
46	7.6858	2.0814	7.6935	5.2507
47	7.69	-1.304	7.7032	8.6445
48	7.7377	32.5494	7.7485	13.6583
49	7.7516	9.8322	7.7632	-8.9161
50	7.7551	-29.6561	7.7678	-10.6568
51	7.7916	-4.7408	7.811	18.535
52	7.8192	30.6025	7.8268	5.1214
53	7.8232	11.8131	7.8442	1.0446
54	7.8787	-18.7462	7.88	-17.2354
55	7.9135	-0.7659	7.9328	-0.0707
56	7.9388	-13.7862	7.9588	-17.902
57	7.9839	-6.1224	7.9664	6.5353
58	8.008	-9.3502	8.0021	-3.5418
59	8.0341	11.17	8.0498	-31.8466
60	8.0514	-32.3674	8.0642	-3.7987

State	C3		C4	
	Excitation energies(eV)	Rotatory Strengths*	Excitation energies(eV)	Rotatory Strengths*
1	3.817	30.351	3.8119	26.256
2	4.2209	35.9547	4.1839	53.5816
3	4.5258	-96.8221	4.513	-96.1712
4	4.8291	-2.6745	4.8057	7.0912
5	4.9563	27.8173	4.9392	25.0237
6	5.1875	-16.9398	5.1719	-18.7709
7	5.4836	5.8712	5.4852	5.8569
8	5.8142	50.7692	5.8232	35.4695
9	5.8347	-6.0745	5.8544	22.876
10	6.1812	-100.1582	6.1952	-59.647
11	6.2133	82.229	6.2221	81.7854
12	6.2674	-66.3713	6.2587	-98.876
13	6.3872	-39.2101	6.3788	-20.057
14	6.4015	7.0454	6.3835	14.8179
15	6.4872	157.7165	6.4835	127.392
16	6.512	62.4326	6.5316	16.2091
17	6.6144	24.7869	6.6201	85.9601
18	6.6216	-18.7913	6.6285	-21.8906
19	6.6687	-103.8906	6.6959	-111.7088
20	6.7428	-2.8685	6.7346	-1.8996
21	6.8909	-15.5527	6.8588	2.9039
22	6.9069	4.4298	6.9074	-15.9731
23	6.9943	-0.9854	7.0112	4.4148
24	7.0286	-3.8821	7.023	-9.6727
25	7.0394	8.1037	7.0622	8.4387
26	7.0753	21.4985	7.0721	10.9973
27	7.0908	-27.6147	7.1006	-1.6444
28	7.204	-1.7592	7.1951	7.374
29	7.2366	-5.0708	7.2431	7.8029
30	7.3031	2.4508	7.297	-1.4334
31	7.3217	-7.0625	7.3506	-1.0275
32	7.3634	3.6031	7.3686	-5.7718
33	7.3871	2.2555	7.4004	-8.9279
34	7.3927	-11.2127	7.4089	-12.2019
35	7.4232	-90.022	7.4248	-41.8177
36	7.4488	0.382	7.4743	-1.5276
37	7.4803	14.1471	7.4779	5.842
38	7.496	-9.7509	7.4952	-6.7573
39	7.5237	9.0654	7.5101	-11.7673
40	7.5739	1.4991	7.5467	-1.3176
41	7.6117	5.3304	7.6015	-3.7926
42	7.6242	11.9684	7.6351	-1.2092
43	7.6498	27.943	7.6581	-3.0176
44	7.6836	4.636	7.6757	11.1435
45	7.7	6.2611	7.6972	18.5592
46	7.7122	16.8363	7.7202	17.9332
47	7.7407	27.0391	7.7412	-21.6908
48	7.7527	14.5971	7.7462	15.4034
49	7.768	-1.1029	7.77	-25.4116
50	7.8068	-2.5328	7.8203	27.4998
51	7.8422	-20.5508	7.8441	-7.2544
52	7.8598	-11.6582	7.8622	-14.3494

53	7.8765	-37.6821	7.87	10.1338
54	7.8886	32.8804	7.908	10.7819
55	7.9359	6.2044	7.9227	-4.9946
56	7.9544	-9.9647	7.9658	-3.026
57	7.9785	5.986	7.9773	7.8884
58	7.9894	-5.1976	8.0013	2.4083
59	8.0353	-4.5062	8.0128	7.6712
60	8.044	13.2327	8.0407	5.8958

	C5		C6	
State	Excitation energies(eV)	Rotatory Strengths*	Excitation energies(eV)	Rotatory Strengths*
1	3.7956	32.2436	3.7975	33.3294
2	4.2637	10.9726	4.2567	10.5599
3	4.5611	-35.5423	4.5649	-37.8976
4	4.845	20.653	4.8428	17.7335
5	4.9251	-26.5438	4.9285	-23.4947
6	5.1293	-19.5398	5.1333	-18.7757
7	5.4516	4.7711	5.4536	4.921
8	5.7823	65.8468	5.7855	72.8499
9	5.8116	-87.7891	5.8128	-95.1751
10	6.1498	65.4293	6.1476	62.902
11	6.218	-18.7344	6.2173	-17.4893
12	6.2594	-3.2142	6.2539	-0.0584
13	6.3425	-55.1036	6.3369	-55.3527
14	6.4604	-10.9691	6.4566	-8.0152
15	6.474	-45.0132	6.477	-51.116
16	6.5193	17.4551	6.5125	16.0141
17	6.6059	4.5831	6.609	18.4402
18	6.6116	14.7104	6.6106	4.2759
19	6.657	4.9427	6.6468	4.9282
20	6.7538	1.9286	6.7471	3.5318
21	6.8802	8.8689	6.8836	8.4192
22	6.9191	-16.8033	6.9202	-17.673
23	6.9602	91.9445	6.9624	105.2711
24	6.9881	-50.5384	6.985	-58.6012
25	7.0167	-3.4186	7.0257	-4.01
26	7.0531	3.9772	7.0528	4.3176
27	7.1162	4.1962	7.1241	2.099
28	7.2296	12.9711	7.2251	5.7403
29	7.2665	-7.0127	7.2416	8.0226
30	7.2782	0.5694	7.2544	-0.6465
31	7.3354	7.1748	7.2916	-13.1819
32	7.344	11.0223	7.3329	8.4485
33	7.3617	-16.7225	7.3494	4.2395
34	7.3962	-21.1076	7.4005	-24.4564
35	7.43	15.6021	7.4306	13.3704
36	7.4581	-40.6985	7.4535	-62.5572
37	7.4723	-1.273	7.4615	19.0905
38	7.5002	-3.5037	7.4756	17.1503
39	7.5122	-11.9535	7.494	-13.049
40	7.5507	3.8162	7.5063	3.1497
41	7.5668	-31.8192	7.518	-33.5559
42	7.5844	-6.618	7.5608	-1.5159
43	7.6263	11.692	7.5845	-16.8358
44	7.6319	8.9567	7.6198	11.0733

45	7.6673	94.5769	7.6271	11.9953
46	7.6941	8.2075	7.6684	87.6494
47	7.7153	7.4666	7.6882	8.3771
48	7.7458	16.1223	7.7462	13.4008
49	7.7649	-22.484	7.7606	-15.6191
50	7.8044	35.4497	7.7631	5.3974
51	7.8069	-1.5531	7.8107	25.9193
52	7.8325	-40.2005	7.8299	-13.3642
53	7.8474	1.8944	7.8482	6.9399
54	7.8677	27.3646	7.8743	17.098
55	7.8868	-11.282	7.8945	-15.1498
56	7.9494	-11.4789	7.9559	-16.9166
57	8.0051	-4.6173	7.9872	2.3752
58	8.0274	-73.2184	8.0206	-4.6203
59	8.0609	-15.0789	8.0262	-60.7422
60	8.0665	1.1216	8.0503	-0.8135

	C7		C8	
State	Excitation energies(eV)	Rotatory Strengths*	Excitation energies(eV)	Rotatory Strengths*
1	3.8096	30.1524	3.8115	29.6878
2	4.2391	28.4647	4.245	28.9051
3	4.5164	-73.3402	4.5186	-72.9043
4	4.8352	-19.9661	4.8385	-20.2388
5	5.0015	28.4077	5.0038	28.0009
6	5.1895	-21.4439	5.1886	-21.2783
7	5.4765	5.4299	5.4775	5.094
8	5.8096	77.0888	5.8107	73.8334
9	5.8162	-48.0363	5.8167	-44.5764
10	6.1664	-91.4608	6.1681	-93.1768
11	6.1947	52.1733	6.1965	51.6611
12	6.2602	-63.5756	6.2644	-66.1814
13	6.3767	-18.1868	6.3791	-16.2407
14	6.4385	16.9516	6.4367	15.559
15	6.4864	206.8489	6.487	204.7677
16	6.5117	89.0225	6.5113	96.2522
17	6.5943	-20.022	6.5936	-20.6354
18	6.629	-73.4372	6.6226	-42.3361
19	6.6536	-59.6096	6.6505	-89.3929
20	6.7354	-14.229	6.7414	-14.1794
21	6.8877	-25.138	6.8924	-23.0461
22	6.9114	0.9064	6.9149	-0.5993
23	6.9624	-14.9818	6.9656	-15.5751
24	7.0398	-0.6614	7.0419	-2.2267
25	7.0544	16.7831	7.0551	19.2162
26	7.0732	3.4505	7.0749	3.5296
27	7.0926	-12.6804	7.0947	-13.611
28	7.2113	-0.2518	7.2193	-1.1524
29	7.2553	-5.1118	7.2433	-4.7385
30	7.3112	-5.9204	7.3087	-6.2832
31	7.3435	3.6528	7.3427	2.7798
32	7.3572	-0.3604	7.3569	4.1351
33	7.3792	-20.6887	7.3812	-19.9248
34	7.3916	-11.7289	7.391	-8.8879
35	7.4161	-33.5577	7.418	-44.329
36	7.4652	-40.4186	7.4684	-27.8619

37	7.477	9.497	7.4787	8.2598
38	7.5008	13.8848	7.5139	-6.3089
39	7.5399	0.7408	7.5233	17.5299
40	7.5721	18.3664	7.5748	7.9177
41	7.5898	-4.5093	7.6078	9.7662
42	7.6074	17.1525	7.6157	17.5208
43	7.6459	11.5468	7.6368	25.5507
44	7.6791	18.3083	7.6901	4.3994
45	7.6999	23.7717	7.6998	-14.4541
46	7.7034	-27.67	7.7032	44.2469
47	7.723	38.7022	7.7117	16.008
48	7.7512	-1.5511	7.7535	1.2895
49	7.7619	8.4448	7.765	10.3919
50	7.7954	-7.2923	7.8105	-3.3844
51	7.8103	7.0559	7.8416	15.0568
52	7.8415	19.827	7.8548	-44.0877
53	7.861	-34.3197	7.8619	-40.622
54	7.8663	-14.4394	7.8728	20.3928
55	7.9209	-5.0488	7.9371	10.5208
56	7.9368	7.9253	7.9592	3.9266
57	7.9886	-4.0559	7.9917	-2.7368
58	8.0039	-8.3878	8.0016	-8.822
59	8.0326	-16.4566	8.0294	-0.9957
60	8.0347	12.2031	8.0401	-12.9143

	C9		C10	
State	Excitation energies(eV)	Rotatory Strengths*	Excitation energies(eV)	Rotatory Strengths*
1	3.8034	24.4188	3.8094	26.1905
2	4.2143	46.2295	4.1838	55.8962
3	4.506	-72.9165	4.5081	-97.4897
4	4.8124	-9.1146	4.8073	5.9757
5	4.9843	28.3535	4.9342	25.5245
6	5.1662	-25.8272	5.1754	-18.842
7	5.4735	4.9614	5.4832	6.0395
8	5.8211	22.679	5.82	37.3467
9	5.8384	18.6468	5.8509	19.0157
10	6.1847	-66.1264	6.1878	-48.7505
11	6.2081	59.6314	6.2218	66.1731
12	6.2544	-92.3136	6.2576	-89.9928
13	6.373	-19.4988	6.3863	-17.0001
14	6.424	29.941	6.3901	12.7078
15	6.4824	214.3725	6.4818	126.8546
16	6.5399	20.2896	6.5326	16.3259
17	6.6148	-10.4008	6.6225	70.1741
18	6.626	52.4632	6.6281	-17.5001
19	6.6667	-130.707	6.6943	-107.0565
20	6.7294	-14.6105	6.7315	-0.5244
21	6.868	7.9523	6.8584	1.5663
22	6.9098	-24.7017	6.8955	-15.2825
23	6.9924	-28.5895	7.0097	7.5024
24	7.0297	-0.9378	7.0146	-9.3714
25	7.0586	12.6392	7.0558	3.9872
26	7.0868	7.3833	7.0811	11.1471
27	7.119	0.6031	7.0931	-3.0405
28	7.2149	8.8794	7.161	5.8581

29	7.2548	6.2511	7.2457	9.122
30	7.3441	5.5921	7.2911	-0.6432
31	7.3559	-12.3705	7.3321	6.9792
32	7.3576	-5.7837	7.369	-4.3484
33	7.3937	-0.9958	7.3999	-7.0829
34	7.4038	-3.8037	7.4084	-27.0768
35	7.4514	-61.6639	7.417	-24.326
36	7.4772	6.7424	7.4692	27.6035
37	7.4898	-4.0383	7.4794	-36.014
38	7.4957	-10.3212	7.5017	1.1554
39	7.5101	4.2991	7.512	-22.6176
40	7.5528	5.5002	7.5562	2.6512
41	7.6014	-7.0845	7.5826	-4.6655
42	7.6254	16.7451	7.6393	1.1411
43	7.6486	6.9263	7.664	11.0146
44	7.6661	-0.8351	7.6658	-3.4928
45	7.6978	19.767	7.7104	-4.2716
46	7.7152	45.3321	7.7411	2.3621
47	7.7358	-25.1559	7.7545	2.4621
48	7.7483	7.2947	7.7788	-8.0951
49	7.7574	-38.8978	7.7861	12.6118
50	7.8147	-9.3049	7.7995	-27.8525
51	7.8271	22.7183	7.8331	24.6466
52	7.8568	-7.8776	7.851	-28.9077
53	7.8772	0.7322	7.8716	50.6259
54	7.8905	-6.056	7.8961	15.8172
55	7.9621	5.3176	7.916	-20.085
56	7.9689	-8.5715	7.9702	16.0797
57	7.9857	17.987	7.9978	3.3208
58	7.9995	-3.3669	8.0033	-2.7558
59	8.0042	8.7896	8.0178	7.7222
60	8.0437	1.3643	8.0642	-6.0996

* R(velocity) 10**-40 erg-esu-cm
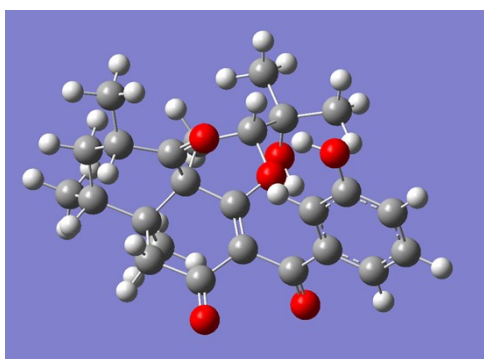
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a1 (22.91%)   (1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a2 (2.25%)
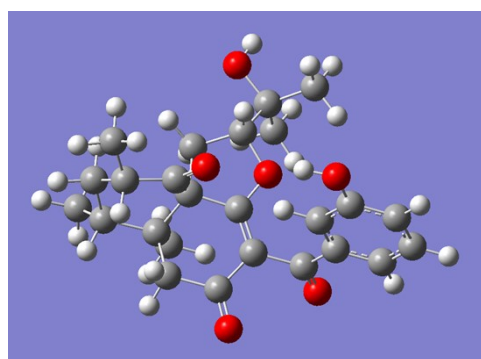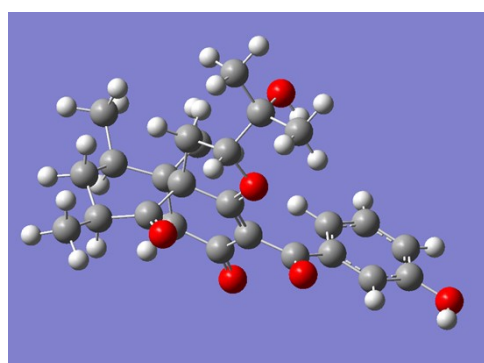
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a3 (37.62%)
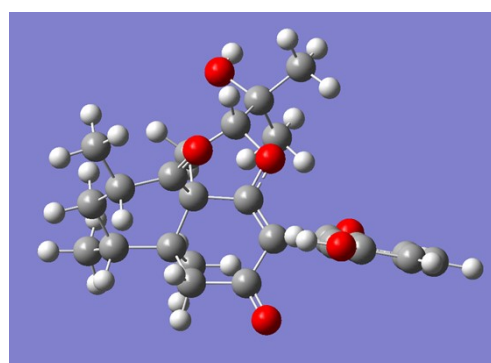
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a4 (10.37%)
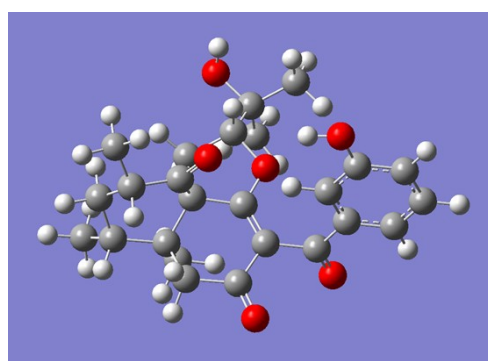
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a5 (3.57%)
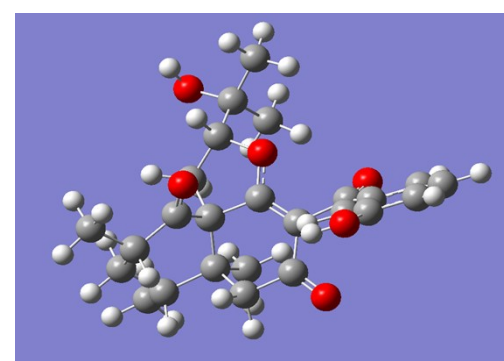
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a6 (15.92%)
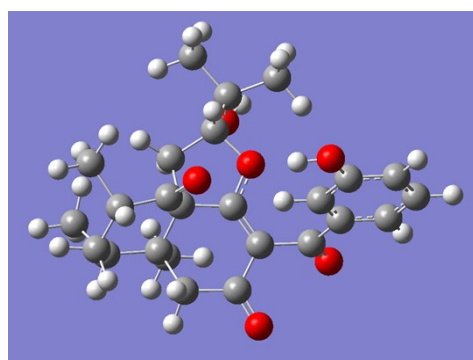
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a7 (1.61%)
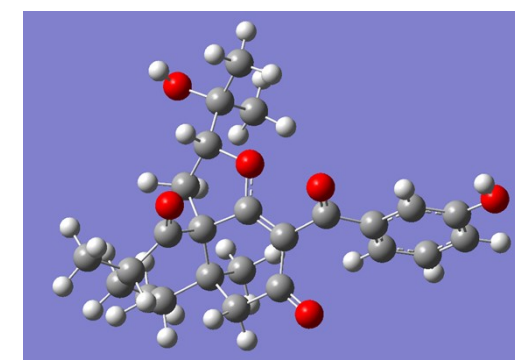
(1*R*,3*S*,5*R*,6*S*,17*R*)-Conf 3a8 (4.34%)

Fig. S40. DFT-optimized structures for low-energy conformers and Boltzmann distributions of compound (1*R*,3*S*,5*R*,6*S*,17*R*)-3a [(1*R*,3*S*,5*R*,6*S*,17*R*)-3a1-(1*R*,3*S*,5*R*,6*S*,17*R*)-3a8].

Table S7. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a1 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-3.88296500	-1.02164500	1.23713100
2	C	-2.63674600	-1.34874800	2.06552400
3	C	-1.40831800	-0.63254600	1.50987400
4	C	-1.47715000	-0.10514900	0.04803300
5	C	-2.33110800	-1.04098100	-0.87519300
6	C	-3.76776400	-1.33256600	-0.27262500
7	C	-0.05666600	-0.00524300	-0.47101500
8	C	0.63761100	-0.99987400	-1.06578200
9	C	-0.05258300	-2.27205400	-1.34117000

Number	Atom	X	Y	Z
10	C	-1.53791500	-2.37639400	-0.95788000
11	C	2.04171600	-0.80734400	-1.59367500
12	C	3.16694200	-0.67505900	-0.61907600
13	O	0.51667400	-3.23800000	-1.82717000
14	C	-2.42545200	-0.47895200	-2.31173800
15	O	-0.41685500	-0.44225900	2.19400400
16	C	-2.81583100	-1.07104300	3.56470800
17	C	-4.94775000	-0.64642600	-0.98478000
18	C	-1.85980800	1.40392800	0.13403800
19	C	-0.51364100	2.10366000	0.36173000
20	O	0.45818800	1.22464300	-0.27765900
21	C	-0.36349700	3.50064600	-0.27896600
22	C	1.05331900	4.04595100	-0.04224700
23	C	-1.41674500	4.45661500	0.28603900
24	O	-0.62988700	3.40530000	-1.68065200
25	O	2.22803800	-0.77548400	-2.79999200
26	C	4.47048200	-0.52662500	-1.11495000
27	C	5.53506800	-0.40259900	-0.22560100
28	C	5.31972100	-0.41897900	1.15322400
29	C	4.01880600	-0.56393800	1.64706000
30	C	2.94549300	-0.69769800	0.76474700
31	O	3.85009400	-0.56834100	3.00469800
32	H	-4.74020400	-1.57046200	1.64579500
33	H	-4.12498100	0.04208800	1.37321200
34	H	-2.41501200	-2.42234200	1.95022800
35	H	-3.92182900	-2.41418100	-0.39069300
36	H	-2.00097000	-3.04742600	-1.68911100
37	H	-1.57491700	-2.91325900	-0.00001400
38	H	-2.93599600	-1.20005900	-2.95836000
39	H	-2.98027500	0.46067700	-2.36825300
40	H	-1.43361200	-0.30935300	-2.73915900
41	H	-3.61790300	-1.69438700	3.97340400
42	H	-3.08109200	-0.02158200	3.73978700
43	H	-1.89350900	-1.28082100	4.11096200
44	H	-5.88444600	-0.92937300	-0.49001700
45	H	-5.03357600	-0.93599500	-2.03521700
46	H	-4.87447500	0.44666900	-0.93933700
47	H	-2.57222400	1.62792600	0.93181400
48	H	-2.28082100	1.74224700	-0.81575700
49	H	-0.25446800	2.14434200	1.42521100
50	H	1.80908500	3.36405700	-0.44511500
51	H	1.25704400	4.17794900	1.02662200
52	H	1.15734200	5.01591700	-0.53812000
53	H	-2.42855200	4.11522000	0.04661800
54	H	-1.32275800	4.54964600	1.37351100
55	H	-1.28389300	5.44758900	-0.15809200
56	H	0.05799200	2.83261300	-2.06032500
57	H	4.62155900	-0.51520800	-2.18864200
58	H	6.54757500	-0.29153600	-0.60433800
59	H	6.14123000	-0.32103000	1.85621000
60	H	1.93895700	-0.80789200	1.15838500
61	H	2.90340600	-0.66052400	3.19850300

Table S8. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a2 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-3.90572400	-0.86720600	1.28140500
2	C	-2.66821800	-1.16799200	2.13210900

3	C	-1.41911800	-0.53071700	1.52813100
4	C	-1.48097200	-0.09012200	0.03765400
5	C	-2.35663000	-1.06453800	-0.82333700
6	C	-3.79793400	-1.28723300	-0.20209900
7	C	-0.05852600	-0.05144100	-0.48956200
8	C	0.61398200	-1.09771000	-1.01941800
9	C	-0.10420100	-2.36952900	-1.21130600
10	C	-1.59086100	-2.41783900	-0.82028400
11	C	2.02227700	-0.97368700	-1.55520200
12	C	3.14587700	-0.76594800	-0.59049500
13	O	0.44130400	-3.37846000	-1.63327900
14	C	-2.44159800	-0.59393000	-2.29295900
15	O	-0.41637900	-0.33824100	2.19476400
16	C	-2.83765600	-0.77603500	3.60693800
17	C	-4.96691800	-0.63379400	-0.96164800
18	C	-1.83594800	1.42931200	0.03477700
19	C	-0.46846200	2.09994900	0.21800200
20	O	0.47982600	1.17722000	-0.37708400
21	C	-0.27466500	3.49326000	-0.41341200
22	C	-0.41332100	3.48605500	-1.94117300
23	C	1.08864500	4.06206300	0.00342300
24	O	-1.33765000	4.25146400	0.18692400
25	O	2.21651000	-1.06055000	-2.75741600
26	C	4.45067400	-0.65835100	-1.09346100
27	C	5.51394900	-0.46845200	-0.21419000
28	C	5.29640200	-0.37977000	1.16160500
29	C	3.99439600	-0.48525400	1.66228800
30	C	2.92241900	-0.68358400	0.79053400
31	O	3.82253000	-0.38746900	3.01617700
32	H	-4.77651000	-1.36450300	1.72593800
33	H	-4.12042100	0.20908700	1.34184900
34	H	-2.47700400	-2.25305700	2.09592300
35	H	-3.97098400	-2.37169300	-0.24252600
36	H	-2.06919900	-3.12623400	-1.50497800
37	H	-1.63671600	-2.88896500	0.17130500
38	H	-2.98329400	0.34827900	-2.40936400
39	H	-1.44710000	-0.46785600	-2.72920100
40	H	-2.96443800	-1.34580800	-2.89299500
41	H	-1.92109900	-0.97234400	4.16773300
42	H	-3.65706000	-1.34435700	4.05927100
43	H	-3.07193900	0.29067700	3.70414500
44	H	-5.90795500	-0.86816800	-0.45006300
45	H	-5.05677500	-0.99349300	-1.98995800
46	H	-4.87775500	0.45871900	-0.99029700
47	H	-2.52551300	1.72852600	0.82624600
48	H	-2.28693800	1.70843000	-0.91944600
49	H	-0.22441500	2.17041200	1.28309300
50	H	-0.26199200	4.50040000	-2.33004500
51	H	-1.41005200	3.15905400	-2.25191600
52	H	0.33244000	2.83393200	-2.40517100
53	H	1.90746500	3.43420700	-0.36115400
54	H	1.22478600	5.06927900	-0.41042000
55	H	1.15651900	4.12705700	1.09441700
56	H	-1.22850500	5.17500900	-0.08999600
57	H	4.60353100	-0.72932300	-2.16462000
58	H	6.52731400	-0.38794700	-0.59848900
59	H	6.11687000	-0.23003800	1.85668200
60	H	1.91544200	-0.76384100	1.19000400
61	H	2.87495300	-0.46216600	3.21342700

Table S9. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a3 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	4.16205100	-1.65902500	0.07659100
2	C	3.59962400	-1.53094100	-1.34381300
3	C	2.48804900	-0.48416800	-1.36932400
4	C	1.70608600	-0.21414400	-0.04357100
5	C	1.68554600	-1.45482300	0.91141400
6	C	3.13119700	-2.05347100	1.15903800
7	C	0.29271400	0.19818000	-0.42307400
8	C	-0.76676800	-0.64158100	-0.56769700
9	C	-0.56282800	-2.07221500	-0.30763400
10	C	0.81539000	-2.52595300	0.19489500
11	C	-2.09543000	-0.12852100	-1.06571800
12	C	-3.34151000	-0.37615800	-0.27167100
13	O	-1.43805100	-2.90832700	-0.49800300
14	C	0.98835400	-1.12322200	2.25034700
15	O	2.25172200	0.17870400	-2.36068600
16	C	4.67452500	-1.22542000	-2.39409000
17	C	3.75687700	-1.75627800	2.53412500
18	C	2.25333300	1.13506200	0.51430500
19	C	1.45300200	2.19048700	-0.25788600
20	O	0.18835100	1.52541800	-0.55767000
21	C	1.11815700	3.48524300	0.51258700
22	C	0.25475400	4.41244100	-0.35648600
23	C	2.40580600	4.18799600	0.94845400
24	O	0.42432000	3.15053300	1.71919100
25	O	-2.14054300	0.52067000	-2.10161800
26	C	-3.33069800	-0.87017900	1.03817800
27	C	-4.53220600	-1.01082700	1.73446600
28	C	-5.74447000	-0.67217000	1.13944400
29	C	-5.75616600	-0.17940600	-0.17241900
30	C	-4.56056100	-0.02508800	-0.86942100
31	O	-6.97223900	0.13862900	-0.71195400
32	H	4.97617400	-2.39404800	0.07904200
33	H	4.63004700	-0.70204100	0.35039000
34	H	3.12437200	-2.48554900	-1.61877500
35	H	3.00744600	-3.14403300	1.10491100
36	H	0.63806200	-3.37711200	0.86128900
37	H	1.33908300	-2.94052700	-0.67573700
38	H	0.88010700	-2.03390700	2.84905000
39	H	1.54108200	-0.39955100	2.85351600
40	H	-0.01439300	-0.71927100	2.08664900
41	H	5.20956900	-0.30035600	-2.14933500
42	H	4.22763400	-1.09986000	-3.38274800
43	H	5.40566800	-2.03968600	-2.43651500
44	H	3.16533200	-2.15302600	3.36341000
45	H	3.89373000	-0.68072600	2.69853600
46	H	4.74864100	-2.22068100	2.58887900
47	H	3.33012900	1.25592800	0.37187000
48	H	2.02794200	1.22646500	1.57950500
49	H	1.91743900	2.42744500	-1.21932400
50	H	-0.66334200	3.90853900	-0.67572800
51	H	0.79225900	4.72777000	-1.25797500
52	H	-0.01457600	5.30414700	0.21811500
53	H	2.98308900	3.56266400	1.63648200
54	H	3.03239900	4.43409800	0.08433500
55	H	2.15515300	5.11683700	1.46952100
56	H	-0.42130800	2.75250400	1.45249300

Number	Atom	X	Y	Z
57	H	-2.39679800	-1.15009100	1.51140000
58	H	-4.52554600	-1.39283400	2.75163900
59	H	-6.68640000	-0.78306500	1.66757600
60	H	-4.54295200	0.37029600	-1.88196000
61	H	-6.83748700	0.44972800	-1.62083900

Table S10. The Cartesian coordinates for the lowest-energy conformer of (1R,3S,5R,6S,17R)-3a4 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-3.47764700	-2.36237700	0.47558300
2	C	-2.33809400	-2.39072300	1.49813400
3	C	-1.45176400	-1.15380400	1.35711400
4	C	-1.51558000	-0.36781500	0.01413400
5	C	-1.77215600	-1.30930600	-1.21210400
6	C	-3.02585400	-2.25634700	-0.99782900
7	C	-0.20142700	0.37354500	-0.15281600
8	C	0.90965100	-0.11105300	-0.76252400
9	C	0.84217900	-1.43257800	-1.39584000
10	C	-0.49374500	-2.18774600	-1.33144400
11	C	2.11122400	0.77693400	-0.98964300
12	C	3.43719200	0.37291300	-0.43832900
13	O	1.79971400	-1.94039900	-1.96848900
14	C	-1.89406000	-0.50204900	-2.52491700
15	O	-0.74874500	-0.76179500	2.26955900
16	C	-2.82436700	-2.56302900	2.94366400
17	C	-4.26733800	-1.93467800	-1.84959100
18	C	-2.49048300	0.82964100	0.24580500
19	C	-1.58528200	1.90428300	0.86457500
20	O	-0.25168800	1.59631500	0.38461900
21	C	-1.89893100	3.37245400	0.50790000
22	C	-1.72425500	3.66803000	-0.98794700
23	C	-1.01618100	4.30550500	1.34796200
24	O	-3.27590900	3.50083200	0.89855500
25	O	1.97361500	1.82186600	-1.61248800
26	C	4.57737400	1.08105800	-0.84214500
27	C	5.82130600	0.74159500	-0.31574200
28	C	5.94263400	-0.28732600	0.61795100
29	C	4.80290200	-0.98763100	1.02852000
30	C	3.55356100	-0.66085200	0.49962900
31	O	4.97447300	-1.98076300	1.95444900
32	H	-4.08978000	-3.26517300	0.59235800
33	H	-4.14457700	-1.52209600	0.71543700
34	H	-1.68228200	-3.24480300	1.26206800
35	H	-2.69311000	-3.25813400	-1.30373200
36	H	-0.54271700	-2.81182300	-2.22990000
37	H	-0.42353900	-2.88616400	-0.48590400
38	H	-1.02804300	0.14772700	-2.67684600
39	H	-1.94093000	-1.18609500	-3.37868500
40	H	-2.79085300	0.12144900	-2.55937000
41	H	-3.52173000	-1.76321200	3.21955400
42	H	-1.98433100	-2.53065100	3.64108100
43	H	-3.34445000	-3.51985400	3.05898700
44	H	-4.67276300	-0.94096700	-1.62490400
45	H	-5.05644500	-2.66333000	-1.62914400
46	H	-4.06819800	-1.98464200	-2.92329000
47	H	-3.32628500	0.59645500	0.90832400
48	H	-2.90887200	1.16756800	-0.70383600
49	H	-1.56300100	1.80399200	1.95416600

Number	Atom	X	Y	Z
50	H	-1.93777200	4.72636100	-1.18221200
51	H	-2.41582800	3.07611700	-1.59556700
52	H	-0.70114200	3.46156500	-1.31666800
53	H	0.04414500	4.14767400	1.12776400
54	H	-1.25352200	5.35436400	1.12926000
55	H	-1.18429200	4.13074200	2.41591600
56	H	-3.52805700	4.42898700	0.77038400
57	H	4.46508300	1.88282800	-1.56332900
58	H	6.70988100	1.28168800	-0.63131800
59	H	6.90529900	-0.56108500	1.03851200
60	H	2.66648800	-1.19781200	0.82633400
61	H	4.11479300	-2.39199200	2.13431600

Table S11. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a5 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-3.90587700	-0.85991800	1.28564000
2	C	-2.66626200	-1.16160800	2.13344900
3	C	-1.42160200	-0.51568500	1.52964100
4	C	-1.48008900	-0.08930000	0.03496500
5	C	-2.35915600	-1.06587100	-0.81989500
6	C	-3.80210500	-1.27651900	-0.19933200
7	C	-0.05713200	-0.06048600	-0.49235600
8	C	0.61123700	-1.11465500	-1.01189600
9	C	-0.11192800	-2.38555900	-1.19208500
10	C	-1.60050800	-2.42321000	-0.80714300
11	C	2.01982000	-1.00096800	-1.54907700
12	C	3.14363900	-0.77815500	-0.58778200
13	O	0.43084900	-3.40171300	-1.59968100
14	C	-2.44058000	-0.60595000	-2.29312400
15	O	-0.42567000	-0.30104800	2.20025000
16	C	-2.83513700	-0.77800300	3.61029300
17	C	-4.96467100	-0.60919600	-0.95667400
18	C	-1.82887300	1.43155200	0.02035700
19	C	-0.45958000	2.10117800	0.19558700
20	O	0.48512000	1.16757600	-0.39296700
21	C	-0.26856300	3.50062200	-0.43369100
22	C	-0.50107800	3.51481200	-1.94477100
23	C	1.12827900	4.03514000	-0.09558200
24	O	-1.28410100	4.34467500	0.13420400
25	O	2.21427000	-1.10774200	-2.74952400
26	C	4.44691200	-0.66701900	-1.09373700
27	C	5.51051600	-0.46304700	-0.21796200
28	C	5.29487300	-0.36479000	1.15745900
29	C	3.99444600	-0.47467400	1.66119100
30	C	2.92217300	-0.68587800	0.79294500
31	O	3.82428300	-0.36745700	3.01486600
32	H	-4.77577100	-1.35745800	1.73153400
33	H	-4.12000500	0.21649300	1.34874200
34	H	-2.47193700	-2.24578300	2.09151100
35	H	-3.98534400	-2.35913900	-0.24337100
36	H	-2.07991300	-3.13163700	-1.49106800
37	H	-1.65310900	-2.89083100	0.18558600
38	H	-2.97409300	0.33986000	-2.41731300
39	H	-1.44526500	-0.49190800	-2.73080100
40	H	-2.97007300	-1.35825000	-2.88678900
41	H	-1.91731200	-0.97330700	4.16935800
42	H	-3.65179900	-1.35168200	4.06071000

Number	Atom	X	Y	Z
43	H	-3.07388200	0.28725900	3.71339400
44	H	-5.90772400	-0.83354300	-0.44429000
45	H	-5.05968400	-0.96682700	-1.98518600
46	H	-4.86333100	0.48227900	-0.98453500
47	H	-2.52073300	1.73587200	0.80820000
48	H	-2.27837800	1.70465300	-0.93613700
49	H	-0.20954700	2.16710400	1.26221200
50	H	-0.29129000	4.51489000	-2.33544400
51	H	-1.54088900	3.27862900	-2.18921700
52	H	0.15391700	2.79651500	-2.44568900
53	H	1.90876300	3.39966600	-0.52430300
54	H	1.24432900	5.05107000	-0.48633100
55	H	1.28432000	4.06243200	0.99159000
56	H	-1.00296600	4.58456100	1.03207200
57	H	4.59841400	-0.74596800	-2.16452700
58	H	6.52262100	-0.37913900	-0.60478200
59	H	6.11563000	-0.20463500	1.84985800
60	H	1.91626200	-0.76884200	1.19461900
61	H	2.87826500	-0.45353200	3.21467800

Table S12. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a6 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-3.46756100	-2.38381200	0.46751700
2	C	-2.32588500	-2.40741000	1.48860100
3	C	-1.46695000	-1.15003900	1.36189000
4	C	-1.51738200	-0.37068800	0.01404800
5	C	-1.76635800	-1.31265500	-1.21302900
6	C	-3.02116600	-2.25885400	-1.00636400
7	C	-0.20155500	0.37020300	-0.14576600
8	C	0.91296200	-0.11505000	-0.74949100
9	C	0.84917600	-1.43733500	-1.38166800
10	C	-0.48767100	-2.19136500	-1.32728100
11	C	2.11094800	0.77815000	-0.97769700
12	C	3.44146700	0.38167600	-0.43165200
13	O	1.81054200	-1.94747700	-1.94581200
14	C	-1.88122300	-0.50651600	-2.52727100
15	O	-0.80139100	-0.73146400	2.29077900
16	C	-2.80714000	-2.60896600	2.93159400
17	C	-4.26542500	-1.92197300	-1.84819000
18	C	-2.49369100	0.82754900	0.23672400
19	C	-1.59403000	1.90710600	0.85555600
20	O	-0.25503400	1.59397900	0.38887100
21	C	-1.91865800	3.37743000	0.49785300
22	C	-1.80495400	3.65770200	-1.00141800
23	C	-1.00393900	4.31752400	1.29180500
24	O	-3.29536300	3.59471800	0.84935000
25	O	1.96502200	1.82341200	-1.59794300
26	C	4.57179100	1.11292300	-0.82209800
27	C	5.82028800	0.78214500	-0.30105500
28	C	5.95626800	-0.26225100	0.61319500
29	C	4.82669800	-0.98681800	1.00942900
30	C	3.57274100	-0.66745300	0.48706400
31	O	5.01265300	-1.99566100	1.91551000
32	H	-4.06964300	-3.29406500	0.57796100
33	H	-4.14306100	-1.55287600	0.71671500
34	H	-1.65570900	-3.24614900	1.23934100
35	H	-2.69201000	-3.25697600	-1.32764200

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Number	Atom	X	Y	Z
36	H	-0.53195200	-2.81160400	-2.22863100
37	H	-0.42174400	-2.89379200	-0.48505500
38	H	-2.77572400	0.11984400	-2.56624300
39	H	-1.01273700	0.14042200	-2.67721900
40	H	-1.92724100	-1.19196100	-3.38000000
41	H	-1.96761600	-2.57221300	3.62940600
42	H	-3.31064200	-3.57611600	3.03325300
43	H	-3.51797000	-1.82547000	3.21983800
44	H	-5.05728300	-2.64871400	-1.63124400
45	H	-4.07202300	-1.96183900	-2.92330200
46	H	-4.66436100	-0.92845700	-1.61132100
47	H	-3.33363000	0.59026800	0.89304700
48	H	-2.90745700	1.16280100	-0.71567700
49	H	-1.57252300	1.80424900	1.94729800
50	H	-0.80785300	3.39928900	-1.36942900
51	H	-1.98820800	4.72041200	-1.18624200
52	H	-2.55125200	3.09376700	-1.56930000
53	H	0.04587100	4.15812900	1.02817700
54	H	-1.26626100	5.35952200	1.08275500
55	H	-1.10653600	4.14456900	2.37207500
56	H	-3.34264800	3.69514600	1.81396300
57	H	4.44813000	1.92585300	-1.52874900
58	H	6.70095400	1.34097000	-0.60596300
59	H	6.92270400	-0.53021800	1.02879900
60	H	2.69420800	-1.22486100	0.80194900
61	H	4.16028300	-2.42731900	2.08161700

Table S13. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a7 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	-3.64190600	-1.86722900	1.27899300
2	C	-2.75297700	-0.99613900	2.19608100
3	C	-1.46906200	-0.49436800	1.52909600
4	C	-1.47233400	-0.14203500	0.01488400
5	C	-2.29843900	-1.18438000	-0.81571000
6	C	-3.71646500	-1.44093700	-0.20604400
7	C	-0.03102600	-0.10179800	-0.46738500
8	C	0.67419800	-1.13909100	-0.97487600
9	C	-0.01263700	-2.42300100	-1.18476800
10	C	-1.48398500	-2.50716700	-0.75964600
11	C	2.09454300	-0.98851700	-1.46884400
12	C	3.18066000	-0.72567900	-0.47263900
13	O	0.54882300	-3.41297500	-1.63021200
14	C	-2.42499100	-0.77431700	-2.29849400
15	O	-0.47214000	-0.30624900	2.20773600
16	C	-3.50557400	0.17954100	2.86503600
17	C	-4.74815800	-0.31974900	-0.44245100
18	C	-1.83510600	1.37326800	-0.08831100
19	C	-0.48712400	2.07534200	0.13406200
20	O	0.49599300	1.12791500	-0.34891000
21	C	-0.30411400	3.41533000	-0.60123400
22	C	1.16278900	3.86275300	-0.54358200
23	C	-1.22669600	4.47415400	0.02680600
24	O	-0.69866200	3.17256200	-1.95722200
25	O	2.33496600	-1.10419000	-2.65981600
26	C	4.49489700	-0.57467000	-0.93829200
27	C	5.52420400	-0.33505100	-0.03106300
28	C	5.26353300	-0.24020200	1.33684800

29	C	3.95224400	-0.38989700	1.80028500
30	C	2.91454100	-0.63751500	0.90026100
31	O	3.73600800	-0.28441300	3.14779900
32	H	-3.27264600	-2.89695700	1.32938400
33	H	-4.65650900	-1.90160200	1.69529000
34	H	-2.38796300	-1.61983100	3.02094100
35	H	-4.10454400	-2.31579300	-0.74802000
36	H	-1.95191000	-3.27271600	-1.38741200
37	H	-1.47218500	-2.91559800	0.26013100
38	H	-1.44579100	-0.68249500	-2.77629100
39	H	-2.98826100	-1.54266100	-2.84097900
40	H	-2.94934700	0.17427800	-2.43606000
41	H	-4.30310200	-0.21819300	3.50200900
42	H	-3.97158300	0.85304000	2.14066600
43	H	-2.82565400	0.76114100	3.49605000
44	H	-4.93953400	-0.16618400	-1.50820800
45	H	-4.44883900	0.64375800	-0.02090300
46	H	-5.70231900	-0.59546000	0.02104300
47	H	-2.57806400	1.69621600	0.64237900
48	H	-2.20286400	1.60945400	-1.08779400
49	H	-0.28505300	2.22724000	1.20060700
50	H	1.49874300	3.99904500	0.49035400
51	H	1.28098200	4.82522400	-1.05813800
52	H	1.80742200	3.12293500	-1.02294100
53	H	-1.10221800	5.42976100	-0.49538200
54	H	-2.27759300	4.18083600	-0.06176800
55	H	-0.99477600	4.64047500	1.08524800
56	H	-0.36202300	3.90161200	-2.50023900
57	H	4.68145900	-0.65183100	-2.00369000
58	H	6.54463800	-0.22032100	-0.38705500
59	H	6.05706700	-0.05223200	2.05361300
60	H	1.89996400	-0.75090400	1.27144100
61	H	2.78650500	-0.39533000	3.31666300

Table S14. The Cartesian coordinates for the lowest-energy conformer of (1*R*,3*S*,5*R*,6*S*,17*R*)-3a8 in the ECD calculations.

Number	Atom	X	Y	Z
1	C	4.13903300	-1.69825100	0.06384600
2	C	3.57815100	-1.53960600	-1.35401200
3	C	2.47159800	-0.48691300	-1.36091400
4	C	1.69476400	-0.23333300	-0.02934500
5	C	1.66418600	-1.49256000	0.90086700
6	C	3.10491100	-2.10697000	1.13775500
7	C	0.28274700	0.19931600	-0.39770100
8	C	-0.78153100	-0.63100300	-0.56344000
9	C	-0.58762400	-2.06749300	-0.33459500
10	C	0.78617600	-2.54197900	0.16217200
11	C	-2.10464000	-0.10053300	-1.05832800
12	C	-3.35626900	-0.35444500	-0.27508000
13	O	-1.46701100	-2.89463700	-0.54551000
14	C	0.96732100	-1.18375800	2.24544600
15	O	2.23712000	0.19198900	-2.34199300
16	C	4.65563600	-1.21962900	-2.39739000
17	C	3.73209600	-1.84192800	2.51875200
18	C	2.26174900	1.09974700	0.55092000
19	C	1.45763100	2.16967100	-0.19822200
20	O	0.18692200	1.52924400	-0.49928000
21	C	1.20099800	3.50845700	0.53101500

| 22	C	0.44909000	3.34060200	1.85161000
23	C	0.45166300	4.46901000	-0.40036600
24	O	2.49148100	4.04029900	0.87456900
25	O	-2.14090100	0.56374000	-2.08485000
26	C	-3.35539600	-0.87408800	1.02472600
27	C	-4.56139500	-1.02227800	1.71147900
28	C	-5.76866800	-0.66554200	1.11670400
29	C	-5.77030300	-0.14681200	-0.18504100
30	C	-4.57010200	0.01448600	-0.87243200
31	O	-6.98176600	0.18863800	-0.72520800
32	H	4.94848100	-2.43835800	0.05257800
33	H	4.61242700	-0.74960700	0.35636200
34	H	3.09813800	-2.48612800	-1.64798500
35	H	2.97290000	-3.19527600	1.06181700
36	H	0.60045900	-3.40436900	0.81166900
37	H	1.30832200	-2.94422100	-0.71510400
38	H	1.52504500	-0.47736600	2.86488100
39	H	-0.03294800	-0.77101400	2.08865000
40	H	0.85335400	-2.10560500	2.82569100
41	H	4.21019000	-1.07203700	-3.38366000
42	H	5.38211000	-2.03711000	-2.45542500
43	H	5.19602000	-0.30284500	-2.13379500
44	H	4.71976700	-2.31586100	2.56496900
45	H	3.13671600	-2.24994000	3.33987100
46	H	3.87873900	-0.77105400	2.70405700
47	H	3.33474600	1.22592000	0.39255100
48	H	2.07818300	1.15440600	1.62559900
49	H	1.92808500	2.38526500	-1.16411500
50	H	-0.50659200	2.83339700	1.69218400
51	H	0.25620100	4.32518500	2.28780100
52	H	1.03839200	2.77042500	2.57580900
53	H	0.31791300	5.43836300	0.09044900
54	H	1.01242700	4.62625400	-1.33166800
55	H	-0.52977600	4.06927500	-0.67222400
56	H	2.88880900	4.39888900	0.06432900
57	H	-2.42522100	-1.16685200	1.49745200
58	H	-4.56240200	-1.42423900	2.72099300
59	H	-6.71410900	-0.78178200	1.63740100
60	H	-4.54472300	0.42935100	-1.87699800
61	H	-6.83933000	0.51774000	-1.62653300

Table S15. The NO inhibitory effects of compounds 1−3 at the maximum safe concentrations on LPS-induced RAW264.7 macrophages.

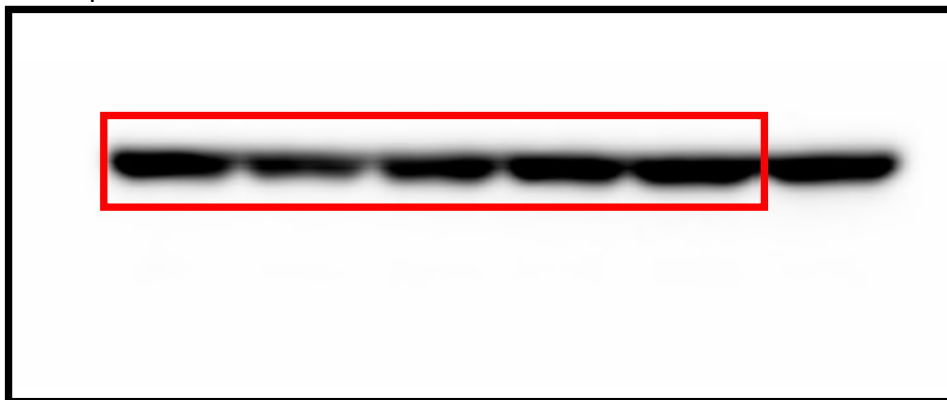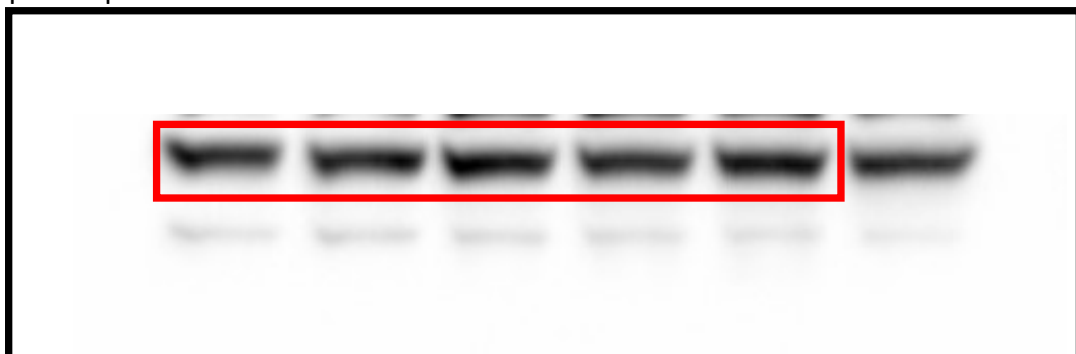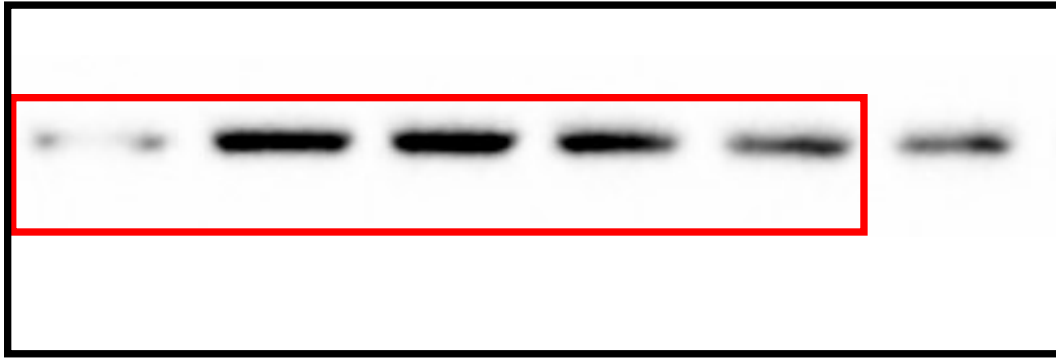| compound	concentration (μM)	NO inhibition rate
1	100	70.88 ± 0.10%
2	5*0*	73.39 ± 0.02%
3	50	26.60 ± 0.23%
DEX	10	71.90 ± 0.10%

cleaved IL-1β
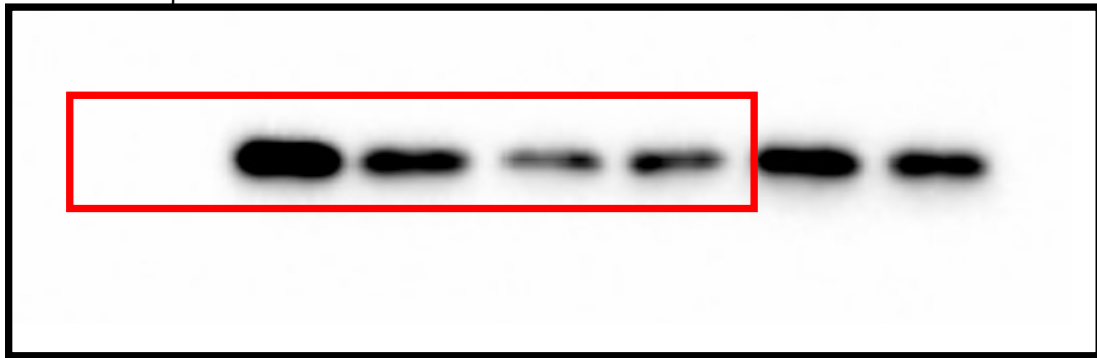
NLRP3
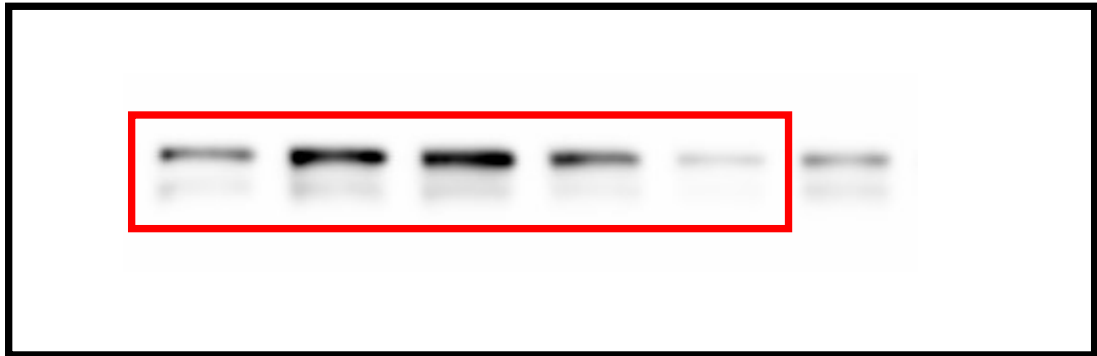
pro-IL-1β

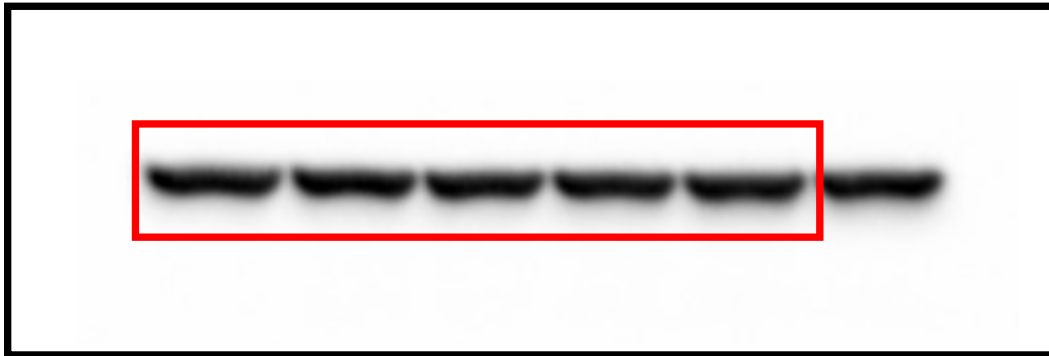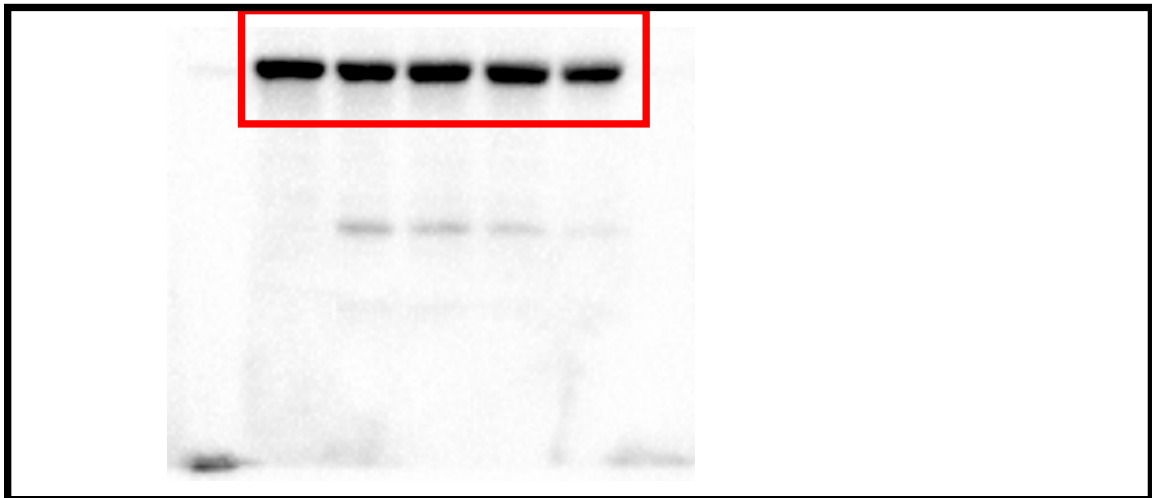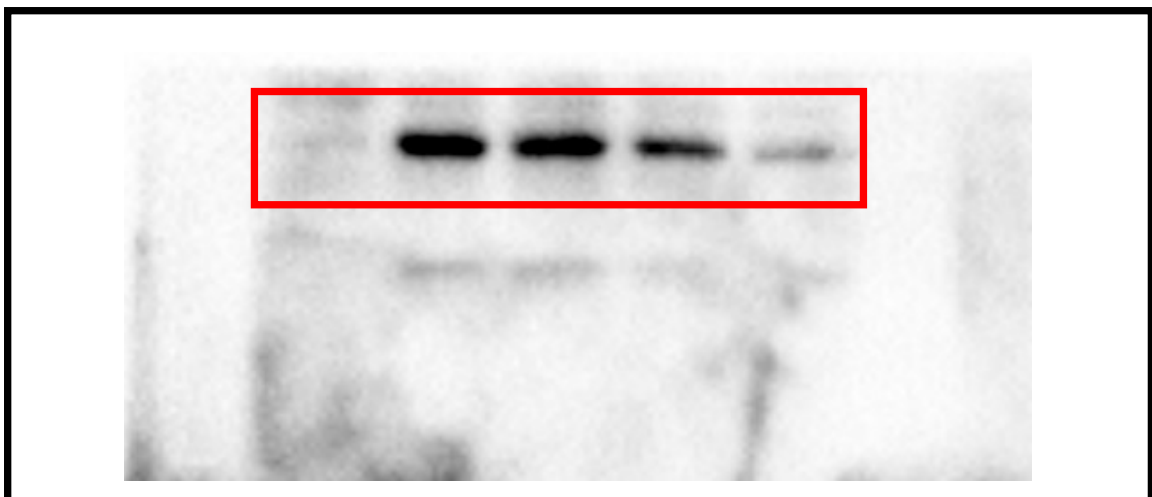
pro-caspase 1
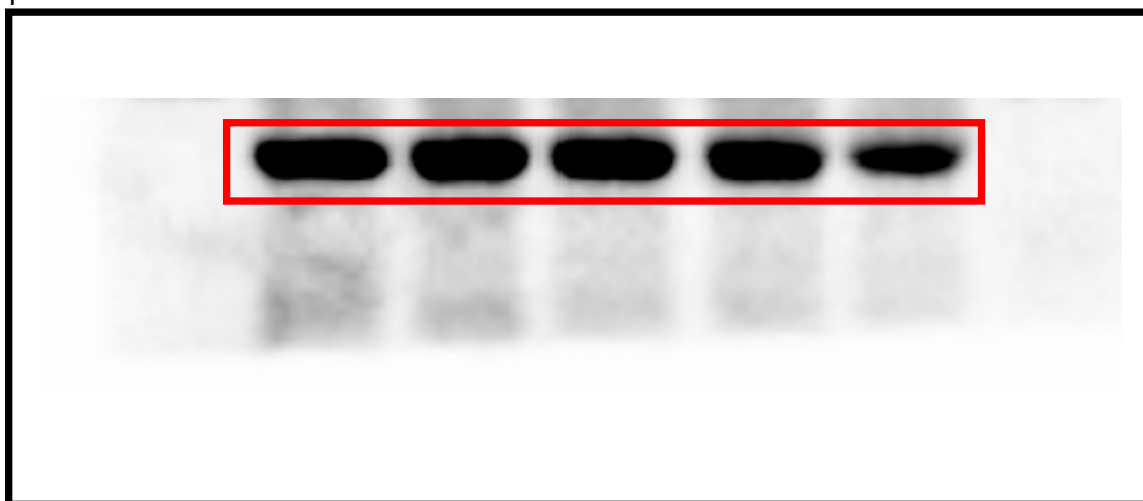
cleaved caspase 1

β-actin

pro-GSDMD

GSDMD-N

β-actin

Fig. S41. Uncropped blots.

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