Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

Laxiflorol A, the First Example of 7,8:15,16-di-*seco*-15-nor-21-homo-*ent*-Kauranoid from *Isodon eriocalyx* var. *laxiflora*

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Contents of Supporting Information

Figure S1. ^{13}C NMR spectrum of laxiflorol A (**1**)

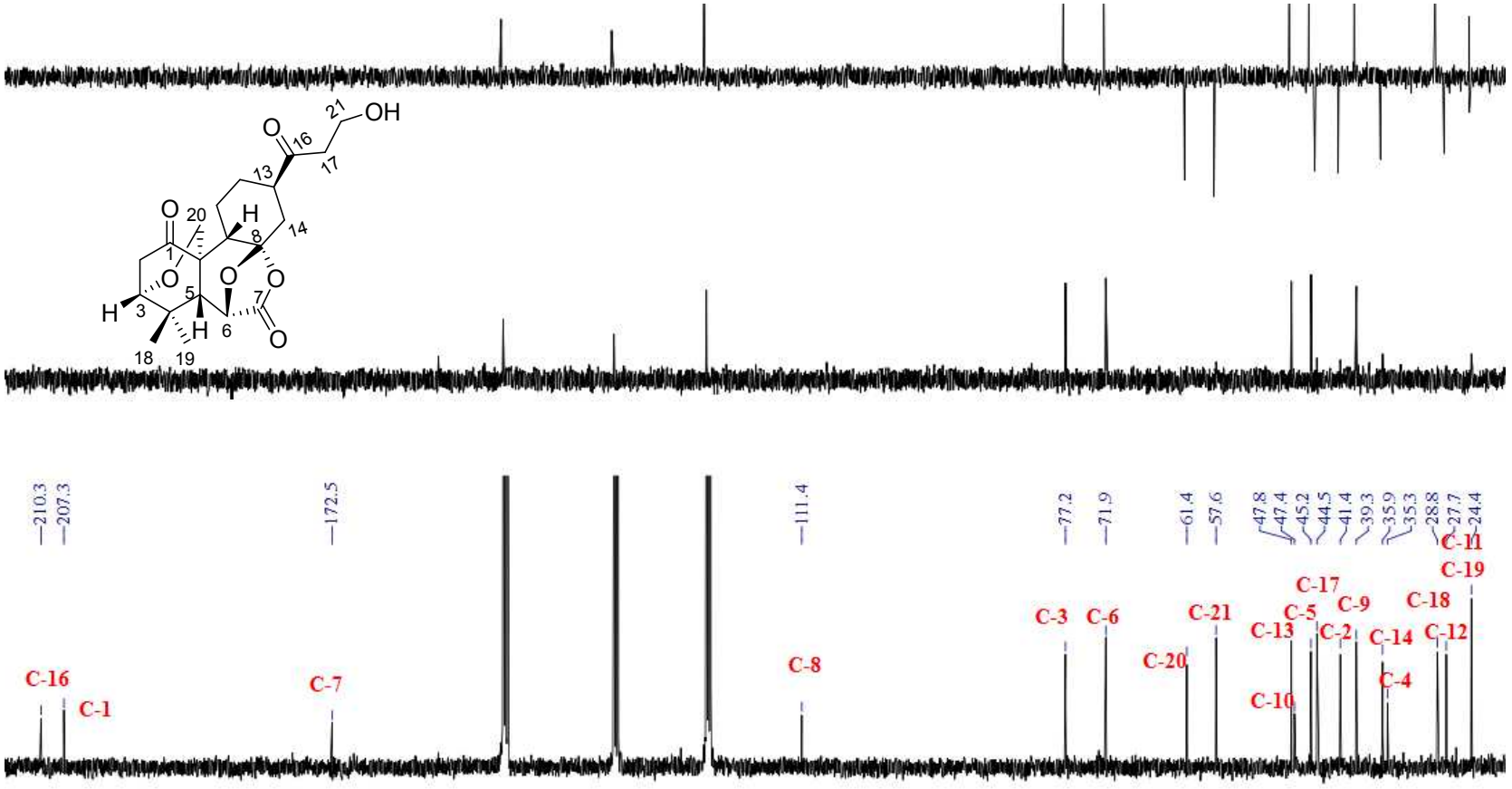


Figure S2. ^{1}H NMR spectrum of laxiflorol A (**1**)

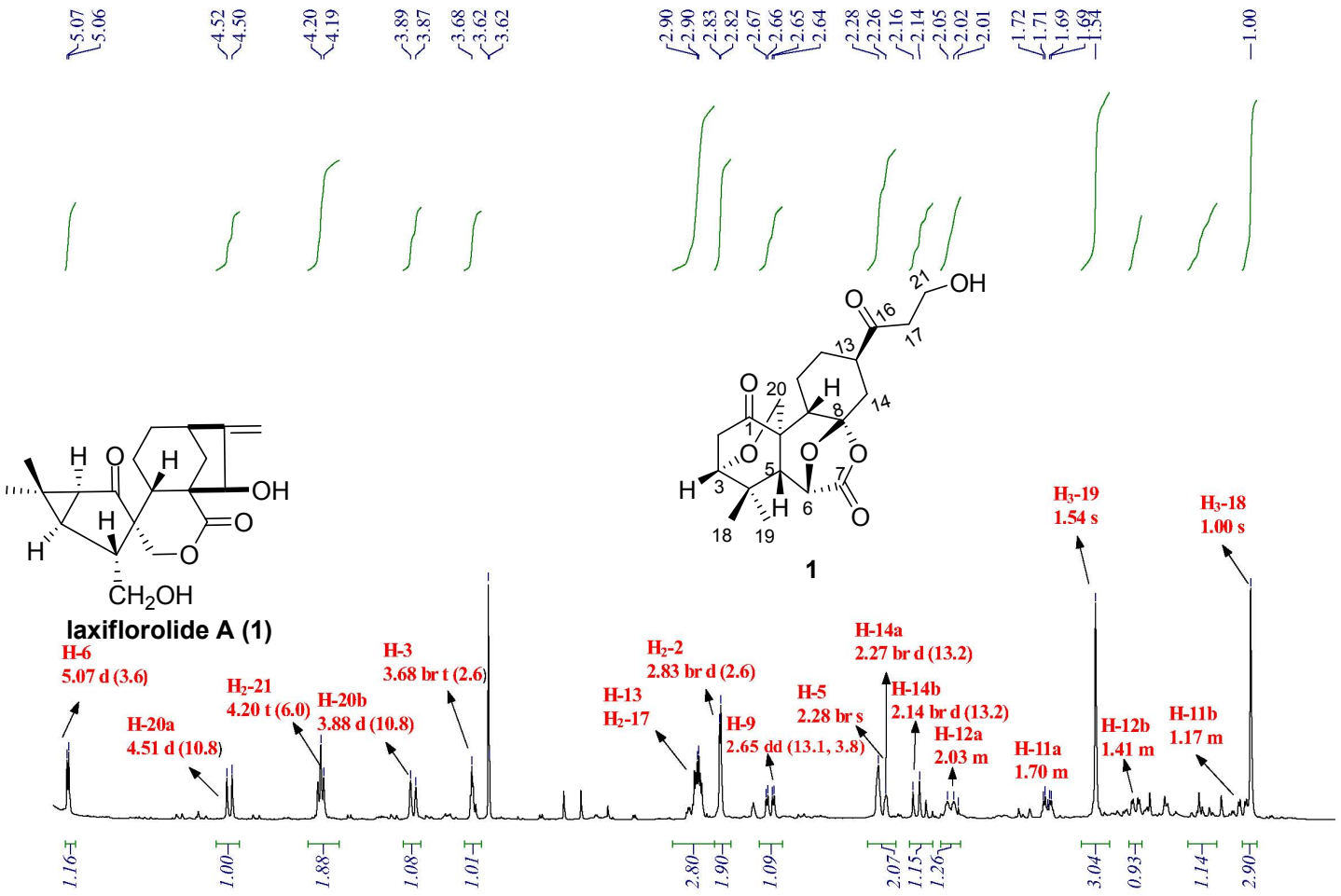

5.07
5.06
4.52
4.50
4.20
4.19
3.89
3.87
3.68
3.62
3.62
2.90
2.90
2.83
2.82
2.67
2.66
2.65
2.64
2.28
2.26
2.16
2.14
2.05
2.02
2.01
1.72
1.71
1.69
1.54
1.00
laxiflorolide A (1)
1
H-6
5.07 d (3.6)
H-20a
4.51 d (10.8)
H2-21
4.20 t (6.0)
H-20b
3.88 d (10.8)
H-3
3.68 br t (2.6)
H-13
H2-17
H2-2
2.83 br d (2.6)
H-9
2.65 dd (13.1, 3.8)
H-5
2.28 br s
H-14a
2.27 br d (13.2)
H-14b
2.14 br d (13.2)
H-12a
2.03 m
H-11a
1.70 m
H3-19
1.54 s
H-12b
1.41 m
H-11b
1.17 m
H3-18
1.00 s
1.16
1.00
1.88
1.08
1.01
2.80
1.90
1.09
2.07
1.15
1.26
3.04
0.93
1.14
2.90

Figure S3. HSQC spectrum of laxiflorol A (**1**)

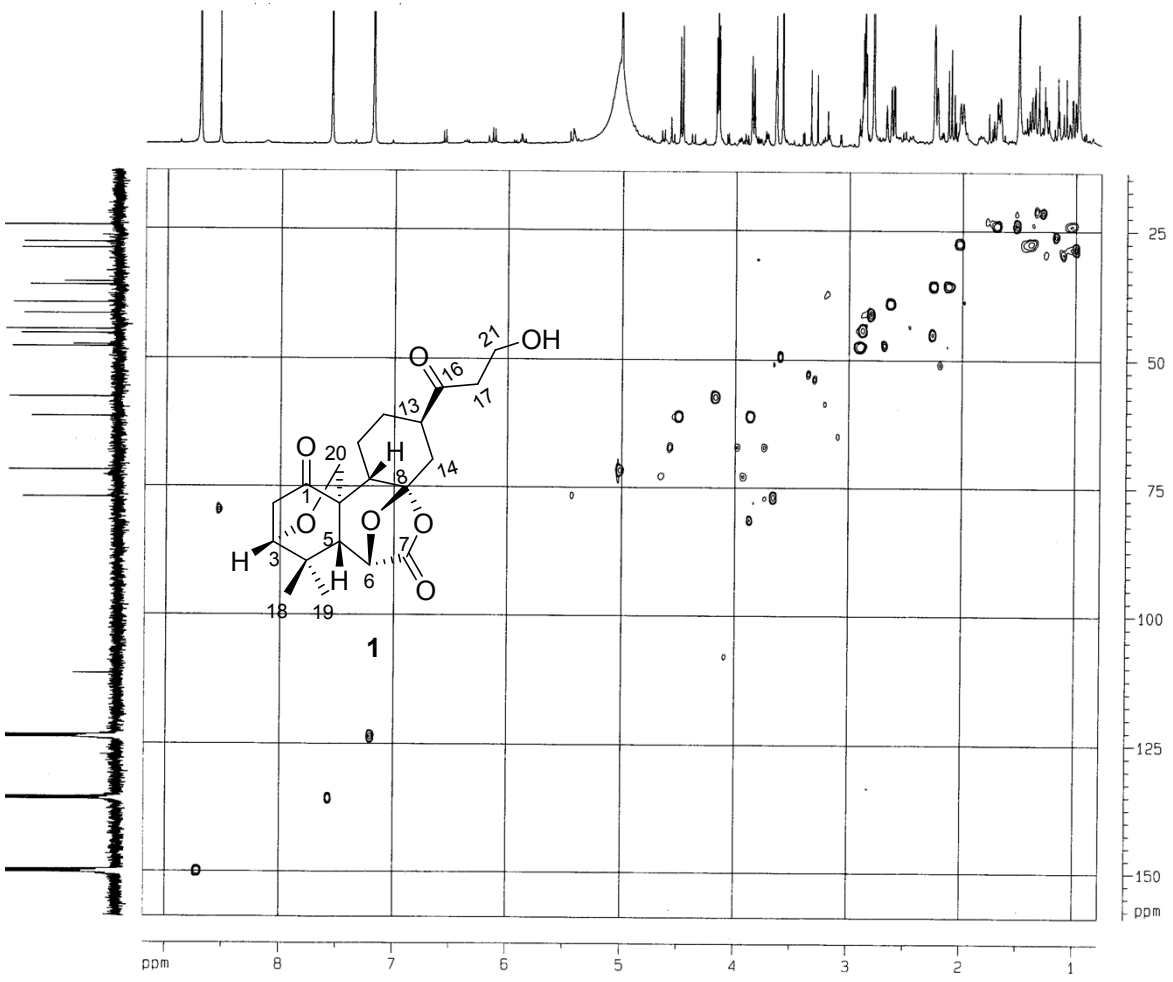


Figure S4. HSQC-TOCSY spectrum of laxiflorol A (**1**)

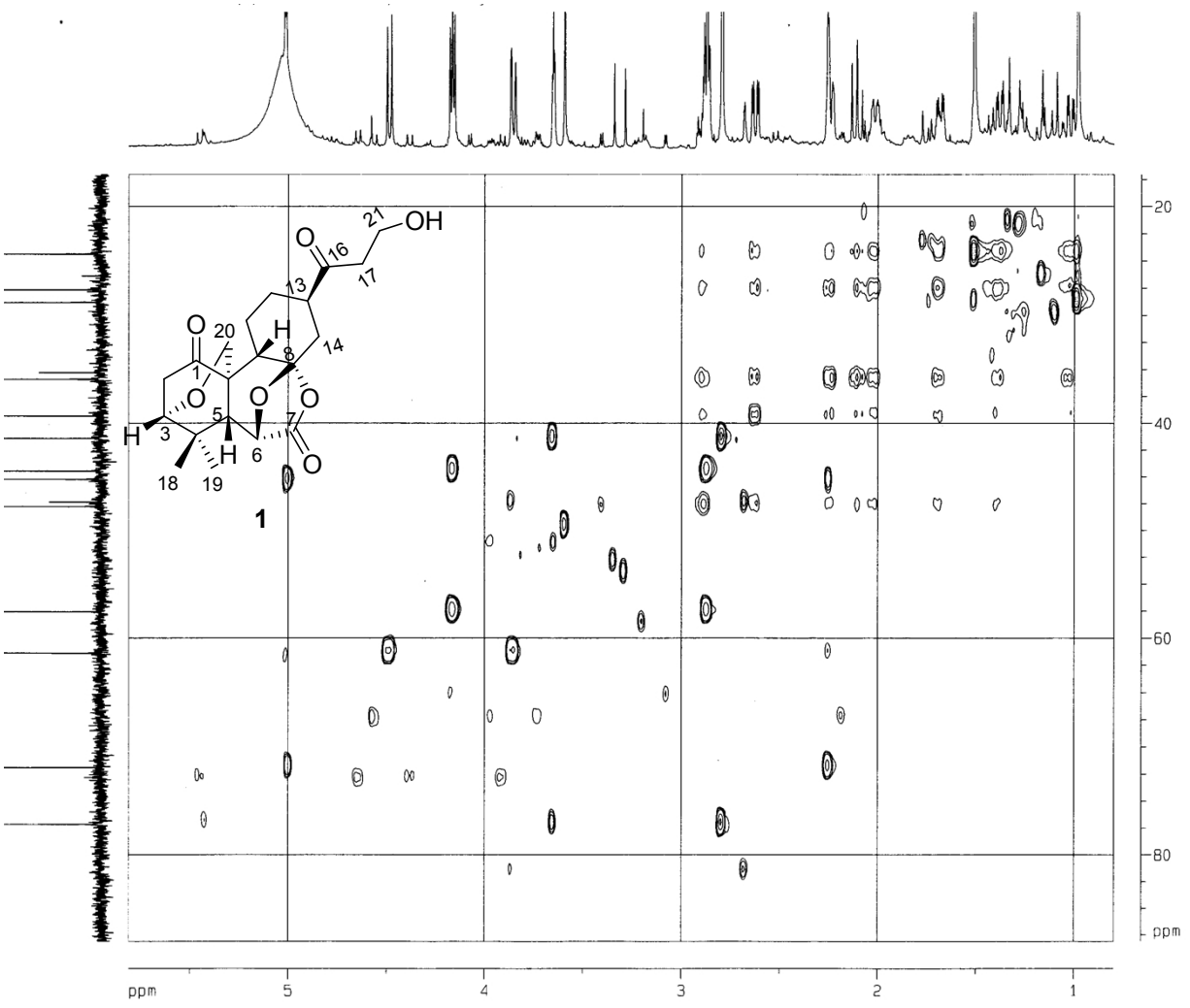
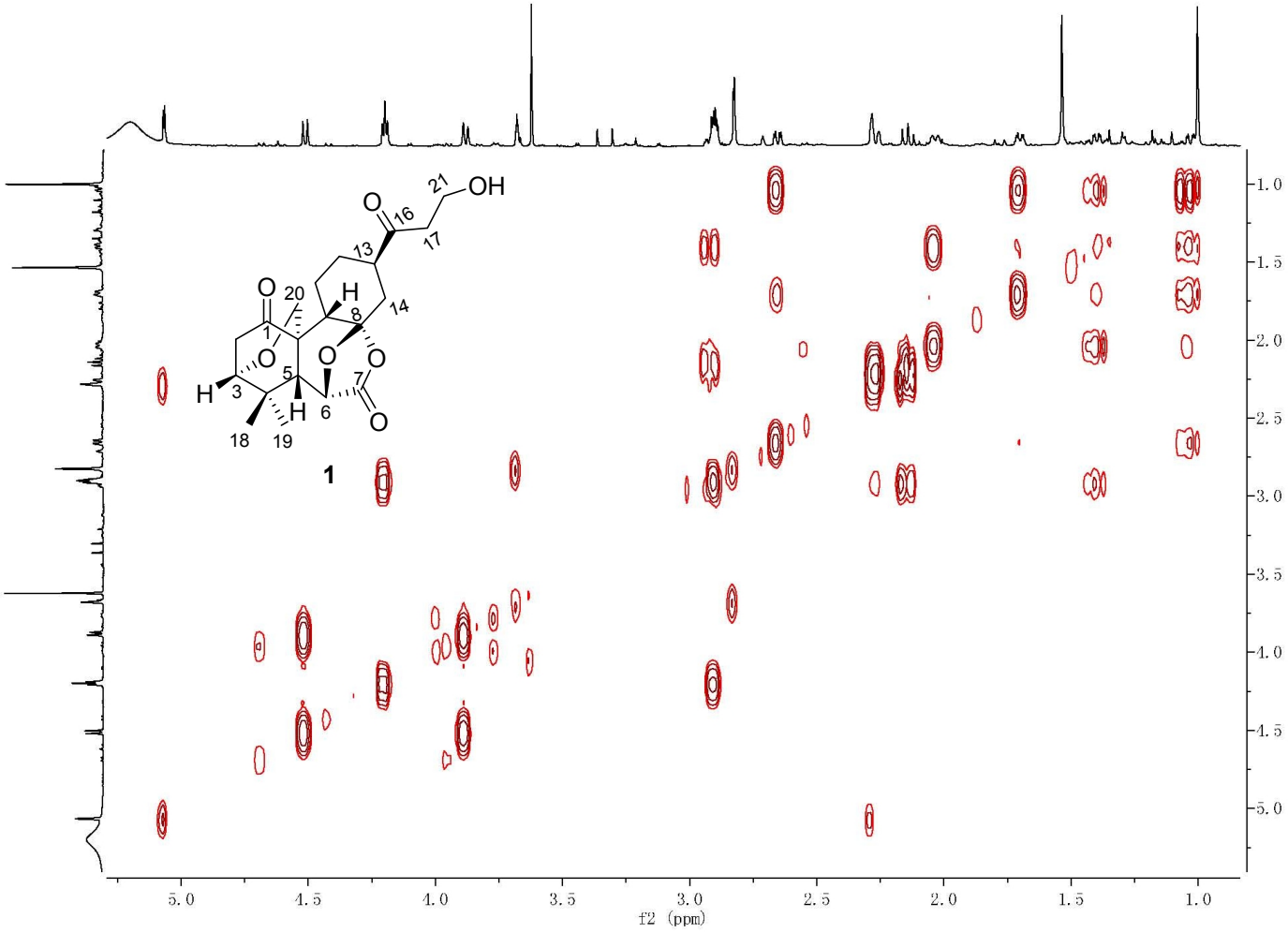
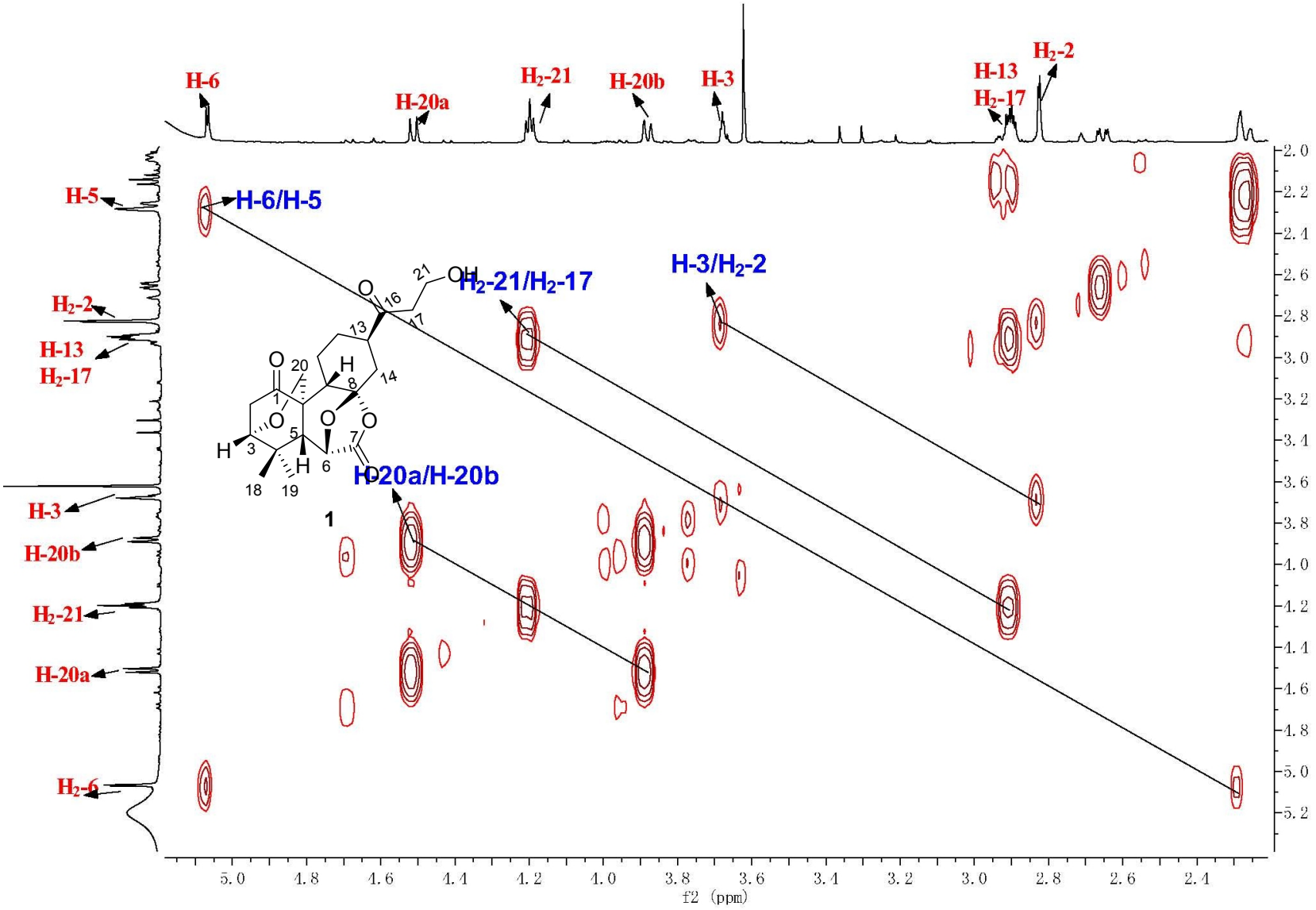


Figure S5. ^{1}H-^{1}H COSY spectrum of laxiflorol A (**1**)




H-6
H-20a
H2-21
H-20b
H-3
H-13
H2-17
H2-2
H-5
H-6/H-5
H2-21/H2-17
H-3/H2-2
H2-2
H-13
H2-17
H-3
H-20b
H2-21
H-20a
H2-6
H-20a/H-20b
1
f2 (ppm)

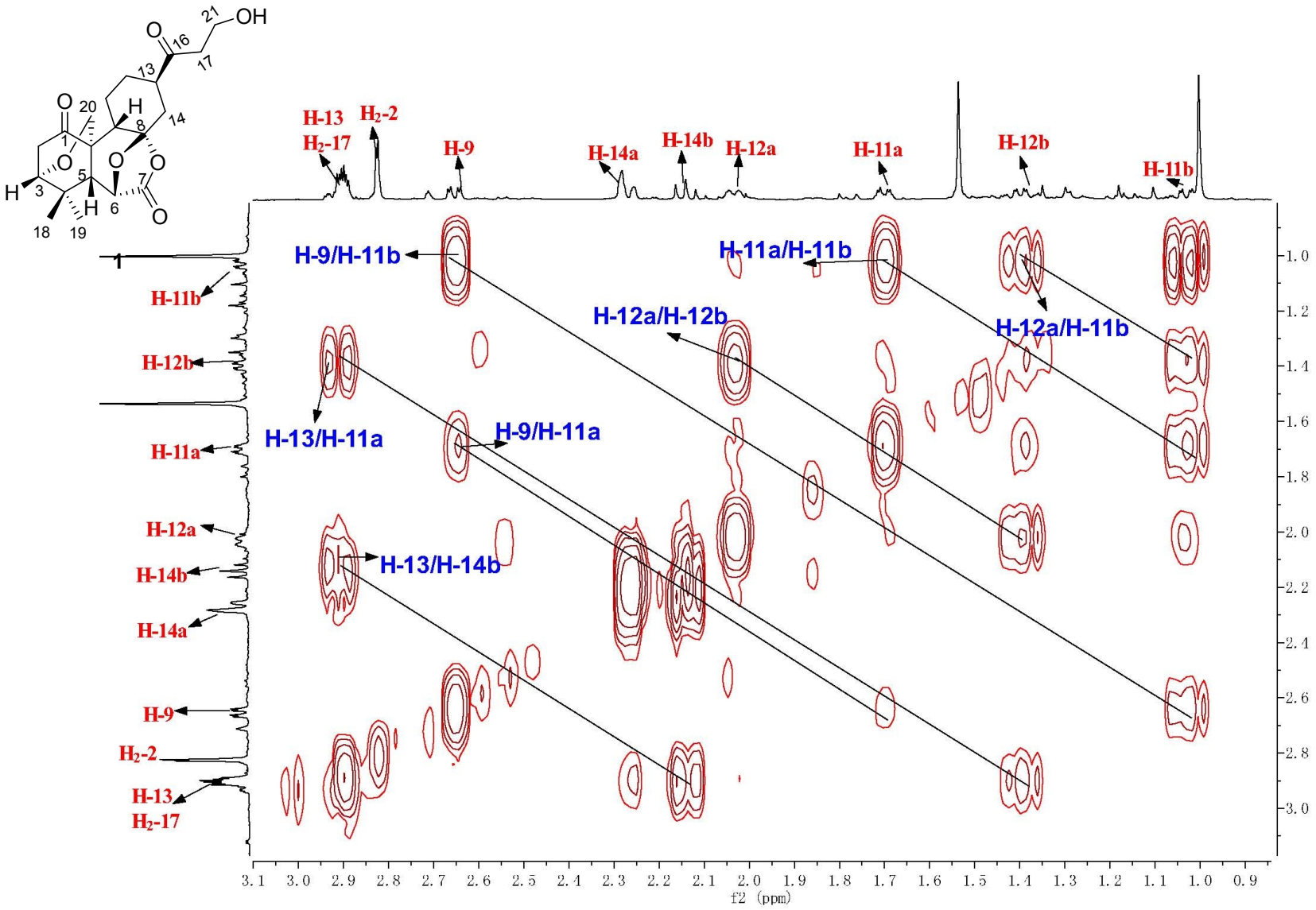
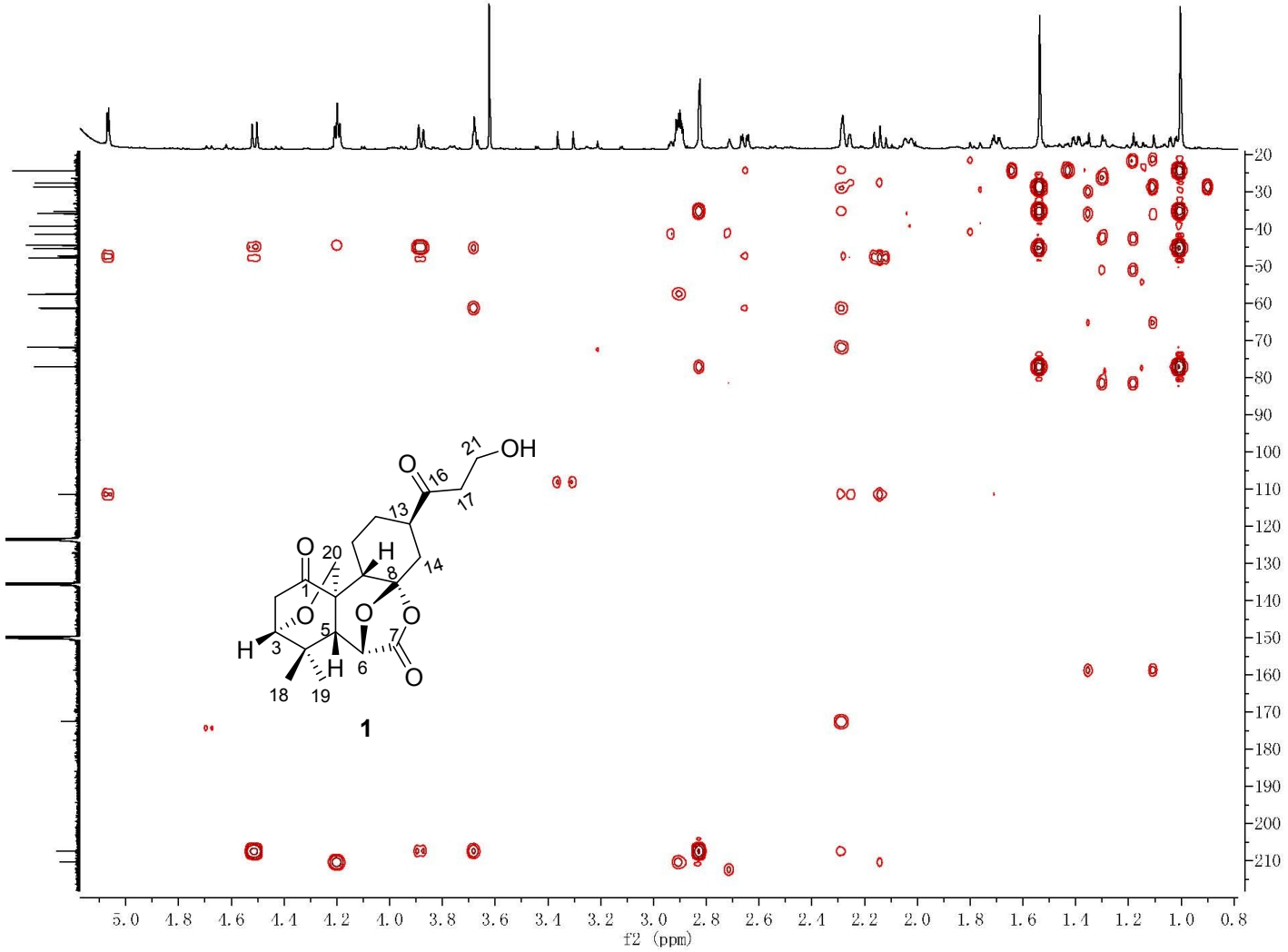
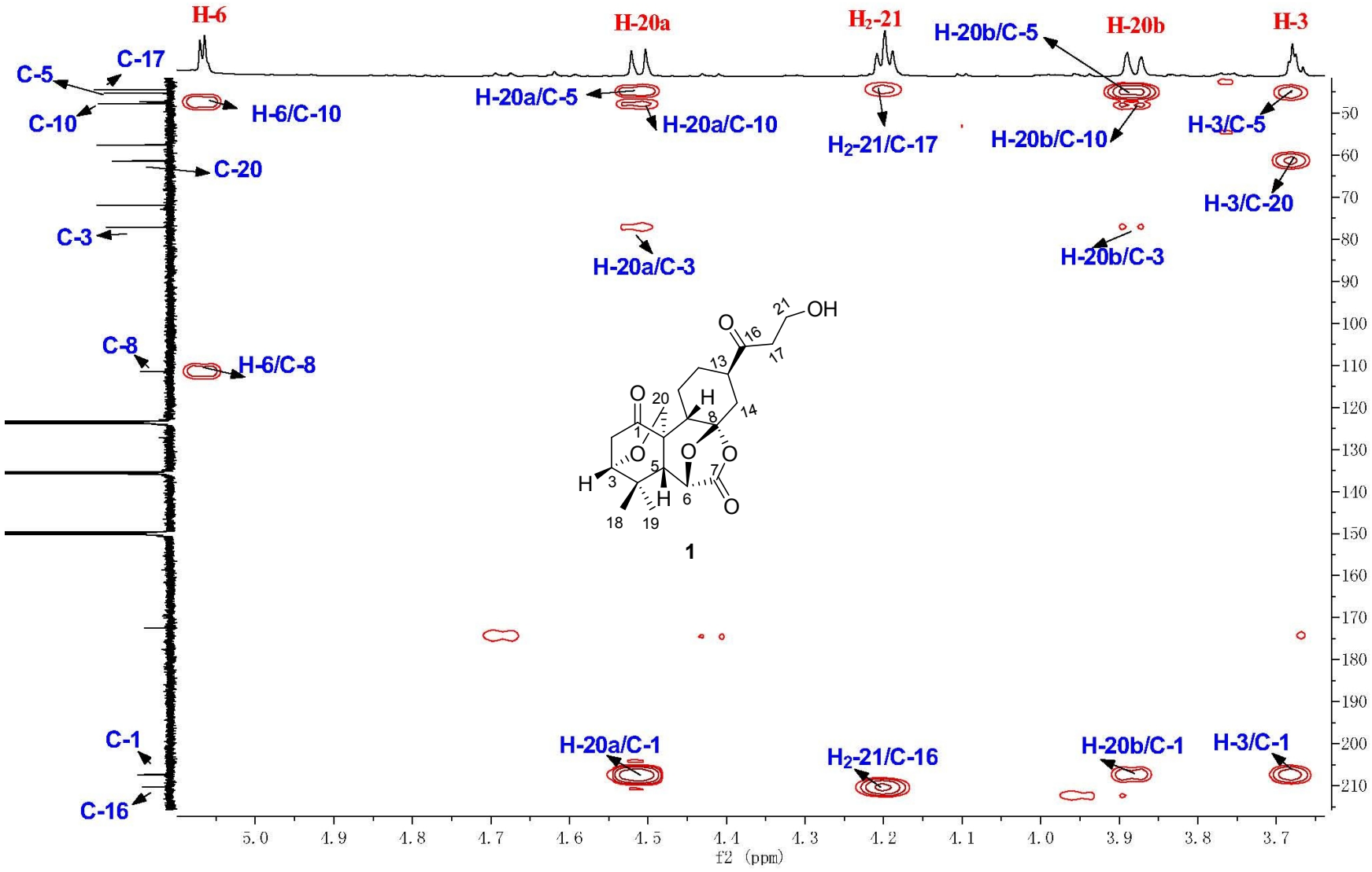
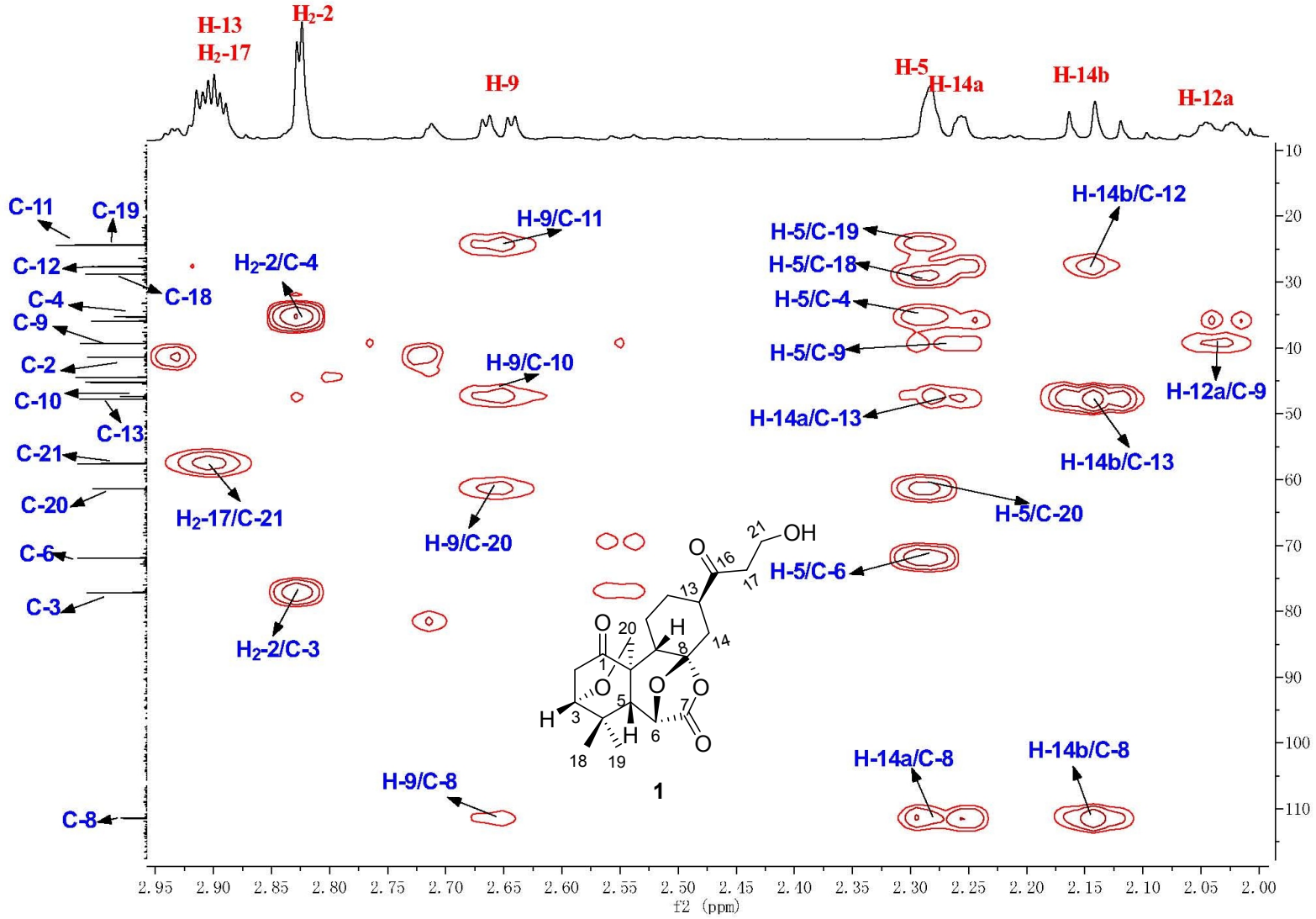
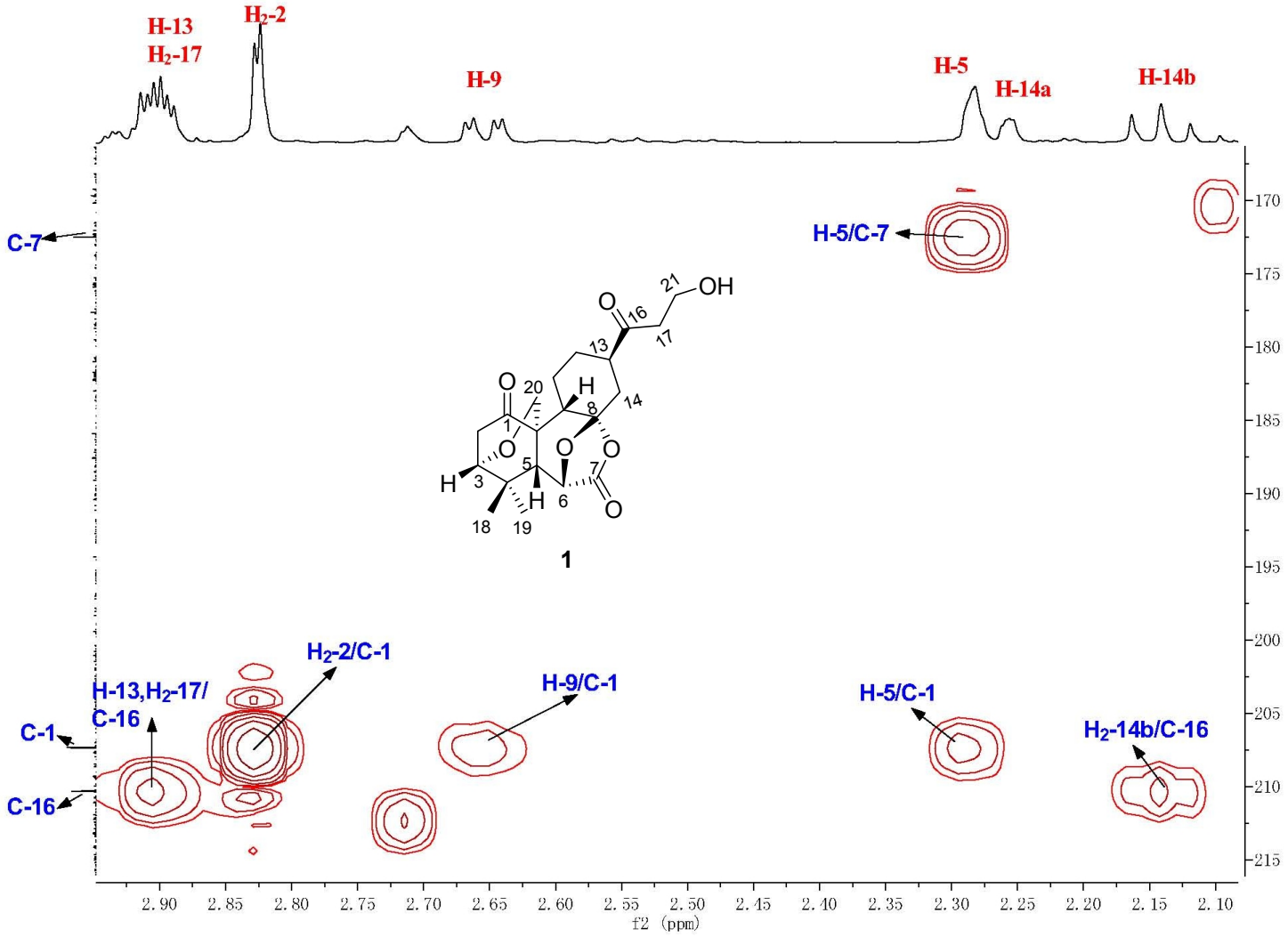

H-13
H2-17
H2-2
H-9
H-14a
H-14b
H-12a
H-11a
H-12b
H-11b
H-9/H-11b
H-11a/H-11b
H-12a/H-12b
H-12a/H-11b
H-13/H-11a
H-9/H-11a
H-13/H-14b
f2 (ppm)

Figure S6. HMBC spectrum of laxiflorol A (**1**)

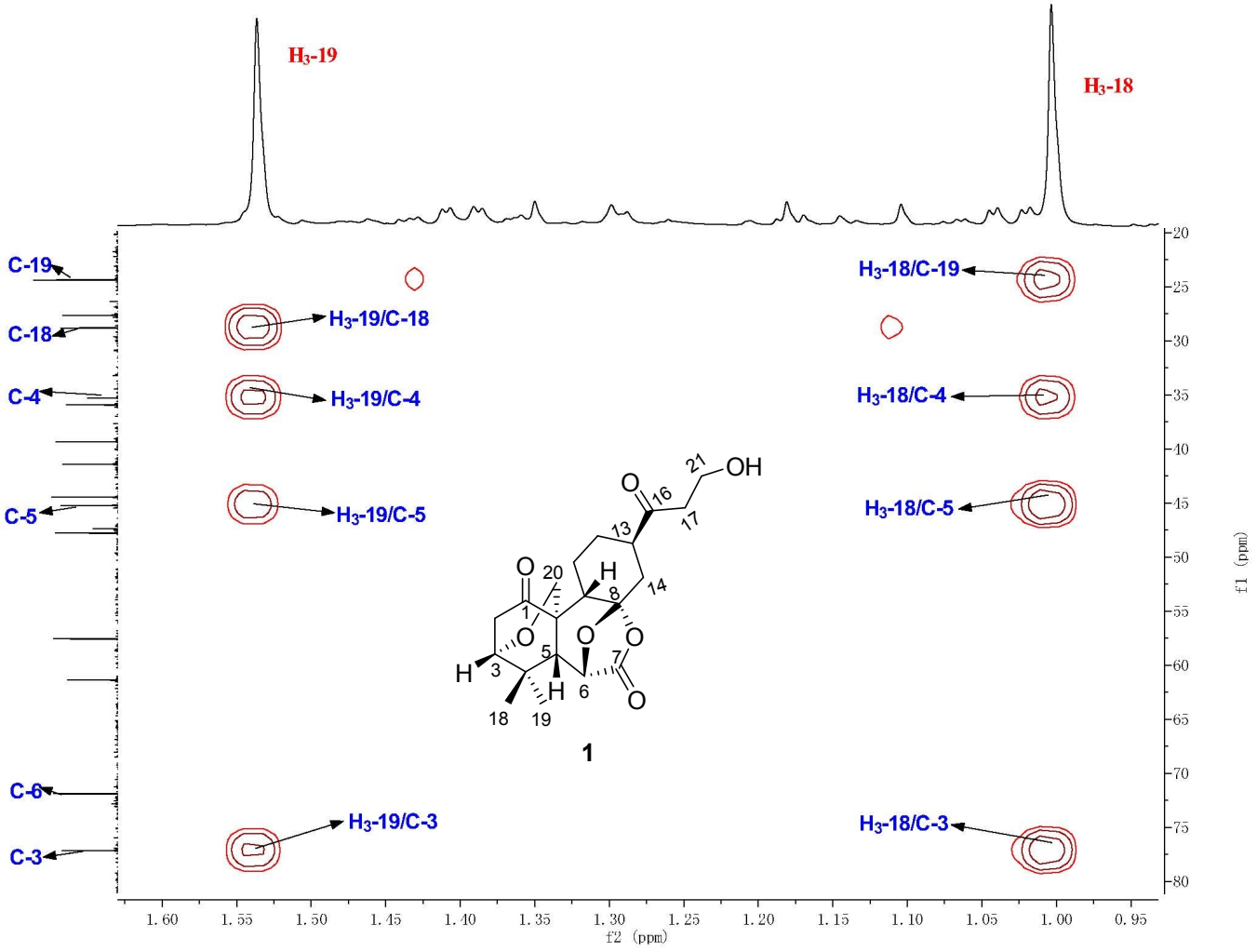



H-6
H-20a
H2-21
H-20b/C-5
H-20b
H-3
C-5
C-17
C-10
H-6/C-10
H-20a/C-5
H-20a/C-10
H2-21/C-17
H-20b/C-10
H-3/C-5
C-20
H-3/C-20
C-3
H-20a/C-3
H-20b/C-3
C-8
H-6/C-8
1
C-1
C-16
H-20a/C-1
H2-21/C-16
H-20b/C-1
H-3/C-1
f2 (ppm)


H-13
H2-17
H2-2
H-9
H-5
H-14a
H-14b
H-12a
C-11
C-19
C-12
C-18
C-4
C-9
C-2
C-10
C-13
C-21
C-20
C-6
C-3
C-8
H2-2/C-4
H-9/C-11
H-9/C-10
H2-17/C-21
H-9/C-20
H2-2/C-3
H-9/C-8
H-5/C-19
H-5/C-18
H-5/C-4
H-5/C-9
H-14a/C-13
H-5/C-20
H-5/C-6
H-14b/C-12
H-12a/C-9
H-14b/C-13
H-14a/C-8
H-14b/C-8
1
f2 (ppm)


H-13
H2-17
H2-2
H-9
H-5
H-14a
H-14b
C-7
H-5/C-7
OH
1
H-13,H2-17/
C-16
H2-2/C-1
H-9/C-1
H-5/C-1
H2-14b/C-16
C-1
C-16
2.90 2.85 2.80 2.75 2.70 2.65 2.60 2.55 2.50 2.45 2.40 2.35 2.30 2.25 2.20 2.15 2.10
f2 (ppm)
170 175 180 185 190 195 200 205 210 215

1


H3-19
H3-18
C-19
C-18
C-4
C-5
C-6
C-3
H3-19/C-18
H3-19/C-4
H3-19/C-5
H3-19/C-3
H3-18/C-19
H3-18/C-4
H3-18/C-5
H3-18/C-3
1
f2 (ppm)
f1 (ppm)

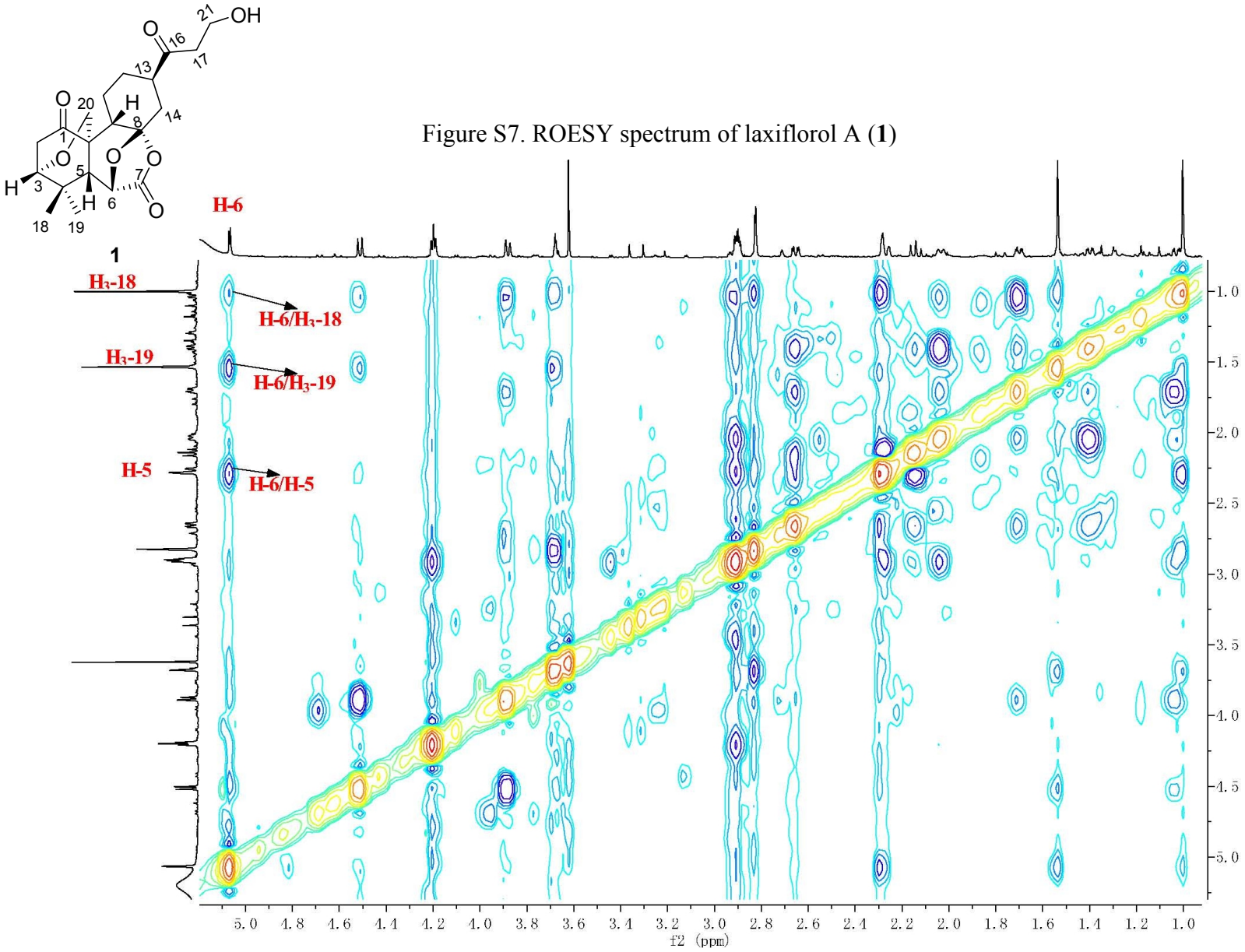


Figure S7. ROESY spectrum of laxiflorol A (**1**)

Figure S8. ESIMS spectrum of laxiflorol A (**1**)

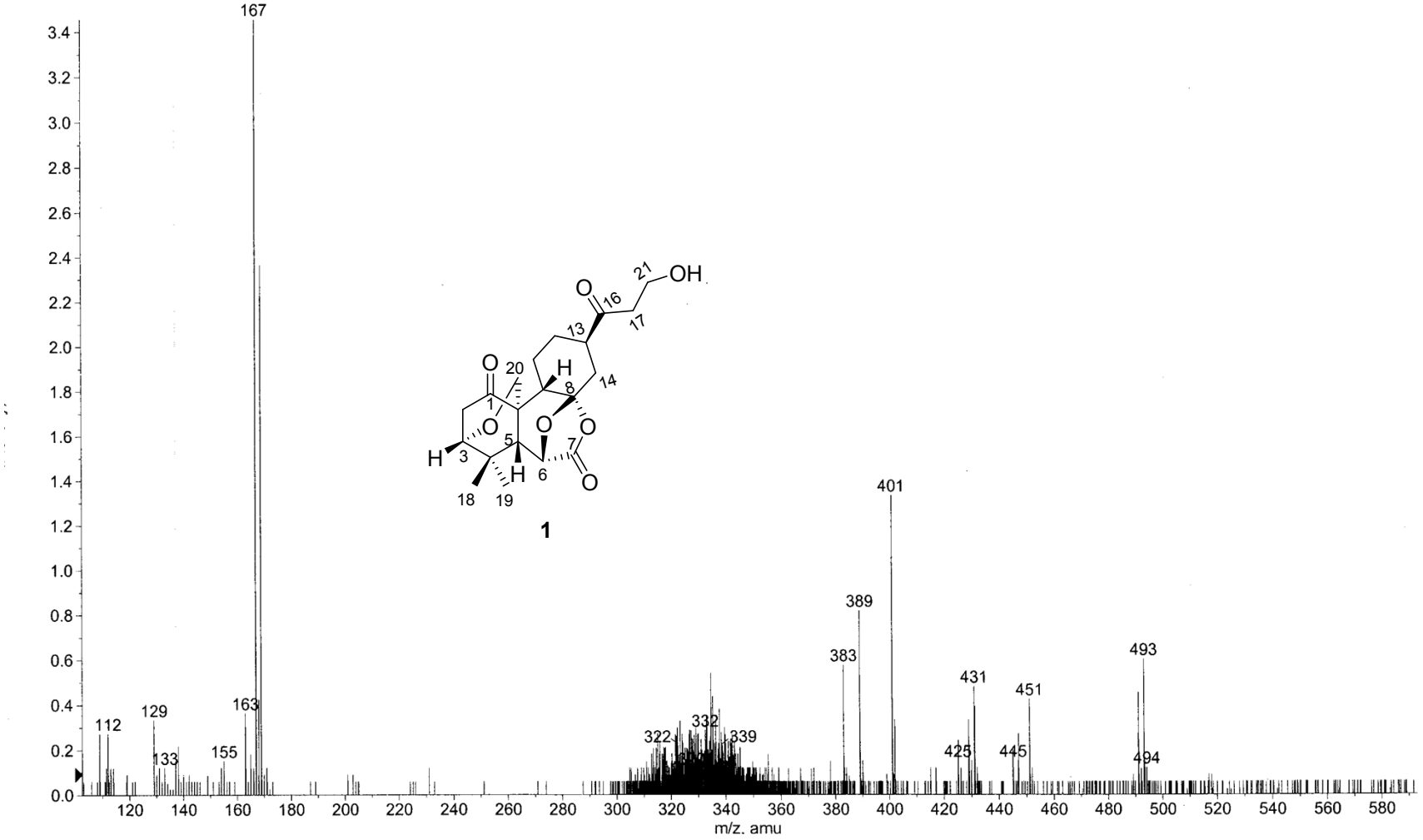
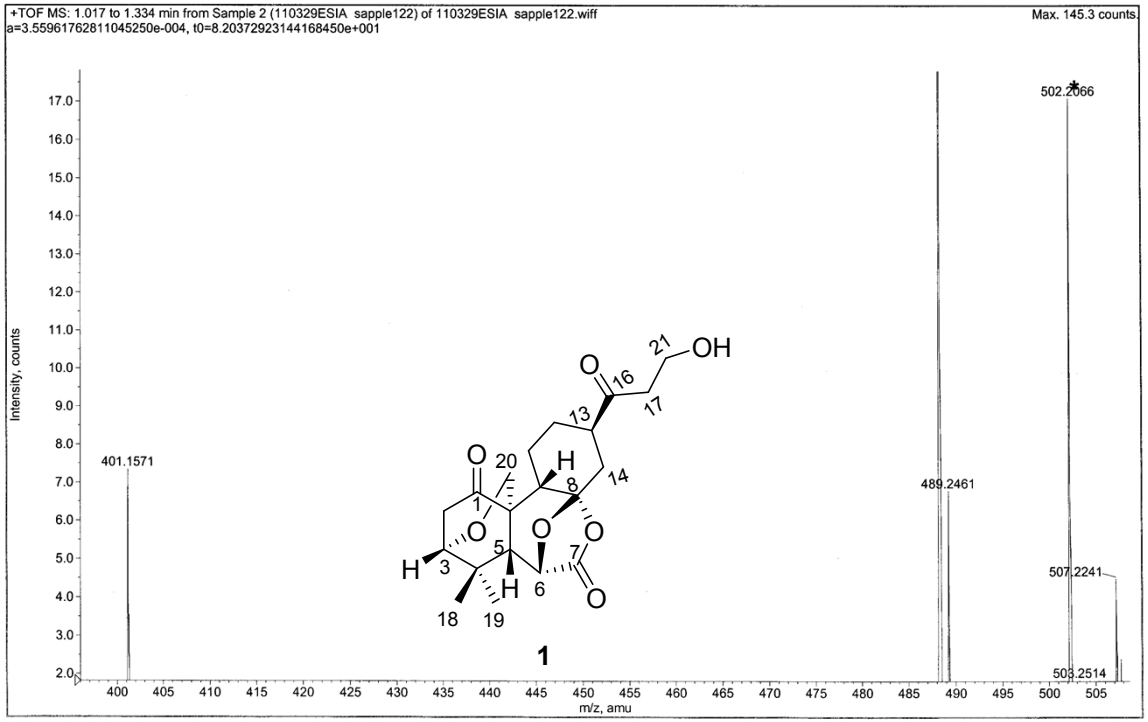


Figure S9. HRESIMS spectrum of laxiflorol A (**1**)



	Elements	Min Number	Max Number
11	Pt	0	0
12	S	0	0
13	Si	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C20 H26 O7 Na	401.1576	-0.5232	-1.3042	7.5

Figure S10. UV spectrum of laxiflorol A (**1**)

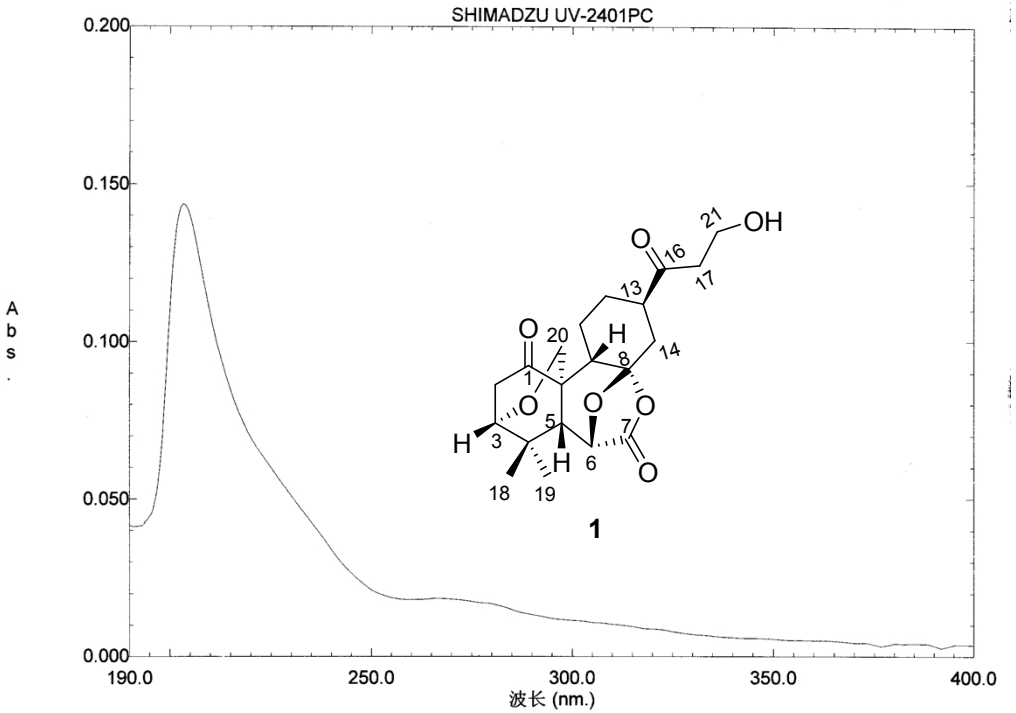


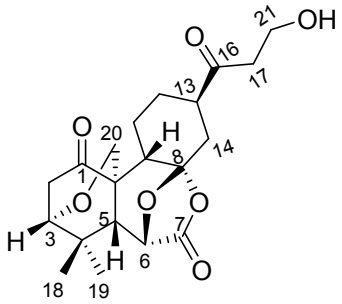
Figure S11. ORD spectrum of laxiflorol A (**1**)

Optical rotation measurement

Model : P-1020 (A060460638)

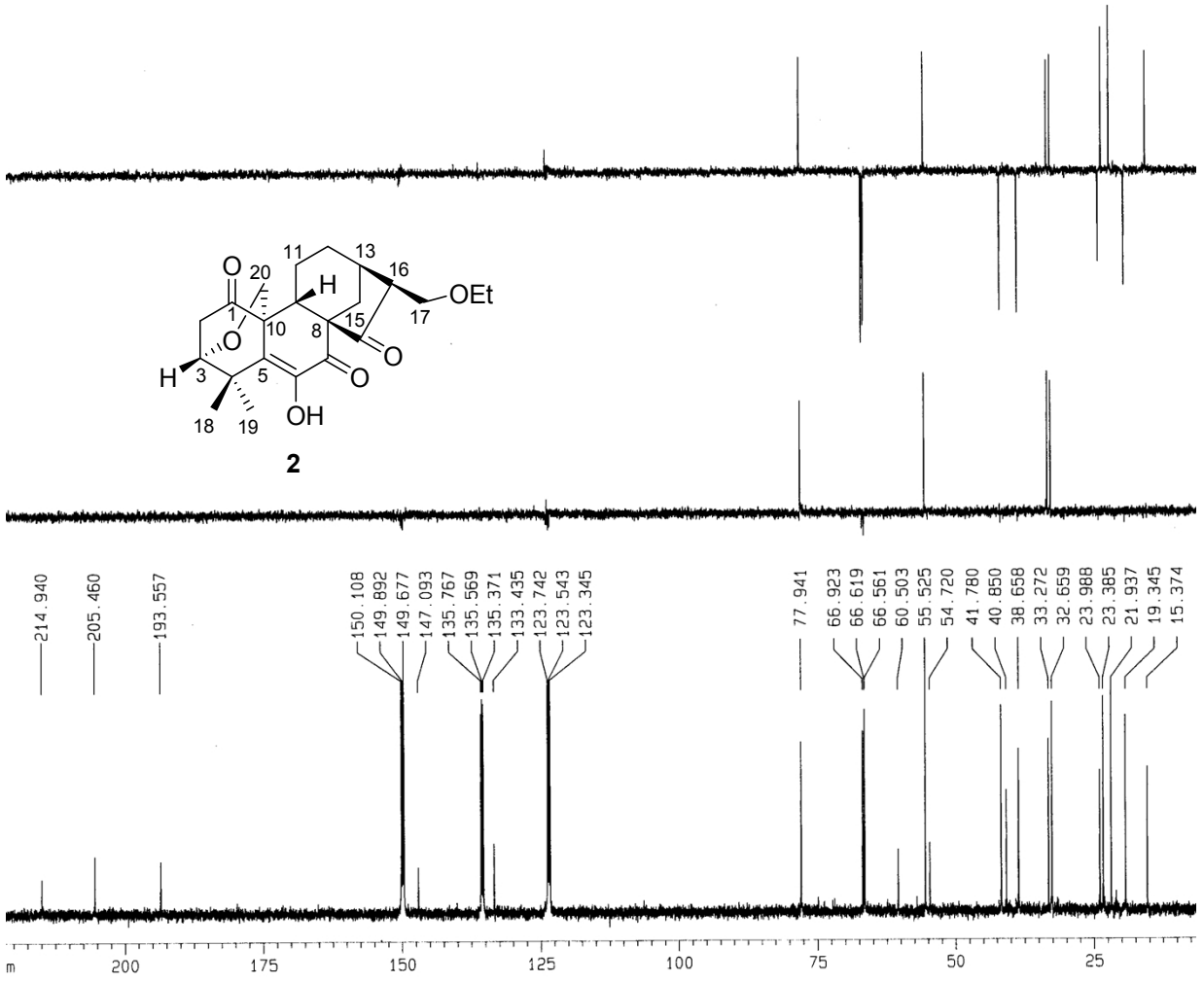
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	1 (1/3)	Sp.Rot	-29.0000	-0.0145 0.0000	12.6 50.00 Cell	Wed Mar 30 13:51:06 2011 0.00100g/mlMeOH SAPPLE122	Na 589nm	2 sec 10 sec
No.2	1 (2/3)	Sp.Rot	-29.2000	-0.0146 0.0000	12.6 50.00 Cell	Wed Mar 30 13:51:19 2011 0.00100g/mlMeOH SAPPLE122	Na 589nm	2 sec 10 sec
No.3	1 (3/3)	Sp.Rot	-30.6000	-0.0153 0.0000	12.6 50.00 Cell	Wed Mar 30 13:51:32 2011 0.00100g/mlMeOH SAPPLE122	Na 589nm	2 sec 10 sec

-29.6000°



1

Figure S12. ^{13}C NMR spectrum of laxiflorol B (**2**)



2

Figure S13. ^{1}H NMR spectrum of laxiflorol B (**2**)

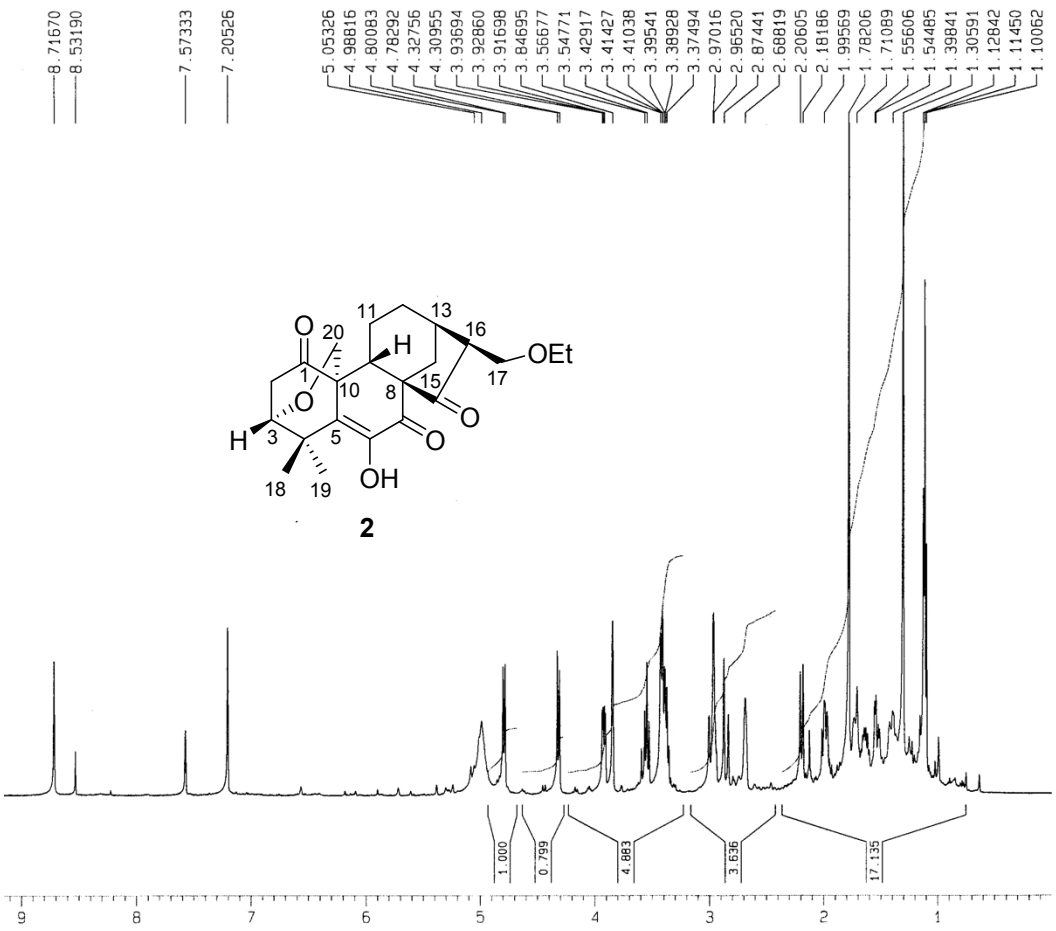


Figure S14. HSQC spectrum of laxiflorol B (**2**)

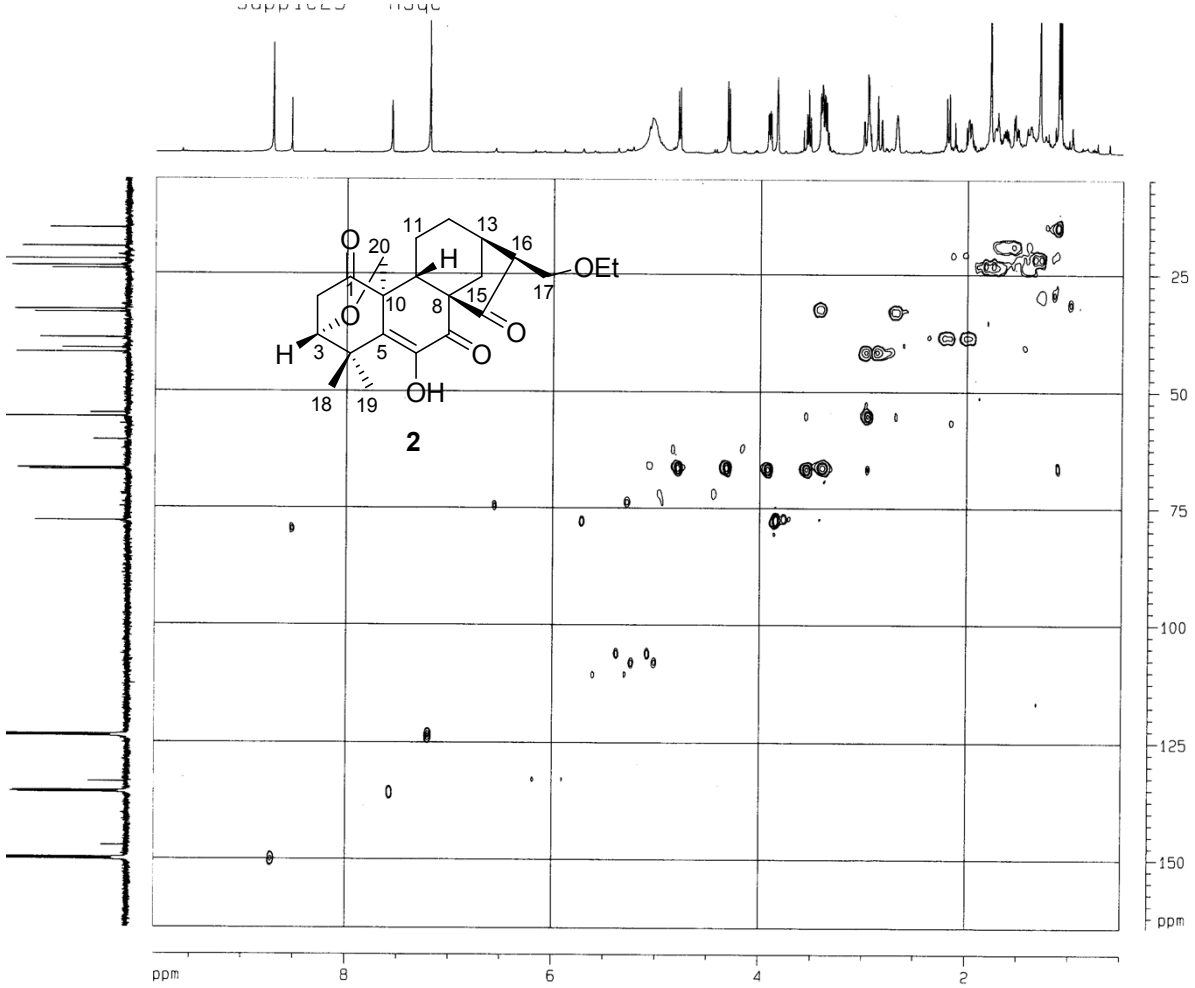


Figure S15. ^{1}H-^{1}H COSY spectrum of laxiflorol B (**2**)

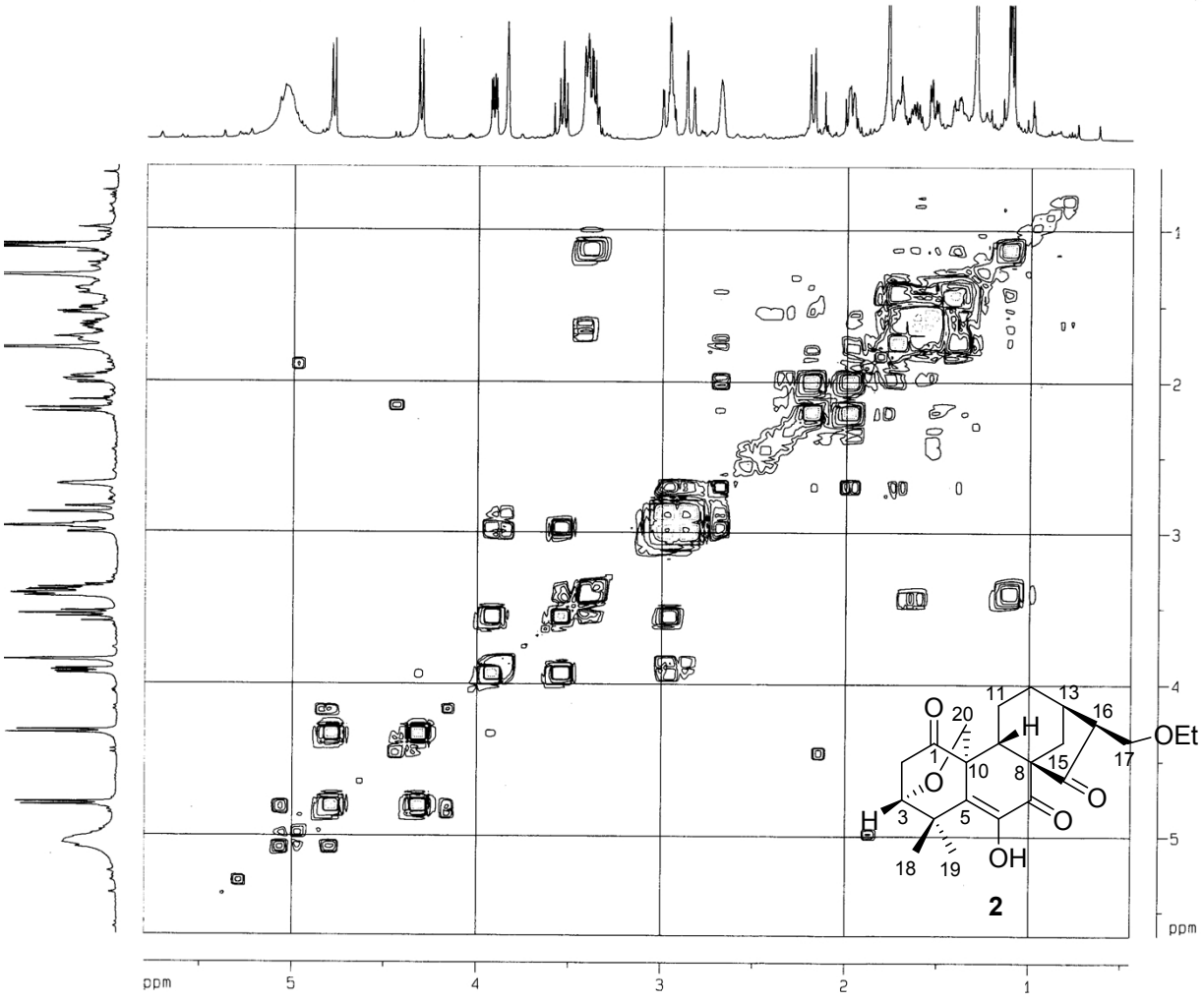


Figure S16. HMBC spectrum of laxiflorol B (**2**)

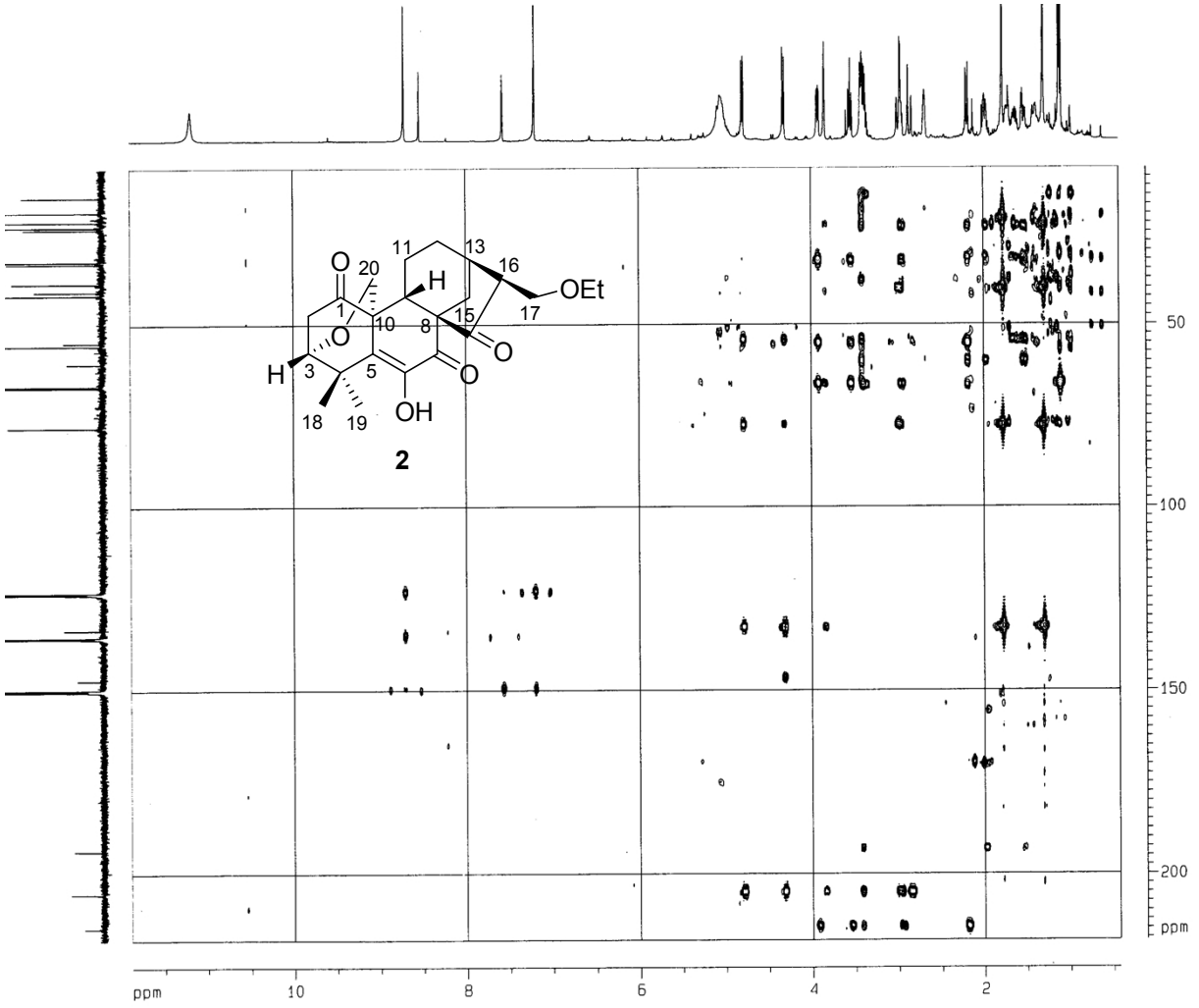


Figure S17. ROESY spectrum of laxiflorol B (**2**)

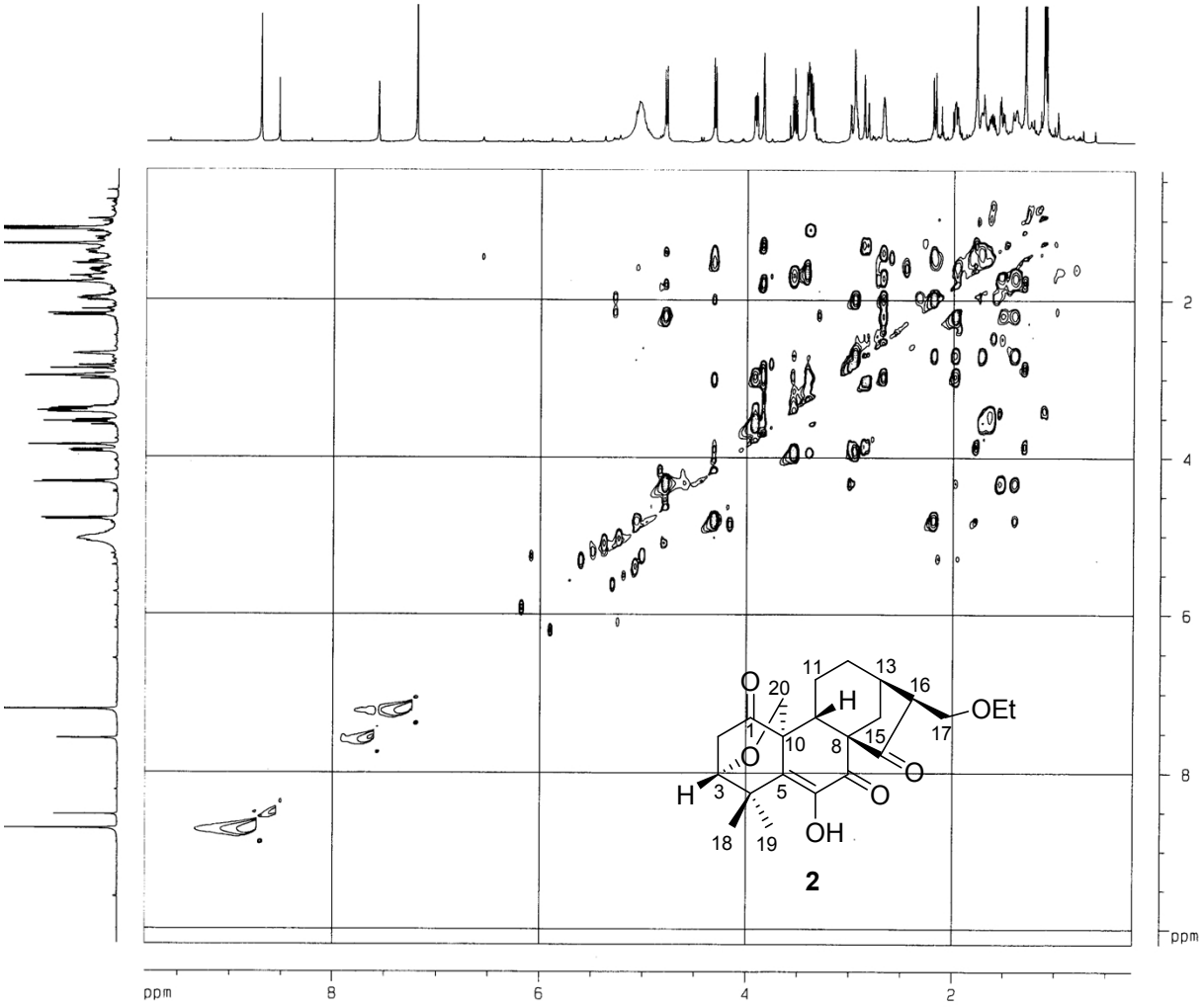
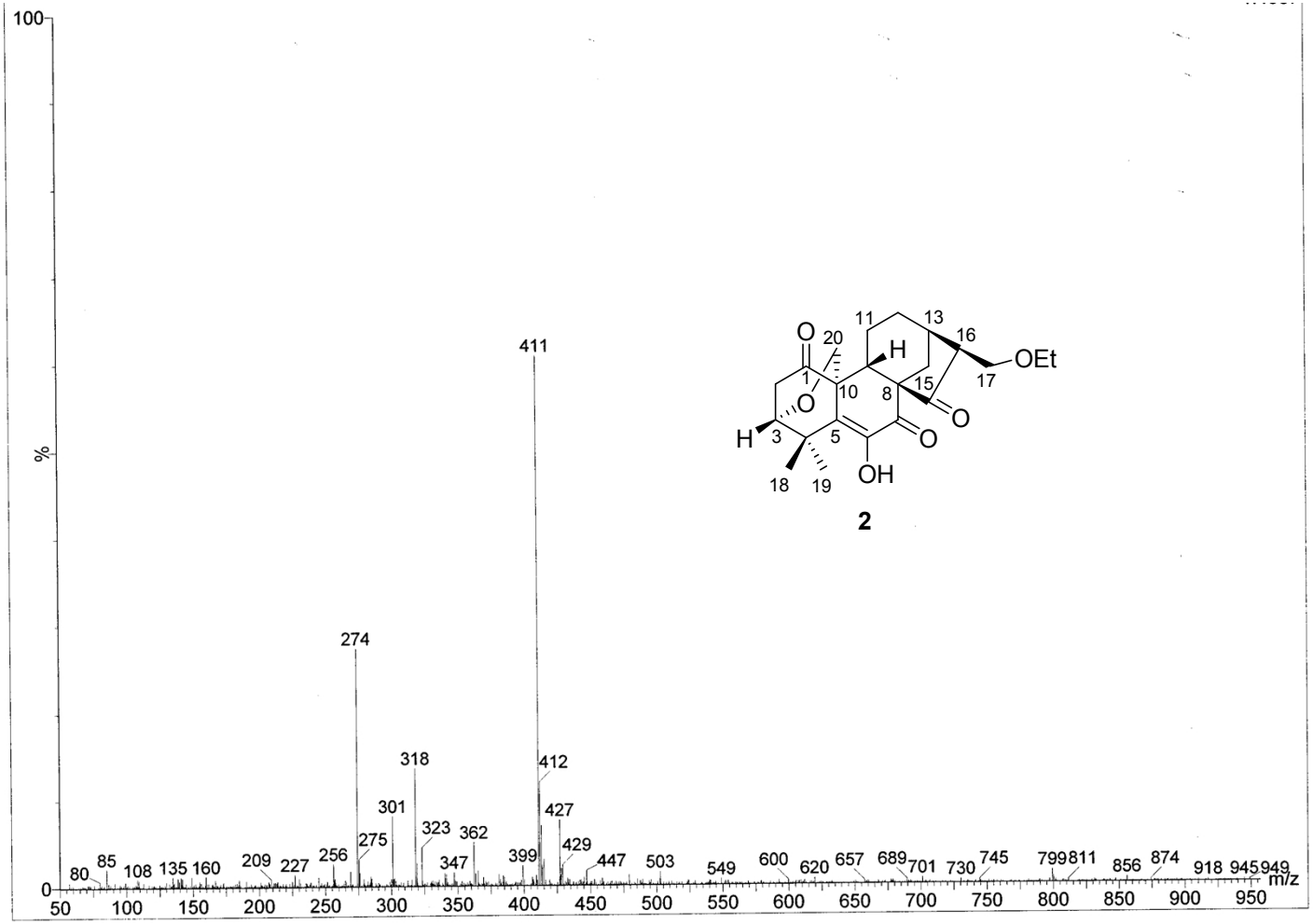


Figure S18. ESIMS spectrum of laxiflorol B (**2**)

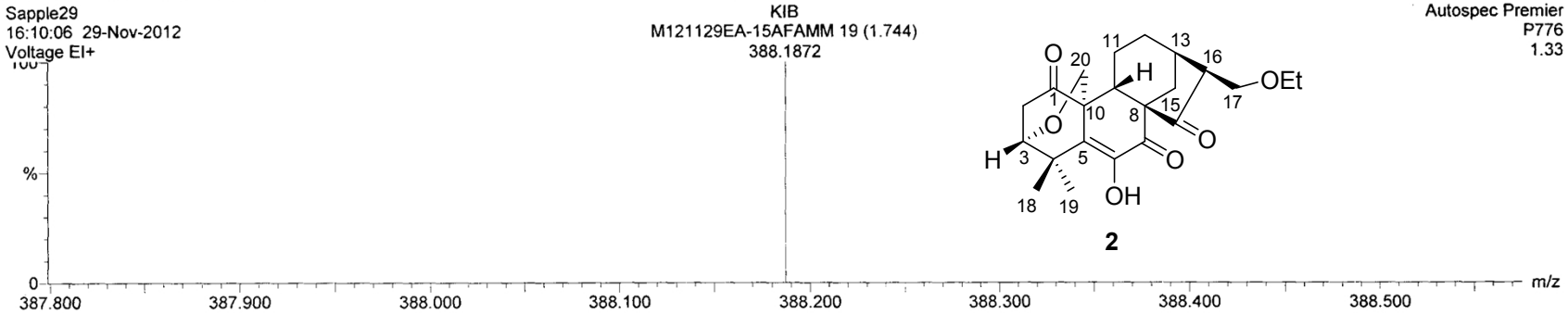


2

Figure S19. HRESIMS spectrum of laxiflorol B (**2**)

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

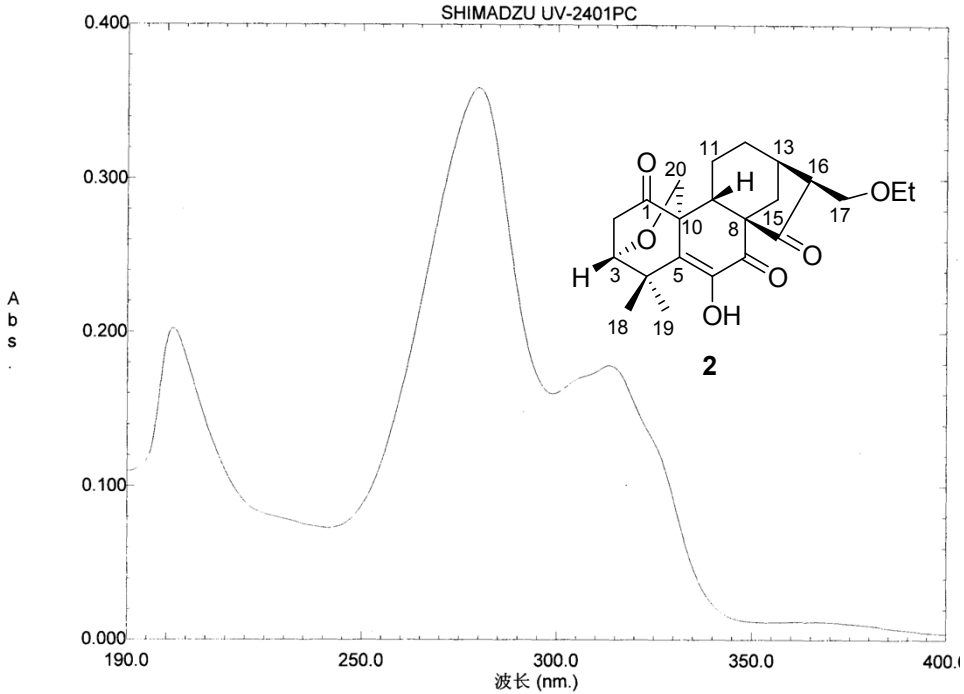
Monoisotopic Mass, Odd and Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 5-7



2

Minimum:				-10.0		
Maximum:		100.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
388.1872	388.1886	-1.4	-3.6	9.0	5546025.5	C22 H28 O6

Figure S20. UV spectrum of laxiflorol B (**2**)



文件名: SAPPLE29

SAPPLE29

样品浓度：0.0338毫克/毫升
溶剂：甲醇

创建于: 16:19 12-11-27
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	313.60	0.1782
2	279.80	0.3589
3	201.60	0.2023

Figure S21. IR spectrum of laxiflorol B (**2**)

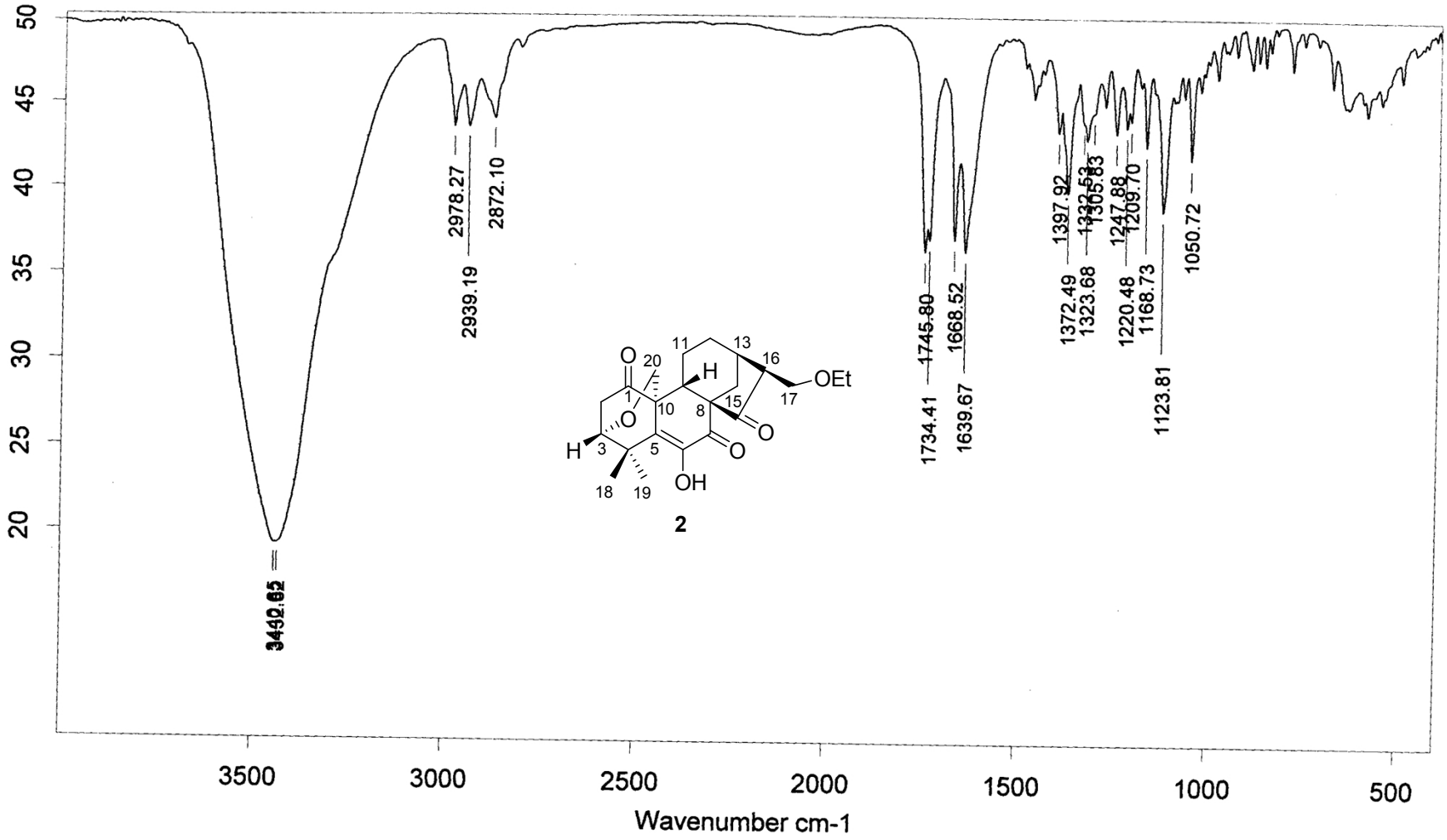


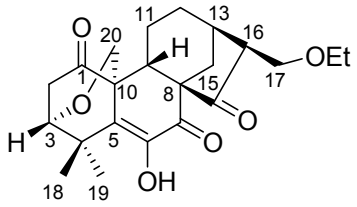
Figure S22. ORD spectrum of laxiflorol B (**2**)

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	1 (1/3)	Sp.Rot	-50.6380	-0.0357 0.0000	18.5 50.00 Cell	Tue Nov 27 14:52:43 2012 0.00141g/mlMeOH SAPPLE29	Na 589nm	2 sec 10 sec
No.2	1 (2/3)	Sp.Rot	-51.0640	-0.0360 0.0000	18.6 50.00 Cell	Tue Nov 27 14:52:57 2012 0.00141g/mlMeOH SAPPLE29	Na 589nm	2 sec 10 sec
No.3	1 (3/3)	Sp.Rot	-50.3550	-0.0355 0.0000	18.5 50.00 Cell	Tue Nov 27 14:53:10 2012 0.00141g/mlMeOH SAPPLE29	Na 589nm	2 sec 10 sec

-50.68°



2

Figure S23. X-ray structure of laxiflorol B (**2**)

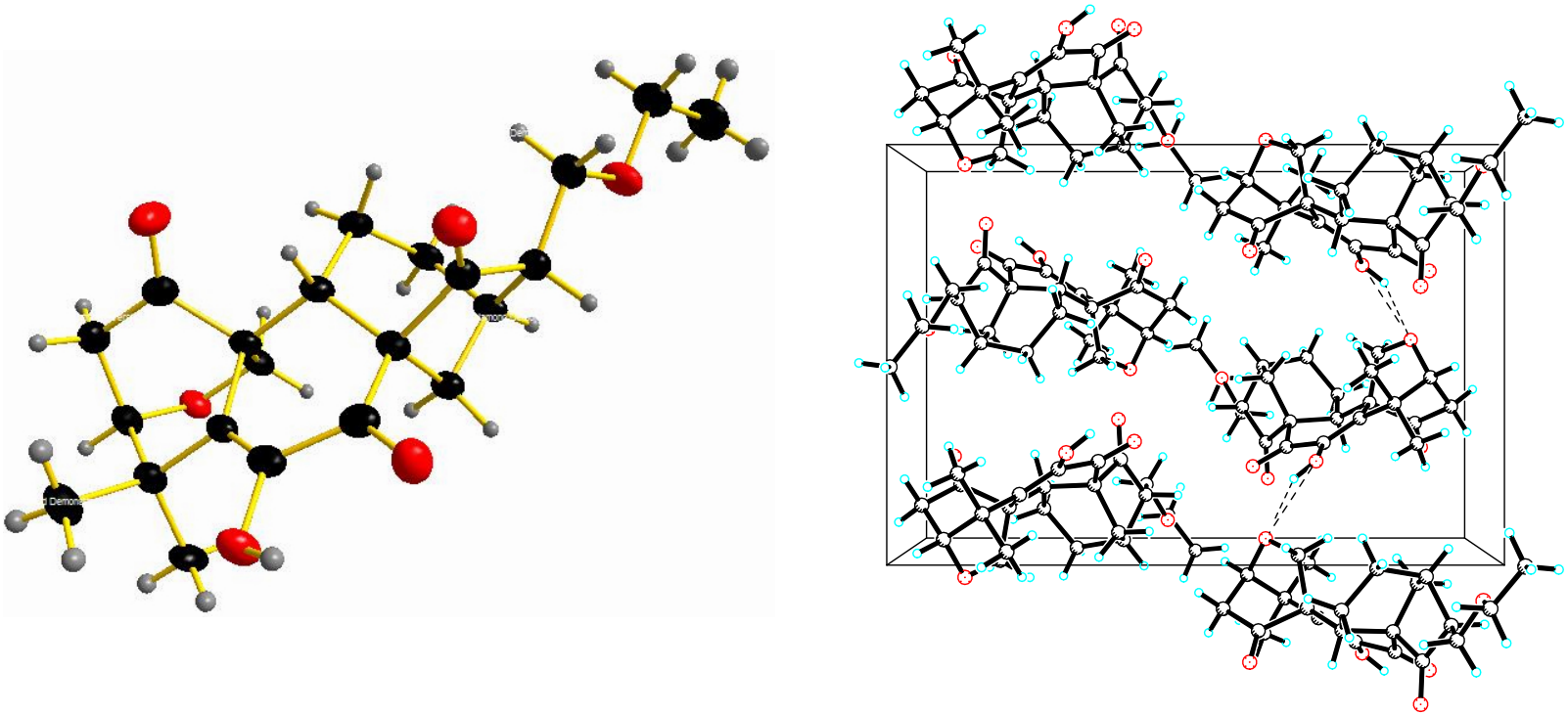


Table S1 NMR Spectroscopic Data (δ in ppm, J in Hz) of Compound **2**[a]

no.	δ_H	δ_C
1	-	205.5 s
2	2.97 br d (19.4)	41.8 t
	2.87 br d (19.4)	
3	3.85 br s	77.9 d
4	-	40.9 s
5	-	133.4 s
6	-	147.1 s
7	-	193.6 s
8	-	60.5 s
9	3.39 overlap	32.7 d
10	-	54.7 s
11	1.55 m	19.3 t
	1.45 m	
12	1.71 m	24.0 t
12	1.40 m	
13	2.69 br s	33.3 d
14	2.19 d (12.0)	38.7 t
	2.00 d (12.0)	
15	-	214.9 s
16	2.97 overlap	55.5 d
17	3.92 m	66.9 t
	3.55 m	
18	1.31 s	23.4 q
19	1.78 s	21.9 q
20	4.79 d (8.9)	66.6 t
	4.31 d (8.9)	
CH_3CH_2O	3.39 overlap	66.6 t
	1.14 d (6.0)	15.4 q

[a]Data were recorded in C_5D_5N on a Bruker AM 500MHz spectrometer

Detailed experimental procedures

1. *General Experimental procedures*

Optical rotations were measured with a JASCO DIP-370 digital polarimeter. UV data were obtained on a Shimadzu UV-2401A spectrophotometer. CD spectra were measured on a Chirascan instrument. A BioRad FtS-135 spectrophotometer was used for scanning IR spectroscopy with KBr pellets. 1D NMR spectra and ^{1}H-^{1}H COSY, HMBC, ROESY spectra were recorded on DRX-600 spectrometers. HSQC and HSQC-TOSY spectra were recorded on DRX-500 spectrometers. Unless otherwise specified, chemical shifts (δ) were expressed in ppm with reference to the solvent signals. High-resolution electrospray-ionization (HRESIMS) were performed on a VG Autospec-3000 spectrometer under 70 eV. Column chromatography was performed with silica gel (100-200 mesh; Qingdao Marine Chemical, Inc., Qingdao, People's Republic of China). Preparative HPLC was performed on a Shimadzu LC-8A preparative liquid chromatograph with a Shimadzu PRC-ODS (K) column. Fractions were monitored by TLC and spots were visualized by heating silica gel plates sprayed with 8% H_2SO_4 in EtOH. All solvents including petroleum ether (60-90 ºC) were distilled prior to use.

2. *Plant material*

The leaves of *Isodon eriocalyx* var. *laxiflora* were collected from Yunnan province, People's Republic of China, in September 2008. Voucher specimens (KIB20080028) were deposited at the State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, and were identified by Prof. Xi-Wen Li.

3. Extraction and isolation

The air-dried leaves of *Isodon eriocalyx* var. *laxiflora* (10 Kg) were extracted with 70% aqueous acetone (3 × 40 L, 2 days each) at room temperature. The solvent was evaporated in vacuo to afford a crude extract (1.2 kg), which was suspended in H_2O, and then extracted successively with EtOAc and n-BuOH. The EtOAc-soluble part (600 g) was decolorized on MCI gel with 90% MeOH/H_2O to obtain a yellow gum (427.5 g). The gum was purified by CC (column chromatography on SiO_2 with $CHCl_3$-Me_2CO gradient system 1:0, 9:1, 8:2, 7:3, 6:4 and 1:1) to yield six main fractions, Fr. A-F. Fr. C ($CHCl_3$/acetone 8:2, 30 g) eluting with $CHCl_3$/CH_3OH (90:1, 60:1 and 30:1), and yield subfractions C1-C5. Subfraction C1 (10 g, $CHCl_3$/ CH_3OH 90:1) was fragmented by repeated CC, first on on RP-18 with a gradien elution of MeOH/H_2O (20:80 to 100:0) to yield fractions C1/1–C1/5, Subsequently fraction C1/3 (3.56 g) was purified by a silica gel column ($CHCl_3$/ isopropyl alcohol 90:1 to 30:1) to give subfractions C1/3/1-C1/3/5. Compound **2** (12 mg) was crystallized from subfraction C1/3/1 (160 mg).

Fr. D ($CHCl_3$/acetone 7:3, 50 g) eluting with $CHCl_3$/CH_3OH (30:1, 20:1 and 10:1), and yield subfractions D1-D3. Subfraction D1 (20 g, $CHCl_3$/ CH_3OH 30:1) was fragmented by repeated CC, first on on RP-18 with a gradien elution of MeOH/H_2O (20:80 to 100:0) to yield fractions D1/1–D1/8, Subsequently fraction D1/3 (2.27 g) was purified by a silica gel column ($CHCl_3$/ MeOH 50:1 to 10:1) to give subfractions D1/3/1-D1/3/8. Compound **1** (3 mg) was precipitated from subfraction D1/3/4 (80 mg) by preparative HPLC (20 mL/min, detector UV λ_{max} 210 nm, MeCN/H_2O 30:70).

3.1 Laxiflorol A (**1**), White, amorphous powder. [α]12.6 D = - 29.6 (*c* 0.10, MeOH). UV (MeOH) λ_{max} (log ε): 203.4 (2.5) nm; Positive ESIMS: *m/z* 401 $[M + Na]^+$; For ^1H and ^{13}C spectroscopic data, see Table 1; positive HRESIMS $[M + Na]^+$ *m/z* 401.1571 (calcd for $C_{20}H_{26}O_7Na$, 401.1576).

3.2 Laxiflorol B (**2**), Colorless needle crystals. [α]18.5 D = - 50.7 (*c* 0.14, MeOH). UV (MeOH) λ_{max} (log ε): 201.6 (2.7), 279.8 (2.9), 313.6 (2.6) nm; IR (KBr) V_{max} 3440, 2978, 2939, 2872, 1746, 1734, 1668, 1639, 1397, 1323, 1220, 1123, 1050 cm^{-1}; For ^{13}C and ^1H spectroscopic data, see Table S1; Positive ESIMS: *m/z* 411 $[M + Na]^+$; positive HREIMS $[M]^+$ *m/z* 388.1872 (calcd for $C_{22}H_{28}O_6$, 388.1886).

X-ray Crystal Structure Analysis of laxiflorol B (**2**): $C_{22}H_{28}O_6$, M = 388.44, orthorhombic, a = 9.4749(3) Å b = 11.6421(3) Å c = 17.1244(5) Å α = 90.00°, β = 90.00°, γ = 90.00°, V = 1888.95(9) $Å^3$, T = 100(2) K, space group $P212121$, Z = 4, 9900 reflections measured, 3262 independ*ent* reflections (R_{int} = 0.0350). The final R_1 values were 0.0354 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0987 ($I > 2\sigma(I)$). The final R_1 values were 0.0354 (all data). The final $wR(F^2)$ values were 0.0988 (all data). Flack parameter = -0.03(15).

The intensity data for laxiflorol B was collected on a Bruker APEX DUO diffractometer using graphitemonochromated Cu Kα radiation. Its structures was solved by direct methods (SHELXS97), expanded using difference Founier techniques, and refined by the program and full-matrix least-squares calculations. The nonhydrogen atoms were refined anisotropically, and hydrogen atoms were fixed at calculated positions. Crystallographic data for the structure of laxiflorol B has been deposited in the Cambridge Crystallographic Data Centre (deposition number CCDC 970056). Copies of the data can be obtained free of charge from the CCDC via www.ccdc.cam.ac.uk.

4. ***Synthesis of acetic ester of 1***

We have try to synthesize the 21-acetic ester of **1** in order to get its single crystal, but we failed.

Compound **1** (2.5 mg) was dissolved in CH_2Cl_2 (1 mL). To this solution, acetic oxide chloride (3 mg), triethylamine (0.1 ml), and DMAP (0.5 mg) were added in small portions over a period of 24 h with stirring at 60 ^oC; then, solvent was evaporated from the resulting mixture. The crude residue has not found the compound **1** and 21-acetic ester of **1**.

5. ***Cellular Proliferation Assay***

Colorimetric assays were performed to evaluate compound activity. The following human tumor cell lines were used: the A549 lung cancer cell line, the HL-60 human myeloid leukemia cell line, the MCF-7 breast cancer cell line, the SMMC-7721 human hepatocarcinoma cell line, and the SW-480 human pancreatic carcinoma. All cells were cultured in RPMI-1640 or DMEM medium (Hyclone, Logan, UT), supplemented with 10% fetal bovine serum (Hyclone) at 37 °C in a humidified atmosphere with 5% CO_2. Cell viability was assessed by conducting colorimetric measurements of the amount of insoluble formazan formed in living cells based on the reduction of 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) (Sigma,St. Louis, MO). Briefly, 100 μL adherent cells were seeded into each well of a 96-well cell culture plate and allowed to adhere for 12 h before drug addition, while suspended cells were seeded just before drug addition, both with initial density of 1×10^5 cells/mL in 100 μL of medium. Each tumor cell line was exposed to the test compound at various concentrations in triplicate for 48 h, with *cis*-Platin (Sigma) as positive control. After the incubation, MTT (100 μg) was added to each well, and the incubation continued for 4 h at 37 °C. The cells were lysed with 100 μL of 20% SDS-50% DMF after removal of 100 μL of medium. The optical density of the lysate was measured at 595 nm in a 96-well microtiter plate reader (Bio-Rad 680). The IC_{50} value of each compound was calculated by Reed and Muench's method.

5. ***ECD Calculation and molecular orbital analysis***

The theoretical calculations of compounds **1** and 6,8-*epi*-**1** were carried out using Gaussian 09.[1] Conformational analysis was initially performed using Discovery

Studio 3.5 Client. The optimized conformation geometries, thermodynamic parameters, and populations of all conformations were provided in Figures S24 and S25 and Tables S2–S8. The conformers were then optimized at B3LYP/6-31G(d,p) level. Room-temperature equilibrium populations were calculated according to Boltzmann distribution law. The theoretical calculation of ECD was performed using time-dependent density-functional theory (TDDFT) at B3LYP/6-31++G(d,p) level in methanol with PCM model and in the gas phase. The ECD spectra of compounds **1** and 6,8-*epi*-**1** were obtained by weighing the Boltzmann distribution rate of each geometric conformation.

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

$$\Delta\varepsilon(E) = \frac{1}{2.297 \times 10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2}$$

where σ represents the width of the band at $1/e$ height, and ΔE_i and R_i are the excitation energies and rotational strengths for transition i, respectively. σ = 0.20 eV and R^{velocity} have been used in this work.

The orbital information (NBO plot files) was generated by NBO program of Gaussian 09.[2] The predominantly populated conformers were selected for molecular orbital (MO) analysis. NBO plot files were used to generate corresponding Gaussian-type grid file by Multiwfn 2.4.[3] After that, the isosurface of generated grid date was afforded by VMD software.[4]

Figure S24. Optimized geometries of conformers of **1** at the B3LYP/6-31G(d,p) level in the gas phase.

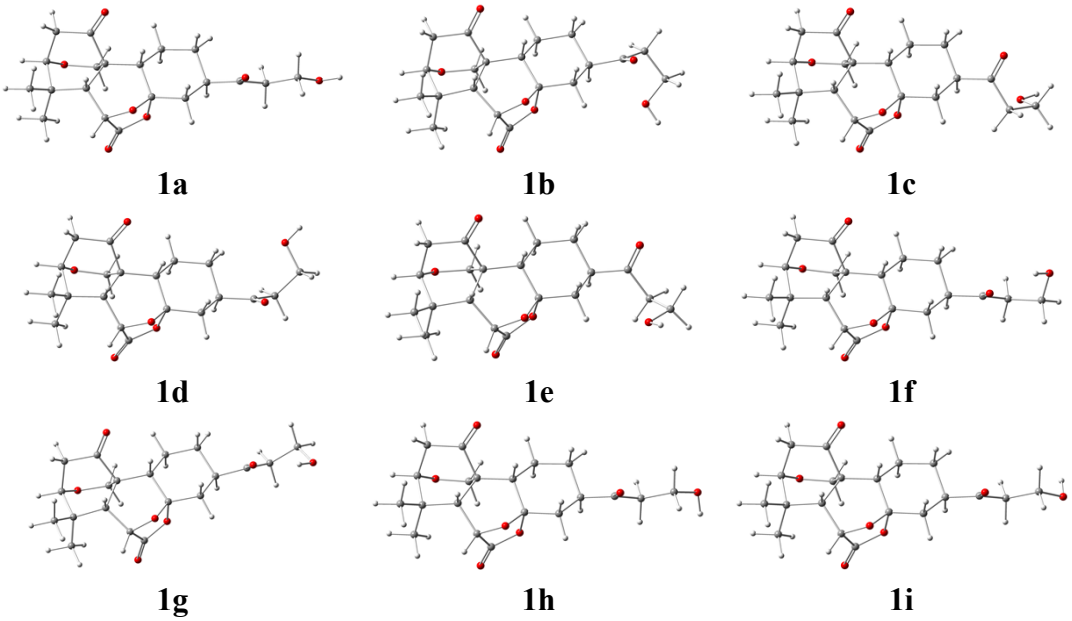


Table S2. Important thermodynamic parameters (a.u.) of the optimized **1** at B3LYP/6-31G(d,p) level in the gas phase.

Species	*E*	*E'=E+ZPE*	*H*	*G*
1a	-1303.902524	-1303.926618	-1303.90158	-1303.979668
1b	-1303.902036	-1303.926008	-1303.901092	-1303.979255
1c	-1303.901131	-1303.925113	-1303.900187	-1303.978558
1d	-1303.903049	-1303.927012	-1303.902105	-1303.979820
1e	-1303.902307	-1303.926234	-1303.901362	-1303.978796
1f	-1303.907035	-1303.930688	-1303.906090	-1303.983080
1g	-1303.907417	-1303.931063	-1303.906473	-1303.983651
1h	-1303.902044	-1303.926137	-1303.9011	-1303.979325
1i	-1303.901911	-1303.925992	-1303.900967	-1303.979133

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy.

Table S3. Conformational analysis of **1**.

Species	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$
1a	3.07	0.3	2.79	0.5	2.50	0.9
1b	3.38	0.2	3.17	0.3	2.76	0.6
1c	3.94	0.1	3.73	0.1	3.20	0.3
1d	2.74	0.6	2.54	0.8	2.40	1.1
1e	3.21	0.3	3.03	0.3	3.05	0.4
1f	0.24	39.2	0.24	39.1	0.36	33.8
1g	0.00	58.9	0.00	58.2	0.00	61.9
1h	3.37	0.2	3.09	0.4	2.71	0.5
1i	3.46	0.2	3.18	0.3	2.84	0.5

[a]Relative energy, [c]relative energy with ZPE, and [e]relative Gibbs free energy in kcal/mol. [b,d,f]Conformational distribution calculated by using the respective parameters above at B3LYP/6-31G(d,p) level in the gas phase. T=298 K.

Table S4. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectra of conformer **1** at B3LYP-SCRF/6-31++G(d,p)//B3LYP/6-31G(d,p) level with PCM model in methanol.

Species	Exited State	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
1f	101->102	4.2793	289.73	0.0005	6.9803	7.3201
	100->103	4.4072	281.32	0.0014	9.4345	8.1872
	99->102	5.0487	245.58	0.0007	-2.7267	-3.1319
	101->104	5.3688	230.94	0.0066	5.0672	5.2544
	101->103	5.4076	229.28	0.0004	-1.3869	-1.4749
	101->104	5.5650	222.79	0.0007	-9.8056	-9.5454
	100->102	5.6033	221.27	0.0001	0.8481	0.9349
	98->103	5.6081	221.08	0.0009	-1.8228	-1.4719
	99->103	5.8446	212.14	0.0001	0.2589	0.2994
	97->102	5.9039	210.00	0.0022	-3.6361	-3.5515
	99->104	5.9360	208.87	0.0073	-3.4002	-3.3726
	100->104	6.0667	204.37	0.0005	2.8597	2.8648
	96->102	6.1368	202.04	0.0074	-0.1886	-0.1887
	101->105	6.1491	201.63	0.0098	1.3188	1.3177
	98->102	6.2181	199.39	0.0001	0.0074	-0.0049
	97->103	6.2570	198.15	0.0001	-0.1781	-0.3106
	100->105	6.3213	196.14	0.0132	7.8507	7.6241
	97->104	6.3644	194.81	0.0084	-15.8251	-16.6947
	101->108	6.4527	192.14	0.0042	-1.8728	-2.0151
	96->103	6.4627	191.85	0.0034	0.2357	-0.0172
	101->106	6.4881	191.10	0.0199	-9.9473	-9.7277
	95->102	6.5053	190.59	0.0018	-0.1440	-1.0519
	101->107	6.5474	189.36	0.0291	-5.2477	-5.3644
	94->102	6.6201	187.29	0.0060	-7.7782	-8.0202
	94->102	6.6283	187.05	0.0094	-7.3993	-7.5107
	98->104	6.6618	186.11	0.0002	0.0841	0.0399
	101->109	6.7346	184.10	0.0023	1.4429	0.3699
	98->105	6.7679	183.19	0.0122	-3.8395	-4.7969
	100->108	6.7877	182.66	0.0005	-0.9503	-1.2997
	101->109	6.8088	182.10	0.0040	7.8774	8.4367
1g	101->102	4.2770	289.88	0.0005	6.9823	7.3606
	100->103	4.4156	280.79	0.0004	12.0133	11.2022
	99->102	5.0442	245.80	0.0007	-2.8132	-3.1579
	101->104	5.3681	230.97	0.0065	5.4327	5.4486
	101->103	5.4131	229.05	0.0015	-1.5773	-1.6802
	101->104	5.5637	222.85	0.0007	-9.9152	-9.6906
	98->103	5.5984	221.46	0.0015	1.8717	1.7219
	100->102	5.6062	221.16	0.0001	-0.1021	0.0150
	99->103	5.8525	211.85	0.0001	0.1088	0.1446
	97->102	5.9026	210.05	0.0023	-3.5201	-3.3648

	99->104	5.9372	208.83	0.0071	-3.1569	-3.1277
	100->104	6.0676	204.34	0.0005	2.5907	2.5832
	96->102	6.1327	202.17	0.0079	-0.0951	-0.1009
	101->105	6.1442	201.79	0.0098	1.1658	1.1614
	98->102	6.1938	200.18	0.0000	0.0333	0.0260
	97->103	6.2673	197.83	0.0001	-0.0034	-0.1083
	100->105	6.3320	195.80	0.0134	5.5122	5.4423
	97->104	6.3651	194.79	0.0079	-15.0914	-16.0251
	99->105	6.4478	192.29	0.0032	0.1237	0.0868
	96->103	6.4748	191.49	0.0021	-1.5313	-1.7351
	101->106	6.4879	191.10	0.0174	-11.4557	-11.3118
	95->102	6.5027	190.67	0.0021	-0.4022	-1.2199
	101->108	6.5539	189.18	0.0345	-5.4822	-5.5753
	101->107	6.6155	187.42	0.0054	-9.7891	-10.0823
	94->102	6.6243	187.17	0.0094	-7.2997	-7.4064
	98->104	6.6333	186.91	0.0001	0.2259	0.2413
	98->105	6.7456	183.80	0.0065	3.9953	5.1631
	101->109	6.7727	183.06	0.0062	-7.1492	-6.6244
	100->107	6.7944	182.48	0.0009	6.4537	6.4953
	101->109	6.8144	181.94	0.0062	14.5595	15.7628

[a]Excitation energy. [b]Wavelength. [c]Oscillator strength. [d]Rotatory strength in velocity form (10^{-40} cgs.). [e]Rotatory strength in length form (10^{-40} cgs.).

Table S5. Optimized Z-matrixes of **1** in the gas phase (Å) at B3LYP/6-31G(d,p) level.

1a				**1b**			
C	-3.698847	2.164622	0.010129	C	3.770331	-1.951908	-0.207545
C	-4.116690	0.847899	-0.656341	C	4.043380	-0.546454	-0.757826
C	-3.900379	-0.393993	0.251894	C	3.734762	0.581248	0.265034
C	-2.401560	-0.314201	0.725917	C	2.265242	0.311901	0.759240
C	-1.592165	0.754373	-0.104865	C	1.536959	-0.747277	-0.154476
C	-2.207462	2.099870	0.318390	C	2.287439	-2.060806	0.127839
C	-1.583221	-1.620326	0.866958	C	1.331183	1.513546	1.042813
O	-0.383348	-1.285682	1.574954	O	0.188069	0.999451	1.735301
C	0.423765	-0.699281	0.567049	C	-0.588972	0.437501	0.689035
C	-0.075073	0.717669	0.234355	C	0.032690	-0.887868	0.212974
O	-1.590486	3.000849	0.849501	O	1.772636	-3.063649	0.579587
C	-1.934998	0.612584	-1.615453	C	1.823936	-0.432269	-1.649980
C	-4.830362	-0.344226	1.480240	C	4.700733	0.514797	1.464388
C	-4.249182	-1.656947	-0.560834	C	3.936507	1.939923	-0.435416
H	-2.120190	-2.391144	1.421092	H	1.808780	2.275767	1.659781
H	-5.159088	0.886563	-0.987431	H	5.075582	-0.454191	-1.109676
O	-3.345777	0.712140	-1.855018	O	3.230981	-0.378770	-1.924707
H	-2.408948	0.051990	1.760172	H	2.337084	-0.147471	1.753215
C	-0.992141	-2.176282	-0.438348	C	0.656266	2.132204	-0.191790
O	0.218956	-1.573151	-0.590664	O	-0.494720	1.432709	-0.382266
O	-1.438236	-2.978969	-1.214015	O	1.005136	3.045192	-0.892236
C	1.880845	-0.754609	0.978909	C	-2.032645	0.313547	1.129650
C	2.801819	-0.062452	-0.038214	C	-2.907290	-0.363455	0.066683
C	2.306857	1.377898	-0.325125	C	-2.292164	-1.717337	-0.368326
C	0.847177	1.387269	-0.801353	C	-0.849675	-1.543168	-0.866167
C	4.239737	-0.005502	0.484599	C	-4.330009	-0.566501	0.576064
C	5.350126	-0.105156	-0.543187	C	-5.427035	-0.814680	-0.459590
C	6.736233	0.146125	0.030918	C	-6.291949	0.437944	-0.600914
O	7.661749	0.010311	-1.041958	O	-5.449180	1.476036	-1.091586
O	4.472745	0.138856	1.672499	O	-4.608885	-0.515378	1.760456
H	2.790253	-0.622006	-0.982288	H	-2.977355	0.283090	-0.818026
H	0.031446	1.283122	1.167939	H	0.004893	-1.546109	1.089806
H	-3.872858	2.999319	-0.678119	H	4.007914	-2.701893	-0.970207
H	-4.250338	2.392243	0.928344	H	4.362617	-2.203506	0.678555
H	-1.580714	-0.340857	-2.018682	H	1.372536	0.518337	-1.949449
H	-1.443310	1.409105	-2.185566	H	1.390464	-1.212653	-2.285480
H	-4.651383	0.533866	2.108066	H	4.626013	-0.428466	2.014076
H	-5.882195	-0.334101	1.174339	H	5.739128	0.635785	1.136887
H	-4.681241	-1.229839	2.107416	H	4.485572	1.322330	2.172661
H	-3.653316	-1.753926	-1.466402	H	3.311388	2.055549	-1.318783
H	-5.303588	-1.615907	-0.855756	H	4.982074	2.031582	-0.749950

H	-4.111699	-2.565607	0.032406	H	3.723668	2.774138	0.239054
H	2.155269	-1.804972	1.114169	H	-2.407264	1.312397	1.368298
H	1.982868	-0.263742	1.951322	H	-2.057371	-0.268843	2.055872
H	2.401855	1.970935	0.593281	H	-2.304262	-2.407294	0.485949
H	2.944447	1.852961	-1.079326	H	-2.899541	-2.176953	-1.155789
H	0.519753	2.419085	-0.962834	H	-0.430889	-2.519331	-1.130526
H	0.782234	0.865025	-1.762963	H	-0.858781	-0.929463	-1.774502
H	5.150978	0.591176	-1.368648	H	-6.054325	-1.640304	-0.108250
H	5.311475	-1.106052	-0.996162	H	-5.010951	-1.076044	-1.437278
H	6.934250	-0.572496	0.838204	H	-6.711236	0.688680	0.383798
H	6.773525	1.150233	0.478384	H	-7.126717	0.237625	-1.289599
H	8.548829	0.148213	-0.687173	H	-5.939447	2.307179	-1.066967
1c				**1d**			
C	3.785998	1.940188	0.204776	C	3.376522	2.357678	-0.196121
C	4.050227	0.535964	0.762467	C	3.929277	1.135811	0.548843
C	3.741748	-0.595102	-0.257040	C	3.829780	-0.178305	-0.273836
C	2.274510	-0.323537	-0.757037	C	2.326385	-0.279198	-0.728130
C	1.547422	0.745786	0.146288	C	1.421484	0.757338	0.043078
C	2.307245	2.051583	-0.148387	C	1.897167	2.123805	-0.481028
C	1.337839	-1.523936	-1.035285	C	1.641470	-1.666542	-0.771233
O	0.197020	-1.009956	-1.734327	O	0.407276	-1.500022	-1.479066
C	-0.576435	-0.436928	-0.691258	C	-0.445210	-0.931439	-0.498284
C	0.044738	0.891390	-0.226126	C	-0.088009	0.547816	-0.266404
O	1.803559	3.047951	-0.625434	O	1.192248	2.918774	-1.068897
C	1.826439	0.442722	1.645427	C	1.790199	0.753026	1.553735
C	4.711728	-0.536581	-1.453501	C	4.740379	-0.117445	-1.516098
C	3.936371	-1.951405	0.449948	C	4.308997	-1.344214	0.613696
H	1.813686	-2.291684	-1.646631	H	2.247874	-2.414675	-1.283381
H	5.080485	0.440759	1.119247	H	4.965669	1.299604	0.860017
O	3.231902	0.375264	1.925677	O	3.186689	1.003726	1.765285
H	2.350900	0.128167	-1.754198	H	2.286579	0.015307	-1.784527
C	0.655996	-2.133191	0.199897	C	1.122509	-2.191197	0.576955
O	-0.493779	-1.426150	0.382693	O	-0.140198	-1.702716	0.710869
O	0.995264	-3.045125	0.905353	O	1.654953	-2.893718	1.394737
C	-2.021070	-0.312343	-1.138538	C	-1.894031	-1.160001	-0.877769
C	-2.895541	0.378335	-0.065150	C	-2.857492	-0.503881	0.119727
C	-2.284303	1.724787	0.343973	C	-2.519811	0.999614	0.295571
C	-0.841234	1.561196	0.842231	C	-1.062615	1.191402	0.738446
C	-4.324918	0.520522	-0.580322	C	-4.308543	-0.645089	-0.325623
C	-5.184214	-0.743328	-0.655530	C	-5.394954	-0.508958	0.743706
C	-6.298105	-0.670829	0.387460	C	-6.480965	0.470585	0.318888
O	-5.671279	-0.647902	1.666752	O	-5.897109	1.771344	0.335312
O	-4.792541	1.596453	-0.904736	O	-4.608624	-0.846593	-1.488279

H	-2.944210	-0.288218	0.807131	H	-2.754049	-0.989832	1.100078
H	0.022728	1.540195	-1.110248	H	-0.260176	1.036313	-1.233229
H	4.016169	2.691054	0.968950	H	3.469713	3.248698	0.434979
H	4.389282	2.188905	-0.674588	H	3.896858	2.579499	-1.133749
H	1.363624	-0.499628	1.953528	H	1.532420	-0.200864	2.023417
H	1.398829	1.234141	2.270955	H	1.228068	1.535072	2.076635
H	4.497024	-1.346714	-2.159007	H	4.675025	-1.052369	-2.083282
H	5.748689	-0.658734	-1.121993	H	5.788404	0.015898	-1.226045
H	4.641291	0.404557	-2.007363	H	4.471107	0.696333	-2.196314
H	3.308420	-2.060328	1.332244	H	3.734422	-1.436146	1.533499
H	4.980559	-2.045581	0.768194	H	5.357471	-1.182301	0.887344
H	3.722974	-2.788055	-0.221456	H	4.253203	-2.299915	0.084608
H	-2.382869	-1.315118	-1.383971	H	-2.063746	-2.238175	-0.947789
H	-2.025397	0.278934	-2.061716	H	-2.058353	-0.742540	-1.875722
H	-2.315603	2.408387	-0.512323	H	-2.686886	1.509056	-0.661929
H	-2.901818	2.182679	1.122974	H	-3.202290	1.463994	1.013370
H	-0.421483	2.540661	1.091949	H	-0.840736	2.260220	0.820444
H	-0.844208	0.961666	1.760352	H	-0.930224	0.750078	1.733378
H	-4.592309	-1.648344	-0.489022	H	-4.974744	-0.202473	1.706479
H	-5.635348	-0.795542	-1.652263	H	-5.837846	-1.504384	0.878927
H	-6.965107	-1.539790	0.281817	H	-7.334208	0.408552	1.011139
H	-6.886566	0.240142	0.209424	H	-6.827302	0.195779	-0.686084
H	-6.347548	-0.478544	2.334421	H	-6.493365	2.378064	-0.120657
1e				**1f**			
C	-3.806591	1.804672	0.546625	C	3.622885	2.211019	-0.067281
C	-4.125736	0.527825	-0.241261	C	4.096972	0.889600	0.551201
C	-3.613295	-0.763091	0.455258	C	3.861429	-0.336889	-0.373025
C	-2.089257	-0.505786	0.751800	C	2.341300	-0.275261	-0.776202
C	-1.560229	0.766208	-0.016702	C	1.551629	0.755790	0.118636
C	-2.292228	1.937145	0.663074	C	2.119034	2.124072	-0.299720
C	-1.084604	-1.675076	0.617071	C	1.542902	-1.593805	-0.913868
O	0.143471	-1.239689	1.213413	O	0.303329	-1.266157	-1.554521
C	0.711618	-0.424272	0.201504	C	-0.464474	-0.722944	-0.493881
C	-0.019642	0.927704	0.123415	C	0.020611	0.695891	-0.148782
O	-1.740462	2.850046	1.242952	O	1.457871	3.025039	-0.774564
C	-2.089007	0.753426	-1.478842	C	1.969735	0.584106	1.607002
C	-4.361559	-1.007161	1.780548	C	4.733061	-0.243344	-1.641258
C	-3.891673	-1.960461	-0.475339	C	4.271557	-1.609873	0.393794
H	-1.425973	-2.578408	1.124261	H	2.067306	-2.338275	-1.514045
H	-5.199549	0.441840	-0.434702	H	5.153060	0.942332	0.833120
O	-3.519185	0.655668	-1.530787	O	3.386922	0.714753	1.781720
H	-2.003142	-0.268343	1.819655	H	2.294212	0.116948	-1.799809
C	-0.608858	-1.981155	-0.811860	C	1.026493	-2.196145	0.402339

O	0.473818	-1.184543	-1.027653	O	-0.187301	-1.621014	0.629154
O	-1.042059	-2.750773	-1.627480	O	1.523311	-3.010404	1.133458
C	2.206313	-0.296698	0.423598	C	-1.939125	-0.800130	-0.835021
C	2.853900	0.631817	-0.633283	C	-2.817763	-0.162061	0.253542
C	2.149775	1.995030	-0.655901	C	-2.344922	1.284887	0.548878
C	0.644852	1.845705	-0.921041	C	-0.862799	1.319035	0.948024
C	4.348851	0.746152	-0.348627	C	-4.283189	-0.131377	-0.178663
C	5.236413	-0.450719	-0.702499	C	-5.340644	-0.328994	0.893652
C	6.087983	-0.879651	0.485585	C	-6.769600	-0.313369	0.341056
O	5.199267	-1.421999	1.459894	O	-7.089681	0.911262	-0.290536
O	4.835483	1.745950	0.146159	O	-4.584307	0.085890	-1.343948
H	2.739635	0.141274	-1.611089	H	-2.731412	-0.745320	1.178559
H	0.139290	1.392932	1.103966	H	-0.141941	1.282735	-1.060931
H	-4.189333	2.678489	0.007480	H	3.817892	3.036709	0.626054
H	-4.251782	1.830156	1.546651	H	4.122034	2.463755	-1.008540
H	-1.662241	-0.076731	-2.049475	H	1.658493	-0.388605	2.000113
H	-1.799098	1.679807	-1.987068	H	1.486457	1.352351	2.221280
H	-4.006762	-1.929153	2.253983	H	5.797290	-0.218115	-1.382825
H	-4.220647	-0.195928	2.501339	H	4.509541	0.643010	-2.242795
H	-5.436883	-1.122992	1.606075	H	4.572968	-1.119190	-2.279411
H	-4.972262	-2.051047	-0.632596	H	3.723540	-1.737811	1.325520
H	-3.546366	-2.899475	-0.033214	H	5.338235	-1.554885	0.637752
H	-3.421025	-1.855990	-1.451257	H	4.121708	-2.508290	-0.211805
H	2.647722	-1.296009	0.423651	H	-2.196262	-1.852199	-0.989712
H	2.359423	0.121431	1.424378	H	-2.101816	-0.280290	-1.783751
H	2.320124	2.499285	0.302036	H	-2.503876	1.895862	-0.348474
H	2.603814	2.633247	-1.421162	H	-2.953148	1.725425	1.346760
H	0.163734	2.828377	-0.891817	H	-0.552376	2.354893	1.116566
H	0.496788	1.438631	-1.928470	H	-0.734767	0.777409	1.892307
H	5.895191	-0.132737	-1.520654	H	-5.214346	0.465191	1.643160
H	4.646090	-1.298766	-1.062768	H	-5.131246	-1.272271	1.417929
H	6.620621	-0.000027	0.870732	H	-7.479052	-0.441818	1.164554
H	6.830903	-1.625390	0.165089	H	-6.900977	-1.167209	-0.341389
H	5.686916	-1.541433	2.284253	H	-6.513215	0.951464	-1.068829
1g				**1h**			
C	3.687245	2.143230	-0.166117	C	-3.697494	2.166956	0.009495
C	4.126586	0.835559	0.504571	C	-4.115344	0.851519	-0.659553
C	3.855509	-0.421208	-0.368372	C	-3.901661	-0.391953	0.247070
C	2.334926	-0.338374	-0.766414	C	-2.403738	-0.313808	0.724307
C	1.577664	0.755028	0.080943	C	-1.591868	0.754902	-0.103844
C	2.182142	2.086477	-0.398532	C	-2.206742	2.100594	0.319864
C	1.500369	-1.640370	-0.835256	C	-1.587004	-1.620750	0.865721
O	0.267291	-1.311613	-1.487551	O	-0.387978	-1.287742	1.576467

C	-0.480896	-0.694792	-0.453448	C	0.421322	-0.701041	0.570872
C	0.045387	0.725792	-0.182779	C	-0.075459	0.716606	0.238168
O	1.545949	2.982571	-0.915161	O	-1.589195	3.000731	0.851655
C	1.993672	0.641053	1.575707	C	-1.932195	0.614703	-1.615071
C	4.721837	-0.402356	-1.643220	C	-4.834176	-0.343728	1.473552
C	4.236419	-1.671449	0.449536	C	-4.249404	-1.653345	-0.568517
H	2.001432	-2.428173	-1.398881	H	-2.125645	-2.391512	1.418323
H	5.184399	0.870815	0.782711	H	-5.157109	0.891618	-0.992491
O	3.415082	0.728452	1.742192	O	-3.342371	0.717047	-1.857139
H	2.291270	0.004884	-1.807626	H	-2.412962	0.051354	1.758937
C	0.973799	-2.160767	0.511747	C	-0.993440	-2.176586	-0.438422
O	-0.222991	-1.541502	0.712825	O	0.218552	-1.574071	-0.588057
O	1.452069	-2.949038	1.282485	O	-1.437772	-2.979194	-1.215136
C	-1.958371	-0.748048	-0.786748	C	1.877731	-0.757980	0.985039
C	-2.814776	-0.027569	0.265728	C	2.799994	-0.068030	-0.032410
C	-2.300622	1.419133	0.484430	C	2.308591	1.373817	-0.318000
C	-0.817081	1.431502	0.879999	C	0.849249	1.386294	-0.795380
C	-4.282008	0.019306	-0.152984	C	4.238892	-0.016179	0.487807
C	-5.327748	0.013111	0.948736	C	5.351454	-0.112470	-0.541790
C	-6.715452	0.456822	0.469884	C	6.744773	0.161148	0.027676
O	-7.250445	-0.410899	-0.508866	O	7.746495	0.142394	-0.981871
O	-4.595747	0.075450	-1.334100	O	4.475276	0.122343	1.675344
H	-2.743471	-0.561021	1.222513	H	2.785066	-0.626906	-0.977027
H	-0.101500	1.268250	-1.124612	H	0.029816	1.281301	1.172388
H	3.902560	2.989796	0.495392	H	-3.869969	3.002788	-0.677781
H	4.193718	2.347129	-1.115251	H	-4.250226	2.393652	0.927219
H	1.649316	-0.299328	2.016408	H	-1.578878	-0.339217	-2.018201
H	1.539164	1.455416	2.151739	H	-1.438276	1.410673	-2.184018
H	5.787903	-0.391879	-1.391395	H	-4.687077	-1.230615	2.099422
H	4.536935	-1.300321	-2.242780	H	-5.885350	-0.332235	1.165438
H	4.515430	0.463008	-2.280230	H	-4.655820	0.533105	2.103309
H	3.690683	-1.743370	1.388478	H	-4.112939	-2.563180	0.023158
H	5.305830	-1.635653	0.685020	H	-3.652278	-1.748588	-1.473486
H	4.058023	-2.590529	-0.116043	H	-5.303355	-1.611584	-0.864961
H	-2.247510	-1.798555	-0.883397	H	2.150488	-1.808634	1.121740
H	-2.108246	-0.278447	-1.763391	H	1.979462	-0.266310	1.957062
H	-2.442142	1.987081	-0.443830	H	2.404233	1.965377	0.601261
H	-2.893196	1.919925	1.258299	H	2.947597	1.848955	-1.070985
H	-0.476574	2.465434	0.992422	H	0.523743	2.418908	-0.955505
H	-0.703069	0.938047	1.852098	H	0.784336	0.865767	-1.757971
H	-4.979287	0.628027	1.789137	H	5.144477	0.575115	-1.372448
H	-5.382565	-1.017316	1.329946	H	5.303872	-1.120418	-0.983454
H	-6.655558	1.494896	0.104952	H	6.963928	-0.545784	0.838708

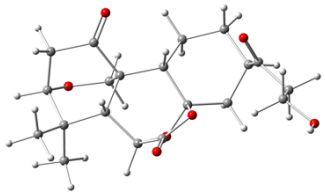
H	-7.410098	0.449968	1.315845	H	6.772671	1.161924	0.466695
H	-6.634702	-0.357940	-1.256593	H	7.855257	-0.771648	-1.274942

1i

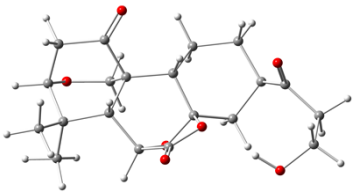
C	-3.698707	2.165445	0.016677
C	-4.116767	0.851369	-0.654853
C	-3.901348	-0.393946	0.248853
C	-2.403047	-0.315771	0.724762
C	-1.592585	0.754501	-0.102704
C	-2.206950	2.099847	0.322559
C	-1.585275	-1.622544	0.863175
O	-0.385874	-1.289970	1.573079
C	0.422285	-0.701610	0.567503
C	-0.075746	0.716321	0.237547
O	-1.588385	3.000317	0.852716
C	-1.934894	0.616016	-1.613720
C	-4.832747	-0.349025	1.476259
C	-4.249110	-1.653780	-0.569166
H	-2.122890	-2.394613	1.414908
H	-5.158932	0.891565	-0.986421
O	-3.345143	0.720321	-1.853751
H	-2.411430	0.047801	1.759927
C	-0.993157	-2.175395	-0.443003
O	0.218545	-1.572218	-0.592595
O	-1.438544	-2.975692	-1.221403
C	1.879061	-0.758278	0.980599
C	2.800593	-0.065399	-0.035529
C	2.306798	1.375883	-0.319537
C	0.847258	1.387633	-0.796282
C	4.238979	-0.010895	0.486525
C	5.353388	-0.114376	-0.540427
C	6.744708	0.169057	0.028469
O	7.770126	-0.053012	-0.931215
O	4.473370	0.131522	1.673840
H	2.787964	-0.623643	-0.980468
H	0.030415	1.279912	1.172284
H	-3.873996	3.003233	-0.667428
H	-4.248913	2.388674	0.936763
H	-1.582976	-0.337901	-2.018058
H	-1.440892	1.412000	-2.182573
H	-4.654451	0.526511	2.107813
H	-5.884188	-0.337600	1.169119
H	-4.684475	-1.237185	2.099996
H	-3.652865	-1.746849	-1.474908

H	-5.303382	-1.612027	-0.864435
H	-4.111450	-2.564788	0.020376
H	2.153126	-1.808864	1.114547
H	1.980841	-0.268789	1.953716
H	2.402187	1.966834	0.600132
H	2.944664	1.852804	-1.072698
H	0.520637	2.420077	-0.955302
H	0.782177	0.867635	-1.759109
H	5.124967	0.556797	-1.381743
H	5.330760	-1.127648	-0.966356
H	6.945978	-0.512694	0.857659
H	6.782508	1.187633	0.440253
H	7.695423	0.630643	-1.609601

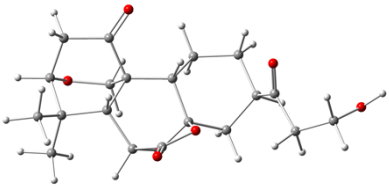
Figure S25. Optimized geometries of conformers of 6,8-*epi*-**1** at the B3LYP/6-31G(d,p) level in the gas phase.



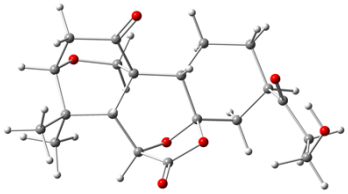
6,8-*epi*-**1a**



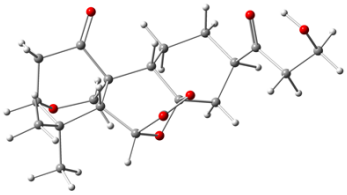
6,8-*epi*-**1b**



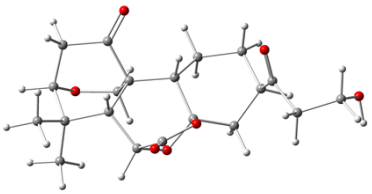
6,8-*epi*-**1c**



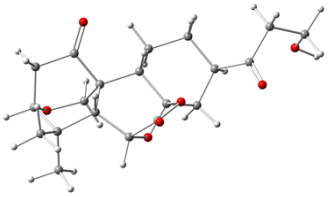
6,8-*epi*-**1d**



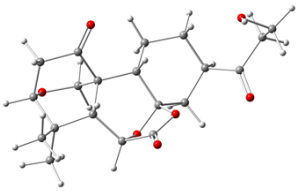
6,8-*epi*-6,8-*epi*-**1e**



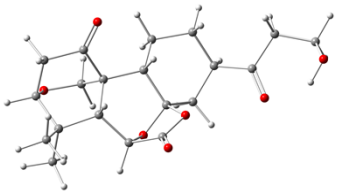
6,8-*epi*-**1f**



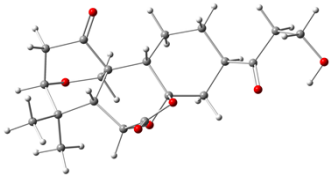
6,8-*epi*-**1g**



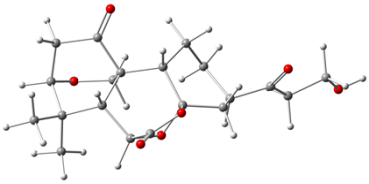
6,8-*epi*-**1h**



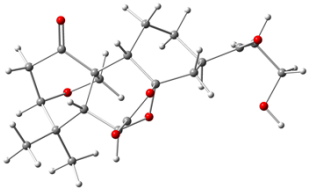
6,8-*epi*-**1i**



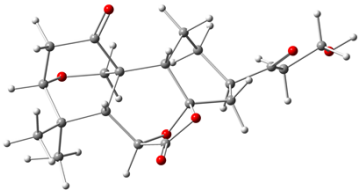
6,8-*epi*-**1j**



6,8-*epi*-**1k**



6,8-*epi*-**1l**



6,8-*epi*-**1m**

Table S6. Important thermodynamic parameters (a.u.) of the optimized 6,8-*epi*-**1** at B3LYP/6-31G(d,p) level in the gas phase.

Species	*E*	*E'=E+ZPE*	*H*	*G*
6,8-*epi*-**1a**	-1303.890679	-1303.914676	-1303.889735	-1303.967908
6,8-*epi*-**1b**	-1303.895613	-1303.919105	-1303.894668	-1303.970560
6,8-*epi*-**1c**	-1303.891566	-1303.915419	-1303.890622	-1303.968586
6,8-*epi*-**1d**	-1303.895765	-1303.919276	-1303.894821	-1303.971763
6,8-*epi*-**1e**	-1303.895484	-1303.918890	-1303.894540	-1303.970991
6,8-*epi*-**1f**	-1303.890234	-1303.914057	-1303.889290	-1303.967302
6,8-*epi*-**1g**	-1303.888487	-1303.912445	-1303.887543	-1303.966037
6,8-*epi*-**1h**	-1303.889093	-1303.913005	-1303.888148	-1303.965767
6,8-*epi*-**1i**	-1303.893229	-1303.916826	-1303.892285	-1303.969612
6,8-*epi*-**1j**	-1303.892961	-1303.916628	-1303.892016	-1303.969891
6,8-*epi*-**1k**	-1303.888356	-1303.912505	-1303.887412	-1303.967005
6,8-*epi*-**1l**	-1303.888029	-1303.911991	-1303.887084	-1303.965601
6,8-*epi*-**1m**	-1303.888356	-1303.912505	-1303.887412	-1303.966993

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy.

Table S7. Conformational analysis of **1**.

Species	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$
6,8-*epi*-**1a**	3.19	0.2	2.89	0.3	2.42	0.8
6,8-*epi*-**1b**	0.10	31.1	0.11	31.3	0.75	13.7
6,8-*epi*-**1c**	2.63	0.4	2.42	0.6	1.99	1.7
6,8-*epi*-**1d**	0.00	36.6	0.00	37.5	0.00	49.0
6,8-*epi*-**1e**	0.18	27.2	0.24	24.9	0.48	21.6
6,8-*epi*-**1f**	3.47	0.1	3.27	0.1	2.80	0.4
6,8-*epi*-**1g**	4.57	0.0	4.29	0.0	3.59	0.1
6,8-*epi*-**1h**	4.19	0.0	3.94	0.0	3.76	0.1
6,8-*epi*-**1i**	1.59	2.5	1.54	2.8	1.35	5.0
6,8-*epi*-**1j**	1.76	1.9	1.66	2.5	1.17	6.9
6,8-*epi*-**1k**	4.65	0.0	4.25	0.0	2.99	0.3
6,8-*epi*-**1l**	4.85	0.0	4.57	0.0	3.87	0.1
6,8-*epi*-**1m**	4.65	0.0	4.25	0.0	2.99	0.3

[a]Relative energy, [c]relative energy with ZPE, and [e]relative Gibbs free energy in kcal/mol. [b,d,f]Conformational distribution calculated by using the respective parameters above at B3LYP/6-31G(d,p) level in the gas phase. T=298 K.

Table S8. Optimized Z-matrixes of 6,8-*epi*-**1** in the gas phase (Å) at B3LYP/6-31G(d,p) level.

6,8-*epi*-**1a**				6,8-*epi*-**1b**			
C	3.651345	-0.913648	1.494078	C	3.713585	-1.178114	1.173281
C	4.064191	-0.205339	0.196018	C	4.024320	-0.357405	-0.086412
C	3.333416	1.145421	-0.026545	C	3.335789	1.034231	-0.097275
C	1.803842	0.837113	0.189671	C	1.826305	0.755910	0.257246
C	1.530962	-0.716946	0.122481	C	1.477780	-0.770014	0.057549
C	2.167801	-1.263174	1.407891	C	2.215317	-1.468060	1.208656
O	1.572898	-1.888462	2.261109	O	1.681457	-2.154863	2.055063
C	2.360944	-1.328674	-1.042779	C	2.155006	-1.284696	-1.244323
C	3.800923	2.203687	0.989930	C	3.956390	1.966701	0.959562
C	3.678954	1.652528	-1.442546	C	3.549288	1.669852	-1.487012
H	5.147252	-0.051886	0.158624	H	5.103787	-0.238843	-0.222672
O	3.767001	-1.093302	-0.886591	O	3.579074	-1.120478	-1.212576
H	1.569605	1.154859	1.213585	H	1.719797	0.967095	1.328932
C	-0.732249	-0.018030	-0.850998	C	-0.843660	0.095104	-0.606373
C	0.014002	-1.046107	0.046794	C	-0.051907	-1.035729	0.110976
C	-1.843388	-0.611699	-1.696352	C	-2.029679	-0.366547	-1.436811
C	-2.699306	-1.619109	-0.891778	C	-2.869999	-1.490700	-0.769853
C	-1.820928	-2.771866	-0.335229	C	-1.988372	-2.625636	-0.186034
C	-0.309927	-2.481952	-0.411742	C	-0.486787	-2.414319	-0.419914
C	-3.500845	-0.911337	0.222366	C	-3.811026	-0.877575	0.281210
C	-4.610895	0.034498	-0.209225	C	-5.016161	-0.088275	-0.225648
H	-0.389408	-0.944494	1.059683	H	-0.342016	-1.010235	1.166835
O	-3.289235	-1.130758	1.400714	O	-3.615232	-0.997811	1.476262
C	-4.886385	1.127856	0.816135	C	-5.059962	1.337752	0.346772
O	-5.988483	1.887655	0.328141	O	-4.017431	2.152709	-0.164421
C	0.797872	1.584288	-0.735024	C	0.760312	1.629231	-0.464299
C	-0.406322	2.030092	0.095924	C	-0.335708	2.014623	0.528198
O	-1.316703	1.027189	-0.002790	O	-1.305314	1.063487	0.404171
O	0.180907	0.693666	-1.672136	O	0.019110	0.870850	-1.425347
O	-0.557867	3.027677	0.748752	O	-0.384162	2.932604	1.300304
H	4.219426	-1.842826	1.609331	H	4.249595	-2.132556	1.139617
H	3.831081	-0.318360	2.395974	H	4.008358	-0.681702	2.104416
H	2.219768	-2.413362	-1.078518	H	1.958302	-2.353435	-1.374891
H	2.022132	-0.910049	-1.996025	H	1.742973	-0.754899	-2.109340
H	4.864384	2.430936	0.857548	H	5.008831	2.169418	0.733022
H	3.650178	1.883853	2.025451	H	3.902490	1.548322	1.969352
H	3.242889	3.136586	0.854810	H	3.430678	2.927492	0.978951
H	3.330480	2.678943	-1.594070	H	3.232593	2.717379	-1.498053
H	4.765873	1.662494	-1.573672	H	4.615093	1.656484	-1.736639
H	3.261224	1.024799	-2.231638	H	3.021661	1.140602	-2.282280

H	-1.379055	-1.128170	-2.542282	H	-1.618837	-0.739125	-2.380187
H	-2.435056	0.209146	-2.107738	H	-2.638244	0.511804	-1.670244
H	-3.450968	-2.015106	-1.587712	H	-3.518399	-1.884379	-1.562264
H	-2.100457	-2.935946	0.708494	H	-2.172073	-2.675286	0.891621
H	-2.034096	-3.696460	-0.881054	H	-2.294149	-3.586954	-0.610670
H	0.045912	-2.641695	-1.436633	H	-0.253613	-2.511877	-1.487284
H	0.227381	-3.190532	0.224718	H	0.077148	-3.191151	0.103956
H	-5.520405	-0.570033	-0.340473	H	-5.909039	-0.634319	0.107623
H	-4.403699	0.482498	-1.185670	H	-5.040012	-0.045832	-1.318957
H	-3.985389	1.746528	0.935158	H	-5.035020	1.282561	1.442711
H	-5.103073	0.666686	1.788287	H	-6.001378	1.812342	0.052428
H	-6.145009	2.608762	0.950485	H	-3.205479	1.947210	0.322359
H	1.236838	2.417903	-1.278669	H	1.171932	2.509886	-0.952964
6,8-*epi*-**1c**				6,8-*epi*-**1d**			
C	3.639842	-1.379391	1.311001	C	3.479273	-1.017611	1.650347
C	4.106688	-0.604147	0.070882	C	4.010538	-0.384833	0.356176
C	3.562162	0.847799	0.013402	C	3.381987	0.999779	0.045578
C	2.012490	0.724354	0.268060	C	1.826481	0.793869	0.187718
C	1.527352	-0.763767	0.058190	C	1.459155	-0.741098	0.148880
C	2.120552	-1.518489	1.256080	C	1.985895	-1.285433	1.483965
O	1.471165	-2.140750	2.070960	O	1.305727	-1.852197	2.314008
C	2.229505	-1.357212	-1.195931	C	2.312796	-1.441368	-0.947169
C	4.200941	1.724511	1.106643	C	3.860532	2.065851	1.048570
C	3.929521	1.446957	-1.360404	C	3.834246	1.430247	-1.365593
H	5.198975	-0.593967	0.001654	H	5.101631	-0.301245	0.378455
O	3.658549	-1.327638	-1.079782	O	3.719336	-1.291706	-0.712697
H	1.857577	0.960193	1.328436	H	1.560444	1.156671	1.188740
C	-0.647351	0.325109	-0.748407	C	-0.700431	0.067008	-0.966366
C	-0.021599	-0.877286	0.016683	C	-0.069582	-0.979638	-0.004064
C	-1.841762	-0.030077	-1.613785	C	-1.801594	-0.479873	-1.854873
C	-2.812966	-0.997100	-0.897260	C	-2.760208	-1.407120	-1.068679
C	-2.087978	-2.287073	-0.430621	C	-1.985051	-2.600351	-0.446128
C	-0.556145	-2.206963	-0.550788	C	-0.456847	-2.404519	-0.446280
C	-3.576258	-0.305288	0.249112	C	-3.569314	-0.620950	-0.018117
C	-4.400105	0.935818	-0.097426	C	-4.594189	0.386013	-0.515937
H	-0.372647	-0.819892	1.052712	H	-0.518765	-0.826505	0.982799
O	-3.553458	-0.728765	1.388201	O	-3.429596	-0.831686	1.177139
C	-5.742391	0.932970	0.619053	C	-4.913661	1.472572	0.522827
O	-6.531631	-0.095705	0.024439	O	-5.552235	0.949615	1.670660
C	1.088214	1.690718	-0.529078	C	0.919954	1.573603	-0.808972
C	-0.022669	2.196769	0.392821	C	-0.295618	2.118213	-0.057317
O	-1.066362	1.342676	0.222795	O	-1.262453	1.169897	-0.179355
O	0.333950	0.994619	-1.526964	O	0.297897	0.695350	-1.755012

O	-0.016977	3.126889	1.153493	O	-0.417770	3.141800	0.559168
H	4.079666	-2.382355	1.312614	H	3.983254	-1.972029	1.835707
H	3.925792	-0.906003	2.256743	H	3.638499	-0.397230	2.539176
H	1.921292	-0.801933	-2.087762	H	2.057971	-1.032692	-1.930691
H	1.940409	-2.404256	-1.330351	H	2.103619	-2.515479	-0.960743
H	3.770028	2.731469	1.089405	H	3.638933	1.794803	2.085254
H	5.280606	1.822868	0.949180	H	3.367433	3.024150	0.852345
H	4.041207	1.322261	2.111729	H	4.941027	2.225505	0.964357
H	3.403417	0.967102	-2.187461	H	3.563398	2.470777	-1.569520
H	3.723259	2.521235	-1.394501	H	4.924721	1.364954	-1.436440
H	5.002528	1.322976	-1.539565	H	3.418343	0.802799	-2.155637
H	-1.457835	-0.509380	-2.519777	H	-1.330194	-1.051157	-2.660528
H	-2.327233	0.898071	-1.924815	H	-2.316541	0.364009	-2.319551
H	-3.597417	-1.246391	-1.624746	H	-3.503083	-1.772364	-1.790465
H	-2.360257	-2.463456	0.613591	H	-2.328420	-2.730504	0.583006
H	-2.447748	-3.145193	-1.006903	H	-2.226443	-3.519302	-0.989507
H	-0.257698	-2.321393	-1.599855	H	-0.057734	-2.611751	-1.446224
H	-0.104839	-3.037285	-0.000410	H	0.000637	-3.127489	0.234576
H	-4.563193	1.018678	-1.177046	H	-4.272018	0.831983	-1.463030
H	-3.812553	1.807858	0.214994	H	-5.512319	-0.179514	-0.733129
H	-6.224334	1.916714	0.511435	H	-5.602043	2.200040	0.080644
H	-5.570922	0.743612	1.686129	H	-3.984803	2.006019	0.775478
H	-7.277031	-0.277160	0.609814	H	-4.918702	0.318040	2.046043
H	1.618815	2.515737	-0.999758	H	1.437737	2.362763	-1.349821
6,8-*epi*-**1e**				6,8-*epi*-**1f**			
C	3.640256	-1.147901	1.471908	C	3.638073	-1.463731	1.194106
C	4.102006	-0.433972	0.192942	C	4.076595	-0.687643	-0.055574
C	3.479849	0.976634	0.016635	C	3.574082	0.780701	-0.073662
C	1.932804	0.782973	0.241174	C	2.032970	0.700391	0.242197
C	1.538730	-0.741118	0.121203	C	1.494734	-0.769699	0.036884
C	2.132959	-1.374867	1.386332	C	2.114442	-1.558511	1.199009
O	1.491265	-1.971191	2.226479	O	1.481003	-2.175099	2.030475
C	2.310813	-1.380892	-1.067285	C	2.126317	-1.366674	-1.252754
C	4.038846	1.962874	1.059005	C	4.282803	1.623790	1.002890
C	3.851367	1.496752	-1.387999	C	3.904198	1.386718	-1.453840
H	5.193615	-0.365521	0.153032	H	5.164858	-0.709129	-0.170575
O	3.731253	-1.261795	-0.914447	O	3.559173	-1.383422	-1.194432
H	1.734074	1.081059	1.278517	H	1.928214	0.927809	1.310550
C	-0.660728	0.157796	-0.838155	C	-0.678389	0.395803	-0.657385
C	0.000785	-0.943151	0.043225	C	-0.057349	-0.837223	0.060217
C	-1.779057	-0.337507	-1.734906	C	-1.928404	0.091294	-1.460782
C	-2.742582	-1.303567	-1.006448	C	-2.886054	-0.847318	-0.691454
C	-1.981019	-2.474383	-0.327043	C	-2.182986	-2.181379	-0.325848

C	-0.451999	-2.341957	-0.416582	C	-0.654771	-2.139392	-0.508647
C	-3.690438	-0.569251	-0.037509	C	-3.510338	-0.162272	0.538661
C	-4.512622	0.588494	-0.583353	C	-4.422414	1.039468	0.305141
H	-0.384745	-0.815695	1.060701	H	-0.364052	-0.788843	1.110542
O	-3.816164	-0.928910	1.123293	O	-3.374970	-0.598946	1.665470
C	-5.840625	0.775868	0.169122	C	-5.895198	0.612040	0.421991
O	-5.656598	1.166883	1.512012	O	-6.278718	-0.310625	-0.594198
C	0.979996	1.637180	-0.643387	C	1.106732	1.704260	-0.505640
C	-0.197662	2.128353	0.202240	C	0.055223	2.235213	0.470354
O	-1.188268	1.208826	0.035702	O	-1.019442	1.413244	0.343189
O	0.312233	0.832216	-1.621584	O	0.285360	1.043531	-1.475032
O	-0.274739	3.096429	0.908098	O	0.124340	3.158246	1.236559
H	4.132929	-2.122617	1.553687	H	4.048159	-2.478832	1.167692
H	3.872232	-0.598016	2.390586	H	3.974941	-1.009506	2.132443
H	2.083120	-2.449711	-1.132510	H	1.800374	-0.788862	-2.123819
H	2.001316	-0.908386	-2.005237	H	1.798843	-2.402080	-1.389295
H	5.115977	2.108237	0.922015	H	4.150841	1.213881	2.008852
H	3.871464	1.624565	2.086178	H	3.882906	2.643532	1.014309
H	3.556816	2.941307	0.957943	H	5.357870	1.690923	0.803224
H	3.585377	2.551908	-1.504695	H	3.329382	0.935704	-2.264522
H	4.934156	1.423013	-1.532044	H	3.731608	2.467407	-1.465687
H	3.376783	0.929279	-2.190396	H	4.964359	1.231414	-1.679120
H	-1.310331	-0.862772	-2.572759	H	-1.616685	-0.393047	-2.391543
H	-2.294570	0.530324	-2.152175	H	-2.393945	1.041019	-1.734741
H	-3.416381	-1.697973	-1.780349	H	-3.749142	-1.036789	-1.343791
H	-2.279740	-2.505574	0.724591	H	-2.414579	-2.407102	0.718259
H	-2.288760	-3.425918	-0.771404	H	-2.593356	-2.994392	-0.932909
H	-0.116698	-2.538421	-1.441934	H	-0.404628	-2.240033	-1.571710
H	0.015030	-3.096608	0.222128	H	-0.204255	-2.993330	0.004874
H	-4.689681	0.456674	-1.658221	H	-4.200054	1.779628	1.080177
H	-3.907757	1.497140	-0.466045	H	-4.253963	1.509157	-0.670092
H	-6.433675	-0.150868	0.089869	H	-6.540764	1.501806	0.418407
H	-6.416370	1.569829	-0.317641	H	-6.042470	0.094355	1.373741
H	-5.111065	0.469459	1.909134	H	-6.352682	0.178601	-1.424074
H	1.474947	2.465478	-1.146116	H	1.642661	2.516272	-0.992601
6,8-*epi*-**1g**				6,8-*epi*-**1h**			
C	-3.702077	-1.752577	-0.965121	C	3.412734	-1.833301	1.066099
C	-4.067866	-1.015024	0.331104	C	3.979938	-0.922687	-0.032558
C	-3.750429	0.504608	0.282613	C	3.608130	0.573042	0.158470
C	-2.272559	0.606248	-0.247493	C	2.055232	0.589711	0.412780
C	-1.534072	-0.783309	-0.095603	C	1.403859	-0.774994	-0.047939
C	-2.192547	-1.654812	-1.172450	C	1.887847	-1.774976	1.009527
O	-1.602969	-2.186349	-2.091688	O	1.162037	-2.426635	1.732877

C	-1.912093	-1.436476	1.262067	C	2.041293	-1.237305	-1.386828
C	-4.702020	1.237613	-0.680983	C	4.342724	1.174059	1.371134
C	-3.951748	1.087879	1.696612	C	4.046407	1.346025	-1.103007
H	-5.121432	-1.166167	0.586358	H	5.066786	-1.027930	-0.108567
O	-3.327444	-1.627570	1.392429	O	3.463631	-1.390850	-1.282773
H	-2.342837	0.812765	-1.323255	H	1.920772	0.655166	1.500170
C	0.548844	0.637025	0.398515	C	-0.603332	0.675589	-0.725978
C	-0.008116	-0.638230	-0.314744	C	-0.141881	-0.677694	-0.094876
C	1.829711	0.441829	1.190135	C	-1.715881	0.573921	-1.754298
C	2.905672	-0.440153	0.525446	C	-2.866462	-0.389695	-1.400377
C	2.308392	-1.582064	-0.351319	C	-2.391536	-1.650736	-0.611639
C	0.846426	-1.874177	0.013735	C	-0.876942	-1.866173	-0.738339
C	3.963608	0.389522	-0.207581	C	-4.026980	0.333218	-0.706241
C	5.084191	-0.359291	-0.934760	C	-5.221967	-0.500741	-0.231901
H	0.124309	-0.474967	-1.390008	H	-0.474484	-0.663203	0.948665
O	3.990199	1.604255	-0.159045	O	-4.047929	1.540669	-0.565428
C	6.398800	-0.175043	-0.179009	C	-5.518614	-0.233138	1.240436
O	6.245317	-0.804176	1.092271	O	-4.445480	-0.783268	2.001740
C	-1.380915	1.730771	0.350015	C	1.250312	1.773443	-0.193437
C	-0.465209	2.316663	-0.733462	C	0.137932	2.205476	0.770938
O	0.723776	1.671484	-0.620993	O	-0.988883	1.567156	0.367417
O	-0.429831	1.193470	1.269164	O	0.495892	1.349890	-1.329511
O	-0.717438	3.157210	-1.555193	O	0.211675	2.936133	1.723264
H	-3.972027	-2.810759	-0.881331	H	3.726283	-2.868083	0.890980
H	-4.214851	-1.364065	-1.851861	H	3.748010	-1.566913	2.074384
H	-1.547916	-0.815299	2.086027	H	1.807156	-0.516110	-2.175703
H	-1.443687	-2.423324	1.346236	H	1.631051	-2.209792	-1.680285
H	-5.738344	1.176529	-0.330928	H	4.130762	0.633276	2.298678
H	-4.663263	0.831553	-1.696486	H	4.036459	2.214206	1.526589
H	-4.436400	2.298251	-0.746911	H	5.427173	1.167570	1.215415
H	-3.213610	0.726340	2.414123	H	3.468714	1.075274	-1.988209
H	-3.912779	2.181399	1.683135	H	3.964365	2.427122	-0.954321
H	-4.940971	0.807737	2.073079	H	5.098239	1.131866	-1.319116
H	1.520172	-0.013034	2.136167	H	-1.230745	0.237519	-2.675851
H	2.241386	1.428081	1.412522	H	-2.106197	1.578283	-1.928676
H	3.485641	-0.912781	1.331275	H	-3.294751	-0.736366	-2.353304
H	2.343342	-1.305034	-1.412876	H	-2.644623	-1.543084	0.449070
H	2.910421	-2.489342	-0.247026	H	-2.924132	-2.537693	-0.968503
H	0.776839	-2.147540	1.073557	H	-0.602651	-1.989249	-1.793232
H	0.479123	-2.724001	-0.567649	H	-0.590140	-2.784037	-0.218159
H	5.187116	0.073530	-1.935487	H	-6.087396	-0.188511	-0.829639
H	4.874405	-1.426947	-1.037551	H	-5.071905	-1.571730	-0.392683
H	6.598075	0.900188	-0.074841	H	-6.476786	-0.696209	1.520072

H	7.223262	-0.627151	-0.750636	H	-5.600905	0.851326	1.384788
H	7.003670	-0.567942	1.640791	H	-4.416580	-0.338934	2.857602
H	-1.948464	2.519371	0.841703	H	1.871105	2.623207	-0.472642
6,8-*epi*-**1i**				6,8-*epi*-**1j**			
C	3.721048	-1.551534	1.204565	C	3.763216	-1.591829	1.094802
C	4.163463	-0.770197	-0.041461	C	4.176617	-0.767250	-0.133159
C	3.709775	0.715635	-0.026588	C	3.725704	0.717309	-0.056060
C	2.176034	0.682847	0.325316	C	2.201872	0.672708	0.335924
C	1.588853	-0.765684	0.094759	C	1.606052	-0.765924	0.065657
C	2.195518	-1.584545	1.241206	C	2.239037	-1.626282	1.166407
O	1.553084	-2.170867	2.088961	O	1.616466	-2.242965	2.007489
C	2.172558	-1.372320	-1.209978	C	2.156968	-1.323719	-1.274329
C	4.475237	1.514679	1.044462	C	4.521367	1.479100	1.019980
C	4.023963	1.332627	-1.405449	C	4.002711	1.380759	-1.421194
H	5.248119	-0.825592	-0.176157	H	5.257580	-0.818835	-0.295855
O	3.604498	-1.433509	-1.180908	O	3.588922	-1.390407	-1.280882
H	2.099552	0.889132	1.400713	H	2.155319	0.836895	1.420347
C	-0.542739	0.464160	-0.637497	C	-0.541861	0.492691	-0.565215
C	0.041786	-0.758635	0.141972	C	0.060763	-0.759822	0.150621
C	-1.703784	0.158021	-1.568075	C	-1.724127	0.223719	-1.480752
C	-2.762645	-0.823992	-1.024567	C	-2.771559	-0.783475	-0.959711
C	-2.169880	-1.898597	-0.064512	C	-2.157304	-1.887813	-0.048206
C	-0.658144	-2.065695	-0.269190	C	-0.651201	-2.049586	-0.292858
C	-3.985244	-0.106733	-0.438467	C	-3.985321	-0.092400	-0.322853
C	-5.046374	-0.961219	0.241016	C	-5.091228	-0.979967	0.233251
H	-0.222798	-0.611519	1.195015	H	-0.177585	-0.653547	1.214832
O	-4.130742	1.100555	-0.552366	O	-4.095890	1.123540	-0.320580
C	-6.399328	-0.245235	0.355881	C	-6.183998	-0.188789	0.962552
O	-6.339573	0.889850	1.193864	O	-6.852275	0.722601	0.112965
C	1.263555	1.725279	-0.380387	C	1.272171	1.742539	-0.302884
C	0.181383	2.227615	0.585419	C	0.215134	2.204286	0.709888
O	-0.925888	1.475997	0.344915	O	-0.898771	1.464159	0.466373
O	0.473577	1.106936	-1.397442	O	0.456215	1.165620	-1.323856
O	0.259242	3.088031	1.420363	O	0.315400	3.029129	1.577877
H	4.088477	-2.581860	1.148775	H	4.128157	-2.619587	0.993383
H	4.096727	-1.131459	2.143975	H	4.162044	-1.206457	2.039585
H	1.847681	-0.780717	-2.071284	H	1.814489	-0.697931	-2.103985
H	1.805493	-2.396556	-1.341625	H	1.783078	-2.340939	-1.436725
H	4.353574	1.093130	2.046923	H	4.424411	1.025546	2.011095
H	4.114096	2.548081	1.082039	H	4.165349	2.511840	1.100432
H	5.546716	1.545932	0.818380	H	5.586691	1.514751	0.766949
H	3.888005	2.418410	-1.393962	H	3.366715	0.993903	-2.218931
H	5.071439	1.145117	-1.663170	H	3.869108	2.465592	-1.368515

H	3.410766	0.917258	-2.206776	H	5.042214	1.201308	-1.714250
H	-1.250056	-0.262647	-2.470502	H	-1.289071	-0.158107	-2.409370
H	-2.175168	1.103458	-1.842629	H	-2.199682	1.180125	-1.704912
H	-3.171045	-1.359885	-1.894949	H	-3.188627	-1.289659	-1.842967
H	-2.336319	-1.606604	0.979422	H	-2.299601	-1.627431	1.008288
H	-2.684199	-2.853975	-0.204168	H	-2.676862	-2.837514	-0.206751
H	-0.448380	-2.332600	-1.312154	H	-0.467007	-2.277330	-1.349800
H	-0.284755	-2.879370	0.357775	H	-0.265078	-2.886690	0.294322
H	-5.146901	-1.916049	-0.291797	H	-4.662288	-1.744952	0.891718
H	-4.687909	-1.208129	1.249426	H	-5.531839	-1.521885	-0.616131
H	-7.131133	-0.928878	0.798140	H	-5.740993	0.318207	1.833658
H	-6.759402	0.010951	-0.653660	H	-6.940281	-0.884502	1.339921
H	-5.708792	1.489084	0.764863	H	-6.176577	1.370642	-0.138876
H	1.812409	2.560493	-0.812238	H	1.809701	2.595606	-0.713728
6,8-*epi*-**1k**				6,8-*epi*-**1l**			
C	3.549395	-1.942709	0.994663	C	-3.632702	-1.766622	-0.731219
C	3.558436	-1.727335	-0.524786	C	-3.378284	-1.587513	0.771964
C	3.575738	-0.231150	-0.933787	C	-3.244170	-0.102186	1.200779
C	2.423699	0.445504	-0.099546	C	-2.218127	0.534432	0.190519
C	1.434673	-0.639083	0.479862	C	-1.396115	-0.588699	-0.556157
C	2.260530	-1.354551	1.560798	C	-2.426282	-1.229315	-1.497171
O	1.942837	-1.432935	2.729866	O	-2.314272	-1.291311	-2.704579
C	1.173332	-1.708737	-0.618398	C	-1.015518	-1.701825	0.459460
C	4.925642	0.422497	-0.583243	C	-4.595702	0.629392	1.099728
C	3.382370	-0.143858	-2.462134	C	-2.784685	-0.063088	2.673564
H	4.398053	-2.251184	-0.992328	H	-4.157398	-2.077179	1.364557
O	2.380667	-2.352527	-1.045821	O	-2.167485	-2.284554	1.083098
H	2.911976	0.916662	0.762809	H	-2.819856	1.044861	-0.572128
C	-0.316613	1.230086	0.255510	C	0.494252	1.153687	-0.558877
C	0.152234	0.004503	1.089615	C	-0.194622	0.002009	-1.348859
C	-1.816124	1.420514	0.189803	C	2.001156	1.189753	-0.675664
C	-2.582459	0.201264	-0.349842	C	2.639098	-0.123706	-0.208783
C	-1.958798	-1.153151	0.132304	C	1.975413	-1.382941	-0.869529
C	-1.026324	-0.970503	1.339226	C	0.850694	-1.021069	-1.859086
C	-4.043965	0.252624	0.112133	C	4.142286	-0.114407	-0.463283
C	-5.069756	-0.367899	-0.816981	C	4.973656	-1.212440	0.203213
H	0.450789	0.383379	2.071318	H	-0.631527	0.452076	-2.245139
O	-4.359005	0.736717	1.185549	O	4.687725	0.736511	-1.141666
C	-6.459088	-0.480958	-0.207698	C	5.761044	-0.625792	1.374862
O	-7.300012	-1.062490	-1.197902	O	4.812906	-0.164657	2.333580
C	1.607986	1.573340	-0.802057	C	-1.238830	1.604258	0.755506
C	1.416154	2.711804	0.198696	C	-1.106977	2.741715	-0.259808
O	0.244828	2.453648	0.833134	O	-0.032681	2.435607	-1.029851

O	0.253850	1.179105	-1.048871	O	0.102759	1.112937	0.810405
O	2.143855	3.635136	0.450202	O	-1.809748	3.705248	-0.413019
H	3.569507	-3.014122	1.220593	H	-3.746527	-2.830125	-0.966716
H	4.407006	-1.494546	1.508506	H	-4.539025	-1.264184	-1.086329
H	0.685422	-1.239368	-1.478766	H	-0.352260	-1.289640	1.226461
H	0.515023	-2.494236	-0.235058	H	-0.487584	-2.512539	-0.052468
H	5.168554	0.334398	0.480068	H	-4.476911	1.688913	1.350963
H	4.906632	1.490964	-0.823698	H	-5.325685	0.202559	1.796212
H	5.741284	-0.033004	-1.155453	H	-5.022030	0.583470	0.092882
H	3.566230	0.871230	-2.827208	H	-1.768895	-0.437249	2.812997
H	4.104014	-0.798113	-2.961803	H	-2.837699	0.951884	3.079224
H	2.385875	-0.451514	-2.783717	H	-3.448822	-0.685557	3.282005
H	-2.015018	2.306641	-0.419249	H	2.371187	2.029193	-0.082287
H	-2.171011	1.637247	1.201480	H	2.269779	1.394080	-1.715657
H	-2.569932	0.210991	-1.444505	H	2.525611	-0.203770	0.878435
H	-2.749389	-1.862893	0.402249	H	2.722723	-1.966683	-1.419478
H	-1.424537	-1.606687	-0.704965	H	1.603879	-2.044837	-0.083616
H	-0.641605	-1.937378	1.675910	H	0.341698	-1.927260	-2.199856
H	-1.617178	-0.582093	2.175804	H	1.310450	-0.592568	-2.756234
H	-4.720098	-1.354603	-1.148037	H	5.681158	-1.606133	-0.533775
H	-5.114685	0.242153	-1.730532	H	4.347241	-2.033274	0.565896
H	-6.808809	0.515434	0.095517	H	6.389765	0.194844	1.001713
H	-6.413986	-1.096576	0.702856	H	6.419795	-1.397212	1.801647
H	-8.191617	-1.120880	-0.832585	H	5.283420	0.334992	3.012355
H	2.048977	1.921676	-1.733285	H	-1.519626	1.979220	1.737619

6,8-*epi*-**1m**			
C	3.549797	-1.942286	0.994531
C	3.557979	-1.727598	-0.525026
C	3.575108	-0.231597	-0.934713
C	2.423584	0.445480	-0.100106
C	1.434843	-0.638821	0.480345
C	2.261297	-1.353788	1.561151
O	1.944292	-1.431584	2.730445
C	1.172824	-1.709018	-0.617208
C	4.925251	0.422135	-0.585239
C	3.380834	-0.144968	-2.462973
H	4.397315	-2.251688	-0.992804
O	2.379897	-2.352972	-1.045124
H	2.912370	0.917009	0.761759
C	-0.316541	1.230257	0.256033
C	0.152744	0.005067	1.090477
C	-1.816087	1.420460	0.190842
C	-2.582141	0.200941	-0.348508

C	-1.958900	-1.153237	0.134977
C	-1.025727	-0.969749	1.341252
C	-4.044016	0.252866	0.112194
C	-5.069021	-0.368797	-0.817046
H	0.451852	0.384415	2.071830
O	-4.359984	0.738327	1.184713
C	-6.458870	-0.481113	-0.208810
O	-7.299023	-1.063594	-1.199111
C	1.607516	1.573038	-0.802665
C	1.416185	2.711925	0.197703
O	0.245132	2.454076	0.832788
O	0.253280	1.178663	-1.048622
O	2.144008	3.635357	0.448485
H	3.569972	-3.013599	1.220933
H	4.407731	-1.493954	1.507688
H	0.684289	-1.240109	-1.477472
H	0.514809	-2.494342	-0.233000
H	5.168807	0.334415	0.477954
H	4.906131	1.490511	-0.826090
H	5.740521	-0.033616	-1.157780
H	4.102154	-0.799470	-2.962785
H	2.384129	-0.452722	-2.783806
H	3.564534	0.869954	-2.828589
H	-2.015373	2.306446	-0.418293
H	-2.170811	1.637291	1.202551
H	-2.568740	0.209972	-1.443172
H	-2.749684	-1.862272	0.406192
H	-1.425261	-1.608032	-0.702001
H	-0.640900	-1.936437	1.678359
H	-1.616079	-0.580779	2.177922
H	-5.113211	0.240167	-1.731359
H	-4.719073	-1.355887	-1.146640
H	-6.808745	0.515623	0.093089
H	-6.414594	-1.095800	0.702418
H	-8.190955	-1.121444	-0.834509
H	2.048038	1.920979	-1.734262

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