Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Vibsanoids A−D, four new subtype vibsane diterpenoids with a distinctive tricyclo[8.2.1.$0^{2,9}$]tridecane core from *Viburnum odoratissimum*

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Contents

Table S1 ^{1}H (600 Hz) and ^{13}C (150 Hz) NMR data of compounds **1**–**4**.

No.	**1**[a]		**2**[a]		**3**[b]		**4**[b]	
	δ_H, mult (*J* in Hz)	δ_C	δ_H, mult (*J* in Hz)	δ_C	δ_H, mult (*J* in Hz)	δ_C	δ_H, mult (*J* in Hz)	δ_C
1	*α* 0.88, m *β* 1.54, dd (9.4, 2.4)	42.3	*α* 1.18, o. *β* 1.46, dd (9.3, 1.7)	44.5	*α* 1.14, dd (10.0, 1.5) *β* 1.21, m	45.2	*α* 1.12, o. *β* 1.59, dd (10.8, 2.5)	43.2
2	2.81, m	39.6	1.78, o.	45.4	2.45, m	42.0	1.80, o.	41.1
3	-	53.7	-	44.9	-	56.0	-	54.2
4	-	95.8	*α* 1.80, o. *β* 1.25, o.	30.3	-	113.3	4.93, dd (9.4, 3.4)	75.3
5	*α* 2.90, dd (15.4, 2.0) *β* 1.85, dd (15.4, 1.9)	36.9	*α* 1.31, o. *β* 2.08, m	25.2	6.24, d (5.8) -	134.2	2.79, o. 2.79, o.	39.6
6	3.15, o.	58.7	2.85, dd (9.6, 5.2)	62.1	6.07, d (5.8)	135.7	-	216.2
7	-	54.8	-	59.8	-	88.9	-	81.8
8	4.31, d (7.6)	70.6	4.72, dd (11.2, 6.3)	74.5	5.27, dd (11.6, 4.1)	75.1	4.68, dd (12.2, 2.7)	74.6
9	4.72, t (7.6)	69.4	*α* 1.61, td (13.5, 6.3) *β* 1.16, o.	24.3	*α* 1.84, o. *β* 1.52, o.	27.4	*α* 1.78, o. *β* 1.27, m	34.0
10	1.23, o.	52.9	1.32, o.	50.9	0.86, m	50.7	1.15, o.	50.1
11	-	47.7	-	47.5	-	48.0	-	46.5
12	*α* 1.20, o. *β* 1.32, o.	36.3	1.37, m 1.75, o.	27.7	*α* 1.85, o. *β* 1.32, m	32.0	*α* 1.33, m *β* 1.48, td (12.2, 2.3)	37.6
13	*α* 1.69, m *β* 1.32, o.	27.8	1.06, m 1.25, o.	27.4	*α* 2.24, m *β* 1.52, o.	28.1	*α* 1.79, o. *β* 1.54, m	27.7
18	3.85, dd (11.5, 5.3) 3.17, o.	65.8	3.40, dd (11.1, 4.5) 3.60, dd (11.1, 4.5)	58.0	3.43, d (10.7) 3.37, d (10.7)	67.9	3.42, d (10.7) 4.05, d (10.7)	66.5
19	1.13, s	22.5	1.17, s	15.7	1.38, s	23.2	1.22, s	19.0
20	0.89, s	18.0	1.00, s	19.8	1.12, s	20.4	0.98, s	19.0

1'	-	165.5	-	165.1	-	165.6	-	165.4
2'	5.71, d (1.4)	115.1	5.72, d (1.3)	115.4	5.61, d (1.3)	116.0	5.70, d (1.3)	115.6
3'	-	158.2	-	157.7	-	157.6	-	158.4
4'	2.12, d (1.4)	20.0	2.12, d (1.3)	20.0	2.16, d (1.3)	20.6	2.16, d (1.3)	20.5
5'	1.89, d (1.4)	27.0	1.89, d (1.3)	26.9	1.89, d (1.3)	27.6	1.89, d (1.3)	27.6
4-OH	5.64, s	-	-	-	-	-	-	-
18-OH	4.05, dd (5.3, 3.3)	-	4.33, t (4.5)	-	-	-	-	-

a: measured in DMSO-d_6.

b: measured in $CDCl_3$.

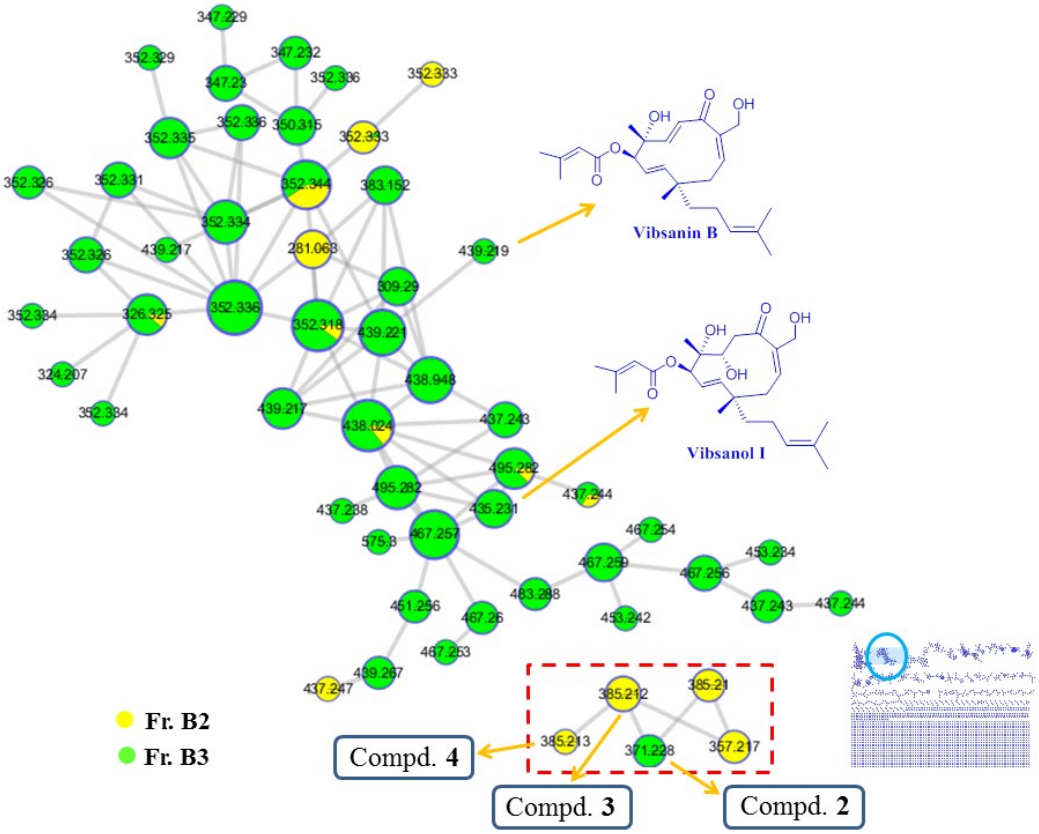


Figure S1 Molecular network of the fractions from *V. odoratissimum*. Node sizes are based on the degree of correlation between compounds. And the nodes with novel skeleton were highlighted using the red frame.

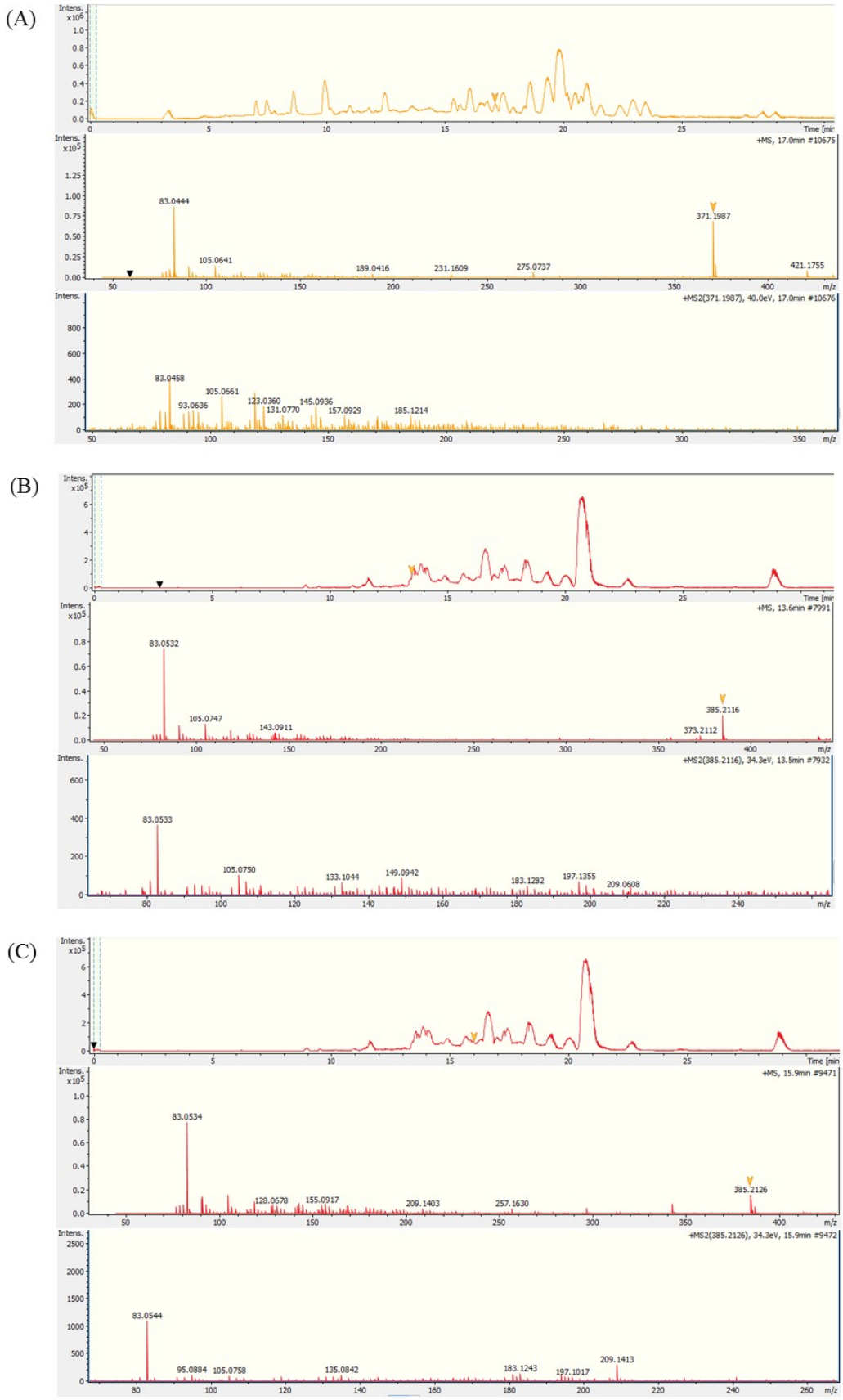


Figure S2 TIC of the fractions from the extract of *V. odoratissimum* and the corresponding MS/MS spectra of compounds **2-4** (A-C).

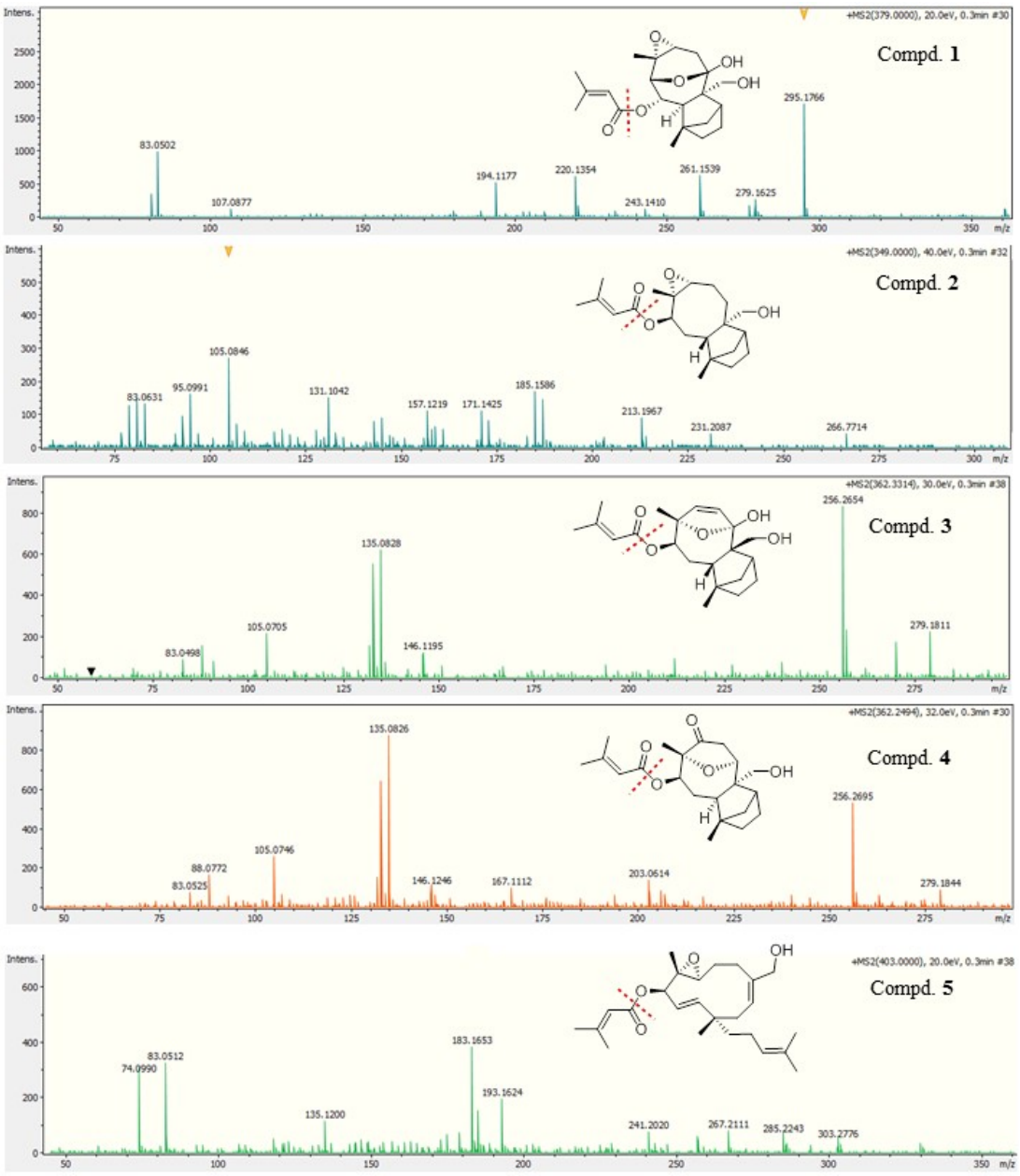
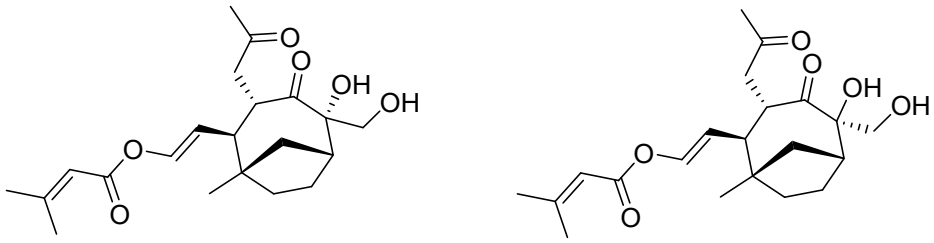


Figure S3 MS/MS spectra of compounds **1-5**.



vibstin A **vibstin B**

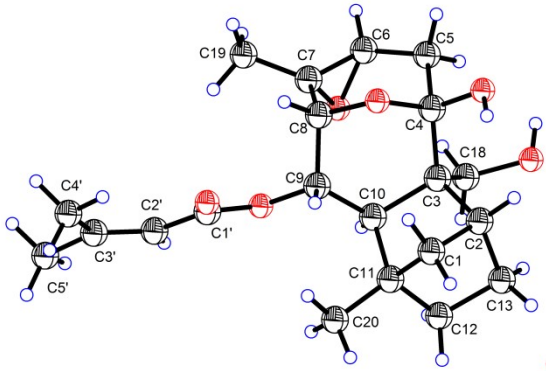
Figure S4 The structures of vibsatins A and B.

Table S2 The cytotoxic effects of compounds on A549, HepG2 and MCF-7 cells (IC_{50}, μM)

Compound	A549	HepG2	MCF-7
1	>50	>50	>50
2	>50	>50	>50
3	>50	>50	>50
4	>50	>50	>50
5	29.10 ± 1.02	9.82 ± 0.12	34.88 ± 0.67
Taxol[a]	0.024 ± 0.001	-	-
Sorafenib[a]	-	6.49 ± 0.24	-
Tamoxifen[a]	-	-	15.65 ± 0.53

[a] Positive control.

Table S3 Crystal data and structure refinement for **1**.



Empirical formula	$C_{21}H_{30}O_6$
Formula weight	378.45
Temperature	153(2) K
Crystal system	monoclinic
Space group	P 1 21 1
a/Å	6.8059(6)
b/Å	11.1722(9)
c/Å	12.3471(11)
α/°	90
β/°	95.962(5)
γ/°	90
Volume/Å	933.76(14)
Z	2
ρ_{calc}g/cm^3	1.346
μ/mm^{-1}	0.799
F(000)	408
Crystal size/mm^3	0.15 × 0.15 × 0.1
Radiation	Cu Kα (λ = 1.54178)
Theta range for data collection/°	3.60 to 67.49
Index ranges	-8≤h≤8, -13≤k≤13, -14≤l≤14
Reflections collected	13150
Independent reflections	3263 [R(int) = 0.1556]
Data/restraints/parameters	3263/1/250
Goodness-of-fit on F^2	1.103
Final R indexes [I>2σ(I)]	R_1 = 0.0671, wR_2 = 0.1715
Final R indexes [all data]	R_1 = 0.1008, wR_2 = 0.1953
Largest diff. peak/hole/e Å^3	0.486/-0.475
Absolute structure parameter	0.3(3)

Table S4 Experimental and calculated ^{13}C NMR data of compound **2** and its possible isomers **2a-2d** (ppm)

No.	**2 (Exp.)**	**Calcd.**			
		2a	**2b**	**2c**	**2d**
1	44.5	47.8	44.6	46.6	44.2
2	45.4	50.5	47.2	50.4	53.9
3	44.9	51.6	54.9	50.7	56.7
4	30.3	33.3	26.8	30.1	29.6
5	25.2	29.4	31.7	28.3	27.5
6	62.1	66.9	68.7	67.9	66.2
7	59.8	64.6	65.3	64.9	65.4
8	74.5	79.6	83.9	79.0	81.6
9	24.3	27.6	31.8	28.1	39.4
10	50.9	54.4	53.4	49.1	54.9
11	47.5	53.5	51.9	54.2	52.7
12	27.7	31.2	44.1	31.8	41.7
13	27.4	31.5	27	27.3	29.2
18	58.0	64.4	67.2	71.3	69.1
19	15.7	18.1	19.5	22.1	18.3
20	19.8	21.4	20.9	22.1	20.8
1'	165.1	175.6	174.8	174.7	175.5
2'	115.4	120.6	120.9	120.6	120.7
3'	157.7	176.3	176.1	176.5	176.2
4'	20.0	21.3	21.3	21.2	21.3
5'	26.9	30.5	30.4	30.4	30.5

Table S5 The results of DP4+ analysis of compound **2**.

A	B	C	D	E	F	G	H
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311+G(d,p)		Unscaled Shifts	
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		99.74%	0.22%	0.04%	0.00%	–	–
sDP4+ (C data)		100.00%	0.00%	0.00%	0.00%	–	–
sDP4+ (all data)		100.00%	0.00%	0.00%	0.00%	–	–
uDP4+ (H data)		15.83%	84.14%	0.01%	0.02%	–	–
uDP4+ (C data)		100.00%	0.00%	0.00%	0.00%	–	–
uDP4+ (all data)		100.00%	0.00%	0.00%	0.00%	–	–
DP4+ (H data)		98.85%	1.15%	0.00%	0.00%	–	–
DP4+ (C data)		100.00%	0.00%	0.00%	0.00%	–	–
DP4+ (all data)		100.00%	0.00%	0.00%	0.00%	–	–

To further validate the relative configurations of C-10 and C-3 for the formation of new bond and confirm the deduced structures of compound **3** and **4**, ^{13}C NMR predictions with DFT method were also performed. The results were as following.

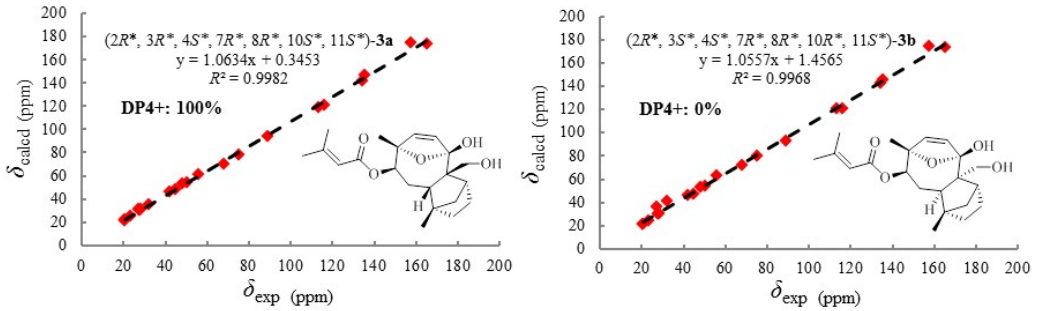


Figure S5 Liner correlation and DP4+ probability analysis between calculated and experimental ^{13}C NMR chemical shifts of compounds **3a–3b**.

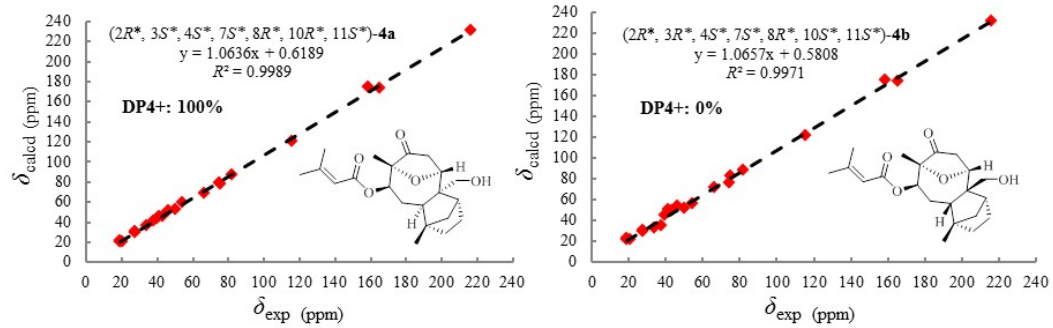


Figure S6 Liner correlation and DP4+ probability analysis between calculated and experimental ^{13}C NMR chemical shifts of compounds **4a–4b**.

Table S6 Experimental and calculated ^{13}C NMR data of compounds **3**, **4** and their possible isomers (ppm)

No.	**3 (Exp.)**	**Calcd.**		**4 (Exp.)**	**Calcd.**	
		3a	**3b**		**4a**	**4b**
1	45.2	47.8	47.3	43.2	45.9	49.4
2	42.0	46.1	45.9	41.1	45.8	50.7
3	56.0	60.8	63.0	54.2	59.7	56.3
4	113.3	119.2	120.2	75.3	78.6	82.5
5	134.2	141.7	142.3	39.6	44.2	44.4
6	135.7	146.5	145.2	216.2	231.1	231.2
7	88.9	94.2	93.2	81.8	86.9	87.7
8	75.1	78.2	79.6	74.6	79.1	76.2
9	27.4	30.8	36.2	34.0	36.6	32.8
10	50.7	54.3	53.9	50.1	52.9	52.1
11	48.0	53.0	52.8	46.5	51.7	53.6
12	32.0	34.7	40.9	37.6	40.9	34.7
13	28.1	31.3	30.3	27.7	31.5	29.8
18	67.9	70.0	71.8	66.5	68.9	71.8
19	23.2	24.9	24.2	19.0	21.8	22.6
20	20.4	22.1	20.9	19.0	20.7	22.2
1'	165.6	173.5	173.4	165.4	173.6	173.6
2'	116.0	121.0	121.0	115.6	121.1	121.4
3'	157.6	174.9	174.9	158.4	174.6	174.7
4'	20.6	21.1	21.1	20.5	21.2	21.2
5'	27.6	30.2	30.3	27.6	30.2	30.2

Table S7 The results of DP4+ analysis of compound **3**.

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	100.00%	0.00%	–	–	–	–
sDP4+ (C data)	99.99%	0.01%	–	–	–	–
sDP4+ (all data)	100.00%	0.00%	–	–	–	–
uDP4+ (H data)	100.00%	0.00%	–	–	–	–
uDP4+ (C data)	99.90%	0.10%	–	–	–	–
uDP4+ (all data)	100.00%	0.00%	–	–	–	–
DP4+ (H data)	100.00%	0.00%	–	–	–	–
DP4+ (C data)	100.00%	0.00%	–	–	–	–
DP4+ (all data)	100.00%	0.00%	–	–	–	–

Table S8 The results of DP4+ analysis of compound **4**.

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	100.00%	0.00%	–	–	–	–
sDP4+ (C data)	100.00%	0.00%	–	–	–	–
sDP4+ (all data)	100.00%	0.00%	–	–	–	–
uDP4+ (H data)	100.00%	0.00%	–	–	–	–
uDP4+ (C data)	100.00%	0.00%	–	–	–	–
uDP4+ (all data)	100.00%	0.00%	–	–	–	–
DP4+ (H data)	100.00%	0.00%	–	–	–	–
DP4+ (C data)	100.00%	0.00%	–	–	–	–
DP4+ (all data)	100.00%	0.00%	–	–	–	–

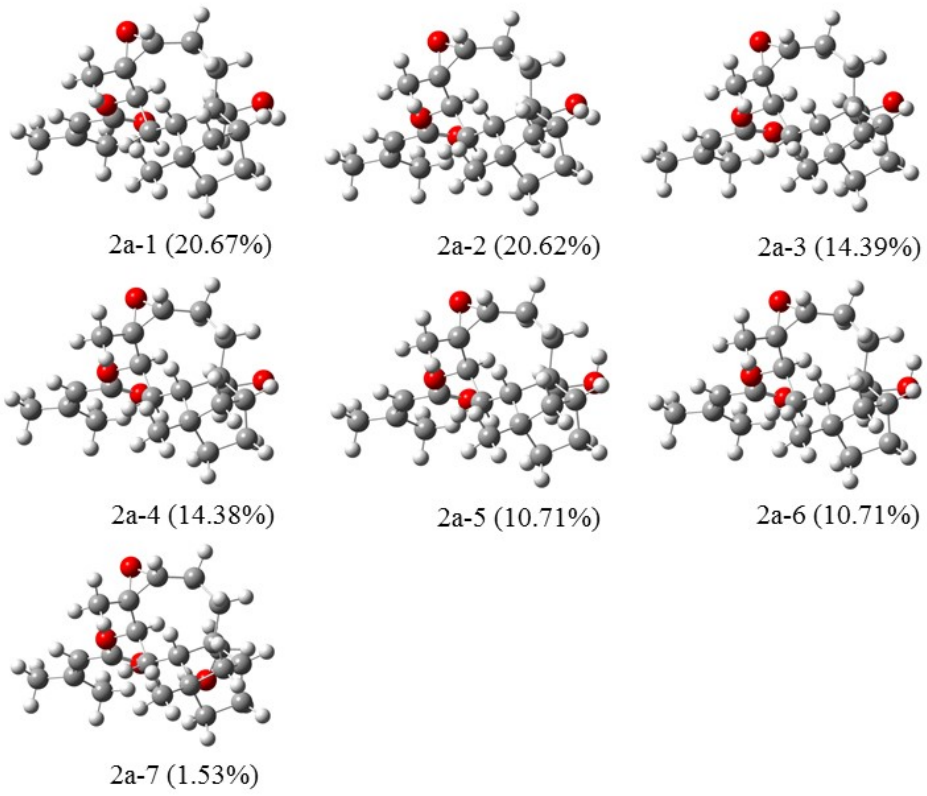


Figure S7 The low-energy conformers of compound **2a**.

Table S9 Conformer analyses of compound **2a**.

Gibbs free energy and Boltzmann distribution of compound **2a** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution
2a-1	-1120.42245332	0	20.67%
2a-2	-1120.42245100	0.00000232	20.62%
2a-3	-1120.42211148	0.00034184	14.39%
2a-4	-1120.41918408	0.00326924	14.38%
2a-5	-1120.42183289	0.00062043	10.71%
2a-6	-1120.42183264	0.00062068	10.71%
2a-7	-1120.41999222	0.00246110	1.53%

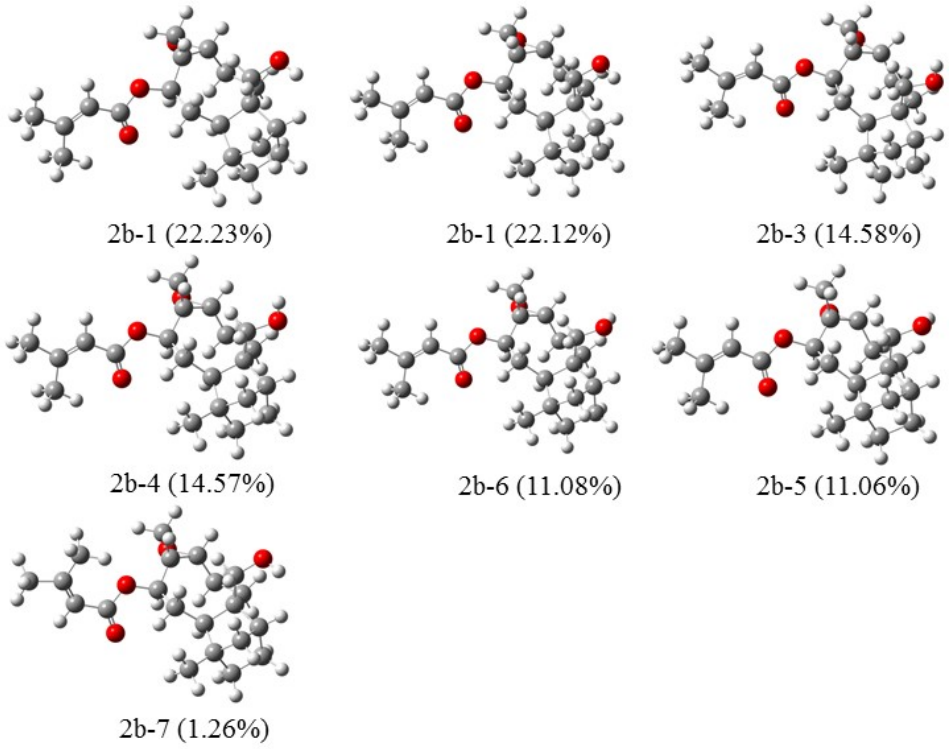


Figure S8 The low-energy conformers of compound **2b**.

Table S10 Conformer analyses of compound **2b**.

Gibbs free energy and Boltzmann distribution of compound **2b** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution
2b-1	-1120.41491463	0	22.23%
2b-2	-1120.41490990	0.00000473	22.12%

2b-3	-1120.41451634	0.00039829	14.58%
2b-4	-1120.41451562	0.00039901	14.57%
2b-5	-1120.41425685	0.00065778	11.06%
2b-6	-1120.41425501	0.00065962	11.08%
2b-7	-1120.41220540	0.00270923	1.26%

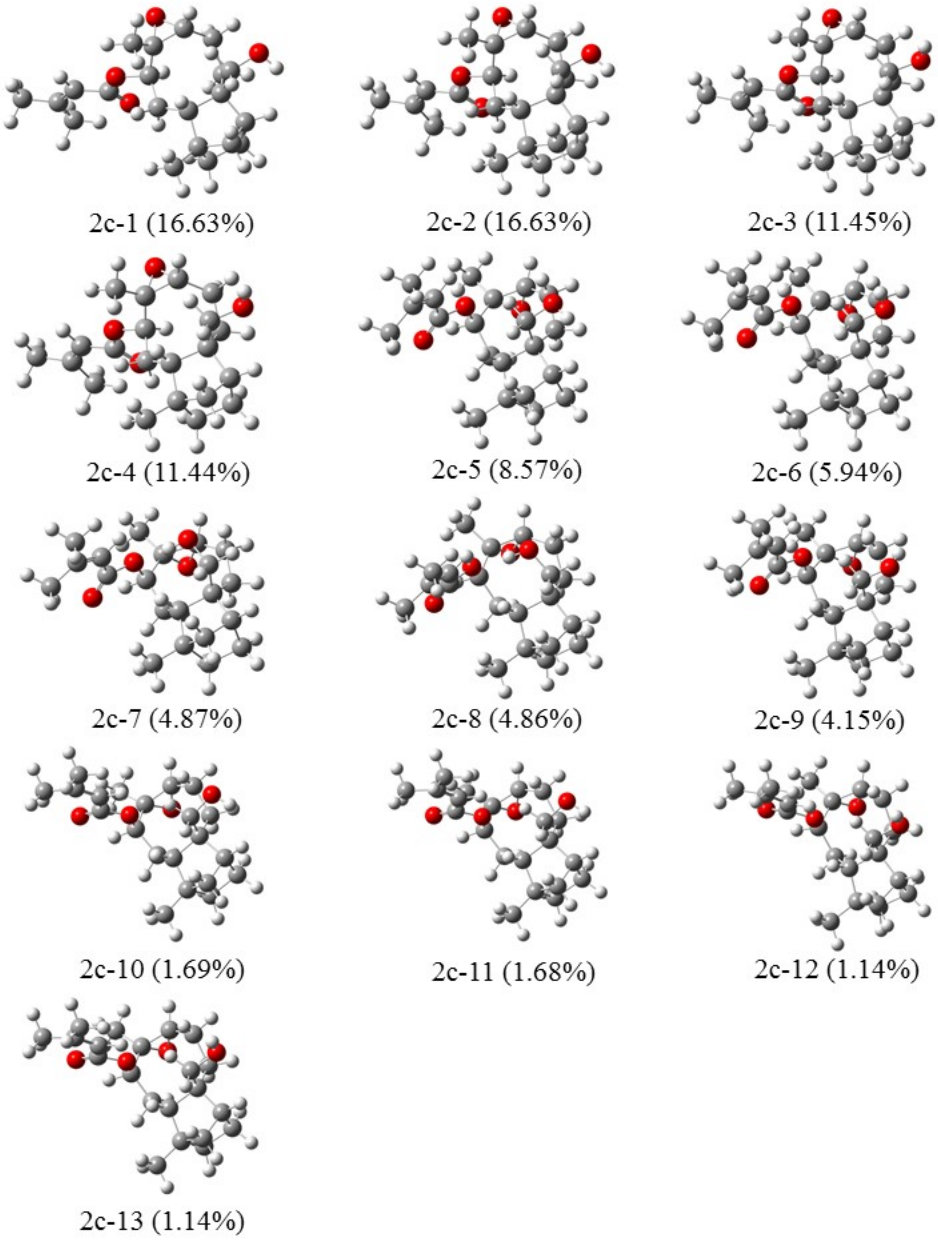


Figure S9 The low-energy conformers of compound **2c**.

Table S11 Conformer analyses of compound **2c**.

Gibbs free energy and Boltzmann distribution of compound **2c** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution

2c-1	-1120.41000748	0	16.63%
2c-2	-1120.41000716	0.00000032	16.63%
2c-3	-1120.40965448	0.00035300	11.45%
2c-4	-1120.40965365	0.00035383	11.44%
2c-5	-1120.40938118	0.00062630	8.57%
2c-6	-1120.40903578	0.00097170	5.94%
2c-7	-1120.40884746	0.00116002	4.87%
2c-8	-1120.40884537	0.00116211	4.86%
2c-9	-1120.40869773	0.00130975	4.15%
2c-10	-1120.40784871	0.00215877	1.69%
2c-11	-1120.40784555	0.00216193	1.68%
2c-12	-1120.40747945	0.00252803	1.14%
2c-13	-1120.40747789	0.00252959	1.14%

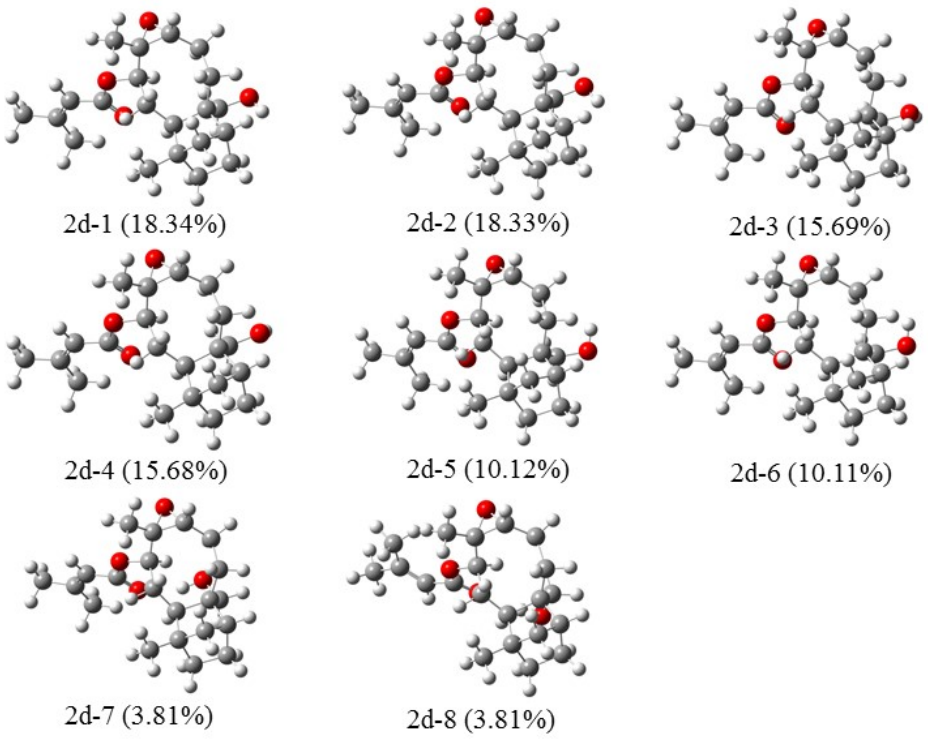


Figure S10 The low-energy conformers of compound **2d**.

Table S12 Conformer analyses of compound **2d**.

Gibbs free energy and Boltzmann distribution of compound **2d** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution

2d-1	-1120.41450112	0	18.34%
2d-2	-1120.41450091	0.00000021	18.33%
2d-3	-1120.41435371	0.00014741	15.69%
2d-4	-1120.41435361	0.00014751	15.68%
2d-5	-1120.41393960	0.00056152	10.12%
2d-6	-1120.41393865	0.00056247	10.11%
2d-7	-1120.41301735	0.00148377	3.81%
2d-8	-1120.41301730	0.00148382	3.81%

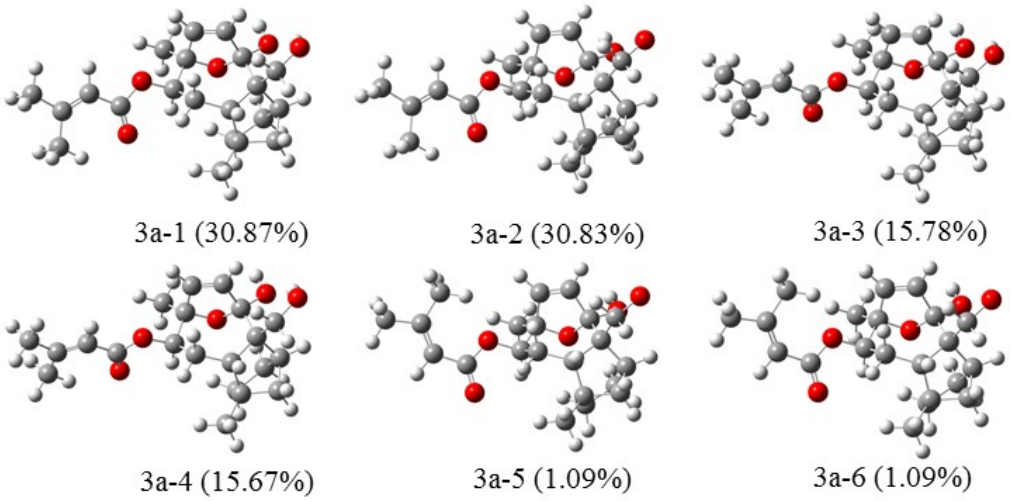


Figure S11. The low-energy conformers of compound **3a**.

Table S13. Conformer analyses of compound **3a**.

Gibbs free energy and Boltzmann distribution of compound **3a** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution
3a-1	-1194.44992764	0	30.87%
3a-2	-1194.44992654	0.00000110	30.83%
3a-3	-1194.44929441	0.00063323	15.78%
3a-4	-1194.44928768	0.00063996	15.67%
3a-5	-1194.44676696	0.00316068	1.09%
3a-6	-1194.44677170	0.00315594	1.09%

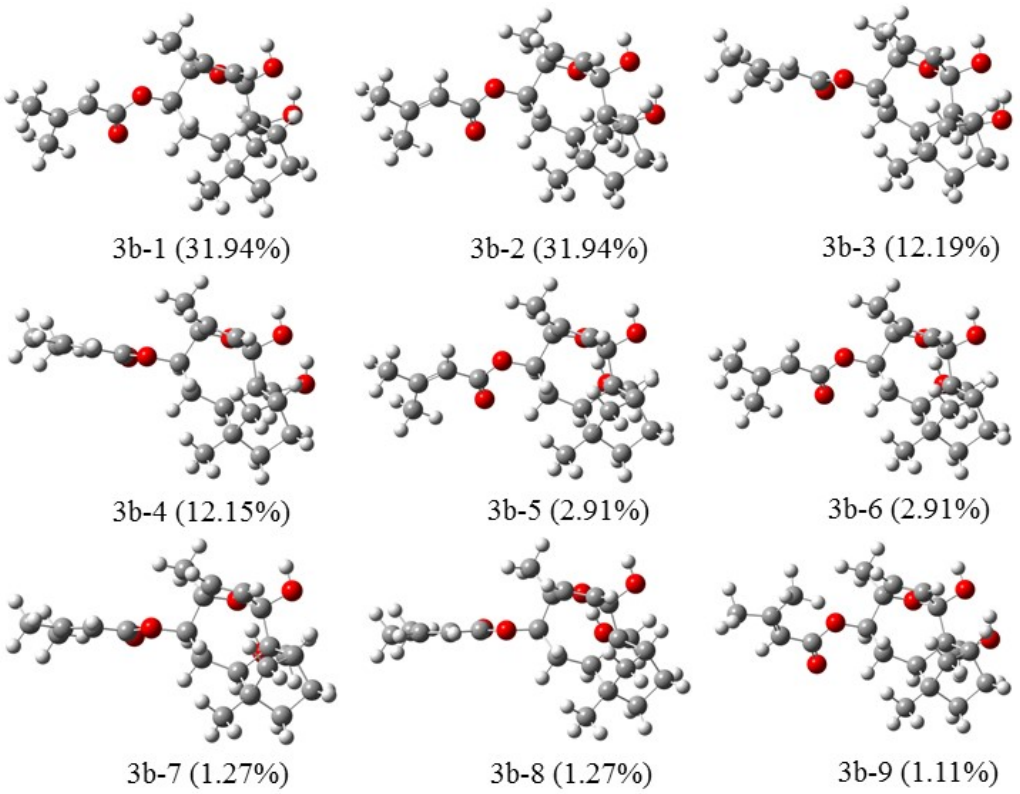


Figure S12. The low-energy conformers of compound **3b**.

Table S14. Conformer analyses of compound **3b**.

Gibbs free energy and Boltzmann distribution of compound **3b** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution
3b-1	-1194.45135648	0	31.94%
3b-2	-1194.45135643	0.00000005	31.94%
3b-3	-1194.45044680	0.00090968	12.19%
3b-4	-1194.45044359	0.00091289	12.15%
3b-5	-1194.44909516	0.00226132	2.91%
3b-6	-1194.44909586	0.00226062	2.91%
3b-7	-1194.44831428	0.00304220	1.27%
3b-8	-1194.44831243	0.00304405	1.27%
3b-9	-1194.44818252	0.00317396	1.11%

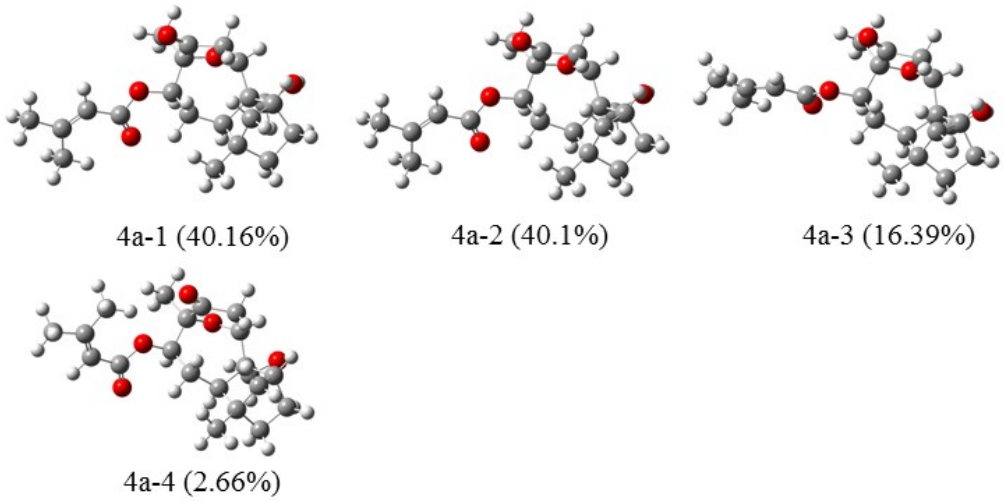


Figure S13. The low-energy conformers of compound **4a**.

Table S15. Conformer analyses of compound **4a**.

Gibbs free energy and Boltzmann distribution of compound **4a** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution
4a-1	-1194.46260719	0	40.16%
4a-2	-1194.46260568	0.00000151	40.1%
4a-3	-1194.46176122	0.00084597	16.39%
4a-4	-1194.46004390	0.00256329	2.66%

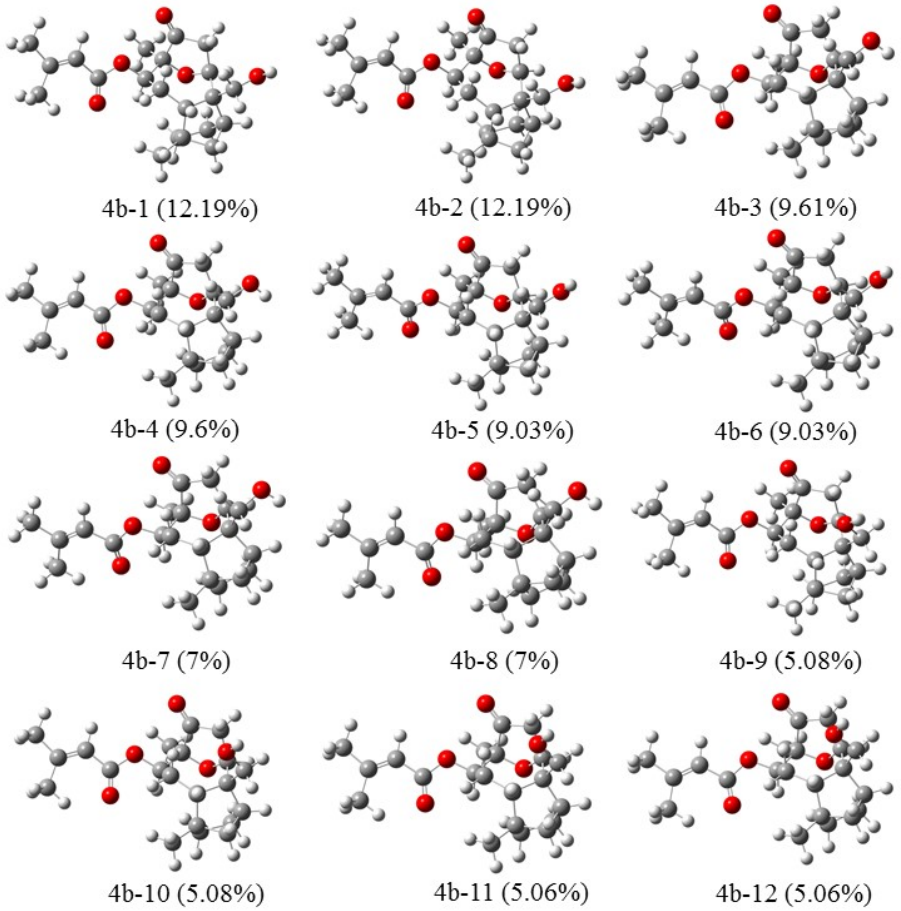
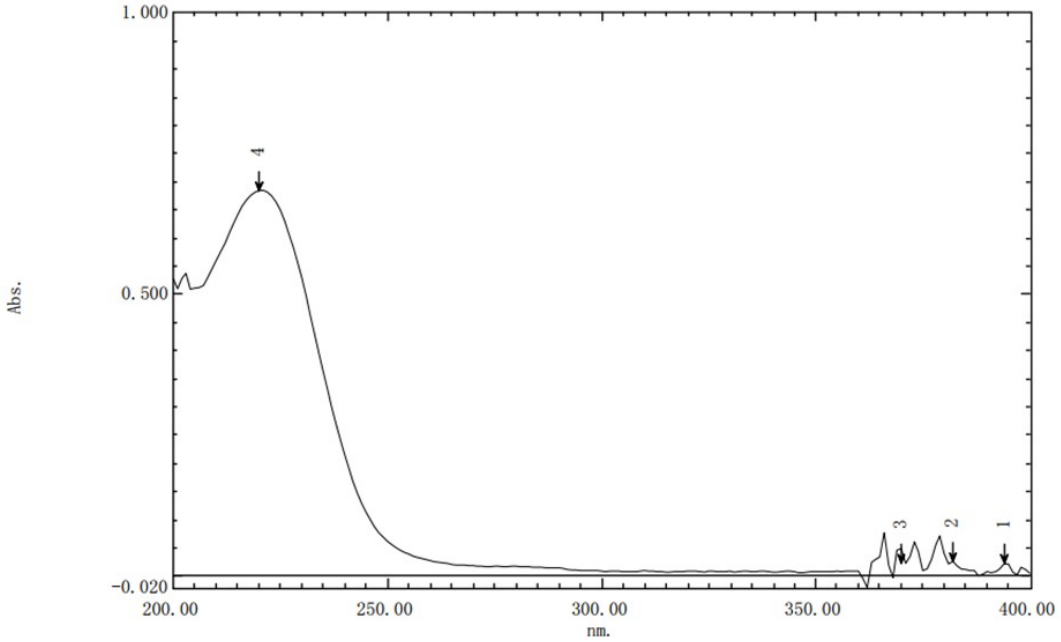


Figure S14. The low-energy conformers of compound **4b**.

Table S16. Conformer analyses of compound **4b**.

Gibbs free energy and Boltzmann distribution of compound **4b** (298.15 K)

Conformations	G (Hartree)	ΔG (Kcal/mol)	Boltzmann distribution
4b-1	-1194.45937152	0	12.19%
4b-2	-1194.45937131	0.00000021	12.19%
4b-3	-1194.45914701	0.00022451	9.61%
4b-4	-1194.45914660	0.00022492	9.6%
4b-5	-1194.45908834	0.00028318	9.03%
4b-6	-1194.45908777	0.00028375	9.03%
4b-7	-1194.45884753	0.00052399	7%
4b-8	-1194.45884703	0.00052449	7%
4b-9	-1194.45854452	0.00082700	5.08%
4b-10	-1194.45854426	0.00082726	5.08%
4b-11	-1194.45854227	0.00082925	5.06%
4b-12	-1194.45854168	0.00082984	5.06%



No.	P/V	Wavelength	Abs.	描述
1	↑	394.00	.022	
2	↑	382.00	.026	
3	↑	370.00	.023	
4	↑	220.00	.684	

Figure S15 UV spectrum of compound **1**.

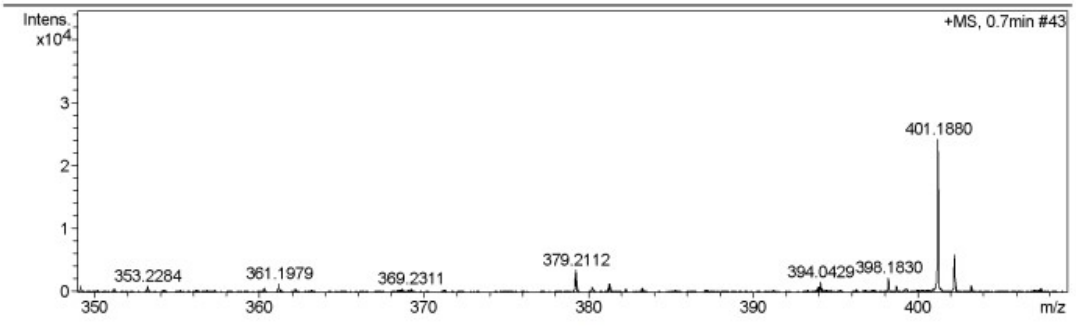
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\20201105 CEYANG\TM-65_1-F,2_01_15417.d	Acquisition Date	11/5/2020 4:38:11 PM
Method	20201105 ceyang.m		
Sample Name	TM-65	Operator	Bruker Customer
Comment		Instrument / Ser#	micrOTOF-Q 125

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
379.2112	1	C 21 H 31 O 6	379.2115	0.8	-21.7	6.5	ok	even	204.75	0.2761	0.0178	0.1792	0.0020	0.8427

Figure S16 HRESIMS spectrum of compound **1**.

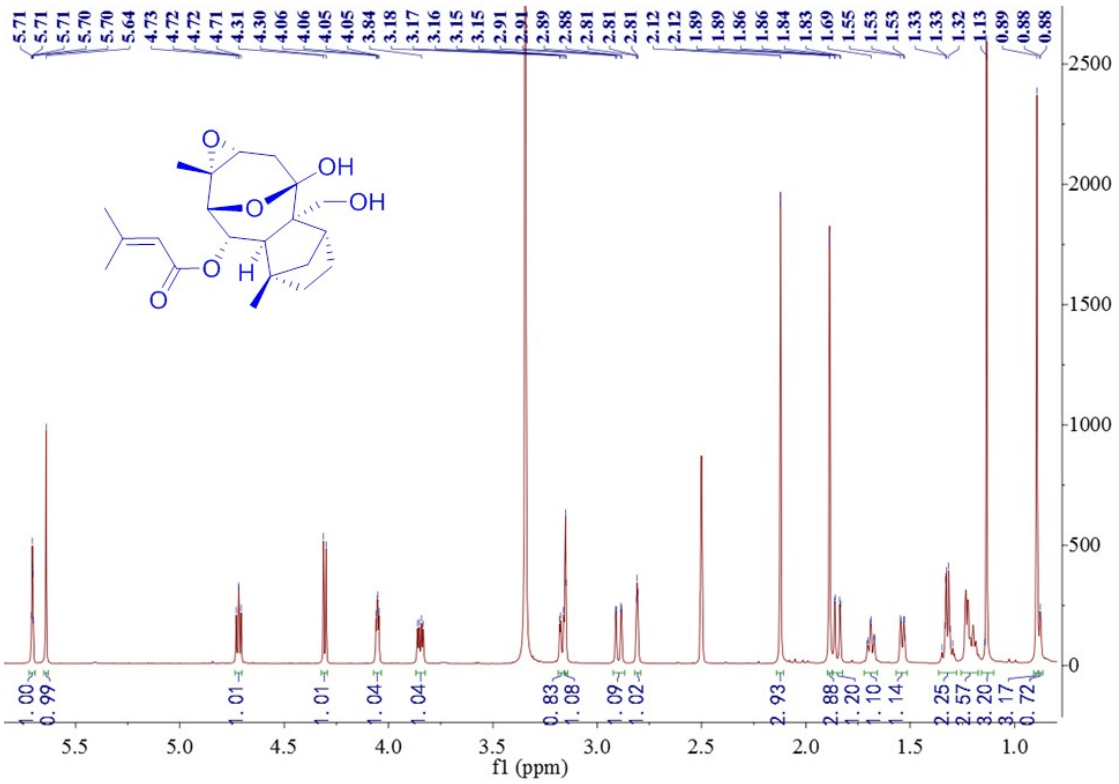


Figure S17 ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **1**.

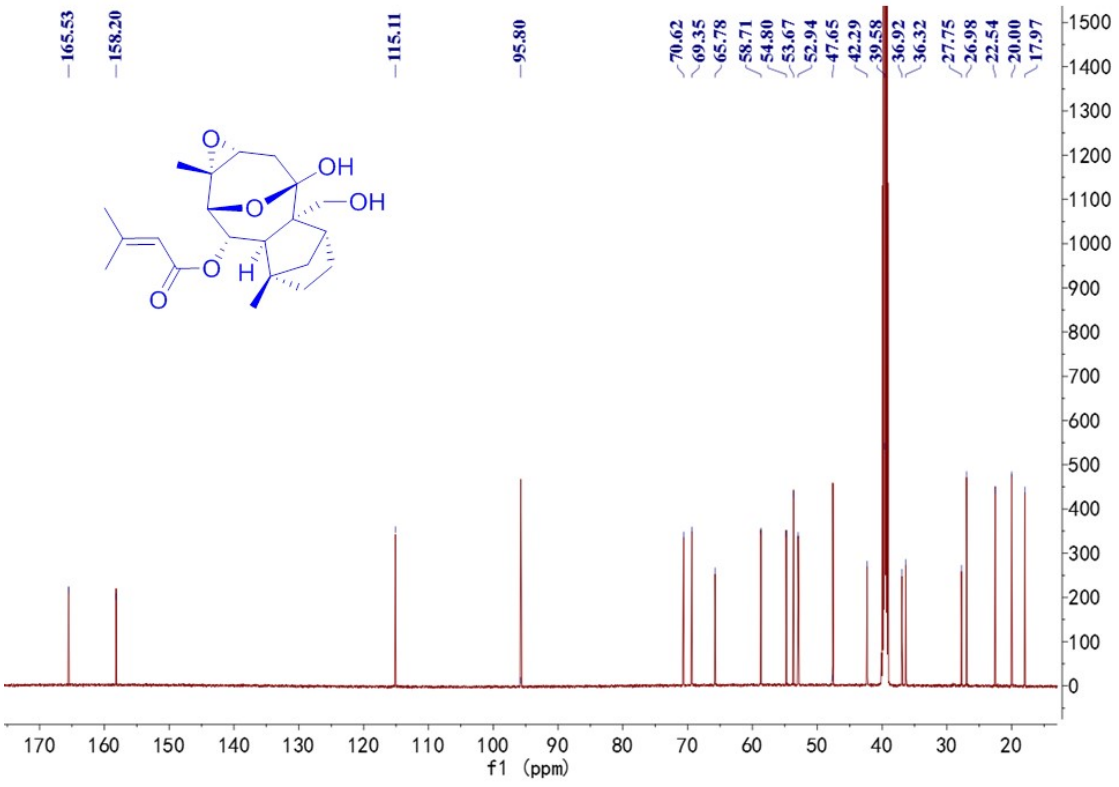


Figure S18 ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of compound **1**.

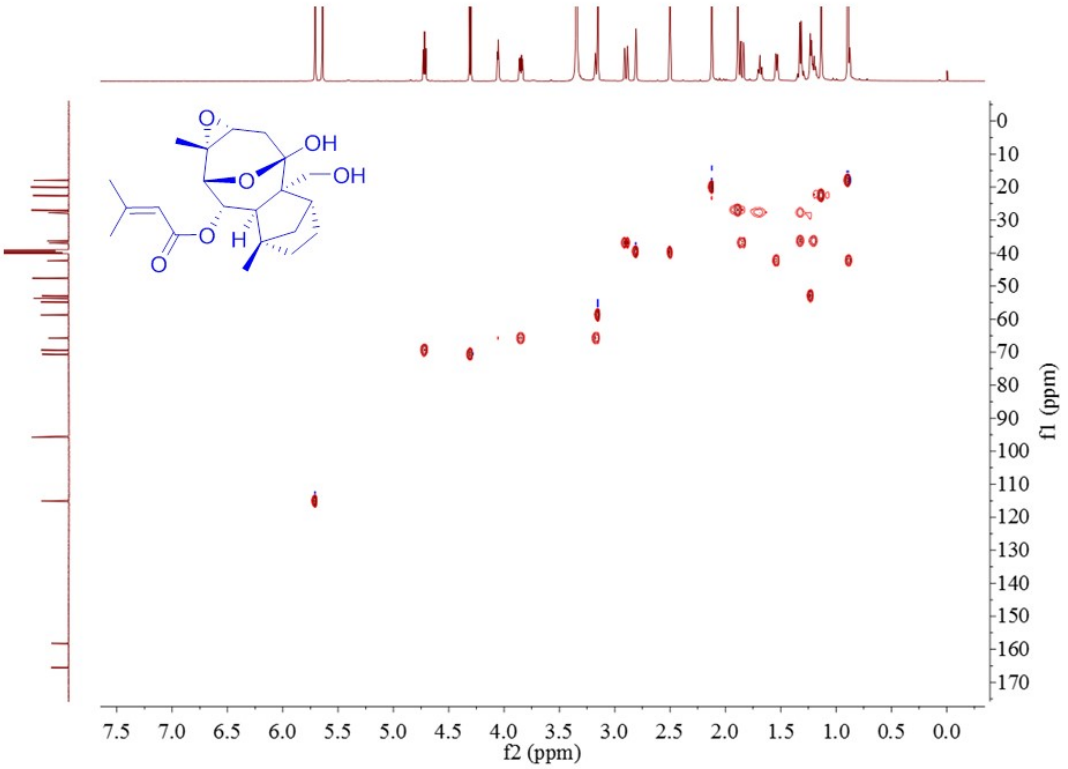


Figure S19 HSQC spectrum (600 MHz, DMSO-d_6) of compound **1**.

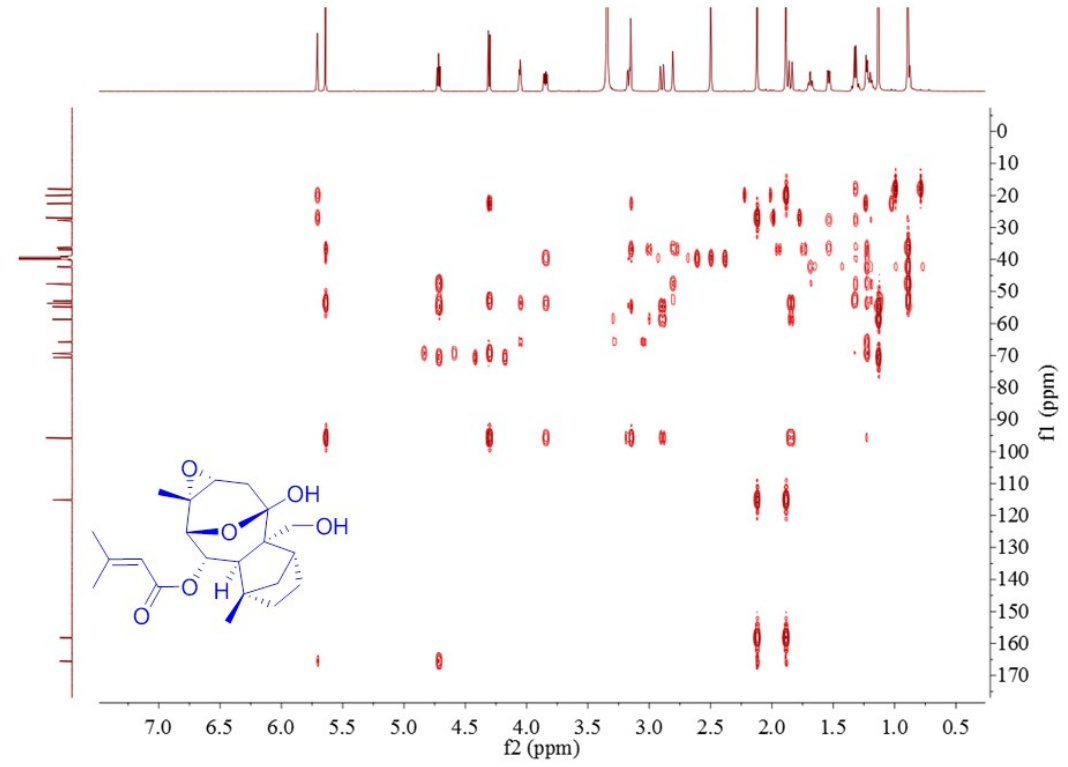


Figure S20 HMBC spectrum (600 MHz, DMSO-d_6) of compound **1**.

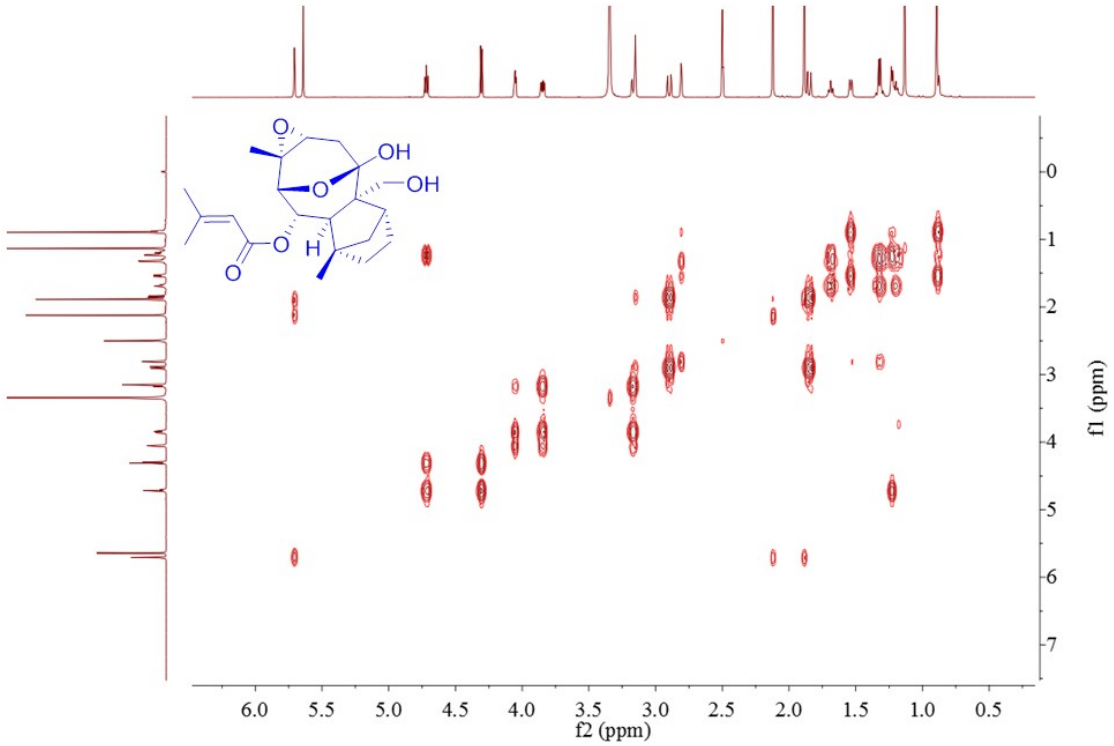


Figure S21 ^{1}H-^{1}H COSY spectrum (600 MHz, DMSO-d_6) of compound **1**.

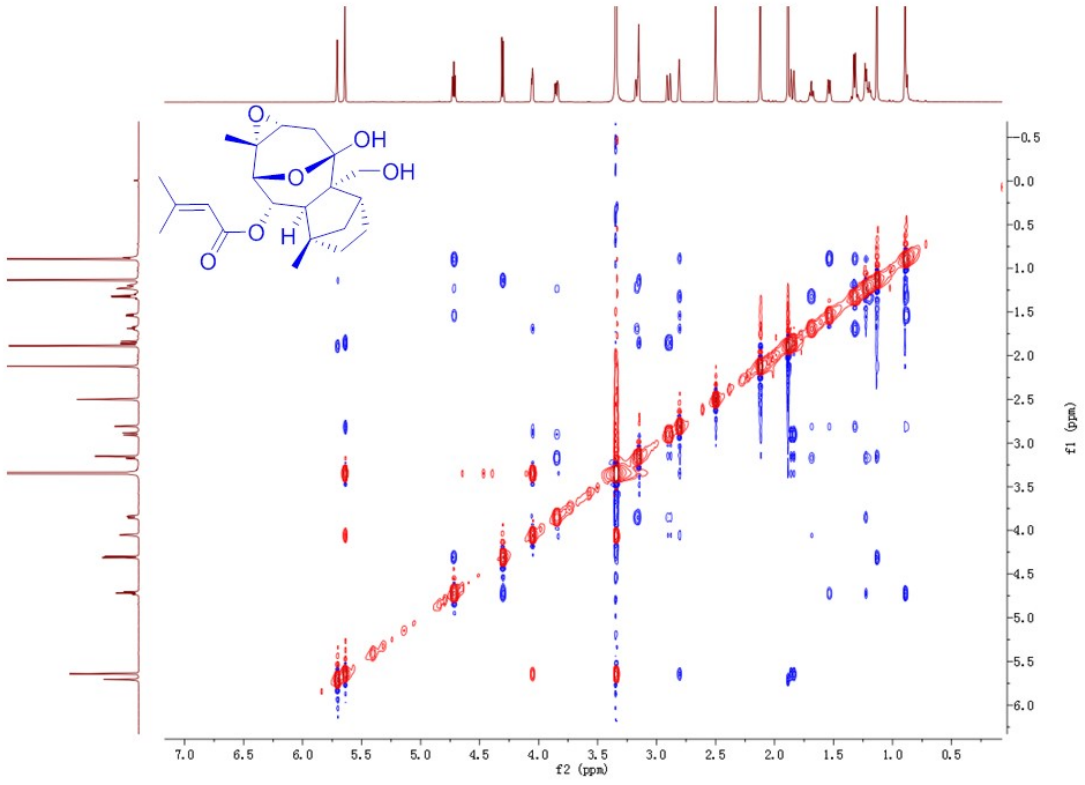


Figure S22 NOESY spectrum (600 MHz, DMSO-d_6) of compound **1**.

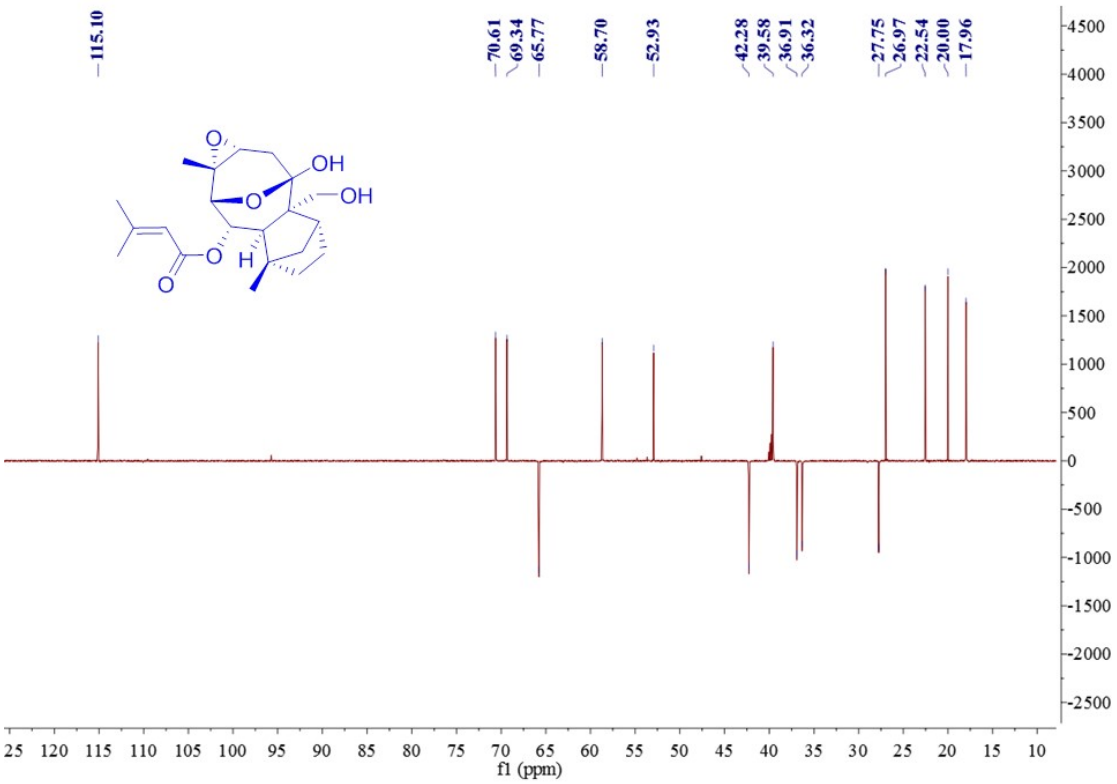
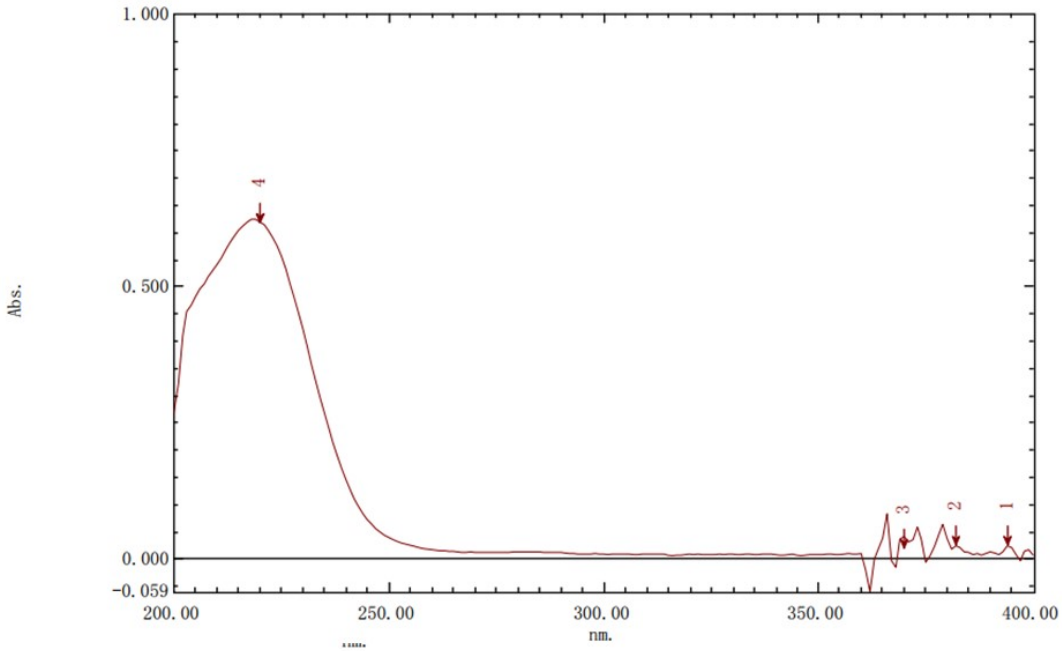


Figure S23 DEPT spectrum (600 MHz, DMSO-d_6) of compound **1**.



No.	P/V	Wavelength	Abs.	描述
1	↑	394.00	.025	
2	↑	382.00	.025	
3	↑	370.00	.019	
4	↑	220.00	.619	

Figure S24 UV spectrum of compound **2**.

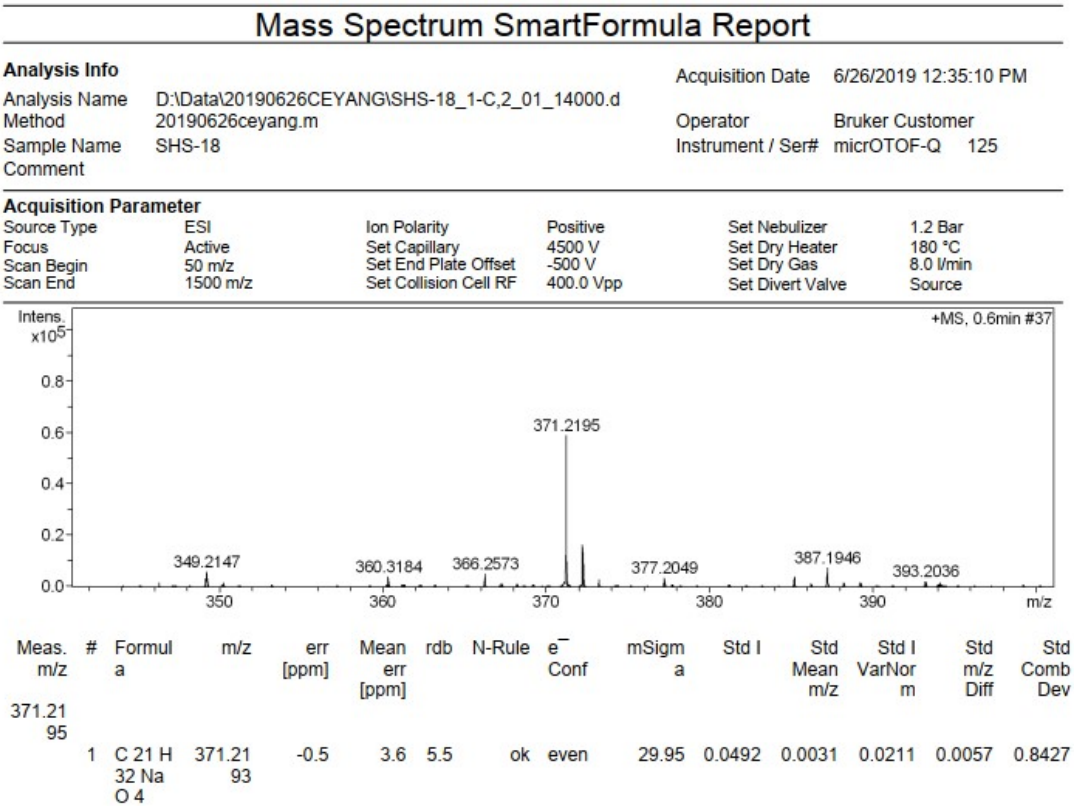


Figure S25 HRESIMS spectrum of compound **2**.

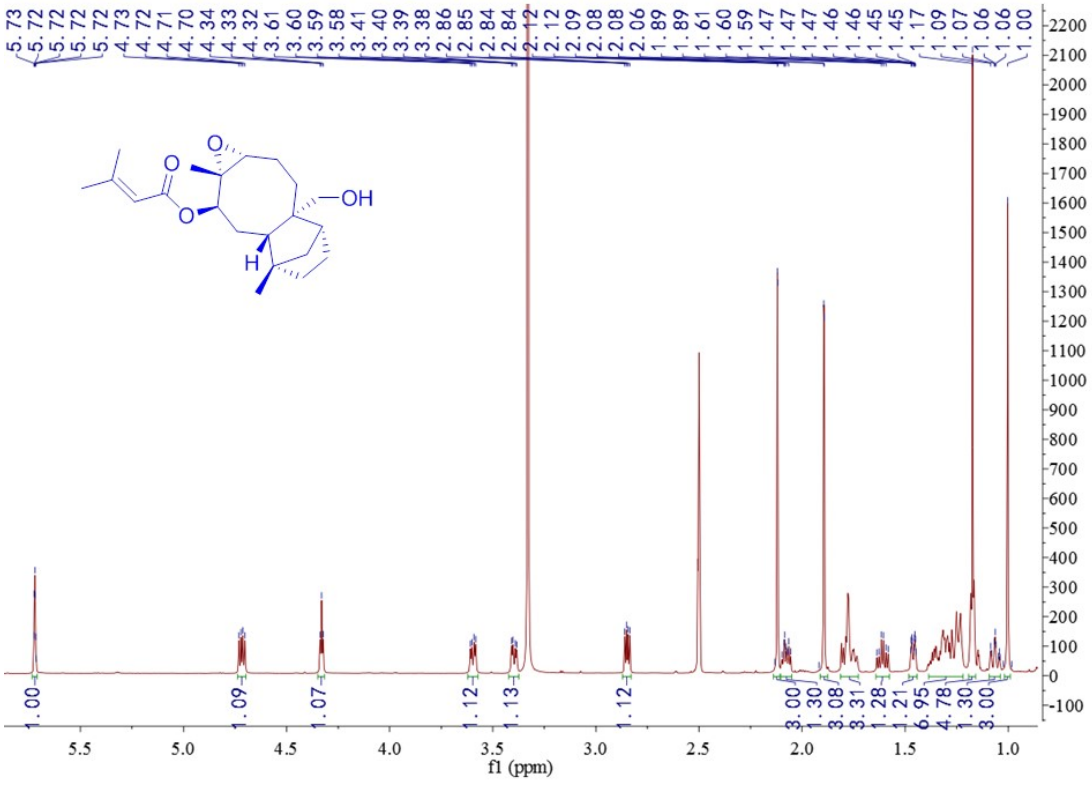


Figure S26 ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **2**.

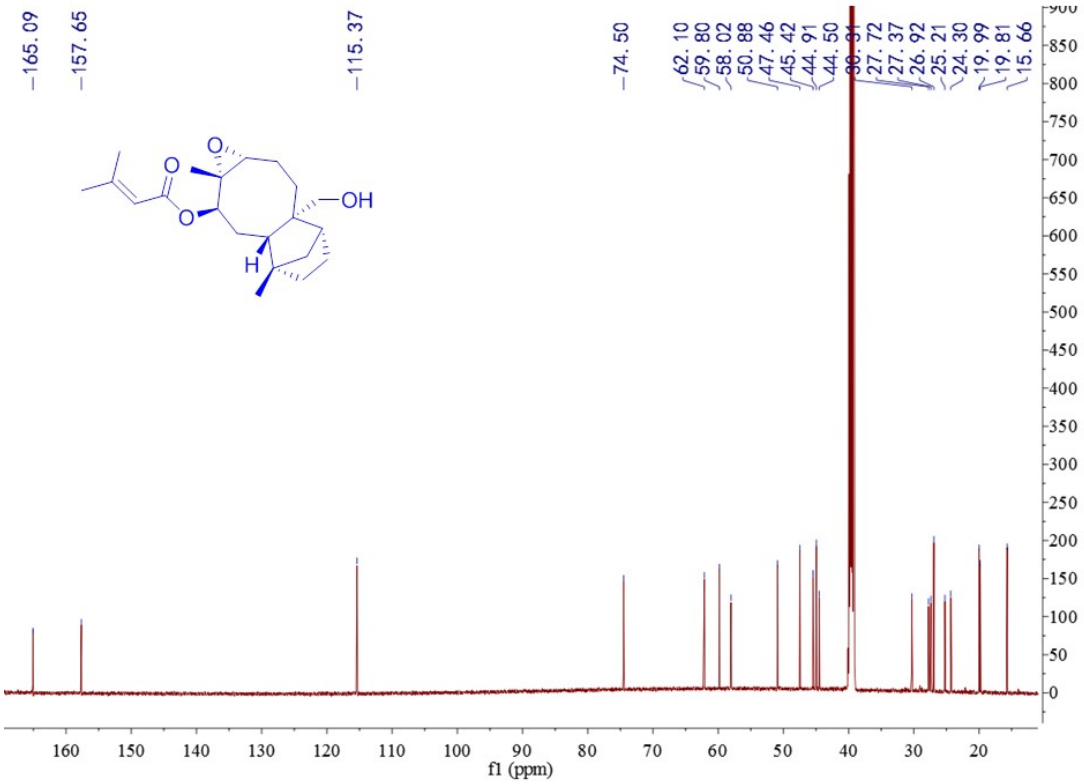


Figure S27 ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of compound **2**.

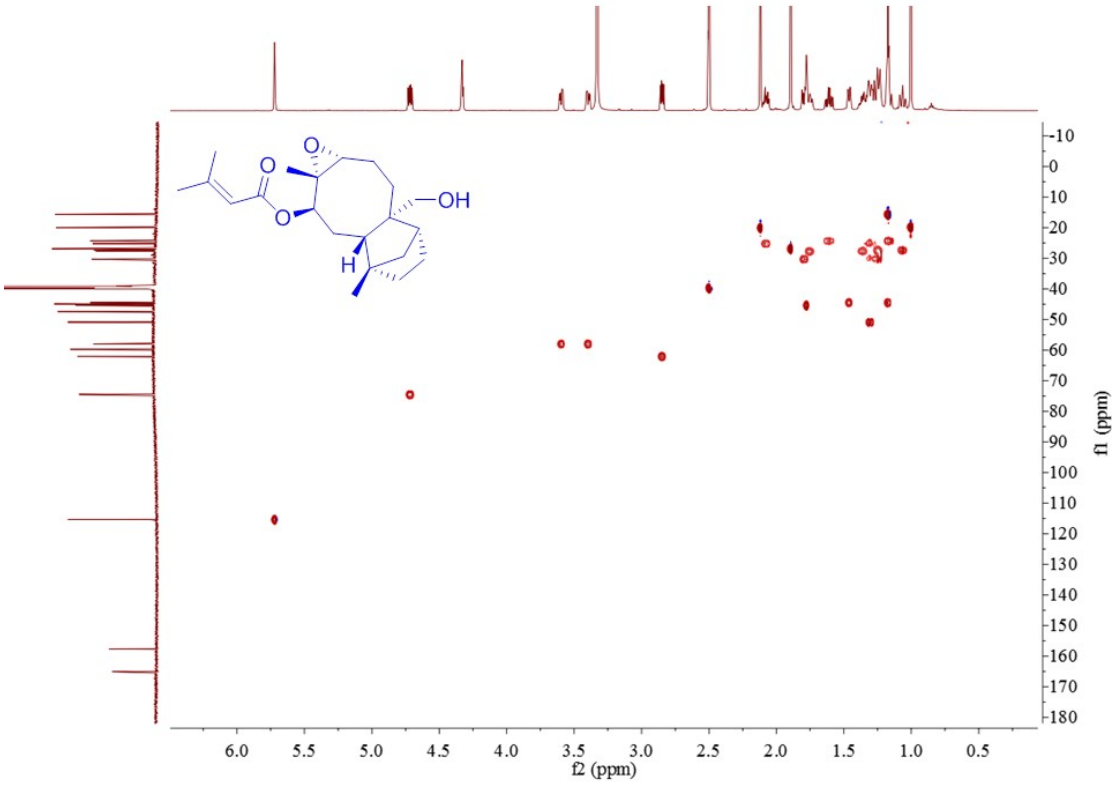


Figure S28 HSQC spectrum (600 MHz, DMSO-d_6) of compound **2**.

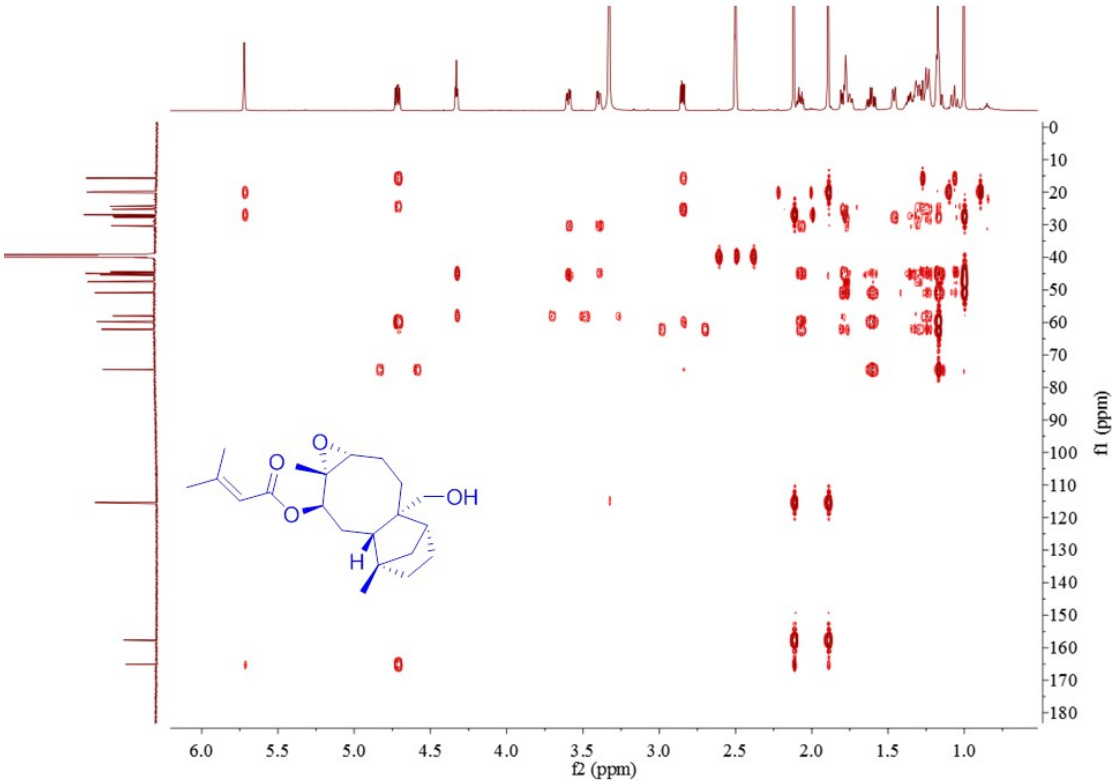


Figure S29 HMBC spectrum (600 MHz, DMSO-d_6) of compound **2**.

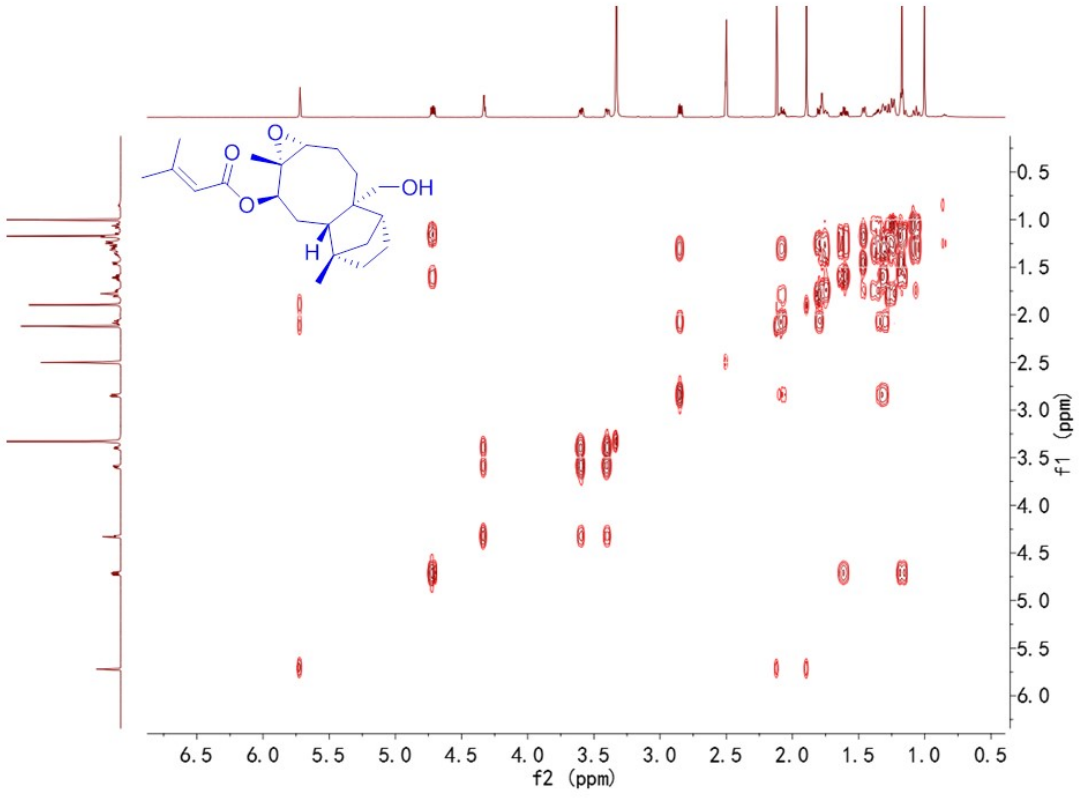


Figure S30 ^{1}H-^{1}H COSY spectrum (600 MHz, DMSO-d_6) of compound **2**.

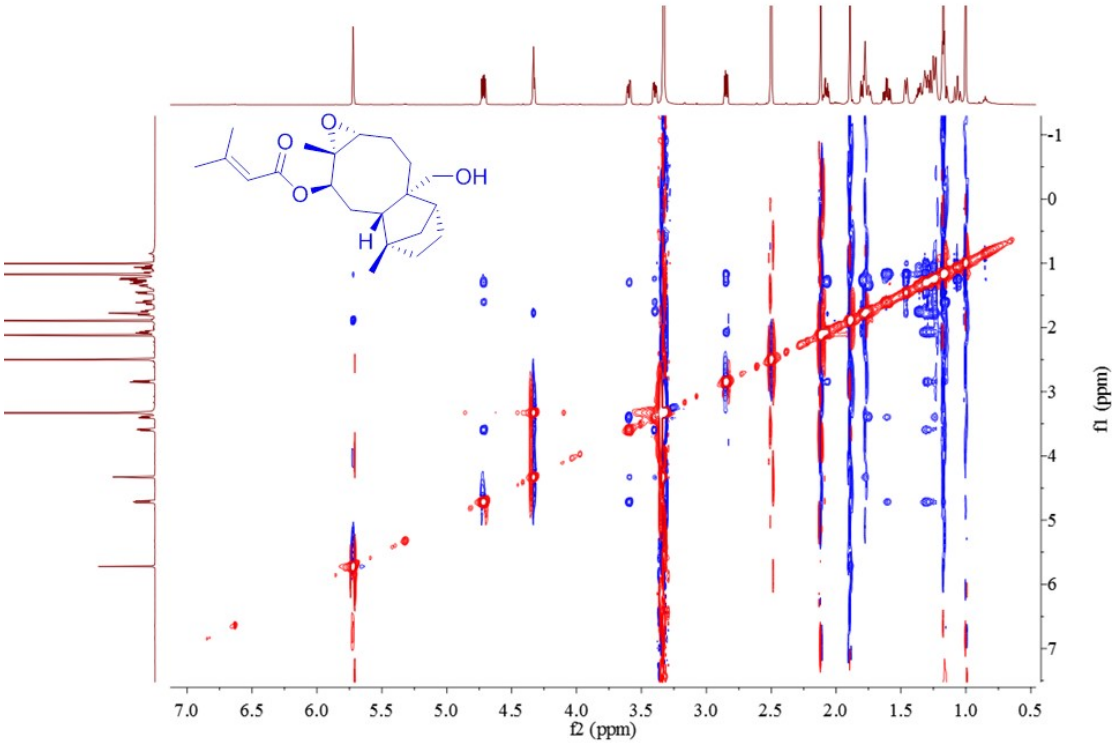


Figure S31 NOESY spectrum (600 MHz, DMSO-d_6) of compound **2**.

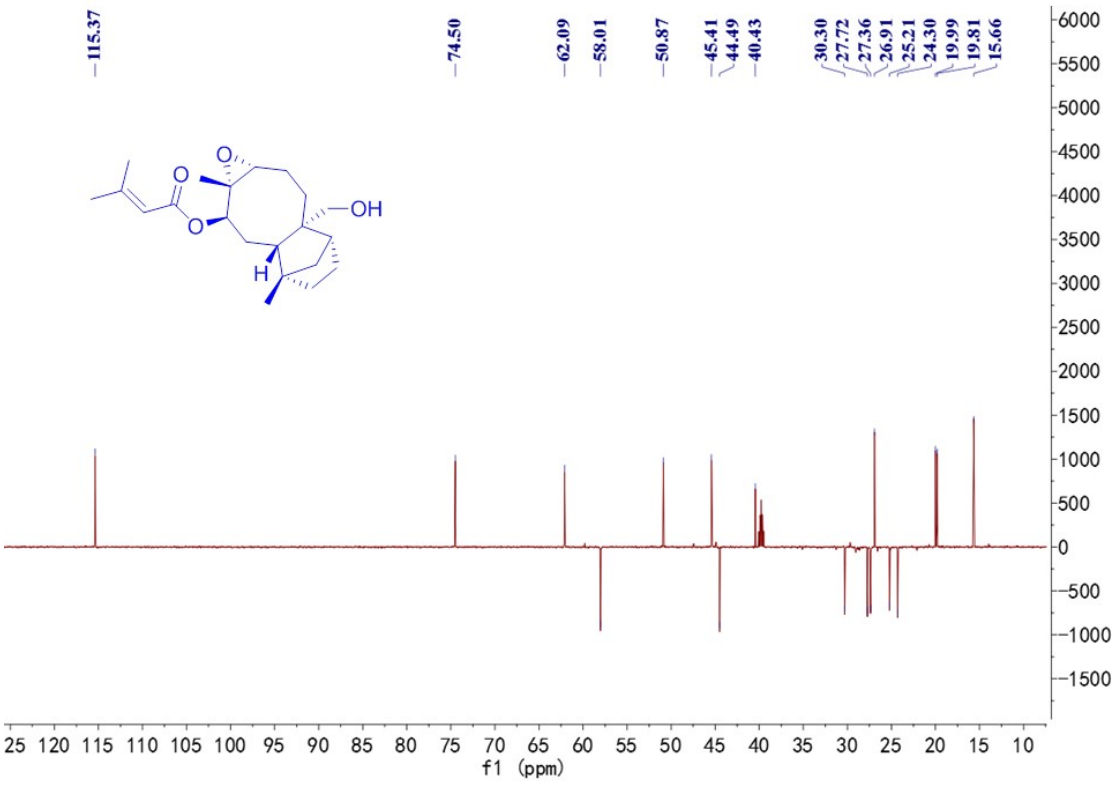
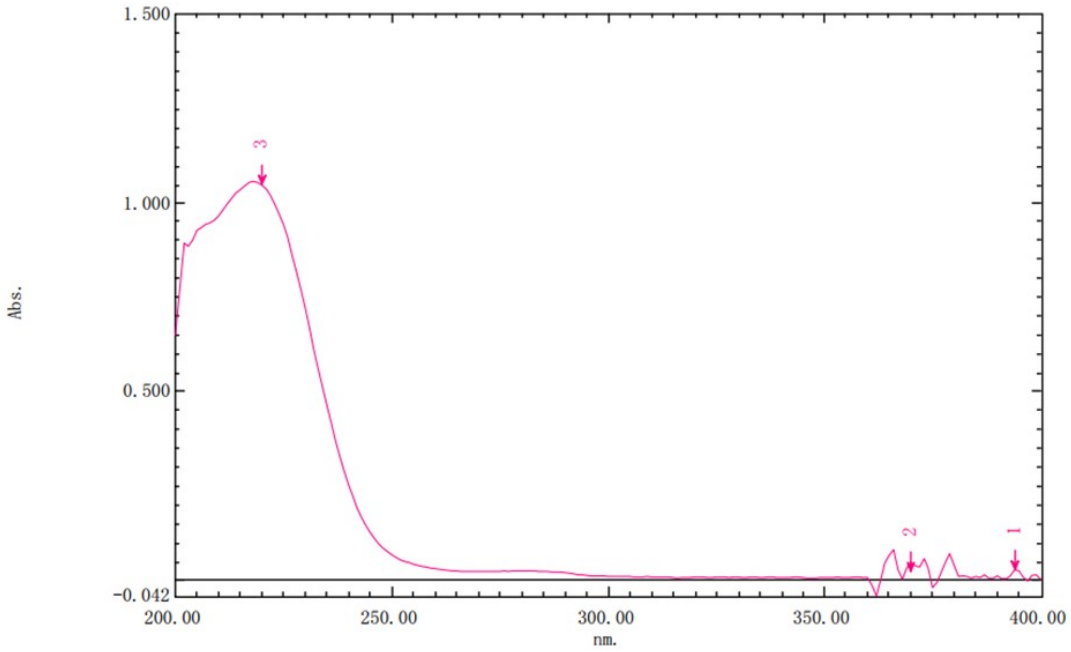


Figure S32 DEPT spectrum (600 MHz, DMSO-d_6) of compound **2**.



No.	P/V	Wavelength	Abs.	描述
1	↑	394.00	.026	
2	↑	370.00	.020	
3	↑	220.00	1.047	

Figure S33 UV spectrum of compound **3**.

Mass Spectrum SmartFormula Report

Analysis Info

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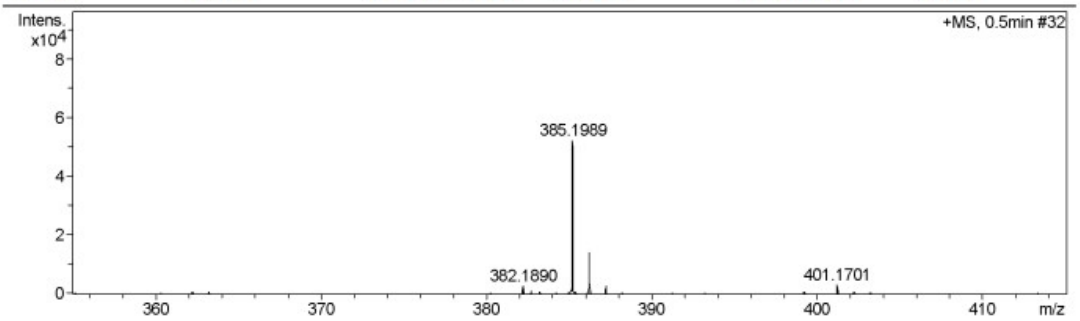
Method	20190425yezhi.m		
Sample Name	SHS-8	Operator	Bruker Customer
Comment		Instrument / Ser#	micrOTOF-Q 125

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
385.1989	1	C 21 H 30 Na O 5	385.1985	-0.8	1.9	6.5	ok	even	25.38	0.0431	0.0020	0.0190	0.0045	0.8427

Figure S34 HRESIMS spectrum of compound **3**.

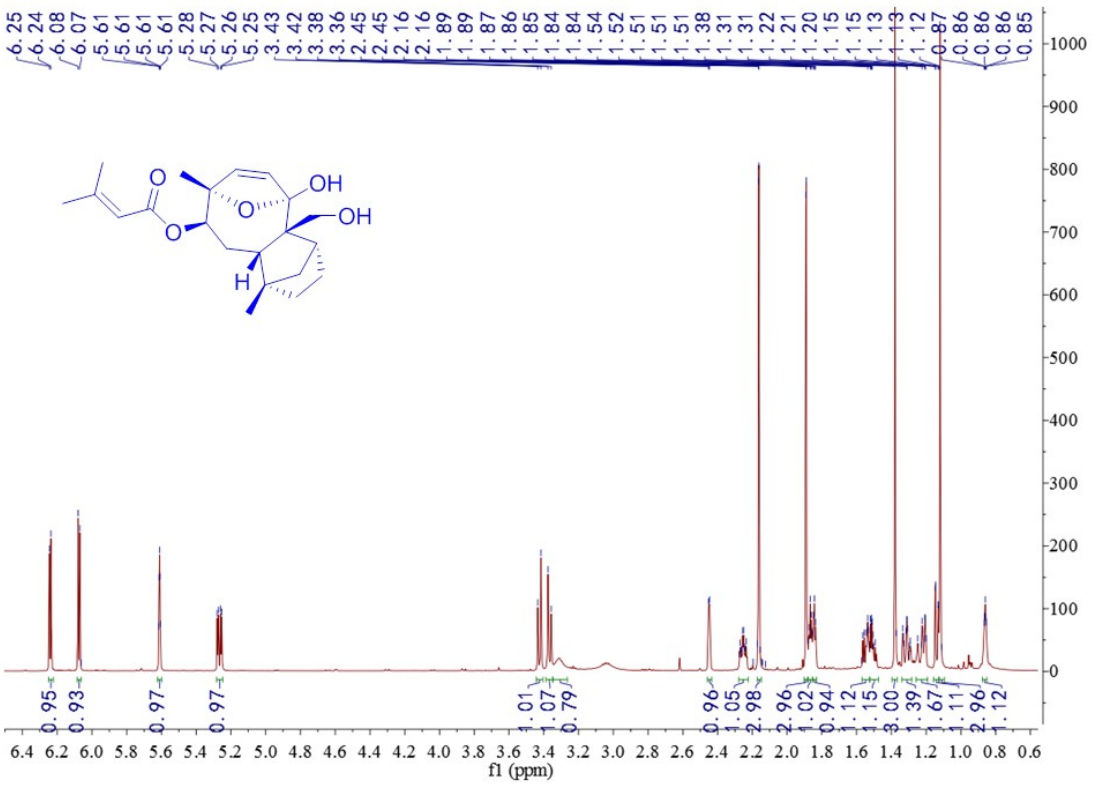


Figure S35 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **3**.

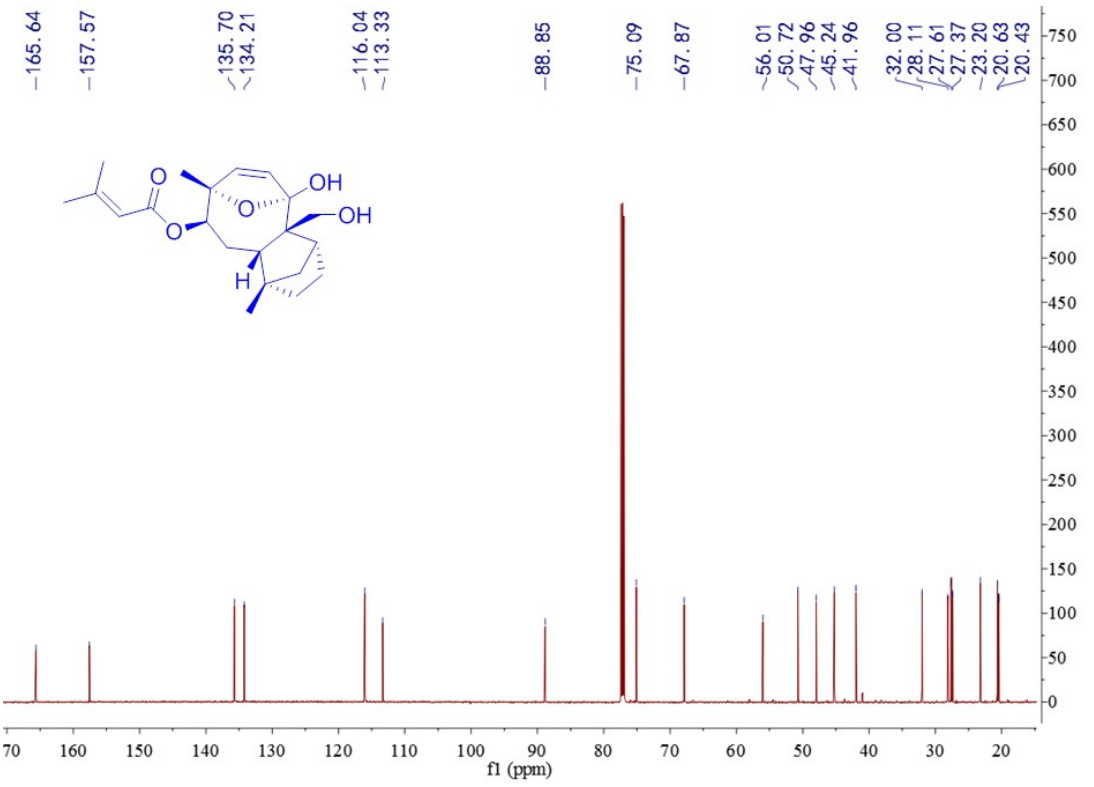


Figure S36 ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **3**.

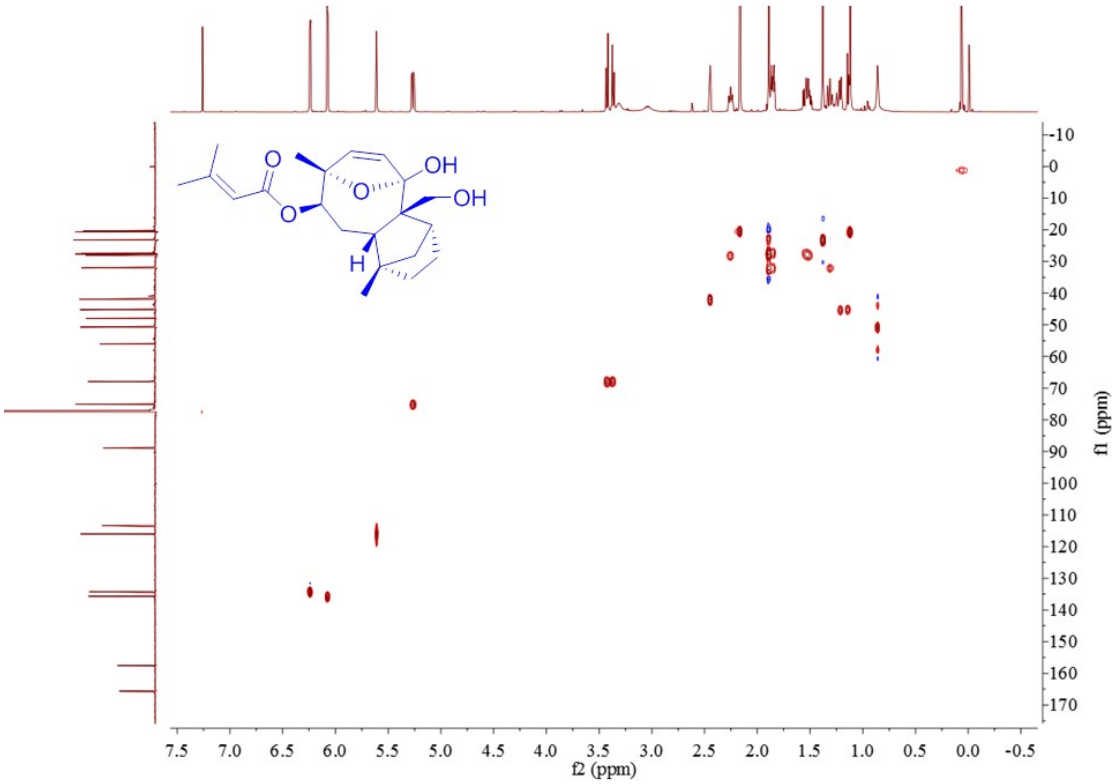


Figure S37 HSQC spectrum (600 MHz, $CDCl_3$) of compound **3**.

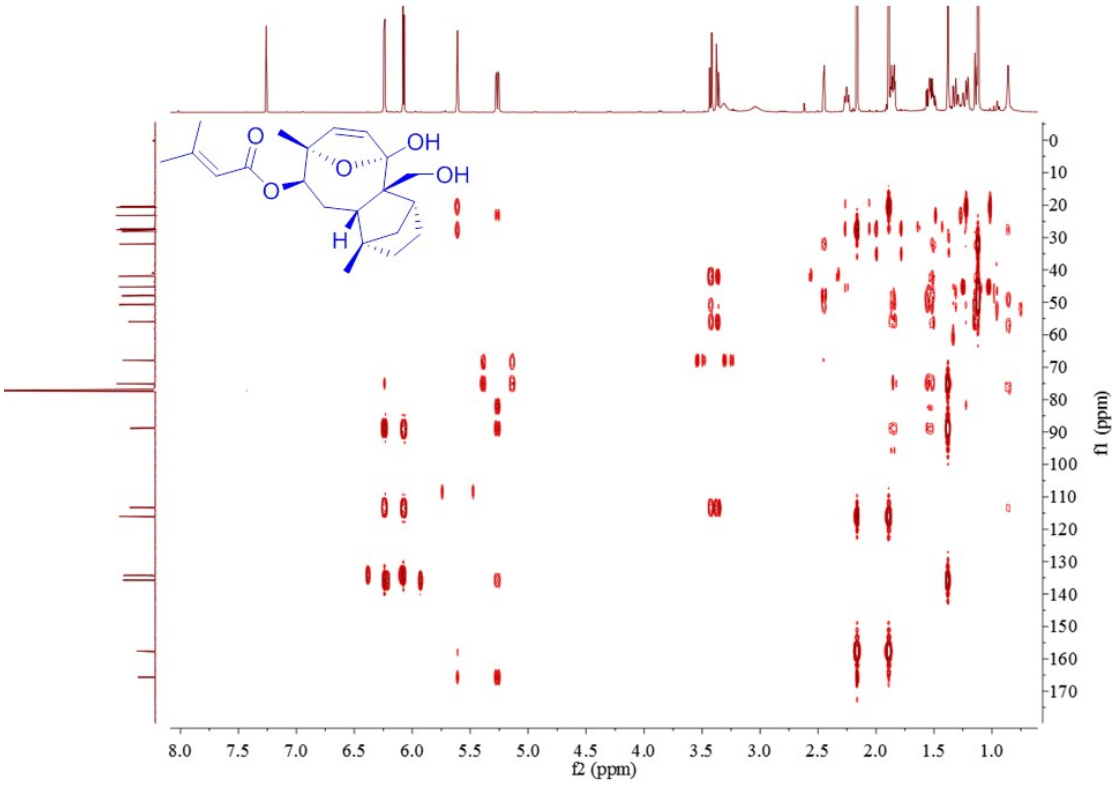


Figure S38 HMBC spectrum (600 MHz, $CDCl_3$) of compound **3**.

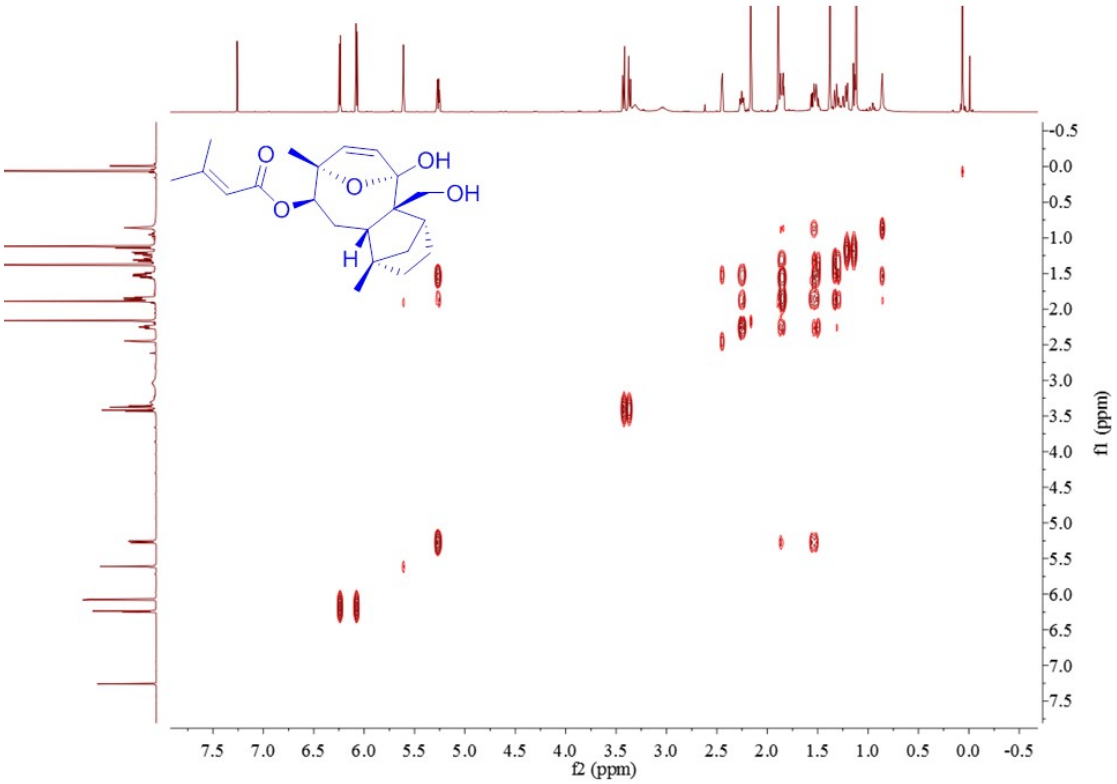


Figure S39 ^{1}H-^{1}H COSY spectrum (600 MHz, $CDCl_3$) of compound **3**.

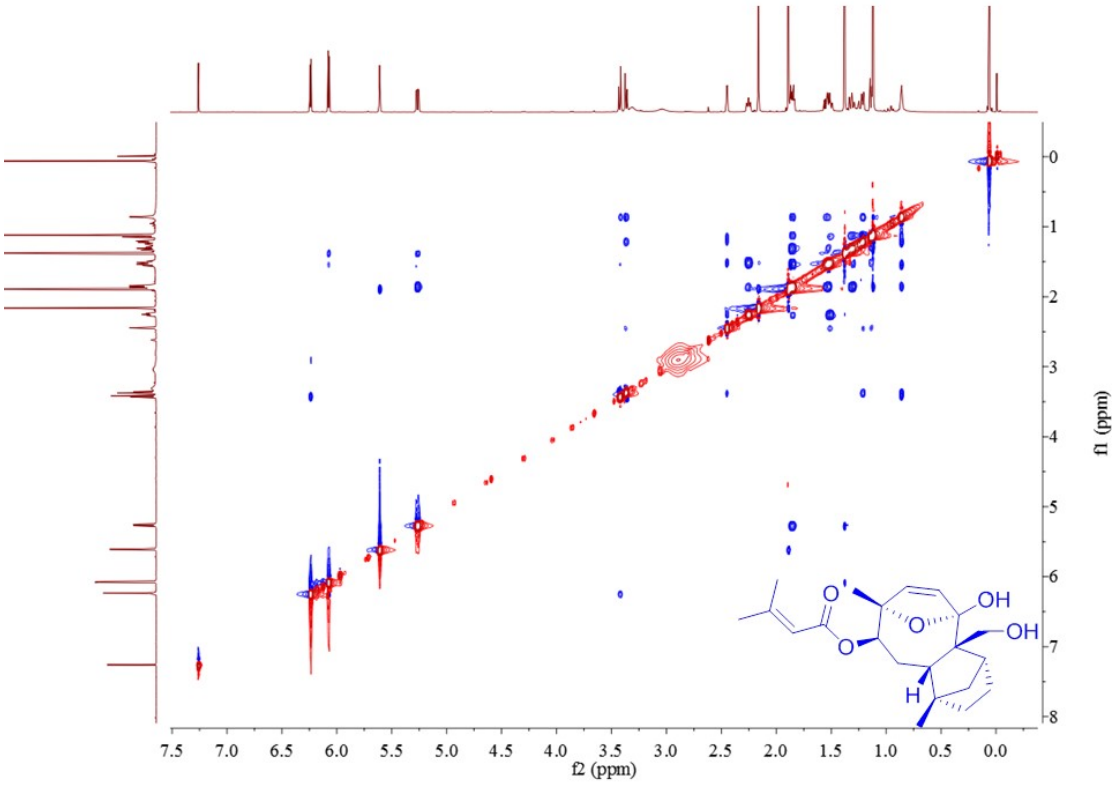


Figure S40 NOESY spectrum (600 MHz, $CDCl_3$) of compound **3**.

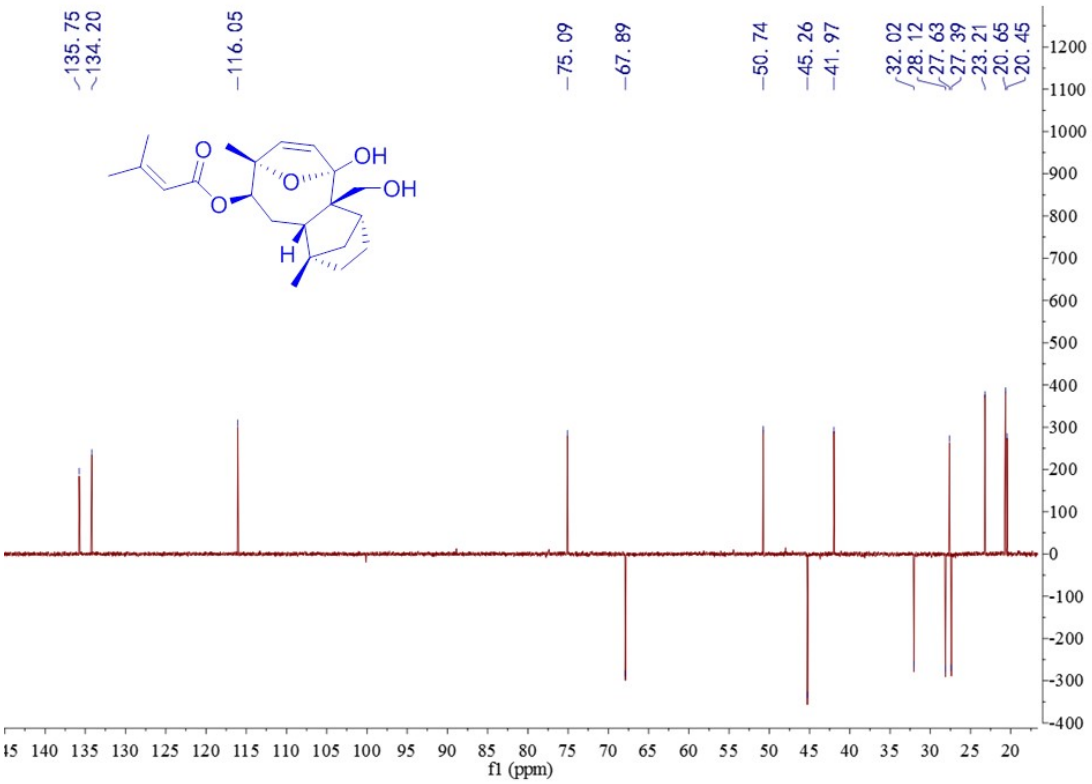
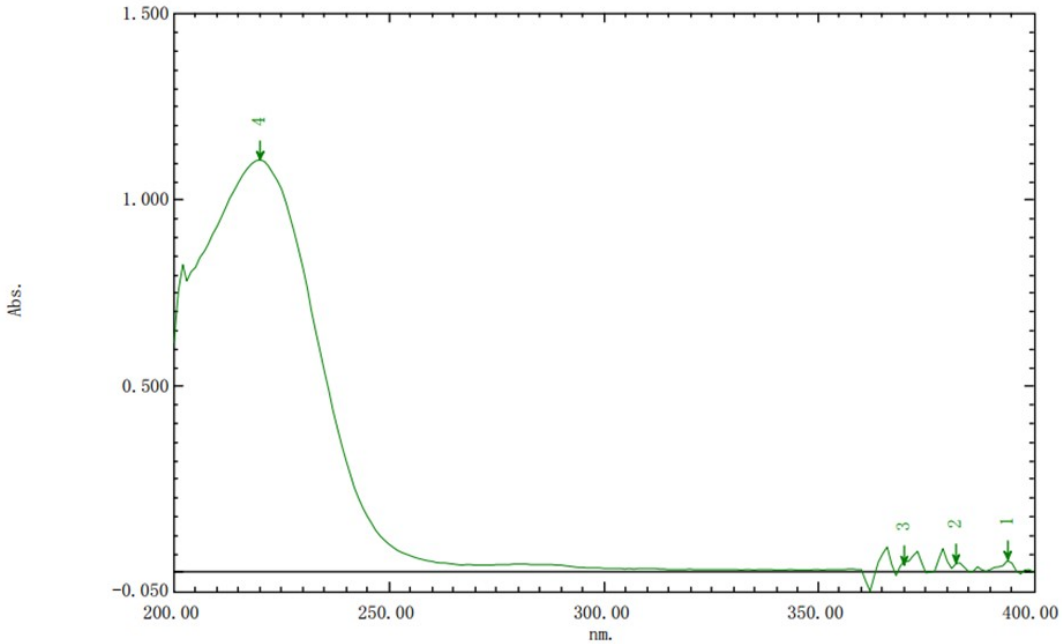


Figure S41 DEPT spectrum (600 MHz, $CDCl_3$) of compound **3**.



No.	P/V	Wavelength	Abs.	描述
1	↑	394.00	.032	
2	↑	382.00	.023	
3	↑	370.00	.017	
4	↑	220.00	1.108	

Figure S42 UV spectrum of compound **4**.

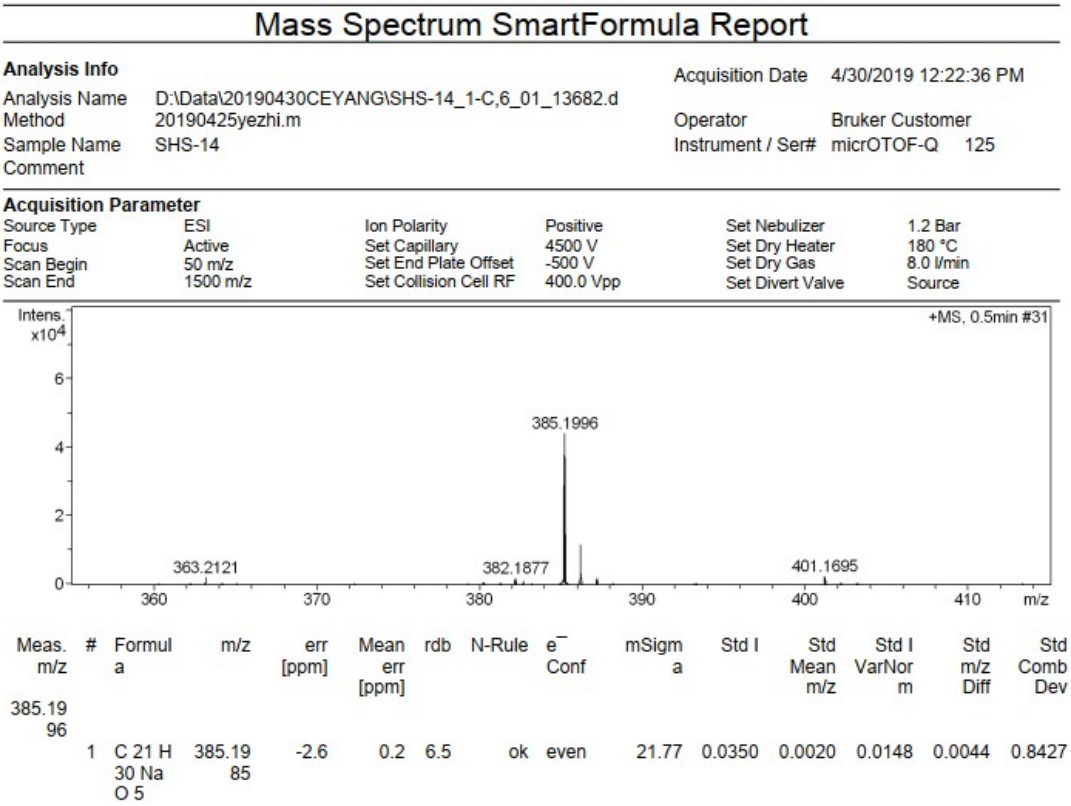


Figure S43 HRESIMS spectrum of compound **4**.

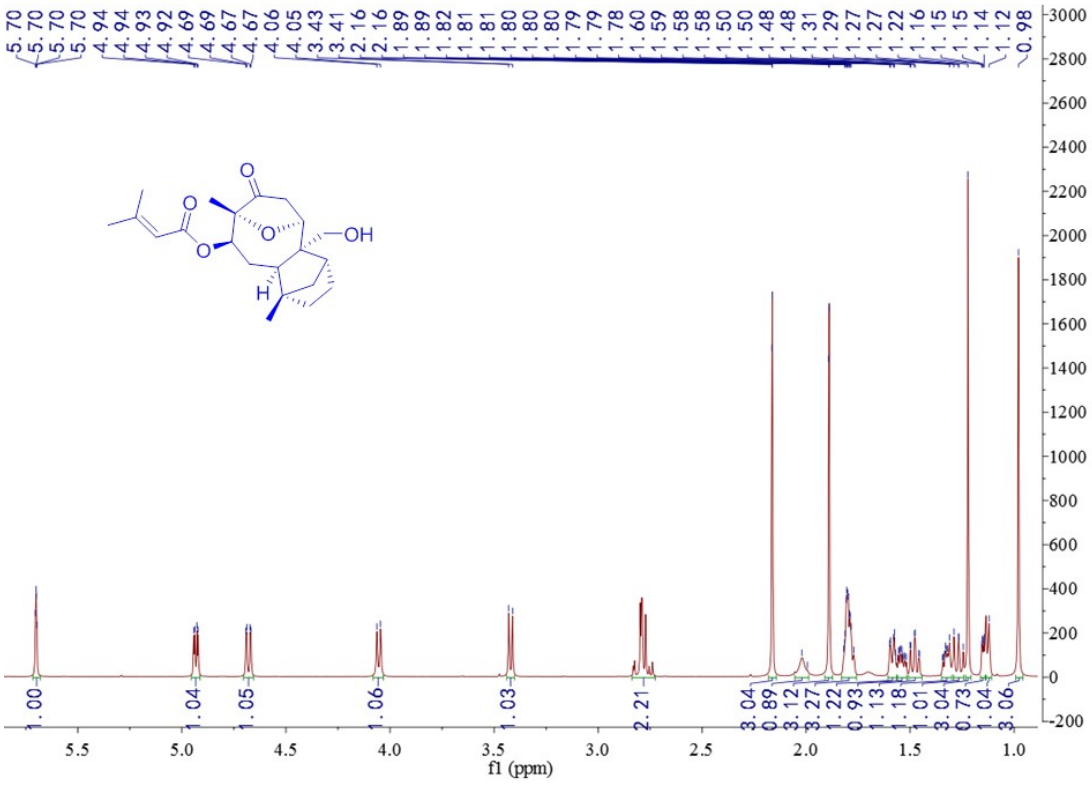


Figure S44 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **4**.

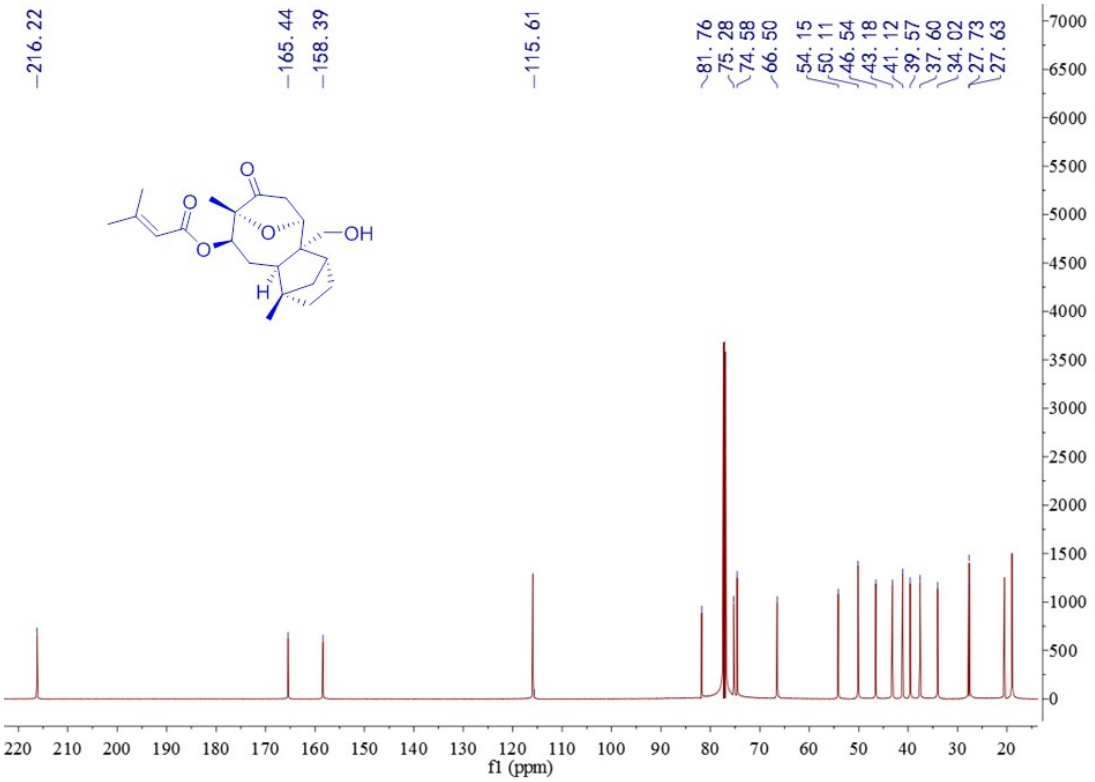


Figure S45 ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **4**.

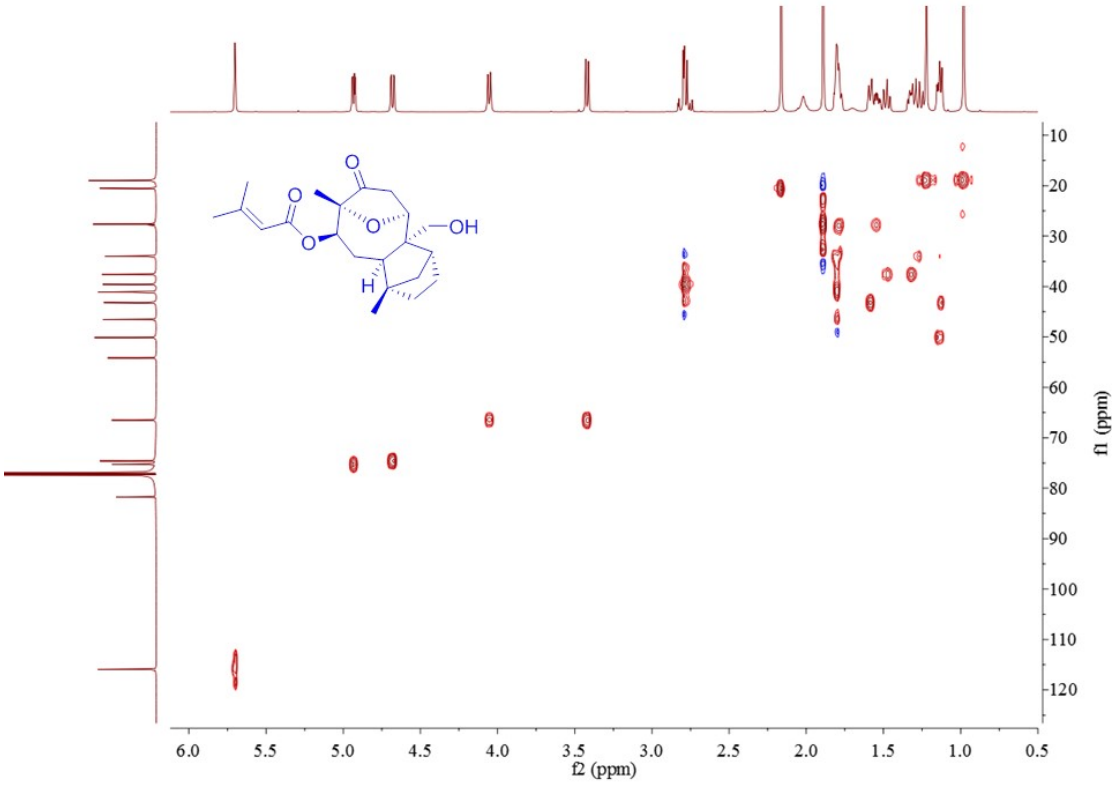


Figure S46 HSQC spectrum (600 MHz, $CDCl_3$) of compound **4**.

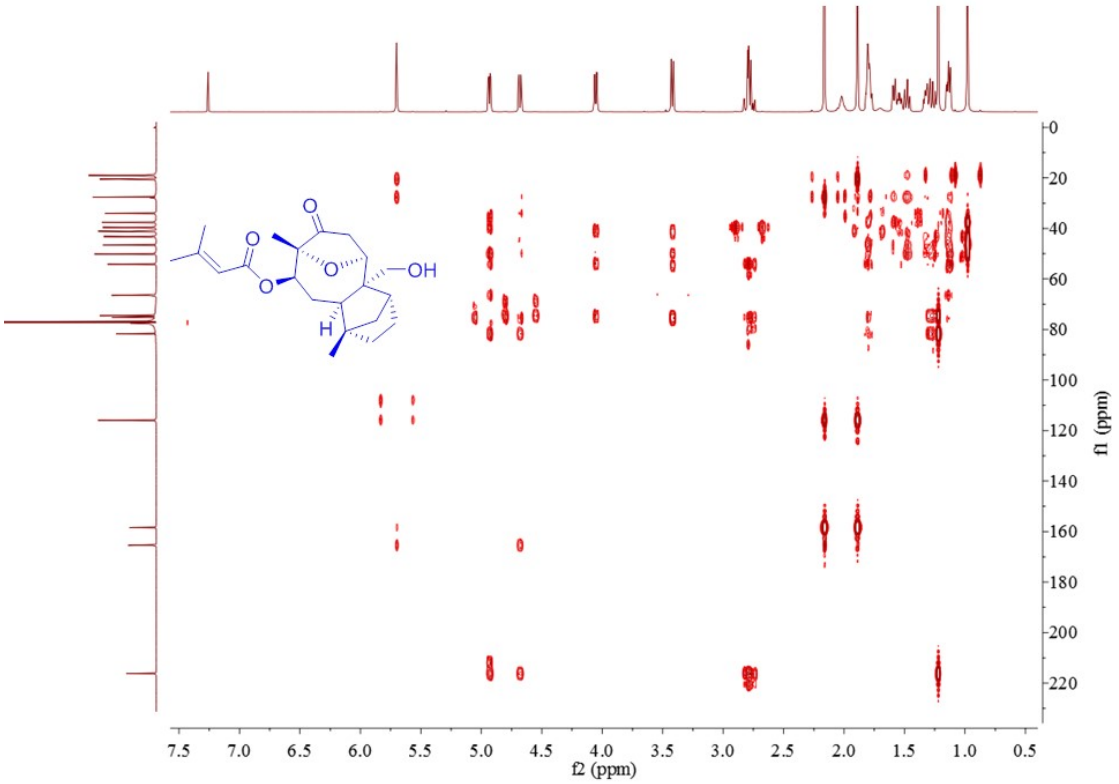


Figure S47 HMBC spectrum (600 MHz, $CDCl_3$) of compound **4**.

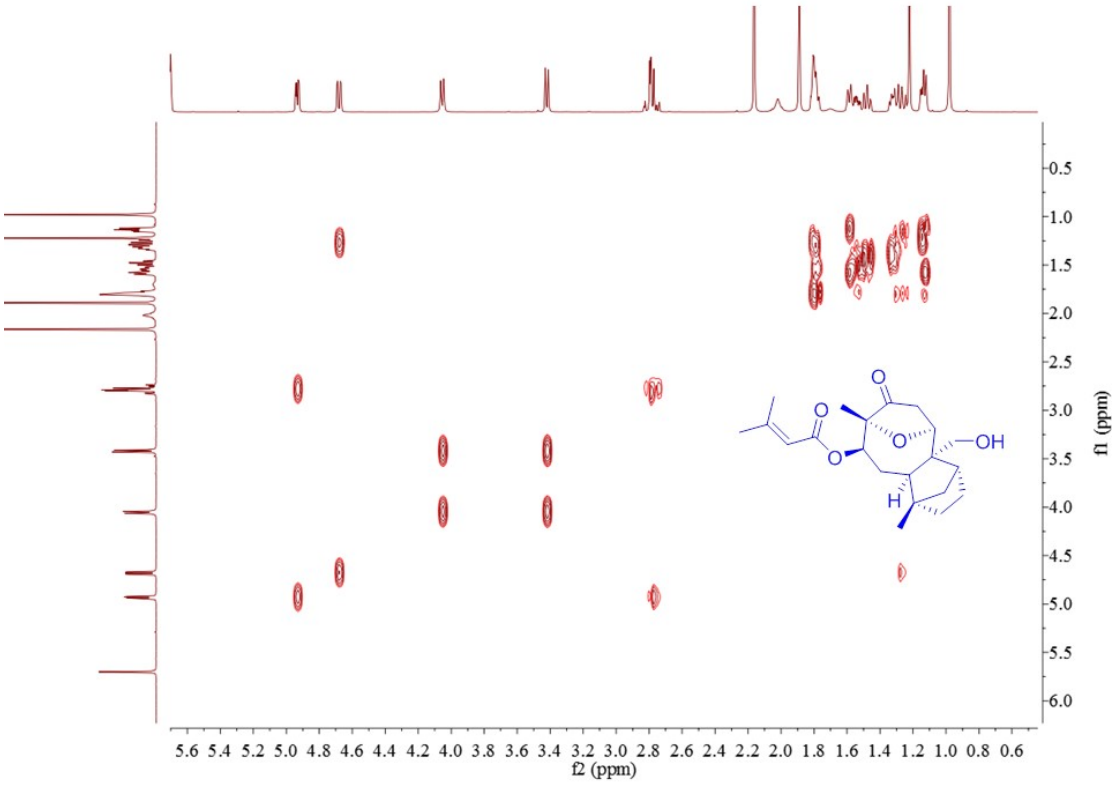


Figure S48 ^1H-^1H COSY spectrum (600 MHz, $CDCl_3$) of compound **4**.

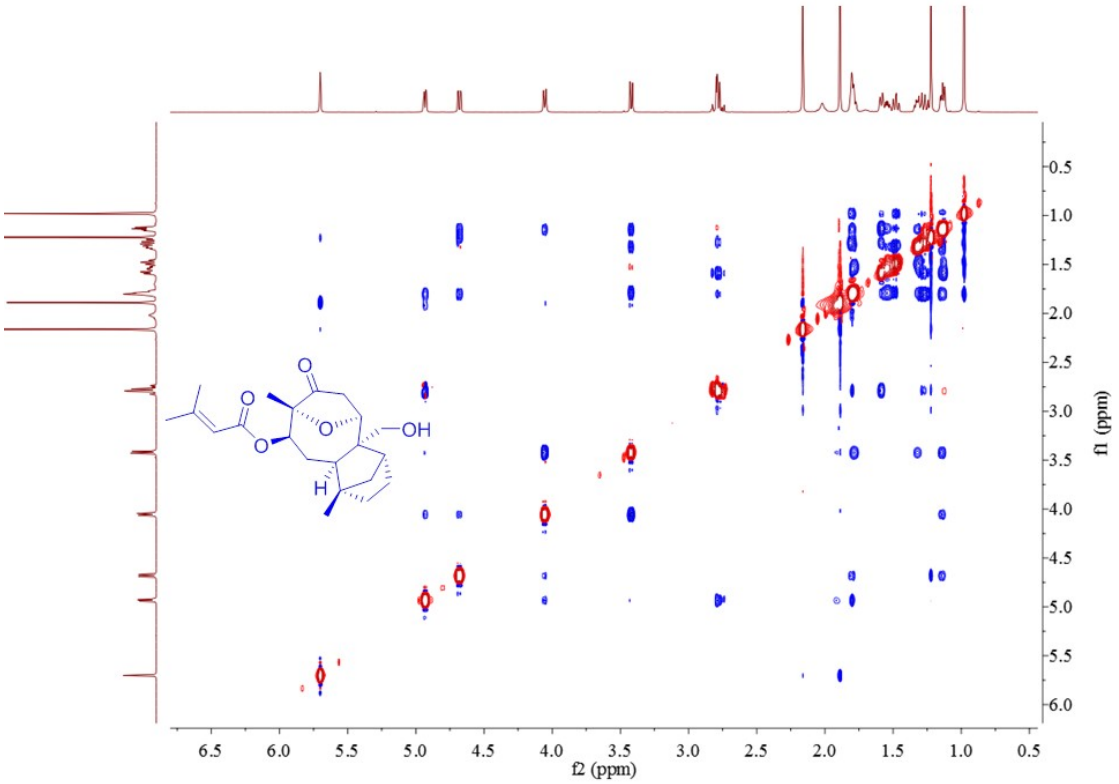


Figure S49 NOESY spectrum (600 MHz, $CDCl_3$) of compound **4**.

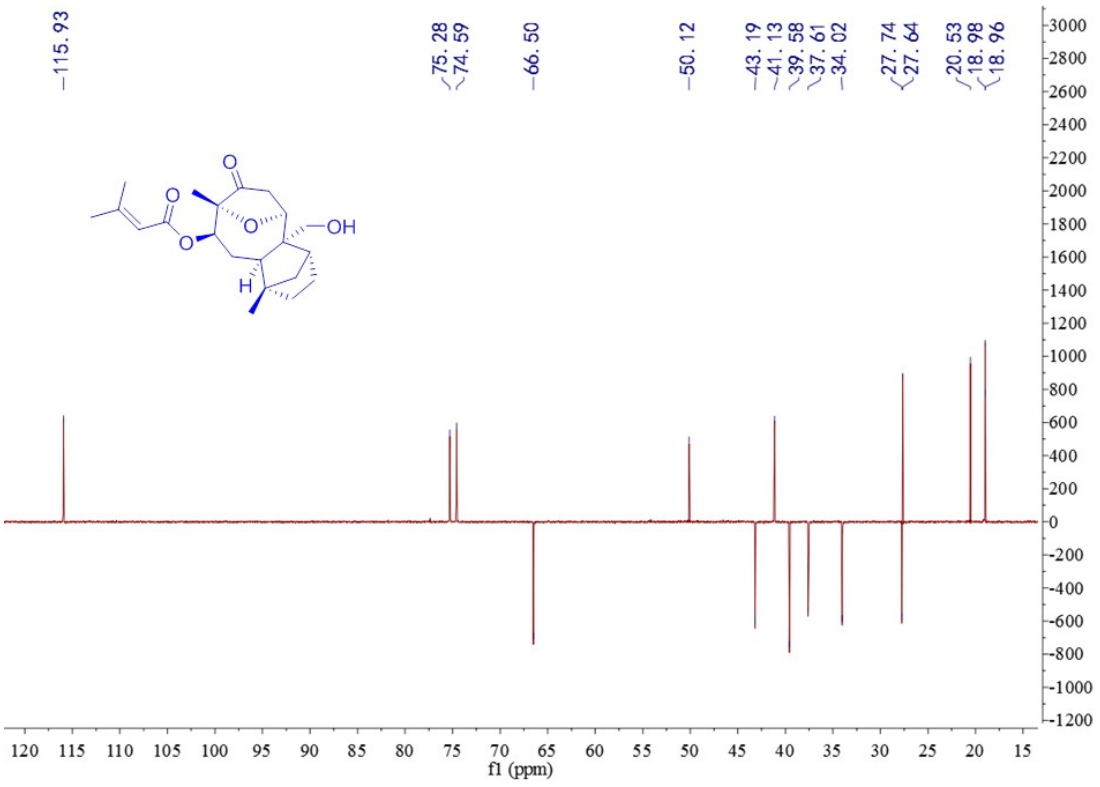


Figure S50 DEPT spectrum (600 MHz, $CDCl_3$) of compound **4**.