Four New Sesquiterpenoids from the Rice Fermentation of *Antrodiella albocinnamomea*

Min Guo [1], Ying-Zhong Liang [1], Xiu-Ming Cui [1, 2], Lin-Jiao Shao [1], Yin-Fei Li [1], and Xiao-Yan Yang [1, 2, *]

[1] Faculty of Life Science and Technology, Kunming University of Science and Technology, Kunming 650500, China, guomin@stu.kust.edu.cn (M. G.); lyz@stu.kust.edu.cn (Y.-Z. L.); 20120094@kust.edu.cn (X.-M. C.); shaolinjiao@stu.kust.edu.cn (L.-J. S.); liyinfei@stu.kust.edu.cn (Y.- F. L.); yangxy@kust.edu.cn (X.-Y. Y.)

[2] Yunnan Key Laboratory of Sustainable Utilization of *Panax Notoginseng*, Kunming 650500, China

[*]Correspondence: yangxy@kust.edu.cn (X.-Y. Y.); Tel.: +86-159-6946-8214 (X.-Y. Y.)

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Table S1 Experimental and calculated ^{13}C data for possible structures of compounds **1**, **2** and **4** (δ in ppm)

NO.	δ_C, Exptl[A]	**1**							
		1a		**1b**		**1c**		**1d**	
		δ_C, calcd[B]	δ_C, $\Delta\delta$[C]	δ_C, calcd[B]	δ_C, $\Delta\delta$[C]	δ_C, calcd[B]	δ_C, $\Delta\delta$[C]	δ_C, calcd[B]	δ_C, $\Delta\delta$[C]
10	38.8	38.3	-0.5	38.6	-0.2	37.9	-0.9	38.6	-0.2
9	35.7	34.9	-0.8	34.8	-0.9	34.7	-1.0	34.8	-0.9
8	213.1	211.8	-1.3	211.5	-1.6	211.8	-1.3	211.4	-1.7
7	91.5	77.7	-13.8	79.0	-12.5	77.6	-13.9	78.9	-12.6
6	45.5	56.8	11.3	56.3	10.8	56.7	11.2	56.6	11.1
11	55.5	37.8	-17.7	37.6	-17.9	37.9	-17.6	37.6	-17.9
1	32.3	39.7	7.4	41.1	8.8	39.8	7.5	41.1	8.8
2	194.7	190.4	-4.3	188.5	-6.2	190.7	-4.0	188.4	-6.3
3	145	140.6	-4.4	141.6	-3.4	140.6	-4.4	141.7	-3.3
4	121.3	112.9	-8.4	105.9	-15.4	112.8	-8.5	105.7	-15.6
5	25.2	28.1	2.9	28.9	3.7	28.2	3.0	28.9	3.7
12	24.3	25.5	1.2	30.9	6.6	34.2	9.9	26.1	1.8
13	24.4	34.0	9.6	26.1	1.7	25.6	1.2	30.7	6.3
14	26.8	25.4	-1.4	26.9	0.1	25.3	-1.5	27.1	0.3

NO.	δ_C, exptl[A]	**2**							
		2a		**2b**		**2c**		**2d**	
		δ_C, calcd[B]	δ_C, $\Delta\delta$[C]	δ_C, calcd[B]	δ_C, $\Delta\delta$[C]	δ_C, calcd[B]	δ_C, $\Delta\delta$[C]	δ_C, calcd[B]	δ_C, $\Delta\delta$[C]
9	36.5	37.0	0.5	36.5	0.00	36.8	0.3	37.0	0.5
8	33.8	34.6	0.8	34.3	0.51	34.3	0.5	34.6	0.8
7	213.4	220.4	7.0	221.2	7.80	221.3	7.9	220.4	7.0
6	80	79.8	-0.2	79.7	-0.34	79.5	-0.5	79.8	-0.2
5	59.7	61.5	1.8	61.8	2.09	61.6	1.9	61.5	1.8
10	37	37.2	0.2	36.8	-0.19	37.0	0.0	37.2	0.2
4	37.6	41.4	3.8	42.1	4.54	42.0	4.4	41.4	3.8
3	150.8	154.7	3.9	155.2	4.43	155.3	4.5	154.7	3.9
2	146.4	146.9	0.5	146.6	0.25	146.6	0.2	146.9	0.5
1	34.3	36.4	2.1	36.4	2.05	36.0	1.7	36.4	2.1
12	24.7	27.2	2.5	27.1	2.38	24.6	-0.1	27.2	2.5
11	26.8	25.0	-1.8	24.4	-2.39	27.4	0.6	25.0	-1.8
14	189.5	188.8	-0.7	188.9	-0.61	188.8	-0.7	188.8	-0.7
13	25.2	25.8	0.6	26.2	1.03	26.3	1.1	25.8	0.6

[A]Recorded in $CDCl_3$ at 150Hz. [B]Calculated in chloroform. [C]$\Delta\delta=\delta$calcd-δexptl

NO.	δ_C, Exptl[A]	**4**			
		4a	**4b**	**4c**	**4d**

		δC, calcd[B]	δC, Δδ[C]	δC, calcd[B]	δC, Δδ[C]	δC, calcd[B]	δC, Δδ[C]	δC, calcd[B]	δC, Δδ[C]
6	207.4	208.8	1.4	209.9	2.5	203.9	-3.5	206.0	-1.4
5	50.6	48.5	-2.1	46.3	-4.3	48.2	-2.4	50.3	-0.3
4	41.2	42.3	1.1	45.4	4.2	52.1	10.9	43.3	2.1
9	78.6	78.8	0.2	78.3	-0.3	73.8	-4.8	74.3	-4.3
8	165	168.1	3.1	169.4	4.4	171.3	6.3	171.3	6.3
7	131.5	129.5	-2.0	129.2	-2.3	131.1	-0.4	130.5	-1.0
3	59.1	56.0	-3.1	55.6	-3.5	55.0	-4.1	54.0	-5.1
2	38.9	37.4	-1.5	37.6	-1.3	37.2	-1.7	37.3	-1.6
1	47.4	45.2	-2.2	45.4	-2.0	45.7	-1.7	45.4	-2.0
15	13.2	14.4	1.2	14.4	1.2	14.6	1.4	14.5	1.3
13	75.5	73.2	-2.3	72.1	-3.4	76.2	0.7	74.9	-0.6
14	18	16.7	-1.3	16.5	-1.5	20.3	2.3	16.2	-1.8
12	26.1	24.2	-1.9	18.7	-7.4	25.5	-0.6	26.2	0.1
10	32.1	31.4	-0.7	31.1	-1.0	28.8	-3.3	28.8	-3.3
11	31.9	31.4	-0.5	31.0	-0.9	29.2	-2.7	29.0	-2.9

NO.	δC, exptl[A]	**4e**		**4f**		**4g**		**4h**	
		δC, calcd[B]	δC, Δδ[C]	δC, calcd[B]	δC, Δδ[C]	δC, calcd[B]	δC, Δδ[C]	δC, calcd[B]	δC, Δδ[C]
6	207.4	208.9	1.5	209.8	2.4	203.9	-3.5	206.2	-1.2
5	50.6	48.7	-1.9	46.4	-4.2	48.5	-2.1	50.1	-0.5
4	41.2	42.1	0.9	45.2	4.0	51.7	10.5	43.3	2.1
9	78.6	78.8	0.2	78.5	-0.1	73.9	-4.7	74.2	-4.4
8	165	168.1	3.1	169.4	4.4	171.2	6.2	171.5	6.5
7	131.5	129.6	-1.9	129.0	-2.5	131.3	-0.2	130.5	-1.0
3	59.1	56.1	-3.0	55.6	-3.5	55.1	-4.0	54.2	-4.9
2	38.9	37.5	-1.4	37.7	-1.2	37.4	-1.5	37.4	-1.5
1	47.4	45.2	-2.2	45.6	-1.8	45.3	-2.1	45.5	-1.9
15	13.2	14.3	1.1	14.4	1.2	14.6	1.4	14.6	1.4
13	75.5	73.2	-2.3	72.3	-3.2	76.3	0.8	74.8	-0.7
14	18	16.9	-1.1	16.2	-1.8	20.3	2.3	16.3	-1.7
12	26.1	24.3	-1.8	18.8	-7.3	25.5	-0.6	26.2	0.1
10	32.1	31.4	-0.7	31.6	-0.5	29.1	-3.0	29.1	-3.0
11	31.9	31.4	-0.5	31.4	-0.5	29.2	-2.7	29.0	-2.9

[A]Recorded in CD_3OD at 150Hz. [B]Calculated in methanol. [C]Δδ=δcalcd-δexptl

Table S2 Regression analysis of ^{13}C NMR chemical displacement calculation and experimental value of eight possible configurations of compounds **1**, **2** and **4**

No.		configuration	R^2	RMSE	DP4+ possibility (%)
1	**1a**	6*R*,7*S*	0.9855	8.01	56.02
	1b	6*R*,7*R*	0.9842	8.54	8.65
	1c	6*S*,7*R*	0.9854	8.03	28.61
	1d	6*S*,7*S*	0.9841	8.59	6.71
2	**2a**	5*S*,6*S*	0.9991	2.63	73.72
	2b	5*S*,6*R*	0.9988	2.96	0.02
	2c	5*R*,6*S*	0.9990	2.81	15.94
	2d	5*R*,6*R*	0.9991	2.64	10.32
4	**4a**	5*R*,9*S*,13*S*	0.9993	1.83	30.72
	4b	5*R*,9*S*,13*R*	0.9975	3.24	0.00
	4c	5*S*,9*S*,13*S*	0.9946	4.07	0.00
	4d	5*R*,9*R*,13*S*	0.9978	2.87	0.00
	4e	5*S*,9*R*,13*R*	0.9993	1.79	69.28
	4f	5*S*,9*R*,13*S*	0.9976	3.18	0.00
	4g	5*R*,9*R*,13*R*	0.9948	3.97	0.00
	4h	5*S*,9*S*,13*R*	0.9978	2.85	0.00

Table S3 DP4+ Analysis

No.	**1** (%)				**2** (%)			
	1a	**1b**	**1c**	**1d**	**2a**	**2b**	**2c**	**2d**
sDP4+ (H data)	-	-	-	-	-	-	-	-
sDP4+ (C data)	56.02	8.65	28.61	6.71	40.66	0.67	34.53	24.14
sDP4+ (all data)	56.02	8.65	28.61	6.71	40.66	0.67	34.53	24.14
uDP4+ (H data)	-	-	-	-	-	-	-	-
uDP4+ (C data)	-	-	-	-	66.22	1.32	16.85	15.61
uDP4+ (all data)	-	-	-	-	66.22	1.32	16.85	15.61
DP4+ (H data)	-	-	-	-	-	-	-	-
DP4+ (C data)	-	-	-	-	73.72	0.02	15.94	10.32
DP4+ (all data)	-	-	-	-	73.72	0.02	15.94	10.32
No.	**4** (%)							
	4a	**4b**	**4c**	**4d**	**4e**	**4f**	**4g**	**4h**
sDP4+ (H data)	-	-	-	-	-	-	-	-
sDP4+ (C data)	39.36	0.00	0.00	0.00	60.63	0.00	0.00	0.00
sDP4+ (all data)	39.36	0.00	0.00	0.00	60.63	0.00	0.00	0.00
uDP4+ (H	-	-	-	-	-	-	-	-

data)								
uDP4+ (C data)	40.53	0.01	0.00	0.04	59.34	0.03	0.00	0.05
uDP4+ (all data)	40.53	0.01	0.00	0.04	59.34	0.03	0.00	0.05
DP4+ (H data)	-	-	-	-	-	-	-	-
DP4+ (C data)	30.72	0.00	0.00	0.00	69.28	0.00	0.00	0.00
DP4+ (all data)	30.72	0.00	0.00	0.00	69.28	0.00	0.00	0.00

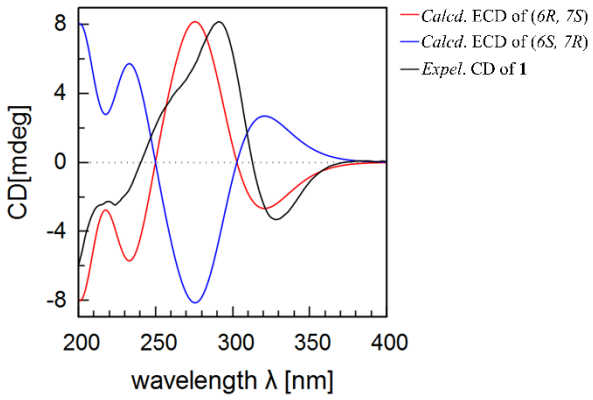


Figure S1. Experimental and calculated ECD spectra of compound **1**

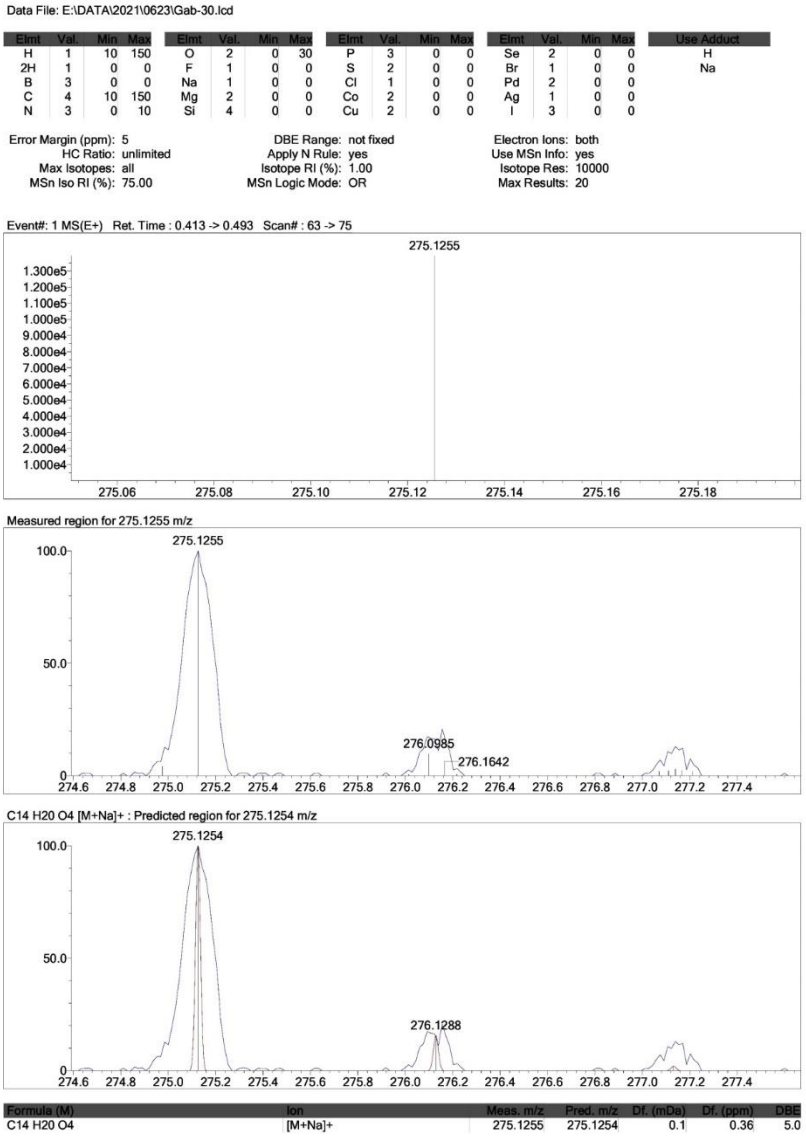
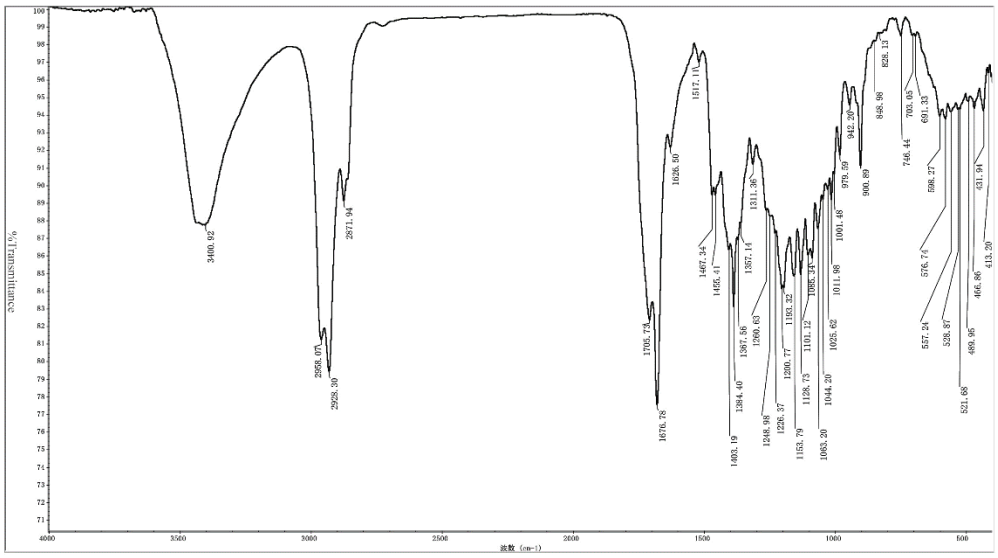


Figure S2. HR-ESI-MS spectrum of compound **1**



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Sampling gain: 1.0
Moving Mirror Speed: 0.4747
Diaphragm: 80.00

Figure S3. IR spectrum of compound **1**

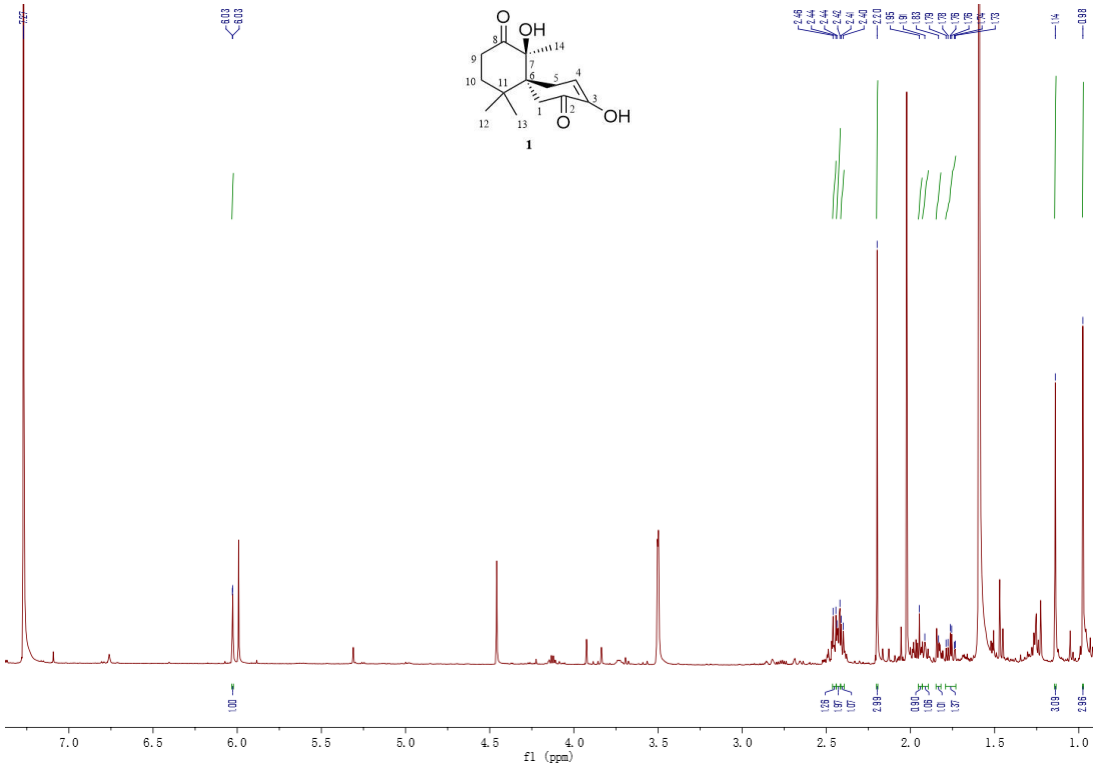


Figure S4. ^{1}H NMR spectrum (600MHz, $CDCl_3$) of **1**

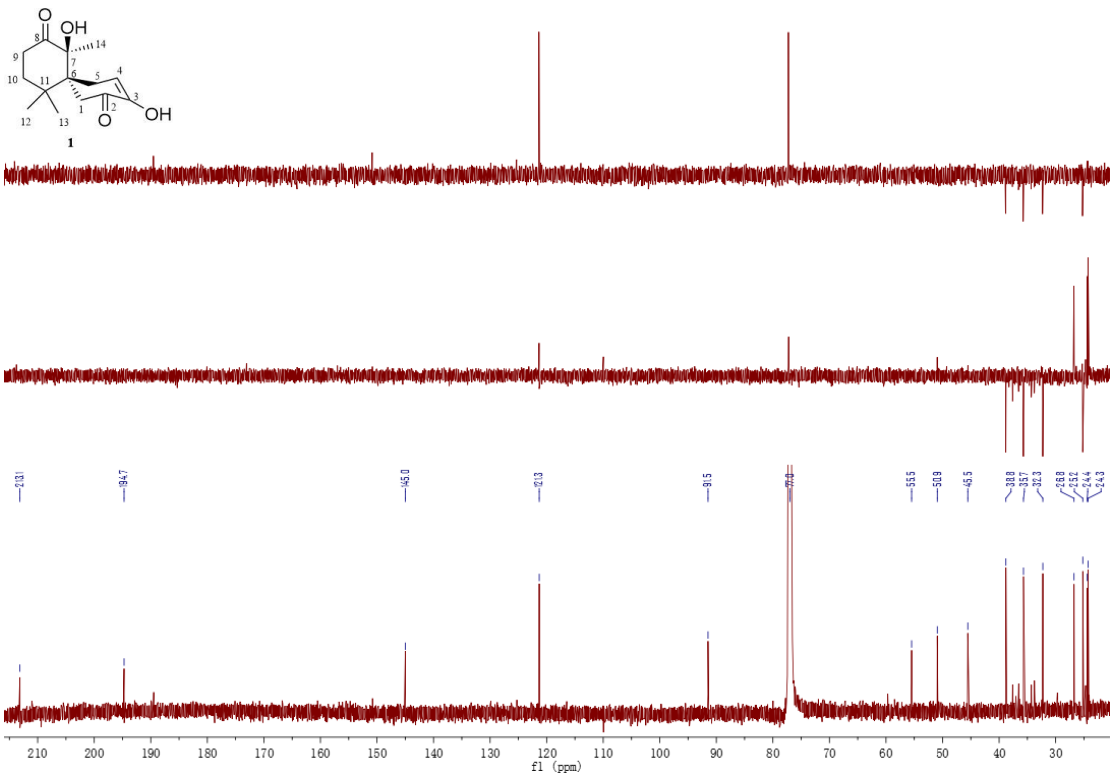


Figure S5. ^{13}C and DEPT spectrum (150MHz, $CDCl_3$) of **1**

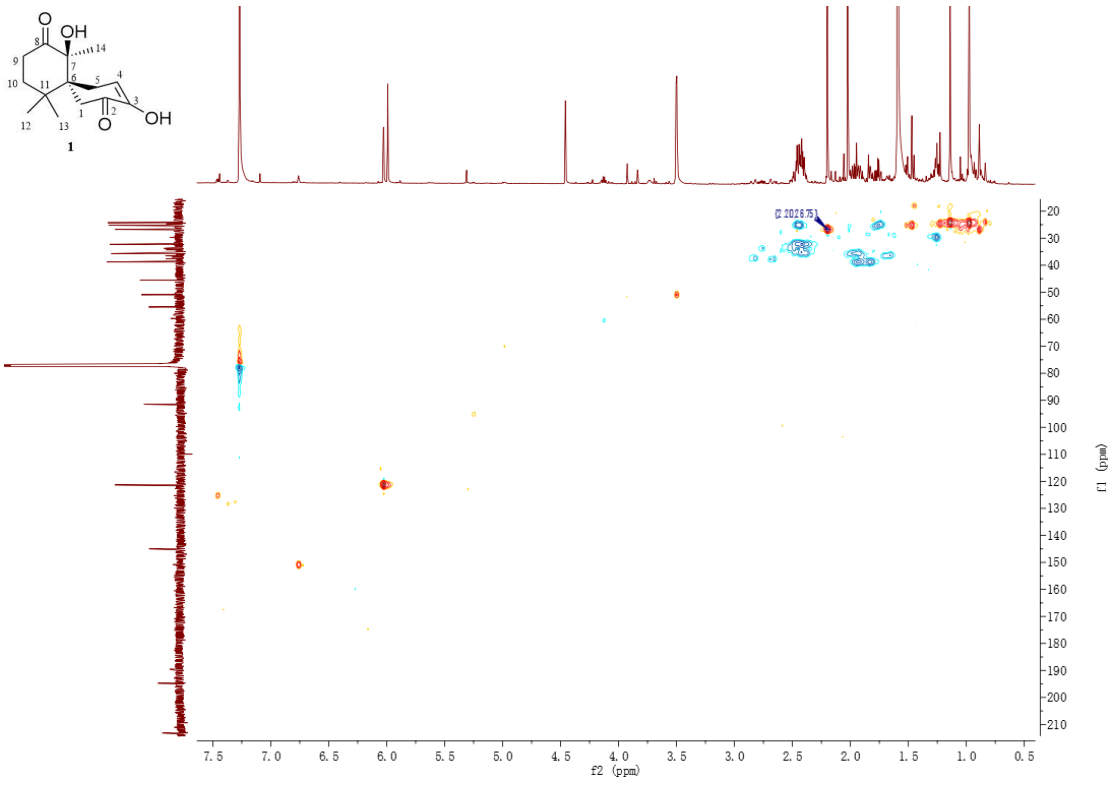


Figure S6. HSQC spectrum of **1**

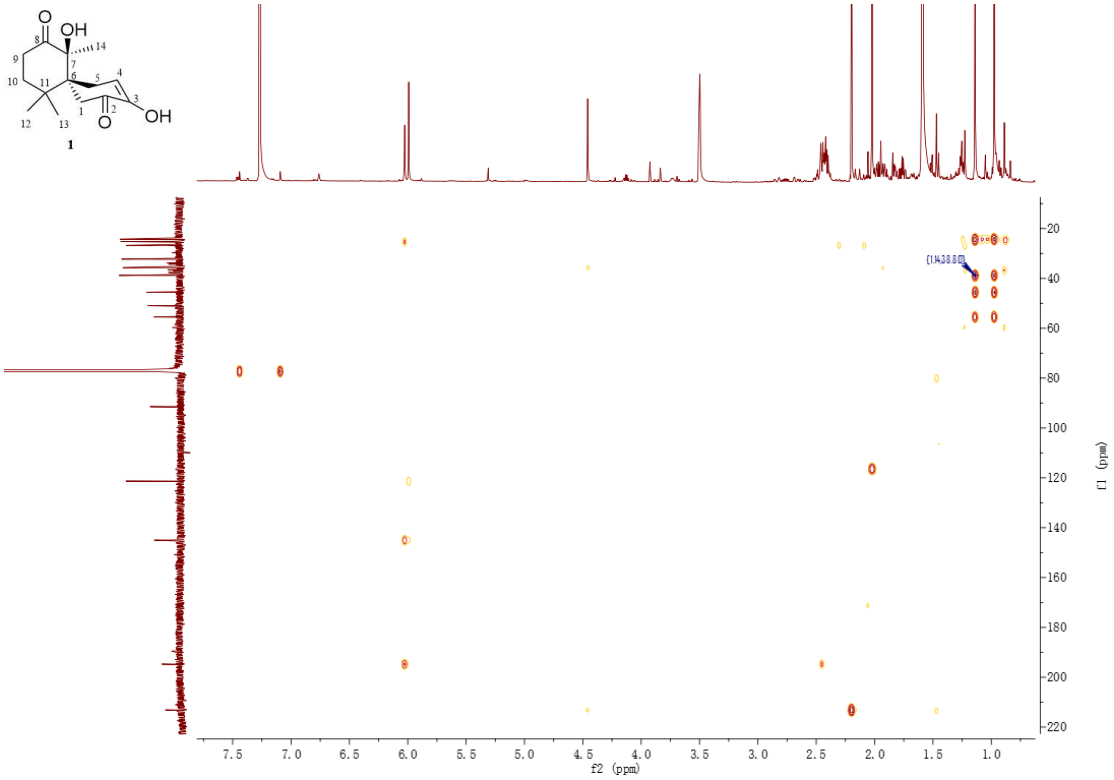


Figure S7. HMBC spectrum of **1**

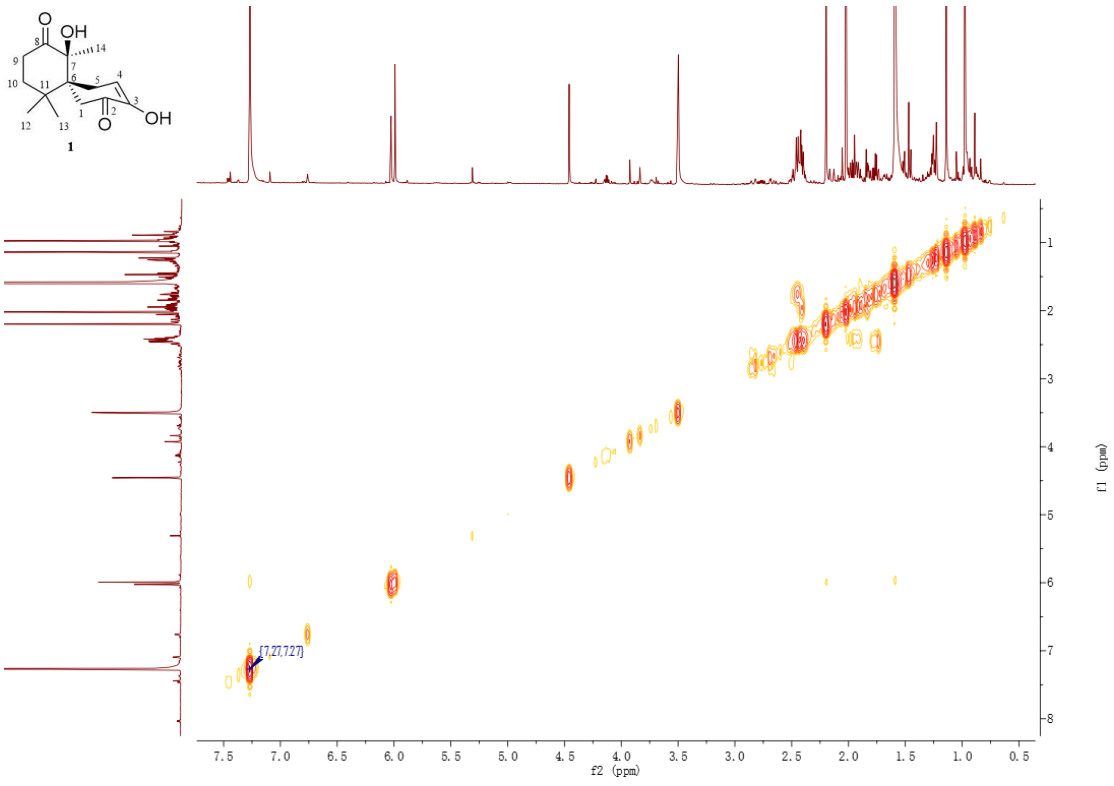


Figure S8. ^{1}H-^{1}H COSY spectrum of **1**

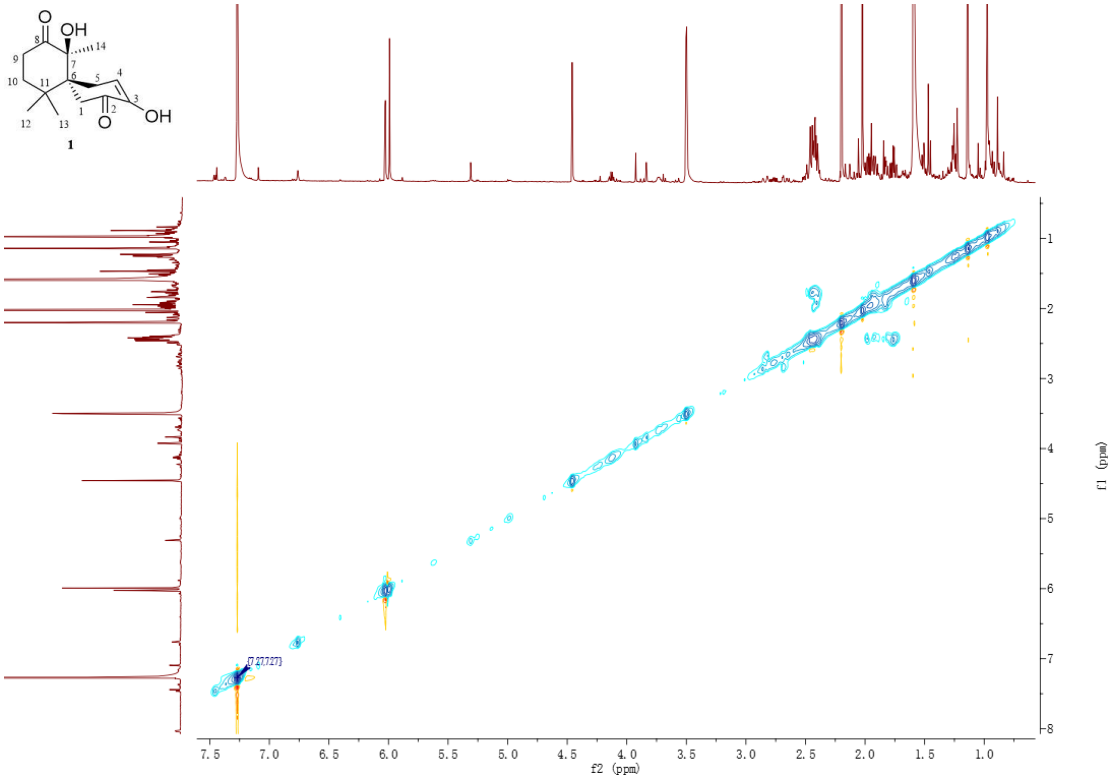


Figure S9. ROESY spectrum of **1**

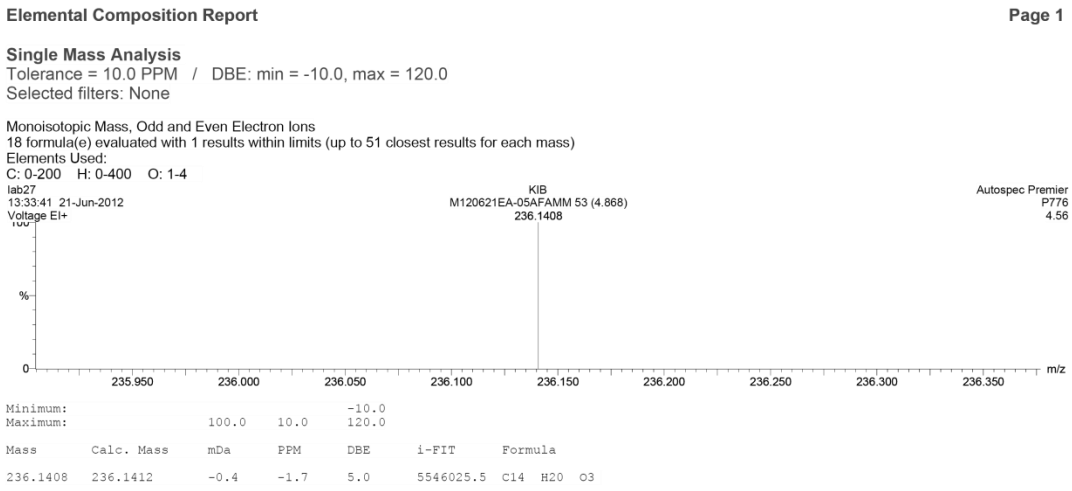


Figure S10. HR-ESI-MS spectrum of compound **2**

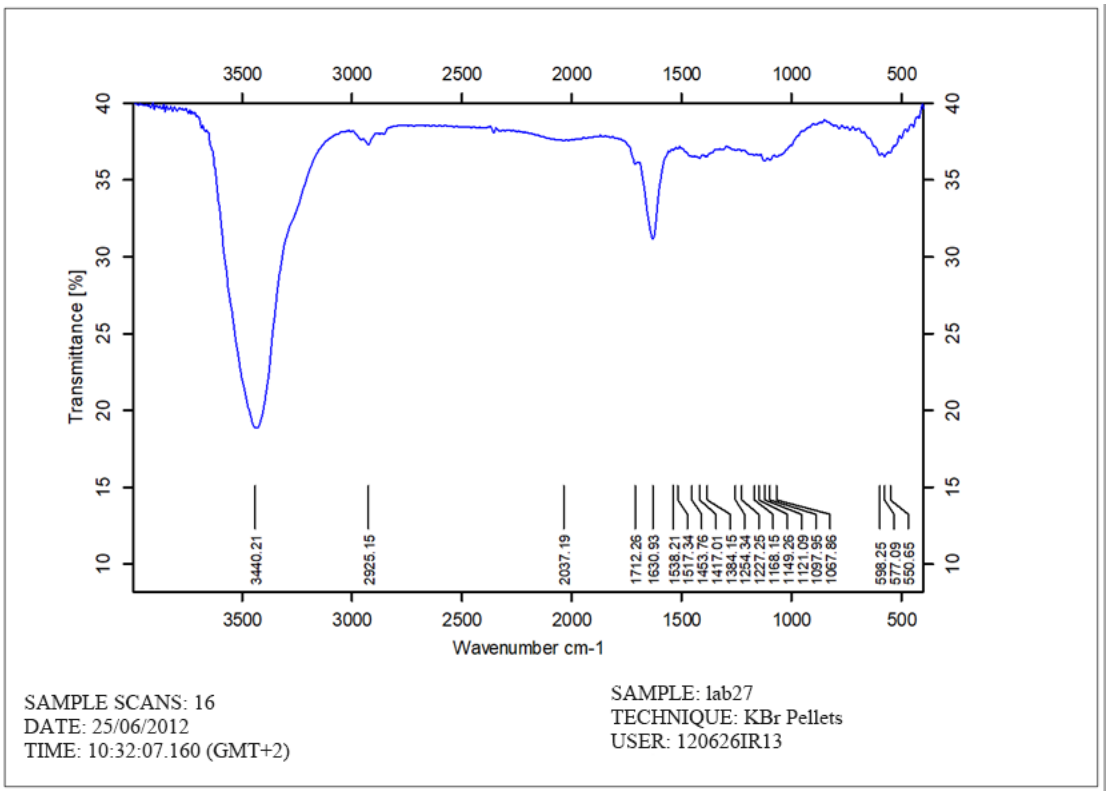


Figure S11. IR spectrum of compound **2**

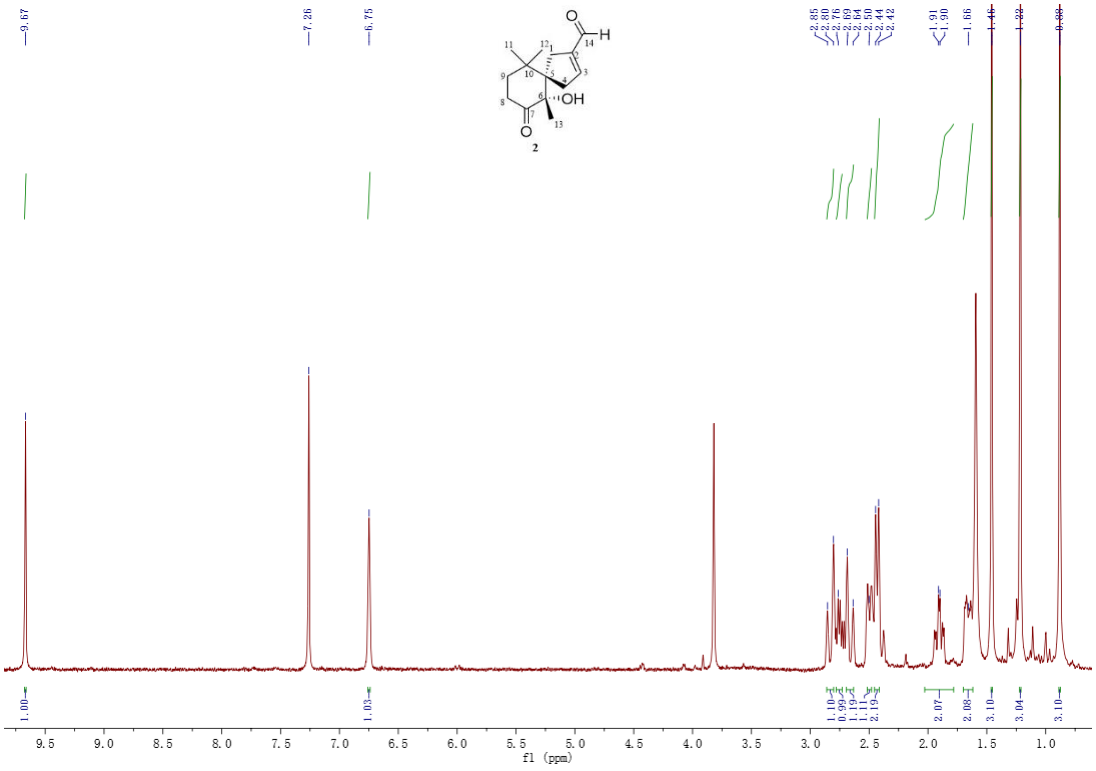


Figure S12. ^{1}H NMR spectrum (600MHz, $CDCl_3$) of **2**

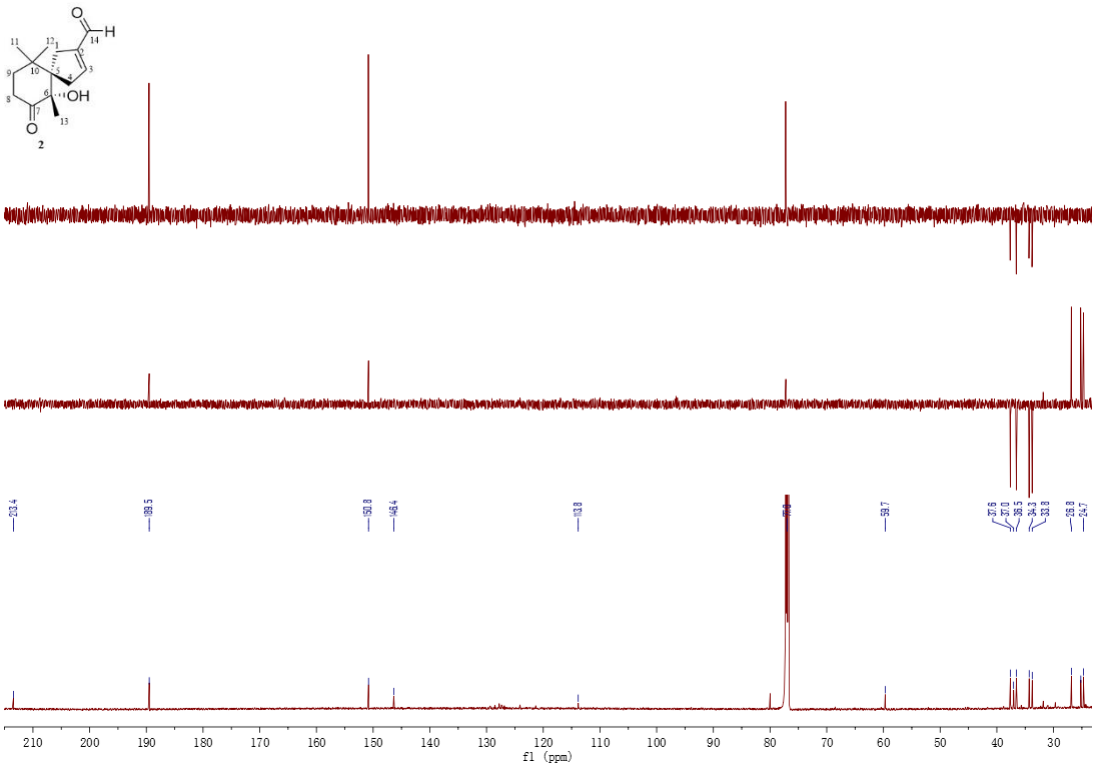


Figure S13. ^{13}C and DEPT spectrum (150MHz, $CDCl_3$) of **2**

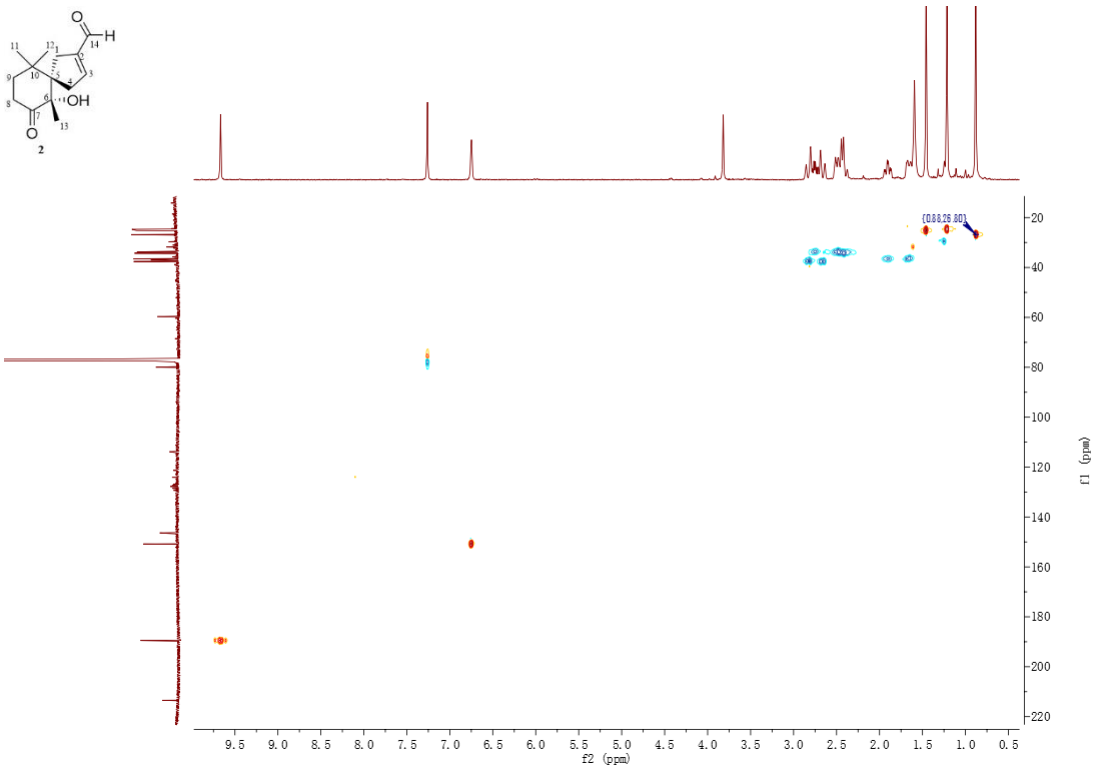


Figure S14. HSQC spectrum of **2**

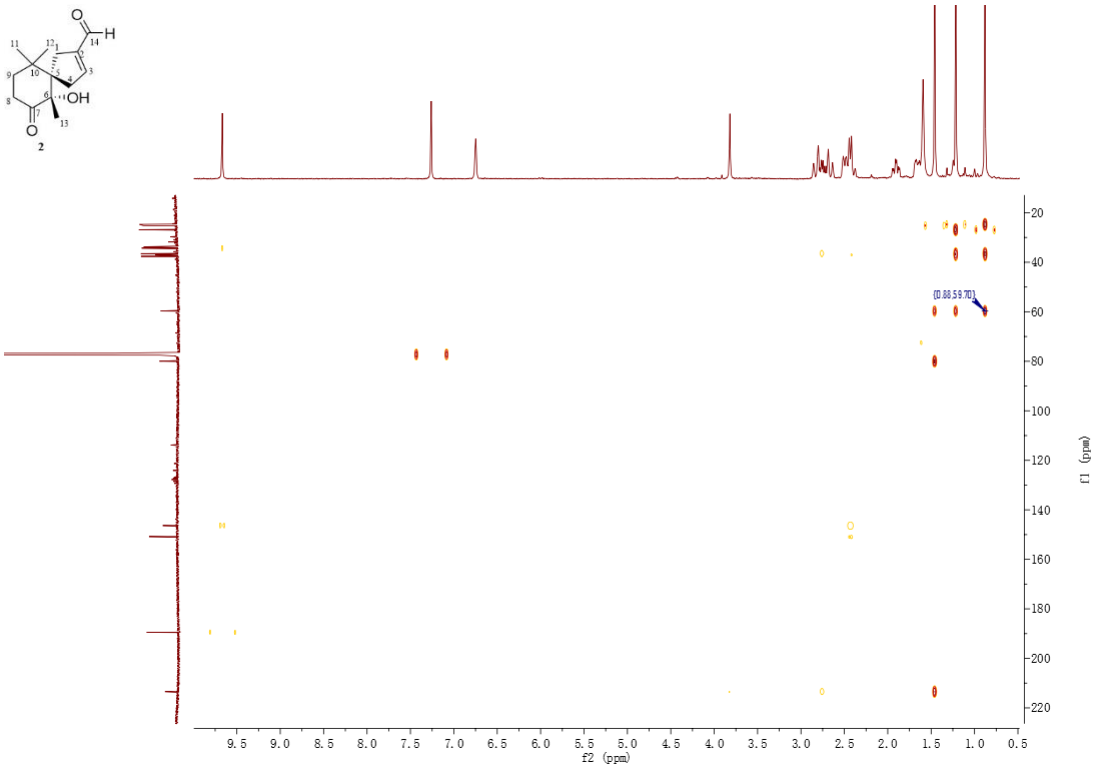


Figure S15. HMBC spectrum of **2**

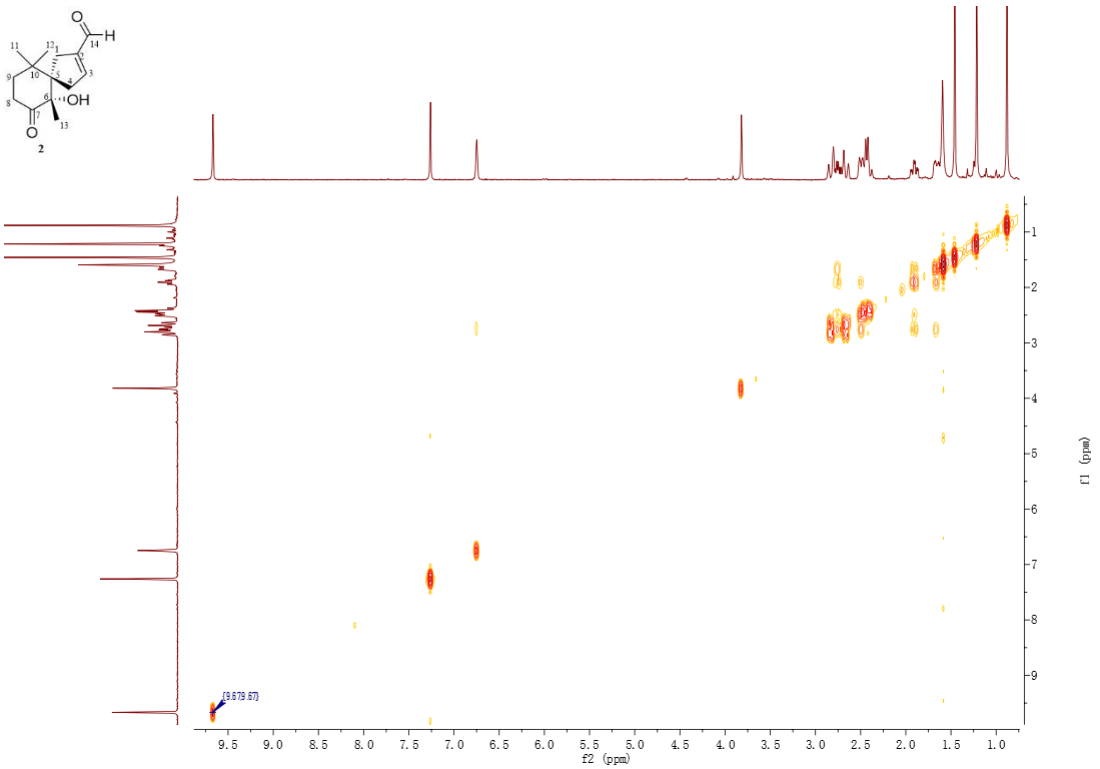


Figure S16. ^{1}H-^{1}H COSY spectrum of **2**

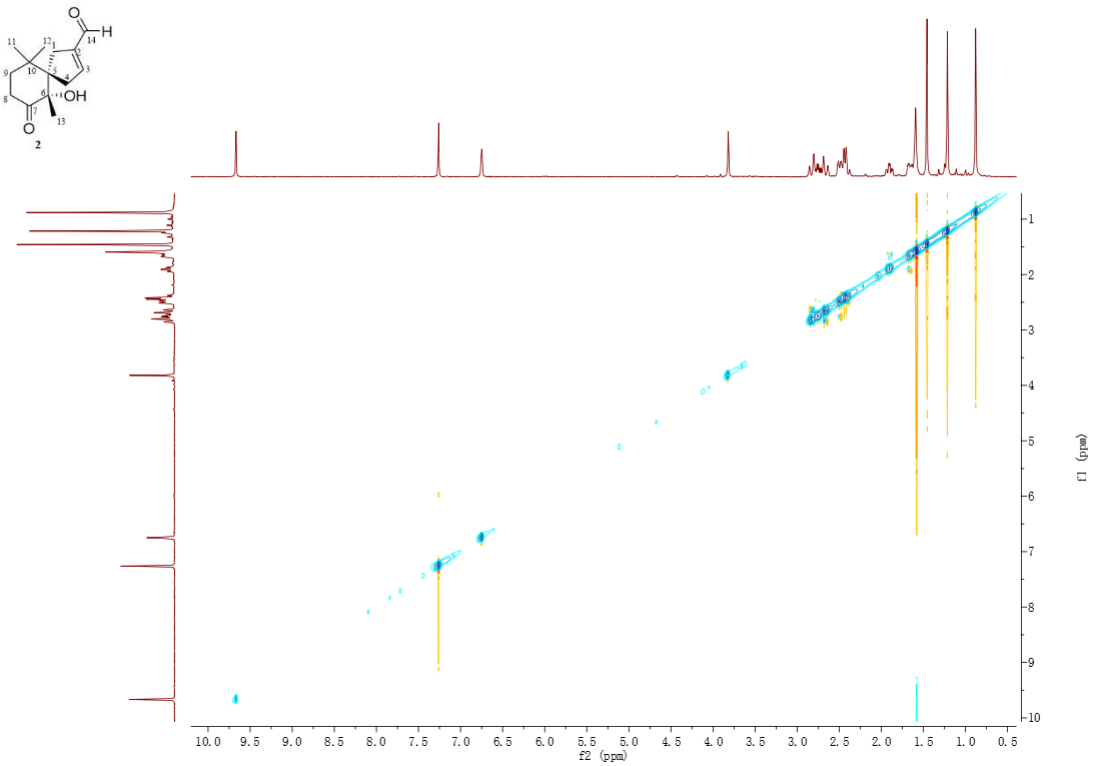


Figure S17. ROESY spectrum of **2**

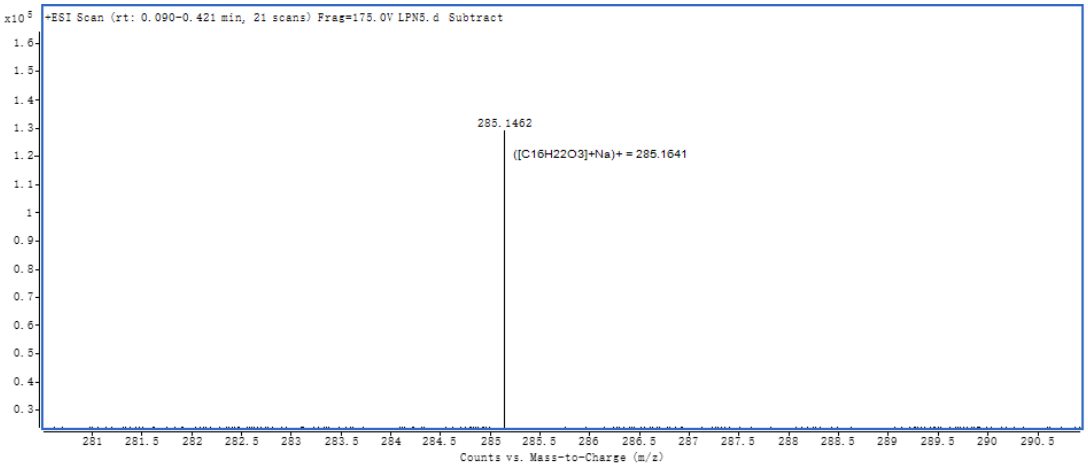
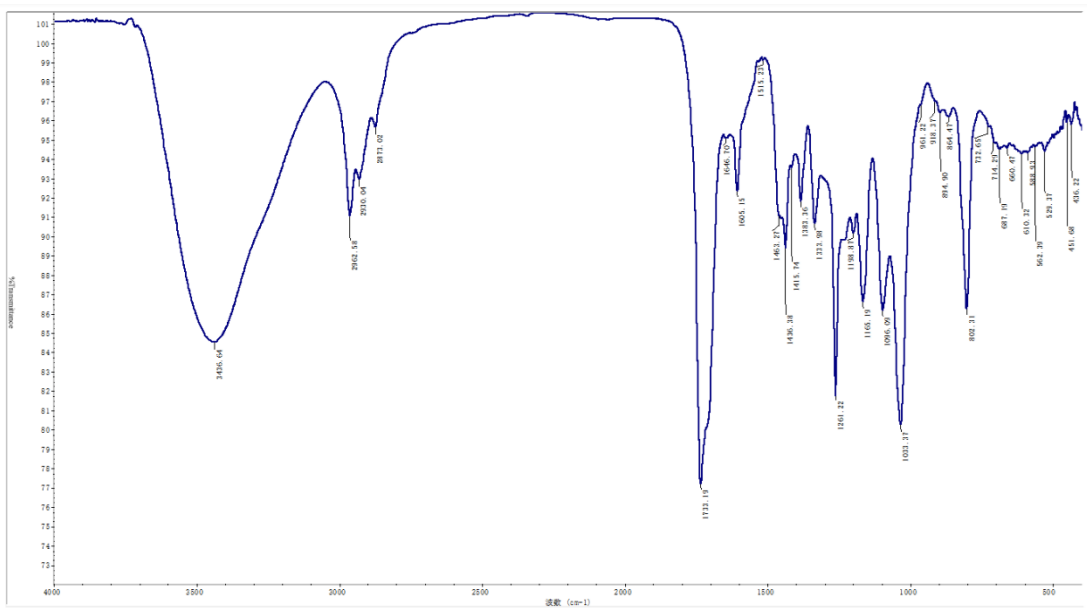


Figure S18. HR-ESI-MS spectrum of compound **3**



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Instrument model: NICOLET iS10
Software version: OMNIC 9.8.372

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Background Scans: 16
resolving Power: 4.000
Sampling gain: 1.0
Moving Mirror Speed: 0.4747
Diaphragm: 80.00

Figure S19. IR spectrum of compound **3**

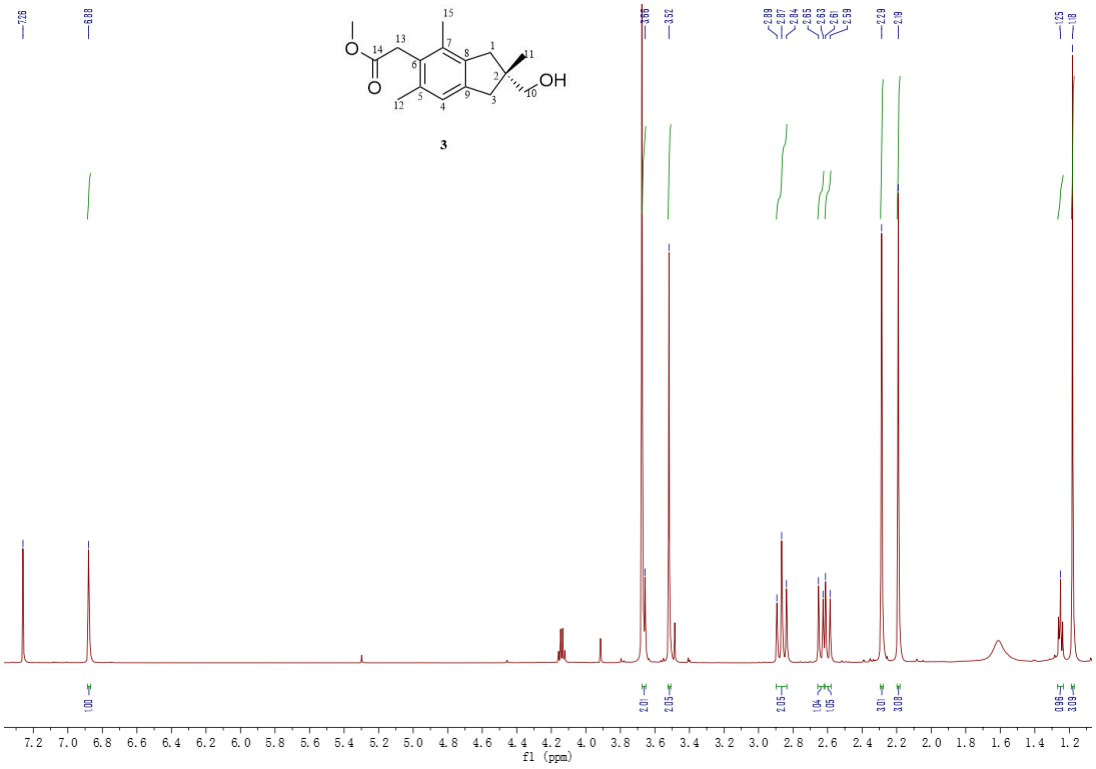


Figure S20. ^{1}H NMR spectrum (600MHz, $CDCl_3$) of **3**

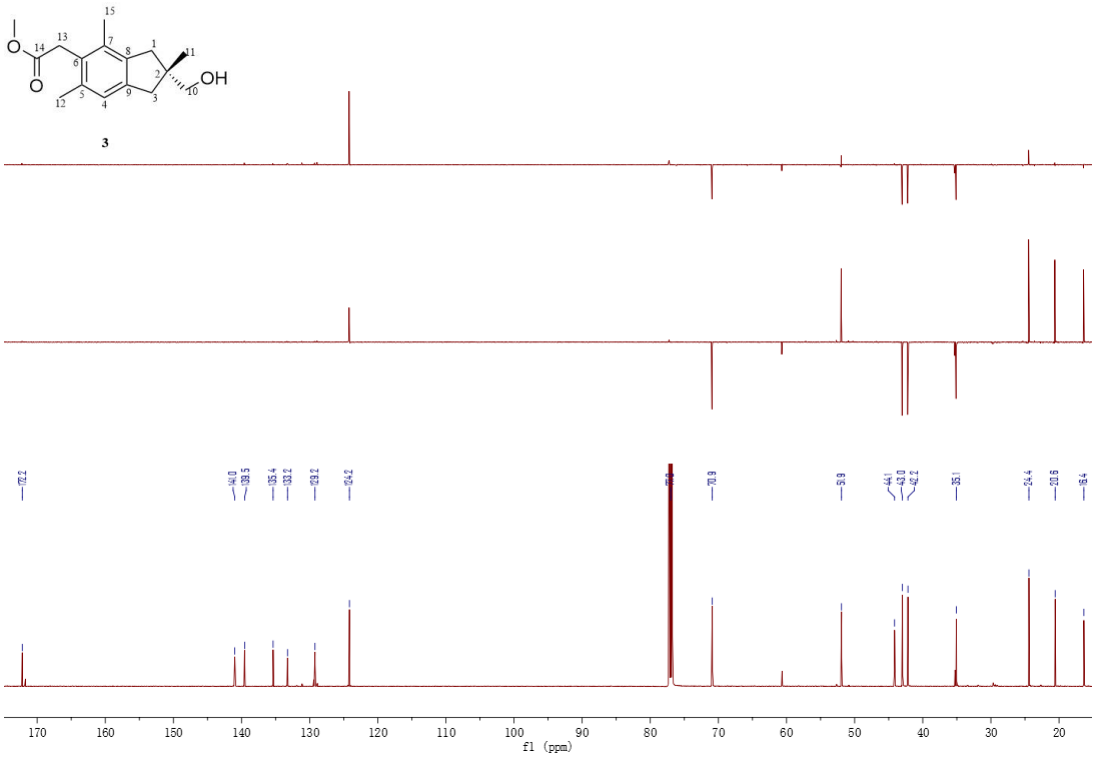


Figure S21. ^{13}C and DEPT spectrum (150MHz, $CDCl_3$) of **3**

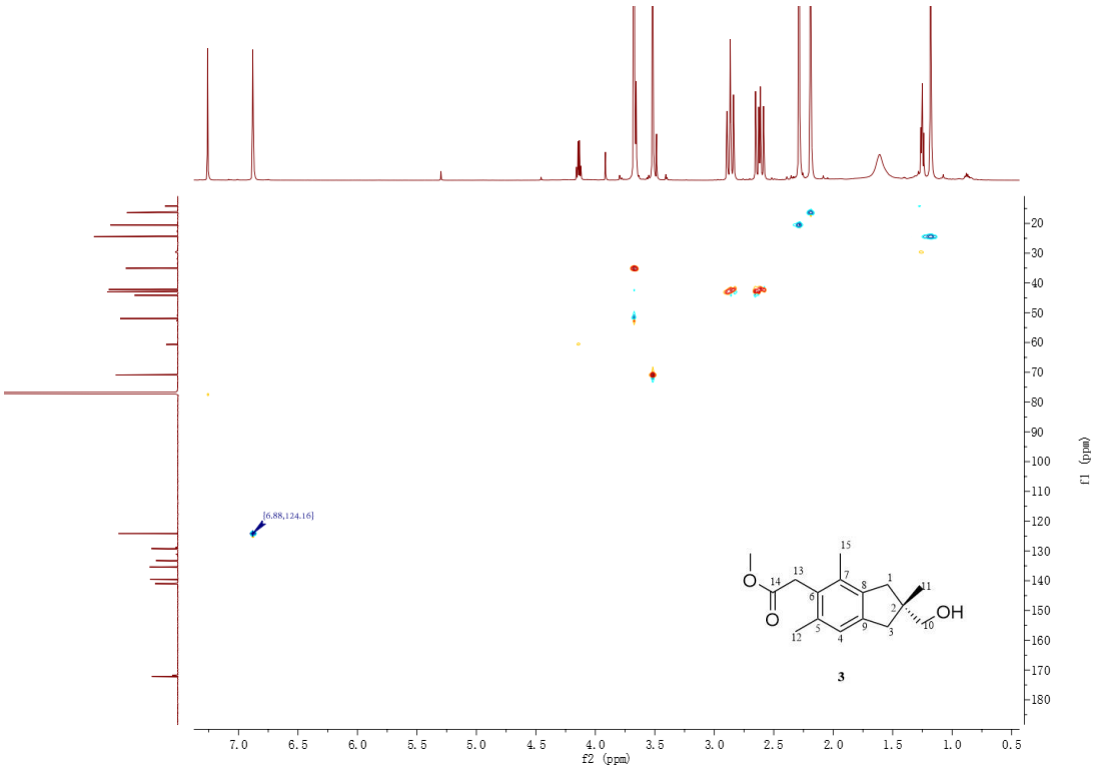


Figure S22. HSQC spectrum of **3**

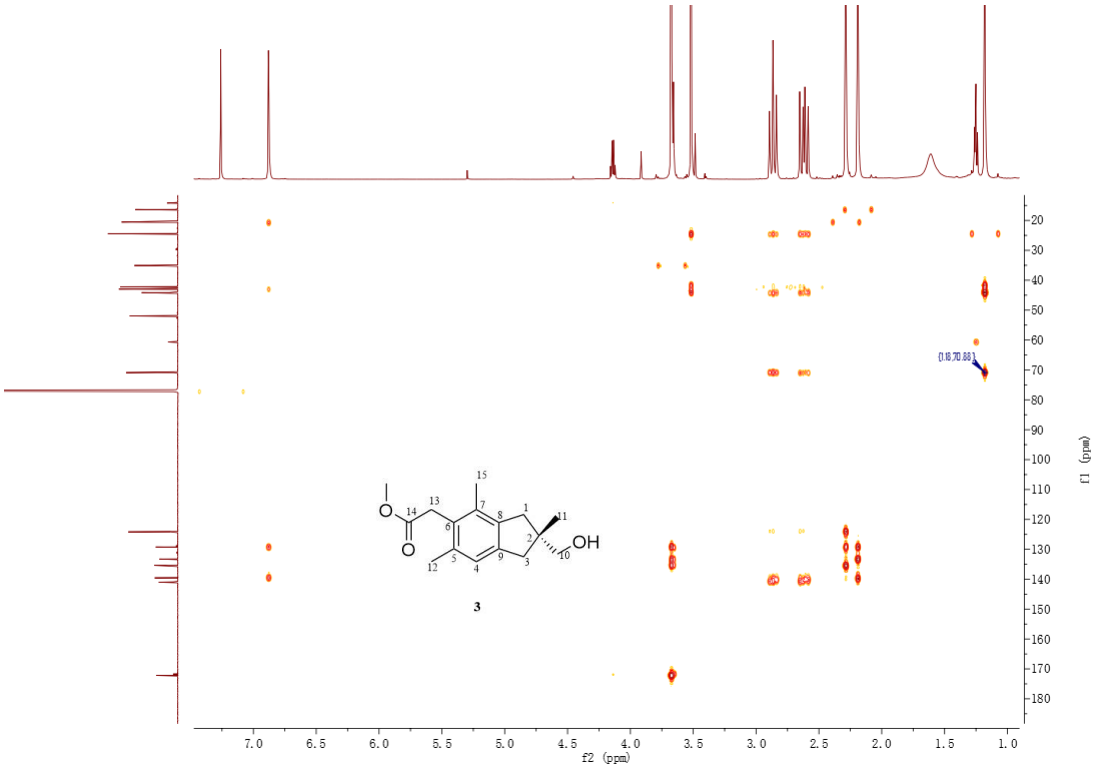


Figure S23. HMBC spectrum of **3**

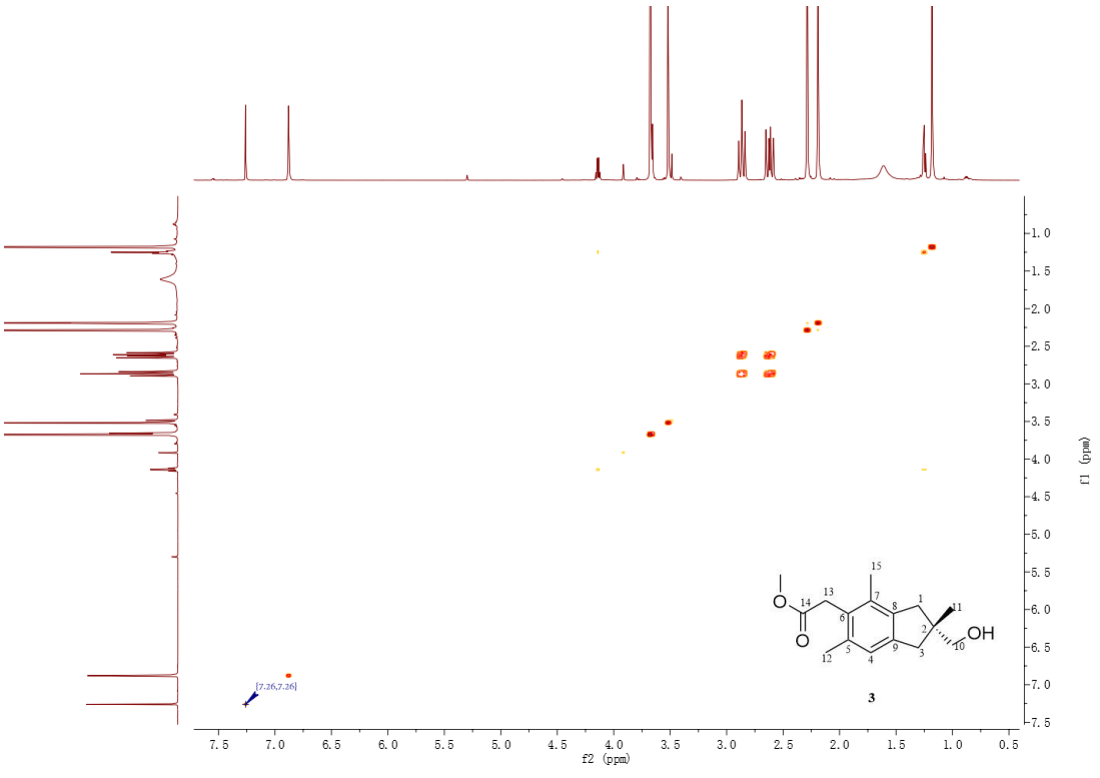


Figure S24. ^{1}H-^{1}H COSY spectrum of **3**

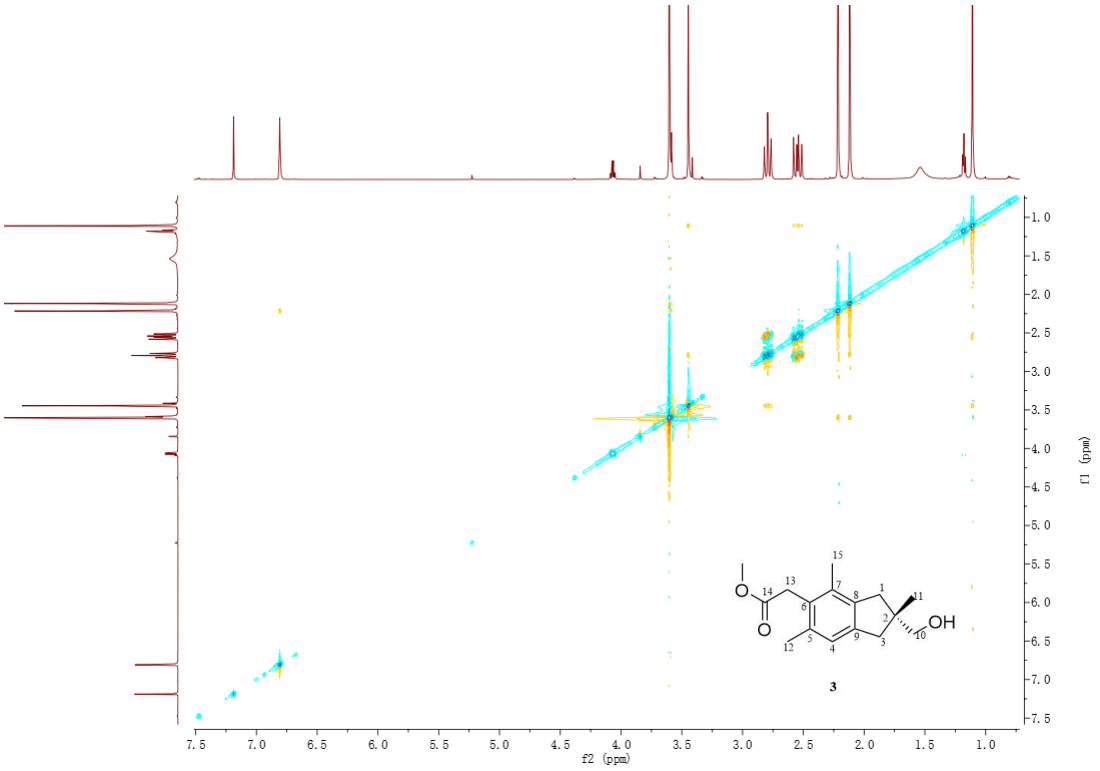


Figure S25. ROESY spectrum of **3**

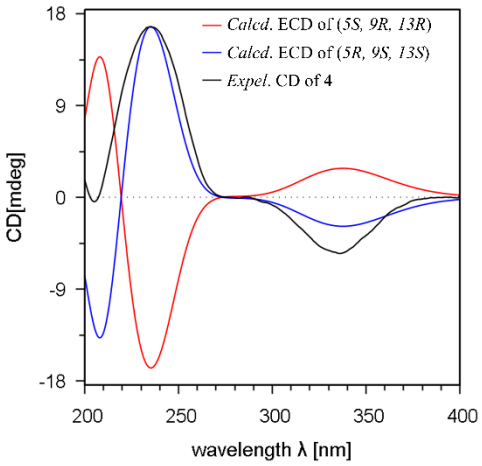


Figure S26. Experimental and calculated ECD spectra of compound **4**

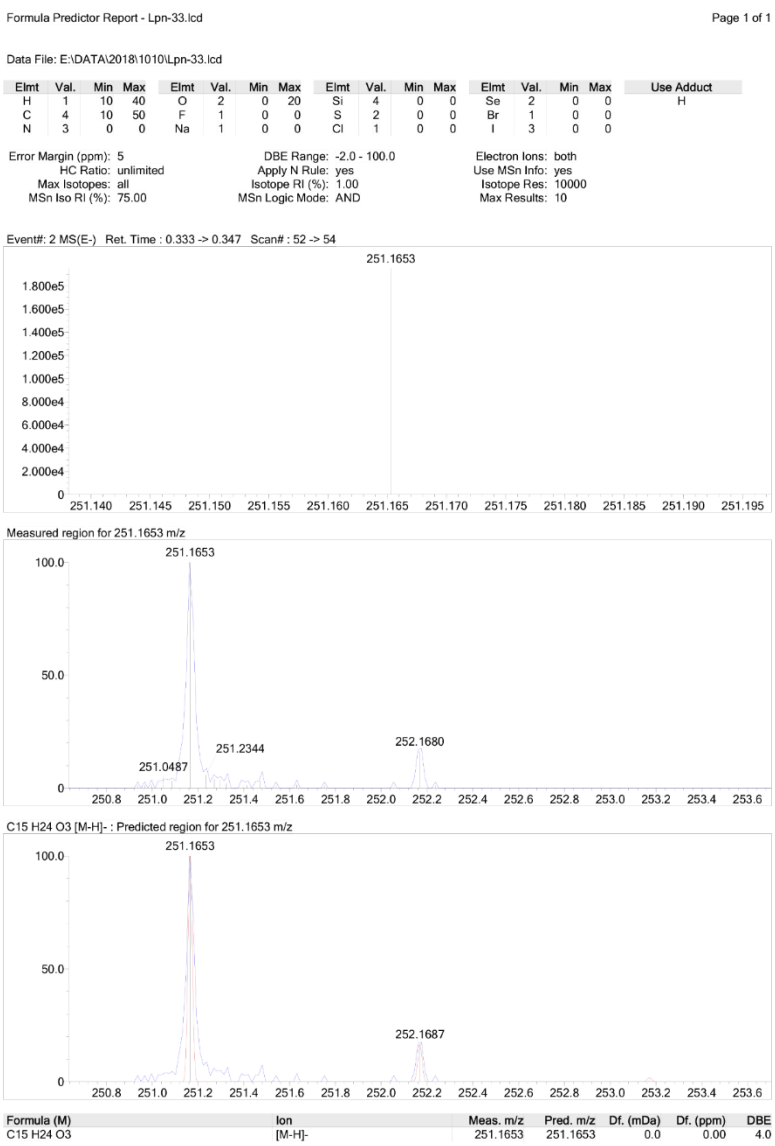


Figure S27. HR-ESI-MS spectrum of compound **4**

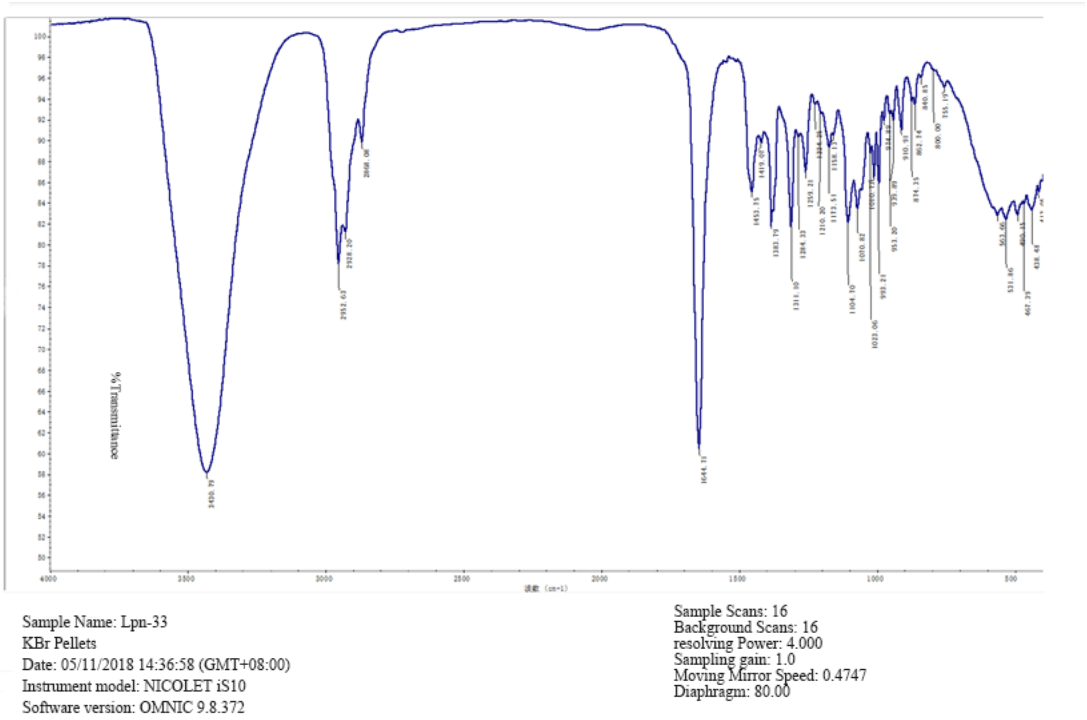


Figure S28. IR spectrum of compound **4**

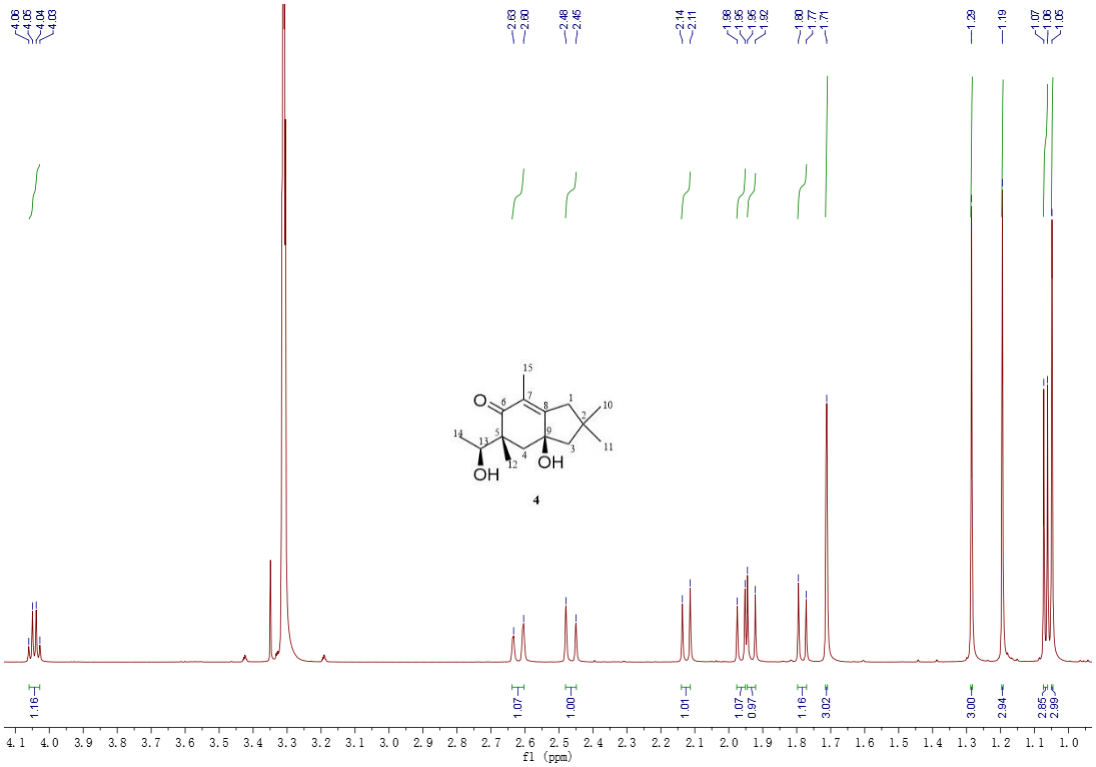


Figure S29. ^{1}H NMR spectrum (600MHz, CD_3OD) of **4**

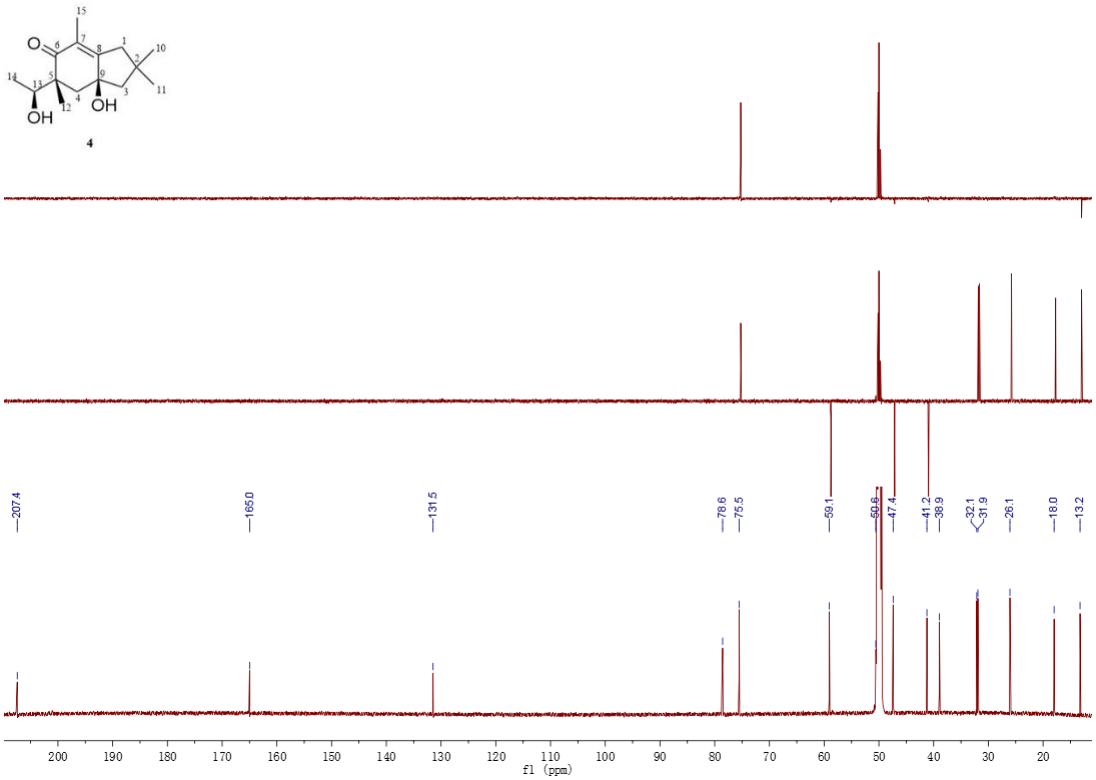


Figure S30. ^{13}C and DEPT spectrum (150MHz, CD_3OD) of **4**

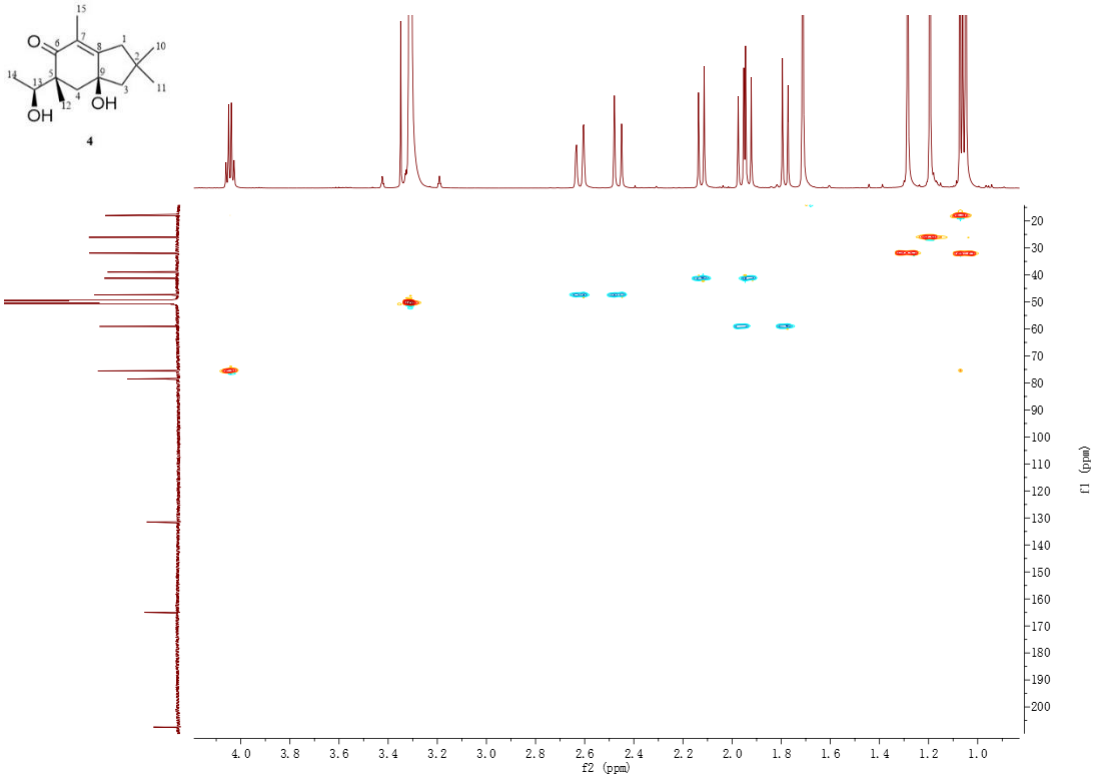


Figure S31. HSQC spectrum of **4**

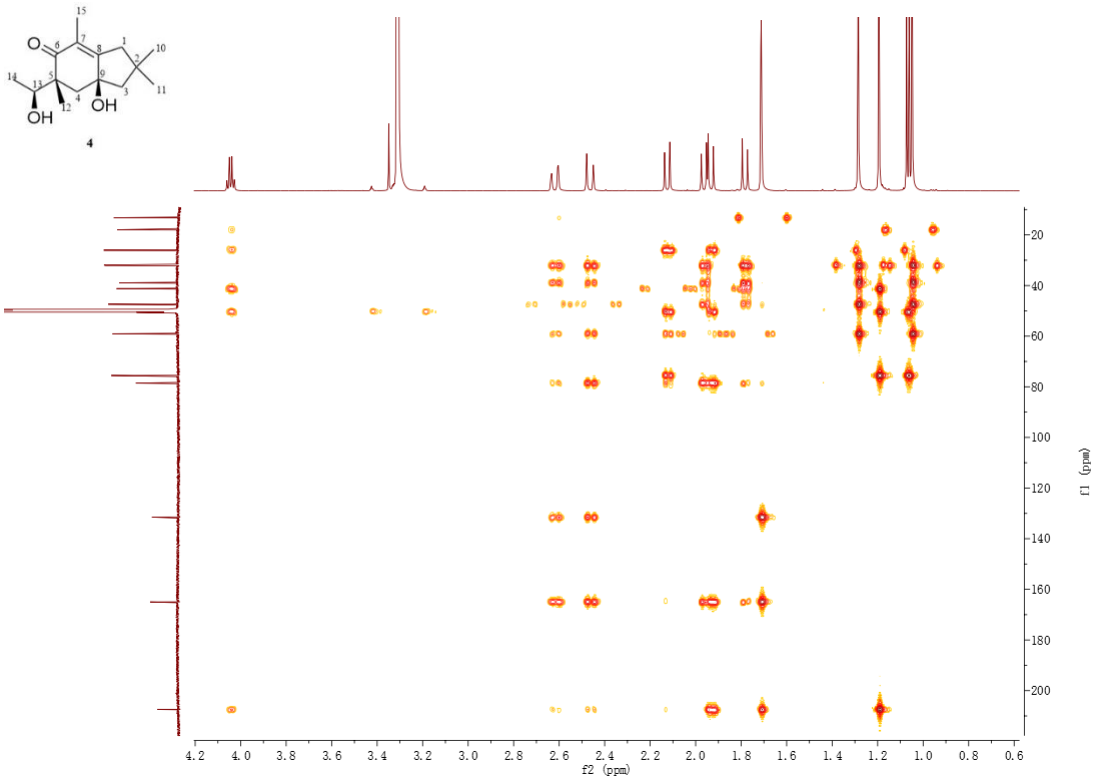


Figure S32. HMBC spectrum of **4**

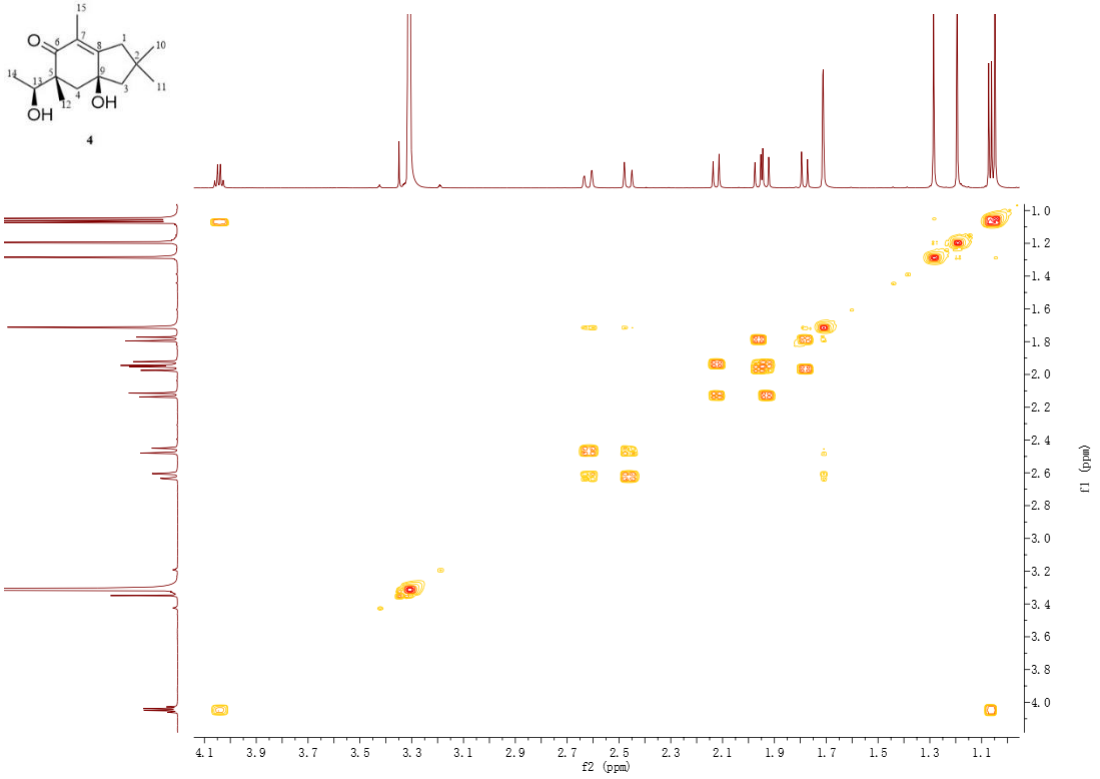


Figure S33. ^{1}H-^{1}H COSY spectrum of **4**

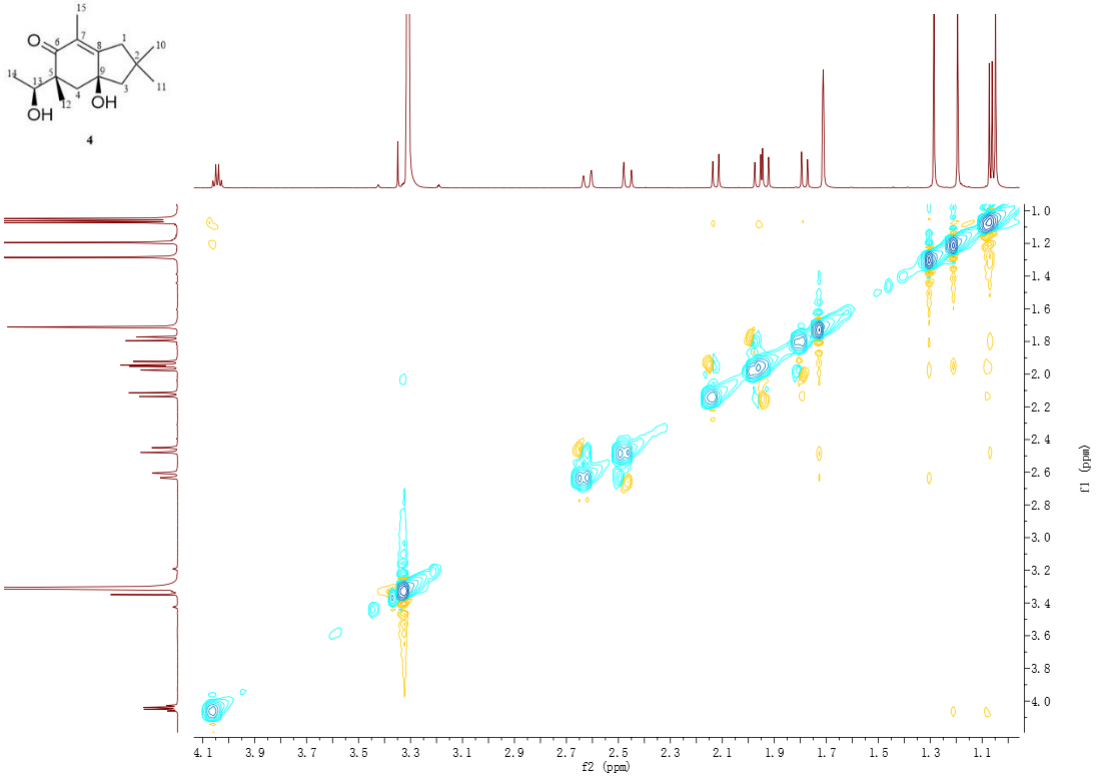


Figure S34. ROESY spectrum of **4**

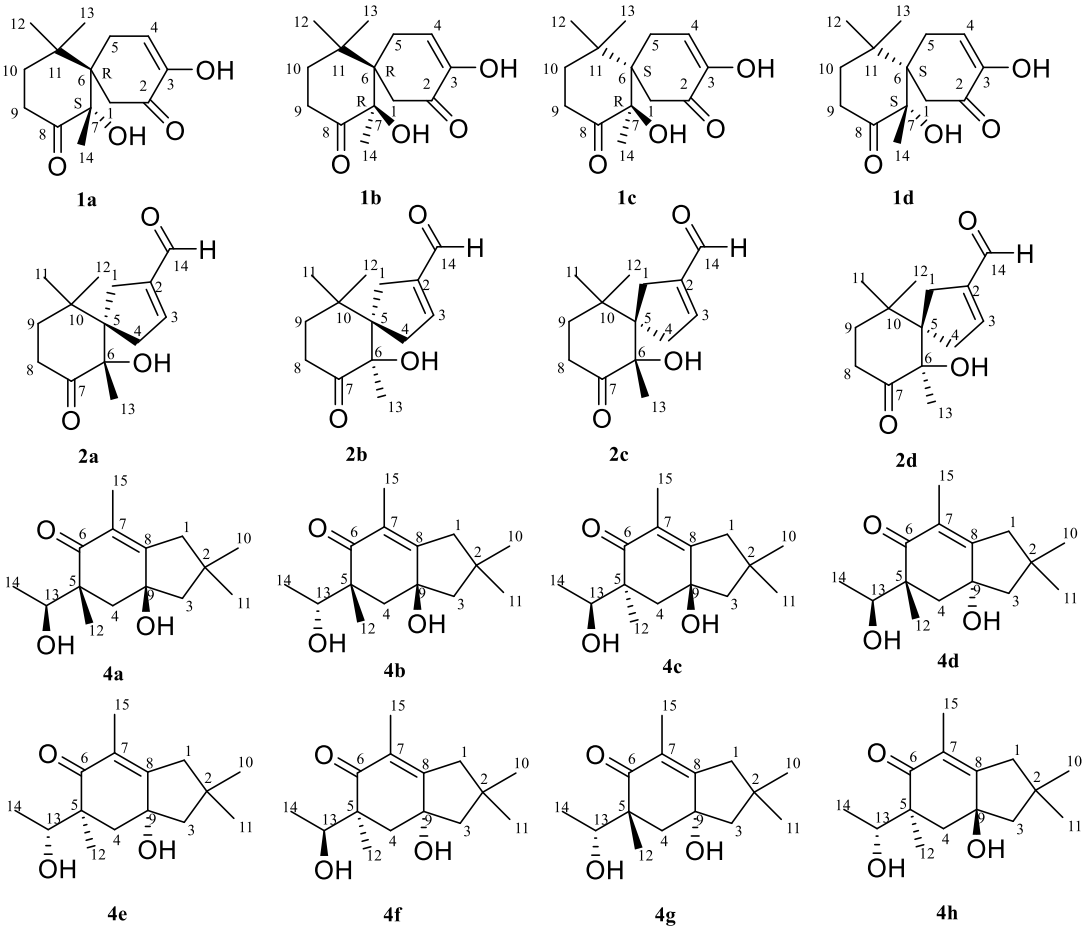


Figure S35. There are possible configurations of compounds **1**, **2** and **4**

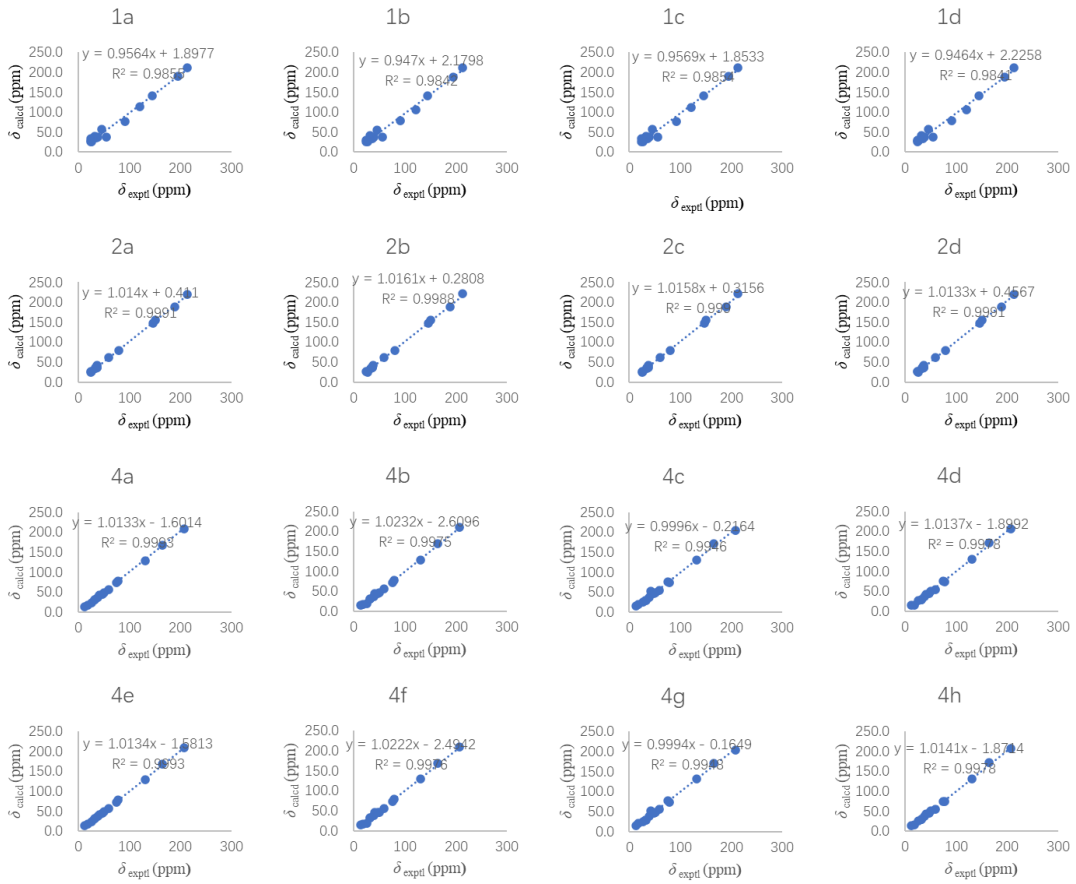


Figure S36. Linear correlation plots of calculate-experimental ^{13}C NMR chemical shift values for (6*R*,7*S*)-**1a**; (6*R*,7*R*)-**1b**; (6*S*,7*R*)-**1c**; (6*S*,7*S*)-**1d**; (5*S*,6*S*)-**2a**; (5*S*,6*R*)-**2b**; (5*R*,6*S*)-**2c**; (5*R*,6*R*)-**2d**, (5*R*,9*S*,13*S*)-**4a**; (5*R*,9*S*,13*R*)-**4b**; (5*S*,9*S*,13*S*)-**4c**; (5*R*,9*R*,13*S*)-**4d**; (5*S*,9*R*,13*R*)-**4e**; (5*S*,9*R*,13*S*)-**4f**; (5*R*,9*R*,13*R*)-**4g**; (5*S*,9*S*,13*R*)-**4h**

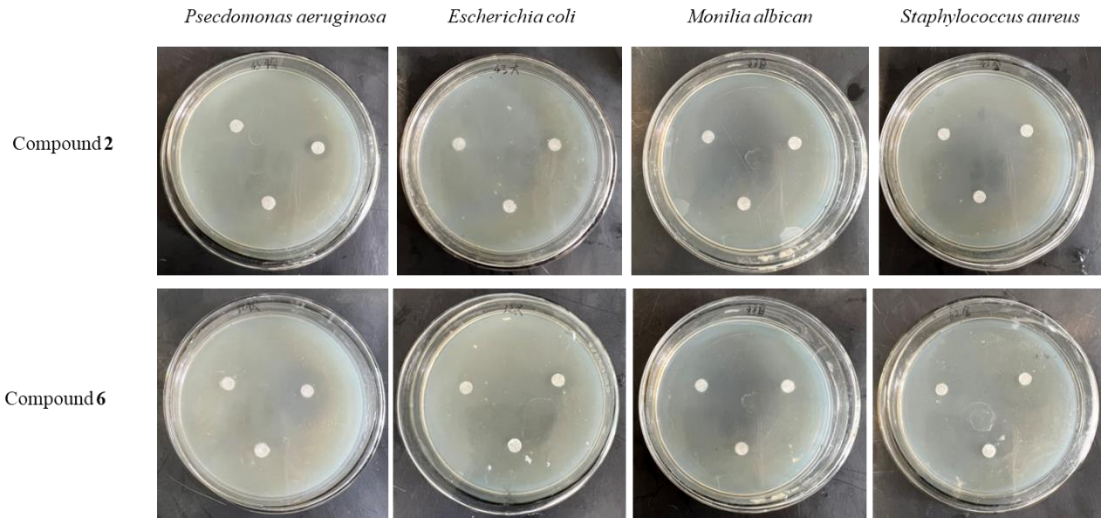


Figure S37. Antibacterial test of compounds **2** and **6**

Calculation of optical rotation of compound **2**:

The conformation search found that compound **2** (5*S*,6*S*) has three conformations, among which the Boltzmann distribution ratio and OR value of each conformation are as follows:

Table S4. The Boltzmann distribution proportion of its dominant conformation of the compound **2** (5*S*,6*S*)

Comformation	Weight (%)	OR
1	99.43	-9.79
2	0.44	-8.32
3	0.12	-8.48

Calculation of optical rotation of compound **3**:

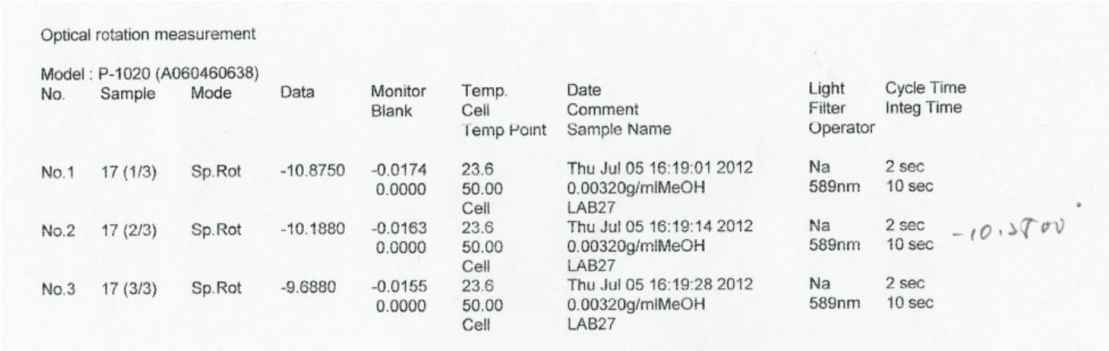
Through conformation search, it is found that there are 124 conformations with the energy threshold of compound **3** (*S*) within 3.0 kcal/mol, and the Boltzmann distribution proportion of its dominant conformation is shown in table S4:

Table S5. Compound **3** (*S*) within 3.0 kcal/mol, and the Boltzmann distribution proportion of its dominant conformation

Comfo-rmation	Weight (%)	OR	Comfo-rmation	Weight (%)	OR	Comfo-rmation	Weight (%)	OR
1	1.56	-7.21	62	1.07	134.05	101	1.16	149.56
3	1.2	-69.09	68	1.08	68.84	102	1.41	17.51

4	1.43	-1.8	69	2	-3.08	103	1.65	22.33
5	1.13	81.11	70	1.02	83.17	104	1.23	87.58
8	1.59	-6.89	72	1.63	-91.08	105	2.18	70.96
17	1.16	82.37	73	1.54	82.4	106	1.69	-58.1
18	1.43	8.31	75	1.17	-248.81	108	1.6	-41.23
20	1.43	31.95	76	1.11	158.47	109	1.16	-266.44
21	1.54	188.75	78	0.99	60.23	110	1.39	-183.21
24	1.24	-64.94	79	1.04	42.8	111	1.62	25.44
27	1.76	84.65	81	2.02	-13.43	112	1.25	-76.34
31	1.53	171.84	84	1.12	155.41	113	1.43	-61.62
37	1.49	107.52	85	1.05	-263.5	114	1.25	97.81
41	1.45	15.27	89	2.16	3.49	115	1.33	-230.92
43	1.02	140.03	90	2.26	166.56	116	1.42	27.8
44	1.02	44.13	91	1.06	133.4	117	1.41	-164.63
50	1.04	73.11	93	1.03	67.55	118	1.58	-37.89
52	2.11	-1.43	94	1.02	40.68	119	1.31	-247.35
53	1.17	-257.65	95	2.22	46.27	120	1.43	-125.95
55	1.51	113.57	96	1.56	-9.98	121	1.39	-52.4
56	1.77	79.7	98	2.07	78.53	122	1.42	-121.11
57	1.27	70.01	99	1.65	-85.72	123	1.24	101.05
60	1	31.15	100	2.18	-5.19	124	1.41	-120.26
61	1.17	-253.2						

The calculation results show that the calculated optical rotation value of **3** (*S*) is +3.01, while the experimental optical rotation value (as shown in the figure S37) is -2.92. Therefore, it is judged that the absolute configuration of compound **3** is *R*.



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	17 (1/3)	Sp.Rot	-10.8750	-0.0174 0.0000	23.6 50.00 Cell	Thu Jul 05 16:19:01 2012 0.00320g/mlMeOH LAB27	Na 589nm	2 sec 10 sec
No.2	17 (2/3)	Sp.Rot	-10.1880	-0.0163 0.0000	23.6 50.00 Cell	Thu Jul 05 16:19:14 2012 0.00320g/mlMeOH LAB27	Na 589nm	2 sec 10 sec
No.3	17 (3/3)	Sp.Rot	-9.6880	-0.0155 0.0000	23.6 50.00 Cell	Thu Jul 05 16:19:28 2012 0.00320g/mlMeOH LAB27	Na 589nm	2 sec 10 sec

Figure S38. Experimental optical rotation of compound **2**

17 (1/3) Specific O.R.	-3.310	24.7	0	Mon Sep 03 18:15:15 2018	0.00290g/mL MeOH LPN-5 ↵
17 (2/3) Specific O.R.	-2.138	24.8	0	Mon Sep 03 18:15:21 2018	0.00290g/mL MeOH LPN-5 ↵
17 (3/3) Specific O.R.	-3.310	24.8	0	Mon Sep 03 18:15:26 2018	0.00290g/mL MeOH LPN-5 ↵

Figure S39. Experimental optical rotation of compound **3**