SUPPLEMENTARY MATERIAL

A new protostane-type triterpenoid from *Alisma plantago-aquatica* subsp. *orientale* (Sam.) Sam.

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A new protostane-type triterpenoid bearing an oxetane ring in the side-chain, named alisol W (**1**), has been obtained from the dried rhizome of *Alisma plantago-aquatica* subsp. *orientale*. The structure and absolute configuration of compound **1** was determined from extensive spectroscopic analysis. In addition, the vasorelaxant activity and the inhibition on 11β-HSD1 of compound **1** were also evaluated, however, it didn't show remarkable effects.

Key words: *Alisma plantago-aquatica* subsp. *orientale*; Alismataceae; protostane triterpenoid; alisol W

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List of Contents

Table S1. ^{1}H- (600 MHz) and ^{13}C-NMR (150 MHz) spectral data of compound **1** (ppm, acetone-d_6)

No.	δ_H [mult., *J* (Hz)]	δ_C	No.	δ_H [mult., *J* (Hz)]	δ_C
1	2.12-2.19 (*m*)	31.4 (t)	15	1.29-1.34 (m)	31.3 (t)
	2.25-2.30 (*m*)			1.90 (*ddd*, 5.0, 10.1, 13.8)	
2	2.12-2.19 (*m*)	34.1 (t)	16	2.03-2.06 (*m*)	30.0 (t)
	2.74-2.79 (*m*)			2.12-2.19 (*m*)	
3		218.8 (s)	17		136.0 (s)
4		47.3 (s)	18	1.04 (*s*)	24.3 (q)
5	2.12-2.19 (*m*)	49.0 (d)	19	1.00 (*s*)	25.7 (q)
6	1.29-1.34 (m)	20.7 (t)	20	2.65-2.71 (*m*)	28.4 (d)
	1.45-1.50 (*m*)		21	1.00 (*d*, 5.9)	20.7 (q)
7	1.24-1.28 (m)	35.0 (t)	22	1.60 (*ddd*, 3.7, 10.1, 13.8)	37.2 (t)
	2.03-2.06 (*m*)			1.74 (*ddd*, 4.8, 9.8, 13.8)	
8		41.3 (s)	23	4.38 (*ddd*, 3.7, 6.4, 9.8)	79.5 (d)
9	1.77 (*d*, 10.9)	50.2 (d)	24	4.27-4.30 (*m*)	73.5 (d)
10		37.7 (s)	25		86.4 (s)
11	3.82 (*ddd*, 5.7, 10.9, 16.4)	69.9 (d)	26	1.23 (*s*)	23.6 (q)
12	1.95-2.01 (*m*)	35.1 (t)	27	1.27 (*s*)	28.5 (q)
	2.65-2.71 (m)		28	1.07 (*s*)	29.6 (q)
13		138.2 (s)	29	1.03 (*s*)	20.4 (q)
14		57.8 (s)	30	1.16 (*s*)	23.8 (q)

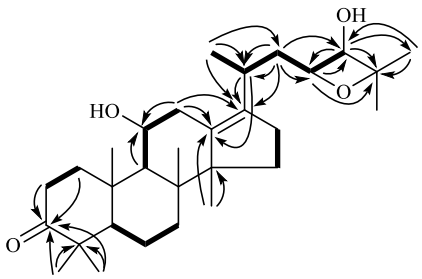


Figure S1. Key HMBC (arrows) and ^{1}H-^{1}H COSY correlations (bold lines) of **1**.

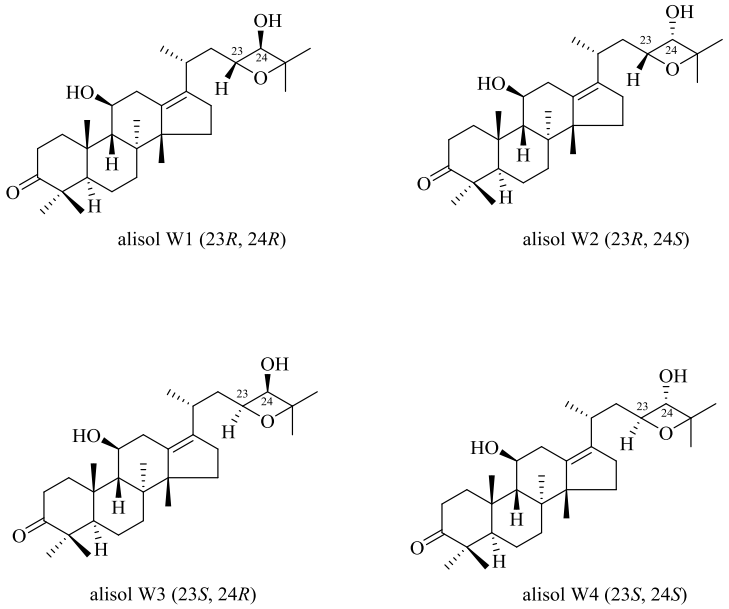


Figure S2. Four possible structures of compound **1**.

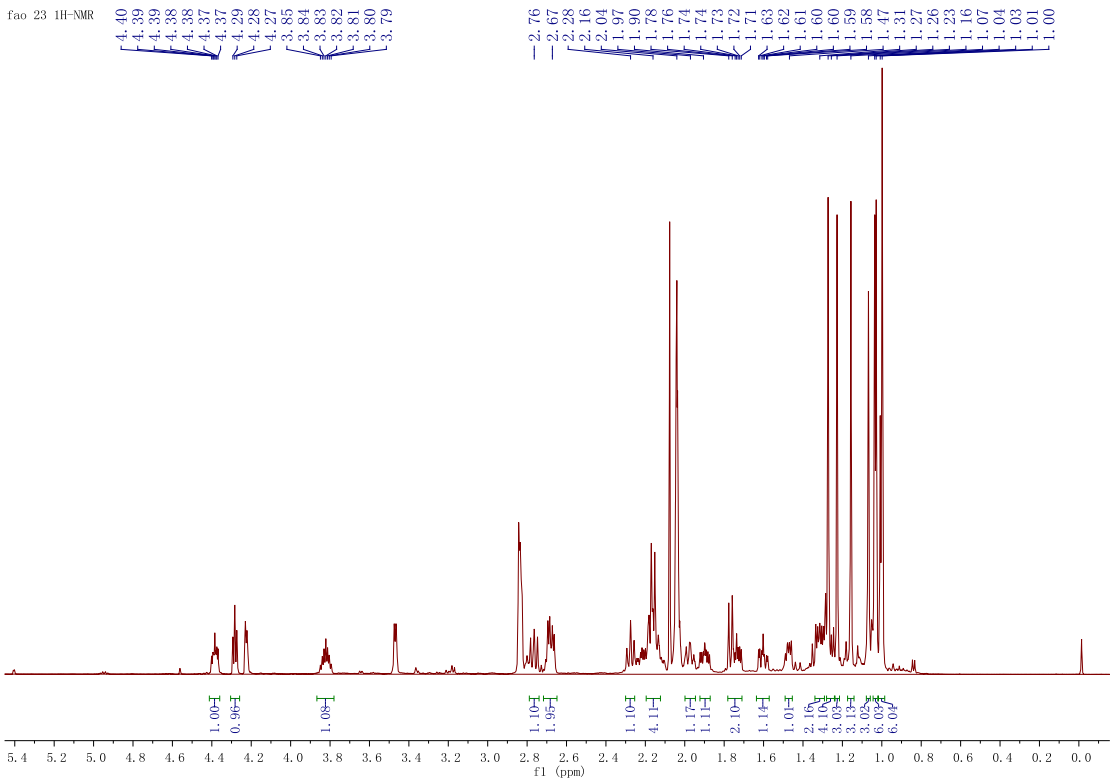


Figure S3. ^{1}H-NMR spectrum (600 MHz, acetone-d_6) of alisol W (**1**).

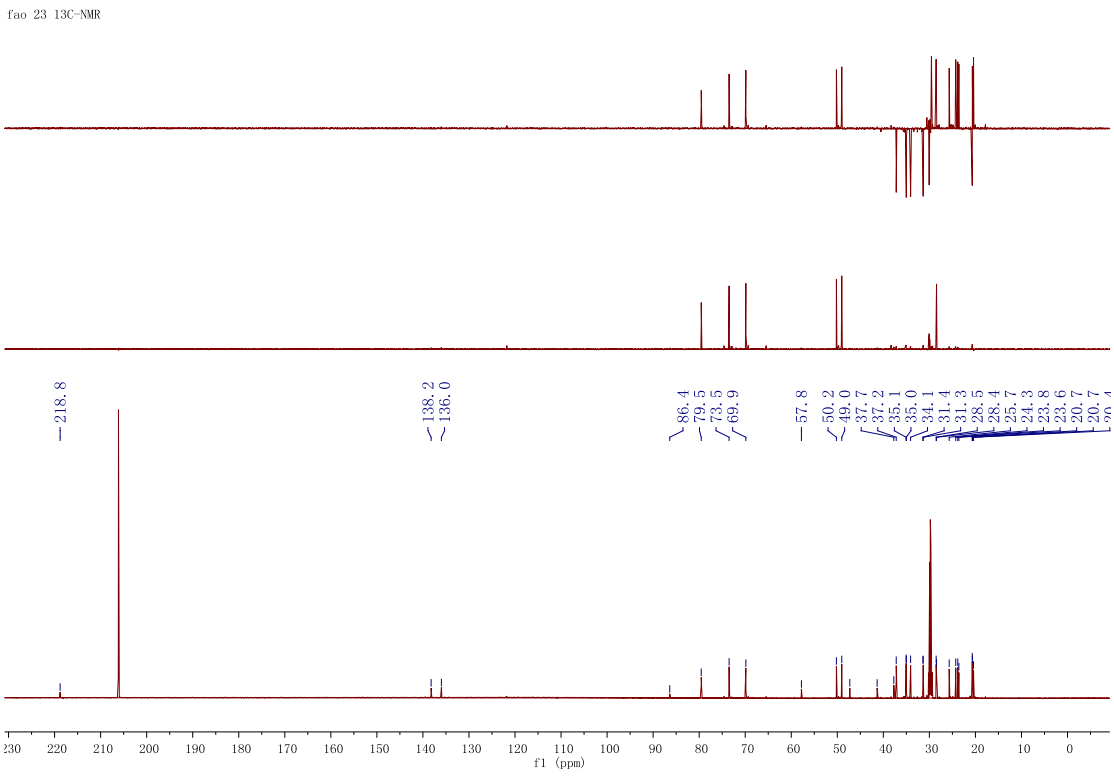


Figure S4. ^{13}C-NMR spectrum (150 MHz, acetone-d_6) of alisol W (**1**).

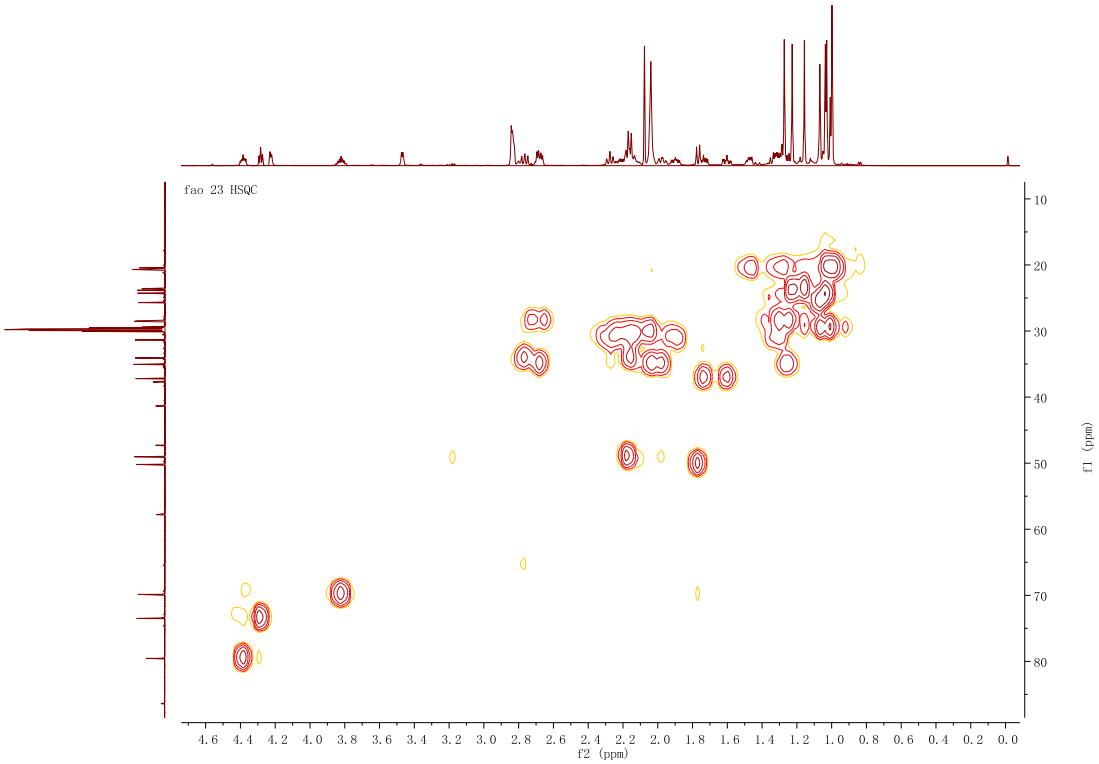


Figure S5. HSQC spectrum of alisol W (**1**).

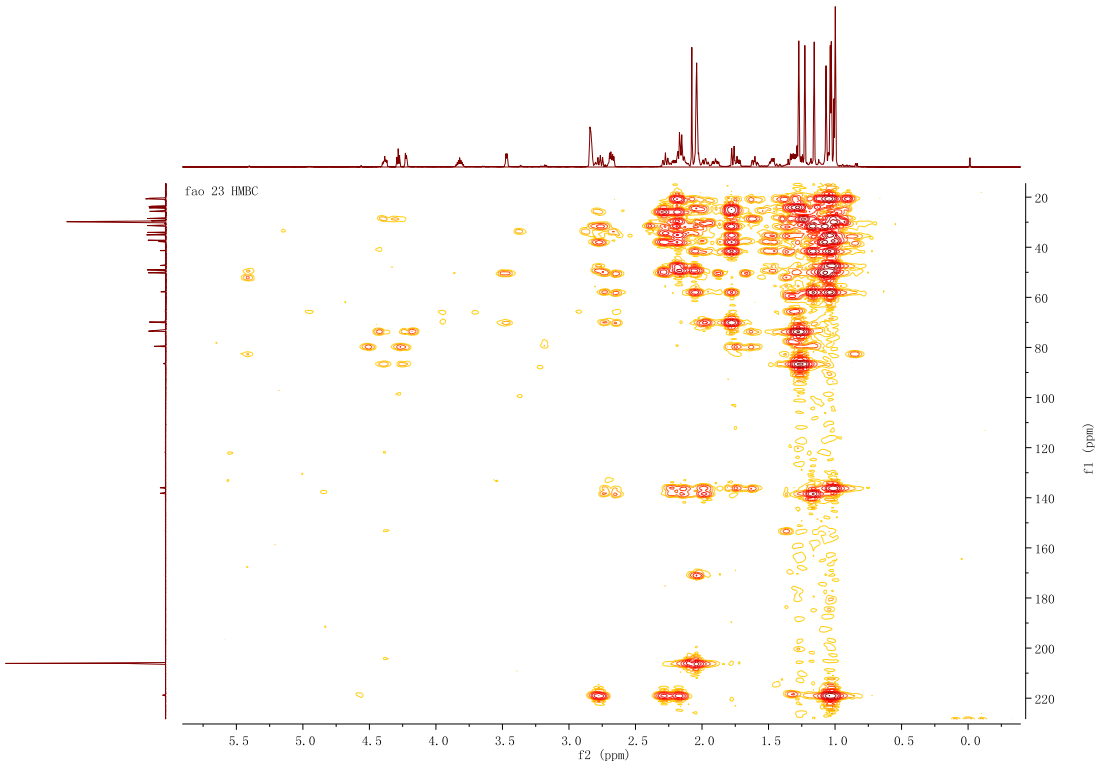


Figure S6. HMBC spectrum of alisol W (**1**).

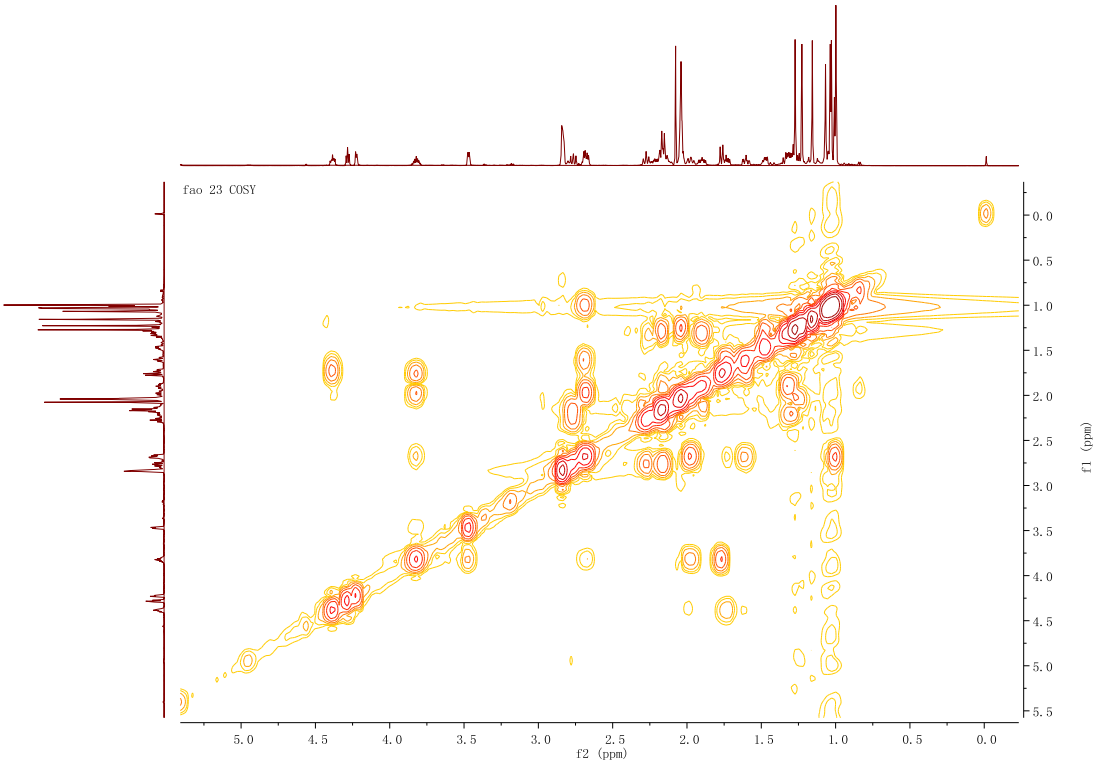


Figure S7. ^{1}H-^{1}H COSY spectrum of alisol W (**1**).

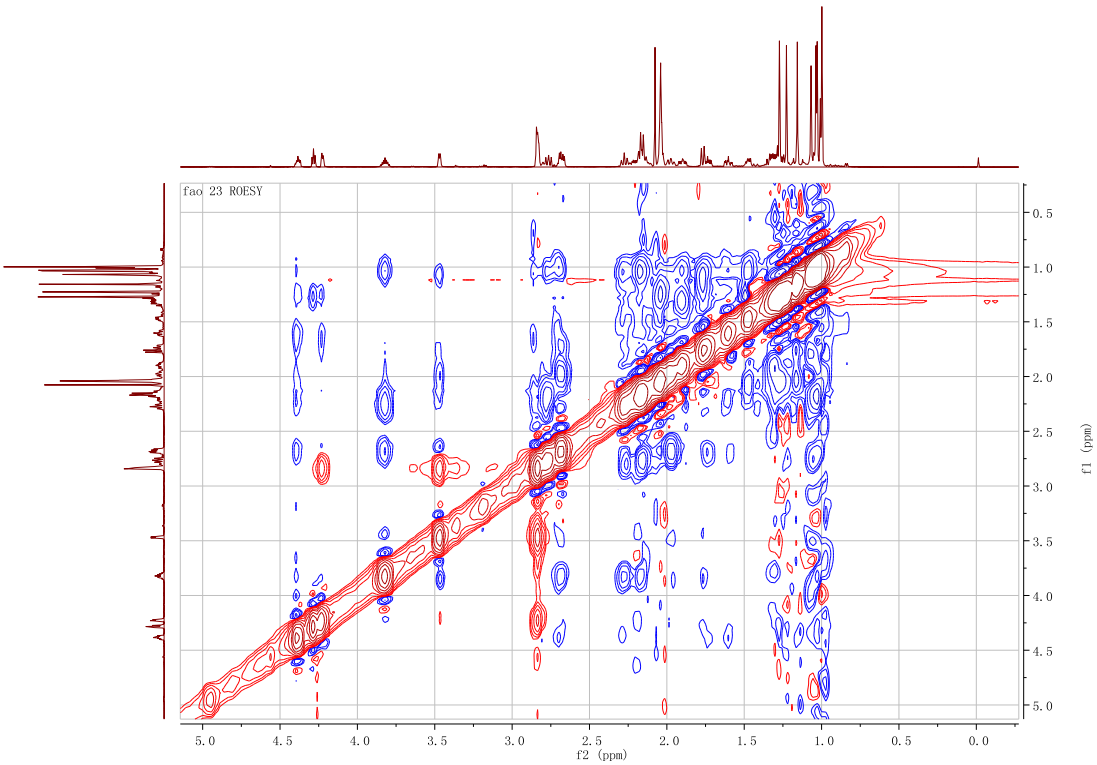


Figure S8. ROESY spectrum of alisol W (**1**).

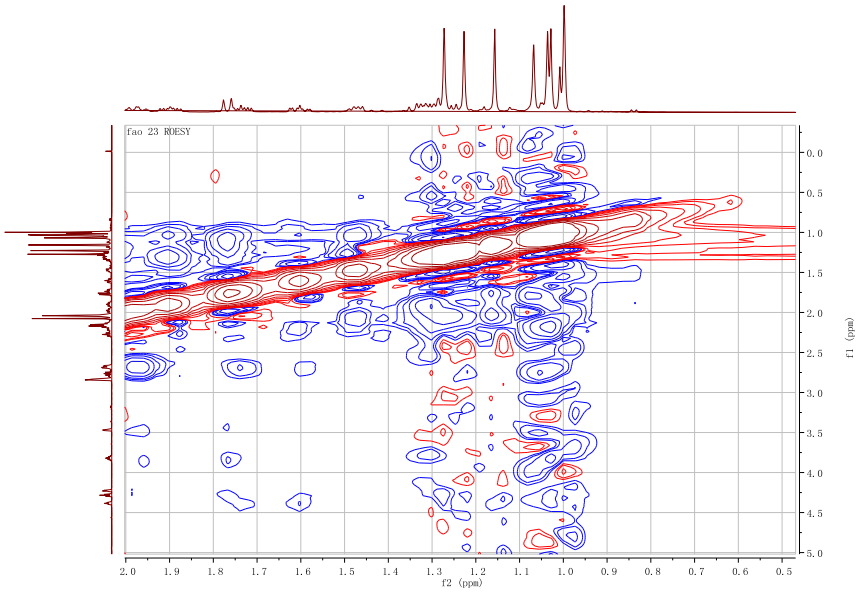


Figure S9. The amplificated ROESY spectrum (from 0.5 to 1.8) of alisol W (**1**).

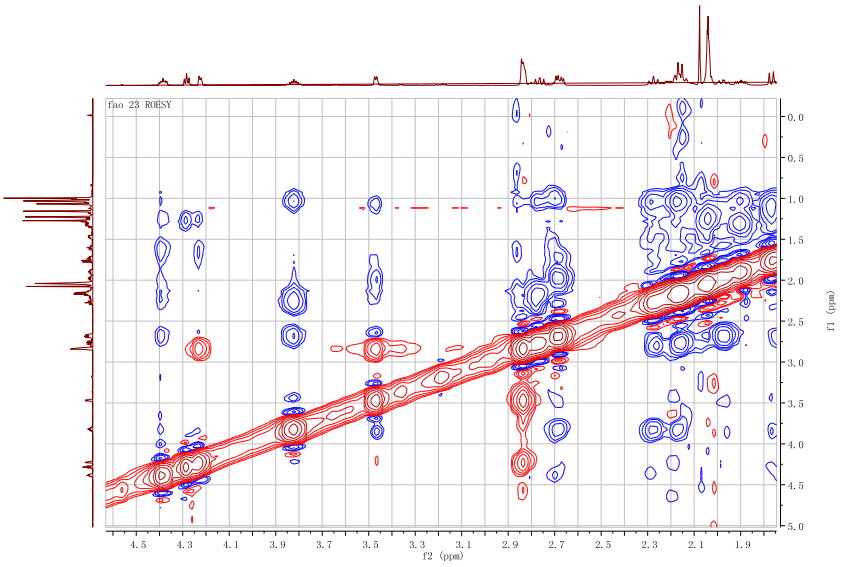


Figure S10. The amplificated ROESY spectrum (from 2.0 to 4.5) of alisol W (**1**).

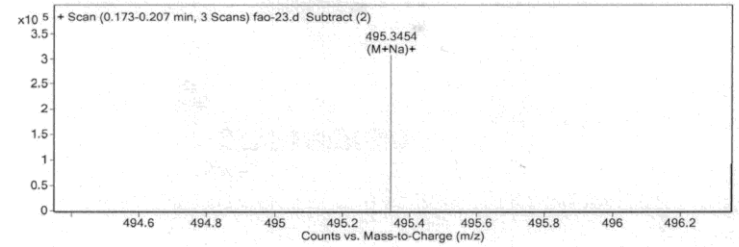
Qualitative Analysis Report

Data Filename	fao-23.d	**Sample Name**	fao-23
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	4/6/2016 3:26:32 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2745	1	39694.54		
318.3007	1	42577.79		
495.3454	1	308706.03	C30 H48 O4	(M+Na)+
496.3486	1	93921.9	C30 H48 O4	(M+Na)+
511.324	1	109950.32		
553.3508	1	92293.79		
569.3254	1	67725.53		
1025.7062	1	51443.74		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H48 O4	472.3553	495.3445	495.3454	-0.9	-1.9	7.0000

--- End Of Report ---

Figure S11. HR-ESI-MS spectrum of alisol W (**1**).