SUPPLEMENTARY MATERIAL

A new kaurane diterpenoid from *Isodon inflexus*

Guang-Hua Xu^{ab*}, Xing-Fu Cai^a, Xuejun Jin^{ab} and Jung Joon Lee^b

^aKey Laboratory of Natural Resources of Changbai Mountain & Functional Molecules, Ministry of Education, College of Pharmacy, Yanbian University, Yanji 133002, P.R. China; ^bMolecular Medicine Research Center, Yanbian University, Yanji 133002, P.R. China

Abstract:

A new 7,20-epoxy kaurane diterpenoid, 15-acetyldemethylkamebacetal A (**1**) and six known kaurane diterpenoids (**2-7**) were isolated from the aerial parts of *Isodon inflexus* in NF- κ B-dependent reporter gene assay-guided fractionation. Their chemical structures were determined on the basis of extensive spectroscopic analysis (UV, IR, MS, 1D- and 2D-NMR) and comparison with literature data. The isolated compounds were evaluated for their inhibitory effects on TNF- α -induced NF- κ B activation, and all compounds exhibited NF- κ B inhibitory activities with IC₅₀ values ranging from 1.91 to 20.15 μ M.

Keywords: *Isodon inflexus*; kaurane diterpenoid; structure elucidation; NF- κ B

*Corresponding author. Email: ghxu@ybu.edu.cn

List of Supplementary Material

Table S1. ^1H - and ^{13}C -NMR data (400 MHz, CD_3OD) for compounds **1** and **2**

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Figure S3. ^1H -NMR spectrum of compound **1**

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Table S1. ¹H- and ¹³C-NMR data (400 MHz, CD₃OD) for compounds **1** and **2**^a

Position	1		2	
	δ_{H} (<i>J</i> in Hz)	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{C}
1 β	3.56 dd (11.2, 5.5)	77.7 d	3.53 dd (11.2, 5.6)	77.2 d
2 α	1.72 ^b	31.2 t	1.74 ^b	31.1 t
2 β	1.69 ^b		1.55 ^b	
3 α	1.55 m	40.0 t	1.51 ^b	39.9 t
3 β	1.35 ^b		1.29 ^b	
4		34.8 s		34.9 s
5 β	1.37 ^b	49.8 d	1.34 ^b	49.7 d
6 α	1.67 ^b	27.8 t	1.71 ^b	26.4 t
6 β	1.48 ^b		2.90 m	
7 β	4.13 m	69.8 d	4.15 m	67.6 d
8		53.4 s		59.6 s
9 β	2.13 m	47.3 d	1.63 m	52.9 d
10		43.6 s		44.2 s
11 α	2.29 m	22.3 t	2.54 m	24.3 t
11 β	1.76 ^b		1.88 m	
12 α	2.35 m	34.4 t	2.45 m	31.1 t
12 β	1.42 ^b		1.46 ^b	
13 α	2.56 d (9.5)	46.4 d	2.96 d (9.2)	44.3 d
14 α	4.62 s	73.5 d	4.94 s	71.6 d
15 α	5.59 br s	76.9 d		207.6 s
16		158.9 s		154.5 s
17	5.09 br s	110.6 t	5.91 br s	116.9 t
	4.93 br s		5.36 br s	
18	0.83 s	32.8 q	0.88 s	32.6 q
19	0.97 s	21.1 q	1.00 s	21.1 q
20	5.77 br s	95.6 d	5.80 br s	95.2 d
OAc		172.6 s		
OAc	2.10 s	21.5 q		

^aThe assignments were based on the DEPT, HSQC, and HMBC experiments. ^bThe multiplicity patterns were unclear due to signal overlapping.

Figure S3. ^1H -NMR spectrum of compound **1**

Figure S4. ^{13}C -NMR spectrum of compound **1**

Figure S5. DEPT spectrum of compound 1

Figure S6. HSQC spectrum of compound 1

Figure S7. HMBC spectrum of compound **1**

Figure S8. NOESY spectrum of compound **1**

Figure S9. ESI-MS spectrum of compound **1**

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\20141020\118-5_P1-A-1_01_14491.d
Method lc-ms-hr-low.m
Sample Name 118-5
Comment

Acquisition Date 10/20/2014 9:33:35 AM

Operator Zhonglin wei
Instrument / Ser# micrOTOF-Q II 10351

Acquisition Parameter

Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 3000 m/z

Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 150.0 Vpp

Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
375.2173	1	C 18 H 27 N 6 O 3	16.84	375.2139	-3.4	-9.1	8.5	8.5	even	ok
	2	C 12 H 27 N 10 O 4	8.42	375.2211	3.8	10.2	20.8	4.5	even	ok
	3	C 22 H 31 O 5	100.00	375.2166	-0.7	-1.9	23.7	7.5	even	ok
	4	C 23 H 27 N 4 O	78.83	375.2179	0.6	1.7	35.6	12.5	even	ok

Figure S10. HR-ESI-MS spectrum of compound **1**