

SUPPLEMENTARY MATERIAL

One new sterpurane sesquiterpene from cultures of the basidiomycete *Pholiota nameko*

Wan-Rong Niu^{a#}, Cong-Liang Guo^{c#}, Deng-Ji Lou^b, Rui-Ting Li^a, Qiao Xiang^a, Yu-Lin Zou^a,
Xiu-Ming Cui^a & Xiao-Yan Yang^{a*}

^a*Faculty of life science and technology, Kunming university of science and technology, Kunming
650201, P.R.China;*

^b*College of Resources and Enviroment, Yuxi Normal University, Xuyi 653100, P.R.China*

^c*Yunnan Institute of Materia Medica, Kunming 650111, P.R.China;*

One new sterpurane sesquiterpene (**1**), named (3R,6S,7S,8R,10S)-3,7,14-trihydroxy-1-sterpurene was isolated from cultures of the basidiomycete *Pholiota nameko*. The structure of new compound was elucidated by extensive spectroscopic. Additionally, a single crystal X-ray diffraction not only confirmed the structure, but also determined the absolute configuration of the new compound. The compound was evaluated for cytotoxicity against five human cancer cell lines, but no significant cytotoxicity were found (IC₅₀ values > 40 μM).

Keywords: basidiomycete, *Pholiota nameko*, sesquiterpene, X-ray, cytotoxicity

*Corresponding author at. E-mail address: yangxiaoyan9999@163.com.

Wan-Rong Niu, Cong-Liang Guo contributed equally to this article.

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Table S1 ^1H NMR (600 MHz) and ^{13}C NMR (150 MHz) spectroscopic data of **1** in CD_3OD (δ in ppm; J in Hz).

No.	δ_{C} , Type	δ_{H} , (J in Hz)
1	136.9, C	
2	128.8, C	
3	77.2, C	
4	33.4, CH_2	2.15, dd (20.6, 10.2)
	20.8, CH_2	1.92, td (10.0, 2.0)
5		1.63, m
6	49.8, C	1.25, m
7	76.7, CH	3.02, br d (9.0)
8	45.4, CH	2.62, m
9	42.8, CH_2	1.84, dd (11.8, 7.0)
10	43.2, C	1.29, m
	40.9, CH_2	2.32, br d (17.0)
11		2.02, br d (17.0)
12	13.1, CH_3	1.62, s
13	19.8, CH_3	1.30, s
14	71.9, CH_2	3.32, m
15	25.0, CH_3	1.11, s

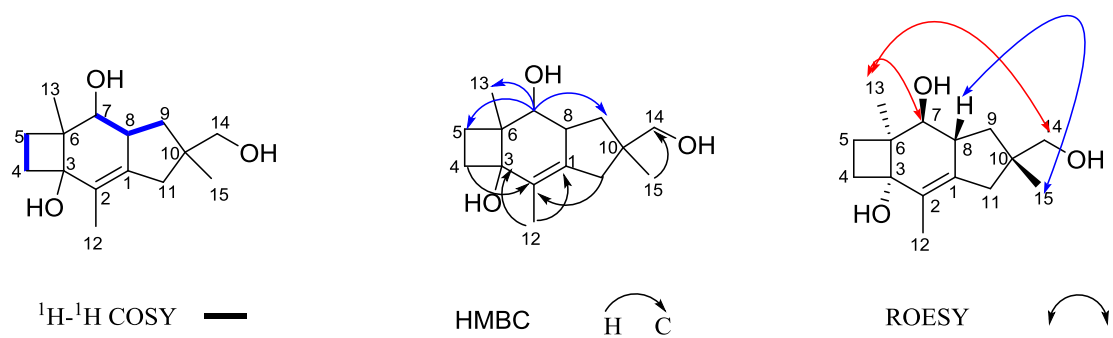


Figure S1. Key 2D NMR correlations of **1**.

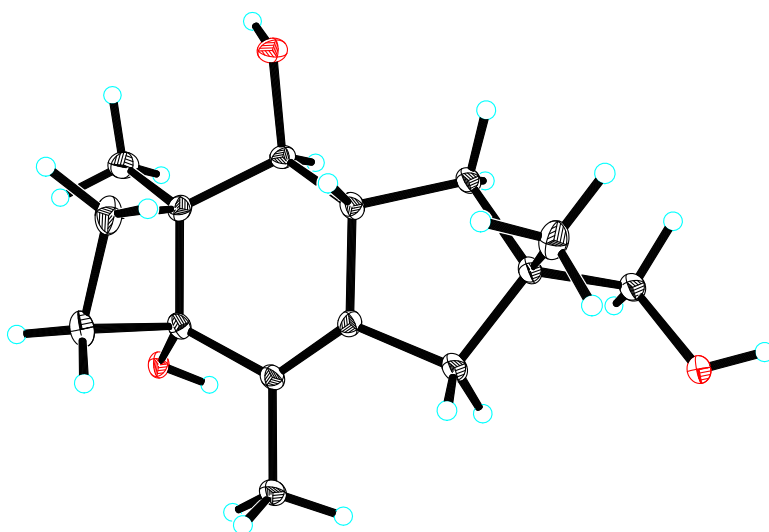


Figure S2. X-ray crystal structure of **1**.

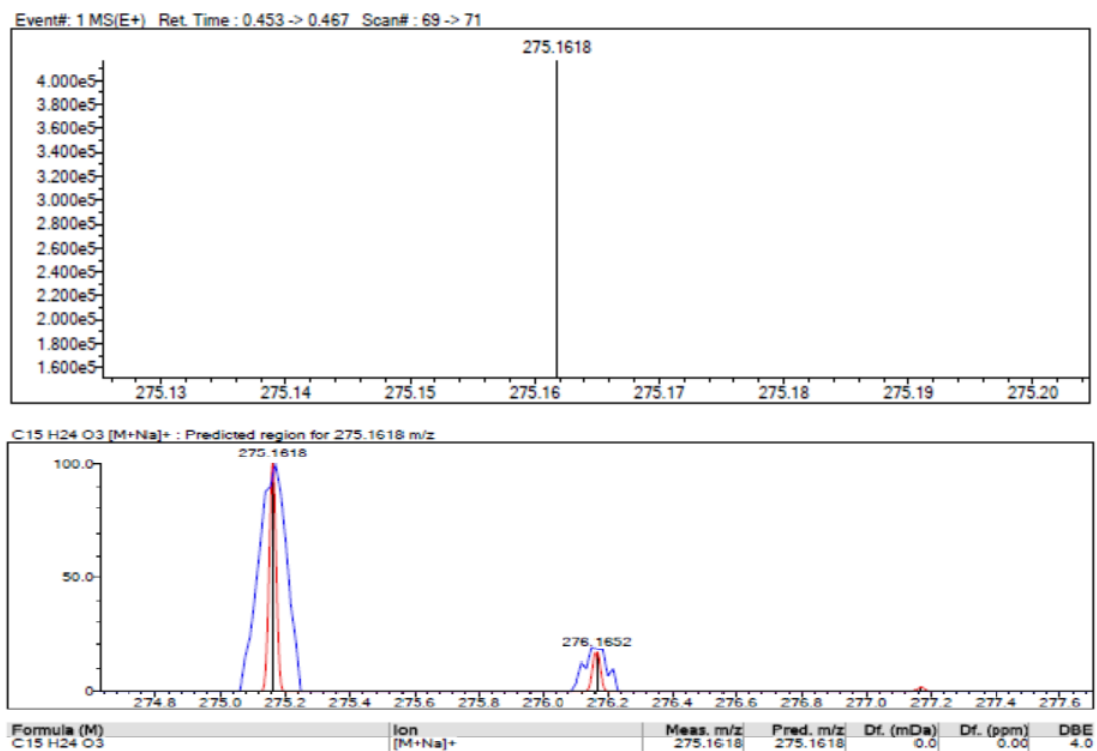
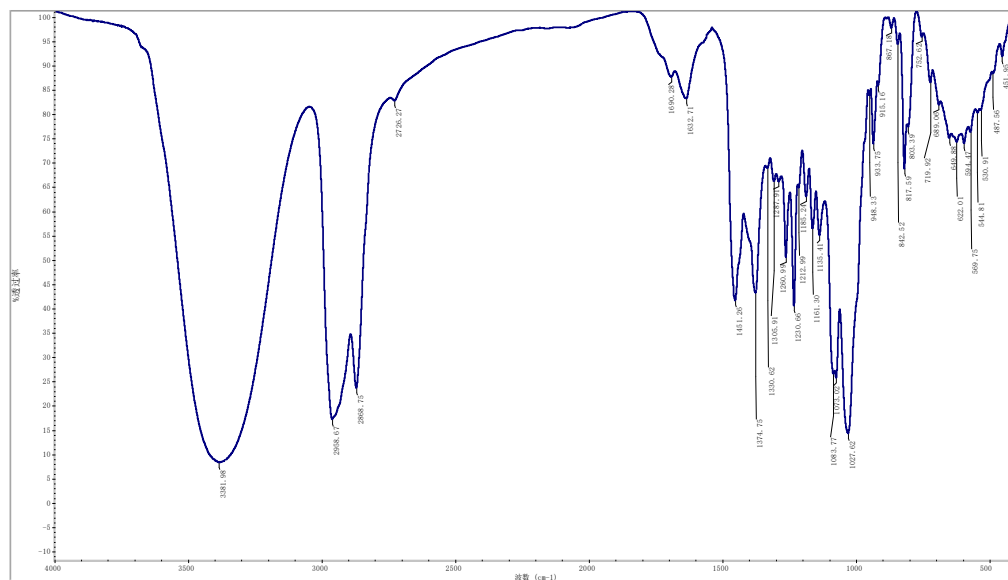


Figure S3. HR-ESI-MS spectrum of compound **1**



Sample Name: Lpn19
 KBr压片
 采集时间: 星期四 11月 15 16:55:53 2018 (GMT+08:00)
 仪器型号: NICOLET iS10
 Software version: OMNIC 9.8.372

样品扫描次数: 16
 背景扫描次数: 16
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.4747
 光阑: 80.00

Figure S4. IR spectrum of compound **1**

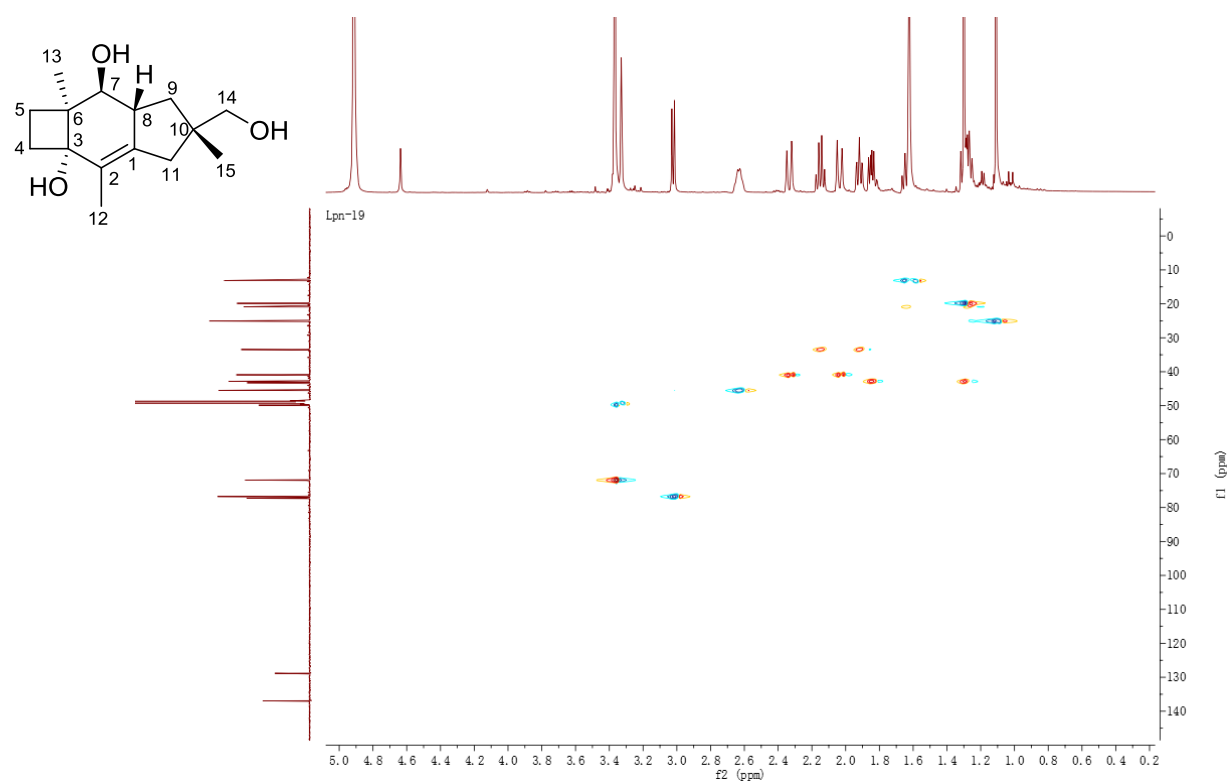


Figure S7. HSQC spectrum of **1**

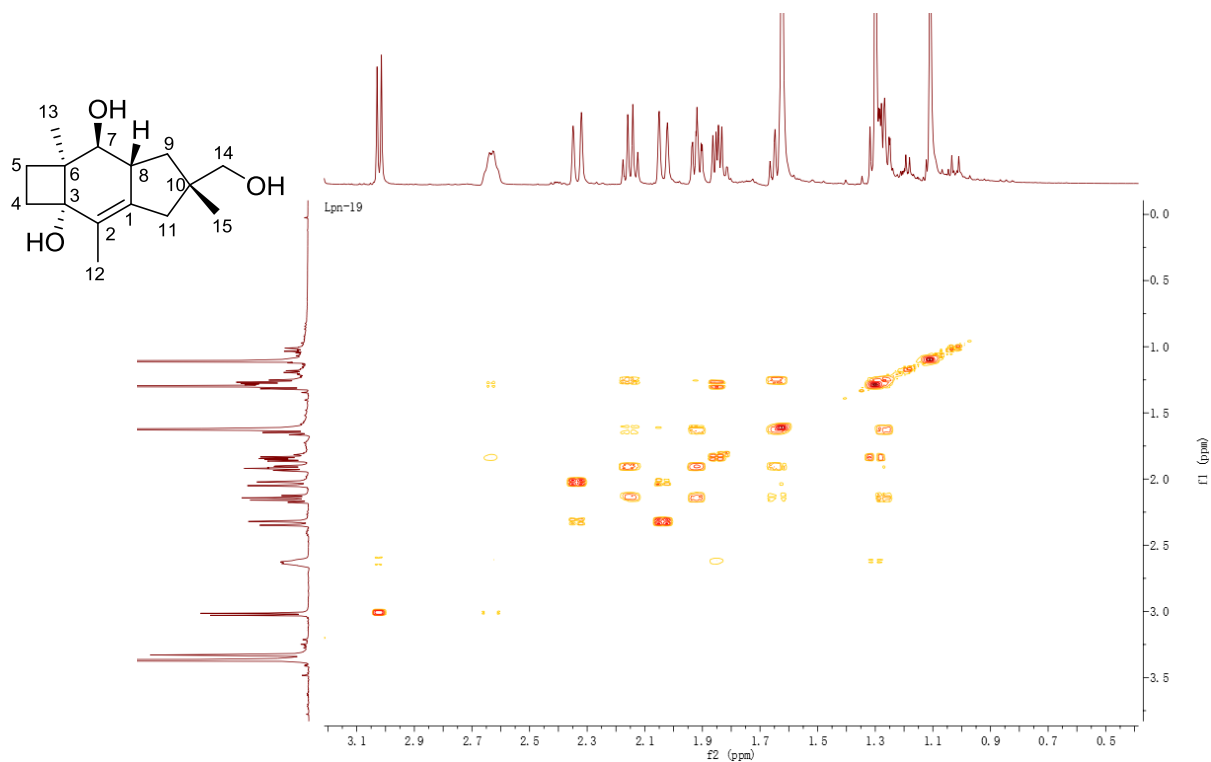


Figure S8. ^1H - ^1H COSY spectrum of **1**

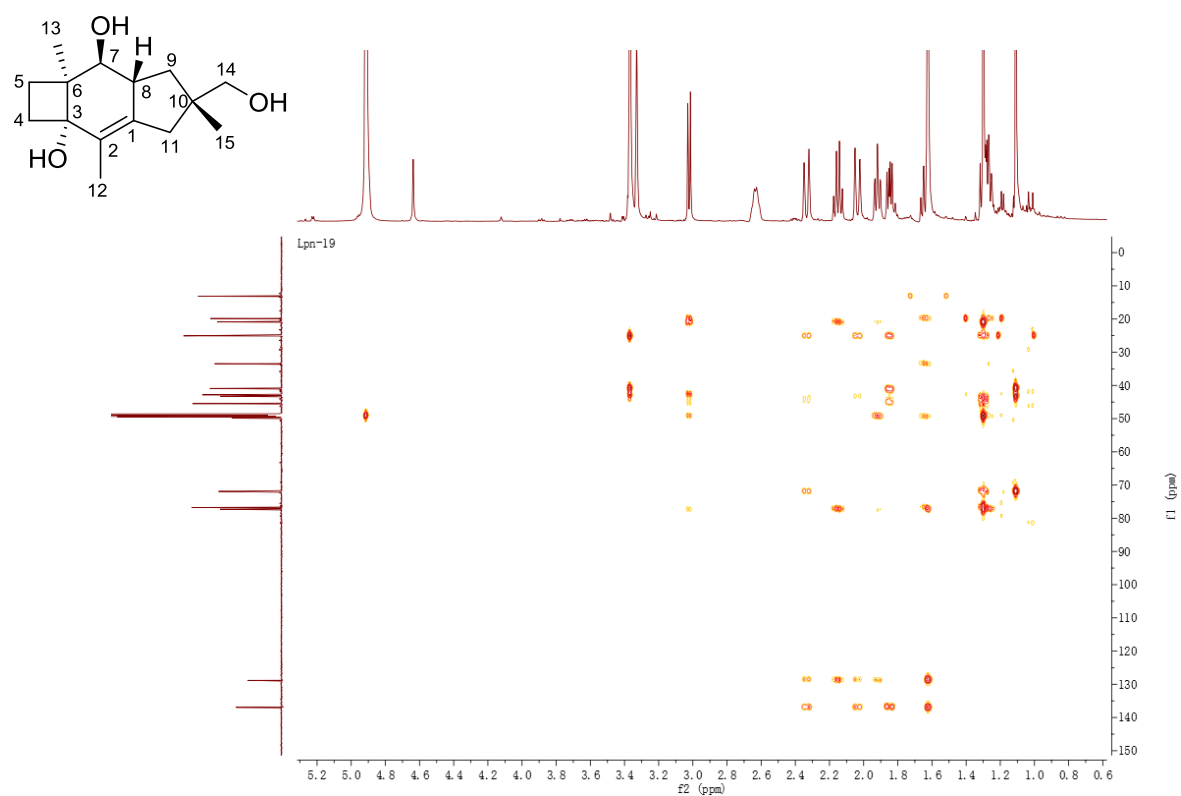


Figure S9. HMBC spectrum of **1**

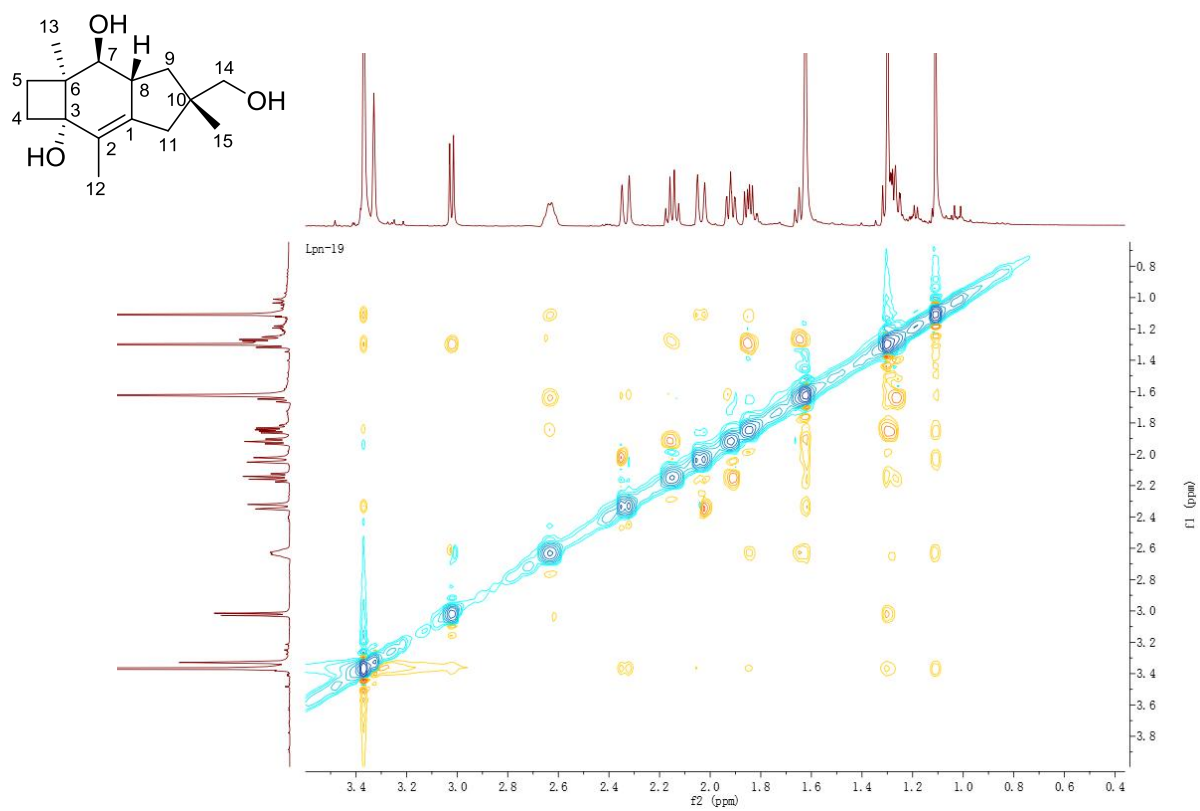


Figure S10. ROESY spectrum of **1**

Table S2. Cytotoxicity of compounds **1** against five human cancer cell lines.

Compounds	IC ₅₀ (μM) for five human cancer cell lines				
	SK-BR-3	SMMC-7721	HL-60	PANC-1	A-549
cisplatin	18.30 ± 0.22	12.71 ± 0.19	1.70 ± 0.08	14.02 ± 0.31	13.36 ± 0.27
1	>40	>40	>40	>40	>40