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SHORT REPORT

Vilmorinine G, a new quassinoid from *Ailanthus altissima*

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Abstract: A new quassinoid, named vilmorinine G (**1**), along with two known congeners (**2** and **3**), has been isolated from the root bark of *Ailanthus altissima* (Mill.) Swingle. The structure of **1** was elucidated through spectroscopic evidence in NMR, HR-ESI-MS, and ECD. The absolute configuration of **1** was further confirmed by X-ray crystallography.

Keywords: Quassinoid, *Ailanthus altissima*, absolute configuration

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1 Plant Source

The root bark of *Ailanthus altissima* utilized in this study was supplied by Sichuan Neautus Pharmaceutical Co., Ltd. This source was chosen to guarantee the accurate identification of the plant material. To further confirm the authenticity of the specimens, they were certified by Guang-Zhi Wang, a botanist with expertise at Chengdu University of TCM. The voucher specimen has been assigned the accession number 20240909/CDCM/SCA and is deposited in the university's herbarium.

2 Previous Studies

The Simaroubaceae family comprises over 170 species and is notably characterized by the presence of quassinoids (Alves et al., 2014). *A. altissima*, a well-known species within this family, has been the subject of research focusing on its phytochemical constituents. Studies have revealed a diverse array of natural substances exhibiting unique structural characteristics, including quassinoids (Tan et al., 2018; Qi et al., 2011; Yang et al., 2014; Tan et al., 2020; Wang et al., 2017), terpenoids (Song et al., 2024), lignans (Tan et al., 2012), coumarins (Hwang et al., 2005), alkaloids (Shao et al., 2023), and various other compounds (Li et al., 2021).

3 Present Study

A total of 50 kg of dried bark from *A. altissima* was powdered and extracted three times using 95% MeOH. After recovering the solvent, 2.75 kg of extract were obtained. The extract was further fractionated using a silica gel column chromatography (CC). It was first eluted with petroleum ether to remove lipophilic components, followed by a gradient of dichloromethane-methanol (from 1:0 to 0:1, v/v), resulting in 16 fractions (Fr.1–Fr.16).

Fr.4 (75.67 g) underwent fractionation through a silica gel CC, utilizing a gradient elution of a petroleum ether and acetone mixture that varied from 15:1 to 1:1 (v/v). This process resulted in the generation of 10 sub-fractions (Fr.4.1–Fr.4.10). The compound Fr.4.8 (8.27 g) was further isolated via Sephadex LH-20 column chromatography, employing a solvent mixture of dichloromethane and methanol at a 1:1 (v/v) ratio, which yielded seven fractions (Fr.4.8.1–Fr.4.8.7). To achieve additional purification of Fr.4.8.4 (842.4 mg), reversed-phase C18 column chromatography was performed, resulting in the production of seven sub-fractions (Fr.4.8.4.1–Fr.4.8.4.7). Crystallization occurred in Fr.4.8.4.7, leading to the isolation of compound **3** (10 mg).

Fraction Fr.5 (248.03 g) underwent separation on a silica gel CC, employing a dichloromethane-methanol gradient (10:0-9:1, v/v), resulting in the production of 10 sub-fractions (Fr.5.1–Fr.5.10). The further purification of Fr.5.4 (57.05 g) was accomplished through reversed-phase C18 CC with a mobile phase comprising methanol and water (60:40, v/v), which yielded 6 sub-fractions (Fr.5.4.1–Fr.5.4.6). The sub-fraction Fr.5.4.1 (2.01 g) was processed via Sephadex LH-20 CC, resulting in 7 fractions (Fr.5.4.1.1–Fr.5.4.1.7). For purification, Fr.5.4.1.3 was treated with silica gel CC, leading to the formation of five sub-fractions (Fr.5.4.1.3.1–Fr.5.4.1.3.5); it is noteworthy that the fractions Fr.5.4.1.3.1 through Fr.5.4.1.3.4 were merged into a single fraction labeled as 3.1. The fraction

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Table 1. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) data for compound **1** in DMSO-d_6

pos	1	
	δ_C, type	δ_H (*J* in Hz)
1	81.9, CH	3.65, overlap
2	70.2, CH	3.76, m
3	126.6, CH	5.36, td (2.8, 1.5)
4	132.7, C	
5	37.9, CH	2.09, m
6	25.0, CH_2	1.89, m
7	75.1, CH	4.62, t (2.9)
8	44.7, C	
9	53.4, CH	3.04, s
10	40.9, C	
11	178.6, C	
12	172.6, C	
13	30.5, CH_2	2.78, m 2.17, m
14	39.8, CH	2.14, overlap
15	35.6, CH	3.10, dd (6.9, 3.7)
16	172.0, C	
18	20.9, CH_3	1.61, s
19	10.1, CH_3	0.84, s
20	70.1, CH_2	4.26, d (7.2) 4.09, d (10.9)
21	13.3, CH_3	1.06, d (6.7)
OCH_3	52.0, CH_3	3.64, s

Fr.5.4.1.3.1 (882.3 mg) was then separated using HPLC, resulting in 12 sub-fractions (Fr.5.4.1.3.1.1–Fr.5.4.1.3.1.12). Crystals obtained from Fr.5.4.1.3.1.2 were collected and thoroughly washed with small quantities of methanol, yielding **1** (2.5 mg).

Fr.8, weighing 73.02 g, underwent dynamic axial compression CC using a methanol-water mixture at a ratio of 40:60 (v/v), resulting in six subfractions identified as Fr.8.1 through Fr.8.6. The subfraction Fr.8.2, with a mass of 3.75 g, was processed through Sephadex LH-20 CC, utilizing a dichloromethane and methanol mixture in equal parts (1:1) for elution. This process produced four subfractions named Fr.8.2.1 to Fr.8.2.4. Crystallization was observed in Fr.8.2.2, yielding 200 mg of **2**.

Compound ***1***: Colorless crystal; $[\alpha]_D^{20}$ = +137.50 (*c* = 0.06, MeOH); UV (MeOH) λ_{max} 200 (3.80); CD (c 0.98 mM, MeOH) λ_{max} ($\Delta\varepsilon$) 205 (2.45), 224 (−0.51) nM; HR-ESI-MS *m/z* 409.1856 $[M+H]^+$ (calcd. For $C_{21}H_{29}O_8^+$, 409.1857); For details on the ^{1}H-NMR and ^{13}C-NMR data, please refer to Table 1.

$C_{21}H_{28}O_8$ (molecular weight = 408.44 g/mol) consists of colorless crystalline structures in a monoclinic arrangement, with lattice parameters a = 11.0242(4) Å, b = 6.9350(2) Å, and c = 12.7985(4) Å. The angles are α = 90.00°, β = 96.3690(10)°, and γ = 90.00°. The volume measures V = 965.40(5) Å^3, and the space group is P1211. The temperature during analysis was T = 293(2) K, with a total of Z = 2. The absorption coefficient μ (Cu Kα) is recorded as 0.899 mm^{-1}, featuring 15,610 measured reflections and 3,547 independent reflections (Rint = 5.66%). The final R indices for significant data (I > 2mσ(I)) are R1 = 0.0432 and wR2 = 0.1259, while the R indices for all observed data are R1 = 0.0466 and wR2 = 0.1333. The Flack parameter is noted as 0.04 (12).

Compound **1** was obtained as a colorless crystal. HR-ESI-MS suggests the molecular formula of **1** is $C_{21}H_{28}O_8$, with 8 degrees of unsaturation. Based on ^{1}H NMR analysis (Table 1), the compound was determined to contain four methyl groups [δ_H: 3.64 (-OCH_3), 1.61 (H-18), 1.06 (H-21), 0.84 (H-19)], three methylene groups [δ_H: 4.26, 4.09 (H-20), 2.78 (H-13), 2.17 (H-13), 1.89 (H-6)], one olefinic proton signal [δ_H: 5.36 (H-3)], and seven methine protons [δ_H: 3.65 (H-1), 3.76 (H-2), 2.09 (H-5), 4.62 (H-7), 3.04 (H-9), 2.14 (H-14), 3.10 (H-15)]. The corresponding carbon atoms for these protons were assigned via the HSQC spectrum. Furthermore, the above spectroscopic data suggest that the compound is likely a quassinoid.

The definitive planar structure of **1** was confirmed by analyzing the 2D NMR data. The ^{1}H-^{1}H COSY spectrum exhibited coupling correlations among H-2 with H-1/H-3, H-6 with H-5/H-7, H-14 with H-13/H-15, and between H-15 and H-21. Additionally, important HMBC correlations were noted from H-18 to C-3/C-4/C-5, H-19 to C-1/C-5/C-9/C-10, and H-20 to C-7/C-8/C-9/C-11/C-14, while both H-7 and H-21 showed connections to C-16, along with -OCH_3 relating to C-12. These findings firmly establish the planar structure, which is completely in agreement with that of vilmorinine B (refer to Figures 1 and 2A) (Takeya et al., 1998).

Compound **1**'s relative configuration was established as 1*S**, 2*S**, 5*S**, 7*R**, 8*S**, 9*R**, 10*S**, 14*S**, and 15*R**. This conclusion relied on notable NOESY correlations (see Figure 2B) observed between H-19 and H-2/H-20/H-6, H-1 and H-5, H-7 and H-20/H-13, as well as between H-13 and H-21.

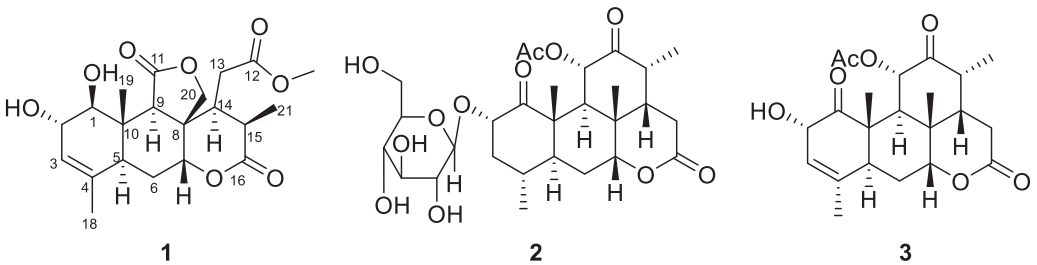

Figure 1. Structures of compounds **1–3**

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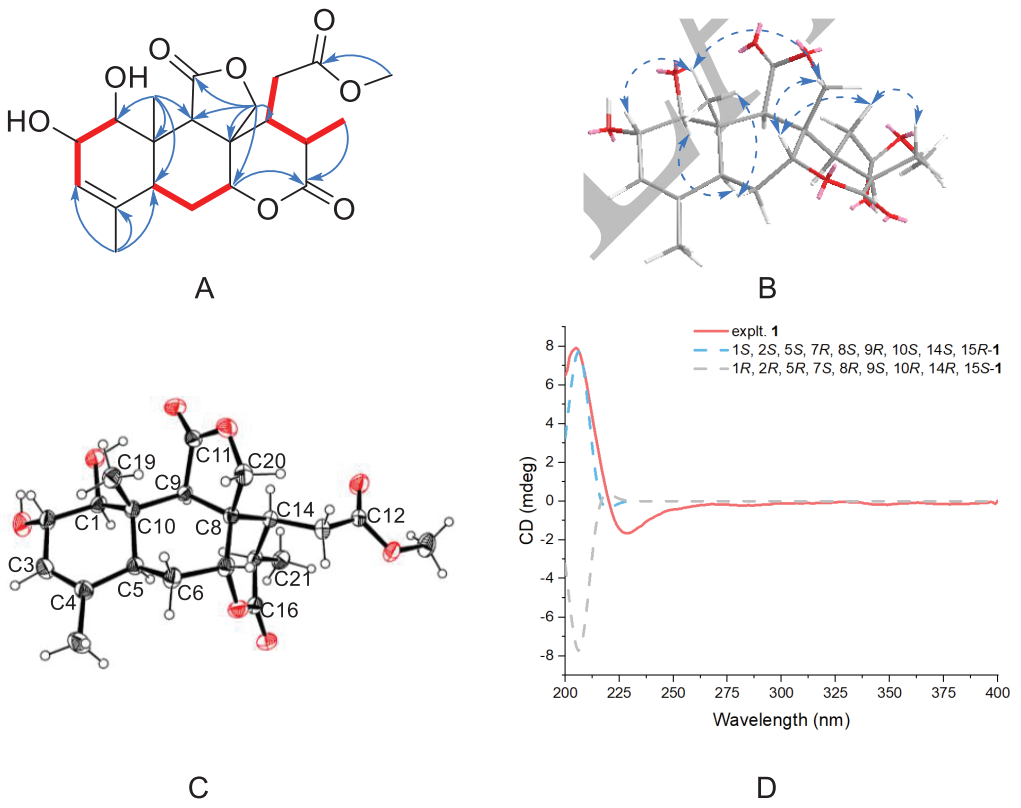

Figure 2. Key ^{1}H-^{1}H COSY (bold lines) and HMBC (arrows) correlations of 1. (B) Key NOESY correlations of 1. (C) ORTEP drawing of 1. (D) The calculated ECD spectra and the experimental spectra of **1** in CH_3OH

Crystals of **1** were successfully obtained through the slow evaporation of a methanol solution. The absolute configuration of **1** was initially established via single-crystal X-ray diffraction analysis (Figure 2C) and subsequently verified to be 1*S*, 2*S*, 5*S*, 7*R*, 8*S*, 9*R*, 10*S*, 14*S*, 15*R* by comparing the experimental ECD spectrum with the calculated ECD curve (Figure 2D). Through a search of the SciFinder database, **1** was characterized as a new quassinoid, and the trivial name was given as vilmorinine G.

Furthermore, compounds **2** and **3** were identified as shinjuglycoside C (Yoshimura et al., 1984) and amarolide 11-acetate (Yoshimura et al., 1984) through a comparative analysis of NMR spectroscopic data from the literature.

Subsequent cytotoxicity assay using a CCK-8 kit indicated compound **1** did not show obviously inhibition against BT549 and CT26 cell lines at the concentration of 60 μM.

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Author Contributions

Lan-Qing Peng: Writing—original draft, Investigation, Data curation, Li Huang: Investigation, Data curation. Li-Lian Zhao: Data curation. Da-Le Guo: Supervision. Zhuo-Hong Li: Validation, Writing—review & editing, Funding acquisition.

Availability of Data and Materials

The authors declare that the data supporting the findings of this study are available within the paper and its Supplementary Information files. Should any raw data files be needed in another format they are available from the corresponding author upon reasonable request. Source data are provided with this paper.

Conflicts of Interest

The authors declare that they do not have any conflict of interest.

Supporting Information

Supporting Information accompanies this paper on http://www.acgpubs.org/journal/records-of-natural-products.

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