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SHORT REPORT

A new benzoin derivative from the medicinal plant *Viscum coloratum*

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Abstract: Chemical investigation of *Viscum coloratum* resulted in the isolation of a new benzoin, named 7-O-demethylamycolabenzoyl (**1**), along with two known isoflavones (**2** and **3**) and two known flavones (**4** and **5**). The structure of **1** was elucidated through extensive NMR and HRESIMS analysis and was further confirmed by ^{13}C NMR calculations. The absolute configuration at the sole chiral center was assigned as *R* by comparison of its experimental ECD spectrum with that of the analogue amycolabenzoyl (**1a**). A plausible biosynthetic pathway for **1** is proposed, suggesting its derivation from the co-isolated isoflavone **2**. Compound **1** showed weak α-glucosidase inhibitory effects.

Keywords: Benzoin derivative, 7-O-demethylamycolabenzoyl, *Viscum coloratum*

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1 Plant Source

The medicinal plant *Viscum coloratum* was collected in July 2022 from Lishui City, Zhejiang Province, China. A sample (202207VISCOL) of the plant material was deposited at Hangzhou Polytechnic University. It was identified according to a voucher specimen (CSH0155894) preserved at Shanghai Chenshan Herbarium (CSH).

2 Previous Studies

Mistletoe, known in Chinese as "Hujisheng", is a medicinal herb derived from the dried stems and leaves of *Viscum coloratum* (Komar.) Nakai (Santalaceae) (Di, Shen, Zhang, Wang, & Guan, 2025). It is also commonly referred to as Northern Mistletoe, Willow Mistletoe, or Mulberry Mistletoe, and is widely distributed across temperate zones of the Northern Hemisphere.

In traditional Chinese medicine, this herb is valued for its ability to dispel wind-dampness, tonify the liver and kidneys, and strengthen the bones and muscles (Di et al., 2025). It has been historically used in the treatment of conditions such as rheumatic arthralgia, lumbar and knee debility, and fetal irritability (Di et al., 2025). Pharmacological studies have further identified a spectrum of bioactive properties in mistletoe, including antitumor (Chen et al., 2022; Hong et al., 2020; Wen et al., 2025; Zhao et al., 2012), antioxidant (Fan et al., 2014; Yao et al., 2006; Yao et al., 2007), antiviral, anti-osteoporosis (Han et al., 2011), and anti-inflammatory (Leu et al., 2006), underscoring its potential in modern therapeutic application.

Previous chemical studies revealed the chemical constituents of this plant were polypeptides (Kong et al., 2004; Liu et al., 2006), flavonoids including chalcone and flavone (Chen et al., 2022; Hwang et al., 2006; Leu et al., 2006; Zhao et al., 2012), flavanone glycosides (Fan et al., 2014; Han et al., 2011; Yao et al., 2006), diarylheptanoids (Chen et al., 2022; Hong et al., 2020; Yao et al., 2007; Zhao et al., 2012), lignans (Chen et al., 2022), terpenoids (Chen et al., 2022), and fatty acids (Chen et al., 2022). It is noteworthy that the curcuminoid analogue (1*E*,4*E*)-1,7-bis(4-hydroxyphenyl)hepta-1,4-dien-3-one demonstrated potent broad-spectrum antitumor activity in vitro, with IC_{50} values below 10 μM against twelve cancer cell lines. It exhibited exceptional potency against the SKBR3 human breast cancer cell line, with an IC_{50} of 1.7 μM. In a mouse model, it significantly outperformed cisplatin in reducing tumor weight and inhibiting tumor growth.

In our research, a chemical study of the medicinal plant revealed the isolation of a new isoflavone derivative (**1**), and four known compounds including two isoflavones (**2** and **3**), and two flavones (**4** and **5**) (Figure 1). This study presents the isolation, structural elucidation, proposed biosynthetic pathway, and bioactivity assessment.

3 Present Study

The air-dried leaves and stems (500 g) of the medicinal plant *Viscum coloratum* were powdered and extracted with MeOH (3 × 2 L). The solvent was removed under reduced pressure to give the residue (35 g), which was suspended in water and extracted with EtOAc to yield an EtOAc fraction (12 g). The EtOAc fraction (12 g) was subjected to silica gel column chromatography and eluted with a stepwise gradient of petroleum ether-EtOAc (100:0 to 0:100, v/v), fractions (200 mL each)

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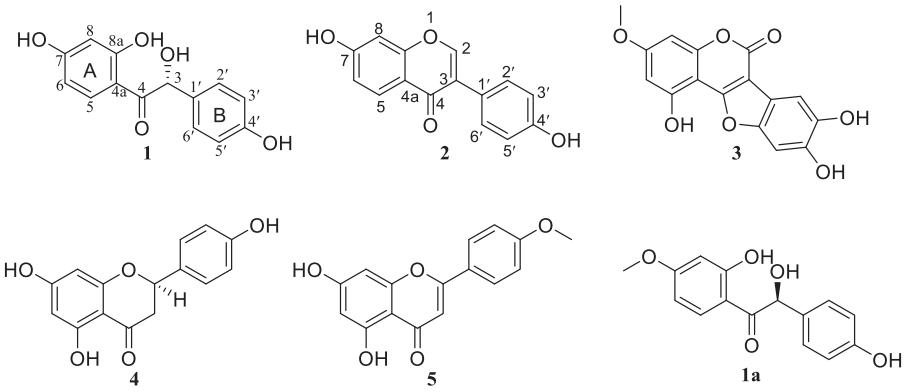

Figure 1. Structures **1**–**5** from the leaves and stems of *Viscum coloratum*

were collected and combined based on TLC analysis to give 10 main fractions (A-1 to A-10). Fraction A-3 (180 mg) was further purified by silica gel column chromatography, eluted with a petroleum ether-EtOAc gradient, to afford compound **2** (3.0 mg). Fraction A-4 (328 mg) was chromatographed on a silica gel column eluted with a gradient of *n*-hexane-EtOAc (7:3 to 1:2, v/v) to yield compound **4** (11 mg) as a yellow solid. Fraction A-5 was subjected to silica gel column chromatography and eluted with a petroleum ether-acetone gradient (2:1 to 1:1, v/v). Subsequent crystallization of the crude product from CH_2Cl_2 afforded compound **3** (150 mg). Fraction A-7 was purified on a silica gel column eluted with a CH_2Cl_2-MeOH gradient (30:1 to 5:1, v/v) to afford compound **5** (2 mg). Fraction A-8 (1.0 g) was chromatographed on a silica gel column eluted with CH_2Cl_2-MeOH gradient (15:1 to 5:1, v/v) to afford compound **1** (1.4 mg).

7-O-Demethylamycolabenzoyl (**1**): Yellow oil; $[\alpha]^{20}_D$ +51 (*c* 0.2, MeOH); UV (MeOH) λ_{max} 320, 280 nm; ^{1}H and ^{13}C NMR data, see Table 1; HRESIMS *m/z* 259.0612 $[M - H]^-$ (calcd. for $C_{14}H_{11}O_5^-$ 259.0611).

Compound **1** was obtained as a yellow oil and assigned the molecular formula $C_{14}H_{12}O_5$ by HRESIMS analysis, corresponding to 9 degrees of unsaturation. The ^{1}H NMR spectrum revealed two distinct sets of aromatic proton signals. One set, consisting of a pair of doublets at δ_H 7.25 (2H, d, *J* = 7.5 Hz) and 6.75 (2H, d, *J* = 7.5 Hz), was characteristic of a para-disubstituted benzene ring (Ring B) (Ji et al., 2025; Lee et al., 2025). The other set displayed signals at δ_H 7.68 (1H, d, *J* = 8.7 Hz), 6.25 (1H, dd, *J* = 8.7, 2.5 Hz), and 6.24 (1H, d, *J* = 2.5 Hz), which is consistent with an ABX spin system indicative of a 1,2,4-trisubstituted benzene ring (Ring A) (Ding et al., 2025; Ji et al., 2025; Li et al., 2023). A key singlet at δ_H 5.93 (1H, s) was assigned to an oxymethine proton. The ^{13}C NMR and HSQC spectra revealed 14 carbon resonances (Table 1): one ketone carbonyl carbon (δ_C 203.4), twelve aromatic carbons (δ_C 103.7, 109.2, 111.8, 116.6, 116.6, 130.1, 130.1, 132.0, 134.0, 158.8, 166.6, 166.9) for two benzene rings, the oxygenated methine carbon (δ_C 75.7). Among the quaternary carbons (δ_C 111.8, 134.0, 158.8, 166.6, 166.9), three were identified as oxygenated aromatic carbons (δ_C 166.9, 166.6, 158.8). The two benzene rings and the one ketone carbonyl group account for all nine degrees of unsaturation, indicating the presence of no additional ring in the structure.

Table 1. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) Data of **1** methanol-d_4 and its analogue (**1a**: 7-methyl derivative) in DMSO-d_6 (*J* in Hz, δ in ppm). [a]

No.	1			1a
	δ_H	δ_C	Cal δ_C	δ_C
3	5.93, s	75.7	74.506	74.9
4		203.4	201.619	203.8
4a		111.8	111.678	112.0
5	7.68, d (8.7)	134.0	135.843	133.3
6	6.25, dd (8.7, 2.5)	109.2	107.493	107.7
7		166.9	165.329	165.9
8	6.24, d (2.5)	103.8	103.411	101.4
8a		166.6	168.169	165.0
1′		132.0	134.715	130.7
2′	7.25, d (7.5)	130.1	132.289	129.0
3′	6.75, d (7.5)	116.6	114.898	115.7
4′		158.8	158.371	157.5
5′		116.6	116.941	115.7
6′		130.1	130.383	129.0

The 1,2,4-trisubstituted pattern of the benzene ring was established by the ^{1}H–^{1}H COSY (Figure 2) correlation between H-8 (δ_H 6.25) and H-8a (δ_H 7.68), coupled with key HMBC correlations (Figure 2) from H-8a to C-7 (δ_C 166.9), and from both H-6 (δ_H 6.24) and H-8 to C-4a (δ_C 111.8). These data confirmed the presence of a 2,4-dihydroxybenzene moiety (ring A). The methine proton H-3 (δ_H 5.93) and H-8a showed HMBC correlations to the ketone carbonyl carbon δ_C 203.4 and to an aromatic carbon C-1′ (δ_C 132.0) of Ring A. This established the fragment -C(O)-CH(OH)- (Xiao et al., 2025) and its connection to Ring A at the quaternary carbon C-4a (111.8). The para-disubstituted benzene ring was confirmed by the ^{1}H-^{1}H COSY correlations between the two doublets (δ_H 7.25 and 6.75) each integrated for two protons, and by the strong three bond correlations from H-2′/H-6′ to C-4′ and from H-3′/H-5′ to C-1′, indicating a 4-hydroxybenzene ring. The

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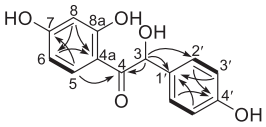

Figure 2. Key ^{1}H-^{1}H COSY and HMBC correlations of **1**

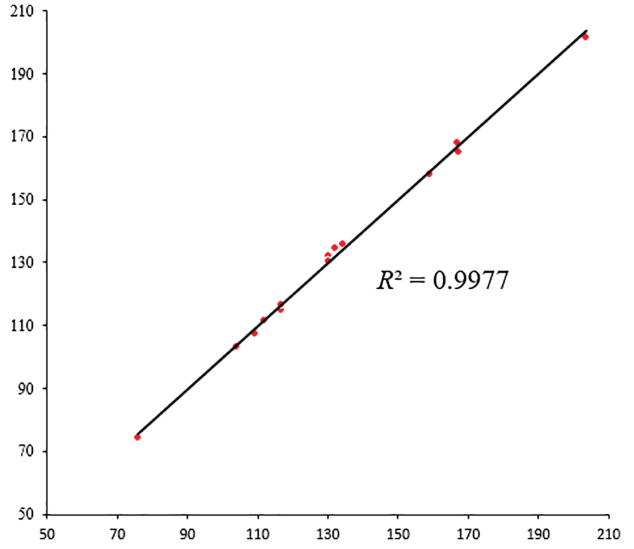

Figure 3. Experimental (X) and calculated (Y) ^{13}C NMR chemical shifts of **1**

HMBC correlations from the oxymethine proton (δ_H 5.93) to C-1′ (δ_C 132.0) and C-2′ (δ_C 130.1) suggested that the 4-hydroxybenzene moiety was connected to C-3 at C-1′ (δ_C 132.0). Thus, the gross structure of compound **1** was determined to be a benzoin derivative (Zhang et al., 2025) with the structure 1-(2,4-dihydroxyphenyl)-2-hydroxy-2-(4-hydroxyphenyl)ethan-1-one.

The observed downfield chemical shifts of C-7 and C-5 were likely attributable to the influence of the carbonyl group at C-4. To confirm the structure of **1**, its ^{13}C NMR chemical shifts were computed at the mPW1PW91/6-311+G(d,p) level of theory. A linear regression analysis between the experimental and calculated chemical shifts afforded a correlation coefficient R^2 = 0.9977 (Figure 3), providing support for the proposed structure. Compound **1** was the 7-demethyl of the dibenzoyl derivative amycolabenzoyl (**1a**), which was isolated from the lichen-associated *Amycolatopsis hippodrome* (Jin et al., 2020). Accordingly, it was named 7-O-demethylamycolabenzoyl.

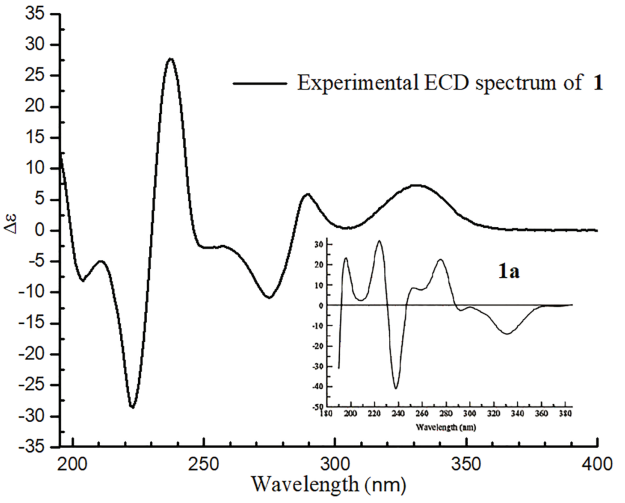

Figure 4. Comparison of the experimental ECD spectra of **1** and **1a**

As for the absolute configuration of the only chiral carbon of C-3, it was determined to be *R* based on the nearly opposite ECD spectrum compared to that of amycolabenzoyl (**1a**) (Figure 4).

The other compounds were identified as daidzein (**2**) (Jalali et al., 2024), wedelolactone (**3**) (Kumar et al., 2018), naringenin (**4**) (Luo et al., 2025), and acacetin (**5**)(Karagecili et al., 2024).

A plausible biosynthetic pathway for compound **1** is proposed as follows (Figure 5): The isoflavone precursor daidzein undergoes reduction of the C-2 and C-3 double bond to form intermediate **a**. Subsequent hydrolysis (ring-opening) of the pyran ring in **a** affords **b**. Oxidation of the hydroxymethyl group in **b** then yields the carboxylic acid **c**. A key transformation involves the conversion of the carboxylic acid at the 3-position in **c** into a methylene group (-CH_2-), likely via a decarboxylation (or decarbonylation) process, to give **d**. The methylene group in **d** is then oxidized to a ketone, producing **e**. Finally, reduction of the ketone in **e** gives the secondary alcohol moiety observed in compound **1**.

The α-glucosidase inhibitory effects of the five compounds were assessed at a concentration of 200 μM following procedures in the literature (Chang et al., 2024; Guo et al., 2024). The evaluation revealed that compound **1** was the sole compound with discernible activity, demonstrating 37% inhibition. In contrast, the inhibitory rates of the other four compounds were all below 20%.

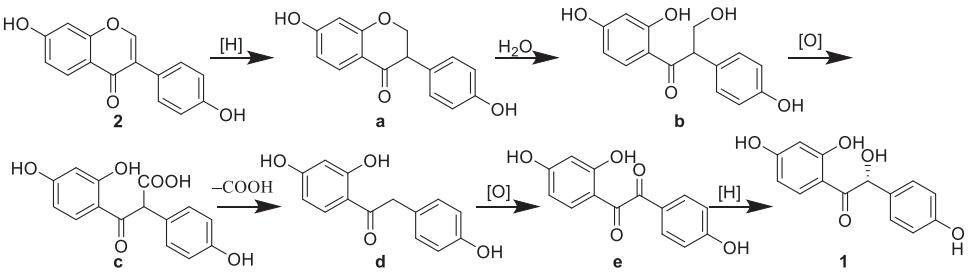

Figure 5. Biogenetic relationships of compounds **1** and **2**

Author Contributions

Ruimin Li: Writing–original draft, Investigation, Data curation. Weiqiang Fei: Investigation, Writing–review & editing, Supervision, Project administration.

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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