

Seven new phenolic compounds from *Lavandula angustifolia*

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ABSTRACT

Seven new phenolic compounds: lavandunat (1), lavandufurandiol (2), lavandufluoren (3), lavandupyrones A (4) and B (5), and lavandudiphenyls A (6) and B (7), along with five known compounds, 4-(1-hydroxy-1-methylethyl) benzoic acid (8), methyl 3-(3,4-dihydroxyphenyl)propanoate (9), 3,4,α-trihydroxyl-ethyl phenylpropionate (10), rosmarinic acid (11), and isosalvianolic acid C (12), were isolated from the ethyl acetate extract of the remaining material, which was obtained from *Lavandula angustifolia* Mill., after the distillation of the essential oil. Their structures were elucidated based on extensive spectroscopic analysis including optical rotation, UV, MS, 1D and 2D NMR spectra. The antioxidant activities of all of the compounds were examined by the 1-1-diphenyl-2-picrylhydrazyl (DPPH) free radical scavenging test. Compared to vitamin C, new compounds 1–3 and 5–7 had stronger activities, which could possibly act as primary antioxidants, and the activity of compound 12 was superior to those of all of the other compounds.

1. Introduction

Lavandula angustifolia Mill. (lavender), of the family Labiatae, was native to the Mediterranean region. In 1965, lavender was introduced from France to the Yili region of Xinjiang (north-western China) for the first time, and since then, it has been intensively cultivated for oil production (Yang and Gao, 2010). Today, Yili, together with the Valensole Plateau and Furano in Hokkaido, have been called “the world's three largest bases of lavender”.

The first record of the use of lavender to treat diseases was in the “Canon of Medicine” of Avicenna (Rastogi et al., 2012), and it has been widely used as a traditional Uighur medicine (TUM) with sedative-hypnotic, spasmolysis, antibacterial, neuroprotective, lipid-decreasing, etc. properties (Chinese Pharmacopoeia Commission, 1999). The majority of experiments in the literature on lavender were conducted with the essential oil, which contains many more than 100 individual components, such as linalool, linalyl acetate, cineole, β-ocimene, p-lavender acetate, lavender alcohol, terpene-4-alcohol and camphor, which confer both aromatic and biological activities (Shi, 2012; Danh et al., 2012). As mentioned in articles, many Lamiaceae plants were rich in phenolic constituents and demonstrated good antioxidant activity (Shan et al., 2005), and a portion of the phenolic compounds in lavender have been

separated (Wu et al., 2007a,b), synthesized (Nitzsche et al., 2004), and identified by GC/MS (Castro-Vázquez et al., 2014).

However, our research has been performed to determine the non-volatile compounds in the remaining material after the essential oils of the plant have been distilled, and only a few phytochemical studies on these compounds which have been found. According to previous research, protocatechuic acid, caffeic acid, chlorogenic acid, rosmarinic acid, apigenin and their derivatives were identified by LC/MS/MS from lavandin waste (Torras-Claveria et al., 2007). In our continuing study for new active constituents, seven new compounds, lavandunat (1), lavandufurandiol (2), lavandufluoren (3), lavandupyrones A (4) and B (5), and lavandudiphenyls A (6) and B (7) (Fig. 1), along with 5 known compounds, 4-(1-hydroxy-1-methylethyl)benzoic acid (8) (Zhang et al., 2015), methyl 3-(3,4-dihydroxyphenyl)propanoate (9) (Wang et al., 2016), 3,4,α-trihydroxyl-ethyl phenylpropionate (10) (Wang et al., 2000), rosmarinic acid (11) (Ly et al., 2006), and isosalvianolic acid C (12) (Qian and Li, 1992), were isolated from the ethyl acetate extract of the remaining material as mentioned, and compounds 8–10 and 12 were first reported in the lavender plant.

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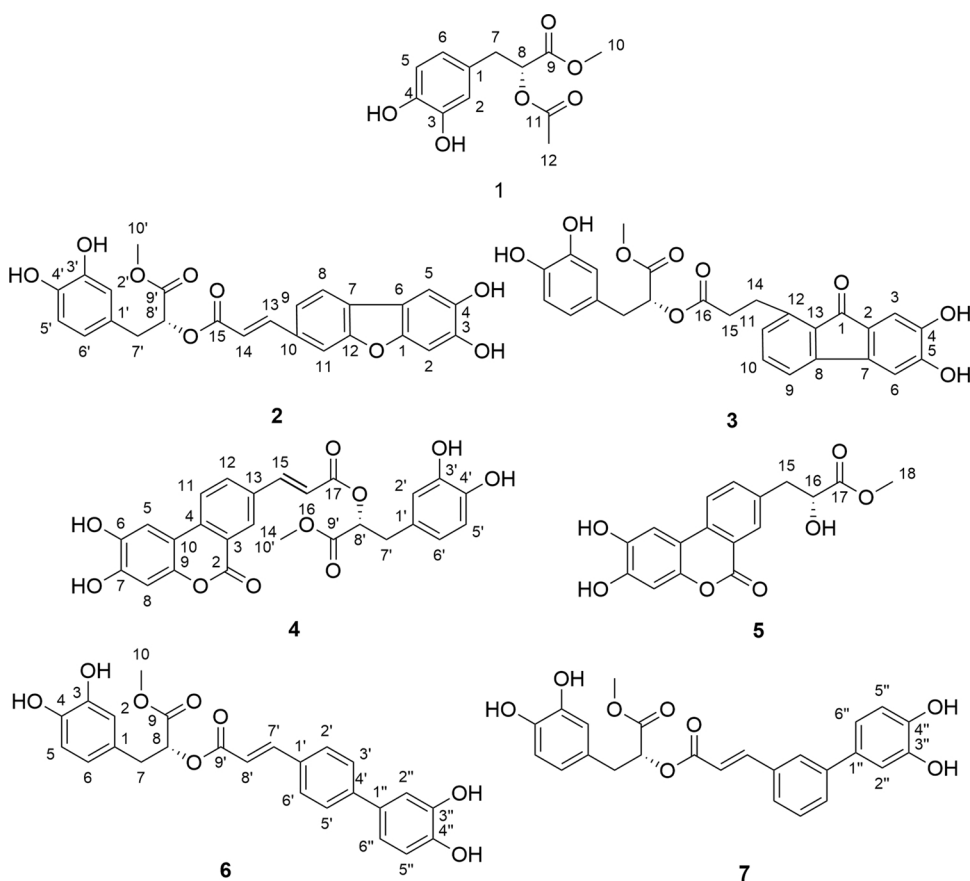


Fig. 1. Chemical structures of new compounds 1–7.

2. Results and discussion

The ethanol extract from the waste of *L. angustifolia* was fractionated with petroleum ether, dichloromethane, ethyl acetate, and *n*-butanol from water, and the ethyl acetate extract was purified by repeated chromatography (silica gel, Sephadex LH-20 and ODS columns with semi-preparative HPLC), to afford 12 phenolic compounds. The identities of the known compounds were confirmed by comparison of mass spectra as well as 1D and 2D NMR spectral data with those reported in the literature.

Compound **1** was obtained as a yellowish amorphous powder with a negative optical rotation of $[\alpha]_D^{25} = -1.0^\circ$ (c 0.1; MeOH). The UV (MeOH) maximum absorption λ (log ϵ) was 280 (3.33) nm. It showed a pseudomolecular molecular ion peak $[M-H]^-$ at m/z 253.0743 (calcd. 253.0790) in the negative mode from its high resolution electrospray ionization mass spectrum (HR-ESI-MS), corresponding to the molecular formula of $C_{12}H_{13}O_6$. The 1H NMR spectrum of **1** (Table 1) had signals from aromatic protons, which were in the ortho- and meta-position, at δ_H 6.62 (1H, d, $J = 8.0$ Hz), 6.59 (1H, d, $J = 2.0$ Hz) and 6.44 (1H, dd, $J = 8.0, 2.0$ Hz), and one signal at δ_H 5.03 (1H, dd, $J = 7.7, 5.2$ Hz) representing the gem acetyl proton, while the signal at δ_H 3.62 (1H, s) was due to the methoxyl group. There were also two signals at δ_H 2.86 (1H, dd, $J = 14.3, 7.7$ Hz), and δ_H 2.91 (1H, dd, $J = 14.3, 5.2$ Hz) appearing from the methylene group, which was characterized as being geminal to the double bond. These facts were confirmed by data of the ^{13}C NMR spectrum of compound **1** (Table 1), which included 12 carbon signals including six signals from aromatic carbons, two carbon signals from the acetyl group, one carbon signal from the methoxyl group, one carbon signal from the carbonyl group, and two carbon signals from the ethylene group. Thus, the structure of **1** had one dihydroxybenzene, one acetyl, one methoxy, one carbonyl and one “ $-CH_2-CH-$ ” group. In addition, based on the correlation peaks observed in the COSY spectrum (Fig. 1) between H-5 (δ_H 6.62)/H-6 (δ_H 6.44), and H-7 (δ_H 2.86, δ_H

Table 1

NMR data for compound **1** (DMSO, δ in ppm, J in Hz, 600 MHz for 1H NMR and 150 MHz for ^{13}C NMR).

No.	δ_C	δ_H
1	126.4	
2	116.5	6.59, d (2.0)
3	145.0	
4	144.1	
5	115.4	6.62, d (8.0)
6	119.9	6.44, dd (8.0, 2.0)
7	36.0	2.86, dd (14.3, 7.7)
		2.91, dd (14.3, 5.2)
8	72.9	
9	169.7	5.03, dd (7.7, 5.2)
10	52.0	3.62, s
11	169.8	
12	20.3	2.03, s
OH		8.78, br. s

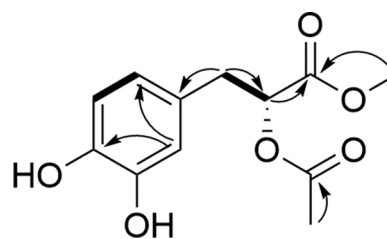


Fig. 2. Structure as well as key COSY (—) and HMBC (H → C) correlations of compound **1**.

2.91)/H-8 (δ_H 5.03) as well as the HMBC correlations (Fig. 2) between H-2 (δ_H 6.59)/C-4 (δ_C 144.1) and C-6 (δ_C 119.9); H-7 (δ_H 2.86)/C-1 (δ_C 126.4), and C-8 (δ_C 72.88); H-8 (δ_H 5.03) and H-10 (δ_H 3.62)/C-9 (δ_C

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