Hydroxyshengmanol-type triterpenoids from the aerial parts of *Cimicifuga simplex* Wormsk

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**ABSTRACT**

New hydroxyshengmanol-type triterpenoids (1–8) were identified from the aerial parts of *cimicifuga simplex* Wormsk by comprehensive 1D and 2D NMR, MS, and single-crystal X-ray diffraction analyses. The absolute configuration of the himeketal carbon (C-16) in hydroxyshengmanol-type constituents from *cimicifuga* spp. was initially determined as R using X-ray diffraction. All compounds were evaluated for their cytotoxicity in a panel of cancer cell lines and acetylcholinesterase inhibitory activity.

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these compounds with 1 showed that they were similar with each other, except for the major differences ascribed to the sugar moiety, the double-bond of C-7 and C-8, and the chiral carbon of C-24. They were elucidated as (23R, 24S)-hydroxyshengmanol-15-one-3-O-β-D-xylopyranoside (2), (23R, 24S)-hydroxyshengmanol-7(8)-en-15-one-3-O-α-L-arabinopyranoside (3), (23R, 24S)-hydroxyshengmanol-15-one-3-O-α-L-arabinopyranoside (4), (23R, 24R)-hydroxyshengmanol-7(8)-en-15-one-3-O-α-L-arabinopyranoside (5), and (23R, 24R)-hydroxyshengmanol-15-one-3-O-α-L-arabinopyranoside (6), respectively (detailed elucidation was showed in S.1.1).

Compounds 7 and 8 were normal hydroxyshengmanol-type triterpenoids with the sugar unit at C-3, a hydroxyl group at C-15, a hemiketal unit at C-16 and an epoxy cyclohexane between C-16, 17, 20, 22 and 23, which are characteristic structural features of these compounds. 7 and 8 were elucidated as 24-epi-24-O-acetylhydroshengmanol-3-O-β-D-glucopyranoside (7) and shengmanol-3-O-β-D-glucopyranosyl-(1→3)-β-D-xylopyranoside (8) (detailed elucidation was showed in S.1.1).

The bioassay results showed that none of them exhibited cytotoxic activity (IC50 > 40 μM) and compounds 7 and 8 showed weak inhibitory activity on AChE (S. Table 3). And the X-ray diffraction result presented here supported the validity of the previous method, which deduced the configurations of C-23 and C-24 in the hydroxyshengmanol, dahurinol and isodahurinol compounds by comparison of the coupling constants with previous literature (Shao et al., 2000). Particularly, for shengmanol-type compounds, the X-ray diffraction method to clarify the absolute configuration of hemiketol group (C-16) is better than NOESY experiment or CD method (Li et al., 1993; Akiko et al., 1996).

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.phytol.2015.04.005.
References


