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PP46. The isovalerate and 2-methylbutanoate of artemisia alcohol–new compounds from *Artemisia annua* L. essential oil

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Artemisia annua L. (sweet wormwood) is an essential oil (EO)-rich, medicinally valuable plant species from the Asteraceae family [1]. During the analysis of the biologically active *A. annua* EO sample (hydrodistilled from the dry aboveground parts of the plants; oil yield 0.2%, w/w; the main components (relative abundance): artemisia ketone (35.7%), α -pinene (16.7%), 1,8-cineole (5.5%), artemisyl alcohol (4.8%), and *trans*-pinocarveol (4.8%) [1]), we have detected two minor compounds, AA1 and AA2 (0.06% and less than 0.05% of the total oil, with RI (DB5-MS) values of 1367 and 1373, respectively) with practically identical mass spectral (MS) fragmentation patterns (EI, 70 eV; m/z (rel. int.)): 169(15), 85(100), 57(38), 41(17). The comparison of GC (\approx 300 unit higher RI values) and MS data of AA1 and AA2 with those of artemisyl acetate (often present in EOs containing artemisia ketone and artemisia alcohol) suggested these might be esters of artemisia alcohol and (isomers of) pentanoic acids. To confirm this tentative identification, and possibly detect some additional AA1 and AA2 homologs, we prepared esters of artemisia alcohol and valeric, isovaleric, 2-methylbutanoic, butanoic, isobutanoic and propanoic acids (Steglich esterification; the starting alcohol was obtained by LiAlH_4 reduction of artemisia ketone isolated from the EO). Co-injection of the EO sample with synthetic standards confirmed AA1 and AA2 were artemisyl isovalerate and artemisyl 2-methylbutanoate (diastereomer not determined), respectively (Fig. 1). Detailed re-analysis of the EO revealed the presence of initially undetected trace amounts of artemisyl acetate. The results of this work once again confirm the importance of natural product-inspired libraries of synthetic compounds in the analysis of EOs, especially when it comes to the detection and identification of trace constituents.

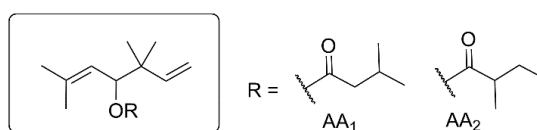


Fig. 1. Structures of artemisyl isovalerate (AA1) and artemisyl 2-methylbutanoate (AA2).

Reference:

[1] Radulović, N.S. et al., 2013. *Food Chem. Toxicol.* 58, 37–49.

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