

RESEARCH ARTICLE

A new longipinane ketone from *Achillea abrotanoides* (Vis.) Vis.: chemical transformation of the essential oil enables the identification of a minor constituent

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Funding information

Ministry of Education, Science and Technological Development of Serbia, Grant/Award Number: 172061

Abstract

Introduction: Minor plant constituents are difficult to identify due to the challenging isolation and acquiring of reliable spectral data. Essential oils abound in such minor constituents that might be of high importance for their (e.g. olfactory) properties. The presence of new minor constituents is usually inferred from gas chromatography mass spectrometry (GC-MS) analyses that provide only a mass spectrum and retention data, which are insufficient to allow a positive identification.

Objective: To identify a minor unknown constituent of the essential oil of *Achillea abrotanoides* (Vis.) Vis. (Asteraceae).

Methodology: The application of chemical transformations (oxidation and reduction) performed directly on crude essential-oil samples, followed by preparative chromatography and detailed spectral analysis, to identify a new longipinane ketone from the mentioned sample.

Results: GC-MS analyses of the essential oil revealed, among other constituents, the presence of a known rare longipinane alcohol (α -longipinen-7 β -ol) representing 2.5% of the total GC-peak areas, and a related unidentified oxygenated sesquiterpene (3.8%). Interpretation of their mass spectra led to an assumption that the unidentified one could represent α -longipinen-7-one. Oxidation of the entire essential-oil sample by pyridinium chlorochromate confirmed the assumed relationship among the compounds and gave a simplified enriched mixture containing the ketone (ca. 16%). A straightforward chromatographic separation of the ketone was followed by corroboration of its structure by nuclear magnetic resonance (NMR) (one- and two-dimensional), infrared (IR) and MS.

Conclusions: The complementing use of chemical transformations of crude essential oils, chromatographic separations, and detailed spectral analysis could have a more general application in the identification of new natural products.

KEYWORDS

Achillea abrotanoides, chemical transformations, essential oil, GC-MS, NMR, structure elucidation, α -longipinen-7-one