

PP88. Misidentification of an essential-oil constituent due to repeated reporting of wrong RI value: 2-methyl-2-nonen-4-one vs. 6-hydroxy-2,6-dimethyl-2,7-octadien-4-oneNiko Radulović^{1*}, Vidak Raičević²*Keywords:* misidentification, retention index, 5-oxolinalool, *Sambucus nigra* L.

In the absence of a reference sample, the majority of essential-oil constituents is identified by GC-MS based on a comparison of their mass spectra (MS) and retention indices (RI) with available/literature ones. Hence, the credibility of literature data is a significant one. Herein we report a case where erroneous data led to an essential-oil constituent misidentification in several different plant species. While analyzing the composition of the essential oil of elderflowers (*Sambucus nigra* L.) we tentatively identified a compound with an MS and an RI (1215 on an HP-5 column) which were in good conformity with those previously reported for 2-methyl-2-nonen-4-one [1]. Up to date, this compound has been reported as an essential-oil constituent, with very similar RI values, at least six times. In order to verify this identification, we performed a crossed aldol condensation reaction between 2-heptanone and acetone, and identified the different addition and condensation products only to conclude that the essential-oil constituent in question cannot be the aforementioned enone as its RI value was notably lower (1143). As aldol-addition products were found to have RI values about 10 units higher than the condensation products, this prompted us to consider the possibility that the unknown compound is a tertiary alcohol. As its MS contained no peak at m/z 59, while a peak at m/z 71 was present, we considered several structural possibilities and concluded that the compound is likely to be 6-hydroxy-2,6-dimethyl-2,7-octadien-4-one (5-oxolinalool), where a tertiary alcohol function exists alongside a double bond, which is consistent with the observed fragmentation. This compound was previously reported to be a constituent of elderflower volatiles [2]. The tentative assignment is also supported by the presence of other oxygenated linalool derivatives in the elderflower essential oil. It follows that one should always approach GC-MS literature data with a degree of caution and rely on co-injections or information gathered from chemical reactions for identification wherever possible.

References:[1] Ceccarini, L. et al., 2004. *Ind. Crop. Prod.* 19, 13–17.[2] Joulain, D., 1987. *Flavour Frag. J.* 2, 149–155.*Acknowledgments:* The authors acknowledge the Ministry of Education, Science and Technological Development of Serbia for the financial support (Project No. 172061).¹Department of Chemistry, Faculty of Sciences and Mathematics, Višegradska 33, 18000 Niš, Serbia;²Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia.*Corresponding author: nikoradulovic@yahoo.com