PP67. Identification and 2D NMR structural elucidation of a C10-polyacetylenic ester, a previously unreported constituent of *Bellis perennis* L. essential oil

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**Keywords:** *Bellis perennis* L., polyacetylenic ester, structural elucidation, 2D NMR, matricaria ester

Common daisy, *Bellis perennis* L., is a widespread herbaceous perennial plant species from the Asteraceae family. Although it has a history of traditional use for the treatment of a variety of health conditions [1], up to now only a few studies dealt with the composition of the essential oil of this plant taxon [1]. Hydrodistillation of the fresh aboveground parts, collected at the beginning of anthesis from a wild-growing population in Serbia (Jelašnica gorge), yielded a small amount of a light green essential oil (0.022%), which was analyzed by GC-MS and a total of 33 compounds was identified (97.1%), with polyacetylenes as one of the major chemical classes detected. The essential oil was chromatographically separated on a 10% AgNO3-coated silica column, which resulted in one polyacetylene-enriched fraction. GC-MS analysis of this fraction revealed the presence of two C10 polyacetylenic compounds. One of them was identified as methyl deca-4,6-diynoate (2,8-tetrahydromatricaria ester), previously reported [1] as one of the main polyacetylenes present in the essential oil of *B. perennis*. Literature data [1] and the mass spectrum of the other polyacetylenic compound, present in the oil in trace amount, suggested that it was likely to be a lachnophyllum ester (8,9-dihydromatricaria ester). Direct analysis of 1H- and 13C-NMR (at 400 MHz, in CDCl3) spectra of the obtained fraction proved to be challenging, due to signal overlap. However, a combination of 2D NMR experiments (gradient 1H-1H COSY, HMBC, and HSQC) enabled a full structural assignment. The compound in question was demonstrated to be methyl (Z)-deca-8-en-4,6-diynoate (i.e. a 2,3-dihydromatricaria ester), which, to the best of our knowledge, has not been reported in *B. perennis* until now. It is possible that the previous reports [1] of lachnophyllum esters in common daisy essential oil, based solely on MS data, are in fact incorrect due to minor differences in the mass spectra of the isomeric esters.

**References:**

**Acknowledgments:** The authors acknowledge the Ministry of Education, Science and Technological Development of Serbia for financial support (project 172061).

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