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PP67. Identification and 2D NMR structural elucidation of a C_{10}-polyacetylenic ester, a previously unreported constituent of *Bellis perennis* L. essential oil

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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% $AgNO_3$-coated silica column, which resulted in one polyacetylene-enriched fraction. GC-MS analysis of this fraction revealed the presence of two C_{10} 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 ^{1}H- and ^{13}C-NMR (at 400 MHz, in $CDCl_3$) spectra of the obtained fraction proved to be challenging, due to signal overlap. However, a combination of 2D NMR experiments (gradient ^{1}H-^{1}H 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:
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