



## New Esters from the Essential Oil Of *Doronicum Columnae* Ten.

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The genus *Doronicum* (Asteraceae) comprises 26 different plant species, mostly distributed in Europe and southwest Asia. Although some of the monoterpenoids, sesquiterpenoids, and diterpenoids from *Doronicum* species possess significant biological activity, the genus is still poorly phytochemically and pharmacologically studied. *Doronicum columnae* Ten. is a perennial representative of this genus, and only non-volatile constituents of this taxon were previously investigated.<sup>1</sup>

Prompted by the lack of data on the secondary metabolites, we decided to investigate the chemical composition of *D. columnae* roots essential oil. GC-MS analysis of the oil showed the presence of 2-isopropyl-4-methylphenyl (isothymyl) and 2-isopropyl-5-methylphenyl (thymyl) isobutyrate (16.4% and 16.3%, respectively) as the main essential-oil constituents. Partial ion current (PIC) chromatograms for *m/z* 135, 150, and 220 or 234 revealed the presence of several additional esters with the same fragmentation pattern in the mass spectrum. To infer the structures of these constituents, we decided to prepare a library of esters of (iso)thymol and (iso)carvacrol (isobutyrate, butyrate, 2-methylbutyrate, 3-methylbutyrate, and valerate), 20 compounds in total, which led to the identification of three new natural products: isothymyl 2-methylbutyrate, isocarvacryl isobutyrate, and isocarvacryl 2-methylbutyrate. The synthesized esters were characterized by spectral (MS, 1D, and 2D NMR) and chromatographic (GC and GC-MS) techniques.

**Keywords:** *Doronicum columnae*, essential oil, esters, spectral characterization

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### References

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