



## The Essential Oil of *Acmella Oleracea* (L.) R.K. Jansen: Structural Elucidation and Acute Toxicity of New Esters

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Amazon rainforest is one of the most significant biodiversity hotspots in the world and represents a phytochemical gold mine with countless plant species with immense pharmacological potential.<sup>1</sup> One of them is paracress (*Acmella oleracea* (L.) R.K. Jansen (Asteraceae)) with already proven pharmacological properties including, but not limited to antinociceptive, anti-inflammatory, antioxidant, immunomodulatory, antimicrobial, antiviral, and diuretic activity.<sup>1</sup> A detailed GC-MS analysis of the chemical composition of the essential oil of paracress revealed, among more than 120 identified constituents, the presence of 12 compounds that were, according to their mass spectral fragmentation, tentatively identified as long-chain  $\alpha$ -keto esters of isobutyric, 2-methylbutanoic, isovaleric, angelic, tiglic, and/or senecioic acids. To determine the exact structure of these minor essential-oil constituents, 18 (completely new) esters were prepared starting from the synthesized 2-oxoundecan-1-ol, 2-oxododecan-1-ol, and 2-oxotridecan-1-ol with the mentioned acids. All synthesized compounds were spectrally and chromatographically characterized. GC-MS, in combination with NMR analyses of the compounds, provided proof of the identity of the mentioned *A. oleracea* constituents. The acute toxicity of these compounds was tested in the *Artemia salina* model to assess the safety of these naturally occurring esters (12 out of 18 synthesized compounds). The obtained results suggest that the intake of these compounds in naturally available amounts, on their own, would probably not represent a risk to human health.

**Keywords:** *Acmella oleracea*, essential oil, esters, spectral characterization

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### References

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