VOLATILE FINGERPRINTS OF BOTANICAL HYDROLATES: HS-GC-MS VERSUS SOLVENT EXTRACTION-GC-MS

Konstantinas Brazinski[1]

[1]Center for Physical Sciences and Technology (FTMC), Department of Organic Chemistry, Vilnius, Lithuania
konstantinas.brazinski@ftmc.lt

Botanical hydrolates are water-based distillates obtained as co-products during essential oil production. They contain a diverse mixture of dissolved volatile organic compounds (VOCs) transferred from plant material during distillation. Because of their pronounced aromas, they are widely used in cosmetics, fragrances, and food flavouring. Profiling of hydrolates is important to verify botanical origin, ensure batch-to-batch consistency, and screen for unexpected or potentially harmful volatile impurities [1]. However, VOC profiles can vary substantially depending on the GC–MS sample preparation method. Headspace (HS) sampling enables VOC determination by analysing the vapour phase above the sample, providing rapid analysis with minimal preparation, but it may under-represent less volatile constituents compared with other approaches.

The aim of this study was to evaluate differences in GC–MS profiles of botanical hydrolates obtained using HS sampling versus liquid–liquid extraction (LLE) with pentane followed by liquid injection. In addition, we aimed to identify marker compounds relevant for both routine screening and more comprehensive chemical fingerprinting. Seven hydrolates were analysed: apple blossom, apple mint, peppermint, two chamomile hydrolates, linden blossom, and rose blossom. Compounds were tentatively identified by mass spectral matching against the NIST mass spectral library.

Overall, HS–GC–MS produced fewer peaks and fewer tentatively identified compounds across samples, indicating reduced coverage of less volatile constituents. In contrast, pentane LLE yielded richer profiles and improved detection of semi-volatile constituents, supporting its use for more robust marker discovery, while HS provides a rapid option for routine screening.

[1] Tavares, C. S., Gameiro, J. A., Roseiro, L. B., & Figueiredo, A. C. “Hydrolates: a review on their volatiles composition, biological properties and potential uses.” Phytochemistry Reviews 21(5) (2022): 1661–1737.