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## Матеріали

*II Науково-практичної Internet-конференції  
з міжнародною участю*

# ФАРМАЦЕВТИЧНІ ТЕХНОЛОГІЇ, СТАНДАРТИЗАЦІЯ ТА ЗАБЕЗПЕЧЕННЯ ЯКОСТІ ЛІКАРСЬКИХ ЗАСОБІВ

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## GC-MS ANALYSIS OF THE ESSENTIAL OIL COMPOSITION OF *RHODODENDRON TOMENTOSUM* HARMAJA: QUALITY CONTROL DURING RESULT PROCESSING

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**Introduction.** *Rhododendron tomentosum* Harmaja, formerly known as *Ledum palustre* (pre-1990), is one of seven species in the subgenus *Rhododendron*, section *Rhododendron*, subsection *Ledum*. Globally, the essential oil of *R. tomentosum* is considered a major target product due to its promising insecticidal, antimicrobial, and antifungal properties.

**Aim** – evaluate the chemical composition of the essential oil extracted from the aerial parts of *R. tomentosum* growing in Ukraine.

**Methods.** Essential oil was obtained by hydrodistillation using a circulatory Clevenger-type apparatus. Gas chromatography–mass spectrometry (GC–MS) analysis was performed using a SHIMADZU GC/MS-QP2010NC system (Shimadzu, Japan). Compound identification was conducted through comparison with mass spectral libraries (NIST14.lib, FFNSC2.lib, and WR10R.lib) and verified using linear retention indices (LRIs) with an Excel-based tool [1, 2]. This tool facilitates LRIs referencing (based on Adams R. P. and Babushok V. I. databases), and calculates experimental LRIs errors while considering the column’s selectivity.

**Results.** The essential oil was predominantly composed of sesquiterpenoids – especially palustrol and ledol – as major secondary metabolites. Monoterpenes such as p-cymene and  $\alpha$ -terpinene were also abundant. Key components included sabinene,  $\beta$ -pinene,  $\delta$ -2-carene,  $\alpha$ -terpinene,  $\beta$ -phellandrene,  $\gamma$ -terpinene, cis-sabinene hydrate, trans-pinocarveol, myrtenol, geranyl acetate, aromadendrene, and germacrene D. Several compounds, including  $\alpha$ -terpinyl acetate, piperitenone oxide, and viridiflorol, were initially misidentified, highlighting the importance of LRIs confirmation.

**Conclusion.** The study demonstrates considerable chemical variability in the essential oil composition of *R. tomentosum*, even within a single geographical region. Moreover, the integration of linear retention index verification tools is essential for accurate compound identification in complex essential oil matrices. A correct understanding and application of retention indices are crucial for drawing valid conclusions regarding chemical identity, mixture composition, and the reliability of data, all of which depend on accurate identification.

### References

- 1 Bizzo, H.; Barboza, E.; Santos, M.; Gama, P. Um conjunto de planilhas eletrônicas para identificação e quantificação de constituintes de óleos essenciais. *Quím. Nova* **2020**. <https://doi.org/10.21577/0100-4042.20170458>.
- 2 Pokajewicz, K. Enhancing Terpene and Other Plant Volatiles Analysis – A Free Spreadsheet Tool “Retentify” for GC–MS Data Processing. *Microchem. J.* **2023**, *193*, 108977. <https://doi.org/10.1016/j.microc.2023.108977>.