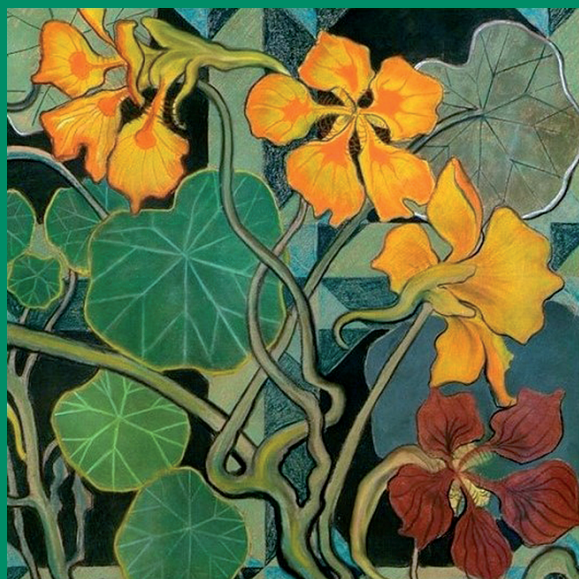


KRAKÓW



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Kraków, 2024, July 13-17

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Posters

S3.P26 *Epilobii herba*: Quality assessment using chromatographic techniques

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The genus *Epilobium* (willow herb) includes ca. 160 species distributed throughout the world. The most rudely used species are *E. angustifolium* L., *E. parviflorum* Schreb., and *E. hirsutum* L. as herbal teas, which have been reported to have prostate-protective and anti-inflammatory properties (1). However, despite their wide use, these plants are not included in key pharmacopoeias. Only the Herbal Medicines Committee (HMPC) has assessed the botanical drug (2, 3) regarding *E. parviflorum*'s medical use, but not in terms of metabolites or analysis.

Here, we focus on a comparative qualitative analysis for *E. hirsutum* herb and the assessment of the homogeneity of samples during a growing season. From April until October 2023 *E. hirsutum* samples (n=78), including leaves and stems, were collected in the United Kingdom. Polyphenols, e.g., chlorogenic acid, gallic acid, caffeic acid, avicularin, guajaverin, isoquercitrin and hyperoside used as reference standards. The analysis was carried out in HPTLC plates Si 60 F254 (Merck) in mobile phase: ethyl acetate: formic acid: water (68:8:8) and 2-aminoethyldiphenylborinate and macrogol 400 for derivatization.

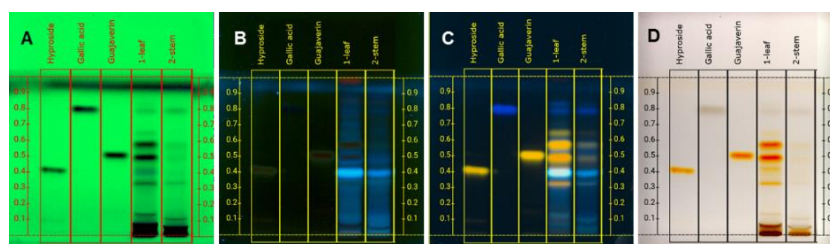


Fig. 1. HPTLC profile under UV 254 nm (A), UV 366 nm (B) prior to derivatization, and under UV 366 nm after derivatization (C), and white light after derivatization (D)

The HPTLC analysis showed all reference substances in *E. hirsutum* extracts but in different concentrations, e.g., yellow fluorescent zones ($R_f=0.4$; $R_f=0.38$; $R_f=0.85$; $R_f=0.52$) were in line with isoquercitrin, hyperoside, avicularin and guajaverin, and these were the dominant compounds in leaves. The light blue, fluorescent zone ($R_f=0.7$) was identified as gallic acid, and it accumulated more in the stems (Fig. 1). The presented method can be used for assessing the *Epilobium* quality, including botanical drugs or finished commercial products.

Keywords: *Epilobium hirsutum*, Onagraceae, quality control, HPTLC

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S3.P70 Exploring potential breast and melanoma cancer drug candidates from *Crocus sativus*: molecular docking insights

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Molecular docking can be particularly useful in identifying potential drug candidates from natural sources, exploring the binding mechanisms of natural products with therapeutic targets, and guiding the optimization of lead compounds derived from natural sources [1]. The current molecular docking aimed the analysis of descriptors with the greatest cytotoxic activity and the study of the possible mechanism of action of selected phenolic compounds of *Crocus sativus*. Previously [2], we identified the following compounds: chlorogenic acid, caffeic acid, mangiferin, isoorientin, ferulic acid, rutin, tectoridin, quercetin, t-cinnamic acid, genistin, apigenin, kaempferol, iristectorigenin B, nigricin and irigenin. The docking simulations were performed with the SCIGRESS software package (Fujitsu, Fukuoka, Japan (license 742F6852C191)). Among estrogen receptors that play an important role in cancer pathogenesis, we selected the human ER α -LBD (PDB ID 3ERT) complex with 4- hydroxytamoxifen, which is an active metabolite of tamoxifen. According to the docking studies, almost all natural compounds showed affinity to the active sites of the selected enzymes that were similar or even better than their native ligands. Such compounds as chlorogenic acid, isoorientin, ferulic acid, tectoridin, quercetin, cinnamic acid, genistin, apigenin, kaempferol, and irigenin showed, better affinity compared with the native ligands of breast cancer proteins 4RJ3, 2IOK, and 4XYF. Moreover, the affinity of many compounds (chlorogenic acid, ferulic acid, cinnamic acid, iristectorigenin B) to the estrogen receptor (3ERT) was comparable to hydroxytamoxifen. Subsequent *in vitro* assays of *Crocus* extracts and individual substances correlated with the results of docking.

Keywords: natural compounds, breast cancer, melanoma, docking studies, drug designing

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- S1.P236 From poison to potential: Nb-methyl usambarensine reveals antiviral activity against SARS-CoV-2
Kristi Leka
- S1.P237 Semi-synthetic ecdysteroids as promising new antichagasic agents
Márton Benedek Háznagy
- S1.P238 Exploring the potential biopesticide application of nemertide alpha-1 on parasitic and disease vector mosquitoes
Quentin Laborde
- S1.P239 Chemical constituents of Sambucus nigra fruit (European Elderberry)
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- S1.P240 Invasive plants as promising solutions against biofilms
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