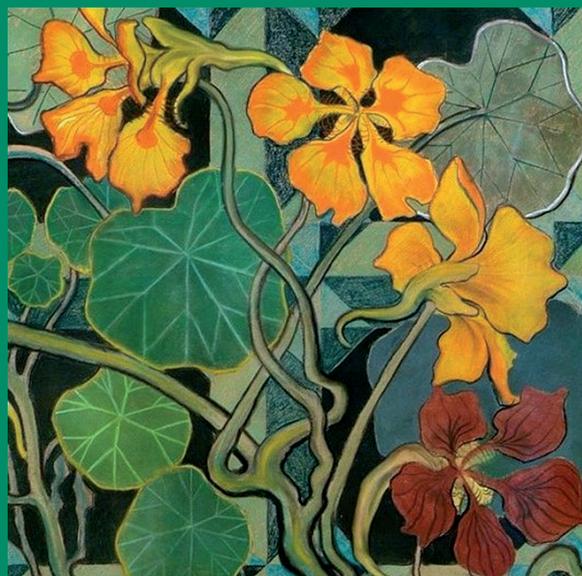


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Kraków, 2024, July 13-17

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Posters

S1.P249 A steroid-rich fraction from parasitic climber *Cocculus hirsutus* (L.) W.Theob inhibits coronavirus disease and neutrophilic inflammation

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Infections from coronavirus diseases and their complications pose significant threats to human health, economies, and societies. Excessive inflammatory responses in human neutrophils are linked to high mortality rates (Chiang et al., 2020). There is a pressing need for affordable and safe treatments, prompting interest in herbal remedies.

Cocculus hirsutus (L.) W.Theob (CH, Menispermaceae) is a perennial climbing plant found widely across Asia and Africa. We have obtained aerial parts of CH from farm in India where it grows as weed and parasite, damaging crops. Notably, various parts of CH are used in folk medicine to treat fever, skin issues, stomach ailments, and urinary disorders. Alkaloid compounds are among major constituents identified in this plant (Logesh et al., 2020). However, other CH secondary metabolites are unexplored.

This study evaluated crude extracts, partitioned layers, and subfractions using SARS-CoV-2 spike/ACE2 pseudovirus neutralization assay (crude CH extract 27.16% and CHEA6 subfraction 54.85% inhibition at 10 µg/mL). Moreover, the anti-inflammatory assays including superoxide anion generation and elastase release in fMLF/CB-induced human neutrophils showed notable activity (crude CH extract 53.95% and 80.39%, respectively; CHEA layer and CHEA6 subfraction >90% inhibition for both assays at 10 µg/mL). Importantly, the bioactivity-guided fractionation of non-alkaloid subfraction CHEA6 (ethyl acetate fraction 6) yielded major steroid triterpenes, including ecdysone type, including 20-hydroecdysone (1), makisterone A (2), and phytosterols, such as β-sitosterol glucoside (3). Additionally, three compounds, including (+)-*proto*-quercitol (4), lutein (5), and formononetin (6) were isolated. The structure of the compounds was confirmed by 1D, 2D NMR, and mass spectroscopic analysis.

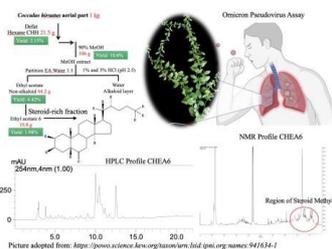


Fig. 1. Steroid-rich fraction isolation scheme, HPLC, and NMR chemical profile

Keywords: *Cocculus*, SARS-CoV-2, human neutrophils, triterpene, phytochemistry

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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.

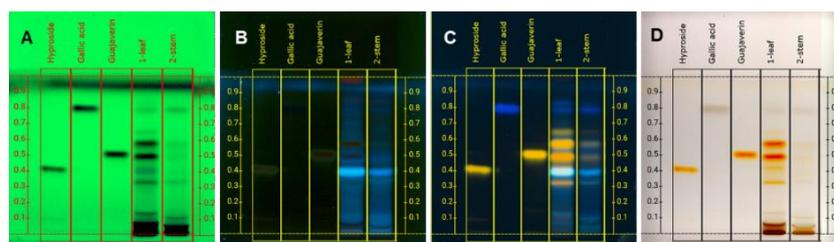


Fig. 1. HPTLC profile under UV 254 nm (A), UV 366 nm (B) prior to derivatization, and under UV 366 nm after derivatization (C), and white light after derivatization (D)

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.

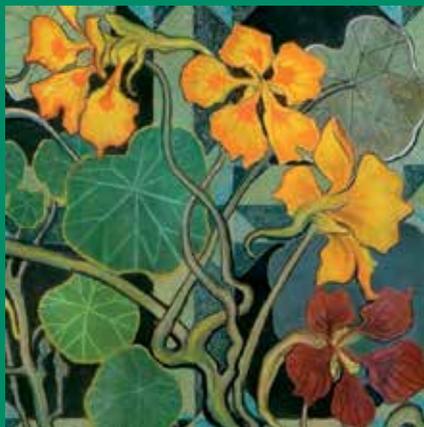
Keywords: natural compounds, breast cancer, melanoma, docking studies, drug designing

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PROGRAMME

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