KRAKÓW

ICNPR 2024

INTERNATIONAL CONGRESS ON NATURAL PRODUCTS RESEARCH

Kraków, 2024, July 13-17

ABSTRACTS BOOK

Posters

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

Vidya Febrasca Tenderly[a*], Thiyagarajan Raviraj[a], Yen Chi Loo[a], Olha Mykhailenko[b], Marcela Safratova[c], Stefan Kosturko[c], Mahendra Jadhao[d], Yu-Li Chen[e], Tsong-Long Hwang[f], Fang-Rong Chang[a*], Michal Korinek[a]

[a] *Graduate Institute of Natural Products, College of Pharmacy, Kaohsiung Medical University, Kaohsiung, Taiwan*

[b] *Department of Pharmaceutical Chemistry, National University of Pharmacy of Ministry of Health of Ukraine, Kharkiv, Ukraine*

[c] *Department of Pharmacognosy and Pharmaceutical Botany, Faculty of Pharmacy, Charles University, Hradec Kralove, Czech Republic*

[d] *Department of Cancer Biology, University of Cincinnati College of Medicine, Cincinnati, OH, USA*

[e] *Research Center for Chinese Herbal Medicine, Graduate Institute of Health Industry Technology, College of Human Ecology, Chang Gung University of Science and Technology, Taoyuan, Taiwan*

[f] *Graduate Institute of Natural Products, College of Medicine, Chang Gung University, Taoyuan, Taiwan*

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.

Cocullus 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 formononentin (**6**) were isolated. The structure of the compounds was confirmed by 1D, 2D NMR, and mass spectroscopic analysis.

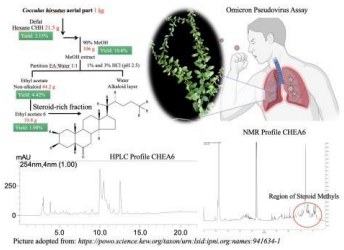

Fig. 1. Steroid-rich fraction isolation scheme, HPLC, and NMR chemical profile

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

References

Chiang, C.-C., Korinek, M., Cheng, W.-J., & Hwang, T.-L. 2020. Targeting Neutrophils to Treat Acute Respiratory Distress Syndrome in Coronavirus Disease. *Frontiers in Pharmacology*, *11*.

Logesh, R., Das, N., Adhikari-Devkota, A., & Devkota, H. P. 2020. Cocculus hirsutus (L.) W.Theob. (Menispermaceae): A Review on Traditional Uses, Phytochemistry and Pharmacological Activities. *Medicines*, *7*(11), 69.

*Presenting author. *E-mail address*: vfebrasca@gmail.com (Vidya Febrasca)

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

Olha Mykhailenko[a,b], Banaz Jalil[a], Michael Heinrich[a,c,*]

[a] *Pharmacognosy and Phytotherapy, UCL School of Pharmacy, 29-39 Brunswick Square, WC1N 1AX, London, UK*

[b] *Department of Pharmaceutical Chemistry, National University of Pharmacy, 4-Valentynivska Str., 61168, Kharkiv, Ukraine*

[c] *Chinese Medicine Research Center, College of Chinese Medicine, China Medical University, Taichung City 404, Taiwan*

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 F_{254} (Merck) in mobile phase: ethyl acetate: formic acid: water (68:8:8) and 2-aminoethyldyphenylborinate and macrogol 400 for derivatization.

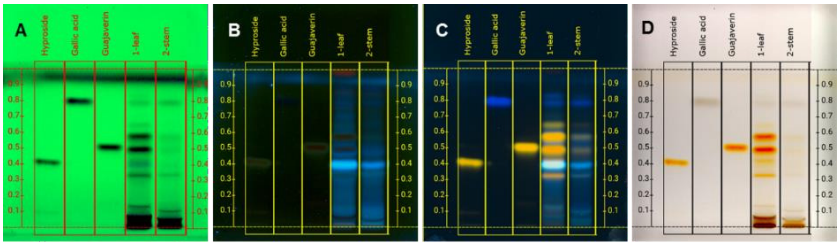

Fig. 1. HPTLC profile under UV 254 nm (A), UV 366 nm (B) prior to derivatization, and under UV 366 nm after derivatization (C), and white light after derivatization (D)

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

References

1. Vlase AM, Toiu A, Tomut˘a I, Vlase, L.; Muntean, D.; Casian, T.; Fizes,an, I.; Nad ˘as, G.C.; Novac, C.S.; T ˘amas,, M.; et al. Epilobium Species: From Optimization of the Extraction Process to Evaluation of Biological Properties. Antioxidants 2023, 12, 91.
2. EMA/HMPC/72238/2022. Call for scientific data for the periodic review of the monograph on Epilobii herba (PDF/107.1 KB), published: 15/02/2022. European Medicines Agency, 2022. Amsterdam, The Netherlands.
3. EMA/HMPC/615965/2022. Addendum to Assessment report on Epilobium angustifolium L. and/or Epilobium parviflorum Schreb., published: 17/11/2022. European Medicines Agency, 2022. Amsterdam, The Netherlands.

* Presenting author. E-mail address: o.mykhailenko@ucl.ac.uk (Olha Mykhailenko)

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

Olha Mykhailenko[a,b,*], Victoriya Georgyiants[b]

[a] *Pharmacognosy and Phytotherapy, UCL School of Pharmacy, 29-39 Brunswick Square, WC1N 1AX, London, UK*

[b] *Department of Pharmaceutical Chemistry, National University of Pharmacy, 4-Valentynivska Str., 61168, Kharkiv, Ukraine*

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 ERα-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 com-pared 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

References

1. Asiamah et al. 2023. Applications of molecular docking in natural products-based drug discovery. Scientific African, 20: e01593.

2. Mykhaolenko et al.2022. Pharmacological Potential and Chemical Composition of *Crocus sativus* Leaf Extracts. Molecules. 27: 10.

* Presenting author. E-mail address: o.mykhailenko@ucl.ac.uk (Olha Mykhailenko)

N

KRAKÓW

ICNPR 2024

INTERNATIONAL CONGRESS ON NATURAL PRODUCTS RESEARCH

Kraków, 2024, July 13-17

PROGRAMME

S1.P235 Bio-guided approach as a valuable tool in the phytochemical investigation of three underexplored Myrtaceae plants
Francesca Guzzo

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)
Zulfiqar Ali

S1.P240 Invasive plants as promising solutions against biofilms
Marion Girardot

S1.P241 Isolation and characterization of antimicrobial compounds from Picralima nitida (Apocynaceae)
Makafui Gbemu

S1.P242 Identification of a Potent Antibiotic Compound from Geodermatophilus Bacteria
Sunmin Woo

S1.P243 Ethnobotany as a tool for targeted discovery of bioactive natural products for emerging infectious diseases
Cassandra Quave

S1.P244 Amaryllidaceae alkaloids as promising anti-dengue phytochemicals
Emmy Tuenter

S1.P245 Multi-target action of volatile compounds from essential oils in the treatment of periodontitis
Ruxandra Ștefănescu

S1.P246 Metabolomic-guided phytochemical investigation and antimicrobial activity of Morus alba L. twigs extract
Giuseppina Chianese

S1.P247 A new approach to study the mechanisms of action of antimicrobial plant-derived molecules in prokaryotic cells
Raffaella Nocera

S1.P248 Harnessing the constrained macrocyclic peptide frameworks for the development of antimicrobial peptides to treat infections
Taj Muhammad

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

S1.P250 Sargassum fusiforme and its components inhibits Respiratory Syncytial Virus replication in vitro and in vivo
Jong-soo Lee

S1.P251 Inhibition of Respiratory Syncytial Virus in vitro and in vivo by Apostichopus japonicus (selenka) extract
Jong-soo Lee

S1.P252 Aster tataricus and its components displays a broad spectrum of antiviral effects in Vitro and in Vivo
Jong-soo Lee

S1.P253 Extracts of Costus speciosus suppresses Influenza A H1N1 activity in Vitro and in Vivo
Jong-soo Lee

S1.P254 Exploring faba bean pods as a potential nutritional supplement for piglet gut health
Inna Vlasova

S1.P255 Anti-inflammatory properties of twelve Norwegian medicinal plants and their protective properties against impairments in the intestinal epithelial barrier
Andrea Angelov

S3.P18 Optimization Formulation of Rhodiola rosea L. Nanoemulsion Containing Natural Oil Using Response Surface Method (RSM): Preparation, Characterization, Stability Test and Antioxidant Activity
Benni Iskandar

S3.P19 Oxidoreductase FSP1-mediated redox-regenerating natural product E18C6 potently suppresses ferroptotic cell death
Minh Bui Hoang

S3.P20 Chinese Traditional Medicine for Prevents Hair Loss in Androgenic Alopecia Mice
Ching-peng Wei

S3.P21 Qualitative and semi-quantitative screening of triterpenes in Vaccinium uliginosum L. fruits using supercritical fluid chromatography
Zuzana Vaneková

S3.P22 Matrix free laser desorption ion mobility mass spectrometry in chemometrics: A new approach to the rapid identification of activity markers in complex mixtures of natural products
Andreas Schinkovitz

S3.P23 Metabolomic study of tea tree oil and Melaleuca spp. using HPTLC, LC-MS and GC-MS
Yi Zhao

S3.P24 Preclinical evaluation of oral nanoformulation based on natural extract as a potential treatment for type 2 diabetes mellitus
Norman Balcazar

S3.P25 Employing Plant-Bacterial Interactions to Access the Metabolic Capacity of Bacteroidetes
Barbara Adaikpoh

S3.P26 Epilobii herba: Quality assessment using chromatographic techniques
Olha Mykhailenko

S3.P27 Phytochemical analysis and quality control study of Dendrobium fimbriatum Hook. Flowers
Anham Abbasi

S3.P28 Identification of chemical defenses of a tropical tree Sextonia rubra using molecular networks from GC-MS, LC-MS/MS and MALDI-MS/MS imaging data
David Touboul

S3.P29 An Ethnobotanical, Pharmacological and Phytochemical Review on Flowers of Shi-hu (Dendrobium spp.)
Anham Abbasi

S3.P30 Study of medicinal plants use among patients of the urology service of Ibn-Sina hospital in Rabat, Morocco, Ethnobotanical, Epidemiological and Toxicological aspects/ Phytovigilance
Khadija Dabra

S3.P31 Unveiling the Multifaceted Efficacy of Gu Sui Bu in Osteoporosis Treatment: Insights from a Zebrafish Model and Advanced Analytical Approaches
Ming-der Lin

S3.P32 Phytochemical profiling and the wound healing potential of five Bulbine species using in vitro and in vivo assays
Ramoagi Segone

S3.P33 Translating community-wide mass spectral libraries into actionable chemical knowledge: A proof of concept with monoterpene indole alkaloids
Sarah Szwarc

S3.P34 Non-targeted Profiling Analysis by GC/MS and LC/MS/MS of extracts derived from Eucalyptus tereticornis with antiobesogenic and antidiabetic activity
Norman Balcazar

S3.P35 Design, synthesis and screening of novel prenylated chalcones as optimised anti-cancer agents
Mouna Hind Laiche

S3.P36 Does the combined effect of natural abietane diterpenes with temozolomide have therapeutic potential against glioblastoma?
Mário Marques

S3.P57 3D printed polymeric scaffolds loaded with antibiotic and anti-inflammatory drugs for tissue engineering applications
Andreana Assimopoulou

S3.P58 ChromAnnot – a webserver for reproducible LC-HRMS/MS chromatogram annotation
Samuel Bertrand

S3.P59 Exploring the anticancer potential of Polygonum barbatum (L.) against colorectal cancer: In vitro and in vivo investigations
Shih-yu Lee

S3.P60 Physical interactions between Streptomyces (Streptomycetaceae) and competing microbes trigger the production of natural products
Heli Tirkkonen

S3.P61 Energy Saving Efficacy and Optimized Condition of Pulse Energy Fields Technology on Centella asiatica extraction
Na Young Lee

S3.P62 Identification of a Leoligin-inspired synthetic lignan as a novel TGR5 agonist
Alexander Perhal

S3.P63 Nano-phytosome delivery system loaded with Crataegus laciniata (Rosaceae) Flowers extract: whitening properties
Shiva Pouramin Arabi

S3.P64 Leoligin derivatives as novel Phosphodiesterase 4 inhibitors
Christine Coffey

S3.P65 The search for nontraditional synergy: pairing in vitro omics and in silico machine learning methods to discover novel combinations of antimicrobial agents from natural products
Katherine Lev

S3.P66 Electron diffraction-guided natural product discovery: identification and isolation of new scaffold class from Podospora australis
David Delgadillo

S3.P67 Metaboseek 2.0: Deconvoluting the complexity of MS/MS Big Data through interactive data processing
Alexandros Polyzois

S3.P68 Cytotoxic activities of terpenoids from genera Euphorbia rowlandii and Euphorbia grandocornis (Euphorbiaceae) against the Triple-negative breast cancer (TNBC)
Jacqueline Tembu

S3.P69 Simultaneous extraction and synthesis of new cannabinoid acid esters and their evaluation on TRPA1, cell proliferation and in MDA-MB-231 xenograft model of cancer
Evangelos Dadiotis

S3.P70 Exploring Potential Breast and Melanoma Cancer Drug Candidates from Crocus sativus: Molecular Docking Insights
Olha Mykhailenko

S3.P71 Metabolic fate of Oleocanthal and Oleacein after oral consumption: Novel biomarkers, human bioactivity insights and TRPA1 channel activation
Nikoleta Anna Madelou

S3.P72 An innovative methodology for the production of a new food supplement enriched in Oleocanthal and Oleacein with multi target protective properties
Prokopios Magiatis

S3.P73 Online dried spot LC-Orbitrap analysis for the quality assessment of cannabis products
Varvara Papaioannou

S3.P74 Anti-prostatic effects of V. album L extracts are influenced by season and the use of hydrogel delivery system
Carla Holandino