KOMISJA CHEMII I FIZYKI
W BIOLOGII I MEDYCYNIE
ODDZIAŁU POLSKIEJ AKADEMII
NAUK WE WROCŁAWIU

POLSKIE
TOWARZYSTWO
CHEMICZNE
ODDZIAŁ WROCŁAWSKI

uprzejmie zapraszają

na posiedzenie naukowe, które odbędzie się w

środę 14 lutego 2024 r. o godz. 11.00

w budynku C3 UPWr Centrum Dydaktyczno-Naukowe (CDN)

w sali Rad Wydziału 018 przy pl. Grunwaldzki 24a.

Podczas posiedzenia, wykład pt.:

Cheminformatics and chemometrics to harness Nature's complexity

wygłosi

Univ.-Prof. Dr. Judith M. Rollinger

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Nature has historically proven to be the best chemist on earth and to ultimately protect its host by the synthesis of a potent chemical arsenal. This is reflected in the chemical complexity of an extract's metabolite profile. Many of these extracts derived from different natural resources have been used since ages as remedies. Today, the information from traditional medicine on the one hand and the tremendous advances in natural product technologies, publicly available data and computational power on the other hand offer new possibilities for the identification of novel drug leads.

Here, I will present and compare some recently developed strategies, which can be used to overcome gaps between knowledge from traditional medicine and the use of artificial intelligence harnessing the tremendous advances in cheminformatics, in analytical, spectral and separation techniques. This ranges from virtual screening for hit identification, machine learning tools to a recently in-house developed 1 H NMR-MS-based biochemometric approach. The effectiveness, strengths and limitations of the presented strategies will be demonstrated on most recent application examples for the identification of novel anti- infective and anti-inflammatory natural lead structures.

Przewodniczący Oddziału Wrocławskiego
Polskiego Towarzystwa Chemicznego
dr hab. inż. Tomasz Olszewski

Przewodnicząca Komisji
Chemii i Fizyki w Biologii i Medycynie
dr hab. Hanna Pruchnik

Cheminformatics and chemometrics to harness Nature's complexity

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Biosketch
Univ.-Prof. Dr. Judith M. Rollinger

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Judith Maria Rollinger is Professor of Pharmacognosy/Pharmaceutical Biology and Head of 'Phytochemistry and Biodiscovery' at the Department of Pharmaceutical Sciences, Faculty of Life Science, University of Vienna, Austria.

After her Ph.D. degree in Pharmacognosy of the University of Innsbruck/Austria dealing with crystal polymorphism, she extended her studies to the fields of phytochemistry, ethnopharmacology, and molecular modeling. Engaged as senior scientist of the software company Inte:Ligand (Maria Enzersdorf, Austria; 2003-2005) she implemented computational approaches in natural product science. In 2007 she received the "venia legendi" as Professor of Pharmacognosy as a result of her habilitation thesis "The Search for Bioactive Natural Products".

Prof. Rollinger is project leader in various national and international projects and has received several awards in her field, e.g. the PHOENIX Science Award 2005, the Science Award 2010 of the Capital Innsbruck, and the Science Award 2020 of the federal state Vorarlberg/Austria. She was appointed full Professor of Pharmacognosy/Pharmaceutical Biology at her present institution in 2014. From 2020 to 2023 she served as president (2018-2020 and currently being vice president) of the largest European learned society, focusing on research on natural products, nature-based drug discovery, medicinal plant research and quality control of herbal medicines – the GA (Society for Medicinal Plant and Natural Product Research). In her role, she leads this global society's efforts to foster research in these important areas, improve networking and communication globally and to support especially younger researchers.

Her research focuses on the interdisciplinary field of integrating big data analytics (cheminformatics, chemometrics) in natural product research as strategy for the discovery of natural lead structures for treating infections, metabolic syndrome, and inflammation. Publications resulting from her research have appeared in highly ranked international journals (~140), and as book contributions and patents.

Budynek C3 Uniwersytetu Przyrodniczego we Wrocławiu, Centrum Dydaktyczno-Naukowe (CDN) przy ulicy pl. Grunwaldzki 24a.

Sala Rad Wydziału 018 (na parterze budynku)