

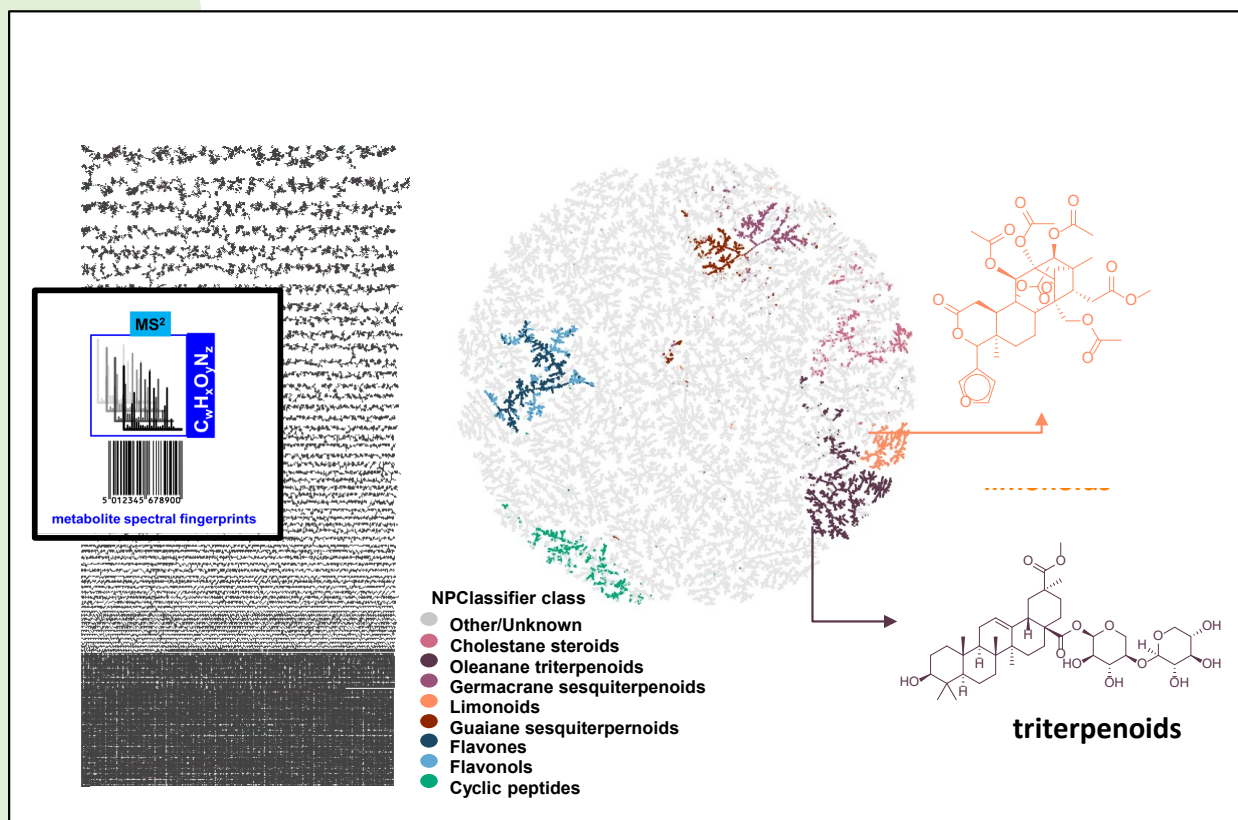
eWorkshop

Society for Medicinal Plant and Natural Product Research



Natural products research in the digital era: Methods for compound annotation and the present status of metabolome characterization

Online, May 23 and 30, June 6 2023
5.00 p.m. – 7 p.m. (CET)



Natural products research in a digital era: compound annotation through computational tools

Natural products (NPs) from plants and micro-organisms are a source of inspiration in drug discovery. They all have their own physical and chemical characteristics and different levels of concentration in extract which makes their comprehensive analysis very challenging. Isolation and complete de novo structural characterization of each compound is necessary for unambiguous identification, but this is a difficult and time-consuming task. In this context, metabolomics is playing an increasingly important role for annotating detected compounds to assess the chemical composition of extracts and dereplication of given metabolites to focus on the discovery of new NPs. Today, with the emergence of advanced liquid chromatography-mass spectrometry (LC-MS) and nuclear magnetic resonance (NMR) metabolite profiling methods, the process of annotating compounds in extracts has been automated and simplified. In this way up to hundreds NPs can be putatively annotated in each extract. Assessing the confidence of annotation however remains a challenge in metabolomics. The proposed online workshop covers the fundamentals of data mining, metabolite profiling and compound annotation using various computational tools. The possibilities and limitations of current metabolomic workflows and computational tools will be discussed. Additionally, we will discuss the exciting possibilities that these advancements offer and show examples of how we've utilized them in our own research to automate annotation and efficiently target the isolation of valuable NPs.

Chairman

Dr. Emerson F. Queiroz, University of Geneva, Switzerland

Invited speakers

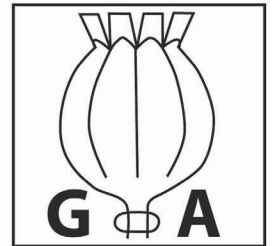
- ✓ **Prof. Jean-Luc Wolfender, University of Geneva (5 to 7 p.m., Mai 23, 2023)**
Topic 1: Introduction on metabolomics and compound annotation
Please use [this link](#) to register.

- ✓ **Dr. Louis-Félix Nothias, University of Geneva (5 to 7 p.m., Mai 30, 2023)**
Topic 2: Generation of molecular networks and spectral annotation
Please use [this link](#) to register.

- ✓ **Dr. Stavros Beteinakis, University of Athens (5 to 6 p.m., June 6, 2023)**
Topic 3: A “driving” force for NMR-based biomarker annotation in natural products metabolomics: STOCSY, SHY & HetCA
Please use [this link](#) to register.

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Society for Medicinal Plant and Natural Product Research



Scientific Committee

Dr. Emerson Ferreira Queiroz (University of Geneva, Geneva, Switzerland)

Prof. Jean-Luc Wolfender (University of Geneva, Geneva, Switzerland)

Prof. Judith Maria Rollinger (University of Vienna, Vienna, Austria)

Prof. Maria Halabalaki (University of Athènes, Greece)

Dr. Olaf Kelber (PSDC, Bayer CH, Darmstadt, Germany)

Organization

GA - Society for Medicinal Plant and Natural Product Research
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Registration

The eWorkshop is free of charge.

Please use the above mentioned links to register. You will receive a Zoom link via e-mail afterwards – please check your spam-folder. If you don't receive any link, please contact events@ga-online.org (Cornelia Kern).

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