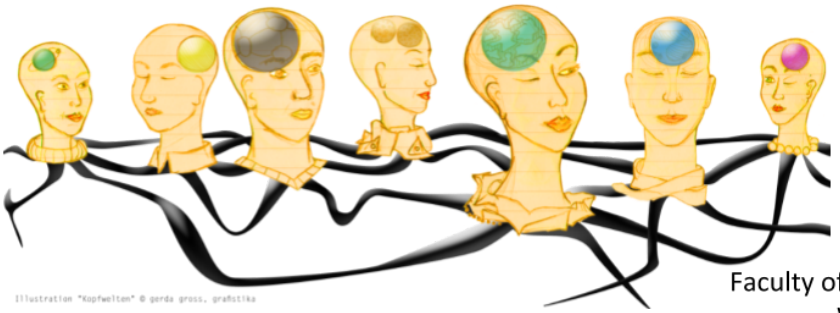


WoChem Symposium 2019

Wednesday April 24, 2019
14:00-18:00
Seminar room 2 (SR2)
Faculty of Chemistry (University of Vienna))
Währinger Straße 42, 1090 Vienna
http://wochem.univie.ac.at/wochem-symposium2019/

Program

14:00 - 14:15	Welcome	
Session 1: Emerging Topics in Chemistry		
14:15 - 14:40	Katharina Pallitsch	Studies on the Biodegradation of P-C Compounds - Synthesis of Phosphonic Acids with High ee
14:40 - 15:05	Esther Heid	Computational solvation dynamics: Possibilities, pitfalls and recent advances
15:05 - 15:30	Giorgia Del Favero	Physical and chemical modulation of the extracellular environment: the biophysical toxicology approach
15:30 - 16:00	Coffee break	
Session 2: Omics and Beyond		
16:00 - 16:25	Evelyn Rampler	Expanding the Analytical Toolbox in Lipidomics
16:25 - 16:50	Astrid Slany	Application of in-depth proteome profiling based on high resolution mass spectrometry to reveal patho-physiological mechanisms
16:50 - 17:15	Andrea Tanzer	RNA Bioinformatics - From Transcriptomics to Structureomics
17:15 - 17:30	Closing remarks	
17:30 - 20:00	Networking & refreshments	

Kindly supported by

universität wien
Faculty of Chemistry

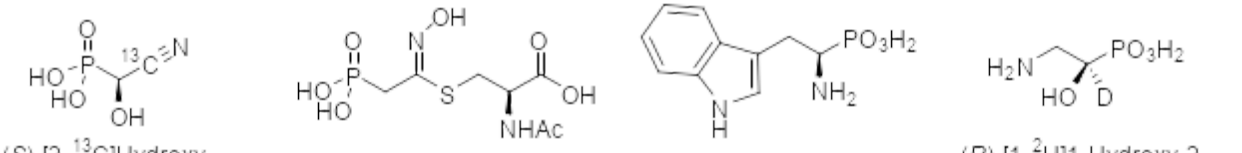
Abstracts

Session 1: Emerging Topics in Chemistry

Studies on the Biodegradation of P-C Compounds - Synthesis of Phosphonic Acids with High ee

Katharina Pallitsch
Department of Organic Chemistry, University of Vienna, Währingerstraße 38, 1090 Vienna, Austria
katharina.pallitsch@univie.ac.at

Biogenic phosphonates have been known for almost 50 years, still they were long time believed to be of limited environmental importance. It has only been recognised during the last decades that they play a crucial role as alternative phosphorus source for microbes, especially in marine ecosystems where phosphate is often the growth limiting nutrient.i However, little is known about the metabolic pathways for the biosynthesis and degradation of phosphonates, which involve a variety of unique enzymatic transformations and unusual intermediates.
Furthermore, phosphonic acid natural products have a commercialisation rate far above the average for other natural product classes and are often very potent enzyme inhibitors.ii α-Aminophosphonic acids proved especially effective in mimicking the tetrahedral transition state of ester/amide bond formation and hydrolysis.



Some selected target structure.

The metabolism and potential bioactivity of newly isolated biogenic and synthetic phosphonates is thus of great importance. However, very elaborate enzymatic and chemical strategies often become necessary for the synthesis of enantiomerically pure compounds. In addition to that, the synthesis of isotopically labelled analogues to these phosphonates, as well as of unstable metabolic intermediates of the proposed degradation pathways is often very complex. We address these problems by developing new, reliable synthetic methods to access the desired phosphonic acids and their analogues in sufficient quantities and in high ee.

Computational solvation dynamics: Possibilities, pitfalls and recent advances

Esther Heid
Department of Computational Biological Chemistry, University of Vienna, Währinger Straße 17, 1090 Vienna, Austria
esther.heid@univie.ac.at

The dynamic behavior of a solvent is characterized by the mechanisms and timescales by which the solvent molecules react to some kind of change or perturbation. Such a perturbation can for example stem from a chemical reaction, where the geometry and electrostatics of dissolved reactants change, a movement of a protein, or a change in electric field. Knowledge of the solvation dynamics of a solvent is thus of importance in a variety of research areas, including spectroscopy of soft matter, chemical reactions in solution, or protein functionality. But how can the dynamic response of a solvent be monitored? A common approach is to measure or calculate the time-dependent Stokes shift of a fluorescent probe molecule which is introduced to the system of interest and excited by a laser pulse. The resulting rearrangement of the nearby solvent molecules to this electrostatic perturbation leads to a change in energy of the emitted fluorescent light. By computer simulation we explore the ability of the time-dependent Stokes shift to reflect local solvation dynamics in a wide variety of systems, ranging from pure polar solvents like water and methanol over pure or aqueous ionic liquids to complex biological systems like protein solutions encapsulated in reverse micelles. Our efforts include exploring new systems, reproducing and interpreting experimental data, improving the accuracy of computer simulations by method and parameter development, as well as relating the obtained information to other observables like NMR experiments or dielectric spectroscopy. Thus, a comprehensive picture of dynamic solvent properties is obtained.

Physical and chemical modulation of the extracellular environment: the biophysical toxicology approach

Giorgia Del Favero
Department of Food Chemistry and Toxicology, University of Vienna, Währinger Straße 38, 1090 Vienna, Austria
giorgia.del.favero@univie.ac.at

In a physiological context, cells are living in a highly dynamic environment. This means that cells are able to “interpret” different signals of chemical and of physical origin and, accordingly, tune their response integrating the different pathways. The biophysical toxicology approach aims to combine the study of toxic substances on cell mechanotransduction to the characterization of the effects of biomechanical stimulation on cytotoxicity processes. In line, the cell membrane has a crucial role in the interface with the extracellular environment and its capability to integrate different signals can be significantly altered in pathological conditions.

Session 2: Omics and Beyond

Expanding the Analytical Toolbox in Lipidomics

Evelyn Rampler
Department of Analytical Chemistry, University of Vienna, Währinger Straße 38, 1090 Vienna, Austria
evelyn.rampler@univie.ac.at

Lipids play a crucial role in cell protection and compartmentalization, fat storage and energy provision, inflammation, temperature maintenance and uptake of essential nutrients. As fats are chemically extremely diverse and lipid handling is impeded by potential oxidation or decay, suitable analytical workflows need to be developed in lipidomics. Chromatography combined with mass spectrometry and isotope dilution strategies represent ideal tools for profound lipid analysis.

Application of in-depth proteome profiling based on high resolution mass spectrometry to reveal patho-physiological mechanisms

Astrid Slany
Department of Analytical Chemistry, University of Vienna, Währinger Straße 38, 1090 Vienna, Austria
astrid.slany@univie.ac.at

Recent advances in proteomics technologies have given us the opportunity to answer complex and clinically relevant questions and better understand cellular processes involved in patho-physiological mechanisms. Especially deep insights are gained from comprehensive in-depth proteome profiling studies investigating not only disease-causing cells, but also cells that may contribute to disease development and progression in an indirect way. Such comprehensive analyses pave the way for the development of improved and, most importantly, of personalized treatment strategies.

RNA Bioinformatics - From Transcriptomics to Structureomics

Andrea Tanzer
Department of Theoretical Chemistry, University of Vienna, Währinger Straße 17, 1090 Vienna, Austria
andrea.tanzer@univie.ac.at

How is genetic information organized and interpreted to drive cellular processes? This is one of the fundamental questions addressed by Bioinformatics. Big Data analysis and omics approaches have kick-started a plethora international research consortia and initiatives to decipher genomes, one of which is the ENCODE project (Encyclopedia of DNA Elements). By integrating results obtained from different omics analysis we try to gain insights on how the individual layers of regulatory networks and their products are interconnected. In my talk I will outline how transcriptomics, genomics and structureomics can be combined to move towards functional genome annotation.