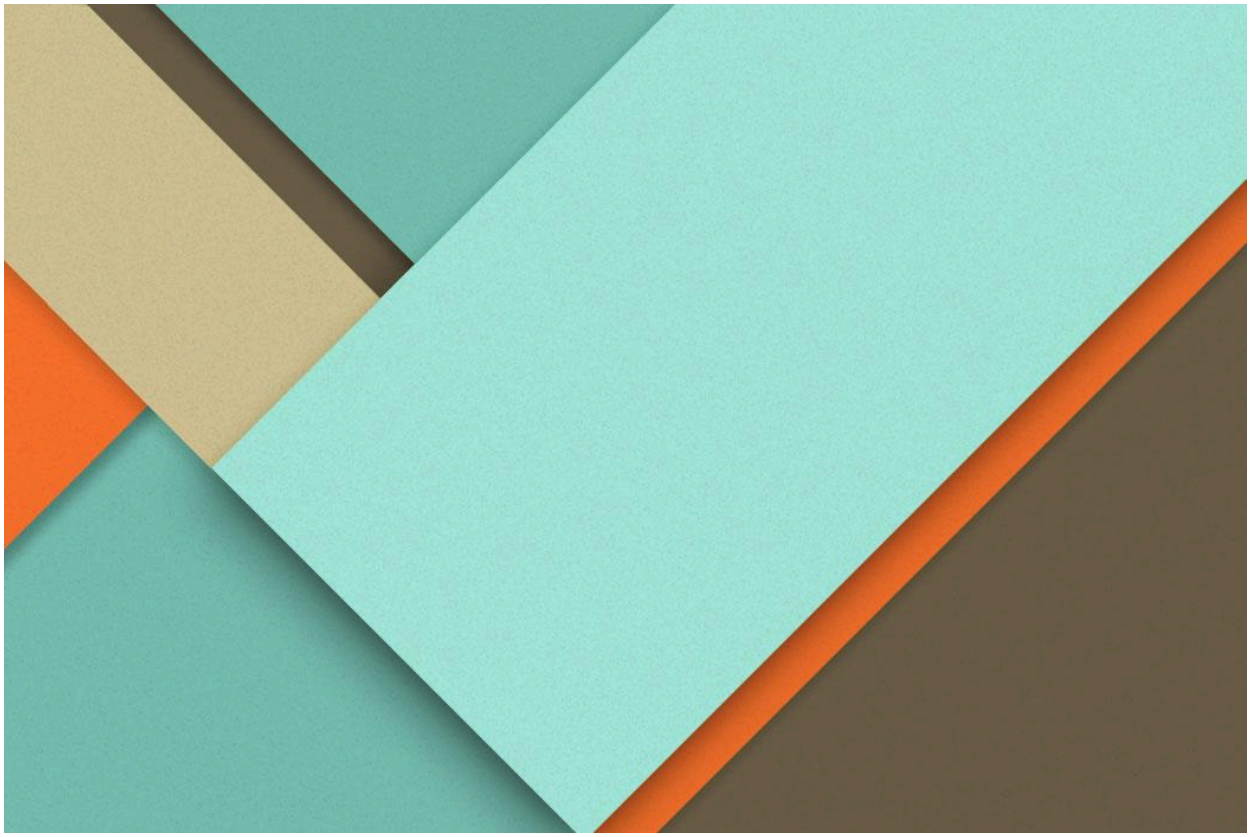

Joint DoSChem Retreat – 2026

Program and Book of Abstracts

Date: 25–27 February 2026 (Wednesday–Friday)

Location: Seehotel Rust, Am Seekanal 2-4, 7071 Rust

Program

1. Practical info
2. Wednesday, 25 February 2026
3. Thursday, 26 February 2026
4. Friday, 27 February 2026

Student Talks

5. First Session, Wednesday 13:30–14:50
    a. Mechanistic investigation of the influence of unsaturated fatty acids on platelet activation using direct infusion and LC-MS/MS, Alexander Eder
    b. New approach methodologies (NAMs) for assessing chemical/mechanical impact on intestinal barrier integrity, Janice Bergen
    c. Polar Bonds, Hot Bands: Anti-Stokes Fluorescence in BN-doped Trapeziumenes , El Czar Galleposo
    d. The UC-MSC Glycolipidomics: Resolving Biological Variability in 3D Models via Cold-Mechanical Homogenization and Multi-staged LC-HRMS, Amirreza Dowlati Beirami
6. Second Session, Thursday 09:00–10:20
    a. N-heterocyclic carbene capped gold nanoparticles. The one-pot reaction to rule them all., Robert Richstein
    b. The Core–Shell Conformational Space of Compartmentalized Single-Chain Nanoparticles by Paramagnetic and Hyperpolarized NMR Spectroscopy, Federico Faglia
    c. A dimetallic rotaxane enabling enzymatic-like photocatalysis, Konstantinos P. Zois
    d. Enhancing spatial resolution in Mass Spectrometry Imaging, Jannik Witte

7. Third Session, Thursday 10:50–12:10

a. Photooxidation of vanillic acid and its structure at the air-water interface, Manuel Hofmann

b. The MTR4-NRDE2 Complex: Structural and Functional Implications in RNA Degradation, Maximilian Mager

c. LSPR-Raman for detailed MIPs characterization, Ester Iatta

d. Hunting for the aggregation culprits: Individual and combined effects of post-translational modifications on tau pathology, Miriam Preissler

Poster Presentations

8. First Poster Session, Wednesday 17:00–18:30

9. Second Poster Session, Wednesday 19:30–21:00

10. Third Poster Session, Thursday 17:00–18:30

Practical info

- **Bus travel meeting point (Wed 25.02. 08:45) at Busparkplatz Schwedenplatz**, 1010 Wien (Google Maps Link, OpenStreetMap Link)
- for Spa/Wellness: bring your swimsuit, for running club and hike: bring suitable shoes and proper clothes, for bird watching: bring a camera (optional)

Wednesday, 25 February 2026

08:45–10:30 — Bus Travel to the Venue

10:30–11:00 — Arrival & Registration

11:00–12:00 — Invited Speaker - **Emanuel Schwarzhans** (University of Malta) - Talk*: Philosophysics: The (Pre-)History of the Foundations of Quantum Physics in the Viennese Cultural Context*

12:15–13:15 — Lunch

13:30–14:50 — Student Talks (1–4 / 12)

14:50–15:20 — Coffee Break

15:20–15:40 — From Admission to your Dissertation - Information session by the study programme director of the Doctoral Study Programme in Chemistry **Prof. Ellen Backus**

15:40–16:40 — Ice Breaker / Housekeeping / Announcements

16:40–17:00 — Coffee Break

17:00–18:30 — Poster Session (1 / 3)

18:30–19:30 — Dinner

19:30–21:00 — Poster Session (2 / 3)

Thursday, 26 February 2026

Morning run

08:00–09:00 — Breakfast

09:00–10:20 — Student Talks (5–9 / 12)

10:20–10:50 — Coffee Break

10:50–12:10 — Student Talks (9–12 / 12)

12:15–13:15 — Lunch

13:30–16:30 — Social / Fun Activity

16:30–17:00 — Coffee Break

17:00–18:30 — Poster Session (3 / 3)

18:30–19:30 — Dinner

19:30–20:00 — Feedback Session

20:00-21:00 — Evening Activity

Friday, 27 February 2026

08:00–09:00 — Breakfast

09:00–10:30 — Soft-skill Workshops

- **PI workshop:** *Communicating Science Beyond the Lab — Coaching for On-Camera and Lay Audience Presentations* – with professional speech coach and ORF moderator **Bernhard Eppensteiner**
- **PhD Workshop A:** *Managing Stress in the Lab — A PhD Survival Guide* - with Dr. **Hannah Tschenett**
- **PhD Workshop B:** *Managing Your Manager* - with **Svitlana Kalitsun**

10:30–11:30 — Coffee Break & informal time to talk to trainers

11:30–12:30 — Invited Speaker - **Thorsten Teutenberg** (Institute of Environment & Energy, Technology & Analysis e.V., Duisburg) – Talk: *The Dark Lab is near - But this is not the end of the analytical scientist*

12:45–13:45 — Lunch

14:15 — Departure for return

Student Talks - First Session, Wednesday 13:30–14:50

Mechanistic investigation of the influence of unsaturated fatty acids on platelet activation using direct infusion and LC-MS/MS

Alexander Eder, Wednesday, 25th February, 13:30 - 13:50

Supervisor: Robert Ahrends

Authors: Alexander Eder [ab], Philipp Mourikis [c], Stefanie Rubenzucker [ab], Cristina Coman [a], Amin Polzin [cd], Robert Ahrends [a]*

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Technical advances in mass spectrometry nowadays enable the analysis of the highly complex lipid space composed of up to 105 different molecules that in many cases only differ in the amount or position of double bonds. [1] Using a combined approach of analyzing low abundant signaling lipids with a comprehensive targeted LC-MS method [2] as well as quantifying the composition of membrane lipids with direct-infusion high-resolution mass spectrometry in untargeted measurements allows us to get a full picture of the molecular mechanisms in cells. Since lipids play a role in many classes of disease, there is strong interest in uncovering metabolic pathways to find new drug targets as well as to find biomarkers to describe the health status of patients. One example is cardiac disease, where recent clinical studies have shown positive effects of omega-3 fatty acids (O3FAs) such as eicosapentaenoic acid (EPA) on plaque formation and the occurrence of cardiac events when supplemented in high-risk patients. [3], [4] However, the underlying mechanisms behind the effects described above are still not fully understood. [5] Ex-vivo experiments with isolated platelets showed that EPA is more effective than other O3FAs in competing with arachidonic

acid for the production of platelet-stimulating thromboxane A2, explaining the varying efficiency of clinical trials on a mechanistical level. Leveraging the unique position of our research group between bioinformatics, analytical method development and practical application future research will focus on quantifying the complete metabolic pathway and tracing the path of individual lipid species throughout platelet activation.

[1] C. Hu, Q. Duan, und X. Han, „Strategies to Improve/Eliminate the Limitations in Shotgun Lipidomics“, PROTEOMICS, Bd. 20, Nr. 11, S. 1900070, 2020, doi: 10.1002/pmic.201900070.

[2] S. Rubenzucker, M.-C. Manke, R. Lehmann, A. Assinger, O. Borst, und R. Ahrends, „A Targeted, Bioinert LC–MS/MS Method for Sensitive, Comprehensive Analysis of Signaling Lipids“, Anal. Chem., Bd. 96, Nr. 23, S. 9643–9652, Juni 2024, doi: 10.1021/acs.analchem.4c01388.

[3] D. L. Bhatt u. a., „Cardiovascular Risk Reduction with Icosapent Ethyl for Hypertriglyceridemia“, N. Engl. J. Med., Bd. 380, Nr. 1, S. 11–22, Jan. 2019, doi: 10.1056/NEJMoa1812792.

[4] M. J. Budoff u. a., „Effect of icosapent ethyl on progression of coronary atherosclerosis in patients with elevated triglycerides on statin therapy: final results of the EVAPORATE trial“, Eur. Heart J., Bd. 41, Nr. 40, S. 3925–3932, Okt. 2020, doi: 10.1093/eurheartj/ehaa652.

[5] X. Wang, S. Verma, R. P. Mason, und D. L. Bhatt, „The Road to Approval: a Perspective on the Role of Icosapent Ethyl in Cardiovascular Risk Reduction“, Curr. Diab. Rep., Bd. 20, Nr. 11, S. 65, Okt. 2020, doi: 10.1007/s11892-020-01343-7.

New approach methodologies (NAMs) for assessing chemical/mechanical impact on intestinal barrier integrity

Janice Bergen, Wednesday, 25th February, 13:50 - 14:10

Supervisor: Giorgia Del Favero

Authors: Janice Bergen[1,2,3], Christian Fellinger[4,5,6], Claudia Iriarte-Mesa[8], Doris Marko[1], Freddy Kleitz[8], Christian Schröder[7], Giorgia Del Favero[1,2]

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3 Vienna Doctoral School in Chemistry (DoSChem), University of Vienna, Vienna, Austria

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6 Vienna Doctoral School of Pharmaceutical, Nutritional and Sport Sciences (VDS PhaNuSpo), University of Vienna, Vienna, Austria

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8 Department of Functional Materials and Catalysis, Faculty of Chemistry, University of Vienna, Vienna, Austria

New approach methodologies (NAMs) are emerging as essential tools to modernize chemical risk assessment by enabling efficient, high-throughput evaluation of both well researched and data-poor substances. These in vitro, in silico and omics-based approaches aim to enhance human relevance by probing mechanistic toxicity pathways, thereby improving the biological plausibility of risk assessments compared to traditional animal tests. NAMs also offer a significant opportunity to reduce reliance on animal (vertebrate) studies, aligning safety assessment practices with ethical, societal and regulatory drivers to implement the 3Rs principle. In addition, the integration of NAM-derived evidence can support smarter testing strategies, improve prioritization, and optimize resource allocation within regulatory decision-making. Here a combined in vitro/in silico application will demonstrate a NAMs approach to elucidate intestinal barrier function using tight junction protein claudin-4 as a target. Collectively, these developments position NAMs as a cornerstone for a more predictive, ethical, and science-driven framework for future chemical safety evaluations.

Polar Bonds, Hot Bands: Anti-Stokes Fluorescence in BN-doped Trapeziumenes

El Czar Galleposo, Wednesday, 25th February, 14:10 - 14:30

Supervisor: Davide Bonifazi

*Authors: El Czar Galleposo†, Nils Pellinger†, Mariel Antonella Lambri, Lorenzo Riccio, Silvina Carla Pellegrinet, and Davide Bonifazi**

Hot-band absorption–induced anti-Stokes fluorescence (HBA-ASF) is commonly observed in organic chromophores. However, no clear structure–property relationship has yet been established to achieve an elicit and resolvable hot-band absorption peak and anti-Stokes fluorescence (ASF). Here, we report a systematic study of HBA-ASF in BN-doped trapeziumenes. We demonstrate that HBA-ASF in these trapeziumenes arises from vibronic bands involving the B–N and N–B–N bonds, with one example exhibiting an elicit and resolvable hot-band with a molar absorption coefficient as high as 1058 M-1 cm-1. Comparison across the molecular series reveals that efficient HBA-ASF arises from a delicate balance between thermal harvesting and the anti-Stokes fluorescence quantum yield, the latter being governed by non-radiative excited-state kinetics. Our results show that an elicit and resolvable hot-band absorption peak and ASF can be achieved by tuning the substituents attached to the B and N atoms in BN-doped trapeziumenes.

The UC-MSC Glycolipidomics: Resolving Biological Variability in 3D Models via Cold-Mechanical Homogenization and Multi-staged LC-HRMS

Amirreza Dowlati Beirami, Wednesday, 25th February, 14:30 - 14:50

Supervisor: Evelyn Rampler

Authors: Amirreza Dowlati Beirami[1,2], Dominik Egger[3], Evelyn Rampler[1]*

1 Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Waehringer Str. 38, 1090, Vienna, Austria;

2 Vienna Doctoral School in Chemistry (DoSChem), University of Vienna, Waehringer Str. 42, 1090, Vienna, Austria;

3 Institute of Cell Biology and Biophysics, Leibniz University, Hannover, Herrenhäuser Str. 2 – Building 4137, 30419 Hannover, Germany.

Glycosphingolipid (GSL) patterns change during the differentiation of mesenchymal stem cells (MSCs). Research by Hohenwallner et al. shows that standard 2D cultures of single-donor human adipose-derived MSCs reveal diverse ganglioside species linked to specific cellular states and lineage commitments (1). Additionally, ganglioside-rich lipid rafts are crucial for multilineage differentiation and signal transduction(2). However, GSL profiles from traditional 2D cultures may not capture the biological variability or three-dimensional microenvironments, especially for more primitive umbilical-cord-derived MSCs (UC-MSCs). This study aims to fill that gap by profiling the glycosphingolipidome of UC-MSCs from multiple donors in 3D-spheroid culture. UC-MSCs (N=3 donors) were differentiated into adipogenic, chondrogenic, and osteogenic lineages using a 3D spheroid culture system. To facilitate lipid extraction from dense spheroids, we employed a mechanical dissociation method with a Beatbox homogenizer. Primary profiling utilized the Orbitrap IQ-X in positive and negative modes. We also established an online 2D-LC-HRMS (HILICxRP) platform linked to EAD-ZenoTOF for high-resolution analysis of isomers and double-bond characterization. Multivariate analysis, revealed high inter-donor consistency with distinct GSL fingerprints for each cell lineage across all biological replicates. Preliminary data show clear lineage clustering, suggesting biologically significant glycolipidomic differences. These results indicate that the 3D spheroid model can yield lineage-specific glycolipidomic profile across diverse human donors. This study

demonstrates the efficacy of cold-mechanical homogenization for the dissociation of 3D spheroids and validates lineage markers across three donors, establishing a foundation for quality control in stem cell therapies. Moreover, the developed 2D-LC-EAD workflow serves as a platform for addressing isomeric ambiguities.

1. Hohenwallner K, Troppmair N, Panzenboeck L, Kasper C, El Abiead Y, Koellensperger G, et al. Decoding Distinct Ganglioside Patterns of Native and Differentiated Mesenchymal Stem Cells by a Novel Glycolipidomics Profiling Strategy. JACS Au. 2022 Nov 28;2(11):2466–80.

2. Santilli F, Fabrizi J, Martellucci S, Santacroce C, Iorio E, Pisanu ME, et al. Lipid rafts mediate multilineage differentiation of human dental pulp-derived stem cells (DPSCs). Front Cell Dev Biol. 2023 Nov 9;11.

Student Talks - Second Session, Thursday 09:00–10:20

N-heterocyclic carbene capped gold nanoparticles. The one-pot reaction to rule them all

Robert Richstein, Thursday, 26th February, 09:00 - 09:20

Supervisor: Michael Reithofer

Authors: Robert Richstein, Constantin Eisen, Dr. Sophie Thomas, Michael Reithofer

N-heterocyclic carbene (NHC) stabilized gold nanoparticles offer superior chemical and thermal stability, making them an attractive candidate for sensing and catalytic applications. However, conventional routes to install NHC ligands on nanoparticle surfaces typically involve multistep procedures and often harsh reagents. Recent work has shown that imidazolium precursors can be activated under mild conditions through transient CO2 adducts, even enabling one step NHC generation so far limited to bulk systems. Here we present an analogous, but mechanistically distinct, approach for gold nanoparticles. Control experiments demonstrate that NHC formation on the nanoparticle surface proceeds without a CO2-adduct intermediate and instead follows a direct mild-base activation pathway. We optimized reaction conditions to minimize ligand rearrangement and particle ripening, yielding highly stable nanoparticles high NHC surface coverage. The method is compatible not only with different wingtip-substituted imidazolium salts but also with various NHC classes, including mesoionic carbenes. These results provide a general, mild, and scalable strategy for preparing robust NHC-functionalized gold nanomaterials. Mechanistic analysis revealed that, unlike prior reports, neither HCO3- nor CO2 adduct intermediates are involved whereas NHC formation on the gold surface proceeds through a direct mild-base activation pathway.

The Core–Shell Conformational Space of Compartmentalized Single-Chain Nanoparticles by Paramagnetic and Hyperpolarized NMR Spectroscopy

Federico Faglia, Thursday, 26th February, 09:20 - 09:40

Supervisor: Dennis Kurzbach

Authors: Federico Faglia, Justus F. Thümmler, Christopher Pötzl, Milan Zachrdla, Ertan Turhan, Dennis Kurzbach, Wolfgang H. Binder

Single-chain nanoparticles (SCNPs) are formed by the collapse of individual polymer chains, generating entities comparable to proteins in size, internal structure, and function. Especially, the formation of hierarchies induced by complex folds of linear polymer chains can result in internalized compartments, reminiscent of pockets in enzymes. However, direct experimental access to their architecture or mode of contact remains a challenge. Here, the conformational organization of a prototypical amphiphilic SCNP is dissected to reveal conformational details of its internally heterogeneous morphology driven by site-specific intramolecular compaction. Using a synergistic combination of unconventional paramagnetic NMR, hyperpolarized water-based dissolution dynamic nuclear polarization (d-DNP), and NMR-guided molecular dynamics simulations, intramolecular structures and solvent accessibility are mapped at atomistic resolution. These findings uncover distinct nanoscopic compartments formed via back-folding of PEG side chains toward the SCNP backbone. Furthermore, these compartments shield internal segments, mimicking hydrophobic pockets found in folded proteins. Thus, this work introduces a transferable methodology for probing functional compartmentalization in synthetic macromolecules. It provides a tool for rationally designing next-generation nanomaterials and enzyme mimetics with programmable internal order via residue-resolved structural information. At the same time, this method's prowess is evidenced through a high-resolution description of the local conformations found within hierarchically structured SCNPs.

A dimetallic rotaxane enabling enzymatic-like photocatalysis

Konstantinos P. Zois, Thursday, 26th February, 09:40 - 10:00

Supervisor: Leticia González

Authors: Konstantinos P. Zois, Marius Müßler, Mohini Semwal, Louis Blechschmidt, Benjamin M. W. Roberts, Linda Zedler, Alexander K. Mengele, Patrick A. Hoffman, L. Dominik Kapp, Max von Delius, Benjamin Dietzek-Ivanšić, Sven Rau, Leticia González

Artificial photosynthesis is a holy grail in catalysis. From a synthetic point of view, the prevention of catalyst degradation is a primary concern and remains an important obstacle. Structural motifs that are ubiquitous in nature, such as membrane and protein integration of the photosynthetic apparatus, are a source of inspiration. Herein, we report a photocatalytically active rotaxane mimicking photosystem I. Chemical and photoinduced degradation is tackled by mechanically interlocking a dimetallic dyad in a cucurbit[7]uril ring, forming a rotaxane system. The dyad consists of a Ru-photosensitiser that is covalently bound to a Rh-catalyst, via an alkyne-based bridging ligand. The ring offers protection to the alkyne groups, enabling an overall efficient and continuous photocatalysis that features enzyme-like behaviour. This talk will provide insights, through the lens of computational chemistry, into the rationally engineered interplay between supramolecular assemblies in (photo)catalysis, serving as a paradigm for sustainable methodologies in artificial photosynthesis. Computational results from density functional theory and molecular dynamics simulations will be discussed in order to understand how structural and solvation characteristics affect photophysics, charge-transfer processes, and catalysis. The interplay between theory and experiment will be stressed throughout the talk.

Enhancing spatial resolution in Mass Spectrometry Imaging

Jannik Witte, Thursday, 26th February, 10:00 - 10:20

Supervisor: Gunda Köllensperger

Authors: Jannik Witte, Patrick Müller, Gunda Köllensperger

Imaging techniques are one of the most relevant tools to evaluate the spatial organization, molecular composition, and dynamics of biological structures in cells and tissues. One emerging technique within bioimaging is the application of mass spectrometry imaging to obtain spatially resolved information. Applications of this range from highly multiplexed antibody labelling strategies for protein localization to untargeted approaches to unravel molecular distributions in metabolites and lipids. The size resolution limit of these techniques is limited by the physical properties of the ionization technique used. To circumvent these limitations, my PhD project focuses on the employment of tissue expansion techniques to physically enlarge samples and resolve finer structures and molecular patterns. Tissue expansion utilises the polymerization of a swellable hydrogel within soft matter. The hydroscopic properties of the formed gel result in isotropic enlargement of the sample upon contact with water. Classically employed in fluorescence microscopy, this technique has been shown to be compatible with mass spectrometry imaging and offers a high improvement in resolution.

Student Talks - Third Session, Thursday 10:50–12:10

Photooxidation of vanillic acid and its structure at the air-water interface

Manuel Hofmann, Thursday, 26th February, first slot, 10:50 - 11:10

Supervisor: Ellen Backus

Authors: Manuel Hofmann[1,2], Ellen H. G. Backus[1,2]

1 University of Vienna, Faculty of Chemistry, Institute of Physical Chemistry, Währinger Str. 42, 1090 Vienna, Austria.

2 University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria.

Phenolic compounds such as vanillic acid are released in the atmosphere by biomass burning and can undergo aqueous phase reactions to form secondary organic aerosols (SOA). Particularly the photooxidation of vanillic acid serves as a potential source of Humic-Like Substances (HULIS), as high-molecular-weight components of this SOA. These HULIS can strongly affect atmospheric chemistry due to light absorption and related processes. As the air-water interface represents a unique chemical environment than can significantly affect structural behaviour and reactivity, these reactions might have very different dynamics at the interface compared to the bulk. To specifically probe this interface, sum-frequency generation (SFG) spectroscopy and surface tension measurements are employed, offering complementary insights into molecular behavior. This study examines vanillic acid at the air-water interface over various pH values, before and after exposure with UV light. Photooxidation is induced by UV irradiation with H2O2 to generate hydroxyl radicals, while control experiments with vanillic acid alone separate direct photolysis from radical mediated processes. Preliminary SFG spectra show pH-dependent vibrational signatures of adsorbed species and significant changes upon photoreaction. The goal is to identify reaction products, structural rearrangements, and pH effects on the photoreaction of vanillic acid.

The MTR4-NRDE2 Complex: Structural and Functional Implications in RNA Degradation

Maximilian Mager, Thursday, 26th February, 11:10 - 11:30

Supervisor: Sebastian Falk

Authors: Maximilian Mager, Marina Pletzer, Sebastian Falk

RNA degradation is essential for maintaining RNA homeostasis and regulating gene expression and thus represents a central component of cellular RNA metabolism. In the nucleus, the RNA exosome cooperates with cofactors such as the RNA helicase MTR4 to mediate the degradation of RNA transcripts. The specificity of RNA targeting is influenced by proteins associated with MTR4, among which NRDE2 has emerged as a potential regulator. The functional role of the NRDE2–MTR4 interaction in nuclear RNA degradation, however, remains poorly understood. Although NRDE2 has previously been described as a negative regulator of RNA decay, our findings indicate that it may instead promote RNA degradation. This apparent discrepancy underscores the need for a more detailed mechanistic understanding of NRDE2 function. Using a combination of cryo-electron microscopy, molecular dynamics simulations, and biochemical assays, we investigate the structural and functional properties of the MTR4–NRDE2 complex. Our biochemical analyses reveal that NRDE2 stimulates MTR4 activity, supporting a role for the complex as a novel RNA-targeting factor. In addition, prior evidence linking NRDE2 to pre-mRNA splicing suggests a functional connection between splicing and nuclear RNA degradation pathways, which we aim to explore further.

LSPR-Raman for detailed MIPs characterization

Ester Iatta, Thursday, 26th February, 11:30 - 11:50

Supervisor: Peter Lieberzeit

Authors: E. Iatta[1,2], P. Lieberzeit[1]*

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*ester.iatta@univie.ac.at

Molecularly Imprinted Polymers (MIPs) are a particular class of polymeric materials designed to be selective for detecting a specific analyte. The main concept behind them is to allow the monomers to arrange around a template thanks to affine functional groups. Once the curing step is complete, the template can be removed and rebound as analyte [1]. Vast literature has been produced on MIP applications in analytical chemistry; however, direct characterization of the MIP selective region (also known as cavity) is very challenging. Indeed, structural models of cavities mostly rely on theoretical calculations and affinity tests. Herein, we aim at developing a method to observe the cavities or selective regions directly. The chosen approach utilizes a peculiar property of noble metals nanomaterials with Raman spectroscopy. In fact, shining a laser with the same wavelength as the one of plasmons' oscillation onto noble metal nanostructures triggers a resonance effect. This phenomenon is known as localized surface plasmon resonance Raman (LSPR-Raman) and results in an enhancement of the Raman signal originated in the nearest surrounding of the nanomaterial [2, 3]. Therefore, we chose to use gold nanostars (AuNSts) to form a self-assembled monolayer to lay on top of a styrene-co-ethylene glycol dimethacrylate MIP layer and then perform Raman measurement to highlight the surface features of the described substrate [4]. This talk will give an overview of the steps we covered so far to develop a characterization method for detailed analysis of MIPs.

1. Leibl, N., et al., Molecularly Imprinted Polymers for Chemical Sensing: A Tutorial Review. chemosensors, 2021. 9(6): p. 19.

2. Mayer, K.M., J.H. Hafer, and Department of Physics and Astronomy, Department of Chemistry,, and Laboratory for Nanophotonics,, Rice University,, Houston,, Texas 77005,, United States,, Localized Surface Plamon Resonance Sensor. American Chemical Society, 2011. 111: p. 3828–3857.

3. Jones, R.R., et al., Raman Techniques: Fundamentals and Frontiers. Nanoscale Research Letters, 2019. 14.

4. Zhang, F., et al., Reproducible fabrication of gold nanostar monolayers for surface-enhanced Raman spectroscopy-based trace detection. Journal of Raman Spectroscopy, 2022. 53(7): p. 1227-1237.

Hunting for the aggregation culprits: Individual and combined effects of post-translational modifications on tau pathology

Miriam Preissler, Thursday, 26th February, 11:50 - 12:10

Supervisor: Christian Becker

Authors: Miriam Preissler, Christian F.W. Becker

As global longevity rises, Alzheimer's disease (AD) is poised to become a defining challenge for medicine and society with up to 140 million people affected by 2050. AD profoundly impacts patients and caregivers while driving escalating healthcare costs. Despite extensive research, its exact molecular etiology remains unclear, and current treatments largely slow progression rather than modify disease. Improving treatment outcome requires earlier, more accurate diagnostics and the identification of actionable biomarkers and drug targets. A pathological hallmark of AD are amyloidogenic protein aggregates of amyloid β and tau. Physiological, monomeric tau promotes tubulin polymerization and stabilizes microtubules, whereas oligomeric and aggregated tau disrupts neuronal structure and plasticity. Tau from AD brains exhibits distinct post-translational modification (PTM) patterns, offering promising avenues for biomarker discovery and therapeutic development. Protein semisynthesis enables generation of site-specifically modified tau variants by ligating synthetic peptides or recombinant fragments. Herein, solid-phase peptide synthesis facilitates precise installation of defined PTMs including phosphorylation, acetylation and succinylation at target residues. Using this platform, we produced tau variants bearing discrete PTMs within the microtubule binding domain and assessed effects on aggregation highlighting the importance of semisynthesis in addressing our current knowledge gap regarding modification-specific effects. Further work will expand upon the biochemical characterization by assessing tubulin polymerization, liquid–liquid phase separation, cellular uptake, and cytotoxicity in SH-SY5Y cells.

First Poster Session, Wednesday 17:00–18:30

Presenter	Title	Poster #
Faissner Maximilian	From Structure to Screen: MD-Ready Enzyme-Substrate Pairs	1
Sommerauer Sophie	A Base-Catalyzed Strategy for the Synthesis of β-Aminoalkylsilanes from Vinylsilanes	2
Czernohlavek Christian	Interaction of polyoxometalates with model membranes	3
Berger Sabrina	Nasal Swab Analysis by LC-HRMS: Method Development and Performance Evaluation	4
Brandstetter Stefanie	Functional insights into Cereblon-mediated targeted protein degradation by chemical crosslinking and quantitative mass spectrometry	5
Staudinger Johannes Nikodemus	Radiolabelling of metal-based Photosensitizers for combined PDT, SPECT and Radiotherapy	6
Brenner Christina	Enhancing Chemical Space Coverage in Biological Matrices Through Orthogonal Ionization Techniques in LC-MS	7
Fritz Sebastian	Small Stereoselectively Deuterated Molecules at the Chemistry–Biology Interface	8
Ölzant Christoph	Examining the Thermal Behavior of Non-Stoichiometric Lithium Nickel Manganese Oxide LiNixMn2-xO4 Cathode Materials	9
Rajkovic Tina	Experimental Design for Robustness Evaluation of an LC-HRMS Workflow for urinary Exposomics	10
Wutschitz Judith	Development of Platinum-Group Metal Complexes with Tumor-Inhibiting Properties	11
Sidl Leonhard Paul	Rational design of mechanically active RNAs: de novo engineering exoribonuclease-resistant RNAs	12
Pusam Patrick	Buffering a biosensor-system enables selective real-time bacteria growth measurements	13

Presenter	Title	Poster #
Ratzer Noah Leon	Mutagenic and topoisomerase-poisoning potential of selected aflatoxin B1 precursors	14
Schweng Paul	Hypercrosslinked Polymers for Volatile and Very Volatile Organic Compound Capture Beyond Commercial Benchmarks	15
Hofmeister Angela	Unified Synthesis of Unconventional α-Polyhalogenated Amines through Hydroaminoalkylation	16
Jacobi Richard Wilhelm	Light-harvesting in DNA-liposomes hybrids: lessons learned	17
Back Hannah Susanne	Potentiating the Anti-Tumor Efficacy of Innate Immune System Engagers (ISErs) through Bispecific Immune Modulation	18
Vezonik Uroš	Direct Alkyl Swap as a Platform for Late-Stage Modification of Amines	19
Kovago Bence	Cross-linking polymers at the air-water interface	20
Königstein Vincent	Developing organic colours through rational mixing of molecular electrochromic hues	21
Vega Ces Sabela	Regioselective Synthesis of β,γ-Unsaturated Amides from Unactivated Alkenes	23
Schmied Sabrina Helena	Semisynthesis of Site-Specifically Phosphorylated Hsp27	24
Castillo Ma Robellene	Glyphosate Detection with Mass-sensitive sensors using Molecularly Imprinted Polymers: Polymerization Strategies and Application.	25
Rímon Martínez María José	Pan genome-scale metabolic modeling of Sulfolobus genus reveals medium - dependent metabolic diversity	26
Gouveia Carvalho Ana Cristina	Towards a novel tetraether lipid producer Haloferax volcanii	27
Stastna Katarina	Bacterial Responses to Biological Nitrification Inhibitors: Efficiency and Structural Insights	28

Presenter	Title	Poster #
Mädge Anna Sophie	Investigation of the Prion Protein: Genetic Code Expansion meets Semisynthesis	29
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