universität wien

Vienna Doctoral School in Chemistry

Book of Abstracts

5th International DoSChem Student Symposium

Sept 25 – 26, 2025

Program

Day 1

8:45 – 9:15	Registration
9:00 – 9:15	Symposium Opening by Dean Prof. Christian Becker & Head of DoSChem Prof. Ellen Backus
9:15 – 10:15	Panel B Keynote Speaker Dr. Andrea Patriarca *"When Chemistry meets Biology: Decoding Mycotoxigenic Fungi"*
10.15 – 10:30	DoSChem New ideas & exchange talks
10:30 – 11:15	Coffee Break
11:15 – 11:30	Patrick Lechner (panel A) *"Spin Frustration: A Key to Stability and Reactivity in Triangular Fe(III) Metal–Organic Frameworks"*
11:30 – 11:45	Julian Libiseller-Egger (panel B) *"Hybrid Modelling in Bioprocess Optimization"*
11:45 – 12:00	Christina Rodler (panel C) *"Synthesis of vincamine derivatives via Pictet-Spengler reaction and investigation of their biological activities"*
12:00 – 12:30	Networking activity
12:30 – 14:00	Lunch Break

Program

Day 1

14:00 – 15:00	Panel A Keynote Speaker Prof. Henrike Müller-Werkmeister *"Exploring Biomolecular Dynamics and Catalysis by 2D-IR Spectroscopy"*
15:00 – 15:15	Lukas Brandfellner (panel A) *"Aggregates and Drag Reduction: Calcium Alginate in Turbulent Flow"*
15:15 – 15:30	Cesar Eduardo Gutierrez Quevedo (panel C) *"Synthesis of Oxindole and Oxoquinoline Compounds and C–H Functionalization of Quinolines"*
15:30 – 16:15	Coffee Break
16:15 – 17:00	Prof. Douglas Stephan *"Frustrated Lewis Pairs: Reactivity across the Periodic Table"*
17:00 – 18:30	Poster Session with drinks (odd numbers)
18:30 – 20:00	Dinner

Program

Day 2

08:30 – 09:00	Registration
09:00 – 10:00	Panel C Keynote Speaker Prof. Jakob Albert *"Sustainable Reaction Concepts for Resilient CO2 and Biomass Valorization Processes"*
10:00 – 11:30	Poster Session with coffee (even numbers)
11:30 – 11:45	Dilara Farkhutdinova (panel A) *"Watching Water Dance Around $[Ru(bpy)_3]^{2+}$ in Real Time"*
11:45 – 12:00	Kirill Zhiliaev (panel C) *"Cationic Selenuranes – Bench-Stable Sources of Se(III) Radicals"*
12:00 – 12:15	Sebastian-Felix Fritz (panel C) *"Small Stereoselectively Deuterated Molecules at the Chemistry–Biology Interface"*
12:15 – 13:30	Lunch Break
13:30 – 14:30	Startup & academic career session with mzio, Vienna Textile Lab & Ass.-Prof. Oana Zeleznik
14:30 – 15:00	Career coaching with Dr. Yasmin Dolak-Struss
15:00 – 15:30	Award Ceremony & Concluding Remarks
15:30 – 18:00	Career Event with AGES, Cytiva, Grünenthal, mzio, Vienna Textile Lab & Dr. Yasmin Dolak-Struss + Pizza

Spin Frustration: A Key to Stability and Reactivity in Triangular Fe(III) Metal–Organic Frameworks

Patrick Lechner,[1,2] Gaurab Ganguly[1], Michael J. Sahre[3], Georg Kresse[3,4], Johannes C. B. Dietschreit[1*] and Leticia González[1*]

[1] *Institute of Theoretical Chemistry, University of Vienna, Währinger Str. 17, 1090 Vienna, Austria*
[2] *University of Vienna, Vienna Doctoral School in Chemistry (DoSChem)* [3]*University of Vienna, Faculty of Physics, Kolingasse 14, A-1090 Vienna, Austria* [4]*VASP Software GmbH, Berggasse 21, A-1090 Vienna, Austria*

[*]*Corresponding author: leticia.gonzalez@univie.ac.at*

High-spin density functional theory is widely used as the defacto standard computational ap- proach for modeling MIL-101(Fe) and related iron-based metal-organic frameworks. However, our research reveals that this convention overlooks a critical electronic feature: a competition between α- and β-spin alignment of the Fe^{3+} in the triangular $Fe_3(\mu_3{-}O)$ nodes, known as spin frustration. Using flip-spin DFT, we show that MIL-101(Fe) exhibits a spin-frustrated ground state, which the conventional high spin approximation fails to capture—leading to structural distortions, incorrect energetics, and misleading predictions of stability and reactivity. By ex- plicitly accounting for spin frustration, we not only recover the correct structure but also provide a unified explanation for the framework's temperature-dependent N_2 and CO fixation behavior. At room temperature, spin frustration enhances N_2 binding, while upon heating its N_2 fixation activity is reduced but facilitates CO adsorption via π-back bonding.[1] These findings chal- lenge the prevailing modeling paradigm and establish spin frustration as an electronic feature that must be considered for accurate description of triangular Fe-MOFs.[2]

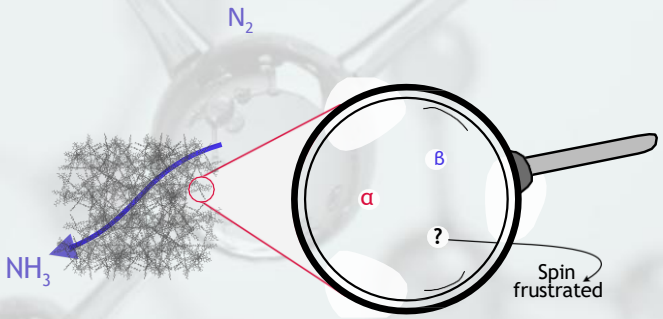


Figure 1: Unit cell of MIL-101(Fe) with enlarged triangular $Fe_3(\mu_3{-}O)$ node. The frustrated spin on the third iron atom, indicated by a question mark, must choose between α and β align- ment, resulting in the phenomenon known as spin frustration.

References

1 G. Li, F. Li, J. Liu, C. Fan, *J. Solid State Chem., 285, 121245 (2020).*

2 P. Lechner, G. Ganguly, M. J. Sahre, G. Kresse, J. C. B. Dietschreit, L. González, *Angw. Chem. Int. Ed. (2025)*, DOI: 10.1002/anie.202514014.

Synthesis of vincamine derivatives via Pictet-Spengler reaction and investigation of their biological activities

Christina Rodler[a,b*], Dominik Wenisch[c], Michael Jakupec[c], Johann Schinnerl[d] and Lothar Brecker[a]

[a]*University of Vienna, Faculty of Chemistry, Department of Organic Chemistry, Währinger Str. 38, 1090 Vienna, Austria;*
[b]*University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria*
[c]*University of Vienna, Faculty of Chemistry, Department of Inorganic Chemistry, Josef-Holaubek-Platz 2 (UZA II), 1090 Vienna, Austria;*
[d]*University of Vienna, Faculty of Life Sciences, Department of Botany and Biodiversity Research, Rennweg 14, 1030 Vienna, Austria;*

- Email: christina.rodler@univie.ac.at

Plant secondary metabolites, especially alkaloids, are famous for their remarkable biological and pharmacological properties. Of particular interest in this substance group is the monoterpene indole alkaloid vincamine, which is mainly isolated from *Vinca minor* and exhibits not only neuroprotective but also vasodilatory and nootropic activities.[1] Recently, vincamine has been investigated as potential cancer treatment[2] as well as potential acetylcholine esterase inhibitor, which plays a role in the treatment of Alzheimer's disease.[3,4]

In this work, derivatives of vincamine bearing various aliphatic, branched, or aromatic residues are produced. By coupling different chloro-substituted aldehydes and tryptamine in a Pictet-Spengler reaction (PSR) a double cyclization leads to tetracyclic vincamine derived substances in a range of 12 % to 66 % yield. Corresponding oxidized side products have been isolated in yields of 7 % to 67 %, and characterized via NMR spectroscopy. Subsequently, some of the synthesized compounds are further functionalized by introducing a Boc-group at the indole nitrogen.

Selected compounds have been subjected to cell viability assays resulting in cytotoxic activities ranging from 19 µM to 55 µM against ovarian teratocarcinoma cancer cell line (CH1/PA-1). Additionally, enzyme inhibition activities have been investigated using acetylcholinesterase and α-glucosidase. For one of the tested compounds an IC_{50} value of 33 uM against α-glucosidase has been observed.

In the future, the compound library will be extended by using 7-azatryptamine as indole component in the PSR as well as subsequent modification reactions. Also, it will be investigated if the same oxidative side reaction occurs. Regarding additional bioassays, it is planned to determine possible interactions of the synthesized compounds with β-amyloid (Aβ42) using CD spectrometry.

References

[1] Fandy T. E.; Abdallah I.; Khayat M.; Colby D. A.; Hassan H. E., In vitro characterization of transport and metabolism of the alkaloids: vincamine, vinpocetine and eburnamonine, *Cancer Chemotherapy and Pharmacology*, **2016**, *77*(2), 259-267. https://doi.org/10.1007/s00280-015-2924-3
[2] Dhyani P.; Quispe C.; Sharma E. *et al.* Anticancer potential of alkaloids: a key emphasis to colchicine, vinblastine, vincristine, vindesine, vinorelbine and vincamine, *Cancer Cell International,* **2022**, *22*(206), 1-20. https://doi.org/10.1186/s12935-022-02624-9
[3] Han J.; Qu Q.; Qiao J.; Zhang J., Vincamine alleviates amyloid-β 25–35 peptides-induced cytotoxicity in PC12 cells, *Pharmacognosy Magazine,* **2017**, *13*(49), 123-128. https://doi.org/10.4103/0973-1296.196309
[4] Syed Sayeed A., Khatoon A.; Sajid Khan M.; Khalid M.; Alharbi A. M.; Siddiqui M. H., Evaluation of vincamine against acetylcholinesterase enzyme: cetylcholinesterase enzyme inhibition, *Cellular and Molecular Biology*, **2022**, *68*(7), 14–21. https://doi.org/10.14715/cmb/2022.68.7.3

Hybrid modelling in bioprocess optimization

DoSChem Symposium Sept. 2025, Julian Libiseller-Egger

Bioprocessing plays a crucial role in producing therapeutics, sustainable materials, and food products, but modelling these complex systems remains challenging due to incomplete mechanistic understanding and limited data. Traditional approaches rely on either physics-based equations (mechanistic models) or purely data-driven methods, each with limitations in accuracy, interpretability, and scalability. Hybrid modelling offers a powerful solution by combining the strengths of both: embedding mechanistic knowledge (e.g., mass balances as ordinary differential equations, ODEs) with flexible data- driven components like neural networks to capture unknown dynamics.

In this talk, I am going to give a brief introduction to bioprocess optimization and hybrid models. We will then explore how recent advances from the wider field of machine learning, such as differentiable ODE solvers, enable end-to-end training of these models, greatly simplifying the process of setting up such models and in extension their utility.

The presentation will focus on intuitive understanding of core concepts and feature basic examples with code snippets and visualizations.

Aggregates and Drag Reduction: Calcium Alginate in Turbulent Flow

L. Brandfellner[1,2*], A. Bismarck[1,2], H. W. Müller[1]
[1]*IMCR, Faculty of Chemistry, University of Vienna, Vienna, Austria*
[2]*DCAFM, Faculty of Physics, University of Vienna, Vienna, Austria*
[*]*lukas.brandfellner@univie.ac.at*

Polymeric drag reduction (DR) is the reduction of flow resistance in turbulent flow of liquids achieved by high molecular weight polymers [1]. Polymers hinder vortex formation, increase flow speed and reduce pumping costs in turbulent flow. At the same time, interaction with turbulent vortices degrades the polymers and diminishes drag reduction [2]. Covalent bonds are broken irreversibly and DR is lost. We explored the potential of noncovalent bonds to provide structures of high molecular weight, which can provide DR and reform after degradation in turbulent flow [3]. Strong noncovalent bonds are needed in order for the structures not to be destroyed already at low shear rates [3]. The polysaccharide alginate forms aggregates in the presence of divalent ions like Ca^{2+}. In un-aggregated state alginate is known as a DR agent albeit limited by its chain rigidity and molecular weight [4]. We performed flow experiments with varying alginate and Ca^{2+} concentration, alginate molecular weight and aggregation time. Aggregates provided increased DR but degraded within a few runs of our flow facility, as seen in Figure 1. Resting at ambient conditions (1 to 7 days) allowed re-aggregation and restored high DR. Cycles of degradation in flow and re-aggregation at ambient conditions were repeated multiple times, proofing the reversibility of the process in contrast to the irreversible loss of DR in systems based solely on covalent bonds.

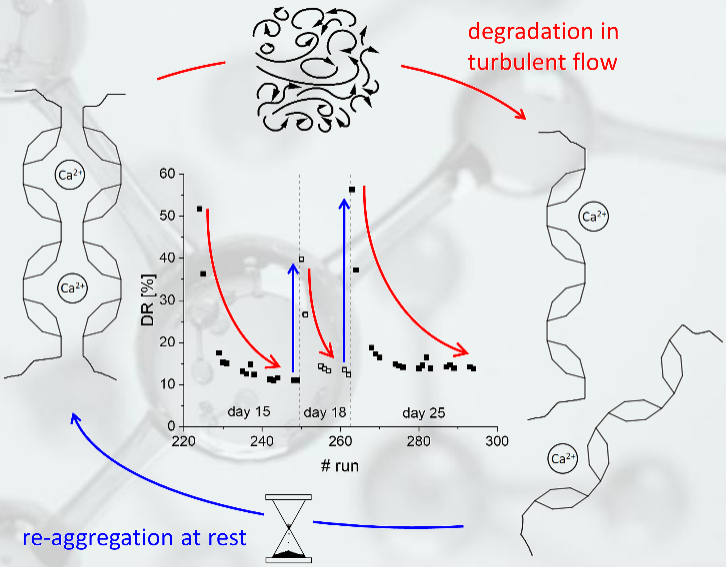


Figure 1: DR of Ca^{2+} alginate solution in multiple degradation and re-aggregation cycles. Aggregates provided high DR during the first cycle of a day while single alginate molecules provided only very low DR.

Acknowledgments

This work was supported by the Doctoral College Advanced Functional Materials (DCAFM) funded by the Austrian Science Fund (FWF, Grant No.: DOC 85 doc. funds).

References

[1] Toms, B.A. *Proceedings of the 1st International Congress on Rheology.* **1948**, 135.
[2] Soares, E. J. Review of mechanical degradation and de-aggregation of drag reducing polymers in turbulent flows. *J. Non-Newt. Fluid Mech.* **2020**, 276.
[3] Muratspahić, E.; Brandfellner L.; Schöffmann, J.; Bismarck, A.; Müller, H. W. Aqueous Solutions of Associating Poly(acrylamide-co-styrene): A Path to Improve Drag Reduction? *Macromolecules* **2022**, 55.
[4] Han, W. J.; Choi, H. J. Role of bio-based polymers on improving turbulent flow characteristics: materials and applications. *Polymers* **2017**, 9.

Synthesis of Oxindole and Oxoquinoline Compounds and C–H Functionalization of Quinolines

Authors: César Eduardo Gutiérrez-Quevedo[1,2], Christian Dank[2]

Institutions: [1]Institute of Applied Synthetic Chemistry, Vienna University of Technology, Vienna, Austria [2] Institute of Organic Chemistry, University of Vienna, Vienna, Austria

Oxo-indoles and oxo-quinolines are heterocyclic scaffolds extensively studied in medicinal chemistry due to their broad spectrum of biological activities such as antifibrotic, antibacterial, antitumor effects, etc. [1-3].

Their therapeutic relevance is evidenced by approved drugs such as Ivacaftor (for cystic fibrosis), Sunitinib (for cancer), and Nintedanib (for pulmonary fibrosis) [1,3]. However, the clinical utility of some of these compounds is often limited by side effects, contraindications, and variable patient response [4].

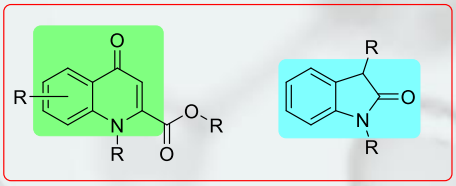


Figure 1: Structures of oxo-indole and oxo-quinoline

Hence, there is a critical need to develop novel analogues with improved efficacy and safety profiles. The application of C–H bond activation for the synthesis and functionalization of these heterocycles is a powerful strategy to access to novel analogues necessary for comprehensive drug discovery [5].

Our research aims to address this need by leveraging innovative synthetic methodologies, particularly Catellani-type C–H functionalization, to develop new lead compounds as potential alternative treatment options for respiratory disorders.

References

[1] P Kaur, A., Anuradha, A., Chandra, T., Tanwar, S. K., Sahu, A., Mittal, A. *Chem. Biol. Drug Des.*; **2022**, 100(6), 765–785. DOI: 10.1111/cbdd.14025

[2] El-mrabet, A. Haoudi, A. Kandri-Rodi, Y. Mazzah, A., *Organics*; **2025**, *6*(2), 1–49. DOI: 10.3390/org6020016

[3] Khetmali, Y.M-, Shivani, M., Murugesan, M., Sekhar, K.V.G.C., *Biomed Pharmacother.141*; 2021, 111842. DOI: 10.1016/j.biopha.2021.111842

[4] Serra López-Matencio, J. M., Gómez, M., Vicente-Rabaneda, E.F., González-Gay, M.A., Ancochea, J., Castañeda, S., Pharmaceuticals; 2021, 14(8), 1–16. DOI: 10.3390/ph14080819

[5] Chen, Z., Zhang, F., Tetrahedron 134; 2023, 133307. DOI:10.1016/j.tet.2023.133307

Watching water dance around $[Ru(bpy)_3]^{2+}$ in real time

Dilara Farkhutdinova, Sebastian Mai, Leticia González

Institute of Theoretical Chemistry, University of Vienna, Währinger Str. 17, 1090 Vienna, Austria

Polypyridine complexes of ruthenium(II), such as $[Ru(bpy)_3]^{2+}$, are central to applications in light- harvesting and photocatalysis, where their efficiency is strongly influenced by interactions with the surrounding solvent. After photoexcitation, the redistribution of energy between solute and solvent determines relaxation pathways, yet simulating the evolution of the solvent explicitly in real time is a formidable challenge. In this work, we present a theoretical investigation of the relaxation dynamics of $[Ru(bpy)_3]Cl_2$ in aqueous solution. Our goal is to time-resolve the evolution of the electronic and nuclear degrees of freedom of solute and solvent, the structural changes within the metal complex, and the solvent reorganization after excitation. To this end, we employed a novel hybrid quantum mechanics/molecular mechanics framework that exploits linear vibronic coupling potentials to generate thousands of trajectories in an affordable manner.

Analysis of the time-dependent electronic wave function provides unprecedented insight into the timescales and mechanisms of excited-state transitions**,** revealing that electronic relaxation occurs predominantly through ultrafast intersystem crossing from singlet to triplet metal-to-ligand charge-transfer states on the order of a few femtoseconds. The solvent undergoes rapid reorganization, with water molecules intercalating into the grooves between the ligands and reshaping the local solvation shell (Fig.1). Furthermore, we investigated temperature changes and the flow of energy from the photoexcited solute into the solvent, which provides a molecular-level view of how energy redistribution occurs during relaxation.

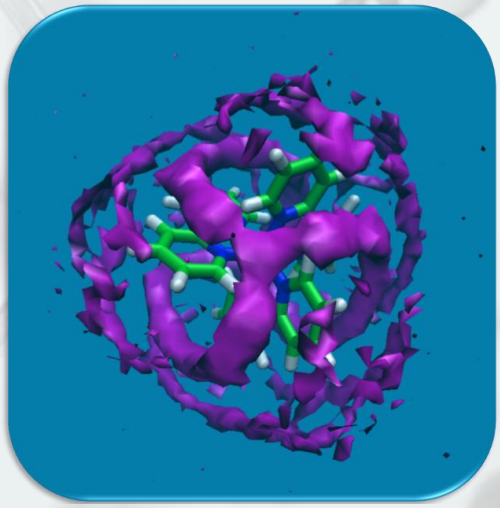


Fig.1. Spatial distribution functions of oxygen solvent atoms around the $[Ru(bpy)_3]Cl_2$ after dynamics simulations.

Our theoretical insights are supported by terahertz spectroscopic experiments**,** which probe the collective solvent response and thus provide an experimental perspective on the observed energy transfer processes. This study sheds light on the fundamental role of the environment in shaping the excited-state relaxation pathways of transition metal complexes and connects atomistic simulations with experimental observables.

Cationic Selenuranes – Bench-Stable Sources of Se(III) Radicals

Kirill Zhiliaev[a*], Boris Maryasin[a,b], Hanspeter Kählig[a], Marcos Gil-Sepulcre[c], Javier Mateos[a]

[a] *Institute of Organic Chemistry, University of Vienna, Währinger Strasse 38-42, 1090 Vienna, Austria*
[b] *Institute of Theoretical Chemistry, University of Vienna, Währinger Straße 17, 1090 Vienna, Austria*
[c] *Departament de Química, Universitat Autònoma de Barcelona Cerdanyola del Valles, 08193 Barcelona, Spain*

* Email: kirill.zhiliaev@univie.ac.at

Organic radicals, particularly stable radicals, play an important role as reagents in organic synthesis, promoting redox reactions and serving as polymer initiators.[1] The first reported stable triphenyl methyl radical persists in solution for several days due to reversible dimerization forming quinoid-type dimer structure.[2] Dimerization is not restricted to C-centered radicals. Bontempelli and co-workers demonstrated that anodic oxidation of dibenzothiophene leads to an irreversible dimerization–deprotonation sequence, yielding a sulfonium salt dimer.[3] In this case, due to the C–S bond formation, radical cation regeneration is not possible. Consequently, one-center/one-electron (1c1e) Ch(III) radicals have hitherto been challenging to access. A reversible oligomerization mechanism would allow the use of heterocyclic radicals with a single heteroatom, unlocking chalcogen radicals for new applications. Dimerization of aryl selenide radicals via Se–Se bond formation between two independent radical subunits enables the generation of chalcogen-centered radicals. Diselenides serve as 1c1e radical precursors, yet Se–Se bond homolysis requires external activation. Electrostatic repulsion in polycationic structures weakens Ch–Ch bond strength.[4] Thus, a rigid polycationic Se–Se bond connecting two discrete subunits, would instead enable radical generation without external activation.

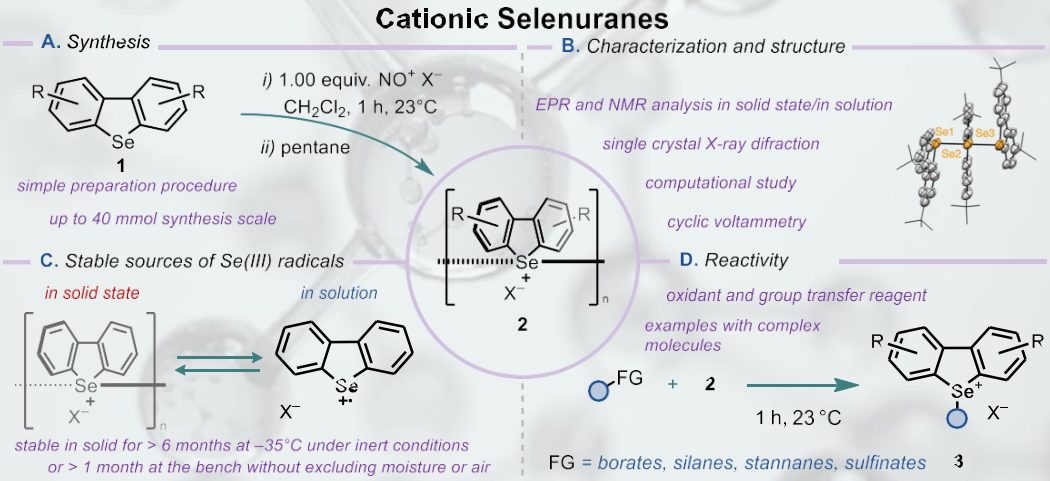


Figure 1. Study of cationic selenuranes

In this talk, we report the synthesis of bench-stable cationic selenurane salts via oligomerization of dibenzoselenophene-based radical cations (**Figure 1**). The salts can be prepared on a multigram scale (>17 g) in two steps from commercial materials. In solution, the electrostatic repulsion of the Se–Se σ-bond promotes dissociation to generate diarylorganoselenium radical cations without external activation. The salt structure has been analyzed in the solid-state and the radical cation properties in solution. Direct access to Se(III) radicals without external activation allows their use as oxidants and group transfer reagents.

References

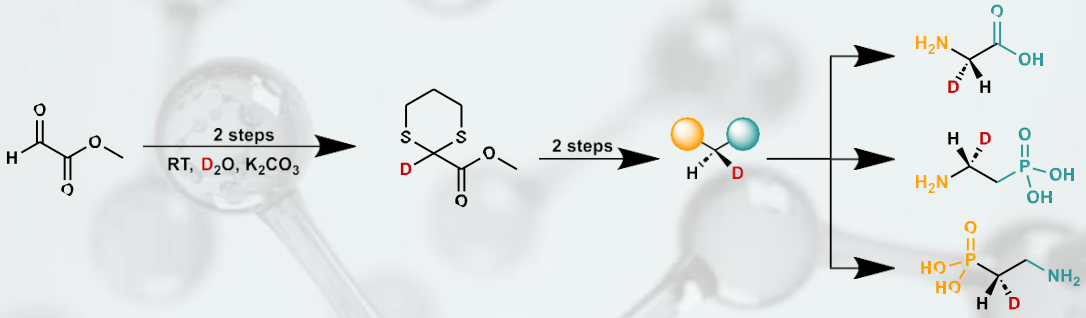
1 Z. X. Chen, Y. Li, F. Huang, Chem **2021**, 7, 288–332.
2 H. Lankamp, Tetrahedron Lett. **1968**, 9, 249–254.
3 G. Bontempelli, Electroanal. Chem. Interf. Electrochem. **1973**, 43, 377–385..
4 N. Furukawa, Bull. Chem. Soc. Jpn. **1997**, 70, 2571–2591.

Small Stereoselectively Deuterated Molecules at the Chemistry–Biology Interface

Sebastian-Felix Fritz, Daphné Brunin, Katharina Pallitsch

Small molecules with high enantioisotopic purity are essential substrates for mechanistic studies in chemical biology, particularly for elucidating enzyme-catalysed transformations and stereospecific interactions. However, generalisable methods for the synthesis of such compounds, as well as reliable strategies for the determination of their absolute configuration, remain limited. [1–4]

In our work, we report the identification of a key synthetic intermediate and a robust, reproducible reaction sequence that enables the efficient preparation of enantioisotopically enriched substrates. These advances provide a versatile platform for probing enzyme mechanisms and broaden the toolkit available for chemical biology at the interface of structure, reactivity, and function.



The key intermediate was efficiently converted into a structurally diverse set of isotopically labelled synthons via stereospecific S_N2 reactions, preserving enantiopurity throughout. This modular approach enables the rapid and economic assembly of chemically and biologically relevant building blocks, thereby broadening the synthetic scope and utility of isotopically labelled probes in chemical biology. The resulting compounds might serve as versatile tools for investigating enzyme mechanisms, metabolic flux, and molecular recognition events.

References

(1) Sonstrom, R. E.; Vang, Z. P.; Scolati, H. N.; Neill, J.L.; Pate, B. H.; Clark, J.R. Rapid Enantiomeric Excess Measurements of Enantioisotopomers by Molecular Rotational Resonance Spectroscopy. *Organic process research & development* **2023**, *27* (7), 1185–1197. DOI: 10.1021/acs.oprd.3c00028. Published Online: Mar. 17, 2023.

(2) Rowbotham, J.S.; Ramirez, M. A.; Lenz, O.; Reeve, H. A.; Vincent, K. A. Bringing biocatalytic deuteration into the toolbox of asymmetric isotopic labelling techniques. *Nature communications* **2020**, *11* (1), 1454. DOI: 10.1038/s41467-020-15310-z. Published Online: Mar. 19, 2020.

(3) Kopf, S.; Bourriquen, F.; Li, W.; Neumann, H.; Junge, K.; Beller, M. Recent Developments for the Deuterium and Tritium Labeling of Organic Molecules. *Chemical reviews* **2022**, *122* (6), 6634–6718. DOI: 10.1021/acs.chemrev.1c00795. Published Online: Feb. 18, 2022.

(4) Mills, M. D.; Sonstrom, R. E.; Vang, Z. P.; Neill, J.L.; Scolati, H. N.; West, C. T.; Pate, B. H.; Clark, J.R. Enantioselective Synthesis of Enantioisotopomers with Quantitative Chiral Analysis by Chiral Tag Rotational Spectroscopy. *Angewandte Chemie (International ed. in English)* **2022**, *c1* (33), e202207275. DOI: 10.1002/anie.202207275. Published Online: Jul. 8, 2022.

Posters

1	**Abel Anne-Susann** Metabolic Engineering for C1-Based Platform Chemical Production
2	**Back Hannah Susanne** Potentiating the Anti-Tumor Efficacy of Innate Immune System Engagers (ISErs) through Bipartite Immune Modulation
3	**Bekzhanov Akzhan** SnS2 and C-SnS2/Si anode active materials for Li ion batteries
4	**Bell Teresa** Peptide functionalization of hybrid polyoxometalates
5	**Berger Sabrina** LC-HRMS-Based Profiling of the Nasal Metabolome and Exposome in a Cohort of Preterm and Full-Term Infants
6	**Blancas Rodríguez Arturo** Study of the catalytic properties of Se (III) species stabilized by intramolecular chalcogen-chalcogen bonds
7	**Bogner Lukas** Construction of a transient absorption setup
8	**Borsos Eszter** Tracing the Mycotoxin Alternariol in the Human Body Using Physiologically Based Kinetic (PBK) Modeling
9	**Brandstetter Stefanie** Computational modeling of protein interactions using chemical crosslinking and mass spectrometry
10	**Brenner Christina** Evaluating Orthogonal Ionization Techniques to Expand Metabolome Coverage in Complex Biological Matrices
11	**Call Florian** Unraveling the effect of *in vitro* digestion on the bioaccessibility, genotoxicity and mutagenicity of a complex *Alternaria* extract
12	**Duran Balsa Alejandra** E-field Assisted Assembly of Metal-Organic Framework Particles with Surface
13	**Preißler Miriam Marta Klara** Hunting for the aggregation culprit(s): Examination of individual and combined effects of select site-specific tau pathology
14	**Eder Alexander** Mechanistic i nvestigation of the influence of unsaturated fatty acids on platelet activation

Posters

Posters

Posters

43	**Netsch Jonathan** Molecular Dynamics Simulation of Functionalized NU-1000 MOF
44	**Nici Venet** Investigating the self-cleavage reaction of polyphenol oxidases from mushroom Agaricus bisporus and apricot Prunus armeniaca
45	**Niedermaier Felix** Improving Lipid Identification and Quantification: Chromatogram Deconvolution
46	**Pan Yingjie** Design of Novel Pathways for Production of High Value-added Chemicals in Multi-Enzyme Cascades
47	**Parlar Etkin** Nucleic Acid Photolithography for the High-Density RNA Microarrays
48	**Partsch Vanessa** Dissecting the immunomodulatory mechanisms of Alternaria mycotoxins: NF-κB signaling alterations in THP-1 monocytes
49	**Pellinger Nils** Zigzag BN-doped Nanoribbons Featuring Thermally Activated Delayed Fluorescence (TADF)
50	**Picha Anna** Architecture independent absolute solvation free energy calculations with neural network potential
51	**Plöchl Konstantin** Phage blocker: Discovery of a novel bacteriophage antiviral for phageome modulation
52	**Pointner Tobias** Lipidomic and Metabolomic Insights from Supplementation with Linseed Oil from Germinated Seeds
53	**Pötzl Christopher** Atomistic structures of early-stage prenucleation clusters by hyperpolarized NMR-validated, quantum mechanical calculations
54	**Duvanova Ella** Synthesis and identification of metal - substituted phosphotungstate with Keggin structure
55	**Puccinelli Chiara** Iron Carbide Nanoparticles for Enhancing CAR-T Cell Therapy in Metastatic Melanoma: Dual Hyperthermia and Surface Eng
56	**Ober Isabell** Bivalent ligands targeting Oxytocin Receptor – Dopamine D2 Receptor Heterodimers

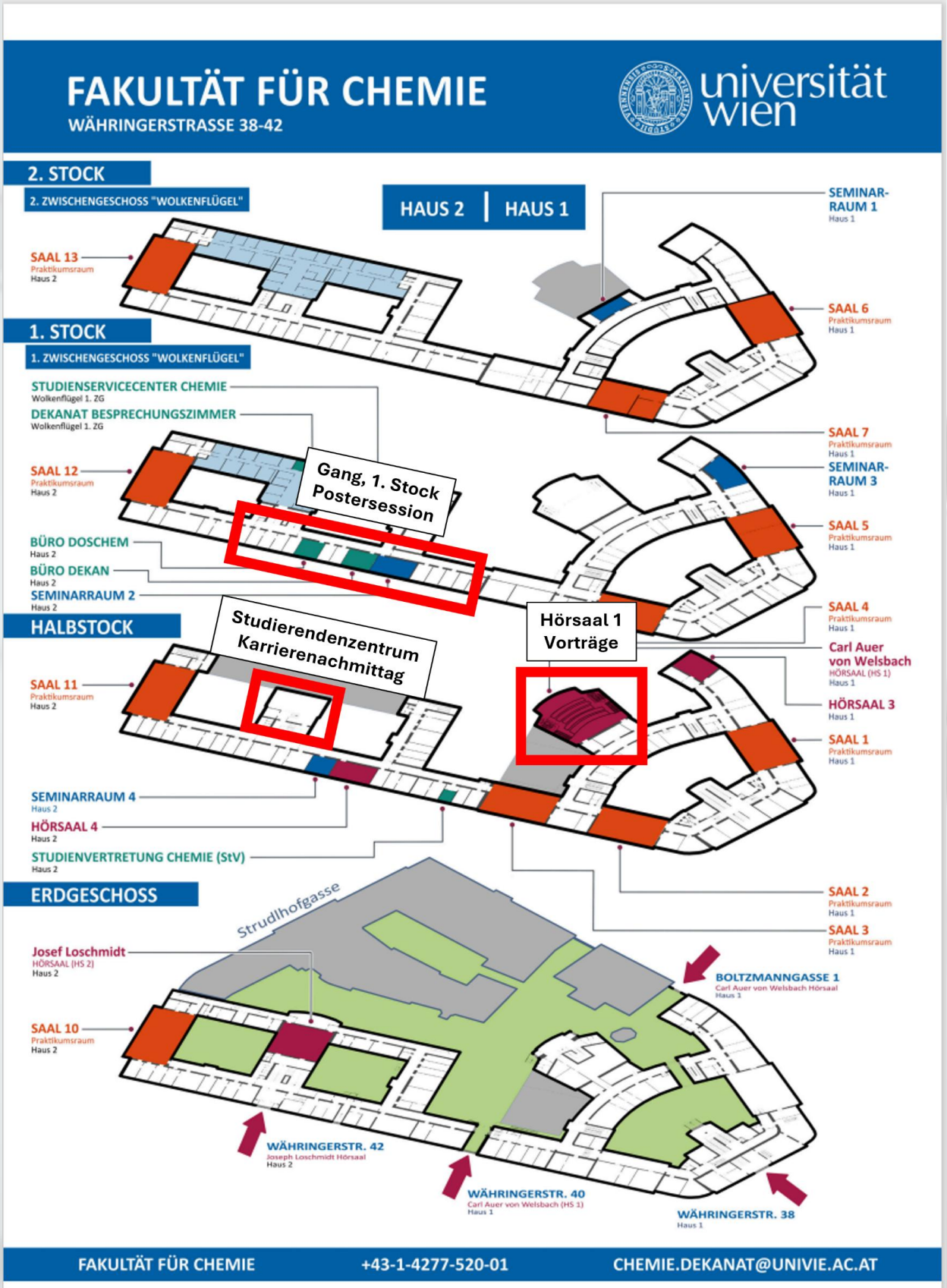
Posters

Posters

71	**Simonelli Federico** Metal Based Catalysts for Borrowing Hydrogen Processes
72	**Skoulikas Nikolas** Facile (Z)-Selective Synthesis of β,γ -Unsaturated Ketones
73	**Smith Joseph Antony** Designing a Multi-Enzyme Cascade Using a Graph-based Approach
74	**Sommerauer Sophie** A Mild and Efficient Route to β-Aminosilanes through Hydroamination Reactions
75	**Stastna Katarina** From soil to structure: electron diffraction reveals crystalline compounds in roots' exudates and their environment
76	**Staudinger Johannes Nikodemus** Progress towards novel theranostic compounds for PDT, SPECT and Radiotherapy
77	**Tiefenbacher Maximilian Xaver** Using neural network potentials to estimate thermal isomerization half-lives of arylazopyrazoles photoswitches
78	**Tiefenbrunner Irmgard Thabea** A surrogate enantioselective Mannich reaction for the synthesis of β-aminoamides and 1,3-diamines
79	**Uhlir Manuel** Predicting Mass Spectra using theoretically derived graph transformation rules
80	**Valovicová Dominika** Development and Utilization of Chiral Base Metal Catalysts for Stereoselective Borrowing
81	**Vavrik Milos** Revisiting the Baddeley reaction: A charge-promoted alkane functionalization
82	**Vezonik Uroš** Direct Alkyl Swap of Unprotected Amines: A Platform for Late-Stage Functionalization
83	**Windisch Dominik** Design, synthesis and biological evaluation of gut-stable peptides targeting intestinal MC4 receptors for metabolic disorders
84	**Wolf Michael** Exploring finger sweat as a proxy biofluid for investigating drug distribution between interstitial fluid and blood

Posters

Site Plan


FAKULTÄT FÜR CHEMIE
WÄHRINGERSTRASSE 38-42
universität wien
2. STOCK
2. ZWISCHENGESCHOSS "WOLKENFLÜGEL"
HAUS 2 | HAUS 1
SAAL 13
Praktikumsraum
Haus 2
SEMINAR-RAUM 1
Haus 1
SAAL 6
Praktikumsraum
Haus 1
1. STOCK
1. ZWISCHENGESCHOSS "WOLKENFLÜGEL"
STUDIENSERVICECENTER CHEMIE
Wolkenflügel 1. ZG
DEKANAT BESPRECHUNGSZIMMER
Wolkenflügel 1. ZG
SAAL 7
Praktikumsraum
Haus 1
SAAL 12
Praktikumsraum
Haus 2
Gang, 1. Stock
Postersession
SEMINAR-RAUM 3
Haus 1
SAAL 5
Praktikumsraum
Haus 1
BÜRO DOSCHEM
Haus 2
BÜRO DEKAN
Haus 2
SEMINARRAUM 2
Haus 2
SAAL 4
Praktikumsraum
Haus 1
HALBSTOCK
Studierendenzentrum
Karrierenachmittag
Hörsaal 1
Vorträge
Carl Auer von Welsbach
HÖRSAAL (HS 1)
Haus 1
SAAL 11
Praktikumsraum
Haus 2
HÖRSAAL 3
Haus 1
SAAL 1
Praktikumsraum
Haus 1
SEMINARRAUM 4
Haus 2
HÖRSAAL 4
Haus 2
STUDIENVERTRETUNG CHEMIE (StV)
Haus 2
ERDGESCHOSS
SAAL 2
Praktikumsraum
Haus 1
SAAL 3
Praktikumsraum
Haus 1
Strudlhofgasse
Josef Loschmidt
HÖRSAAL (HS 2)
Haus 2
BOLTZMANNGASSE 1
Carl Auer von Welsbach Hörsaal
Haus 1
SAAL 10
Praktikumsraum
Haus 2
WÄHRINGERSTR. 42
Joseph Loschmidt Hörsaal
Haus 2
WÄHRINGERSTR. 40
Carl Auer von Welsbach (HS 1)
Haus 1
WÄHRINGERSTR. 38
Haus 1
FAKULTÄT FÜR CHEMIE
+43-1-4277-520-01
CHEMIE.DEKANAT@UNIVIE.AC.AT