



WHERE: [HERNSTEIN Castle](#), Berndorfer Str. 32, 2560 Hernstein

PROGRAM DAY 1 – Wednesday, 28.09.2022

07:30 Meeting point Schwedenplatz, Night-Bus stop (vis-avis “Motto am Fluss”, see next page)
07:50 Departure by Bus (exactly on time!)
09:05 Arrival at the Hotel
09:25 Begin, Opening Address by Speaker **Gerhard Ecker**
Key note lecture by [Trevor Smart](#):
Probing GABA_A receptor structure and function in health and disease (Appendix I)
Introduction and Q&A Moderation: Margot Ernst

10:25 Coffee Break (20 min)

10:45 Progress Reports á 18 minutes – 7 students (1 short break; Appendix II)
Moderation: Nathalie Agudelo Dueñas & Mojtaba Tavakoli

13:00 Start of Lunch Break

14:30 Poster Pitch Session - 9 posters á 3 minutes (Appendix II)

15:00 Poster Session, 10 Posters

15:50 Coffee Break (30 min) – **Check in: go to reception and pick up your room key!**

16:20 Progress reports á 18 minutes – 6 students (1 short break; Appendix II)
Moderation: Theres Friesacher & Michael Bründl-Jirout

19:00 Dinner

PROGRAM DAY 2 – Thursday, 29.09.2022

From 07:00 Breakfast & **Check out (until 11:00 !)**

09:45 Challenging Medicinal Chemistry as part of successful Translation of Academic Research into Industrial Drug Development
Lecturers: Peter Nussbaumer; Lead Discovery Center and Thierry Langer; University of Vienna (Appendix III)
Moderation and Q&A: Margot Ernst

10:50 Coffee Break (25 minutes)

11:15 Panel discussion:
“Careers beyond Academia - A discussion with founders and supporters about practical implications of start-ups and career options after PhD” (Appendix III)
Kick off and moderation: Gerhard Ecker; Panelists: Chris Ahern, Sharon Bryant, Ingrid Kelly-Spillmann, Thierry Langer, Peter Nussbaumer

From 12:30 Lunch buffet

14:00 Return option to Vienna by bus for Faculty/SAB
 For students: **“Escape the Hotel”** (team building challenge;
 we meet **14:15** at reception!; **Bus back to Vienna goes 16:00 !**



September 28: Progress Report Sessions

The students present their PhD project results either in an oral presentation or in a poster presentation with a previous poster pitch.

a) Oral Presentations (18 min per student including Q&A)

Oral Report with a **13 min project presentation** followed by Discussion (**max 5 min**) with Faculty and SABs: C. Ahern, D. Belelli, T. Langer, P. Nussbaumer, C. Oostenbrink, M. Van der Heyden and guest lecturer T. Smart. Further guest: Kelly-Spillman I.

Presentations Part 1 (10:45 – 12:50)

Moderation: Nathalie Agudelo Dueñas & Mojtaba Tavakoli

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|---|--|---|---|
| Slot 1 (10:45) | BRÜNDL-JIROUT Michael | Visualizing individual protonation events in Kir2 channels | Anna Weinzinger, UniVie Life |
| Slot 2 (11:03) | FRIESACHER Theres | In silico investigation of ion channels in connection with rare diseases | Anna Weinzinger, UniVie Life |
| Slot 3 (11:21) | SINGER Nadja | Computer-aided investigation and rational design of photosensitive compounds bound to ion channels and transporters | Leticia González, UniVie Chemistry |
| Short break, max 5 minutes | | | |
| Slot 4 (11:45) | KNITTL-FRANK Christian | Enantioselective assembly of congested carbon-carbon bonds | Nuno Maulide, UniVie Chemistry |
| Slot 5 (12:03) | BELLEZA Oliver | Pharmacological characterization of fluorescent probes for imaging monoamine transporters | Harald Sitte, MedUni Wien |
| Slot 6+7 (12:21) | SCHLÖGL Katharina and GRADISCH Ralph | Synthesis of Serotonin Derivatives with different sidechain lengths for Serotonin Neurotransmitter Transporter Investigations Looking from the other side – What converts a full substrate to a partial substrate, releaser or even a blocker? | Marko Mihovilovic, TU Wien Harald SITTE, MedUni Wien |
| End ca. 12:50, 13:00: Lunch at restaurant! Program continues 14:30 with Poster Pitches (see b) | | | |

Presentations Part 2 (16.20 – ca. 18:32)

Moderation: Theres Friesacher & Michael Bründl-Jirout

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|-------------------------------------|--------------------------|---|--------------------------------|
| Slot 1 (16:20) | VOGEL Florian | Characterization of a <i>de novo</i> GABRA4 variant | Margot Ernst, MedUni Wien |
| Slot 2 (16:38) | GARIFULINA Aleksandra | Modulation of Ligand-Gated Ion Channels by Peptides and Low-Molecular-Weight Compounds | Steffen Hering, UniVie Life |
| Slot 3 (16:56) | SCHNALZER Dominik | Developing (Non)-Labeled Ligands as Tool Compounds for Mechanistic Studies on the GABA _A -Receptor | Marko Mihovilovic, TU Wien |
| Short break (max 5 min) | | | |
| Slot 4 (17:38) | KNAUS Lisa | Large neutral amino acids tune perinatal neuronal excitability and survival | Gaia Novarino, ISTA |
| Slot 5 (17:56) | MICHALSKA Julia | A versatile toolbox for the comprehensive analysis of nervous tissue organization with light microscopy | Johann Danzl, ISTA |
| Slot 6 (18:14) | TAVAKOLI Mojtaba | Towards optical connectomics at single synapse level with expansion microscopy | Johann Danzl, ISTA |
| End ca. 18:32, Dinner: 19:00 | | | |



b) Poster Pitch (á 3 min) and Poster Session

The students shall present their PhD project or project results **both in a 3-minutes short communication at the podium – and additionally in a classical poster session.**

The pitch session has the goal **to inform the audience about the topic of your poster and to motivate to visit you during the poster session.** These presentations are strictly limited to **3 minutes each**. After this time, the presentation will be stopped. In depth discussions will be held later, right in front of the (paper) posters.

The **STUDENTS** of each non presenting session **choose the posters they visit.**

SAB and Faculty Members got the abstracts 2 weeks before the meeting and will choose whose posters they are going to visit.

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|-------------------|------------------|---|------------------------------------|
| Slot 1 (14:30) | SCHWARZ Lena | Hidden targets of Autism Spectrum Disorders: dissecting convergent causal paths in the ubiquitin-proteasome system and beyond | Gaia Novarino, IST-A |
| Slot 2 (14:33) | AGUDELO Nathalie | Decoding the transcriptional landscape at nanoscale resolution | Johann Danzl, IST-A |
| Slot 3 (14:36) | TIEFENBACHER Max | Excited-state dynamics of furan in explicit solvent using machine-learned potentials | Leticia González, UniVie Chemistry |
| Slot 4 (14:39) | NETZER Michael | Electrophysiological characterization of cardiac organoids | Steffen Hering, UniVie Life |
| Slot 5 (14:42) | BALTOV Bozhidar | Organ on a chip technology for cardiotox studies and drug development | Steffen Hering, UniVie Life |
| Slot 6 (14:45) | HUANG Jiahui | Structure landscape analysis and functional mapping of disease-relevant mutations on SLC transporters | Gerhard Ecker, UniVie Life |
| Slot 7 (14:48) | KASTNER Nina | Characterization of the structure-activity relationship of α -pyrrolidinovalerophenone derivatives at monoamine transporters | Harald Sitte, MedUni Wien |
| Slot 8 (14:51) | XIAO Yi | Development of Novel Fluorescent Dyes and Their Application as Probes to Study Biological Processes | Nuno Maulide, UniVie Chemistry |



September 29, 09:45 – 10:50

Challenging Medicinal Chemistry as part of successful Translation of Academic Research into Industrial Drug Development

By Peter Nussbaumer and Thierry Langer



Peter Nussbaumer has about 35 years of industry experience in medicinal chemistry and drug discovery. Since 2008, he is Managing Director and Head of Medicinal Chemistry at the Lead Discovery Center GmbH (LDC) in Dortmund, Germany and since 2019 also Managing Director of the wings4innovation GmbH in Vienna. Both organisations operate at the interface of academia and industry. Before joining LDC, Peter was Executive Director at the Novartis Institutes for BioMedical Research in Vienna, Austria, heading the Chemistry Department. During his 23 years at Sandoz/Novartis, he held various positions in the area of medicinal chemistry and interdisciplinary project leadership.

Peter Nussbaumer is member of the MolTag Scientific Advisory Board since the 1st funding period and serves as advisor to private and public funding bodies. He is (co)author of more than 80 peer-reviewed publications and more than 25 patent applications, referee to various journals, and holds a Dr. degree in organic chemistry from the TU Wien, Austria.

Thierry Langer holds an MSc degree in Pharmacy (1988) and a PhD in Pharmaceutical Chemistry (1991) from University of Vienna. He began his academic career at Leopold-Franzens-University of Innsbruck in 1992 after completing a post doctoral fellowship at the Université Louis Pasteur, Strasbourg, France with Prof. C.-G. Wermuth. In 1997, he was appointed Associate Professor of Pharmaceutical Chemistry at University of Innsbruck. In 2003, with colleagues, he founded the company Inte:Ligand GmbH which develops scientific software for computer aided molecular design, and served as the CEO until 2008. Then he was appointed CEO of Prestwick Chemical, Inc., a world renown contract research organization specialized in medicinal chemistry services, located in Strasbourg, France. Under his leadership, several drug discovery programs in different research target sectors successfully progressed into pre-clinical and clinical development. In 2013, he was nominated full professor for medicinal chemistry at University of Vienna, where he currently heads the Department of Pharmaceutical Chemistry at the Faculty of Life Sciences. Thierry Langer is member of the MolTag Scientific Advisory Board since the 2nd Funding period.



September 29, 11:15 – ca. 12:25

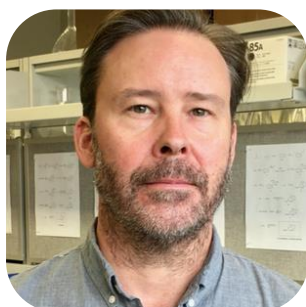
Panel discussion: **“Careers beyond Academia - A discussion with founders and supporters about practical implications of start-ups and career options after PhD”**

Moderated by **Gerhard Ecker**



The Ecker lab is partner in several projects of the Innovative Medicines Initiative, which are based on a public-private partnership between the European Commission and EFPIA (comprising the top 50 Pharma companies with research sites in Europe). Phenaris is a spin-off from the Pharmacoinformatics group at the University of Vienna and deals with all aspects of molecular modeling with a focus on drug transporters, data mining and in silico toxicology. The team applies its more than 20 years of chemical informatics and data analysis experience to concrete products to support toxicologists and medicinal chemists in their daily work.

Panelists: **Peter Nussbaumer, Thierry Langer and**



Chris Ahern: The Ahern lab works at the interface of membrane biophysics and chemical biology. Our particular expertise is in the synthesis and expression of tailor made non-natural amino acids and the application of chemical biological approaches to the study of membrane proteins. We have had success in expressing synthetic amino acids in many channel and receptor types for pharmacological studies of ligand and drug interactions as well as structure function relationships. We are currently developing synthetic amino acid spin labels and fluorophores for use in cellular and cell-free expression systems. Chris Ahern is MolTag SAB member since the 3rd funding period.



Sharon Bryant is CEO at Inte:Ligand, a company that develops computer aided molecular design software and provides research consulting services to pharmaceutical and life science industries in 88 countries worldwide. She has more than 30 yrs experience in computer-aided molecular design, molecular modeling and research consulting with pharmaceutical, cosmetic and nutrition industries involving a variety of targets, including cancer, antivirals and GPCRs. Sharon is also a Guest Professor at the University of Vienna, where she teaches courses in Drug Discovery and Pharmacy programs. She is involved in [NeuroDeRisk](#), an [IMI](#) project, where she co-leads a work package on developing an in silico toolbox for derisking drugs and compounds for neurotoxic adverse outcomes



Ingrid Kelly-Spillmann joined the IST Tech Transfer team in 2018 after spending a number of years at the University of Vienna, where she was responsible for managing the life sciences technology portfolio and supporting spin-out companies. Ingrid worked as a patent attorney in and for the pharma industry for more than a decade in different countries before moving into technology transfer. At IST cube she is primarily involved with biotech, pharma and chemistry startups, with a particular emphasis on intellectual property and legal matters. Ingrid holds a PhD in molecular biology from the University of Cambridge. She is a qualified European patent attorney with RTPP (registered technology transfer professional) certification.