MolTag Graduates 2016 – 2018

- Peter Lukács, Medical University Vienna
- Kusumika Saha, Medical University Vienna
- Laurin Wimmer, TU Wien
- Roshan Purackal, née Puthenkalam, Medical University of Vienna
- Vaibhavkumar S. Gawali, Medical University of Vienna
- Eva Zangerl-Plessl, University of Vienna
- Felix Mayer, Medical University of Vienna
- Eva Gschaider-Reichhart, IST Austria
- David Siebert, TU Wien and Medical University of Vienna
- Kumaresan Jayaraman, Medical University of Vienna
- Dominik Dreier, TU Wien
- Catherine McKenzie, IST Austria
- Sankalp Jain, University of Vienna

Der Wissenschaftsfonds.

Péter LUKÁCS

Finishing year: 2016

Supervisor: Hannes Todt, Medical University of Vienna

Thesis title: Exploring the extracellular access pathway for charged local anaesthetics in voltage-gated sodium channels.

Current Position and Employer: PI at Plant Protection Institute, Centre for Agricultural Research, Martonvásár, Hungary (after Postdoc at Eötvös Lorand University, Budapest, Hungary)

MolTag alumni page:

Peter Lukacs (univie.ac.at)

Social network:

Péter Lukács | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

Our bacterial channel based Voltage-gated sodium channel homology model predicted a large hydrophilic cavity when a key residue in the mammalian NaV1.4 (W1531) at the pore loop was mutated to smaller sidechains. The mutant protein indeed had altered selectivity demonstrating that a nonselective channel opened towards the pore. In addition, charged lidocaine derivative QX-222 became effective on the mutant, demonstrating that the new pathway is large enough to let large organic ions into the central cavity.

What did you do after your PhD?

I was invited as Postdoc to Eötvös Loránd University, Dept. of Biochemistry, Opto-Neuropharmacology Research Group. Here my project was to test photoreactive sodium channel inhibitor analogs. After we successfully finished this project, I moved to the Centre for Agricultural Research. **Here I am the leader of a multidisciplinary research project aiming to develop an olfactory receptor based volatile organic compound sensor**. The goal is to develop a simple but sensitive system at least as sensitive as the recent gold standard, the gas chromatograph coupled to a mass spectrometer. This new system is based on deep-learning analysis methods we develop with the help of an IT company.

What was the impact of the MolTag program on your further career?

MolTag is a great background for me to handle such complex projects as the program itself was built on the principle to discover several fields of science and integrate the interesting and useful parts into your research.

What did you particularly like about the MolTag program?

The **lab rotations and the retreats were great opportunities** to get new skills, and do networking

MEDICAL UNIVERSITY OF VIENNA

Kusumika SAHA

Finishing year: 2016

Supervisor: Harald Sitte, Medical University of Vienna

Thesis title: Unraveling the molecular pharmacology of 4-MEC and 4-MePPPInsights into their mode of action.

Current Employer: PostDoc in the group of Stefano Marullo, Institute Cochin, Biomedical research Institute, INSERM, Paris, France

MolTag alumni page:
Kusumika Saha (univie.ac.at)

How would you summarize your thesis results in 3 sentences?

My thesis focused on elucidating the mechanism of action for two "second generation" synthetic cathinones 4-MEC and 4-MePP; 4-MEC had a "hybrid" profile wherein it acted as a blocker for dopamine transporter (DAT) and substrate releaser for serotonin transporter (SERT). 4-MePP was a blocked both SERT and DAT with a higher efficacy at DAT. Our work also emphasized the importance of structural modifications on the drugs and its impact on its pharmacology.

What are you doing now?

My present work is in the field of Cell Biology and focuses on the intracellular trafficking of Cystic Fibrosis Transmembrane Regulator (CFTR) within the framework of Cystic Fibrosis.

What was the impact of the MolTag program on your further career?

MolTag program is unique in the way of allowing PhD students under different supervisors from interdisciplinary fields to come together and learn from one another. I had the honor of interacting with other supervisors who were a constant source of inspiration and guidance. The interdisciplinary environment I experienced has helped a lot in my research career in terms of scientific collaborations and embracing diverse scientific approaches to answer questions.

What did you particularly like about the MolTag program?

Being mentored by Harald Sitte I learned a lot, not only in the realm of my project but also as a researcher. **MolTag provided a strong support system both academically and administratively allowing me to focus on learning during my PhD.**

MEDICAL UNIVERSITY OF VIENNA

Laurin WIMMER

Finishing year: 2016

Supervisor: Marko Mihovilovic, TU Wien

Thesis title: Synthesis of bioactive molecules for the investigation of ion channels and transporters.

Current Position and Employer: Principal Investigator and Project Leader in the Process Chemistry Dept. at Novartis, Basel, Switzerland (after a PostDoc in the lab of Phil Baran at The Scripps Research Institute, CA, USA)

MolTag alumni page:

Laurin Wimmer (univie.ac.at)

Social network:

Laurin R. Wimmer | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

For my PhD work I investigated structure-activity relationships across subtypes of $GABA_A$ receptors identifying elusive subtype selective compounds. In a second project we were interested in the metabolic fate of metcathinones, a common class of recreational drugs, and their interaction with transporters. In both projects we were able to deepen the understanding of compound-receptor interactions

What was the impact of the MolTag program on your further career?

It gave me **a sense of appreciation for other disciplines in the drug discovery and development arena.** In industry, teams are very divers and working together well is one of the most important things. Having gained a basic understanding of disciplines outside of my core area of expertise helps me today to better understand and collaborate in interdisciplinary teams.

Did you keep connections with some former colleagues? I do - with some we became good friends and we keep in touch regularly. For others I follow them on Linkedin and other platforms and I am always glad to see how well their careers are going.

What did you particularly like about the MolTag program?

The program offered a unique opportunity to work in an interdisciplinary team as PhD student. Besides the opportunity for personal growth this setting also sparked scientific ideas, some of it later turned into researchprojects.

What is your recommendation for current MolTag PhD students?
Take full advantage of what the program has to offer. Lab roations and internships abroad were really valuable experiences. Secondly, **start planning for the time after PhD early on**. This can be difficult with all the stress and workload but it is very important since e.g. applying for scholarhip can take a long time.

TECHNISCHE UNIVERSITÄT WIEN

Roshan PURACKAL née Puthenkalam

How would you summarize your thesis results in 3 sentences?

$GABA_A$ receptor homology models were generated based on superfamily members, in the light of experimental evidence. The models served as a basis for binding site confirmation, binding mode confirmation and ultimately, structure-guided drug design. Experiments were designed to test if the models correctly depict $GABA_A$ receptors.

What was the impact of the MolTag program on your further career?

I learned during the program to obtain and value feedback from professors and students who were close to my PhD project but also from fellow students from other disciplines who were interested in my work. I am not working in research anymore, however my experience gained during the Moltag program is helping me in my current role to exchange constructive feedback which is something I need to apply in my daily work in Regulatory Affairs.

Did you keep connections with some former colleagues?

Yes I have contact with few of my fellow students and my PhD supervisor (Margot Ernst).

What did you particularly like about the MolTag program?

I liked the possibility to do lab rotations in other disciplines as they added value to my PhD project.

What is your recommendation for current MolTag PhD students?

Start building a good network during your PhD time. **A strong network is highly beneficial in identifying and exploring career opportunities.**

Finishing year: 2016

Supervisor: Margot Ernst, Medical University of Vienna

Thesis title: Understanding subtype-selective allosteric modulation of $GABA_A$ receptors.

Current Employer: Regulatory Affairs Manager at Ascensia Diabetes Care, Basel, Switzerland

MolTag alumni page:

Roshan Puracкal (née Puthenkalam) (univie.ac.at)

Social network:

Roshan Puracкal, PhD | LinkedIn

MEDICAL UNIVERSITY OF VIENNA

Vaibhavkumar S. GAWALI

Finishing year: 2016

Supervisor: Hannes Todt, Medical University of Vienna

Thesis title: The mechanism of interaction of local anesthetic drugs with voltage-gated sodium channels.

Current position and employer: PostDoc in the Conforti Lab, College of Medicine, University of Cincinnati, Cincinnati, OH, USA.

MolTag alumni page:

Vaibhavkumar S. Gawali (univie.ac.at)

Social networks:

Vaibhavkumar Gawali, Ph.D. | **LinkedIn**

Vaibhavkumar Gawali, PhD (@vaibhavkumar_g) / **Twitter**

How would you summarize your thesis results in 3 sentences?

Local anesthetics bind to voltage-gated sodium channels that are important for the treatment of neurological and cardiac disorders. My thesis work identified and characterized the critical interactions of local anesthetics with various inactivation states of these channels using single cell patch-clamp electrophysiology. This work laid the foundation for the discovery of new local anesthetics with prolonged effects.

What did you do after your PhD?

I am doing translational research in immuno-oncology to discover new & safer therapies with a focus on ion channels.

What was the impact of the MolTag program on your further career?

Training in electrophysiology & ion channels helped me lead the projects independently and become an expert in this area.

Did you keep connections with some former colleagues?

Yes, I am glad to mention here that I got some lifetime “friends” during my MolTag endeavor.

What did you particularly like about the MolTag program?

Great interdisciplinary training by connecting students with other labs and an opportunity to do summer internship abroad.

What is your recommendation for current MolTag PhD students?

This is your best opportunity to get maximum out of it. **Be proactive and reach out to your colleagues, faculty, and alumni to form new collaboration,** discuss, and share your ideas.

MEDICAL UNIVERSITY OF VIENNA

Eva-Maria ZANGERL-PLESSL

Finishing year: 2016

Supervisor: Anna Weinzinger, Faculty of Life Sciences, University of Vienna

Thesis title: Investigation of drug receptor interactions in inward rectifier and hERG potassium channels and modulations by “lipids”.

Current Position and Employer:
PI in the FWF-Zukunftskolleg „PeptAIDes“, currently on maternity leave

MolTag alumni page:

Eva Zangerl-Plessl (univie.ac.at)

Social network:

Eva-Maria Plessl | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

Crystal structures of proteins lead to their better understanding; however, all ion channels undergo poorly understood conformational changes during gating. Thus, my thesis focused on exploring their gating dynamics using molecular dynamics simulations, in cooperation with experimentalists. In these simulations, we made use of single point mutations which reached the open state within a feasible timeframe and were later crystalized.

What did you do after your PhD?

I started a PostDoc position at Prof. Herings lab and am now a PI in a Zukunftskolleg funded by the FWF.

What was the impact of the MolTag program on your further career?

During my time in the program, **I had the financial possibility to do an internship at one the most renown scientist in the field** of the hERG channel in the USA. His recommendation letters and word-to-mouth advertising should never be underestimated.

What did you particularly like about the MolTag program?

For me, it was the financial support to go to conferences and visit international labs. Also, the **easy access to a variety of different expertise’s within MolTag to perform interdisciplinary research within Vienna** was a great advantage.

What is your recommendation for current MolTag PhD students?

Don’t take it for granted! The possibilities within MolTag are almost unlimited and you will have a lot of colleagues that won’t have the opportunity to visit one or more international conferences per year. Use this possibility!

Felix P. MAYER

Finishing year: 2017

Supervisor: Harald Sitte, Medical University of Vienna

Thesis title: Unraveling the mechanism of action of new psychoactive substances and their phase 1 metabolites.

Current Position and Employer: PostDoc in the Lab of Randy D. Blakely, Brain Institute, Florida Atlantic University, Boca Raton, FL, USA (after a PostDoc period at MedUni)

MolTag alumni page:

Felix Mayer (univie.ac.at)

Social network:

Felix Mayer (@felixpmayer) / **Twitter**

How would you summarize your thesis results in 3 sentences?

My project focused on the molecular mechanism of action of new psychoactive substances and d-amphetamine at monoamine transporters, i.e. the high-affinity transporters for dopamine (DAT), norepinephrine (NET) and serotonin (SERT) and the low-affinity/high-capacity transporter OCT3. We were able to show that the phase-1 metabolites of mephedrone exert bioactive effects and that stereochemistry dictates their mode of action at DAT, NET and SERT. The latter finding served as a starting point for a complex and promising project that should aid the discovery/characterization of a novel class of therapeutics.

What was the impact of the MolTag program on your further career?

Numerous interactions with students from other labs from different fields broadened my scientific background. Moreover, the program provided me with a solid basis of contacts for ongoing and future collaborations.

Did you keep connections with some former colleagues?

Yes. I am in close contact with my former supervisor and we are still working on unpublished projects from my PhD-thesis which will ultimately benefit from the techniques I learned during my postdoctoral training.

What did you particularly like about the MolTag program?

The social and scientific events enabled us to interact with PIs and the members of the SAB. These interactions did not only support the formation of potential collaborations but also **enabled us to discuss our projects from an academic and industrial perspective**. The financial support for traveling was excellent.

What is your recommendation for current MolTag PhD students?

Going to conferences, networking, go abroad, **seek international collaborations (not only within the Moltag program).**

MEDICAL UNIVERSITY OF VIENNA

Eva GSCHAIDER-REICHHART

Finishing year: 2017

Supervisor: Harald Janovjak, IST Austria
Co-Supervisor: Gaia Novarino, IST Austria

Thesis title: Optical and Optogenetic Control of Cell Proliferation and Survival.

Current Position and Employer: Operational Managment Trainee, Takeda Pharmaceutical Company, Vienna, Austria (after a PostDoc year at Monash University, Melbourne, Australia)

MolTag alumni page:

Eva Gschaider-Reichhart (univie.ac.at)

Social network:

Eva Gschaider-Reichhart | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

The goal of the thesis was the development of new strategies for optical and optogentic control of proliferation and pro-survival signalling. These new light-based systems have unique features, such as red light as an activator, or the avoidance of gene delivery. A special focus was placed to implement these new light-based approaches in pancreatic beta-cells, the key players in diabetes.

What was the impact of the MolTag program on your further career?

It was a great opportunity to learn more about different scientific fields, allowing me to gain a broad scientific background.

Did you keep connections with some former colleagues?

I am in contact with some of my colleagues from IST, who were also MolTag colleagues.

What did you particularly like about the MolTag program?

I enjoyed the opportunity to **learn more about different scientific fields and to get challenged from colleagues with another scientific background**. I also liked organizing the Symphosion together with my MolTag colleagues and the evenings together at the Heurigen.

What is your recommendation for current MolTag PhD students?

Be **open-minded for new and different things and aspects**.

IST AUSTRIA
Institute of Science and Technology

David Chan Bodin SIEBERT

Finishing year: 2018

Supervisors: Margot Ernst, Medical University of Vienna;

Marko Mihovilovic, TU Wien

Thesis title: Towards Selective Ligands for the $GABA_A$Receptor α+/β- Interface.

Current Position and Employer: Senior Account Manager at Schrödinger Drug Discovery Group, Munich, GER.

MolTag alumni page:

David Siebert (univie.ac.at)

Social network:

David Siebert, PhD | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

In my thesis we focused on the synthesis of a systematic library of differently substituted pyrazoloquinolinones to examine molecular determinants which trigger potency and efficacy at the α+/β- and the α+/γ2- sites of $GABA_A$ receptors. Here, we applied computational chemistry to create *in silico* models as well as mutational studies to shed light on the overall understanding of structural protein-ligand interactions. All in all, we identified several lead compounds for the design of subtype selective ligands at α+/β- interface which will be improved in future studies.

What else did you do after your PhD?

I am CEO and CoFounder of Craft Collective which is an internet platform to support local micro-breweries in Germany. We advertise their events and beer and create a new customer base for local brewers. Vice versa, we provide an overview for customers over the local beer scene in different cities.

What was the impact of the MolTag program on your further career?

The interdisciplinary program supported me to select from a broad range of job opportunities. Currently, I am working in a more biology field even though I am a chemist. Also, I am looking at a new position in the area of computational chemistry right now due to my knowledge gained at MolTag lab rotations.

What did you particularly like about the MolTag program?

Interdisciplinary and international program with a lot of **opportunities to get to know different working techniques as well as different work places**. Also, the individual educational budget helps to set the focus in areas you really interested in.

What is your recommendation for current MolTag PhD students?

Stay open-minded and **try to get as much out of MolTag as possible regarding extra education.** It really is a unique opportunity and you should be happy to be part of it :).

TECHNISCHE UNIVERSITÄT WIEN

MEDICAL UNIVERSITY OF VIENNA

Kumaresan JAYARAMAN

Finishing year: 2018

Supervisor: Harald Sitte, Medical University of Vienna

Thesis title: A biophysical study to investigate oligomer orientations and interface of the human dopamine transporter.

Current Position and Employer: PostDoc in the group of Prof. Holger Gohlke, Computational Pharmaceutical Chemistry and Molecular Bioinformatics, H.H. University, Düsseldorf, Germany

MolTag alumni page:

Kumaresan Jayaraman (univie.ac.at)

Social network:

Kumaresan Jayaraman | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

I have studied the bacterial homolog of NSS Leucine transporter (LeuT) and found the environment mediated structure and function variation in transporters. Moreover, the transport cycle was studied using steered molecular dynamics simulations combined with umbrella sampling. Further, I have studied the oligomeric nature of human dopamine transporter (hDAT) and elucidated an unique model in transporter oligomerization.

What was the impact of the MolTag program on your further career?

I am trained as a computational structural biologist. In the MolTag program, I got the opportunity to interact with many experimental researchers from various fields. **I have gained knowledge in the fields where I don't have expertise.** The journal club, progress presentations and symposiums are the places where the knowledge share happened. It helped and helping me to grasp concepts in diverse fields in better way. **Also, it's really helpful while writing grant proposals and to come up with new ideas.**

Did you keep connections with some former colleagues?

Yes! I am in contact with my former colleagues.

What did you particularly like about the MolTag program?

Interdisciplinary nature of the program.

What is your recommendation for current MolTag PhD students?

Hard work is the key to success. Interact more with your fellow PhD students in the program. Make healthy discussions during the presentations**.**

MEDICAL UNIVERSITY OF VIENNA

Dominik DREIER

Finishing year: 2018

Supervisor: Marko Mihovilovic, TU Wien

Co-Supervisor: Harald Sitte, Medical University of Vienna

Thesis title: Synthesis and Evaluation of Photoswitchable Monoamine Transporter Inhibitors.

Current Position and Employer: Consultant at the Boston Consulting Group, Austria, Vienna

MolTag alumni page:

Dominik Dreier (univie.ac.at)

Social network:

Dr. Dominik Dreier | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

A photoswitchable molecule's structure (and hence, biological activity) changes upon irradiation with light. We synthesized small molecules to inhibit different monoamine transporters. Ultimately, some of the compounds were both, active and inactive, dependent on whether you would apply light or not.

What did you do after your PhD?

After some vacation I became a Junior Consultant at BCG where we help corporations to solve challenging business problems. A systematic approach and analytical thinking trained in a PhD program are of great advantage.

What was the impact of the MolTag program on your further career?

In my current role at BCG I need to collaborate with people from many different backgrounds and industries. **The MolTag program prepared me well to always consider various perspectives and comfortably navigate a multidisciplinary environment**.

Did you keep connections with some former colleagues?

Yes, indeed. With many of my cohort we stayed in touch and I am very happy to regularly meet and catch up.

What did you particularly like about the MolTag program?

I appreciated the **regular interaction with many motivated people from different fields** and the rewarding opportunity to spend a semester at Columbia University.

TECHNISCHE UNIVERSITÄT WIEN

Catherine McKENZIE

Finishing year: 2018

Supervisor: Harald Janovjak, IST Austria

Thesis title: Design and characterization of methods and biological components to realize synthetic neurotransmission.

Position after PhD: Post-doctoral fellow in the group of Prof. Olivier Thoumine; Interdisciplinary Institute for Neuroscience (IINS), Bordeaux, France

MolTag alumni page:

Catherine McKenzie (univie.ac.at)

Social network:

Catherine McKenzie | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

My PhD thesis was highly interdisciplinary in terms of components and experimental approach. I employed molecular biology, chemogenetics, electrophysiology and imaging throughout my thesis. I focus and result was on building biological methods to specifically address how tangible elements of the mammalian brain (ie synaptic communication) translate to cognitive processes and behavioral output.

What are you doing now?

I am in my second year as a post-doctoral fellow at IINS, where I focus on employing 3D super-resolution microscopy, optogenetics, and electrophysiology to understand the role of adhesion proteins in real-time by optical recruitment and reassembly of these proteins at synapses.

What was the impact of the MolTag program on your further career?

I gained a lot of support from the faculty throughout my PhD research as well as how to proceed into a post-doctoral fellow.

Did you keep connections with some former colleagues?

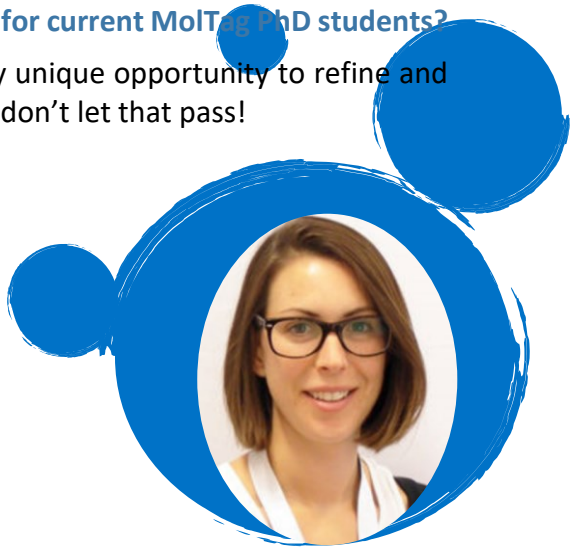
Yes! **and it is so nice to share what the next steps after finishing PhD are like and what are the similarities and difference are for each of us.**

What did you particularly like about the MolTag program?

The interdisciplinary approach was the most impactful on my PhD research. **I was exposed, through MolTag, to experimental approaches and expertise that was not available at my host institution**. This exposure created creative avenues in which to think about next steps in my PhD work.

What is your recommendation for current MolTag PhD students?

MolTag gives you the incredibly unique opportunity to refine and extend your scientific network, don't let that pass!



IST AUSTRIA
Institute of Science and Technology

Sankalp JAIN

Finishing year: 2018

Supervisor: Gerhard Ecker, Faculty of Life Sciences, University of Vienna

Thesis title: Ligand-based and Structure-based Studies to Understand the Molecular Basis of Inhibition of ABC Transporters Expressed in the Liver.

Current Position and Employer: Postdoctoral Research Fellow; Division of Preclinical Innovation Early Translation Branch, NCATS, NIH, Bethesda, MD, USA

MolTag alumni page:

Sankalp Jain (univie.ac.at)

Social networks:

Sankalp Jain | **LinkedIn**

Sankalp Jain (@Sankinator) / **Twitter**

How would you summarize your thesis results in 3 sentences?

My Ph.D. focused on structure-based drug design studies on three major ABC transporters—BSEP, BCRP and P-glycoprotein—that helped in identifying the molecular features responsible for the inhibitory activity of ligands at these transporters.

What did you do after your PhD?

Currently I am a postdoctoral research fellow in the Early Translation Branch at NCATS-NIH. I serve as a computational chemist, specializing in chemoinformatics, machine learning and molecular modeling. I apply and develop artificial intelligence-based machine learning prediction and classification models and perform virtual screening for various therapeutic endpoints.

What was the impact of the MolTag program on your further career?

Moltag brings experts/researchers from diverse (yet related) domains of drug-design together; **this really helped me in expanding my knowledge and skills in those areas.**

Did you keep connections with some former colleagues?

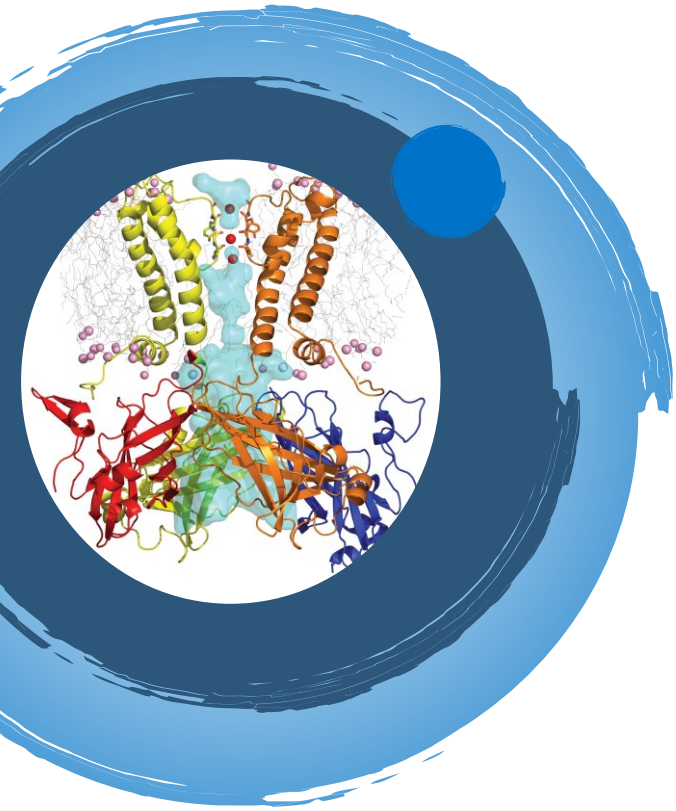
For Sure! The people and connection we made during the MolTag period happens to stay connected 😉

What did you particularly like about the MolTag program?

What I liked most are the **guest lectures and journal clubs** organized for MolTag. And also the retreats were the best part of MolTag, where we can exchange science over great food and drinks 😋

What is your recommendation for current MolTag PhD students?

Well my recommendation would be to take the complete benefit of the MolTag program by attending the lectures and presentations. **Also do focus on networking from different conferences and project meetings.**



MOLTAG COMMUNICATION

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Univ.Prof.Mag.Dr**. Gerhard Ecker**
University of Vienna
Division of Pharmaceutical Chemistry
Pharmacoinformatics Research Group (univie.ac.at)

Deputy Speakers:
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Medical University of Vienna
Dept. of Neurobiology of the Nervous System
Margot Ernst (meduniwien.ac.at)

Assoz.Prof.Mag.Dr. Anna Weinzinger
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Dept. of Pharmacological Toxicology
Molecular modelling of ion channels (Prof. Weinzinger) (univie.ac.at)

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MolTag Doctoral Program | **LinkedIn**

MolTag Doc Program (@MoltagDK) / **Twitter**

FINANCIAL SUPPORT BY:

FWF Der Wissenschaftsfonds.