MolTag Graduates 2013 - 2015

- **Thomas Steinkellner**, Medical University of Vienna

- **Tobias Linder**, University of Vienna

- **Song Ke**, University of Vienna

- **Lukas Rycek**, TU Wien

- **Andreas Jurik**, University of Vienna

- **Amir Seddik**, University of Vienna

- **Juliane Faschang** née Hintersteiner, University of Vienna

- **Angela Schöffmann**, University of Vienna

- **Denise Kogler** (née Luger), University of Vienna

- **Priyanka Saxena**, University of Vienna

Thomas STEINKELLNER

Finishing year: 2013

Supervisors: Harald Sitte, Medical University of Vienna

Thesis title: Amphetamine action at dopamine and serotonin transporters is modulated by aCaMKII.

Current Position and Employer: Assistant Prof. at Institute of Pharmacology, Med. University of Vienna (after a PostDoc at Hnasko-Lab, Neurosciences, UCSD, San Diego, USA)

MolTag alumni page:
Thomas Steinkellner (univie.ac.at)

Social networks:
Thomas Steinkellner | **LinkedIn**
Thomas Steinkellner (@TomSteinkellner) / **Twitter**

How would you summarize your thesis results in 3 sentences?

The psychostimulant properties of amphetamines require CamKII-dependent interaction and modulation of monoamine transporters to exert their full-fledged effects. Pharmacological inhibition or genetic deletion of CaMKII abolish transporter-mediated substrate release and result in behavioral alterations in mice. While the addictive properties of amphetamines are preserved, the motor-stimulating effects are diminished suggesting that these effects are mediated partly by different molecular processes.

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

MolTag enabled me to train in theoretical and practical skills related to drug development and pharmacology through ample interactions with experts in different disciplines and helped informing me about different ways of tackling down a research question from both an academic- as well as industry-point of view.

What did you particularly like about the MolTag program?

MolTag offered **many occasions that allowed me to interact with both, my student fellows as well as the individual PIs. Our frequent seminars covered many exciting topics and offered insights into both, academic science as well as industry**. Finally, the multidisciplinary science branches participating in the program offered valuable insights in the various processes involved in drug development.

What is your recommendation for current MolTag PhD students?

Use the frequent opportunities to attend seminars and interact with you colleagues. **The lab rotations are particularly exciting to learn new techniques and look at research questions from different angles.** They are also good ways to start new collaborations, and get a feeling of how science is done in other labs. Most importantly, use the opportunity to go abroad and **experience some outside-the-box thinking outside your comfort zone.**

MEDICAL UNIVERSITY OF VIENNA

Tobias LINDER

How would you summarize your thesis results in 3 sentences?
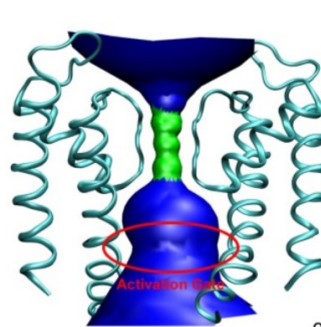
My thesis provided novel insights into K$^+$ channel specific movements on amino acid level of the opening and closing behavior of these channels which is crucial for ion conduction and the importance of these movements to drug binding. In all studied K$^+$ channels, the prototypical bacterial K$^+$ channel KcsA, the bacterial inward rectifier K$^+$ channel KirBac1.1, and the human Kv channel hERG, aromatic amino acids were found to play crucial roles in gating by unlocking channels from a specific state (F114 in KcsA), by forming the pore gate (F146 in KirBac1.1) and by shaping the drug binding site (Y652 and F656 in hERG). Specifically, studies on the hERG channel disclosed the important role of F656 for drug trapping which is characterized by the drug's retention in its binding site upon channel closure.

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

It affected to a high degree the way of how I pursue my goals and **always reminds me to keep an open mind**.

What did you particularly like about the MolTag program?

The opportunity to get insights into different research areas and to **discuss research questions from different perspectives** with scientists from all around the world. Also the possibility of research stays in Germany and the USA was great.

Finishing year: 2014

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

Thesis title: Pore gating of potassium channels and its relevance for drug effects.

Current Employer: Self-employed Pharmacist (owner), Dornbirn, Vorarlberg, Austria

MolTag alumni page:

Tobias Linder (univie.ac.at)

Social network:

Tobias Linder | **LinkedIn**

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Song KE

Finishing year: 2015

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

Thesis title: Selectivity and conduction studies in bacterial voltage-gated sodium channels by molecular dynamics simulations.

Current Employer: Medical Advisor at Beigene, Shanghai, China

MolTag alumni page:

Song Ke (univie.ac.at)

Social network:

Song Ke | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

We performed the MD analysis of the sodium ion conduction in sodium channels; analyzed the kinetics and thermodynamics of the sodium ions inside channel's selectivity filter at atomic level.

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

It provides sufficient basic training, freedom and funding resources to conduct research. Through these trainings, I developed rigorous and strategic scientific thinking and acumens which ensures a fine career as medical science liaison and medical advisor in pharma-industry.

Did you keep connections with some former colleagues?

Not too much, but look forward to reconnecting with Moltag Alumni.

What did you particularly like about the MolTag program?

A. **Sufficient funding sources** to support us to participate into the exchange program and international conferences
B. **Enough freedom and good interdisciplinary platform to expand our vision** of various cross-functional and cutting-edge knowledge and techniques

What is your recommendation for current MolTag PhD students?

Don't forget to carry out aerobic sports & extensive reading in philosophy during busy studies, which makes you even more energetic and creative.

Lukas RYCEK

Finishing year: 2016

Supervisor: Marko Mihovilovic, TU Wien

Co-Supervisor: Margot Ernst, Medical University of Vienna

Thesis title: Synthesis and Biological Evaluation of Natural Products and Derivatives as potential Anti-Inflammatory Agents and $GABA_A$ Receptor Modulators.

Current Position and Employer: Assistant Prof., Dept. of Organic Chemistry, Charles University Prague, Czech Republic

MolTag alumni page:

Lukas Rycek (univie.ac.at)

Social network:

Lukas Rycek, PhD. | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

We synthesized several derivatives of natural products. In the collaboration with MolTag partners (and others) we evaluated them as modulators of $GABA_A$ receptors and for potential anti-inflammatory activity. We developed few compounds with superior activity and selectivity towards the targets of interest compared to the lead natural products.

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

MolTag is a great opportunity to learn about different, yet somehow related disciplines. One more thing is that **MolTag was all about cooperation between groups**. This is not easy, because different people have different priorities. The cooperation in MolTag worked mostly well and I could learn, how to deal with such a challenge. **All this made me realize, what is the role of my own discipline in the broader perspective** and based on it, I can better understand what I want to do within my field and my current career develops accordingly.

What did you particularly like about the MolTag program?

The multidisciplinarity. We had to attend all kind of seminars and listen to many presentations. And to be honest, in the beginning I quite often had difficulties to understand what my colleagues or specialists from different fields were presenting. But with time, I started to understand their "language" and out of sudden, things started to make much more sense. **So what looked in the beginning like a waste of time turned out to be a great investment of it. The coin has of course two sides.** I tried to do my best to make others understand the "language I was speaking" and make them aware of what my field is about. I also have to mention the financial side. There were always resources.

TECHNISCHE UNIVERSITÄT WIEN

Andreas JURIK

Finishing year: 2015

Supervisor: Gerhard Ecker, Faculty of Life Sciences, Univ. of Vienna

Thesis title: In Silico Evaluation of Inhibitor Binding Modes in the Gamma-Aminobutyric Acid Transporter System.

Current Position and Employer: Senior Regulatory Affairs Manager at AOP Orphan Pharmaceuticals AG, Vienna, Austria

MolTag alumni page:
Andreas Jurik (univie.ac.at)

Social network:
Andreas Jurik | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

Making use of the individual toolboxes of institutions participating in MolTag, it was possible to elaborate and experimentally challenge hypotheses based on in-silico calculations. This helped gaining insights to the molecular determinants of ligand recognition and transporter subtype differentiation in the GABA reuptake system.

What are you doing now?

Managing marketing authorization applications and lifecycle strategies for medicinal products with a focus on cardiology and intensive care on European and global level.

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

The MolTag program helped **me to broaden the picture on possible strategies to approach complex questions**. Deeper understanding of – back then – current trends in science and big pharma is also now facilitating **to bridge the worlds of cutting-edge pharmaceutical development to established frameworks in regulatory authorities**.

Did you keep connection with some former colleagues?

I am happy that the contact with some former colleagues is still active, and I hope it will stay like this.

What is your recommendation for current MolTag students?

Challenge yourself, your goals and your project on a regular basis. If you don't go forwards, you go backwards.

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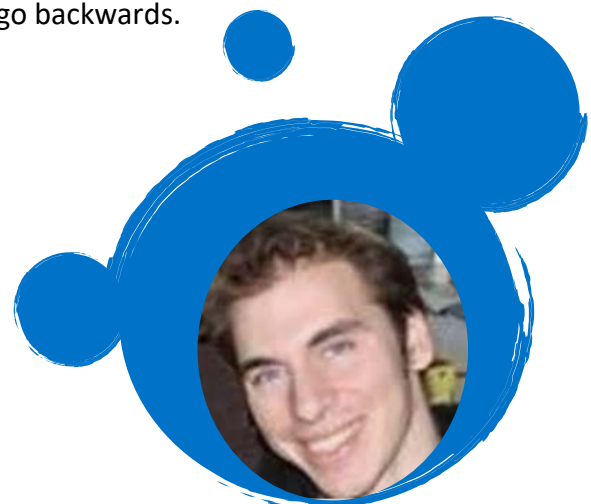
Amir
SEDDIK

Finishing year: 2015

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

Thesis title: Substrate selectivity profiling of the human monoamine transporters

Current Position and Employer: Data scientist at Visa Consulting & Analytics, Kuala Lumpur, Malaysia

MolTag alumni page:

Amir Seddik (univie.ac.at)

Social network:

Amir Seddik | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

My doctorate research has contributed to a better understanding of how monoamine molecules selectively bind to transporter proteins. Such research is fundamental to the improvement of currently used medication. The methods I used were primarily computational modelling, such as genetic algorithms, regression, classification, moleducular dynamics simulations and binding free energy calculations. I supervised other students in applying these techniques, and reported my findings to post-doctorates, professors and at (international) conferences.

What are you doing now?

I help Malaysian banks improving their analytical capabilities.

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

I learned to manange different stakeholders, networking, programming, machine learning.

Did you keep connections with some former colleagues?

Yes definitely! I keep contact regularly with many former colleagues who are all around the world.

What did you particularly like about the MolTag program?

The fact that people come from different parts of the world, the courses on pharmacology and chemistry, **getting to know Austrian culture, the possibility to attend European and international conferences and much more.**

What is your recommendation for current MolTag PhD students?

To **think well about where you want to see yourself after the PhD, because you should see your PhD as a preparation for the next step in your career**. To come for yourself and to participate in (steering) comittees with professors and express your opinions and ideas…

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Juliane
FASCHANG née Hintersteiner

Finishing year: 2015

Supervisor: Steffen Hering, Faculty of Life Sciences, University of Vienna

Thesis title: In vivo characterization of natural product GABA$_A$ modulators and their derivatives.

Current Employer: Private Pharmacy, Upper Austria, Austria

MolTag alumni page:

Juliane Faschang née Hintersteiner (univie.ac.at)

How would you summarize your thesis results in 3 sentences?

The aim of my thesis was to analyze anxiolytic, sedative, and anticonvulsive effects of Valerenic Acid, Piperine and selected derivatives, which positively modulate GABA$_A$ receptors comprising β2- or β3- subunits. The studied Valerenic Acid derivatives may serve as scaffolds for the development of novel anxiolytics and/or anticonvulsants. Piperine derivatives SCT-66 and compound 23 induced more pronounced anxiolysis in mice than piperine and thus may be an interesting starting point for the development of novel anxiolytics.

What are you doing now?

I worked in a hospital pharmacy, where I practiced clinical pharmacy. After parental leave, I continued working in privately owned pharmacy. Currently, I am in parental leave again and enjoy the time with my family.

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

I learned much about scientific writing and presenting my scientific work. After finishing my PhD, I worked in a hospital pharmacy, where I benefited a lot from this knowledge.

What did you particularly like about the MolTag program?

When the program started, I felt like I was not a lone fighter any more. I found it very interesting to see how others work on their thesis. We were in constant contact and if you had a problem you could ask the others and get some input.

What is your recommendation for current MolTag PhD students?

Conducting a PhD is a lot of work. You need staying power, tenacity, and diligence. **Team-up with like-minded people, exchange your thoughts and ideas, and do not forget to have fun during this time!**

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Angela SCHÖFFMANN

Finishing year: 2015

Supervisor: Steffen Hering, Faculty of Life Sciences, University of Vienna

Thesis title: Natural Products as Scaffold for the Development of $GABA_A$ Receptor Ligands.

Current Position and Employer: Country Safety Lead, sanofi-aventis GmbH, Vienna, Austria

MolTag alumni page:

Angela Schöffmann (univie.ac.at)

How would you summarize your thesis results in 3 sentences?

Discovery of more potent $GABA_A$ ligands,
Investigation of derivatives on vanilloid receptor-1,
Elucidation of SAR and pharmacophore modell,
Development of new scaffold for antiepileptic drugs.

What are you doing now?

From a professional perspective: Country Safety Lead, sanofi-aventis GmbH, Vienna, Austria.

From a personal perspective: Enjoying maternity leave and taking care of a lovely not-yet-a-year-old baby boy.

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

I significantly improved my (scientific) English and greatly benefited from experience in project management, from great team work and international collaboration with top scientists.

Did you keep connections with some former colleagues?

Yes.

What did you particularly like about the MolTag program?

The spirit - motivated, open-minded, skilled and open-hearted people working together

What is your recommendation for current MolTag PhD students?

Enjoy a great time together and **make use of any occasion to take a glance into your peer's field of work**. Travel. Stay in touch.

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Denise
KOGLER née Luger

Finishing year: 2015

Supervisor: Steffen Hering, Faculty of Life Sciences, Univ. of Vienna

Thesis title: Molecular determinants of $GABA_A$ receptor modulation by valerenic acid.

Current Position and Employer: Hospital Pharmacist at the Wiener Gesundheitsverbund (Klinik Favoriten), Vienna, Austria; University Lecturer

MolTag alumni page:

Denise Kogler (née Luger) (univie.ac.at)

Social network:

Denise Kogler 🖉 | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

I combined electrophysiology, animal behavioural testing and computational biology to investigate amino acids necessary for efficient modulation of $GABA_A$ receptors by Valerenic acid (VA). By doing so, I localized the potential binding site of VA on $GABA_A$ receptors and showed that it overlaps with binding sites for known anaesthetics such as etomidate. Based on this findings, we then generated novel $GABA_{\underline{A}}$ receptor ligands together with the group of Prof. Mihovilovic with enhanced $GABA_A$ receptor activity and increased anxiolytic and anticonvulsant potential.

What are you doing now?

After a PostDoc at UniVie, I joined AstraZeneca as a Medical Scientfic Liaison Manager, responsible for scientific communication and KOL management. In 2017 I moved back to the hospital sector. Since then, I work as a hospital pharmacist. My main tasks are the initiation and management of oncology and Covid-19 clinical trials in the hospital pharmacy, providing medical and scientific information about the effective and safe drug use to doctors as well as the supervision of the sterile compoundig of individual drug preparations for cancer patients. Additionally, I lecture courses on drug development, clinical trial management, applied pharmacology and clinical pharmacy at Universities in the Vienna area.

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

It broadened my horizons by collaborating with various research groups from different universities and countries. I also got insight into drug synthesis and computational biology by joining research groups at TU Wien and MedUni. Further, I had the great opportunity to spend 6 months at UCL London, where I gained experiences on patch-clamp physiology of isolated neurons.

What is your recommendation for current MolTag students?

Take advantage of the MolTag network and build relationships to researchers all over the world!

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Priyanka SAXENA

Finishing year: 2015

Supervisors: Steffen Hering and Evgeny Timin; Faculty of Life Sciences, University of Vienna

Thesis title: hERG channel pharmacology – relation to proarrhythmia and novel molecular determinant.

Current Position and Employer: Research Associate at the Institute of Cardiovascular and Medical Sciences, University of Glasgow, UK

MolTag alumni page:

Priyanka Saxena (univie.ac.at)

Social network:

Priyanka Saxena | **LinkedIn**

How would you summarize your thesis results in 3 sentences?

In my thesis I was involved in studying structure, function and pharmacology of cardiac hERG potassium channel and one of my major finding is identification of new molecular binding determinant of hERG potassium channel.

What did you do after PhD?

After completing PhD I have joined department of Cardiovascular Sciences, University of Glasgow as a post-doctoral research assistant and recently I have been promoted as a Research Associate.

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

MolTag being an international PhD programme gave me an **opportunity to network and recognition with in the scientific community along with the scientific knowledge and experience** which together helped in my career

Did you keep connections with some former colleagues?

Yes I am in touch with some of my colleagues and friends within the programme who was with me in the journey

What did you particularly like about the MolTag program?

MolTag programme is one of the best international PhD programme and I find myself very fortunate to be an alumni of the same.

What is your recommendation for current MolTag PhD students?

You are in one of the best place make the best out of this amazing programme and gain as much experience as you can to advance your future research career.
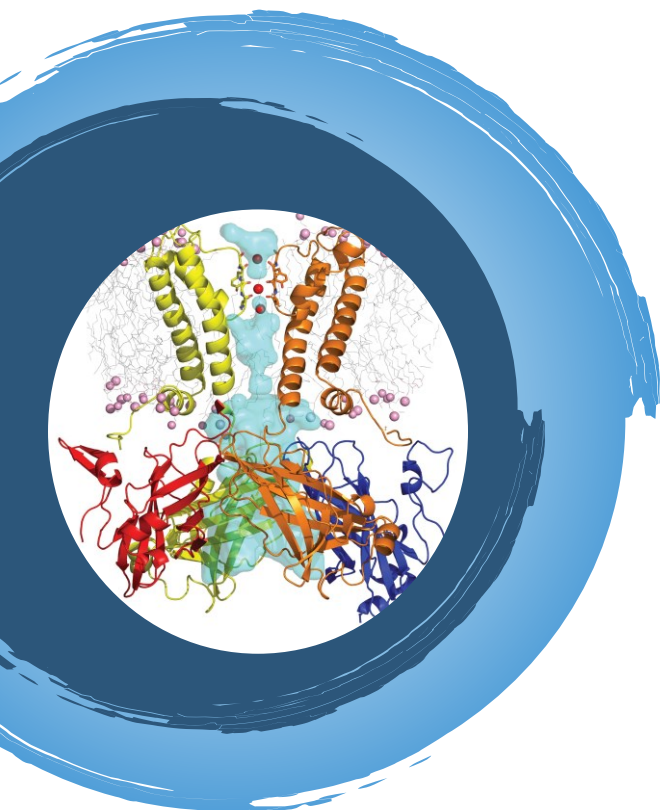
MOLTAG COMMUNICATION

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

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

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

MolTag Program Management:
Susanne Menschik-Zunzer
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MolTag Doctoral Program | **LinkedIn**

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