



## MolTag Graduates 2019 - 2020

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## Yong CHEN



**Finishing year:** 2019

**Supervisor:** Nuno Maulide,  
Faculty of Chemistry,  
University of Vienna

**Co-Supervisor:** Harald  
Janovjak, IST Austria

**Thesis title:** Total Synthesis of  
Cicutoxin and FR252921 via a  
Unified Pericyclic Approach.

**Current Position and  
Employer:** PostDoc in the lab  
of Prof. Buno De Geest, Lab  
for Biopharmaceutical  
Sciences, University of Ghent,  
Belgium

**MolTag alumni page:**  
[Yong Chen \(univie.ac.at\)](#)

**Social network:**  
[Yong Chen | LinkedIn](#)

### How would you summarize your thesis results in 3 sentences?

We achieved the most efficient and short total synthesis of an immunosuppressant metabolite FR252921 to date. The key to this success is based on the  $4\pi$ -electrocyclic ring opening of a cyclobutene moiety. This ring opening reaction can serve as a general strategy for the synthesis of other polyene natural products.

### What are you doing now?

My current research topic focuses on the materials engineering in the field of immunotherapy and vaccine development. I like my research a lot as it involves interdisciplinary skills, and most importantly it is quite crucial to help to cure diseases, such as COVID-19.

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

MolTag is a family harboring people with different backgrounds. The seminars and outreaches organized by MolTag program definitely help me to broaden my horizons. **I myself am a trained organic chemist, but through my PhD study with MolTag program, I developed a strong interest in biology.** Guess what? The more I am involved in the problems of biology now, the more I believe in the power of chemists.

### What did you particularly like about the MolTag program?

I am very grateful for the opportunity to do an internship abroad. After my internship in Berlin, **I am determined to do research in the interface of chemistry and biology.**

### What is your recommendation for current MolTag PhD students?

I would recommend to **focus on what you are good at**, in the meantime appreciate the developments from other scientific areas.





## Marco STADLER

**Finishing year:** 2019

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

**Co-Supervisor:** Margot Ernst,  
Medical University of Vienna

**Thesis title:** Interaction of  
GABA<sub>A</sub> Receptors with Natural  
Compounds and Protons.

**Current Position and Employer:**  
Medical Science Liaison,  
BioMarin Pharmaceuticals,  
Vienna, Austria

**MolTag alumni page:**  
[Marco Stadler \(univie.ac.at\)](http://MarcoStadler.univie.ac.at)

**Social network:**  
[Marco Stadler, PhD | LinkedIn](#)

### How would you summarize your thesis results in 3 sentences?

We elucidated structural components of GABA<sub>A</sub> receptors required for modulation through selected natural compounds and leveraged these new insights for developing novel, simple, synthetic compounds with enhanced activity. In addition we described for the first time that selected GABA<sub>A</sub> receptor subtypes can be activated under acidic conditions.

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

It helped me understand **how to wrap up and present content to people of different backgrounds.**

### Did you keep connections with some former colleagues?

Sure. We created a network that we can draw on any time.

### What did you particularly like about the MolTag program?

I think the guest lectures belong to those assets of Moltag I appreciated the most. Because they enabled to engage with renowned scientists very easily for collaborations, internships,...

### What is your recommendation for current MolTag PhD students?

Exchange with other colleagues as often as possible, also attend lectures which have little to do with your thesis - there is always something you can take away... **AND work hard in silence, but celebrate success.**





## Martin BERGER



**Finishing year:** 2019

**Supervisor:** Nuno Maulide,  
Faculty of Chemistry, University  
of Vienna

**Co-Supervisor:** Harald Janovjak,  
IST Austria

**Thesis title:** Synthesis of Natural  
Products and Analogues by  
Directed C-H Activation and  
Unified Synthesis of Cicutoxin  
and Virol A *via* Electrocyclic  
Cyclobutene Ring Opening.

**Current Position and Employer:**  
PostDoc in the group of Paolo  
Melchiorre at the ICIQ  
Tarragona, Spain

**MolTag alumni page:**  
[Martin Berger \(univie.ac.at\)](https://univie.ac.at)

**Social network:**  
[Martin Berger | LinkedIn](#)

### How would you summarize your thesis results in 3 sentences?

During my doctoral studies I focused on the total synthesis of biologically active natural products. The most dominant synthetic strategy was C-H activation, which allowed furthermore the preparation of biologically active analogues. This resulted in the preparation of the alkaloid quinine, polyhydroxylated triterpenoids or analogues of dehydroabietic acid amongst others.

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

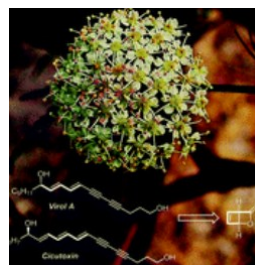
The interdisciplinary collaborations within the program were very beneficial on the outcome of my projects and the resulting publications. This approach will remain a steady part in my further career and when the research allows I will happily contact previous collaborators from the MolTag program again.

### Did you keep connections with some former colleagues?

I have sporadically contact with former colleagues.

### What did you particularly like about the MolTag program?

Talking chemistry to non-chemists cannot be learned from books or in the own research group. It is best learned in the MolTag program.





# Stanislav ANDRANOVITŠ



**Finishing year:** 2019

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

**Co-Supervisor:** Anna  
Weinzinger, Faculty of Life  
Sciences, University of Vienna

**Thesis title:** Probing the role of  
voltage sensors in calcium  
channel inactivation and  
inhibition by antagonists.

**Current Position and Employer:**  
Affiliate Pharmacovigilance QC  
Associate at Cognizant,  
Budapest, Hungary

**MolTag alumni page:**

[Stanislav Andranovits \(univie.ac.at\)](#)

**Social network:**

[Dr. Stanislav Andranovič | LinkedIn](#)

## How would you summarize your thesis results in 3 sentences?

In my dissertation I tried to answer the question how charge neutralization in voltage sensors affects activation and inactivation processes in Cav1.2 voltage-gated channels. To understand the role of the voltage sensors in those processes the charges of voltage sensors were gradually neutralized. The main result of my study was the significant effect of the first segment on the gating processes.

## What did you do after your PhD?

I started my career in ChanPharm GmbH, where my work was focused on drug screening projects. Nowadays, I work in drug safety field, managing data on the safety of medicines

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

The Moltag program gave me a chance to grow as a person and as a worker. It taught me to take responsibilities in my work, improved my presentation and communication skills.

## Did you keep connections with some former colleagues?

I am in very close contact with Daniela Cintulova. During our PhD time we did not communicate as much as now, but nowadays we are colleagues and very close friends.

## What did you particularly like about the MolTag program?

Moltag program was very different from a simple PhD program. Especially I liked the yearly gatherings, that kept us fit. **The possibility to have an internship abroad, was also a huge advantage of the program.**

## What is your recommendation for current MolTag PhD students?

My recommendation to the students would be to **build as many connections as possible, not only in academia but also in the industry.** Try to think in advance about your career development and find corresponding contacts. Don't forget to network





# Eva HELLSBERG



**Finishing year:** 2019

**Supervisors:** Gerhard Ecker and Anna Weininger, Faculty of Life Sciences, University of Vienna

**Co-Supervisors:** Harald Sitte, Medical University of Vienna

**Thesis title:** Computational studies of molecular interactions in the human serotonin and dopamine transporters.

**Current Position and Employer:** PostDoc in the group of Prof. Lucy Forrest, Computational Structural Biology Unit, NINDS, NIH, Bethesda, MD, USA

**MolTag alumni page:**  
[Eva Hellsberg \(univie.ac.at\)](http://Eva.Hellsberg@univie.ac.at)

## How would you summarize your thesis results in 3 sentences?

The overall goal of my thesis was to enhance our understanding of crucial molecular interactions in the human serotonin and dopamine transporters (hSERT and hDAT) by using computational methods. My thesis provided useful findings about (i) the selectivity profiles of hSERT and hDAT, and (ii) important molecular characteristics of the substrate-bound outward-occluded state of hSERT. These predictive models of protein-ligand interactions can serve as a valuable starting point for future development of neuropharmacological treatments during the early stage of the drug discovery pipeline and have the potential to impact studies of many mechanistically related proteins, as the monoamine transporters adopt a protein fold common among transporters beyond the solute carrier 6 (SLC6) family.

## What did you do after your PhD?

I started a Postdoc in Dr. Lucy Forrest's lab at the National Institutes of Health (NIH).

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

I was in the main organization team of the Moltag Science Day in 2016. **We invited Dr. Forrest as one of our speakers, and so I connected for the first time with her through the Moltag program.**

## Did you keep connections with some former colleagues?

Yes, I did and still do – with both PIs and several of my peers all over the world!

## What did you particularly like about the MolTag program?

I like its **interdisciplinarity, the exposure to various research fields, and the training possibilities it offered.**





## Konstantina BAMPALI

**Finishing year:** 2019

**Supervisor:** Margot Ernst,  
Medical University of Vienna

**Co-Supervisor:** Harald Sitte,  
Medical University of Vienna

**Thesis title:** Structural basis of  
allosteric GABA<sub>A</sub> receptor  
modulation.

### **Current Position and**

**Employer:** PostDoc in the  
Center of Brain Research,  
Medical University of Vienna,  
Austria

### **MolTag alumni page:**

[Konstantina Bampali \(univie.ac.at\)](https://www.univie.ac.at)

### **Social network:**

[Konstantina Bampali | LinkedIn](#)

### **How would you summarize your thesis results in 3 sentences?**

The aim was to improve the understanding of the molecular and structural rules which underlie allosteric modulation of GABA<sub>A</sub> receptors, in part also applied to subtype selective ligands. Defining structural determinants of binding of characterized compounds, such as benzodiazepines, as well as binding site hypotheses were the main findings of my thesis work.

### **What are you doing now?**

I am participating in the IMI Horizon 2020 research and innovation program and EFPIA: "Neurotoxicity De-Risking in Preclinical Drug Discovery".

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

The interdisciplinary nature of MolTag allowed me to grow my knowledge further and be more equipped for the challenging projects of my Postdoc studies. Most importantly, it has allowed me to establish invaluable connections and collaborations that not only reinforce my current research, but also provide immense support for my further career development.

### **What did you particularly like about the MolTag program?**

I feel very lucky to have met wonderful people and brilliant scientists and grateful to have been part of such a cooperative and supportive environment. MolTag gave me the opportunity to have one of the greatest experiences of my life, which was a research internship at Harvard Medical School. I was able to gain amazing new experiences, grow my scientific skillset further, as well as meet distinguished scientists.

### **What is your recommendation for current MolTag PhD students?**

Invest in building scientific, as well as personal relationships within MolTag and beyond. **Projects can become a lot stronger when you join forces!** Most of all, just enjoy it, and have fun!





## Xingyu CHEN

**Finishing year:** 2019

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

**Co-Supervisor:** Thierry Langer,  
Faculty of Life Sciences,  
University of Vienna

**Thesis title:** *In silico*  
investigations of KATP-  
channels

**Current Position and  
Employer:** PostDoc with the  
topic of enzyme engineering,  
in the group of Thomas  
Simonson, the Structural  
Biology of the Cell Laboratory,  
Ecole Polytechnique,  
Palaiseau, France.

**MolTag alumni page:**

[Xingyu Chen \(univie.ac.at\)](https://www.univie.ac.at)

### How would you summarize your thesis results in 3 sentences?

The rare disease Cantú syndrome is caused by gain-of-function mutations in KATP channels. In my thesis, I have investigated the KATP channels using structure-based and multiple computational methods. We gain more insight about the Cantú mutation mechanism. Our computational drug-repurposing strategy provides novel possibilities for development of Cantú treatment options and can be applied to explore novel therapies for other rare diseases.

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

The interdisciplinary of MolTag gave me different views from other related fields, which makes me adapt to the new job faster. Also, I've learned how to explain my topic in an easy way to the people in other fields.

### Did you keep connections with some former colleagues?

Yes.

### What did you particularly like about the MolTag program?

We had a lot of chances to attend the conferences we were interested in and the internships/lab rotations. We could invite guest lecturers and attend so many cool guest lectures. We met a lot of people and discussed our topic with them.

### What is your recommendation for current MolTag PhD students?

Take the benefit to attend conferences and to internships abroad (maybe after the pandemic), which is not normal in other doctoral programs. Also, take the chance to discuss your topic with other people, which would help a lot to develop the presentation- and discussion skills.







# Harald BERNSTEINER

**Finishing year:** 2019

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

**Co-Supervisor:** Gerhard Ecker,  
Faculty of Life Sciences,  
University of Vienna

**Thesis title:** Atomistic insight  
into function and dysfunction  
of inward-rectifier potassium  
channels.

**Current Position and  
Employer:** Clinical Assessor at  
the Austrian Agency for  
Health and Food Safety  
(AGES), Vienna, Austria

**MolTag alumni page:**  
[Harald Bernsteiner \(univie.ac.at\)](https://univie.ac.at)

## How would you summarize your thesis results in 3 sentences?

Molecular dynamics simulations with an applied electrical field revealed novel insights into gating, conduction mechanism and selectivity of K<sup>+</sup> channels. Our simulations captured the opening transition of two different Kir channels in presence of the modulating phospholipid PIP<sub>2</sub> and suggest a major importance of a conformationally stable selectivity filter for continuous ion flux. Further, these simulations provided insights into the role of charged residues in the ion channel pore.

## What are you doing now?

My job is to evaluate safety & efficacy of new medicines in frame of centralised European market authorisation applications. Additionally, I work on EMA Scientific Advice procedures. Both tasks are usually team efforts that are done by several assessors who work on clinical, non-clinical, quality and statistical methodology questions.

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

Working with different disciplines is also a fundamental part of my current job.

## What did you particularly like about the MolTag program?

The possibility to go abroad and to attend international conferences with scientifically top-level speakers. Further, **learning about the PhD projects of fellow MolTag students automatically results in less narrow-mindedness.**

## What is your recommendation for current MolTag PhD students?

Basically, as a PhD student **you often have to solve problems you didn't know about before by (self-)learning new methods and techniques** you maybe didn't know that they existed. **Do not underestimate the skills and experiences you gain during this process.**





## Daniela CINTULOVÁ



**Finishing year:** 2019

**Supervisor:** Marko Mihovilovic, TU Wien

**Co-Supervisor:** Harald Sitte, Medical University of Vienna

**Thesis title:** Synthesis and biological profiling of bioactive molecules for the investigation of monoamine transporters.

**Current Position and Employer:** Pharmacovigilance associate at Cognizant Technology Solutions, Budapest, Hungary

**MolTag alumni page:**  
[Daniela Cintulova \(univie.ac.at\)](#)

**Social network:**  
[Daniela Cintulova | LinkedIn](#)

### How would you summarize your thesis results in 3 sentences?

In my thesis we carried out chiral chemical synthesis of metabolites of a party drug mephedrone. We then investigated their neuropharmacological profile on monoamine transporters and identified metabolites that could contribute to the overall effect of the parental drug. We also confirmed stereo- and enantioselective metabolism of mephedrone in the human body.

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

Right now I am working in pharmacovigilance and therefore reading tons of medical literature every day. I am a chemist by training but thanks to Moltag I was working on a project which was highly interdisciplinary - apart from chemistry I did pharmacology, neurology, biological analysis, analytics, computational simulation. Now I have no problem to navigate myself through medical and pharmacology terms and publications.

### What did you particularly like about the MolTag program?

The interdisciplinary aspect of it. **I love learning new things and Moltag enabled me to do this. There was no problem to reach out for cooperation.** I enjoyed the interdisciplinary meetings, brainstormings, coordination of the projects across many fields. **I think it prepared me perfectly for any job afterwards.**

### What is your recommendation for current MolTag PhD students?

**If you can, become friends with your fellow Moltag students. Apart from gaining like-minded friends, the projects will proceed exponentially.** The best ideas came out of hanging out together. Moltag is not a competition, it is a cooperation. Most importantly, have fun at what you are doing, even if things are not going smoothly. You are here to try out, make mistakes, learn and eventually become an independent scientist.





## Marco NIELLO



**Finishing year:** 2019

**Supervisor:** Harald Sitte,  
Medical University of Vienna

**Co-Supervisor:** Margot Ernst,  
Medical University of Vienna

**Thesis title:** Pharmacological  
characterization and  
selectivity profile of different  
synthetic cathinones among  
monoamine transporters.

### Current Position and

**Employer:** PostDoc at the  
Institute of Pharmacology,  
Medical University of Vienna

### MolTag alumni page:

[Marco Niello \(univie.ac.at\)](https://www.univie.ac.at)

### Social networks:

[Marco Niello | LinkedIn](#)

[Marco Niello \(@MarcoNiello\) /  
Twitter](#)

### How would you summarize your thesis results in 3 sentences?

I have studied the chemical determinants of monoamine transporter substrate-selectivity. Substrates of monoamine transporters, such as MDMA ('ecstasy') and fenfluramine are becoming always more popular as innovative medical strategy for the treatment of neuropsychiatric disorders. I have worked in close contact with the Mihovilovic group (organic chemistry) and the Ecker group (docking, in silico prediction of compounds) to develop new monoamine transporter substrates. I have found that specific chemical substitution of the DAT-selective substrate methcathinone could lead to partial substrates of SERT and that the partial efficacy could be explained by the interaction with the allosteric site of SERT.

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

**The interdisciplinary nature of MolTag pushed me in improving my communication skills.** Having the need to explain what you are doing to people with a completely different background forces you to better understand what you are doing in the first place. Moreover, the numerous meetings with other groups, largely broadened my knowledge in different fields of science. **Being able to properly convey and collect information to and from different audiences is a crucial point in every career and in daily life.**

### Did you keep connections with some former colleagues?

Yes, we are still in touch and we meet from time to time to get a beer in Vienna with those that are still here and exchange some messages/emails with those who left Vienna already.

### What did you particularly like about the MolTag program?

I have really enjoyed the will of participating in the program that was present in most of the students and the **highly international environment.**





# Maria Teresa IORIO



**Finishing year:** 2020

**Supervisor:** Marko Mihovilovic,  
TU Wien

**Co-Supervisor:** Margot Ernst,  
Medical University of Vienna

**Thesis title:** New Modifications  
of an old Scaffold: Pyrazolo-  
quinolinone Derivatives and  
Analogues as Active Compounds  
on GABA<sub>A</sub> Receptors.

**Current Position and Employer:**  
Research Scientist at Takeda  
Pharmaceutical Company,  
Research and Development;  
Vienna, Austria

**MolTag alumni page:**  
[Maria Teresa Iorio \(univie.ac.at\)](https://univie.ac.at/mariateresiaiorio)

**Social network:**  
[Maria Teresa Iorio, PhD | LinkedIn](#)

## How would you summarize your thesis results in 3 sentences?

We designed, synthesized and evaluated a library of pyrazoloquinolinone (PQ) derivatives and analogues, as active compounds on GABA<sub>A</sub> receptors. The aim was to modify the general PQ scaffold in order to accomplish compounds with better properties in terms of selectivity, potency and detectability. This study yielded a new scaffold with improved properties. To investigate the binding and mechanism of action of the new scaffold, we performed functional and mutational studies, as well as radioligand displacement assay.

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

Practically, **it gives you a good leverage in job interviews**. If you use all the opportunities, it also gives you a lot of experience. It shows potential employers that you are fit to work in many different teams, and on a variety of topics.

## Did you keep connections with some former colleagues?

Yes, many actually...with the colleagues in Vienna we meet quite regularly, and with the others I am still in touch.

## What did you particularly like about the MolTag program?

The lab rotations, or better the strong collaboration with other labs and scientists. The travelling opportunities. The lively exchange of ideas, and the possibility of having colleagues with different expertise.

## What is your recommendation for current MolTag PhD students?

The interaction with experts in other areas of science and with students with varying tenure can be challenging. **Use it as a learning opportunity and do not get discouraged by comparing to others**. Also, take advantage of all the opportunities: visit other labs, create a network, go abroad, meet the other scientists and learn techniques that are not used in your lab. It will all be incredibly helpful. And last but not least, stay strong :)





## Stefanie KICKINGER



**Finishing year:** 2020

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

**Co-Supervisor:** Margot Ernst,  
Medical University of Vienna

**Thesis title:** Computational  
Studies of SLC Transporters  
with Special Focus on the  
GABA Transporter Subfamily.

**Position after PhD:** PostDoc  
at the Dept. of Pharmaceutical  
Chemistry, UniVie; currently  
applying for Grants and  
international PostDoc  
positions

**MolTag alumni page:**  
[Stefanie Kickinger \(univie.ac.at\)](https://www.univie.ac.at/stefanie-kickinger)

**Social networks:**  
[Stefanie Kickinger | LinkedIn](#)  
[Stefanie Kickinger \(@zmuvas\) / Twitter](#)

### How would you summarize your thesis results in 3 sentences?

GABA transporters are emerging drug targets implicated in epilepsy and stroke. Within my thesis we generated and validated the first binding hypotheses of selective competitive and noncompetitive GABA transporter inhibitors by computationally guided mutagenesis studies. Our findings will lay the basis for the rational design of future inhibitors.

### What did you do after your PhD?

I started to work as a post doc where I was stepping into the field of machine learning. I also got the chance to work on my first own grants for future research projects.

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

We were embedded in an interdisciplinary research community which not only **created a supportive and collaborative environment, but also broadened our scientific horizon**. Due to the generous travel budget I was able to attend more than 10 international conferences and to perform research internships at Yale and Copenhagen. These **experiences were tremendously important for building my scientific network**.

### Did you keep connections with some former colleagues?

Yes, of course. We have our own WhatsApp group where we keep tabs on each other and plan to meet for beers.

### What did you particularly like about the MolTag program?

I believe the best value of MolTag was that it gave us a sense of community. Working on your PhD can be at times quite demanding and consuming. **Knowing that you are not alone in this journey and that you have colleagues sharing the same experience really helps you to keep up with all the ups and downs of a thesis.**

### What is your recommendation for current MolTag PhD students?

My recommendation is to make use of the travel budget! Get involved in your scientific community and be bold to **ask inspiring researchers for internships!**





# Jasmin MORANDELL



**Finishing year:** 2020

**Supervisor:** Gaia Novarino, IST Austria

**Co-Supervisor:** Harald Sitte, Medical University of Vienna

**Thesis title:** Illuminating the Role of *Cul3* in Autism Spectrum Disorder Pathogenesis.

**Current position and employer:** Currently on Maternity leave from IST Austria

**MolTag alumni page:**

[Jasmin Morandell \(univie.ac.at\)](#)

**Social network:**

[Jasmin Morandell](#) | [LinkedIn](#)

## How would you summarize your thesis results in 3 sentences?

My thesis project investigated the molecular and cellular consequences of mutations in the high-risk autism gene *CUL3*. Employing a mouse model we could show that *Cul3* heterozygous deletion leads to behavioral, electrophysiological and brain anatomical deficits that are rooted in early development: newly generated neurons in the embryonic cortex fail to properly migrate to their target location due to an abnormal accumulation of cytoskeletal proteins, of which the actin bundling protein Pls3 appears to be the most important one.

## What are you doing now?

Currently, I am on maternity leave. For my professional future I am planning to continue my work as a researcher and will soon be looking for an interesting PostDoc position.

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

Thanks to MolTag I had the opportunity to attend several scientific meetings and conferences over the course of my PhD. Giving talks and presenting posters at these conferences **allowed me to meet a number of interesting researchers that may eventually become future employers.**

## What did you particularly like about the MolTag program?

The interdisciplinary environment and the students' community. **Interacting with chemists and pharmacologists broadened my scientific horizon as a molecular biologist significantly.**

## What is your recommendation for current MolTag PhD students?

**Stay connected to the MolTag community** and talk to your fellow MolTag students, also if from a different field- **they may give you new perspectives on your research question.**





# Julia WESTERMAYR



**Finishing year:** 2020

**Supervisor:** Leticia González,  
Faculty of Chemistry,  
University of Vienna

**Co-Supervisor:** Chris  
Oostenbrink, University of  
Natural Resources and Life  
Sciences, Vienna

**Thesis title:** Machine Learning  
for Excited-State Molecular  
Dynamics Simulations.

**Current Position:** "Erwin  
Schrödinger" (FWF)-PostDoc  
Reinhard Maurer group,  
Computational Surface  
Chemistry, Dept. of Chemistry,  
Univ. of Warwick, UK

**MolTag alumni page:**

[Julia Westermayr \(univie.ac.at\)](https://www.univie.ac.at/moltag/alumni/julia-westermayr)

**Social network:**

[Julia Westermayr \(@JWestermayr\) /  
Twitter](https://twitter.com/JWestermayr)

## How would you summarize your thesis results in 3 sentences?

I developed machine learning models to investigate photo-initiated reactions. Due to the computational efficiency of machine learning, simulations could be speed up such that better statistics and long time scale molecular dynamics simulations were achieved. The developed method was applied to small molecules.

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

The MolTag program **helped me a lot in communicating with researchers from different disciplines**, i.e., it improved my communication as a theoretician with experimental scientists. The interdisciplinary activities and the discussions/talks we had to explain our research to others were definitely helpful. Furthermore, the **tips for our future career of SAB members and PIs helped me a lot in deciding on the next steps after my PhD.**

## Did you keep connections with some former colleagues?

Yes, especially because I plan to come back to Vienna for one year due to a fellowship I received.

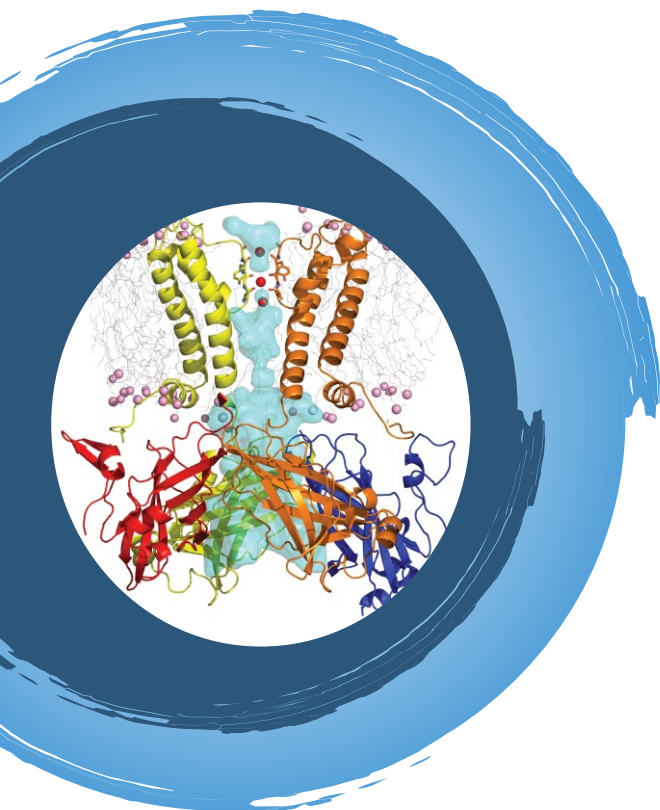
## What did you particularly like about the MolTag program?

I liked the fact that **it brings together scientists from different disciplines who might not have met without this program.** I especially enjoyed the research internship at the lab of one of the SAB members, where I could learn about simulations of metalloproteins.

## What is your recommendation for the MolTag PhD students?

**Never compare yourself to others** – in performance, number of publications, etc. Always remember that you are the only one who knows most about your project, that you are the most suitable person to solve related problems. No doctoral thesis is similar to another.





## MOLTAG COMMUNICATION

### MolTag Speaker:

Univ.Prof.Mag.Dr. **Gerhard Ecker**  
University of Vienna  
Division of Pharmaceutical Chemistry  
[Pharmacoinformatics Research Group \(univie.ac.at\)](http://univie.ac.at)

### Deputy Speakers:

Ass.Prof.Priv.Doiz.Dr. Margot Ernst  
Medical University of Vienna  
Dept. of Neurobiology of the Nervous  
System  
[Margot Ernst \(meduniwien.ac.at\)](http://meduniwien.ac.at)

Assoz.Prof.Mag.Dr. Anna Weinzinger  
University of Vienna  
Dept. of Pharmacological Toxicology  
[Molecular modelling of ion channels \(Prof. Weinzinger\)  
\(univie.ac.at\)](http://univie.ac.at)

### MolTag Program Management:

Susanne Menschik-Zunzer  
University of Vienna  
Division of Pharmaceutical Chemistry

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