



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 \(univie.ac.at\)](#)

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.**

