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
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MolTag alumni page:
Sankalp Jain (univie.ac.at)

Social networks:
Sankalp Jain | **LinkedIn**
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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.**

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