

# Valerij Talagayev

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## Experience

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**PJ Researcher | University of Marburg: Institute of Pharmacy – Kolb Lab**

MAY 2020 – OCTOBER 2020

Research Work: Docking of antipsychotics to aminergic receptors; Supervision of students

**PHD Student | Free University of Berlin: Institute of Pharmacy – Wolber Lab**

From OCTOBER 2021

PhD Thesis: In silico design and optimization of toll-like receptor modulators

Research Work: Virtual screening and discovery of novel Toll-like receptor agonists and antagonists,

Optimization of compounds, In silico mutational studies

**Google Summer of Code participant | MDAnalysis**

June 2024 - July 2024

Developed a new MDAKits package for the MDAnalysis

Package: 2D small molecule visualization for MDAnalysis

Mentors: Richard Gowers, Yuxuan Zhuang & Cédric Bouysset

## Education

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**Pharmacy | University of Marburg, Germany**

OCTOBER 2014 – FEBRUARY 2021

Grade Pharmacy: 2.2; Grade Approbation: 2.51

**MSc Medicinal Chemistry | University of Marburg, Germany**

From OCTOBER 2019

Master's Thesis: Docking of antipsychotic drugs and ligands to aminergic receptors

Current Grade: 1.59

## Internships

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**Intern | University of Marburg: Institute of Pharmacy – Schlitzer Lab**

AUGUST 2018 – OCTOBER 2018

Peptide synthesis

**Intern | University of Marburg: Institute of Pharmacy – Kolb Lab**

FEBRUARY 2020 – MARCH 2020

Docking, Virtual screening

**Intern | University of Marburg: Institute of Chemistry – Geyer Lab**

APRIL 2021 – JUNE 2021

Peptide synthesis

**Intern | University of Warsaw: Faculty of Chemistry – Filipek Lab**

JUNE 2021 – JULY 2021

Homology modelling and MD simulations of histamine receptor dimers

## Research Stay | Technical University of Berlin: Faculty of Chemistry – Nunes Lab

From AUGUST 2023

Pathway unbinding prediction of TLR8 Agonists and Antagonists

## Research Stay | Leiden University: LACDR Medicinal Chemistry – Van Westen Lab

FEBRUARY 2024 – APRIL 2024

Discovery of novel TLR9 Antagonists through Machine learning with further selectivity prediction towards TLR7/8

## Skills

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**Software/ Operating Systems:** Linux, MOE, PyMol, LaTeX, Chimera, Mogul, Amber, NAMD, VMD, Yasara, Ligandscout, GOLD, Schrödinger (Maestro, Desmond), KNIME, ACEMD, Gromacs, TauRAMD

**Web Servers:** GPCRdb, Uniprot, BLAST, ChEMBL, RCS PDB, OPM, CHARMM-GUI, GPCRmd

**Python Libraries:** Pandas, NumPy, rdkit, flask, MDAnalysis, MDTraj, OpenMM, Openforcefield, Scikit-learn, Matplotlib, PLIP, Prolif, QSPRPred

**Techniques:** Molecular Docking, Virtual Screening, Homology modelling, MD Simulations, Organic Chemistry, Drug Optimization, Method development, Machine Learning

## Software Projects

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[OpenMMDL](#): An OpenMM Interface for easy setup of molecular dynamic simulations of protein-ligand complexes.

Author & Maintainer

[MDonatello](#): 2D small molecule visualization for MDAnalysis with jupyter notebook

Author & Maintainer

[MDAnalysis](#): Python library to analyze molecular dynamics simulations

Contributor

## Publications

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### Publications:

- **Talagayev, V.**, Chen, Y., Doering, N. P., Obendorf, L., ... & Wolber, G. (2024). OpenMMDL Simplifying the Complex: Building, Simulating, and Analyzing Protein-Ligand Systems in OpenMM. *Manuscript in Preparation*
- **Talagayev, V.**, Wolber, G., & Nunes Alves, F. A. (2024) Unbinding Pathways of Toll-like receptor 8 agonists and antagonists. *Manuscript in Preparation*
- Fuchs, N., Calvo-Barreiro, L., **Talagayev, V.**, Pach, S., Wolber, G., & Gabr M. (2024) From Virtual Screens to Cellular Target Engagement New Small Molecule Ligands for the Immune Checkpoint LAG-3, *BioRxiv (Preprint)*
- Li, F., ..., **Talagayev, V.**, ..., & Schapira, M. CACHE Challenge #1: targeting the WDR domain of LRRK2, a Parkinson's Disease associated protein, *BioRxiv (Preprint)*
- Gaitonde, S. A., Avet, C., de la Fuente Revenga, M., Blondel-Tepaz, E., Shahraki, A., Pastor, A. M., **Talagayev, V.**, ... & Bouvier, M. (2024). Pharmacological fingerprint of antipsychotic drugs at the serotonin 5-HT<sub>2A</sub> receptor. *Molecular Psychiatry*, 1-12.

- Abdel-Rahman, S. A., **Talagayev, V.**, Pach, S., Wolber, G., & Gabr, M. T. (2023). Discovery of Small-Molecule TIM-3 Inhibitors for Acute Myeloid Leukemia Using Pharmacophore-Based Virtual Screening. *Journal of Medicinal Chemistry*, 66(16), 11464-11475.
- Calvo-Barreiro, L., **Talagayev, V.**, Pach, S., Abdel-Rahman, S. A., Wolber, G., & Gabr, M. (2023). Discovery of ICOS-targeted small molecules using pharmacophore-based screening. *ChemMedChem*, e202300305.
- Maccari, R., Wolber, G., Genovese, M., Sardelli, G., **Talagayev, V.**, Balestri, F., ... & Ottanà, R. (2023). Designed multiple ligands for the treatment of type 2 diabetes mellitus and its complications: Discovery of (5-arylidene-4-oxo-2-thioxothiazolidin-3-yl) alkanolic acids active as novel dual-targeted PTP1B/AKR1B1 inhibitors. *European Journal of Medicinal Chemistry*, 252, 115270.
- Noonan, T., Denzinger, K., **Talagayev, V.**, Chen, Y., Puls, K., Wolf, C. A., ... & Wolber, G. (2022). Mind the Gap—Deciphering GPCR Pharmacology Using 3D Pharmacophores and Artificial Intelligence. *Pharmaceuticals*, 15(11), 1304.

## Awards

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- August 2024 - 2nd Poster Prize Award - **MDAnalysis UGM 2024**

## Talks & Posters

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- **ICCS**, July 12-16 2022: An innovative approach of Toll-like receptor dynamics exploitation for structure optimization through 3D pharmacophore analysis. **Talk**
- **Europin**, *Vienna Summer School* September 10-15 2023: Discovery, Optimization and Exploration of Toll like receptor 8 Antagonist. **Europin Application Talk**
- **EFMC-YMCS 2023**, September 7-8 2023: A novel approach of Toll-like receptor dynamics application for structure optimization through 3D pharmacophore analysis, **Poster**
- **EMBO Workshop Computational structural biology**, December 6-9 2023: OpenMMDL A workflow for molecular dynamic simulations of protein-ligand complexes setup, simulation and analysis. **Flash Talk + Poster**
- **MDAnalysis UGM 2024**, August 21-23 2024: OpenMMDL A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis. **Lightning Talk + Poster**



