Valerij Talagayev

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Employment

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

Education

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

Intern | University of Marburg: Institute of Pharmacy – Schlitzer Lab
MARCH 2018
Synthesis of drugs against schistosomiasis

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

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

Open Source

OpenMMDL: An OpenMM Interface for easy setup of molecular dynamic simulations of protein-ligand complexes.
Google Summer of Code 2024: MDAnalysis Contributor: 2D visualization for small molecules

Publications and Talks

Publications:

- 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-HT2A 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) alkanoic 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.

Talks:

- **ICCS**, July 12-16 2022: An innovative approach of Toll-like receptor dynamics exploitation for structure optimization through 3D pharmacophore analysis
- **Europin**, *Vienna Summer School September* 10-15 2023: Discovery, Optimization and Exploration of Toll like receptor 8 Antagonist