

Georgiy Andreev

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EXPERIENCE

Lead Developer

Dec 2022 – Present

InSilico Medicine

Abu Dhabi, AE

- Engineered and delivered **Alchemistry**, a physics-based binding free energy optimization tool that increases binder prioritization efficacy, achieving an **8x increase in the probability** of selecting superior binders over traditional medicinal chemistry approaches
- Achieved benchmark accuracy of **1.5 kcal/mol** across diverse targets at **30% costs** compared to traditional methods
- Facilitated the adoption of Alchemistry by the internal user base and the onboarding of **4 partners**
- Prepared visualizations and 3D animations for promotional materials and 2 webinars to communicate the capabilities and benefits of the Alchemistry to stakeholders

Structural Biologist

Apr 2020 – Dec 2022

InSilico Medicine

Shanghai, CN

- Collaborated on the development of **ISM001-055**, a small molecule inhibitor targeting Idiopathic pulmonary fibrosis. Extracted molecular insights and formulated hypotheses to support the pre-clinical team
- Enhanced outcomes of **3 external** collaborations and **2 internal** drug discovery projects by providing insights into mechanisms of actions and interactions of small molecules

Alumnus

Sep 2019 – Jun 2023

Virtual Structural Biology Group

Moscow, RU

- Applied hybrid models combining MM and ML for **RBF calculations**. Improved MUE from 2 kcal/mol to **1.2 kcal/mol**
- Developed an approach for BFE-guided generative hit-optimization as a part of thesis work. This approach converged to **500 nM range hits** in 4 active learning cycles
- Published a paper in a Q1 journal together with colleagues, published abstracts for Biocatalysis-2019 international conference

EDUCATION

Lomonosov Moscow State University

Moscow, RU

Master's degree in Bioengineering and Bioinformatics

May 2023

TECHNICAL SKILLS

Molecular Modeling, Chemoinformatics: OpenMM, Gromacs, Amber, Plumed, Psi4, MOE, Martini, RDKit, openff-toolkit

Molecular Visualization: PyMol, Blender, VIAMD, Mol*, Plotly, Dash, Ngview, MDAnalysis

Machine Learning: PyTorch, PyG, Diffusion, Flow-matching, AL, GNNs, MLOps

Compute, Databases, VCS: Docker, Kubernetes, AWS, Ray, Dask, Git(Lab), Neo4j, MongoDB, SurrealDB

Programming Languages: Python, Rust, JS/TS, C++

Languages: Russian (native), English (fluent), Chinese (upper intermediate), Georgian (intermediate)

PUBLICATIONS

Andreev, G., Kovalenko, M., Bozdaganyan, M. E. & Orekhov, P. S. *Colabind: A Cloud-Based Approach for Prediction of Binding Sites Using Coarse-Grained Simulations with Molecular Probes.* *J. Phys. Chem. B*, 128, 3211–3219 (2024).

Aladinskiy, V. et al. *Discovery of Bis-imidazolecarboxamide Derivatives as Novel, Potent, and Selective TNIK Inhibitors for the Treatment of Idiopathic Pulmonary Fibrosis.* *J. Med. Chem.* (2024) doi:10.1021/acs.jmedchem.4c01580.

PROJECTS

Alchemistry: SOTA Alchemical free energy calculations for drug discovery.

ISM001-055: AI-discovered drug now in Phase 2 clinical trials for IPF. The structural biology department played a significant role in reaching this milestone.

Generative Hit-Opt with Alchemistry: A diffusion-based generative model for small molecule design, focusing on optimizing affinity in an Active Learning Cycle.

Colabind: A cloud-based approach for predicting binding sites using CG cosolvent simulations, identifying druggable, orthosteric, and cryptic pockets in experimental and AI-predicted structures for 10 out of 13 tested targets.

YoungFace: Winners of LongHack 2022. Guided a team in developing a pipeline to identify skin-aging related targets and generate natural-like hits in two weeks.

CNNs for Enzymes: Exploratory research project on the applicability of CNNs for enzyme activity prediction. Presented at Biocatalysis-2019.

NN-Enhanced ABFE: A hybrid ML/MM approach for binding free energy calculations with ANI2x neural network potentials, achieving chemical accuracy of 1 kcal/mol for affinity estimation on a small set of protein-complex systems.

OpenFE Ecosystem: Participated in open-source development, contributing 3 PRs and opening 6 issues to gufe and alchemiscale.