Georgy Andreev

+971501169750 | yawner@pm.me | in/georgiy-andreev | github.com/LilDojd

Experience

Research Engiener Apr 2025 – Present
GenBio AI *Abu Dhabi, AE*

- Working on foundational models for structural biology

Lead Developer Dec 2022 – Apr 2025
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**
- Ported in-house tools to a tailored high-throughput execution and orchestration system for use with cloud providers, improving GPU utilization by **20%**, in some cases reaching **60% decrease in Time to Solution**
- Prepared visualizations and 3D animations for promotional materials and 2 webinars to communicate the capabilities and benefits of the Alchemistry to stakeholders

Structual 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 **4 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 **RBFE 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, Nglview, MDAnalysis
Machine Learning: PyTorch, PyG, Diffusion, Flow-matching, Active Learning, GNNs, MLOps
Orchestration, Databases, VCS: Docker, Kubernetes, AWS, Ray, Dask, Git(Lab), Neo4j, MongoDB, PostgreSQL, SQLite, SurrealDB
Compute: CUDA, WGPU, SIMD
Frameworks: Axum, Actix, Dioxus, Flask, FastAPI
Programming Languages: Python, Rust, JS/TS, C++, C
Languages: English (fluent), Russian (fluent), Chinese (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 and contributions

Alchemistry: SOTA Alchemical free energy calculations for drug discovery.

ISM001-055: A small-molecule 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.

labour: An experimental extensible open-source software suite for performing Molecular Dynamics with heterogeneous hardware acceleration (TBA).

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.

Burn: Contributed backend-agnostic implementations of tensor operations to this Rust Deep Learning Framework.