Georgy Andreev

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EXPERIENCE

InSilico Medicine **Dec 2022 – Current**
Lead Developer Abu Dhabi. UAE

- 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** big pharma partners
- Prepared visualizations and 3D animations for **promotional materials** and **2 webinars** to communicate the capabilities and benefits of the Alchemistry to stakeholders

InSilico Medicine **Apr 2020 – Dec 2022**
Structural Biologist Shanghai

- 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

Virtual Structural Biology Group **Sep 2019**
Student → Alumnus Moscow, Russia

- 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 **May 2023**
Master's degree in Bioengineering and Bioinformatics Moscow, Russia

MADE: Big Data Academy **May 2021**
Mail.ru, Russia

OTHER

- **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, AL, GNNs, MLOps
  Compute, DBs, 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)

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 has played a significant role in reaching this milestone

Generative Hit-Opt with Alchemistry
A diffusion-based generative model for small molecule design with a focus on optimizing affinity in an Active Learning Cycle

Colabind
A Cloud-based approach for prediction of binding sites with CG cosolvent simulations that identifies druggable, orthosteric and cryptic pockets in experimental and AI-predicted structures in 10 out of 13 tested targets

YoungFace
Winners of LongHack 2022. Guided a team that has developed a pipeline for identifying skin-aging related targets and generating natural-like hits in just two weeks

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

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

dioxus-spline
A small project that allows to export and use Spline scenes directly in Dioxus websites. 700 downloads from crates.io as of 09.05.2024