Vladislav Cherdantsev

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Education

Massachusetts Institute of Technology Sep 2021 - May 2025
B.S. in Chemistry and B.S. in Computer Science

Experience

Broad Institute — Supervised by Wengong Jin Cambridge, MA
Undergraduate Researcher May 2024 - Present

- Developed and trained an SE(3) denoising score-matching model for unsupervised binding energy prediction using the DiffDock codebase.
- Designed and trained a graph neural network to predict small molecule-protein binding using molecular SMILES and protein sequences as inputs. Led decisions on data featurization and implemented the model codebase.

Connor Coley Group Cambridge, MA
Undergraduate Researcher Mar 2023 - Mar 2024

- Developed an automated pipeline (shell and Python scripts) to set up relative binding free energy calculations in GROMACS for an antitubercular drug.
- Implemented an efficient lookup algorithm that uses locality-sensitive hashes to improve molecular similarity search. Integrated the algorithm as an API endpoint into the web-based ASKCOS software using Docker and MongoDB.

Pfizer Sponsored Research Experience (Klavs Jensen Group) Cambridge, MA
Undergraduate Researcher Jun 2022 - Sep 2022

- Contributed to the creation of a tool capable of predicting site selectivity in electrochemical oxidation reactions. Collected and preprocessed a dataset containing DFT calculations to train the initial model for regioselectivity prediction.
- Used a machine learning-based tool (ChemProp) to analyze extracted data for predicting molecular properties. Conducted evaluations of various NMR deconvolution software packages to assess their compatibility with the tool.

Kiessling and Dinca Groups Cambridge, MA
Undergraduate Researcher Sep 2021 - May 2022

- Designed and performed multistep synthesis of mucin-mimetic polymers (ROMP), organic linkers, and metal-organic frameworks (MOFs), involving solvothermal techniques, purification, and characterization.

Awards and Certifications

- D. E. Shaw Research Undergraduate Fellowship (Aug 2023)
- Free Energy Calculations for Drug Design with FEP+, Schrödinger (Nov 2023)
- Introduction to Molecular Modeling in Drug Discovery, Schrödinger (Jul 2023)
- International Chemistry Olympiad 2019, Silver Medal

Technical Skills

- **Programming:** Linux, Shell Scripting, PyTorch, torch_geometric, e3nn, RDKit, Biopython
- **Molecular Modeling:** GROMACS, FEP+, PyMOL, VMD, DiffDock