

Sergei Evteev, PharmD

Results-driven medicinal chemist with over 7 years of experience in computer-aided drug design (CADD) and software development within commercial biotech settings. Proven expertise in drug discovery, molecular modeling, chemoinformatics, and machine learning. Author of 20+ patents and scientific articles, h-index of 9.



Areas of Interest

- Drug Design
- Medicinal Chemistry
- Molecular Modeling
- Chemoinformatics
- Machine Learning
- Software Development

Selected publications

1. Evteev S. et al. Integrating modern computational techniques elevates binding mode identification for molecular fragments. *Molecular Diversity*, 2026.
2. Evteev S. et al. AlphaFold Kinase Optimizer: Enhancing Virtual Screening Performance through Automated Refinement of AlphaFold-Based Kinase Structures. *Proteins*, 2025.
3. Ershchenko A. et al. Enhancing accuracy of virtual kinase profiling via application of graph neural network to 3D pharmacophore ensemble. *J Comput Aided Mol Des*, 2025.
4. Evteev S. et al. Skittles: GNN-Assisted Pseudo-Ligands Generation and Its Application for Binding Sites Classification and Affinity Prediction. *Proteins*, 2025.
5. Evteev S. et al. Quantum-assisted Fragment-based Automated Structure Generator (QFASG) for small molecule design: an in vitro study. *Frontiers in Chemistry*, 2024.
6. Evteev S.A. et al. SiteRadar: Utilizing Graph Machine Learning for Precise Mapping of Protein–Ligand-Binding Sites. *JCIM*, 2023.
7. Ivanenkov Ya. et al. The Hitchhiker's Guide to Deep Learning Driven Generative Chemistry. *JMCL*, 2023.
8. Evteev S. et al. Bifunctional inhibitors of influenza virus neuraminidase: molecular design of a sulfonamide linker, *IJMS*, 2021.