	SEROV, Nikita S. PhD
Research interests	✓ Applied artificial intelligence ✓ Cheminformatics ✓ Molecular biology ✓ Structural biology
Features of the PhD program	The program will enable students to acquire skills in applying data science and artificial intelligence to solve chemical problems such as synthesis planning, drug and diagnostic molecule design, modeling the properties of multicomponent systems, and exploring chemical spaces to find molecular systems with a given set of properties and activities.
List of the supervisor's research projects (participation/supervision)	✓ Generative design of RNA aptamers with high affinity for small organic molecules ✓ Biopolymer knowledge graph for repurposing, property prediction, and biosensor generation ✓ Hybrid approach based on AI and molecular dynamics for generating first-in-class antibiotic biosensors based on cyclic peptides ✓ Transformer model for conditional generation of protein-binding aptamers through knowledge transfer from the antibody domain ✓ Evolutionary optimization algorithm based on a meta-regressor model for the design of highly effective chemically modified miRNAs for gene knockdown ✓ Generation of cell-penetrating peptides for targeted delivery of drug molecules, taking into account cell line types ✓ A physically informed full-cycle model for in silico design of DNAzyme catalytic centers with increased activity ✓ A model for improving the quality of X-ray structural analysis results for resolving difficult-to-crystallize protein structures ✓ Training of joint representations of proteins based on chemical, spectral, and structural data ✓ BiLSTM-AE model with contrastive learning for the formation of task-independent, stable, and interpretable peptide embeddings ✓ In silico design of aptamers with high affinity and selectivity for protein toxins in biological fluids
List of potential thesis topics	✓ Physical informing of neural networks for modeling biomacromolecules in conditions of insufficient quality data ✓ Interpretable algorithms for the targeted design of biosensors and therapeutic biomacromolecules ✓ Development of transfer learning strategies for modeling rare and poorly studied systems ✓ Reinforcement learning algorithms for optimizing the properties and activities of biopolymers

	✓ Development of versatile mathematical representations of biomacromolecular systems
Publications in the last five years	16 (Scopus / Web of Science / RSCI)
Key publications	1. Eremeyeva, M., Din, Y., Shirokii, N., & Serov, N. (2025). SequenceCraft: machine learning-based resource for exploratory analysis of RNA-cleaving deoxyribozymes. BMC bioinformatics, 26(1), 2 2. Shirokii, N., Din, Y., Petrov, I., Seregin, Y., Sirotenko, S., Razlivina, J., ... & Vinogradov, V. (2023). Quantitative prediction of inorganic nanomaterial cellular toxicity via machine learning. Small, 19(19), 2207106 3. Gubina, N., Dmitrenko, A., Solovev, G., Yamshchikova, L., Petrov, O., Lebedev, I., ... & Vinogradov, V. (2024). Hybrid generative AI for de novo design of co-crystals with enhanced tabletability. Advances in Neural Information Processing Systems, 37, 84606-84644 4. Jyakhwo, S., Serov, N., Dmitrenko, A., & Vinogradov, V. V. (2024). Machine learning reinforced genetic algorithm for massive targeted discovery of selectively cytotoxic inorganic nanoparticles. Small, 20(6), 2305375 5. Serov, N., & Vinogradov, V. (2022). Artificial intelligence to bring nanomedicine to life. Advanced Drug Delivery Reviews, 184, 114194
Key IPs	✓ Currently, IP is being registered for the SeQuant model developed in the laboratory for the formation of stable interpretable peptide embeddings
Supervisor's specific requirements	✓ Personal presence ✓ Participation in the life of the laboratory and the Center ✓ Willingness and ability to supervise master's students ✓ Commitment and competent time management
Code of the subject area of the PhD program	1.4.4 Physical Chemistry 1.4.5 Chemoinformatics