

Nikita Polomoshnov is an undergraduate student of the Department of Bioengeneering and Bioinformatics of Lomonosov MSU, working under the supervision of Anastasia Rudik in the Laboratory of Structural and Functional Drug Design at IBMC. His current work is related to computational methods for predicting xenobiotic metabolism. The main scientific interests are deep learning as applied to chemoinformatics problems, structural bioinformatics, organic chemistry and drag design. He is currently working on the application of graph neural networks and transformers to the task of predicting possible metabolites of drug compounds.