Dmitry Shulga biosketch

Dr. Dmitry Shulga graduated from Moscow State University in 2002, defended his PhD in 2009. He also graduated from RANEPA's Institute of Business Studies with MBA degree in 2018. Currently leads a research group of graduate and undergraduate students at Department of Chemistry of Lomonosov Moscow State University.

The areas of scientific focus are fragment-based drug discovery, inter- and intra-molecular interactions, electrostatic interactions (including anisotropic models for halogen bonding), force field and scoring function development and refinement, structure-based pharmacophore modeling via characterization of a binding site with fragment "basis", QSAR/QSPR, chemoinformatics, machine learning, molecular dynamics, FEP and quantum chemistry.

The applied expertise includes hit finding, hit-to-lead and lead optimization using the relevant in silico tools for several targets, including factor Xa/thrombin, SortaseA (*Staphylococcus aureus*), prostaglandin EP1-4 receptors, melatonin MT3/QR2 receptor, CDK1/2, EFGR, GSK3β, AchE/BchE, hTG2, Myosin and others.

Additional expertise and focus of interest lies in startup, customer development, IT, software development, Agile/Scrum, project and risk management.

Open to scientific shulga@qsar.chem.msu.ru and applied shulga@molmodel.com collaborations.