

Dmitry Shulga biosketch

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



His areas of scientific expertise are computer-aided drug discovery in general and, in particular, fragment-based drug discovery; inter- and intramolecular 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 a fragment “basis” approach; QSAR/QSPR; chemoinformatics; machine learning; molecular dynamics; FEP; and quantum chemistry.

The current focus of his research is the *in silico* Reverse Fragment-Based Drug Discovery (R-FBDD) approach; ensemble representation of protein structures for modeling; building target-structure-based pharmacophores using characterization of the binding site with a “fragment basis” approach; the empirical DENR and DENR+POL schemes for calculating atomic charges and electrostatic interactions between species relevant to biomolecular context and drug discovery, by correctly and physically soundly taking into account known electronic effects, e.g., inductive and polarization effects.

His applied expertise includes hit finding, hit-to-lead, and lead optimization using relevant *in silico* tools for several targets, including factor Xa/thrombin, Sortase A (*Staphylococcus aureus*), prostaglandin EP1–4 receptors, melatonin MT3/QR2 receptor, CDK1/2, EGFR, GSK3 β , AChE/BChE, hTG2, viral neuraminidase, myosin, and others. In these applied projects, conventional CADD methods were used; for a subset of targets, they were complemented by selected elements of our newly developed approaches, such as R-FBDD and ensemble-based representation of protein structures. Further development of these approaches remains a current methodological focus.

Additional expertise and interests include startups, customer development, IT, software development, Agile/Scrum, and project and risk management.

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