Dmitrii Shkil

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Education

Master of Science, Lomonosov Moscow State University
Faculty of Chemistry, Fundamental and Applied Chemistry, Department of Organic Chemistry

Work experience

1. Head of Data Science Department (present, 0.5 yrs of experience), Syntelly LLC
Projects:
Organization and holding of the hackathon on Digital Pharmacology and Predictive Modelling
Development of new approaches for toxicity prediction using ML and AI
Technical supervision of the platform and provision of chemical data audit
Optical entity recognition from unstructured documents related to chemistry
Creation of algorithms for predicting the physicochemical properties of small molecules

2. Medicinal Chemist (2 yrs of experience), Insilico Medicine, Skolkovo Innovation Center
Projects:
Protein-ligand complex library preparation for QSAR validation
Chemistry42 generation study of selective covalent inhibitors against one of the tyrosine kinase isoform
Development of novel structure generation approach based on CADD

3. Medicinal Chemist (1.5 yrs of experience), The Federal State Unitary Enterprise Dukhov Automatics Research Institute
Projects:
Synthesis and molecular modeling of *de novo* designed serin-threonine kinase inhibitors
Development of algorithm to predict small colloidally aggregating molecules

4. Organic Chemist (5+ yrs of experience), Lomonosov Moscow State University
Department of Chemistry, Lab of Biologically Active Organic Compounds (BAOC)
Projects:
Discovery of new selective ligands for targeted delivery via ASGPR
Synthesis of ribavirin-based antiviral prodrugs with triterpenoid moiety
Efficient synthesis of nitrodopamine under mild acid catalysis

Publications related to Organic and Medicinal Chemistry

1. Discovery of Bivalent GalNAc-Conjugated Betulin as a Potent ASGPR-Directed Agent against Hepatocellular Carcinoma
Bioconjugate Chemistry, 2021, 32, 4, 763-781. doi: 10.1021/acs.bioconjchem.1c00042

2. Synthesis and cytotoxicity of new alkyne derivatives of pentacyclic triterpenoids
Russian Chemical Bulletin, (68):855–861, 2019. doi: doi.org/10.1007/s11172-019-2496-1

3. Synthesis and Evaluation of New Trivalent Ligands for Hepatocyte Targeting via the Asialoglycoprotein Receptor *Bioconjugate Chemistry*, 2020, 31, 5, 1313–1319. doi: doi.org/10.1021/acs.bioconjchem.0c00202.

4. Aprotinin – Drug against Respiratory Diseases *International Journal of Molecular Science*, 2023, 24(13):11173. doi: 10.3390/ijms241311173

5. Resistance profile of investigational neuraminidase inhibitor AV5080 against influenza A and B viruses *Antiviral Research, 2023,* 217:105701. doi: 10.1016/j.antiviral.2023.105701.

Participation in conferences and competitions

1. "Search for a drug against cytokine storm", 2nd place
ChemDiv Business Championship, October 27, 2021, Khimki, Russia

2. "Novozymes Enzyme Stability Prediction", 16th rank / 2483 participants
Kaggle, September 21, 2022 - January 3, 2023

3. "AMP®-Parkinson's Disease Progression Prediction", 93th rank / 1805 participants
Kaggle, February 16, 2023 - May 18, 2023

4. "Synthesis of trivalent conjugates of ribavirin and N-acetylgalactosamine for targeted drug delivery to hepatocytes"
Markovnikov Readings. Organic chemistry: from Markovnikov to the present day, January 17-20, 2020, Krasnovidovo, Russia

Competencies

Cheminformatics and medicinal chemistry: preparation of protein computer models (homology modeling, preprocessing, minimization), high-throughput virtual screening of small molecules, work with molecular databases, pharmacophore analysis, docking, prediction of ADME properties, QSAR/QSPR analysis, conformational analysis, quantum chemistry methods, methods of molecular mechanics and molecular dynamics, machine learning models and the use of neural networks (PyTorch), writing Python scripts for solving problems of chemoinformatics, *de novo* design of drug molecules based on computer modeling and medicinal chemistry approaches.
Organic chemistry:
Methods of organic synthesis, purification of small molecules using liquid chromatography, physicochemical analysis and subsequent interpretation of spectral data, retrosynthetic analysis.

Knowledge of computer programs and databases

Visualization of molecules and spectral data: ChemDraw3D, PyMol, Jmol, ACDLabs, Mestrenova, BIOVIA, ChemSketch, SMARTSEditor

Molecular modeling: Maestro, MOE, Corina, Autodock Vina

Programs for database processing: KNIME, Chemosoft, Alvadesc, Openbabel

Databases: RCSB Protein Data Bank, SciFinder, Reaxys, ZINC, Clarivate Integrity, Google Scholar, Google Patents, PubMed, PubChem, ChEMBL

IDE and additional software: RStudio, PyCharm, Visual Studio, Jupyter Notebook, Google Colab, Anaconda, Docker

Libraries that I often use on Python: rdkit, deepchem, numpy, pandas, sklearn, xgboost/catboost/lgbm, pytorch, tabpfn

Programming languages: Python, SQL (RDBMS PostgreSQL), C++, R, Bash