**Name:** Aleksandra Ivanova

**Date of birth:** 14.09.1996

**Place of birth:** Volgograd, Russia

**E-mail:** aleksandra.ivanova@upol.cz

**ORCID profile:** <https://orcid.org/0000-0002-8064-7845>

**Github profile:**  <https://github.com/avnikonenko>

**EDUCATION:**

**2019 – present**  student, PhD in computational chemistry “In silico design of compounds with desired properties”

Faculty of Medicine and Dentistry, Institute of Molecular and Translational Medicine, Palacky University Olomouc (supervisor Dr. Pavel Polishchuk)

**2014 - 2019** Specialist’s degree in Bioengineering and Bioinformatics “Modeling the Structure-Activity Relationship using an ensemble of stereoisomers and conformers of molecules".

Volgograd State University, Department of Bioengineering and Bioinformatics, Russia

**WORK EXPERIENCE**

2017 – 2019 laboratory assistant

Laboratory of the chemistry and biochemistry, Volgograd State University, Russia

**RESEARCH INTERESTS:**

chemoinformatics, drug design, de novo design, molecular biology, medicinal chemistry, bioinformatics, molecular modeling, machine learning, data mining, data analysis

**PROFESSIONAL SKILLS**

- **Molecular modeling:** QSAR modeling, molecular docking, molecular dynamics

- **Programming languages and technologies:** Python (scikit-learn, multiprocessing, numpy, scipy, sqlite3, pandas, BioPython), R, SQL

- **Graphical visualisation:** R (ggplot2, plotly), Python (matplotlib, seaborn, plotly, Bokeh)

- **OS:** Linux, Windows

**- Software knowledge:** RDKit, Autodock Vina, Glide, Maestro, Chimera, PyMOL, MarvinTools, Gromacs, Amber, MDAnalysis

- statistical analysis

- parsing data from databases (API/HTML)

**- Languages:** English (intermediate), Russian (native)

### **Publications:**

1) Michal Jurášek, Jiří Řehulka, Lenka Hrubá, Aleksandra Ivanová, Soňa Gurská, Olena Mokshyna, Pavel Trousil, Lukáš Huml, Pavel Polishchuk, Marián Hajdúch, Pavel B. Drašar, Petr Džubák. Triazole-Based Estradiol Dimers Prepared via CuAAC from 17α-Ethinyl Estradiol with Five-Atom Linkers Causing G2/M Arrest and Tubulin Inhibition. Bioorganic Chemistry. 2023, https://doi.org/10.1016/j.bioorg.2022.106334

2) Rehulka, J., Subtelna, I., Kryshchyshyn-Dylevych, A., Cherniienko, A., Ivanova, A., Matveieva, M., Polishchuk, P., Gurska, S., Hajduch, M., Zagrijtschuk, O., Dzubak, P., Lesyk, R., Anticancer 5-arylidene-2-(4-hydroxyphenyl)aminothiazol-4(5H)-ones as tubulin inhibitors. *Arch. Pharm.* 2022, e2200419. <https://doi.org/10.1002/ardp.202200419>

3)Zankov D.V., Shevelev M.D., Nikonenko A.V., Polishchuk P.G., Rakhimbekova A.I., Madzhidov T.I. (2020) Multi-instance Learning for Structure-Activity Modeling for Molecular Properties. In: van der Aalst W. et al. (eds) Analysis of Images, Social Networks and Texts. AIST 2019. Communications in Computer and Information Science, vol 1086. Springer, Cham. <https://doi.org/10.1007/978-3-030-39575-9_7>

4) Nikonenko, A., Zankov, D., Baskin, I., Madzhidov, T. and Polishchuk, P. (2021), Multiple Conformer Descriptors for QSAR Modeling. Mol. Inf. <https://doi.org/10.1002/minf.202060030>

5) QSAR Modeling Based on Conformation Ensembles Using a Multi-Instance Learning Approach Dmitry V. Zankov, Mariia Matveieva, Aleksandra V. Nikonenko, Ramil I. Nugmanov, Igor I. Baskin, Alexandre Varnek, Pavel Polishchuk, and Timur I. Madzhidov. Journal of Chemical Information and Modeling DOI: 10.1021/acs.jcim.1c00692