

CURRICULUM VITAE



1. PERSONAL DATA

NAME: OLEG TINKOV

DATE OF BIRTH: September 5, 1984.

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Web of Science ResearcherID: Q-4699-2017

ResearchGate <https://www.researchgate.net/profile/Oleg-Tinkov>

GitHub: <https://github.com/ovttiras>

2. EDUCATION AND POSITIONS HELD:

2017 - PhD in organic chemistry: "Quantitative analysis of the impact of structural factors on toxicity, lipophilicity, and water solubility of environmentally hazardous organic compounds."

Institute of physiologically active compounds of Russian Academy of Sciences, Chernogolovka, Russia (supervisor Prof. V.E. Kuz'min)

2001 - 2006: Master's degree in chemistry, T.G. Shevchenko Transdnistria State University, Transdnistria, Moldova

07.2025-present: researcher, Ligand Pro, Russia, Moscow.

3. SCIENTIFIC INTERESTS:

Data Science, machine learning, QSAR/QSPR, molecular and drug design, computational toxicology, medicinal and bioorganic chemistry.

Developed approaches:

1) ***The use of artificial intelligence for the study of antitumor drugs*** (Tinkov, O. V., Grigorev, V. Y., Grigoreva, L. D., Osipov, V. N., Kolotaev, A. V., & Khachatryan, D. S. (2023). HDAC6 detector: online application for evaluating compounds as potential histone deacetylase 6 inhibitors. SAR and QSAR in environmental research, 34(8), 619–637)

Result: Web services for virtual screening of HDAC inhibitors have been developed:

- a) <https://ovttiras-hdac6-detector-hdac6-detector-app-yzh8y5.streamlit.app/>
- b) <https://ovttiras-hdac1-inhibitors-hdac1-predictor-app-z3mrbr.streamlitapp.com/>
- c) <https://hdac2scan.streamlit.app/>
- d) <https://hdac3-vs-assistant.streamlit.app/>
- e) <https://htpredict.streamlit.app/>

2) ***Structural and physico-chemical interpretation of QSAR models*** (O.V. Tinkov, V.Y. Grigorev, A.N. Razdolsky, L.D. Grigoryeva & J.C. Dearden (2020) Effect of the structural factors of organic compounds on the acute toxicity toward *Daphnia magna*, SAR and QSAR in Environmental Research, 31:8, 615-641, DOI: 10.1080/1062936X.2020.1791250).

Result: identification of molecular patterns which constantly increase acute and reproductive toxicity, as well as more detailed studying of known toxicophores.

3) ***Development of QSAR/QSPR models for avermectins***. (O.V. Tinkov, V.Y. Grigorev, L.D. Grigoryeva, (2021) QSAR analysis of the acute toxicity of avermectins towards *Tetrahymena pyriformis*, SAR and QSAR in Environmental Research, Vol. 32, Issue 7, 541-571)

Result: New QSAR/QSPR models for virtual screening avermectins.