Dmitry Zankov

PhD in Chemoinformatics (University of Strasbourg)

Postdoctoral Researcher, Aix-Marseille Université, France

KagakuAI GoogleScholar LinkedIn

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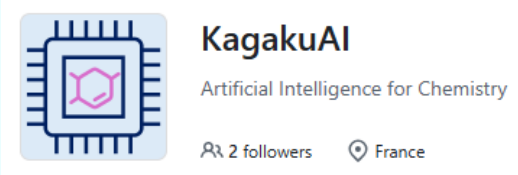
Background

2013 - 2017	**4y**	**BA | Chemistry**	Irkutsk State University | Russia
2017 - 2019	**2y**	**MS | Chemoinformatics**	Kazan Federal University | Russia
2017 - 2018	**1y1m**	**Chemoinformatics Data Scientist**	Science Data Software LLC (remote) | USA
2020 - 2023	**2y6m**	**PhD | Chemoinformatics**	University of Strasbourg | France
2023 - 2025	**1y11m**	**Postdoctoral Researcher**	Hokkaido University | Japan
2025 - now	**0y5m**	**Postdoctoral Researcher**	Aix-Marseille Université | France

Expertise

General	General Chemistry, Medicinal Chemistry, Artificial Intelligence, Deep Learning, AutoML, High-Performance Python, Software Design
Advanced	Quantum Chemistry, Chemoinformatics, Bioinformatics, Machine Learning, Search/Optimization Algorithms, QSAR, Computer-Aided Synthesis Planning (CASP), Python, Docker, RDKit, PyTorch/Keras,
Master	Conjugated Machine Learning, Multi-Instance Machine Learning, Genetic Algorithms

Projects/Tools



QSARmil QSARcons SEQmil
SynPlanner CoLearn
milearn

KagakuAI – a collection of tools for AI/ML in chemistry (created by author).

Quantum Chemistry	Reaction mechanism elucidation with quantum chemistry methods
Genetic Algorithm	Optimization of molecule structure and polymer properties, de novo design, synthesis planning
Conjugated ML	Integrating fundamental chemical laws and machine learning algorithms
Multi-Instance ML	Application of multi-instance machine learning to the molecular property prediction
SynPlanner	An open-source tool for computer-aided synthesis planning

*Main developer only