ALINA DENZLER

M.Sc. in Computational Chemistry

+41784411678 alina.denzler5@gmail.com

Swiss B permit Lehenmattstrasse 141, 4052 Basel, CH

I am a Computational Chemist with a background in molecular modeling and machine learning. I have worked on ligand- and structure-based drug discovery using Python and AI tools. My experience spans academic research across multiple countries. Currently, I explore GenAI.

LinkeIn • GitHub

SKILLS

Python | SQL | LLMs | Drug Discovery | Machine Learning | Data Mining | Statistical Analysis | Cross-Functional Collaboration

LANGUAGES

English – fluent ●●●●●

Russian – fluent ●●●●●

German – beginner ●○○○○

EDUCATION

2016 – 2018

M.Sc. in computational chemistry

Kazan Federal University, Russia

2012 – 2016

B.Sc. in pharmaceutical technology

Saint Petersburg Chemical Pharmaceutical Academy, Russia

EXTRACURRICULAR ACTIVITIES

➢ Drawing

A space for creative exploration through new techniques, materials, and visual storytelling

➢ Hiking

A way to recharge, stay grounded, and enjoy expansive views

WORK EXPERIENCE

GenAI Explorer 01/2025 — Now

Self-employed Basel, Switzerland

- Leading AI research pipelines with a focus on data collection, cleaning, analysis, and preparation for modeling.

GitHub Repo (in progress)

Sabbatical Break 03/2024 — 12/2024

Career break Switzerland & Abroad

- Explored new countries and cultures
- Established a Swiss presence and expanded professional network through biotech and pharma events

Chemical Data Scientist 08/2019 — 02/2024

Palacký University Olomouc, Czech Republic

- Built an end-to-end pipeline to identify selective MARK4 inhibitors for Alzheimer's research, combining ML, docking, and chemical similarity analysis over **1.78M compounds**, resulting in **18% experimental validation** and novel scaffold discovery.

Article · GitHub Repo

- Co-developed a virtual screening pipeline based on 4D pharmacophore modeling and molecular dynamics, enabling hit identification across 28,000 compounds and achieving **10–20× better enrichment** than conventional methods.

Article · GitHub Repo

- Co-developed a de novo compound generation tool producing **10,000+ synthetically feasible molecules in 12 hours** with **>70% novelty**, validated on **818K structures** and benchmarked across diverse protein families.

GitHub Repo

- Led data analysis for CACHE Challenge #1, targeting the LRRK2 protein (Parkinson's); applied MD simulations and feature space mapping to prioritize compounds, contributing to a **top 3 finish out of 23 global teams**.

Article

- Delivered a **Python workshop** for drug discovery scientists (Olomouc, 2023), covering data analysis, QSAR, and machine learning, and translating complex concepts for a multidisciplinary audience.

GitHub Repo

Junior Researcher 02/2017 — 07/2019

Kazan Federal University Kazan, Russia

- Developed and validated a ligand-based virtual screening tool, outperforming traditional 2D methods across targets like AChE and CYP3A4; tool adopted by **Insilico Medicine** for commercial use.

Article · GitHub Repo

- Applied machine learning to pharmacophore-based screening using one-class classifiers, improving compound ranking accuracy and early enrichment; results published and deployed as a **public web tool**.

Article · GitHub Repo · Public Web Tool

Lab Assistant 06/2015 — 07/2015

Biocad Moscow, Russia

- Supported monoclonal antibody production through cell culture; authored documentation for Rituximab manufacturing in accordance with GMP standards.