Establishing a benchmarking platform for AI/ML predictive models for bioactivity and toxicity in agrochemistry.

Modern agriculture faces a number of serious challenges. Pests and weeds are increasingly developing resistance to existing chemical treatments, while at the same time, public expectations and legal regulations are demanding that new substances be safer for humans, animals, and the environment. In addition, climate change is causing plant protection issues to emerge in new regions and on an unprecedented scale. Meanwhile, the development of new pesticides remains a costly and time-consuming process, still largely based on trial and error.

This is why we need more precise modern tools that can help identify substances that are not only effective but also safe for people and the environment. The goal of our project is to create an open-access platform to support scientists and companies in designing safer and more efficient crop protection agents, such as herbicides and other pesticides. To achieve this, we will apply advanced technologies in molecular data analysis, artificial intelligence (AI), and machine learning (ML) that enable computers to learn from large datasets. Based on curated data and our own experimental results, we will build a so-called benchmark: a structured collection of datasets that allows researchers to consistently test and compare the performance of different predictive models. We will also train our own, openly available models designed to predict key properties of novel chemical substances, such as their impact on living organisms, persistence in the environment, and likelihood of accumulating in biological tissues

This project addresses real-world needs in both agriculture and environmental protection. By creating an open platform for AI model testing in agrochemistry, we will foster international scientific collaboration and knowledge sharing. At the same time, industry partners will be able to bring improved solutions to market faster and more effectively.