IKTOS

Artificial Intelligence
for new drug design

Iktos is an applied artificial intelligence startup that helps chemistry researchers improve their molecular discovery, drug design process and synthetic planning.

Our technology leverages many advances in machine and deep learning to generate novel molecules that satisfy the end user's criteria in a fraction of the time and effort. A second area of research is related to data-driven retrosynthetic analysis and empowers organic chemists with exhaustive analyses in minutes.

To support Iktos' fast-growing team and keep pace with our high number of cutting-edge projects, we are recruiting passionate AI interns. If you wish to join a young team, experience the startup mindset and be mentored by top-notch scientists while working on exciting projects, reach out to us !

Profile

We are looking for students in their final year of a MSc in data science or Engineering degree. Candidates should have a computer science/software engineering or a probability/statistics/data science background, provided that they are motivated to expand their skill set.

- Knowledge in supervised/unsupervised learning methods
- Advanced level in Python language and being familiar with a deep learning framework (tensorflow, pytorch …)
- Ease with communication/explanation of your work and results (both in French and in English)
- Knowledge in deep learning and optimisation is a plus
- Understanding of basic concepts in chemistry is a plus

Mission

Our R&D team is focused on various subjects to directly improve what we offer to our customers, depending on your interest and skills you could work on:

- Some molecule properties used to select the most active drug candidates can be very heavy to compute, often the heavier is one, the more correlated with activity it is. As a result, we would like to design an active learning strategy to improve how we select the most active candidate without having to compute the properties on all the available molecules or all the generated molecules. This work will cover among other topics: active learning, bayesian batch optimisation, multi-fidelity optimisation, models ensembling, uncertainty quantification, generative models…

- In in silico drug discovery, one of the main challenge relies on understanding the relationship between the structure of the molecules and their desired properties, even though we only y have very few measured data points compared to the possible molecules in the data space. We aim at exploring and improving state-of-the-art predictive models with a good generalisation power. This work will cover among other topics: supervised predictive models, domain generalisation[1], few shot learning, uncertainty quantification…

- In target-based drug discovery, the goal is to find a set of molecules which are “actives” for the target, which means that the structure of the molecule builds strong interactions with the target protein. Hence, the 3D structure of the molecule should be considered when modelling the activity. However, most of the state-of-the art machine learning methods does not take into account this spatial information. We aim at including this spatial information on top of the structural information in order to build more robust predictive models. This work will cover among other topics: transformers, multi-modal learning, attention mechanism, representation learning, generative models, graph neural network …

Details

- Start date: from or after January 2022
- Duration: 6 months (4 months minimum).
- Location: Paris (17th district) with remote work flexibility
- Contact: nicolas.drizard@iktos.com

Please send your resume and availability by email.