[Senior] Scientist Machine Learning in Computational Chemistry (80-100%)

Deep Learning for structure-based drug design and cell signaling prediction

Overview

One cannot predict output of a neural network if the weights of only a few nodes are specified, while weights of others are allowed to vary. Yet, this happens in drug development: drug effects on cellular networks are analyzed for a couple of network nodes, while others remain ignored. Such shallow analysis in part contributes to the current 90% drug failure rate in clinical trials.

InterAx Biotech is pioneering experimental and computational systems biology approaches, combined with machine learning, for quantification of drug effects on signaling networks. This gives deeper insight into drug network effects before the drugs enter clinical trials.

The company is a growing Biotech based between Zurich and Basel, two important pharma/biotech hubs in Switzerland. We are a friendly, dynamic, inter-disciplinary and multi-national team aiming to transform preclinical drug discovery with new tools focusing on cellular networks. We currently focus on the largest class of drug targets – GPCRs. In addition to the technology platform, InterAx runs an in-house anti-cancer drug discovery program.

InterAx seeks to recruit an experienced, self-driven and creative machine learning scientist to join the computational chemistry team. You will help to connect chemistry with biology using deep learning methods, to rationally design novel patentable therapies at the forefront of drug discovery. Remote work is possible.

Responsibilities include

- Development and deployment of ML approaches to predict drug cell signaling based on 3D drug-target structures and cell signaling data. Current focus is on convolutional networks and transfer learning.
- Interactions with chemists, structural biologists and cell biologists to support in-house and pharma partner drug discovery programs at various stages.
- For the senior level – lead and develop the computational chemistry team; scout for new technologies and continue to grow the CADD, AI capabilities and ML infrastructure; help to refine company vision and strategy.

Qualifications

- PhD in Computational Chemistry or related field; or M.Sc. with 5+ years practical experience in computational chemistry machine learning.

Required:

- Good knowledge of modern statistical and machine learning techniques.
- Experience in implementing, debugging, and extending convolutional neural networks (preferably 3D).
- Skilled in ligand-protein docking algorithms and results evaluation.
- Experience with DL frameworks, e.g. TensorFlow/Keras or PyTorch/Fastai.
- Self-driven, proactive, and forward-thinking attitude.

Considered a plus:

- Hands-on experience with Transfer Learning or Multi-objective learning.
- Track record in computational / medicinal chemistry role, focusing on compound optimization towards a clinical candidate.
- Experience in several areas from ligand- and structure-based virtual screening, multi-parameter optimization, conformational analysis, pharmacophore development, QSAR, data mining and target assessment strategies.
- Experience in analysis of Molecular Dynamics or other time-resolved data.
- Familiarity with generative models, graph-convolutional neural networks.

Personal attributes

- Highly organized, conscientious, and reliable team player, with strong attention to detail.
- Excellent communication and presentation skills to share complex ideas and results with non-experts.
- Fluency in English.

Your benefits

- Exceptional possibilities for the discovery of innovative drugs against cancer and other diseases.
- Competitive salary, and ample support to grow your skills.
- Dynamic and motivated team with flat hierarchy.
- Support in publishing new ML & structure-based drug discovery approaches.
- Swiss Alps nearby.
- Possibility of remote work (in Switzerland or another country).

Please send your CV, motivation letter and references to **recruiting[at]interaxbiotech.com**, adding “ID-2022-42” to the subject of your email.

Applications will be evaluated continuously, with anticipated deadline on March 15th.