Senior Computational Chemist / Team Leader
Deep Learning in Drug Design

Overview

Characterization of drug effects on cell signaling is challenging and is most often ignored in pre-clinical drug discovery. The limited drug biology characterization strongly contributes to the 90% drug failure rates in clinical trials. The future drug discovery will have to consider the inner workings of cells in more detail. With this vision, InterAx is establishing an integrated pre-clinical GPCR drug discovery platform with a strong focus on early optimization of drug effects on cell signaling. InterAx pioneering experimental and computational systems biology approaches, combined with machine learning, already yield deeper insight into drug effects on signaling, and help to select low-risk drug candidates before the start of clinical trials.

The company is a growing Biotech based between Zurich and Basel, two important pharma/biotech hubs in Switzerland. We are a dynamic and multi-national team, combining inter-disciplinary scientists from cell biology to chemistry to mathematical modeling. In addition to the technology platform, InterAx runs in-house anti-cancer drug discovery program, and is launching an anti-ageing program.

After early successes InterAx seeks to recruit an experienced and self-driven scientist to lead the future developments of the computational chemistry AI team. If you are a skilled and ambitious scientist, this role will provide you a unique opportunity for personal growth and development, and ample ways to influence the strategy of a computation-driven biotech company on a quest to deliver safer and more efficacious therapeutics.

Primary responsibilities

- Develop and apply innovative cheminformatics/ML approaches at all pre-clinical drug discovery stages: target identification, hit finding, H2L, and LO.
- Particular ML focus is on direct analysis of 3D drug-target structures for binding/activity prediction, and leveraging unique InterAx cell signaling datasets for lead optimization towards safer and more efficacious drugs.
- Contribute to in-house and pharma partner GPCR drug discovery projects within multidisciplinary teams.
- Lead and strategically develop InterAx computational chemistry / AI team.
- Scout for best practices and develop next-generation CADD solutions for drug discovery challenges, e.g. in structure-driven AI generative models, chemogenomics and polypharmacology-focused screening, utilization of ultra-large on-demand libraries, explainable AI.
- Use good programming practices, documentation and reproducible research.

Additional responsibilities

- Support data organization and integration into databases for efficient data analytics.
- Communicate project results internally and externally (e.g. to clients) via presentations and publications.
- Interact with business development team to identify new opportunities, refine company strategy, and prepare scientific proposals.

Qualifications

Required:

- PhD in Computational Chemistry or related discipline.
- 4+ years applying CADD in multi-disciplinary pharma/biotech environment aimed at optimization of compounds towards a clinical candidate.
- Proven track record with first- or senior-author publications/patents in cheminformatics/ML.
- Working knowledge and proven experience in CADD structural analysis of proteins and protein-ligand interactions, including homology modeling, docking algorithms and structure-based virtual screening.
- Experience in several of the following areas: molecular modeling (e.g. Schrödinger, MOE), phamacophore modeling, virtual library design, hit and lead finding, ligand-based virtual screening, diversity analysis, molecular dynamics, free energy perturbations, multi-parameter optimization, QSAR.
- Experience in implementing and optimizing deep neural networks, using modern DL frameworks (e.g. TensorFlow/Keras or PyTorch/Fast.ai).
- Good knowledge of modern statistical and machine learning techniques.
- Programming experience in at least one scripting language (e.g., Python), toolkits (e.g. RDKit), and knowledge of pipelining tools (e.g. KNIME).

Experiences considered a plus:

- Cheminformatics or AI techniques for de novo molecular design (e.g. fragment-based methods, generative chemistry models).
- Transfer Learning, Multi-objective learning, Graph neural networks.
- GPCR structural modelling and structure-based ligand design.
- Managing and mentoring scientists and/or involvement in drug discovery project leadership roles.

Personal attributes

- Highly organized, attentive to detail, conscientious, and reliable team player.
- Self-driven, proactive, with creative problem-solving skills and forward-thinking attitude.
- Excellent oral and written communication and presentation skills: to share complex ideas and results with non-experts.

Your benefits

- Deep dive into pharmacology, biology & chemistry of the largest class of drug targets – GPCRs, and possibility to discover innovative drugs against cancer and other diseases.
- Possibility to directly influence the strategy of a biotech company.
- Competitive salary and stock compensation, commensurate with experience.
- Active support to grow your skills and abilities.
- Support in publishing new CADD/ML approaches.
- Dynamic and motivated team with flat hierarchy.
- 25 workdays annual leave in addition to public holidays.
- Scenic Swiss Alps at your door.
- Flexible working hours and possibility of remote work.

Please send your CV and motivation letter to **recruiting[at]interaxbiotech.com**,
adding “ID-2022-72” to the subject of your email.