NOVARTIS

Senior Specialist, Data Science & AI

Job ID
REQ-10087864
Sep 25, 2026
LOC_US

About the Role

Purpose of the role

Senior Expert (Applied AI, LMW Drug Discovery):

- Work within a global team of AI researchers and SME with core domain expertise in applying AI to low molecular weight drug discovery.
- Contribute to the conceptualization of AI methods and their applications for hit generation, lead optimization, pre-clinical analysis, including safety and PK/PD
- Develop, adapt and evaluate state-of-the-art AI/machine learning models, including foundation models, generative AI, multimodal AI, and agentic systems
- Establish rigorous evaluation and benchmarking frameworks to assess the robustness and scientific validity of models deployed in drug discovery applications
- Define translatable metrics that connect model performance to downstream scientific decisions, including assay-level or prioritization improvements, and experimental efficiency
- Help integrate of AI approaches into design-make-test-analyze (DMTA) cycles to accelerate LMW drug discovery
- Facilitate delivery of AI solutions through collaboration with Engineering and Product Development teams
- Communicate progress and impact to stakeholders and multidisciplinary audiences

Collaboration & partnership

- A respectful team-player attitude is an absolute must
- Regularly communicate, engage, align with AI4R teams, broader data science community, and senior scientists
- Collaborate cross-functionally (medicinal chemists, DMPK, structural biology, and disease-area scientists, engineers and other AI experts) complementing complex projects with AI-based approaches to LMW drug discovery
- Excellent interpersonal and communication skills, with ability to translate analytical concepts for diverse audience and stakeholders (English is our primary language)

What you'll bring to the role:

- A deep curiosity and passion for biomedical sciences driven therapeutic discovery.
- 4+ years of significant experience in innovation, development, deployment and continuous support of Machine Learning data management and modeling
- Strong hands-on coding proficiency in Python and deep learning frameworks
- Strong understanding and experience in using version control systems for developing software (e.g. GitHub, git, subversion, bitbucket, etc.)
- Demonstrated expertise / experience in several of molecular AI/ML areas, such as generative chemistry; structure-

based drug design across hit finding, hit to lead, lead optimization, and candidate selection; protein-ligand modelling, co-folding; docking, scoring, and pose assessment with rigorous model validation and tight coupling to experimental follow up; QSAR; multi-objective property optimization (uncertainty estimation, active learning concepts); free energy and affinity prediction
- Demonstrated expertise / experience with AI driven molecular design applied to the areas above Experience working in a large Research organization & deep understanding of drug development a plus
- Passion for understanding emerging technologies with pragmatic insight into where those technologies can be integrated into business solutions
- Ability to balance requirements, manage expectations, and drive effective results using a proactive attitude towards identifying and resolving issues
- Strong organizational and problem-solving skills, with ability to execute and prioritize well in a complex matrixed environment.

Relevant areas of desired expertise:

Molecular representation learning for small molecules, graph neural networks, geometric deep learning, property prediction for ADME PK, physiochemical properties, safety, de novo design, chemical space exploration, foundation models for chemistry, uncertainty quantification, active learning, agentic AI, generative chemistry, counterfactuals and explainability, multi-objective optimization.

Role Requirements

Division
DIV_RE
Business Unit
Information Technology
Location
LOC_US
Site
Cambridge (USA)
Company / Legal Entity
U175 (FCRS = US175) Novartis Institutes for BioMedical Research, Inc.
Functional Area
FCT_DD
Job Type
Full time
Employment Type
Regular
Shift Work
No
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