

Senior Expert Data Science, Modeling & Simulation

Job ID REQ-10049332

8月 11, 2025

India

摘要

As a Data Science expert, you will join our Modeling & Simulation Data Science team in the Translational Medicine Unit and help us to unleash the power of data science for drug discovery. You will bring your curious, innovative, and collaborative mindset to effectively harness the absorption, distribution, metabolism, excretion (ADME) and pharmacokinetics (PK) / pharmacodynamics (PD) data generated within our department and master the use of our in-house applications and state-of-the-art machine learning (ML) methods and statistical techniques to accelerate drug design. Our group is growing, and we hope you will join our dynamic, enthusiastic and forward-thinking team!

About the Role

Key responsibilities

Your responsibilities will include, but are not limited to:

- Act as the M&S Data Science representative on drug discovery and lead optimization programs by collaboratively contributing to project team discussions, using dryand wet-lab data to provide scientific and strategic input to guide decisions such as compound progression and in vivo study prioritization
- Master and advocate the use of in silico models and in-house tools, applications and data to accelerate and streamline decision making
- Apply data mining to understand relationships between structure and molecular properties for programs involving small molecules, peptides, RNAs
- Identify opportunities to create custom, project- or modality-specific in silico models and data strategy, and contribute to their development and implementation
- Proactively seek opportunities to increase the impact and awareness of M&S Data Science through clear and concise communications with internal and external audiences or various expertise
- Monitor and stay up to date on developments within the field of AI/ML applied to ADME and PK/PD, and data science methods applied to drug discovery

Role requirements Essential requirements:

- Advanced degree in life sciences with multidisciplinary background (cheminformatics, bioinformatics, biomedical engineering, AI/ML in drug discovery or life sciences, data science, computational biology, computational chemistry or related field)
- PhD with 2+ years or MSc with 6+ years of relevant work experience with deep knowledge on drug discovery and development processes
- Experience in the application of (reproducible) data science methods, tools and practices to drug discovery
- Strong understanding of statistics, machine learning and deep learning
- Demonstrated knowledge of data visualization and exploratory analysis

- Solid skills in programming languages, i.e. Python and R, including software development practices such as version control, testing, documentation, etc.
- Knowledge of machine learning/deep learning libraries such as scikit-learn, keras or pytorch
- Excellent communication skills and ability to translate analytical concepts for diverse audience and stakeholders (English is our primary language)

Desirable:

- Expertise with discovery-stage PK modeling for small molecule compounds (e.g., relating ADME properties to in vivo PK; scaling of preclinical PK to human) is a plus
- Experience with generative algorithms and explainable Al

Languages:

• English.

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Job Type Full time
Employment Type Regular
Shift Work No

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