

# Senior Expert Data Scientist, Modeling & Simulation

Job ID  
REQ-10051140  
May 25, 2025  
USA

## Summary

#LI-Hybrid

This position will be located at our Cambridge, MA site and will not have the ability to be located remotely. 200! This is the number of experimental data generated every single day in the Pharmacokinetic Sciences (PKS) department at Novartis Biomedical Research on drug discovery projects. We need your expertise, experience, and unwavering passion to help us leverage this wealth of information for decision making and shape the future of medicine.

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 lead optimization. Our group is growing, and we hope you will join our dynamic, enthusiastic and forward-thinking team!

## About the Role

### Key Responsibilities:

- Act as the M&S Data Science representative on drug discovery and lead optimization programs by collaboratively contributing to project team discussions, using dry- and 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

### 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 Requirements:**

- 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 AI

**Novartis Compensation and Benefit Summary:** The pay range for this position at commencement of employment is expected to be between: \$119,700 to \$222,300/year; however, while salary ranges are effective from 1/1/25 through 12/31/25, fluctuations in the job market may necessitate adjustments to pay ranges during this period. Further, final pay determinations will depend on various factors, including, but not limited to geographical location, experience level, knowledge, skills, and abilities. The total compensation package for this position may also include other elements, including a sign-on bonus, restricted stock units, and discretionary awards in addition to a full range of medical, financial, and/or other benefits (including 401(k) eligibility and various paid time off benefits, such as vacation, sick time, and parental leave), dependent on the position offered. Details of participation in these benefit plans will be provided if an employee receives an offer of employment. If hired, employee will be in an “at-will position” and the Company reserves the right to modify base salary (as well as any other discretionary payment or compensation program) at any time, including for reasons related to individual performance, Company or individual department/team performance, and market factors.

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Division

Biomedical Research

Business Unit

Pharma Research

Location

USA

State

Massachusetts

Site

Cambridge (USA)

Company / Legal Entity

U175 (FCRS = US175) Novartis Institutes for BioMedical Research, Inc.

Functional Area

Data and Digital

Job Type

Full time

Employment Type

Regular

Shift Work

No

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