

## Senior Scientist, Cheminformatics

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Our ability to excel depends on the integrity, knowledge, imagination, skill, diversity and teamwork of an individual like you. To this end, we strive to create an environment of mutual respect, encouragement and teamwork. As part of our global team, you'll have the opportunity to collaborate with talented and dedicated colleagues while developing and expanding your career.

The department of Computational & Structural Chemistry is seeking a creative and self-motivated cheminformatics data scientist to join our team. The successful candidate will work closely with discovery scientists to drive towards a 'design first' culture, supporting project medicinal chemists with the proper predictive models and workflows. In addition to leveraging rapid advances in machine learning towards the interpretation of complex *in vitro* and *in vivo* biological data, the candidate will make informed decisions to de-risk safety liabilities and understand the mechanisms of toxicity at both lead selection and throughout the lifecycle of a discovery project.

### Responsibilities include and are not limited to the following:

- Drive a 'predict first' culture in hit-to-lead and lead optimization
- Develop and apply computational tools, including machine learning
- Characterize the toxicology profile of lead molecules and mitigate potential adverse effects
- Design and implement deeper informatics methods to address specific project challenges

### Education Minimum Requirement:

Ph.D. (or close to completion) in Chemistry, Mathematics, Physics, Computer Science, Biology or commensurate career experience.

### Required Experience and Skills:

- Competency in programming, scripting, and databases (e.g. Python, R, MySQL)
- Background in methods for cheminformatics, statistical analysis, visualization tools, and machine learning techniques
- Strong communication skills, both written and oral
- Ability to work well in multidisciplinary teams

**Preferred Experience:**

- Experience with workflow applications and data analytics software (Pipeline Pilot, Knime, Spotfire, ...)
- External scientific visibility through multiple publications and/or presentations
- A basic understanding of the drug discovery processes and medicinal chemistry