

Title: Cheminformatics Scientist

Company:

X-Chem, Inc. is a privately held biotechnology company based in Waltham, Massachusetts, established in 2009 to apply its innovative drug discovery capabilities to the generation of novel small molecule therapeutics

Education/Experience:

Ph.D. or commensurate experience in Cheminformatics, Chemistry, Scientific Computing
5+ years relevant experience in Biotech/Pharma industry or academic informatics.

Job Description:

The Cheminformatics position will report to the Group Leader of Scientific Computing, Scientific Software & Databases. With a DNA encoded library consisting of 100 Billion+ molecules and 10s-100s of millions of data points capturing enrichment of encoded structures per each experiment, a broad range of cheminformatic questions remain to be explored. The novel combination of the ability to generate rich information across numerous experimental conditions coupled with the unprecedented amount of data generated by next generation sequencing creates a significant opportunity to develop new approaches to further drive the drug discovery potential of this technology. This role will lead exploration in a broad range of cheminformatics areas: automation of structure categorization and exploitation of selection derived SAR; application of property predictions, in silico reactions, and diversity analyses of reactions schemes included or proposed for the X-Chem library; expansion of the use of enrichment data to influence downstream series optimization. This role will maintain and enhance X-Chem proprietary cheminformatics solutions. The role will interact with individual scientific staff and project teams to develop capabilities and data analyses that have direct impact on successful completion of partner and internal project goals.

Candidate Qualities:

Successful candidate will demonstrate the ability to draw on a broad range of multi-disciplinary information in order to develop and apply innovative approaches to cheminformatic analysis on large scale data. Candidate will be able to demonstrate creative problem-solving abilities and adaptability to new technologies as well as the ability to work independently and drive a project from proof of concept through deployment and production. Candidate must show effective direct communication with scientific staff at all levels. Candidate must be able to work in a fast paced environment while maintaining the high level of accuracy in computational results required.

Desired Skills/Background:

- Core cheminformatic expertise e.g. similarity, diversity, SAR analysis; definition of in silico reactions; use of software e.g. ChemAxon, CambridgeSoft; SMARTS, SMILES, structure searching; property prediction
- Programming skills in a relevant coding language (C#, java, Python) with experience developing for non-trivial applications in a scientific industry or academic laboratory setting.

- Data Analytics capabilities, e.g. large scale data analysis, data-mining, Oracle, SQL and PL/SQL, predictive model building, machine-learning, clustering, statistical analysis, Vortex/Spotfire, Excel.
- Molecular modelling, docking, pharmacophore analysis, computational chemistry a plus

About X-Chem:

X-Chem is a privately held biotechnology company whose mission is to harness the power of DEX technologies to create medicines that transform patients' lives.

X-Chem offers a stimulating, casual, and fun working environment; plus a competitive salary and benefits package, stock option incentives, and the opportunity for all employees to grow with the Company. X-Chem is an equal opportunity employer that complies with all applicable national, state and local laws governing nondiscrimination in employment as well as employment eligibility verification requirements of the Immigration and Nationality Act. All applicants must have authorization to work in the United States.

No Employment Agencies please, the Company is not responsible for **any fees related to** candidates that are unsolicited.

Job Code – MGP41 (Use Job Code in subject line of all communications)

Apply Now

- **Company** [X-Chem, Inc.](#)
- **Contact Name** Human Resources
- **Email** careers@x-chemrx.com
- **Position Location** Waltham, MA
- **Position** Cheminformatics Scientist
- **Minimum Preferred Education** Ph.D. or commensurate experience
- **Years of Experience** 5+
- **Career Level** non-manager
- **Availability** Immediate