

Cheminformatics Software Engineer

The Opportunity:

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 maintain and enhance X-Chem proprietary cheminformatics solutions. This role will lead exploration in a broad range of cheminformatics areas such as:

- 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.
- Library enumeration
- Chemical entity registration enhancements
- Molecule collections analysis (PCA, diversity, properties, etc.)
- Fingerprints and other representations (e.g. shape based, scaffold analysis)
- ChemAxon, CambridgeSoft management
- Refinement of large molecule sets to subsets of representative molecules.
- Large scale similarity, substructure search

The Cheminformatics Software Engineer will report to the Associate Director of Scientific Computing. The 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. The candidate will be asked to work independently to build software systems required to support X-Chem's platform. This role will be responsible for the full system development life cycle. This will include requirements gathering, design, planning, software development, testing, enhancement, and maintenance of a variety of chemistry related software functionalities. These projects may also include database design/programming, integration of purchased software, etc. The role will require becoming an expert user/analyst of existing and new software systems with the ability to train scientific staff. The Scientific Computing group promotes a dynamic, engaging and empowering work environment to match X-Chem's core values and would look to this role to bring a fresh perspective to the team with the goal of enhancing user experience.

Candidate Qualities:

The successful candidate will be a self-starter with the ability to work independently and drive a project from conception through deployment and production. The candidate must show effective direct communication with scientific staff at all levels. The candidate must be able to work in a fast paced environment while maintaining the high level of quality in delivered products. The candidate must be able to maintain confidentiality as required by partner contracts. The candidate will be able to demonstrate creative problem-solving abilities and adaptability to new problems, technologies, and system requirements.

Required 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
- Data Analytics capabilities, e.g. large scale data analysis, data-mining, predictive model building, machine-learning, clustering, statistical analysis, Vortex/Spotfire.
- Programming skills in a relevant coding language (C#, C++, Java, Python) with experience developing for non-trivial applications in a scientific industry or academic laboratory setting.
- .NET 4.5 or higher (desktop application development preferred, web development a plus)
- WinForms, WCF and/or WPF
- Experience with chemistry software implementation
- Experience with user driven custom application development
- Proven ability to gather requirements
- Experience in a small team environment
- Strong capabilities in use of Excel

Desired Skills/ Background:

- Experience with TFS administration
- Experience with Oracle, SQL, PL/SQL
- Experience with Design Models
- Molecular modelling, docking, pharmacophore analysis, computational chemistry
- VSTO Excel programming desirable
- RDKit, Knime, PipelinePilot, Python
- Scripting in MOE and Schrodinger

Education/Experience: B.S. or M.S. in Chemistry or commensurate experience in cheminformatics software development. 5+ years relevant experience in Biotech/Pharma industry or academic cheminformatics.

About X-Chem

X-Chem is a privately held biotechnology company whose mission is to apply its innovative drug discovery capabilities to the discovery of compounds against novel therapeutic targets.

Our chemical strategy can be applied broadly to most targets in any therapeutic area, including the most challenging ones. We have built a strong team of leading experts with proven track records in innovative drug discovery and biotechnology partnering.

Why join X-Chem?

X-Chem offers highly competitive compensation based on prior experience and qualifications as well as comprehensive benefits in order to best support our people. Benefits we offer includes: 100% Paid Medical, Dental, STD/LTD and Life Insurance; 12 Paid Holidays; 22 days PTO; Tuition Reimbursement; Stock Options; Flexible Spending account for both medical and dependent care; weekly social hour; Summer Hours and company events. Our work environment includes casual dress, bike storage, free parking, and wellness perks.

EEO Statement

X-Chem is an equal opportunity employer and all qualified applicants will receive consideration for employment without regard to race, color, religion, sex, national origin, disability status, protected veteran status, gender identity, sexual orientation, pregnancy and pregnancy-related conditions, or any other characteristic protected by law.

Job Code: MAG47**Apply Now****X-Chem Pharmaceuticals Careers Page****Contact Name** Marie-Aude Guié**Email** careers@x-chemrx.com**Position Location** Waltham, MA