

Job Title: Cheminformatics Software Engineer

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.

Job Description:

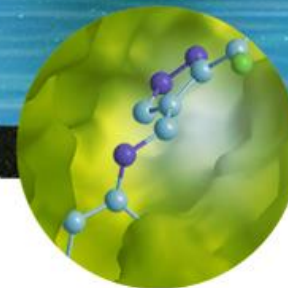
With a DNA encoded library consisting of 200 Billion+ molecules and 100s of millions of data points capturing enrichment of encoded structures per experiment, a broad range of cheminformatics questions remain to be explored. The ability to generate rich information across numerous experimental conditions coupled with the unprecedented amount of data generated by X-Chem's platform creates a significant opportunity to develop new approaches to further drive the drug discovery potential of this technology.

The Cheminformatics Software Engineer will report to the Senior Director of Scientific Computing. 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. The successful candidate will demonstrate the ability to draw on a broad range of multi-disciplinary information in order to develop and drive the implementation of innovative approaches to cheminformatics analysis on large scale data. These approaches may also include integration of purchased software, etc.

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

- Automation of structure categorization and exploitation of experimentally derived SAR (with the goal of refining large molecule sets down to representative molecules).
- Creation of tools for:
 - o the generation/application of property predictions, in silico reactions, and diversity analyses of reactions schemes included or proposed for the X-Chem library and commercial molecule collections
 - o molecule collections analysis (PCA, diversity, properties, etc.)
- Enhancement of existing systems and/or proposal of novel systems:
 - o library enumeration algorithms
 - o implementation of chemical fingerprint approaches and other representations (e.g. shape based, scaffold analysis)
- Large scale similarity and substructure searching

This role will be responsible for the full system development life cycle. This will include requirements gathering, design, planning, software development (or supervision thereof), testing, maintenance (or



supervision thereof), proposal of enhancements for a variety of chemistry related software functionalities. The candidate will:

- be able to demonstrate creative problem-solving abilities and adaptability to new technologies.
- be asked to work independently to drive the implementation of software systems required to support X-Chem's platform.
- become an expert user/analyst of existing and new software systems with the ability to train scientific staff.

Candidate Qualities:

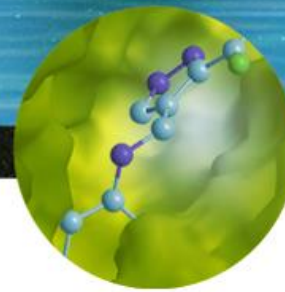
The successful candidate will be a self-starter with the ability to work independently and drive a project from conception through deployment and production. The candidate must show effective direct communication with scientific staff at all levels. The candidate must be able to work in a fast paced 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:

- Expert knowledge of chemistry in the context of drug discovery
- Core cheminformatics 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
- Experience with chemistry software implementation
- 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.
- Experience with user driven custom application development
- Proven ability to gather requirements
- Experience in a small team environment

Desired Skills/ Background:

- WinForms, WCF and/or WPF
- .NET 4.5 or higher (desktop application development preferred, web development a plus)
- TFS administration
- Oracle, SQL, PL/SQL
- Design Models
- Molecular modelling, docking, pharmacophore analysis, computational chemistry
- RDKit, Knime, PipelinePilot, Python
- Scripting in MOE and Schrodinger



About X-Chem

X-Chem is the industry-leading provider of DNA-Encoded Library (DEL)-based discovery services. DEL technology, allowing customers to screen billions of compounds simultaneously against a single biological target, is an innovative and high growth segment of the market as pharmaceutical companies look for access to cutting edge scientific expertise to support an increasingly challenging drug discovery process. From its Waltham, US headquarters and leveraging a proprietary DEL platform with libraries containing over 200 billion small molecules, X-Chem has supported drug discovery programs for partners throughout the US, Europe and Japan and has licensed over seventy research programs, comprising hundreds of novel chemical entities, to companies.

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; Flexible Spending account for both medical and dependent care; onsite fitness classes; 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.

Apply Now

Company: [X-Chem, Inc](#)

Contact Name Marie-Aude Guié

Job Code: MAG47 (Please include on all correspondence)

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Position Location Waltham, MA