1.1 PROBLEM STATEMENT

To avoid high cost and to provide safety during exploratory stages, most manufacturers of drugs run simulations of molecular interactions and analyze the movements of atoms (in the context of multiple molecules that they belong to). The main purpose is to detect whether certain events of interest occur – which, in turn, would mean that certain properties of the drug under development are satisfied (or not). For this project's purposes, our event of interest is the formation of a Hydrogen Bond (HB) during the evolution of the chemical compound, and its persistence for a set amount of time. Our project aims to develop a system that will allow users to analyze the simulation datasets and: (1) detect the occurrence of such long-lasting HBs; (2) provide a detailed report to the user; (3) provide a visual representation of the persistent HBs, if they occur within the data set.

1.2 REQUIREMENTS & CONSTRAINTS

Functional Requirements:

- Take input from user regarding data set, algorithm, parameters. Parameters will change depending on the algorithm selected. The system needs to ensure that the correct parameters are provided.
- Output the results of the algorithm so that the user can clearly see the clusters that persist over time.
- System needs to scale well with multiple users as well as larger datasets.
- Computations need to be done on a server rather than the client's machine due to high intensity computations.
- Validation needs to be done on user input parameters to ensure that the system does not crash.
- Runtime of the algorithms needs to be reasonably efficient (Algorithms provided)
- Access to data should be fast and reliable.

Environmental:

- System should not make excessive/unnecessary computations and should be power efficient.

Economic:

- System should not make excessive/unnecessary computations and should be power efficient and should be extensible so that other datasets can be easily incorporated, and other criteria be added.
- Guarantees of quality of output so that drug companies can clearly see the results as real-world testing involves high costs and risks.

UI:

- UI needs to provide ease of navigation.
- It should be intuitive to understand the (purpose and use of) different components.
- It should provide input validation.

1.3 ENGINEERING STANDARDS

What Engineering standards are likely to apply to your project? Some standards might be built into your requirements (Use 802.11 ac Wi-Fi standard) and many others might fall out of design. For each standard listed, also provide a brief justification.

IEEE/ISO/IEC 12207-2017

- Covers the common framework for the software development life cycle.

IEEE/ISO/IEC 90003-2018

- supply, development, operation and maintenance of computer software and related support services.

ISO/IEC 27001

- Standard dealing with information security and practices that should be followed.

V. Phoha, "A standard for software documentation," in Computer, vol. 30, no. 10, pp. 97-98, Oct. 1997, doi: 10.1109/2.625327.

- Based on ANSI/ANS 10.3-1995 a standard used for the documentation of computer software and development

1.4 INTENDED USERS AND USES

There are several classes of stakeholders that could potentially benefit from the results of this project.

Chemical scientists and engineers:

- How will they use our project?
    - o Easily filter received data and visualize results in a way that is useful to chemists.
    - o Display easy to understand information about properties regarding reactions of chemical compounds to peers and others.
- What do they gain from our project?
    - o Speeds up the process of drug development.
    - o Reduces time and effort on evaluating the data our application does for them.

Pharmaceutical Investors and Businesses:

- How will they use our project?
    - o Easy, high-level tool to understand drug interactions without needing to understand the details.

- What do they gain from our program?
    - o Reduce the risks when investing in development for potential drugs.

Educators:

- How will they use our project?
    - o Safe environment for demonstrating properties of chemical reactions to students.