The Computational Molecular Biomedicine group is pursuing N major research topics as well as collaborative projects in diverse biomedical research areas. Most projects combine broad knowledge of molecular biology with state-of-the-art mathematical modeling and machine learning techniques.

1. Proteomics data analysis method and software development

The goal of this project is to develop high-performance, high-throughput analysis methods and software tools for proteomics datasets. We are particularly interested in applying machine learning techniques on both CPU and GPU architectures to improve peptide identification and quantification from mass spectrometry data. Example application areas include identification of (i) crosslinked peptides whose mass spectra are generally 3-4 times more complex than those found in typical proteomics studies and (ii) novel peptide sequences and modifications that currently do not exist in reference databases.

Parts of this project will be performed in collaboration with the Systems Biology Center at Chulalongkorn University (CUSB), whose characterizations of novel proteomes will greatly benefit from improved *de novo* identification of unknown peptides and proteins, and Dr. David W. Speicher’s proteomics research laboratory at the Wistar Institute in Philadelphia, PA USA, where zero-length crosslinking is being routinely utilized to probe the structure of red cell membrane proteins and other complex systems.

1. Integrative analysis of high-throughput biomedical datasets

[Public datasets + internal datasets]

[Computational analyses + biological interpretation]

[What are primary biological topics]

1. Mathematical modeling and simulation of chromatin folding process

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1. Visualization of biomedical data using virtual reality

Even though we can perceive three dimensions, our visualization of data has largely been limited to 2-dimension media such as monitor screen or a piece of paper. With the emergence of affordable virtual reality technology, we can now explore the possibility of representing structural and non-structural biomedical data in 3-dimensional space and subsequent visualization in virtual reality. A primary goal of this project is to develop novel visualization methods and tools that facilitate comprehensive integration, visualization, and interpretation of complex biomedical datasets.