Undergraduate research opportunities (Winter/Summer 2024) for Chemistry & Biochemistry/Biology//Physics/Chemical & Materials Engineering students

In silico T-cell epitope identification targeting *Treponema pallidum* mediated Congenital Syphilis

In silico T-cell epitope identification represents a promising strategy for developing preventive and therapeutic measures against harmful pathogens. Syphilis, caused by the spirochete bacterium *Treponema pallidum*, is a sexually transmitted infection that can lead to severe health complications if left untreated. Among its various forms, infectious syphilis poses a risk to individuals who contract the disease, while congenital syphilis affects newborns when the bacterium is transmitted from an infected mother. Developing effective preventive and therapeutic strategies is crucial in combatting this global public health challenge in North America. In this context, *in silico* T-cell epitope identification emerges as a valuable approach for designing vaccines and immunotherapies against *Treponema pallidum* infections.

Our immuno-informatics team focuses on integration of immunomics and clinical data, and computational techniques for identification of epitopes. These epitopes should be selected based on their likelihood to induce a robust T-cell immune response. In addition, we evaluate the immunogenicity of predicted epitopes through *in silico* simulations. This involves predicting the binding affinity of epitopes to major histocompatibility complexes (MHCs) and assessing their potential to stimulate T-cell responses. The potential cross-reactivity of identified epitopes with host proteins must then be investigated to ensure specificity and avoid autoimmune responses.

In the proposed research project, the student will collect comprehensive datasets containing immunomic, genomic and proteomic data related to *Treponema pallidum*. Moreover, the student will learn and use different databases, tools and techniques for pathogen nucleotide and protein sequence retrieval, BLAST search, multiple sequence alignment, allele database, MHC types, epitopes, T-cell mediated immune response and population coverage analysis. To facilitate this investigation, the student will have access to cutting-edge computing resources within the Centre for Research in Molecular Modeling (CERMM) and the Digital Research Alliance of Canada (formerly Compute Canada). Additionally, they will benefit from the collective expertise of our scientific and technical team, participate in team meetings, and engage in scientific discussions throughout the project's duration. By predicting and validating epitopes that can elicit potent T-cell immune responses, this approach offers a pathway toward more effective vaccines and immunotherapies. Such interventions are crucial in the global effort to combat syphilis, particularly in regions like North America, where the disease remains a significant public health concern. This collaborative and technologically advanced environment will provide an ideal platform for the student to contribute meaningfully to the field of *in silico* immunotherapeutics design against *Treponema pallidum* infections.

Keywords: Allele selection; BLAST; Epitope prediction; multiple sequence alignment; T-cell; homology modeling;