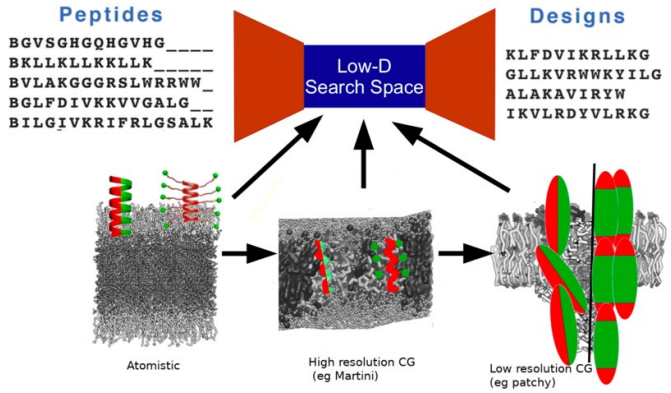
Concordia University
Arts and Science
Department of Physics

Graduate student position will be available, starting in the Fall 2021 / Winter 2022, in the group of Professor Rachael Mansbach
Department of Physics, Concordia University, Montreal, Canada.



Proteins are the building blocks of living things, miniature motors that make all of your cells function. Proteins embedded in cell membranes filter out toxic materials or uptake necessary nutrients. Meanwhile, malfunctioning proteins are responsible for a slew of disorders, including Alzheimer's, type II diabetes, and Parkinson's. Therefore, it is of great interest to be able to study the molecular mechanisms of various proteins, either to correct when things go wrong, or to design drug molecules to inhibit the proteins of damaging cells such as bacteria or cancerous cells.

My primary scientific interests lie in designing small molecules and peptides (short proteins) for therapeutic applications: killing bacteria and drugging human cells in beneficial ways—for example to find new analgesics for treatment of chronic pain disorders, or to correct dysregulation of pathways involving the intrinsically disordered proteins that lead to Alzheimer's. In order to do this, I employ theoretical and computational biophysics tools. I am particularly interested in the burgeoning field of deep learning as applied to molecular dynamics and drug design. Over the past decade, generative deep learning (training an AI to create by pattern-matching to a large amount of data) has demonstrated a fascinating ability to create images and text, and there has been an explosion in the past three years over its application to drug design and molecular dynamics, but it still suffers from lack of interpretability and scalability. As a physicist, I am particularly interested in the interpretability issue.

Drug Design for Antibiotics

With dwindling drug leads and increasing fatalities from multidrug-resistant bacteria, we are teetering on the brink of the post-antibiotic era. New design techniques and approaches for both understanding of antibiotic resistance and design of novel therapeutics are urgently needed. Recently, there has been promising experimental work in the field of antibiotic hybrids, in which sets of different pharmacophores are linked in novel ways, which may lead to molecules with enhanced efficacy or even entirely novel properties.

I am looking for a student interested in exploring the use of a fragment-based approach for novel antibiotic hybrid design through generative deep learning, in which a library of fragments relevant to antibiotic applications will be used as a basis for a generative model that produces novel antibiotic hybrids through linking, growth, and merging, with a particular emphasis on interpretability as well as candidate generation.

Desired qualifications. I am looking for strongly-motivated graduate student candidates interested in theoretical biophysics and deep learning. Physics or Biophysics BA or BS is preferred but I am happy to take CS, biomedical engineering or related fields if the match is good. Experience with coding will be valuable, particularly in Python, and prior experience with molecular dynamics simulations will also be useful. I would like to cultivate an ***inclusive, diverse and collaborative*** lab environment and I would particularly like to encourage members of traditionally underrepresented groups in STEM to apply. I am happy to work with students on their own ideas—as long as they fall within the broad scope of my work—and/or to tailor projects to suit specific strengths and interests.

Concordia Department of Physics is a growing department in a university with rapidly increasing rating. We offer research-based M.Sc. and Ph.D. programs. Our faculty members conduct research in the areas of Condensed Matter Physics (theoretical and experimental), Molecular Biophysics, Medical Physics / Imaging, Photonics, Theoretical High Energy Physics, Computational Physics and Physics Education.
Successful applicants will be offered financial packages consisting of RA, TA and various awards of at least 20,000 CAD per year (often more), for 4 years (Ph.D.) or 2 years (M.Sc.). International students will be offered tuition remissions or other awards to compensate for the international tuition fees.
Please contact Professor Rachael Mansbach (re.mansbach@concordia.ca) or Valter Zazubovits (valter.zazubovits@concordia.ca; Graduate Program Director) for more information.