

Funded Graduate Student Position Available, starting in Fall 2022 / Winter 2023

Group of Professor Mansbach

Department of Physics, Concordia University, Montreal, Canada.



We do computational research on physics-based rules for creating interpretable design spaces for therapeutics. We use cutting-edge deep learning techniques combined with molecular dynamics simulations to tease out basic science underlying biomolecules and their interactions. My goal for our group is to work hard, have fun, maintain a good work-life balance, and cultivate a just and equitable environment where students of many different backgrounds can thrive.

Antimicrobial peptide design through interpretable deep learning

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. A promising line of research for novel drugs with antimicrobial action is the design of peptides with antimicrobial properties that preferentially disrupt the membranes of bacterial cells while displaying a lower affinity for mammalian cells. This is still an active area of research, with only a few candidate peptides having reached clinical trials, due to the continued existence of unwanted side effects such as serum binding or the requirement of potentially-toxic concentrations to be effective.

We are working on designing a deep learning model informed by multi-scaled molecular dynamics, wherein generative learning is used to iteratively create potential AMP candidates that are assessed on multiple scales using molecular dynamics, from high-resolution atomistic molecular dynamics to assess detailed properties on short time scales, to low resolution "spherical peptide in a vacuum" models to assess penetration of candidates into the cell membrane. Interested candidates should have a strong background in statistical and computational physics, with knowledge of biochemistry or molecular biology a plus.

Concordia's Department of Physics is growing rapidly in size, impact, and diversity. We have over 170 undergraduate students, 45 graduate students, several postdocs, and are regularly hiring new faculty members in cutting edge research fields such as Condensed Matter and Nanomaterial Physics (theoretical, computational, and experimental), Biophysics and Biomedical Physics (computational and experimental, from molecular-scale



up to human-scale), Theoretical Particle Physics, and Physics Education. Successful MSc/PhD applicants will be offered complete financial packages consisting of research bursaries, teaching assistantships, and various awards totaling at least 20,000 CAD per year (often more) and additional tuition support for international students. For information about this specific position, please contact Professor Mansbach (re.mansbach@concordia.ca).