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ROADMAP: Reflectometry-driven Optimization And Discovery of Membrane Active Peptides

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The COVID-19 pandemic underscores the urgent need for swift advancements in therapeutic discovery against emerging health threats. Membrane-active peptides (MAPs) are a class of bioactive compounds with diverse applications in antimicrobial activity and drug delivery across cell membranes. Despite their immense potential, the sheer complexity of the space of possible MAPs presents challenges in discovery efforts. Understanding the structure-function relationship of MAPs is pivotal, yet remains incompletely elucidated.

In response to these challenges, we initiated the ROADMAP project to establish a robust measurement framework for membrane-associated MAPs. The project involves the complete automation of neutron reflectometry (NR) measurements and sample preparation at the CHRNS CANDOR reflectometer, NCNR. The approach accelerates measurement times through experimental optimization using information theory before and active learning during data acquisition. Predictive ML models, derived from sequentially collected data, guide efficient future measurements, facilitating rapid refinement of the structure-function relationship.

The ultimate objective of ROADMAP is to curate an extensive NR dataset encompassing over 1000 MAP sequences. Our approach emphasizes autonomous experimentation and model building, demonstrating the ability to derive meaningful insights from sparse data. By bridging the gap between theory and experimentation, ROADMAP represents a pioneering effort in the quest for novel therapeutics with potential implications for combating infectious diseases and addressing public health challenges.

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