Generative AI in Peptide Discovery

Daniela Kalafatović

daniela.kalafatovic@uniri.hr

University of Rijeka, Faculty of Engineering, 51000 Rijeka, Croatia

In an era increasingly shaped by artificial intelligence, peptide discovery is transitioning from a resource-intensive, trial-and-error process reliant on human intuition toward a data-driven paradigm characterized by high predictive accuracy and scalability. The immense size of peptide sequence space, coupled with a limited understanding of sequence-to-function relationships, makes the identification of new functional peptides inherently challenging [1]. To address this, we integrate machine learning with a genetic algorithm-based exploration strategy to efficiently identify sequences with strong self-assembly propensity [2]. A neural network trained on experimentally validated peptides and coarse-grained molecular dynamics data achieves an accuracy of 81.9%, enabling the discovery of self-assembling peptides in previously unexplored regions of the sequence space with low similarity to the training set. This framework is readily extendable to therapeutic peptide discovery through a multi-objective optimization that balances antimicrobial activity and toxicity. Beyond improving the exploration of unknown peptide spaces, we employ generative AI to accelerate discovery, supporting continued innovation in the field.

References:

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