



In silico screening of bilayer-lipid-membranepenetrable peptide

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Method

- Actor: "sequence generator" by sampling GRU-RNN training with positive data
- Critic: "sequence classifier" of antimicrobial or not antimicrobial training with both positive and negative data.
- Policy improvement:
 - 1. Predicted antimicrobial sequence will be put to homology modeling and MD simulations for validating (parallelizable)
 - 2. Updating Actor (new-found antimicrobial seq) and Critic network (new-found antimicrobial and non-antimicrobial seq).





Actor-critic RL

Method (GAN)



Method Training GRU-RNN



Probability cut-off 0.999 (GAN)

Amino acid type distribution of the generated peptide



Probability cut-off 0.999 (GAN)



Actor-critic AMP design

- Dataset:
 16648 exp.-validated AMP sequences
 5583 exp.-validated nonAMP sequences
 1000 exp.-validated AMP sequences for performance test.
- Natural amino acid only
- max length 55 residues.

