SUPPLEMENTARY INFORMATION

Molecular Dynamics Based Antimicrobial Activity Descriptors for Synthetic Cationic Peptides
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Figure S1. The SASA and volume over 10 ns simulation shows the system gets stabilized within 10 ns. Only 10 peptides are shown as an example.
Figure S2. The model predicted using the parameters calculated from the last 5 ns of total 10 ns simulation. It shows very poor prediction for the test set.