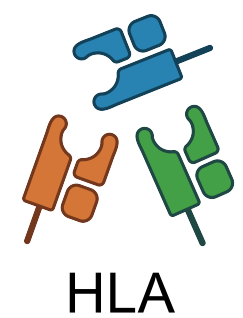
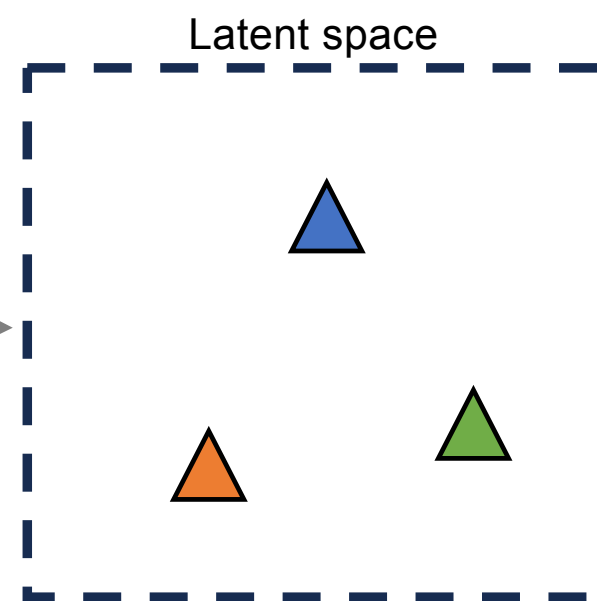
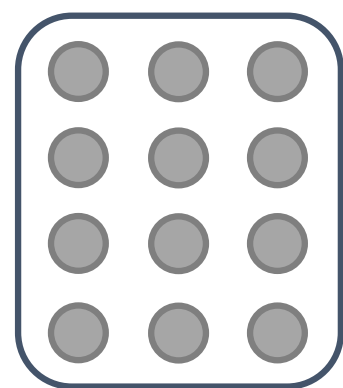


a

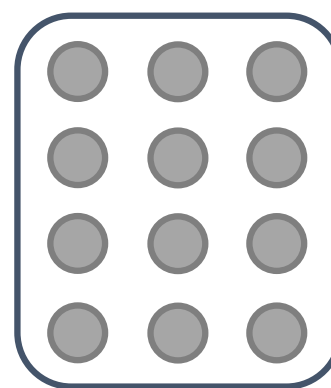
H dataset



BLOSUM50



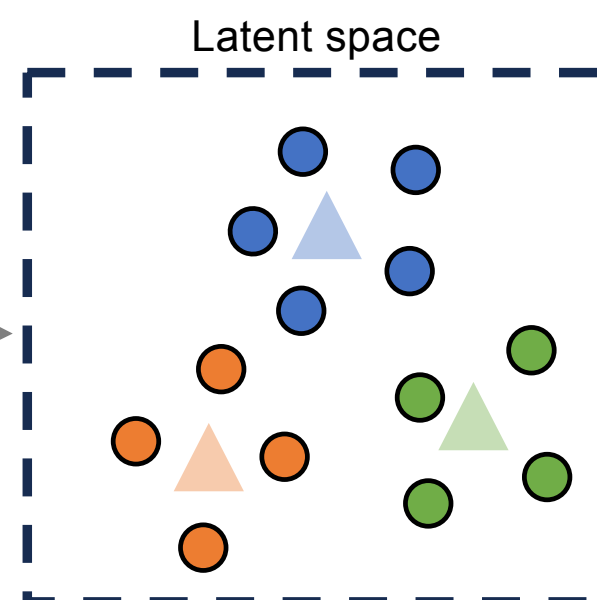
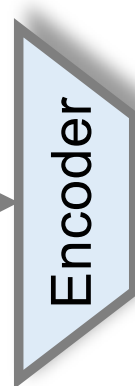
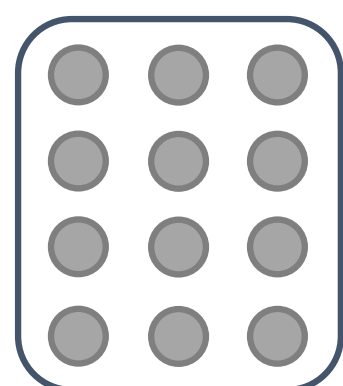
Reconstruction



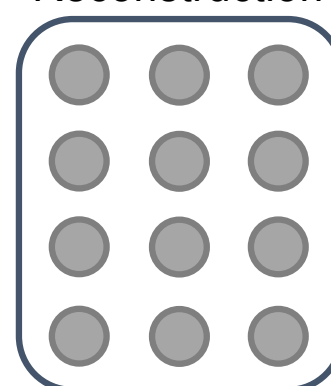
P-H dataset



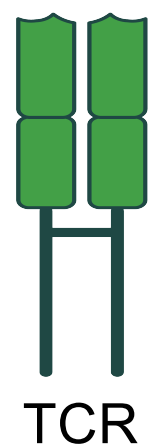
BLOSUM50



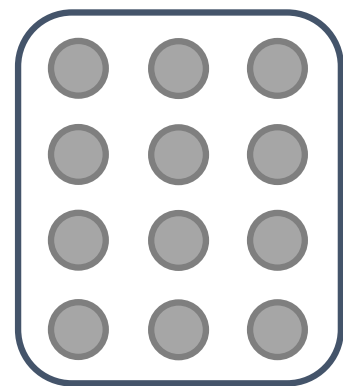
Reconstruction



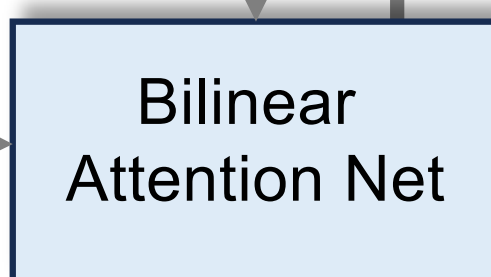
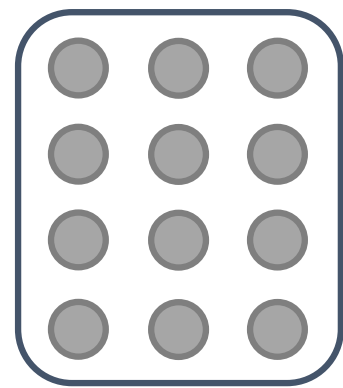
T-P-H dataset



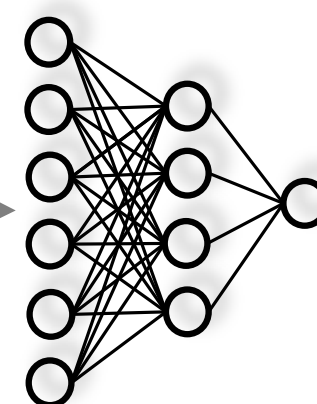
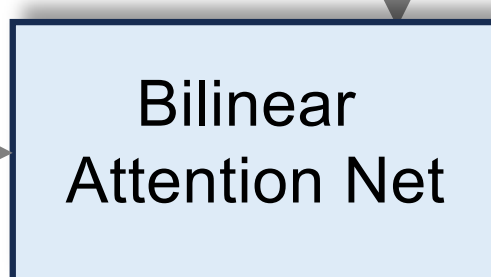
PLM



PLM



concatenate



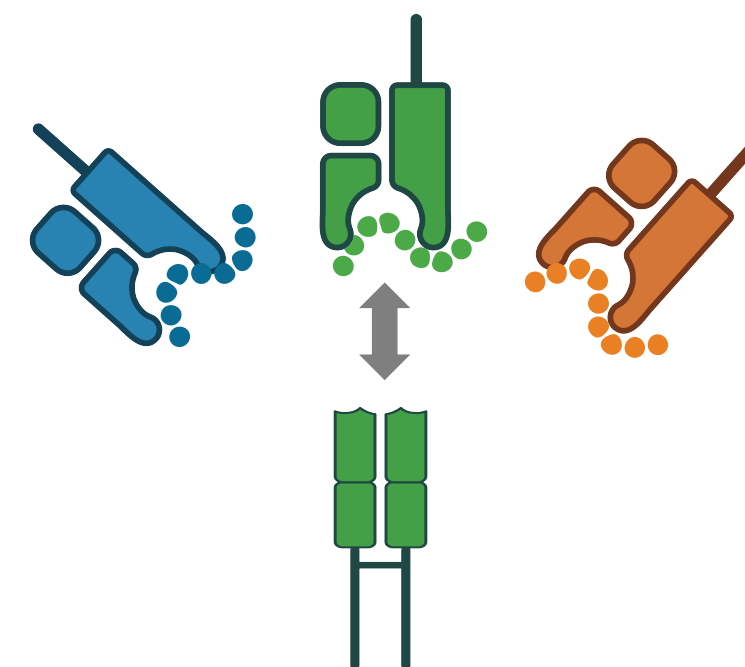
Binding probability



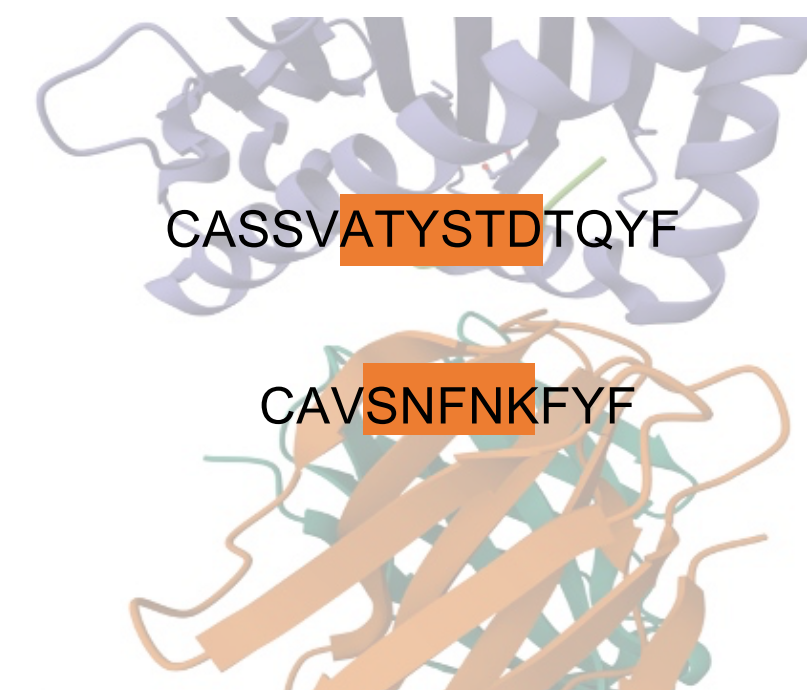
$$\begin{aligned}
 & \begin{bmatrix} \mathbf{E}^T \mathbf{U} \\ 1 \cdot \mathbf{q}^T \end{bmatrix} \cdot \mathbf{V}^T \mathbf{T} = \mathbf{I} \quad \mathbf{U}^T \mathbf{E} \cdot \mathbf{I} \cdot \mathbf{T}^T \mathbf{V} = \text{vector} \\
 & \text{U, V, q: Learnable parameters} \\
 & \text{E: Peptide representation} \\
 & \text{T: TCR representation} \\
 & \text{I: Multi-head Attention}
 \end{aligned}$$

b

- Predict TCR-pHLA interactions



- Identify the most important residues in TCR interactions



- Discover immunogenic peptides via high-throughput screening

