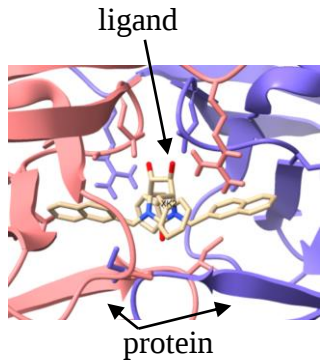
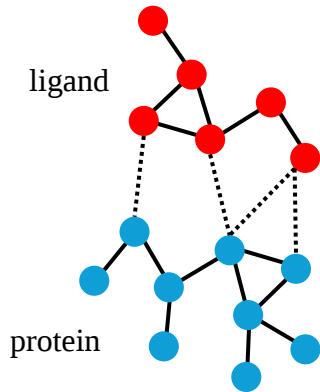




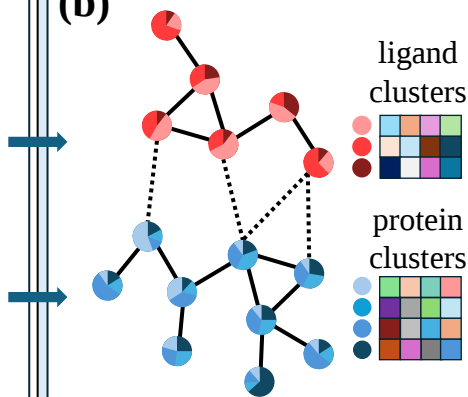
Protein-ligand
complex

(a)



GNN encoder

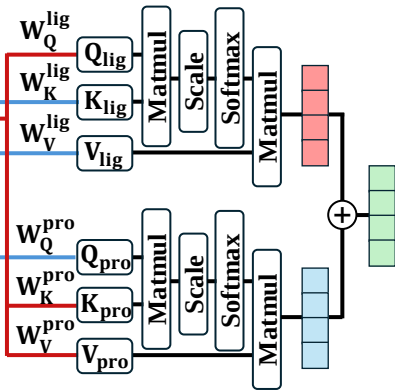
(b)



Functionality-based
Clustering

Cluster-Attention Mechanism

(c)



Cross-attention