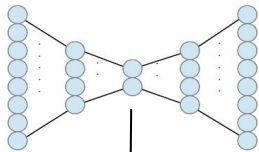
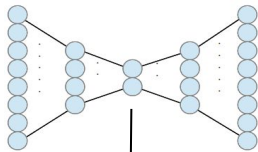


RMSD



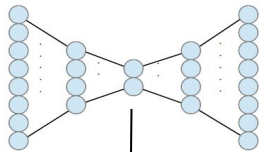
KNN

Chi1



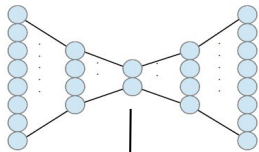
KNN

Chi2



KNN

H-bond



KNN

Compare with ground-truth (labeled data)