Blocking the Binding Interface

Spike Binding Domain

Full Length ACE2

Receptor

Linker

TMD

Intra-cellar (Host)

RBD

Build from Scratch (RCSB:6m17)

Residue distance matrix (RBD)

Residue Num

Residue Num

t=9Å

t=9Å

Predicted score vs. score (lr)   Predicted score vs. score (fcn)   Predicted score vs. score (cnn)   Predicted score vs. score (gcn)

Performance (test set)

conv1   conv2   conv3   dense
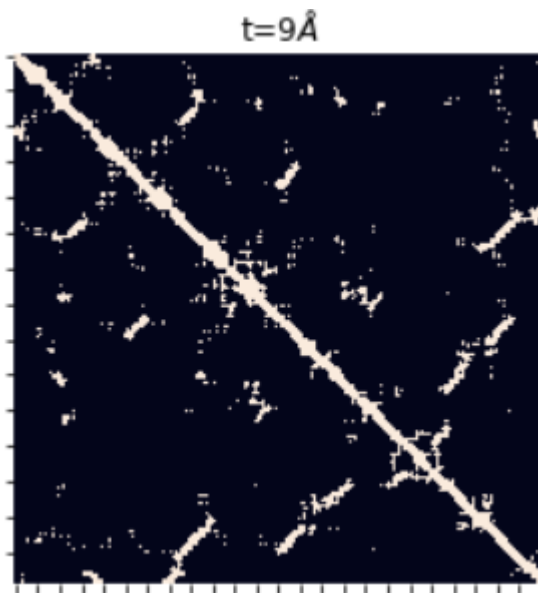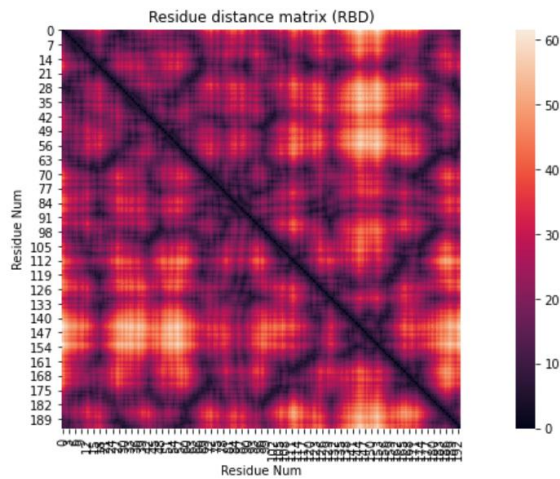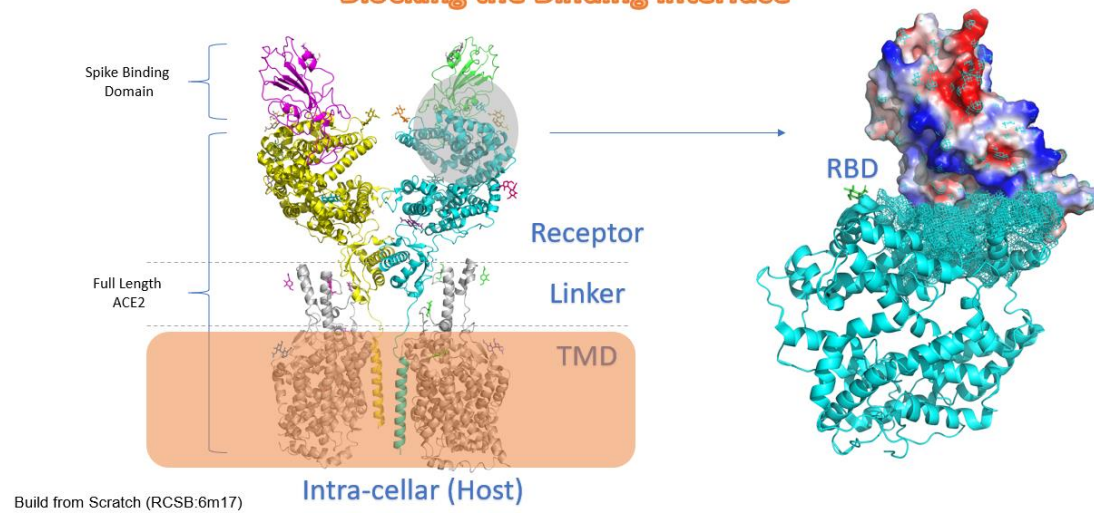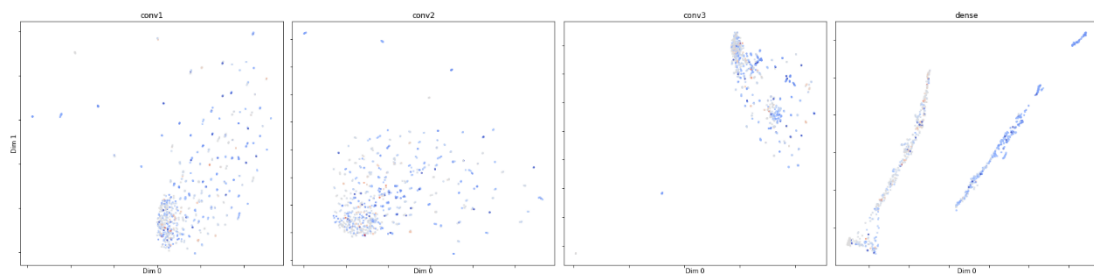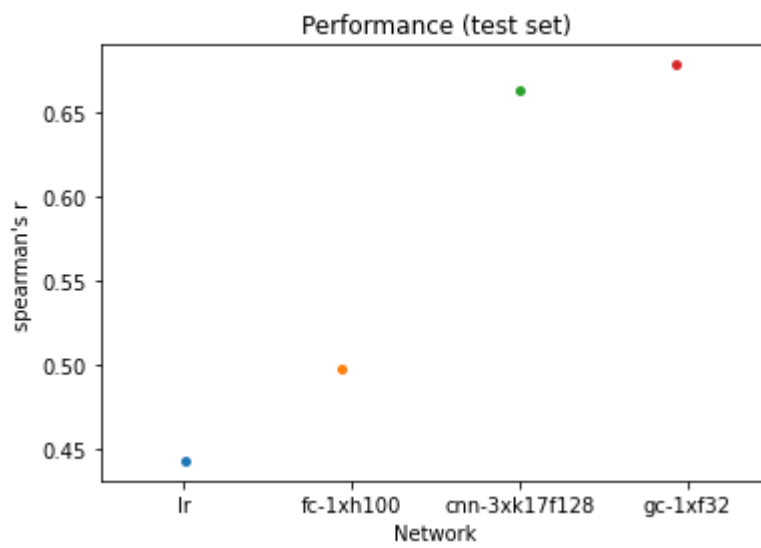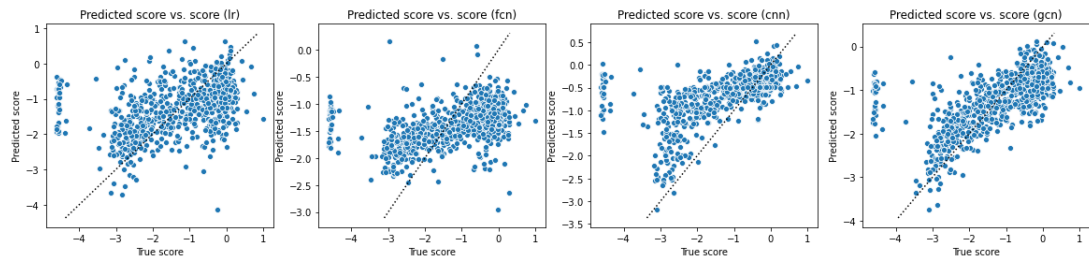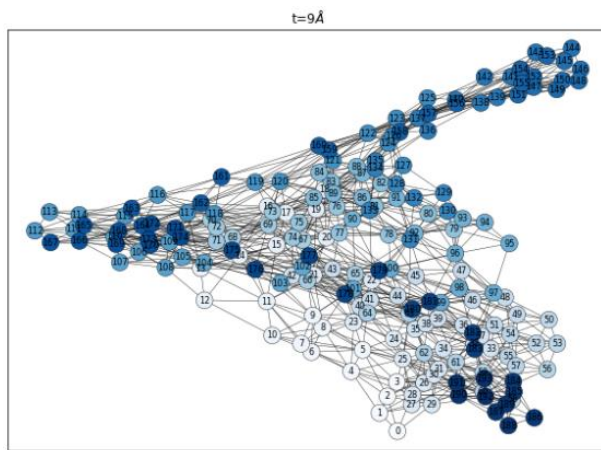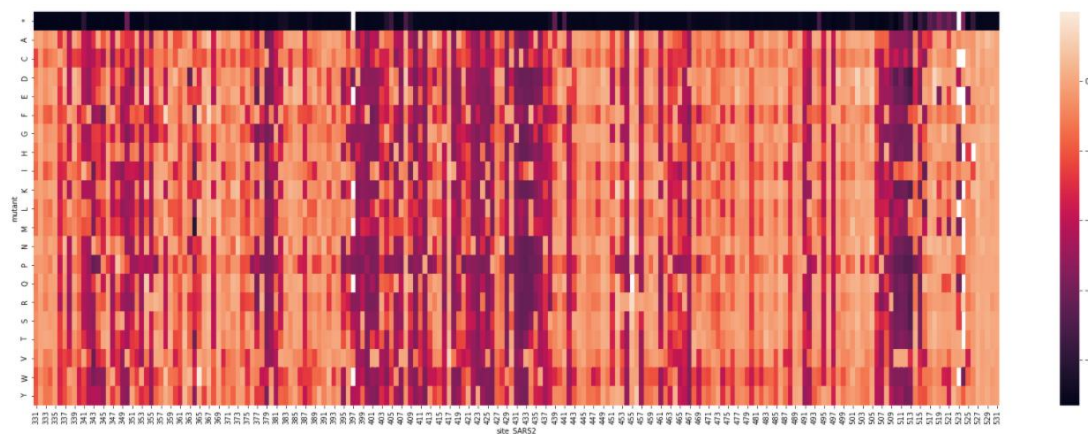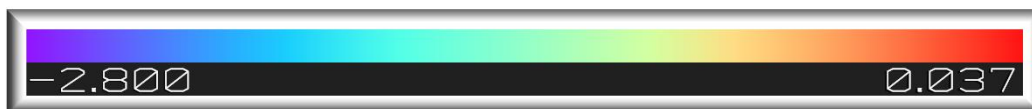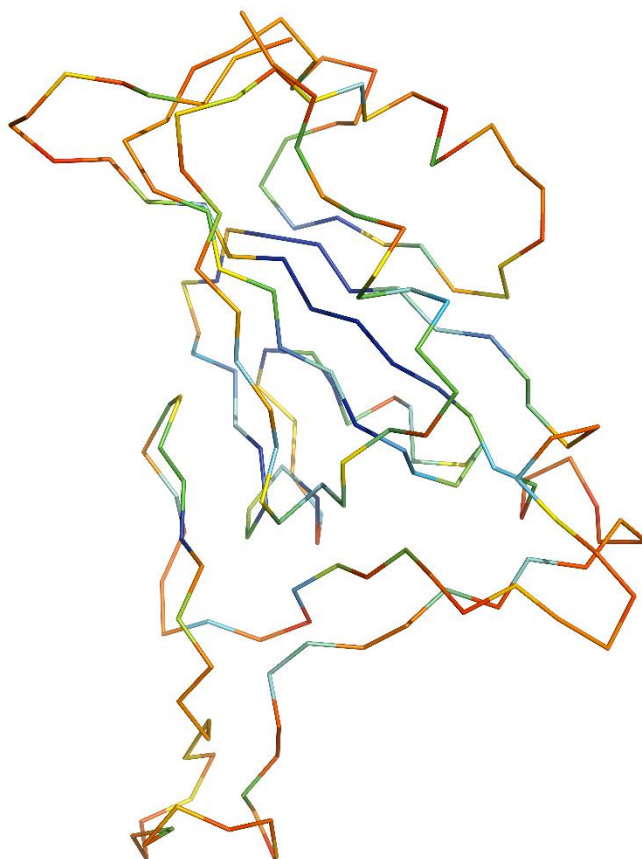
In CNN (Sigmoid (.62)> Relu6 (.59) > LeakyRelu(.578) > SeLu~eLu > tanh(.39))