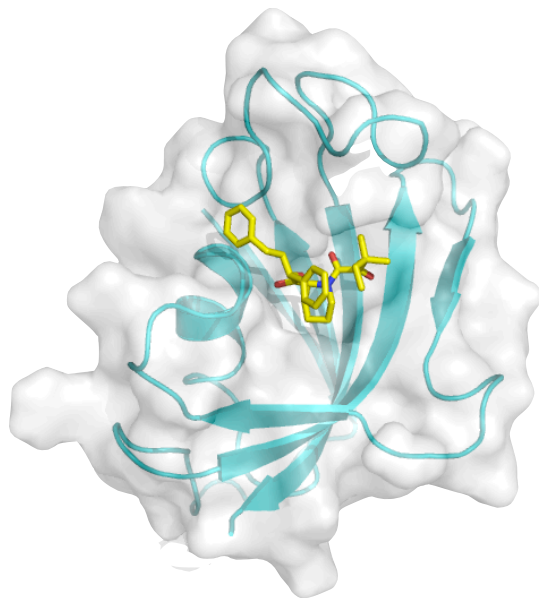


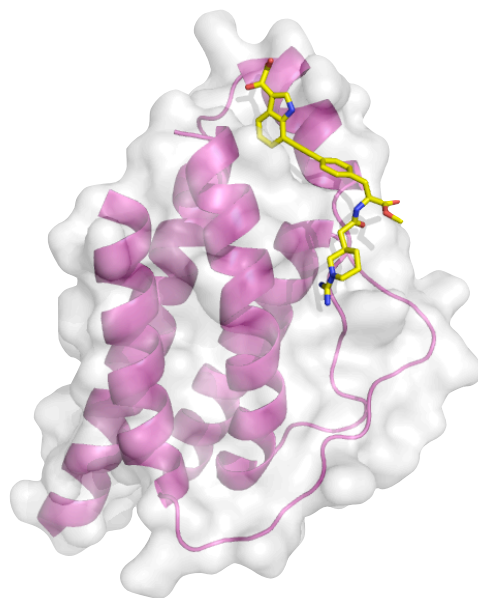
**T4 lysozyme L99A
and L99A/M102Q**

small, rigid protein
small, neutral ligands
fixed protonation states
multiple sidechain orientations
multiple ligand binding modes



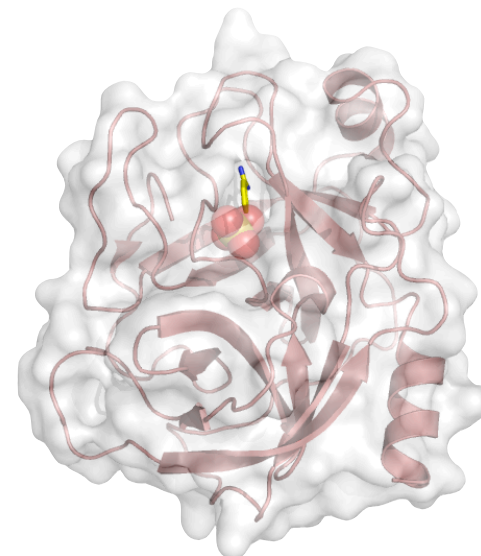
FKBP12

small, rigid protein
fixed protonation states
larger natural product-like
ligands with rotatable bonds



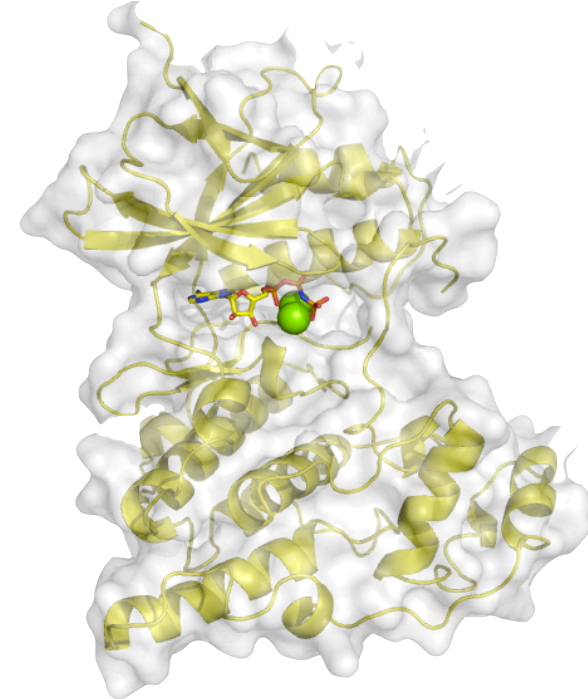
IL-2

small protein
fixed protonation states
some allostery and
binding site plasticity



trypsin

small, rigid protein
small ligands
charged ligands
potential protonation state changes



p38 kinase

large protein, multiple conformations
large drug-like ligands, rotatable bonds
multiple protonation states?
tautomers?
phosphorylation and activation
peptide substrate?
MgCl₂ salt effects?