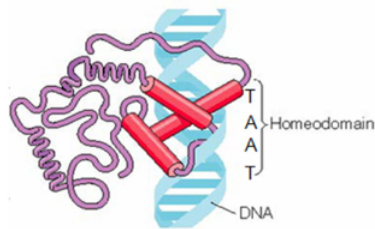
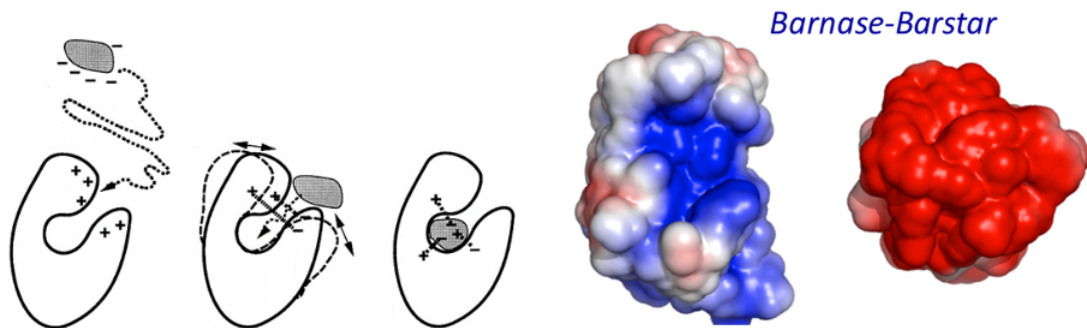


21.7: Forces Guiding Binding

Electrostatics

- Electrostatics play a role at long and short range
 - Long-range nonspecific interactions accelerate diffusive encounter
 - Short range guides specific contacts
- Electrostatic complementarity
- Electrostatic steering
- van der Waals, π - π stacking



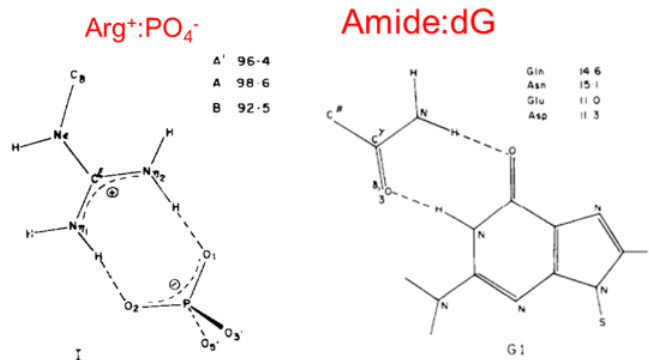
Repressors: Helix-turn-helix
TAAT homeodomain

Shape and Geometry

- Shape complementarity
- Orientational registry
- Folding
- Anchoring residues

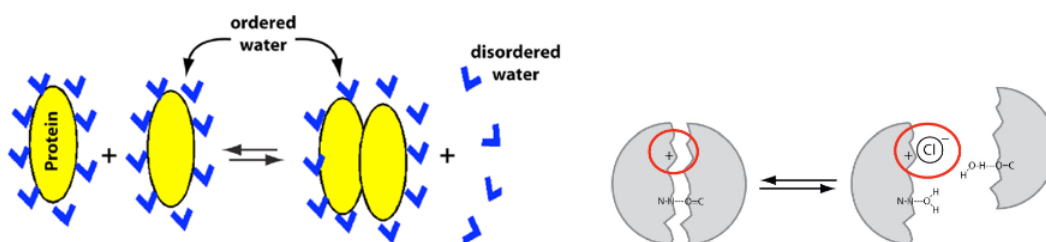
Hydrogen Bonding

- Short range
- Cross over from electrostatic to more charge transfer with strong HBs (like DNA, protein–DNA binding)
- Important in specificity



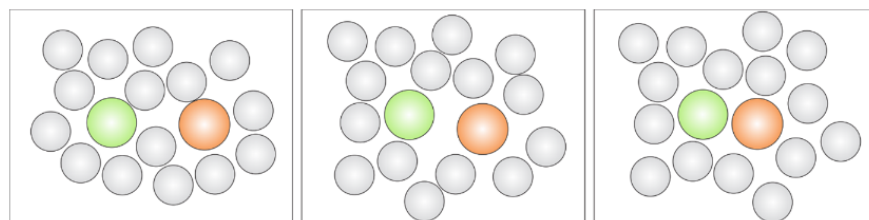
Solvation/Desolvation

- To bind, a ligand needs to desolvate the active site
- Bimolecular contacts will displace water
- Water often intimate binding participant (crystallographic waters)
- Hydrophobic patches
- Charge reconfiguration in electrolyte solutions at binding interface
- Electrostatic forces from water

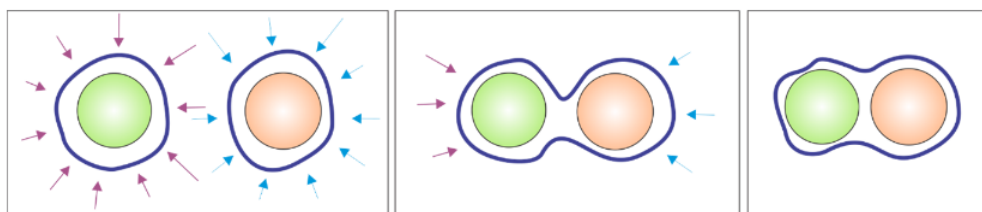


Depletion Forces

- Entropic effect
- Fluctuations that lead to an imbalance of forces that drives particles together
 - Crowding/Caging

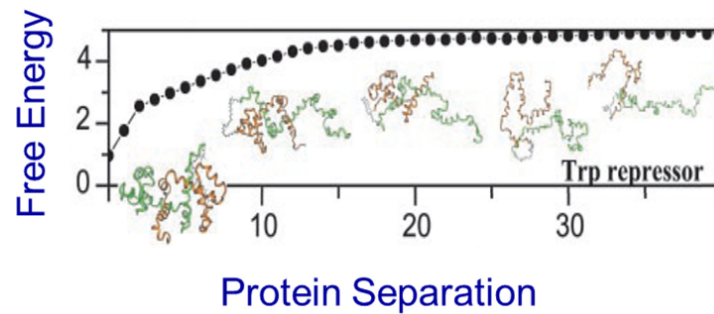


- Hydrophobicity
 - Dewetting and Interfacial Fluctuations



Folding/Conformational Change

- Disorder increases hydrodynamic volume
- Coupled folding and binding
 - Fly-casting mechanism
 - Partially unfolded partners
 - Long-range non-native interaction
 - Gradual decrease in free energy



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