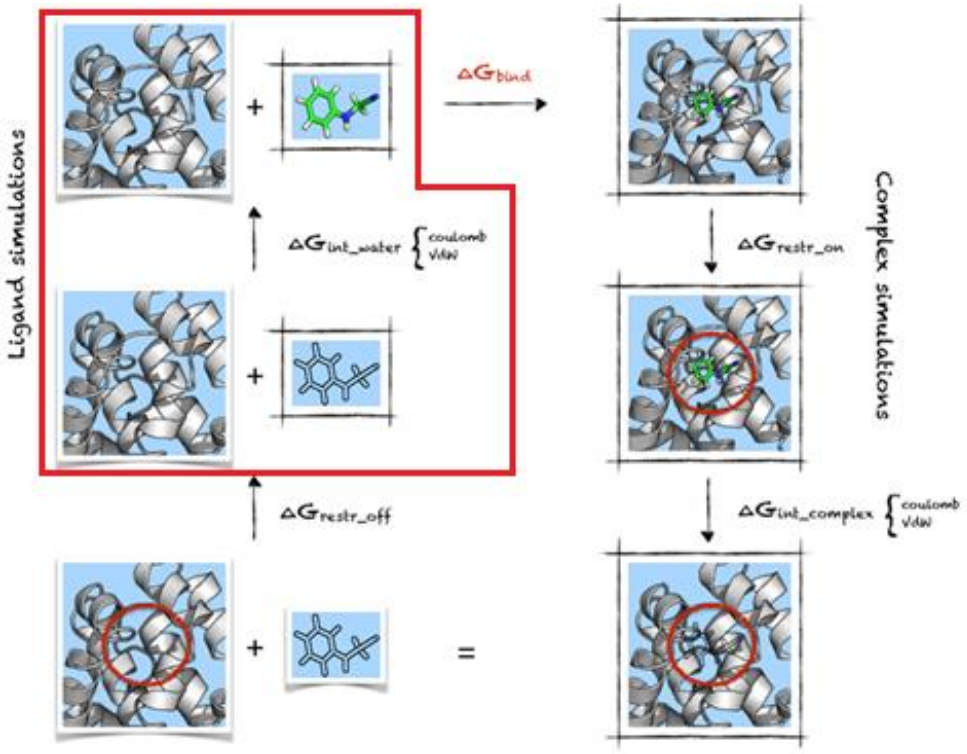
# Measuring Free Energy Change of Solvation of Glucose and Galactose as Part of Glucose/Galactose Binding Protein Thermodynamic Cycle

Phuc Vo, Austin Holmes, and Amil Anderson
Department of Chemistry, Wittenberg University, Springfield OH

D-Glucose / D-Galactose Binding Protein plays an important role in chemotaxis in many bacterial species. It binds with glucose and galactose primarily forming hydrogen bonds with OH groups on these sugars, and these bonds are crucial in determining the binding strength between the protein and its ligand. One method of determining the free energy change of binding for this interaction is through the use of a thermodynamic cycle performed with molecular dynamic simulations. Here, the intermolecular interactions (van der Waals' and Coulombic forces) of the sugar are slowly disabled while it is bound to a protein, and then slowly enabled as the sugar is grown back into a separate box of water. The free energy change of this entire process is then equal to the free energy change of dissociation. This research focuses on the second half of the cycle, where glucose and galactose molecules are grown into their own respective systems. The free energy change of this process, $\Delta G_{int\_water}$ from the diagram, is also effectively the free energy change of solvation of these sugars in water. Molecular dynamics simulations were done with GROMACS version 4.6.5 using the GROMOS43a1 force field. So far, the free energy change of solvation of glucose and galactose are calculated to be -76.03 +/- 0.29 kJ/mol and - 82.54 +/- 0.12 kJ/mol, respectively.




**A sample thermodynamic cycle for T4 lysozyme and n-phenylglycinonitrile**

Adapted from: Aldeghi, Matteo. "GROMACS 4.6 example: n-phenylglycinonitrile binding to T4 lysozyme." – AlchemistryWiki. (http://www.alchemistry.org/wiki ,accessed July 9, 2014)