SJSU | DEPARTMENT OF CHEMISTRY

CHEMISTRY Departmental Seminar

Fall 2017
CHEM 285 Schedule
Tuesdays at 4:30-5:45PM
Room Duncan Hall 250

October 10, 2017

Ms. Caroline R. Harmon
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MS Final Oral Seminar

Biophysical approaches for studying desolvation energy in DNA:DNA binding systems

Hydration spheres have unique water behavior compared to the disorder of the bulk water phase. These hydration spheres have been shown to be crucial for structural and conformational stability, yet their effect on binding association has been largely ignored. For a one-to-one binding system, we propose to append the classical Gibbs-free energy equation as follows: $\Delta G^0 = -RT\ln(K_i) - [AB]\Delta G_i^{H_2O}$. Having a stronger grasp on how desolvation energy affects binding will ultimately aid studies from drug development and metabolism, to interpretation of structural models. To test our equation, we studied two small oligonucleotides that follow Watson-Crick base pairing using two techniques. (1) Isothermal Titration Calorimetry (ITC); a well-established binding method that measures the heat from direct binding interactions as one reactant is titrated into the system, and (2) MicroScale Thermophoresis (MST); a new method that directly measures the movement of a fluorescently-labeled molecule as heat is applied. In each case, as the concentration of bound DNA increased, we found the binding affinity weakened linearly in terms of the quantity –RTln(K), with $R^2 > 0.90$ and $R^2 > 0.80$ for ITC and MST, respectively. Thus the desolvation energy had an unfavorable impact on DNA:DNA binding and, interestingly, this energy is orders of magnitude larger than that of our published model system, chelation of calcium(II) by EDTA. The larger energy value for DNA:DNA binding is not too surprising given (a) the much larger surface area of the DNA binding interface relative to EDTA and calcium, and (b) recent reports of a water spine in the minor groove of the DNA double helix.

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