Andrew Torda
Björn Hansen

Zentrum für Bioinformatik
Übung zur Vorlesung
Grundlagen der Strukturanalyse
Wintersemester 2011/2012

Universität Hamburg

24.01.2012

Übung 7: Revision 2

Dies ist die zweite von drei Übungen, welche Ihnen die Prüfungsvorbereitung erleichtern soll. Auf den folgenden Seiten finden Sie typische Fragen, wie sie in einer Klausur gestellt werden könnten. Dies ist aber kein Fragenkatalog, sondern nur eine kleine Sammlung möglicher Prüfungsfragen. Die Prüfungsfragen der Klausur werden auf Deutsch gestellt.

Um diese Übungseinheit möglichst interaktiv zu gestalten, wird darum gebeten, die folgenden Fragen bereits vor dem 24. Januar gründlich zu studieren. Die Antworten werden dann gemeinsam diskutiert.

Fragenblock 5 (Protein Stability):

- As a chemist, you would expect ΔG to refer to some reaction.
  What is the relevant reaction in protein folding?
- I define ΔH as the enthalpy change upon a protein folding.
  Name and explain two different energetic terms which would contribute to this.
- In the reaction above, I imagine there is something called the “unfolded state”.
  Why is this a simplification?
- I can measure the stability of a protein. I change the pH of the system and the protein becomes more stable.
  Give one example of contributions to the ΔG which could explain this.

- I have a small molecule which causes a protein to unfold. According to all evidence, the small molecule does not interact with the native protein. How could the small molecule be causing a change in stability?
- If I say ΔG is for the reaction A→ B is 10 kJ mol^{-1}, do I have more A or B at equilibrium?
- Forget entropy. What would be the balance of energies which make a protein stable?

Fragenblock 6 (Harmonic Oscillators):

- Given the coordinate of a particle in a harmonic oscillator is $x(t) = A\cos(\omega t + \delta)$ and given that kinetic energy is ½ mv^2, write an expression for the kinetic energy of a harmonic oscillator. Is the energy constant? If not, is energy still conserved?
- I consider the motions within a protein, treating them as harmonic oscillators.
  I claim that most particles in a protein have similar kinetic energy. Consider the expression for kinetic energy. The relationship of kinetic energy, frequency and amplitude is given by

  $$E_{kin} = \frac{1}{2}mv^2 = \frac{1}{2}mA^2\omega^2 \sin^2(\omega t + \delta)$$

  Is the kinetic energy really a constant with time?
  Are the larger amplitude motions associated with the low or high frequencies? Explain.
- In a harmonic oscillator, the force depends on the coordinates x as in

  $$m\frac{d^2x}{dt^2} = -kx \, .$$

  Show that $x(t) = A\cos(\omega t + \delta)$ is a valid solution.
- If I have a two-state system, what does the frequency of the motions mean?
- Why does the frequency of motions increase with increasing temperature in a two-state model?
- Why does the frequency of the motions not increase in a harmonic oscillator model?
- A crystallographer does not usually speak about harmonic oscillators. They normally use a wave equation, $y(x) = F\cos\left(\frac{2\pi}{\lambda}x + \alpha\right)$. How does this correspond to the harmonic oscillator equation $x(t) = A\cos(\omega t + \delta)$? What are the meanings of $\boldsymbol{\alpha}$ and λ?