Andrew Torda
Björn Hansen

Zentrum für Bioinformatik
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Übung 5: Revision 1

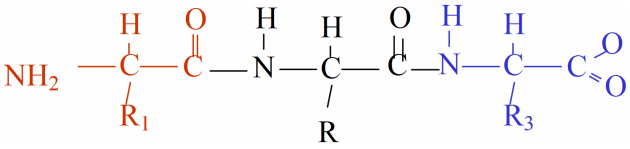
Dies ist die erste von drei Übungen, welche Ihnen die Prüfungsvorbereitung erleichtern soll. Auf den folgenden Seiten finden Sie typische Fragen, wie sie in einer Klausur gestellt werden könnten. Dies ist aber kein Fragenkatalog, sondern nur eine kleine Sammlung möglicher Prüfungsfragen. Die Prüfungsfragen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

Diese Übungseinheit gilt als bestanden, wenn Sie entweder

a) am 20. Dezember 2011 für mindestens 2 Aufgaben die korrekte Lösung vorstellen oder
b) mindestens 50% der Aufgaben richtig beantworten und diese spätestens am 16. Januar 2012 an **hansen@zbh.uni-hamburg.de** schicken.

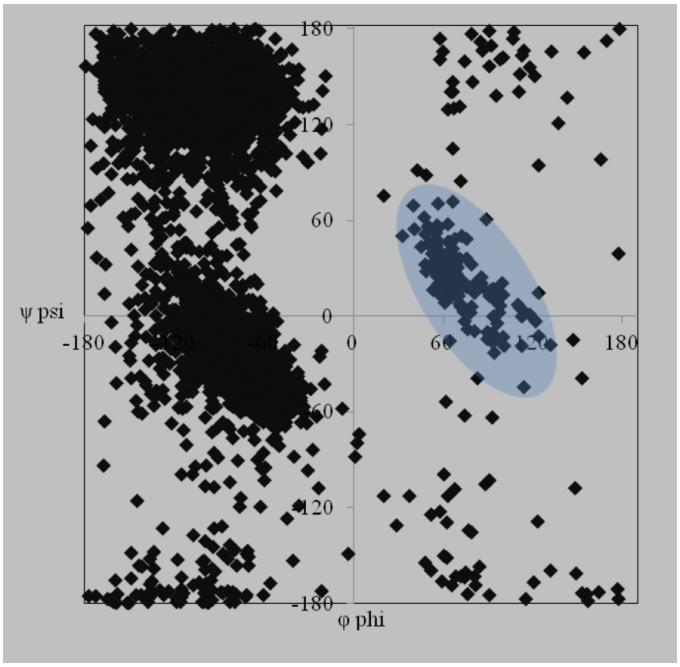
Fragenblock 1 (Protein Structure):

- What order of magnitude is a chemical bond (in Å)?
- On the diagram, mark the two backbone angles which can rotate in a normal protein. You only need do this for one residue.



- Mark the angle which is nearly planar (flat).
- Why can I not have a short α-helix which is only 2 residues long?
- Name a large hydrophobic amino acid, a small amino acid and a polar (but uncharged) amino acid.
- Name the amino acid which often forms covalent bonds from its side-chain.

- If you consider a Ramachandran plot for a protein, there is a region where only one amino acid is found, marked on the diagram by the grey oval.
  Which amino acid is this? Why can it occupy this area?



- Why can proline not be part of a perfect α-helix?

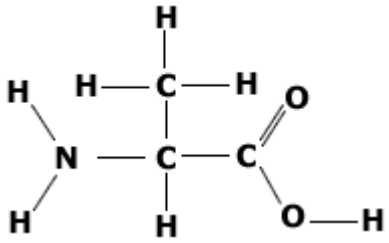
Fragenblock 2 (Crystallography):

- A crystallographer has a model for uncertainty in atomic coordinates.
  How is this uncertainty represented?
- The R-factor used by protein crystallographers is given by $R = 100 \frac{\sum_{hkl} \left| |F_{obs}| - |F_{calc}| \right|}{\sum_{hkl} |F_{obs}|}$

  What is the purpose of the equation / when does a crystallographer use it?
- What is the difference between *R* and R_{free}?
- Write a wave equation in any format you like. Explain each term.
- Given $F_{hkl} = \sum_{j=1}^{n} e^{2\pi i (hx_j + ky_j + lz_j)}$, explain what F_{hkl} is. What are *x*, *y* and *z*?
- Given $\rho_{x,y,z} = V^{-1} \sum_h \sum_k \sum_l F_{h,k,l} e^{-2\pi i (hx+ky+lz)}$, explain what each of the terms are.
- Explain why you cannot simply Fourier transform to recover $\rho_{x,y,z}$.
- In MIR (heavy atom phasing), you have recorded data of protein alone and protein with heavy atoms.
  What is the first step to using this for phasing?

Fragenblock 3 (NMR):

- How is uncertainty in protein coordinates from NMR represented?
- Name three elements, with the correct nuclei, which are relevant to biochemistry and NMR.
- In an NMR spectrum, the hydrogen in the hydroxyl group is not normally seen. Why?
- In the structure of alanine, which protons would be *J* (spin/spin) coupled to another?



- When calculating a protein structure based on NMR data, what information does one get from the size of a *J* (spin-spin) coupling constant?
- Why are only some values of the coupling constant useful?
- Which experimental phenomenon provides most of the structural information for determining a structure by NMR?
- What structural information may be provided by ^{3}J coupling measurements? Which atoms are involved?

Fragenblock 4 (Distance Geometry):

- Draw three atoms with distances between them, which are not possible in 3-dimensional space.
- Aside from experimental distance information, what information does one add to a metric matrix distance geometry calculation, before applying the triangle inequality (bound smoothing).
- Why is the triangle inequality applied twice during a metric matrix distance geometry calculation?
- In the metric matrix distance geometry method, one generates a trial matrix. Imagine you have no experimental errors. All your distance measurements are correct to 10^{-20} m. Would you expect the trial matrix to correspond to a set of 3-dimensional coordinates?
- What is the running time of the bound smoothing step in this kind of distance geometry?
- You use the metric matrix method to calculate the structure of a protein, but you do not have any experimental data.
  What would you expect if you generate 20 structures?
- In a distance geometry calculation, I have a set of atoms *i-j-k-l-m-n*. What stops atoms *i* and *n* ending on top of each other? If I know nothing about the angles in the structure, what is the minimum distance d_{ik}?
- Draw a graph that corresponds to this distance matrix.

	A	B	C	D	E
A	0		4		
B		0	2	5	3
C			0	2	1
D				0	
E					0

  What is the maximum distance between points D and E?

- Name an advantage of the variable target function method, compared to the metric matrix method for distance geometry.
- The metric matrix method has $O(n^3)$ running time. Explain in one sentence.
- What is the running time of the variable target function method?