



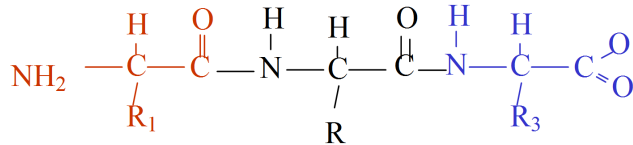
Übung 5: Revision 1

Dies ist die erste von zwei Übungen, welche Ihnen die Prüfungsvorbereitung erleichtern sollen. 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. Im Gegensatz zu dieser Übung werden die Prüfungsfragen der Klausur auf Deutsch gestellt.

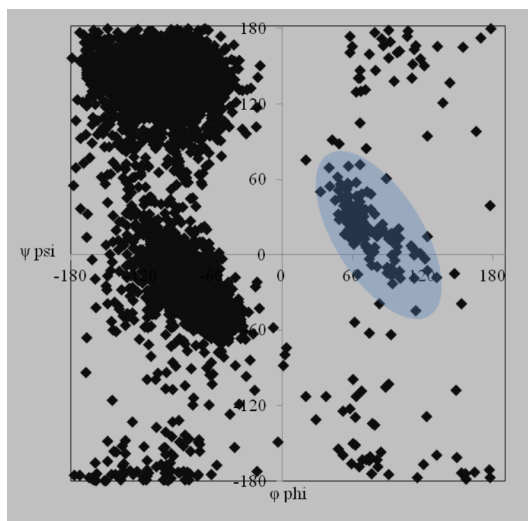
Bitte beantworten Sie mit Hilfe Ihrer Übungs- und Vorlesungsunterlagen alle gestellten Fragen und bringen Sie Ihre Antworten für die gemeinsame Besprechung in der Übung am **28.11.2015** mit. Welche Studenten ihre Antworten zu den einzelnen Übungsfragen vorstellen, wird zufällig bestimmt.

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 type of 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?
- For length N , do all / many / few of the 20^N sequences form specific structures?
- You synthesized a 100 amino acid long protein consisting entirely of aspartate: $(\text{Asp})_{100}$
What are its properties? Is it soluble? Is it acidic? Is it basic?
Would it form a compact regular structure?
- If you have a protein of poly-Trp (polytryptophan), would it form a specific structure?
How would it behave in solution?
- Why would you want to represent a protein by its surface?
- Why might you draw a protein as a ribbon representation in *Chimera*?
- What is the biggest chain in the protein data bank?
What is the average size of a protein?

Fragenblock 2 (Crystallography):

- Why are some atoms essentially invisible in the X-ray diffraction? Which atoms?
- A crystallographer has a model for uncertainty in atomic coordinates.
How is this uncertainty represented?
- A crystal structure represents a space and time average. Explain!
- If a crystallographer wants to crystallize a protein, there are several problems he might face. Name one of them!
- What is the requirement for constructive interference?

- The R-factor used by protein crystallographers is given by
$$R = \frac{\sum_{hkl} |F_{hkl}^{obs} - F_{hkl}^{calc}|}{\sum_{hkl} |F_{hkl}^{obs}|}$$

What is the purpose of the equation / when does a crystallographer use it?

Hypothetically: What is the R-factor for a perfect model?

- 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 $\rho_{x,y,z} = \sum_{hkl} |F_{h,k,l}| e^{-2\pi i(hx + ky + lz)}$, explain what each of the terms are.
- What is the purpose of multiple isomorphous replacement?
- Explain why you cannot simply Fourier transform to recover $\rho_{x,y,z}$.

Fragenblock 3 (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 single set of 3-dimensional coordinates?
- What is the running time of the bound smoothing step in the metric matrix method? Explain in one sentence.
- 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?
- 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

Add the missing values to the distance matrix and the corresponding edges to your graph. Is there some value in the distance matrix that can be improved?

What is the shortest path between points D and E?

- Name an advantage of the variable target function method, compared to the metric matrix method for distance geometry.
- What is the running time of the variable target function method?

Fragenblock 4 (NMR):

- How is uncertainty in protein coordinates from NMR represented?
- Name three elements, with the correct nuclei, which are relevant to biochemistry and NMR.
- When calculating a protein structure based on NMR data, what information does one get from the size of a J (spin-spin) coupling constant?
Which atoms are involved?
- 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?