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DER FORSCHUNG | DER LEHRE | DER BILDUNG

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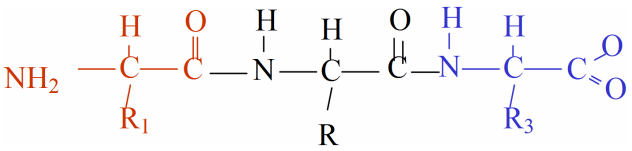
Übung 5: Revision 1

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.

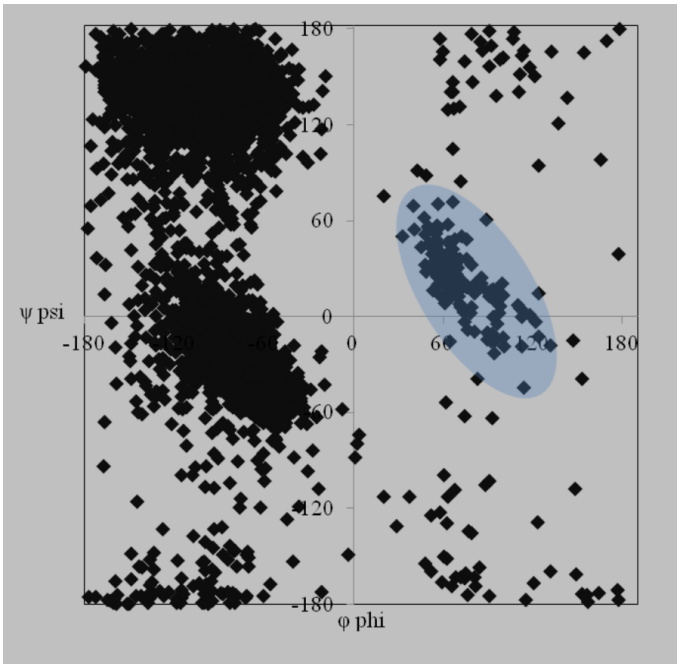
Bitte beantworten Sie mit Hilfe Ihrer Übungs- und Vorlesungsunterlagen alle gestellten Fragen und bringen Sie Ihre Antworten für die gemeinsame Besprechung in der Übung am **18.12.2012** (Raum 16) mit. Welche Studenten die einzelnen Übungsaufgaben vorstellen, wird zufällig festgelegt werden.

Fragenblock 1 (Protein Structure): (8 P)

- 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?

Fragenblock 2 (Distance Geometry): (11 P)

- 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? 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.

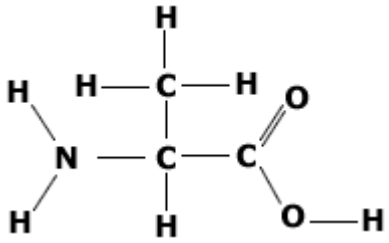
	A	B	C	D	E
A	0		4		
B		0	2	5	3
C			0	2	1
D				0	
E					0

  What is the 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 3 (NMR): (8 P)

- 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 a 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?
  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?

Fragenblock 4 (Modelling): (3 P)

- You have built an initial structural model for a sequence. You have a very simple model for the energy of the system. Describe a method to find a reasonable arrangement of side-chains.
- You want to use distance geometry to generate possible conformations of a loop in a protein. You have endpoints for the loops. Describe how you would cast this into a problem suitable for the metric matrix method.