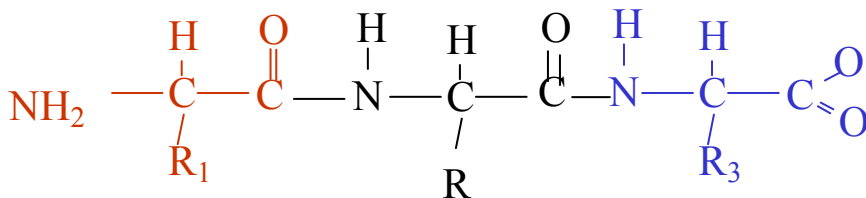


Revision Übung GST

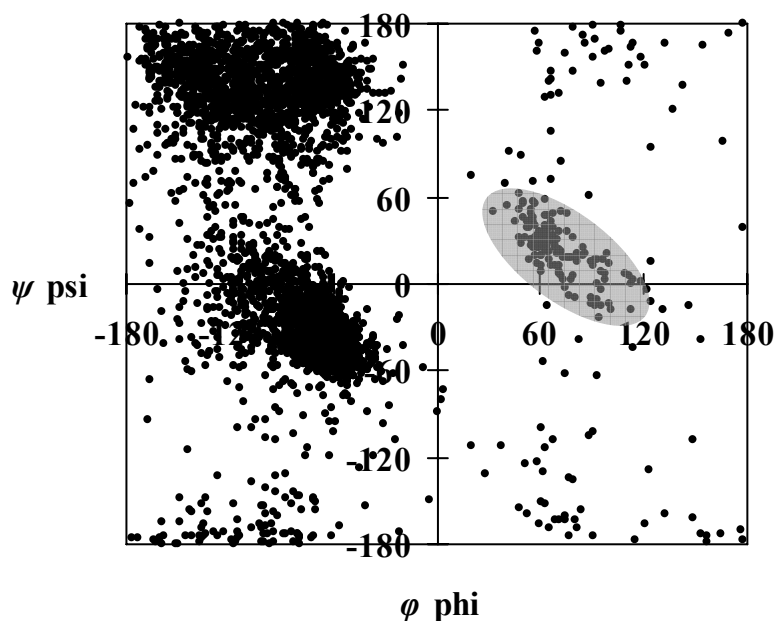
For 8 Dec 2008

- Could you be ready to answer questions 1-20 ?
 - We probably use the time from 10:15 for the questions and from 12:15 for Manfred Weiss' Vorlesung.
1. What order of magnitude is a chemical bond (in Å) ?
 2. On the diagram, mark the two backbone angles which can rotate in a normal protein. You only need do this for one residue.
 3. Mark the angle which is nearly planar (flat).



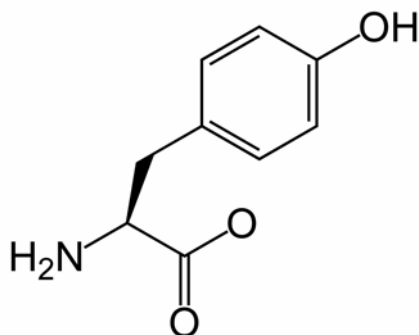
4. Why can I not have a short α -helix which is only 2 residues long ?
5. Name a small amino acid.
6. Name a large hydrophobic amino acid.
7. Name the amino acid which often forms covalent bonds from its side-chain.

8. 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.



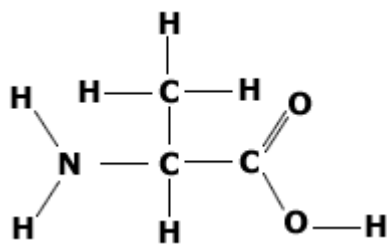
Which amino acid is this ? Why can it occupy this area ?

9. Why can proline not be part of a perfect α -helix ?
10. Name three elements, with the correct nuclei, which are relevant to biochemistry and NMR.
11. In an NMR spectrum, the hydrogen in the hydroxyl group is not normally seen.



Why ?

12. In the structure of alanine, which protons would be J (spin/spin) coupled to another ?



13. When calculating a protein structure based on NMR data, what information does one get from the size of a J (spin-spin) coupling constant ?
14. Why are only some values of the coupling constant useful ?

15. You use the metric matrix method to calculate the structure of a protein, but you do not have any experimental data.
- a. What would you expect if you generate 20 structures ?
16. 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} ?
17. 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 ?

18. What is an advantage of the variable target function method compared to the metric matrix method of distance geometry ?
19. The metric matrix method has $O(n^3)$ running time. Explain in one sentence.
20. What is the running time of the variable target function method ?
21. Given the coordinate of a particle in a harmonic oscillator is $x(t) = A \cos(\omega t + \delta)$ and given that kinetic energy is $\frac{1}{2} m v^2$, write an expression for the kinetic energy of a harmonic oscillator. Is the energy constant ? If not, is energy still conserved ?
22. 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. Are larger motions a
The relationship of kinetic energy, frequency and amplitude is given by $E_{kin} = \frac{1}{2} m v^2 = \frac{1}{2} m A^2 \omega^2 \sin^2(\omega t + \delta)$
Are the larger amplitude motions associated with the low or high frequencies ?
Explain.
23. In a harmonic oscillator, the force depends on the coordinates x as in $m \frac{d^2 x}{dt^2} = -kx$
Show that $x(t) = A \cos(\omega t + \delta)$ is a valid solution.