You should be able to solve the following questions right away without the use of any textbook

1. Ligand A has a binding constant of $5 \cdot 10^9$. For ligand B an exptl. energy of $-51.7$ kJ/mol at 298K was measured upon binding. Which ligand shows a higher affinity? (calculator required)

2. Mark the polar hydrogen atoms in this molecule:

![Molecule Diagram]

3. Assign the protonation state of arginine at pH 7.

4. Assign the protonation state of cysteine at pH 10.

5. The one letter code for lysine is …

6. The one letter code E denotes the amino acid …

7. The amino acids that contain an aromatic ring as part of their side chain are …

8. Which is the largest amino acid?

9. Which is the smallest amino acid?

10. Which amino acid is a typical structure breaker of α-helices?

11. What is the (structural) difference between a loop and a turn?

12. The Cartesian coordinates of atoms in .pdb files are separated by a single space _, separated by a single tab stop _, in a fixed format _

13. Which of the following alignments is more reasonable?

   target VSNVIASLTGRRFEYDDPRWRLDLLAQEGLKEESGFLREVLANPVLHIPA
   align1 ISNVLASISCAR-YDYEDPWRV-ELGQDGKDDGFLRDG-NAPIPG-LHVPG
   align2 VTQVLGSLSCGDGFY-GPLYR-DLANEGLG--RSGFLREVQLGIPEGLKIPG
14. What is the difference between the PAM250 and the BLOSUM62 matrix?

15. Order the following solvents according to their dielectric constant: benzene, water, DMSO, ethanol.

16. How many chiral atoms/stereo centers are in the following molecule? How many stereoisomers are possible?

\[ \text{H}_2\text{C} \quad \text{C} \quad \text{C} \quad \text{F} \]
\[ \text{Br} \quad \text{Cl} \]

17. To determine the energy difference between these stereoisomers one can use: force fields, semi-empirical methods, quantum chemical methods.

18. To determine the energy difference of isomers in general one can use: force fields, semi-empirical methods, quantum chemical methods.

19. To determine the heat of formation of a molecules one can use: force fields, semi-empirical methods, quantum chemical methods.

20. Which methods will yield reliable dipole moments: CNDO, AM1, PM3, RHF/6-31G*.

21. Name two optimization algorithms that are useful to local the global minimum.

22. Name the experimental method to determine the following quantities/properties: 
- $^{13}$C chemical shift
- hyperfine coupling constants
- valence orbital energies
- electron densities

23. Why is it more difficult to crystallize membrane proteins than soluble proteins?

24. Order the following organisms according to the size of their genome: fruit fly, yeast, mouse, bacteriophage lambda, Salmonella typhimurium.

25. Which UNIX command joins two files horizontally: cat, dog, cut, paste.