selftest Modern Methods in Drugs Discovery WS06/07
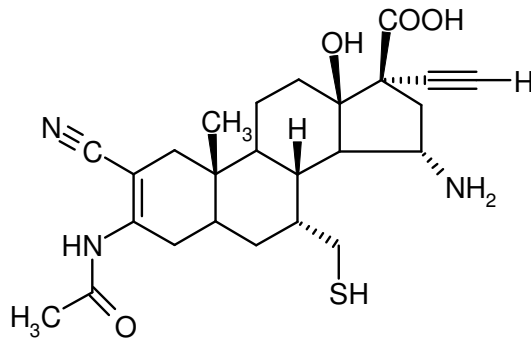
You should be able to solve the following questions right away without the use of any textbook

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 molecules

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
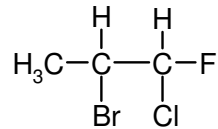separated by a single space _ , separated by a single tab stop _ , in a fixed format _

13. Which of the following alignments is more reasonable ?

```
target VSNVIASLTCGRRFEYDDPRWRLLDLAQEGLKEESGFLREVLNAVPVLLHIPA
align1 ISNVLASISCAR-YDYEDPKWRV-ELGQDGIKDDSGFLRDG-NAIPG-LHVPG
align2 VTQVLGSLSCGDGFEY-GPLYR-DLANEGLG--RSGFLREVLQGIPEGLKIPG
```

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 ?

$$H_3C-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle Br}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle Cl}{|}}{C}}-F$$

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 _