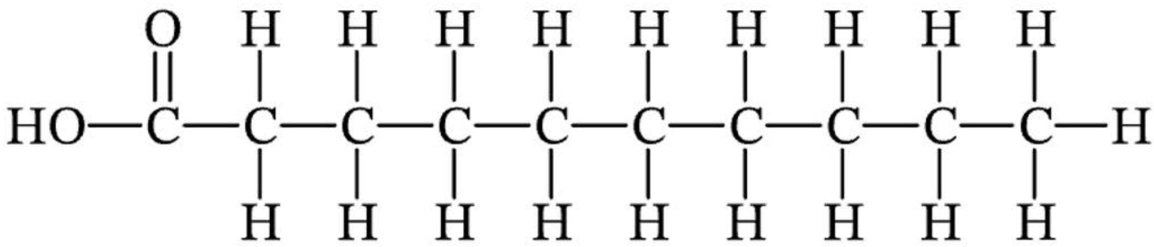
Exercise 1:
Atoms, bonds and non-covalent interactions

Question 1:

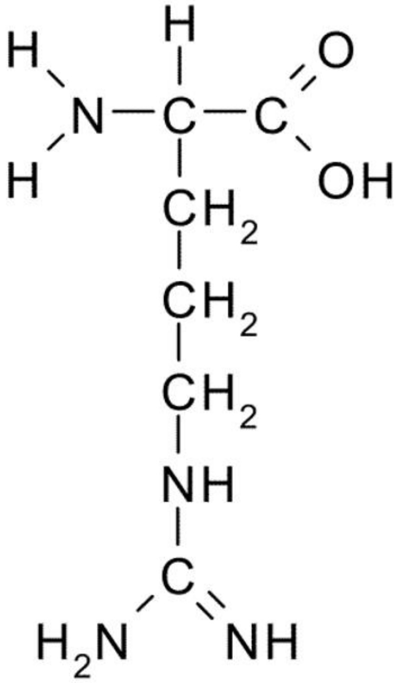
Below are some examples of biomolecule building blocks.

A



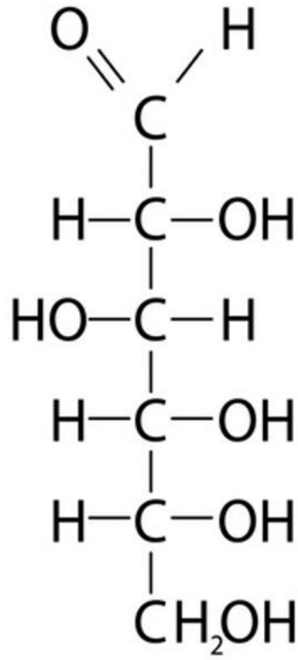
Capric acid

B



Arginine

C



Glucose

a) Can you identify and name different chemical groups in them?

b) Can you differentiate polar vs non-polar bonds?

c) Assuming aqueous solution at pH 7, what groups would be suitable for electrostatic interactions?

d) What about hydrogen bonds?

e) What about vdW interactions?

f) Which of these molecules has the highest capacity to be hydrophobic?

Question 2:

Here we classify bonds in four categories based on their dissociation energy (the change in energy when atoms are moved away from each other).

Strong:	>200 kJ/mol
Medium:	20-200 kJ/mol
Weak:	5-20 kJ/mol
Very weak:	0-5 kJ/mol

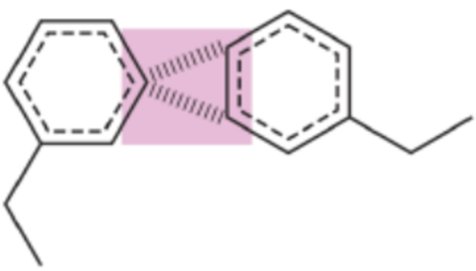
Below four bond types are shown in purple.

(a) Name each bond-type and classify them into the four categories given above (in vacuum).

(b) Consider what happens when these molecules are immersed in water (fully solvated). For each bond, indicate whether the bond becomes weaker, stronger, or stays the same.

(c) Which of these bonds can be broken by just the thermal fluctuations in water with energy of 2.5 kJ/mol?

1



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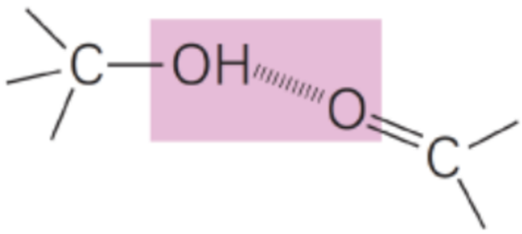

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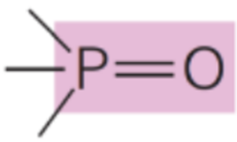
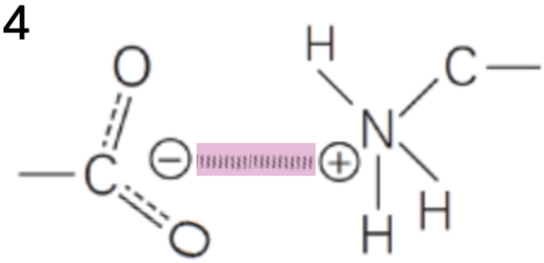


4



Question 3:

For each statements write whether it is true or false and please explain why:

a) When two atoms come close together, the energy increases due to repulsion between their nuclei.

b) Ionic interactions are weaker in nonpolar solvents (such as heptane) as compared to polar solvents (such as water).

c) Free atoms can also participate in vdW interactions since they can be polarized by other atoms or groups.

d) The strength of an N-H•••O=C hydrogen bond is at its maximum when all the atoms are in a straight line.

e) Under standard lab conditions (atmospheric pressure, room temperature), noble gases such as He, Ne, Ar, Kr, Xe can engage other atoms/molecules via vdW forces but not hydrogen bonds or electrostatic interactions.

Question 4:

Imagine two functional groups in a protein that are at 3Å from each other interacting via (a) van der Waals, (b) hydrogen bonds or (c) electrostatic interactions. The conformational change in the protein changes their relative orientation to 5Å. Assume that all environmental conditions are the same and the only change was the distance.

What is the relative change in the interaction energy potential (U) induced by this conformational change in case of (a), (b) and (c)? Which interaction type reduces its potential most rapidly.

Question 5:

Magnesium ions (Mg^{2+}) play a crucial role in stabilizing DNA structure and are essential cofactors for DNA polymerases during replication. Mg^{2+} binds to the phosphate groups of the DNA backbone to neutralize and stabilize the DNA helix. The positively charged Magnesium is surrounded by two negatively charged phosphate backbones. Assume that all charges lie on the same line. Calculate the electrostatic energy potential (U) of the entire system involving these 3 charged groups in the following two conditions:

a) The interaction takes place in water (D=78.5).

b) The interaction takes place in vacuum (D=1).

Assume the permittivity of the vacuum $\epsilon_0 = 8.854 \times 10^{-12}$ $F \cdot m^{-1}$ ($C^2 \cdot J^{-1} \cdot m^{-1}$) and the unit charge is 1.602×10^{-19} C. To determine the energy potential for one mole of ion combinations (i.e., J/mol) you will need the Avogadro's number 6.02×10^{23} mol^{-1}.