FB 08 Informatik
Lehrstuhl f. Software-Technik und Bioinformatik

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BIOINFORMATICS II - SS 16

3. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 15-05-2016

	Exercise	Points
Practical	1	10
Practical	2	10
Theoretical	3	10
Theoretical	4	10

Exercise 1: Rotation – `Ball` (10 Points)
In many PDB, there are many different models for the same protein. Download the PDB file (`http://tinyurl.com/cjjf9w`) and extract the first model. Rotate the position of all the atoms around the axis x of an angle $\frac{\pi}{3}$ and save the obtained protein in a PDB file.

Exercise 2: Creation of a molecule – `Ball` (10 Points)
Create a molecule of ammonia. For the sake of this exercise, assume that ammonia (NH_3) is a planar molecule. Generate the bond lengths correctly, and assume that the angle between the bonds is $\frac{2\pi}{3}$. Save the molecule in a PDB file. You may want to revise how to use polar coordinates, and consult: `http://tinyurl.com/znpf453`

Exercise 3: The ∇ operator (10 Points)
Consider the following vector $\mathbf{F}$ and scalar V:

$$\mathbf{F} = [3x + y]\mathbf{i} + [z + 3x]\mathbf{j} + [x + y + z]\mathbf{k}$$

$$V = \frac{1}{(x^2 + y^2 + z^2)^3} - \frac{1}{(x^2 + y^2 + z^2)^3}$$

Calculate (if it is possible!) $\nabla \cdot \mathbf{F}$, $\nabla \times \mathbf{F}$, $\nabla \times V$, $\nabla \cdot V$, ∇V.

Exercise 4: Calculation of a potential (10 Points)
Remembering the definition of potential as:

$$\mathbf{F} = -\nabla V,$$

determine a potential V that corresponds to the force:

$$\mathbf{F} = [6x - y\sin(xy)]\mathbf{i} + [z - x\sin(xy)]\mathbf{j} + \left[y + \frac{1}{1 + z^2}\right]\mathbf{k}$$