FB 08 Informatik
Lehrstuhl f. Software-Technik und Bioinformatik

Prof. Dr. Andreas Hildebrandt
Dr. Marco Carnini

BIOINFORMATICS II - SS 16

10. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 10-07-2016

	Exercise	Points
Theoretical	1	10
Practical	2	10

Exercise 1: Protein docking (10 Points)
Assume that you know that your protein should look like a long string of 6 repeated monomers interleaved with another string of the same 6 monomers. You experimentally know the structure of the monomer. Assume that the command `ROSETTA` generate a candidate for the docking, once two input PDB files are provided (the structures to be docked). Describe with pseudo code what will be your approach to build a candidate structure for the 6-mer. In your pseudo code, you can refer to `GROMACS`, specifying the main input parameters. Consider the case that the docking procedure may generate a candidate decoy with clashes; in this case, generate a new decoy. The docking procedure, as it involves energy minimization, can lead to different results. Take this into account in your pseudo-code.

Exercise 1: Score calculation (10 Points)
ClusCo is a popular program for clustering and comparison of protein models. Download the code (`http://tinyurl.com/zxhj79d`) and read the manual. Then, extract the first model of `1L2Y` file, performe molecular dynamics simulation and optimization on it with BALL. Finally, compared all the different models in the `1L2Y` PDB file with the results of molecular dynamics simulation. What is the model in `1L2Y` that is closest to the refined structure? Consider all possible scores. Write all the commands for ClusCo that you use; consider all avaialable scores.