module code / module title	Module D-AMB / Atomistic modelling of biomacromolecules
date / version of the module description	16.12.2020

1	**INFORMATION ON THE MODULE**	
1a	module code	Module D-AMB
1b	module title *(German title)*	Atomistische Modellierung von Biomakromolekülen
1c	module title *(English title)*	Atomistic modelling of biomacromolecules
1d	credit points	6
1e	responsible for the module	Dr. Susan Köppen
1f	type of module	elective module
1g	programs using the module	M.Sc. Biochemistry and Molecular Biology
1h	organizational unit offering the module	Hybrid Materials Interfaces Group, Faculty of Production Engineering
1i	content-related prior knowledge or skills	Fundamental knowledge about structural setup of biomacromolecules is recommended
1j	learning contents	**Lecture:** • 3D visualization of bio-macromolecules like proteins and lipids • Building protein 3D structures from their amino acid using homology modeling algorithms • Introduction into statistical mechanics and molecular mechanics • Basics of molecular dynamics simulations with the usage of force field based methods

Seminar:

- Introduction to basic terminal commands (Linux)

- Guided walk-through through the GROMACS tutorial setting up a protein simulation under physiological conditions

- Calculation of a protein isosurface

- Introduction into common analysis tools for protein structural models (RDF, RMSD, h-bond-, secondary structure-, dipole-, charge distribution analysis etc.

Practical work:

- Reproduction of GROMACS online tutorial with a selected protein:

  1. Homology modelling for 3D structure determination

  2. setup of simulation cell using GROMACS

  3. Performing a molecular dynamics simulation of the protein in aqueous ionic solution using GROMACS

  4. Post-processing of obtained trajectories for dynamic characterisation using VMD and processing scripts by GROMACS

1k	learning outcomes/ competencies/ targeted competencies	Students have a detailed understanding of biomacromolecules three-dimensional structure and knowledge that can be derived from the analysis.

Computational Toolbox: Students …

- can construct protein 3D structures based on homology modelling

- understand and are able to visualize macromolecules

- can apply atomistic calculation tools independently to perform molecular dynamics simulation and physiological conditions of thermodynamically stable systems

- have a fundamental theoretical background knowledge about the physical calculations implemented in these algorithms

1l — calculation of student workload

(part a: calculation of presence time and working hours)

The total amount of the presence time and working hours of the module has to be calculated additionally in the detailed calculation a) to c).

a) detailed calculation:
  SWS / presence time/working hours in each course of the module

☒	1	lecture(s) with	2	SWS/ contact hours	28	hours of presence time
☒	1	seminar(s) with	1	SWS/ contact hours	14	hours of presence time
☒	1	exercise(s) with	2	SWS/ contact hours	28	hours of presence time
☐		internship(s) with		sum of working hours		
☐		seminar(s) with		SWS/ contact hours		total hours of presence time

☐ laboratory/laboratories with	SWS/ contact hours	total hours of presence time
☐ tutorial(s) with	SWS/ contact hours	
☐ excursion(s) with	SWS contact hours in total	working hours

☐ other form of course (e.g. block seminar), namely this:

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with	SWS / with totaly	contact hours	☐ presence time	☐ working hours

= sum of presence time and working hours:

70 hours

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b) working hours for preparation/follow-up work of the course(s) and/or self-study

= sum of working hours:

- Lecture: 25 hours
- Seminar: 20 hours
- Practical: 35 hours

80 hours in total

calculation of student workload

(part b: preparation time and follow-up work/self-study)

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calculation of student workload

(part c: exam preparation etc.)

c) exam preparation (incl. examination)

= sum of working hours:

30 hours

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calculation of student workload

(total amount of hours including a) - c))

Total amount of the presence time and working hours a) to c):
180 hours

1m

description of possible optional courses in the module

<u>Can a student choose between different courses within the module?</u>

NO

<u>Short description of selection option</u>

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1n	language(s) of instruction	☐ German ☒ English ☐ Spanish ☐ French ☐ Other, namely this: *Klicken Sie hier, um Text einzugeben.*
1o	frequency	*(regular cycle module is offered) e.g.: winter semester, yearly or summer semester, yearly or each semester* summer semester yearly *Klicken Sie hier, um Text einzugeben.*
1p	duration	one semester module *Klicken Sie hier, um Text einzugeben.*
1q	Literature (*optional*)	*Klicken Sie hier, um Text einzugeben.*
1r	more information on the module (*optional*)	Instructors: Susan Köppen, Isabell Louise Grothaus, Limited to 8 students

2	**INFORMATION ON THE MODULE EXAMINATION** (see also AT Art. 5 section 8)	
2a	type of examination	☐ module exam; i.e. exam with only one component (MP) ☒ combination exam, i.e. exam with several components (administered by instructors) (KP) ☐ partial exam; i.e. exam with several components (administered by registrar) (TP)
2b	exam components or prerequisites *(type, number)*	*PL* = *graded component of the examination* *SL* = *ungraded component of the examination, coursework* *PVL* = *prerequisite of the examination (see AT Art. 5 Section 10)* ☒ PL | 2 ☐ SL | ☐ PVL | justification If necessary, further explanations:
2c	Give this information for combination examinations only: Weights (in percentage) of component grades	PL 1: 50 % project report PL 2: 50 % oral examination PL 3: *Klicken Sie hier, um Text einzugeben.* PL 4: *Klicken Sie hier, um Text einzugeben.* If necessary, further comments: *Klicken Sie hier, um Text einzugeben.*

2d	form of examination (see AT BPO/AT MPO Art. 8, 9 and 10)	☐ Assignment	☐ Oral examination (single)	☐ Presentation, oral
		☐ Written examination	☒ Group examination, oral	☐ Presentation and written assignment
		☐ Portfolio	☒ Project report	☐ Bachelor Thesis
		☐ Internship report	☐ Colloquium	☐ Master Thesis
		☐ Other (concrete definition is given in the examination regulations):		

2e	language(s) of instruction	☐ German	☒ English	☐ Spanish	☐ French
		☐ Other, namely this:			
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