

module code /  
module title

## D-AMB / Atomistic Modelling of Biomacromolecules

 date / version of the module  
description

26.10.2021

1 INFORMATION ON THE MODULE		
1a	module code	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	<p><b>Lecture:</b></p> <ul style="list-style-type: none"> <li>• 3D visualization of bio-macromolecules like proteins and lipids</li> <li>• Building protein 3D structures from their amino acid using homology modeling algorithms</li> <li>• Introduction into statistical mechanics and molecular mechanics</li> <li>• Basics of molecular dynamics simulations with the usage of force field based methods</li> </ul>

		<p><b>Seminar:</b></p> <ul style="list-style-type: none"> <li>• Introduction to basic terminal commands (Linux)</li> <li>• Guided walk-through through the GROMACS tutorial setting up a protein simulation under physiological conditions</li> <li>• Calculation of a protein isosurface</li> <li>• Introduction into common analysis tools for protein structural models (RDF, RMSD, h-bond-, secondary structure-, dipole-, charge distribution analysis etc.</li> </ul> <p><b>Practical work:</b></p> <ul style="list-style-type: none"> <li>• Reproduction of GROMACS online tutorial with a selected protein: <ol style="list-style-type: none"> <li>1. Homology modelling for 3D structure determination</li> <li>2. setup of simulation cell using GROMACS</li> <li>3. Performing a molecular dynamics simulation of the protein in aqueous ionic solution using GROMACS</li> <li>4. Post-processing of obtained trajectories for dynamic characterisation using VMD and processing scripts by GROMACS</li> </ol> </li> </ul>																																			
1k	learning outcomes/ competencies/ targeted competencies	<p>Students have a detailed understanding of biomacromolecules three-dimensional structure and knowledge that can be derived from the analysis.</p> <p>Computational Toolbox: Students ...</p> <ul style="list-style-type: none"> <li>• can construct protein 3D structures based on homology modelling</li> <li>• understand and are able to visualize macromolecules</li> <li>• can apply atomistic calculation tools independently to perform molecular dynamics simulation and physiological conditions of thermodynamically stable systems</li> <li>• have a fundamental theoretical background knowledge about the physical calculations implemented in these algorithms</li> </ul>																																			
1l	<p>calculation of student workload</p> <p><i>(part a: calculation of presence time and working hours)</i></p>	<p><b>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).</b></p> <p><b>a) detailed calculation:</b></p> <p><b>SWS / presence time/working hours in each course of the module</b></p> <table border="1"> <tr> <td><input checked="" type="checkbox"/></td> <td>1</td> <td>lecture(s) with</td> <td>2</td> <td>SWS/ contact hours</td> <td>28</td> <td>hours of presence time</td> </tr> <tr> <td><input checked="" type="checkbox"/></td> <td>1</td> <td>seminar(s) with</td> <td>1</td> <td>SWS/ contact hours</td> <td>14</td> <td>hours of presence time</td> </tr> <tr> <td><input checked="" type="checkbox"/></td> <td>1</td> <td>exercise(s) with</td> <td>2</td> <td>SWS/ contact hours</td> <td>28</td> <td>hours of presence time</td> </tr> <tr> <td><input type="checkbox"/></td> <td></td> <td>internship(s) with</td> <td></td> <td>sum of working hours</td> <td></td> <td></td> </tr> <tr> <td><input type="checkbox"/></td> <td></td> <td>seminar(s) with</td> <td></td> <td>SWS/ contact hours</td> <td></td> <td>total hours of presence time</td> </tr> </table>	<input checked="" type="checkbox"/>	1	lecture(s) with	2	SWS/ contact hours	28	hours of presence time	<input checked="" type="checkbox"/>	1	seminar(s) with	1	SWS/ contact hours	14	hours of presence time	<input checked="" type="checkbox"/>	1	exercise(s) with	2	SWS/ contact hours	28	hours of presence time	<input type="checkbox"/>		internship(s) with		sum of working hours			<input type="checkbox"/>		seminar(s) with		SWS/ contact hours		total hours of presence time
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		<input type="checkbox"/> laboratory/laboratories with SWS/ contact hours total hours of presence time <hr/> <input type="checkbox"/> tutorial(s) with SWS/ contact hours <hr/> <input type="checkbox"/> excursion(s) with SWS contact hours working hours in total <hr/> <input type="checkbox"/> other form of course (e.g. block seminar), namely this: Klicken Sie hier, um Text einzugeben.  with SWS / with total contact hours <input type="checkbox"/> presence time <input type="checkbox"/> working hours  = sum of presence time and working hours:  70 hours
	calculation of student workload  <i>(part b: preparation time and follow-up work/self-study)</i>	<b>b) working hours for preparation/follow-up work of the course(s) and/or self-study</b> = sum of working hours: <ul style="list-style-type: none"> <li>Lecture: 25 hours</li> <li>Seminar: 20 hours</li> <li>Practical: 35 hours</li> </ul> 80 hours in total
	calculation of student workload  <i>(part c: exam preparation etc.)</i>	<b>c) exam preparation (incl. examination)</b> = sum of working hours:  30 hours
	calculation of student workload  <i>(total amount of hours including a) - c)</i>	<b>Total amount of the presence time and working hours a) to c):</b> 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>  Klicken Sie hier, um Text einzugeben.

1n	language(s) of instruction	<input type="checkbox"/> German <input checked="" type="checkbox"/> English <input type="checkbox"/> Spanish <input type="checkbox"/> French <input type="checkbox"/> Other, namely this: Klicken Sie hier, um Text einzugeben.
1o	frequency	<i>(regular cycle module is offered) e.g.: winter semester, yearly or summer semester, yearly or each semester</i> <b>summer semester yearly</b> Klicken Sie hier, um Text einzugeben.
1p	duration	<b>one semester module</b> Klicken Sie hier, um Text einzugeben.
1q	Literature <i>(optional)</i>	Klicken Sie hier, um Text einzugeben.
1r	more information on the module <i>(optional)</i>	Instructors: Susan Köppen, Isabell Louise Grothaus, Limited to 8 students
<b>2</b>	<b>INFORMATION ON THE MODULE EXAMINATION</b> (see also AT Art. 5 section 8)	
2a	type of examination	<input checked="" type="checkbox"/> module exam; i.e. exam with only one component (MP) <input type="checkbox"/> combination exam, i.e. exam with several components (administered by instructors) (KP) <input type="checkbox"/> partial exam; i.e. exam with several components (administered by registrar) (TP)
2b	exam components or prerequisites <i>(type, number)</i>	<i>PL = graded component of the examination</i> <i>SL = ungraded component of the examination, coursework</i> <i>PVL = prerequisite of the examination (see AT Art. 5 Section 10)</i> <input checked="" type="checkbox"/> PL   1 <input type="checkbox"/> SL   <input type="checkbox"/> PVL   justification  If necessary, further explanations:  PL = Portfolio, consisting of: project report (50%) and oral examination (50%)
2c	Give this information for combination examinations only: Weights (in percentage) of component grades	PL 1:  PL 2:  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)	<input type="checkbox"/> Assignment <input type="checkbox"/> Oral examination (single) <input type="checkbox"/> Presentation, oral <input type="checkbox"/> Written examination <input type="checkbox"/> Group examination, oral <input type="checkbox"/> Presentation and written assignment <input checked="" type="checkbox"/> Portfolio <input type="checkbox"/> Project report <input type="checkbox"/> Bachelor Thesis <input type="checkbox"/> Internship report <input type="checkbox"/> Colloquium <input type="checkbox"/> Master Thesis <input type="checkbox"/> Other (concrete definition is given in the examination regulations):
2e	language(s) of instruction	<input type="checkbox"/> German <input checked="" type="checkbox"/> English <input type="checkbox"/> Spanish <input type="checkbox"/> French <input type="checkbox"/> Other, namely this: Klicken Sie hier, um Text einzugeben.