Innholdskrav	Utdypende opplysninger og kommentarer
Name	Biomolecular modeling
Course code	KJE-3xxx
Course type	Theoretical and practical subject. The course is available as a singular or elective course independent of study program, also to exchange students and free-movers. The course is offered on condition that a minimum number of students register for the course.
No of ECTS	10 stp
Recommended previous knowledge	KJE-1005 is recommended.
Content	Computer modeling and simulations have now become important tools to study complex systems in many areas of chemistry and biology. With todays high performance computers and advanced software it is possible to study the atomic level details of ribosomes and virus capsids, and to explore biological function with computational modeling. Computational modeling is frequently used to obtain novel insights into ligand binding and design, protein folding, enzyme catalysis and protein-membrane interactions. The course will introduce the basic concepts of computer modeling techniques with main focus on molecular interactions: • Intermolecular forces • Molecular mechanics • Energy minimization • Molecular dynamics simulations • Monte Carlo simulations • Solvation models • Free energy calculations and ligand binding • Enzyme catalysis
Learning outcome	**Knowledge:** The student… • will understand the principles of the methods • will have knowledge of how to apply the methods • will understand the limitation of the methods • will have knowledge to search the literature to present a chosen subject at the research front both written and orally **Skills:** The student will be able to… • write concise reports • discuss and evaluate theoretical predictions with experimental data • conduct independent modeling of binding affinities • make models of biological complexes • analyze the results from the methods **Competence:** The student… • understands the relationship between molecular structure and function in biological systems • can apply his/her knowledge and skills to solve relevant problems • can communicate both in writing and orally terms, theories and problems related to the methods
Teaching	Lecuters: 30 hours, Seminars/exercises 40 hours.
Quality control	Student and teacher evaluation every second or third year
Exam qualification	Five practical exercise needs to be approved.

Exam and evaluation	Five practical exercises will be evaluated, and contribute 30 % of the final grade. The remaining 70 % will be assessed from an oral exam. Passed/not passed.
Re-sit exam	Candidates that receive the grade F can repeat the oral exam the following semester.
Course material	Andrew Leach: Molecular modeling: Principles and applications
Teaching language	The language of instruction is English and all of the syllabus material is in English. The reports will be written in English.
Other	