

SAMMANFATTANDE KURSVÄRDERINGSRAPPORT AV LÄKEMEDELSKEMI  
MED DATORBASERAD LÄKEMEDELSDESIGN (3FK219)

Course name	Läkemedelskemi med datorbaserad läkemedelsdesign (3FK219)
Points	7,5 hp
Course was taken	vt18
Programme and semester	apo,kemiteknik,frifarm,vt18
Separate course	Ja
Number of replies	14
Number of registered students	33
Frequency of replies (%)	42
Date of course evaluation meeting	2018-09-28
Reviewer comments	

Utöver kvantitativa resultat, inkludera centrala synpunkter från fritextsvaren och synpunkter som framkommit i muntlig kursvärdering i helkurs eller i formativa kursvärderingar. (Gör tydligt vad som är resultat från kvantitativa svar och vad som är från kvalitativa svar, såsom fritextsvar.)

1. General opinion of the course, mean value: 5.1  
79 percent chose option 5 or 6  
0 percent chose option 1 or 2
2. The students have particularly appreciated:  
- *Most students liked the practical approach of the course. - Students appreciated an introduction to each computer lab, as it helped them to understand beforehand what would be taught during the lab. Explicit instructions for the Maestro labs were also highly appreciated. - Students appreciated the course "kompendium". - Teacher assistants were very helpful and provided individual guidance to all students. - Students appreciated using commercial software used in industry, and exercises that emulated early drug screening in the industry.*
3. What the students think can be improved:  
- *Given time constraints, some students would have appreciated having more free training time in the lab to finish computer labs or work on the assignment. - There are mixed feelings regarding the necessity of the final exam. Some students liked the structure of the course (with some theoretical lectures in the beginning and practical labs afterwards), while others believe that the theoretical part could be scrapped entirely arguing that the course is meant to be practical (and hence the exam being unnecessary). - Some students were caught off-guard by the exam questions. We believe this stems from some students expecting the final exam to be more similar to the old exam, and not preparing extensively some parts of the course. - Some students believe that lab instructions were unclear, particularly for the SIMCA labs. Some students were a bit lost since the instructions were not step-by-step instructions but rather questions to be answered. Perhaps it would be easier for students to answer the questions if they had a stronger background in multivariate analysis (which the biomedicine students apparently saw for the first time during this course). - While in general students appreciated working with an industry-standard software like Maestro, some are concerned about their dependence on it.*
4. Head teachers reflections of the course and of students opinions on the course:  
*The exam will remain and is carefully written to cover the Learning outcomes as stated on Studentportalen. There is a balance in writing lab instructions as too much focus on*



*step-by-step instructions will make the exercises less educational. We want the students to think by themselves and to apply the theory taught to practical examples. We are constantly trying to improve the lab instructions to get them more clear every year. Although there is some freeware available for modelling, these softwares usually require much more of the user. However, for next year we can provide a list of available softwares.*

5. Suggestions on measures that could improve the course:

Comments from students:

*- Provide some free time in the lab to allow students to finish computer labs or work on the project. - Provide either more old exams or an explicit list of topics to prepare for the final exam to avoid any sort of confusion. - Organize an additional seminar on multivariate analysis with particular focus on PCA so that all students have sufficient knowledge for the SIMCA labs. - Showcase/mention some alternatives to Maestro during the lectures, preferably some open-license software.*

Comments from head teacher:

*Next year there will be even less opportunities for students to spend extra time in the computer lab as the period for the course is shortened. This is unfortunate. The learning outcomes are clearly listed here: <http://www.uu.se/en/admissions/master/selma/kursplan/?kpid=37316type=1>  
On completion of the course, the student should be able to: **KNOWLEDGE AND UNDERSTANDING** - explain how a molecular mechanics force field is constructed - account for the basics in PCA and PLS modelling - account for the basics in molecular recognition - describe strategies to convert peptides to drug-like molecules **COMPETENCE AND SKILLS** - apply 3D-QSAR methodology to predict biological effects - dock molecules to a target protein - carry out conformational analysis studies - carry out a database search to identify molecules that satisfy different pharmacophore criteria - calculate physico-chemical descriptors and use these in QSAR analyses - use multivariate techniques to select datasets based on molecular diversity - build and use in silico models to predict drug absorption - rank and select molecules based on their predicted biological effects and properties - orally present and discuss scientific results in English **JUDGEMENT AND APPROACH** - demonstrate insight of the use of predictive models to promote sustainable development  
Content The course gives an introduction to methods and strategies that are used in drug discovery with a focus on computer-aided drug design. The course includes components such as conformational analysis, ligand-based design, peptide modelling, structure-based design, multivariate analysis, and 3D-QSAR. The exams are written on the basis of this information. This year four old exams were uploaded to Studentportalen. The intention was to show how an exam could look like, not to give a list of every possible question that can appear on a future exam. However, the questions will always cover the topics listed in the Learning outcomes as listed on Studentportalen. I will forward the request for a PCA seminar to Christian Sköld. I will also ask him to review the lab instructions for the Simca exercise.*

The document has been signed by following persons :

Anna Postovskaya (kursrepresentant), Alan Kerstjens Medina (kursrepresentant), Peter Brandt (kursansvarig),

Date: 2018-10-24