18

How can I teach to maximize the learning of "Roberts" (slow/nonambitious) and "Susans" (fast/ambitious)?

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Introduction

The project deals with how to adapt the teaching to suit different students (slow/fast, ambitious/nonambitious. . .) i.e. those referred to by the adjunktpædagogikum course book as "Roberts" and "Susans" (Biggs and Tang; 2007).

The project involves planning of some of my teaching for the coming semester (fall 2009). I only have isolated parts of the courses and can thus not freely chose TLAs based on topics but rather have to improve on existing lecture and exercises. In this project I describe representative examples of a (1) lecture, (2) group exercise/workshop and (3) master project supervision in light of the problem formulation.

The lecture setting

The lecture that I have chosen to include in this project has the title "sequence alignments and phylogenetic analysis" and is held for a class of approximately 150 pharmacy students at their third year. I have had this lecture once, last fall, and it was part of my teaching supervised during adjunktpædagogikum. At that time I had taken over an existing set of lecture slides which were then to the greatest extent are made. The pedagogic considerations were discussed in the "reflection paper" upon my teaching, also written as part of adjunktpædagogikum . Now, I have revisited the presentation (Appendix A) by examining it through the eyes of Robert and Susan.

Slides 2 & 27

I added these two slides already last year and they do not need to be updated. I just want to note here that they explain the relevancy and use of two main subjects and that this is important, especially for “Roberts”.

Slides 3-4

The lecture overview slide was too detailed. I have now updated it so that it does not included details of which the students have not yet heard. I believe an overview is good as it tells the students what is coming, however if being too detailed with new complex terms it might “scare” some students to think that is lecture will be very difficult and that they will not be able to understand it. I want to avoid expectations of failure.

Slide 7

This year I judged the “dot-plot” slide as not being of central importance and it was thus removed.

Slides 9-10 and slide 34

Pedagogic project in the “KNUD” course in natural sciences university pedagogics and didactics. The lecture contains two questions to be discussed in pairs. They have been chosen to cover the most important topics;

1) how to construct sequence alignments and
2) how to interpret a phylogenetic tree.

The question (1a-b) on slide 9 was good for the students to self process and work with the calculation of alignment scoring. However, I felt that another question should be added that can challenge Susans and also lead to higher-taxonomy considerations leading to a deeper understanding. For this reason I added question 2: “Why is it better to use the similarity than distance scores? “ to the updated slide (no 10).

Slides 12-13

I wanted to make the point clearer on this slide and also integrate it better with previous ones. To do this I changed the title and color-coding the text that corresponds to the residue color-coding in the alignment. This is probably a clarifying change for everyone, not Roberts or Susans in particular.

Slides 22-25

Similarly, to previous comment these slides have just been clarified. The main message is to explain protein sequence profiles and this was better done by changing both slide titles and updating the text and illustration for the first slide.

Slides 28-32

The making of phylogentic trees is probably the most difficult part of the lecture and yet a very central theme. I made new slides for this section last fall and, although I wanted to make a special effort to improve them again, I could only think of small layout improvements increasing the clarity but no new pedagogical approaches.

Slides 37-38

I do not give ILOs at the beginning of the lecture as they would probably not be understood before the lecture, – this is what I reasoned for the lecture overview above (slides 3-4). This finishing slide is the closest to ILOs in this lecture. By grading the topics of the lecture I have designed it so that the student can him/herself 1) prioritize and focus home studies and also 2) choose a level of ambition. Another important addition is the references for Susans so that they can find more information. I believe that challenging Susans in a lecture and at the same time be understood by Roberts requires home work for the former type of student.

After the lecture

Students can download all lectures of this course from the course web site and my email address is available on the slides so that questions can be sent. I have tried to make it possible to understand the slides without my oral presentation, at least together with the book. After the lecture I invite for questions in whole class or individually at the desk. Giving room for individual questions is beneficial for meeting the different needs of Roberts and Susans.

Reflections from last year and tips for next year

Last year I enjoyed having this lecture and the response from the class was very good. I got answers for every question posed during the lecture, applauds when finished and one student walked up to me to ask questions afterwards. The fact that most students looked as if they were concentrated and listened well suggests that they also gained new knowledge, but it is difficult to assess to what extent I could reach them. Furthermore, several students may have understood less because I spoke English, but the class also contained ca 6 Icelandic students that prefer English to Danish. I have decided to take a Danish course for Scandinavians this fall. I also got a very good pedagogic tip from my external pedagogic supervisor, Per Geckler, that I will use this year. The advice was to ask the students to give me the Danish word for central, new English terms such as "sequence alignment" and "phylogeny". That would increase the understanding of these new concepts.

The group exercise/workshop setting

I have the main responsibility for one computer-based exercise and the pedagogical work on this is described in my reflection paper. However, for this project I work with a new group exercise, which I will only be co-managing. This is "Toolbox Exercise 2 – Conformational analysis and conformational energy penalty of binding". This is part of an elective course for Pharmacy Master students. There are usually ca 20 students on the course, most of which are relatively motivated. They have 2 hours to complete the exercise. The purpose of the exercise is to equip the students with skills in the "Schrodinger" software necessary to conduct their projects.

Introduction to exercise

For the group exercise described in my reflection paper I produced a 15 minute introduction summarizing the knowledge needed (the corresponding lecture had been 1-2 weeks ago and did not cover all topics of the exercise). I had planned to do the same thing for this new exercise. However, it is scheduled right after the corresponding lecture which has the same responsible teacher and provides full cover. What I believe can actually be

improved would be to spend some time before the exercise to take questions from the lecture and also suggestively let the students in small groups define key words, such as “solvation” and “force field”. These terms are used repeatedly in the exercise.

Written instructions for exercise

For the group exercise described in my reflection paper I made multiple pedagogic improvements to the instructions. It is my experience that spending time on formulating clearer instructions pays off by increasing the understanding and decreasing the frustrations of students and at the same time saving time as students tend to get stuck less often. However, for this exercise also the instructions were very clear already from the beginning. It is structured in goal, background theory, methodology and then the actual exercise containing questions that I judge can adequately encourage high-level learning. However, I have made some improvements to the instructions that are found in appendix B. The track changes function has been used to document my updates. A short note is that it is nice to have some factual background about the molecule being worked on, Glutamate. I added parentheses to two words that I am not sure that the students would otherwise have understood the meaning of; conformational space (possible compound 3D structures) and complete (converged) search. To better explain the concept of electrostatic collapse I will add a picture of a collapsed molecule.

Giving help during the exercise

When answering students’ questions during labs I try to get a picture of how much the student has understood and to provide guidance at the right level and in simple words. One technique that I often use is to ask the student to self formulate an explanation for me as far as she/he can and then I fill in the parts where the understanding was limited. I strive to address all the students in a group to make sure that all of them participate and have understood. An observation I have made is that different students understand things in different ways and it is good if the support can be individualized. For example some students prefer to go through practical examples, whereas others like analogies or just a presentation of the background theory. I want the students to comprehend and do therefore not give answers for questions directly. Instead I share the information that the student needs

to answer the question him/her self. When students have asked for help on a particular question I sit by until they have completed it. In this way I can be assured that they have understood and also avoid frustration resulting from getting stuck at a certain question.

After the exercise

Home studies are not possible as the software is very expensive, -it is essential that the students learn how to use the software during the scheduled exercises. I will suggest that the teachers goes through all questions in the exercise individually with each group when they are finished. This gives the opportunity to make sure that the students have understood and which parts are the most difficult. This is also a good time to ask what the students have learned, what was difficult and what can be improved. My experience from the other computer-based exercise is that students finish at different times and that the post-exercise talk is relatively successful in meeting different students at their level and also gaining information about how the exercise can be improved.

Master project supervision

Previous experience

Supervision of students is the type of teaching that I have the most experience of and it is also my favorite type of teaching. During the last year of my PhD I supervised three Master project students that all continued doing research in the group also after completing the project. Two of the students came so far that they influenced the development of their ongoing projects. All three chose to take on PhD studies, one in my group and two in other groups.

Explaining the project and aligning expectations

September 2009 to June 2010 (35 points) I will supervise my first master project student at the University of Copenhagen. The student chose me as he recognized me from classes and a computer-based project matched his skills, having worked with programming and web design. The first main

concern of the student was that it is very difficult to get a good understanding of projects and how they will be to work with. Sending complex texts such as articles or project applications would probably just have scared him and I decided to book a meeting to explain the project and to let him ask questions. I also initiated a discussion about expectations on each other and about results. In short the discussion I emphasized that scientific results can never be ascertained on beforehand, I will not count clock-hours but want to see an honest attempt to carry out the project and that results are as depending on my effort as his i.e. without adequate help even the brightest student will have difficulties.

Supervision attitudes and techniques

Our first meeting (Dec 07) has been followed up with new meetings every 6th week to provide updates of my project, which is similar to the master project. The meetings have given the student some insight into how running a project works, the type of problems that may be encountered and how a computational chemist work together with organic chemists and pharmacologists. During a master project I make sure that students have understood what to do I often ask them to self explain the next steps. Furthermore, this time I want to test letting the student write a draft of the introduction and project plan of master thesis already when starting. This PBL element, if it works, could encourage independent thinking at an early stage and personal “ownership” of the project.

Special master project considerations for Roberts and Susans

Many of the considerations apply to all students. A master project should be well defined and separated into an independent (sub?)task, feasible within the given time-frame and contain elements of “learning-by-doing”. The supervisor should provide help at a level appropriate for the student and stimulate the use of the students own innovation and creativity. However, a Susan could probably handle more freedom and faster-pace challenges. A Robert would need more frequent guidance and a larger effort in ascertaining that the tasks and the relevancy (project and skills) have been understood. I as the supervisor, need to accept that publishable results are not necessarily a goal of the student and that the ambition may often only be too get the desired grade.

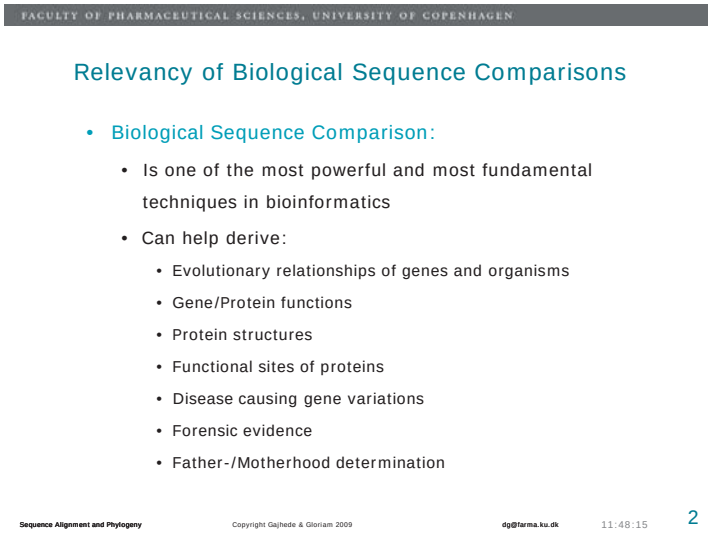
Ethical discussion about the prioritization of teaching resources

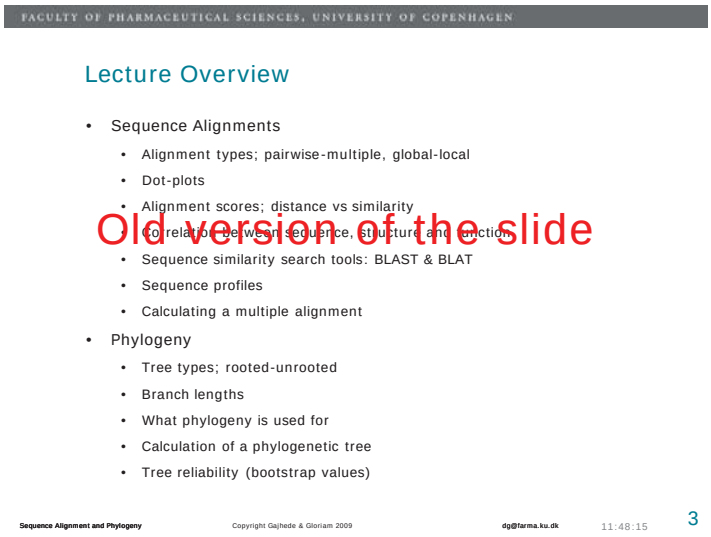
Ethical discussion was initially planned to be a primary part of the project, however the instructions have been clear on that the project must directly relate to specific courses and therefore this topic is only touched upon. I think that what can be concluded within the frames of this project and from adjunktpædagogikum is that by carefully designing TLAs much can be done to increase the learning outcome of Roberts and Susans without extra resources.

Should time and money be spent on the students which have the ability to learn the most, an "elite", or should the university focus on making sure that no one is left behind?

The adjunktspedagogikum course book has a reference on page 14 on this topic (Buckridge, Guest; "A conversation about pedagogical responses to increased diversity in university classrooms"). Due to the project instructions and time limitations I have not read it, but might do so later. My stand point (the only result here) is that for societal, humanistic and ethical reasons there is a need to reach as many as possible of the students. However, teachers should not forget to make the effort to provide the extra challenges needed for Susans. I think that "elite" classes, such as those currently introduced at the Danish Niels Brock high school (http://www.brock.dk/om-niels-brock/nyhederpresse/her-kommereliten.html) can increase the learning outcome of Susans. I suspect that many people fear that elite classes might foster personalities with a 'besserwisser' attitude that look down on others. This is a problem on the individual level, but not on the institutional, and I believe it also can to some extent be dealt with by providing the right teaching environment. As a contrasting perspective, this is not better than letting the "jantelov" make Susan-like students reduce their ambitions to not stand out from the crowd.

A Appendix: Slides from lecture on “sequence alignments and phylogenetic analysis” (excerpt)





Lecture Overview

- Sequence Alignments
  - Different types of sequence alignments
  - How to make a sequence alignment
  - Online alignment tools
  - Connection between sequence, structure and function
- Phylogeny
  - Types of phylogenetic trees
  - How to make a phylogenetic tree
  - What phylogeny is used for

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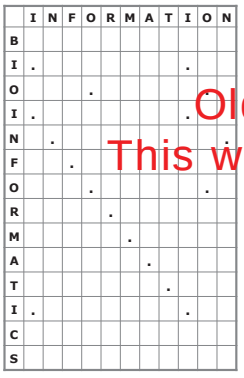
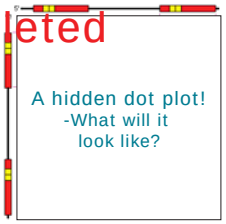
"Dot Plots" - Graphical Illustrations of Aligned Regions Within 2 Sequences



Old slide
This was deleted

- Dot plot of a retroviral vector aligned against itself



A hidden dot plot!
-What will it look like?

  dg@farma.ku.dk 11:48:15

11/30/2009

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Which is the Best Alignment?

- A) Using a distance measurement?
- B) Using similarity score?

1) 2) 3)

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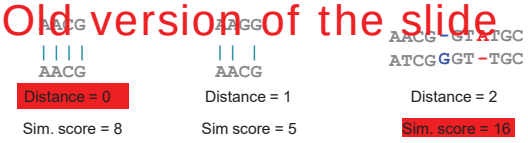

Distance = 0 | Distance = 1 | Distance = 2

Sim. score = 8 | Sim score = 5 | Sim. score = 16

- Distance:
  - Hamming distance: Number of mismatches
  - Levenshtein distance: Number of edits required to turn one string into another
- Similarity score calculation:
  - aligned position: +2
  - mismatch: -1
  - gap: -1

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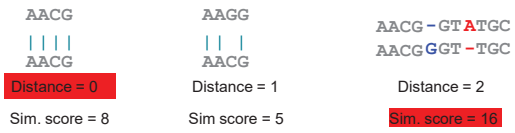
Q1) Which of 1-3 below is the Best Alignment?

- A) Using a distance measurement?
- B) Using similarity score?

Q2) Why is it better to use the similarity than distance scores?

1) 2) 3)



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Multiple Alignment Advantages

- Sequence alignment between multiple sequences can help to find functional sites (e.g., active sites) in a protein sequence
- Functional sites are conserved (un-mutated) in evolution

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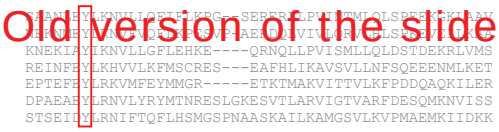
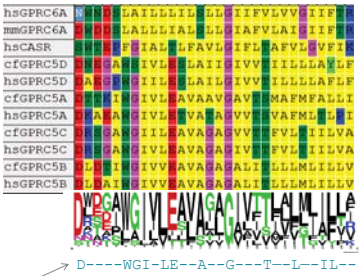


- Alignment profiles
  - Made based on multiple alignments
  - Can be use in sequence searches to increase sensitivity and selectivity (PSI-BLAST, Hidden Markov Models)

Alignment profiles

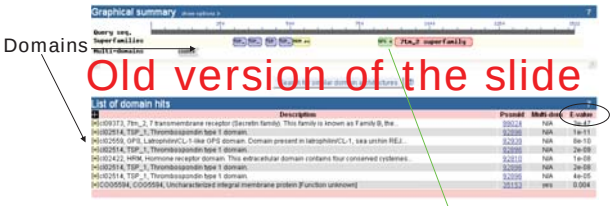
- Functionally important sites are evolutionary conserved (less mutated)
- A profile ranks highly conserved sites as more important
- Sequence searches using profiles have higher sensitivity and selectivity (PSI-BLAST, Hidden Markov Models)



11/30/2009

Example of Protein Profiles & Functional Sites

Result from a “Conserved Domain Search”
(a variant of BLAST) at NCBI web site



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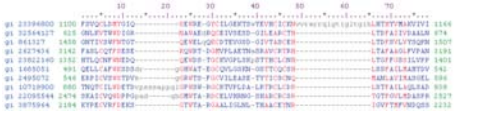
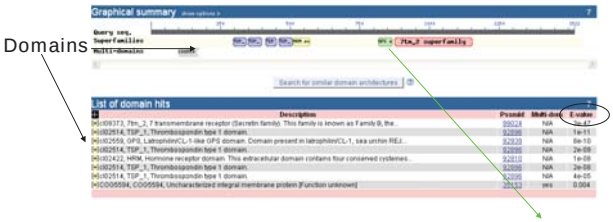
The profile of one of the domains (GPS) found above

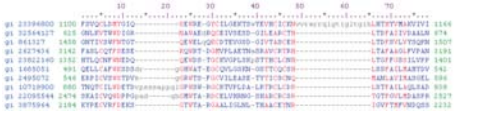


Database of Protein Domains Profiles

Result from a “Conserved Domain Search”
(a variant of BLAST) at NCBI web site



Example of profile for one functional domain (GPS)



What is Phylogeny Used For?

Species Comparisons:

- Evolutionary analyses e.g. protein family evolution
- Selection of appropriate (genetically similar) model organisms

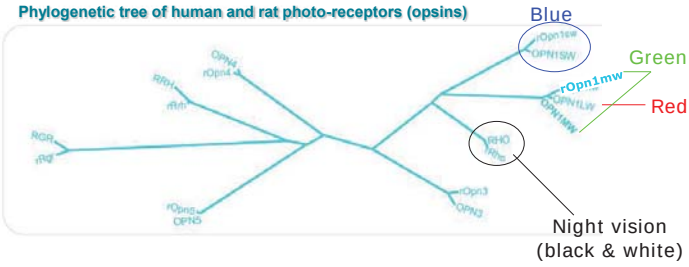
Protein Family Comparisons:

Based on protein relatedness it is possible to predict:

- Physiological functions of proteins with unknown functions
- Pharmaceutical data such as ligands

Question

- Which difference is there in the color vision of humans and rats?



11/30/2009

Summary

- Sequence Alignments
  - Alignment types; pairwise-multiple, global-local
  - Dot-plots
  - Alignment scores; distance vs similarity
  - Correlation between sequence, structure & function
  - Sequence similarity search tools: BLAST & BLAT
  - Sequence profiles
  - Calculating a multiple alignment
- Phylogeny
  - Tree types; rooted-unrooted
  - Branch-lengths
  - What Phylogeny is used for
  - Calculation of a phylogenetic tree
  - Tree reliability (bootstrap values)

Old version of the slide

Basic knowledge
Very useful
Advanced

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Basic knowledge
Very useful
Advanced

- If you want to know more consult the course book. Wikipedia also has good entries on sequence alignments and phylogeny.

B Appendix: Changes to written instructions for excercise (excerpt)

Toolbox Exercise 2 – Conformational analysis and conformational energy penalty of binding

Goal

~~The aim of this exercise is to demonstrate:~~ After this exercise you should have learned how to:

- ~~How to~~ perform a conformational search on small molecules.
- ~~How to~~ identify and handle electrostatic collapse.
- ~~How to~~ calculate conformational energy penalties of binding.

Calculation of conformational energy penalties of binding

When a ligand binds to a protein it usually has to change conformation from the most stable one in solution to a conformation that fits the active site. This change in conformation may cost energy, which subtracts from the free energy of binding and decrease the binding affinity. We call it the conformational energy penalty of binding (Epenalty) and it is the difference in conformational energy between the most stable conformation in water and the binding conformation. If Epenalty is significantly higher than 3 kcal/mol **for high affinity ligands** it is considered an unlikely binding conformation.

~~The procedure~~ Epenalty is calculated as follows:

1. Calculate Eglobal:
   ~~1~~a. Perform a conformational search of your compound in water to identify the global energy minimum conformation.
   ~~2~~b. Calculate the energy of the conformation from step 1 in vacuum. This is ~~to get~~ Eglobal.
2. Calculate Ebinding
   ~~3~~a. Perform a constrained energy minimization of the binding conformation in water constraining each atom to only be allowed to move ~~only~~ 0.5 Å before a force constant of 500 kcal/mol is applied.
   ~~4~~b. Calculate the energy of the conformation from step 3 in vacuum. This is ~~to get~~ Ebind
3. Calculate Epenalty
   ~~5~~a. Subtract the energy of the global energy minimum conformation from the energy of the binding conformation (Epenalty = Ebind – Eglobal).

Comment [d1]: After AdjPed no teacher can miss that the important thing is not what the teacher does, but what the student learns.

Comment [d2]: I just think the numbers 1-5 are categorized under the Energy term they are part of calculating.

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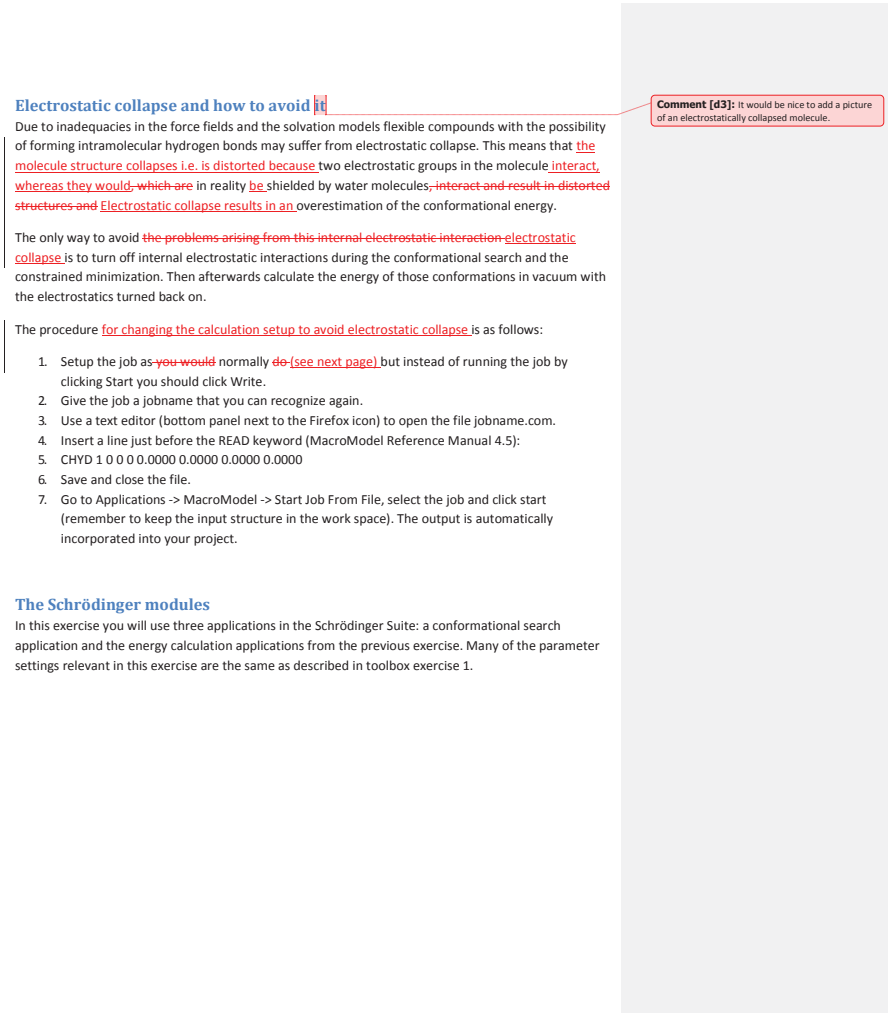

Electrostatic collapse and how to avoid it

Comment [d3]: It would be nice to add a picture of an electrostatically collapsed molecule.

Due to inadequacies in the force fields and the solvation models flexible compounds with the possibility of forming intramolecular hydrogen bonds may suffer from electrostatic collapse. This means that the molecule structure collapses i.e. is distorted because two electrostatic groups in the molecule interact, whereas they would~~, which are~~ in reality be shielded by water molecules~~, interact and result in distorted structures and~~ Electrostatic collapse results in an overestimation of the conformational energy.

The only way to avoid ~~the problems arising from this internal electrostatic interaction~~ electrostatic collapse is to turn off internal electrostatic interactions during the conformational search and the constrained minimization. Then afterwards calculate the energy of those conformations in vacuum with the electrostatics turned back on.

The procedure for changing the calculation setup to avoid electrostatic collapse is as follows:

1. Setup the job as ~~you would~~ normally ~~do~~ (see next page) but instead of running the job by clicking Start you should click Write.
2. Give the job a jobname that you can recognize again.
3. Use a text editor (bottom panel next to the Firefox icon) to open the file jobname.com.
4. Insert a line just before the READ keyword (MacroModel Reference Manual 4.5):
5. CHYD 1 0 0 0 0.0000 0.0000 0.0000 0.0000
6. Save and close the file.
7. Go to Applications -> MacroModel -> Start Job From File, select the job and click start (remember to keep the input structure in the work space). The output is automatically incorporated into your project.

The Schrödinger modules

In this exercise you will use three applications in the Schrödinger Suite: a conformational search application and the energy calculation applications from the previous exercise. Many of the parameter settings relevant in this exercise are the same as described in toolbox exercise 1.

All contributions to this volume can be found at:

http://www.ind.ku.dk/publikationer/up_projekter/2008-1/

The bibliography can be found at:

http://www.ind.ku.dk/publikationer/up_projekter/kapitler/2008_vol1_bibliography.pdf/