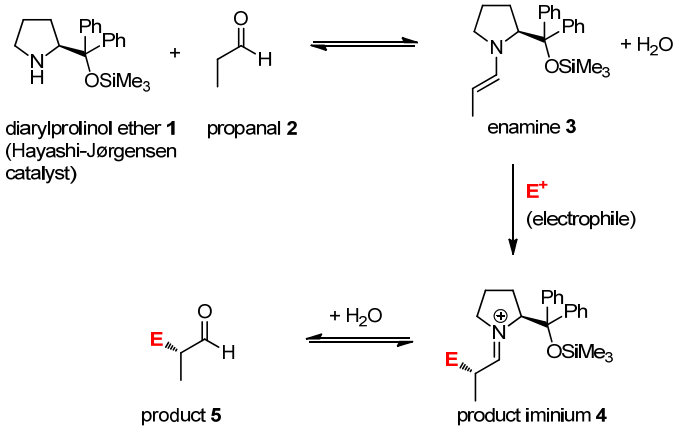
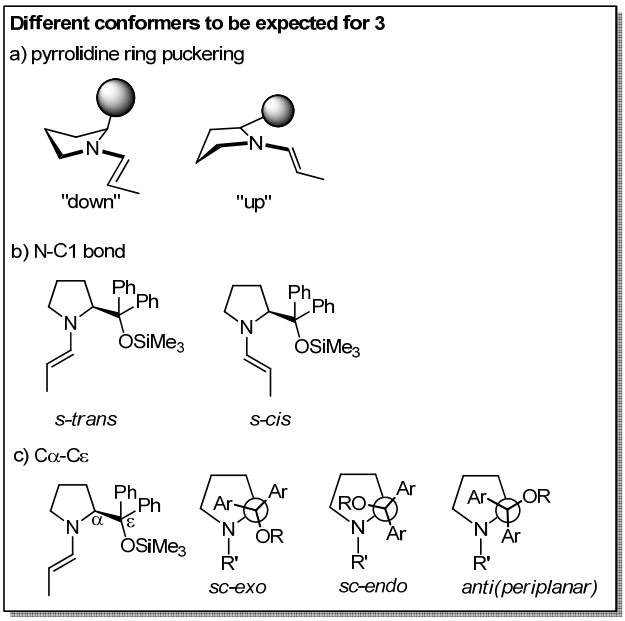
Please return your report and the answers to the Home Exam questions by Friday 24 August to ***Petri.Pihko@jyu.fi***

Report of the Computational Exercise

Please prepare a short report in the following format:

1. Write a short description of the computational procedure – at least mention the force field used(MMFFs), how many structures were obtained from the initial screen, and how many of these were further optimized by DFT (using B3LYP/6-31G** level of theory).
2. Prepare a short table of results (you can simply copy and paste the table you have prepared in Excel according to the instructions).
3. Comment on the conformers you have found and their relative stabilities according to these calculations. Are the results in line with the experimental work by Gschwind and coworkers? The Gschwind paper is available in Koppa together with the other course materials.





Home Exam Questions

1. Briefly outline the strengths of *three* methods/approaches to solution phase structures and/or conformational analysis. You can select from the following list or suggest your own:
   - Computational methods: force fields
   - Computational methods: DFT calculations
   - NMR methods: NOE (NOESY/ROESY) experiments
   - IR methods
   - X-ray crystallography
   - Circular dichroism
   - X-ray crystallography (note also how this method could yield insights into what happens in *solution*)