C7790 Computational Chemistry and Molecular Modeling I
TSM Modeling of molecular structures

C7800 Computational Chemistry and Molecular Modeling I - seminar

Project III

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Dynamics of a small organic molecule

(Almost) Individual project

- **Reference manuals**
  - AMBER (molecular dynamics)
  - VMD (visualization)
  - Infinity (submitting jobs)

Requirements for processing results

I recommend processing the results in the form of a brief protocol, which should have the following requirements:

- Name and surname, name of the exercise and date
- For each thematic area:
  - Brief summary of the topic, including a reaction scheme, if appropriate
  - Software used, including versions
  - Results (tables and graphs)
  - Discussion of results according to the assignment
  - Used literature (e.g., for experimental values)

Tasks

1) Build a model of a molecule of your choice (e.g., an active substance of ibuprofen).
2) Prepare the input topology (parm7) and coordinates (rst7) for the molecular dynamic simulation in vacuum according to the procedure described in the AMBER reference manual.
3) Perform equilibration and subsequently a production dynamics (10 ns) at 300 K.
4) Visualize the obtained trajectory in VMD. Qualitatively characterize the dynamics of the molecule.
5) Select the characteristic geometric parameter(s) (e.g., distance, angle, dihedral angle), which best capture(s) the observed conformational transformations. Display the course of the selected parameter in time, the graph will be part of the protocol.
6) Perform a histogram analysis of the selected parameter, the resulting graph will be part of the protocol. Determine the number of substates (conformers) by analyzing the histogram and estimate their relative representation.