# Computational analysis of chain flexibility and fluctuations in Rhizomucor miehei lipase - DTU Orbit (08/11/2017)

## Computational analysis of chain flexibility and fluctuations in *Rhizomucor miehei* lipase

We have performed molecular dynamics simulation of Rhizomucor miehei lipase (Rml) with explicit water molecules present. The simulation was carried out in periodic boundary conditions and conducted for 1.2 ns in order to determine the concerted protein dynamics and to examine how well the essential motions are preserved along the trajectory. Protein motions are extracted by means of the essential dynamics analysis method for different lengths of the trajectory. Motions described by eigenvector 1 converge after approximately 200 ps and only small changes are observed with increasing simulation time. Protein dynamics along eigenvectors with larger indices, however, change with simulation time and generally, with increasing eigenvector index, longer simulation times are required for observing similar protein motions (along a particular eigenvector). Several regions in the protein show relatively large fluctuations and in particular motions in the active site lid and the segments Thr57-Asn63 and the active site hinge region Pro101-Gly104 are seen along several eigenvectors. These motions are generally associated with glgcine residues, while no direct correlations are observed between these fluctuations and the positioning of prolines in the protein structure. The partial opening/closing of the lid is an example of induced fit mechanisms seen in other enzymes and could be a general mechanism for the activation of Rml.

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