Analysis of Molecular Dynamics Simulation - For Small Polypeptides and Proteins

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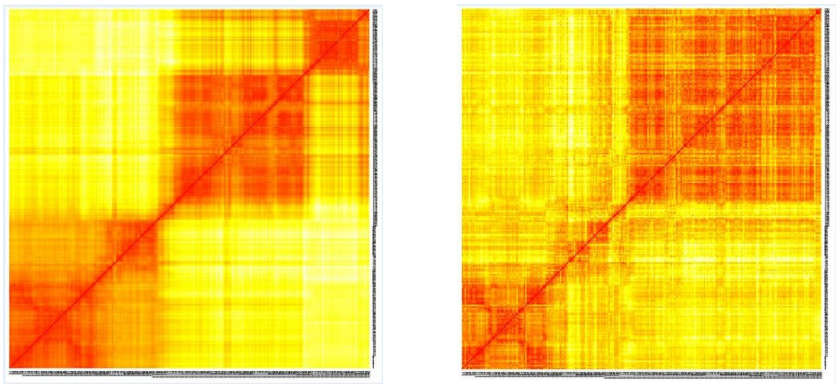
The aim of this project to analyze the molecular dynamics simulation generated structures, group them in to different clusters according to their relative conformations and hence to identify and display the major structural changes during MD simulation. Since the standard parameter like root mean square deviation (RMSD) does not reveal the most interesting properties of the dynamics, we use C-alpha torsion angle – pseudo dihedral angle defined by four successive C-alpha atoms. [1].



Managing the large amount of data and presenting them in a comprehensive manner are the major challenges here. The results of C-alpha torsion angle method were compared with that of RMSD matrix method. We used heat-maps to visualize the symmetric nxn matrix. RMSD heatmap (left) and C-alpha torsion angle heatmap (right) are shown in the above picture. The same method of comparison have been extended and tested for bigger proteins. To handle the huge amount of data, we use KNIME [2], a user-friendly and comprehensive open-source data integration, processing, analysis and exploration platform.

[1] Maria M. Flocco, Sherry L. Mowbary, Protein Science, **1995**, 4, 2118-2122.
[2] KNIME: The Konstanz Information Miner. (http://www.knime.org)