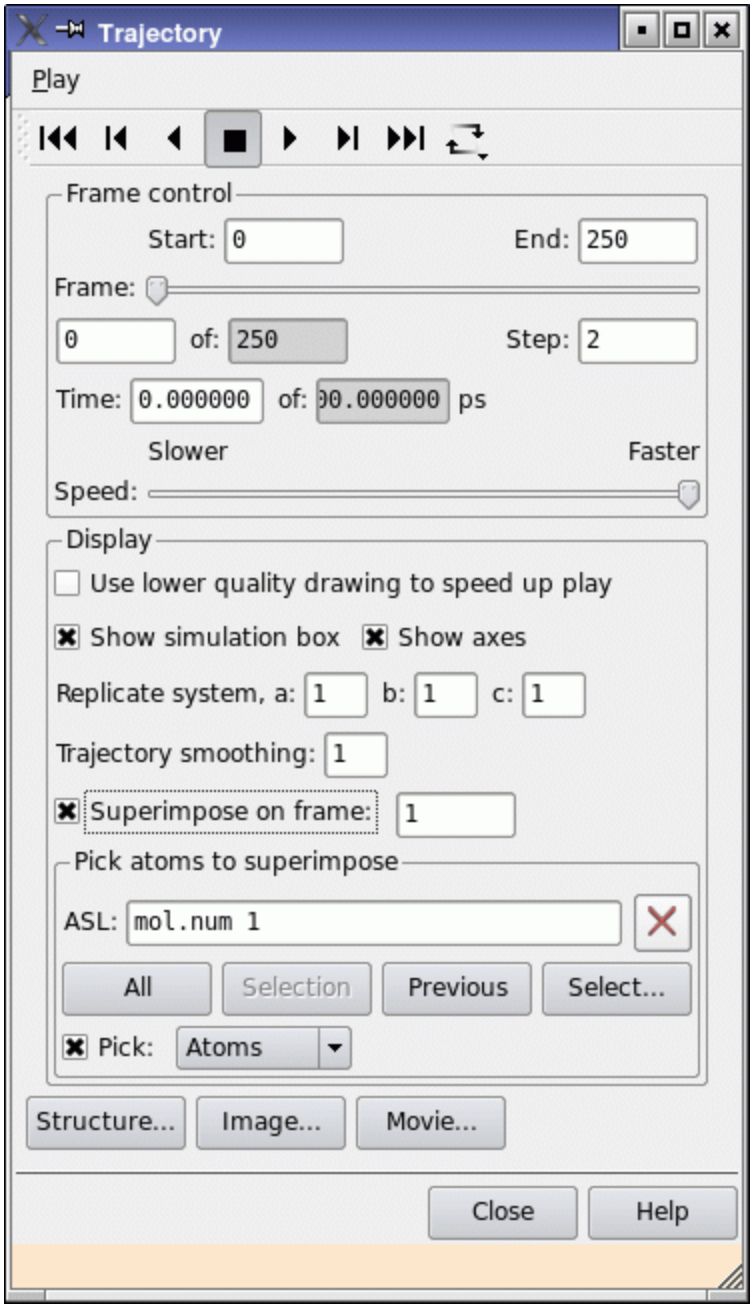
Molecular dynamics Trajectories for activated processes

Introduction

- Molecular dynamics simulation methods produce trajectories of atomic positions as a function of time
- Optionally velocities and energies can also be produced in trajectories
- Simulations on 10-100ns were carried out which gives trajectories with large amounts of data.

Desmond trajectories

- Trajectories of different frames can be visualized and analyzed.
- Difference in interactions, conformational positions can be visualized.



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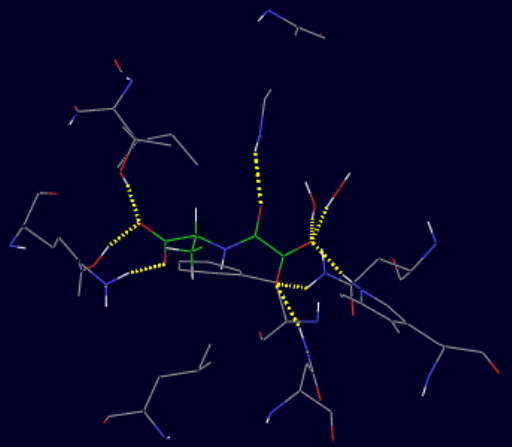

Atoms:0/180/18596 Entries:1/1 Res:5654 Chn:2 Mol:5562 Chg:0 Jobs: 0/0

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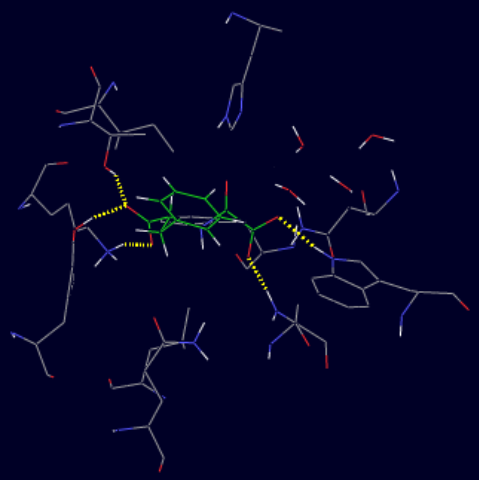

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Jobs: 0/0

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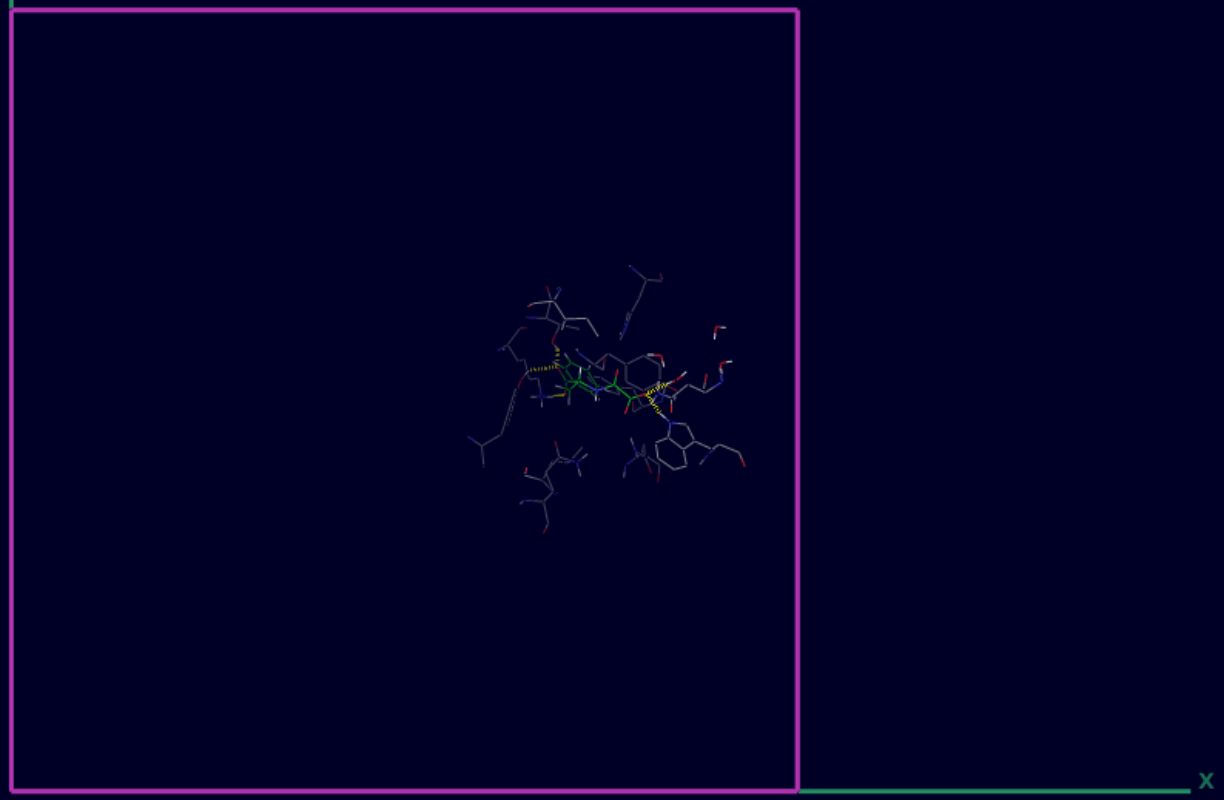
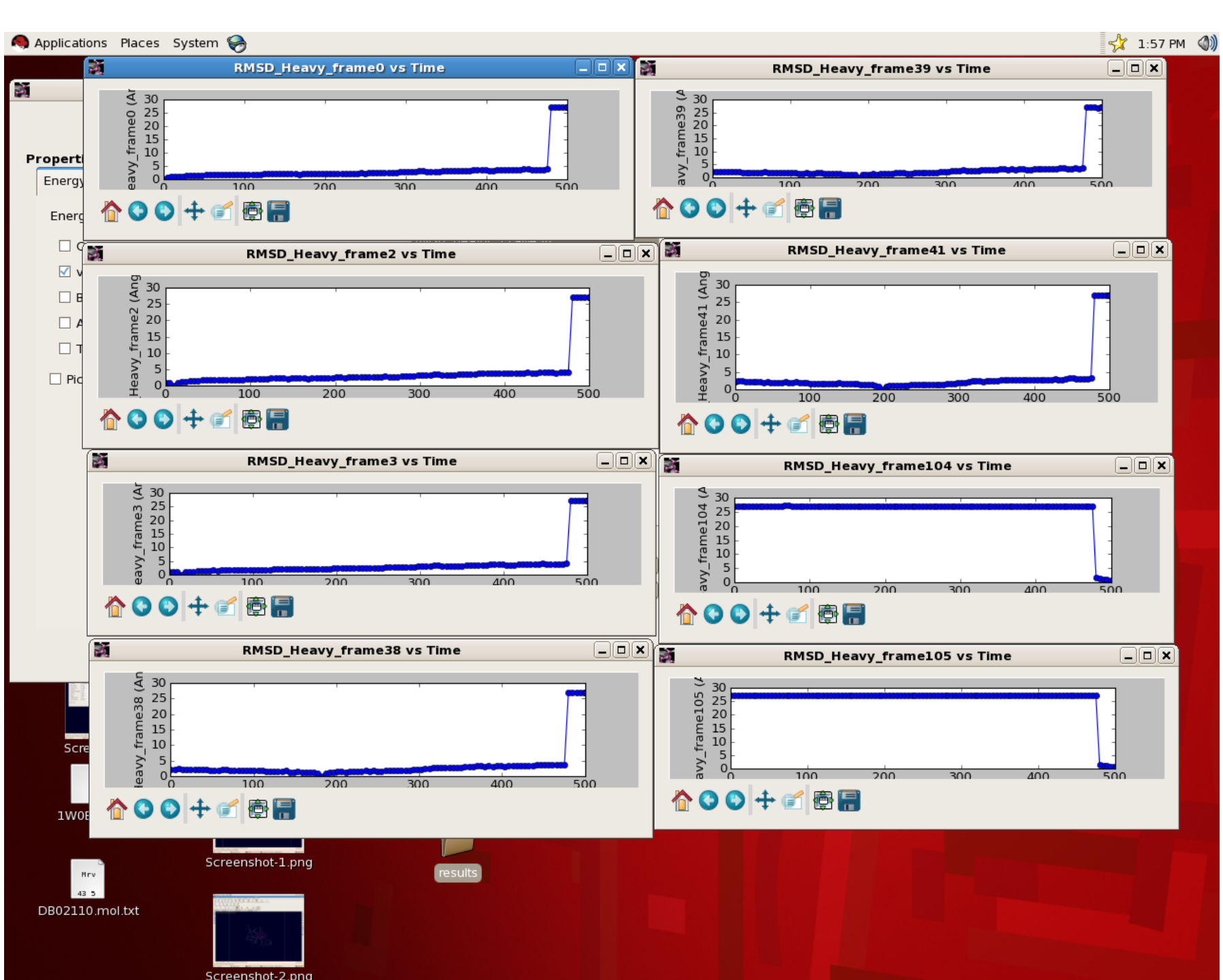


- Trajectories can be analyzed by RMSD, RMSF,calculations.Also we can analyse
- Coloumbic interactios
- Covalent bond interactions
- Vanderwaals interactions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RMSD_Heavy_frame104 vs Time
RMSD_Heavy_frame38 vs Time
RMSD_Heavy_frame105 vs Time
Screenshot-1.png
results
DB02110.mol.txt
Screenshot-2.png

Clustering MD trajectories

J. Chem. Theory Comput. **2007,** *3,* 2312−2334

JCTC Journal of Chemical Theory and Computation

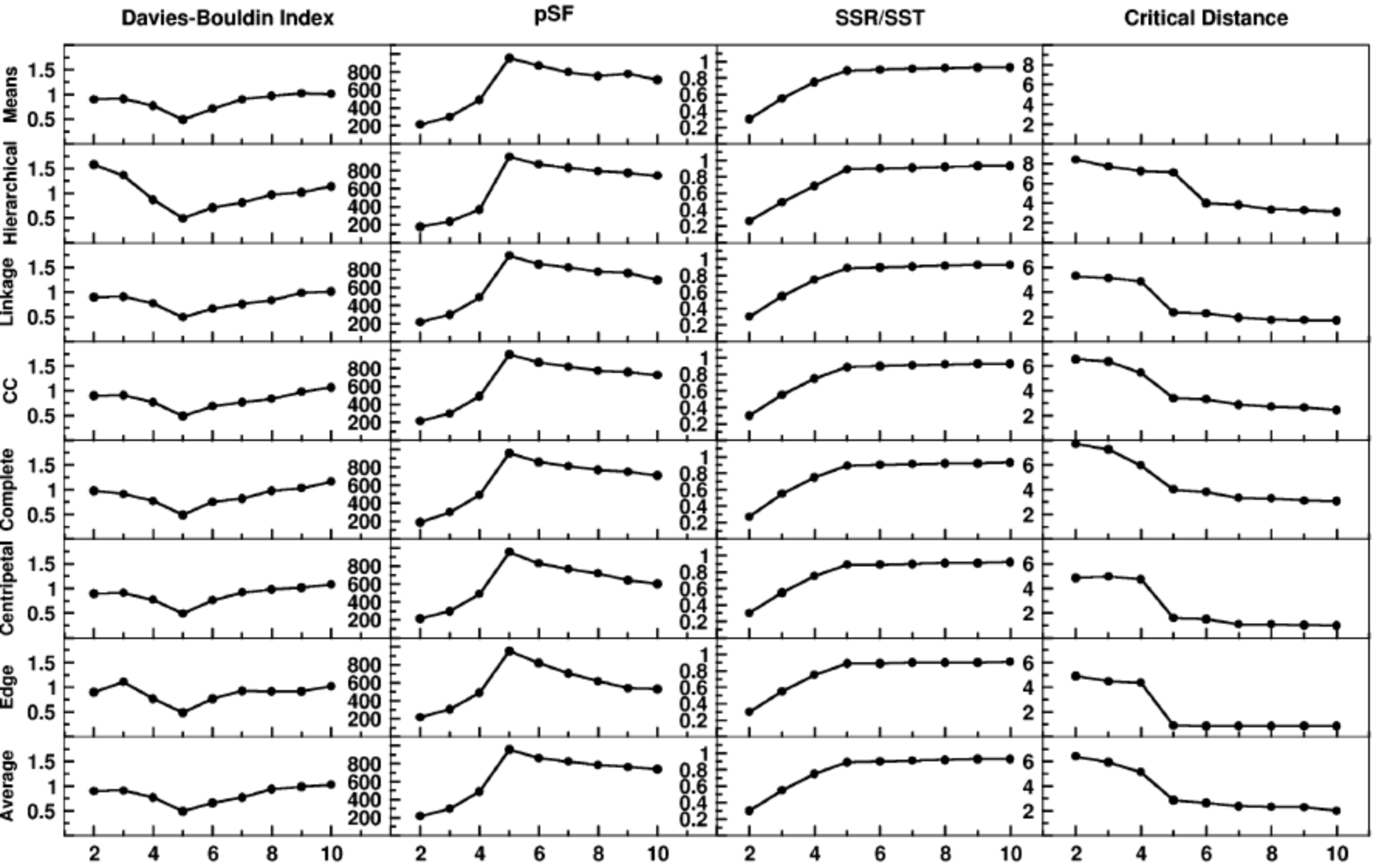
Clustering Molecular Dynamics Trajectories: 1. Characterizing the Performance of Different Clustering Algorithms

Jianyin Shao, Stephen W. Tanner,[†] Nephi Thompson,[‡] and Thomas E. Cheatham, III*

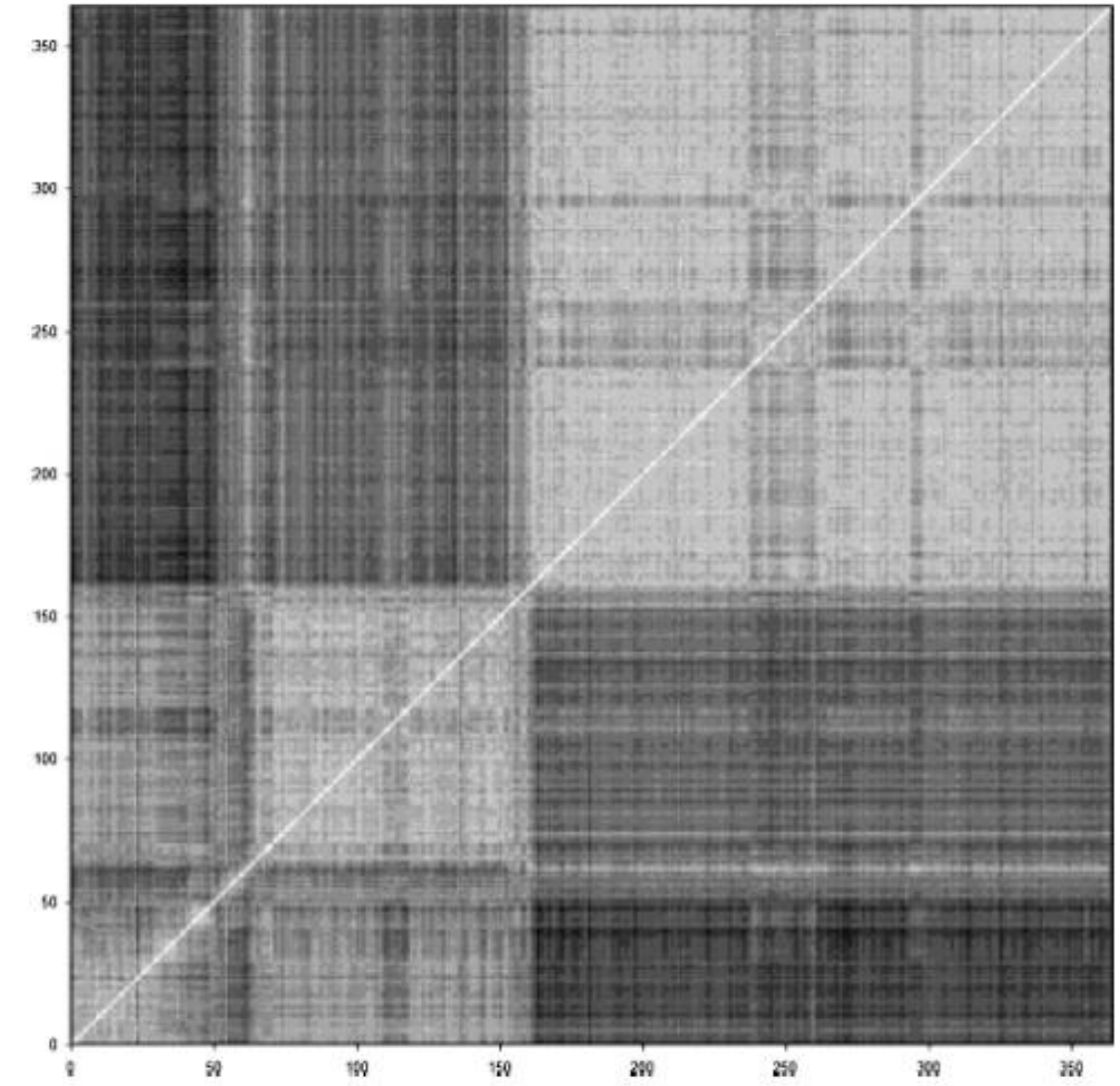
Departments of Medicinal Chemistry, Pharmaceutics and Pharmaceutical Chemistry, and Bioengineering, College of Pharmacy, University of Utah, 2000 East 30 South, Skaggs Hall 201, Salt Lake City, Utah 84112

Received May 17, 2007

Cluster metrics for MD trajectory

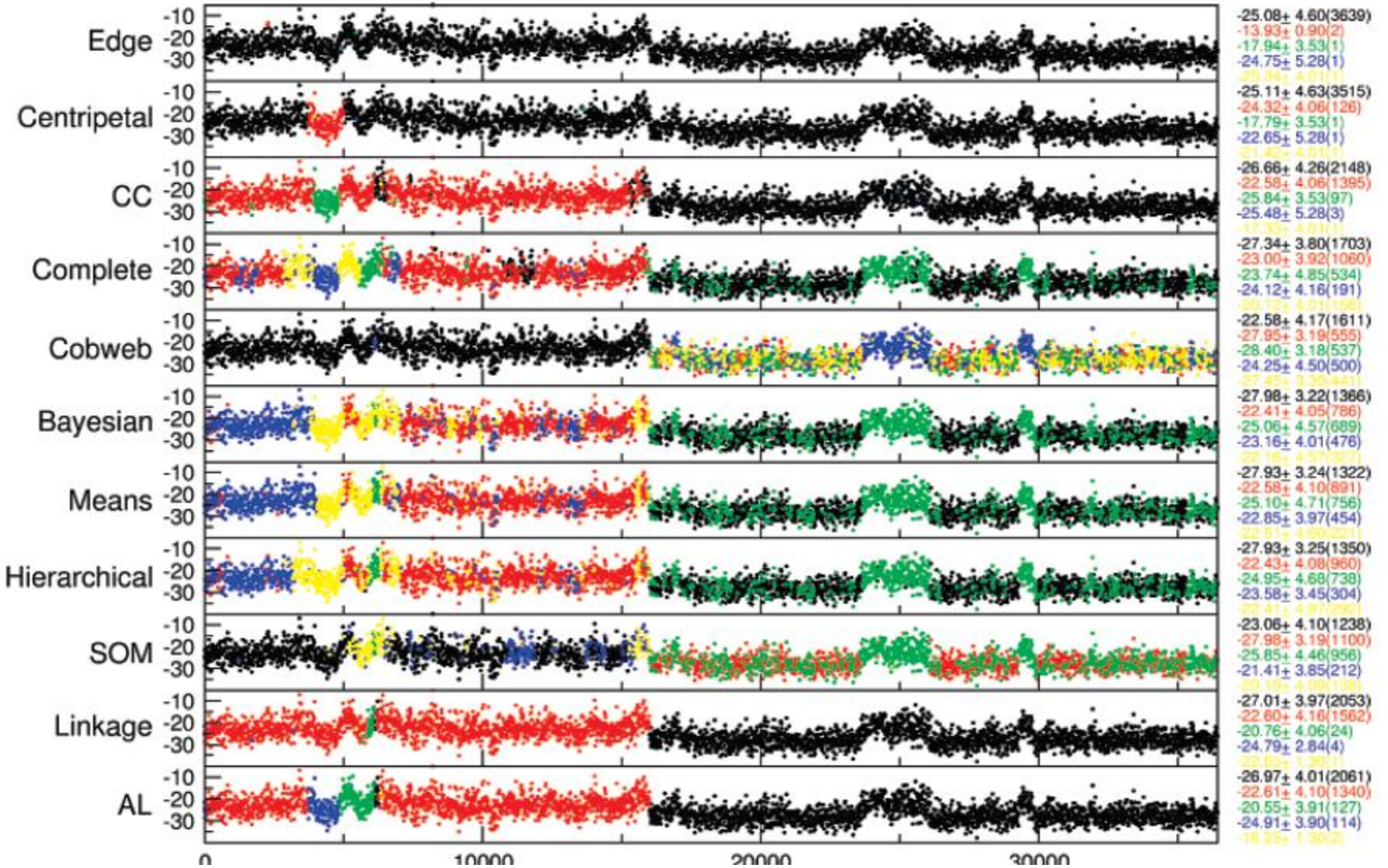


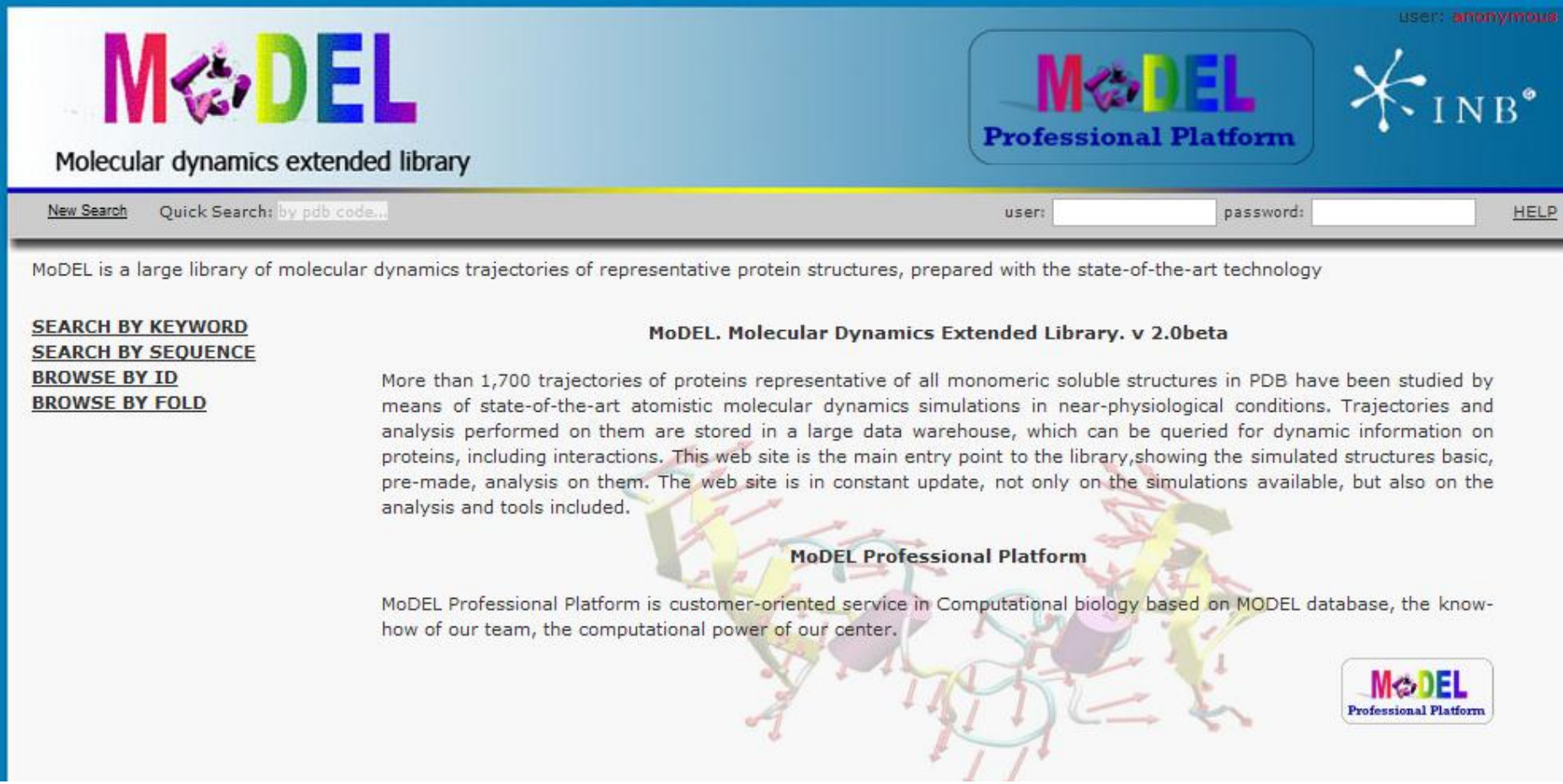
luster metrics for a subset of the algorithms investigated for the constructed polyA trajectory of five distinct equ
s as a function of cluster count (*x*-axis). At the optimal cluster count of 5, DBI is at a minimum, pSF is at a maxim



RMSD plot for frames

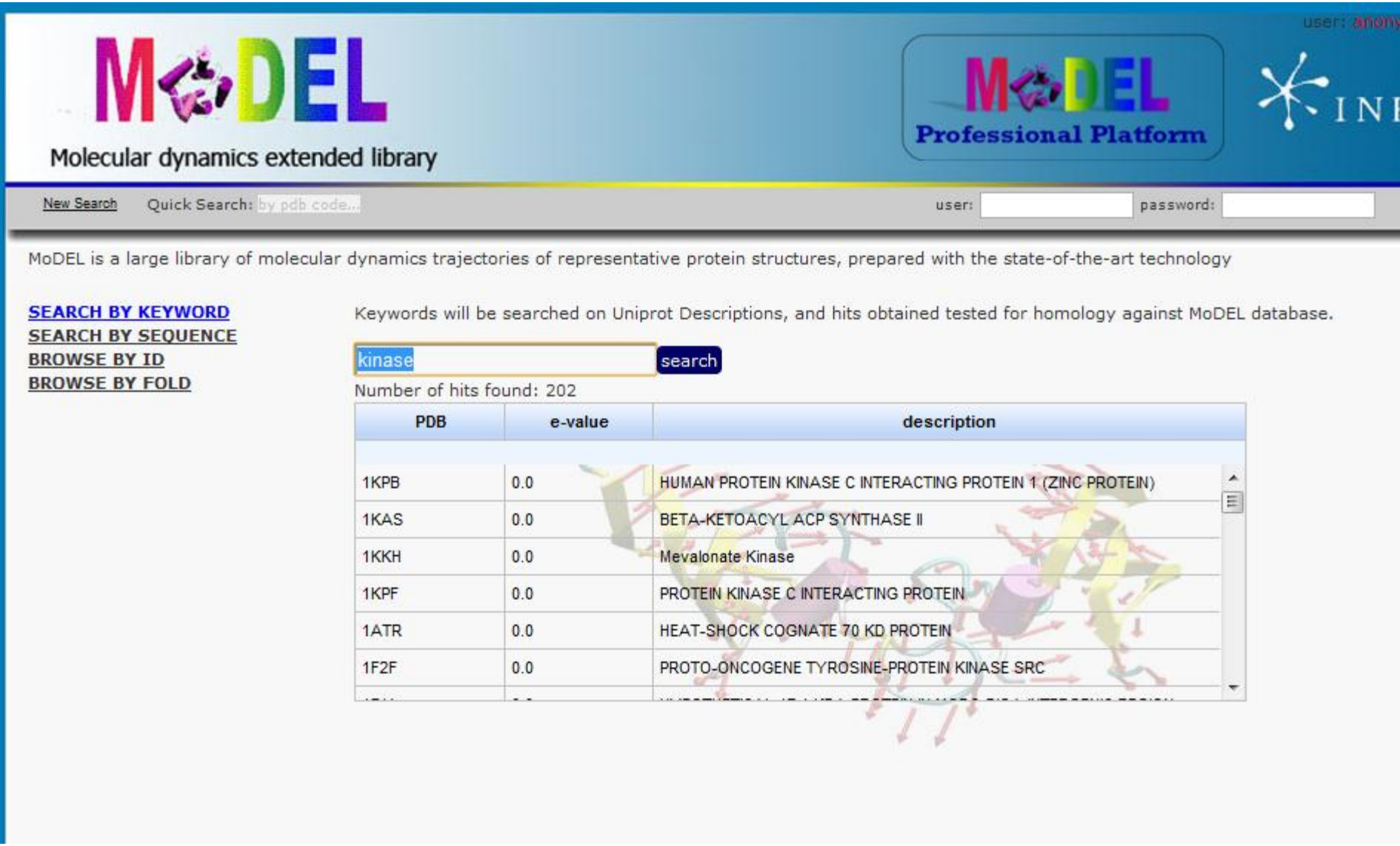
Plot for trajectories for different clustering algorithms





More than 1,700 trajectories of proteins representative of all monomeric soluble structures in PDB

Trajectories and analysis performed on them are stored in a large data warehouse, which can be queried for dynamic information on proteins, including interactions.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user:
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MoDEL is a large library of molecular dynamics trajectories of representative protein structures, prepared with the state-of-the-art technology
SEARCH BY KEYWORD
SEARCH BY SEQUENCE
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Keywords will be searched on Uniprot Descriptions, and hits obtained tested for homology against MoDEL database.
kinase
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Number of hits found: 202
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HUMAN PROTEIN KINASE C INTERACTING PROTEIN 1 (ZINC PROTEIN)
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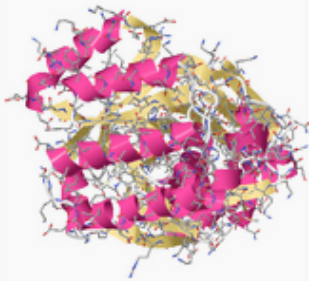
1KKH. Crystal Structure of the Methanococcus jannaschii Mevalonate Kinase



PDBSum
MSD
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Simulation: AMBER 8.0 P99 (T3P), 10000

Time Slice: 1 - 10000

Structure Fragment: (PRO A1 - ASN A317)

Program Version	AMBER8.0
Simulation time	10000 ps
Total atoms	55837
Force field	parm99 tip3P

more details:

GEOMETRY
SECONDARY STRUCTURE
FLEXIBILITY & DYNAMICS
INTERACTIONS & CONTACTS

Switch to 3D (Jmol)

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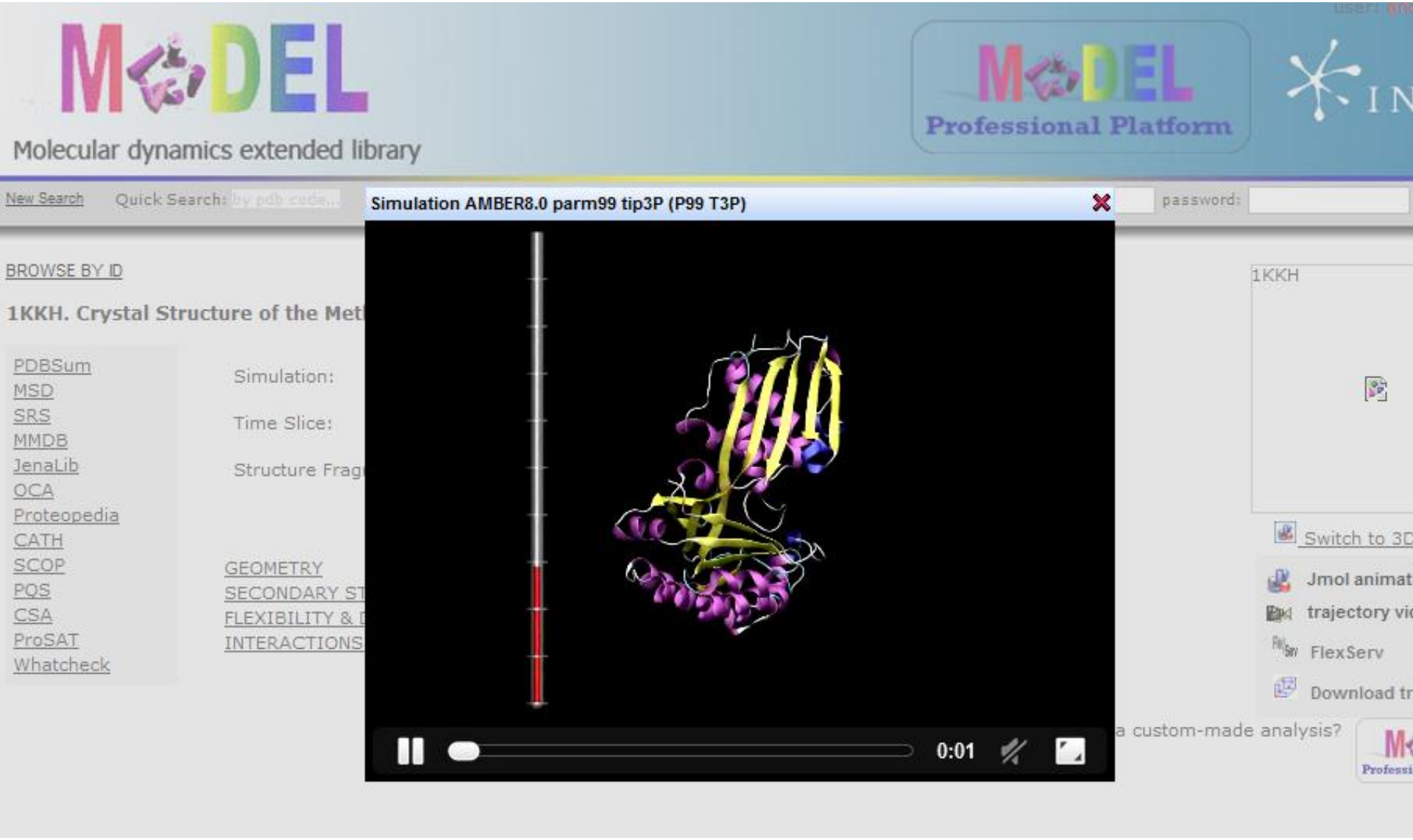
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a custom-made analysis?

References

- http://mmb.pcb.ub.es/MoDEL/
- http://oldcompbio.biosci.uq.edu.au/mediawiki/upload/6/6a/Clustering_molecular_dynamics_trajectories-I._Characterizing_the_performance_of_different_clustering_algorithms.pdf

THANK YOU