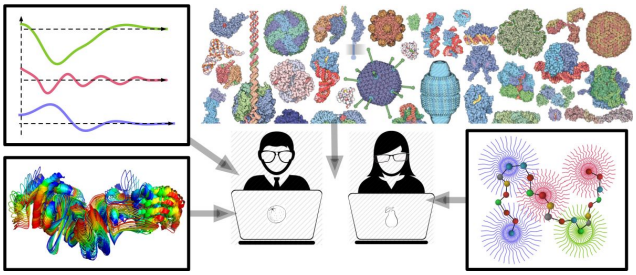

Contribution ID: **22** Type: **Poster**

Detailed analysis of a thermostable protein-DNA complex: the case of Sac7d as a prototype for protein-DNA interaction

Sac7d is a 7kDa protein belonging to the class of the small chromosomal proteins from archeon Sulfolobus acidocaldarius. Sac7d was discovered in 1974 in Yellowtone National Parks geysers, and studied extensively since then for its remarkable stability at large pH and temperature ranges. Sac7d binds to DNA minor groove to protect DNA from these extreme conditions by increasing its melting temperature.
In this study, we analyzed the Sac7d-DNA complex using 1 µs molecular dynamics simulations. The interaction energy ofthe interface was decomposed using Molecular Mechanics Generalized Born Surface Area (MM/GBSA) to determine at the amino acids level which residue contributed most to DNA binding. Twelve amino acids are essential for DNA binding, out of which three were not identified previously by former studies.
One of these new aminoacids, R63, may be involved in a dynamic protein-DNA interaction. Our analysis provides novel insights into how the Sac7d chaperones allows to protect DNA from degradation in extreme conditions.

Submitting to:

8th CAPRI assessment meeting

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