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MSSP: simultaneous comparison of the same structure descriptor for different protein structures

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Short Abstract: The Multiple Structures - Single Parameter STING module allows a user to compare variety of structure parameters from different protein structures in a simple yet intuitive 2D plot. The parameters which can be used for the analysis are those stored in the STING_DB (Neshich et al., 2005).

Long Abstract:
Investigation of similarities and differences in structural parameters, cross referenced to sequence, stability and function parameters of proteins, can be a starting point for the classification of proteins and understanding of the variation in biological function originating from the subtle differences in their structure.

Multiple Structure Single Parameter (MSSP) is a web based tool to visually survey, in different protein structures, differences and/or similarities in a certain structure descriptor/parameter. For each chain selected among the query structures, a graphics is presented showing the numerical values of the chosen parameter in the Y-axis and the sequence residue numbers in the X-axis. The parameters to be displayed can be chosen from the Sting database, which contains data for 310 different parameters. The choice for parameters range from electrostatic potential, conservation, temperature factor, accessibility, hydrophobicity, distance from N-terminal, amino-acid co-evolution, order of cross links and others.

Owing to the structural genomics initiatives there will be increasing numbers of proteins whose structures are available and their biological function waiting to be determined. The availability of objective protein analysis at the residue level can help the high-throughput computational structure analysis. The MSSP module makes it easy to quickly grasp differences and/or similarities in protein structures, regarding one chosen structural parameter.
In this work we present number of co-related parameters, chosen to be presented each at the time for number of structures, grouped as homologous and non-homologous ones to the main query structure. The results are presented in terms of protein classification and in terms of importance of each parameter for classification characterization of structures.
As an example of use of this tool, a graphical visualizations of four PDB files: 1gwd (chain A),

1jkc (single chain), 1vgc (chain B) and 1aks (chain A), and the parameters: distance from N-Terminal, electrostatic potential at surface and relative entropy, clearly distinguished the proteins in two different families: proteins 1vgc and 1aks are serine proteases, and proteins 1gwd and 1jkc are lysozymes.