

STING - A web server for comprehensive analysis of protein structure and sequence

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STING is a web based suite of programs that brings together a number of analysis tools at a single web server for a comprehensive analysis of the relationship between protein sequence, structure, function and stability. Using STING it is possible to analyze: sequence to structure relationships, quality of the structure, nature and volume of atomic contacts of intra and inter chain type, relative conservation of amino acids at the specific sequence position based on multiple sequence alignment, indications of folding essential residues based on relationship of the residue conservation to the intra-chain contacts, cavities in the protein structure, etc.. The STING server can handle local files containing protein structures (either modeled or not yet deposited to the PDB) so that they can be used by the principal STING components: ^{Java}Protein Dossier (JPD) and STING Report. JPD not only displays and quantifies physicochemical properties of proteins at a residue-by-residue level but also allows mapping these properties on the three-dimensional structure. Structurally aligned macromolecules can be displayed and analyzed.

STING has the capability to present the largest number of descriptors for the sequence, structure, function, stability and binding in a concise and visually compelling way, as well as the capability to select/focus for/at those residues which satisfy a user defined parameter/descriptor values. This feature allows that some very interesting and important questions can be answered, such as: Is there a set of parameters (protein structure descriptors) which can define UNIQUELY an amino acid ensemble coinciding with the active site of a given protein or coinciding with amino acids identified experimentally as crucial for the folding / stability.

The demonstration will cover:

- Accessing basic and advanced STING features
- Applications: identification of active sites and folding essential residues by STING
- Sting key components: JavaProtein Dossier and STING Report
- Local file submission to STING server: generating 306 different structure/function parameters

The STING database is updated weekly, in synchrony with the PDB updates. STING is public available at <http://sms.cbi.cnptia.embrapa.br> and <http://trantor.bioc.columbia.edu/SMS>. The requirements to run STING are: a web server, Java plug-in 1.3.1 and Chime plug-in.

References:

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