Laboratory of Structural Biology & Bioinformatics

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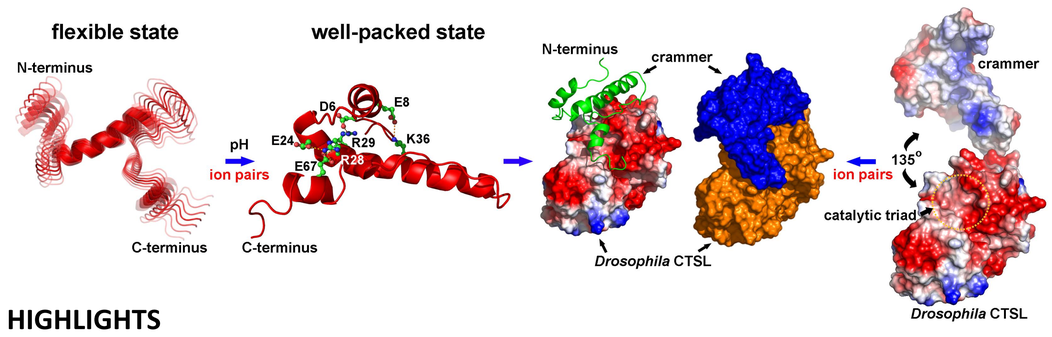
Structural Biology

Our laboratory concentrates on the structure, function and design of peptides and proteins.

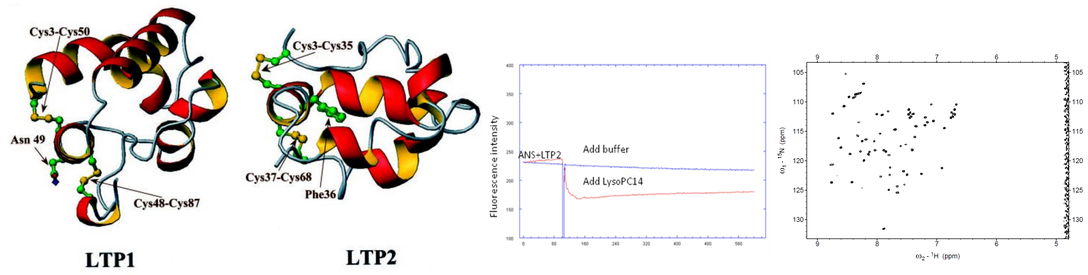
Characterization of a Novel Cysteine Protease Inhibitor, Crammer, from *Drosophila melanogaster* and its Potential Role in Cathepsin Regulation



HIGHLIGHTS

1. Cys72 in crammer is essential for cathepsin inhibition and dimer formation.
2. Monomeric crammer is a strong competitive inhibitor of Drosophila cathepsin.
3. We present the first 3D structure of a propeptide-like protease inhibitor.
4. To function, crammer undergoes a molten globule-to-ordered structure transition.

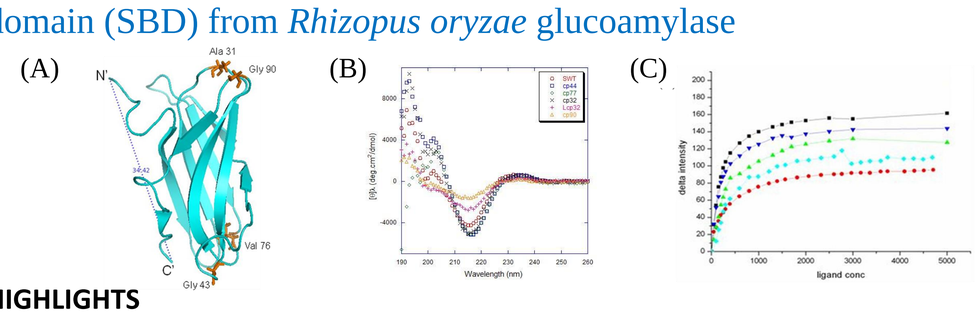
Purification, Characterization and Functional Comparison of Rice Non-specific Lipid Transfer Protein 2 (nsLTP2) and nsLTP3



HIGHLIGHTS

1. Plant nsLTPs are small and basic proteins and can be divided into LTP1 and LTP2.
2. Some anther-specific proteins which are named as LTP3 have considerable homologies with plant nsLTPs.
3. LTP2 displays both lipid binding and transfer activities while LTP3 do not interact with lipid.

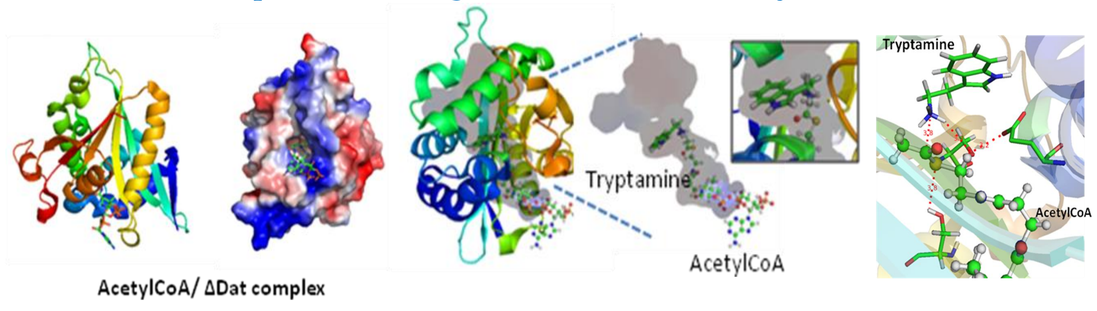
Investigation of the effects of circular permutation on starch-binding domain (SBD) from *Rhizopus oryzae* glucoamylase



HIGHLIGHTS

1. A protein engineering strategy, circular permutation, can be applied to SBD and viable cp mutants can be created.
2. One of the permutants, cp90, exhibits superior biological function to the wild type.

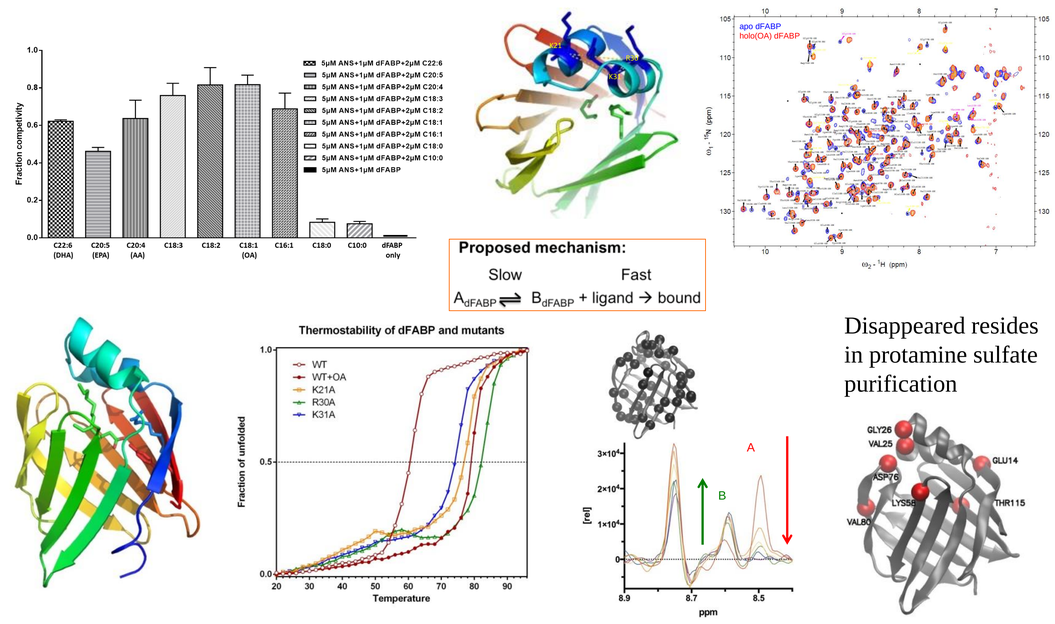
Crystal Structure of Dopamine *N*-acetyltransferase in Complex with Acetyl CoA from *Drosophila Melanogaster* Reveals a Catalytic Mechanism



HIGHLIGHTS

1. The X-ray structure of dopamine *N*-acetyltransferase bound to acetyl coenzyme A (AcCoA) has been determined at 1.46 Å .
2. Based on complex structure and ternary complex docking model, the potential catalytic triads are proposed.
3. The results of site-directed mutagenesis studies and kinetic analysis support the proposed reaction mechanism of catalysis of dopamine *N*-acetyltransferase.

Role of Drosophila Memory Related Fatty Acid Binding Protein on Transporting Fatty Acids



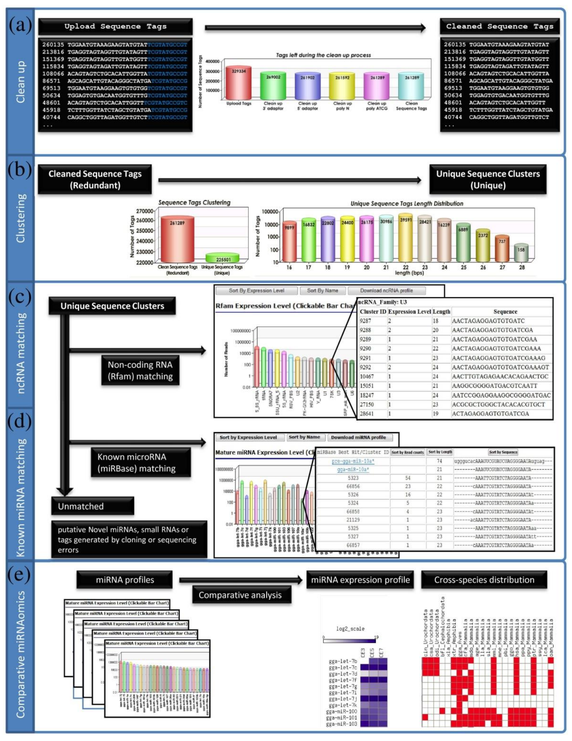
HIGHLIGHTS

1. X-ray structure of fatty acid-binding protein (FABP) has been determined of 1.86 Å .
2. Ligand binding conserved sites, R125 and Y127, within beta clamps were identified.
3. The binding affinity of dFABP is carefully **balanced between structural stability and flexibility**.
4. apo-dFABP may accommodate ligands (long chain fatty acids) from membrane and then dissociate as holo-dFABP.

Structural Bioinformatics

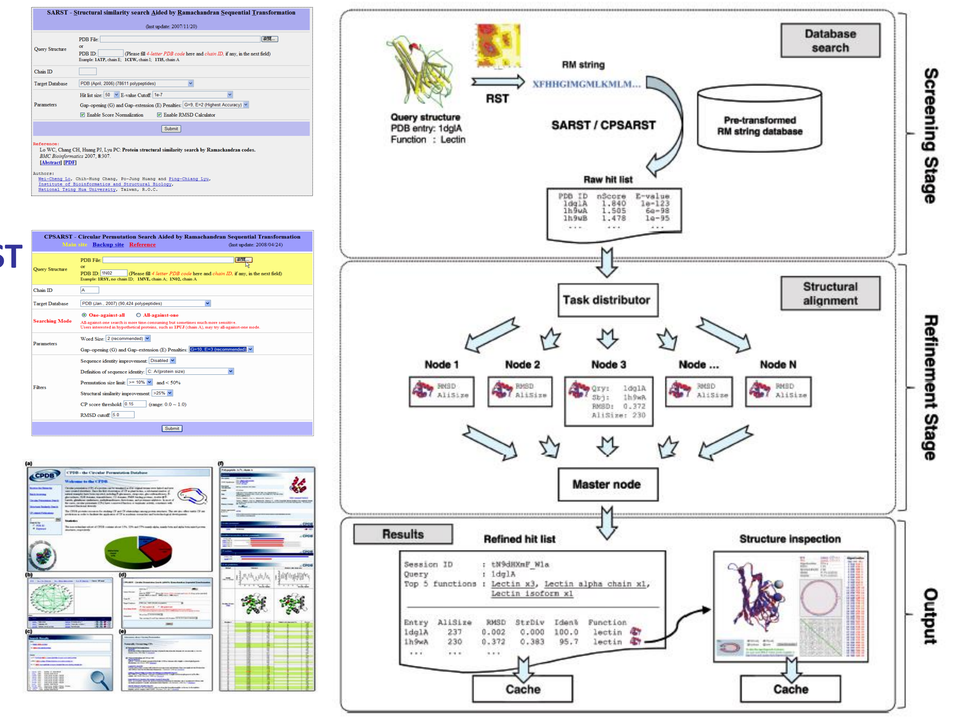
Our research focuses on bio-database construction, protein structure comparison, protein structure modeling, and computer-aid drug design.

DSAP- Deep-Sequencing Small RNA Analysis Pipeline



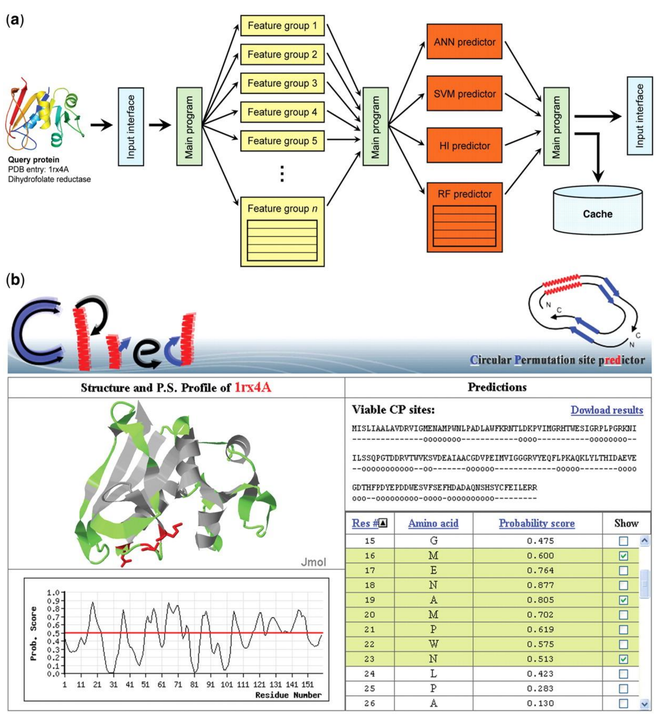
http://dsap.life.nthu.edu.tw/

iSARST: an Integrated SARST Web Server for Rapid Protein Structural Similarity Searches



http://sarst.life.nthu.edu.tw/isarst/

CPred: a web server for predicting viable circular permutations in proteins



http://sarst.life.nthu.edu.tw/CPred/