Web Predictors at http://www.biocomp.unibo.it

CORNET/ Predictor of Residue Contacts in Proteins

CYSPRED/ Predictor of Bonding State of Cysteines in Proteins

DCON/ Predictor of Disulfide Connectivity in Proteins

RCNPRED/ Predictor of Residue Coordination Numbers in Proteins

SECPRED/ Predictor of Secondary Structures of Proteins

ISPRED/ Predictor of Protein Interaction Sites

I-MUTANT/ Predictor of Protein Stability Changes upon Single Point Mutation

B2TMR/ Predictor of Transmembrane Topology of all-beta Membrane Proteins (Neural Network-based)

HMM-B2TMR/ Predictor of Transmembrane Topology of all-beta Membrane Proteins (Hidden Markov Model-based)

HTMR/ Predictor of Transmembrane Topology of all-alpha Membrane Proteins (NN based)

SPEPLip/ Predictor of Signal Peptide and Lipoprotein Cleavage Sites in Proteins

Curated Databases at http://www.biocomp.unibo.it

ZenPatches/ Predicted Protein-Protein Interacting Surface Patches in collaboration with BioDec (www.biodec.com)

TOPDB/ Proteins from thermophiles and their counterparts in mesophiles

The research interests of **The Biocomputing Group** focus on different aspects of protein sequence analysis, mainly the implementation of predictive algorithms based on different machine learning approaches. The Biocomputing Group organises International Advanced Schools on Bioinformatics at the Bologna University since 1999.

The Biocomputing Group is presently also:

> Node of the BioSapiens Network of Excellence

> Italian node of the FIRB project "Bioinformatics for Genomics and Proteomics"

> Member of the European Computational Biology Community (ECCB)

The **Biocomputing Group** of the University of Bologna

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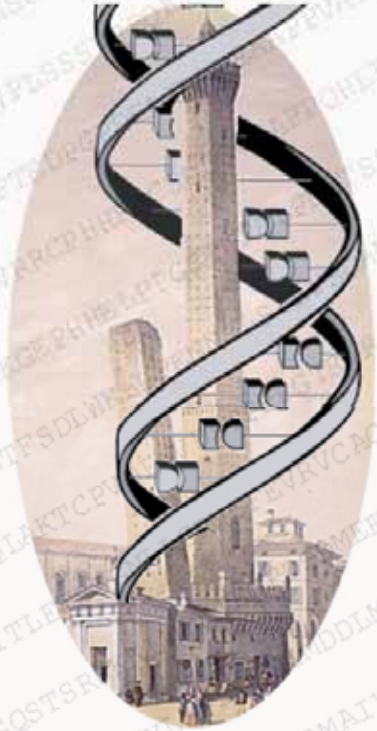
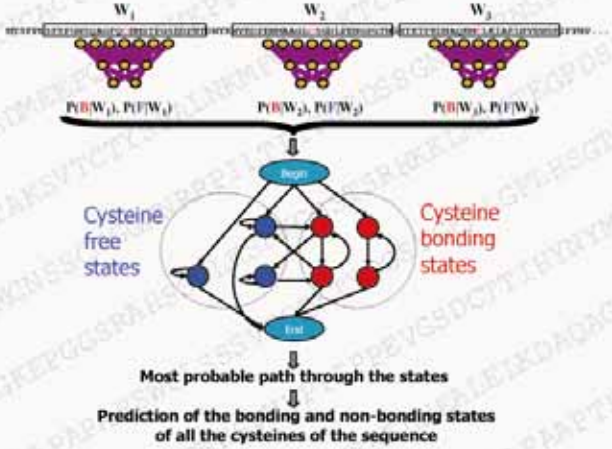


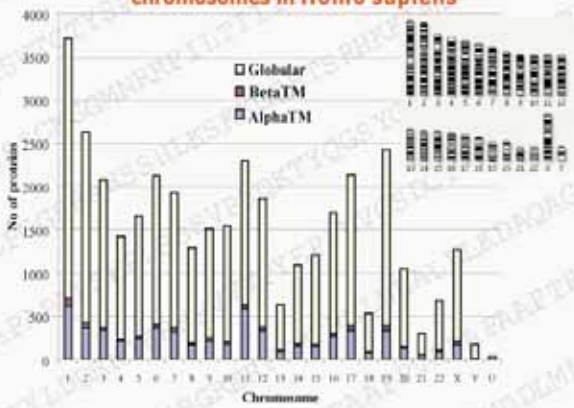
> Protein Biosequence Analysis
> Protein Modelling
> Prediction of
  - Protein Secondary Structure
  - Contact Map
  - Protein Folding
  - Bonding State of Cysteines
  - Topology of Disulfide Bridges
  - Protein Stability upon Mutation
> Protein and Peptide Design
> Molecular Docking
> Molecular Dynamics

CYSPRED2 predicts the disulfide-bonding state of cysteines in proteins at 88% accuracy starting from the residue sequence. It is a new hybrid system that combines a neural network and a hidden Markov model (Hidden Neural Network).



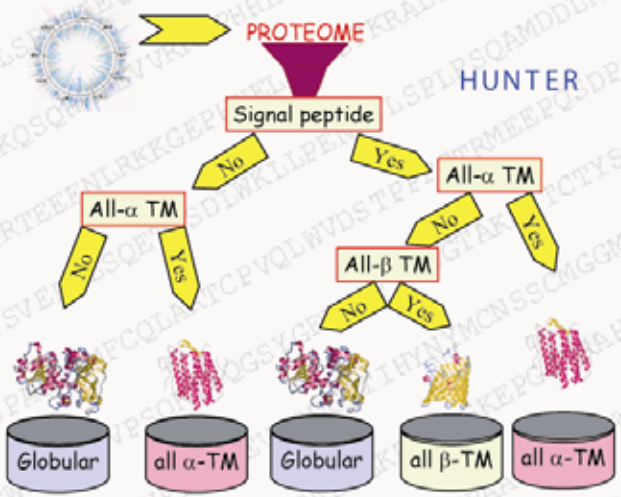
MANHUNTER is a suite of programs for the annotation of the human genome on the basis of structure prediction, including membrane proteins.

Distribution of the different protein structures among the chromosomes in Homo sapiens

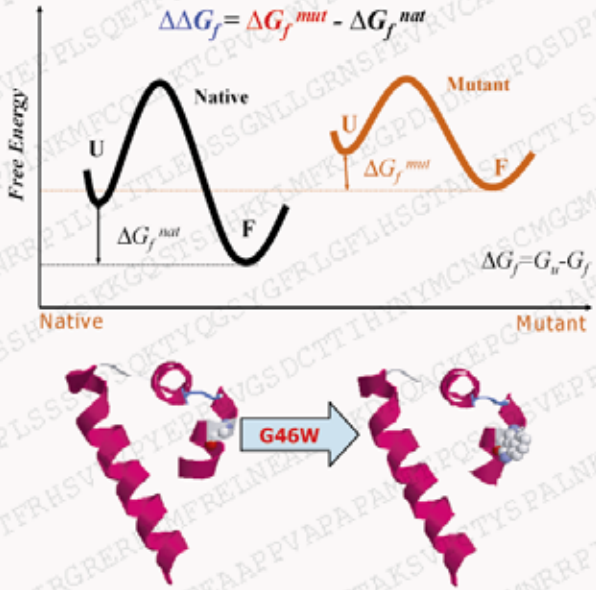


TOPDB is a novel derived database of proteins for highlighting determinants of thermostability in proteins via a direct structural comparison of similar proteins in thermophilic and mesophilic organisms. TOPDB contains about 2200 protein structures from 102 different species.

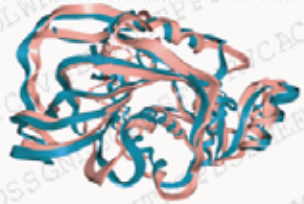
HUNTER is an integrated suite of programs specifically developed for predicting the occurrence of signal peptides in proteins of Gram-negative bacteria, the topography of all-alpha and all-beta membrane proteins, and the genome annotation on structural bases.



I-Mutant is a Support Vector Machine-based web server for the automatic prediction of protein stability changes upon single-site mutations.



Molecular Modelling with expert-driven procedures: models when sequence identity is below 30%. A success story: the low-resolution 3D model of the tetrameric alcohol dehydrogenase from Sulfolobus solfataricus was computed before the 3D structure was available (the root mean square deviation of the model to the structure is 0.25nm).



ZenPatches is a database containing the protein-protein interacting surface patches predicted for the whole PDB.