Haloalkane dehalogenases:
phylogenetics, characterization, modelling, engineering

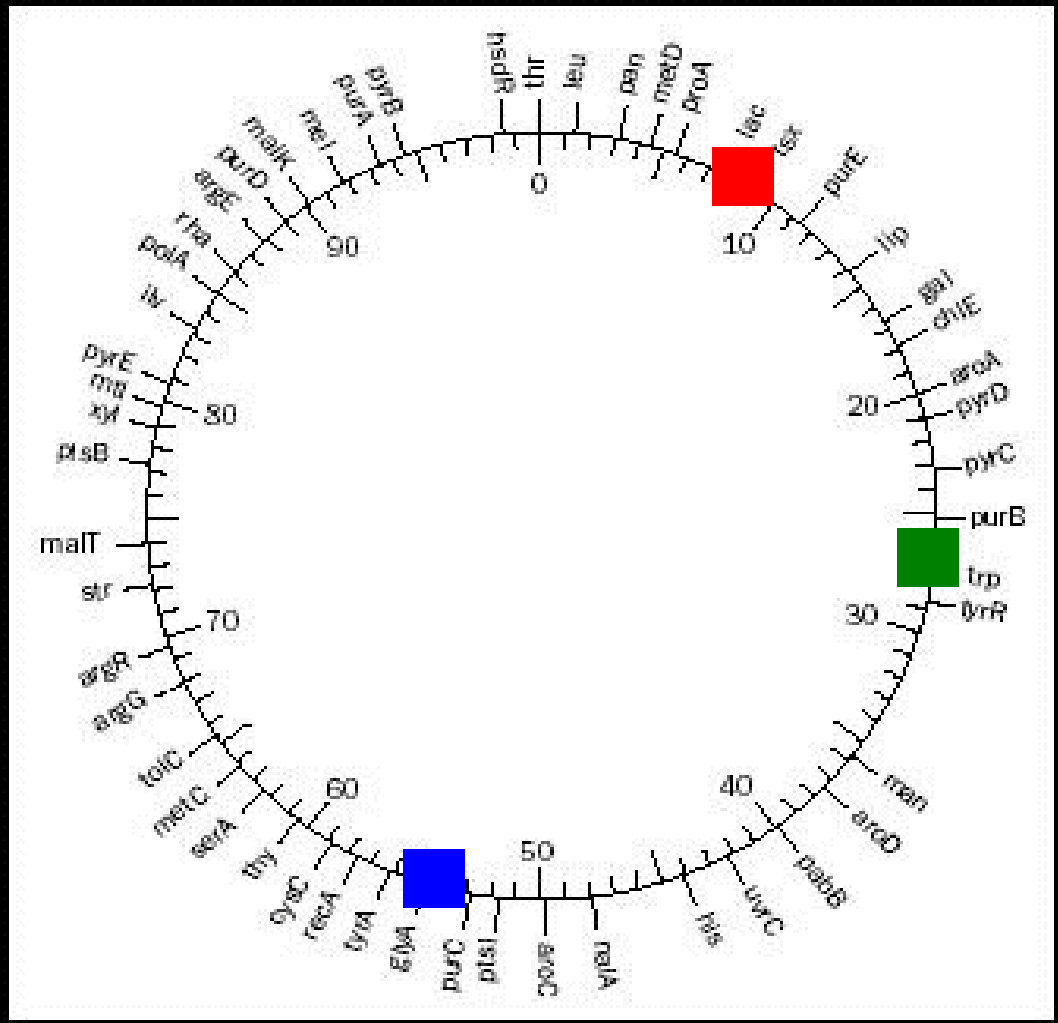
Protein Engineering Group

Loschmidt Laboratories, Masaryk University

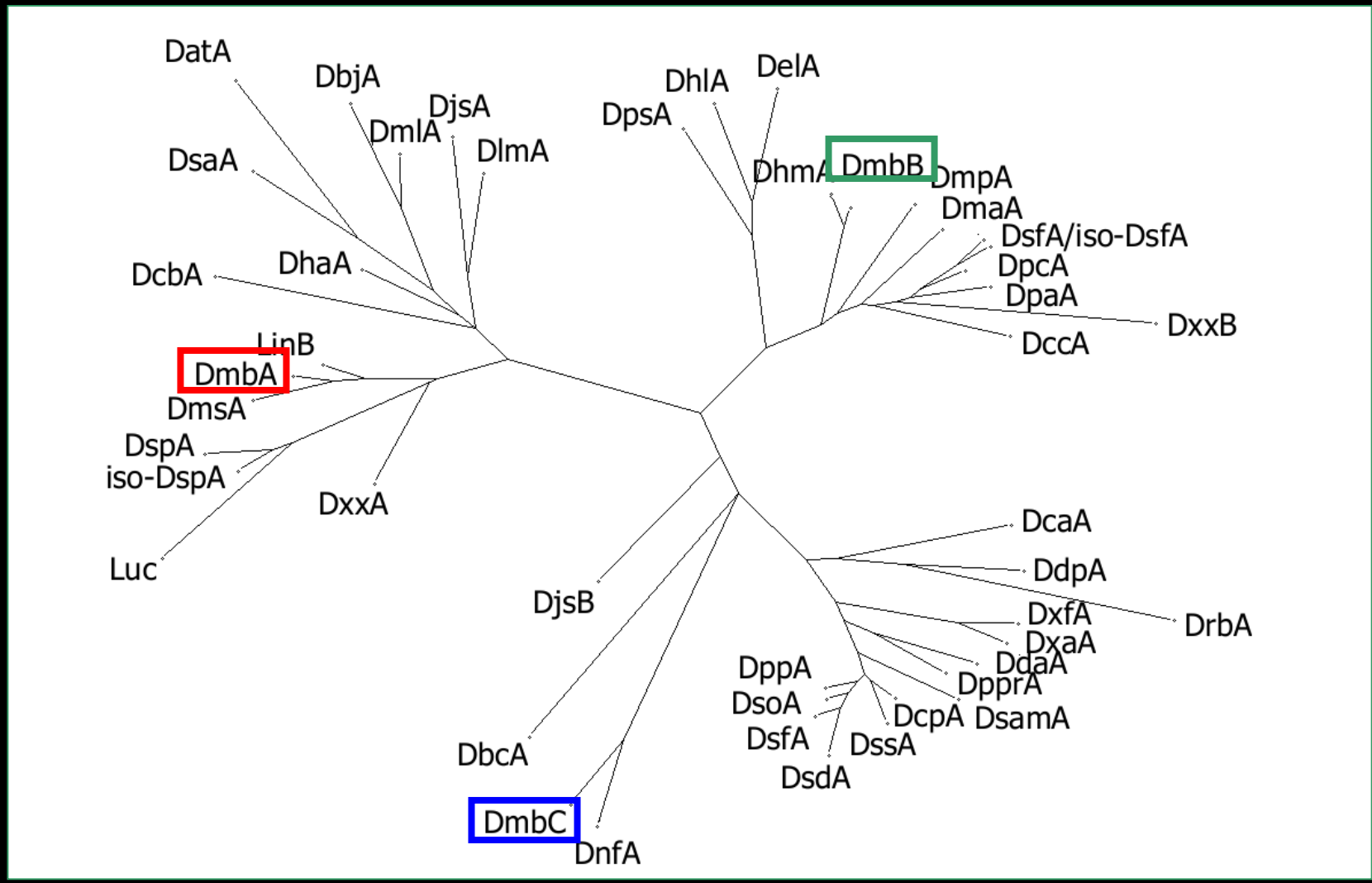
Projects

- Phylogenetics
  - screening of sequences in protein databases
  - re-construction of phylogenetic tree
  - identification of new family members
  - prediction of novel activities, catalytic promiscuity
- Isolation of novel enzymes
  - DbeA from *Bradyrhizobium elkani*
  - DmbC from *Mycobacterium tuberculosis*
  - DrbA from *Rhodopirullela baltica*
  - purification, biochemical & structural characterization

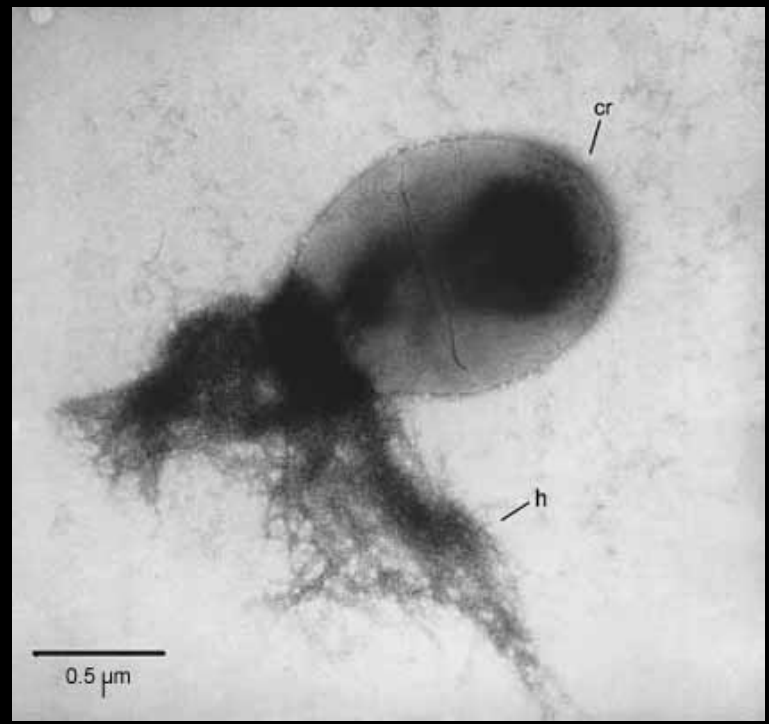
DmbA, DmbB and DmbC from *Mycobacterium tuberculosis*



DmbA, DmbB and DmbC from *Mycobacterium tuberculosis*



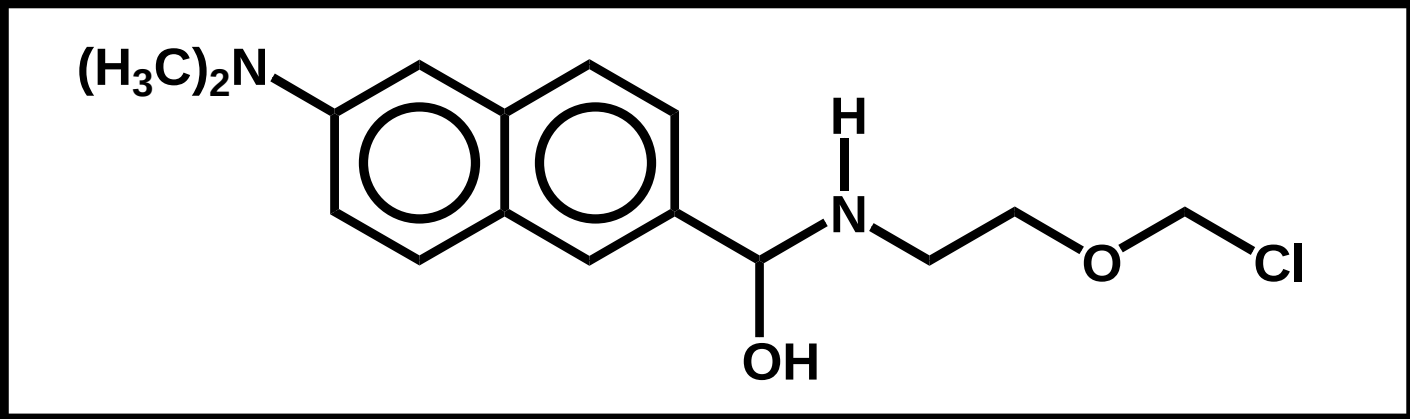
DrbA from *Rhodopirullela baltica*

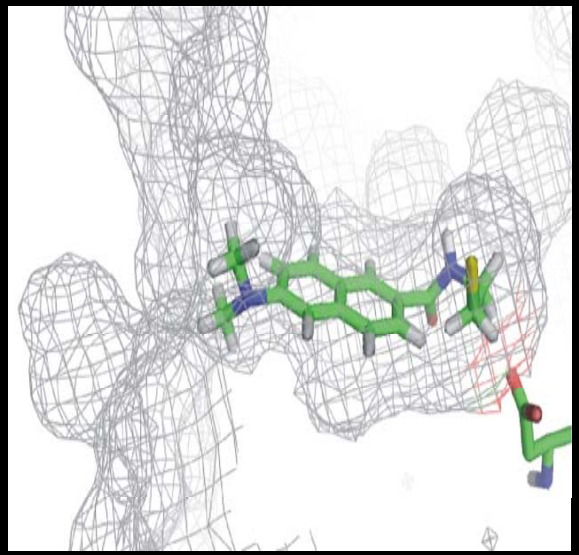


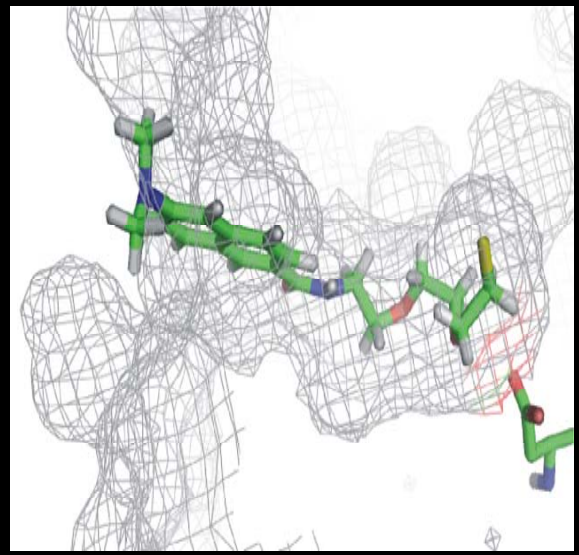
Projects

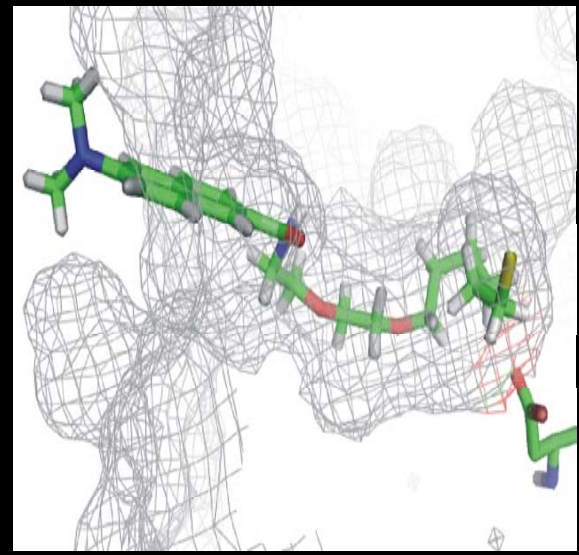
- Enantioselectivity
  - substrate mapping
  - structural analysis of DbjA and its mutant
  - site-directed mutagenesis & directed evolution
- Solvent relaxation
  - design of fluorescence probes
  - construction of mutants
  - chemical synthesis of probes
  - femtosecond spectroscopy, molecular dynamics

Fluorescence probes

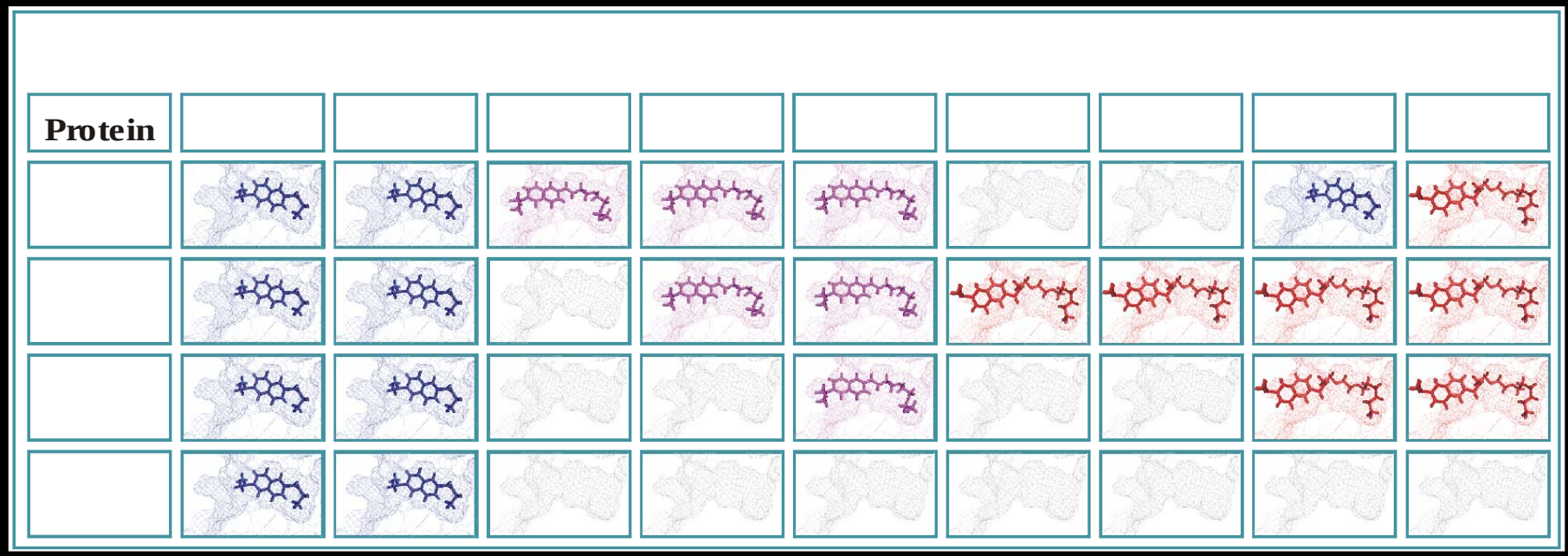








Fluorescence probes



Projects

- Engineering for 1,1-dichloromethane
  - design of mutation L263W (Rebecca)
  - COMBINE analysis of L263W protein
  - construction of mutant → negative result
  - plan: directed evolution
- Engineering for 1,2,3-trichloropropane
  - modelling of DhaA mutants
  - dissecting mechanism (access paths)
  - RAMD, identification of hot-spots
  - directed evolution

Projects

- Development of COMBINE
  - data matrix prepared for “classical” COMBINE for DhlA and DhaA [data Schindler]
  - data matrix prepared for “ab initio” COMBINE for DhlA and LinB [data Brno]

- Development of virtual reality for proteins
  - development of program CAVER
  - new algorithm based on Voronoi diagram
  - new software for engineering of import/export paths
  - virtual reality

Program CAVER

Caver - Microsoft Internet Explorer

Soubor Úpravy Zobrazit Oblíbené Nástroje Nápověda

Zpět Hledat Oblíbené

Adresa http://loschmidt.chemi.muni.cz/caver/ Přejít

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CAVER ... *secure caving in the world of biomolecules*

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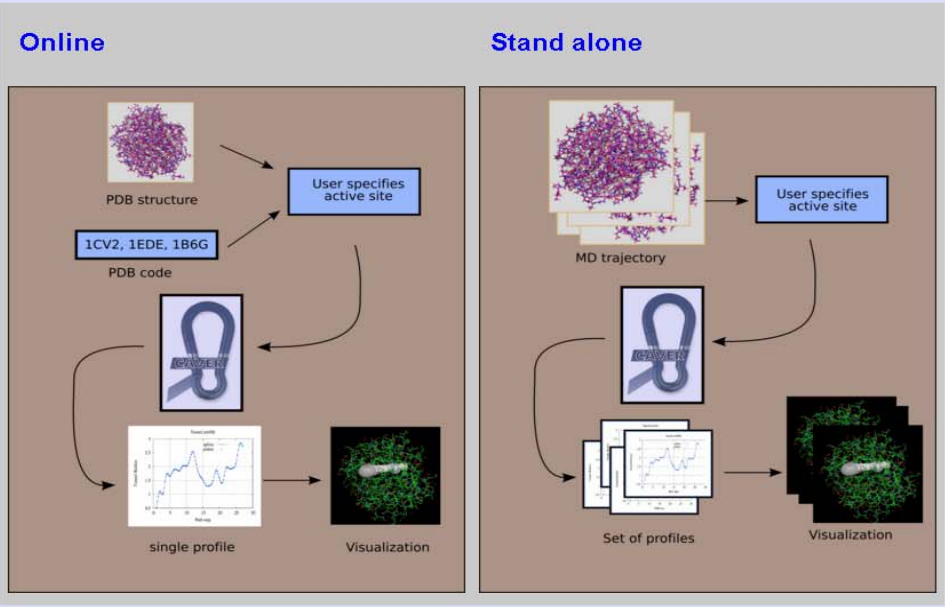
59 registrated users

Main

CAVER provides rapid, accurate and fully automated calculation of pathways leading from buried cavities to outside solvent in static and dynamic protein structures. Study of these pathways is important in *drug design* and *molecular enzymology* to understand binding of inhibitors to the receptors, substrate binding and product egress from the enzyme active sites. Calculated pathways can be visualized by graphic program PyMol dissecting anatomy and dynamics of entrance tunnels.

CAVER is available as online version or PyMol plugin suitable for calculation of pathways in discrete protein structures and stand alone version enabling analysis of trajectories from the molecular dynamics simulations.



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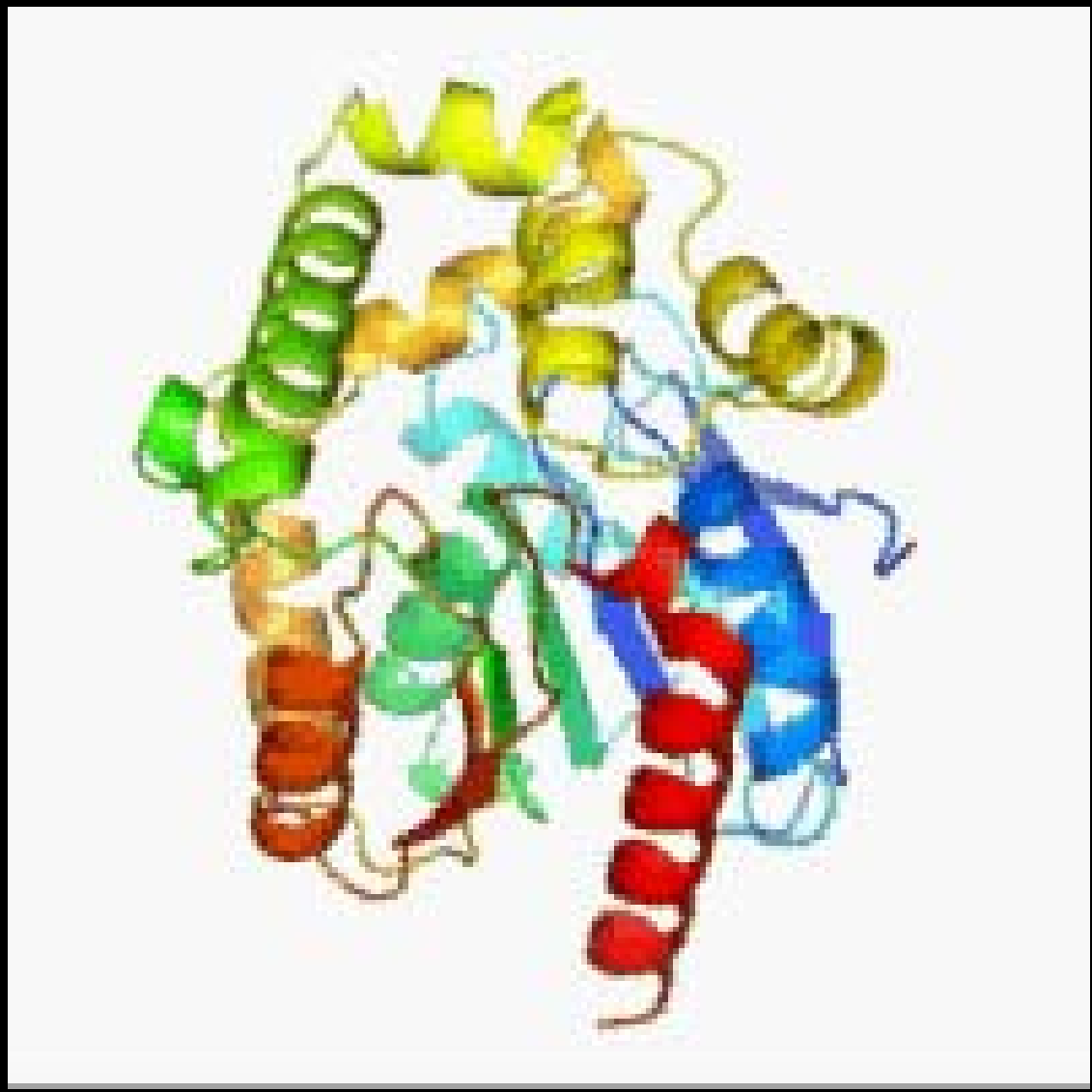
Hotovo Místní intranet

CAVER Methodology



CAVER Visualisation