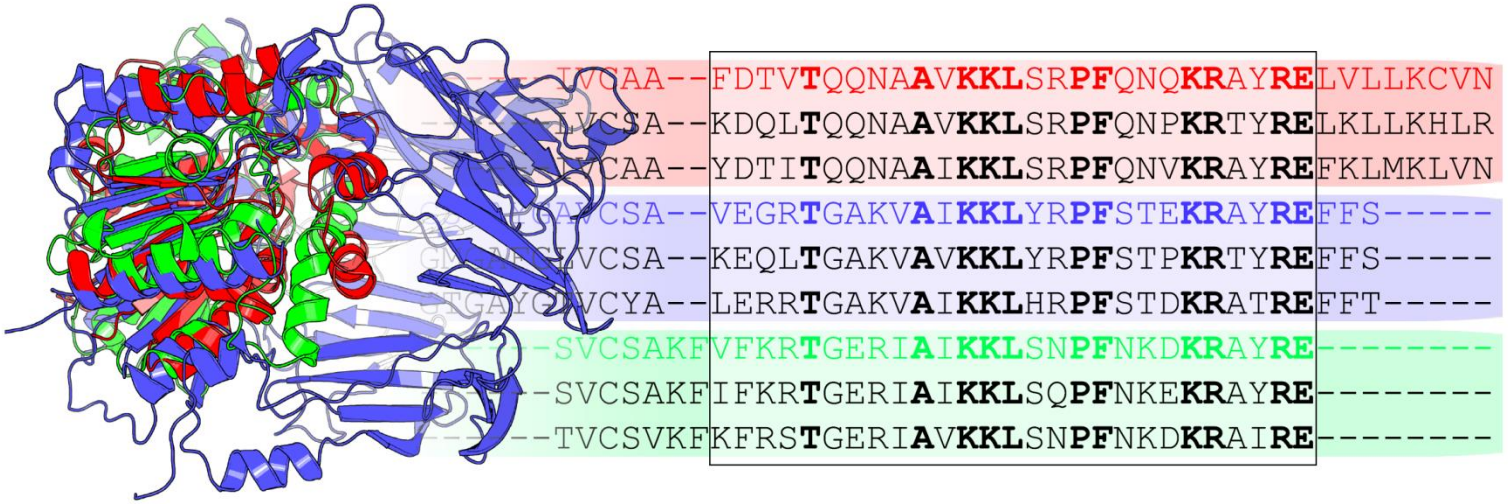
Mustguseal

Open-access on-line platform for bioinformatic analysis in computational enzymology



https://biokinet.belozersky.msu.ru/m-platform

Introductory presentation
by Dmitry Suplatov
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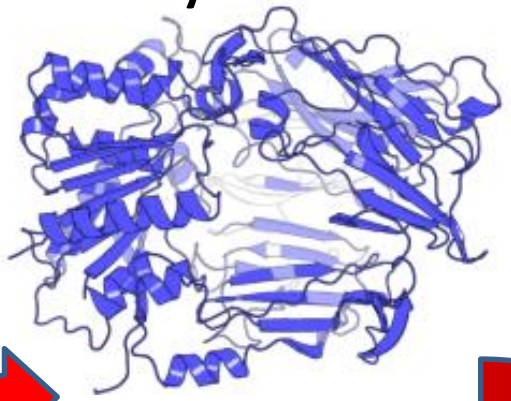
Lomonosov Moscow State University
Moscow, Russia
July 1st, 2020

The key concept

is to study the structure-function relationship of a particular protein by systematic bioinformatic analysis of the corresponding superfamily

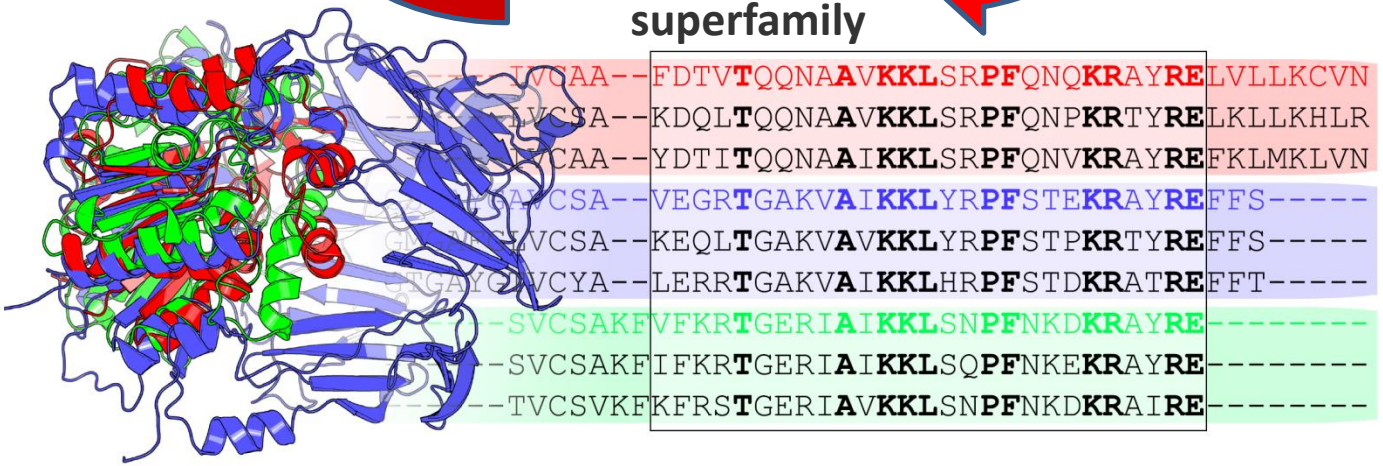


Protein of interest

Conclusions regarding the sequence/structure-function relationship in the particular protein

Collection and analysis of all the available sequence and structural data corresponding to the superfamily

Corresponding superfamily

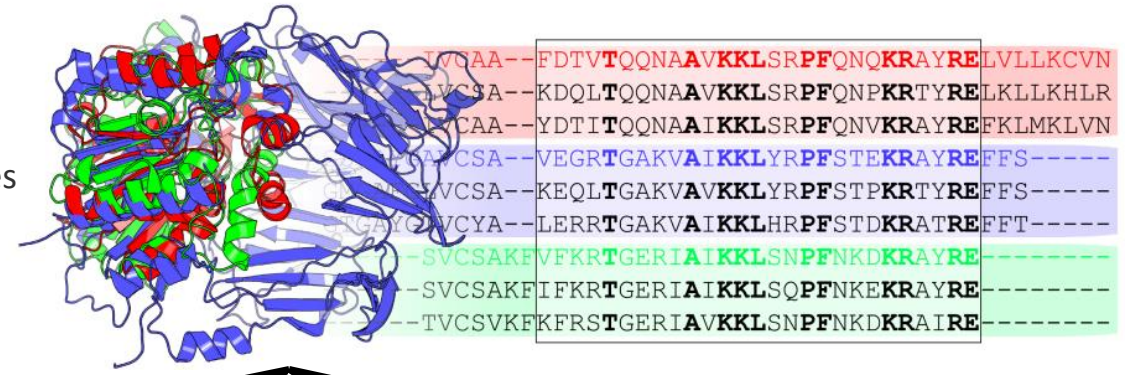


Open-access on-line platform for bioinformatic analysis in computational enzymology

Mustguseal

can automatically collect from public databases and align thousands of sequences and structures of proteins within a superfamily to produce a large structure-guided sequence alignment

Bioinformatics, 2018



Zebra2

To identify and prioritize **subfamily-specific and conserved positions** as the determinants of functional diversity and key catalytic/structural residues, respectively

Nucleic Acids Res., 2020

pocketZebra

To identify and rank **binding sites** in proteins by functional significance and select particular positions in the structure that are important for selective binding of substrates and ligands

Nucleic Acids Research, 2014

Yosshi

To systematically classify and study **disulfide bonds** in diverse protein families, and to assist at selecting hot-spots for disulfide engineering

Nucleic Acids Research, 2019

visualCMAT

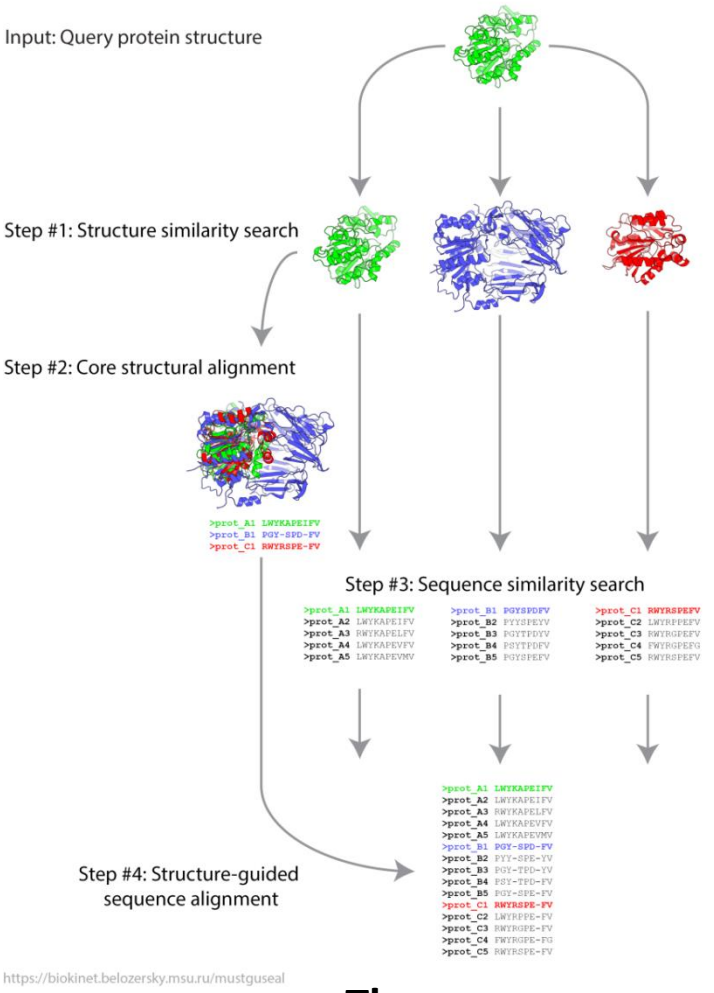
To predict and visualize **correlated mutations/co-evolving residues** in protein structures as a mechanism of allosteric communication, and a source of compensatory mutations for rational design

J Bioinform Comput Biol., 2018

https://biokinet.belozersky.msu.ru/m-platform

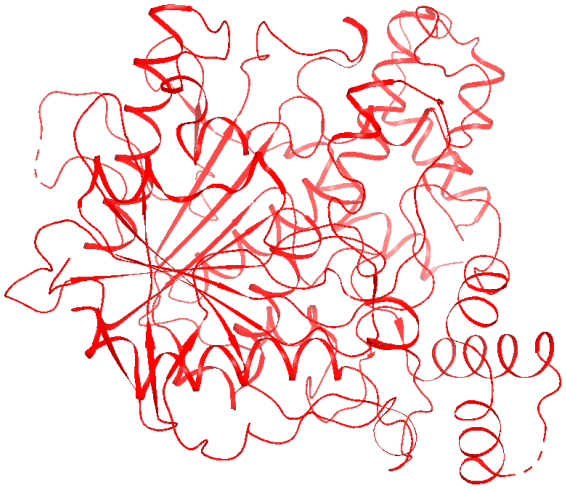
Automatic construction of a large structure-guided sequence alignment of your protein family by the Mustguseal

The input:
PDB structure of human acetylcholinesterase

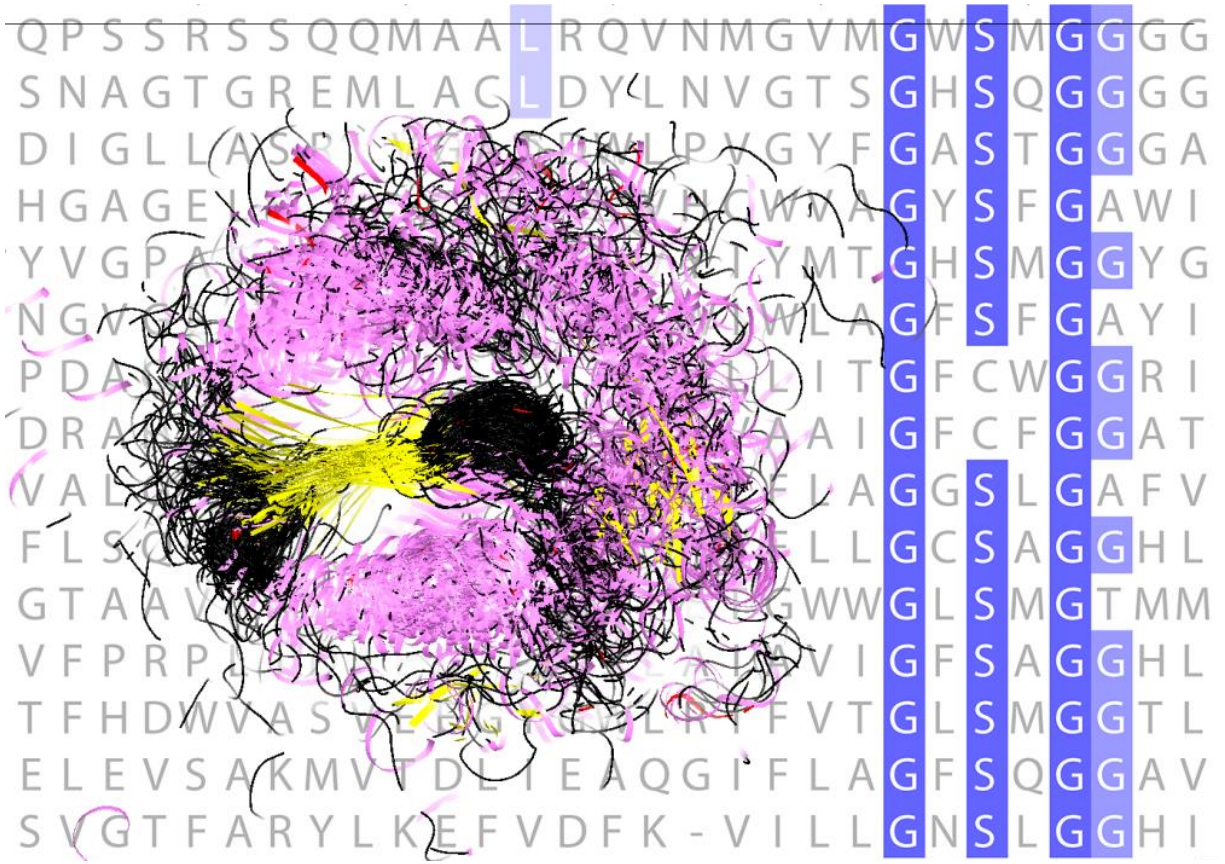


The process:
Automatic collection and alignment of all the available protein sequences and structures from public databases

Automatic construction of a large structure-guided sequence alignment of your protein family by the Mustguseal

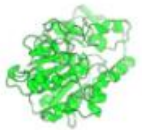


The input:
PDB structure of human acetylcholinesterase



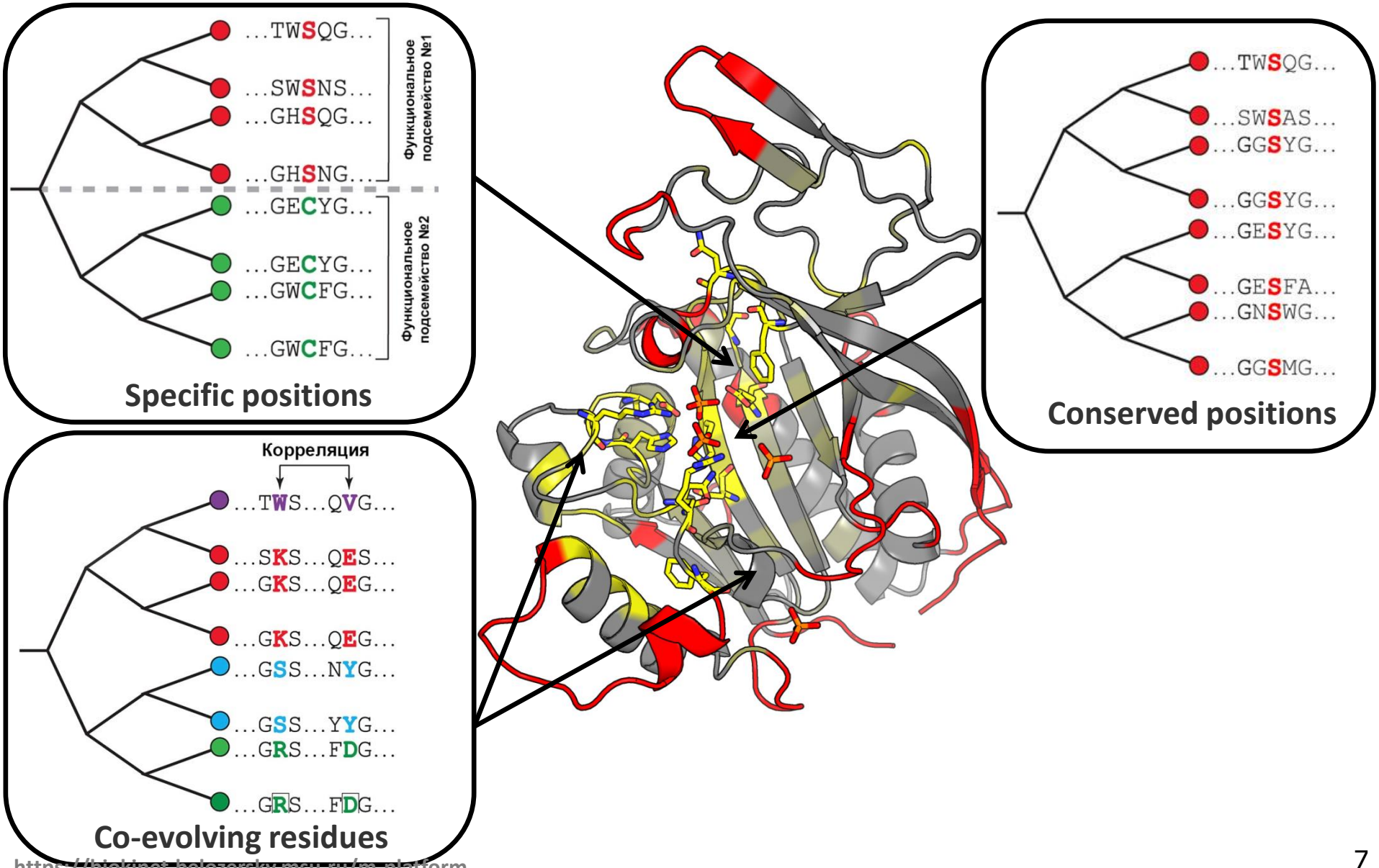
The output:
Structure guided-sequence alignment of human acetylcholinesterase and its homologs from the α/β-hydrolase superfamily

Submit the final Mustguseal alignment for further analysis

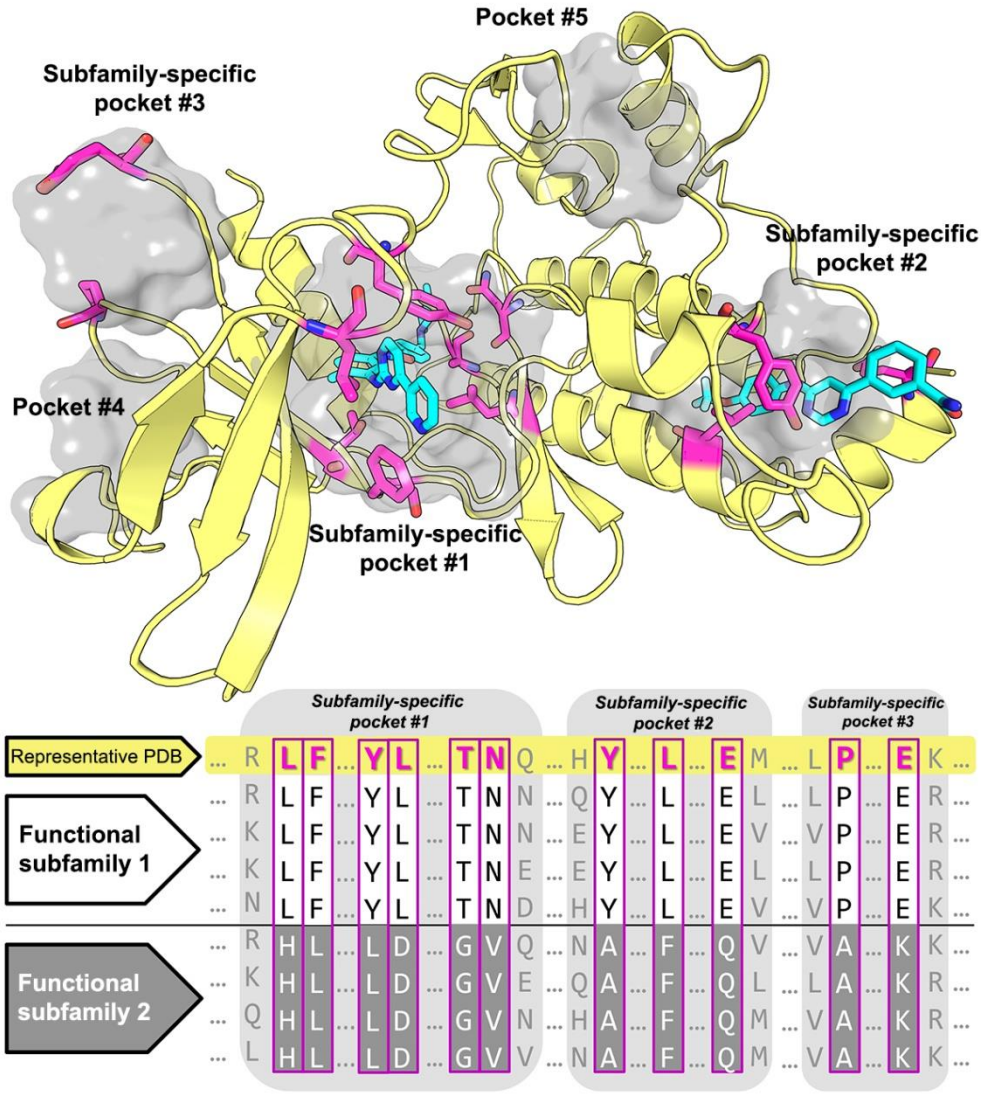
Submit the Final Mustguseal alignment	FINAL_A-ditxcb9jvnyuqz.fasta	12.0 MB		Submit to **Zebra**
Submit the Final Mustguseal alignment and a PDB structure of the representative protein	FINAL_A-ditxcb9jvnyuqz.fasta	12.0 MB		Submit to **Zebra**
				Submit to **pocketZebra**
	0_1u8f_O.pdb	166 KB		Submit to **visualCMAT**

- A new submission to Zebra, pocketZebra, visualCMAT, and Yosshi can be made directly from the Mustguseal Results page.

Annotation of the protein of interest according to the bioinformatic analysis of the superfamily



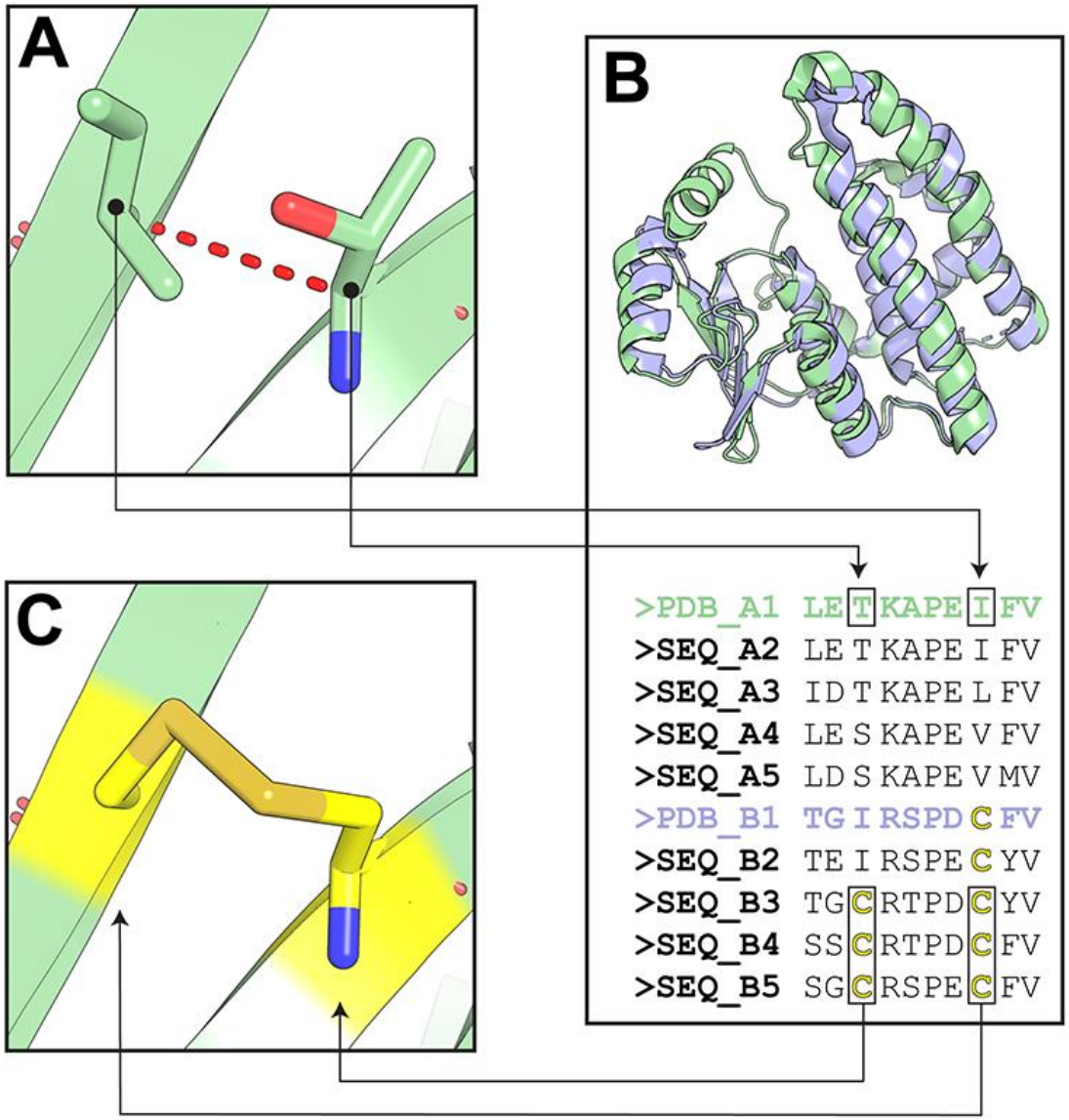
Identify and study the conserved and subfamily-specific positions



- The **Zebra** web-server can be used to identify and prioritize subfamily-specific and conserved positions in a functionally diverse superfamily and to select hot-spots for rational design of the query protein;
  Suplatov D., et al. (2020) *Nucl. Acids Res.*

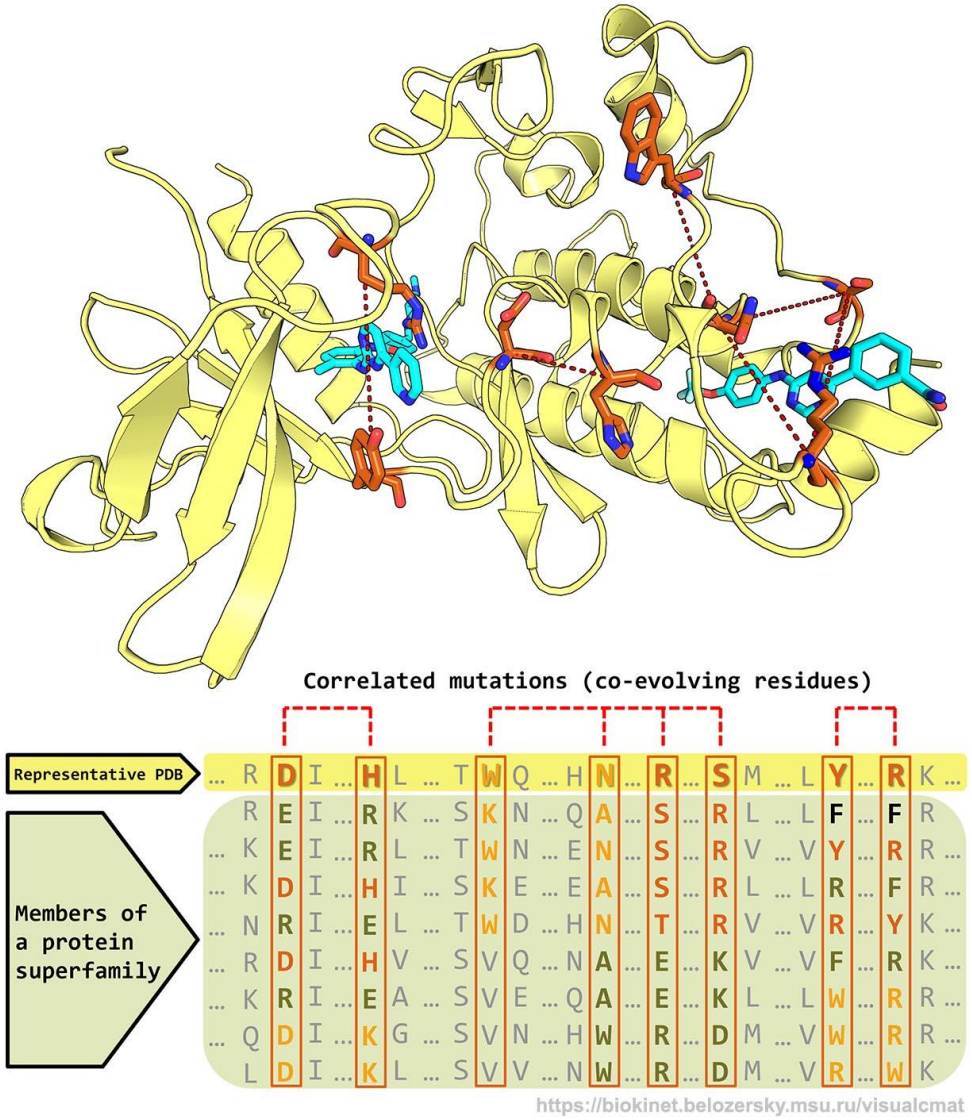
- The **pocketZebra** web-server can be used to identify and rank binding sites in proteins by functional significance and select particular positions in the structure that are important for selective binding of substrates/inhibitors/effectors;
  Suplatov D., et al. (2014) *Nucl. Acids Res.*

Systematically classify and study disulfide bonds in diverse protein families



The **Yosshi** web-service can be used to systematically classify and study disulfide bonds in diverse protein families, and to assist at selecting hot-spots for disulfide engineering in the structure of your query protein. The "**YO**ur web-server for **S-S** bond **H**arvest**I**ng" is a new highly automated on-line tool for a systematic homology-driven analysis and engineering of disulfide bonds that can be easily used by a general biologist at a daily laboratory routine. The Yosshi facilitates a broader interpretation of disulfides not just as a factor of structural stability, but rather as a mechanism to implement diversity within a superfamily; Suplatov D., et al. (2019) *Nucl. Acids Res.*

Predict and visualize the correlated mutations (co-evolving residues)



- The **visualCMAT** web-service can be used to predict and visualize correlated mutations/co-evolving residues in protein structures. The visualCMAT can be used to understand the relationship between structure and function and identify co-evolution patterns in protein superfamilies, implemented at selecting hotspots and compensatory mutations for rational design and directed evolution experiments to produce novel enzymes with improved properties, and employed at studying the mechanism of selective ligand's binding and allosteric communication between topologically independent sites in protein structures;
  Suplatov D., et al. (2018) *J Bioinform Comput Biol*.

Contacts

- Support and collaboration
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- Press to ask your question on-line

Ask for help

Lomonosov Moscow State University, the Main building