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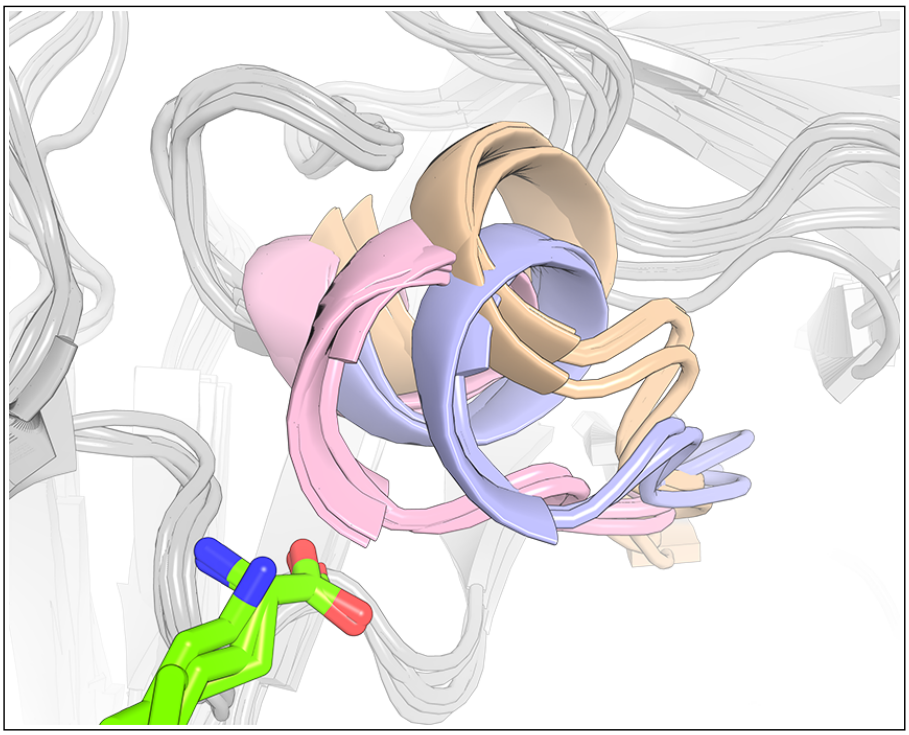
Zebra3D

Tool for bioinformatic analysis of 3D-determinants of functional diversity in protein superfamilies using machine learning



This software is free and open to all users with no login requirement

Download Zebra3D

... to run on you local computer for full flexibility ...

Mustguseal it NOW!

... or use Mustguseal web-server to run Zebra3D on-line with default settings ...

... to **identify and prioritize subfamily-specific regions** in the common fold of a protein superfamily **as 3D-determinants of functional diversity**, and to use this information for protein design and drug discovery

Version **1.1** since October 27th, 2020

Publication: Timonina D., Sharapova Y., Švedas V., Suplatov D. (2021) Bioinformatic analysis of subfamily-specific regions in 3D-structures of homologs to study functional diversity and conformational plasticity in protein superfamilies. *Comput. Struct. Biotechnol. J.*, 19, 1302-1311; DOI: **10.1016/j.csbj.2021.02.005**

Navigation:

Highlights:

- Zebra3D is a novel bioinformatic tool for a systematic assessment of 3D-alignments of protein superfamilies to study 3D-structural determinants of functional diversity;
- The new algorithm can identify the subfamily-specific regions (SSRs) in 3D-structures of homologs – patterns of local 3D-structure (e.g., single residues, loops, or secondary structure fragments) that are spatially equivalent within families/subfamilies, but are different between them;
- SSRs represent plausible determinants of functional diversity in a superfamily. Knowledge of SSRs in your superfamily can help to understand how enzymes perform their natural functions, and can also assist the design of proteins with novel properties by implementing insertions/deletions, and help to assess function-related conformational plasticity in binding sites to provide insight into drug-binding interaction;
- A companion **Mustguseal web-server** is available to alleviate the burden on the end-user of identifying suitable homologs and performing a resource-consuming 3D-superimposition. That bioinformatic tool can handle the automatic collection and alignment of protein PDB entries belonging to the superfamily of interest, which reduces the minimal input required to operate the Zebra3D to single a PDB code. The automatically constructed 3D-alignment will be subjected to Zebra3D analysis with default settings on-line. The user can then download both the automatically constructed 3D-alignment and the default Zebra3D results from that web-server;
- Assessment of the 3D-specificity, which is the primary focus of Zebra3D, does not replace, but rather complements the sequence-based assessment of specificity (i.e. identification of "specific positions" in multiple sequence alignments). Thus, we suggest to use Zebra3D together with the **Zebra2** sequence-based bioinformatic tool to assess all categories of subfamily-specific determinants of functional diversity in a protein superfamily. The results of the two tools are qualitatively different, as they assess mutually exclusive parts of a multiple alignment. See the **Zebra3D publication** for a further detailed discussion.

Contacts and support

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