

Protein Folding Nuclei Database

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Folding nucleus is a structured part of the protein in the transition state of folding process. Thus, folding nucleus formation is a rate-limiting step of the whole process. The involvement of a certain amino acid residue into the folding nucleus is measured separately (the residue is mutated, and the influence of this point mutation on folding rate and on protein stability is measured), and is represented as a Φ -value which reflects a fraction of contacts formed by this residue in the folding nucleus.

We collected a database of proteins (or rather, protein domains) with experimentally investigated folding nuclei. For each protein, the following data were collected: size of experimentally investigated protein, its amino acid sequence, 3D structure of the experimentally investigated protein or (if its 3D structure is unknown) the structure of the closest homolog with known structure, list of experimentally investigated amino acid residues and their Φ -values.

Now, our database comprises over 40 different wild-type proteins as well as their point mutations (in average, about 15 mutant forms for each protein). In the database, proteins of all main structural classes (α -helical, β -structural, α/β , and $\alpha+\beta$) are present.

Using folding nuclei prediction methods, we predicted the positions of folding nuclei in the proteins of our database. A comparison of the results of the prediction with experimental data shows that the tested methods allow successful prediction of folding nuclei.

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