Progress of ProTherm: Thermodynamic Database for Proteins and Mutants

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1   Introduction

Thermodynamic data for proteins are important for understanding the mechanism of protein stability. Pfeil [1] collected a set of thermodynamic data on protein folding and stability from experimental studies. Recently, we have developed an electronically accessible Thermodynamic Database for Proteins and Mutants (ProTherm) [2], which includes several thermodynamic data (unfolding Gibbs free energy change, enthalpy change, heat capacity change, transition temperature, activity, etc.), structural information (secondary structure, solvent accessibility, etc.), measuring methods, experimental conditions and literature information. We have developed a WWW interface to facilitate searching the database and sorting outputs. At present, the number of data has been increased to more than 5,500 covering the latest experimental data and several new features have been included in the database.

2   New features and additional information in ProTherm

In the recent version of the database, we have included the following information [3]: (i) updated the database with 5,542 entries, an increase of 67% over the previous version, (ii) additional information about reversibility, (iii) details about buffers and ions and their concentrations, (iv) information about the surrounding residues around each mutant in space for specific radius (0-4 Å and 4-8 Å) and (v) display option to view all mutants and surrounding residues through RasMol.

3   Contents of the database and search options

Each entry in the database contains (i) structural information, (ii) thermodynamic data obtained from thermal and denaturant denaturation experiments, (iii) experimental methods and conditions, (iv) functional and (v) literature information. The details about the computation of solvent accessibility have been described in our earlier article [4]. A WWW interface has been developed to facilitate searching the database on various conditions with different sorting options for outputs. Further, the database statistics and detailed tutorials describing the usage of the present ProTherm database are available at the home page.

4   Links to other databases

At present, cross references to NCBI PUBMED literature database, Protein Mutant Database (PMD), Enzyme code (EC), Protein Data Bank (PDB) structural database and 3DinSight (integrated database for structure, function and property of biomolecules) can be directly accessed from ProTherm web page.

5   Availability

The ProTherm database is freely available at the URL, http://www.rtc.riken.go.jp/protherm.html. Suggestions and other materials for inclusion in the database are welcome and should be sent to Akinori Sarai (sarai@rtc.riken.go.jp).

References

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