Current Status of ProTherm: Thermodynamic Database for Proteins and Mutants

M. Michael Gromiha1  Hatsuo Uedaira1
  gromiha@rtc.riken.go.jp  uedaira@rtc.riken.go.jp
Jianghong An2  Samuel Selvaraj1
  jianghon@scripps.edu  selvaraj@rtc.riken.go.jp
Ponraj Prabakaran1  Akinori Sarai1
  Praba@rtc.riken.go.jp  sarai@rtc.riken.go.jp

1 RIKEN Tsukuba Institute, Institute of Physical and Chemical Research, 3-1-1 Koyadai, Tsukuba, Ibaraki 305-0074, Japan
2 Scripps Research Institute, La Jolla, California, USA

Keywords: protein stability, protein mutants, database, free energy change, solvent accessibility

1 Introduction

Thermodynamic data for proteins are essential for understanding the mechanism of protein folding and stability, and for designing stable mutants. The compilation of thermodynamic data along with the sequence, structural, functional and literature information would be a valuable resource for such studies [7, 8]. Pfeil [9] collected a set of several thermodynamic parameters from experimental studies. We have designed an electronically accessible database, ProTherm [5, 6], including several thermodynamic parameters (unfolding Gibbs free energy change, enthalpy change, heat capacity change, transition temperature etc.), along with sequence and structural information, experimental methods and conditions, and literature information. Further, we have provided a WWW interface to facilitate searching the database, sorting and visualizing the results. Recently, we have updated ProTherm and included several new features in the database.

2 Recent Developments

1. Release 3.0 contains about 10,000 entries, 300% of the release 1.0 (3317 entries).
2. PDB code can be used for searching thermodynamic data associated with the structure.
3. The source of the protein is included.
4. Enthalpy change, ΔH, from calorimetric measurements is classified into van't Hoff enthalpy change, ΔHvH and calorimetric enthalpy change, ΔHcal.
5. Concentration of protein for each experiment is added
8. NMR category is added to the “Measure” item and can be searched.
9. Quick search is provided, covering all the text fields.
3 Database Statistics

We update Protherm frequently. At present, it contains 9784 entries from 463 proteins with 3982 wild type, 4896 single and 661 double mutations. In terms of secondary structures, 2194 mutations are in helical segments, 1617 in strand, 649 in turn and 1540 in coil region. Based on solvent accessibility, 2776 mutations are at buried, 1488 mutations are at partially buried and 1516 are at exposed regions. A majority of data are obtained by circular dichroism (3791), followed by scanning calorimetry (2988) and fluorescence (2130). Further, 5072 data are obtained with thermal denaturation, and 2525 and 1906 data from GdnHCl and urea denaturation, respectively.

4 Links to other Databases

ProTherm is directly linked to PUBMED literature database, Protein Mutant Database (PMD), Enzyme code (EC), BRENDA, PIR, SWISS-PROT, PDB and 3DinSight, an integrated database for structure, function and property of biomolecules [1].

5 Availability of ProTherm

ProTherm is freely available at http://www.rtc.riken.go.jp/jouhou/protherm/protherm.html. Suggestions and other materials for inclusion in the database are welcome and should be sent to protherm@rtc.riken.go.jp.

References