

Current Status of ProNIT: Thermodynamic Database for Protein-Nucleic Acid Interactions

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1 Introduction

Understanding the mechanism by which protein interacts with nucleic acid is of great importance since these interactions occur in many vital cellular processes including replication, recombination, repair, transcription and translation. Whether proteins bind to nucleic acids or not is determined by the law of thermodynamics. In this regard, thermodynamic factors which control the binding are of fundamental importance. Although databases for the sequence and structure of proteins, nucleic acids and the complexes are developed and available, databases for thermodynamic data on the interaction of protein-nucleic acid are few. Thus, we have developed electronically freely accessible thermodynamic database for protein-nucleic acid interactions, ProNIT [2, 3]. ProNIT aims to provide researchers information about the experimentally determined thermodynamic parameters involved in protein-nucleic acid interactions, published in the literature. It contains several important thermodynamic parameters along with experimental conditions, methods, etc. In addition, the supplementary information such as sequence, structure and the other functional details are also given. We have provided a Web interface to help users searching for the data with required conditions and sorting formats, and visualizing the results through the Internet. We report here the current status of the ProNIT database.

2 Contents of the Database

Each entry in the database is referred by a serial number and has thermodynamic data together with the other information as below:

- (1) *Protein Information*: name, source, fragment and sequence, biological unit, details of mutation with secondary structure information and accessibility at the mutant sites, Enzyme Commission (EC) number, Protein Information Resource (PIR) number, Protein Data Bank (PDB) code for wild proteins
- (2) *Nucleic acid information*: name, source and sequence of the nucleic acid, details of mutation and sequence of mutant nucleic acid, and Gene Bank accession number
- (3) *Complex information*: codes for PDB, NDB, and Protein-Nucleic Acid Complex Database number, ligand molecules, accessibility for the wild-type residues corresponding to mutation sites in the complex and conformational changes of protein and nucleic acid upon binding.
- (4) *Experimental conditions*: temperature (T), pH, detailed information about buffer, ions, additives and experimental method.
- (5) *Binding data*: dissociation

constant (K_d), association constant (K_a), changes in Gibbs free energy (ΔG), enthalpy (ΔH) and heat capacity (ΔC_p) for wild and mutant entities, stoichiometry of binding, activity (K_m and k_{cat}).
(6) *Literature information*: reference, authors, keywords and remarks.

3 Database Statistics and Recent Developments

We update ProNIT frequently. At present, it contains 3619 entries from 135 proteins. Majority of data are obtained by Gel shift (768), Fluorescence (706), Calorimetry (674) and Filter binding (550). Further, about 900 data are obtained by Footprinting and other techniques. A new field “Related entries” was added. This will help users to obtain similar entries from the same reference. Now that an increasing number of thermodynamic data on protein-RNA interactions are available in the literature, we are planning to include these data also in the database from the next update. Recently, ProNIT is linked with the “ProTherm” database [1, 4] with respect to the particular protein involved in the protein-nucleic acid interaction.

4 Links to Other Databases

ProNIT is cross-linked with other relevant databases we have developed, Protein-Nucleic Acid Recognition Database [5] through 3DinSight [6]. This enables users to examine conformational properties of DNA, and to search for specific pairs of base and amino acid involved in the protein-nucleic acid complex. ProNIT is also hypertext-linked with EC, PIR, PDB, NDB, GenBank and NCBI PubMed literature database.

5 Availability of ProNIT

ProNIT is freely available at <http://gibk26.bse.kyutech.ac.jp/jouhou/pronit/pronit.html>. Suggestions and other materials for inclusion in the database are welcome and should be sent to pronit@rtcmain.bse.kyutech.ac.jp.

References

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