NMR Data of Biological Macromolecules

The Protein Data Bank ("PDB", http://www.rcsb.org/pdb/) is well known as the central data depository of protein structures by most internet users interested in biological macromolecules. Its younger cousin, the Biological Magnetic Data Bank ("BioMagResBank") is mainly supported by the NIH (US National Institute of Health). The BioMagResBank is the international repository for biological NMR data from primary literature. The database collects ^{1}H, ^{13}C, ^{15}N, and ^{31}P NMR chemical shifts of amino acids, peptides, proteins, and nucleic acids. Currently (March 2002), the database contains about 2000 peptides and proteins, 52 data sets of DNA, and 19 data sets of RNA parameters. In addition to the chemical shift parameters, some data sets also contain information about scalar and dipolar couplings and T_1 and T_2 relaxation times. Most data sets include direct links to the structure files in the PDB. These links enable the user to investigate the spatial structure of the protein and thus draw conclusions from both chemical shift and molecular conformation.

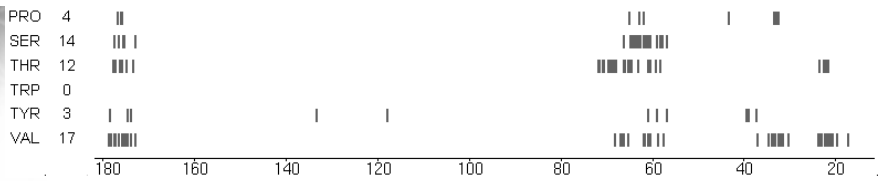

Figure 2. Excerpt of ^{13}C chemical shift data of the individual amino acid residues in a phosphotransferase complex.

The BioMagResBank has several built-in search tools. The most simple and intuitive search tool is found behind the links Retrieve and Query Grid Interface from the home page. The information is stored as a rectangular grid (like a chess board) of mouse-selectable table entries. The horizontal axis of the grid specifies the class of the biopolymer and the vertical axis shows the NMR parameters. This grid allows an easy selection, in particular of a desired subset of the database. The second and most powerful search tool is found behind the links Retrieve and NMR Data Browser. Selection of this link opens a very versatile input form (Figure 1). Here, the user can specify search criteria, such as author, name of the compound, temperature, or pH. The search parameters can be linked with a logical AND or OR. Finally, there is a third query tool (links Retrieve, FASTA Search) to search for sequence similarities. Here, the sequence is specified by one-letter codes.

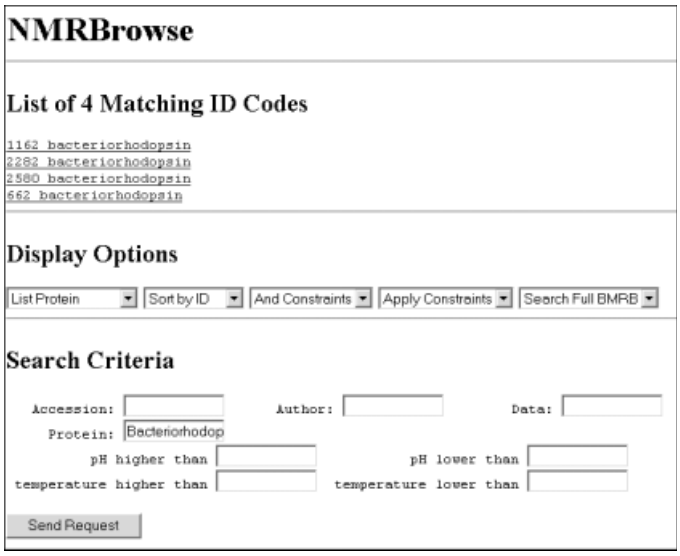

Figure 1. Query mask of the BioMagResBank.

The data can be accessed in several ways. An interactive Java application allows for a graphical display and analysis of the data (Figure 2). This tool should be sufficient for the needs of most users. For a more complex data analysis beyond the capabilities of the Java tools, it is possible to download the data sets as text files. The structure of these files is documented under the links Tools, Documentation. In addition to the pure documentation of these files, there is also a downloadable library with routines which help to write customized data analysis programs.

Suggest a web site or submit a review:
angewandte@wiley-vch.de

With its large collection of protein data, the BioMagResBank probably is the largest free resource of biological NMR data. Primarily, this collection is of interest for NMR spectroscopists and users who study this class of systems. Owing to its versatile search and analysis tools, its intuitive usage, and its interactive graphical data display, the BioMagResBank is also a valuable resource for educational purposes, for example in courses on Instrumental Analytical Chemistry.

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