PROPHET—a national computing resource for life science research

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ABSTRACT

PROPHET is a national computing resource tailored to meet the data management and analysis needs of life scientists working in a wide variety of disciplines, ranging from pharmacology to molecular biology. The PROPHET system offers a fully integrated graphics-oriented environment designed for the manipulation and analysis of tabular data, graphs, molecular structures, biological simulation models, and protein and nucleic acid sequences, and it includes access to molecular structure and sequence databases.

INTRODUCTION

The PROPHET system was first conceived in the late 1960's as a computing facility that would provide easily used interactive tools for studying the interactions of chemical and biological systems(1). The initial design, development, and testing stage for the system was completed by 1972, when it was made available on a regular basis to a few approved groups of pharmacologists and pharmaceutical chemists. The PROPHET system currently serves scientists at over 40 universities, medical schools, research foundations, chemical and pharmaceutical companies, working in chemistry, biology, pharmacology, epidemiology, microbiology, molecular biology, and biochemistry.

The PROPHET system offers a broad spectrum of integrated, graphics-oriented information-handling tools to aid research scientists in the manipulation and analysis of data through tables, statistics, and graphs. There are tools to facilitate biological simulation and modeling, molecular modeling, and protein and nucleic acid sequence analysis. The system incorporates interfaces to such molecular databases as the Cambridge Crystallographic Files(2), the GenBank® Genetic Sequence Data Bank(3), the Protein Data Bank from Brookhaven National Laboratory(4), and the Protein Identification Resource Database from the National Biomedical Research Foundation(5). With easy-to-understand English-like commands and its own programming language, PROPHET can be used with ease by the computer novice as well as by those with strong computer backgrounds. A hallmark of PROPHET is the sense of sharing and communication that exists among PROPHET users and with the PROPHET support staff. The resulting PROPHET system reflects current user research needs and continues to evolve with the increasing sophistication of biomedicine and computer technology.

CAPABILITIES

The PROPHET system employs natural data types such as tables, graphs, molecules, and sequences. They are easy to create and modify, without any concern for the details of internal file structures or storage management.

The two-dimensional table enables easy data storage and retrieval. Graphs are easily made from the data in PROPHET tables or from arbitrary functions. Many different graph types are supported, including two- and three-dimensional graphs, scatterplots, bargraphs, and histograms. Statistical tools can be applied to the data in PROPHET tables and PROPHET graphs, ranging from simple descriptive measures through analysis of variance, contingency table analysis, and non-parametric testing to linear and non-linear regression and pharmacokinetic modeling.

Figure 1. PROPHET's van der Waals dot surface representation of morphine.

Figure 2. The linear sequence of a yeast phenylalanine transfer RNA molecule(6) retrieved from the GenBank database(3), a secondary structure for the same molecule generated using PROPHET, and a three-dimensional projection abbreviated from a crystal structure(7) in the Protein Data Bank(4). A uniform base pair coloring scheme is applied to all three representations.

PROPHET provides extensive capabilities for storing and manipulating molecular structure information. Display methods include Dreiding models, ball and stick models, space-filling models, and van der Waals surfaces (Figure 1). PROPHET also contains tools for handling and displaying nucleotide and amino acid sequence data. These tools focus on analysis and manipulation of primary sequence data, but they are incorporated in the PROPHET environment, which includes RNA secondary structural modeling software and access to three-dimensional structural databases (Figure 2).

AVAILABILITY

PROPHET is a fully distributed system for high-performance graphics workstations. Network connections to the central facility provide access to the latest versions of scientific databases, facilitate information sharing, code development and distribution, and, in the future, will make available specialized computing resources. PROPHET software is now available for any Sun 3 workstation or for any VAX running Ultrix. Additional workstations will be supported in the near future. The software is available for a nominal charge to cover distribution costs. Support services are available on a cost-recovery basis.

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