WINNER

1998 R&D 100 Awards Winner

SOLVE—Creating Three-Dimensional Pictures of Protein Molecules from X-Ray Diffraction Spots

Features

Because three-dimensional (3-D) pictures of proteins provide important information about the way in which proteins operate, they are indispensable to applications in biotechnology and health care. SOLVE is the first expert system that produces 3-D pictures of protein structure by automatically solving for the missing information in x-ray crystallography. Its speed—it is faster than any other available method—and ease of operation make it suitable for the rapid analysis of the shapes of protein molecules.

Applications

Currently used in government, academic, and commercial laboratories, our technology can be applied to

- rational drug discovery and thus to the design of new, improved drugs,
- the engineering of enzymes with new catalytic properties useful in the rapid breakdown of toxic waste and in rapid chemical synthesis, and
- the engineering of robust, heat-tolerant enzymes useful in chemical manufacture.

Benefits

- Creates accurate pictures of proteins from x-ray diffraction data.
- Constructs pictures fast (typically 6 minutes to 5 hours versus 1 to 2 days).
- Is automated (even the analysis and evaluation of starting solutions, that is, educated guesses about the arrangement of the heavy atoms in a protein).
- numerous solutions (500 to 1,000 versus 1 to 10).
- Is easy to operate (a novice technician can operate the system, whereas an expert in crystallography is required for other related software applications).