ELVES--AN EXPERT SYSTEM FOR X-RAY CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

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ABSTRACT

Elves is a computer expert system for X-ray crystallography of biological macromolecules. Elves automates and accelerates every step of X-ray data analysis, from processing X-ray diffraction images to guiding and refining a molecular model. Elves requires the use of CCP4, which must be obtained under separate license from a third party. Elves also uses common data analysis programs such as Mosflm. Elves also has novel functionalities, such as Spotter to identify and display particular diffraction spots, sendhome to transmit data frames over the internet, and table1.com to tabulate statistics for publication.

Elves sequentially runs each step of X-ray structure determination using a generalized regimen. The problem-solving strategy is based on empirical rules and procedures for overcoming common problems. Optimized parameters are passed from each program to the next. These values can be evaluated by the user or simply accepted automatically at each stage. The overall effect is to systematize, optimize and accelerate the process of X-ray structure analysis in biomedical research.

Elves can accept English language inputs or shell script inputs. After locating the data and the necessary programs on the file system, Elves writes program-input scripts, runs programs, examines the output and iteratively repeats this cycle to optimize input parameters. This optimization is generally beyond the capability of human users of the underlying programs.

This systematic X-ray data analysis reduces the frequency of mistakes. In addition, Elves operates faster and more reliably than a human user, even when the user employs a graphical interface. Complicated analytical calculations that can take months for human users to complete can be performed in a matter of hours using Elves. To date, Elves has been used to help determine the crystal structure of over fourteen proteins. Novel structures have been solved in as little as five hours from the start of X-ray data collection at a synchrotron source; a typical investigator not using Elves would take weeks to months to complete the same work.

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OTHER INFORMATION

KEYWORDS

copyright, genomics, proteomics, bioinformatic, protein sequencing, research tool

CATEGORIZED AS

- **Computer**
  - Software
- **Research Tools**
  - Other

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