Automating Crystallographic Structure Determination Calculations

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Structural genomics efforts require a high throughput at all stages of the structure determination process. Simultaneously, it is important to reduce the cost per structure, which means reducing the time spent on each structure. We have focused on the structure determination calculations going from processed, merged data through to initial model. The Automated Crystallography System (ACrS) utilizes existing software and algorithms but a distributive program interface administers the programs for determining protein structures. A relational data base stores initial data for starting the process as well as harvesting and warehousing data generated during the structure determination process.

The ACrS default mode of operation is to try several defined pathways in parallel. Analysis of the results in the database provides information for improving the pathways and for selecting software with complementary strengths.

An example is a recently determined structure of a member of the ROK family of transcription regulators that used a “native” data set and SAD phasing from one bound zinc to automatically built 384 residues of 405 without any intervention or optimization of parameters.

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