The *Xtaldb* System for Project salvaging in high-throughput Crystallization

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Over the past 15 years, advances in protein crystallography have continuously redefined the concept of "low-hanging fruit". Salvaging proteins that do not crystallize in high-throughput environments has become increasingly important for structural coverage of major protein families with sufficient granularity to allow 3-D homology modeling. To address this problem, we have created *Xtaldb*, a scalable, cross-platform, networked expert system for tracking and statistical analysis of crystallization experiments. *Xtaldb* records detailed information about each crystallization, including chemical and biochemical data about reagents and macromolecules, crystal images, annotated observations, and diffraction data. These data are gathered with a minimum of researcher input with the aid of touchscreens, barcode scanners, digital cameras, and other forms of automation.

Using these data, the *Xtaldb* system organizes experiments and overall target status information into projects and provides tools for data mining and statistical analysis of the crystallization data both on the project and database-wide levels. To test these tools, we used the system in the salvage of a group of ten targets that previously failed to produce a structure in the MCSG pipeline. To date, two structures have been solved and deposited in the PDB, and three others diffract natively: two to 2.7Å, and one to 3.6Å.

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