



Crystallographic Information System

Crystallographic Information System (CrysIS) manages the data and workflow of X-Ray protein crystallography from a request for a protein-compound, through the experiment and final deposition of a protein-ligand structure, and the subsequent exploitation of that structure data.

Business and IT challenge

A typical pharmaceutical organization will produce hundreds of protein-ligand (PDB) structures per year. The workflow associated with this process is complex and results in a large quantity of data that is utilized by structural medicinal, and computational chemists alike. Planning the work of structural chemists across multiple projects within an organization can therefore be a difficult task. Identifying those attributes that lead to a successful experiment is difficult without ready access to previous experimental results. With such a complex workflow and without the use of appropriate tools, the possibility for manual transcription errors is increased.

The Crystallography Environment

- Complex workflow, incorporating multiple steps and functional specializations
- Manual data transcription
- Large volumes of data
- Time critical to the drug discovery process

CrysIS delivers capabilities across several key areas:

- Management of requests for protein-ligand structures
- Performing of crystallization experiments
- Management of the process of crystallography
- Exploitation of the resultant structure data



Request Management

CrysiS enables users to make requests for protein-ligand structures and to track the progress of those structures as the experimental work is performed by structural chemists. This enables medicinal and computational chemists to plan, prioritize and organize their work.

Chemists can readily search the database for requests in the system for a chemically similar compound or structures that exist in the data already.

"I want the structure of compound X solving against this target. Does a request for a chemically similar compound exist?"

Crystallization Experiments

CrysiS can integrate with a number of crystallization systems used during the protein crystallization process: Crymon and RockMaker for example. This enables seamless data transfer as an experiment progresses and reduces manual input of data.

CrysiS contains a rich graphical user interface to manage the work of the laboratory scientist in performing soak, co-crystallization and APO experiments.

"What were the ideal soaking conditions when I used this target with a similar compound in the past?"

The scientist is able to readily annotate, modify and set the status of all crystals within an experiment. The system has many features for the location tracking of various entities:

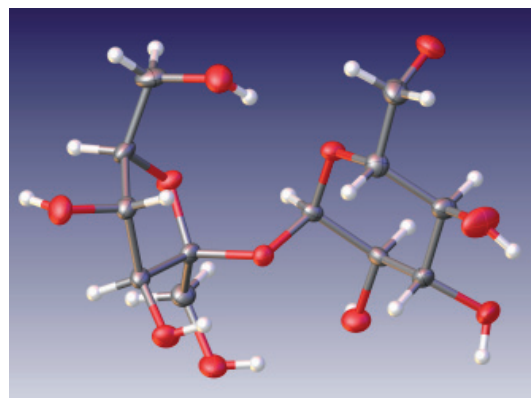
- Crystals within pucks (ACTOR and ESRF) and canes
- Racks and dewars
- Compound plates
- Protein batches

The system prevents users from having to re-enter data multiple times into different systems as an experiment progresses. This therefore reduces the likelihood of transcription errors and saves time handling such data.

Crystallography

Following production of a crystal complex, CrysiS takes the experiment forward and has support for a number of features:

- Integration with ACTOR robots
- Workflow management through data collection, reduction, refinement and deposition
- Support for complex experiments concerning multiple proteins and/or compounds
- Management of synchrotron data and integration with ISPyB data formats
- Validation and annotation of structures





Exploitation

CrySiS serves as a repository for all protein structure data following deposition or can be integrated with an existing structure repository. The system includes a number of features to facilitate the exploitation of structure data:

- Integration with Astex Viewer
- Display of electron density and manipulation of compound, protein and water parts of the structure
- Ability to perform overlays of two or more different structures
- Search for structures that contain a chemically similar compound or protein with a similar binding site to a reference structure.

Benefits

- Improved quality of service of structural-chemistry groups to their customers
- Improved quality of data through checking and validation of inputs
- Improved decision making through better planning and greater visibility of projects
- Process Improvement through the ability to mine data
- Economy through the use of a streamlined interface

CRYSTAL LOCATION ADMINISTRATION

Crystal Locations	
Blue-1 Crystals: 2 Actor Puck	Blue-2 Crystals: 0 Actor Puck
Blue-3 Crystals: 0 Actor Puck	Blue-4 Crystals: 0 Actor Puck
Blue-5 Crystals: 0 Actor Puck	ESRF-151A Crystals: 1 ESRF Puck
ESRF-152A Crystals: 0 ESRF Puck	ESRF-153A Crystals: 0 ESRF Puck
ESRF-154A Crystals: 0 ESRF Puck	ESRF-155A Crystals: 0 ESRF Puck
Red-1 Crystals: 0 Actor Puck	Red-2 Crystals: 0 Actor Puck
Red-3 Crystals: 0 Actor Puck	Red-4 Crystals: 0 Actor Puck
Red-5 Crystals: 0 Actor Puck	

Blue-1
Crystals: 2
Actor Puck

Contents
1. C14orf29-TSS0000002-1
7. C14orf29-TSS0000002-6

ESRF-151A
Crystals: 1
ESRF Puck

Contents
4. p35BP-TSS0000023-1

Export Actor Puck Data



Technology

CryslS is a web-based system that uses a variety of technologies:

- Oracle database (8i or above)
- Microsoft ASP.Net utilising Microsoft Internet Information Services
- Java applets, MDL Chime Pro, Astex Viewer
- Web Services
- Custom Oracle, SQL Server, PostgreSQL etc databases for integrated systems
- Internet Explorer 6+/Firefox 1.5+ compatible

Why Tessella?

- We provide IT and consulting services based on scientific methods and rigorous quality procedures
- We have 25 plus years of experience in working with some of the biggest names in R&D, science, and engineering and we understand the industry issues
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