

# *MyCrystals* – a simple visual data management program for laboratory-scale crystallization experiments

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Received 17 February 2009  
Accepted 28 April 2009

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*MyCrystals* is designed as a user-friendly program to display crystal images and list crystallization conditions. The crystallization conditions entry fields can be customized to suit the experiments. *MyCrystals* is also able to sort the images by the entered crystallization conditions, which presents a unique opportunity to easily assess the effect of, for example, changing pH or concentration and thus establish the best conditions to be used for optimization.

## 1. Introduction

Macromolecular structure determination by X-ray diffraction requires a successful crystallization. This can be a difficult task where numerous crystallization experiments lead to a large amount of data. Crystallization projects can be worked on by several people over long periods of time, and keeping track of, as well as sharing, results can be made much easier by the use of a database.

There are many available systems and programs that can be used to store crystallization data. In connection with crystallization robots there is usually commercial software available to handle the large amount of data. Some of the free programs are *XtalBase* (Meining, 2006), *XAct* (Brodersen *et al.*, 1999), *Xtrack* (Harris & Jones, 2002), *CLIMS* (Fulton *et al.*, 2004) and *LISA* (Haebel *et al.*, 2001). *XtalBase* (Meining, 2006) is a comprehensive system that amongst many other features can manage and display images of the results, and *CLIMS* (Fulton *et al.*, 2004) is able to store visual observations of the drops. Images combined with scores afford a simple way to assess crystallization results and simplify the optimization procedure because of the transparency of the results. Laboratory information management systems like the *Protein Information Management System (PiMS; https://www.compbio.dundee.ac.uk/pims2\_0/)* are designed to manage various types of data, such as target, construct and experimental data, through a web interface. We have developed a program named *MyCrystals* with the main purpose of managing and storing images and crystallization conditions and sorting them to give an overview of the results.

*MyCrystals* is simple to use, easy to navigate and requires minimal time investment by the researcher to utilize the software. The unique feature of *MyCrystals* is its ability to display and sort crystallization images. The images are stored locally or on external media, and the program creates a database with file paths to identify the images. *MyCrystals* is also able to sort the images by the entered data to view the effect of, for example, changing the pH or precipitant. This makes it easier to establish the best conditions and to assess how they can be optimized. *MyCrystals* can also be used as a notebook program to keep track of attempted crystallization conditions without necessarily using the image-viewing part. Furthermore, *MyCrystals* may be useful in other experimental optimization procedures, such as purification, where a lot of slightly different procedures are usually tested. These

may be stored in the database and linked to an image file containing the resulting chromatogram.

## 2. Program description and use

*MyCrystals* is primarily designed for viewing and sorting images in a simple and intuitive user interface.

The File menu is used for creating new databases and loading or saving existing databases. Creating a new database in the File menu will auto-generate a standard set of conditions.

The user interface of *MyCrystals* is divided into three simple main tabs: Filter Data, Edit Data and Data Table.

### 2.1. Data structure

The data consist of two parts. The first part is an XML database that contains all entered conditions including the appropriate image path for each set of conditions (data entries). The second part is the images themselves, which are placed in a directory on the hard drive. *MyCrystals* recognizes graphics file formats JPEG, GIF, PNG and TIFF.

The full path to each image consists of two parts, a project directory and a relative image path. The image path is unique for each data entry, while the project directory is shared. This arrangement facilitates the moving of all images to another location, as only the project directory needs to be changed.

### 2.2. Filter Data

The Filter Data tab is used for viewing and sorting images entered into the database. The sorting options are available in a drop-down menu and consist of all entered data. First, a condition is selected, and then a filter option is applied. Text strings can be sorted as absolutes, while numerical strings also can be sorted using >, <, ≥, ≤ and ≠. It is possible to apply 15 filters simultaneously. A list of entries that match the criteria is generated and displayed in the tab (see Fig. 1).

The information shown for each data entry in the list can be customized using the field Filter text. Writing [1] will list the data entered in the first field in the Data Entry area of the Edit Data tab, [2] will list the data in the second field, and so forth.

Selecting one of the listed entries will display the matching image to the right of the tab, as shown in Fig. 1.

# computer programs

## 2.3. Edit Data

The database can be edited in the Edit Data tab. The tab consists of three parts: Project Directory, Column Properties and Data Entry.

The project directory is the path to a directory where all the images used in the database are placed. The rest of the path is stored as a property (image path) for each data entry.

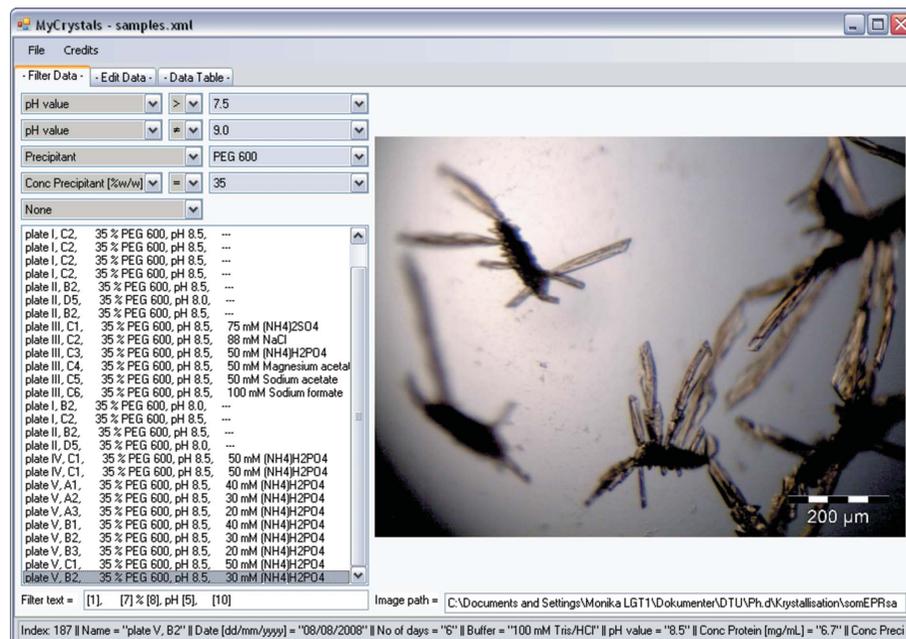


Figure 1

A screenshot showing how the Filter Data tab of *MyCrystals* can appear. Data with  $\text{pH} > 7.5$  and  $\text{pH} \neq 9.0$  in 35% PEG 600 have been selected. For the displayed image, the conditions are  $\text{pH} = 8.5$  and 30 mM  $\text{NH}_4\text{H}_2\text{PO}_4$ . The scalebar is part of the depicted image.

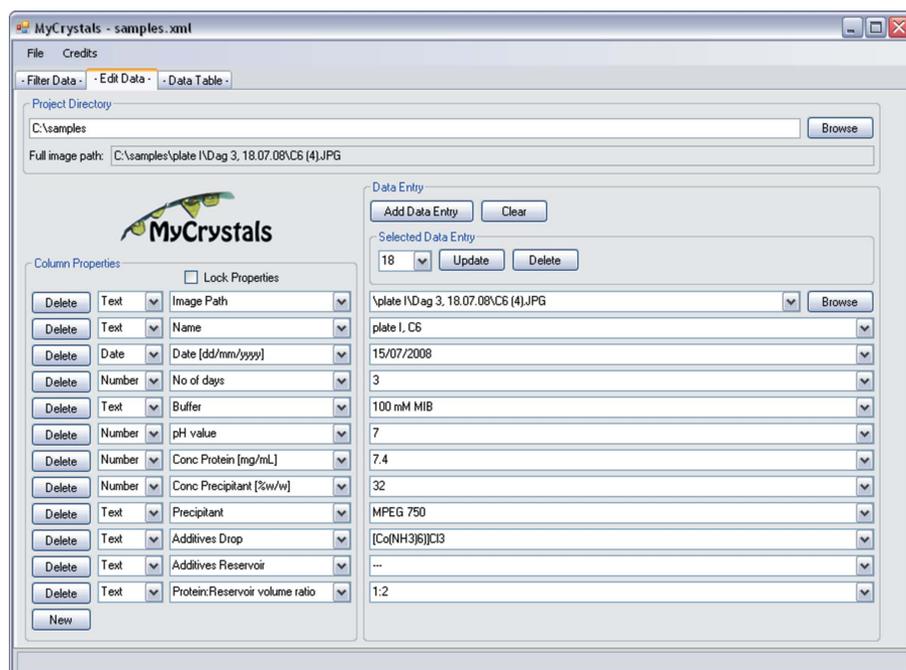


Figure 2

A screenshot showing how the Edit Data tab of *MyCrystals* can appear. Checking the Lock Properties option will simplify the Column Properties by only showing the name.

Column Properties makes it possible to change the data columns of the database. It is possible to delete or add columns, change the names and types, and switch the positions of two columns. An intuitive user interface renders this possible (see Fig. 2).

The Data Entry area is used to add, change and remove data entries in the database. The Selected Data Entry area operates on an existing data entry. To add a new data entry into the database, use the Add Data Entry button, which creates a new data entry with a consecutive index number. The data entry fields are empty when the first data are typed in, and after Add Data Entry has been used, the entry fields will contain the information of the latest data entry. Drop-down menus of previously entered data are available when entering or correcting database entries. The Selected Data Entry area can advantageously be used when entering data, as an entire set of previously entered conditions can be loaded by giving the index number. Minor changes can be applied to the set of conditions and Add Data Entry will generate a new entry in the database.

## 2.4. Data Table

The Data Table tab lists all entered data to give an overview of the contents of the database.

## 3. Platforms and availability

The program is written in C# as a Windows Form in Microsoft Visual Studio. The program consists of a single executable file, and no installation is needed. *MyCrystals* runs under Windows and has no special hardware requirements.

*MyCrystals* is available free of charge for download from <http://xray.kemi.dtu.dk/mycrystals/>.

## 4. Conclusions

The unique main feature of the program *MyCrystals*, presented here, is the displaying and sorting of crystallization images based on the entered crystallization conditions. This enables the user to view the effect of changing conditions, which helps to identify parameters for optimization.

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