

DEVELOPMENT OF A SOFTWARE APPLICATION FOR HANDLING PROTEIN CRYSTALLISATION CONDITIONS AND TRIALS

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The new automated high throughput approaches applied in the field of macromolecular crystallization during the last decade have resulted in the generation of a huge amount of information¹. To meet the emerging need for handling this information a number of tools has been developed. Our work focuses on the organization of commercial crystallization conditions as well as those derived from a crystallization lab routine in a database to support the crystal optimization process. We have developed a computer software application for handling protein crystallization conditions and trials. The new tool facilitates organization and storage of crystallization related data in a database comprising three main areas of interest: a) commercially available and home-designed screens of crystallization conditions used in each trial, b) Optimization conditions: Keeping record of all the deviations made from the initial crystallization solution in order to achieve the optimum result. c) Evaluation of the crystallization trial results by applying a score (number). In addition, users can make their own search queries and retrieve valuable information for (e.g. crystallization conditions of homologous proteins) the design of further optimization crystallization experiments² (Figure 1). Additional utilities, such as filing of protein samples allow users submit targeted queries (e.g. crystallization conditions of homologous proteins) and manage such relational database more efficiently.

Crystallization Kit Database & Screening diary							
----- Home----- How to Use----- About us----- Contact form-----							
Crystallization Conditions <ul style="list-style-type: none"> • Submit New Conditions • Search for Conditions • Make Corrections Protein Stocks <ul style="list-style-type: none"> • New Protein Batch • Search for Protein Samples • Make Corrections Screening Experiments <ul style="list-style-type: none"> • Enter a Screening Experiment • Search for Experiments • Edit an experiment Optimization Experiments <ul style="list-style-type: none"> • Enter an optimization Experiment • Search for Experiments • Edit an Experiment 	Crystallization Conditions meeting the requirements						
Condition Code	Kit Description	Well	Company	Precipitant Description	Precipitant C (mM)	Precipitant C (%w/V)	2nd Precipitant Description
molecular dimensions-Structure Screen 1 & 2 HT-96-A01	Structure Screen 1 & 2 HT-96	A01	molecular dimensions	PEG 1000	0	30	PEG 3000
molecular dimensions-Structure Screen 1 & 2 HT-96-A02	Structure Screen 1 & 2 HT-96	A02	molecular dimensions	MPD	1.45	0	PEG 2000
molecular dimensions-Structure Screen 1 & 2 HT-96-A05	Structure Screen 1 & 2 HT-96	A05	molecular dimensions	sodium formate	0	30	PEG 3000

Figure 1. The Crystallization database manager: results of a query

[1] I.M. Berry et al., Acta Cryst. (2006). D62, 1137–1149

[2] C. E. Kundrot, CMLS, Cell. Mol. Life Sci. Vol. 61, 2004