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 information[1]. 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 experiments[2] (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.

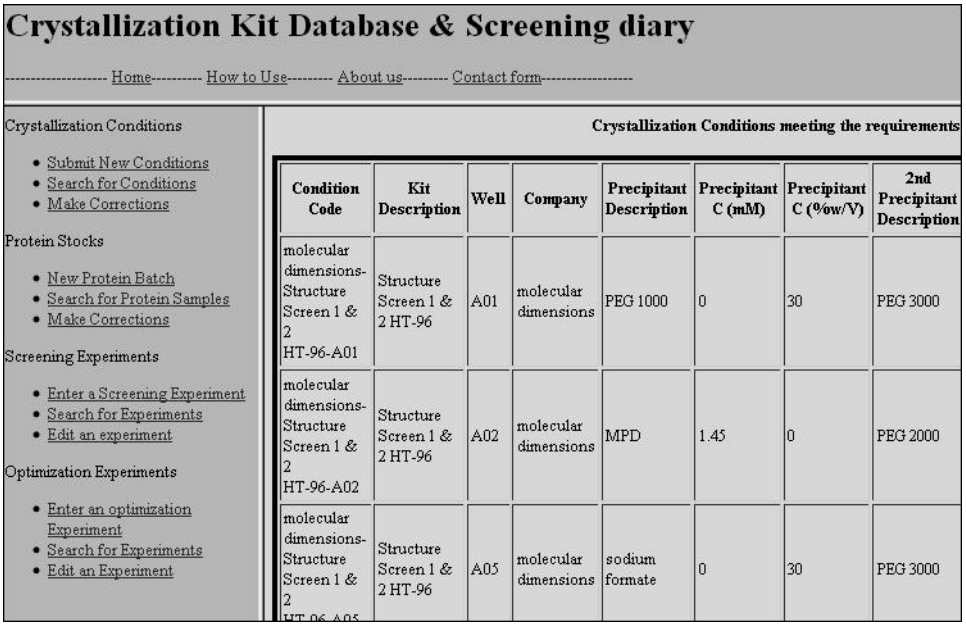

Figure 1. The Crystallization database manager: results of a query

[1] I.M. Berry et al., Acta Cryst. (2006). D62, 1137–1149
[2] C. E. Kundrot, CMLS, Cell. Mol. Life Sci. Vol. 61, 2004