physiological conditions the most stable calcium phosphate is hydroxyapatite ($Ca_5(PO_4)_3OH$, HAP). The growth mechanism of HAP has received considerable attention in view of its importance in understanding the mechanism of hard tissue calcification such as bone and teeth and in many undesirable cases of pathological mineralization of articular cartilage, dental caries and kidney stones [2].

In this work that we investigate the individual effect of polymeric additives for the hydroxyapatite (HAP) crystallization as a model for biomineralization. The higher affinity of PAA for HAP corresponds to the more significant effect of this polymer on the rate of HAP crystal growth.

The results indicate that polyelectrolyte concentration and the larger number of negatively charged functional groups markedly affect the growth rate. The fit of the Langmuir adsorption model to the experimental data supports a mechanism of inhibition through molecular adsorption of polymers on the surface of growing crystals.

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Keywords: hydroxyapatite, biomineralization, crystallization

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Morphological Control of Calcium Oxalate by Hydrophilic Block Copolymers

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Biomineralization processes have attracted considerable attention due to their importance in life sciences, especially with respect to pathological effects[1]. On the aspect of biomineralization, it is of interest to study the crystallization of calcium oxalate monohydrate (COM), because COM crystals have been known as a possible source of urinary and kidney stones[2]. Previous works have shown that the significant influence of urinary macromolecules on calcium oxalate crystallization[3]. Both inhibition and promotion of crystal growth and crystal aggregation by these biopolymers has been reported [4]. An understanding of biological solid-state interactions would be of immense value in many areas.

In this study, we prepared a range of acrylic polymers with different architectures to explore their relative effectiveness in inhibiting crystal growth of calcium oxalate. We investigated the effect of polymers on the particle size, morphology and precipitation of crystals. The presence of copolymers inhibited the crystal growth of calcium oxalate possibly through adsorption onto the active growth sites for crystal growth due to the charge and hydrophilic effects.

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Keywords: calcium oxalate, crystallization, morphology

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Searching the Crystallisation Parameter Space using Evolutionary Algorithms

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When trying to crystallize a new protein, the researcher usually explores a multi-dimensional parameter space using a sparse-matrix or other type of screen. Frequently, the results of such a search consist in a small number of 'promising' conditions. The researcher then conducts a finer mesh search, centered at each of the 'promising' points of the parameter space. If this fails to produce diffracting crystals, other screening conditions must be thought up.

We propose the further probing of such 'promising' conditions, using small-scale Evolutionary (Darwinian) Optimisation Algorithms. Each promising condition is pictured as a 'chromosome', the values of the various parameters (type of precipitant, buffer, pH, temperature, ...) being the alleles on that chromosome. The original 'promising' conditions of the screen constitute a 'first generation' of experiments. A second generation is constituted by random 'recombination' of these 'alleles', i.e. by combining successful values of parameters from different conditions. The most successful of the second generation of experiments will in turn be the 'parent conditions' of a third generation. 'Mutations', i.e. as yet untried values of parameters, can be sparsely introduced in each generation.

This method will not be as robust as for the purely computational optimisation problems for which it is normally used, due to the limitations on the number of 'generations'. It can however lead to optimal combinations of parameters, provided judicious choice of the conditions that will be the parents to each successive generation.

Keywords: biocrystallization, crystallogenesis, crystallization strategies

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Crystallization Platform Integrating Screening & a Novel Optimization Strategy

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Obtaining diffraction quality crystals is a common bottleneck in macromolecular crystallography. With the number of projects increasing exponentially, searching for the right crystallization conditions is a time consuming effort. We have now setup a medium-throughput crystallization platform at the main laboratory in Heidelberg in order to centralize resources, cut costs, and provide efficient and rapid service to EMBL-Heidelberg research groups using X-rays.

The platform is based on use of a nanoliter dispensing robot, standardized crystallization screens with a total of 1800 different conditions, and a database linked to an imaging system for data archiving. The advantages of the service are multiple. It significantly reduces crystallization setup costs by using fewer crystallization solutions and fewer samples. It also saves valuable time. What started as a medium throughput crystallization platform has rapidly grown and 300,000 crystallization drops have already been set up.

As a standard and simple approach for crystal optimization, we are now using the prefilled Nextal Opti-Salts crystallization microplates. This tool allows us to rapidly generate our own new subset of conditions expanded around the hits obtained at initial screening. It works using a combinatorial optimization approach. We will present three projects where the Opti-Salts generate a significant improvement with minimum efforts and investment.

Keywords: crystallization robots, optimization, biomacromolecular crystallization

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$Li_{3.17}(P_{0.69}Ge_{0.24}Mo_{0.07})O_4$: Growth under Electrical Field and the Structure

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The influence of electrical field on crystal growth from flux has been studied in the system Li_3PO_4-Li_4GeO_4-Li_2MoO_4-LiF. Growth occurs on the Pt-rod (anode) immersed into the flux due to temperature decrease with the simultaneous application of direct electrical current. The starting molar ratio between the starting components of the system (Li_3PO_4 : Li_4GeO_4 =1: 1) corresponded to the ratios which provided the stable crystallization of solid solution $Li_{3+x}P_{1-x}Ge_xO_4$ with x=0.31 at the absence of electrical field. When electrical current (V=0.08V) was applied to the growth system, the