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Making the most out of typical crystallization screening experiments

Jia Tsing Ng
University of Oxford

Abstract:
We present computational tools that extract information from standard sparse-matrix screens, to help experimenters make informed decisions in subsequent crystallization effort, even if there were no crystals in the initial screen.

Firstly, we aid in the identification of crystals or microcrystals by ranking droplets according to their likelihood of containing crystalline behaviour. This allows users to view droplets in a more meaningful order and prioritise attention and time to what is likely to matter most.

Secondly, we describe screening experiments by the collective precipitation patterns across the screen. This enables us to cluster historical experiments at the Structural Genomics Consortium, Oxford by their precipitation behaviour. Each cluster has a different distribution of crystallization conditions that gave hits, which is then used to identify conditions for optimization for a new protein that falls into the same cluster.

Thirdly, we automatically generate an analysis of conditions that produced clear drops. These conditions can be used to design an alternative protein formulation buffer for further stabilization of the sample. A stable formulation allows for crystallization experiments at higher protein concentration. We present cases for each of these applications and how they have enabled the crystallization of difficult targets, and/or improved the crystal quality. A centralised software called TeXRank