Poster Presentation

MS100.P03

Computational analysis of early stage crystallization based on UV fluorescence

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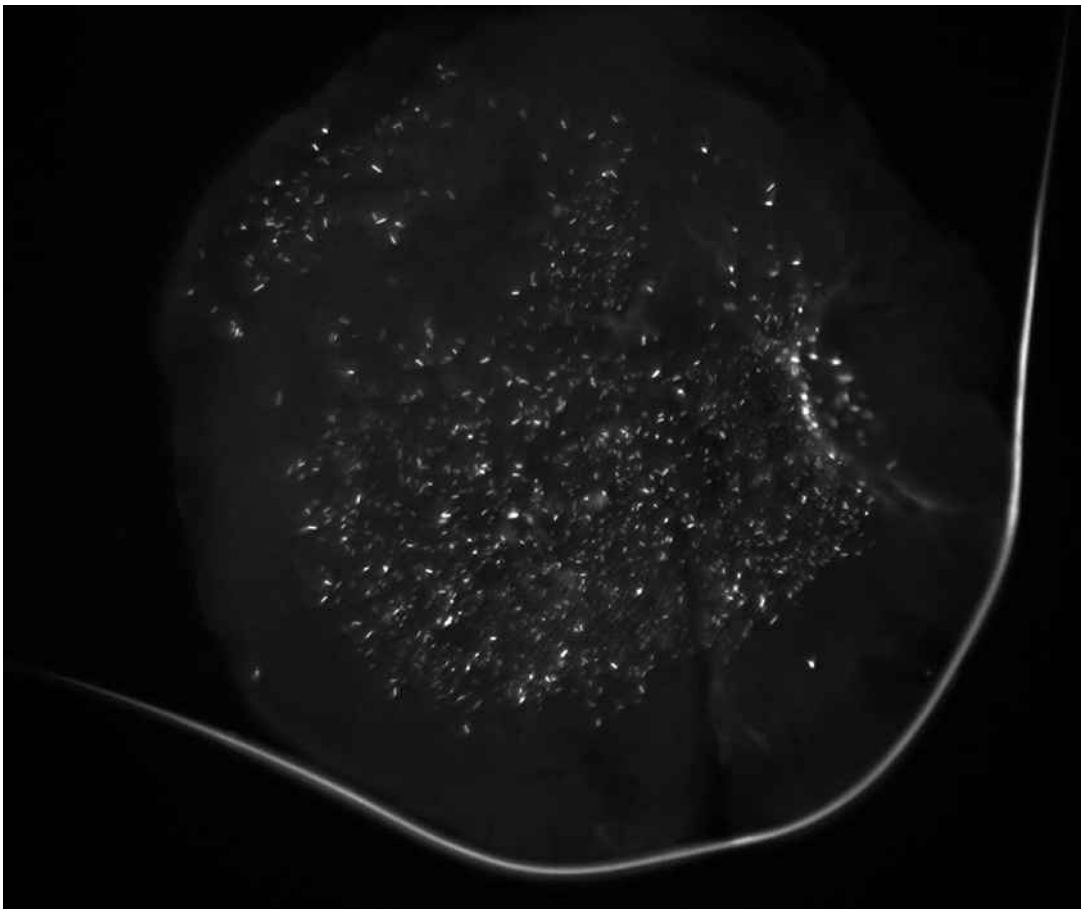
Detection of initial crystal hits during de novo attempt of structure determination of a macromolecule is a critical step in the crystallization process. The most common strategy during the initial matrix screening is to identify a condition that can grow crystals readily. Such occurrences are rare events for difficult to crystallize samples, which led Rigaku Automation to focus on methods to identify microcrystalline precipitation and marginally interesting conditions for further expansion trials from a high throughput (HTP) environment. Usually, the initial crystals observed for tough to crystallize samples are microcrystalline and buried within precipitated samples. UV imaging is proven to be a powerful tool to analyze the microcrystalline nucleation in crystallization trials. To further analyze UV imaging results we developed FluorScore, a numerical method that reduces the UV image to a single numeric metric that can be used to categorize the drops in terms of their type and intensity of fluorescence signal. This study will analyze the usefulness of the algorithm for successful detection of promising conditions for tough to crystallize novel samples along with some standard proteins for comparison. An evaluation of the challenges of analyzing the results of crystallization trials by exhaustive manual inspection compared to FluorScore's algorithm results will be presented. In situations of HTP crystallization trials, the described algorithm is a very useful tool that can be used to identify conditions that harbor microcrystal nuclei and help Crystallographers make confident decisions on expansion trials.



Keywords: Crystallization, microcrystallography, UV fluorescence