Modeling and machine learning tools to improve image processing in crystallization screening

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Imaging methods are vital to the process of screening for successful crystallization hits. When screening is carried out in a high-throughput manner, the sheer volume of images needing processing is enormous, requiring a large commitment of time and effort to locate successful crystallization conditions. In addition, different imaging modes are subject to different complications, including optical aberrations, resolution limitations, and behavior with respect to obstruction, etc. We discuss our recent work on computational and modeling approaches to improve image processing and analysis for crystallization screening. These include wavelet transforms for image reconstruction, denoising, and registration, and machine learning approaches to process and classify image content, enabling easier identification of crystal hits. We discuss applications of our methods to standard brightfield imaging, as well as explore their capabilities in multimodal image integration, combining information from UV-TPEF (two-photon excited ultraviolet fluorescence) and SHG (second harmonic generation) nonlinear imaging modes. These computational tools are developed to facilitate steps towards automated imaging to streamline crystal detection and acquisition.