Autoscoring of Protein Crystallization Drops in ROCK MAKER using MARCO

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Over the past decade, the use of automation and specialized software for protein crystallization have become general practice in both academic and industrial settings alike. Advancements in both crystallization automation and software have allowed for higher experiment throughput and an increase in the number and rate of structures determined. With automated imaging systems, researchers can now run even more experiments and program a schedule for capturing images of their protein drops to see how those conditions are performing over time. One bottleneck to this process is manually scoring those protein drop images, which is often very time-consuming and most certainly boring.

With the advent of machine learning has come the ability to have a computer algorithm analyze and score protein drop images. One such technology is the MAchine Recognition of Crystallization Outcomes or MARCO, that can score a 96 well- 1 drop plate in under 3 minutes, with an accuracy of ~94%. MARCO automatically provides a probability of a drop image being either a crystal, precipitate, clear, or other. Although MARCO currently works with images taken using visible light path only, research to make it more versatile and work with other light paths such as UV fluorescence, visible light fluorescence, and Second Harmonic Generation (SHG) is being carried out at Formulatrix.

We present how machine learning and MARCO are being integrated into our ROCK MAKER® Crystallization Software to allow for even greater throughput than ever before. Having machine learning integrated with ROCK MAKER will provide researchers access to this powerful new tool and keep their all of their experimental data in one place.