Crystal Ranking: Automatic Analysis of Screening Images.

Q. Xu[1,2], Z. Zhang[1,2], N. Sauter[3], H. van den Bedem[1,2], A. Gonzalez[2], C. Smith[2], A. Deacon[1,2]

The ability to screen crystals and find ones suitable for crystallographic studies is essential to any crystallographic project. The rapid adoption of crystal mounting robots at synchrotron beamlines allows automatic screening of hundred of crystals in a couple of hours. Quick and automatic analysis of the diffraction images from such screening is essential in order to reduce human labor and make efficient usage of beam time. The goals are to collect the diffraction properties of screened crystals and select ones suitable for further structural studies. We attempt to address this problem by a two-step process. The first step is to conduct a statistical analysis of the diffraction images, through the identification of diffraction peaks and the detection of ice rings. The statistics include a resolution estimation, spot shape analysis, diffraction strength, spot split percentage, and ice ring strength/location. A score is assigned to each image based on these statistics. This step is implemented in a C++ library DISTL (Diffraction Image Scoring Tools Library). Autoindexing is then used to provide a more accurate picture of the crystal quality for promising crystals.

[1] Joint Center for Structural Genomics
[2] SSRL, Stanford Univ., Menlo Park, CA
[3] Dept. of Physical Biosciences, LBL, Berkeley, CA