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Probability-based Cryo Condition Optimization Procedure for High-throughput X-ray Crystallography. M. Yu¹, E.H. Bursey¹, T. Radhakannan¹, L-W. Hung^{1,2}, ¹Physical Biosciences Div., Lawrence Berkeley National Lab, Berkeley, CA 94720 USA, ²Physics Div., Los Alamos National Laboratory, Los Alamos, NM 87545 USA.

An empirical probability-based cryo condition selection procedure for high-throughput diffraction screening and data collection has been developed at the ISFI/TBSGC X-ray crystallography facility at the Lawrence Berkeley National Laboratory. This method is based on (1) diffraction experiments from about 3000 crystals of 62 unique TBSGC targets conducted in 2004-2005, and (2) empirical compatibilities between cryo-additives and crystallization reagents. The results have been cross-validated with over 700 independent data from the Cryoprotectant Database (http://idb.exst.jaxa.jp/db_data/protein/200304E02478000.html) with highly positive correlations. Our procedure selects 2-20 cryoprotectant candidates for initial diffraction screening according to the contents of the crystallization mother liquor. A 'score of merit' (SOM) combining the diffraction resolution, the mosaicity, and the presence of ice rings are used to track the successfulness of each cryo condition. Using this procedure, we have obtained high success rate to rapidly determine an optimal cryo condition for crystals from a board range of proteins.