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Function-Biased Choice of Additives for Optimization of Protein Crystallization. M. Chruszcz¹, M.D. Zimmerman¹, K. Koclega¹, J. Raynor¹, J.J. Petkowski¹, M. Cymborowski¹, X. Xu², T. Skarina², E. Evdokimova², A. Savchenko², A. Edwards², Z. Otwinowski³, W. Minor¹, ¹Univ. of Virginia, Charlottesville, Virginia 22908, USA, ²Univ. of Toronto, Toronto, Ontario M5G 1L6, Canada, ³UT Southwestern Medical Center at Dallas, Dallas, Texas 75390, USA.

Well-diffracting single crystals of macromolecules are one of the most valuable pieces of matter. Production of crystals suitable for structure solution is still a bottleneck of the structure determination process. We present an approach to optimization of protein crystallization that is based on the LabDB knowledge database. LabDB keeps information on all experiments that were performed in order to obtain crystals. Crystallization optimization is based on application of different so-called 'additives' that may lead to better quality crystals in the same or a different crystal form. The choice of chemicals is based on the analysis of protein function and information stored in LabDB. The presented approach substantially increased the diffraction resolution limit for several crystals and in some cases its application gave different crystal form(s). The approach was also successfully used to prevent or reduce twinning. In one of the most successful applications of the optimization protocol (thioesterase from *Pseudomonas aeruginosa*; PDB code: 2AV9) three new crystals forms were obtained by a small variation of the original crystallization conditions. The resolution limit was extended from 2.4Å to 1.9Å.