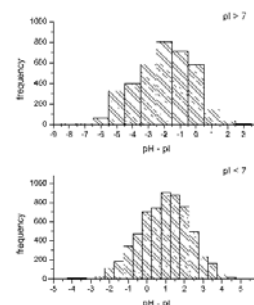


## W0153

**Designing More Efficient Crystallization Screening Experiments: Consider Protein Isoelectric Point.** K.A. Kantardjieff<sup>1</sup>, B. Rupp<sup>2</sup>, <sup>1</sup>Keck Center for Molecular Structure, CSU Fullerton, <sup>2</sup>UC Lawrence Livermore National Laboratory.

Increased efficiency in initial crystallization screening reduces cost and material requirements in structural genomics involving high throughput crystallographic structure determination. Because pH is one of the few consistently reported parameters in the Protein Data Bank, the isoelectric point, pI, of a protein has been explored as a useful indirect predictor for optimal choice of range and distribution of pH sampling in crystallization trials. We have analyzed 9596 unique protein crystal forms from the August 2003 PDB and found a significant relationship between the calculated pI of successfully crystallized proteins and the difference between pI and reported crystallization pH. These preferences provide strong prior information for the design of crystallization screening experiments with significantly increased efficiency. A prototype screen design and efficiency estimator program, CrysPred, is available at <http://www-structure.llnl.gov/cryspred/>.



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