

W0197

Mapping the Dimensionality of Crystallization Parameter Space by Success Rate Comparison. Brent Segelke, Timothy Lakin, Dominique Toppani, BBRP, LLNL, Livermore, CA 94551.

At the TBSGC crystallization facility, we have developed a metric for quantifying the similarity of parameters used in crystallization experiments based on pair wise success rate comparisons. We are pursuing a research plan to accumulate a large data set to enable pair wise success rate comparisons of a large number of reagents commonly used in crystallization experiments. To date we have accumulated success rates from >100,000 random screening experiments. Since our experiments are designed by random combination, we can treat each parameter as independent and compare success rates of individual reagents. We have completed an extensive success rate analysis on individual reagents and have now begun extensive pair-wise success rate comparisons. While success rate analysis of individual components is very useful for design of initial screens with maximized efficiency, having a metric for quantitatively comparing the similarity or dissimilarity, or orthogonality, of experimental conditions provides something much more useful. A few examples of the application for such a metric are: the convenient display of the diversity of a given set of experiments; the development of more sophisticated optimization strategies; but most significantly, the mapping of the dimensionality of the crystallization parameter space itself and the development of a minimum basis set of reagents that most efficiently spans crystallization parameter space. We are currently developing an application on the Screenmaker 96+8 (Innovadyne) to speed the accumulation of success rate data.