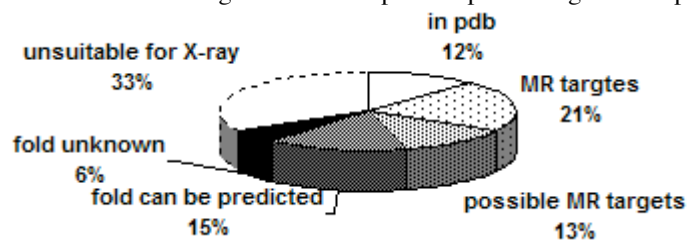


W0365

Improved Success Rate of Molecular Replacement. Lukasz Jaroszewski, Robert Schwarzenbacher, Adam Godzik, Joint Center for Structural Genomics, TBI, 10901 N. Torrey Pines Rd. La Jolla, CA 92037, USA

The most important goals of the Structural Genomics Initiative are: determining new protein folds and extending “structural coverage” of large protein families with known structures. It is possible to significantly reduce the costs of the second goal by using molecular replacement (MR) phasing method.

We have recently shown (Schwarzenbacher, et. al., 2004) that the success rate of MR can be improved by using advanced modeling methods and parallel processing of multiple MR searches.



Here we present a full analysis of over 70 successful and 15 unsuccessful MR trials performed at the Joint Center for Structural Genomics. We show that in the most difficult cases several variants of alignments and search models had to be used. We present the method of predicting probability of successful MR phasing based on the features of the alignment between the

protein and its modeling template. We predict the number of MR targets in the proteome of *t. maritima* and show that about 30% of structures from typical bacterial proteome can be solved with MR:

Structural coverage of the proteome of *t.maritima*.

References

Schwarzenbacher, R., Godzik, A., Grzechnik, S.K., Jaroszewski, L. (2004). The importance of alignment accuracy for molecular replacement. Acta Cryst. D60, 1229-1236.