Molecular Replacement At SSGCID

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The Seattle Structural Genomics Center for Infectious Disease (SSGCID) expresses all targets by default as native, non-SeMet protein. While the majority of structures can readily be solved by Molecular Replacement (MR), several structures will not solve using the most likely search model. This can be due to low homology, conformational changes, proteolytic cleavage or a simple sample mix up.

Using a larger pool of homologs and homologues domains as provided by MorDa has significantly increased our success rate for MR and has streamlined our structure solution pipeline.

For weaker MR solutions, reduction of model bias via density modification, followed by automated model building into the density modified maps has streamlined solving a number of structures.

MR searches against the entire PDB via Simbad, MR searches for smaller secondary structure fragments via Acrimboldo, or target identification via anomalous scattering have enabled us to solve several proteolyzed or mislabeled targets.