

## W0466

**Gene Composer: A Tool for Designing and Optimizing Protein Constructs for X-ray Crystallography.** Mark Mixon, J. Walchli, K. Post, P. Nollert, L. Stewart, A. Burgin, deCODE biostructures and Emerald BioSystems, Bainbridge Island, WA.

The diligent crystallographer will often consult many different software packages in order to make decisions about how to design a protein construct and to maximize the likelihood of success for crystallizing a protein. Since information that impacts the design process comes from disparate sources, it is often a laborious task to assemble a unified view of sequence and structural information. We have developed software and a database, called Gene Composer that neatly bundles the process into one package. The Protein Design Module contains alignment as well as web access tools that allow users to rapidly place sequence information in the context of homologous structural models. Information about solvent accessible regions, crystal contacts, B-factors, as well as ligand, and water contacts are displayed so that important structural and functional regions of homologous sequences can be rapidly identified. The Protein-to-DNA Design Module allows users to design a novel nucleic acid coding sequence with optimized open reading frame features for different heterologous expression systems (preferred codon usage, minimized mRNA secondary structure, eliminated or introduced restriction sites, regulatory elements, etc.). Various features of the software will be discussed together with examples of how Gene Composer can aid researchers in designing protein constructs and nucleic acid coding sequences for improved protein expression and crystallization.