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Assigning Protein Fold on the Basis of Wide-Angle Solution Scattering Data. L. Makowski^{1*}, D.J. Rodi¹, R.F. Fischetti^{1,2}, ¹Biosciences Div.,²GM/CA-CAT, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439.

Secondary and tertiary structure motifs have characteristic distributions of inter-atomic distances that produce features buried within the solution scattering pattern from a protein in solution. Wide angle solution scattering patterns predicted in silico from crystallographic coordinates were employed as the basis for the dissection of scattering patterns into individual elements using a principal components analysis. Patterns from a test set of 100 proteins were used to construct linear relationships between percentage alpha/beta structure and features in the diffraction patterns. This analysis produced a set of coefficients that were applied to a set of 400 diffraction patterns derived from protein crystal structures to predict their alpha/beta content, with an average error rate of 11%. A similar approach is being used to position proteins in 'fold space' on the basis of their actual and calculated solution scattering patterns.