

KS12 - Willie Taylor (National Institute for Medical Research - UK)

Ideal Protein Forms and their Application to De-Novo Structure Prediction

Abstract:

An abstract representation, similar to a Periodic Table, was used to generate a large number of idealised protein folds. Each of these was taken as a framework onto which a variety of predicted secondary structures were mapped and the resulting models constructed at a more detailed level. The best of these were refined and rescored. On a set of five proteins, the correct fold was scored highly in each with the top models having a low root-mean-square deviation from the known structure.