Inverse protein folding: design of stable proteins

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The inverse protein folding problem is that of designing an amino acid sequence which has a particular native protein fold. This problem arises in drug design where a particular structure is necessary to ensure proper protein-protein interactions. In this talk, we show that in the 2D HP model of Dill it is possible to solve this problem for a broad class of structures. These structures can be used to closely approximate any given structure. One of the most important properties of a "good" fold is its stability - the aptitude not to fold simultaneously into other structures. This is a necessary condition in for drug design, for example. We show that for a number of basic structures, our sequences have a unique fold.

This is a joint work with A. Gupta and L. Stacho.