

TT2 - Willie Taylor (National Institute for Medical Research - UK)

Protein Folds, Knots and Tangles

Saturday – 10:40-12:00

English (Translation provided by R. Dilão and R. Mondaini)

Abstract:

The backbone chain of a protein (called its fold) can be considered as a simple directed chain with one point representing each amino acid in the sequence. Repeated local smoothing of the chain coordinate set (without chain passage) leads to a simple method to detect knots in open chains. With each step in the smoothing the chain shrinks and close points can be removed. If the chain can be reduced to two points, it is not knotted: otherwise a knot exists. A trefoil and figure-of-eight protein knot are described. Extension of the algorithm to incorporate hydrogen-bond cross-links allows protein pseudo-knots to be considered. The general connectivity of a protein chain is considered as a graph and a novel concept of topological accessibility described. These ideas are then applied to semi-random folds.