

THE RAP SEMINAR SERIES

NCAR

Modeling of Complex Systems: Application to Cancer Therapy

by

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*Thursday, September 12, 2002, 3:30 p.m.
Foothills Lab, Building 1, Atrium*

In recent years, modeling of complex systems has become a reality and has been applied to fields as diverse as atmospheric research or theoretical chemistry. Therefore, although molecular dynamics simulations of proteins is far from UCAR's research, the hope is that interesting comparisons between the methods used to solve our different problems might be drawn.

This presentation will, therefore, focus on some of the techniques currently used in computer analysis of proteins, like molecular dynamics simulations, free energy simulations, conformational space search using simulated annealing or genetic algorithms.

These methods will be presented in the frame work of cancer research and, more specifically, in the design of peptidic vaccines aimed at building an efficient immune response against the patient's tumor. An example of such in silico design will be given together with preliminary clinical trials results conducted on melanoma patients.