PROFILE

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PROFESSIONAL FOCUS

Numerical Methods in Genomics, Proteomics, and Metabolic Network Analysis.

MAJOR PROJECTS

- Structural analysis of Cyclodextrin host:guest complexes as models for enzyme - substrate interaction
- Combination of structure and circular dichroism computation in a Monte Carlo Simulated Annealing framework
- Computation of peptide folding with special focus on solvation effects
- Simulation of the assembly of micellar / membraneous structures
- Dynamical hierarchies as a formal framework for complex systems theory
- Simulation of intracellular reaction networks
- Differential gene expression and promoter analysis
- Antigenicity profiling of disease associated proteins

PROGRAM SUITES

- MultiMize: Macromolecular structure optimizer
- LMA: Lattice Molecular Automaton, CA based simulator
- discoveryBASE: Framework for lead discovery combining genomics and structural bioinformatics
- GAnalyze: Genetic algorithm based promoter analysis

ACADEMIC BACKGROUND

1993. MS, Molecular Biology, University of Vienna, Austria 1995. PhD, Theoretical Chemistry, University of Vienna, Austria

1996-2000. Research positions at University of Vienna (A), CNR

Bologna (I), Los Alamos National Lab. (USA)

2004. Venia docendi in Structural Biology, University of

Vienna; Adjunct Professor at the Department of

Theoretical Chemistry and Molecular Structural Biology

Over 100 full papers, book / conference contributions and invited talks in the area of Molecular Recognition, Differential Gene Expression Analysis, and Applied Computational Biology.