3rd Workshop on Molecular Theories and Simulations

Gaeta, 14-16 May 2004

Organizing committee:

A. Amadei (Roma, TOV)
M. Aschi (L'Aquila)
A. Di Nola (Roma, La Sapienza)

Program

Friday 14

afternoon: welcome and rooming in.

Saturday 15

9:20 opening

9:30-10:10 **Cecilia Bossa** (Roma)
Extended Molecular Dynamics Simulation of the Carbon Monoxide Migration in Sperm Whale Myoglobin.

10:10-10:50 **Alessandro Grottesi** (Oxford)
Permeation and Gating in KIRBAC1.1: Insights from Molecular Dynamics Simulations.

Coffee break

11:10-11:50 **Steven Hayward** (Norwich)
Identification of Specific Interactions that Drive Ligand-Induced Closure in Domain Enzymes.

11:50-12:30 **Isabella Daidone** (Roma)
Free Energy Landscape of a Beta-Hairpin Peptide in Solution: a Molecular Dynamics Study.

13:00 Lunch

15:30-16:10 **Marco D'Abramo** (Roma)
On the Use of the Quasi-Gaussian Entropy Theory in the Study of Simulated Dilute Solutions.

16:10-16:50 **Maira D'Alessandro** (Roma – l'Aquila)
Theoretical Modelling of Enzyme Reactions Chemistry: the Electron Transfer in Cu-Zn Superoxide Dismutase.

Coffee break

17:10-17:50 **Riccardo Spezia** (Paris)
Environmental Effects on Conical Intersections.

17:50 Discussion

Sunday 16

10:00-10:40 **Tsjerk Wassenaar** (Groningen)
The Molecular Shaped Box: Determination, Usage and Validation.

Coffee break

11:00-11:40 **Mario Compiani** (Camerino - Bologna)
Toward a Unified Model of the Folding Mechanism of Small All-Alpha Proteins.

11:40-12:20 **Martin Ulmschneider** (Roma)
Properties of Integral Membrane Protein Structure: Derivation of an Implicit Membrane Potential.

13:00 Lunch

Hotel Summit - Gaeta (LT)
Via Flacca Km 23 – Tel. 0771-741741