7th Workshop on Molecular Theories and Simulations

Gaeta (Latina), Hotel Summit, 16-18 May 2008

Organizing committee:

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

Friday 16

18:00-18:35 **Ambra Tarquini.** **Università di Roma 'La Sapienza'**

Theoretical and computational characterization of dilute ionic solutions under the effect of external electric field.

18:35-19:10 **Stephan Lutz.** **University of Basel**

Ligand migration in heme-proteins.

Saturday 17

9:30-10:05 **Markus Meuwly.** **University of Basel**

The role of higher CO-multipole moments in understanding the dynamics of photodissociated carbon monoxide in Myoglobin.

10:05-10:40 **Marco D'Abramo.** **IRB Barcelona**

Protein dynamics in electrospray conditions.

10:40-11:20 **Coffee Break**

11:20-11:55 **Isabella Daidone.** **IWR Uni-Heidelberg**

Hydrogen-bond driven loop closure kinetics in unfolded polypeptide chains.

11:55-12:30 **Paolo Foggi.** **LENS Firenze**

Time-resolved spectroscopy: what we learn about structure and dynamics of complex molecules.

13:00 **Lunch**

15:30-16:05 **Modesto Orozco.** **IRB Barcelona**

Simulation in nucleic acids, going to the genomic scale.

16:05-16:40 **Antonella Fontana.** **Università di Chieti**

Study of the aggregation behaviour of a series of block co-polymers in water.

16:40-17:20 **Coffee Break**

17:20-17:55 **Massimiliano Anselmi. Università di Roma 'La Sapienza'**

The kinetics of ligand migration in crystalized Myoglobin as revealed by MD simulations.

17:55-18:30 **Alessandro Grottesi. CASPUR Roma**

Essential dynamics of the mitochondrial ADP/ATP carrier: dynamical role of odd-numbered helices.

18:30-19:05 **Guoyng Qi. University of Norwich**

Role of interdomain bending regions in ligand induced domain closure.

Sunday 18

9:00-9:35 **Costantino Zazza. CASPUR Roma e Università di L'Aquila**

An Electrochemical Controllable Nanospring.

9:35-10:10 **Stephen Hayward. University of Norwich**

New results on well-known biomolecular complexes using DynDom3D.

10:10-10:45 **Riccardo Spezia. Universite' d'Evry Val d'Essonne**

Modelling Collision Induced Dissociations by Direct Dynamics Simulations.

10:45-11:15 **Coffee Break**

11:15-11:50 **Georgios Patargias. University of Leeds**

Calculation of a Protein dielectric response using Molecular Dynamics simulations

11:50-12:25 **Laura Zanetti. Università di Roma 'La Sapienza'**

Structural and Thermodynamic Characterization of a Beta-Hairpin Peptide in Solution: a MD Study of a Synthetic Analogue of Gramicidin S

12:25-13:00 **Massimiliano Aschi. Università di L'Aquila**

On the UV spectrum of water in condensed phase: a different interplay between experimentalists and theoreticians?

13:30 **Lunch**

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