8th Workshop on Molecular Theories and Simulations

Gaeta (Latina), Hotel Summit, 24-26 May 2010

Via Flacca Km 23 Gaeta (Latina) Tel. +39-0771-741741

Organizing committee:

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

Monday 24
Afternoon : Chair - Alfredo Di Nola
16.00-16.40
Isabella Daidone - Università di L'Aquila (Italia)
On the origin of infrared spectral changes upon protein folding
16.40-17.20
Enrico Bodo - Università di Roma 'La Sapienza' (Italia)
The stereochemistry of sulphoxides: theoretical treatments of the inversion process.
Coffee Break
18.00-18.40
Laura Zanetti-Polzi - Università di Roma 'La Sapienza' (Italia)
Analysis of computed infrared spectra: an application to peptides
18.40-19.20
Massimiliano Anselmi - Università di Roma 'La Sapienza' (Italia)
On the use of MD simulations of globins in different environments for an effective comparison with structural and kinetic experimental data.
Tuesday 25
Morning: Chair - Sylvio Canuto
9.30-10.10
Carles Pons - Barcelona Supercomputing Center (Espana)
Modelling of protein-protein and protein-RNA interactions by computational docking
10.10-10.50
Francois Dehez - Nancy Universite (France)
Some aspects of the association of ADP3-to the mitochondrial ADP/ATP carrier (AAC).
Coffee Break
11.30-12.10
Tsjerk Wassenaar – Utrecht University (The Nederlands)
Potpurri
12.10-12.50
Steven Hayward – University of Norwich (United Kingdom)
The effect of end constraints on protein loop kinematics

13.30 Lunch

Afternoon: Chair - Andrea Amadei
15.30-16.10
Sylvio Canuto - Cidade Universitaria, São Paulo (Brasil)

Effect of the Liquid Environment in the Electronic Spectroscopy and Reactivity of Molecular Systems.
16.10-16.50
Kaline Coutinho - Cidade Universitaria, São Paulo (Brasil)
Relative Free Energy Calculation in Solution: Applications in Reaction and Aggregation
Coffee Break
17.30-18.10
Antonino Polimeno – Università di Padova (Italia)
Modeling NMR spin relaxation in proteins via stochastic methods: semi-analytical and computational approaches
18.10-18.50
Costantino Zazza - CASPUR Roma (Italia)
Theoretical modelling of molecular machines.
Wednesday 26
Morning: Chair - Steven Hayward
9.30-10.10
Francesco Gervasio - Biophysics Group at the Spanish National Cancer Research Center (CNIO)
Multiscale Modeling of Cancer
10.10-10.50
Bert De Groot – MPI Göttingen (Deutschland)
Mechanisms underlying molecular recognition
Coffe Break
11.30-12.10
Alessandro Grottesi – CASPUR Roma (Italia)
Conformational Dynamics of a Voltage-Gated K^+ Channel Chimera Kv1.2/Kv2.1: Insights from full Atomistic Molecular Dynamics Simulations
13.30 Lunch

Please note that each speaker has 30 minutes of talk and additional 10 minutes of discussion.