
2nd Workshop on Molecular Theories and Simulations

13-15 May 2003

Summit hotel

Via Flacca Km 23 – Gaeta (LT)

Tel. 0771-741741

Organizing committee:

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

Program

Tuesday 13

afternoon: welcome and rooming in.

Wednesday 14

9:30-10:00 G. Brancato (New York) '**Modelling Proton Transfer in Condensed Phase: a Multi-State EVB Approach**'

10:00-10:30 R. Spezia (Paris) '**Mixed Quantum-Classical Molecular Dynamics Study of A Hydrated Electron and Cation Pairs in Bulk Water**'

10:30-11:00 C. Benzi (Napoli) '**Effective Procedures for Calculating NMR Parameters on Large Molecular Systems in Solution**'

11:00-11:30 Coffee break

11:30-12:00 A. R. Bizzarri (Viterbo) '**Molecular Dynamics Simulation of Copper Plastocyanin Immobilized on Gold Surface**'

12:00-12:30 I. Daidone (Roma – 'La Sapienza') **'Solvent Induced Alpha to Beta Conformational Transition of the Prion Protein Peptide H1 Studied by Molecular Dynamics Simulations.'**

13:00 Lunch

16:00-16:30 C. Zazza (Roma – 'La Sapienza') **'Electronic Properties in Complex Molecular Systems: from Simple Solutes to Enzyme Reactions'**

16:30-17:00 M. D'Abramo (Roma – 'La Sapienza') **'Statistical Mechanics of Solute-Solvent Systems: the Thermodynamics of Formaldehyde in Water'**

17:00-17:30 Coffee Break

17:30-18:00 E. Langella (Napoli) **'Environmental Effects on The Conformational Behavior of Human Prion Protein'**

18:00-18:30 D. Roccatano (L'Aquila) **'A Statistical Mechanical Approach to Protein Folding Problem'**

Thursday 15

10:00-10:30 C. Bossa (Roma – 'La Sapienza') **'Molecular Dynamics Simulation Study of Myoglobin: Cavities Fluctuations and Ligand Motion Relationship.'**

10:30-11:00 G. Colombo (Milano – 'CNR') **'Combining Simplified and All Atom Methods to Investigate Small Protein Folding'**

11:00-11:30 Coffee Break

11:30-12:00 A. Grottesi (Oxford) **'Docking of TC1 Toxin onto Shaker K Channel: a Molecular Dynamics Study'**

12:00-12:30 M. D'Alessandro (Roma – 'La Sapienza'/'TOV') **'Dynamical and Statistical Mechanical Characterization of a Peptide in Water'**

13:00 Lunch

