Preface

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This special Issue of the International Journal of Molecular Sciences contains selected papers from the US-Czech-Polish workshop on **Modeling Interaction in Biomolecules** that took place between 15-th and 20-th September, 2003 in Nové Hrady, Czech Republic. 65 participants from 8 countries attended this conference.

The workshop focused on recent computational techniques and advanced methodology used to model various biological systems and processes. The meeting was divided into several parts, morning lectures delivered by invited lecturers were designed to introduce particular topics. This was continued by junior speakers and PhD students in the afternoon sessions.

The introductory address given by D. Štys from the leading local experimental group from Institute of physical biology, University of South Bohemia was devoted to general questions of mutual cooperation between theoretical and experimental community.

Following lecture of R. Zahradník contained valuable overview of recent progress in this interdisciplinary area and this contribution opens the Special IJMS Issue.

First session was devoted to modeling of catalytic processes with lectures delivered by M. Blomberg, W.L. Jorgensen, S. Zaric, S. Záliš, and S.Lee. The topics discussed at afternoon session were related to metaloorganic and bioinorganic complexes.

Next morning session dealt with problems in classical molecular dynamics and main contributions were presented by J. Šponer, E. Fadrná, J. Koča, N. Gresh, and S. Raugei.

Third session was devoted further extension of modeling catalytic activities by E. Broclawik, W. A. Sokalski, and T. Wesolowski.

A trip to UNESCO heritage – city and castle of Český Krumlov provided a sightseeing opportunities during the Thursday afternoon.

Last two morning lectures on techniques for QSPR (T. Clark), weak and non-covalent interactions (P. Politzer, J. Leszczynski, and P. Hobza), electron spectra calculations (Z. Havlas) and organization of available structural databases (B. Schneider) concluded our meeting.

In addition 17 shorter (20 minutes) oral contributions and 34 posters were presented in the afternoon sessions.