# MATH/CHEM/COMP 2003

# Dubrovnik June 23-28, 2003

Inter-University Center, Dubrovnik, Croatia, "Ruder Bošković" Institute, Zagreb, Croatia
Universities of Zagreb & Split

International Society for Mathematical Chemistry, International Society for Theoretical Chemical Physics

### **Scientific Committee**

B. Borštnik (Ljubljana) D. J. Klein (Galveston) I. Simon (Budapest) T. Braun (Budapest) S. McGlynn (Baton Rouge) P. F. Stadler (Leipzig) J. Brickmann (Darmstadt) W. A. Milne (Williston) D. Svrtan (Zagreb) D. Butina (Cambridge) V. Ostrovskii (St. Petersburg) N. Trinajstić (Zagreb) R. Ponec (Prague) I. Ugi (Garching) J. Cioslowski (Tallahassee) H. Hosoya (Tokyo) M. Randić (Des Moines) H. Vančik (Zagreb) P. Fowler (Exeter) D. Veljan (Zagreb) H. Sachs (Ilmenau)

# **Organizing Committee**

A. Graovac (Zagreb), director

D. Butina (Cambridge), co-dir.

M. V. Diudea (Cluj)

D. Plavšić (Zagreb)

D. Janežič (Ljubljana)

E. C. Kirby (Pitlochry), co-dir.

I. Lukovits (Budapest)

T. Pisanski (Ljubljana), co-dir.

D. Plavšić (Zagreb)

D. Plavšić (Zagreb)

N. Štambuk (Zagreb)

D. Vikić-Topić (Zagreb), co-dir.

J. Žerovnik (Maribor)

# Venue

The MATH/CHEM/COMP 2003 (MCC'03) will be held from June 23-28, 2003, in Dubrovnik in the Inter-University Centre (IUC), don Frana Bulića 4. Dubrovnik is situated on Adriatic Coast at the far south of the Republic of Croatia, and due to its beauty and harmony it is designated by UNESCO as a world heritage.

## **Conference Scope**

The MCC'03 is the 18<sup>th</sup> in the series of MCC meetings which started in 1986. Any subject pertinent in an interdisciplinary way to mathematics and/or computer sciences and chemistry and related sciences is a legitimate topic to be presented at the MCC'03. The meeting is open to all aspects of current research in the applications of computer modeling, combinatorics, graph theory and topology to any area of chemistry, physics, materials and life sciences.

### Sessions

Three special sessions will be held during the first three days of the MCC'03. The first one on Chemometrics (organized by Tom Solmajer) will cover topics like chemical descriptors, similarity, diversity, fingerprints, data storage, registration, compound selection, integration of measured and calculated molecular properties, data mining, in silico screening, statistical tools, etc. The Session on Drug Discovery (organized by Darko Butina) will cover subjects like QSAR, SAR, QSPR, 3D-methods, in vitro screening, ADME-TOX, high throughput screening and combinatorial chemistry, and new paradigms in drug discovery processes. The Session on Bioinformatics (organized by Istvan Simon & Peter Stadler) will present recent developments in the field of proteomics, comparative sequence analysis, structure and function prediction, and related fields of computational biology and biophysics.

# **Organizer**

All correspondence concerning the meeting should be addressed to:

**Prof. Ante Graovac** 

Ruđer Bošković Institute, HR-10002 Zagreb, POB 180, Croatia

phone: (385)-(1)-46-64-565; fax: (385)-(1)-46-80-245; e-mail: graovac@rudjer.irb.hr

REGISTRATION SUBMISSION DEADLINE: April 15, 2003 ABSTRACT SUBMISSION DEADLINE: May 1, 2003

www page: http://mcc.irb.hr