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## **FOREWORD**

The MATH/CHEM/COMP 2004 Dubrovnik International Course & Conference (MCC 2004) on the Interfaces among Mathematics, Chemistry and Computer Sciences was held from June 21–26, 2004, in Dubrovnik, Croatia, under the joint auspices of the Inter-University Centre, Dubrovnik, Ruđer Bošković Institute, Zagreb, Universities of Zagreb & Split, International Society for Mathematical Chemistry, and International Society for Theoretical Chemical Physics. MCC 2004 was the nineteenth in a series of annual meetings that we started in 1986, and it attracted 100 participants from 20 countries, a large number of them students and young researchers.

The MCC meetings are traditionally focused on discussions about the interplay among mathematics, chemistry and computer sciences, and this continues. However, to keep pace with »hot« subjects and practical needs, we incorporate into our meetings special sessions that vary from year to year. Two such sessions were offered at MCC 2004: *Bioinformatics* (organized by Istvan Simon and Peter Stadler) and *Chemoinformatics and Drug Discovery* (organized by Darko Butina).

From the very beginning, due care has taken to publish the results presented in Dubrovnik. As a result, twenty-seven MCC Proceedings have been printed up to

now in various distinguished scientific journals. The first part of the results presented at MCC 2004 are published in this special and refereed issue of Croatica Chemica Acta, and the rest will appear in No. 4 (2005) of the same journal. All these papers are dedicated to Dr. Edward C. Kirby in happy celebration of his 70<sup>th</sup> birthday. Some of the papers reported at the MCC 2004 *Session on Bioinformatics* were edited by Ante Graovac and Peter Stadler and are published as Vol. 124, No. 4 (2005) of the eminent journal *Theory in Biosciences*.

The organization of MCC 2004 was in the first place possible owing to the help of the Inter-University Centre in Dubrovnik, Ruđer Bošković Institute Zagreb, University of Zagreb, and University of Split. The financial support of the Ministry of Science, Education and Sports of the Republic of Croatia, Croatian Academy of Sciences and Arts, and PLIVA d.d. (Zagreb) is gratefully acknowledged. Special thanks for partial financial support go to SMS (Split), Profil (Zagreb), and Wolfram Research-Systemcom (Zagreb). Many thanks are also due to the CCA Editor-in-Chief, Academician Nenad Trinajstić, Mrs. Nada Trajkov, and Dr. Miro Bajić for their patience and understanding as well as to the contributors and referees for their assistance.

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