

## FOREWORD

The MATH/CHEM/COMP 2001 Dubrovnik International Course & Conference (MCC 2001) on the Interfaces between Mathematics, Chemistry and Computer Sciences was held from June 25-30, 2001, in Dubrovnik, Croatia, under the joint auspices of the Inter-University Centre, Dubrovnik, Ruđer Bošković Institute, Zagreb, Universities of Zagreb and Split, International Society for Mathematical Chemistry, and International Society for Theoretical Chemical Physics. MCC 2001 was the sixteenth in the series of annual meetings that we started in 1986, and it attracted 120 participants from 15 countries, a large number of them being students and young researchers. We are especially glad and proud that two leading figures of the chemical graph theory, Prof. Frank Harary and Prof. Alexandru T. Balaban, participated in MCC 2001, and we dedicated the meeting to them in happy celebration of their birthdays. Their achievements and CVs are displayed at: <http://www.cs.nmsu.edu/~fnh/> and <http://www.tamug.tamu.edu/mars/faculty/balaban.htm>.

The MCC meetings are traditionally oriented to discussion 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, which vary from year to year. Four such sessions were offered at MCC 2001: Session on Advanced Materials (organized by Zorica Crnjak Orel, Ante Graovac and Aleksandra Turković), Session on Bioinformatics (organized by Davor Juretić, Gábor Náray-Szábo and Andrej Sali), Session on Proteomic Modelling of Bioactive Molecules (organized by Nikola Štambuk), and Session on Drug Design (organized by Darko Butina, Vesna Gabelica and Tom Šolmajer). The fifth one, the Session on Philosophy of Chemistry (organized by Edward C. Kirby and Hrvoj Vančik) was a return to the fundamentals whence our research originated.

From the very beginning, due care has been given to publishing the results presented in Dubrovnik. As a result, twenty MCC Proceedings have been printed up to now in various distinguished scientific journals. The results presented at MCC 2001 are published in this special and refereed issue of *Croatica Chemica Acta*, and the same number of papers have been printed in the first four issues of Vol. 42 (2002) of *Journal of Chemical Information and Computer Sciences*. The contributions presented at the MCC 2001 Session on Philosophy of Chemistry appeared in the September 2002 issue of *Kemija u industriji (Zagreb)*.

MATH/CHEM/COMP meetings are of an interdisciplinary character and are not just a sum of the MATH(ematics), CHEM(istry) and COMP(uter) Sciences but are trying to establish a synergy of these and related disciplines, which are of importance to modern chemists and related researchers.

The present issue contains four papers on discrete mathematics in chemistry, two on bioinformatics, four on modelling in chemistry and medicine, and two on quantum chemistry.

The organization of MCC 2001 was possible in the first place due to the help of the Inter-University Centre in Dubrovnik, Ruđer Bošković Institute in Zagreb (on the occasion of its 50<sup>th</sup> anniversary), University of Zagreb and University of Split. The financial support from the Ministry of Science and Technology of the Republic of Croatia, PLIVA d.d. (Zagreb), Camitro (Cambridge, UK), and Hrvatski Telekom (HT) is gratefully acknowledged. Special thanks for partial financial support go to the Deutscher Akademischer Austauschdienst (DAAD), Krka d.d. (Novo Mesto), Office of the President of the University of Split, SMS (Split), Profil (Zagreb), Sava (Kranj), and Croatia Airlines. Many thanks are also due to the Editor-in-Chief Professor Nenad Trinajstić, Mrs. Nada Trajkov and Mr. Miro Bajić for their patience and understanding as well as to the contributors and referees for their assistance.

We dedicate this issue to Professor Frank Harary and Professor Alexandru T. Balaban wishing them all the best in the coming years.

*Ante Graovac (Zagreb & Split)*

*Biserka Pokrić (Zagreb)*

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