

FOREWORD

The MATH/CHEM/COMP 2002 Dubrovnik International Course & Conference (MCC 2002) on the Interfaces between Mathematics, Chemistry and Computer Sciences was held from June 24–29, 2002, 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 2002 was the seventeenth in a series of annual meetings 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 the two leading figures of chemical graph theory, Professor Milan Randić and Academician Nenad Trinajstić, participated actively in many MCC conferences, and we dedicated the MCC 2002 meeting to them in happy celebration of their birthdays.

The MCC meetings are traditionally oriented to discussion of the interplay between 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 2002: Session on Drug Design (organized by Darko Butina and Tom Šolmajer) and Session on Bioinformatics (organized by Davor Juretić and István Simon).

From the very beginning, due care was taken of publishing the results presented in Dubrovnik. As a result, twenty MCC Proceedings have been printed up to now in various distinguished scientific journals. A part of the results presented at MCC 2002 are published in this special and refereed issue of *Croatica Chemica Acta*, and the same number of papers are to appear in the forthcoming issues of the *Journal of Chemical Information and Computer Sciences*.

The present issue contains papers on mathematical chemistry, theoretical and experimental chemistry, and modelling in science and technology. It opens with a feature article by Marija, Nađa and Tomislav Došlić, which in an amusing way questions the mathematical content of the MCC meetings and estimates it to range from 0–43 % with an indication that the meetings are only 15 % mathematical in an average taken over the last eleven years. This is good news as the 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 between these and related disciplines that are of importance to modern chemists and related researchers.

The organization of MCC 2002 was possible in the first place due to the help of the Inter-University Centre in Dubrovnik, Ruđer Bošković Institute in Zagreb, University of Zagreb and University of Split. The financial support of the Ministry of Science and Technology of the Republic of Croatia, PLIVA d.d. (Zagreb), and ArQule (Cambridge, UK) is gratefully acknowledged. Special thanks for partial financial support go the Deutscher Akademischer Austauschdienst (DAAD), Krka d.d. (Novo Mesto), The City Council of Split, Pharmacia (Zagreb), SMS (Split), Profil (Zagreb), Wolfram Research-Systemcom (Zagreb), Dr. Etlinger d.o.o. (Zagreb), and Croatia Airlines. Many thanks are also extended to the Editor-in-Chief Academician Nenad Trinajstić, Mrs. Nada Trajkov and Dr. Miroslav Bajić for their patience and understanding as well as to the contributors and referees for their assistance.

We dedicate this issue to Profesor Milan Randić and Academician Nenad Trinajstić wishing them all the best in the coming years.

Ante Graovac (Zagreb & Split)

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