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On the Cover

Spatial view of the dopamine D_2 receptor. The Chimera program has been used as a graphic interface, Fig. 5, page 12, Andujar et al.

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FROM THE EDITOR

The Journal is paying in this issue a deserved homage to Professor Csizmadia with the help of his former students and collaborators. As detailed in the preface, Professor Csizmadia's works and positive influence span several countries, his prestige being internationally recognized in the field of theoretical chemistry.

The Journal would like to express its satisfaction for having been chosen as a means to draw attention to the figure of Professor Csizmadia and his legacy.

This number also underlines, peering into the future, the growing significance of physical/chemical simulation and modeling software that nowadays cover areas as wide ranging as quantum chemistry, nanotechnology, biomedicine, fluid dynamics, automotive industry, colliding galaxies etc. Computing power has become less of a limiting factor with the advent of cheaper clusters, multi-core chips and parallel processing that brought supercomputing to the desktop. Despite some obstacles in parallelizing software, the increase in accuracy and speed allow nowadays solutions to complex problems previously considered impossible.

Next issue, due out at the end of 2006, will deal with regular works on general topics.

The Journal is indexed in Chemical Abstracts and in the Scielo database (Scientific Electronic Library on Line).

Thanks to guest and associate editors plus anonymous referees who spare part of their valuable time to keep this publication going.

Keep in touch.

Reynaldo O. Lezna
Editor-in-Chief

PREFACE

Dedicated to Prof. Imre G. Csizmadia

Imre G. Csizmadia was born in Budapest, Hungary, on October 30th, 1932. The 75th anniversary of his birth is a timely occasion to highlight his outstanding personality, his scientific career, greatly acknowledged by the international community, and his profound influence on young investigators, particularly those of the National University of San Luis (UNSL), Argentina.

Csizmadia began his Chemistry studies at the Polytechnical University of Budapest, where he graduated as B.Sc. in 1956, his Ph.D. degree was obtained in 1962 at the University of British Columbia in Canada. From 1962 to 1964 he was a NATO Science Fellow in Quantum Physics at MIT. Later on he started teaching as Chemistry Professor at the University of Toronto, where he is Emeritus Professor since 1998. Over the years, he has been Visiting Scientist and Visiting Professor of numerous and well-known Universities all over the world, such as London, Queen's and York in England; Bologna in Italy; Nancy, Paris and Sorbonne in France; Budapest and Szeged in Hungary; Erlangen in Germany; Barcelona in Spain and San Luis in Argentina.

Furthermore, he is a Fellow of the Chemical Institute of Canada since 1970, Member of the European Academy since 1979, Honorary Member of the Hungarian Chemical Society since 1986 and Honorary Professor at Tianjin Normal University, China, since 1988. Professor Csizmadia was distinguished as Honorary Doctor from the Eötvös University of Budapest in 1988, recipient of the E.W.R. Steacie Award in Chemistry from The Chemical Institute of Canada in 1990, Angelo Mangini Gold Medal from the Italian Chemical Society in 1992, Martin Kajtar Medal from the Hungarian Academy of Sciences in 1999 and "Dr. Honoris Causa" of San Luis National University since 2005. In 1985, he co-founded the World Association of Theoretically Oriented Chemists (WATOC) and was its President during the period 1985-1990.

Professor Csizmadia collaborated with Professor Orville Thomas in the founding of the "Journal of Molecular Structure (THEOCHEM)" and was its Editor-in- Chief until 2004. In addition, he is a member of the Editorial Board of "Topics in Molecular Organization and Engineering" and "The Journal of the Argentine Chemical Society". Professor Csizmadia has published 12 books either as author, co-author, editor or co-editor, and more than 350 papers in international journals.

Imre G.Csizmadia developed a school in Computational Chemistry. He directed 12 MSc theses and 15 PhD theses, two of them (Dr. G. N. Zamarbide, 1999 and Dr. M. A. Zamora, 2001) in UNSL, Argentina.

Most of Prof. Csizmadia´s former PhD students are now full Professors who made a name for themselves in science and education in several Universities and Research Centers of Europe and America.

Without any doubt, Professor Csizmadia is a world reference on Molecular Computational Chemistry, the discipline he developed and in which he worked, with life and soul, for more than five decades.

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