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Editorial

Introduction and Foreword to the Special Issue on Molecular Modeling of Carbohydrates

INTRODUCTION

Two years ago, when the Executive Committee of the Computers in Chemistry (COMP) Division of American Chemical Society selected me as their editorial representative for JMGM, one of my first duties was to appoint half the members of the new International Editorial Board. Professor Rod Hubbard, editorial representative of the Molecular Graphics and Modelling Society in the United Kingdom, had responsibility for appointing the other half of the new board. My sphere of responsibility included the continents of North America, South America, Australia, and the Pacific Rim. To select dynamic and prominent computational chemists in each of these regions, I surveyed publication records and citation data. To learn who was highly respected in the more far-flung regions, opinions of computational chemists in those regions were solicited.

Out of this careful process, one of the outstanding individuals selected was Professor Dr. José Raúl Grigera, Director of the Instituto de Fisica de Liquidos y Systemas Biologicos, La Plata, Argentina. His service on the board is greatly appreciated. In May 1999, when he proposed organizing a special issue on the topic of molecular modeling of carbohydrates, I readily accepted his offer. I welcome him as Guest Editor of this issue.

Dr. Grigera is clearly an American: he was born in the small town of América, Argentina, in 1941. He began his studies in physics, but expanded his interests to biophysics and biochemistry. He did most of his Ph.D. research in Groningen, The Netherlands, under the guidance of Prof. Herman J. C. Berendsen, although the thesis was presented in the University of La Plata in 1972. The doctoral thesis was a study of collagen hydration using nuclear magnetic resonance, dielectric relaxation, and sorption isotherms. Dr. Grigera became assistant professor of biophysics at La Plata in 1973 and full professor in 1980.

In 1981 Prof. Grigera moved to the newly funded Institute for Physics of Liquids and Biological Systems. In 1987 he was appointed as assistant director and in 1988, director. Along with conducting research and teaching, he was several times head of the Department of Biology of the Faculty of Sciences, the National University of La Plata. The main line of his research evolved around the structure-function relationship of macromolecules emphasizing the role of the environment, particularly of the water molecules. Thus, the hydration of proteins, carbohydrates, and other macromolecules was studied by both experimental and computational research, including especially molecular dynamics simulations. He helped pioneer simulations of carbohydrates in aqueous solution.

Professors Grigera and Berendsen continued their collaboration at both La Plata and Groningen, and developed the famous, widely used SPC/E water model.[1] Prof. Grigera is a visiting professor at the University of Groningen, Columbia University, and the University of San Luis, Argentina. He has maintained research exchanges with Prof. H. E. Stanley (Boston University), Prof. Lesser Blum (University of Puerto Rico), Prof. J. Fischbarg (Columbia University, New York), Prof. M. Silbert (University of East Anglia, UK) and Dr. A. Podjarny (Institute de Genetique et Biologie Molecular et Cellulaire, Strasbourg, France).

Prof. Grigera has promoted biophysics, not only through the teaching which he does in undergraduate and graduate courses (the latter include international courses), but also through active participation in scientific organizations. He is a founding member of the Argentine Biophysical Society and has occupied several offices, including the position of President. He is a member of the Argentine Physical Society, the American Physical Society, the American Biophysical Society, the Royal Society of Chemistry (UK), the Carbohydrate Division of the American Chemical Society, and the Council of the International Union for Pure and Applied Biophysics (IUPAB). He has organized numerous conferences and workshops.

Prof. Grigera was honored with the Prize "Consagración Provincia de Buenos Aires" in Mathematical Sciences (1989) by the Province of Buenos Aires, Argentina. In addition, he was awarded an Antorchas Fellowship (1997) and a John Simon Guggenheim Memorial Foundation Fellowship (1998).

Besides directing the research of 13 Ph.D. students, he has authored nearly 90 papers in journals and contributed to 9 books on various aspects of hydration, carbohydrates, DNA, molecular dynamics simulations, and biophysics.

Prof. Grigera is married with four children. His free time (if any) is occupied with writing short stories (never published) and doing carpentry, wood carving, and machine work.

It is thus my pleasure and honor to introduce this special issue by Prof. Grigera. I thank him for suggesting the topic and splendidly carrying the idea to fruition. He has assembled

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research leaders in the field from Brazil, England, Spain, Germany, Italy, the United States, and France. The material that he forwarded to me for this issue was extremely well organized, making my job easy. We trust our readers will enjoy the articles and learn much from them for their own research endeavors.

I am also happy to announce that other exciting special issues are planned for the year 2000 and beyond.

Donald B. Boyd, Ph.D.
Editor, *Journal of Molecular Graphics and Modelling*

FOREWORD

Carbohydrates are commonly recognized as a significant source of biosphere energy reserves and as a primary food source. The functions of carbohydrates are not limited to these; the molecules have many other functions of major importance in living systems. A more comprehensive list would include carbohydrates as part of structural elements of plants and cell walls, as key molecules for molecular recognition, and as participants in protection under water stress. Carbohydrates comprise the basis of the economically significant food, paper, and textile industries.

Traditionally the study of carbohydrates was almost an exclusive subject of organic chemistry. Recently, new fields — with strong interdisciplinary content — have emerged. Glycobiology, glycochemistry, glycoimmunology, glycotechnology, glycobiochemistry, and others are terms in the new taxonomy of science, because the terminology of the classical disciplines of science inadequately described the actual complexity of the problems under consideration.

Molecular modelling is clearly able to solve (or to help solve) many problems and broaden our knowledge of molecular properties. Molecular modelling consists of methodologies that are neither experimental nor theoretical but complement both.

It is not surprising that modelling became an important component for the study of carbohydrates. The well-known 1990 American Chemical Society book[2] collected the papers of a symposium held in Dallas in 1989 and is probably the first volume devoted specifically to the field. Its contents reflect the state-of-the-art at that time, and other specialized symposia and publications followed. It is now 10 years later, and the field has been expanded.

This special issue on modelling of carbohydrates harvests papers from recognized scientists in the area and conveys the strong research activity on modelling of carbohydrates by physicists, chemists, biochemists, and biologists. It is hoped that this issue will be a cornerstone in the "reinvention" of JMGM as a forum for presenting significant modelling of important molecules.

I thank the authors who contributed their interesting and high quality work. This issue could not have been completed without the valuable and rigorous help of anonymous referees, whom I want to heartily acknowledge. On the editorial side, thanks are due to Elsevier Science, which is publishing this special issue, and to Don Boyd, who helped me with his advice, support, and kindness.

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REFERENCES

1 Berendsen, H.J.C., Grigera, J.R., and Straatsma, T.P. The missing term in effective pair potentials. *J. Phys. Chem.* 1987, **91,** 6169–6271
2 French, A.D., and Brady, J.W., Eds. *Computer modeling of carbohydrate molecules.* ACS Symposium Series 430, American Chemical Society, Washington, DC, 1990.