

Guest Editorial

**Special Issue Dedicated to Professor Marvin Charton –
Correlation Analyst *Par Excellence***

Tadeusz M. Krygowski

Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland, Phone/Fax:
(+48) 22 822 28 92; E-mail: tmkryg@chem.uw.edu.pl

Received: 18 January 2005 / Published: 31 January 2005

The collection of papers dedicated to Marvin Charton that we present in this special issue of *IJMS* covers a variety of fields of scientific research and well represents his wide range of interests – all the contributors are his friends or users of his ideas and the results of his scientific work and have often also been partners in subtle and very fruitful discussions with Marvin. The wide scope of the topics also reflects the great potential of correlation analysis and modeling – as methods which allows one to reach a better understanding of chemical phenomena in many very different areas of chemical research. They are also useful ways of interpreting results from everyday practice in chemistry.

The issue starts with an obvious topic – a short biography of Marvin Charton by his old friend – Dr John Shorter. Apart of a historical outline of Marvin's path through various problems and topics of physical organic chemistry – there is also included a list of most important works done by Marvin over only slightly less than a half century.

The problems closest to the Marvin early field of research – those associated with substituent effects – are represented by papers by J. Oszczapowicz, M. Hirota, J. Svoboda and T. M. Krygowski and their respective co-workers, who clearly demonstrate that the various aspects of this field are still very much alive as a research topic of great current interest. First, substituent effects are tackled using ¹³C-NMR spectroscopy, then, a reexamination of the steric substituent constants is presented, followed by a study of the kinetics and mechanism of acetoxymercuration and hydration of α -alkylstyrenes and finally, an analysis of how substituents affect pi-electron delocalisation in the ring of meta and para substituted benzoic acids and their anions is presented.

Close to these problems is the work by Gawinecki *et al.*, where the electronic and steric interactions in variously substituted aromatic amines are studied by means of ¹³C-NMR. Not far away from these topics is the paper by A. Cherkasov on the use of inductive QSAR descriptors for

distinguishing compounds with antibacterial activity using artificial neural networks. Dennis Kevill *et al.* present a paper dealing with an application of the extended Grunwald – Winstein equation to solvolyses of n-propylchloroformate. The solvent and ligand effects on the tandem addition-lithiation-electrophilic substitution of phenyllithium on α,β -unsaturated carbonyl compounds is presented by N. S. Nudelman and his colleagues. Jan Engberts *et al.* show in their contribution the influence of long-tailed alcohols on the solubilisation of cationic di-n-hexadecyldimethylammonium bromide, while the thermodynamics of water – octanol and water – cyclohexane partitioning of some aromatic compounds is subject of study by J. C. Dearden *et al.*

Eduardo Humeres *et al.* present studies on the salt catalyzed reduction of sulfur dioxide on carbons. Finally, we have a pair of theoretical studies. In the first, Raczyńska and co-workers present their *ab initio* studies on the protonation of the alkaloid Cytisine in the gas phase and water and in the second, a very theoretical study by G. Haefelinger *et al.* deals with *ab-initio* post HF CCSD(T) computations for triplet and singlet methylene.

Looking forward, it seems clear that the field of classical Physical Organic Chemistry represented so nicely by Marvin is actually understood as a much wider field of research, and most of authors contributing to the special issue illustrate this to great effect in their papers. The Guest Editor would like to conclude by thanking all the participants for answering his call to put together this special issue to celebrate a truly memorable occasion and Dr. Derek McPhee, Editor-in-Chief of Molecules, for his help in bringing it to fruition.

Tadeusz M. Krygowski
Department of Chemistry, University of Warsaw