

Milan Randić, Professor Emeritus, Drake University, Des Moines, Iowa, USA;

Visiting Professor, National Institute of Chemistry, Ljubljana, Slovenia

Milan Randić, studied Theoretical Physics in the University of Zagreb (1949-1953), obtained Ph. D. in Cambridge, England, in 1959, for his work on molecular vibrational spectroscopy. On return to the Rudjer Bošković Institute in Zagreb he founded the Theoretical Chemistry Group at the Institute and continued with research in Theoretical Chemistry. In 1971 he left for USA. In 1973, during a visit with Professor E. Bright Wilson at Harvard, he became interested in application of Discrete Mathematics and Graph Theory to molecular structure and chemistry. He has been one of the pioneers of Chemical Graph Theory. Since the year 2000, he became interested in quantitative characterization of graphical approaches to modeling of DNA and proteins, as well as proteomics and is one of the leading authorities in this field of Graphical Bioinformatics.

His contributions in Chemical Graph Theory and Graphical Bioinformatics are numerous and diverse: He introduced the “Conjugated Circuit Model,” which gave important insights on the nature of the aromaticity of conjugated hydrocarbons, and lead to computational scheme for calculation of molecular resonance energies in hydrocarbons and fullerenes. More recently he introduced algebraic (numerical) Kekulé valence and characterization of rings of benzenoid hydrocarbons based on partitioning of  $\pi$ -electrons in such systems, as well as, calculating ring currents in such systems.

His work in this area has been summarized in a giant review article “Aromaticity of Polycyclic Conjugated Hydrocarbons,” published in *Chemical Reviews* (2003, vol. 103, pp. 3449-3605). His contributions to Graphical Bioinformatics has been reviewed in the article entitled: Graphical Representation of Proteins, *Chemical Reviews* (2011), vol. 111, pp. 790-862. Most recently he co-authored (an invited) review article entitled: Milestones in Graphical Bioinformatics, *Int. J. Quantum Chem.* (2013) vol-113, pp. 2413-2446, which gives a summary on the most recent results in Graphical Bioinformatics, which has been crowned by his paper: “Very Efficient Search for Protein Alignment—VESPA” *J. Comput. Chem.* 33 (2012) 702-707. In this article is reported the **exact** solution of the protein alignment problem, that is, solution without use of

approximations, such as penalties for gaps, insertion and deletions of amino acids in sequences, without use of empirical parameters or statistical data, and most importantly, without shifting pairs of sequences relative one to the other )a trial-and-error methodology), which characterize most computer programs, including BLAST (of 1990) and its update of (1997) the two most widely used computer packages for protein alignment, together having 80,000 citations (annually about 5,000). The problem which has been around for over 45 years, believed by many not to have exact (i.e., without approximations) solution. But it has!

M. Randić has diverse interests in structural chemistry which covers molecules having several atoms as well as lengthy DNA structures and proteins. Moreover, he contributed to characterization of complex experimental results such as proteome maps. He has written several review chapters in various books, including:

- (1) On Topological Indices in: *The Encyclopedia of Computational Chemistry*. (Schleyer, P. v. R., Editor-in-chief; J. Wiley and Sons, London (1998), pp. 3018-3032);
- (2) On quantitative characterization of proteome maps, in: *Handbook of Proteomic Methods*, (edited by P. M. Conn, Humana Press: Totowa, N. J., (2003), pp. 429-450);
- (3) On application of Graph Theory Chemistry, in: *Geometry at Work*, C. A. Gorini, Ed., Math. Assoc. America, Washington, D. C. (2000), pp. 174-194;
- (4) On characterization of three-dimensional molecular structure, in: *From Chemical Topology to Three-Dimensional Geometry*, pp. 159-236, Editor A. T. Balaban, Plenum Press, New York, (1997).
- (5) On similarity methods of interest in chemistry, in: *Mathematical Methods in Contemporary Chemistry*, S. I. Kuchanov (ed.), Gordon and Breach Publ. (1996) pp. 1-100.
- (6) On design of molecules with desired properties (A molecular similarity approach to property optimization, in: *Concepts and Applications of Molecular Similarity*, M. A. Johnson and G. Maggiora, eds., New York: John Wiley & Sons; 1990, pp. 77-145.

## Awards

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| 1966 | Annual Science Award of City of Zagreb (Capitol of Croatia)           |
| 1986 | Centenial Professorship, Drake University                             |
| 1987 | Boris Kidrič Science Award (Republic of Slovenia)                     |
| 1988 | Ellis & Nelle Levitt Professorship, Drake University                  |
| 1988 | Governor of Iowa Annual Science Award                                 |
| 1996 | Skolnik Award (Am. Chem. Soc.: Computers in Chemistry Division)       |
| 1996 | Croatian Chemical Society Award                                       |
| 1996 | Honorary Mmember of Croatian Chem. Soc.                               |
| 1997 | Member of Croatian Academy of Sciences and Arts                       |
| 2007 | Honorary Member of Mathematical Chemistry International Academy       |
| 2008 | Honorary Member of Slovenian Chem. Soc.                               |
| 2009 | Honorary Member of the National Institute of Chemistry, Ljubljana     |
| 2010 | Grand Pregel Award of the National Institute of Chemistry of Slovenia |

Milan Randić served or serving on the Editorial Boards of the following journals:

*Croatica Chemica Acta*

*Chemical Physics Letters*

*Journal of Mathematical Chemistry*

*Journal of Chemical Information and Computer Science*

*SAR & QSAR in Environmental Research*

*Acta Chimica Slovenica*

*Current Computer-Aided Drug Design*

For a photo and brief curriculum vita see *Chem. Rev.* **2003**, *103*, p. 3449

For more details information on M. Randić see the special issue of *Croatica Chemica Acta* on Mathematical Chemistry, (*Croat. Chem. Acta*, year **2002**, vol. 75,

number 2), dedicated to Professor Milan Randić “*to mark his 70<sup>th</sup> birthday and to acknowledge his distinguished research in mathematical chemistry.*”