MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **73** (2015) 271-272

ISSN 0340 - 6253

BOOK REVIEW

Advances in Mathematical Chemistry and Applications (Volume 1)

edited by

Subhash C. Basak, Guillermo Restrepo & José L. Villavaces

Bentham Science Publishers, Sharjah, U. A. E., 2014, XVI+337 pp.
eISBN 978-1-60805-928-7, ISBN 978-1-60805-929-4, 79US$ (person), 316 US$ (library)

In his *Foreword*, Alexandru Balaban says that this e-book adds a new brick to the edifice of Mathematical Chemistry. Indeed, the book provides a representative cross section of ideas, results, methods, and techniques of contemporary research in a field of science in which chemistry and mathematics meet, and which justly is referred to as *Mathematical Chemistry*. In the book we find both "pure" and "applied" aspects of this science.

After Balaban's *Foreword* comes the *Preface* written by the three editors, explaining how the book was created, but also outlining a short history of Mathematical Chemistry. Volume 1 contains 13 chapters, and from the *Foreword* and *Preface* we learn that there will also a Volume 2, with additional 13 chapters.

The contributions to this e-book are written by a total of 29 authors, each chapter having an exhaustive list of references:

1. S. C. Basak, *Mathematical structural descriptors of molecules and biomolecules: Background and applications* (pp. 3–23)
2. G. Restrepo, *Ordering thinking in chemistry* (pp. 24–41)
3. D. Bonchev, *On the concept of overall topological representation of molecular structure* (pp. 42–75)

4. B. Lučić et al., *The four connectivity matrices, their indices, polynomials and spectra* (pp. 76–91)
5. S. M. Arif et al., *The use of weighted 2D fingerprints in similarity–based virtual screening* (pp. 92–112)
6. R. Gugisch et al., *MOLGEN 5.0, a molecular structure generator* (pp. 113–138)
7. M. Dehmer and L. Sivakumar, *On comparability graphs: Theory and applications* (pp. 139–160)
8. J. Gálvez et al., *Basic concepts and applications of molecular topology to drug design* (pp. 161–195)
9. P. K. Chattaraj and D. R. Roy, *Conceptual density functional theory of chemical reactivity* (pp. 196–221)
10. M. Vračko, *Mathematical (structural) descriptors in QSAR: Applications in drug design and environmental toxicology* (pp. 222–250)
11. H. Rajesh et al., *Recent advances in the assessment of druglikeness using 2D-structural descriptors* (pp. 251–272).
12. A. K. Bhattacharjee, *Role of in silico stereoelectronic properties and pharmacophores in aid of discovery of novel antimalarials, antileishmanials, and insect repellents* (pp. 273–305)
13. R. Hefferlin, *Molecular taxonomy* (pp. 306–319).

Basak's Chapter 1 and Bonchev's Chapter 3 provide introductions to what usually is called "*Chemical Graph Theory*". These two chapters should be strongly recommended for first–reading by neophytes and less informed readers, noting that Chapter 1 contains surprisingly little mathematical formalism (and it therefore most suitable for chemistry students). Restrepo's Chapter 2 is on the mathematical theory and chemical applications of partially ordered sets. Hefferlin's Section 13 is concerned with objects "*other than normal molecules*": sub-atomic particles, mesons, barions, quarks, strings, ..., with emphasis on their periodicities. The contents of the other chapters is evident from their titles.

The book ends with a detailed *Subject Index* (pp. 320–337).

In summary, the e-book "*Advances in Mathematical Chemistry and Applications*" is a valuable, state-of-the-art, treatise, outlining the contemporary activities in this field of science. It will be useful for both experts and beginners. It should be a must for any decent science library. We eagerly wait for the appearance of its Volume 2.

Ivan Gutman, Boris Furtula