Guest Editorial Preface

Special Issue on Applications of QSPR/QSAR in Toxicology, Ecology, and Drug Discovery: Problems and Solutions

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Any topic of Natural Sciences involves many aspects. Actually, majority of fields of research works are more or less connected with the quantitative structure – property / activity relationships (QSPRs/ QSARs): this is true for physics, chemistry, biology, and medicine.

It is very important to be able to select unexpected or vice versa expected research objects connected systematically, for practical applications and economic benefits. In this issue, the selection of topics is the following: toxicology – ecology – drug discovery.

The theoretical and practical results of the research activity of a variety of laboratories constitute the gigantic labyrinth for possible successful applications in the QSPR/QSAR analyses. However, manifold tests of the suggested results are necessary in order to improve the acceptability. In other words, the combination of similar but non-identical approaches of QSPR/QSAR analyses is a promising heuristic idea.

"The historically first approach" and the basis of the QSPR/QSAR analysis are molecular descriptors, which are mathematical functions derived from the molecular graphs. "The historically second basic conception" of the QSPR/QSAR analyses are descriptors calculated with quantum mechanics. Finally, most young conception of the QSPR/QSAR analysis are so-called optimal descriptors. All above-mentioned conceptions of the QSPR/QSAR analyses are collected in this special issue. Endpoints examined in the special issue are related to toxicological problems, to the risk assessment, and drug discovery. Hopefully, the reader can discover interesting results related to the above problematics.

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