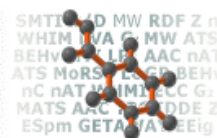


Molecular Descriptors

the free online resource



What is a molecular descriptor

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"The molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment.

.....

Attention is paid to the term "useful" with its double meaning: it means that the number can give more insight into the interpretation of the molecular properties and / or is able to take part in a model for the prediction of some interesting property of other molecules.

..... The field of molecular descriptors is strongly interdisciplinary and involves a mass of different theories. For the definition of molecular descriptors, a knowledge of algebra, graph theory, information theory, computational chemistry, theories of organic reactivity and physical chemistry is usually required, although at different levels.

For the use of the molecular descriptors, a knowledge of statistics, chemometrics, and the principles of the QSAR/QSPR approaches is necessary in addition to the specific knowledge of the problem. Moreover, programming, sophisticated software and hardware are often inseparable fellow-travelers of the researcher in this field.

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The historical development of molecular descriptors reflects some of the distinctive characteristics of the most creative scientists, i.e. their capability of being at the same time engaged and/or detached, rational and/or queer, serious and/or funny. Science is a game and the best players appreciate not only the beauty of a discovery by a precise and logical reasoning, but also the taste of making a guess, of proposing eccentric hypotheses, of being doubtful and uncertain in front of new and complex problems. Molecular descriptors constitute a field where the most diverse strategies for scientific discovery can be found."

From the introduction to the "[Handbook of Molecular Descriptors](#)"
by Roberto Todeschini and Viviana Consonni, Wiley-VCH, 2000.