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.

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.