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relevant literature over

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added to the list, and

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AMW = MW /nAT (3)

wherenAT is the
number of atoms.

The mean volume (Mv)
is calculated by
dividing the sum of the
van der Waals volumes
by the number of
atoms: $Mv = Sv/nAT$
(4) The mean
electronegativity (Me)

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and mean

polarizability(Mp) are

calculated using

formulas similar to

equation 4.

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Descriptors Guide

September 2012

Roberto Todeschini and

Viviana Consonni,

Molecular Descriptors

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(2 volumes), Wiley-

VCH, 2009. Mati

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& Sons, 2000. James

Devillers and
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(Eds.), Topological
indices and related
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Molecular descriptor - Wikipedia

A molecular descriptor
is a structural or
physicochemical
property of a molecule
or part of a molecule. A
QSAR model for

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predictive toxicology is
a mathematical
relationship between a
chemical's quantitative
molecular descriptors
and its toxicological
endpoint

[9,44].Molecular
descriptors derived
from atomic or
molecular properties
that translate
physicochemical,
topological, and
surface ...

Molecular Descriptor

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Descriptors For

- **an overview** |

ScienceDirect Topics

There are currently a large number of molecular descriptors, which can be classified into three broad categories: 1-, 2-, and 3D descriptors that encode chemical composition, topology, and 3D shape and functionality, respectively. 2 A descriptor can be simple, like molecular volume, which encode

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only one feature of a compound, or can be complex, like 3D-MoRSE, which encode multiple physicochemical and structural properties of a compound.

**PaDEL-descriptor:
An open source
software to
calculate ...**

Molecular descriptors are widely employed to present molecular characteristics in

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cheminformatics.

Various molecular-

descriptor-calculation

software programs

have been developed.

However, users of

those programs must

contend with several

issues, including

software bugs,

insufficient update

frequencies, and

software licensing

constraints.

Mordred: a

molecular descriptor

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Meanwhile, the types of the descriptors are of high diversity.

Applying different kinds of molecular descriptors are very necessary for a specific research problem. For example, molecular volume descriptors or those characterizing molecular polarity would be more relevant to study the LogD.

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alvaDesc is the next generation tool for the calculation of a wide range of molecular descriptors and a number of molecular fingerprints.. Molecular Descriptors.

Specifically it calculates almost 4000 descriptors independent of 3-dimensional information such as

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constitutional,
topological,
pharmacophore.

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The integrals $V(n_1, n_2, n_3) = \int dr x^{n_1} y^{n_2} z^{n_3}$,

where $\int dr$ represents integration over the volume of a body, such as a molecule, where x , y , and z are Cartesian coordinates of a point in the interior of the body relative to an arbitrary reference

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frame, and where n_1 ,

n_2 , and n_3 are integers

greater than or equal

to zero, constitute

moments of the

volume distribution of

the body ...

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