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Molecular descriptors
are mathematical
values that describe
the structure or shape
of molecules, helping
predict the activity and

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properties of molecules
in complex
experiments. This book
describes the
equations known as
QSAR (quantitative
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relationships), showing
how they can be used
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step in QSAR/QSPR is
to quantify the
molecular structures so

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as to build a correlation
model between the
chemical structures of
various chemical
compounds and the
corresponding...

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Molecular descriptors
have become the most
significant features
used in QSAR/QSPR
modeling. The
information encoded

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by descriptors
generally depends on
the kind of molecular
representation and the
defined algorithm for
its calculation. Some of
these include:

topological indices, and
geometrical,
constitutional and
physicochemical
descriptors.

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**Statistical Modelling
of Molecular
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QSAR/QSPR**

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play a fundamental
role in QSAR and other
in silico models since
they formally are the
numerical
representation of a
molecular structure. ...
include the hydrogen
atoms, the ...

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approaches including
quantum chemical
methods and molecular

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enable the definition of
a large number of
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characterizing the
reactivity, shape, and
binding properties like
atomic charges,
molecular orbital
energies, frontier
orbital densities,
superdelocalizabilities,
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polarizabilities,
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complete molecule as
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Principal steps of
QSAR/QSPR including
(i) Selection of Data set
and extraction of
structural/empirical
descriptors (ii) variable
selection, (iii) model
construction and (iv)

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validation evaluation."

SAR and the SAR
paradox. The basic
assumption for all
molecule based
hypotheses is that
similar molecules have
similar activities.

Quantitative structure-activity relationship - Wikipedia

Molecular fingerprints
are property profiles of
a molecule, usually in
forms of bit or count

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vectors with the vector
elements indicating the
existence or the
frequencies of certain
properties,
respectively. Both
molecular descriptors
and fingerprints play a
fundamental role in
QSAR/SAR analysis,
virtual molecule
screening, similarity-
based compound
search, target
molecule ranking, drug
ADME/T prediction and
the other drug

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play a fundamental
role in chemistry,
pharmaceutical
sciences,
environmental
protection policy, and
health researches, as
well as in quality
control, being the way

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molecules, thought of
as real bodies, are
transformed into
numbers, allowing
some mathematical
treatment of the
chemical information
contained in the
molecule. This was
defined by Todeschini
and Consonni as:

Molecular descriptor - Wikipedia

Abstract Background:
Molecular descriptors
and fingerprints have

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been routinely used in
QSAR/SAR analysis,
virtual drug screening,
compound
search/ranking, drug
ADME/T prediction and
other drug discovery
processes.

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"In summary,
Statistical Modelling of
Molecular Descriptors
in QSAR/QSPR" is a

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valuable treatise,
aimed at practitioners,
useful both for
beginners and experts.
It should be a must for
any decent science
library.” (Match, 1
November 2012)

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...

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play a fundamental
role in chemistry,
pharmaceutical

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sciences,
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protection policy, and
health researches, as
well as in quality
control, being the way
molecules, thought of
as real bodies, are
transformed into
numbers, allowing
some mathematical
treatment of the
chemical information
contained in the
molecule. This was
defined by Todeschini
and Consonni as:

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- Wikipedia

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fundamental role in
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well as in quality
control, being the way
molecules, thought of

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as real bodies, are
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numbers, allowing
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treatment of the
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contained in the
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Chemical descriptors
are used to calculate
and to develop
methods for chemical
property calculations

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(QSPR - quantitative structure-property relationship) or chemical activity (QSAR - quantitative structure-activity relationship)

calculations. A common classification method for descriptors can be taken from ChemInformatics textbooks and a collection of common molecular descriptors in the Handbook of molecular descriptors [

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Dragon calculates
5,270 molecular
descriptors, covering
most of the various
theoretical approaches.
The list of descriptors
includes the simplest
atom types, functional
groups and fragment
counts, topological and
geometrical

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descriptors, three-
dimensional

descriptors, but also
several properties
estimation (such as
logP ... 02 04

Kode -

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2. M. Dehmer, F.
Emmert?Streib (eds.)

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