Milano Chemometrics and QSAR Research Group

Roberto Todeschini
Viviana Consonni
Andrea Mauri
Davide Ballabio
Alberto Manganaro

chemometrics
molecular descriptors
QSAR
multicriteria decision making
environmetrics
experimental design
artificial neural networks
statistical process control

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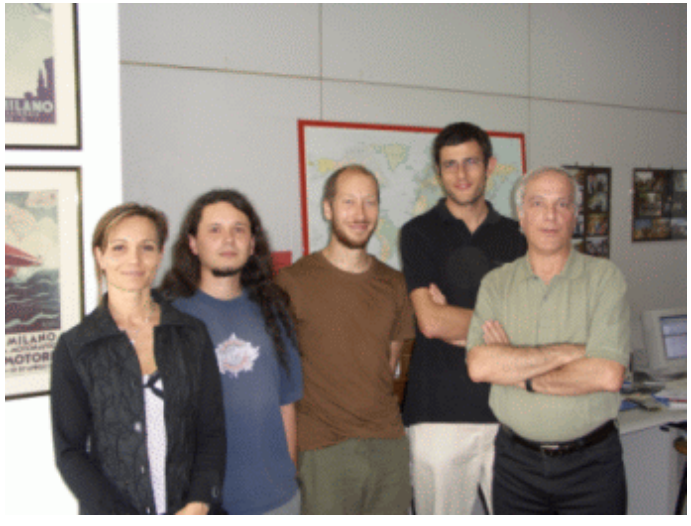

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Research activities

- Chemometrics
- Molecular Descriptors
- Quantitative Structure-Activity Relationships (QSAR)
- Quantitative Structure-Property Relationships (QSPR)
- Environmetrics
- Design of Experiments
- Multicriteria Decision Analysis

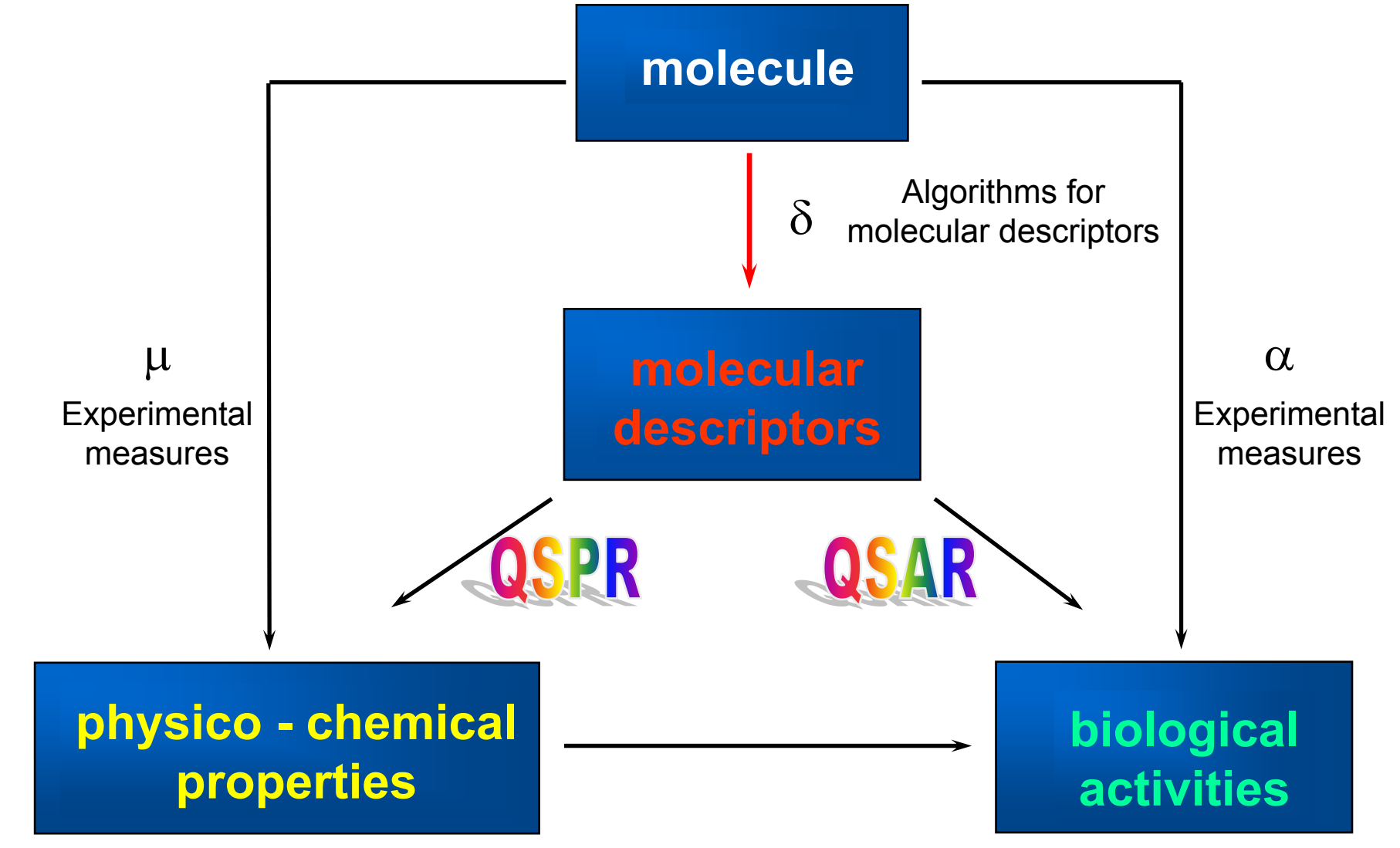
QSAR/QSPR strategy

The QSAR field is one of the most interesting fields where molecular descriptors and chemometric methods can be applied.

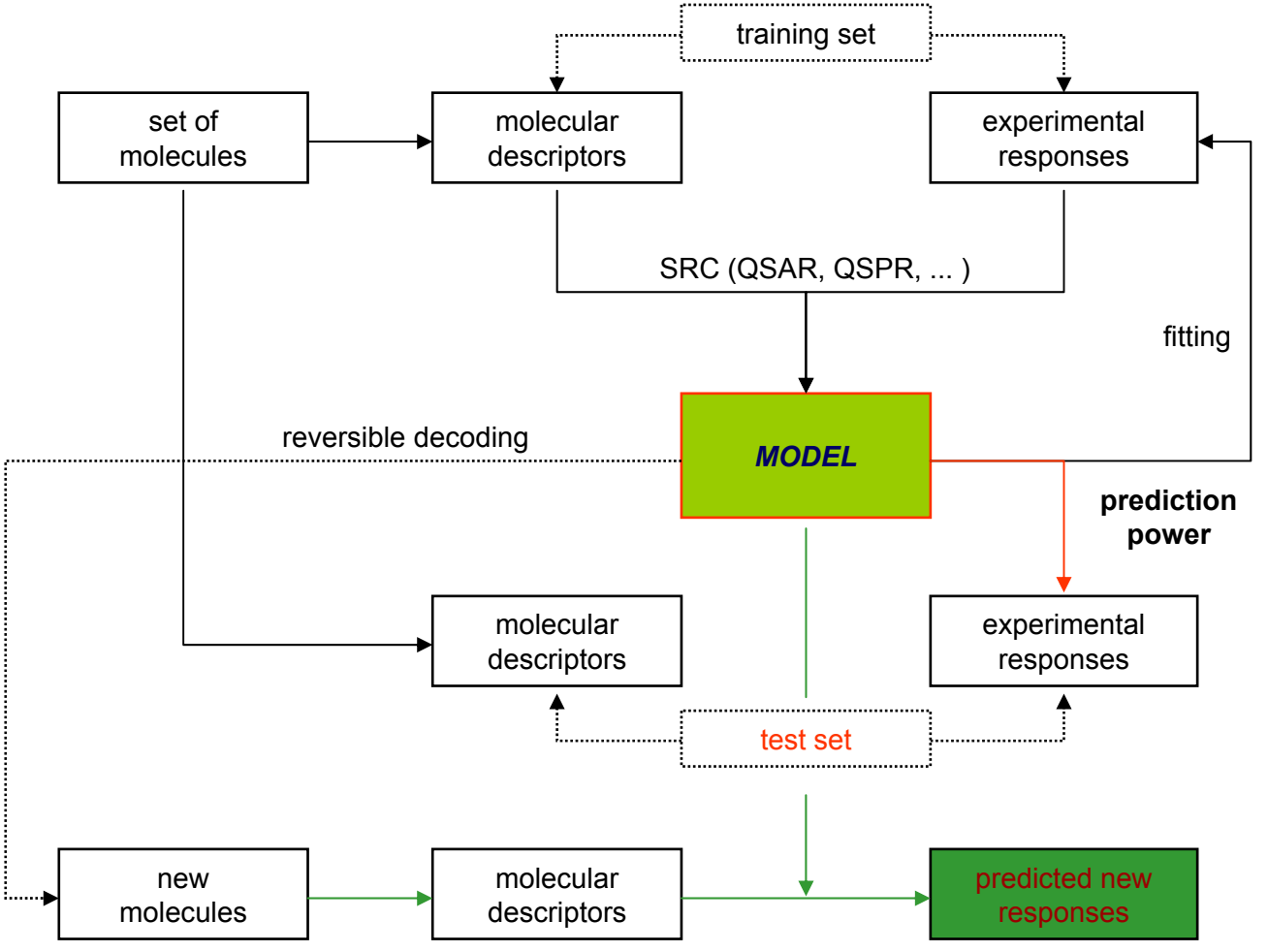
End-points

- physico-chemical properties
- biological activities
- toxicological and ecotoxicological end-points
- environmental end-points
- technological properties

QSAR/QSPR strategy



QSAR/QSPR strategy



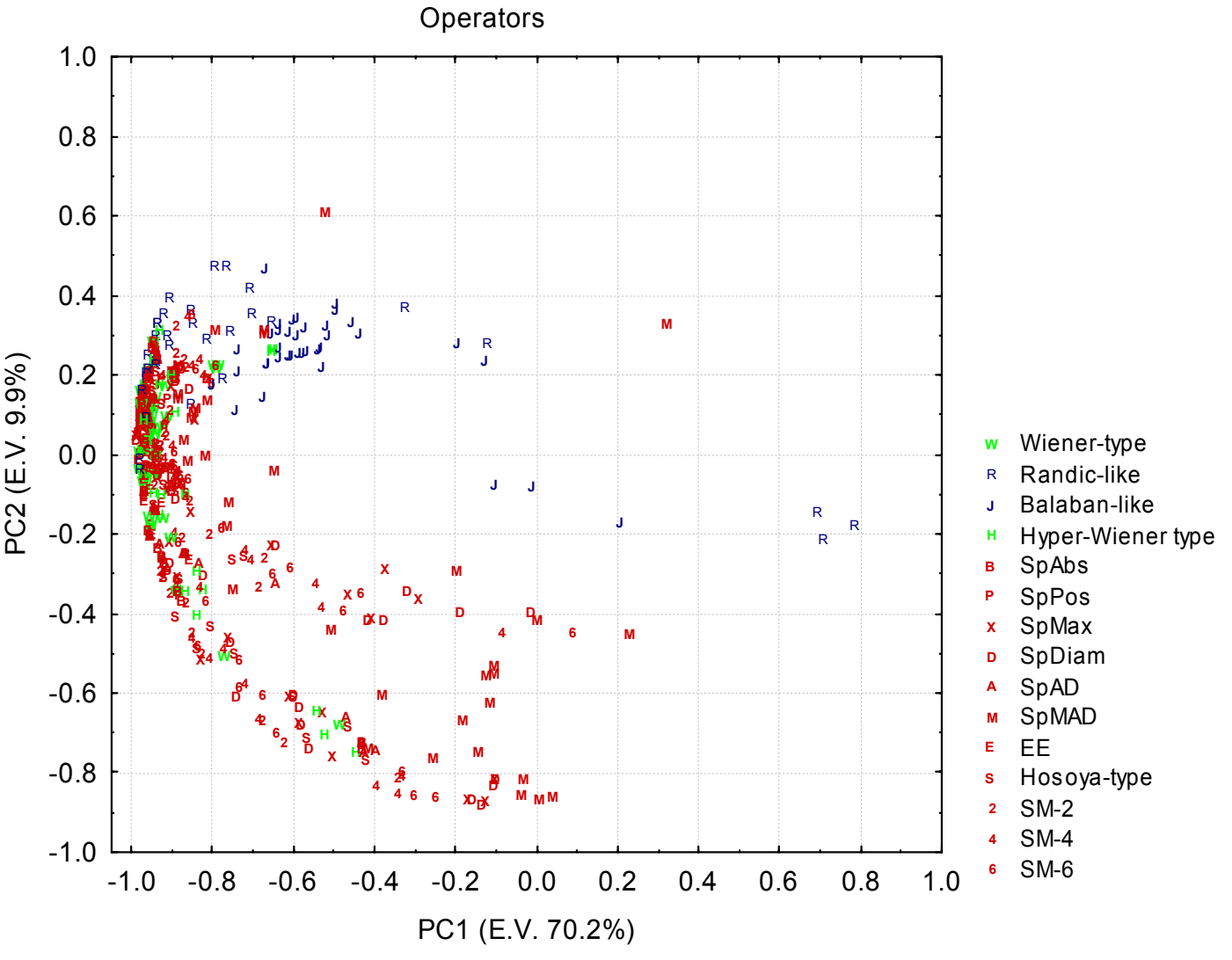
Exploratory data analysis

- Principal Component Analysis (PCA)
- Similarity/Diversity analysis

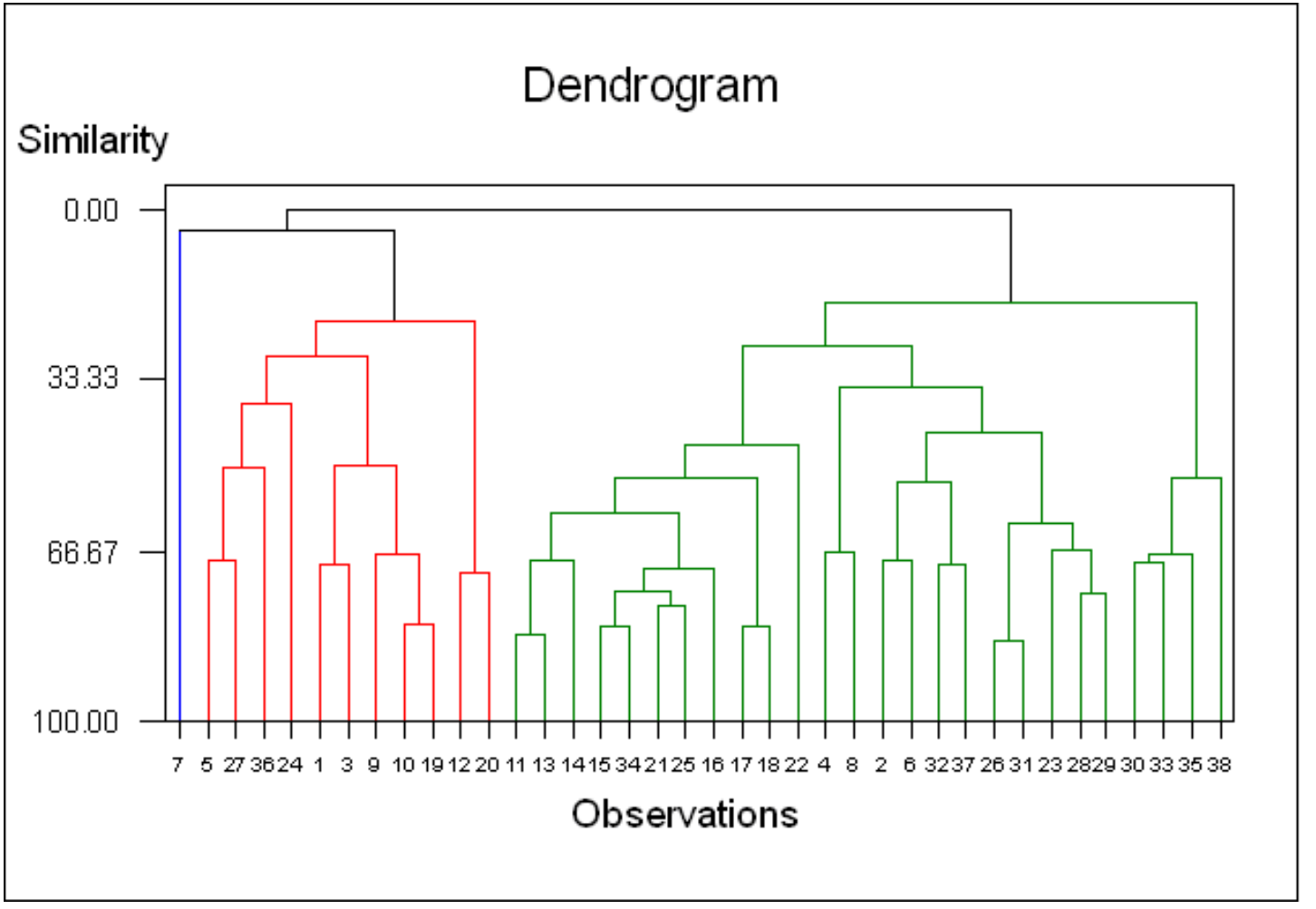
Models

- regression models (quantitative response)
- classification models (qualitative response)
- ranking models (ordered response)

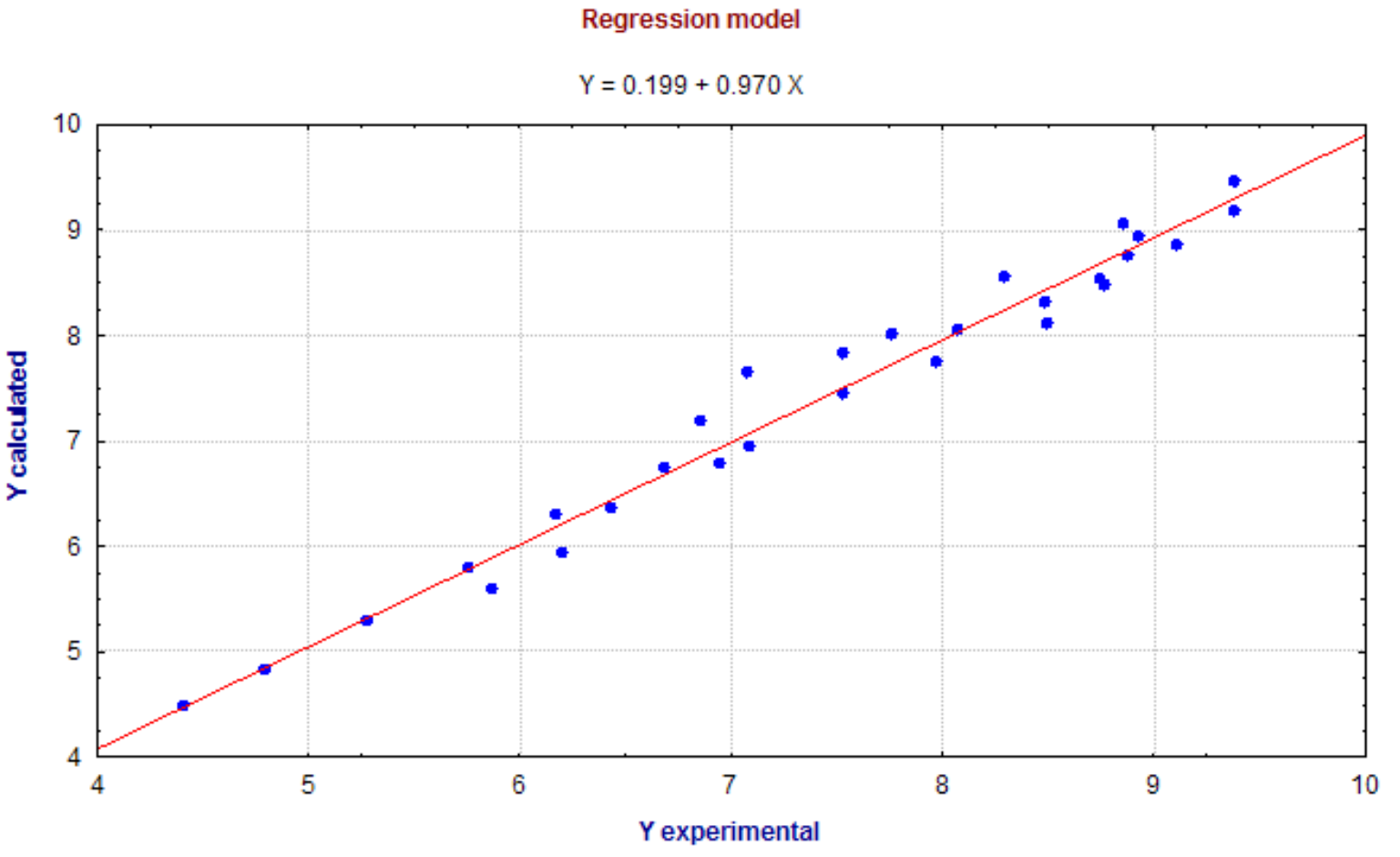
Chemometrics – PCA



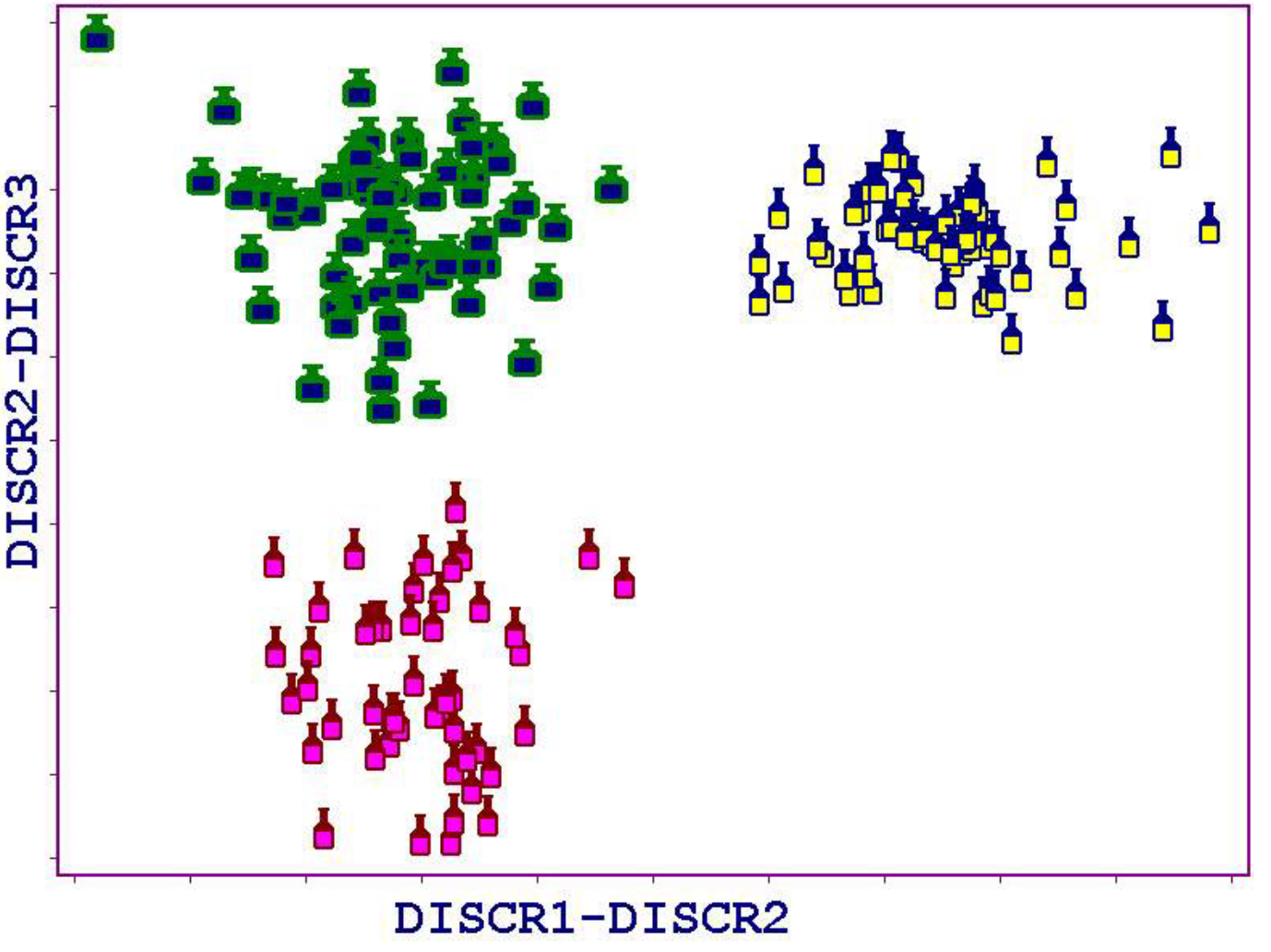
Chemometrics – Cluster Analysis



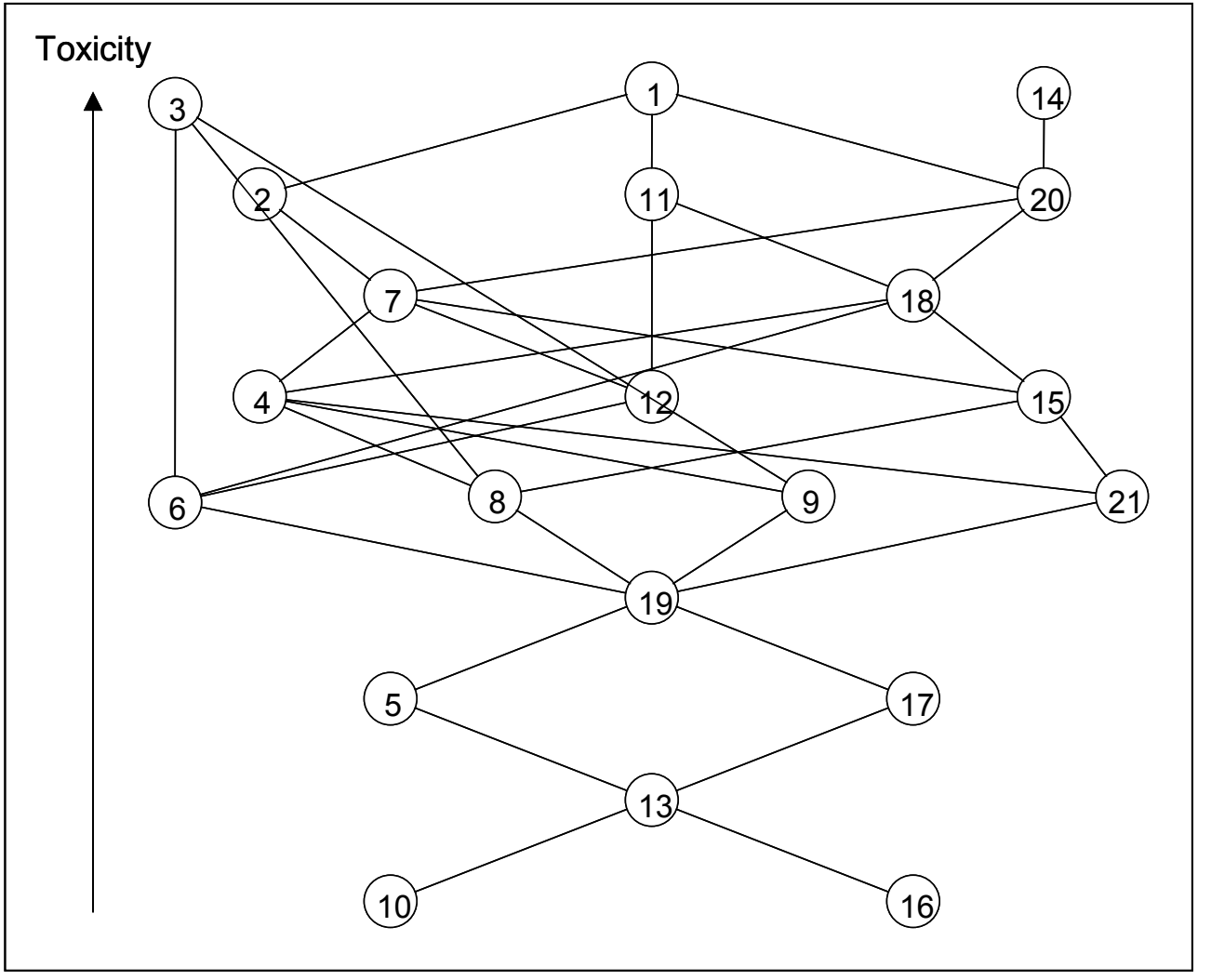
Chemometrics – Regression



Chemometrics – Classification



Chemometrics – Ranking



Molecular descriptors

Molecules are the most reach source of experimental chemical information

Molecular structures are the most reach source of theoretical chemical information encoded in molecules

Molecular descriptors are the way to encompass chemical information encoded in the molecular structures

Molecular descriptors

Definition of molecular descriptor

"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."

R. Todeschini and V. Consonni

***Handbook of Molecular Descriptors*, WILEY-VCH, 2000**

Molecular descriptors

graph theory discrete mathematics physical chemistry
information theory quantum chemistry organic chemistry
differential topology algebraic topology

derived from ….

Molecular descriptors

processed by ….

statistics
chemometrics
chemoinformatics

applied in ….

QSAR/QSPR medicinal chemistry pharmacology genomics
drug design toxicology proteomics analytical chemistry
environmetrics virtual screening library searching

Atom list

0D

counting

summing

Substructure list

1D

counting

structural keys

molecular graph

2D

graph invariants

topographic descriptors

topostructural descriptors

topochemical descriptors

topological information indices

molecular geometry x, y, z coordinates

3D

geometrical descriptors

bulk descriptors

quantum-chemical descriptors

molecular surface descriptors

grid-based QSAR techniques

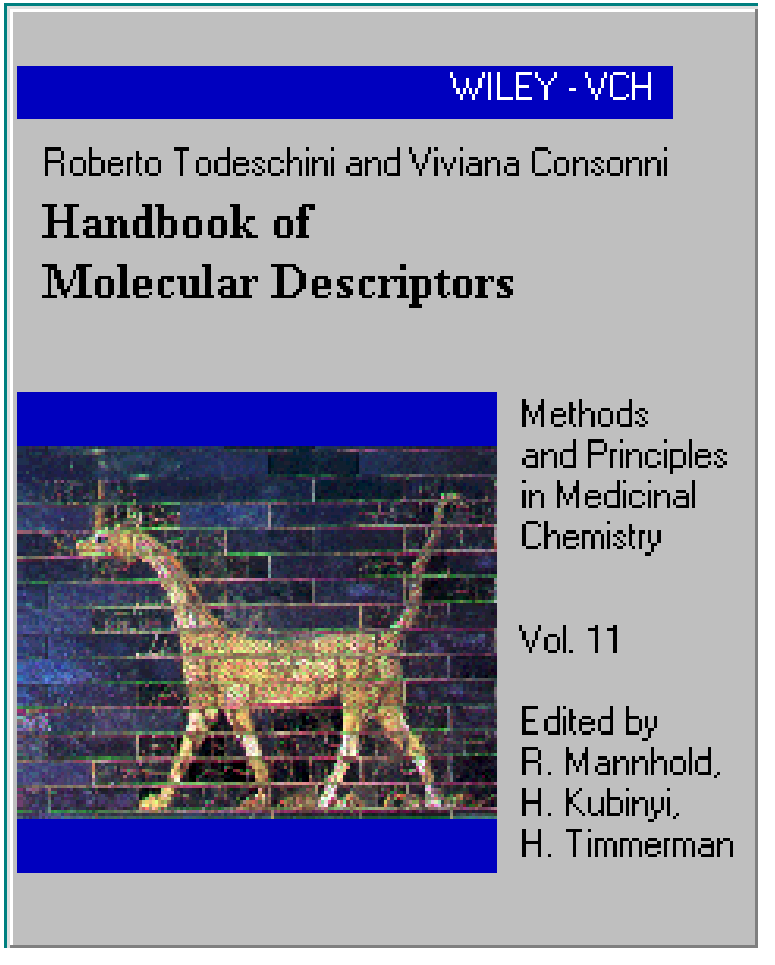
4D

interaction energy values

Molecular descriptors

Wiley-VCH, 2000

≈ 3300 bibliographic references



≈ 3000 molecular descriptors

Molecular descriptors

41 Methods and Principles in Medicinal Chemistry

As every chemist knows, there is a direct (if complex) relationship between the molecular structure of a compound and its chemical behavior. Predicting such behavior is possible by an abstract representation of its structure in terms of chemical similarity parameters, so-called 'descriptors'. These are most useful in predicting the pharmacological properties of drug candidates, but are also used in predicting reactivity, toxicity and other important chemical characteristics.

The number-one reference on the topic now contains a wealth of new data: The entire relevant literature over the past eight years has been pain-stakingly surveyed, resulting in more than 100 new descriptors being added to the list, and some 3,000 new references in the bibliography section.

Volume 1 contains an alphabetical listing of around 3300 terms for the chemoinformatic analysis of chemical compound properties, while the second volume contains 6343 references selected from 450 journals with about 7000 authors quoted covering the period from the beginning of molecular descriptor research until the year 2008.

In this second edition, the greatly expanded introductory section has been completely re-written and now contains several "walk-through" reading lists of selected keywords to make the data even more accessible for novice users.

Roberto Todeschini is full professor of chemometrics at the Department of Environmental Sciences of the University of Milano-Bicocca (Milano, Italy), where he constituted the Milano Chemometrics and QSAR Research Group. His main research activities concern chemometrics in all its aspects, QSAR, molecular descriptors, multicriteria decision making and software development. President of the International Academy of Mathematical Chemistry, president of the Italian Chemometric Society and "ad honorem" professor of the University of Azuay (Cuenca, Ecuador), he is author of more than 160 publications in international journals and of the books "The Data Analysis Handbook", by I.E. Frank and R. Todeschini, 1994 and "Handbook of Molecular Descriptors", by R. Todeschini and V. Consonni, Wiley-VCH, 2000.

Viviana Consonni received her PhD in Chemical Sciences at the University of Milano in 2000 and is now full researcher of chemometrics at the Department of Environmental Sciences of the University of Milano-Bicocca (Milano, Italy). She is a member of the Milano Chemometrics and QSAR Research Group and has 10 years experience in multivariate analysis, QSAR, molecular descriptors, multicriteria decision making and software development. She is author of more than 25 publications in peer reviewed journals and of the book "Handbook of Molecular Descriptors", by R. Todeschini and V. Consonni, Wiley-VCH, 2000. In 2006 she obtained the International Academy of Mathematical Chemistry Award for distinguished young researchers.

Volume I of II

ISBN 978-3-527-31852-0

www.wiley-vch.de

Todeschini - Consonni

Vol. I

Molecular Descriptors for Chemoinformatics

WILEY-VCH

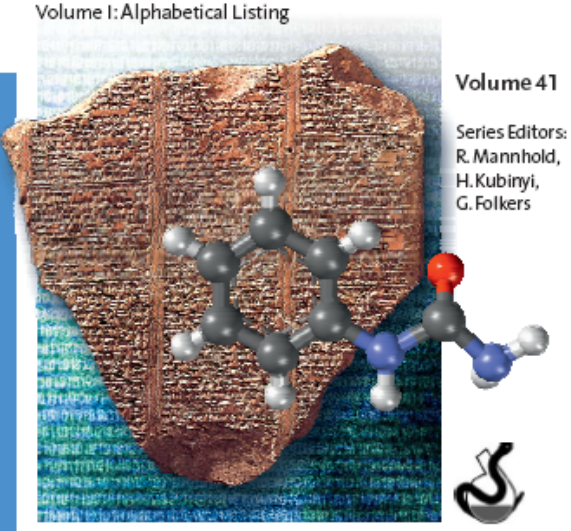
Roberto Todeschini, Viviana Consonni

WILEY-VCH

Molecular Descriptors for Chemoinformatics

Second, Revised and Enlarged Edition

Volume I: Alphabetical Listing



Volume 41

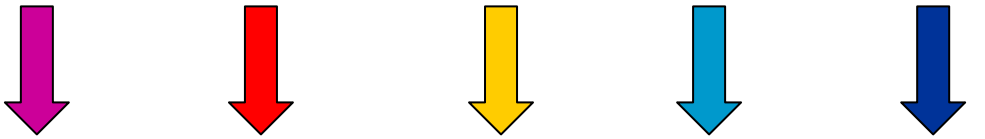
Series Editors:
R. Mannhold,
H. Kubinyi,
G. Folkers

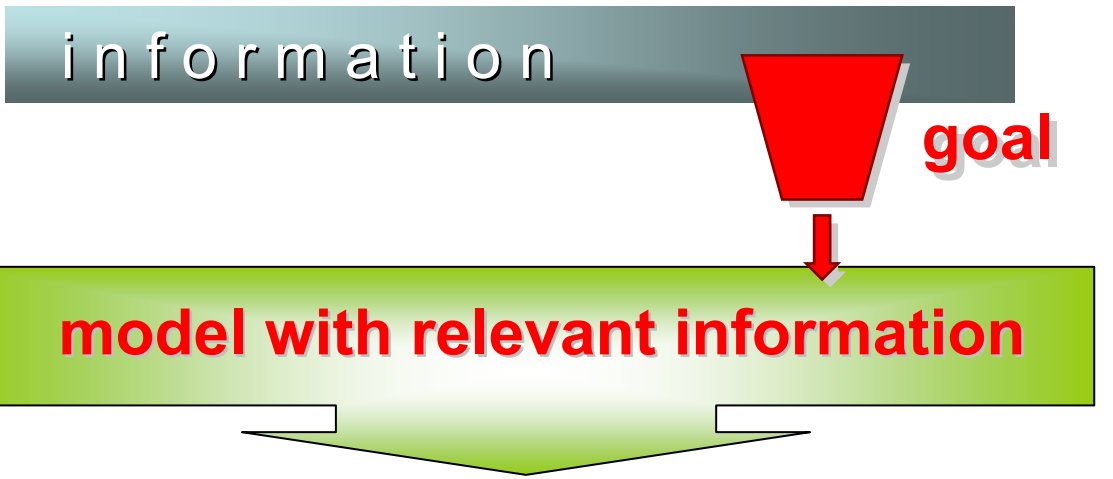
≈ 6300 bibliographic references

Wiley-VCH,2009 – 2 volumes

From information to knowledge

system description by several variables





stability → model under control

interpretability → knowledge of the problem

predictive power → future use of the model

From information to knowledge

Quality of the models

representation of the chemical information

DATA QUALITY

mathematical methods to extract the information

METHOD QUALITY

Software

Milano Chemometrics and QSAR Research Group developed two main software to calculate molecular descriptors and deal with regression models selected from the huge number of molecular descriptors.

These software are commercialized by the company TALETE srl, for which Todeschini is the scientific responsible.

Talete srl

DRAGON

Software for the calculation of 3224 molecular descriptors (version 5.5) from molecular structures

Talete srl

MobyDigs

Software for the calculation of regression models by genetic algorithms (GA) for variable selection aimed to search for predictive models

MOBYDIGS

www.moleculardescriptors.eu

Molecular Descriptors

the free online resource

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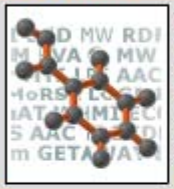
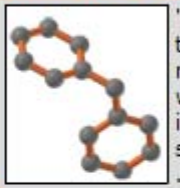
Welcome to moleculardescriptors.eu

Editorial



moleculardescriptors.eu is a website dedicated to all the scientists who propose new molecular descriptors and/or apply molecular descriptors in scientific research. [more]

What is a molecular descriptor ?

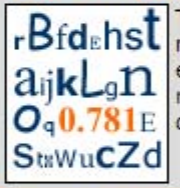


"The molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of ... [more]

Forum

The **Molecular Descriptor Forum** is a virtual place where you can discuss, ask questions or give answers on molecular descriptors.

News & Events



This section is dedicated to meetings, workshops, events and general **news** related to molecular descriptors.

On-line resources

In this section you can find a collection of links to on-line **free tools and resources** related to molecular descriptors.

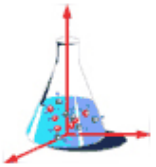
Tutorials

In this section you can find **tutorials** and examples about molecular descriptors.

Top News

● **IAMC meeting**
The next meeting of the International Academy of Mathematical Chemistry (IAMC '2007) will be held in Dubrovnik June 07-09, 2007.

michem.disat.unimib.it/chm/



Milano Chemometrics and QSAR Research Group

Prof. Roberto Todeschini

Dipartimento di Scienze dell'Ambiente e del Territorio
Università degli Studi di Milano - Bicocca

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contacts

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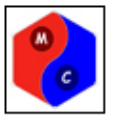
Prof. Todeschini is the new president of the IAMC

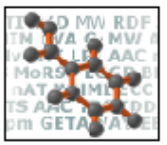


At the 3rd Meeting of the International Academy of Mathematical Chemistry (Dubrovnik, June 7-9, 2007), Prof. Roberto Todeschini has been elected as new president of the Academy, in place of Prof. Alexandru Balaban. [**read more...**]

MOLE db - Molecular Descriptors Data Base

The MOLE db - Molecular Descriptors Data Base is a free on-line database constituted of 1124 molecular descriptors calculated on 234773 molecules, released by Milano Chemometrics and QSAR Research Group: **explore the MOLE db data base here!**

New website about molecular descriptors



A new website dedicated to molecular descriptors has been released by Milano chemometrics and QSAR research group. You can find it here: **www.moleculardescriptors.eu**

Download software and code

```
if strcmpi(
  in_out =
  for i=1:s
    W_out =
  end
```

Visit our download page, where you can find softwares and MATLAB routines you can freely download: **Kohonen and CPANN toolbox**, **MOLMAP multiway toolbox**, **Variable Reduction Testbench**, **CAIMAN** (Classification And Influence Matrix ANalysis), **Molecular Descriptor Correlations**, **Similarity measure based on Hasse matrices**.

E-DRAGON software for molecular descriptor calculations

Quick Info

- **New website about molecular descriptors** by Milano Chemometrics
- **Molecular Descriptors Data Base** by Milano Chemometrics
- **iamc-online.org**, website of the International Academy of Mathematical Chemistry
- **Ranking Methods in Chemical Sciences**, PhD thesis by Manuela Pavan
- **VCC-LAB**, Virtual Computational Chemistry Laboratory
- **Handbook of Molecular Descriptors**
- **Gruppo di Chemiometria della SCI**
- **Past and present visitors list**