

# Roberto TODESCHINI

Milano Chemometrics and QSAR Research Group



## CONTACT

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## EDUCATION

### Master in Chemistry

Università degli Studi di Milano,  
1972

### Researcher

Università degli Studi di Milano.  
1975

### Full Researcher

Università degli Studi di Milano,  
1982

### Associate Professor

Università degli Studi di Milano,  
1991

### Full Professor

Università di Milano-Bicocca,  
2001

## PROFILE

Roberto Todeschini, was graduated in chemistry in 1972 at the University of Milan. He was then enrolled as researcher at the same university and worked in the field of theoretical chemistry, with special focus on conformational analysis, until the first '80s. Then, his research interests shifted towards chemometrics and multivariate data analysis applied to different scenarios. In particular, the use and application of multivariate statistical models to analytical and cheminformatics data lead to the development of different research outputs in the field of analytical chemistry and Quantitative - Structure Activity Relationships (QSAR). These new research interests arose from the participation to an educational project carried out at Escuela Politecnica del Chimborazo (Riobamba, Ecuador) in the framework of an official cooperation action between the Foreign Minister of Ecuador and Italy, aimed to propose up-to-date and low cost research activities in developing countries.

At the beginning of the '90s, Todeschini became associate professor at the University of Milano-Bicocca (Milan, Italy) and then, in 2001, full professor of analytical chemistry and chemometrics at the Department of Earth and Environmental Sciences, recently awarded as one of the excellent Italian Departments. Here he founded the *Milano Chemometrics and QSAR Research Group* (<http://www.michem.unimib.it/>), which actually includes as permanent staff Davide Ballabio, Viviana Consonni and Francesca Grisoni. His research group hosted more than twenty visiting foreign students in the last 10 years, as a result of the several international cooperation projects and programs with research group located all over the world. Finally, Todeschini organized several national and international meetings and high education courses on different topics related to multivariate analysis, molecular descriptors, multi-criteria decision-making, chemometrics, and experimental design.

## AKNOWLEDGEMENTS and AWARDS

- In 2004 he was among the founders of the International Academy of Mathematical Chemistry (IAMC), which includes four Nobel Prizes among its members, and served as President of the Academy from 2008 to 2013. He is now an Honorary Member.
- He currently is the President of the Italian Chemometric Society and "ad honorem" professor of the University of Azuay (Cuenca, Ecuador) since 2006.
- Todeschini served for several years as coordinator of the Chemometric Group of the Analytical Chemistry Division of the Italian Chemical Society.
- Todeschini has collaborations with several foreign universities and research centres, such as ETH (Zurich, Switzerland), University of Sheffield (UK), Universidad Catolica de Azuay (Cuenca, Ecuador), Universidad de Granada, Universidad de Burgos and Universidad de Valencia (Spain), Aix Marseille Université (France), Linnaeus

## EDITORIAL BOARDS

- SAR and QSAR in Environmental Research
- International Journal of Chemical Modeling
- International Journal of Chemical Sciences
- MATCH
- Iranian Journal of Mathematical Chemistry

## BIBLIOMETRIC INDICES

*Source: Google Scholar, October 2018*

Citations: 15429

h-index: 49

g-index: 122

i10: 134

University (Kalmar, Sweden), Vienna University of Technology (Austria), Joint Research Center (Ispra, Italy), EPA (USA).

- Todeschini held several invited and plenary lectures and, among these, the opening lecture at the 30° Congreso Argentino de Química, Buenos Aires (2014). He was also invited professor for a tour of conferences at some universities in Japan (Tokyo and Osaka, 2009), in Iran (Zanjan, Shiraz, Isfahan, 2008), in Colombia (Bogotá and Pamplona, 2010) and several times at universities in Ecuador (Riobamba and Cuenca).
- Todeschini is in the editorial boards of SAR & QSAR in Environmental Chemistry, MATCH Communications in Mathematical and in Computer Chemistry, International Journal of Chemical Modeling, Iranian Journal of Mathematical Chemistry, Chemical Processes and Materials, International Journal of Molecular Sciences (section Molecular Informatics).
- The research of Todeschini and his group has been acknowledged (2 pages) in a recent Italian book on the history of chemistry in last century ("Bella e Potente: La chimica dagli inizi del Novecento ai giorni nostri" by Luigi Cerruti, Editori Riuniti/University Press, 2016), where their research on molecular descriptors was presented as one of the relevant contributions to chemistry in the last century.

## FUNDED PROJECTS

Todeschini has acted as responsible of research unit in several national and European funded projects. In particular:

1) The SafeRubber project (Grant agreement no.: 2-243756 - Funded by the EU Call: SME-2008 - Univ. of Milano-Bicocca funded by: € 393120.00, Period: 2008-2011) has received EC funding under the FP7 framework to develop a new, safe, multifunctional accelerator curative molecule which can replace thiourea-based accelerators in the vulcanisation process. Thirteen partners (a mix of SME-AGs and research institutes) participated in the research project. In particular, the unit coordinated by Todeschini was responsible of one of the project work packages, devoted to the analysis and prediction of toxicological properties of accelerator curative molecules by means of computational tools.

2) The Environmental ChemOinformatic (ECO) Marie Curie Initial Training Network (Grant agreement no.: 238701 - Funded by the EU: Marie Curie ITN Call: FP7-PEOPLE-ITN-2008 – Univ. of Milano-Bicocca funded by: € 518332.00, Period: 2008-2012) was a collaborative action of seven institutions from five EU countries (Germany, The Netherlands, Spain, Sweden, Italy) with the primary objective to contribute to the education of environmental chemo-informaticians in both environmental sciences and computational in-silico methods.

3) The Virtual Institute for Chemometrics and Industrial Metrology (VICIM, Grant agreement no.: GTC1-2001-43030 - Period: 2001-2004) was a virtual organisation for the promotion of cost-effective chemical measurement practices by making use of modern chemometric approaches and procedures for adequate assessment of the quality of methods and measurement results. VICIM brought together experts from different European institutes with knowledge in a wide-range of chemometric and multivariate statistics competencies applied in the fields of pharmaceuticals industry, food & drink industry, petrochemical industry and environmental issues.

4) Finally, Todeschini was Principal Investigator and coordinated the PRIN project "Development of chemoinformatics tools for screening

and identification of Persistent Bioaccumulable and Toxic (PBTs) compounds and Endocrine Disruptors (EDs) for REACH regulation." funded by MIUR (PRIN 2007, Univ. of Milano-Bicocca funded by € 55000.00) in the period from 2008 to 2009.

The total funding of the projects goes over 1 million of euro.

## INTERNATIONALIZATION

Beside the European projects, Todeschini gave a contribution to the internationalization of his University giving courses on Design of Experiments and Chemometrics in Ecuador (several times) and Colombia (two times), a tour of invited conferences in Japan, Colombia and Iran. He co-signed the bilateral agreement with his University and the University of Riobamba (Ecuador). Several Visiting Professors, Post-doc researchers and PhD students participated to stages (from one month to one year) at his research group at the University of Milano-Bicocca from Spain, Argentina, Ecuador, Colombia, Iran, Germany, Holland, Denmark, Roumania, Belgium. Several of these stages gave origin to useful scientific collaborations with foreign research groups. Todeschini published more than 40 papers together with foreign researchers and participated to more than 150 congresses, several of them as invited speaker.

## ACADEMIC RESPONSABILITIES

Todeschini was the Coordinator of the Doctorate in Chemistry from 2010 to 2014 and was member of the PhD Board for the Doctorate in Chemistry since its constitution and for the Doctorate in Environmental, Geological and Chemical Sciences (2015 – 2018).

He was also in charge for several official commissions of the Department of Environmental and Heart Sciences.

## TEACHING in ACADEMIC COURSES

Since the end of '80 until today, Todeschini give the course of Chemometrics, before for the Master in Chemistry at the University of Milan and later for the Masters both in Chemical Sciences and Technologies and in Environmental Sciences at the University of Milano-Bicocca.

In the first years of '90, Todeschini gave a course of Physical Chemistry for the Master in Biology at the University of Milan.

Since the first years of 2000, Todeschini teaches also Analytical Chemistry for the Masters both in Chemical Sciences and Technologies and in Environmental Sciences.

## RESEARCH ACTIVITIES

His main past and present research activities include chemometric approaches applied to analytical and cheminformatics scenarios, such as QSAR, molecular descriptors, multicriteria decision-making, software development, and proposals of multivariate methods for the analysis of analytical data. In particular, he has experienced the application of

chemometrics to analytical, spectroscopical, ecotoxicological, toxicological, pharmaceutical, and environmental data.

In order to solve specific problems dealing with data arising from complex systems, Todeschini proposed different novel chemometric and cheminformatics approaches based on multivariate analysis and advanced statistical tools. An important part of his research has been dedicated to QSAR, i.e. Quantitative Structure-Activity Relationships, aimed to find relationships (i.e. models) relating the chemical structure, described by molecular descriptors, and biological activities or environmental/toxicological properties of the molecules. The several papers on the WHIM molecular descriptors received more than 1000 citations as well as those on the GETAWAY descriptors, with almost 700 citations. Moreover, Todeschini proposed several new multivariate methods and indicators, such as new classification methods (CAIMAN, N3 and BNN), ranking approaches and parameters/indices to detect multivariate correlation, evaluate model predictive ability, establish the applicability domain of multivariate models. In particular, the K multivariate correlation index was accepted as the exact measure of the correlation present in a multivariate data set.

Several researches were dedicated to study new distance and similarity measures, such as, for example, new binary similarity measures, a Housdorff-like distance between metabolites, a distance between Hasse matrices, a distance taking into account a higher-order similarity, and a quasi-distance derived from the Mahalanobis distance. Moreover, in multicriteria decision-making, he proposed a detailed description of the Hasse diagrams, introduced weighting schemes in Hasse diagrams, and a flexible strategy to obtain a family of Hasse diagrams and of total ordering by the Power-Weakness Ratio.

Several software toolbox (more than 15) were developed and are free available at the website of his research group (<http://michem.disat.unimib.it/chm/>).

As a result of the research activities, he is author of more than 250 publications in international scientific peer-reviewed journals and author/co-author of the books:

- "The Data Analysis Handbook (I.E. Frank and R. Todeschini, Elsevier, 1994),
- "Handbook of Molecular Descriptors" (R. Todeschini and V. Consonni, Wiley-VCH, 2000), which is among the most cited scientific books, with almost 4000 citations (October 2018),
- "Molecular Descriptors for Chemoinformatics" (R. Todeschini and V. Consonni, Wiley-VCH, two volumes, 2009),
- "Handbook of Bibliometric Indicators" (R. Todeschini and A. Baccini, Wiley-VCH, 2016).
- "Introduzione alla chemiometria" (R. Todeschini, EdiSes, 1994)
- "La Metodologia della Ricerca Sperimentale" (R. Todeschini, V. Consonni, D. Ballabio and A. Mauri, 2007, electronic book).

Todeschini is also co-editor of the book

- "Scientific Data Ranking Methods: Theory and Applications" (M. Pavan and R. Todeschini, Eds., Elsevier, 2008)

## PUBLICATIONS

The complete list of publications of Roberto Todeschini can be accessed in Google Scholar, where more than 15000 citations and an h-index of 49 are recorded (October 2018).

Note that Scopus and WoS do not take into account the books, some book chapters and software officially released for scientific research, thus providing lower h-indices and citations.

*Link to Google Scholar:*

"<https://scholar.google.com/citations?user=RCrPb5YAAAAJ&hl=en>"