CV

Roberto Todeschini

Roberto Todeschini, responsible of this unit, 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 Ministers 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://michem.disat.unimib.it/chm/), 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 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 Universitè (France), Linnaeus 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 Quimica, Buenos Aires (2014). He was also invited professor at some universities in Japan (Tokyo and Osaka, 2009), in Iran (Zanjan, Shiraz, Isfahan, 2008), in Colombia (Bogotà and Pamplona, 2010) and several times at universities in Ecuador (Riobamba and Cuenca).
- Todeschini is in the editorial board of SAR & QSAR in Environmnetal Chemistry, MATCH Communications in Mathematical and in Computer Chemistry, International Journal of Chemical Modeling, Iranian Journal of Mathematical Chemistry, Chemical Processes and Materials.
- The research of Todeschini and his group has been aknowledged (2 pages) in a recent Italian scientific book ("Bella e Potente: La chimica dagli inzizi del Novecento ai giorni nostri" by Luigi Cerruti), 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.

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 proposal of multivariate methods for the analysis of analytical data. In particular, he has experienced the application of chemometrics to analytical, spectroscopical, pharmaceutical, toxicological, ecotoxicological 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 fine 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 descriptors received more than 1000 citations as well as those on the GATAWAY descriptors, almost 700. Moreover, Todeschini proposed several new multivariate methods and indicators, such as new classification methods (CAIMAN, N3 and BNN), distance and similarity measures, ranking approaches and parameters/indices to detect multivariate correlation, evaluate model predictive ability and establish the applicability domain of multivariate models.
Several software toolbox were proposed and are free available at the website of his group (http://michem.disat.unimib.it/chm/).
As a result of the research activities, he is author of more than 230 publications in international scientific peer-reviewed journals and 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 more than 3600 citations (February 2018),
- “Molecular Descriptors for Chemoinformatics” (R. Todeschini and V. Consonni, Wiley-VCH, 2009),

- “Handbook of Bibliometric Indicators” (R. Todeschini and A. Baccini, Wiley-VCH, 2016).

The complete list of publications of Todeschini can be accessed in Google Scholar at “https://scholar.google.com/citations?user=MNyEfBcAAAAJ” with more than 14000 citations and an h-index of 48 (March 2018). Note that Scopus and WoS do not take into account the books, some book chapters and software officially released on the market, thus calculating lower H-indices.