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Autobiography of Roberto Todeschini

ROBERTO TODESCHINI•

Milano Chemometrics and QSAR Research Group, Department of Earth and Environmental Sciences, University of Milano Bicocca, Milan, Italy
Website: http://michem.disat.unimib.it/chm/

Born in Rome (Italy) in 1949, Roberto Todeschini graduated in chemistry at the University of Milan (Italy) in 1972 with a thesis in theoretical chemistry. He got married to Marilena in 1973 and soon had a daughter Alessia (1975) and some years later a son Edoardo (1982).

In 1975, he was appointed to the position of researcher at the same university in Milano and worked in the field of theoretical chemistry, with special focus on conformational analysis, until the first '80s. Then, since 1985 his research interests have shifted towards chemometrics, multivariate analysis and applied statistics, QSAR, molecular descriptors, multicriteria decision making, software development, starting to publish on these topics. The 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 over there up-to-date but low cost researches. In the beginning of '90s, Todeschini became associate professor at the University of Milano-Bicocca (Milan, Italy) and then, in 2001, full professor of chemometrics at the Department of Earth and Environmental Sciences in the same Institution, where he founded the *Milano Chemometrics and QSAR Research Group*. The actual staff of the research group includes Davide Ballabio, Viviana Consonni and Francesca Grisoni, while past-researchers of the

•Corresponding author (Email: roberto.todeschini@unimib.it)
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group are Paola Gramatica, Manuela Pavan, Andrea Mauri, Matteo Cassotti, Kamel Mansouri, and Faizan Sahigara.

He was one of the founders of the International Academy of Mathematical Chemistry in 2004 and served as President of the Academy from 2008 to 2013. He is also President of the Italian Chemometric Society and “ad honorem” professor of the University of Azuay (Cuenca, Ecuador) since 2006.

He is author of more than 200 publications in international peer-reviewed journals and co-author of the books: “The Data Analysis Handbook”, by I.E. Frank and R. Todeschini (Elsevier, 1994); “Handbook of Molecular Descriptors”, by R. Todeschini and V. Consonni (Wiley-VCH, 2000); “Molecular Descriptors for Chemoinformatics” by R. Todeschini and V. Consonni (Wiley-VCH, 2009); “Handbook of Bibliometric Indicators” by R. Todeschini and A. Baccini (Wiley-VCH, 2016). The first book about the molecular descriptors (2000) is among the most cited scientific books, with more 3300 in 2016.

Todeschini, together with his research group, organized several national and international meetings and schools about molecular descriptors, multi-criteria decision making, chemometrics, experimental design.

The complete list of publications of Todeschini can be accessed in Google Scholar at “https://scholar.google.com/citations?user=MNyEfBcAAAAJ” with more than 11000 citations and an h-index of 44 (January 2017).His main scientific results were organized in different topics and presented below.

1. CHEMOMETRICS

The interests of Todeschini about chemometrics include all its theoretical aspects. Critical reviews about Q^2 metrics proposed in literature for evaluating prediction ability of regression models were published and earned a big success. More recently, an extended comparison about the different proposals to estimate Q^2 was published and a reliable solution was proposed.

About classification methods, he proposed three new methods, called CAIMAN, N3 and BNN; in particular, the last two methods, proposed together with Ballabio, Cassotti and Consonni, were demonstrated to give very good quality classification results. Moreover, studies were also made on the KNN classification method, about its dependence on scaling and distance measures and for evaluating missing values.

Several studies were also performed on the concept of the applicability domain of classification and regression models and on the topic of variable selection, for which some novel methods were also proposed.

In 1993, Todeschini along with Ildiko Frank released the software SCAN (Software for Chemometric Analysis) andin 1994 Todeschini, still with Ildiko Frank, published the book “The Data Analysis Handbook” (Elsevier).

2. MOLECULAR DESCRIPTORS

Todeschini proposed in 1994 a set of 3D molecular descriptors, called WHIM, based on the Principal Component Analysis and, in 2000 with Consonni, the GETAWAY descriptors, based on the statistical concept of leverage. Starting from the publication of the first book on molecular descriptors, already mentioned afore, Consonni and Todeschini published several reviews and book chapters in this field. About topological descriptors, they published a paper where a generalization of graph energy was proposed analysing the spectral indices defined in literature as well as the different kinds of topological vertex degree. Still with Consonni, a review was also dedicated to analyse all the weighted and unweighted topological matrices defined in literature.

The software DRAGON was also developed by Todeschini and his research group since 2000, collecting from time to time always more molecular descriptors.

3. STATISTICS

Among the main results in statistics, the K multivariate correlation index was proposed in two papers, giving the exact definition of an index able to give a measure of global correlation in a multivariate dataset.

Several papers were also dedicated to similarity/diversity measures. Among these, a paper with Consonni, Peter Willett *et al*., on all the binary similarity measures proposed in the literature, some papers about canonical distances and similarities between datasets, an original variant of the Mahalanobis distance, a similarity measure for DNA sequences, a new similarity measure taking into account higher order similarities, a Hausdorff-like similarity measure to evaluate the similarity between sets (i.e. molecules) when they are partitioned in different constituents (i.e. ionic liquids, metabolites, sub-structures) and a review about similarity/diversity measures for the Encyclopaedia of Analytical Chemistry by Wiley & Sons.

4. QUANTITATIVE STRUCTURE-ACTIVITY (-PROPERTY) RELATIONSHIPS (QSAR/QSPR), DRUG DESIGN

Several chemometric applications were developed by Todeschini's research group in QSAR/QSPR and related fields.

In the environmental and human health fields, studies were performed on biodegradability, aquatic toxicity, tropospheric degradation, bioconcentration factor,

bioaccumulation, water quality, non-ionic surfactants, mutagenicity and environmental priority settings. In chemistry, studies were performed on the phisico-chemical and toxicological behaviour of PAH, PCB, PCDD and PCDF compounds. In food chemistry, studies were performed on olive oils, sweetness, dairy cream, spirits, and food quality analysis, while in drug design, studies were performed on Cytochrome P450, Ca2+ channel antagonists, non-peptide angiotensin II receptor antagonists and virtual compound screening for sets of pharmacological targets.

5. MULTICRITERIA DECISION MAKING

He was the editor, together with Manuela Pavan, of a book for Elsevier about the ranking methods and decisions based on multi-criteria. In this field, papers were published about indices for the evaluation of Hasse diagrams, generalization of the Power-Weakness Ratio (PWR) measure and Hasse theory.

6. BIBLIOMETRIC INDICATORS

In 2016 he published the “Handbook of Bibliometric Indicators” together with Alberto Baccini (Wiley-VCH), following the same encyclopaedic approach used in the past for the books about molecular descriptors.

This topic is actually particularly warm, due to the large interest of researchers, institutions, countries, etc. for the research evaluation.

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