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CARRIERA ACCADEMICA	<p>Dal 1975 al 1992 è stato prima contrattista e poi ricercatore confermato presso il Dipartimento di Chimica-Fisica ed Elettrochimica dell'Università degli Studi di Milano.</p> <p>Nel 1992 è diventato professore associato di Chimica Fisica presso il Dipartimento di Chimica-Fisica ed Elettrochimica dell'Università degli Studi di Milano. Dal 2000 è professore ordinario presso il Dipartimento di Scienze dell'Ambiente e del Territorio della Facoltà di Scienze Matematiche, Fisiche e Naturali dell'Università degli Studi di Milano-Bicocca.</p>
DIDATTICA	<p>Titolare dei seguenti insegnamenti nei corsi di laurea di Scienze e Tecnologie Chimiche e Scienze e Tecnologie dell'Ambiente e del Territorio:</p> <ul style="list-style-type: none"> - Chimica Analitica (mod.2) / Lab. Chimica Analitica II - Chimica Analitica II / / Lab. Chimica Analitica II - Chemiometria Applicata - Chemiometria
ATTIVITA' DI RICERCA	<p>I principali campi di interesse sono gli studi relativi alla chemiometria, alle relazioni quantitative tra struttura molecolare e attività biologiche (QSAR) e proprietà chimico-fisiche (QSPR) e allo sviluppo di descrittori molecolari.</p> <p>Attuali attività di ricerca specifiche:</p> <ol style="list-style-type: none"> 1) Sviluppo di strumenti chemoinformatici per la selezione ed identificazione di composti Persistenti Bioaccumulabili e Tossici (PBTs) ed Interferenti Endocrini (EDs) nell'ambito del Regolamento REACH. (PRIN 2007) 2) Libro "Molecular Descriptors for Chemoinformatics", R. Todeschini and V. Consonni - Wiley-VCH (in stampa) 3) Creazione di un data base di molecole con le relative proprietà chimiche e strutturali. 4) Collaborazione scientifica su "Analysis of molecular descriptors and chemical modelling" nell'ambito dei programmi per lo scambio di ricerche con la Croazia. 5) Elaborazione di immagini cellulari mediante algoritmi di classificazione.

	6) Studi sulla correlazione per l'analisi multivariata dei dati.
PRINCIPALI PUBBLICAZIONI RELATIVE AGLI UTLIMI CINQUE ANNI	<p>Ballabio D. and Todeschini R. (2008). Multivariate Classification for Qualitative Analysis. In <i>Infrared Spectroscopy for Food Quality Analysis and Control</i>. (Da-Wen Sun, Ed.), Elsevier, Amsterdam.</p> <p>Consonni V. and Todeschini R. (2008). New Spectral Indices for Molecule Description. <i>MATCH</i>, 60, 3-14.</p> <p>Gutman I., Indulal G. and Todeschini R. (2008). Generalizing the McClelland Bounds for Total π-Electron Energy. <i>Zeitschrift fur Naturforschung A</i>, 63a, 280-282.</p> <p>Manganaro A., Ballabio D., Consonni V., Mauri A., Pavan M. and Todeschini R. (2008). The DART (Decision Analysis by Ranking Techniques) software. In <i>Scientific Data Ranking Methods: Theory and Applications</i>. (Pavan M. and Todeschini R., Eds.), Elsevier, Amsterdam (The Netherlands), pp. 193-207.</p> <p>Mauri A., Ballabio D., Consonni V., Manganaro A. and Todeschini R. (2008). Peptides multivariate characterisation using a molecular descriptor based approach. <i>MATCH Commun. Math. Comput. Chem.</i>, 60, 671-690.</p> <p>Todeschini R. and Pavan M., Eds. (2008). <i>Scientific Data Ranking Methods: Theory and Applications</i>. Elsevier, Amsterdam (The Netherlands), 180 pp.</p> <p>Pavan M. and Todeschini R. (2008). Total order ranking methods. In <i>Scientific Data Ranking Methods: Theory and Applications</i>. (Pavan M. and Todeschini R., Eds.), Elsevier, Amsterdam (The Netherlands), pp. 51-72.</p> <p>Tetko I. V., Sushko I., Pandey A. K., Zhu H., Tropsha A., Papa E., Öberg T., Todeschini R., Fourches D. and Varnek A. (2008). Critical assessment of QSAR models of environmental toxicity against <i>Tetrahymena pyriformis</i>: Focusing on applicability domain and overfitting by variable selection. <i>Journal of Chemical Information and Modeling</i>, 48, 1733-1746.</p> <p>Todeschini R., Ballabio D., Consonni V. and Mauri A. (2008). A new similarity/diversity measure for the characterization of DNA sequences. <i>Croatica Chemica Acta</i>, 81.</p> <p>Ballabio D., Consonni V. and Todeschini R. (2007). Classification of multiway analytical data based on MOLMAP approach. <i>Anal. Chim. Acta</i>, 605, 134-146.</p> <p>Ballabio D., Kokkinofa R., Todeschini R. and Theocharis C. R. (2007). A classification model built by means of Artificial Neural Networks for the characterization of the traditional Cypriot spirit Zivania. <i>Chemometrics & Intell. Lab. Syst.</i>, 87, 78-84.</p> <p>Todeschini R., Ballabio D., Consonni V. and Mauri A. (2007). A new similarity/diversity measure for sequential data. <i>MATCH</i>, 57, 51-67.</p> <p>Todeschini R., Ballabio D., Consonni V., Mauri A. and Pavan M. (2007). CAIMAN (Classification And Influence Matrix Analysis): A new approach to the classification based on leverage-scaled functions. <i>Chemometrics & Intell. Lab. Syst.</i>, 87, 3-17.</p> <p>Ballabio D., Cosio M. S., Mannino S. and Todeschini R. (2006). A chemometric approach based on a novel similarity/diversity measure for the characterization and selection of electronic nose sensors. <i>Anal. Chim. Acta</i>,</p>

578, 170-177.

Ballabio D., Mauri A., Todeschini R. and Buratti S. (2006). Geographical classification of wine and olive oil by means of CAIMAN (Classification And Influence Matrix Analysis). *Anal. Chim. Acta*, 570, 249-258.

Mauri A., Consonni V., Pavan M. and Todeschini R. (2006). DRAGON software: an easy approach to molecular descriptor calculations. *MATCH*, 56, 237-248.

Pavan M., Consonni V., Gramatica P. and Todeschini R. (2006). New QSAR modelling approach based on ranking models by Genetic Algorithms - Variable Subset Selection (GA-VSS). In *Partial Order in Environmental Sciences and Chemistry*. (Brüggeman R. and Carlsen L., Eds.), Springer Verlag, pp. 185-224.

Pavan M., Todeschini R. and Orlandi M. (2006). Data mining by total ranking methods: a case study on optimization of the "pulp and bleaching" process in the paper industry. *Annali di Chimica*, 96, 13-27.

Todeschini R., Consonni V., Mauri A. and Ballabio D. (2006). Characterization of DNA primary sequences by a new similarity/diversity measure based on the partial ordering. *Journal of Chemical Information and Modeling*, 46, 1905-1911.

Todeschini R. (2006). Molecular Descriptors and Chemometrics. *G. I. T. Laboratory Journal*, 5, 40-42.

Pavan M., Consonni V. and Todeschini R. (2005). Partial Ranking Models by Genetic Algorithms Variable Subset Selection (GA-VSS) approach for environmental priority settings. *MATCH*, 54, 583-609.

Tetko I. V., Gasteiger J., Todeschini R., Mauri A., Livingstone D., Ertl P., Palyulin V. A., Radchenko E. V., Zefirov N. S., Makarenko A. S., Tanchuk V. Y. and Prokopenkov V. V. (2005). Virtual Computational Chemistry Laboratory -- Design and Description. *J. Computer-Aided Mol. Des.*, 19, 453-463.

Pavan M., Mauri A. and Todeschini R. (2004). Total ranking models by the Genetic Algorithms Variable Subset Selection (GA-VSS) approach for environmental priority settings. *Analytical and Bioanalytical Chemistry*, 380, 430-444.

Pavan M. and Todeschini R. (2004). New indices for analyzing partial ranking diagrams. *Anal. Chim. Acta*, 515, 167-181.

Todeschini R., Consonni V. and Pavan M. (2004). A Distance Measure between Models: a Tool for Similarity/Diversity Analysis of Model Populations. *Chemometrics & Intell. Lab. Syst.*, 70, 55-61.

Todeschini R., Consonni V. and Pavan M. (2004). Distance Measure between Models: a Tool for Model Similarity/Diversity Analysis. In *Designing Drugs and Crop Protectants: processes, problems and solutions*. (Ford M., Livingstone D., Deardean J. and van de Waterbeemd H., Eds.), Blackwell, Oxford (UK), pp. 467-469.

Todeschini R. (2004). Reality and Models. Concepts, strategies and tools for QSAR. In *Designing Drugs and Crop Protectants: processes, problems and solutions*. (Ford M., Livingstone D., Deardean J. and van de Waterbeemd H., Eds.), Blackwell, Oxford (UK), pp. 235-242.

Todeschini R., Consonni V., Mauri A. and Pavan M. (2004). Detecting "bad" regression models: multicriteria fitness functions in regression analysis. *Anal. Chim. Acta*, 515, 199-208.

Backhaus, T., Altenburger, R., Arrhenius, A., Blanck, H., Faust, M., Finizio, A., Gramatica, P., Grothe, M., Junghans, M., Meyer, W., Pavan, M., Porspring, T., Scholze, M., Todeschini, R., Vighi, M., Walter, H., and Grimme, L. H. (2003). The BEAM-project: prediction and assessment of mixture toxicities in the aquatic environment. <[11] Journal Name>, 23, 1757-1769.

Lleti R., Sarabia L., Ortiz M. C., Todeschini R. and Colombini M. P. (2003). Application of the Kohonen Artificial Neural Network in the identification of Proteinaceous Binders in Samples of Panel painting Using Gas Chromatography-Mass Spectrometry. *The Analyst*, 181, 281-286.

Mezzanotte V., Castiglioni F., Todeschini R. and Pavan M. (2003). Study on anaerobic and aerobic degradation of different non-ionic surfactants. *Bioresource Technology*, 87, 87-91.

Todeschini R., Consonni V. and Pavan M. (2003). Distance measure between models: a tool for model similarity/diversity analysis. In *Designing Drugs and Crop Protectants: processes, problems and solutions*. (Ford M., Livingstone D., Deardean J. and van de Waterbeemd H., Eds.), Blakwell, Oxford (UK), pp. 467-469.

Todeschini R., Consonni V., Mauri A. and Pavan M. (2003). New fitness functions to avoid bad regression models in variable subset selection by Genetic Algorithms. In *Designing Drugs and Crop Protectants: processes, problems and solutions*. (Ford M., Livingstone D., Deardean J. and van de Waterbeemd H., Eds.), Blakwell, Oxford (UK), pp. 323-325.

Todeschini R., Consonni V. and Pavan M. (2003). MobyDigs: Software for Regression and Classification Models by Genetic Algorithms. In *Nature-inspired Methods in Chemometrics: Genetic Algorithms and Artificial Neural Networks*. (Leardi R, Ed.), Elsevier, Amsterdam (The Netherlands), pp. 141-167.

Todeschini R. and Consonni V. (2003). Descriptors from Molecular Geometry. In *Handbook of Chemoinformatics - Vol.3*. (Gasteiger J., Ed.), WILEY-VCH, Weinheim (GER), vol. 3, pp. 1004-1033.