ANDREA MAURI

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Sex: Male
Nationality: Italian

EDUCATION

2004 - 2007:	University of Milano-Bicocca, Milano, Italy PhD project in Chemical Sciences. Thesis title: "Protein and peptide multivariate characterisation using a molecular descriptor based approach"
1994 - 2000:	University of Milano-Bicocca, Milano, Italy Degree in Environmental Sciences Final grade: 110/110
1989 - 1994:	IT High School, A. Badoni, Lecco Final grade: 52/60

PROFESSIONAL EXPERIENCES

October 2010 - Now	EC funding at the Milano Chemometrics and QSAR Research Group (University of Milano - Bicocca) under the FP7 framework to develop a new, safe, multifunctional accelerator curative molecule which can replace thiourea-based accelerators in the vulcanisation process (http://www.saferubber.eu/). Scientific consultant for Talete: chemometric consulting and collaboration in the realization of software of multivariate analysis. Scientific consulting and software development at Talete (http://www.talete.mi.it) company.
November 2007 – September 2010	Post-doc grant at Milano Chemometrics and QSAR Research Group led by Professor Roberto Todeschini, at University of Milano-Bicocca; research related to Multivariate statistical analysis techniques and statistical software development.
May 2008 – September 2008	Stage at Istituto di Ricerche Farmacologiche Mario Negri in collaboration with University of Milano-Bicocca, Milano, Italy

November 2004 – November 2007	PhD project in Chemical Sciences on a molecular descriptor-based approach for protein characterization, University of Milano-Bicocca, Department of Environmental Sciences. PhD thesis title is: "Protein and peptide multivariate characterisation using a molecular descriptor based approach"
	Scientific consulting and software development at Talete (http://www.talete.mi.it) company.
	Ongoing collaboration with Milano Chemometrics and QSAR Research Group led by Professor Roberto Todeschini, at University of Milano-Bicocca; research related to Multivariate statistical analysis techniques and statistical software development.
	Visiting PhD student for 6 months (October 2006- April 2007) at the National Chemistry Institute, Ljubljana
April 2002 - April 2004:	Collaboration in the project for the creation of the Virtual Insitute for Chemometrics and Industrial Metrology (VICIM)
	Collaboration in the INTAS project for the creation of the Virtual Computational Chemistry Laboratory (VCCLAB) with respect to the E-DRAGON application.
March 2004	Teaching-Assistant in the Second Italian School on Molecular Descriptors, Talete srl, University of Milano-Bicocca, Milano (Italy)
January 2001 - November 2001	Civil Service with Associazione Comunità Papa Giovanni XXIII, Rimini. March 2001, Chiapas, Mexico. June – November 2001, Ndola, Zambia.
June 2000	Teaching-Assistant for the graduate course of "Diseño Experimental y Optimizacion de Procesos" in the Ecuadorian Master "Programa de Postgrado de Maestría en Gestíon Tecnologíca", Universidad Del Azuay (UDA), Cuenca (Ecuador)

SOFTWARE DEVELOPED

- Author of **DRAGON, dragonX** and **dProperties** software. DRAGON is a software package for the calculation of molecular descriptors distributed by Talete srl (http://www.talete.mi.it).
- Author of **SmartEdit Plus** software distributed by Ideatech srl (http://www.ideatechsrl.com)

PUBLICATIONS AND CONGRESSES

Papers on peer reviewed international journals

- Comparison of Different Approaches to Define the Applicability Domain of QSAR Models (2012), F. Sahigara, K. Mansouri, D. Ballabio, A. Mauri, V. Consonni, R. Todeschini, *Molecules* **17** (5), 4791-4810
- Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 3. Variable selection in classification (2010). D. Ballabio, V. Consonni, A. Mauri, R. Todeschini, *Analytica Chimica Acta*, **657**, 116-122
- Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 2. Variable reduction. (2009), V. Consonni, D. Ballabio, A. Manganaro, A. Mauri, R. Todeschini, *Analytica Chimica Acta*, **648**, 45-51
- Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 1. Theory and simple chemometric applications.(2009), R. Todeschini, D. Ballabio, V. Consonni, A. Manganaro, A.

Mauri, *Analytica Chimica Acta*, **648**, 52-59

- Introduction to MOLE DB - on-line Molecular Descriptors Database (2009), D. Ballabio, A. Manganaro, V. Consonni, A. Mauri and R. Todeschini. *MATCH, communications in mathematical and in computer chemistry*, **62**, 199-207
- A New Similarity/Diversity Measure for the Characterization of DNA Sequences (2008), R. Todeschini, D. Ballabio, V. Consonni and A. Mauri. *Croatica Chemica Acta*, **81**, 657-664
- Peptides multivariate characterisation using a molecular descriptor based approach (2008), A. Mauri, D. Ballabio, V. Consonni, A. Manganaro and R. Todeschini. *MATCH, communications in mathematical and in computer chemistry*, **60**, 671-690
- CAIMAN (Classification And Influence Matrix Analysis): a new approach to the classification based on leverage-scaled functions (2007). R. Todeschini, D. Ballabio, V. Consonni, A. Mauri, M. Pavan. *Chemometrics and Intelligent Laboratory Systems*, **87**, 3-17
- A new similarity/diversity measure for sequential data (2007). R. Todeschini, D. Ballabio, V. Consonni, A. Mauri. *MATCH, communications in mathematical and in computer chemistry*. **57**, 51-67
- Characterization of DNA primary sequences by a new similarity/diversity measure based on the partial ordering (2006). R. Todeschini, V. Consonni, A. Mauri, D. Ballabio. *Journal of Chemical Information and Modeling*, **46**, 1905-1911
- DRAGON Software: An Easy Approach to Molecular Descriptor Calculations (2006). A. Mauri, V. Consonni, M. Pavan, R. Todeschini. *MATCH, communications in mathematical and in computer chemistry*. **56**, 237-248
- Geographical classification of wine and olive oil by means of CAIMAN (Classification And Influence Matrix Analysis) (2006). D. Ballabio, A. Mauri, R. Todeschini, S. Buratti. *Analytica Chimica Acta*. **570**, 249-258
- Virtual computational chemistry laboratory – design and description (2005). I.V. Tetko, J. Gasteiger, R. Todeschini, A. Mauri, D. Livingstone, P. Ertl, V.A. Palyulin, E.V. Radchenko, N.S. Zefirov, A.S. Makarenko, V.Y. Tanchuk and V.V. Prokopeko. *Journal of Computer-Aided Molecular Design.* **19,** 453-456
- Detecting 'bad' regression models: multicriteria fitness functions in regression analysis. (2004). R. Todeschini, V. Consonni, A. Mauri and M. Pavan. *Analityca Chimica Acta*. **515**, 199-208
- Total ranking models by Genetic Algorithms Variable Subset Selection (GA-VSS) approach for environmental priority settings. (2004). M. Pavan, A. Mauri and R. Todeschini. *Analytical and Bioanalytical Chemistry*

Book Chapters

- The DART (Decision Analysis by Ranking techniques) software, A. Manganaro, D. Ballabio, V. Consonni, A. Mauri, M. Pavan, R. Todeschini in "Ranking methods" (R. Todeschini and M. Pavan, Eds.), Elsevier, 2008
- Similarity/diversity measure for sequential data based on Hasse Matrices: Theory and applications, A. Mauri, D. Ballabio in "Ranking methods" (R. Todeschini and M. Pavan, Eds.), Elsevier, 2008
- MobyDigs: software for regression and classification models by geneic algorithms. (2004). R.Todeschini, V. Consonni, A.Mauri and M.Pavan in "Nature-inspired methods in chemometrics: genetic algorithms and artificial neural networks" (R. Leardi Ed.), Chapter 5, p.141-167, Elsevier, 2004
- New fitness functions to avoid bad regression models in variable subset selection by Genetic Algorithms. (2004). R. Todeschini, V. Consonni, A. Mauri and M. Pavan in "Designing Drigs and Crop Protectants: processes, problems and solutions." (M. Ford, D. Livingstone, J. Deardean, H. van de Waterbeemd Ed.), Chapter 5, p.323-325, Blackwell, 2004

Other papers

- Evaluation of multivariate classification and variable selection for the distinction of cachaça and rum samples (2007). R. Todeschini, D. Ballabio, C. Rojas, A. Manganaro, A. Mauri, V. Consonni, and P. Tripaldi. *Alimentos,*

Ciencia e Ingeniería, Vol. 16(2): 113-115

Posters

- "A (Q)SAR study on ready biodegradability", T. Ringsted, K. Mansouri, D. Ballabio, A. Mauri, V. Consonni, R. Todeschini, *15th International Workshop on Quantitative Structure-Activity Relationships (QSAR2012)* in Environmental and Health Sciences, Tallinn (Estonia), 18-22 June 2012
- "Read-across methodology in aquatic ecotoxicology and ready biodegradation", T. Ringsted, E. Giagloglou, D. Ballabio, A. Mauri, M. Cassotti, V. Consonni, R. Todeschini, *ECO winter school*, Madrid (Spain), 27 February -2 March 2012
- "QSAR study for the prediction of LogP coefficient", K. Mansouri, A. Mauri, D. Ballabio, V. Consonni, R. Todeschini, *6th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2011)*, Maribor (Slovenia), 3-7 September 2011
- "Molecular descriptors by Dragon software", A. Mauri, A. Manganaro, D. Ballabio, V. Consonni, R. Todeschini, *XII Convegno della Divisione di Chimica Analitica della Società Chimica Italiana*, Como (Italy), 13-16 September 2010
- "MOLE DB - on-line Molecular Descriptors Data Base", D. Ballabio, A. Manganaro, V. Consonni, A. Mauri, R. Todeschini, *MATH/CHEM/COMP 2008* Conference, Verbania (Italy), 10-13 June 2008
- "Evaluation of multivariate classification and variable selection for the distinction of cachaca and rum samples", R. Todeschini, D. Ballabio, C. Rojas, A. Manganaro, A. Mauri, V. Consonni, P. Tripaldi, *Ibero-American Congress in Food Engineering*, Ambato (Ecuador), 5-8 November 2007
- "Novel XML-based Electronic Format for QSAR Models Exchange and Application", A. Manganaro, R. Todeschini, V. Consonni, D. Ballabio, A. Mauri, *6th World Congress on Alternatives & Animal Use in the Life Sciences*, Tokyo (Japan), 21-25 August 2007
- "On the characterization of proteomic maps by a novel similarity/diversity", A.Mauri, V.Consonni and R.Todeschini. *Chemoinformatics in Europe: Research and Teaching*, Obernai (France), 29 May - 1 June 2006
- "Comparison of several different fitness functions in regression models." A.Mauri, D.Ballabio, V.Consonni, M.Pavan and R.Todeschini. *Colloquium Chemometricum Mediterraneum*, Ustica (Italy), 25 – 27 June 2003
- "Data mining by a partial ranking strategy (Hasse Diagram Tecnique, HDT)" M.Pavan, A.Mauri, V.Consonni, D.Ballabio and R.Todeschini. *Colloquium Chemometricum Mediterraneum*, Ustica (Italy), 25 – 27 June 2003
- "New fitness functions to avoid bad regression models in variable subset selection by Genetic Algorithms." R.Todeschini, V.Consonni, A.Mauri, M.Pavan *14 TH European Symposium on quantitative structure-activity relationships*, Bournemouth (UK), 8-13 September 2002.

Talks

- "How to build a predictive QSAR model", *ECO summer school*, Verona (Italy), 11 June 2012
- "Proteins and peptides multivariate characterization using a molecular descriptors based approach", A. Mauri, R. Todeschini, D. Ballabio, V. Consonni andA.Manganaro. *Colloquium Chemiometricum Mediterraneum*, Saint maximin (France) September 5-7, 2007
- "A similarity/diversity measure based on partial ordering", R. Todeschini, D. Ballabio, A. Manganaro, A. Mauri. *Workshop di Chemometria*, Modena (Italy) February 15-16, 2007
- "A molecular descriptor-based approach for protein characterization using DRAGON descriptors", A. Mauri. *IBAAC meeting*. Bologna (Italy), December 1-2, 2006
- "Characterization of proteomic maps by means of Hasse distances", A. Mauri. *Workshop on Ranking Methods and Multicriteria Decision Analysis in Environmental Sciences*, Verbania (Italy), October 2-3, 2006
- "On the characterization of proteomic maps by a novel similarity/diversity measure", A. Mauri, V. Consonni and R. Todeschini. *MATH/CHEM/COMP 2006. The 21st International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences*, Dubrovnik (Croatia), June 19-24, 2006

Courses and Congresses

- ECO summer school, Verona (Italy), 11-15 June 2012, Member of the organizing committee
- VII Colloquium Chemiometricum Mediterraneum, Granada (Spain), 21-24 June 2010
- MATH/CHEM/COMP 2008 Conference, Verbania (Italy), June 10-13, 2008. Member of the organizing commitee
- Italian Chemometric Workshop, Pisa (Italy), May 14-15, 2008
- VI Colloquium Chemiometricum Mediterraneum, Saint-Maximin (France), September 5-7, 2007
- Italian Chemometric Workshop, Modena (Italy), February 15-16, 2007
- Workshop on Ranking Methods and Multicriteria Decision Analysis in Environmental Sciences, Verbania (Italy), October 2-3, 2006
- MATH/CHEM/COMP 2006. The 21st International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik (Croatia), June 19-24, 2006
- Chemoinformatics in Europe: Research and Teaching, Obernai (France), 29 May - 1 June 2006
- "Scuola Nazionale di Chimica Analitica per Dottorandi", School of Analytical Chemistry for PhD Students, Rocca di Papa (RM) (Italy), October 3-7, 2005
- Introduction to methods of Experimental Design, Chemometric School, Milano (Italy) June 29, 2004
- Colloquium Chemometricum Mediterraneum, Ustica (Italy), June 25-27, 2003
- First Italian School on Molecular Descriptors, Italian Society of Chemometrics, Gargnano del Garda (Italy), September 28-30, 1998

LANGUAGES AND INFORMATIC SKILLS

- Good knowledge of spoken and written English
- Good knowledge of spoken Spanish
- Good knowledge of Windows and Linux operating systems
- Good programming skills in Pascal (Delphi/Kylix, Lazarus/FPC), Visual Basic, MatLab and SQL
- Basic programming skills in Java and C
- Excellent knowledge of Microsoft Office, OpenOffice and of some statistical software: Statistica, SIMCA, MODDE and Scan.

FIELDS OF INTEREST

- *Primary:* Chemometrics, QSAR, Software development
- *Secondary:* Algorithms, Multicriteria decision making.