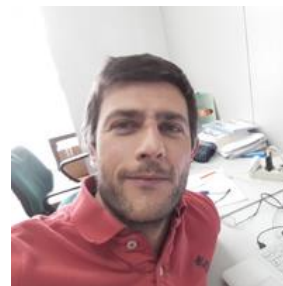


# Davide Ballabio

davide.ballabio@gmail.com



## Education

- |                    |   |
|--------------------|---|
| <b>2003 - 2006</b> | University of Milano<br>PhD project in food biotechnology   |
| <b>1996 - 2002</b> | University of Milano - Bicocca<br>Degree in Environmental Sciences (final grade: 110/110 cum laude) |
| <b>1990 - 1995</b> | High School: Liceo Classico Zucchi, Monza   |

## Professional experiences

- |                            |  |
|----------------------------|--|
| <b>Sep 2015 - Now</b>      | Researcher in chemometrics, QSAR and analytical chemistry at the Milano Chemometrics and QSAR Research Group (Department of Earth and Environmental Sciences, University of Milano - Bicocca).   |
| <b>Mar 2014 - Feb 2015</b> | Funding by Reach and Colour Italia srl at the Milano Chemometrics and QSAR Research Group (University of Milano - Bicocca) for the quantitative analysis of relationships between molecular structures and toxicological and chemical-physical properties of dyes.<br>Scientific consultant for Talete: chemometric consulting and collaboration in the realization of software of multivariate analysis.  |
| <b>Jan 2011 - Feb 2014</b> | 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 ( <a href="http://www.saferubber.eu/">http://www.saferubber.eu/</a> ).<br>Scientific consultant for Talete: chemometric consulting and collaboration in the realization of software of multivariate analysis.  |
| <b>Jan 2007 - Dec 2010</b> | Post-doc grant (Milano Chemometrics and QSAR Research Group, University of Milano - Bicocca) for the development of an on-line database of molecular structures, available at: <a href="http://michem.disat.unimib.it/mole_db">http://michem.disat.unimib.it/mole_db</a>   |
| <b>Jan 2004 - Oct 2006</b> | PhD project in food biotechnology (University of Milano): Chemometric characterisation of physical-chemical fingerprints of food products.<br>Consultant for Tecnogalenica: calibration of NIR instruments by means of chemometrics.<br>Scientific consultant for Talete: chemometric consulting and collaboration in the realization of software of multivariate analysis.<br>Visiting PhD student for 8 months (Jan-May 2005 and Jul-Sep 2006) at the Spectroscopy and Chemometrics Group (The Royal Veterinary and Agricultural University, Copenhagen), world leader in multi-way analysis and chemometrics.<br>Ongoing collaboration with Milano Chemometrics and QSAR Research Group (University of Milano - Bicocca) on researches related to multivariate statistical analysis and statistical software development. |

<b>Jan 2003 - Dec 2003</b>	Scholarship (University of Milano - Bicocca) for the analysis of quality indices applicable on soils in Lombardia by means of multivariate analysis.
<b>Oct 2002 - Dec 2002</b>	Stage at Synergia S.r.l., consulting company specializing in workplace safety and environmental protection.
<b>Apr 2002 - Sep 2002</b>	Scholarship (University of Milano - Bicocca) for the evaluation, selection and development of softwares concerning university didactical tests.

## Teaching experiences

<b>31 May - 1 June 2017</b>	Lecturer in the PhD course (14 hours) on Classification methods in chemometrics at Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).
<b>Apr - May 2017</b>	Teaching assistant at the course of Analytical Chemistry (20 hours), Department of Chemistry, University of Milano - Bicocca.
<b>Jan 2017</b>	Teaching assistant at the course of Chemometrics (12 hours), Department of Chemistry, University of Milano - Bicocca.
<b>Nov 2016</b>	Teaching assistant at the course of Analytical Chemistry (20 hours), Department of Environmental Sciences, University of Milano - Bicocca.
<b>Oct - Dec 2016</b>	Laboratory of Instrumental Analytical Chemistry (36 hours) and lecturer at the course of Instrumental Analytical Chemistry (14 hours), Department of Chemistry, University of Milano - Bicocca.
<b>21-24 June 2016</b>	Seminar "Chemometric analysis for the evaluation of analytical data" at the State General Laboratory (Nicosia, Cyprus) and lecturer in the course "SIMCA for isotopic and analytical data regarding food and drink authenticity" at the NMR laboratory of the State General Laboratory (Nicosia, Cyprus).
<b>Apr - May 2016</b>	Teaching assistant at the course of Analytical Chemistry (20 hours), Department of Chemistry, University of Milano - Bicocca.
<b>25 Jan - 10 Feb 2016</b>	Lecturer in the course (80 hours) on Chemometrics and QSAR applied to molecules of biological interest at the University of Azuay (Cuenca, Ecuador).
<b>Dec 2015</b>	Teaching assistant at the course of Chemometrics (12 hours), Department of Chemistry, University of Milano - Bicocca.
<b>Dec 2015</b>	Teaching assistant at the course of Instrumental Analytical Chemistry (36 hours), Department of Chemistry, University of Milano - Bicocca.
<b>Nov 2015</b>	Teaching assistant at the course of Analytical Chemistry (20 hours), Department of Environmental Sciences, University of Milano - Bicocca.
<b>15-16 June 2015</b>	Lecturer in the PhD course (14 hours) on Classification methods in chemometrics at Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).
<b>May 2015</b>	Lecturer in the PhD course (module of Principal Component Analysis, 6 hours) at the Department of Pharmaceutical Sciences, University of Milan (Italy).
<b>Apr 2015 - May 2015</b>	Teaching assistant at the course of Analytical Chemistry (20

hours), Department of Chemistry, University of Milano - Bicocca.

- Dec 2014** Lecturer in the MSc course of Multivariate Analysis (module on multivariate classification, 4 hours) at the Department of Biotechnology, University of Milano - Bicocca (Italy).
- 7-10 July 2014** Lecturer in the PhD course (28 hours) on Classification methods in chemometrics at Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).
- May 2014** Lecturer in the course of Basics of Statistical Analysis and Multivariate Analysis (16 hours) at the Department of Material Science, University of Milano - Bicocca (Italy).
- 5 May 2014** Seminar on multivariate analysis of isotopic data at the Department of Science and Technology, University of Bolzano (Italy).
- Oct 2013 - Jan 2014** Teaching assistant at the course of Analytical Chemistry (20 hours) and Chemometrics (10 hours), Department of Chemistry, University of Milano - Bicocca (Italy).
- Nov 2013** Lecturer in the MSc course of Multivariate Analysis (module on multivariate classification, 8 hours) at the Department of Biotechnology, University of Milano - Bicocca (Italy).
- October 2013** Lecturer in the course of Multivariate Analysis applied to Electronic Nose data (10 hours) at Demetra.
- 26-27 Sept 2013** Lecturer in the PhD course (16 hours) on Classification methods in chemometrics at Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).
- 9 May 2013** Seminar on Multivariate Analysis as a tool for the development and control of bioprocesses at the Pontificia Universidad Javeriana in Bogota (Colombia).
- 6-7 May 2013** Lecturer in the course of Multivariate Analysis applied to Microbiological data (12 hours) at the Pontificia Universidad Javeriana in Bogota (Colombia).
- Apr 2013** Lecturer in the course of Basics of Statistical Analysis and Multivariate Analysis (18 hours) at the Department of Material Science, University of Milano - Bicocca (Italy).
- Nov 2012** Lecturer in the MSc course of Multivariate Analysis (module on multivariate classification, 8 hours) at the Department of Biotechnology, University of Milano - Bicocca (Italy).
- Oct 2012 - Jan 2013** Teaching assistant at the course of Analytical Chemistry (24 hours) and Chemometrics (24 hours), Department of Chemistry, University of Milano - Bicocca.
- 27 Mar - 5 Apr 2012** Lecturer in the Chemometrics and Experimental Design course (16 hours) at the Master in Materials for Energy and Environment, Università degli Studi del Piemonte Orientale (Italy).
- 13 - 15 Dec 2011** Lecturer in the Advanced Chemometrics MSc course (module on multivariate classification) at the Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).
- 14 Dec 2011** Seminar on Classification methods in chemometrics at Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).

<b>22 Feb - 4 Mar 2011</b>	Consulting on data analysis and course on chemometrics (12 hours) at the National University of Colombia in Bogota (Colombia).
<b>23-24 Nov 2010</b>	Lecturer in the course on multivariate classification for PhD students and industry partners (12 hours) at the Quality & Technology Research Group, Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark).
<b>Sep - Oct 2010</b>	Assistant in the training course on Experimental Design (32 hours) in the project Formulation and developing of new products in cosmetic companies.
<b>4-19 Feb 2010</b>	Consulting on the data analysis and course on chemometrics (20 hours) in the project Selection of physical chemical indicators for cataloguing Colombian apicultural products at the National University of Colombia in Bogota (Colombia).
<b>Oct - Dec 2009</b>	Teaching assistant at the course on Analytical Chemistry (56 hours), department of Chemistry, University of Milano - Bicocca.
<b>11-12 Nov 2008</b>	Lecturer in the course (16 hours) on chemometrics and basic multivariate modelling, University of Loja (Ecuador)
<b>20-31 Oct 2008</b>	Lecturer in the full course (30 hours) of advanced modelling and applications on environmental and technological problems (modelistica superior aplicada a problemas tecnologicos y gestion ambiental) for the Master of technological management, University of Cuenca (Ecuador)
<b>Oct 2007</b>	Lecturer in the on-line course (4 hours) of chemometrics for the master: Diplomado Superior en Analisis de Datos y Sistemas Complejos, Universidad del Azuay, Cuenca (Ecuador)
<b>04-11 Nov 2006</b>	Lecturer in the course on chemometrics (20 hours) at the National University of Colombia in Bogota, during the cooperation program between IILA (Institute Italo - Latino Americano) and the National University of Colombia.
<b>03-05 Mar 2004</b>	Teaching assistant during the Second Italian School on Molecular Descriptors (University of Milano - Bicocca).
<b>Jan 2003 - Dec 2003</b>	Teaching assistant during the Master level sessions of: <ul style="list-style-type: none"> <li>- Environmental Management and Sustainability (University of Milano - Bicocca)</li> <li>- Cultural Goods management (University of Milano)</li> <li>- Quality and Safety of alimentary Products: analytical, statistical and managerial aspects (University of Milano).</li> </ul>
<b>Mar 2003 - Jun 2003</b>	Lecturer in the course on Operative Research, Probability and Statistics (Department of Computer Sciences, University of Milano - Bicocca)

## Languages and Informatic Skills

<b>Languages</b>	Excellent spoken and written English Basic spoken and written Spanish
<b>Informatic skills</b>	Excellent knowledge of Microsoft Office, Macromedia Flash 5, Macromedia DreamWeaver, Photoshop, FrontPage. Good skills in WEB sites development  Excellent knowledge of the main statistical softwares: Statistica, SPSS, Unscramble and MATLAB.  Excellent programming skills in MATLAB and Visual Basic.

## Software developed

Author of several MATLAB toolboxes, available at:  
<http://michem.disat.unimib.it/chm>  
- Kohonen and CPANN toolbox  
- Classification toolbox for MATLAB  
- PCA toolbox for MATLAB

## Referee activity

Continuative activity as referee for the following peer reviewed international journals:

African Journal of Agricultural Research  
Algorithms for Molecular Biology  
Analyst  
Analytica Chimica Acta (top referee 2008)  
Analytical Chemistry  
Analytical & Bioanalytical Chemistry  
Atmospheric Environment  
Central European Journal of Chemistry  
Chemical Reviews  
Chemometrics and Intelligent Laboratory Systems  
Environmental Pollution  
European Food Research and Technology  
Food and Bioprocess Technology: An International Journal  
IEEE Transactions on Systems, Man, and Cybernetics--Part C: Applications & Reviews  
International Journal of Molecular Sciences  
International Journal of Pharmaceutics  
Iranian Journal of Mathematical Chemistry  
Journal of Agricultural and Food Chemistry  
Journal of Biomedical Science and Engineering  
Journal of Chemical Information and Modeling  
Journal of Chemometrics  
Journal of Chromatography A  
Journal of Computational Chemistry  
Journal of Computer-Aided Molecular Design  
Journal of Pharmaceutical and Biomedical Analysis (top referee 2006)  
Journal of the Iranian Chemical Society  
Mechanical Systems and Signal Processing  
Molecular informatics  
SAR and QSAR in Environmental Research  
Science of the Total Environment  
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy  
Talanta  
Trends in Analytical Chemistry

## Supervision MSc

Simona Cappellini, Studio di nuovi algoritmi per la valutazione del dominio di applicabilità di modelli QSAR (New algorithms for the applicability domain evaluation in QSAR models), University of Milano - Bicocca (Italy), July 2010

Matteo Cassotti, Evaluation of performance and toxicological relevance of accelerators used in the vulcanization process of polychloroprene rubbers, University of Milano - Bicocca (Italy), October 2011

Advisor for: Mohammad Shahbazy, Exploratory analysis of excitation-emission fluorescence data from colorectal cancer with oblique rotation of factors and self-organizing maps, Institute for Advanced Studies in Basic Sciences (Iran), September 2013

Filippo Gravino, Design of chemometric and QSAR solutions to develop inhibitors of trehalase as insecticides, University of Milano - Bicocca (Italy), October 2015

Fabrizio Biganzoli, Comparison of recent advances in consensus modelling of environmental and toxicological QSAR predictions, University of Milano - Bicocca (Italy), November 2016

Alessandro Fabbrica

Chemoinformatic strategy for the development of in silico models related to the molecular interaction with androgen receptor, , University of Milano - Bicocca (Italy), July 2017

## Supervision PhD

Faizan Sahigara, Tools for prediction of environmental properties of chemicals by QSAR/QSPR within REACH. An applicability domain perspective. University of Milano-Bicocca, June 2013, Marie Curie ITN Environmental Chemoinformatics (ECO) project

Kamel Mansouri, New molecular descriptors for estimating degradation and fate of organic pollutants by QSAR/QSPR models within REACH. University of Milano-Bicocca, June 2013, Marie Curie ITN Environmental Chemoinformatics (ECO) project

Matteo Cassotti, QSAR study of aquatic toxicity by chemometrics methods in the framework of REACH regulation. University of Milano-Bicocca, March 2015

External reviewer for Ainara Lopez, Near-infrared spectroscopy and hyperspectral imaging for non-destructive quality inspection of potatoes. University of Navarre (Spain), 2016

## Publications

### PhD Thesis

Chemometric characterisation of physical-chemical fingerprints of food products

D. Ballabio

PhD thesis, University of Milano (2006), discussed on 22/01/2007

### Papers on peer reviewed international journals:

68. Non linear classification of commercial Mexican tequilas.

J.M. Andrade, D. Ballabio, M.P. Gómez-Carracedo, G. Pérez-Caballero

Journal of Chemometrics (2017), accepted for publication

67. Qualitative consensus of QSAR ready biodegradability predictions

D. Ballabio, F. Biganzoli, R. Todeschini, V. Consonni

Toxicological & Environmental Chemistry (2017), 99, 1193-1216,

66. A QSTR-based Expert System to Predict Sweetness of Molecules

C. Royas, R. Todeschini, D. Ballabio, A. Mauri, V. Consonni, P. Tripaldi, F. Grisoni

Frontiers in Chemistry (2017), 5, 53

65. Principal Component Analysis to interpret changes in chromatic parameters on paint dosimeters exposed long-term to urban air

A. Herrera, D. Ballabio, N. Navas, R. Todeschini, C. Cardell

Chemometrics and Intelligent Laboratory Systems (2017), 167, 113-122

64. Valorization of side streams from a SSF biorefinery plant: Wheat straw lignin purification study

L. Zoia, A. Salanti, E.L. Tolppa, D. Ballabio, M. Orlandi

Bioresources (2017), 12, 1680-1696

63. Beware of unreliable  $Q^2$ ! A comparative study of regression metrics for predictivity assessment of QSAR models.

R. Todeschini, D. Ballabio, F. Grisoni

Journal of Chemical Information and Modeling (2016), 56, 1905-1913

62. Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems

A. Mauri, D. Ballabio, R. Todeschini, V. Consonni

Journal of Cheminformatics (2016), 8:49, 1-3

61. A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods

R. Todeschini, D. Ballabio, F. Grisoni, V. Consonni

Chemometrics and Intelligent Laboratory Systems (2016), 157, 50-57

60. Oblique rotation of factors: A novel pattern recognition strategy to classify fluorescence

- excitation-emission matrices of human blood plasma for early diagnosis of colorectal cancer  
M. Shahbazy, M. Vasighi, M. Kompany-Zareh, D. Ballabio  
Molecular BioSystems (2016), 12, 1963-1975
59. Multimethod approach to trace the geographical origin of alpine milk: a case study of Tyrol region  
M. Scampicchio, D. Eisenstecken, L. De Benedictis, C. Capici, D. Ballabio, T. Mimmo, P. Robatscher, L. Kerschbaumer, M. Oberhuber, A. Kaser, C. Huck, S. Cesco  
Food Analytical Methods (2016), 9, 1262-1273
58. Quantitative structure-activity relationships to predict sweet and non-sweet tastes  
C. Rojas, D. Ballabio, V. Consonni, P. Tripaldi, A. Mauri, R. Todeschini  
Theoretical Chemistry Accounts (2016), 135, 66
57. N3 and BNN: Two new similarity based classification methods in comparison with other classifiers.  
R. Todeschini, D. Ballabio, M. Cassotti, V. Consonni  
Journal of Chemical Information and Modeling (2015), 55, 2365-2374
56. A MATLAB toolbox for Principal Component Analysis and unsupervised exploration of data structure  
D. Ballabio  
Chemometrics and Intelligent Laboratory Systems (2015), 149 Part B, 1-9
55. The use of diagnostic ratios, biomarkers and 3-way Kohonen Neural Networks to monitor the temporal evolution of oil spills  
R. Fernández-Varela, M.P. Gómez-Carracedo, D. Ballabio, J.M. Andrade  
Marine Pollution Bulletin (2015), 96, 313-320
54. A similarity-based QSAR model for predicting acute toxicity towards the fathead minnow (*Pimephales promelas*)  
M. Cassotti, D. Ballabio, R. Todeschini, V. Consonni  
SAR and QSAR in Environmental Research (2015), 26, 217-243
53. Impact of medium-distance pollution sources in a Galician suburban site (NW Iberian peninsula)  
M.P. Gómez-Carracedo, J.M. Andrade, D. Ballabio, D. Prada-Rodríguez, S. Muniategui-Lorenzo, V. Consonni, M. Piñeiro-Iglesias, P. López-Mahía  
Science of the Total Environment (2015), 512-513, 114-124
52. Towards global QSAR model building for acute toxicity: Munro database case study  
S. Chavan, I. Nicholls, B. Karlsson, A. Rosengren, D. Ballabio, V. Consonni, R. Todeschini  
International Journal of Molecular Sciences (2014), 15, 18162-18174
51. Validation and extension of a similarity-based approach for prediction of acute aquatic toxicity towards *Daphnia Magna*  
M. Cassotti, V. Consonni, A. Mauri, D. Ballabio  
SAR and QSAR in Environmental Research (2014), 25, 1013-1036
50. K-CM: a new artificial neural network. Application to supervised pattern recognition  
M. Buscema, V. Consonni, D. Ballabio, A. Mauri, G. Massini, M. Breda, R. Todeschini  
Chemometrics and Intelligent Laboratory Systems (2014), 138, 110-119
49. A novel variable reduction method adapted from space-filling designs  
D. Ballabio, V. Consonni, A. Mauri, M. Claeys-Bruno, M. Sergent, R. Todeschini  
Chemometrics and Intelligent Laboratory Systems (2014), 136, 147-154
48. Prediction of acute aquatic toxicity towards *daphnia magna* by using the GA-kNN method  
M. Cassotti, D. Ballabio, V. Consonni, A. Mauri, I. Tetko, R. Todeschini  
Alternatives to Laboratory Animals (2014), 42, 31-41
47. Assessing the validity of QSARs for ready biodegradability of chemicals: an Applicability Domain perspective  
F. Sahigara, D. Ballabio, R. Todeschini, V. Consonni  
Current Computer-Aided Drug Design (2014), 10, 137-147
46. QSPR study of rheological and mechanical properties of Chloroprene rubber accelerators  
R. Todeschini, V. Consonni, D. Ballabio, A. Mauri, M. Cassotti, S. Lee, A. West, D. Carlidge

Rubber Chemistry and Technology (2014), 87, 219-238

45. Oxygen consumption in South African Sauvignon blanc wines: role of glutathione, sulphur dioxide and certain phenolics

D. Fracassetti, C. Coetzee, A. Vanzo, D. Ballabio, W.J. du Toit  
South African Journal of Enology and Viticulture (2013), 34, 156-169

44. Classification tools in chemistry. Part 1: Linear models. PLS-DA

D. Ballabio, V. Consonni  
Analytical methods (2013), 5, 3790-3798

43. Locally-centred Mahalanobis distance: a new distance measure with salient features towards outlier detection

R. Todeschini, D. Ballabio, V. Consonni, F. Sahigara, P. Filzmoser  
Analytica Chimica Acta (2013), 787, 1-9

42. Defining a novel k-Nearest Neighbours approach to assess the applicability domain of a QSAR model for reliable predictions

F. Sahigara, D. Ballabio, R. Todeschini, V. Consonni  
Journal of Cheminformatics (2013), 5:27, 1-9

41. Quantitative Structure - Activity Relationship models for ready biodegradability of chemicals

K. Mansouri, T. Ringsted, D. Ballabio, R. Todeschini, V. Consonni  
Journal of Chemical Information and Modeling (2013), 53, 867-878

40. Particle size, chemical composition, seasons of the year and urban, rural or remote site origins as determinants of biological effects of particulate matter on pulmonary cells

M.G. Perrone, M. Gualtieri, V. Consonni, L. Ferrero, G. Sangiorgi, E. Longhin, D. Ballabio, E. Bolzacchini, M. Camatini  
Environmental Pollution (2013), 176, 215-227

39. Effects of supervised Self Organising Maps parameters on classification performance

D. Ballabio, M. Vasighi, P. Filzmoser  
Analytica Chimica Acta (2013), 765, 45-53

38. A MATLAB Toolbox for Self Organizing Maps and supervised neural network learning strategies

D. Ballabio, M. Vasighi  
Chemometrics and Intelligent Laboratory Systems (2012), 118, 24-32

37. Screening oil spills by mid-IR spectroscopy and supervised pattern recognition techniques

M.P. Gomez-Carracedo, R. Fernandez-Varela, D. Ballabio, J.M. Andrade  
Chemometrics and Intelligent Laboratory Systems (2012), 114, 132-142

36. Comparison of different approaches to define the Applicability Domain of QSAR models

F. Sahigara, K. Mansouri, D. Ballabio, A. Mauri, V. Consonni, R. Todeschini  
Molecules (2012), 17, 4791-4810

35. Chemometric analysis of gas chromatography with flame ionisation detection chromatograms: A novel method for classification of petroleum products

N.J. Nielsen, D. Ballabio, G. Tomasi, R. Todeschini, J.H. Christensen  
Journal of Chromatography A (2012), 1238, 121-127

34. Relationships between apple texture and rheological parameters by means of multivariate analysis

D. Ballabio, V. Consonni, F. Costa  
Chemometrics and Intelligent Laboratory Systems (2012), 111, 28-33

33. Monitoring of Alcoholic Fermentation using NIR and MIR Spectroscopy combined with Electronic Nose and Electronic Tongue

S. Buratti, D. Ballabio, G. Giovanelli, C.M. Zuluaga Dominguez, A. Moles, S. Benedetti, N. Sinelli  
Analytica Chimica Acta (2011), 697, 67-74

32. Genetic Algorithms for architecture optimisation of Counter-Propagation Artificial Neural Networks

D. Ballabio, M. Vasighi, V. Consonni, M. Kompany-Zareh  
Chemometrics and Intelligent Laboratory Systems (2011), 105, 56-64

31. Comparing roadsoils pollution patterns extracted by MOLMAP and classical 3-way



decomposition methods

M.P. Gomez-Carracedo, D. Ballabio, J.M. Andrade, J. Aires-de-Sousa, V. Consonni  
*Analytica Chimica Acta* (2010), 677, 64-71

30. Self Organizing Maps For Analysis Of Polycyclic Aromatic Hydrocarbons 3-Way Data From Spilled Oils

R. Fernandez-Varela, M.P. Gomez-Carracedo, D. Ballabio, J.M. Andrade, V. Consonni, R. Todeschini  
*Analytical Chemistry* (2010), 82, 4264-4271

29. A chemometric approach to the environmental problem of predicting toxicity in contaminated sediments

M. Alvarez-Guerra, D. Ballabio, J. M. Amigo, J. R. Viguri, R. Bro  
*Journal of Chemometrics* (2010), 24, 379-386

28. Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 3. Variable selection in classification.

D. Ballabio, V. Consonni, A. Mauri, R. Todeschini  
*Analytica Chimica Acta* (2010), 657, 116-122

27. Evaluation of model predictive ability by external validation techniques

V. Consonni, D. Ballabio, R. Todeschini  
*Journal of Chemometrics* (2010), 24, 104-201

26. Development of models for predicting toxicity from sediment chemistry by partial least squares-discriminant analysis and counter-propagation artificial neural networks

M. Alvarez-Guerra, D. Ballabio, J. M. Amigo, R. Bro, J. R. Viguri  
*Environmental Pollution* (2010), 158, 607-614

25. Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 2. Variable reduction.

V. Consonni, D. Ballabio, A. Manganaro, A. Mauri, R. Todeschini  
*Analytica Chimica Acta* (2009), 648, 45-51

24. Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 1. Theory and simple chemometric applications.

R. Todeschini, D. Ballabio, V. Consonni, A. Manganaro, A. Mauri  
*Analytica Chimica Acta* (2009), 648, 52-59

23. The Kohonen and CP-ANN toolbox: a collection of MATLAB modules for Self Organising Maps and Counterpropagation Artificial Neural Networks

D. Ballabio, V. Consonni, R. Todeschini  
*Chemometrics and Intelligent Laboratory Systems* (2009), 98, 115-122

22. Comments on the definition of the  $Q^2$  parameter for QSAR validation.

V. Consonni, D. Ballabio, R. Todeschini  
*Journal of Chemical Information and Modeling* (2009), 49, 1669-1678

21. Dairy cream response in instrumental texture evaluation processed by multivariate analysis

L. Piazza, J. Gigli, C. Rojas, D. Ballabio, R. Todeschini, P. Tripaldi  
*Chemometrics and Intelligent Laboratory Systems* (2009), 96, 258-263

20. Introduction to MOLE DB - on-line Molecular Descriptors Database

D. Ballabio, A. Manganaro, V. Consonni, A. Mauri, R. Todeschini  
*MATCH, communications in mathematical and in computer chemistry* (2009), 62, 199-207

19. Fatty acid composition of lipid classes in commercial breast muscle of capons as a marker of the dietary fat source

F. Carcione, L.M. Chiesa, D. Ballabio, S. Soncin, P.A. Biondi, P. Cattaneo, C. Cantoni  
*Italian Journal of Food Science* (2009), 21, 149-156

18. A new similarity/diversity measure for the characterization of DNA sequences

R. Todeschini, D. Ballabio, V. Consonni, A. Mauri  
*Croatica Chemica Acta* (2008), 81, 657-664

17. Classification of GC-MS measurements of wines by combining data dimension reduction and variable selection techniques

D. Ballabio, T. Skov, R. Leardi, R. Bro

Journal of Chemometrics (2008), 22, 457-463

16. Peptides multivariate characterisation using a molecular descriptor based approach  
A. Mauri, D. Ballabio, V. Consonni, A. Manganaro, R. Todeschini  
MATCH, communications in mathematical and in computer chemistry (2008), 60, 671-690
15. Multiblock Variance Partitioning. A new approach for comparing variation in multiple data blocks.  
T. Skov, D. Ballabio, R. Bro  
Analytica Chimica Acta (2008), 615, 18-29
14. Amperometric Electronic Tongue for Food Analysis  
M. Scampicchio, D. Ballabio, A. Arecchi, M.S. Cosio, S. Mannino  
Microchimica Acta (2008), 163, 11-21
13. Classification of multiway analytical data based on MOLMAP approach  
D. Ballabio, V. Consonni, R. Todeschini  
Analytica Chimica Acta (2007), 605, 134-146
12. Interactions between oral burn, meat flavour and texture in chili spiced pork patties evaluated by Time-Intensity  
H. C. Reinbach, L. Meinert, D. Ballabio, M. D. Aaslyng, W.L.P. Bredie, K. Olsen, P. Moller  
Food Quality and Preference (2007), 18, 909-919
11. Characterization of the traditional Cypriot spirit Zivania by means of Counterpropagation Artificial Neural Networks  
D. Ballabio, R. Kokkinofa, R. Todeschini, C. R. Theocharis  
Chemometrics and Intelligent Laboratory Systems (2007), 87, 78-84
10. On the Application of Chemometrics for the study of Acoustic-Mechanical properties of Crispy Bakery products  
L. Piazza, J. Gigli, D. Ballabio  
Chemometrics and Intelligent Laboratory Systems (2007), 86, 52-59
9. A new similarity/diversity measure for sequential data  
R. Todeschini, D. Ballabio, V. Consonni, A. Mauri  
MATCH, communications in mathematical and in computer chemistry (2007), 57, 51-67
8. CAIMAN (Classification And Influence Matrix Analysis): a new approach to the classification based on leverage-scaled functions  
R. Todeschini, D. Ballabio, V. Consonni, A. Mauri, M. Pavan  
Chemometrics and Intelligent Laboratory Systems (2007), 87, 3-17
7. Evaluation of different storage conditions of extra virgin olive oils with a innovative recognition tool built by means of electronic nose and electronic tongue  
M.S. Cosio, D. Ballabio, S. Benedetti, C. Gigliotti  
Food Chemistry (2007), 101, 485-491
6. Prediction of Italian red wine sensorial descriptors from electronic nose, electronic tongue and spectrophotometric measurements by means of Genetic Algorithms regression models  
S. Buratti, D. Ballabio, S. Benedetti, M.S. Cosio  
Food chemistry (2007), 100, 211-218
5. Characterization of DNA primary sequences by a new similarity/diversity measure based on the partial ordering  
R. Todeschini, V. Consonni, A. Mauri, D. Ballabio  
Journal of Chemical Information and Modeling (2006), 46, 1905-1911
4. A chemometric approach based on a novel similarity/diversity measure for the characterization and selection of electronic nose sensors  
D. Ballabio, M.S. Cosio, S. Mannino, R. Todeschini  
Analytica Chimica Acta (2006), 578, 170-177
3. Geographical classification of wine and olive oil by means of classification and influence matrix analysis (CAIMAN)  
D. Ballabio, A. Mauri, R. Todeschini, S. Buratti  
Analytica Chimica Acta (2006), 570, 249-258

2. Geographical origin and authentication of extra virgin olive oils by an electronic nose in combination with artificial neural networks.  
M.S. Cosio, D. Ballabio, S. Benedetti, C. Gigliotti  
*Analytica Chimica Acta* (2006), 567, 202-210

1. Classification of ancient Etruscan ceramics using statistical multivariate analysis of data  
P. Fermo, F. Cariati, D. Ballabio, V. Consonni, G. Bagnasco  
*Applied Physics A* (2004), 79, 299-307

#### **Book chapters:**

9. Distances and other dissimilarity measures in chemometrics

R. Todeschini, D. Ballabio, V. Consonni

in *Encyclopedia of Analytical Chemistry*, R.A. Meyers (ED) John Wiley & Sons, 2015

8. Enhancing chemical information in QSAR: Generalized Graph-Theoretical Matrices

V. Consonni, D. Ballabio, R. Todeschini

in *Novel Molecular Structure Descriptors - Theory and Applications II*, I. Gutman, B. Furtula (Eds.), University of Kragujevac and Faculty of Science Kragujevac, 2010, 21-55

7. Novel molecular descriptors based on functions of new vertex degrees

R. Todeschini, D. Ballabio, V. Consonni

in *Novel Molecular Structure Descriptors - Theory and Applications I*, I. Gutman, B. Furtula (Eds.), University of Kragujevac and Faculty of Science Kragujevac, 2010, 73-100

6. Applications of Selforganizing Maps to Address Environmental Studies

M.P. Gomez-Carracedo, D. Ballabio, J.M. Andrade, R. Fernandez-Varela, V. Consonni

in *Soft Computing Methods for practical Environmental solutions: techniques and studies*, M. Gestal, D. Rivero (EDs), IGI Global Publishers, 2010, 332-353

5. Geographical characterisation of olive oil by means of multivariate classification: application of CAIMAN

D. Ballabio, R. Todeschini

in *Olives and Olive Oil in Health and Disease Prevention*, V.R. Preedy, R.R. Watson (EDs), Elsevier, 2010, 129-137

4. The DART (Decision Analysis by Ranking Techniques) software

A. Manganaro, D. Ballabio, V. Consonni, A. Mauri, M. Pavan, R. Todeschini

in *Scientific Data Ranking Methods: Theory and Applications*, R. Todeschini, M. Pavan (EDs), Elsevier, 2008, 193-209

3. Multi-Criteria Decision Making (MCDM) Methods: A Tool for Assessing River Ecosystem Health using Functional Macroinvertebrate Traits

S. Canobbio, V. Mezzanotte, D. Ballabio, M. Pavan

in *Scientific Data Ranking Methods: Theory and Applications*, R. Todeschini, M. Pavan (EDs), Elsevier, 2008, 169-188

2. Similarity/diversity measure for sequential data based on Hasse matrices: Theory and applications

A. Mauri, D. Ballabio

in *Scientific Data Ranking Methods: Theory and Applications*, R. Todeschini, M. Pavan (EDs), Elsevier, 2008, 111-137

1. Multivariate Classification for Qualitative Analysis

D. Ballabio, R. Todeschini

in *Infrared Spectroscopy for Food Quality Analysis and Control*, Da-Wen Sun (ED), Elsevier, 2008, 83-104.

#### **Other papers:**

9. Prediction of Toxicity from Contaminated Sediments using PLS-DA and CP-ANN Models

M. Alvarez-Guerra, D. Ballabio, J.M. Amigo, R. Bro, J.R. Viguri

8th World Congress of Chemical Engineering, Abstract Book (2009) Abstract No. 699

8. 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  
*Alimentos, Ciencia e Ingenieria* (2007), 16, 113-115

7. Analisis multivariante de propiedades fisicas y quimicas de aceites y grasas vegetales del Ecuador

C. Rojas, J. Alvarado, D. Ballabio, R. Todeschini, P. Tripaldi  
*Alimentos, Ciencia e Ingenieria* (2007), 16, 38-40

6. Mapping of dairy cream shelf-life by means of mechanical measurements combined with multivariate analysis

L. Piazza, J. Gigli, C. Rojas, D. Ballabio, R. Todeschini, P. Tripaldi  
*Alimentos, Ciencia e Ingenieria* (2007), 16, 218-220.

5. Tecniche innovative combinate naso elettronico e lingua elettronica per la predizione di descrittori sensoriali di vini rossi secchi mediante uso degli Algoritmi Genetici

S. Buratti, S. Benedetti, D. Ballabio  
*Ingredienti Alimentari* (2006), 29, 6-9

4. Geographical characterization of extra virgin olive oils by electronic nose

M.S. Cosio, C. Gigliotti, D. Ballabio, S. Benedetti, S. Buratti  
7th congresso di scienza e tecnologia degli alimenti (ciseta), 19 September 2005, congress proceedings.

3. Multi-way analysis on sensory data: application on time-intensity evaluation of chilli spiced pork patties

D. Ballabio, A. Schiraldi  
10th Workshop on the developments in the Italian PhD Research in Food Science Technology, Foggia (Italy), 7-9 September 2005, workshop proceedings.

2. Gli indici di Desirability e Utility nel processo

D. Ballabio, C. Regazzoni, S. Mannino  
*ICP n11*, novembre 2004, 38-40

1. Oltre il Plug and Play: uso e abuso dell'ICT a supporto delle decisioni manageriali

D. Ballabio, M. Magni  
*Ticonzero*, web journal, 2005, num. 57

### **Posters:**

43. Non linear classification of commercial mexican tequilas

J.M. Andrade, D. Ballabio, M.P. Gómez Carracedo, G. Pérez-Caballero  
IX Colloquium Chemiometricum Mediterraneum, 27-30 June 2017, Arles (France)

42. Data fusion strategies for enhancing classification performance: a case study on cytochrome P450

S. Nembri, F. Grisoni, V. Consonni, D. Ballabio, R. Todeschini  
XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (Italy), 18-22 September 2016

41. A chemometric approach: quality assessment for foodstuffs using high-data fusion methods

M. Coppolino, M. Gandolfi, D. Ballabio, V. Consonni, R. Todeschini, E. Robotti, E. Marengo, F. Gosetti, M. Manfredi  
XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (Italy), 18-22 September 2016

40. A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods

R. Todeschini, D. Ballabio, V. Consonni, F. Grisoni,  
XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (Italy), 18-22 September 2016

39. Classification parameters: an extended multivariate comparison

D. Ballabio, F. Grisoni, V. Consonni, R. Todeschini  
XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (Italy), 18-22 September 2016

38. Exploiting the potential of molecular descriptors through data-fusion strategies: A case study

on Cytochrome P450

F. Grisoni, S. Nembri, V. Consonni, D. Ballabio, R. Todeschini  
21st European Symposium on Quantitative Structure-Activity Relationship (EuroQSAR 2016),  
Verona (Italy), 4-8 September 2016

37. Integration of QSAR ready biodegradability by means of qualitative consensus  
D. Ballabio, F. Biganzoli, R. Todeschini, V. Consonni,  
21st European Symposium on Quantitative Structure-Activity Relationship (EuroQSAR 2016),  
Verona (Italy), 4-8 September 2016

36. Impact of UV radiation and urban atmospheric aerosols in paint dosimeters over time using  
Principal Component Analysis  
A.Herrera, D. Ballabio, R. Todeschini, N. Navas, C. Cardell  
XVI Chemometrics in Analytical Chemistry (CAC 2016), Barcelona (Spain), 6-10 June 2016

35. Preliminary studies of ultraviolet radiation over time in paint mock-ups  
A. Herrera, F. Grisoni, D. Ballabio, R. Todeschini, N. Navas, C. Cardell  
2nd International Conference on Innovation in Art Research and Technology, Ghent (Belgium),  
21-25 March 2016

34. Principal component analysis of chromatic parameters measured on atmospheric aged paint  
dosimeters  
A. Herrera, D. Ballabio, R. Todeschini, N. Navas, C. Cardell  
2nd International Conference on Innovation in Art Research and Technology, Ghent (Belgium),  
21-25 March 2016

33. N3 and BNN: Two new similarity based classification methods in comparison with other  
classifiers.  
R. Todeschini, D. Ballabio, M. Cassotti, V. Consonni  
XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste  
(Italy), 13-17 September 2015

32. QSAR Study for Modelling the Sweetness and Bitterness Tastes  
C. Rojas, D. Ballabio, P.R. Duchowicz, R. Todeschini, P. Tripaldi  
Congress of Theoretical Chemists of Latin Expression (CHITEL2015), Torino (Italy), 26-31 July  
2015

31. Uso de relaciones diagnostico, biomarcadores y redes neurales de Kohonen de 3 vias para la  
monitorizacion de la evolution temporal de los vertidos de petroleo  
M.P. Gómez-Carracedo, R. Fernández-Varela, D. Ballabio, J.M. Andrade  
XX reunion de la Sociedad Espaniolan de Química Analitica, Santiago de Compostela (Spain), 1-3  
July 2015

30. A GC-MS based environmental metabolomics approach to detect oil hydrocarbon stress  
response of marine polychaetes  
R. Fernández-Varela, D. Ballabio, G. Tomasi, N.J. Nielsen, J. H. Christensen  
Metabolomics2014, Japan, 23-26 June 2014

29. Modelling of acute aquatic toxicity towards daphnia magna using GA-kNN method  
M. Cassotti, D. Ballabio, V. Consonni, A. Mauri, I. Tetko, R. Todeschini  
ECO conference, September 2013

28. A comparative study on different methods for applicability domain assessment  
V. Consonni, D. Ballabio, F. Sahigara, A. Mauri, M. Cassotti, F. Grisoni, R. Todeschini  
VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italy), 30 June - 4 July 2013

27. K-Contractive Map (K-CM) for classification  
M. Buscema, D. Ballabio, V. Consonni, M. Breda, G. Massini, L. Galli, M. Fabrizi, R. Todeschini  
VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italy), 30 June - 4 July 2013

26. Sviluppo di un metodo veloce, economico e non distruttivo per la quantificazione della  
componente ionica nel particolato atmosferico  
U. Molteni, D. Ballabio, P. Fermo, A. Piazzalunga  
XIV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, Rimini (Italy), 2-5 June  
2013

25. QSAR study on ready biodegradability of chemicals  
K. Mansouri, T. Ringsted, V. Consonni, D. Ballabio, R. Todeschini

3rd Strasbourg Summer School in Chemoinformatics, Strasbourg (France), 25-29 June 2012

24. Multi criteria variable selection for QSARs

K. Mansouri, D. Ballabio, V. Consonni, A. Mauri, R. Todeschini  
Euro QSAR 2012, Vienna (Austria), 26-30 August 2012

23. QSAR study on ready biodegradability of chemicals

K. Mansouri, T. Ringsted, V. Consonni, D. Ballabio, R. Todeschini  
Euroscience Open Forum 2012, Dublin (Ireland), 11-15 July 2012

22. 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

21. 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

20. 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

19. Comparison of approaches to define Applicability Domain for the application of QSAR models

F. Sahigara, K. Mansouri, D. Ballabio, V. Consonni, R. Todeschini  
SETAC Europe 21st Annual Meeting, Milan (Italy), 15-19 May 2011

18. 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

17. Use of Self Organizing Maps with polycyclic aromatic hydrocarbons 3-way data from spilled oils

R. Fernandez-Varela, M.P. Gomez-Carracedo, J.M. Andrade, D. Ballabio, V. Consonni, R. Todeschini  
7th Colloquium Chemiometricum Mediterraneum, Granada (Spain), 21-24 June 2010

16. Comparing different 3-way decomposition methods applied to roadsoils pollution

M.P. Gomez-Carracedo, D. Ballabio, J.M. Andrade, R. Fernandez-Varela, J. Aires-de-Sousa, R. Todeschini  
7th Colloquium Chemiometricum Mediterraneum, Granada (Spain), 21-24 June 2010

15. Regression and Classification QSAR Models for the prediction of Bioconcentration Factor in fish

E. Papa, M. Luini, P. Gramatica, V. Consonni, D. Ballabio, R. Todeschini  
SETAC Europe 20th Annual Meeting, Sevilla (Spain), 23-27 May 2010

14. 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

13. Analisis multivariante de propiedades físicas y químicas de aceites y grasas vegetales del Ecuador

C. Rojas, J. Alvarado, D. Ballabio, R. Todeschini, P. Tripaldi  
Ibero-American Congress in Food Engineering, Ambato (Ecuador), 5-8 November 2007

12. 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

11. Mapping of dairy cream shelf-life by means of mechanical measurements combined with multivariate analysis

L. Piazza, J. Gigli, C. Rojas, D. Ballabio, R. Todeschini, P. Tripaldi  
Ibero-American Congress in Food Engineering, Ambato (Ecuador), 5-8 November 2007

10. Novel XML-based Electronic Format for QSAR Models Exchange and Application  
A. Mangano, 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
9. Application of chemometrics to improve texture analysis: the case of the combined acoustic-mechanical measurements  
L. Piazza, R. Todeschini, J. Gigli, D. Ballabio.  
IUFoST 13th World Congress of Food Science and Technology, Nantes (France), 17-21 September 2006
8. Tecniche innovative ed analisi statistica multivariata per la autenticazione di oli extravergini di oliva DOP  
M.S. Cosio, D. Ballabio, S. Benedetti.  
Oli e Grassi Alimentari: innovazioni Tecnologiche e Ricerca Chimica, Bologna (Italy), 30 June 2006
7. Fatty Acid Composition in Broiler Meat as Marker of Traceability  
F. Carcione, L.M. Chiesa, D. Ballabio, C. Cattaneo, C. Cantoni, P.A. Biondi.  
29th international symposium on capillary chromatography, Riva del Garda (Italy), 29 May-2 June 2006
6. Time-Intensity evaluation of chilli spiced pork patties  
Helene C. Reinbach, Lene Lauridsen, Davide Ballabio, Margit D. Aaslyng, W.L.P. Bredie, Karsten Olsen, Per Moller  
LMC International Food Congress 2006, Copenhagen (Denmark), 15-16 March 2006
5. Multi-way analysis on sensory data: application on time-intensity evaluation of chilli spiced pork patties  
D. Ballabio, A. Schiraldi  
10th Workshop on the developments in the Italian PhD Research in Food Science Technology, Foggia (Italy), 7-9 September 2005
4. Application of the PARAFAC2 model on sensory data: Time-Intensity evaluation of meat taste and chilli burn  
D. Ballabio, A. Schiraldi  
Conferentia Chemometrica 2005 and Chemometrics VII, Hajduszoboszlo (Hungary), 28-31 August 2005
3. Comparison of several different fitness functions in regression models  
A. Mauri, D. Ballabio, V. Consonni, M. Pavan, R. Todeschini  
Colloquium Chemiometricum Mediterraneum, Ustica (Italy), 25-27 June 2003
2. Data mining by a partial ranking strategy (Hasse Diagram Techniques, HDT)  
M. Pavan, D. Ballabio, V. Consonni, A. Mauri, R. Todeschini  
Colloquium Chemiometricum Mediterraneum Ustica (Italy), 25-27 June 2003
1. Classification of ancient Etruscan ceramics using statistical multivariate analysis of data  
P. Fermo, F. Cariati, D. Ballabio, V. Consonni, G. Bagnasco  
MRS Spring Meeting 2003 Strasbourg, France, 10-13 June 2003

## Attended congresses and courses

### Oral presentation and lectures:

26. High-level data fusion: perspectives in QSAR and analytical applications  
IX Colloquium Chemiometricum Mediterraneum, 27-30 June 2017, Arles (France), invited lecture
25. Data integration to increase quality and reliability of QSAR predictions  
SETAC Europe 27th Annual Meeting, 7-11 May 2017, Bruxelles (Belgium)
24. Development of QSAR models to predict environmental and toxicological properties of chemicals  
Symposium on QSAR modelling, 9 March 2017, Copenhagen, (Denmark)
23. PCA toolbox for MATLAB  
Italian Chemometric workshop, 15-17 February 2017, Vietri sul mare (Italy)

22. High-level fusion methods to classify samples associated to multiple analytical sources  
XVI Chemometrics in Analytical Chemistry (CAC 2016), Barcelona (Spain), 6-10 June 2016
21. Recent advances in consensus modelling of multiple analytical chemical data  
XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste (Italy), 13-17 September 2015
20. A novel unsupervised method for reducing the dimensionality of large QSAR datasets  
16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014), Milan (Italy), 16-20 June 2014
19. Multivariate analysis applied to bioprocesses  
V International Congress of Industrial Microbiology, Bogotá (Colombia), 8-10 May 2013
18. How to build a predictive QSAR model  
ECO summer school, Verona (Italy), 11 June 2012
17. Kohonen and CP-ANN toolbox for MATLAB  
Italian Chemometric workshop, Albano laziale, Roma (Italy), 26-28 May 2011
16. Optimisation of neural network architectures by means of genetic algorithms  
XII Convegno della Divisione di Chimica Analitica della Società Chimica Italiana, Como (Italy), 13-16 September 2010
15. Optimisation of Counter-Propagation Artificial Neural Networks by means of genetic algorithms  
VII Colloquium Chemiometricum Mediterraneum, Granada (Spain), 21-24 June 2010
14. Principal component analysis (PCA), theory and examples  
Introductory course on multivariate analysis and quantitative structure - activity relationships (QSAR), Milan (Italy), 19 May 2009
13. Kohonen Maps and Counterpropagation Artificial Neural Networks Toolbox for MATLAB  
8th Iranian Workshop on Chemometrics, Zanjan (Iran), 7-9 February 2009, invited speaker
12. MOLMAP: chemometric strategy based on Kohonen Maps  
8th Iranian Workshop on Chemometrics, Zanjan (Iran), 7-9 February 2009, invited speaker
11. Introduction to the application of multivariate analysis in food science  
III Jornadas de Ciencia y Tecnología, Universidad del Azuay, Cuenca (Ecuador), 12 November 2008
10. Multivariate analysis applied to food science  
Segundo Congreso Ecuatoriano de Ingeniería en Alimentos, Loja (Ecuador), 5-7 November 2008, invited speaker
9. Chemometric application for the quality monitoring of rheological profiles: case study  
Italian Chemometric workshop, Pisa (Italy), 14-15 May 2008
8. Statistic tools for PQR (Product Quality Review)  
Product Quality Review, Milan (Italy), 4 March 2008
7. Moderne tecniche di analisi multivariata applicate ai processi alimentari - Multivariate Analysis and food processes (PAT)  
Metodi Analitici Rapidi per il Settore Agro Alimentare, Milan (Italy), 2 October 2007
6. Classification of multiway data based on the MOLMAP approach  
VI Colloquium Chemiometricum Mediterraneum, Saint-Maximin (France), 5-7 September 2007
5. Selection and characterisation of electronic nose sensors by means of Hasse distances  
Italian Chemometric workshop, Modena (Italy), 15-16 February 2007
4. Characterisation and selection of electronic nose sensors by means of Hasse distances  
Workshop on Ranking Methods and Multicriteria Decision Analysis in Environmental Sciences, Verbania (Italy), 2-3 October 2006
3. Chemometrics for the authentication and characterization of food products  
11th Workshop on the Developments in the Italian PhD Research on Food Science and Technology, Teramo (Italy), 27-29 September, 2006



2. Introduction to Chemometrics. Tools for multivariate analysis of chemical data  
Joint PAT Workshop, Pomezia (Italy), 6 April 2006

1. 3-way chemometric application on sensory data: the chilli flavoured meat balls experience  
Italian Chemometric workshop, Varenna (Italy), 26-27 May 2005

**Attended courses:**

21 June 2011  
Parallel computing in MATLAB and C code generation with MATLAB Coder, Milano (Italy)

19 May 2011  
Writing success full FP7 cooperation proposals, Milano (Italy)

6-8 September 2010  
School of Experimental Design, Genova (Italy)

13 May 2010  
ERC starting grant: becoming independent research leaders. A one-day training session, Milano (Italy)

6 September 2006  
Multivariate Image Analysis for Statistical Process Control, Copenhagen (Denmark)

1-3 April 2005  
ERCIM: European Consortium on Informatics and Mathematics - Working Group on Matrix Computations and Statistics, Sixth workshop, Copenhagen (Denmark)

14-17 February 2005  
PARVUS chemometric school, Genova (Italy)

10-25 January 2005  
Advanced Chemometrics/Multi-way analysis course - Copenhagen (Denmark)

29 June 2004  
Chemometric School - Introduction to methods of Experimental Design, Milano (Italy)

3- 5 March 2004  
II Italian School on Molecular Descriptors, Milano (Italy)

**Attended congresses:**

27-30 June 2017  
IX Colloquium Chemiometricum Mediterraneum, Arles (France)

7-11 May 2017  
SETAC Europe 27th Annual Meeting, Bruxelles (Belgium)

15-17 February 2017  
Italian Chemometric workshop, Vietri sul mare (Italy)

4-8 September 2016  
21st European Symposium on Quantitative Structure-Activity Relationship (EuroQSAR 2016), Verona (Italy)

6-10 June 2016  
XVI Chemometrics in Analytical Chemistry (CAC 2016), Barcelona (Spain)

13-17 September 2015  
XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste (Italy)

16-20 June 2014  
16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014), Milan (Italy)

30 June - 4 July 2013

VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italy) - member of the organizing committee

8-10 May 2013  
V International Congress of Industrial Microbiology, Bogotá (Colombia)

11-15 June 2012  
ECO summer school, Verona (Italy)

26-28 May 2011  
Italian Chemometric workshop, Albano laziale, Roma (Italy)

13-16 September 2010  
XII Convegno della Divisione di Chimica Analitica della Società Chimica Italiana, Como (Italy)

21-24 June 2010  
VII Colloquium Chemiometricum Mediterraneum, Granada (Spain)

7-9 February 2009  
8th Iranian Workshop on Chemometrics, Zanjan (Iran), invited speaker

5-7 November 2008  
Segundo Congreso Ecuatoriano de Ingenieria en Alimentos, Loja (Ecuador), invited speaker

10-13 June 2008  
MATH/CHEM/COMP 2008 Conference, Verbania (Italy) - member of the organizing committee

14-15 May 2008  
Italian Chemometric workshop, Pisa (Italy)

5-7 September 2007  
VI Colloquium Chemiometricum Mediterraneum, Saint-Maximin (France)

15-16 February 2007  
Italian Chemometric workshop, Modena (Italy)

2-4 October 2006  
Workshop on Ranking Methods and Multicriteria Decision Analysis in Environmental Sciences, Verbania (Italy)

27-29 September, 2006  
11th Workshop on the Developments in the Italian PhD Research in Food Science Technology, Teramo (Italy)

30 June 2006  
Oli e Grassi Alimentari: innovazioni Tecnologiche e Ricerca Chimica , Bologna (Italy)

7 March 2006  
La spettroscopia NIR e i prodotti alimentari (workshop), Milano (Italy)

7-9 September 2005  
10th Workshop on the developments in the Italian PhD Research in Food Science Technology, Foggia (Italy)

28-31 August 2005  
Conferentia Chemometrica 2005 and Chemometrics VII, Hajduszoboszlo (Hungary)

26-27 May 2005  
Italian Chemometric workshop, Varenna (Italy)

25-27 June 2003  
V Colloquium Chemiometricum Mediterraneum, Ustica (Italy)