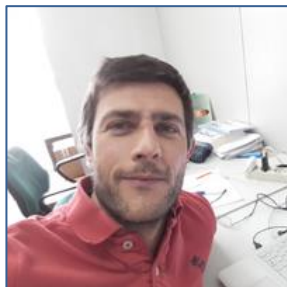


Davide Ballabio

associate professor in chemometrics, QSAR and analytical chemistry



CONTACT

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SOCIAL

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7749a43a

EDUCATION

PhD in food biotechnology

Università degli Studi di
Milano
2003 - 2006

Master Degree in Environmental Sciences

(110/110 cum laude)
Università degli Studi di
Milano-Bicocca
1996 - 2002

LANGUAGES

English: excellent spoken and
written

Spanish: basic spoken and
written

PROFILE

Davide Ballabio graduated in Environmental Sciences in 2002 and since then he has been working in chemometrics, analytical chemistry and Quantitative Structure Activity Relationship (QSAR). He is associate professor at the Milano Chemometrics and QSAR Research Group (Department of Earth and Environmental Science, University of Milano - Bicocca).

He is author of more than 70 peer reviewed papers and he has a continuative activity as referee for several international scientific journals. He has experience in multivariate data analysis (especially supervised classification) applied to both analytical and QSAR data; he also likes to code MATLAB toolboxes for the calculation of multivariate models and share them publicly.

PROFESSIONAL EXPERIENCES

Associate professor

September 2018 – now

Associate professor in chemometrics, QSAR and analytical chemistry at the Milano Chemometrics and QSAR Research Group (Department of Earth and Environmental Sciences, University of Milano - Bicocca).

Full researcher

September 2015 - August 2018

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).

Post-doc

March 2014 - February 2015

Post-doc grant by Reach and Colour Italia 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.

I was a solicitor in the property department dealing with a busy workload of residential conveyancing transactions. I also mentored new members of the firm joining the property department, acting as a go-to person.

EC project funding

January 2011 - February 2014

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.

Post-doc

January 2007 - December 2010

Post-doc grant (Milano Chemometrics and QSAR Research Group, University of Milano - Bicocca) for the development of an on-line database of molecular structures.

PhD

January 2004 - October 2006

PhD project in food biotechnology (University of Milano): Chemometric characterisation of physical-chemical fingerprints of food products.

Consultant for Tecnogalenica: calibration of NIR instruments by means of chemometrics.

INFORMATIC SKILLS

Statistical software:

Statistica, SPSS, MODDE, SIMCA, Unscramble and MATLAB.

Programming skills

MATLAB and Visual Basic.

Author of MATLAB toolboxes for multivariate analysis, available at:
<http://www.michem.unimib.it/>

Co-author of HYPER-Tools Free Graphical User Interface for Hyperspectral Image Analysis
<https://www.hypertools.org/>

Scientific consultant for Talete: chemometric consulting and collaboration in the realization of software of multivariate analysis.

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. Ongoing collaboration with Milano Chemometrics and QSAR Research Group (University of Milano - Bicocca) on researches related to multivariate statistical analysis and statistical software development.

Scholarship

January 2003 - December 2003

Scholarship (University of Milano - Bicocca) for the analysis of quality indices applicable on soils in Lombardia by means of multivariate analysis.

Stage

October 2002 - December 2002

Stage at Synergia S.r.l., consulting company specializing in workplace safety and environmental protection.

Scholarship

April 2002 - September 2002

Scholarship (University of Milano - Bicocca) for the evaluation, selection and development of softwares concerning didactical tests.

SCIENTIFIC PROJECTS and CONSULTANCIES

SafeRubber

Role in the project: research assistant. The SafeRubber project (ga 2-243756, founded by the European Community, Call: SME-2008) 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.

Environmental ChemOinformatics

Role in the project: research assistant, co-supervisor of long-term and short-term fellows. Environmental ChemOinformatic (ECO) Marie Curie Initial Training Network (ga 238701, founded by the European Community: Marie Curie Initial Training Networks, Call: FP7-PEOPLE-ITN-2008) was a collaborative action of 7 institutions from 5 EU countries to contribute to the education of environmental chemo-informaticians who will receive an advanced training in both environmental sciences and computational in silico methods.

Research activities and coordination in the following **scientific consultancies**:

- REACH&Colours Italia (2013-2016): QSAR software for the study of dyes properties
- Ruffino s.r.l. (2013-2017), chemical characterisation and advanced statistical tools for the geographical identification of red wines by ICP-MS elemental analysis.
- Athlon Car Lease Italy s.r.l. (2016), multivariate statistical models for the analysis of car price in relation to different marketing scenarios.
- Total Marketing Service France (2014-2015), QSPR to evaluate the relationships between molecular structure and lubrication properties of gasoil additives.
- ENI S.p.A. (2013), scientific consultancy and training course on the use of statistical modelling to characterize raw oils through analytical profiles.
- Demetra s.r.l. (2013), training course on statistic-mathematical methods for the analysis of electronic nose-detected chemical data.

TEACHING: PhD COURSES

Lecturer in the PhD course "Copenhagen School of Chemometrics"

Department of Food Science, Faculty of Life Sciences, University of Copenhagen

Module on classification methods: **May 2019 (14 hours)**, May 2018 (14 hours), May 2017 (14 hours), June 2015 (14 hours), July 2014 (28 hours), September 2013 (16 hours), November 2010 (12 hours)

Lecturer in the PhD course of Pharmaceutical Sciences

Department of Pharmaceutical Sciences, University of Milan

Module on Principal Component Analysis: May 2015 (6 hours)

TEACHING: MASTER and BACHELOR

Lecturer in the course of Instrumental Analytical Chemistry

Bachelor degree in chemical science and technology, University of Milano - Bicocca

October 2018 (14 hours), October 2017 (14 hours), October 2016 (14 hours)

Laboratory of Chemometrics

Master degree in chemical science and technology, University of Milano - Bicocca

January 2018 (12 hours), January 2017 (12 hours), December 2015 (12 hours), January 2014 (10 hours), January 2013 (24 hours)

Laboratory of Instrumental Analytical Chemistry

Bachelor degree in chemical science and technology, University of Milano - Bicocca

December 2017 (30 hours), December 2016 (36 hours), December 2015 (36 hours)

Laboratory of Analytical Chemistry

Bachelor degree in chemical science and technology, University of Milano - Bicocca

April 2018 (20 hours), April 2017 (24 hours), April 2016 (20 hours), April 2015 (20 hours), October 2013 (20 hours), October 2012 (24 hours), October 2009 (56 hours)

Bachelor degree in environmental science and technology, University of Milano - Bicocca

November 2017 (20 hours), November 2016 (20 hours), November 2015 (20 hours)

Lecturer in the course of Advanced Chemometrics

Master degree at the Department of Food Science, Faculty of Life Sciences, University of Copenhagen (Denmark)

Module on multivariate classification: December 2011 (7.5 ECTS)

Lecturer in the course of Multivariate Analysis

Master degree in industrial biotechnology, University of Milano - Bicocca

Module on multivariate classification: December 2014 (4 hours), November 2013 (8 hours), November 2012 (8 hours)

Lecturer in the course of Basics of Statistical and Multivariate Analysis

Bachelor Degree in Optics and Optometry, University of Milano - Bicocca

May 2014 (16 hours), April 2013 (18 hours)

TEACHING: SEMINARS and INVITED COURSES

NMR laboratory of the State General Laboratory (Nicosia, Cyprus)

June 2016

Seminar "Chemometric analysis for the evaluation of analytical data" at the State General Laboratory (Nicosia, Cyprus) and course "SIMCA for isotopic and analytical data regarding food and drink authenticity".

University of Azuay (Cuenca, Ecuador)

January 2016

Course (80 hours) on Chemometrics and QSAR applied to molecules of biological interest.

University of Bolzano (Italy)

May 2014

Seminar on multivariate analysis of isotopic data at the Department of Science and Technology.

Pontificia Universidad Javeriana (Bogota, Colombia)

May 2013

Seminar on Multivariate Analysis as a tool for the development and control of bioprocesses.

Pontificia Universidad Javeriana (Bogota, Colombia)

May 2013

Course of Multivariate Analysis applied to Microbiological data (12 hours).

Università degli Studi del Piemonte Orientale (Italy)

March 2012

Chemometrics and Experimental Design course (16 hours) at the Master in Materials for Energy and Environment.

University of Copenhagen (Denmark)

December 2011

Seminar on Classification methods in chemometrics at Department of Food Science, Faculty of Life Sciences.

National University of Colombia (Bogota, Colombia)

March 2011

Course on chemometrics (12 hours).

University of Milano - Bicocca

October 2010

Assistant in the training course on Experimental Design (32 hours) in the project Formulation and developing of new products in cosmetic companies.

National University of Colombia (Bogota, Colombia)

February 2010

Course on chemometrics (20 hours) in the framework of the project Selection of physical chemical indicators for cataloguing Colombian apicultural products.

University of Loja (Ecuador)

November 2008

Course on chemometrics and basic multivariate modelling (16 hours),

University of Cuenca (Ecuador)

October 2008

Course (30 hours) of advanced modelling and applications on environmental and technological problems (modelística superior aplicada a problemas tecnológicos y gestión ambiental) for the Master of technological management.

National University of Colombia (Bogotá, Colombia)

November 2006

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.

SUPERVISION PhD

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

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

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

SUPERVISION BACHELOR and MSc

Master degree in environmental sciences

Matteo Mastropiero, Multivariate analysis of environmental omics data for an untargeted freshwater quality alarm, University of Milano - Bicocca (Italy), October 2018

Cecile Valsecchi, Chemoinformatic protocol to search for relevant structural alerts of environmental interest, University of Milano - Bicocca (Italy), October 2017

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

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

Master degree in chemistry

Claudio Marchesi, Metodi chemiometrici per il pretrattamento e l'elaborazione multivariata di profili cromatografici per la valutazione della shelf-life di prodotti alimentari, University of Milano - Bicocca (Italy), October 2018

Chiara Arienti, Chemoinformatic approaches for the prediction of molecular toxicologic activity, University of Milano - Bicocca (Italy), July 2018

Mattia Coppolino, Study and application of chemometric "data fusion" techniques for the integration of chemical data, University of Milano - Bicocca (Italy), September 2017

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

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

Bachelor degree in chemistry

Emanuele Baffi, Taratura di spettrometro ottico per la determinazione del bario in matrice di piombo e caratterizzazione di un sottoprodotto del ciclo produttivo del piombo, University of Milano - Bicocca (Italy), September 2018

Erika Colombo, Characterisation of pollen with vibrational spectroscopy and chemometrics, University of Milano - Bicocca (Italy), July 2018

Maria Cairolì, Evaluation of NIR data pretreatment for the characterisation of pharmaceutical tablets, University of Milano - Bicocca (Italy), July 2018

Giorgia Conti, Acque destinate al consumo umano. Analisi dei microinquinanti emergenti: screening mediante HPLC-HRMS di composti farmaceutici persistenti, University of Milano - Bicocca (Italy), March 2018

Mattia Pagnoncelli, Determinazione di azoto totale in acque reflue e scarichi industriali: confronto tra ossidazione catalitica ad alta temperatura e metodo ossidativo con persolfato, University of Milano - Bicocca (Italy), November 2017

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

Advisor activities

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

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

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

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:

73. On the Misleading Use of Q2F3 for QSAR Model Comparison
V. Consonni, R. Todeschini, D. Ballabio, F. Grisoni
Molecular Informatics (2018), in press
72. Structural alerts for the identification of bioaccumulative compounds
C. Valsecchi, F. Grisoni, V. Consonni, D. Ballabio
Integrated Environmental Assessment and Management (2018), in press
71. Chemical profiling and multivariate data fusion methods for the identification of the botanical origin of honey
D. Ballabio, E. Robotti, F. Grisoni, F. Quasso, M. Bobba, S. Vercelli, F. Gosetti, G. Calabrese, E. Sangiorgi, M. Orlandi, E. Marengo
Food Chemistry (2018), 266, 79-89
70. Mapping of Activity through Dichotomic Scores (MADS): a new chemoinformatic approach to detect activity-rich structural regions.
R. Todeschini, V. Consonni, D. Ballabio, F. Grisoni
Journal of Chemometrics (2018), 32, e2994
69. Multivariate comparison of classification performance measures
D. Ballabio, F. Grisoni, R. Todeschini
Chemometrics and Intelligent Laboratory Systems (2018), 174, 33-44
68. Nonlinear classification of commercial Mexican tequilas.
J.M. Andrade, D. Ballabio, M.P. Gómez-Carracedo, G. Pérez-Caballero
Journal of Chemometrics (2017), 31, e2939
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 Q2! 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. Cartlidge
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 Q2 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:

10. Molecular Descriptors for Structure–Activity Applications: A Hands-On Approach
F. Grisoni, V. Consonni, D. Ballabio, R. Todeschini

in Computational Toxicology. Methods in Molecular Biology, O. Nicolotti (eds), vol 1800. Humana Press, New York, NY

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

ORAL PRESENTATIONS AND POSTERS AT CONGRESSES

Oral presentation and lectures:

28. Multivariate classification of chianti red wines based on massive sampling and ICP-MS element composition
D. Ballabio, B. Bronzi, C. Brilli, G.M. Beone, M.C. Fontanella, R. Todeschini, V. Consonni
XXVII Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Bologna (Italy), 16 -20 September 2018
27. QSAR models to predict properties of dyes for regulatory use
D. Ballabio, V. Consonni, A. Mauri, V. Alberti, M. Locatelli, R. Todeschini
QSAR 2018, 11-15 June 2018, Bled (Slovenia)
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), invited lecture

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

Posters

46. QSAR models to predict Acute Oral Systemic Toxicity

C. Arienti, C. Valsecchi, V. Consonni, R. Todeschini, D. Ballabio
QSAR 2018, 11-15 June 2018, Bled (Slovenia)

45. Structural alerts for the identification of bioaccumulative compounds

C. Valsecchi, F. Grisoni, V. Consonni, R. Todeschini, D. Ballabio
QSAR 2018, 11-15 June 2018, Bled (Slovenia)

44. A Dynamic MOLMAP approach for pattern classification in three-way data

M. Vasighi, M. Talebi, D. Ballabio
6th Iranian Joint Congress on Fuzzy and Intelligent Systems, 28 February-2 March 2018, Kerman (Iran)

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 diagnóstico, biomarcadores y redes neurales de Kohonen de 3 vías para la monitorización de la evolución temporal de los vertidos de petróleo

M.P. Gómez-Carracedo, R. Fernández-Varela, D. Ballabio, J.M. Andrade
XX reunion de la Sociedad Espaniolan de Quimica 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. 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
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:

- 16 -20 September 2018
XXVII Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Bologna (Italy)
- 11-15 June 2018
QSAR 2018, Bled (Slovenia)
- 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 Ingeniería 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)

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

Il Italian School on Molecular Descriptors, Milano (Italy)