Davide Ballabio

associate professor in chemometrics, QSAR and analytical chemistry

CONTACT

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SOCIAL

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RESEARCH ID

Orcid ID:
0000-0002-5748-147X
Scopus Author ID:
13408766700
WoS Researcher ID:
B-7470-2014

EDUCATION

PhD in food biotechnology
Università degli Studi di Milano
2003 - 2006

Master Degree in Environmental Sciences
(110/110 cum laude)

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 90 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).

Since March 2020, member of the board of the Ph.D. Course in Chemical, Geological and Environmental Sciences. Since June 2020, coordinator of the chemical curriculum of the PhD course.

Since January 2020, member of the scientific and didactical council of the University of Milano-Bicocca unit for the inter-university center for the replacement, reduction and refinement of animal testing (3R)

Since November 2019, member of the research quality committee at the Department of Earth and Environmental Science, University of Milano - Bicocca.

Since February 2019, member of the board of the Gruppo divisionale di Chemiometria della Divisione di Chimica Analitica della Società Chimica Italiana.

Since November 2018, member of the Council of the Department of Earth and Environmental Science, University of Milano - Bicocca.

Since October 2018, quality insurer at the Bachelor degree in chemical science and technology, 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.

EC project funding

Università degli Studi di Milano-Bicocca
1996 – 2002

LANGUAGES

English: excellent spoken and written
Spanish: basic spoken and written

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 Graphical User Interface for Hyperspectral Image Analysis
https://www.hypertools.org/

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.
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 "Machine learning for multivariate data analysis"
Department of Earth and Environmental Sciences, University of Milano-Bicocca
July 2020 (16 hours)

Lecturer in the PhD course "International School of Chemometrics"
University of Bilbao and Copenhagen
Module on classification methods: October 2020 (14 hours)

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 Chemical Sciences
Department of Pharmaceutical Sciences, University of Milan
Module on Principal Component Analysis: July 2019 (1 hour)

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 Analytical Chemistry
Bachelor degree in chemical science and technology, University of Milano - Bicocca
March-May 2021 (35 hours), March-May 2020 (35 hours)

Lecturer in the course of Analytical Methods for the Formulation Chemistry
Master degree in chemical science and technology, University of Milano - Bicocca
March-May 2021 (48 hours)

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 2021 (12 hours), January 2020 (12 hours), January 2019 (12 hours), 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 2018 (30 hours), 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 2021 (32 hours), April 2020 (40 hours), April 2019 (52 hours), 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 2019 (20 hours), November 2018 (20 hours), 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

IV Winter School of Chemometrics
August 2019
Course on multivariate classification at the IV Winter School of Chemometrics Universidade Federal do Rio Grande do Sul (Porto Alegre, Brasil)

Winter School (combining NIR spectroscopy and Chemometrics)
January 2019
Course on multivariate classification in the framework of NIR spectroscopy (Univeristà degli Studi di Milano).

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 (modelistica superior aplicada a problemas tecnologicos y gestion 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

Supervisor:
Giacomo Baccolo, Integration of omics-data based on advanced chemometric approaches. PhD in chemistry, University of Milano-Bicocca / University of Copenhagen, to be discussed on 2022

Cecile Valsecchi, Novel machine learning approaches to detect nuclear receptors modulators. PhD in chemistry, University of Milano-Bicocca, to be discussed on 2022

Co-supervisor:
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

External reviewer:
Giorgia Orlandi, Development of Multivariate Image Analysis Methods for Food Colour Characterization. University of Modena and Reggio Emilia, 2019

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

SUPERVISION BACHELOR and MSc

Master degree in environmental sciences
Matteo Mastropierro, 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
Francesca Gritti, Sviluppo, ottimizzazione e convalida di un metodo analitico per la determinazione di impurezze di NDMA in ranitidina, University of Milano - Bicocca (Italy), September 2020

Pietro Bertani, A multivariate approach at the thermodynamic properties of polyamino polycarboxylic complexes with paramagnetic and other endogenous metal ions, University of Milano - Bicocca (Italy), September 2020

Magda Collarile, Multi-target qsar models to predict nuclear receptor modulation, University of Milano - Bicocca (Italy), July 2020

Genny Cau, In silico modelling for androgen and estrogen disrupting potential of chemicals, University of Milano - Bicocca (Italy), March 2019, (Erasmus at Helmholtz Zentrum München)

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 releated 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
Giovanni Caccamo, Sviluppo di metodi analitici per l'estrazione di composti organici da matrici polimeriche e da poli(ossido di 2,6 difenil-p-fenilene), University of Milano - Bicocca (Italy), November 2019

Davide Boldini, Development of a chemometric algorithm for classification of stains via spectroscopic approaches, University of Milano - Bicocca (Italy), September 2019

Carlo Gariboldi, Development of a chemometric data fusion model for predicting quality parameters of micellar solutions, University of Milano - Bicocca (Italy), September 2019

Martina Basili, Studio delle interferenze derivanti dalla matrice e dalla procedura preparativa per l'analisi di campioni ambientali mediante tecnica ICP-OES, University of Milano - Bicocca (Italy), September 2019

Federica Porta, Sviluppo di metodiche spettroscopiche IR per l'analisi di microplastiche in ambiente marino, University of Milano - Bicocca (Italy), September 2019

Gianluca Beretta, Analisi dei parametri di qualità di prodotti esistenti, denominati masterbatch bianchi, nel trasferimento delle produzioni da una linea standard ad un nuovo impianto ad alta automazione, University of Milano - Bicocca (Italy), February 2019

Lorenzo Guaita, Caratterizzazione reologica di poliammide 6.6, University of Milano - Bicocca (Italy), February 2019

Alessio Minghinelli, Sviluppo di metodiche analitiche mediante GCMS per la determinazione di parametri non tabellati del D.LGS. 152/06, University of Milano - Bicocca (Italy), February 2019

Emanuele Baffi, Taratura di quantometro 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 Cairoli, 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

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

PARTECIPATION TO SCIENTIFIC COMMITTEE

The International Conference on Contemporary Issues in Data Science, 5-8 March 2019, Zanjan (Iran)

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:

87. NURA: a curated dataset of nuclear receptor modulators
C. Valsecchi, F. Grisoni, S. Motta, L. Bonati, D. Ballabio
Toxicology and Applied Pharmacology (2020), accepted for publication

86. Traceability of soybeans produced in Argentina based on their trace element profiles
M.J. Hidalgo, D.C. Fechner, D. Ballabio, E.J. Marchevsky, R.G. Pelleran
Journal of Chemometrics (2020), accepted for publication

85. Diabetes mellitus type 2: Exploratory data analysis based on clinical reading
M. Nedyalkova, S. Madurga, D. Ballabio, R. Robeva, J. Romanova, I. Kichev, A. Elenkova, V. Simeonov
Open chemistry (2020), 18, 1041–1053

84. Self-Organizing Map and Relational Perspective Mapping for the Accurate Visualization of High-Dimensional Hyperspectral Data
W. Gardner, R. Maliki, S.M. Cutts, B.W. Muir, D. Ballabio, D.A. Winkler, P.J. Pigram
Analytical Chemistry (2020), 92, 10450–10459

83. Deep Ranking Analysis by Power Eigenvectors (DRAPE): a polypharmacology case study
C. Valsecchi, D. Ballabio, V. Consonni, R. Todeschini
Chemometrics and Intelligent Laboratory Systems (2020), 203, 104001

82. ToF-SIMS and Machine Learning for Single-Pixel Molecular Discrimination of an Acrylate Polymer Microarray
W. Gardner, A.L. Hook, M.R. Alexander, D. Ballabio, S.M. Cutts, B.W. Muir, P.J. Pigram
Analytical Chemistry (2020), 92, 6587-6597

81. Consensus versus individual QSARs in classification: comparison on a large-scale case study
C. Valsecchi, F. Grisoni, V. Consonni, D. Ballabio
Journal of chemical information and modelling (2020), 60, 1215-1223

80. CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity
K. Mansouri, N. Kleinstreuer, A.M. Abdelaziz, D. Alberga, V. Alves, P. Andersson, C. Andrade, F. Bai, I. Balabin, D. Ballabio, E. Benfenati, B. Bhhatarai, S. Boyer, J. Chen, V. Consonni, S. Farag, D. Fourches, A.T. García-Sosa, P. Gramatica, F. Grisoni, C.M. Grulke, H. Hong, D. Horvath, X. Hu, R. Huang, N. Jeliazkova, J. Li, X. Li, H. Liu, S. Manganelli, G.F. Mangiatordi, U. Maran, G. Marcou, T. Martin, E. Muratov, D. Nguyen, O. Nicolotti, N.G. Nikolov, U. Norinder, E. Papa, M. Petitjean, G. Piir, P. Pogodin, V. Poroikov, X. Qiao, A.M. Richard, A. Roncaglioni, P. Ruiz, C. Rupakheti, S. Sakkiah, A. Sangion, K. Schramm, C. Selvaraj, I. Shah, S. Sild, L. Sun, O. Taboureau, Y. Tang, I.V. Tetko, R. Todeschini, W. Tong, D. Trisciuzzi, A. Tropsha, G. Van Den Driessche, A. Varnek, Z. Wang, E.B. Wedebye, A.J. Williams, H. Xie, A.V. Zakharov, Z. Zheng, R.S. Judson
Environmental Health Perspectives (2020), 128, 2

79: Geographical identification of Chianti red wine based on ICP-MS element composition
B. Bronzi, C. Brilli, G.M. Beone, M.C. Fontanella, D. Ballabio, R. Todeschini, V. Consonni, F. Grisoni, F. Parri, M. Buscema
Food chemistry (2020), 315, 126248

78. Integrated QSAR models to predict acute oral systemic toxicity
D. Ballabio, F. Grisoni, V. Consonni, R. Todeschini
Molecular Informatics (2019), 38, 1800124

77. Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making
R. Todeschini, F. Grisoni, D. Ballabio
Chemometrics and Intelligent Laboratory Systems (2019), 191, 129-137

76: Machine Learning Consensus to Predict the Binding to the Androgen Receptor within the CoMPARA project.
F. Grisoni, V. Consonni, D. Ballabio
Journal of chemical information and modelling (2019), 59, 1839–1848

75. Capsaicinoids in chili habanero by flow injection with coulometric array detection
K. Morozova, I. Rodríguez-Buenfil, C. López-Domínguez, M. Ramírez-Sucre, D. Ballabio, M. Scampicchio

Electroanalysis (2019), 31, 844-850

74. On the misleading use of Q2F3 for QSAR model comparison
V. Consonni, R. Todeschini, D. Ballabio, F. Grisoni
Molecular Informatics (2019), 38, 1800029

73. Structural alerts for the identification of bioaccumulative compounds
C. Valsecchi, F. Grisoni, V. Consonni, D. Ballabio
Integrated Environmental Assessment and Management (2019), 15, 19-28

72. Classification-based QSAR models for the prediction of the bioactivity of ACE-inhibitor peptides
P. Tripaldi, A. Pérez-González, C. Rojas, J. Radax, D. Ballabio, R. Todeschini
Protein & Peptide Letters (2018), 25, 1015-1023

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
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M. Cassotti, D. Ballabio, R. Todeschini, V. Consonni
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M.P. Gómez-Carracedo, J.M. Andrade, D. Ballabio, D. Prada-Rodríguez, S. Muniategui-Lorenzo, V. Consonni, M. Piñeiro-Iglesias, P. López-Mahía
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S. Chavan, I. Nicholls, B. Karlsson, A. Rosengren, D. Ballabio, V. Consonni, R. Todeschini
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M. Cassotti, V. Consonni, A. Mauri, D. Ballabio
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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

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D. Ballabio, V. Consonni, A. Mauri, M. Claeys-Bruno, M. Sergent, R. Todeschini
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M. Cassotti, D. Ballabio, V. Consonni, A. Mauri, I. Tetko, R. Todeschini
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F. Sahigara, D. Ballabio, R. Todeschini, V. Consonni
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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
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D. Ballabio, V. Consonni
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R. Todeschini, D. Ballabio, V. Consonni, F. Sahigara, P. Filzmoser
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F. Sahigara, D. Ballabio, R. Todeschini, V. Consonni
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41. Quantitative Structure - Activity Relationship models for ready biodegradability of chemicals
K. Mansouri, T. Ringsted, D. Ballabio, R. Todeschini, V. Consonni
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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
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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
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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

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F. Sahigara, K. Mansouri, D. Ballabio, A. Mauri, V. Consonni, R. Todeschini
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N.J. Nielsen, D. Ballabio, G. Tomasi, R. Todeschini, J.H. Christensen
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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
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R. Fernandez-Varela, M.P. Gomez-Carracedo, D. Ballabio, J.M. Andrade, V. Consonni, R. Todeschini
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M. Alvarez-Guerra, D. Ballabio, J. M. Amigo, J. R. Viguri, R. Bro
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V. Consonni, D. Ballabio, R. Todeschini
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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
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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

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D. Ballabio, V. Consonni, R. Todeschini
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22. Comments on the definition of the Q2 parameter for QSAR validation.
V. Consonni, D. Ballabio, R. Todeschini
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L. Piazza, J. Gigli, C. Rojas, D. Ballabio, R. Todeschini, P. Tripaldi
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D. Ballabio, A. Manganaro, V. Consonni, A. Mauri, R. Todeschini
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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
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18. A new similarity/diversity measure for the characterization of DNA sequences
R. Todeschini, D. Ballabio, V. Consonni, A. Mauri
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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
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16. Peptides multivariate characterisation using a molecular descriptor based approach
A. Mauri, D. Ballabio, V. Consonni, A. Manganaro, R. Todeschini
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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
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13. Classification of multiway analytical data based on MOLMAP approach
D. Ballabio, V. Consonni, R. Todeschini
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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
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11. Characterization of the traditional Cypriot spirit Zivania by means of Counterpropagation Artificial Neural Networks
D. Ballabio, R. Kokkinofta, R. Todeschini, C. R. Theocharis
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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
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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
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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
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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
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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
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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
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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
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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
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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:

13. Chemometrics for QSAR Modeling

R. Todeschini, V. Consonni, D. Ballabio, F. Grisoni
in Comprehensive Chemometrics (Second Edition), S. Brown, R. Tauler, B. Walczak (Eds.), Elsevier, 2020

12. Distances and Similarity Measures in Chemometrics and Chemoinformatics
R. Todeschini, D. Ballabio, V. Consonni
in Encyclopedia of Analytical Chemistry, R.A. Meyers (Ed.), Wiley, 2020

11. Recent advances in High-Level Fusion Methods to classify multiple analytical chemical data
D. Ballabio, R. Todeschini, V. Consonni
in Data Fusion Methodology and Applications, M. Cocchi (eds.), vol 31, Elsevier, Netherlands, 2019

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, 2018

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.

ORAL PRESENTATIONS AND POSTERS AT CONGRESSES

Oral presentation and lectures:

29. Consensus prediction of Androgen receptor activity within the CoMPARA project
D. Ballabio, C. Valsecchi, F. Grisoni, V. Consonni, K. Mansouri, R. Todeschini
IX Colloquium Chemiometricum Mediterraneum, 12 -14 June 2019, Menorca (Spain)

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, Bogotà (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
Introductive 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 Cienca y Tecnologia, Univesidad del Azuay, Cuenca (Ecuador), 12 November 2008

10. Multivariate analysis applied to food science
Segundo Congreso Ecuatoriano de Ingenieria 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 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 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. Ballabioa, 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 fisicas y quimicas 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