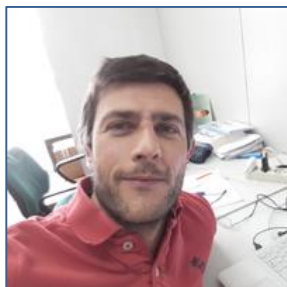


Davide Ballabio

associate professor in chemometrics, QSAR and analytical chemistry



CONTACT

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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)

Università degli Studi di
Milano-Bicocca

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).

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

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.

1996 – 2002

LANGUAGES

English: excellent spoken and written

Spanish: basic spoken

INFORMATIC SKILLS

Programming skills

Python and MATLAB

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/>

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.

ACADEMIC INSTITUTIONAL OFFICES

December 2021 - now

Member of the *Commissione revisione offerta formativa* at the degree in chemical science and technology, University of Milano - Bicocca.

September 2021 - now

Member of the departmental "*commissione paritetica*" at the Department of Earth and Environmental Science, University of Milano - Bicocca.

February 2021 - now

Vice coordinator of the Ph.D. Course in Chemical, Geological and Environmental Sciences at the University of Milano - Bicocca.

June 2020 - now

Coordinator of the chemical curriculum of the Ph.D. Course in Chemical, Geological and Environmental Sciences at the University of Milano - Bicocca.

March 2020 - now

Member of the board of the Ph.D. Course in Chemical, Geological and Environmental Sciences at the University of Milano - Bicocca.

January 2020 - now

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)

November 2019 - now

Member of the research quality committee at the Department of Earth and Environmental Science, University of Milano - Bicocca.

February 2019 - now

Member of the board of the Gruppo divisionale di Chemiometria della Divisione di Chimica Analitica della Società Chimica Italiana.

November 2018 - now

Member of the Council (*giunta*) of the Department of Earth and Environmental Science, University of Milano - Bicocca.

October 2018 - January 2022

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 2021 (16 hours), July 2020 (16 hours)

Lecturer in the PhD course "International School of Chemometrics"

University of Bilbao and Copenhagen
Module on classification methods: June 2021 (14 hours), 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 "The principles of 3Rs in biomedical studies"

School of Medicine and Surgery, University of Milano-Bicocca
Module on Development of QSAR in silico models for the studies on the relationship between structure and molecular properties: June 2021 (2 hour)

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
October-November 2021 (30 hours), October-November 2020 (30 hours), 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

Winter School (combining NIR spectroscopy and Chemometrics)

January 2022

Course on multivariate classification and regression in the framework of NIR spectroscopy (SISNIR).

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 chemistry

Martina Barbagallo, Development and validation of deep-learning strategies for the prediction of the molecular structure by LC-MS/MS spectra, University of Milano - Bicocca (Italy), November 2021

Leonardo Fedrigotti, Experimental Design and Chemometrics for innovative formulation of fragrance in Fast Moving Consumer Goods, University of Milano - Bicocca (Italy), November 2021

Davide Crucitti, Consensus based Multi-Target classification of drugs interaction with P-glycoprotein, University of Milano - Bicocca (Italy), November 2021

Martina Caserta, Enhancing compound identification: application of deep learning to predict molecular structures from mass spectra, University of Milano - Bicocca (Italy), July 2021

Maria Cairoli, Multicolor flow cytometry and chemometrics for understanding the effects of prolonged physical exercise on the human innate immune system, University of Milano - Bicocca (Italy), February 2021

Erika Colombo, NMR spectroscopy and chemometric methods applied to heparin: detection of contaminants and comparison of production sites, University of Milano - Bicocca (Italy), February 2021

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 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

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

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

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

Cristian Rojas Villa, Aplicación del aprendizaje automático para la predicción del gusto de moléculas orgánicas, Universidad Nacional de Córdoba, November 2021

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

Young researcher forum on sustainable biomass and climate change, 19-22 October 2021, Milan (Italy)

Chemometrics Open Day - La Chemiometria oggi: un confronto aperto, 16 June 2021, on line workshop

CHEMINFOICD3-03: Chemoinformatics North Carolina Workshop Series and International Conference on Drug Design & Discovery 2021, on-line event, Bilbao, Spain-München, Germany-Chapell Hill, Durham, USA

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:

97. NMR spectroscopy and chemometric models to detect a specific non-porcine ruminant contaminant in pharmaceutical heparin

E. Colombo, L. Mauri, M. Marinozzi, T. R. Rudd, E.A. Yates, D. Ballabio, M. Guerrini

Journal of Pharmaceutical and Biomedical Analysis (2022), 214, 114724

96. ChemTastesDB: A Curated Database of Molecular Tastants

C. Rojas, D. Ballabio, K. Pacheco Sarmiento, E. Pacheco Jaramillo, M. Mendoza, F. Garcia

Food Chemistry: Molecular Sciences (2022), 4, 100090

95. Predicting molecular activity on nuclear receptors by multitask neural networks

C. Valsecchi, M. Collarile, F. Grisoni, R. Todeschini, D. Ballabio, V. Consonni

Journal of Chemometrics (2022), 36, e3325

94. Expanding antineoplastic drugs surface monitoring profiles: enhancing of zwitterionic hydrophilic interaction methods
S. Dugheri, N. Mucci, D. Squillaci, E. Bucaletti, G. Cappelli, L. Trevisani, C. Valsecchi, V. Consonni, F. Gosetti, D. Ballabio, G. Arcangeli
Separations (2022), 9, 34
93. Evaluation of the predictivity of Acute Oral Toxicity (AOT) structure-activity relationship models
K. Gromek, W. Hawkins, Z. Dunn, M. Gawlik, D. Ballabio
Regulatory Toxicology and Pharmacology (2022), 129, 105109
92. Parsimonious optimization of multitask neural network hyperparameters
C. Valsecchi, V. Consonni, R. Todeschini, M. Orlandi, F. Gosetti, D. Ballabio,
Molecules (2021), 26, 7254
91. A MATLAB toolbox for multivariate regression coupled with variable selection
V. Consonni, G. Baccolo, F. Gosetti, R. Todeschini, D. Ballabio
Chemometrics and Intelligent Laboratory Systems (2021), 213, 104313
90. CATMoS: Collaborative Acute Toxicity Modeling Suite
K. Mansouri, A.L. Karmaus, J. Fitzpatrick, G. Patlewicz, P. Pradeep, D. Alberga, N. Alepee, E.H. Allen, D. Allen, V.M. Alves, C.H. Andrade, T.R. Auernhammer, D. Ballabio, S. Bell, E. Benfenati, S. Bhattacharya, J.V. Bastos, S. Boyd, J.B. Brown, S.J. Capuzzi, Y. Chushak, H. Ciallella, A.M. Clark, V. Consonni, P.R. Daga, S. Ekins, S. Farag, M. Fedorov, D. Fourches, D. Gadaleta, F. Gao, J.M. Gearhart, G. Goh, J.M. Goodman, F. Grisoni, C.M. Grulke, T. Hartung, M. Hirn, P. Karpov, A. Korotcov, G.J. Lavado, M. Lawless, X. Li, T. Luechtefeld, F. Lunghini, G.F. Mangiatordi, G. Marcou, D. Marsh, T. Martin, A. Mauri, E.N. Muratov, G.J. Myatt, D. Nguyen, O. Nicolotti, R. Note, P. Pande, A.K. Parks, T. Peryea, A.H. Polash, R. Rallo, A. Roncaglioni, C. Rowlands, P. Ruiz, D.P. Russo, A. Sayed, R. Sayre, T. Sheils, C. Siegel, A.C. Silva, A. Simeonov, S. Sosnin, N. Southall, J. Strickland, Y. Tang, B. Teppen, I.V. Tetko, D. Thomas, V. Tkachenko, R. Todeschini, C. Toma, I. Tripodi, D. Trisciuzzi, A. Tropsha, A. Varnek, K. Vukovic, Z. Wang, L. Wang, K.M. Waters, A.J. Wedlake, S.J. Wijeyesakere, D. Wilson, Z. Xiao, H. Yang, G. Zahoranszky-Kohalmi, A.V. Zakharov, F.F. Zhang, Z. Zhang, T. Zhao, H. Zhu, K.M. Zorn, W. Casey, N.C. Kleinstreuer
Environmental Health Perspectives (2021), 129, 47013
89. Application of DNA mini-barcoding and infrared spectroscopy for the authentication of the Italian product "*bottarga*"
J. Frigerio, C. Marchesi, C. Magoni, F. Saliu, D. Ballabio, V. Consonni, T. Gorini, F. De Mattia, P. Galli, M. Labra
LWT - Food Science and Technology (2021), 139, 110603
88. 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. Pellerano
Journal of Chemometrics (2020), 34, e3252
87. Analyzing 3D Hyperspectral ToF-SIMS Depth Profile Data Using Self-Organizing Map-Relational Perspective Mapping
W. Gardner, D.A. Winkler, D. Ballabio, B.W. Muir, P.J. Pigram
Biointerphases (2020), 15, 061004
86. NURA: a curated dataset of nuclear receptor modulators
C. Valsecchi, F. Grisoni, S. Motta, L. Bonati, D. Ballabio
Toxicology and Applied Pharmacology (2020), 407, 115244
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
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- 79: Geographical identification of Chianti red wine based on ICP-MS element composition
B. Bronzi, C. Brillì, G.M. Beone, M.C. Fontanella, D. Ballabio, R. Todeschini, V. Consonni, F. Grisoni, F. Parri, M. Buscema
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78. Integrated QSAR models to predict acute oral systemic toxicity
D. Ballabio, F. Grisoni, V. Consonni, R. Todeschini
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77. Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making
R. Todeschini, F. Grisoni, D. Ballabio
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- 76: Machine Learning Consensus to Predict the Binding to the Androgen Receptor within the CoMPARA project.
F. Grisoni, V. Consonni, D. Ballabio
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V. Consonni, R. Todeschini, D. Ballabio, F. Grisoni
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67. Qualitative consensus of QSAR ready biodegradability predictions
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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
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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
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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
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R. Todeschini, D. Ballabio, F. Grisoni
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61. A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods
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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
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56. A MATLAB toolbox for Principal Component Analysis and unsupervised exploration of data structure
D. Ballabio
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55. The use of diagnostic ratios, biomarkers and 3-way Kohonen Neural Networks to monitor the temporal evolution of oil spills
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D. Ballabio, V. Consonni, F. Costa
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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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M.P. Gomez-Carracedo, D. Ballabio, J.M. Andrade, J. Aires-de-Sousa, V. Consonni
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M. Alvarez-Guerra, D. Ballabio, J. M. Amigo, R. Bro, J. R. Viguri
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R. Todeschini, D. Ballabio, V. Consonni, A. Manganaro, A. Mauri
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L. Piazza, J. Gigli, C. Rojas, D. Ballabio, R. Todeschini, P. Tripaldi
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F. Carcione, L.M. Chiesa, D. Ballabio, S. Soncin, P.A. Biondi, P. Cattaneo, C. Cantoni
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R. Todeschini, D. Ballabio, V. Consonni, A. Mauri
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D. Ballabio, T. Skov, R. Leardi, R. Bro
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A. Mauri, D. Ballabio, V. Consonni, A. Manganaro, R. Todeschini
MATCH, communications in mathematical and in computer chemistry (2008), 60, 671-690
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T. Skov, D. Ballabio, R. Bro
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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
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
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D. Ballabio, R. Kokkinofa, 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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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
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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
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
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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
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:

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 AT CONGRESSES

Oral presentation and lectures:

31. High-Level Data Fusion to classify chemical data from multiple analytical sources
D. Ballabio
XI Argentine Conference of Analytical Chemistry, 30 November - 3 December 2021, Corrientes (Argentina) held on line, invited lecture

30. Quantitative Structure Activity Relationships (QSARs): introduction and applications
D. Ballabio
Application of Artificial Intelligence to nuclear forensics, 17 - 18 November 2021 (on line), invited lecture

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. Brillì, 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, Univesidad 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