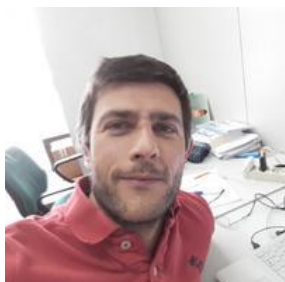


# Davide Ballabio

full professor in chemometrics, QSAR and analytical chemistry



## CONTACT

### Address

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Università degli Studi di  
Milano-Bicocca  
P.zza della Scienza, 1  
20126 Milano, Italy  
Building U1 - 3th floor

### Email

davide.ballabio@unimib.it

## 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  
1996 - 2002

## INFORMATIC SKILLS

Programming skills

## PROFILE

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

I have experience in multivariate data analysis (especially supervised classification) applied to both analytical and QSAR data; I also like to code MATLAB toolboxes for the calculation of multivariate models and share them publicly. I am author of more than 100 peer reviewed papers and have been included in the Top 2% Scientists list according to DOI:10.17632/btchxktzyw.5

## PROFESSIONAL EXPERIENCES

### Full professor

*October 2023 – now*

Full 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).

### Associate professor

*September 2018 – September 2023*

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 funded 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

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/>

*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.

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.

#### **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

*March 2023 – now*

Member of the *Presidio della Qualità - Ramo Ricerca (PQA Ricerca)* of the University of Milano – Bicocca.

*June 2022 - now*

Coordinator of the *Gruppo divisionale di Chemiometria della Divisione di Chimica Analitica della Società Chimica Italiana*.

*June 2022 – now*

Member of the scientific committee of EURIS, Centre for the sustainable use and risk assessment of chemicals at the Department of Earth and Environmental Science, University of Milano – Bicocca.

*December 2021 - now*

Member of the *Commissione revisione offerta formativa* at the degree in chemical science and technology, 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 – June 2022*

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

*November 2018 - September 2024*

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

*September 2021 – September 2024*

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

*October 2018 - January 2022*

Quality insurer at the Bachelor degree in chemical science and technology, University of Milano - Bicocca.

## 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*

February 2024 (20 hours), July 2023 (16 hours), July 2022 (16 hours), 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 2023 (14 hours), June 2022 (14 hours), 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 2022 (2 hour), 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 2024 (35 hours), March-May 2023 (35 hours), March-May 2022 (35 hours), 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 2024 (52 hours), March-May 2023 (48 hours), March-May 2022 (48 hours), 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 2024 (12 hours), January 2023 (12 hours), January 2022 (12 hours), 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 2024 (32 hours), April 2023 (32 hours), April 2022 (32 hours), 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 2023 (20 hours), October-November 2022 (30 hours), 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****University of the Basque Country**

September 2024

Beyond linear in classification. An introduction to Support Vectors Machine, Random Forest and Artificial Neural Networks, course on advanced classification methods at the University of the Basque Country (Bilbao) supported by Erasmus+ program

September 2023

Chemometrically Speaking 5 – Classification, course on advanced classification methods at the University of the Basque Country (Bilbao) supported by Erasmus+ program

**Scuola Superiore di Chimica Analitica per Dottorandi**

12 June 2025

Introduction to Chemometrics: principles and methods

Chemometric strategies for the fusion and multiblock analysis of data from different analytical platforms

**University of Burgos**

October 2023

Invited lecture: An introduction to classification for modelling chemical data

Short course: A deep insight into Support Vector Machines (SVM)

**Chemometric Group of Copenhagen, University of Copenhagen**

January 2023

On-line seminar "Chemometrics and molecular fingerprints to enhance LC-MS/MS spectral match"

**NIEHS Clustering Classification Virtual Workshop - National Institutes of Health (NIH)**

October 2022

On-line seminar on unsupervised clustering and supervised classification

**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 ILLA (Institute Italo - Latino Americano) and the National University of Colombia.

**Supervisor:**

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

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

**Tutor**

Enmanuel Cruz Munoz, Geochemical study of sulfide minerals persistence in the sedimentary records, University of Milano-Bicocca

Valentina Bellotti, Synthesis and characterization of amphiphilic block-copolymer nano-object prepared by PET-RAFT PISA polymerization as confined systems for up conversion, University of Milano-Bicocca, 2024

**External reviewer:**

Fabio Fornari, Innovative materials for miniaturized sample preparation techniques, environmental and food packaging applications. University of Parma, 2023

Martina Foschi, Geographical traceability of traditional food products by multi-elemental and spectroscopic profiling methods combined with chemometrics, University of l'Aquila

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

Eleonora Amante, Eleonora Amante:

Title of the Thesis: Chemometric interpretation of targeted and untargeted metabolomics for the investigation of clinical diseases and sport induced deviations. University of Torino, 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 Peracchi, Valutazioni delle funzionalità di un nuovo polimero di origine naturale in prodotti make-up, University of Milano - Bicocca (Italy), July 2023

Alberto Azrak, New anti-perspirant deodorants for cosmetic applications, University of Milano - Bicocca (Italy), November 2022

Alessandro Bordin, Formulazione di una sospensione stabile di PTFE micronizzato in basi minerali e sintetiche, University of Milano - Bicocca (Italy), November 2022

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 and EDITORIAL BOARD ACTIVITY**

Editorial Board Member, Chemometrics and Intelligent Laboratory Systems (peer-reviewed, Elsevier)

Review Editor, Frontiers in Analytical Science – Chemometrics (peer-reviewed, Frontiers)

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)

#### PARTECIPATION TO ORGANISING COMMITTEE

Symposium of Young Chemometricians 2025, bertinoro (Italy), 3-6 febraury 2025

Workshop di Chemiometria 2024, Ravenna (Italia), 27-29 may 2024

Centro 3R IV annual meeting, Milano (Italia), 13-15 september 2023

XI Colloquium Chemiometricum Mediterraneum, Padova (Italia), 27-30 june 2023

Chemometrics Open Day - La Chemiometria oggi, on-line, 9 february 2023

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

VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italia), 30 giugno - 4 july 2013

## 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:

116. Development of Quantitative Structure–Anti-Inflammatory Relationships of Alkaloids

C. Rojas, D. Muñoz, I. Corder, B. Tenesaca, D. Ballabio

Chemistry Proceedings, 2024, 16, 77

115. Condensed phase membrane introduction mass spectrometry: A new frontier for the real-time monitoring of hazardous chemical migration from food contact materials

M. Piergiovanni, V. Termopoli, C. Maffezzoni, N. Riboni, V. Consonni, F. Bianchi, M. Mattarozzi, D. Ballabio, M. Careri

Green Analytical Chemistry, 2025, 12, 100199

114. Oxidative weathering of pyrite in acidic environments: Data-driven experimental evaluation coupled with Raman hyperspectral imaging

E. Cruz Muñoz, F. Gosetti, S. Andò, D. Ballabio, E. Garzanti

Science of The Total Environment, 2024, 954, 176284

113. Extended multivariate comparison of 68 cluster validity indices. A review

R. Todeschini, D. Ballabio, V. Termopoli, V. Consonni

Chemometrics and Intelligent Laboratory Systems 2024, 251, 105117

112. Effectiveness of molecular fingerprints for exploring the chemical space of natural products.

D. Boldini, D. Ballabio, V. Consonni, R. Todeschini, F. Grisoni, S.A. Sieber

Journal of Cheminformatics 2024, 16, 35

111. Kernel-based mapping of reliability in predictions for consensus modelling

V. Consonni, R. Todeschini, M. Orlandi, D. Ballabio

Chemometrics and Intelligent Laboratory Systems 2024, 246, 105085

110. Artificial Intelligence and Machine Learning Methods to Evaluate Cardiotoxicity following the Adverse Outcome Pathway Frameworks

E. Viganò, D. Ballabio, A. Roncaglioni

Toxics 2024, 12, 87

109. Comparison of machine learning approaches for the classification of elution profiles

G. Baccolo, H. Yu, C. Valsecchi, D. Ballabio, R. Bro

Chemometrics and Intelligent Laboratory Systems 2023, 243, 105002

108. Enhanced Visualization and Interpretation of XMCD-PEEM Data Using SOM-RPM Machine Learning

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Microchimica Acta (2008), 163, 11-21
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. Kokkinofa, R. Todeschini, C. R. Theocharis  
Chemometrics and Intelligent Laboratory Systems (2007), 87, 78-84
10. On the Application of Chemometrics for the study of Acoustic-Mechanical properties of Crispy Bakery products  
L. Piazza, J. Gigli, D. Ballabio  
Chemometrics and Intelligent Laboratory Systems (2007), 86, 52-59
9. A new similarity/diversity measure for sequential data  
R. Todeschini, D. Ballabio, V. Consonni, A. Mauri  
MATCH, communications in mathematical and in computer chemistry (2007), 57, 51-67
8. CAIMAN (Classification And Influence Matrix Analysis): a new approach to the classification based on leverage-scaled functions  
R. Todeschini, D. Ballabio, V. Consonni, A. Mauri, M. Pavan  
Chemometrics and Intelligent Laboratory Systems (2007), 87, 3-17
7. Evaluation of different storage conditions of extra virgin olive oils with a innovative recognition tool built by means of electronic nose and electronic tongue  
M.S. Cosio, D. Ballabio, S. Benedetti, C. Gigliotti  
Food Chemistry (2007), 101, 485-491
6. Prediction of Italian red wine sensorial descriptors from electronic nose, electronic tongue and spectrophotometric measurements by means of Genetic Algorithms regression models  
S. Buratti, D. Ballabio, S. Benedetti, M.S. Cosio  
Food chemistry (2007), 100, 211-218
5. Characterization of DNA primary sequences by a new similarity/diversity measure based on the partial ordering  
R. Todeschini, V. Consonni, A. Mauri, D. Ballabio  
Journal of Chemical Information and Modeling (2006), 46, 1905-1911

4. A chemometric approach based on a novel similarity/diversity measure for the characterization and selection of electronic nose sensors

D. Ballabio, M.S. Cosio, S. Mannino, R. Todeschini  
*Analytica Chimica Acta* (2006), 578, 170-177

3. Geographical classification of wine and olive oil by means of classification and influence matrix analysis (CAIMAN)

D. Ballabio, A. Mauri, R. Todeschini, S. Buratti  
*Analytica Chimica Acta* (2006), 570, 249-258

2. Geographical origin and authentication of extra virgin olive oils by an electronic nose in combination with artificial neural networks.

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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:**

18. Statistical Process Control (SPC)

D. Borda, L. Wilson, I. Banu, I. Bleoanca, D. Ballabio, S. Mannino, I. Zheleva, T. Todorov, H. Bozkurt, F. Göğüş  
in *Statistics in Food and Biotechnology. Integrating Food Science and Engineering Knowledge Into the Food Chain*, Schleining, G., Mannino, S., Suwannaporn, P. (eds) Springer 2024

17. Statistic for Food Product and Process Development

M. Cortez Vieira, S. Quispe-Condori, P. Suwannaporn, D. Ballabio, F. Gosetti, S. Mannino, V. Consonni  
in *Statistics in Food and Biotechnology. Integrating Food Science and Engineering Knowledge Into the Food Chain*, Schleining, G., Mannino, S., Suwannaporn, P. (eds) Springer 2024

16. Chemical space and Molecular Descriptors for QSAR studies

V. Consonni, D. Ballabio, R. Todeschini  
In *Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development*, Roy, K. (Eds), Elsevier, 2023

15. Multitask Learning for Quantitative Structure–Activity Relationships: A Tutorial.

C. Valsecchi, F. Grisoni, V. Consonni, D. Ballabio, R. Todeschini  
In *Machine Learning and Deep Learning in Computational Toxicology. Computational Methods in Engineering & the Sciences*, Hong, H. (Eds), Springer, 2023

14. Authenticity and Chemometrics basics

V. Consonni, R. Todeschini, F. Gosetti, D. Ballabio  
In *Chemometrics and Authenticity of Foods of Plant Origin*, S. Agriopoulou, M. Tarapoulouzi, T. Varzakas (Eds.), CRC Press, 2023

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:

35. Multitask modelling for QSAR and analytical applications

D. Ballabio

9th Iranian Chemical Society Biennial Chemometrics Seminar, 18-19 October 2023, Qazvin (Iran), invited lecture

34. Univariate vs Multivariate for Clustering and Classification

D. Ballabio

Clustering and Classification Workshop, 3-4 October 2022, National Institute of Environmental Health Sciences, invited lecture

33. Enhancing LC-MS/MS spectral searching with multi-task neural networks and molecular fingerprints  
D. Ballabio, V. Consonni, F. Gosetti, V. Termopoli, R. Todeschini  
18th Chemometrics in Analytical Chemistry Conference, 29 August – 1 September 2022, Rome (Italy)
32. Tailoring supervised classification to data: an overview  
D. Ballabio  
Second Chemometric Symposium of Iranian Chemical Society, 11 – 12 May 2022, Tabriz (Iran), held on line, invited lecture
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. Brilli, G.M. Beone, M.C. Fontanella, R. Todeschini, V. Consonni  
XXVII Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Bologna (Italy), 16 -20 September 2018
27. QSAR models to predict properties of dyes for regulatory use  
D. Ballabio, V. Consonni, A. Mauri, V. Alberti, M. Locatelli, R. Todeschini  
QSAR 2018, 11-15 June 2018, Bled (Slovenia)
26. High-level data fusion: perspectives in QSAR and analytical applications  
IX Colloquium Chemiometricum Mediterraneum, 27-30 June 2017, Arles (France), invited lecture
25. Data integration to increase quality and reliability of QSAR predictions  
SETAC Europe 27th Annual Meeting, 7-11 May 2017, Bruxelles (Belgium)
24. Development of QSAR models to predict environmental and toxicological properties of chemicals  
Symposium on QSAR modelling, 9 March 2017, Copenhagen, (Denmark), invited lecture
23. PCA toolbox for MATLAB  
Italian Chemometric workshop, 15-17 February 2017, Vietri sul mare (Italy)
22. High-level fusion methods to classify samples associated to multiple analytical sources  
XVI Chemometrics in Analytical Chemistry (CAC 2016), Barcelona (Spain), 6-10 June 2016
21. Recent advances in consensus modelling of multiple analytical chemical data  
XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste (Italy), 13-17 September 2015
20. A novel unsupervised method for reducing the dimensionality of large QSAR datasets  
16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014), Milan (Italy), 16-20 June 2014
19. Multivariate analysis applied to bioprocesses  
V International Congress of Industrial Microbiology, Bogotá (Colombia), 8-10 May 2013

18. How to build a predictive QSAR model  
ECO summer school, Verona (Italy), 11 June 2012
17. Kohonen and CP-ANN toolbox for MATLAB  
Italian Chemometric workshop, Albano Laziale, Roma (Italy), 26-28 May 2011
16. Optimisation of neural network architectures by means of genetic algorithms  
XII Convegno della Divisione di Chimica Analitica della Società Chimica Italiana, Como (Italy), 13-16 September 2010
15. Optimisation of Counter-Propagation Artificial Neural Networks by means of genetic algorithms  
VII Colloquium Chemiometricum Mediterraneum, Granada (Spain), 21-24 June 2010
14. Principal component analysis (PCA), theory and examples  
Introductory course on multivariate analysis and quantitative structure - activity relationships (QSAR), Milan (Italy), 19 May 2009
13. Kohonen Maps and Counterpropagation Artificial Neural Networks Toolbox for MATLAB  
8th Iranian Workshop on Chemometrics, Zanjan (Iran), 7-9 February 2009, invited speaker
12. MOLMAP: chemometric strategy based on Kohonen Maps  
8th Iranian Workshop on Chemometrics, Zanjan (Iran), 7-9 February 2009, invited speaker
11. Introduction to the application of multivariate analysis in food science  
III Jornadas de Ciencia y Tecnología, Universidad del Azuay, Cuenca (Ecuador), 12 November 2008
10. Multivariate analysis applied to food science  
Segundo Congreso Ecuatoriano de Ingeniería en Alimentos, Loja (Ecuador), 5-7 November 2008, invited speaker
9. Chemometric application for the quality monitoring of rheological profiles: case study  
Italian Chemometric workshop, Pisa (Italy), 14-15 May 2008
8. Statistic tools for PQR (Product Quality Review)  
Product Quality Review, Milan (Italy), 4 March 2008
7. Moderne tecniche di analisi multivariata applicate ai processi alimentari - Multivariate Analysis and food processes (PAT)  
Metodi Analitici Rapidi per il Settore Agro Alimentare, Milan (Italy), 2 October 2007
6. Classification of multiway data based on the MOLMAP approach  
VI Colloquium Chemiometricum Mediterraneum, Saint-Maximin (France), 5-7 September 2007
5. Selection and characterisation of electronic nose sensors by means of Hasse distances  
Italian Chemometric workshop, Modena (Italy), 15-16 February 2007
4. Characterisation and selection of electronic nose sensors by means of Hasse distances  
Workshop on Ranking Methods and Multicriteria Decision Analysis in Environmental Sciences, Verbania (Italy), 2-3 October 2006
3. Chemometrics for the authentication and characterization of food products  
11th Workshop on the Developments in the Italian PhD Research on Food Science and Technology, Teramo (Italy), 27-29 September, 2006
2. Introduction to Chemometrics. Tools for multivariate analysis of chemical data  
Joint PAT Workshop, Pomezia (Italy), 6 April 2006
1. 3-way chemometric application on sensory data: the chilli flavoured meat balls experience  
Italian Chemometric workshop, Varenna (Italy), 26-27 May 2005