

Davide Ballabio

full professor in chemometrics, QSAR and analytical chemistry



CONTACT

Address

Dipartimento di Scienze
dell'Ambiente e della Terra
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

Python and MATLAB

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

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

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.

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.

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.

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.

November 2018 - now

Member of the Council (*giunta*) of 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.

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 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 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 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 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 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 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

Chemometrically Speaking 5 - Classification

September 2023

Course on advanced classification methods at the University of the Basque Country (Bilbao) supported by Erasmus+ program

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 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, 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

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, to be discussed in 2024

Enmanuel Cruz Munoz, Geochemical study of sulfide minerals persistence in the sedimentary records, University of Milano-Bicocca, to be discussed in 2025

Sofia Nizzolo, Derivatization and characterization of polysaccharides to be used for the functionalization of biomaterials, University of Milano-Bicocca, to be discussed in 2026

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 with Chemometrics and Intelligent Laboratory Systems (peer-reviewed, Elsevier)

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-Chapel Hill, Durham, USA

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

PARTECIPATION TO ORGANISING COMMITTEE

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

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

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

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

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

MATH/CHEM/COMP Conference 2008, Verbania (Italia), 10-13 giugno 2008

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:

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, in press

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

S.Y. Wong, S.L. Harmer, W. Gardner, A.K. Schenk, D. Ballabio, P.J. Pigram

Advanced Materials Interfaces 2023, 2300581

107. Effect of data preprocessing and machine learning hyperparameters on mass spectrometry imaging models

W. Gardner, D.A. Winkler, D.L.J. Alexander, D. Ballabio, B.W. Muir, P.J. Pigram

Journal of Vacuum Science and Technology A 2023, 41, 063204

106. Classification-based machine learning approaches to predict the taste of molecules: A review

C. Rojas, D. Ballabio, V. Consonni, D. Suárez-Estrella, R. Todeschini

Food Research International 2023, 171, 113036

105. Characterization of pyrite weathering products by Raman hyperspectral imaging and chemometrics techniques

E. Cruz Muñoz, F. Gosetti, D. Ballabio, S. Andò, O. Gómez-Laserna, J.M. Amigo, E. Garzanti, E.

Microchemical Journal 2023, 190, 108655

104. Exploring the relationship between polymer surface chemistry and bacterial attachment using ToF-SIMS and self-organizing maps

S.Y. Wong, A.L. Hook, W. Gardner, C.Y. Chang, Y. Mei, M.C. Davies, P. Williams, M.R. Alexander, D. Ballabio, B.W. Muir, D.A. Winkler, P.J. Pigram

Advanced Materials Interfaces 2023, 10, 2202334

103. Condensed phase membrane introduction mass spectrometry: a direct alternative to fully exploit the mass spectrometry potential in environmental sample analysis

V. Termopoli, M. Piergiovanni, D. Ballabio, V. Consonni, E. Cruz Muñoz, F. Gosetti

Separations 2023, 10, 139

102. From the streets to the judicial evidence: determination of traditional illicit substances in drug seizures by a rapid and sensitive UHPLC-MS/MS-based platform

F. Gosetti, V. Consonni, D. Ballabio, M.E. Orlandi, A. Amodio, M.V. Picci, M. Visentin, V. Termopoli

Molecules (2023), 28, 164

101. Response surface methodology approach to evaluate the effect of transition metals and oxygen on photo-degradation of methionine in a model wine system containing riboflavin
D. Fracassetti, D. Ballabio, M. Mastro, A. Tirelli, D. Jeffery
Journal of Agricultural and Food Chemistry (2022), 70, 16347-16357
100. Improving bitter pit prediction by the use of X-ray fluorescence (XRF): a new approach by multivariate classification
C. Moggia, M.A. Bravo, R. Baettig, M. Valdés, S. Romero-Bravo, M.A. Zúñiga, J. Cornejo, F. Gosetti, D. Ballabio, R.A. Cabeza, R. Beaudry, G.A. Lobos
Frontiers Plant Science (2022), 13:1033308.
99. Identification of photodegradation products of Escitalopram in surface water by HPLC-MS/MS and preliminary characterization of their potential impact on the environment
V. Termopoli, V. Consonni, D. Ballabio, R. Todeschini, M. Orlandi, F. Gosetti
Separations (2022), 9, 289
98. Multi-task neural networks and molecular fingerprints to enhance compound identification from LC-MS/MS data
V. Consonni, F. Gosetti, V. Termopoli, R. Todeschini, C. Valsecchi, D. Ballabio
Molecules (2022), 27, 5827
97. NMR spectroscopy and chemometric models to detect a specific non-porcine ruminant contaminant in pharmaceutical heparin
E. Colombo, L. Mauri, M. Marinuzzi, 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
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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:

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. 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 Tecnologia, Universidad 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

47. Predicting molecular activity on nuclear receptors with deep and machine learning
C. Valsecchi, F. Grisoni, V. Consonni, D. Ballabio, R. Todeschini
QSAR 2021, 7 -9 June 2021, on-line meeting
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. Ballabio, V. Consonni, A. Mauri, I. Tetko, R. Todeschini
ECO conference, September 2013
28. A comparative study on different methods for applicability domain assessment
V. Consonni, D. Ballabio, F. Sahigara, A. Mauri, M. Cassotti, F. Grisoni, R. Todeschini
VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italy), 30 June - 4 July 2013
27. K-Contractive Map (K-CM) for classification
M. Buscema, D. Ballabio, V. Consonni, M. Breda, G. Massini, L. Galli, M. Fabrizi, R. Todeschini
VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italy), 30 June - 4 July 2013
26. Sviluppo di un metodo veloce, economico e non distruttivo per la quantificazione della componente ionica nel particolato atmosferico
U. Molteni, D. Ballabio, P. Fermo, A. Piazzalunga
XIV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, Rimini (Italy), 2-5 June 2013
25. QSAR study on ready biodegradability of chemicals

K. Mansouri, T. Ringsted, V. Consonni, D. Ballabio, R. Todeschini
3rd Strasbourg Summer School in Chemoinformatics, Strasbourg (France), 25-29 June 2012

24. Multi criteria variable selection for QSARs

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

23. QSAR study on ready biodegradability of chemicals

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

22. A (Q)SAR study on ready biodegradability

T. Ringsted, K. Mansouri, D. Ballabio, A. Mauri, V. Consonni, R. Todeschini
15th International Workshop on Quantitative Structure-Activity Relationships (QSAR2012) in Environmental and Health Sciences, Tallinn (Estonia), 18-22 June 2012

21. Read-across methodology in aquatic ecotoxicology and ready biodegradation

T. Ringsted, E. Giagloglou, D. Ballabio, A. Mauri, M. Cassotti, V. Consonni, R. Todeschini
ECO winter school, Madrid (Spain), 27 February - 2 March 2012

20. QSAR study for the prediction of LogP coefficient

K. Mansouri, A. Mauri, D. Ballabio, V. Consonni, R. Todeschini
6th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2011), Maribor (Slovenia), 3-7 September 2011

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

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

18. Molecular descriptors by Dragon software

A. Mauri, A. Manganaro, D. Ballabio, V. Consonni, R. Todeschini
XII Convegno della Divisione di Chimica Analitica della Società Chimica Italiana, Como (Italy), 13-16 September 2010

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

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

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

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

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

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

14. MOLE DB - on-line Molecular Descriptors Data Base

D. Ballabio, A. Manganaro, V. Consonni, A. Mauri, R. Todeschini
MATH/CHEM/COMP 2008 Conference, Verbania (Italy), 10-13 June 2008

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

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

12. Evaluation of multivariate classification and variable selection for the distinction of cachaca and rum samples

R. Todeschini, D. Ballabio, C. Rojas, A. Manganaro, A. Mauri, V. Consonni, P. Tripaldi
Ibero-American Congress in Food Engineering, Ambato (Ecuador), 5-8 November 2007

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

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

10. Novel XML-based Electronic Format for QSAR Models Exchange and Application

A. Manganaro, R. Todeschini, V. Consonni, D. Ballabio, A. Mauri
6th World Congress on Alternatives & Animal Use in the Life Sciences, Tokyo (Japan), 21-25 August 2007

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

Attended congresses:

- 11 - 15 September 2022
XXIX Congresso della Divisione di Chimica Analitica (Milazzo, Italy)
- 29 August – 2 September 2022
18th Chemometrics in Analytical Chemistry Conference (Roma, Italy)
- 30 May - 1 June 2022
Italian Chemometric workshop, L'Aquila (Italy)
- 14 – 23 September 2021
XXVII Congresso Nazionale della Società Chimica Italiana, on-line
- 12 -14 June 2019
IX Colloquium Chemiometricum Mediterraneum, Menorca (Spain)
- 25-27 February 2019
Italian Chemometric workshop, Bergamo (Italy)
- 16 -20 September 2018
XXVII Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Bologna (Italy)
- 11-15 June 2018
QSAR 2018, Bled (Slovenia)
- 27-30 June 2017
IX Colloquium Chemiometricum Mediterraneum, Arles (France)
- 7-11 May 2017

SETAC Europe 27th Annual Meeting, Bruxelles (Belgium)

15-17 February 2017

Italian Chemometric workshop, Vietri sul mare (Italy)

4-8 September 2016

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

6-10 June 2016

XVI Chemometrics in Analytical Chemistry (CAC 2016), Barcelona (Spain)

13-17 September 2015

XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste (Italy)

16-20 June 2014

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

30 June - 4 July 2013

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

8-10 May 2013

V International Congress of Industrial Microbiology, Bogotá (Colombia)

11-15 June 2012

ECO summer school, Verona (Italy)

26-28 May 2011

Italian Chemometric workshop, Albano laziale, Roma (Italy)

13-16 September 2010

XII Convegno della Divisione di Chimica Analitica della Società Chimica Italiana, Como (Italy)

21-24 June 2010

VII Colloquium Chemiometricum Mediterraneum, Granada (Spain)

7-9 February 2009

8th Iranian Workshop on Chemometrics, Zanzan (Iran), invited speaker

5-7 November 2008

Segundo Congreso Ecuatoriano de Ingenieria en Alimentos, Loja (Ecuador), invited speaker

10-13 June 2008

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

14-15 May 2008

Italian Chemometric workshop, Pisa (Italy)

5-7 September 2007

VI Colloquium Chemiometricum Mediterraneum, Saint-Maximin (France)

15-16 February 2007

Italian Chemometric workshop, Modena (Italy)

2-4 October 2006

Workshop on Ranking Methods and Multicriteria Decision Analysis in Environmental Sciences, Verbania (Italy)

27-29 September, 2006

11th Workshop on the Developments in the Italian PhD Research in Food Science Technology, Teramo (Italy)

30 June 2006

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

7 March 2006

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

7-9 September 2005

10th Workshop on the developments in the Italian PhD Research in Food Science Technology, Foggia (Italy)

28-31 August 2005

Conferentia Chemometrica 2005 and Chemometrics VII, Hajduszoboszlo (Hungary)

26-27 May 2005

Italian Chemometric workshop, Varenna (Italy)

25-27 June 2003

V Colloquium Chemiometricum Mediterraneum, Ustica (Italy)

Attended courses:

21 June 2011

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

19 May 2011

Writing success full FP7 cooperation proposals, Milano (Italy)

6-8 September 2010

School of Experimental Design, Genova (Italy)

13 May 2010

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

6 September 2006

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

1-3 April 2005

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

14-17 February 2005

PARVUS chemometric school, Genova (Italy)

10-25 January 2005

Advanced Chemometrics/Multi-way analysis course - Copenhagen (Denmark)

29 June 2004

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