

CURRICULUM VITAE ET STUDIORUM
Dr. FEDERICO MARINI

Personal information:

Date and place of birth: Rome March 9th 1977
University address: Dept. of Chemistry, University of Rome "La Sapienza"
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Education:

1995: High school diploma at Liceo Classico Terenzio Mamiani in Rome (mark: 60/60)
2000: Laurea (equivalent to MSc degree) in Chemistry at the University of Rome "La Sapienza" (mark 110/110 cum laude). Title of the thesis: "Analytical characterization of mono-cultivar extra virgin olive oils and their discrimination by means of multivariate statistical analysis and artificial neural networks".
2004: PhD in Chemical Sciences at the University of Rome "La Sapienza". Title of the thesis: "A chemometric approach to the evaluation of the quality of foodstuff".
2004-2008: Post-doc in Analytical Chemistry at the University of Rome "La Sapienza". Title of the project: "Multivariate analysis of quality".
2008-present: Researcher in Analytical Chemistry (permanent faculty) at the Department of Chemistry of the University of Rome "La Sapienza".
2013: National habilitation as Associate Professor
2014: National habilitation as Full Professor

Visits and stays:

1997: Short stay at the Chemical Laboratories of B.A.S.F. (Ludwigshafen, Germany) for a training stage (2 weeks).
2003: Visiting researcher at the National Institute of Chemistry (Ljubljana, Slovenia) to cooperate with prof. Jure Zupan (1 month).
2003: Marie Curie Fellow at the National Institute of Chemistry (Ljubljana, Slovenia). Title of the project: "Chemometric treatment of endocrine disrupter compounds", responsible: dr. Mariana Novič (3 months).
2007: Visiting researcher at the Faculty of Life Science of the University of Copenhagen to cooperate with prof. Rasmus Bro (3 weeks).
2008: Visiting researcher at the Faculty of Life Science of the University of Copenhagen to cooperate with prof. Rasmus Bro (5 months).
2009-2010: Visiting researcher at the Faculty of Life Science of the University of Copenhagen to cooperate with prof. Rasmus Bro (2 months).
2014: Visiting professor at the University of Stellenbosch (South Africa, 2 weeks).
2015: Visiting professor at the University of Silesia (Poland, 2 weeks).

- 2016: Visiting professor at the University of Stellenbosch (South Africa, 2 weeks).
Visiting professor at the University of Lille (France, 2 weeks).
Visiting professor at the University of Silesia (Ktowice, Poland, 1 week).

Teaching activity:

- 2003-2004: Professor of Computational Chemistry I (Chemometrics) at the University of L'Aquila (Degree Courses in Chemistry and Environmental Sciences).
- 2004-2007: Professor of Chemometrics at the University of L'Aquila (Degree Course in Chemistry).
- 2006-2008: Professor of Complements of Analytical Chemistry at the University of L'Aquila (Degree Course in Chemistry).
- 2006-present: Teacher of the module "Artificial Neural Networks for data analysis" at the University of Modena and Reggio Emilia (PhD Course in Multiscale modelling, computational simulations and characterization in Material and Life Sciences).
- 2008-2010: Professor of Water Chemistry at the University of Rome "La Sapienza" (Degree Course in Chemistry).
- 2008-present: Professor of Chemometrics at the University of Rome "La Sapienza" (Degree Course in Chemistry).
- 2009-present: Professor of Elements of chemometrics with MATLAB at the University of Rome "La Sapienza" (PhD Course in Sciences for the Conservation of Cultural Heritage).
- 2010-present: Teacher of the module "Chemometrics" for the PhD school in Analytical Chemistry organized by the Analytical Division of the Italian Chemical Society.
- 2012-2013: Teacher of the module "Advanced classification methods" for the Copenhagen School of Chemometrics (University of Copenhagen, Denmark).
- 2013: Coordinator and Teacher of the module "Classification and regression" for the 1st school on multi-way, multi-set and multi-block methods, organized in Rome (Italy).
- 2014-present: Professor of Advanced Chemometrics with Matlab for the PhD course in Chemical Sciences at the University of Rome "La Sapienza" (Degree Course in Chemistry).

Other teaching activity:

- 2001-present: Teacher of different modules of "Chemometrics", "Statistics", or "Instrumental Analytical Chemistry" for several public and private institutions, such as Italian National Research Council, Italian Ministry of Agriculture, Italian Customs' Chemical Laboratories, Italian Air Force.

Membership and awards:

- 2001: Prize for the best thesis in Analytical Chemistry awarded by the

- Analytical Division of the Italian Chemical Society.
- 2006: Young Researcher Prize (prize for the best researcher under 35 in Analytical Chemistry) awarded by the Analytical Division of the Italian Chemical Society.
- 2012: Chemometrics & Intelligent Laboratory Systems Award for contribution to the development of chemometrics in the last 5 years.
- 2006: Award for the best oral communication in chemometrics at the International Conference CM4CH06 – Chemometrics and Multivariate Analysis Applied to Cultural Heritage and Environment (Nemi, Italy).
- 2001-present: Member of the Italian Chemical Society.
- 2006-present: Member of the American Chemical Society.
- 2007-present: Session chairman in several national and international conferences.
- 2008-present: Member of several national and international PhD committees and evaluation boards.
- 2009-present: Member of the Editorial Board of Chemometrics and Intelligent Laboratory Systems (Elsevier).
- 2010-present: Member of the Scientific Committee of the series of conferences CMA4CH – Chemometrics and Multivariate Analysis Applied to Cultural Heritage and Environment.
- 2010-present: Member of the Scientific Committee of the series of conferences WSC – Winter Symposium on Chemometrics.
- 2011-2015: Member of the Board of the Chemometrics group of the Italian Chemical Society.
- 2011-present: Member of the Editorial Board of *Analytica Chimica Acta* (Elsevier).
- 2012-present: Member of the Chemometrics study group of the Division of Analytical Chemistry of the EuCheMS.
- 2012: Member of the Scientific Committee of the conference AFRODATA2012.
- 2013: Member of the Scientific Committee of the conferences 8th Colloquium chemiometricum mediterraneum (Bevagna, Italy) and 13th Scandinavian Symposium of Chemometrics (Stockholm archipelago, Sweden)
- 2013-present: Associate Editor for Chemometrics of the *Encyclopedia of Analytical Chemistry* (John Wiley and Sons).
- 2014-present: Member of the Editorial Board of *Frontiers in Medicine*.
- 2014-present: Member of the Board of the Italian Society for NIR spectroscopy (SISNIR).
- 2014: Guest Editor of the Virtual special issue of Chemometrics and Intelligent Laboratory Systems collecting the proceedings of the CCM2013 conference.
- 2014: Co-chairman of the conference IASIM-14 (Rome, Italy).
- 2015: Co-chairman of the conference TRICAP2015 (Pecol (BL), Italy)
- 2015: Member of the Scientific Committee of the conferences 14th Scandinavian Symposium of Chemometrics (Chia Laguna, Italy) and XV Chemometrics in Analytical Chemistry (Changsha, China).
- 2015-present: Coordinator of the Chemometrics group of the Italian Chemical Society.
- 2015-present: Member of the Editorial Board of the *Journal of Near Infrared Spectroscopy*.
- 2016: Member of the Scientific Committee of the conferences NTCA2016

(Side-Antalya, Turkey), XVI Chemometrics in Analytical Chemistry (Barcelona, Spain) and IASIM2016 (Chamonix, France).

2016-present: Member of the Editorial Board of the Journal of Spectral Imaging.

Refereeing activity:

Referee for several international journals, among which: Analytical Chemistry, Trends in Analytical Chemistry, Chemometrics and Intelligent Laboratory Systems, Analytica Chimica Acta, Talanta, Journal of Chemometrics, Food Chemistry, Journal of Agricultural and Food Chemistry, Analytical Methods, Analytical Letters, MATCH, Journal of the American Chemical Society, Journal of Chemical Information and Modeling, Journal of the American Oil Chemists' Society, Journal of the Association of Official Analytical Chemists, Journal of Chromatography, Metabolomics.

Reviewer of International project proposals for the European Research Council (ERC), Flanders Research Foundation (FWO), South African National Research Foundation (NRF), Dutch Research Foundation (NWO).

Funding:

- 2008: 7000€ from the University of Rome "La Sapienza" (FARI2008). Title of the project: Chemometrics and multivariate analysis for chromatography.
- 2010: 7500€ from the University of Rome "La Sapienza" (FARI2010). Title of the project: Chemometrics for -omics data.
- 2010: 15000€ from the University of Rome "La Sapienza" (ATENEO2010). Title of the project: Development of chemometric methods for the interpretation of analytical data.
- 2012: 2500€ from the University of Rome "La Sapienza" (CONGRESSI2012). Cofinancing for the organization of the conference VIII Colloquium Chemiometricum Mediterraneum.
- 2012: 12000€ from the University of Rome "La Sapienza" (UNIVERSITÀ2012). Title of the project: Development of chemometric methods and their application to food chemical problems.
- 2013: 6800€ from the University of Rome "La Sapienza" (UNIVERSITÀ2013). Title of the project: Innovative chemometrics-based analytical approaches for the evaluation of food quality.
- 2014: 10000€ from the University of Rome "La Sapienza" (UNIVERSITÀ2014). Title of the project: Coupling of novel chemometric methods to NIR spectroscopy for a rapid and non-destructive characterization of complex matrices.
- 2014-2016: 11000€ from the JPI "Healthy diet for a healthy life (JPI-HDHL). Title of the project: European Nutritional Phenotype Assessment Data Sharing Initiative (ENPADASI).
- 2015: 11000€ from the University of Rome "La Sapienza" (RICERCA2015). Title of the project: Design and application of advanced chemometric methods for food quality control.
- 2015-2017: 41700€ from Fondazione Roma. Title of the project: BIOmarkers

associated with Sarcopenia and PHysical frailty in EldeRly pErsons: the BIOSPHERE study.

Brief description of the research activity

My research work is mainly focused on all the different aspects of chemometrics, particularly with regard to both the build up and the development of new methods and algorithms and to the application of models to solve real problems. In particular, the main areas my research work is articulated in, are:

A. Development of new methods for quality control of food and pharmaceutical products.

A substantial part of my research has focused on the possibility of making profitable use of the coupling between different instrumental analytical techniques and appropriate chemometric tools for the development of innovative methods of analysis in the food and pharmaceutical fields. In particular, the aim was to exploit the full potential arising from the use of chemometrics in order to develop methodologies which were as non-invasive/non-destructive as possible, which would require the use of a limited amount of reagents, if not even their complete absence, and that in some cases did not require any pretreatment of the sample, allowing a considerable saving in terms of time and cost of analysis and resulting perfectly in line with the principles of green chemistry. In this context, from the analytical point of view, particular attention has been paid to the use of spectroscopic techniques - primarily in the infrared region.

B. Metabolomics and Proteomics

Recent years have seen the emergence of the "omics" life sciences of life, by concepts such as genomics, proteomics or metabolomics/metabonomics. The new aspects captured by these concepts are a global vision and large-scale surveys, in contrast to the problem-oriented reductionist vision, prevalent in previous studies. In this context, the automated acquisition of large amounts of -omic data represents a challenge in terms of exploration and interpretation. The abundance of data is not in itself a guarantee of obtaining useful information on the main events that take place in a system under investigation. On the contrary, the -omic data must be processed and analyzed, in order to highlight the relevant information, embedded in the measures. Because these data are highly multivariate in nature, there is the need to use data analysis techniques that are able to meet the challenges inherent in such large masses of data, in particular noise, collinearity and missing observations. Only with a careful analysis of the data, one may be able to address key issues such as the effects of treatment on the metabolism of a patient or the identification of biomarkers.

A part of my research work is situated in this framework and, through the collaboration with several national and international research groups, involves the use of different chemometric methods for metabolomic and proteomic studies. In particular, topics such as the search for plasma biomarkers of ovarian cancer, of the study of the effects of the supplementation of probiotics on the gut microbiota and on

the host/guest metabolism have been addressed. Moreover, also in the field of nutritional metabolomics, the effect of apple intake on rat metabolism and that of the supplementation of a sport drink to professional athletes were also investigated.

C. Cultural Heritage

The preservation of cultural heritage is a field for its multidisciplinary nature, involving knowledge of chemical, physical, historical, archaeological, architectural and engineering nature (to name only the major disciplines). The interrelationship between these different fields makes science applied to the conservation of cultural heritage an inherently multivariate context that, as such, is particularly suitable to be studied through the use of chemometric tools. In recent years, this need has been felt by a growing number of research groups engaged in the study of cultural heritage, some of whom I had recently the opportunity to work with. As a result of these collaborations, a part of my research is focused on the use of chemometrics in support of the analytical techniques used for the study of the artistic heritage.

D. Development of new chemometric methods

My research is not limited only to the application of already existing chemometric methods to solve real problems of different nature but a part of it is also focused on the build up and the development of innovative methods. In this context, particular interest has been directed to the class of algorithms generically referred to as "nature-inspired" (the functioning of which is inspired by biological models and/or behavioral problems), to the so-called multi-way methods (i.e., those methods who are able to deal with the cases in which, for each sample, a two- or higher-dimensional landscape is recorded), and to non-linear pattern recognition (classification and class-modeling).

Summary of scientific production.

94 publications on scientific journals.

13 book chapters

2 proceedings in book.

1 edited book (Chemometrics in Food Chemistry, Elsevier, 2013)

131 communications in national and international conferences (oral + poster), of which:

- 28 invited

- 16 plenary

h-index: 23

number of citations (February 2017): 1368

PUBLICATIONS

1) Scientific journals

- P01 R. Bucci, A.D. Magri, A.L. Magri, D. Marini, F. Marini "Chemical authentication of extra-virgin olive oil varieties by supervised chemometric procedures", *J. Agric. Food Chem.*, **50** (2002), 413-418
- P02 R. Bucci, A.D. Magri, A.L. Magri, F. Marini "Comparison of three spectrophotometric methods for the determination of γ -oryzanol in rice bran oil", *Anal. Bioanal. Chem.*, **375** (2003), 1254-1259
- P03 F. Marini, F. Balestrieri, R. Bucci, A.L. Magri, D. Marini "Supervised pattern recognition to discriminate the geographical origin of rice bran oils: a first study", *Microch. J.*, **74** (2003), 239-248
- P04 F. Marini, A.L. Magri, D. Marini, F. Balestrieri "Characterization of the lipid fraction of niger seeds (*Guizotia Abyssinica* Cass.) from different regions of Ethiopia and India and chemometric authentication of their geographical origin", *Eur. J. Lipid Sci. Tech.*, **105** (2003), 697-704
- P05 F. Marini, J. Zupan, A.L. Magri "On the use of counterpropagation artificial neural networks to characterize Italian rice varieties", *Anal. Chim. Acta*, **510** (2004), 231-240
- P06 F. Marini, A.L. Magri, F. Balestrieri, F. Fabretti, D. Marini "Supervised pattern recognition applied to the discrimination of the floral origin of Italian honey samples", *Anal. Chim. Acta*, **515** (2004), 117-125
- P07 D. Mott, F. Biasioli, F. Gasperi, E. Aprea, F. Marini, T.D. Märk "Characterization of strawberry genotypes by PTR-MS spectral fingerprinting", *Acta Horticulturæ*, **649** (2004), 65-68
- P08 F. Marini, F. Balestrieri, R. Bucci, A.L. Magri, D. Marini "Supervised pattern recognition to authenticate Italian olive oil varieties", *Chemom. Intell. Lab. Syst.*, **73** (2004), 85-93
- P09 F. Biasioli, F. Gasperi, G. Odorizzi, E. Aprea, D. Mott, G. Autiero, F. Marini, T.D. Märk "PTR-MS monitoring of odour emissions from composting plants", *Int. J. Mass Spectrom.*, **239** (2004), 103-109
- P10 F. Biasioli, F. Gasperi, G. Odorizzi, E. Aprea, D. Mott, F. Marini, G. Autiero, G. Rotondo, T.D. Märk "Studio sull'applicabilità del PTR-MS al controllo degli odori negli impianti per il trattamento dei rifiuti", *Rifiuti Solidi*, **18** (2004), 220-229
- P11 F. Marini, J. Zupan, A.L. Magri "Class-modeling using Kohonen artificial neural networks", *Anal. Chim. Acta*, **544** (2005), 306-314
- P12 F. Marini, A.L. Magri, R. Bucci, F. Balestrieri, D. Marini "Class-modeling techniques in the authentication of PDO Italian oils from Sicily", *Chemom. Intell. Lab. Syst.*, **80** (2005), 140-149
- P13 F. Marini, A. Roncaglioni, M. Novič "Variable Selection and Interpretation in Structure-Affinity Correlation Modeling of Estrogen Receptor Binders", *J. Chem. Inf. Model.*, **45** (2005), 1507-1519
- P14 F. Biasioli, F. Gasperi, E. Aprea, I. Endrizzi, V. Framondino, F. Marini, D. Mott, T.D. Märk "Correlation of PTR-MS spectral fingerprint with sensory characterization of flavour and odour profile of 'Trentingrana' cheese", *Food Qual. Pref.*, **17** (2006), 63-75
- P15 R. Bucci, F. Balestrieri, A.D. Magri, A.L. Magri, F. Marini "UV-Vis spectrophotometric method for the quantitation of all the components of Italian general denaturant and its application to check the conformity of alcohol samples", *Talanta*, **68** (2006), 781-790

- P16 V. Vinciguerra, R. Bucci, F. Marini, A. Napoli “Thermal behaviour of iminodiacetic, oxydiacetic and thiodiacetic acids”, *J. Therm. Anal. Calorim.*, **83** (2006), 475-478
- P17 F. Biasioli, F. Gasperi, E. Aprea, D. Mott, F. Marini, T.D. Märk “Characterization of strawberry genotypes: a three years study”, *Acta Horticulturae*, **708** (2006), 497-500
- P18 F. Marini, R. Bucci, A.L. Magri, A.D. Magri “Authentication of Italian CDO wines by class-modeling techniques”, *Chemom. Intell. Lab. Syst.*, **84** (2006), 164-171
- P19 E. Aprea, F. Biasioli, F. Gasperi, D. Mott, F. Marini, T.D. Märk “Assessment of Trentingrana cheese ageing by proton transfer reaction-mass spectrometry and chemometrics”, *Int. Dairy J.*, **17** (2007), 226-234
- P20 F. Marini, A.L. Magri, R. Bucci “Multilayer feed-forward neural networks for class-modeling”, *Chemom. Intell. Lab. Syst.*, **88** (2007), 118-124
- P21 F. Marini, A.L. Magri, R. Bucci, A.D. Magri, “Use of different artificial neural networks to resolve binary blends of monocultivar Italian olive oils”, *Anal. Chim. Acta*, **599** (2007), 232-240
- P22 F. Marini, R. Bucci, A.L. Magri, A.D. Magri, R. Acquistucci, R. Francisci “Classification Of 6 Durum Wheat Cultivars From Sicily (Italy) Using Artificial Neural Networks”, *Chemom. Intell. Lab Syst.*, **90** (2008), 1-7
- P23 F. Marini, A.L. Magri, R. Bucci, A.D. Magri, “Artificial Neural Networks in Chemometrics: History, Examples and Perspectives”, *Microch. J.*, **88** (2008), 178-85
- P24 L. Campanella, E. Gregori, F. Marini, M. Tomassetti, “Biosensors, colorimetric tests and chemometrics to check antioxidant and prooxidant properties of several animal feeds”, *J. Agric. Food. Environ.*, **6** (2008), 326-332
- P25 M.S. Simonetti, F. Damiani, L. Gabrielli, L. Cossignani, F. Blasi, F. Marini, D. Montesano, A. Maurizi, E. Ventura, A. Bosi, P. Damiani, “Characterization of triacylglycerols in *Arbutus Unedo* L. seeds”, *Italian J. Food Sci.*, **20** (2008), 49-56
- P26 L. Cossignani, F. Damiani, L. Gabrielli, D. Montesano, M.S. Simonetti, T. Petrosino, F. Ventura, F. Marini, P. Damiani, “Structural characteristics of the triacylglycerol fraction from the seed fat of *Mangifera Indica* L.”, *Italian J. Food Sci.*, **20** (2008), 263-271
- P27 F. Marini, R. Bucci, I. Ginevro, A.L. Magri, “Coupling of IR measurements and multivariate calibration techniques for the determination of enantiomeric excess in pharmaceutical preparations”, *Chemom. Intell. Lab Syst.*, **97** (2009), 52-63.
- P28 F. Marini, “Artificial neural networks in food analysis: trends and perspectives”, *Anal. Chim. Acta*, **635** (2009), 121-131.
- P29 M. West-Nørgaard, R. Bro, F. Marini, E.V. Høgdall, C.K. Høgdall, L. Nedergaard, N.H.H. Heegaard, “Feasibility of serodiagnosis of ovarian cancer by mass spectrometry”, *Anal. Chem.*, **81** (2009), 1907-1913.
- P30 A. Miccheli, F. Marini, G. Capuani, A. Tomassini Miccheli, M. Delfini, M.E. Di Cocco, C. Puccetti, M. Paci, M. Rizzo, A. Spataro, “The influence of a sports drink on the postexercise metabolism of elite athletes as investigated by NMR-based metabolomics”, *J. Am. Coll. Nutr.*, **28** (2009), 553-564.
- P31 M. Ritota, F. Marini, P. Sequi, M. Valentini, “Metabolomic characterization of Italian sweet pepper (*Capsicum annum* L.) by means of HRMAS-NMR spectroscopy and multivariate analysis”, *J. Agric. Food Chem.*, **58** (2010), 9675-9684.
- P32 L. Mannina, F. Marini, M. Gobino, A.P. Sobolev, D. Capitani, “NMR and chemometrics in tracing European olive oils: the case study of Ligurian samples”, *Talanta*, **80** (2010), 2141-2148.

- P33 F. Marini, "Classification methods in chemometrics", *Curr. Anal. Chem.*, **6** (2010), 72-79.
- P34 C. Cavaliere, P. Foglia, F. Marini, R. Samperi, D. Antonacci, A. Laganà, "The interactive effects of irrigation, nitrogen fertilization rate, delayed harvest and storage on the polyphenol content in red grape (*Vitis Vinifera*) berries: A factorial experimental design", *Food Chem.*, **122** (2010), 1176-1184.
- P35 F. Marini, A. D'Aloise, R. Bucci, F. Buiarelli, A.L. Magrì, A.D. Magrì, "Fast analysis of 4 phenolic acids in olive oil by HPLC-DAD and chemometrics", *Chemom. Intell. Lab. Syst.*, **106** (2011), 142-149.
- P36 S. Bellato, V. Del Frate, R. Redaelli, D. Sgrulletta, R. Bucci, A.D. Magrì, F. Marini, "Use of Near Infrared Reflectance and Transmittance coupled to Robust Calibration for the evaluation of nutritional value of naked oats", *J. Agric. Food Chem.*, **59** (2011), 4349-4360.
- P37 F. Marini, B. Walczak, "Finding relevant clustering directions in high-dimensional data using Particle Swarm Optimization", *J. Chemom.*, **25** (2011), 366-374.
- P38 A.A. Gowen, F. Marini, C. Esquerre, C. O'Donnell, G. Downey, J. Burger, "Time series hyperspectral chemical imaging data: Challenges, solutions and applications", *Anal. Chim. Acta*, **705** (2011), 272-282.
- P39 M. Bevilacqua, R. Bucci, A.D. Magrì, A.L. Magrì, F. Marini, "Tracing the origin of extra virgin olive oils by infrared spectroscopy and chemometrics: A case study", *Anal. Chim. Acta*, **717** (2012), 39-51.
- P40 M. Favaro, A. Guastoni, F. Marini, S. Bianchin, A. Gambirasi, "Characterization of lapis lazuli and corresponding purified pigments for a provenance study of ultramarine pigments used in works of art", *Anal. Bioanal. Chem.*, **402** (2012), 2195-2208.
- P41 C. Ruiz-Samblás, F. Marini, L. Cuadros-Rodríguez, A. González-Casado, "Quantification of blending of olive oils and edible vegetable oils by triacylglycerol fingerprint gas chromatography and chemometric tools", *J. Chromatogr. B*, **910** (2012) 71-77.
- P42 F. Marini, M. Tomassetti, S. Vecchio, "Detailed kinetic and chemometric study of the cellulose thermal breakdown in artificially aged and non aged commercial paper. Different methods for computing activation energy as an assessment model in archaeometric applications", *Chem. Centr. J.*, **6 Suppl.2** (2012), S7.
- P43 M. Ritota, S. Cozzolino, S. Marconi, P. Sequi, M. Valentini, F. Marini, "Metabolic profiling of sweet pepper (*Capsicum annuum L.*) by means of HRMAS-NMR spectroscopy", *Acta Horticulturae*, **932** (2012) 279-284.
- P44 M. Tomassetti, F. Marini, L. Campanella, A. Coppa, "Study of modern or ancient collagen and human fossil bones from an archaeological site of middle Nile by thermal analysis and chemometrics", *Microch. J.*, **108** (2013) 7-13.
- P45 R. Vitale, M. Bevilacqua, R. Bucci, A.D. Magrì, A.L. Magrì, F. Marini, "A rapid and non-invasive method for authenticating the origin of pistachio samples by NIR spectroscopy and chemometrics", *Chemometr. Intell. Lab. Syst.*, **121** (2013) 90-99.
- P46 M. Bevilacqua, R. Bucci, S. Materazzi, F. Marini, "Application of near infrared (NIR) spectroscopy coupled to chemometrics for dried egg-pasta characterization and egg content quantification", *Food Chem.*, **140** (2013) 726-734.
- P47 E. Salvatore, M. Cocchi, A. Marchetti, F. Marini, A. de Juan, "Determination of phenolic compounds and authentication of PDO Lambrusco wines by HPLC-DAD and chemometric techniques", *Anal. Chim. Acta*, **761** (2013) 34-45.

- P48 S. Serranti, D. Cesare, F. Marini, G. Bonifazi, "Classification of oat and groat kernels using NIR hyperspectral imaging", *Talanta*, **103** (2013) 276-284.
- P49 D. Rago, M. Kristensen, G. Gürdeniz, F. Marini, M. Poulsen, L.O. Dragsted, "A LCMS metabolomics approach to investigate the effect of raw apple intake in the rat plasma metabolome", *Metabolomics*, **9** (2013), 1202-1215.
- P50 E. Brasili, E. Mengheri, A. Tomassini, G. Capuani, M. Roselli, A. Finamore, F. Sciubba, F. Marini, A. Miccheli, "Lactobacillus acidophilus La5 and Bifidobacterium lactis Bb12 Induce Different Age-Related Metabolic Profiles Revealed by ¹H-NMR Spectroscopy in Urine and Feces of Mice", *J. Nutr.*, **143** (2013) 1549-1557.
- P51 F. Marini, R. Bro, "SCREAM: A novel method for multi-way regression problems with shifts and shape changes in one mode", *Chemometr. Intell. Lab. Syst.*, **129** (2013) 64-75.
- P52 A.R. Sprocati, C. Alisi, V. Pinto, M.R. Montereali, P. Marconi, F.Tasso, K. Turnau, G.De Giudici, K. Goralska, M. Bevilacqua, F. Marini, C. Cremisini, "Assessment of the applicability of a "tool-box" designed for microbially assisted phytoremediation: the case study at Ingurtosu mining site (Italy)", *Environ. Sci. Pollut. Res.*, **21** (2014) 6939-6951.
- P53 M. Bevilacqua, R. Nescatelli, R. Bucci, A.L. Magrì, A.D. Magrì, F. Marini, "Chemometric classification techniques as a tool for solving problems in analytical chemistry", *J. AOAC Int.*, **97** (2014) 19-28.
- P54 R. Calvani, E. Brasili, G. Praticò, G. Capuani, A. Tomassini, F. Marini, F. Sciubba, A.Finamore, M. Roselli, E. Marzetti, A. Miccheli, "Fecal and urinary NMR-based metabolomics unveil an aging signature in mice", *Exp. Gerontol.*, **49** (2014) 5-11.
- P55 C. Mazzuca, L. Micheli, F. Marini, M. Bevilacqua, G. Bocchinfuso, A. Palleschi, "Rheoreversible hydrogels in document restoration processes: a versatile tool", *Chem. Centr. J.*, **8** (2014) 10.
- P56 M. Tomassetti, F. Marini, L. Campanella, A. Coppa, "Archaeometric classification of ancient human fossil bones, with particular attention to their carbonate content, using chemometrics, thermogravimetry and ICP emission", *Chem. Centr. J.*, **8** (2014) 26.
- P57 T. Gatta, E. Gregori, F. Marini, M. Tomassetti, G. Visco, L. Campanella, "New approach to the differentiation of marble samples using thermal analysis and chemometrics in order to identify provenance", *Chem. Centr. J.*, **8** (2014), 35.
- P58a R. Tauler, F. Marini, B. Walczak, L. Buydens, R.G. Brereton, W. Buchberger, P.J. Worsfold, "European Analytical Column Number 42", *J. Anal. Chem.*, **69** (2014) 812-816.
- P58b R. Tauler, F. Marini, B. Walczak, L. Buydens, R.G. Brereton, W. Buchberger, P.J. Worsfold, "European Analytical Column Number 42", *Accr. Qual. Assur.*, **19** (2014) 225-229.
- P58c R. Tauler, F. Marini, B. Walczak, L. Buydens, R.G. Brereton, W. Buchberger, P.J. Worsfold, "European Analytical Column Number 42", *Anal. Bioanal. Chem.*, **406** (2014) 3525-3529.
- P58d R. Tauler, F. Marini, B. Walczak, L. Buydens, R.G. Brereton, W. Buchberger, P.J. Worsfold, "European Analytical Column Number 42", *Trends Anal. Chem.*, **56** (2014) IX-XIII.
- P58e R. Tauler, F. Marini, B. Walczak, L. Buydens, R.G. Brereton, W. Buchberger, P.J. Worsfold, "European Analytical Column Number 42", *J. Serbian Chem. Soc.*, **79** (2014) 509-516.

- P59 L. Rigoni, S. Venti, M. Bevilacqua, R. Bucci, A.D. Magrì, A.L. Magrì, F. Marini, “Quantification of the enantiomeric excess of two APIs by means of near infrared spectroscopy and chemometrics”, *Chemom. Intell. Lab. Syst.*, **133** (2014) 149-156.
- P60 A. Biancolillo, R. Bucci, A.L. Magrì, A.D. Magrì, F. Marini, “Data-fusion for multiplatform characterization of an Italian craft beer aimed at its authentication”, *Anal. Chim. Acta*, **820** (2014), 23-31.
- P61 M. Bevilacqua, F. Marini, “Local classification: Locally weighted-partial least squares-discriminant analysis (LW-PLS-DA)”, *Anal. Chim. Acta*, **838** (2014) 20-30.
- P62 J. Casado, R. Nescatelli, I. Rodriguez, M. Ramil, F. Marini, R. Cela, “Determination of benzotriazoles in water samples by concurrent derivatization-dispersive liquid-liquid microextraction followed by gas chromatography-mass spectrometry”, *J. Chromatogr. A*, **1336** (2014) 1-9.
- P63 A.P. Sobolev, S. Carradori, D. Capitani, S. Vista, A. Trella, F. Marini, L. Mannina, “Saffron Samples of Different Origin: An NMR Study of Microwave-Assisted Extracts”, *Foods*, **3** (2014) 403-419.
- P64 E. Marzetti, F. Landi, F. Marini, M. Cesari, T.W. Buford, T. M. Manini, G. Onder, M. Pahor, R. Bernabei, C. Leeuwenburgh, R. Calvani, “Patterns of circulating inflammatory biomarkers in older persons with varying levels of physical performance: a Partial Least Squares–Discriminant Analysis (PLS–DA) approach”, *Frontiers Geriatr. Med.*, **1** (2014) 27.
- P65 R. Calvani, E. Brasili, G. Praticò, F. Sciubba, M. Roselli, A. Finamore, F. Marini, E. Marzetti, A. Miccheli, “Application of NMR-based metabolomics to the study of gut microbiota in obesity”, *J. Clin. Gastroenterol.*, **48 Suppl.1** (2014) S5-S7.
- P66 E. Brasili, G. Praticò, F. Marini, A. Valletta, G. Capuani, F. Sciubba, A. Miccheli, G. Pasqua, “A non-targeted metabolomics approach to evaluate the effects of biomass growth and chitosan elicitation on primary and secondary metabolism of *Hypericum perforatum* in vitro roots”, *Metabolomics*, **10** (2014) 1186-1196.
- P67 R. Nescatelli, R.C. Bonanni, R. Bucci, A.L. Magrì, A.D. Magrì, F. Marini, “Geographical traceability of extra virgin olive oils from Sabina PDO by chromatographic fingerprinting of the phenolic fraction coupled to chemometrics”, *Chemometr. Intell. Lab. Syst.*, **139** (2014) 175-180.
- P68 E. Marzetti, R. Calvani, M. Lorenzi, F. Marini, E. D'Angelo, A. M. Martone, M. Celi, M. Tosato, R. Bernabei, F. Landi, “Serum levels of C-terminal agrin fragment (CAF) are associated with sarcopenia in older hip fractured patients”, *Exp. Gerontol.*, **60** (2014) 79-82.
- P69 A. Tomassini, A. Vitalone, F. Marini, G. Praticò, F. Sciubba, M. Bevilacqua, M. Delfini, A. Di Sotto, S. Di Giacomo, P. Mariani, C.L. Mammola, E. Gaudio, A. Miccheli, G. Mazzanti, “¹H NMR-based urinary metabolic profiling reveals changes in nicotinamide pathway intermediates due to postnatal stress model in rat”, *J. Prot. Res.*, **13** (2014) 5848-5859.
- P70 A.A. Gowen, F. Marini, Y. Tsuchisaka, S. De Luca, M. Bevilacqua, C. O'Donnell, G. Downey, R. Tsenkova, “On the feasibility of near infrared spectroscopy to detect contaminants in water using single salt solutions as model systems”, *Talanta*, **131** (2015) 609-618.
- P71 A. Guelpa, M. Bevilacqua, F. Marini, K. O'Kennedy, P. Geladi, M. Manley, “Application of Rapid Visco Analyser (RVA) viscograms and chemometrics for maize hardness characterisation”, *Food Chem.*, **173** (2015) 1220-1227.
- P72 A. Miccheli, G. Capuani, F. Marini, A. Tomassini, G. Praticò, S. Ceccarelli, D. Gnani, G. Baviera, A. Alisi, L. Putignani, V. Nobili, “Urinary ¹H-NMR-based

- metabolic profiling of children with NAFLD undergoing VSL#3 treatment”, *Int. J. Obesity*, **39** (2015) 1118-1125.
- P73 M. Tomassetti, F. Marini, L. Campanella, M. Positano, F. Marinucci, “Suitable classification of mortars from ancient Roman and Renaissance frescoes using thermal analysis and chemometrics”, *Chem. Centr. J.*, **9** (2015) 23.
- P74 E. Ghanem, H. Hopfer, A. Navarro, M. Ritzer, L. Mahmood, M. Fredell, A. Cubley, J. Bolen, R. Fattah, K. Teasdale, L. Lieu, T. Chua, F. Marini, H. Heymann, E. Anslyn, “Predicting the composition of red wine blends using an array of multicomponent peptide-based sensors”, *Molecules*, **20** (2015) 9170-9182.
- P75 R. Calvani, F. Marini, M. Cesari, M. Tosato, S.D. Anker, S. von Haehling, R.R. Miller, R. Bernabei, F. Landi, E. Marzetti, “Biomarkers for physical frailty and sarcopenia: state of the science and future developments”, *J. Cachexia Sarcopenia Muscle*, **6** (2015) 278-286.
- P76 F. Marini, D. de Beer, E. Joubert, B. Walczak, “Analysis of variance of designed chromatographic data sets: The Analysis of Variance-Target Projection approach”, *J. Chromatogr. A*, **1405** (2015) 94-102.
- P77 F. Marini, N.B. Gallagher, “Meeting report: ICRM-2014 international chemometrics research meeting”, *Chemometr. Intell. Lab. Syst.*, **146** (2015) 147-148.
- P78 F. Westad, F. Marini, “Validation of chemometric models – A tutorial”, *Anal. Chim. Acta*, **893** (2015) 14-24.
- P79 F. Marini, B. Walczak, “Particle swarm optimization (PSO). A tutorial”, *Chemometr. Intell. Lab. Syst.*, **149** (2015) 153-165.
- P80 M. Tomassetti, F. Marini, R. Bucci, A. Coppa, L. Campanella, “Human fossil bones: archaeometric classification using chemometrics and thermogravimetry. Influence of skeleton fossilization and its anatomical parts”, *Microch. J.*, **124** (2016) 396-401.
- P81 G. Tranfo, E. Pignini, E. Paci, F. Marini, R.C. Bonanni, “Association of exposure to benzene and smoking with oxidative damage to nucleic acids by means of biological monitoring of general population volunteers”, *Environ. Sci. Pollut. Res.*, in press. doi:10.1007/s11356-016-6366-1
- P82 M. Tomassetti, F. Marini, R. Bucci, L. Campanella “A survey on innovative dating methods in archaeometry with focus on fossil bones”, *Trends Anal. Chem.*, **79** (2016) 371-379.
- P83 E. Brasili, A. Miccheli, F. Marini, G. Praticò, M.E. Di Cocco, F. Sciubba, V. Cechinel-Filho, N. Tocci, A. Valletta, G. Pasqua “Metabolic profile and root development of *Hypericum perforatum* L. in vitro roots under stress conditions due to chitosan treatment and culture time”, *Front. Plant Sci.*, **7** (2016) 507.
- P84 C.E. Eskildsen, P.W. Hansen, T. Skov, F. Marini, L. Nørgaard “Evaluation of multivariate calibration models transferred between spectroscopic instruments: Applied to near infrared measurements of flour samples”, *J. Near Infrared Spectrosc.*, **24** (2016) 151-156.
- P85 L. Mannina, F. Marini, R. Antiochia, S. Cesa, A. Magrì, D. Capitani, A.P. Sobolev “Tracing the origin of beer samples by NMR and chemometrics: Trappist beers as a case study”, *Electrophoresis*, **37** (2016) 2710-2719.
- P86 R. Calvani, F. Marini, M. Cesari, T.W. Bruford, T.M. Manini, M. Pahor, C. Leeuwenburgh, R. Bernabei, F. Landi, E. Marzetti “Systemic inflammation, body composition, and physical performance in old community-dwellers”, *J. Cachexia Sarcopenia Muscle*, in press. doi: 10.1002/jcsm.12134
- P87 S. De Luca, M. De Filippis, R. Bucci, A.D. Magrì, A.L. Magrì, F. Marini, Characterization of the effects of different roasting conditions on coffee samples of

different geographical origins by HPLC-DAD, NIR and chemometrics, *Microch. J.*, **129** (2016) 348-361.

P88 S. Hugelier, P. Firmani, O. Devos, M. Moreau, C. Pierlot, F. Marini, C. Ruckebusch, Weighted fuzzy clustering for (fuzzy) constraints in multivariate image analysis– alternating least square of hyperspectral images, *J. Spectral Imaging*, **5** (2016) a7.

P89 F. Marini, M. Tomassetti, M. Piacentini, L. Campanella, P. Flamini, Application of near infrared spectroscopy (NIR), X-ray fluorescence (XRF) and chemometrics to the differentiation of marmora samples from the Mediterranean basin, *Nat. Prod. Res.*, in press. doi: 10.1080/14786419.2016.1190717.

P90 A. Vignoli, D.M. Rodio, A. Bellizzi, A.P. Sobolev, E. Anzivino, M. Mischitelli, L. Tenori, F. Marini, R. Priori, R. Scrivo, G. Valesini, A. Francia, M. Morreale, M.R. Ciardi, M. Iannetta, C. Campanella, D. Capitani, C. Luchinat, V. Pietropaolo, L. Mannina, NMR-based metabolomic approach to study urine samples of chronic inflammatory rheumatic disease patients, *Anal. Bioanal. Chem.*, **409** (2017) 1405-1413.

P91 A. Guelpa, F. Marini, A. du Plessis, R. Slabbert, M. Manley, Verification of authenticity and fraud detection in South African honey using NIR spectroscopy, *Food Contr.* **73** (2017) 1388-1396.

P92 R. Nescatelli, S. Carradori, F. Marini, V. Caponigro, R. Bucci, C. De Monte, A. Mollica, L. Mannina, M. Ceruso, C.T. Supuran, D. Secci, Geographical characterization by MAE-HPLC and NIR methodologies and carbonic anhydrase inhibition of Saffron components, *Food Chem.*, **221** (2017) 855-863.

P93 F. Marini, D. de Beer, N.A. Walters, A. de Villiers, E. Joubert, B. Walczak, Multivariate analysis of variance of designed chromatographic data. A case study involving fermentation of rooibos tea, *J. Chromatogr. A*, in press. doi: 10.1016/j.chroma.2017.02.007.

P94 R. Calvani, F. Marini, M. Cesari, M. Tosato, A. Picca, S.D. Anker, S. von Haehling, R.R. Miller, R. Bernabei, F. Landi, E. Marzetti. For the SPRINTT Consortium, Biomarkers for physical frailty and sarcopenia, *Aging Clin. Exp. Res.*, in press. doi 10.1007/s40520-016-0708-1

2) Book chapters

B01 F. Marini, “Non-linear modeling: neural networks”. In: B. Walczak, R. Taulèr, S.D. Brown (eds.), *Comprehensive Chemometrics*, vol. 3, Elsevier, Amsterdam, The Netherlands, 2009, pp.477-505.

B02 F. Marini, R. Bucci, A.D. Magrì, A.L. Magrì, “Multivariate analysis of NMR data”. In: E. Brosio (ed.), *Basic NMR in food characterization*, Research Signpost, Kerala, India, 2009, pp.79-92.

B03 F. Marini, R. Bucci, A.L. Magrì, A.D. Magrì, “An overview of the chemometric methods for the authentication of the geographical and varietal origin of olive oils”. In: V.R. Preedy, R.R. Watson (eds.), *Olives and olive oil in health and disease prevention*, Academic Press, Oxford, UK, 2010, pp.569-579.

B04 D. Marini, F. Marini, “Neutral Lipids”, In: L.M.L. Nollet, F. Toldra (eds.), *Food analysis by HPLC*, 3rd ed., CRC Press, Boca Raton, FL, 2013, pp. 139-218.

B05 F. Marini, “Introduction”. In: F. Marini (ed.), *Chemometrics in Food Chemistry*, Elsevier, Amsterdam, The Netherlands, 2013, pp. 1-5.

- B06 F. Westad, M. Bevilacqua, F. Marini, "Regression". In: F. Marini (ed.), *Chemometrics in Food Chemistry*, Elsevier, Amsterdam, The Netherlands, 2013, pp. 127-170.
- B07 M. Bevilacqua, R. Bucci, A.D. Magri, A.L. Magri, R. Nescatelli, F. Marini, "Classification and Class-Modelling". In: F. Marini (ed.), *Chemometrics in Food Chemistry*, Elsevier, Amsterdam, The Netherlands, 2013, pp. 171-233.
- B08 J.M. Amigo, F. Marini, "Multiway Methods". In: F. Marini (ed.), *Chemometrics in Food Chemistry*, Elsevier, Amsterdam, The Netherlands, 2013, pp. 265-313.
- B09 E. Salvatore, M. Bevilacqua, R. Bro, F. Marini, M. Cocchi, "Classification methods for multi-way arrays as a basic tool for food PDO authentication". In: M. de la Guardia, A. Gonzalves (eds.), *Food Protected Designation of Origin. Methodologies and applications*, Elsevier, Oxford, UK, 2013, 339-382.
- B10 M. Bevilacqua, F. Biasioli, F. Gasperi, F. Marini, "Advances in analysis of instrumental food sensory quality data". In: D. Kilcast (ed.), *Instrumental assessment of food sensory quality: A practical guide*, Woodhead Publishing, Cambridge, UK, 2013, pp. 313-351.
- B11 A. Raffo, A. D'Aloise, E. Lardschneider, F. Paoletti, F. Marini, R. Bucci, M. Kelderer, "Effect of soil nutrition on aroma compound formation in organically grown apples (cv. Golden delicious)". In: V. Ferreira, A. Lopes (eds.), *Flavour science*, Elsevier, Oxford, 2014, pp. 173-176.
- B12 F. Marini, "Chemometrics". In: B. Caballero, P. Finglas, F. Toldrá (eds.), *Encyclopedia of food and health*, Elsevier, Oxford, UK, Academic Press, Oxford, UK, 2016, vol. 2, pp. 1-9.
- B13 F. Marini, "Triacylglycerols. Characterization and determination". In: B. Caballero, P. Finglas, F. Toldrá (eds.), *The Encyclopedia of Food and Health*, Academic Press, Oxford, UK, 2016, vol. 5, pp. 345-350.

3) Books edited.

L01 F. Marini, *Chemometrics in Food Chemistry, Data Handling in Science and Technology series*, vol. 28, Elsevier, Amsterdam, The Netherlands, 2013. ISBN 978-0444595287.

4) Proceedings in book.

- A01 F. Marini, "Non-linear class-modeling using Artificial Neural Networks", *Sixth International Conference on Fuzzy Systems and Knowledge Discovery, 2009. FSKD '09*, vol.7, IEEE Computer Society, Piscataway, NJ, 2009, pp.271-273.
- A02 S. Bellato, V. Del Frate, A. Conciatori, A. Cammerata, D. Sgrulletta, E. De Stefanis, A. D. Magri, F. Marini, "Comparison of near infrared transmittance and near infrared reflectance spectroscopy to select high nutritional value naked oats", In: S. Saranwong, S. Kasemsumran, W. Thanapase, P. Williams (eds), *Near Infrared Spectroscopy: Proceedings of the 14th International Conference*, IM Publication, Chichester, UK, 2010, pp.415-420.