



Straightforward approach in cultural heritage and environment studies—multivariate analysis and chemometry

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For the 6th edition of the biennial Mediterranean meeting CMA4CH, held in Rome (Italy) from 18th to 19th of December 2016, this special issue was produced containing a selection of nine articles. From the first edition, the Meeting has the following patrons: UNESCO, La Sapienza University of Rome, Ministry of Cultural Heritage and Activities, Italian Chemical Society, National Research Council (CNR), and Federchimica. Also for this edition we have obtained sponsorship from Umetrics, ArsMensurae, and Marco Valerio Editions. The main guideline and theme of the Meeting was the multivariate and chemometric analysis used as a direct approach to the study of cultural heritage and the environment. The biennial meetings were born in 2006 to bring together researchers from all over the Mediterranean basin; in these years, they have received considerable interest also from researchers distant from the Mediterranean area and we could have welcome the interesting research of people from Spain, Romania, Bulgaria, Germany, the USA, Iran, Brazil, and Cuba. Precious information and knowledge, contained in over 400 oral and poster contributions, were produced. In addition, together with the meetings, the course on chemometric methods is held by internationally renowned chemometers that deal with all chemometric methods applied in different fields: materials sciences, nanotechnologies, physical sciences, chemistry, and medical studies. In the 2 days of this edition we have been confronted with the participating researchers on the use of statistical methods, multivariate, and chemometric approaches to solve or, at least, to help solve environmental and cultural problems, remembering that the two fields are closely related to each other. The presentations, based on plenary lectures and oral and poster communications, covered different aspects, some of which are innovative also from

the technological point of view. All abstracts (collected in a proceeding book with ISBN) passed a double-blind peer review. The selection made by the scientific committee has been difficult and we apologize to all the researchers who are not present in this special issue: the editors are firmly convinced that the other documents may merit publication. Without prejudice to the main theme set out above, the selected articles can be divided into three sections: the first on environmental analyzes, the second on cultural heritage and the third on chemistry; constituted respectively by four, three, and two articles. The articles dealing with environmental problems are three out of four focusing on the PAH survey, indicating considerable interest in this class of polluting compounds. Ielpo et al. performed PM_{2.5} samples in a bakery laboratory from 7 to 19 April 2013. On the daily samples, one every 6 hours, some polycyclic aromatic hydrocarbons (PAH) were determined. The comparison of the average PAH concentrations (obtained with GC-MS-MS analysis) in the four sampling intervals revealed the times with higher values. Furthermore, 3D CFD (Computational Fluid Dynamics) simulations were performed to obtain information on the dynamics of pollutants and on the dispersion in the bakery store products. Mistaro et al. used exploratory data analysis techniques on the results of the PM₁₀ analyzes collected in four locations in Friuli Venezia Giulia (Italy). The compulsory elements plus other seven additional were investigated; BaP plus other 15 PAHs congeners. The analysis techniques showed useful information in the data set: similarities and differences between the different areas, defining the predominantly urban or predominantly industrial characteristic; chemical signatures of the different point or areal sources, both industrial (foundries and coke oven) and urban (traffic and domestic heating). Tomassetti et al. underline one of the negative points of the use of ethanol in fuels and biofuels, whose use is aimed at reducing pollution due to fossil fuels. The presence of ethanol in natural waters increases the solubility of BTX and simultaneously exerts diauxic effects during the biodegradation of BTX. An economic method is proposed for the analytical determination of ethanol; based on an enzymatic direct catalytic fuel cell (DMFC). The PCA representation allowed to identify the sub-clusters due to the different

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ethanol content in the samples. Tranfo et al. quantified five hydroxy-PAHs and cotinine (nicotine metabolite) in human urine by HPLC-MS-MS. Comparing the results of urine samples from 445 non-smokers and 153 smokers (from the same area of Central Italy) information on levels and different sources of exposure was obtained. 6-OHNP_y and 3-OHBaPy are not influenced by the status of smoker and are particularly suitable biomarkers for the study of exposure to environmental pollution. Furthermore, a significant difference was observed in diesel exhaust exposure between males and females. The articles concerning cultural heritage are representative of three research fields on whose data it is possible to carry out restoration and conservation interventions. De Lorenzi Pezzolo et al. carried out a preliminary investigation for the identification of possible sources of materials used by the Romans in the construction of a building of the Imperial age located in Lio Piccolo (Venice). Five diffuse mortar fragments were analyzed using diffuse reflectance infrared Fourier transform spectroscopy, whose DRIFT spectra were compared by analysis of the main components with those of 15 sand samples from the lagoon bottom, from the sea shore, and from the Brenta and Piave river be. Siani et al. carried out a preliminary analysis of the thermal behavior of the La Polledrara paleontological site in Cecanibbio (Rome), carrying out a long-term microclimatic monitoring campaign combined with a simulation model of the entire building calibrated using only measurements of the hourly internal temperature and different thermo-physical properties of external walls and soil. Preliminary results of the simulated thermal behavior were compared with the measured data using the Taylor diagram. The articles concerning purely chemiometry illustrate how it can be applied to any field of investigation. Marini et al. after having characterized, both qualitatively and quantitatively, samples of green coffee of Arabica (23) and Robusta (14), of different geographical origin, have shown that the use of different chemometric methods for the optimization of experimental procedures and processing and the interpretation of spectroscopy (NIR spectroscopy) and chromatographic (HPLC-DAD) data is a valid, versatile, and very promising strategy for quality control of coffee samples. Always Marini et al. have developed a non-destructive methodology based on near infrared and able to authenticate the hazelnuts, since the collection area can define small variations in the chemical composition of the fruits, influencing their quality. Two different classification approaches have been tested, a discriminant one, a partial analysis of the least squares and one of class modeling, an independent soft modeling of class analogies. Both methods led to a very high prediction capacity in external validation on a test set. We conclude by thanking each author for his generous commitment to contribute to the realization of this special issue and the editors of the magazine who have managed the proposals and suggested to all readers to be present in the 2018 edition of the CMA4CH Meeting.



Giovanni Visco is currently a contract professor at the University La Sapienza in Rome, Italy. Since 2001, he teaches in the degree course “Technologies for the Preservation and Restoration of Cultural Heritage” of the Faculty of Mathematical, Physical, and Natural Sciences. He is the creator, organizer, and coordinator of the biennial International Meeting CMA4CH (Chemometrics and Multivariate Analysis applied to Cultural Heritage and Environment) from 2006 until today. In

the past work as coordinator of teachers and lecturers in the Regional Training Course on Chemometrics-Data-Evaluation of the International Atomic Energy Agency (IAEA), held in Tirana, Albania, 10–14 December 2007. He is a guest editor of Special Issues, related to editions of the Meeting CMA4CH, in international journal such as *Microchemical Journal*, *Chemistry Central Journal*, *Current Analytical Chemistry*, and *Environmental Science and Pollution Research*. He is already a teaching owner “Data processing and Chemometrics in the chemical and agro-food Automation Tools and Information in the product laboratory” at the University of Cassino; already an adjunct professor for the supplementary course “Applications of Computer in Laboratory” at La Sapienza University; already a contract professor in the supplementary course “Application of Computer in Analytical Chemistry Program” at La Sapienza University; already holds a research grant “Monitoring via screening and confirmatory methods, using sensors and biosensors, the quality of drinking water with the use of chemometric methods of calculation and multivariate,” by La Sapienza University. He is a professional contract at the Department of Chemistry, La Sapienza University “Data processing for the classification of archaeological findings using pattern recognition analysis.” He is the author of about 60 publications for which the statistical treatment of the data was within its exclusive competence.



Emanuele Dell'Aglio received his Master in Science and Technology for the Conservation of Cultural Heritage, with honors, in 2017 at the “La Sapienza” University of Rome. Currently he is continuing his studies by attending the course Degree in Analytical Chemistry at the same University. He is a member of research groups whose objectives are the preservation of Cultural Heritage through the production of innovative methodologies and tools for conservation and restoration, in this regard since

2018 participates in the Italian national project “Smart Cities.” He is actively involved in the field of scientific dissemination as a member of the jury of national awards for scientific dissemination; moreover, he writes from 2017 articles published on the blog “Research for Cultural Heritage.” From the 6th edition of the Mediterranean meeting CMA4CH (2016) he is part of the organizing committee. He is author of articles and posters on new methods of restoration and environmental monitoring of natural waters.