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Short communication

Conference report: The first "food and drug testing workshop" (FDT-2018), 12–14 December, Genoa, Italy

Cristina Malegori[a], Paolo Oliveri[a], Alexey Pomerantsev[b,c], Oxana Rodionova[b,c,*]

[a] Department of Pharmacy, University of Genoa, Viale Cembrano, 4, I-16148 Genoa, Italy
[b] N.N. Semenov Institute of Chemical Physics RAS, Kosygin 4, 119991 Moscow, Russia
[c] Institute of Natural and Technical Systems RAS, 354024 Sochi, Russia

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The first Food and Drug Testing 2018 conference was held in Genoa (Italy), 12–14 December 2018. The aim of the conference was to establish an international platform of experts from academia, regulatory institutions and industry, for the definition and discussion of key aspects and issues in the analysis of food and pharmaceutical products, with a specific focus on the verification of authenticity claims. All the parts of the analytical workflow – from sampling design to instrumental measurements and multivariate data processing – were critically examined and debated. The meeting was intended to provide a unified, open, cross-disciplinary and interactive forum for the exchange of information and ideas within the scientific community operating in the field of targeted and non-targeted analytical techniques and chemometric strategies (both method development and applications) for the verification of authenticity and counterfeiting of food and pharmaceutical products. Researchers from several areas (analytical methods, data processing, regulatory aspects, agro-food, drugs and pharma) attended the workshop for discussion of new trends and challenges in the field. The Scientific Committee was composed by Alexey Pomerantsev and Oxana Rodionova (Institute of Chemical Physics, Russian Academy of Sciences, Moscow), Paolo Oliveri and Cristina Malegori (Department of Pharmacy, University of Genoa).

Three days of scientific sessions, with oral presentations and in-depth discussions, resulted in the exchange of ideas and new collaborations. To provide an opportunity for wider debate, a reduced number of recognized experts on food and drug authentication was invited to contribute with an oral communication.

The purpose of this meeting report is to briefly present the relevant contribution of each expert to the Workshop; for the detailed program, please visit the website http://www.sisnir.org/food-testing-2018.

Claudia Paoletti from the European Food Safety Authority (EFSA) talked about the critical role of representative sampling before analysis. She outlined the necessary-and-sufficient theory of sampling (TOS) principles and sampling unit operations that will guarantee a full understanding and full acceptance of the need for relevant sampling before adequate analysis, in order to be able to secure only representative analytical results. Moreover, she provided a comprehensive overview on the role of EFSA in the food safety and authenticity fields.

Alessandra Biancolillo from the University of Rome "La Sapienza" discussed the chemometric tools used for food authentication. She presented the classification approaches that can be combined with spectroscopy in order to authenticate specific food items.

This topical issue was continued by *Cristina Alamprese* from the University of Milan who debated a fingerprinting workflow for food authentication, from the experimental design to data processing, passing through representative sampling and analytical measurements, and showing the way forward to filling some gaps in the regulations.

Pierre Dardenne, from Belgium, reported on the untargeted contaminant detection by FTIR and window PCA. He talked about a novel approach that is to check new spectra *vs*. a clean library and looking at the X-residues not from a global PCA model, but with double local procedures. The first procedure is done by selecting the most similar samples among the clean spectra of the product library. The second local PCA models are calculated along the selected spectra by moving windows. The proposed method seems to be sensitive to get low level of

* Corresponding author at: N.N. Semenov Institute of Chemical Physics RAS, Kosygin 4, 119991 Moscow, Russia.
E-mail address: rcs@chph.ras.ru (O. Rodionova).

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contaminants

Oxana Rodionova from the Institute of Chemical Physics, Russian Academy of Sciences talked about the discriminant analysis in comparison with the class modeling in authentication. In general, authentication is the process of determining whether an object is, in fact, what it is declared to be. Class-modeling methods are well suited for solving such type of problems. The main drawback of the discriminant analysis is inability of proper classification of new samples, which do not belong to any of the predefined classes. To manage this shortcoming a soft allocation approach can be applied.

Paolo Oliveri from the University of Genoa contributed to the discussion with the talk 'Recent chemometric trends for the verification of authenticity: a real alternative to class-modeling?' He presented novel approaches from the literature, which were evaluated in depth, and critically compared with standard class-modelling strategies, verifying whether they actually represent or not a reliable and more efficient alternative for addressing authentication problems.

Claudia Beleites from the Julius-Kühn-Institut (Berlin), reported on the sample structures in NIR spectroscopy of cacao beans. She presented experimental designs that allow estimating the size of nested confounders and combined them with iterative selection of reference analyses. She also discussed the implications of the observed data structures for internal and external validation of the models.

Federico Marini from the University of Rome "La Sapienza" talked about the recent advances in class-modeling for single and multiple blocks. He presented a possibility of extending class-modeling approaches and, specifically, the SIMCA algorithm, to deal with irregular shapes of the class spaces. Both the kernel methods and the extended local approaches to class-modeling were discussed, using real and simulated data as benchmark.

Marina Cocchi from the University of Modena and Reggio Emilia presented preliminary results for authentication of *Parmigiano Reggiano* cheese obtained by a handheld Raman spectrometer. This technology allows measuring the intact sample also without removing it from the bag. The results obtained by class-modeling (SIMCA) are extremely promising, showing sensitivity and specificity of 100% for the test set.

Cristina Malegori from the University of Genoa talked about the potential of an innovative analytical strategy, based on hyperspectral imaging in the near infrared region (HSI-NIR), coupled with multivariate pattern recognition techniques, for the identification of defects in green coffee. The developed models demonstrated possibility not only to separate defective beans but also to classify various defects, with a high percentage of correct assignations for each class.

Authentication of green coffee by means of NIR hyperspectral imaging was also considered in the talk given by *Rosalba Calvini* from the University of Modena and Reggio Emilia. She reported on discrimination between Arabica and Robusta coffee species that can be achieved using the NIR hyperspectral imaging, since it allows to obtain chemical information of large sample amounts in real time.

Giovanna Esposito from the Istituto Zooprofilattico Sperimentale (IZS) del Piemonte e della Valle D'Aosta presented the activities of the IZS in the field of food fraud detection. In particular, she talked about alteration of fish by monitoring the levels of trimethylamine (TMA) and about the olive oil authentication by means of mass spectrometry.

Viacheslav Artyushenko, from ArtPhotonics GmbH gave a talk on the advantages of fiber spectroscopy in the 300 nm–16 μm range for real-time food analysis. He explained that, in cases when no single spectroscopic method can be selected, two or three methods may be united in one combi-fiber probe for the synergy fusion of multi-spectral data. This approach enables to achieve the most sensitive and precise process control parameters on-line or even in-line.

Alexey Pomerantsev from the Institute of Chemical Physics, Russian Academy of Sciences reported on the case study of detection of the 'high quality' falsified medicines using *VisCam* and NIR-based analysis. The counterfeits were recognized using a model that had been previously developed and stored in a library for everyday monitoring in drugstores. Additionally, he presented a new instrument, *VisCam*, which was applied to a visual analysis of the primary and secondary packages. This instrument helps revealing hidden violations in the primary and secondary packages.

Emiliano Genorini, from VIAVI Solutions talked about using handheld NIR for identification of street drugs and especially narcotics. He reported that MicroNIR OnSite is a perfect solution for this request. Heroin, cocaine, methamphetamine and different marijuana are easily identified and quantified with a cloud prediction app on mobile phones based on Android or iOS.

Remo Simonetti from Janssen Pharmaceutical Companies, reported on the content uniformity evaluation in a pharmaceutical continuous manufacturing line. He presented methodology of the quality control that utilizes a NIR test method for the uniformity of dosage units test. This method allows the determination of the content uniformity for both API's from one single NIR spectrum and consists of two calibration models (one for each API).

The concluding talk was given by *Riccardo Leardi* from University of Genoa. He presented a brilliant example of multivariate evaluation of particle size distribution of an active principle ingredient. It was demonstrated that the Principal Component Analysis applied to the granulometric distribution curves detects two significant components; the first one being related to the average particle size, and the second one being related to variability of the particle size. The PCA scores can be used as X variables in the case of experimental design.

An interactive round table, coordinated by *Marina Cocchi* and *Alexey Pomerantsev*, provided the occasion for creating a wide and open debate on current limitations and challenges in the strategies for the verification of authenticity of food and drug products, with a special focus not only on technical and scientific issues, but also on regulatory aspects.

The workshop took place in an evocative location inside the *Convento di Santa Maria di Castello*, a church and religious complex located in the *Castello* hill in Genoa. The church, in Romanesque style, was erected before 900 CE. It houses many artworks commissioned by the main noble families of Genoa to the famous artists from the 15th and 16th century Genoese school.

FDT-2018 was accompanied with series of very interesting social events: the guided tours (in Italian, English, and Russian) in the *Santa Maria di Castello* complex, a brilliant exhibition of paintings by the renowned Genovese artist *Gian Marco Crovetto*, and a social dinner in the hearth of the medieval vicoli, where food testing naturally turned into food tasting. The closing discussion confirmed a high evaluation of the results achieved by the Organizing Committee headed by Paolo Oliveri and Cristina Malegori, and revealed a unanimous consent to continue the series of these Christmas workshops on Food and Drug Testing. It was decided that the next edition will be held in Germany in 2020.

Declaration of interests

None.

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