

Exploring common and distinct information among three different kinds of NIR instruments by means of chemometrics

Original

Exploring common and distinct information among three different kinds of NIR instruments by means of chemometrics / Cavallini, N., Giraud, A., Pennisi, F., Esposito, G., Pezzolato, M., Savorani, F.. - ELETTRONICO. - (2021), pp. 89-90. (National Symposium of NIR Spectroscopy - NIR Italia online online 24-25 febbraio 2021) [10.5281/zenodo.4550844].

Availability:

This version is available at: 11583/2874003 since: 2021-03-11T15:04:19Z

Publisher:

InnoRenew CoE

Published

DOI:10.5281/zenodo.4550844

Terms of use:

This article is made available under terms and conditions as specified in the corresponding bibliographic description in the repository


Publisher copyright

(Article begins on next page)

National Symposium of NIR Spectroscopy


NIR Italia online

24-25 February 2021

 waiting for Slovenia 2022

Book of abstracts



Welcome / Benvenuto

Gentili Soci, Colleghi ed Amici SISNIR,

sono molto felice di porgervi, a nome di tutto il Direttivo e mio personale, un caloroso benvenuto a questo importante appuntamento per la nostra Società.

Come prima cosa vorrei ringraziare tutto il Comitato Organizzatore di 'NIRItalia online 2021, waiting for Slovenia 2022', in particolar modo la nostra collega Anna Sandak per il grande lavoro svolto. Vorrei ringraziare tutti Voi per essere presenti così numerosi e ringraziare i relatori che interverranno in queste due giornate, in particolare gli invited speaker Dr. José Manuel Amigo e Dr. Ingunn Burud e la Prof.ssa Dolores Perez-Marin.

Un ringraziamento speciale va infine alle aziende che da sempre sostengono SISNIR e che hanno sponsorizzato questo evento: Bruker, Buchi, Hellma, Termo Fisher e Viavi.

Il programma scientifico di questo Congresso è ricco e stimolante e, nello specifico, accanto a tematiche di consolidata tradizione per la nostra Società, approfondirà anche argomenti e sfide più recenti.

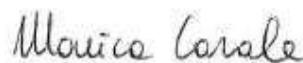
Ci auguriamo che questo evento, grazie alle relazioni scientifiche e ai numerosi momenti di confronto, possa offrire validi spunti di discussione concorrendo al raggiungimento degli obiettivi della Società, ossia quelli della formazione e divulgazione scientifica.

Quello che sicuramente ci mancherà sarà l'aspetto umano...prima di essere colleghi, siamo un gruppo di amici e il Simposio NIRItalia ha sempre rappresentato un momento unico di scambio scientifico ma anche di 'scambio di abbracci'.

L'Italia sta attraversando uno dei periodi più difficili dal secondo dopoguerra; ognuno di noi è stato toccato più o meno da vicino da questa triste situazione, ma se un lato positivo in tutto questo può esserci, è che questa pandemia ha fatto capire che la Ricerca Scientifica è il solo strumento di cui disponiamo per fronteggiare simili problemi su scala mondiale. Ci auguriamo che una volta usciti da questa emergenza l'attenzione nei confronti della Ricerca Scientifica, e dell'Istruzione e Cultura in genere, non cali.

Tornando alla nostra Società, noi del Direttivo crediamo che tanta strada sia stata fatta ma che tanta ne rimanga ancora da percorrere, anche in un'ottica di rafforzamento del rapporto e della collaborazione fra ricerca accademica e industria.

Pertanto, con la soddisfazione per le mete raggiunte e con lo sguardo rivolto ai nuovi obiettivi che cercheremo di realizzare grazie all'impegno e la partecipazione attiva di tutti, Vi auguriamo un buon NIRItalia online 2021, waiting for Slovenia 2022!



Monica Casale
(Presidente SISNIR)

NIRItalia online 2021 host welcome / Benvenuto dall'ospitante NIRItalia online 2021

We are very pleased to welcome you to “NIRItalia online 2021, waiting for Slovenia 2022” Organising the NIRItalia conference has been a point of pride for us at the University of Primorska and InnoRenew CoE. While we will miss having you all visit us for the event this year, we are happy that we could still manage to organize the conference for all the presenters and attendees to share and to continue moving the field ahead.

The NIRItalia online 2021 programme is filled with novel research, and we are looking forward to hearing all about it. We are sure the online conference will foster the open discussion and knowledge-sharing of past conferences and encourage you to reach out to your peers and carry on the discussions after the conference.

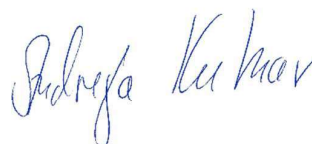
NIR spectroscopy is an exciting field with opportunities for many disciplines to contribute to its use and development. This sort of interdisciplinary field is exciting for us, and why the University of Primorska and InnoRenew CoE have invested in personnel and NIR spectroscopy equipment to help shape the future of its use in science and industry. We look forward to 2022, when NIRItalia will return to its usual form and be hosted in Slovenia. At that point, construction of the new InnoRenew CoE building will be complete and we are eager to invite you to visit.

On behalf of both the University of Primorska and the InnoRenew CoE, we would like to thank the organizing committee for their hard work, the participants for submitting their work, and all attendees for their patience and interest in NIR spectroscopy. We wish you well and welcome you to “NIRItalia online 2021, waiting for Slovenia in 2022.”



Michael Burnard, PhD
Deputy Director
InnoRenew CoE

Assistant Professor
Programme Coordinator, Data Science
Master's Degree Programme
University of Primorska



Andreja Kutnar, PhD
Director
InnoRenew CoE

Professor
Programme Coordinator,
Renewable Materials and Healthy
Built Environment PhD
Programme
University of Primorska

NIRItalia online 2021 organizing committee welcome / Benvenuto dal comitato organizzativo NIRItalia online 2021

Following the pandemic situation that continues to affect Europe and the whole World, Consiglio Direttivo SISNIR decided to postpone our regular NIRItalia Symposium to year 2022. In the meantime, we agreed that it is important to organize an additional event entitled “NIRItalia online 2021, waiting for Slovenia 2022”, which we do believe is a great opportunity to see each other, at least virtually, to present works, as well to exchange ideas, opinions, and future perspectives.

We are especially pleased to present you two distinguished keynote speakers, and dear Friends, Dr Ingunn Burud and Dr José Manuel Amigo who will share with us their years of experiences with NIR spectroscopy by presenting the cutting-edge research in our field. We are also happy to have with us Prof Dolores Perez-Marin who will introduce the new COST action CA19145 “European Network for assuring food integrity using non-destructive spectral sensors”, that is closely related to our SISNIR activities.

Please notice that abstracts submitted by you are available in SISNIR community at Zenodo.org repository. You can access these with the QR code provided below. We do hope that the content of this virtual event will be interesting for you and may encourage you to join us next year in Koper.

Wishing you a fruitful and inspirational time,



Anna Sandak on behalf of “NIRItalia online 2021” organizing committee



Conference chairpersons / Presidenti di conferenza

- Monica Casale, *University of Genoa, DIFAR*
- Anna Sandak, *InnoRenew CoE, University of Primorska, FAMNIT*

Scientific committee / Comitato scientifico

- Monica Casale, *University of Genoa, DIFAR*
- Silvia Grassi, *University of Milan, DeFENS*
- Cristina Malegori, *University of Genoa, DIFAR*
- Federico Marini, *Sapienza University of Rome, Chemistry Department*
- Anna Sandak, *InnoRenew CoE, University of Primorska, FAMNIT*
- Jakub Sandak, *InnoRenew CoE, University of Primorska, IAM*
- Alessandro Ulrici, *University of Modena and Reggio Emilia, Department of Life Sciences*

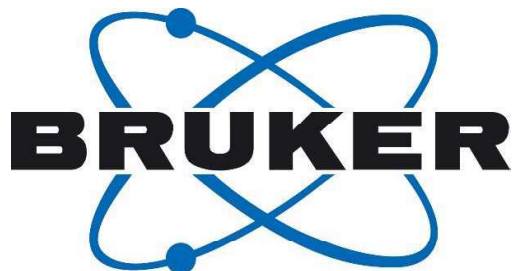
Organizing committee / Comitato organizzatore

- Liz Dickinson, *InnoRenew CoE*
- Oihana Gordobil, *InnoRenew CoE*
- René Herrera, *InnoRenew CoE, University of the Basque Country*
- Veerapandian Ponnuchamy, *InnoRenew CoE*
- Faksawat Poohphajai, *InnoRenew CoE*
- Lea Primožič, *InnoRenew CoE*
- Hana Remešová, *InnoRenew CoE*
- Nežka Sajinčič, *InnoRenew CoE, University of Primorska, PEF*
- Anna Sandak, *InnoRenew CoE, University of Primorska, FAMNIT*
- Amy Simmons, *InnoRenew CoE, University of Primorska, IAM*
- Tine Šukljan, *InnoRenew CoE, University of Primorska, IAM*
- Domen Vake, *InnoRenew CoE*

Editors / Editrici

- Anna Sandak, *InnoRenew CoE, University of Primorska, FAMNIT*
- Nežka Sajinčič, *InnoRenew CoE, University of Primorska, PEF*
- Hana Remešová, *InnoRenew CoE*
- Elizabeth Dickinson, *InnoRenew CoE*

Sponsors / Sponsor



VIAVI Solutions



Patronage / Patrocini



Program / Programma

Day 1 24.02.2021

Hour	Presenter	Title
09:15	Monica Casale	Welcome from SISNIR, InnoRenew CoE and organizing committee
09:25	Tine Šukljan	Explanation how to use ZOOM
09:30	José Manuel Amigo	Keynote 1: To what Extent can We detect Microplastics with NIR Imaging
10:00		Discussion
10:10		Break



Agro-food oral session 1, chair Silvia Grassi

10:20	Alessandro Giraud	NIR and Visible Spectroscopies coupled with chemometrics for the evaluation of edible seed oils quality evolution during storage under different illumination conditions
10:30	Marilena Paolini	Durum Wheat quality prediction for breeding purposes with NIRS
10:40	Francesca Di Donato	Sequential data fusion techniques for the authentication of the P.G.I. Senise ("Crusco") pepper bell
10:50		Discussion
11:00		Sponsors session #1 BUCHI
11:10		Break



Agro-food oral session 2, chair Silvia Grassi

11:20	Lorenzo Strani	Assessment of frying oil quality by FT-NIR spectroscopy
11:30	Stefania Costa	Selection of intact garlic cloves for in-field sowing based on NIR spectroscopy attribution of grade of infection
11:40	Andrea Casson	Near infrared spectroscopy as a green technology for more sustainable analyses on intact olive and olive oil
11:50		Discussion
12:00		Sponsors session #2 Thermo Fisher Scientific



Agro-food poster session, chair Silvia Grassi

12:10	Marco Bragolusi	A data fusion model of NIR and RAMAN techniques for the geographical screening of Italian extra virgin olive oil
12:12	Ilaria Lanza	NIR spectroscopy application for assessment of the PDO Asiago cheese variety
12:14	Eleonora Loffredi	Development of a Diffuse Reflectance FT-NIR Spectroscopy Method for the Shell Egg Quality Assessment
12:16	Valentina Giovenzana	Packaging influence in optical analysis of minimally processed and ready to eat <i>Valerianella locusta</i> L. by visible/near infrared (vis/NIR) spectroscopy to monitor shelf life
12:18	Cristina Alamprese	Prediction of Olive Chemical Characteristics by FT-NIR Spectroscopy
LUNCH UNTIL 14:00		



Functional NIR oral session, chair Federico Marini

14:00	Nežka Sajinčič	Brain Imaging with Functional Near-Infrared Spectroscopy in Educational Research
14:10	Abimbola Y. Ikoyi	Impact of Sample Volume and Wavelength Region on Near Infrared Reflectance Spectroscopy (NIRS) Prediction of Inorganic Nutrient Components in Equine Faeces
14:20		Discussion
14:30		Sponsors session #3 BRUKER
14:40		Break



Imaging oral session, chair Cristina Malegori

14:50	Rosalba Calvini	NIR-Hyperspectral Imaging for the quantification of rind percentage in grated Parmigiano Reggiano cheese
15:00	Jakub Sandak	Characterization of heritage objects with NIR hyperspectral imaging
15:10	Giorgia Sciotto	Clustering-based automated data-reduction for the processing of hyperspectral data on paintings
15:20		Discussion
15:30	Mohamad Ahmad	Recovering biological fluids signature from near-infrared hyperspectral images
15:40	Vicky Caponigro	Identification of dried bacteria related to dairy industry using NIR Spectral Imaging at different spatial scales
15:50		Discussion
16:00		Break



Forestry-wood oral session, chair Jakub Sandak

16:10	Manuela Mancini	Use of infrared spectroscopy for a sampling study of waste wood samples in a panel board industry
16:20	Veerapandian Ponnuchamy	Stability of cellulose in water cluster – insight from density functional theory and infrared spectroscopy
16:30	Oihana Gordobil	Study of lignin-water molecular interactions using NIR spectroscopy: the effect of the drying process of the hardwood kraft lignin
16:40	Jakub Sandak	Off-line timber sorting with portable NIR spectrometer – feasibility study for glulam production
16:50		Discussion
17:00		Closing of the day 1

Day 2 25.02.2021

Hour	Presenter	Title
09:15	Monica Casale	Welcome from SISNIR, and organizing committee
09:25	Tine Šukljan	Explanation how to use ZOOM
09:30	Ingunn Burud	Keynote 2: NIR spectral imaging as a tool in basic and applied research, from astronomy to wood science
10:00		Discussion
10:10	Lola Perez Marin	Presentation of the COST Action CA 19145
10:20		Break



Portable instruments, PAT & Industry oral session, chair Alessandro Ulrici

10:30	Alessio Tugnolo	Stand-alone LED sensors for future field monitoring of grape (<i>Vitis vinifera</i> L.) ripeness
10:40	Morandise Rubini	Applicability of a Handheld NIR spectrometer to determine the quality of maritime pine resin (<i>Pinus pinaster</i>) in situ forest
10:50	Paolo Berzaghi	Performances of handheld NIR instruments on wet and dry forages
11:00		Discussion
11:10	Silvia Grassi	A PAT approach for common wheat with IIoT NIR devices
11:20	Monica Casale	NIR spectroscopy for Engine Oil characterisation
11:30		Discussion
11:40		Sponsors session #4 VIAVI
11:50		Break



Chemometrics, aquaphotomics and pharma oral session, chair Monica Casale

12:00	Nicola Cavallini	Exploring common and distinct information among three different kinds of NIR instruments by means of chemometrics
12:10	Federico Marini	Preprocessing revisited
12:20	Tiziana Cattaneo	NIRS and Aquaphotomics for the Evaluation of the Efficiency of Solar Dehydration Processes
12:30	Ilaria Lanza	Bee pollen pyrrolizidine alkaloids detection by NIR spectroscopy
12:40		Discussion
12:50		Sponsors session #5 Hellma



Portable instruments, PAT & Industry poster session, chair Alessandro Ulrici

13:00	Valentina Giovenzana	Experimentation of an optical prototype for monitoring the ripening of table tomatoes (<i>Solanum lycopersicum</i> L., Marinda F1) and oil olives (<i>Olea europaea</i> L.)
13:02	Paolo Berzaghi	Forage calibration transfer between near infrared laboratory and handheld instruments
13:04	Daniela Summa	NIR spectroscopy-based determination of carotenoids content in ice-cream supplemented with carrot lyophilized extract
13:06	Silvia Grassi	SUPERCHILL! Study of ice crystal formation in beef

13:08	Best oral and best poster voting
	LUNCH UNTIL 14:30
14:30	SISNIR assembly
16:30	Closing of the conference

Exploring common and distinct information among three different kinds of NIR instruments by means of chemometrics

N. Cavallini^{1*}, A. Giraud¹, F. Pennisi², G. Esposito², M. Pezzolato², F. Savorani¹

¹ Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24 – 10129 Torino, Italy; nicola.cavallini@polito.it

² Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, via Bologna 148 – 10154 Torino, Italy

Food fraud is an old but still common and widespread problem that affects almost any type of food commodity sold on the market. Products may be mislabelled or counterfeit and, in many cases, it can be very difficult to detect these illegal practices. For this reason, quick and reliable methods are needed for efficiently tackling this problem. Due to its ease of use and rapidity, near-infrared (NIR) spectroscopy is particularly suitable for the purpose. In this study, the subtle differences between fresh and thawed cephalopods were investigated using different NIR instruments to collect the data and different chemometric approaches to perform the data analysis.

Fifty fresh cephalopod specimens of both cuttlefish (*Sepia officinalis*) and musky octopus (*Eledone spp.*) were collected directly at the food distribution warehouse and immediately analysed at refrigeration temperature (~5°C). Then, the specimens were kept frozen at -20°C for at least 48 hours and eventually thawed and analysed once again. Data collection was performed by measuring the same specimens using three different NIR spectrometers: one portable low-cost instrument (SCiO by Consumer Physics), one portable moderately high-cost instrument (MicroNIR by Viavi), and one benchtop instrument (MPA by Bruker). The common and distinct information among the three data sources was investigated by means of a mid-level data fusion approach (Borràs et al., 2015) and by means of methods such as CovSel (Covariance Selection–Roger et al., 2011) and ComDim (Common Dimensions–Cariou et al., 2019).

Differently from other traditional techniques employed for counteracting fraud, NIR spectroscopy coupled with chemometrics proves a robust approach for distinguishing between fresh and frozen cephalopods. Similarities and differences among the three NIR datasets, unravelled by the tested chemometric tools, reflect the building characteristics of each instrument and provide a complementary picture of the specimens' evolution during the freeze-thaw process.

Keywords: chemometrics, data fusion, cephalopods, authenticity, NIR instruments

Acknowledgements: This study is supported by the Italian Ministry of Health under Grant nr. IZSPLV 02-18 - RC.

REFERENCES

Borràs, E., Ferré, J., Boqué, R., Mestres, M., Aceña, L., Busto, O., 2015. Data fusion methodologies for food and beverage authentication and quality assessment – A review. *Anal. Chim. Acta* 891, 1–14. <https://doi.org/10.1016/j.aca.2015.04.042>

Cariou, V., Jouan-Rimbaud Bouveresse, D., Qannari, E.M., Rutledge, D.N., 2019. ComDim Methods for the Analysis of Multiblock Data in a Data Fusion Perspective, in: Data Handling in Science and Technology. Elsevier Ltd, pp. 179–204. <https://doi.org/10.1016/B978-0-444-63984-4.00007-7>

Roger, J.M., Palagos, B., Bertrand, D., Fernandez-Ahumada, E., 2011. CovSel: Variable selection for highly multivariate and multi-response calibration. Application to IR spectroscopy. Chemom. Intell. Lab. Syst. 106, 216–223. <https://doi.org/10.1016/j.chemolab.2010.10.003>

DOI: <https://doi.org/10.5281/zenodo.4550844>

NIRItalia online 2021 - Book of abstracts

Online conference, 24-25 February 2021

Kataložni zapis o publikaciji (CIP) pripravili v Narodni in univerzitetni knjižnici v Ljubljani
COBISS.SI-ID=53127939
ISBN 978-961-95303-0-6 (pdf)

This work is available for free on the NIRItalia online website:
<https://niritalia2020.sisnir.org/en/book-of-abstract/>

Editors: Anna Sandak, Nežka Sajinčič, Hana Remešová, Elizabeth Dickinson
Publisher: InnoRenew CoE, Livade 6, 6310 Izola, Slovenia
First Published: 25 February 2021

InnoRenew CoE is funded by the European Commission under Horizon 2020, the EU Framework Programme for Research and Innovation (H2020 WIDESPREAD-2-Teaming #739574), and by investment funding from the Republic of Slovenia and the European Regional Development Fund.

This publication and the abstracts within are published under the [Creative Commons Attribution 4.0 International License](#). Abstract copyrights belong to their authors.

