NIR Italia 2022

7-9 June 2022

beyond spectral range

Book of abstracts

Benvenuto

Gentili Soci, Colleghi ed Amici SISNIR,

è per me un grande piacere essere qui oggi: questo evento rappresenta oltre ad un importante appuntamento per la nostra Società, anche una nuova ripartenza in presenza dopo 2 anni difficili.

Come prima cosa vorrei ringraziare tutto il Comitato Organizzatore di 'NIRITALIA2022', in particolar modo la nostra collega Anna Sandak per il lavoro svolto. Vorrei ringraziare tutti Voi per essere presenti e ringraziare i relatori che interverranno in queste due giornate, in particolare gli invited speaker Jean-Michel Roger, Krzysztof B Bec e Justyna Grabska.

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

Sono molto felice di porgerVi, a nome di tutto il Direttivo e mio personale, un caloroso benvenuto, Vi auguriamo di trascorrere giornate ricche sotto tanti punti di vista.

In particolare, 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.

Ci auguriamo inoltre di poter trascorre giornate piacevoli assieme in questa magnifica cornice di Isola e di ritrovare i momenti di socialità che tanto ci sono mancati.

Vi auguro un Buon NIRITALIA2022!

Monica Casale
(Presidente SISNIR)

9th National Symposium host welcome

We are very pleased to welcome you to the 9th National Symposium of the Italian Society for Near Infrared Spectroscopy (SISNIR). Organising the conference has been a point of pride for us at the University of Primorska and InnoRenew CoE. We are particularly pleased to organise this event in our new building, which we hope you will have an opportunity to see and will inspire you to visit us again in the near future.

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

NIR spectroscopy is widely applicable in various disciplines. This sort of interdisciplinary science is exciting for us, and this is why the University of Primorska and InnoRenew CoE have invested in personnel and spectroscopic equipment to help shape the future of spectroscopy in science and industry.

On behalf of both the University of Primorska and InnoRenew CoE, we would like to thank the organising committee for their hard work, the participants for submitting their work, the sponsors for their support, and all attendees for their interest in this topic. We wish you a productive conference that will inspire you in your future research.

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

9th National Symposium organising committee welcome

Despite the pandemic that continues to affect Europe and the whole world, and the difficult political situation in Europe related to the ongoing war in Ukraine, we are very pleased to be able to organise the 9th National Symposium of SISNIR in Izola, Slovenia. We do believe it is a great opportunity to meet each other face to face, to present our work, as well as exchange ideas, opinions, and future research topics.

We are especially pleased to present our four distinguished keynote speakers and dear friends, Dr. Jean-Michel Roger, Dr. Justyna Granska, and Dr. Krzysztof Bec who will share with us their years of experience in NIR spectroscopy and present cutting-edge research in this field. We are also thankful to our sponsors Bruker, Buchi, Hellma, itphotonic, QuantumDesign and VIAVI Solutions for their generous support.

Wishing you a fruitful and inspirational time,

Anna Sandak
on behalf of the 9th National Symposium
organising committee

Conference chairpersons

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

Scientific committee

- 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

- Albert Kravos, InnoRenew CoE
- Amy Simmons, InnoRenew CoE, University of Primorska, IAM
- Anna Sandak, InnoRenew CoE, University of Primorska, FAMNIT
- Benjamin Božič, InnoRenew CoE
- Faksawat Poohphajai, InnoRenew CoE
- Gertrud Fábián, InnoRenew CoE
- Jakub Sandak, InnoRenew CoE, University of Primorska, IAM
- Lea Primožič, InnoRenew CoE
- Liz Dickinson, InnoRenew CoE
- Nežka Sajinčič, InnoRenew CoE
- Oihana Gordobil, InnoRenew CoE
- René Herrera, InnoRenew CoE, University of the Basque Country
- Richard Acquah, InnoRenew CoE
- Sasikala Perumal, InnoRenew CoE
- Tine Šukljan, InnoRenew CoE, University of Primorska, IAM
- Veerapandian Ponnuchamy, InnoRenew CoE

Editors: Anna Sandak, Nežka Sajinčič, Monica Casale

Program / Programma

Tuesday, 07.06.2022

10:00 12:00		**Training 1: Practical exercise with NIR instruments** Sponsors
12:00 14:00		Lunch break
14:00 16:00		**Training 2: Theoretical course – data pre-treatment** Jean Michel Roger
16:15 18:00		Ice breaker – welcome reception

Wednesday, 08.06.2022

09:00		Registration
09:40		Welcome
10:00	Keynote #1: Krzysztof Beć & Justyna Grabska	In silico simulation of NIR spectra: fundamental insights, new discoveries and emerging possibilities for analytical applications
11:00		Coffee break sponsored by **Bruker**
		Session #1: Environment & Agriculture *Session chair: Jakub Sandak*
11:20	Elena Leoni	Performance evaluation of NIR prediction models of moisture content on industrial woodchip
11:40	Gasparini Andrea	Evaluation of the antioxidant capacity of the hydrophilic and lipophilic extract of hemp seed cake of different varieties
12:00	Myriam Catalá	Metabolomic analysis of the global molecular fingerprint and aquaphotomic analysis of the dehydration-rehydration cycle of the symbiotic aeroterrestrial microalga Asterochloris erici
12:20		**Sponsor presentation** **Bruker**
12:40 13:40		Lunch break

13:40 14:00		Poster session
		Session #2: Imaging *Session chair: Silvia Grassi*
14:00	Danial Fatchurrahman	Prediction of nutritional quality and the astringency of Black chokeberry (Aronia melanocarpa L.) using a Hyperspectral Imaging System in the Visible-NIR and Near-Infrared regions
14:20	Rosalba Calvini	NIR Hyperspectral imaging for on-field detection of Halyomorpha halys
14:40	Cristina Malegori	Near infrared hyperspectral imaging and multivariate image analysis for microplastics identification and haracterisation in aquatic samples
15:00	Maria Luisa Amodio	Potential application of hyperspectral imaging and FT-NIR spectroscopy for discrimination of soilless tomato according to cultivation practices with different level of sustainability
15:20		Sponsor presentation **Buchi**
15:40		Coffee break sponsored by **Buchi**
16:00 17:40		**SISNIR general assembly**
17:40-19:00		Free time

Thursday, 09.06.2022

09:00		Registration
10:00	Keynote #2: Jean-Michel Roger	**Increasing the robustness of chemometric models by calibration transfer, orthogonal projections, domain adaptation**
		Session #3: Pharmaceutical *Session chair: Federico Marini*
10:20	Remo Simonetti	The central role of NIR spectroscopy in the oral solid dosage Real Time Release testing
10:40	Monica Casale	A moving-block-PCA based approach for real time monitoring of a powder blending process using a miniaturized near infrared sensor

11:00	Coffee break	
	Session #4: PAT & chemometrics *Session chair: Alessandro Ulrici*	
11:20	Eleonora Mustorgi	Multivariate qualitative approaches for on-line monitoring of a mixing process using a miniaturized NIR probe
11:40	Lorenzo Strani	On-line prediction of ABS quality parameters fusing NIR and process sensors data using different multiblock approaches
12:00	Federico Marini	Strategies for non-linear modelling of NIR data
12:20 13:40	Lunch break	
13:40 14:00	Poster session	
	Session #5: Food part 1 *Session chair: Cristina Malegori*	
14:00	Alessandro Giraudo	3-2-1: Three NIR instruments, two fish species, one chemometric approach
14:20	Marco Bragolusi	Combination of NIR spectroscopy and LASSO modelling for black pepper authentication: development of the method, exploration of validation strategies and build-up of a user-friendly online application for large-scale screening
14:40	Silvia Grassi	FT-NIR spectroscopy for vinegar adulteration assessment
15:00	Sponsor presentation **Hellma**	
15:20	Coffee break sponsored by **Helma**	
	Session #6: Food part 2 *Session chair: Monica Casale*	
15:40	Giuseppina Marello	Validation and accreditation of automatic method in NIR Near Infrared Spectroscopy on butter matrix
16:00	Alessia Pampuri	Grape polyphenol content prediction through vis/NIR spectroscopy in a view of real time application at winery consignment
16:20	Nicola Cavallini	Measure your bratwurst: quantifying the content of mechanically separated meat by means of NIR spectroscopy and chemometrics

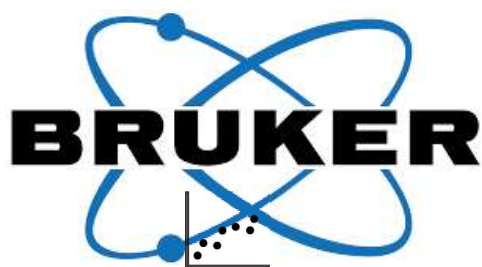| 16:40 17:40	🏆	**Best oral and poster presentation award & closing of the conference**

Friday, 10.06.2022

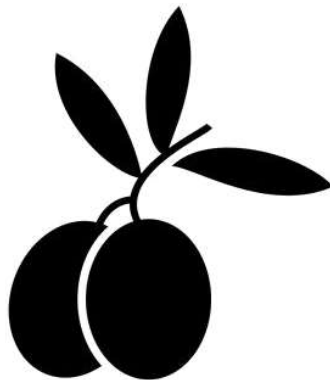| 11:15 15:00	⛰️	Post-conference tour

Sponsor Gold

Sponsor Silver

Session #5:
Food part 1

Sessione #5:
Alimenti – prima parte

Alessandro Giraudo

3-2-1: Three NIR instruments, two fish species, one chemometric approach

A. Giraudo[1*], N. Cavallini[1], F. Pennisi[2], G. Esposito[2], M. Pezzolato[2], F. Geobaldo[1], F. Sa-vorani[1], E. Bozzetta[2]

[1] Department of Applied Science and Technology, Polytechnic of Turin, Corso Duca degli Abruz-zi, 24, 10129, Turin, Italy
[2] Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, via Bologna 148 – 10154, Turin, Italy
*Corresponding author (alessandro.giraudo@polito.it)

Fish identification on the market can be very challenging for both consumers and experienced inspectors in the cases of fish sold as fillets (Acutis et al., 2019). In this field, reference, and gold standard analyses to identify animal species generally require rather long processing times, but quick decision-making is fundamental in preventing and counteracting frauds (Grassi et al., 2018).

This study investigated the performance of NIR spectroscopy as a fast and non-destructive method to distinguish between two very similar flatfish species, namely the Guinean sole (Synaptura cadenati) and European plaice (Pleuronectes platessa). Fifty fillets of each species were analysed using three near-infrared (NIR) instruments: the handheld SCiO (by Consumer Physics) and MicroNIR (by VIAVI), and the benchtop MPA (by Bruker). All the collected spectra were processed by applying the same chemometric approach, i.e., pre-processed and used to build PLS-DA classification models, whose performances were evaluated and compared. All the three instruments provided very good results, showing high accuracy: both SCiO and MicroNIR reached 94.1 % accuracy, while MPA spectrometer reached 90.1 %. Moreover, a thorough interpretation of actual chemical signals, as recorded by the three NIR instruments, was provided. The good results in classification obtained by combining NIR spectroscopy and simple chemometric modelling techniques suggest a direct applicability of the method, also using cheap portable instruments, both in the context of real-world marketplaces and in official control plans.

Keywords: food frauds, Guinean sole, European plaice, NIR spectroscopy, chemometrics

REFERENCES
Acutis, P.L., Cambiotti, V., Riina, M.V., Meistro, S., Maurella, C., Massaro, M., Stacchini, P., Gili, S., Malandra, R., Pezzolato, M., Caramelli, M., Bozzetta, E., 2019. Detection of fish species substitution frauds in Italy: A targeted National Monitoring Plan. Food Control 101, 151–155. https://doi.org/10.1016/j.foodcont.2019.02.020
Grassi, S., Casiraghi, E., Alamprese, C., 2018. Handheld NIR device: A non-targeted approach to assess authenticity of fish fillets and patties. Food Chem. 243, 382–388. https://doi.org/10.1016/j.foodchem.2017.09.145

Alessandro Giraudo

3-2-1: Tre strumenti NIR, due specie di pesce, un approccio chemiometrico

A. Giraudo[1*], N. Cavallini[1], F. Pennisi[2], G. Esposito[2], M. Pezzolato[2], F. Geobaldo[1], F. Sa-vorani[1], E. Bozzetta[2]

[1]Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino,
Corso Duca degli Abruz-zi, 24, 10129, Torino, Italia
[2] Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta,
via Bologna 148 – 10154, Torino, Italia
*Corresponding author (alessandro.giraudo@polito.it)

L'identificazione del pesce presente sul mercato può risultare molto complessa, sia per il consumatore sia per valutatori esperti, nel caso in cui il pesce venga venduto a filetti (Acutis et al., 2019). In questo contesto, le analisi di riferimento e gli standard volti all'identificazione delle specie solitamente richiedono tempistiche piuttosto lunghe, ma la rapidità di intervento decisionale è fondamentale nella prevenzione e nel contrasto delle frodi (Grassi et al., 2018). Questo studio ha indagato le prestazioni della spettroscopia NIR come metodo rapido e non distruttivo per differenziare tra due specie di filetti di pesce molto simili, ossia la sogliola della Guinea (Synaptura cadenati) e la platessa europea (Pleuronectes platessa). Cinquanta filetti di ciascuna specie sono stati analizzati utilizzando tre strumenti nel vicino infrarosso (NIR): il palmare SCiO (Consumer Physics), il portatile MicroNIR (VIAVI) e quello da banco MPA (Bruker). Tutti gli spettri acquisiti sono stati elaborati utilizzando il medesimo approccio chemiometrico, ossia pretrattati ed impiegati per l'implementazione di modelli di classificazione PLS-DA, le cui prestazioni sono state valutate e confrontate. Tutti e tre gli strumenti hanno fornito risultati molto buoni, mostrando un'elevata accuratezza: sia lo SCiO sia il MicroNIR hanno raggiunto il 94,1% di accuratezza, mentre lo spettrometro MPA ha raggiunto il 90,1%. Inoltre, è stata fornita un'interpretazione approfondita dei segnali chimici effettivi ottenuti dai tre strumenti NIR.
I buoni risultati in classificazione ottenuti combinando la spettroscopia NIR e semplici tecniche di modellazione chemiometrica suggeriscono un'applicabilità diretta del metodo, anche tramite dispositivi portatili economici, sia in ambito commerciale, sia nei piani di controllo ufficiali.

Parole chiave: frodi alimentari, sogliola della Guinea, platessa europea, spettroscopia NIR, chemiometria

Riferimenti bibliografici:
Acutis, P.L., Cambiotti, V., Riina, M.V., Meistro, S., Maurella, C., Massaro, M., Stacchini, P., Gili, S., Malandra, R., Pezzolato, M., Caramelli, M., Bozzetta, E., 2019. Detection of fish species substitution frauds in Italy: A targeted National Monitoring Plan. Food Control 101, 151–155. https://doi.org/10.1016/j.foodcont.2019.02.020
Grassi, S., Casiraghi, E., Alamprese, C., 2018. Handheld NIR device: A non-targeted approach to assess authenticity of fish fillets and patties. Food Chem. 243, 382–388. https://doi.org/10.1016/j.foodchem.2017.09.145