



# NIR Italia 2022

7-9 June 2022

beyond spectral range

## Book of abstracts



Società Italiana di Spettroscopia NIR



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# 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
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- Tine Šukljan, InnoRenew CoE, University of Primorska, IAM
- Veerapandian Ponnuchamy, InnoRenew CoE







# Program / Programma







## Tuesday, 07.06.2022

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


## Wednesday, 08.06.2022

|   |   |   |
|---|---|---|
| 09:00   |  | Registration  |
| 09:40   |   | Welcome   |
| 10:00   | Keynote #1:<br>Krzysztof Beć &<br>Justyna Grabska                                   | In silico simulation of NIR spectra: fundamental insights, new discoveries and emerging possibilities for analytical applications   |
| 11:00   |  | Coffee break sponsored by <b>Bruker</b>   |
|  | Session #1: Environment & Agriculture<br><i>Session chair: Jakub Sandak</i>         |   |
| 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 <i>Asterochloris erici</i> |
| 12:20   |  | Sponsor presentation<br><b>Bruker</b>   |
| 12:40<br>13:40  |   | Lunch break   |






|   |   |   |
|---|---|---|
| 13:40<br>14:00  |    | Poster session  |
|  <b>Session #2: Imaging</b><br><i>Session chair: Silvia Grassi</i> |   |   |
| 14:00   | Danial Fatchurrahman  | Prediction of nutritional quality and the astringency of Black chokeberry ( <i>Aronia melanocarpa</i> 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 <i>Halyomorpha halys</i>  |
| 14:40   | Cristina Malegori   | Near infrared hyperspectral imaging and multivariate image analysis for microplastics identification and characterisation 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<br><b>Buchi</b>  |
| 15:40   |   | Coffee break sponsored by <b>Buchi</b>  |
| 16:00<br>17:40  |  | <b>SISNIR general assembly</b>  |
| 17:40-<br>19:00   |  | Free time   |

## Thursday, 09.06.2022

|  |                                  |   |
|--|----------------------------------|---|
| 09:00  | Registration                     |   |
| 10:00  | Keynote #2:<br>Jean-Michel Roger | Increasing the robustness of chemometric models by calibration transfer, orthogonal projections, domain adaptation                |
|  <b>Session #3: Pharmaceutical</b><br><i>Session chair: Federico Marini</i> |                                  |   |
| 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   |   |
|  <b>Session #4: PAT &amp; chemometrics</b><br><i>Session chair: Alessandro Ulrici</i> |  |   |
| 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<br>13:40   |  Lunch break                              |   |
| 13:40<br>14:00   |  Poster session                           |   |
|  <b>Session #5: Food part 1</b><br><i>Session chair: Cristina Malegori</i>            |  |   |
| 14:00  | Alessandro Girauda   | 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<br><b>Hellma</b>  |   |
| 15:20  |  Coffee break sponsored by <b>Helma</b> |   |
|  <b>Session #6: Food part 2</b><br><i>Session chair: Monica Casale</i>              |  |   |
| 15:40  | Giuseppina Marellò   | 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

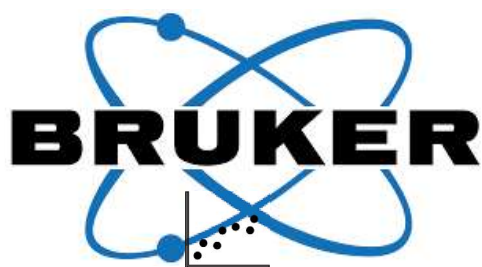
Friday, 10.06.2022

11:15  
15:00



Post-conference tour

## Sponsor Gold



## Sponsor Silver



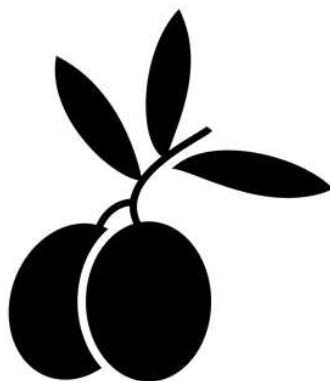
Quantum Design  
ITALY





# Session #6: Food part 2

## Sessione #6: Alimenti - seconda parte





Nicola Cavallini

## Measure your bratwurst: quantifying the content of mechanically separated meat by means of NIR spectroscopy and chemometrics

Nicola Cavallini<sup>1\*</sup>, A. Giraud<sup>1</sup>, F. Pennisi<sup>2</sup>, G. Esposito<sup>2</sup>, M. Pezzolato<sup>2</sup>, F. Savorani<sup>1</sup>

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<sup>2</sup> Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, via Bologna 148, 10154 Torino, Italy

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Any food chain can be affected by food frauds, from mislabelling to authentication counterfeiting. The meat chain is no exception: in the case of processed meat, especially when it is sold minced or in sausage form, it becomes very difficult to distinguish the different ingredients, therefore mislabelling and meat substitution can easily occur. This is especially true with the famous German bratwurst, a type of sausage produced from minced or mechanically separated meat (MSM). MSM is obtained through a high-pressure process aimed at separating the bone from the edible meat tissue: the resulting pureed material is then formed into sausages and cooked. MSM meat is less expensive and of lesser quality compared to selected meat cuts, thus providing an economic incentive for the substitution fraud.

The present study was developed with the aim of determining whether NIR spectroscopy could be used for identifying meat products containing MSM, by means of chemometrics modelling. Alongside the main classification aim, a parallel research line regarding the actual quantification of MSM was developed and is the subject of this study. Bratwursts containing different percentages of MSM were minced and mixed with meat from non-MSM products, with the aim of obtaining new samples with specific MSM percentages. A calibration set of 30 samples spanning the content range between 0 % and 91% (in steps of 10 %) was built, together with a set of 27 samples corresponding to the “5 %” percentages (also in steps of 10 %). All samples were measured using three NIR instruments: the benchtop MPA (Bruker), the portable MicroNIR (Viavi) and the handheld SCiO sensor (Consumer Physics).

One PLS regression (Wold et al., 2001) model for each NIR dataset was developed and validated, and all three analytical techniques yielded good performances in calibration and prediction, with R<sup>2</sup> values above 0.95.

**Keywords:** food fraud, mechanically separated meat, chemometrics, quantification

**Acknowledgements:** The Italian Ministry of Health is greatly acknowledged for funding this research project (Grant nr. IZSPLV 02-18-RC).

### REFERENCES

Wold, S., Sjöström, M., Eriksson, L., 2001. PLS-regression: a basic tool of chemometrics. *Chemom. Intell. Lab. Syst.* 58, 109–130. [https://doi.org/10.1016/S0169-7439\(01\)00155-1](https://doi.org/10.1016/S0169-7439(01)00155-1)

**Nicola Cavallini****Measure your bratwurst: quantifying the content of mechanically separated meat by means of NIR spectroscopy and chemometrics**Nicola Cavallini<sup>1\*</sup>, A. Giraudo<sup>1</sup>, F. Pennisi<sup>2</sup>, G. Esposito<sup>2</sup>, M. Pezzolato<sup>2</sup>, F. Savorani<sup>1</sup><sup>1</sup>Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino<sup>2</sup> Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, via Bologna 148, 10154 Torino, Italy

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Qualsiasi filiera alimentare può essere soggetta a frodi, dalle etichettature errate alla contraffazione di autenticità. La filiera della carne non fa eccezione: nel caso della carne processata, specialmente quando viene venduta macinata o come salsiccia, diventa molto difficile distinguere i diversi ingredienti che la costituiscono, e pertanto risulta più facile sostituire parte della carne impiegata con varietà meno costose e di qualità più bassa. Ciò risulta particolarmente vero nel caso del famoso wurstel tedesco, generalmente prodotto da carne macinata o separata meccanicamente (CSM). La CSM viene prodotta mediante un processo ad alta pressione che separa le ossa dai tessuti edibili: il risultato è una purea che viene modellata nella forma di salsiccia e quindi cotta. La CSM è meno costosa e di qualità inferiore rispetto a tagli selezionati di carne, e ciò può fornire un incentivo economico per la frode della sostituzione. Questo studio è stato sviluppato con l'obiettivo di determinare se la spettroscopia NIR possa venire utilizzata per identificare la presenza di CSM in prodotti a base di carne, mediante modellazione chemiometrica. Parallelamente all'obiettivo principale di classificazione è stata sviluppata una seconda linea di ricerca riguardante la quantificazione della percentuale di CSM: tale linea è l'oggetto di questo studio. Sono stati analizzati due set di campioni preparati appositamente mescolando carne macinata di wurstel contenente CSM in varie percentuali e wurstel senza CSM aggiunta. Sono stati preparati e analizzati: un set di 30 campioni di calibrazione con percentuali nell'intervallo 0 % - 91 % (a passi del 10 %), un test set di 27 campioni con percentuali nel medesimo intervallo, ma corrispondenti agli intermedi fra le decine. Tutti i campioni sono stati misurati con tre strumenti NIR: lo spettrofotometro da banco MPA (Bruker), il portatile MicroNIR (VIAMI) e l'ultra-portatile SCiO (Consumer Physics).

È stato sviluppato e validato un modello di regressione PLS (Wold et al., 2001) per ogni dataset NIR acquisito, ottenendo in tutti e tre i casi buone performance in calibrazione e in predizione, con R<sup>2</sup> superiori a 0.95.

**Parole chiave:** food fraud, mechanically separated meat, chemometrics, quantification**Ringraziamenti:** The Italian Ministry of Health is greatly acknowledged for funding this research project (Grant nr. IZSPLV 02-18-RC).**Riferimenti bibliografici:**Wold, S., Sjöström, M., Eriksson, L., 2001. PLS-regression: a basic tool of chemometrics. *Chemom. Intell. Lab. Syst.* 58, 109-130. [https://doi.org/10.1016/S0169-7439\(01\)00155-1](https://doi.org/10.1016/S0169-7439(01)00155-1)

