# NIR Italia 2022

7-9 June 2022

beyond spectral range

# Book of abstracts
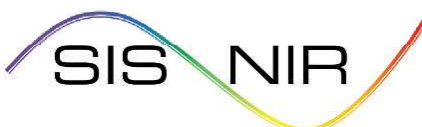
SIS NIR
Società Italiana di Spettroscopia NIR

UP UNIVERSITÀ DEL LITTORALE
UNIVERZA NA PRIMORSKEM

INNORENEW COE

# 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.

<div align="center">

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

</div>

# 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

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- Richard Acquah, InnoRenew CoE
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- 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<br><br>Sponsors |
| --- | --- | --- |
| 12:00 14:00 | | Lunch break |
| 14:00 16:00 | | Training 2: Theoretical course – data pre-treatment<br><br>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<br>*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<br>**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 |

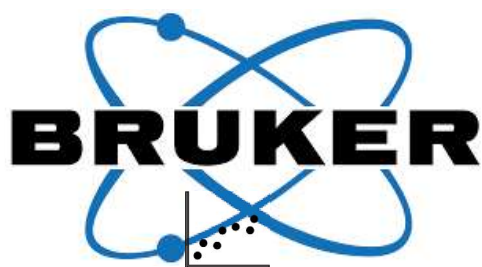| 16:40 17:40 | 🏆 | **Best oral and poster presentation award & closing of the conference** |
|---|---|---|

## Friday, 10.06.2022

| 11:15 15:00 | | Post-conference tour |
|---|---|---|

# Sponsor Gold



# Sponsor Silver

# Francesco Savorani

# Lipids in a nutshell: quickly assess the lipidic content in hazelnuts using NIR spectroscopy

F. Savorani[1]*, E. Cazzaniga[1], Nicola Cavallini[1], A. Giraudo[1]

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Hazelnuts (Corylus avellana L.) are one of the most consumed dry fruits all over the world (Oliveira, et al., 2008). Their success is correlated with their nutraceutical properties, which show a high content in lipids with high nutritional value (Köksal, Artik, Şimşek, & Güneş, 2006). In the present work, we investigate the possibility of using near infrared (NIR) spectroscopy, using both an expensive benchtop spectrometer and a cheap portable instrument, to obtain information concerning the lipids and polyphenols contents of 57 samples of hazelnuts, mainly differing by country of origin (Italy, South America, Turkey, Georgia and Azerbaijan). To this aim, two near-infrared (NIR) instruments were used: a benchtop FT-NIR spectrometer (Multi-Purpose Analyser–MPA, by Bruker) equipped with an integrating sphere and the handheld, battery powered SCiO Pocket molecular sensor (by Consumer Physics).

The collected NIR spectra were inspected through multivariate data analysis. Firstly, a Principal Component Analysis (PCA) model was built to explore the information contained in the samples. Then, a Partial Least Square (PLS) regression model was developed to predict the lipids and polyphenols contents. The MPA instrument showed the best results both for PCA and regression models. The PLS-regression results regarding the lipids content showed much better performances than the polyphenols. The robustness of the model was tested through cross-validation and the regression parameters were $R2 = 0.807$ and $RMSE = 0.839$ (% of lipidic content) in calibration and $RMSEP = 0.609$ in prediction for the lipids, while the same parameters for the polyphenols were much lower, respectively $R2 = 0.606$ and $RMSE = 0.621$ (mg GAE/g nut) in calibration and $RMSEP = 1.071$ in prediction. Due to its limited NIR spectral range, the results obtained through the SCiO portable instrument were not considered suitable for a reliable application to these purposes.

**Keywords:** food, hazelnuts, chemometrics, NIR calibration

REFERENCES
Köksal, A. I., Artik, N., Şimşek, A., & Güneş, N. (2006). Nutrient composition of hazelnut (Corylus avellana L.) varieties cultivated in Turkey. Food Chemistry, 99, 509-515.
Oliveira, I., Sousa, A., Sa Morais, J., Ferreira, I. C., Bento, A., Estevinho, L., & Pereira, J. A. (2008). Chemical composition, and antioxidant and microbial activities of three hazelnut (Corylus avellana L.) cultivars. Food and Chemical Toxicology, 1801-1807.

# Francesco Savorani

## Lipidi "in a nutshell": valutazione rapida del contenuto lipidico di nocciole attraverso spettroscopia NIR

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Le nocciole (Corylus avellana L.) rappresentano uno dei tipi di frutta secca più consumata in tutto il mondo (Oliveira, et al., 2008). Questo successo è dovuto alle loro proprietà nutraceutiche, dovute, tra l'altro, ad un elevato contenuto in lipidi ad alto valore nutrizionale (Köksal, Artik, Şimşek, & Güneş, 2006). In questo lavoro, è stata investigata la possibilità di usare la spettroscopia nel vicino infrarosso (Near Infra-Red spectroscopy), usando sia un costoso spettrometro da banco, sia un economico strumento portatile, per ottenere informazioni riguardanti il contenuto in lipidi e polifenoli su 57 campioni di nocciole, diversi tra loro principalmente in base all'origine (Italia, sud America, Turchia, Georgia e Azerbaijan). A tal fine, sono stati usati due strumenti NIR differenti: uno spettrometro FT-NIR da banco (Multi Purpose Analyser–MPA, Bruker), equipaggiato con una sfera d'integrazione, e uno spettrometro portatile e alimentato a batteria, SCiO Power Molecular Sensor (Consumer Physics).
Gli spettri infrarossi acquisiti sono stati ispezionati attraverso analisi multivariata. Inizialmente è stato costruito un modello esplorativo attraverso Principal Component Analysis (PCA), per evidenziare l'informazione contenuta nei campioni. Successivamente è stato sviluppato un modello di regressione attraverso Partial Least Square (PLS), per predire il contenuto in lipidi e polifenoli. Lo strumento MPA ha dato i risultati migliori sia per PCA che per i modelli di regressione. I risultati ottenuti con PLS in riferimento al contenuto lipidico sono migliori rispetto a quelli per il contenuto di polifenoli. La robustezza del modello è stata testata attraverso cross-validation e i parametri di regressione ottenuti sono $R^2 = 0.807$ e RMSE = 0.839 (% contenuto lipidi) in calibrazione e RMSEP = 0.609 in predizione per i lipidi, mentre gli stessi parametri per i polifenoli sono decisamente più bassi, rispettivamente $R^2 = 0.606$ e RMSE = 0.621 (mg GAE/g nocciola) in calibrazione e RMSEP = 1.071 in predizione. A causa del suo range spettrale limitato nella zona vicino infrarosso, i risultati ottenuti con lo strumento portatile SCiO non sono stati considerati idonei a un'applicazione affidabile per questi scopi.

**Parole chiave**: cibo, nocciole, chemiometria, calibrazione NIR

**Riferimenti bibliografici:**
Köksal, A. I., Artik, N., Şimşek, A., & Güneş, N. (2006). Nutrient composition of hazelnut (Corylus avellana L.) varieties cultivated in Turkey. Food Chemistry, 99, 509-515.
Oliveira, I., Sousa, A., Sa Morais, J., Ferreira, I. C., Bento, A., Estevinho, L., & Pereira, J. A. (2008). Chemical composition, and antioxidant and microbial activities of three hazelnut (Corylus avellana L.) cultivars. Food and Chemical Toxicology, 1801-1807.