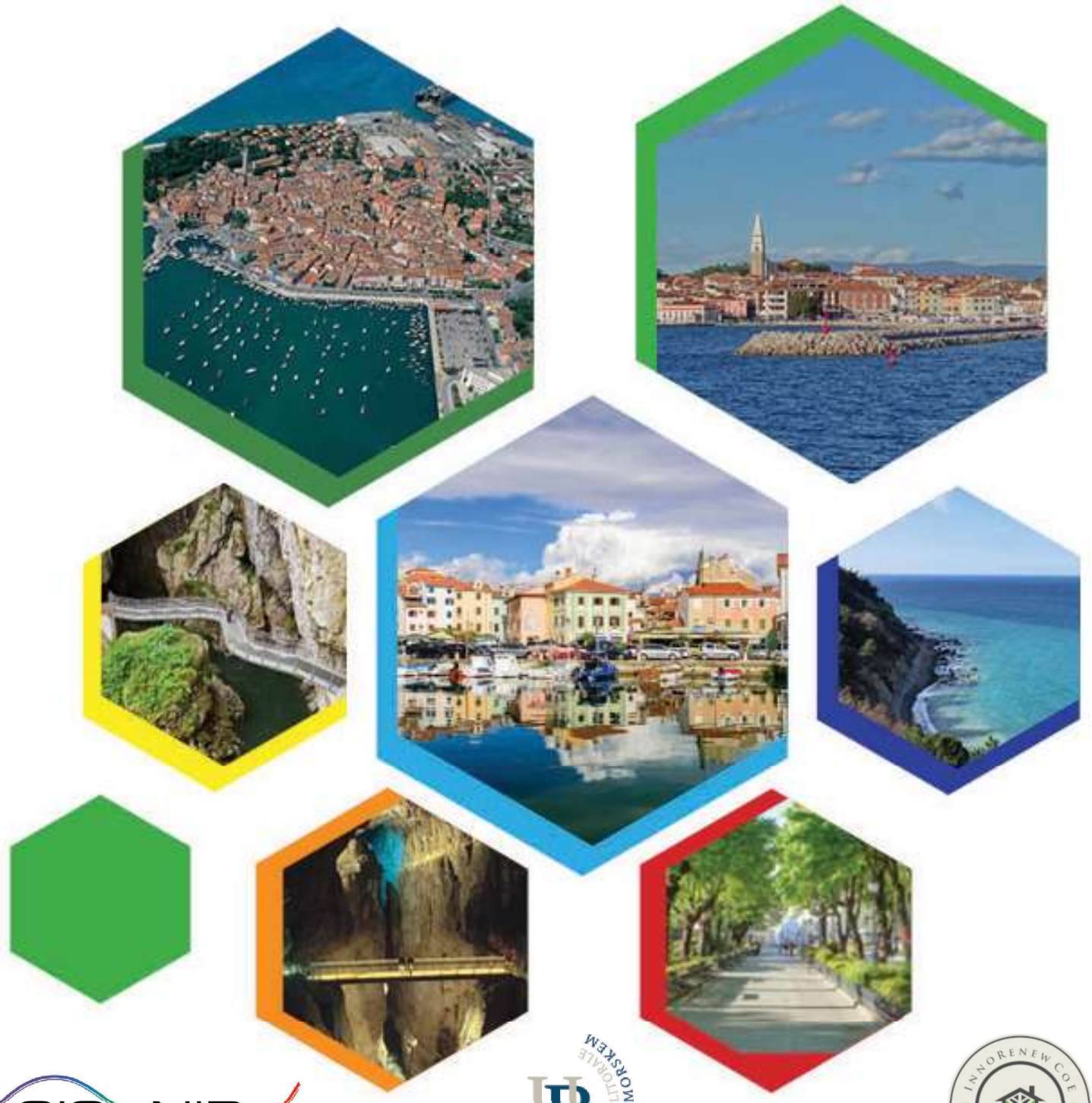
NIR Italia 2022

7-9 June 2022

beyond spectral range

Book of abstracts



SIS NIR

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

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

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- 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

Giovanna Esposito

Discrimination among different fish fillets with NIR spectroscopy

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

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Fish and related products have become categories of food among the most vulnerable to frauds (FAO, 2018). Examples of fraudolent practices are species substitution or mislabelling. Until now several spectroscopic techniques in conjunction with chemometrics have been used to evaluate the quality or the authenticity of seafood products such as vibrational, fluorescence and ultraviolet/visible absorption. Based on this background, in this study a method to distinguish between different types of fish fillets was developed. Five species were selected: Epinephelus costae; Gadus morhua; Pleuronectes platessa; Synaptura cadenati and Chelidonichthys lucerna. The analyses were performed by using three different types of NIR instrument: a bench NIR, a portable micro-NIR and a handheld NIR (SCiO) on 50 samples for each category. Using a chemometric approach to analyse the NIR data, good identification performances were obtained, in fact each NIR instrument allowed to classify fish fillets with an overall accuracy ranging from 65% up to 93%. The proposed method can help in fighting commercial frauds in fish market throughout the entire commercial chain.

Keywords: fish fillets, food frauds, NIR, chemometrics

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

REFERENCES

Food and Agriculture Organization of the United Nations. 2018. OVERVIEW OF FOOD FRAUD IN THE FISHERIES SECTOR. FAO Fisheries and Aquaculture Circular No. 1165

Giovanna Esposito

Discriminazione tra diverse specie di filetti di pesce mediante spettroscopia

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

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Il pesce e i prodotti correlati sono diventati categorie di alimenti tra i più vulnerabili alle frodi (FAO, 2018). Esempi di pratiche fraudolente sono la sostituzione o l'errata etichettatura delle specie. Finora sono state utilizzate diverse tecniche spettroscopiche in combinazione con la chemiometria per valutare la qualità o l'autenticità dei prodotti ittici come la spettroscopia vibrazionale, della fluorescenza e dell'assorbimento nelll' ultravioletto/visibile. Sulla base di queste conoscenze, in questo studio è stato sviluppato un metodo per distinguere tra diversi tipi di filetti di pesce. A tale scopo sono state selezionate cinque specie: Epinephelus costae ; Gadus morhua; Pleuronectes platessa; Synaptura cadenati e Chelidonichthys lucerna. Le analisi sono state eseguite utilizzando tre diversi tipi di strumenti NIR: un NIR da banco, un micro-NIR portatile e un NIR portatile (SCiO), selezionando 50 campioni per ogni categoria. Attraverso un approccio chemiometrico dati NIR sono stati analizzati, ottenendo buone prestazioni di identificazione, infatti ogni strumento NIR ha permesso di classificare i filetti di pesce con un'accuratezza complessiva che va dal 65% al 93%. Il metodo proposto può quindi essere un valido stumento per aiutare a combattere le frodi commerciali nel mercato ittico lungo l'intera catena commerciale.

Parole chiave: filetti di pesce, frode alimentare, NIR, chemiometria

Ringraziamenti: Questo studio è stato supportato dal Ministero della Salute Italiano Grant nr. IZSPLV 02-18 - RC.

Riferimenti bibliografici:

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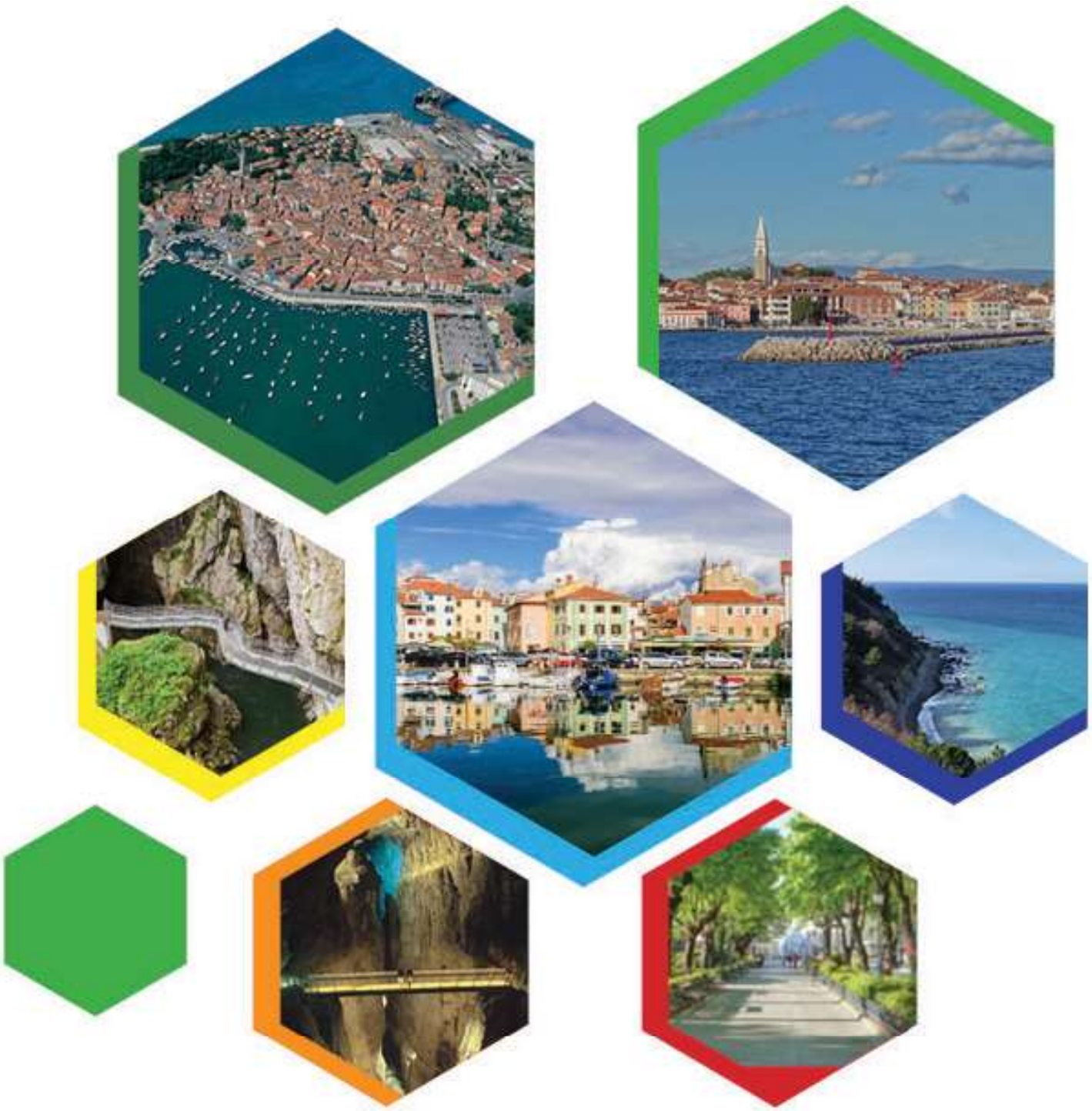

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