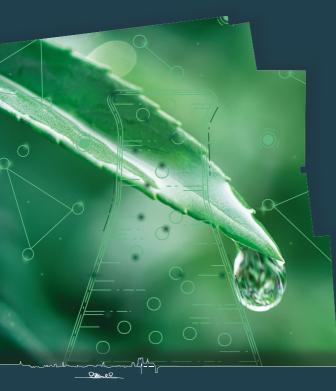
## LE STUDIUM WEBINARS



## 06-07 September 2022 **NaDES** for biomass valorization: new insight of a green technology



### CONVENORS

### Dr Duangjai Tungmunnithum

2021-2022 LE STUDIUM RESEARCH FELLOW / ARD CVL COSMETOSCIENCES PROGRAMME

Mahidol University - TH

### Dr Christophe Hano

Laboratory of Woody Plants and Crops Biology (LBLGC) / INRAe, University of Orléans - FR

### Prof. Leslie **Boudesocque-Delaye**

Synthesis and Isolation of Bioactive Molecules (SIMBA). University of Tours - FR









### **CONVENORS**

### Dr Duangjai Tungmunnithum

2021-2022 LE STUDIUM RESEARCH FELLOW // ARD CVL COSMETOSCIENCES PROGRAMME Mahidol University - TH

Dr Christophe Hano Laboratory of Woody Plants and Crops Biology (LBLGC) / INRAe, University of Orléans - FR

**Prof. Leslie Boudesocque-Delaye** Synthesis and Isolation of Bioactive Molecules (SIMBA), University of Tours - FR

### ORGANIZING COMMITTEE

Sophie Gabillet, General Secretary

Dr Aurélien Montagu, Scientific Manager

Maurine Villiers, Communication & Events Manager

LE STUDIUM Loire Valley Institute for Advanced Studies • Région Centre-Val de Loire • FR

## LE STUDIUM WEBINARS 06-07 SEPTEMBER 2022

### ABSTRACTS

## NaDES for biomass valorization: new insight of a green technology

3

# EDITO

Created in 1996 in the Centre-Val de Loire region, LE STUDIUM Loire Valley Institute for Advanced Studies (IAS) offers a multidisciplinary environment to highly qualified international scientists. LE STUDIUM holds exceptional facilities in the city centre of Orleans, in a newly renovated 17th century building. Its activities cover the entire spectrum of scientific disciplines represented in the Centre-Val de Loire region. LE STUDIUM Loire Valley IAS develops programmes to build new or strengthen existing IAS collaborative relationships with the local and the international community of researchers, developers and innovators.

LE STUDIUM IAS offers to international competitive research scientists the opportunity to discover and work in one of its affiliate laboratories within the University of Tours, the University of Orleans, the National Institute of Applied Sciences (INSA) Centre Val de Loire, the University Hospital of Tours, the Social & Human Sciences Val-de-Loire Centre and the Art & Design Institute ESAD of Orléans, as well as within national research institutions located in Centre-Val de Loire such as BRGM, CEA, CNRS, INSERM, INRAE). The goal is to develop and nurture transdisciplinary approaches as innovative tools for addressing some of the key scientific, socio-economic and cultural questions of the 21st century. LE STUDIUM IAS encourages researchers' exchanges between them and with industries through its links with poles of competitiveness, thematic clusters, technopoles and innovation labs and together with DEV'up, the regional economic development agency. Its various programmes and a large portfolio of events create a virtuous circle of interactions.

Thanks to the faithful partnership and support of the Centre-Val de Loire Regional Council, Orleans Metropole and academic and research partners, LE STUDIUM actions have opened wide arrays of internationalisation and exchanges in the region. Over the past 25 years, LE STUDIUM has welcomed nearly 250 scientists coming from 47 countries for long-term residencies. In addition to their contribution in their host laboratories, researchers participate in the scientific life of the IAS through attendance at monthly interdisciplinary meetings called LE STUDIUM THURSDAYS. Their presentations and debates enrich the regional scientific community at large and are a place of knowledge sharing and scientific awareness. With the IAS's support, and in collaboration with their host laboratory, fellows have the opportunity to organise different types of events: CONFERENCES, WORKSHOPS, SUMMER SCHOOLS and WEBINARS. Experience has shown that these conditions facilitate the development or extension of existing regional and international collaborations and enable the creation of productive new research networks. These events also consist in a real contribution to knowledge sharing and open science. For the period 2015-2021, LE STUDIUM has operated with an award from the European Commission, a programme supporting the mobility of international researchers, the Marie Skłodowska-Curie Actions (MSCA) COFUND programme. For the period 2022-2025, LE STUDIUM has joined the FIAS Programme (French Institute for Advanced Study) alongside five other institutes in France, also supported by the MSCA Actions.

Since 2013, LE STUDIUM is an official partner of the Ambition Research and Development programmes initiated by the Centre-Val de Loire Regional Council to support the smart specialisation strategy (S3) around priority domains: biopharmaceuticals, renewable energies, cosmetics, environmental metrology, digital twins, materials, forestry and natural and cultural heritage. Furthermore, LE STUDIUM recently joined the ATHENA European University Consortium as a partner of the University of Orléans to welcome international fellows from its ten European university partners. All programmes aim to include all major societal challenges with an interdisciplinary approach.

The present LE STUDIUM WEBINAR named "NaDES for biomass valorization: new insight of a green technology" is organised in the framework of the regional COSMETOSCIENCES Ambition Research and Development CVL Programme. With the growing interest in more environmentally friendly solvents and processes, the introduction of Natural Deep Eutectic Solvents (NaDES) as low cost, non-toxic and biodegradable solvents represents a new opportunity for green and sustainable chemistry. This research is critical to address current societal challenges around a more sustainable environment.

We thank you for your participation and we hope scientific presentations will bring knew knowledge, and be intellectually stimulating for your research projects.

### Yves-Michel GINOT

Chairman LE STUDIUM

VITIO

# INTRODUCTION

The principles of 'green chemistry' are gaining traction in many sectors, including cosmetics, due to the need to reduce pollution from toxic chemicals, make industrial processes safer and more sustainable, and provide consumers with 'clean-labeled products'. During the last decade, green technology is moving from an option to a must in modern industrial processing. Plants produce a rich and diverse array of natural products that have been extracted and used by humans for millennia.

With the growing interest in more environmentally friendly solvents and processes, the introduction of Natural Deep Eutectic Solvents (NaDES) as low cost, non-toxic and biodegradable solvents represents a new opportunity for green and sustainable chemistry. Thanks to their remarkable advantages, NaDES are now arousing growing interest in many fields of research such as food, health, cosmetics and biofuels. Around the world, NaDES are seen as a promising alternative to commonly used petrochemical solvents.

This webinar takes place over two half-days, and offers an overview of recent advances in biomass extraction, from raw materials to the latest advances in processes and modeling. The first day is devoted to new perspectives in terms of plant valorization, in particular by addressing biomass, biological activities and bio-transformations. The second day is devoted to advances in extractive processes and the modeling of NaDES.

## PROGRAMME

### TUESDAY 06TH SEPTEMBER (08:45-12:15 GMT+2 PARIS)

**08:45** Official Opening by Aurélien Montagu (LE STUDIUM) & Alexia Soussen (Cosmétosciences Programme)

08:45 Opening conference : Dr Alena Stupar - NADES-solvents of the future

### SESSION 1 : EXTRACTION AND BIOTRANSFORMATION

**09:45 Dr Duangjai Tungmunnithum** - Green NaDES-Based Ultrasound-Assisted Extraction of Antioxidant and Anti-aging Flavonoids from *Opuntia ficus-indica* Oil Seed Cakes (Byproducts)

**10:15** Dr Nemanja Teslic - Carotenoids and ellagic acid extraction with Natural deep eutectic solvents – potential application for cosmetic industry?

**10:45 Dr Gorawit Yusakul -** Therapeutic microemulsion based on hydrophobic-NaDES for Curcuma longa L. extraction and anti-inflammation

**11:15 Dr Erwann Durand** - NaDES (Natural Deep Eutectic Solvents): a new approach inspired by nature to promote the biomass (bio)transformation

**11:45 Prof. Jeongmi Lee -** Applications of deep eutectic solvents for efficient preparation of biopolymers and nanoparticles from natural resources

WEDNESDAY 07TH SEPTEMBER (09:00-12:00 GMT+2 PARIS)

### SESSION 2: INNOVATION PROCESSES AND MODELING

**09:00 Dinis Abranches -** Modelling Deep Eutectic Solvents with Sigma Profiles: from COSMO-RS to Deep Learning

**09:30 Prof. Leslie Boudesocque-Delaye** - Natural Deep Eutectic Solvents in microalgae biorefinery: a bioinspired technology for sustainable multistep processes

**10:05 Prof. Ana Rita Duarte -** Innovation in extraction processes using natural deep eutectic systems

10:30 Dr Nicolas Papaiconomou - TBC

SESSION 3: ROUND TABLE : COLLABORATION NETWORKING

11:00 ->12:00

## ARD CVL COSMETOSCIENCES PROGRAMME



In an international framework characterised by changing regulatory regimes and increasing harsh competition, research and innovation are key factors to ensure smart specialisation and sustainable economic development of territories and stakeholders. In the very well-established perfume and cosmetic industry of the Centre-Val de Loire region, the COSMETOSCIENCES Programme aims at giving a significant impetus to research projects with a strong character of innovation to unlock industrial development blockages by opening the door to new concepts and enabling the creation of new startups and link with industries. It fosters French leadership in the sector and the leadership of the Centre-Val de Loire region, particularly with regard to sustainable cosmetics.

Anchored in the Centre-Val de Loire region, the Cosmetosciences Programme revolves around the structuring of research at the national level on this cosmetic theme. It brings twelve laboratories and twenty-three research teams together, and is driven by the University of Orléans. It strives to increase the visibility of cosmetic research and funding with the recruitment of PhD students and postdoctoral fellows for collaborative projects between academia and the cosmetic industry. The programme covers the whole value chain of cosmetic products.

The scientific scope has been defined to specifically respond to the scientific challenges of the cosmetic fields according to 3 three development axes:

- Naturalness and ecofriendly processes
- Characterisation of biological activity and product safety
- Formulation & sensoriality

8



LE STUDIUM WEBINARS NaDES for biomass valorization: new insight of a green technology | 06-07 September 2022

## **TABLE OF CONTENTS**

### CONVENORS

Dr Duangjai Tungmunnithum
Green NaDES-Based Ultrasound-Assisted Extraction of Antioxidant and Anti-aging Flavonoids from <i>Opuntia ficus-indica</i> Oil Seed Cakes (Byproducts)
Prof. Leslie Boudesocque-Delaye
Natural Deep Eutectic Solvents in microalgae biorefinery: a bioinspired technolo- gy for sustainable multistep processes
Dr Christophe Hano
SPEAKERS
Dinis Abranches
Modelling Deep Eutectic Solvents with Sigma Profiles: from COSMO-RS to Deep Learning
Prof. Ana Rita Duarte14
Innovation in extraction processes using natural deep eutectic systems
Dr Erwann Durand
Prof. Jeongmi Lee
Applications of deep eutectic solvents for efficient preparation of biopolymers and nanoparticles from natural resources
Dr Nicolas Papaiconomou
Developing greener biphasic systems for the separation of natural compounds using CPC
Dr Alena Stupar
NADES-solvents of the future
Dr Nemanja Teslic
Carotenoids and ellagic acid extraction with Natural deep eutectic solvents – potential application for cosmetic industry ?
Dr Gorawit Yusakul
Therapeutic microemulsion based on hydrophobic-NaDES for <i>Curcuma longa</i> L. extraction and anti-inflammation

# CONVENORS



### Dr Duangjai Tungmunnithum

2021-2022 LE STUDIUM Research Fellow Mahidol University

447 Sri-Ayuthaya Road Rajathevi, Bangkok 10400 - TH

Email: duangjai.tun@mahidol.ac.th Phone: +662 6448677-91 ext 5549, 5551

Assistant Professor Dr. Duangjai Tungmunnithum completed her Ph.D. from Chulalongkorn University in 2016, and won the DPST Postdoctoral Fellowship to conduct her Postdoctoral research in Japan at the National Museum of Nature and Science collaborate with the University of Tokyo focusing on medicinal plant and phytochemistry in the same year. After completing her research in Japan, she was soon getting a permanent lecturer position at the Faculty of Pharmacy, Mahidol University, Thailand. She experts in Pharmaceutical Botany, biochemistry, innovative green extraction methods, biological activity both antioxidant and anti-aging from plant extracts and pure phytochemical compounds for cosmetic and pharmaceutical applications both in vitro, in vivo and in cellulo models. According to her research profiles, she has awarded by many outstanding research grants from both national and international funding sources e.g. the Junior Research Fellowship from French Embassy and Campus France, Sakura Science Program from Japanese Government, Franco-Thai Mobility Programme 2020-2021 funding by French and Thai Governments, LE STUDIUM Research Fellowship, and so forth.

### Green NaDES-Based Ultrasound-Assisted Extraction of Antioxidant and Anti-aging Flavonoids from *Opuntia ficus-indica* Oil Seed Cakes (Byproducts)

Plants have long been used as the potential source of active ingredients for pharmaceuticals and cosmeceuticals. Nowadays, pharmaceuticals and cosmeceuticals industries continuously innovate their extraction and optimization processes to increase efficacy, ensure the safety and environmentally friendly of their products. Extraction solvents are one of the most important factors to get the rich active ingredients from the selected plants for pharmaceuticals and cosmeceuticals. The natural deep eutectic solvents (NaDES) - natural product-based green liquids became the most actively studied as potential green extraction solvents. NaDES are considered the promising alternative to conventional organic solvents, suitable for green extraction since they have high solvency, high flash points with low toxicity and low environmental impacts, easily biodegradable, obtained from renewable (non-petrochemical) resources at a reasonable price and easy to recycle without any deleterious effect to the environment. The PIERIC (CosmetoSciences) project aim to create green NaDES-based extraction methodologies for various plant natural product from diverse plants for cosmetic applications. The chemical characterization as well as biological evaluation of these extracts are also considered. For this presentation, an example of extraction methods and optimization of Opuntia ficus-indica oil seed cakes (byproducts) using NaDES will be illustrated that NaDES is more than just simple (green) solvents.



### Prof. Leslie Boudesocque-Delaye

### University of Tours EA 7502 SIMBA

Faculté de Pharmacie 31 avenue Monge 37200 Tours - FR

Email: boudesocque@univ-tours.fr Phone: (+) 33 2 47 36 71 75

Pr L Boudesocque Delaye is a graduate of the Faculty of Pharmacy of Reims Champagne Ardenne, where she validated her PharmD in 2008. She carried out her PhD on purification processes using Centrifugal Partition Chromatography for natural peptides under the direction of Pr JH Renault, which she obtained in 2010. After a post-doctorate in 2011 within the company Lonza (Visp, Switzerland), she joined the University of Tours as assistant professor in September 2011. She was promoted to full professor in 2020. Her research themes revolve around the development of innovative and eco-designed processes to facilitate access to metabolites of biological interest, within plant or microalgal biomass. In particular, it has recognized know-how in the design of apolar natural eutectic solvents.

### Natural Deep Eutectic Solvents in microalgae biorefinery: a bioinspired technology for sustainable multistep processes

NaDES appeared at the end of the 2010s following the work of Dai et al. Since then, the enthusiasm for these new green solvents linked to ionic liquids has continued to grow. Indeed, the unique properties of these solvents (solubilization capacity, biocompatibility, selectivity, stabilization) make them alternatives to classical solvents. While academic research is intense, few industrial applications have emerged, due to several technological obstacles: tedious preparation, extractive processes not well suited to the industrial scale, and limited options in terms of composition, in particular for non-polar system. At the SIMBA laboratory, we are specialized in the design of NaDES dedicated to extraction of bioactives compounds from microalgae. Spirulina (*Arthrospira platensis*) has been particularly studied within our group. At the same time, our laboratory has recognized know-how in the development of eco-designed extractive processes, which has enabled us to design innovative processes that simplify the use of NaDES while improving extractive performances. Especially, sequential or biphasic processes were designed, using both polar and non-polar NaDES, paving the way of full NaDES-based biorefinery scheme.



### Dr Christophe Hano

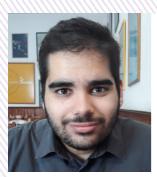
### University of Orleans

Eure et Loir Campus Chartres - FR

Email: hano@univ-orleans.fr Phone: (+) 33 237-309-53

Christophe Hano, completed his Ph.D. in 2005 in Plant Biochemistry and Molecular Biology, is currently Assistant Professor at the University of Orleans. His research focuses on applied plant metabolism and biotechnology. He has written more than 200 scientific peer-review papers, reviews, and book chapters in internationally renowned journals, and he edited a variety of journal topical issues on plant secondary metabolism, including polyphenols as well as books on the anti-aging action of polyphenols. He is Academic Editor and Editorial Board Member of several renowned Q1 Journals in Biochemistry and Biotechnology. He is working on research projects targeted at analyzing plant secondary metabolites in order to produce natural extracts with cosmetic applications.

# **SPEAKERS**



### Dinis Abranches

**University of Notre Dame** 

Department of Chemical and Biomolecular Engineering University of Notre Dame, Notre Dame, Indiana 4655 - USA

Email: abranches@nd.edu Phone: +1 574-514-6401

Dinis O. Abranches is a PhD student in Chemical Engineering and research assistant at the University of Notre Dame, USA. His research interests include thermodynamics, computational chemistry, molecular dynamics, and machine learning, which he explores to predict physicochemical phenomena and understand non-covalent interactions in soft matter. He is active in green-chemistry-related fields, namely deep eutectic solvents, hydrotropy, and ionic liquids.

He obtained his BSc (2018) and MSc (2020) in Chemical Engineering at the University of Aveiro, Portugal, winning several prizes for outstanding academic achievement. He defended the thesis entitled "Unveiling the Mechanism of Hydrotropy: Towards a Sustainable Future". Part of the work developed was highlighted in Nature Reviews Chemistry.

## Modelling Deep Eutectic Solvents with Sigma Profiles: from COSMO-RS to Deep Learning

Deep eutectic solvents (DESs), and the closely related Natural Deep Eutectic Solvents (NaDESs), are eutectic-type liquid mixtures prepared by physically mixing solid precursors. Their melting temperature depression arises due to strong negative deviations from thermodynamic ideality, a trait that distinguishes DESs from other eutectic systems. These deviations constitute the cornerstone of DES design and are frequently attained by selecting hydrogen bond donors (HBDs) and acceptors (HBAs) as precursors. However, not all HBD/HBA combinations result in the formation of DESs, and accurate predictive methodologies are crucial to avoid time-consuming trial and error approaches.

Grounded on solid-liquid equilibrium (SLE) thermodynamics, this work provides qualitative and quantitative pathways to design DESs and NaDESs. To do so, the concepts of asymmetric HBDs and lone HBAs are introduced and the intermolecular interactions that lead to liquid phase nonideality are discussed. Particular attention is given to COSMO-RS, a fully predictive excess Gibbs energy model, showing how it can be used to successfully estimate the activity coefficients of DES components and, thus, their SLE phase diagrams. Finally, sigma profiles (unnormalized histograms of the screened charges of molecules) are also leveraged outside of the scope of COSMO-RS, both to develop heuristic rules to aid in the preselection of DES components, as well as to function as a feature space for machine learning applications.



### Prof. Ana Rita Duarte

### LAQV-REQUIMTE, Departamento de Química, Faculdade Ciências e Tecnologia, Universidade Nova de Lisboa,

2829-516 Caparica, Portugal Des Solutio, Avenida Tenente Valadim nº 17 2ºF 2560-265 Torres Vedras - PT

Email: aduarte@fct.unl.pt

Associate Professor with habilitation at the Chemistry Department from Nova School of Science and Technology. In 2006 she completed her PhD by the same University and in 2007 ISASF granted her thesis the Best Thesis Award. She has been working in different international laboratories, including TU Delft and MIT. She has been the involved in 5 Projects funded by Fundação para a Ciência e Tecnologia. In 2016 she was awarded an ERC consolidator grant entitled: DES.solve – When Solids Become Liquids. In 2018, co-founded Des Solutio, which aims to develop safer and greener alternatives to the chemicals used in the production of beauty, pharmaceutical, personal care and other products. She is the Action Chair of COST Action Greenering. At the moment, she has 145 papers listed in web of knowledge with a total of 4981 citations, and an h-index of 35.

### Innovation in extraction processes using natural deep eutectic systems

Sugars, aminoacids or organic acids are typically solid at room temperature. Nonetheless when combined at a particular molar fraction they present a high melting point depression, becoming liquids at room temperature. These are called Natural Deep Eutectic Solvents – NADES. NADES are envisaged to play a major role on different chemical engineering processes in the future, playing a significant role towards the development of greener and sustainable processes. Nonetheless, there is a significant lack of knowledge on fundamental and basic research on NADES, which is hindering their industrial applications. For this reason it is important to extend the knowledge on these systems, boosting their application development. NADES applications go beyond chemical or materials engineering and cover a wide range of fields from biocatalysis, extraction, electrochemistry, carbon dioxide capture or biomedical applications. In this presentation we will explore how can we develop higher yield processes for the production of novel functional extracts and is there still room for innovation in the field. Within our approach NADES they are proposed for the extraction of natural products and to contribute towards the bio-refinery and circular economy concepts particularly focusing on Mediterranean agro-industrial wastes.



### **Dr Erwann Durand**

### **CIRAD / UMR QUALISUD**

Maison de la Technologie / Bât 16 73 rue Jean-François Breton 34398 Montpellier Cedex 05 - FR

Email: Erwann.durand@cirad.fr

I received a multidisciplinary formation in organic and analytical chemistry. My expertise and research interests are focused to implement new antioxidant strategies for preserving oxidation of lipid-based formulation products. I am doing my researches in the context of green chemistry, with the willingness to design less harmful processes using mild conditions and renewable resources, they encompass the extraction of bioactive molecules (phenolic compounds, lipids, proteins, etc.) from biomass, along with their purification, (bioltransformation and characterization. In this context, I went to investigate for many years the Natural Deep Eutectic Solvents in different research areas [extraction, biocatalysis, formulation, etc.]. I have authored 55 publications in peer-reviewed scientific journals, 3 book chapters, and gave about 40 communications at international conferences. My H-index is 17 and, combined together, my articles have been cited 1600 times (source: Scopus).

## NaDES (Natural Deep Eutectic Solvents): a new approach inspired by nature to promote the biomass (bio)transformation.

Natural Deep Eutectic Solvents (NaDES) are liquid mixtures resulting from the association of metabolites such as sugars, organic acids, amino acids, polyols or vitamins. The singularity of NaDES, compared to all the other conventionally encountered solvents, remains in the biological and physiological roles that these mixtures could have in living organisms. Although the presence of NaDES in cells has not yet been demonstrated, we present how these liquid phases could form in-situ and contribute to the cellular functions of living organisms. In the era of green chemistry, NaDES is therefore of particular interest for developing more efficient and sustainable processes in the fields of food industries. Through this talk, we want to show how an approach based on the concept of biomimicry thanks to NaDES could respond to the challenges of transformation (especially using enzymes) and sustainable use of biomass, and open up great eco-innovative opportunities.



### Prof. Jeongmi Lee

#### Sungkyunkwan University

2066 Seoburo, Jangan-gu, Suwon Gyeonggi 16419 Republic of Korea - KR

Email: jlee0610@skku.edu Phone: (+) 82 31 290 7784

Jeongmi is a Full Professor of Sungkyunkwan University School of Pharmacy [Suwon, Republic of Korea] where she joined as a faculty member in 2010. She earned B.S. (1997) and M.S. (1999) from Seoul National University [Seoul, Republic of Korea] and Ph.D. (2008) from UT Southwestern Medical Center (TX, USA). Her research group aims to: (1) perform application and fundamental studies on deep eutectic solvents, (2) discover biomarkers and understand underlying mechanisms of diseases and drugs via metabolomics, and (3) develop green sample preparation methods for analysis of endogenous and exogenous molecules. She has been serving as an [Associate] Editor of J Anal Sci Technol, Arch Pharm Res, and J Ginseng Res and as an Editorial Board Member of Sci Rep and Molecules.

### Applications of deep eutectic solvents for efficient preparation of biopolymers and nanoparticles from natural resources

Deep eutectic solvents (DESs) have shown to serve as eco-friendly and safe solvents in replacement of toxic volatile solvents and even ionic liquids in diverse areas. Recently, my research group has attempted to apply DESs in the preparation of valuable materials out of natural resources. First, DESs were applied to prepare fungi-derived chitin materials. Specifically, DESs were used to pretreat white button mushrooms in order to prepare chitin-glucan complexes (CGCs) for the first time. Thanks to diverse combinations of hydrogen-bond donors and acceptors in DESs, CGCs with various properties and structures could be prepared using our DES-based method. Importantly, certain DESs could help produce CGCs that appeared preferable to further functionalization and application for subsequent biomaterial preparations. Moreover, the preparation procedure was simple under mild and ecologically benign conditions. Secondly, DESs were applied in the plant extract-based biogenic synthesis of metallic nanoparticles. Specifically, green tea leaves were extracted with DESs, producing various green tea extracts (GTEs). The resulting DES-based GTEs were found to promote the biosynthesis of silver nanoparticles by playing diverse roles depending on the unique properties of the DESs and their constituents. DESs could serve not only as green solvents to efficiently extract the natural reductants, phytochemicals, but also as effective surface modifiers of silver nanoparticles for stabilization.



### Dr Nicolas Papaiconomou

### Cote d'Azur University, UMR 7272

parc Valrose, 28 avenue Valrose 06108 Nice - FR

Email: Nicolas.PAPAICONOMOU@univ-cotedazur.fr Phone: (+)33 4 89 15 01 41

Nicolas Papaiconomou is a physical chemist who has obtained his PhD in Germany and France. He is an associate Professor since 2007 and has always been interested in developing sustainable solvents, applying them to the extraction of value materials, such as metal ions or natural compounds, and describing the thermodynamics of extraction of such systems. He is currently focusing on developing sustainable solvents such as Deep Eutectic Solvents and mixtures based on these solvents in extraction and separation processes of natural compounds from plant raw material.

With the aim of gaining better insights in the extraction processes and understanding their mechanisms, he uses COSMOTherm as a predictive model for the thermodynamic description of complex solutions. Typical applications of this model is calculating phase diagrams, solubilities of solutes in solvents and partition coefficients of a solute between two immiscible phases.

### Developing greener biphasic systems for the separation of natural compounds using CPC

Recently, organic biphasic systems based on heptane, ethanol and a deep eutectic solvent and their application to the extraction of natural compounds have been reported in the literature. [1] Data are however very scarce, and no insight into the influence of these compounds on phase diagrams or partition of natural compound in these systems are available.

In order to gain better insights into such organic biphasic systems, phase diagrams of these systems as well as partition of a given natural compound added into a biphasic mixture, several biphasic systems containing butanol, ethyl acetate and type III or V DES have been studied. Phase diagrams, partition coefficients of apigenin, coumarin, -ionone, retinol and -tocopherol were measured. Starting from the results gathered here, application of a biphasic system in CPC in order to separate natural compounds was successfully carried out.

Finally, COSMO-RS was used in order to describe phase compositions of several biphasic mixtures, as well as partition coefficients, confirming its interest as a predictive tool for optimizing extraction systems for natural compounds.

<sup>1</sup> Chagnoleau, J.-B., N. Papaiconomou, M. Jamali, D.O. Abranches, J.A.P. Coutinho, X. Fernandez, et T. Michel. « Toward a Critical Evaluation of DES-Based Organic Biphasic Systems: Are Deep Eutectic Solvents so Critical? » ACS Sustainable Chemistry and Engineering 9, 29 (2021): 9707 16.



### **Dr Alena Stupar**

### Institute of Food Technology, University of Novi Sad

Buulevar cara Lazara 1 21000 Novi Sad, Serbia - RS

Email: alena.tomsik@fins.uns.ac.rs Phone: (+)38163662076

Dr. Alena Stupar is a research associate at the Institute of food technology in Novi Sad, She earned her PhD degree in 2018 at the Department of Biotechnology and Pharmaceutical Engineering at University of Novi Sad. During the research career, Alena Stupar, have collaborated with many researchers and received several scientific related trainings abroad. Focus of her research is isolation of bioactive compounds from natural resources by novel extraction techniques and green solvents, encapsulation of natural extracts and their potential application in food and/or cosmetics products. Until now, she was engaged in several national and international projects. The latest projects are based on green concept: "Natural Deep Eutectic Solvents for Green Agri-Food Solutions", where she was a team leader of WP and participat on project "Novel extracts and bioactive compounds from under-utilized resources for high-value applications.

### NADES-solvents of the future

The principles of 'green chemistry' are gaining importance in different sectors due to the need to reduce pollution from toxic chemicals, make industrial processes safer and more sustainable, and to offer 'clean-labeled products' required by the consumers. The appropriate selection of solvents is crucial to tackle new challenges such as the circularity of manufactured products to achieve sustainable development goals. The application of natural deep eutectic solvents (NADES) is considered promising alternative to conventional organic solvents. As the demand for sustainable, green products is growing, NADES present opportunities to develop innovative extracts with unique phytochemical footprints and biological activities. Possibilities to design tailor-made solvents for specific utilization, their high solubilisation ability for poorly soluble natural compounds, ability to enhance stability of extracted compounds and in some cases, promotion of their biological activities makes NADES economic solvents with relatively higher environmental and health safety, suitable for applications in pharmaceutical, cosmetic and food industry. However, their potential for industrial scale-up utilization is not completely investigated; additional data and thorough understanding on physicochemical properties of NADES are still needed as they are relevant for industrial applications.



### Dr Nemanja Teslic

### Institute of food technology, University of Novi Sad, Serbia

Bulevar cara Lazara 1 21000 Novi Sad, Serbia - RS

Email: nemanja.teslic@fins.uns.ac.rs

Dr. Teslić is a research associate at the Institute of food technology. In 2018 he earned PhD at the Department of agricultural and food science, University of Bologna. He was a team leader of WP on project "Natural Deep Eutectic Solvents for Green Agri-Food Solutions" and participating on project "Novel extracts and bioactive compounds from under-utilized resources for high-value applications". Current field of research is valorization of bioactive compounds from food industry by-products and agricultural waste by novel green extraction techniques and solvents. In 2019 he received award R. Ferrarini for the best PhD in viticulture issued by Italian association of enology and viticulture. In 2021 he received award for the best young investigator issued by Institute of Food Technology.

## Carotenoids and ellagic acid extraction with Natural deep eutectic solvents – potential application for cosmetic industry ?

The cosmetic industry faces the challenges of sustainable production due to high negative impact of the industry on the environment. To tackle such challenges cosmetic industry requires development of innovative and eco-friendly solutions to exploit agro-food waste and as natural resources for the next generation of cosmetic products. These solutions should also be aligned with the principles of "green chemistry". One of the potential solutions could be the usage of natural deep eutectic solvents (NADES) composed only of edible, recyclable, non-toxic compounds which are present in nature. More precisely, organic acids, water, sugars, fatty acids, amino acids, terpenes, alcohols, and other compounds some of which are already used by the cosmetic industry, can be mixed in the certain ratio to create solvents with specific features suitable for a wide range of applications. Since large number of NADES combinations can be made these solvents can be used as extraction medium for natural polar/non-polar compounds, stabilization medium of extracted compounds etc. Due to NADES edible and nontoxic properties obtained extracts are ready-to-use and in certain cases may be applied in cosmetic products without additional separation technology which reduces cost of production. Some of the examples are application of NADES is carotenoids recovery from pumpkin pulp and ellagic acid from by-product raspberry seeds which could be potentially incorporated in anti-aging and skin repair products.



### Dr Gorawit Yusakul

### Walailak University

Nakhon Si Thammarat - TH

Email: gorawit.yu@mail.wu.ac.th Phone: (+)66-65-348-3484

Dr. Gorawit Yusakul is a lecturer at Walailak University after receiving Ph.D. from Kyushu University in Japan. Dr. Yusakul received a Pharmacy bachelor's degree from Khon Kaen University, Thailand. I am passionate about researching green chemistry and developing novel green solvents. Unexpectedly, honeybees produce great NaDES with sugars, organic acids, minerals, enzymes, etc. As mentioned above, our team work on NaDES to extract turmeric and other medicinal plants. We aim to make NaDESs for herb extracts, NaDESs for improving pharmacology, NaDES-based microemulsions, and NaDESs that can be used as biocompatible solvents.

## Therapeutic microemulsion based on hydrophobic-NaDES for *Curcuma longa* L. extraction and anti-inflammation

The hydrophobic NaDESs and their microemulsions have been created to enhance the extraction and delivery of hydrophobic curcuminoids while producing their own therapeutic effects. Fatty acids and menthol are utilized to create hydrophobic NaDESs (HNaDES), which can then be applied to microemulsion systems. HNaDES (octanoic acid:menthol) was found to be effective extraction of Curcuma longa L. In these circumstances, the yields of bisdemethoxycurcumin, demethoxycurcumin, curcumin, and ar-turmerone were 2.49, 5.61, 9.40, and 3.83% (w/w, dry basis), respectively, while the yields from the HNaDES-based microemulsion were 2.10, 6.31. 12.6, 2.58%. Compared to curcumin prepared in dimethyl sulfoxide, curcumin in HNaDES-based microemulsion had superior NO inhibitory action that was > 7.5 times more potent. The cytotoxicity of curcumin was also reduced in RAW264.7 cells when coupled with hydrophobic NaDES of menthol:oleic acid, which completely inhibited NO secretion (anti-inflammation). These findings clearly show that HNaDESs can dissolve curcuminoids and confer anti-inflammatory effects. In terms of chemical stability, more than 90% of the curcumin was still present after a month of storage in HNaDES and HNaDES-based microemulsion. HNaDES and its microemulsions are more efficient and environmentally benign than traditional organic solvents, and these solvents are also compatible with food and pharmaceutical formulations.

### CONTACT

### Dr Aurélien Montagu

Scientific Manager +33 2 38 21 14 86 aurelien.montagu@lestudium-ias.fr

### LE STUDIUM

Loire Valley Institute for Advanced Studies

www.lestudium-ias.com 1, rue Dupanloup • 45000 Orléans • FR

