Book of Abstracts

23 - 26 June 2025, Lisbon

Welcome,

The Organizing Committee of the 4th International Meeting on Deep Eutectic Systems is very pleased to welcome you back to Lisbon. This year, we have planned an enriching scientific program in a new location in the city center (Sana Metropolitan Hotel), between 23-26th of June 2025 and the social program will be hosted in a relaxed environment, with a magnificent sunset over the Atlantic Ocean.

We are happy to meet you again and see old time friends and scientists who continue to trust us on this mission to disseminate the work developed in Eutectic Systems from all around the globe. It is our expectation that this the 4th meeting exceeds the previous series of fruitful meetings. The numerous abstract submissions are the proof that the International Meeting on Deep Eutectic Systems, is, now, eight years after its first edition, after plenty of hard but rewarding work, a renowned event in the field. Never forgetting the fundamental knowledge that is the foundation of further innovative application developments, it is interesting to see how the spectrum of submitted contributions continues to grow.

The organization committee aims to offer a unique opportunity, in an informal environment not only to hear the newest developments and discoveries, but also a place for sharing knowledge, brainstorm new ideas and where the participants interact, network and build new bridges towards successful collaborations.

We hope that the 4th IMDES will motivate and leave you inspired to pursue your work, and we could not finish without thanking you for your contribution, without which we could not organize such a high scientific level meeting.

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Special Issue Opportunity

We are excited to announce that if you are a participant in the 4th International Meeting on Deep Eutectic Systems, you have the chance to submit a **Special Issue** to the journal *Sustainable Chemistry and Pharmacy* (Impact Factor 5.5).

Topic: Advancing Sustainable Chemistry and Chemical Engineering through (Natural) Deep Eutectic Systems

This issue aims to highlight innovative research that goes beyond the simple application of so-called green and sustainable processes. While Natural Deep Eutectic Systems are often presented as green alternatives, it is essential to critically assess the **actual greenness and sustainability** of these technologies.

Therefore, we strongly encourage submissions that incorporate:

- Green chemistry metrics
- Life Cycle Assessment (LCA)

Submission Open date: July 1, 2025

Submission Deadline: September 30, 2025

Program

	23/jun	24 June	25 June	26 June
09:00		Opening Remarks	PL2- Leslie Boudesocque-Delaye (B)	PL2- Mara Freire (P)
09:15		PL1- Christoph Held (F)		
09:30				
09:45			OC16- Roberto Canales (B)	OC28- Joyce Cavalcante (P)
10:00		OC1- Dinis Abranches (F)	OC17- Ana Carolina Costa (B)	OC29- Joana Pereira (P)
10:15		OC2- Cristian Malebran (F)	OC18- Zhiwen Qi (B)	OC30- Vasiliki Kakokefalou (P)
10:30		OC3- Santiago Aparicio (F)	OC19- Valentin Diez-Cabanes (B)	**Coffee Break**
10:45		**Coffee Break**	**Coffee Break**	
11:00				KN5- Dharamachi Rabari (M)
11:15		KN1- Andreia Farinha (B)	KN3- Carlos Garcia (F)	
11:30				OC31- Cláudio Fernandes (M)
11:45		OC4- Jeongmi Lee (B)	OC20- Marina Cvjetko Bubalo (F)	OC32- Phil Hunt (M)
12:00		OC5- Matteo Bonomo (B)	OC21- Gangqiang Yu (F)	OC33- Cristina Prieto (M)
12:15		OC6- Mariana Rodrigues (B)	OC22- Laura Falivene (F)	OC34- Marcin Wysokowski (M)
12:30		OC7- Jian Shi (B)	OC23- Santiago Aparicio (F)	OC35- Maria Luisa Ferrer (M)
12h45		**Lunch**	**Lunch**	Closing Remarks
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13:30				
13:45				
14:00		KN2 - Ivana Radojcic Redovnikovic (E)	KN4- Matteo Tiecco (B)	
14:15				
14:30		OC8- Luiz Castro (E)	OC24- Lamya Al Fuhaid (B)	
14:45		OC9- Clarice Amaral (E)	OC25- Tiancheng Mu (B)	
15:00		OC10- Marta Marques (E)	OC26- Maria-Anna Karadendrou (B)	
15:15		OC11- Filipe Sosa (E)	OC27- Maria Enrica di Pietro (B)	
15:30		**Poster Session/Coffee Break**	**Poster Session/Coffee Break**	
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16:45		OC12- Benoit Caprin (B)		
17:00		OC13- Laura Divoux (B)		
17:15		OC14- Boris Popovic (B)		
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18:00	**Opening Cocktail, registration**		**Gala Dinner**	
18:15				
18:30				
18:45				
19:00				
20:00				
22:00/23				

Venue

Hotel Sana Metropolitan Lisboa

Rua Soeiro Pereira Gomes, 2, 1600-198 Lisboa

Registration, Welcome Cocktail, Coffee Breaks and Lunches

1st Floor Hall

Presentations and Poster Sessions

Paris Room and 1st Floor Hall

Gala Dinner

Waikiki, Praia da Sereia, Costa da Caparica

Transportation to and from the Gala Dinner

Bus available – Meeting place at entrance of Sana Metropolitan Hotel, at 17h45. Return to the same place at 23h.

Wi-Fi

Sana Metropolitan hotel *Wi-Fi* network

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Plenary Lectures

PL1 - How can thermodynamics assist in the design of DES?

Christoph Held
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Thermodynamic fundamentals enable the design of separation steps and reaction steps in biochemical and chemical processes. They allow building physically-based prediction tools to screen conditions that give an optimal process window with respect to a certain property such as solubility of a reactant or yield of a reaction. This talk will highlight some examples of optimizing biochemical and chemical reactions and highlight the importance of the process window on the process efficiency, evaluated by maximum reaction yield or reaction kinetics. The process window can be dramatically manipulated by temperature/pressure, concentration, solvents, and additives. This is a huge matrix that needs to be understood. I will then show how thermodynamics (in most cases, a hybrid approach between modeling at different scales and experiments) enables to find the sweet spot for such reactions or separations and which challenges are met in general. Special focus is chemical reactions under elimination of water, since these require a reaction medium that keeps thermodynamic water activity as low as possible in order to overcome yield limitations caused by thermodynamic equilibrium, while the thermodynamic reactant activity and thermodynamic catalyst activity (e.g., proton's activity) must be as high as possible. The use of single solvents usually allows tuning only one of these properties, e.g. decreasing water activity in water-elimination reactions might be possible only at cost of decreased kinetics by negative impact on the activity of reactant or catalyst. Thus, DESs might be an opportunity here. The multi-facetted influence of DESs on phase behavior and reaction efficiency on top of other parameters (temperature, pressure, pH) will be shown with the overall goal to boost the efficiency of liquid-phase reactions and to make the reaction conditions greener.

PL2 - Eutectic Matrixes: A Game-Changer for Sustainable Ingredient Development

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In the context of the ongoing transformation toward more sustainable practices in the nutraceutical, cosmetic, and pharmaceutical industries, the demand for natural ingredients is experiencing significant growth. These ingredients—sourced from plants, marine environments, or biotechnology—are typically extracted using organic solvents derived from petrochemicals. In this regard, natural eutectic solvents offer a promising alternative to support the industry's transition.[1] Since their initial identification in 2013 as extraction solvents, Natural Deep Eutectic Solvents (NaDES) have garnered increasing interest, not only in academic literature but also within the cosmetic industry.[2] However, their growing popularity has led to semantic confusion and marketing-driven misuse of the term "NaDES," often applied to mixtures that do not meet the strict thermodynamic criteria.[3] Scientifically, NaDES are characterized by a pronounced depression of melting points compared to thermodynamic ideality.[3] To more accurately describe mixtures lacking this behavior, new terminology such as "Mixture of Natural Compounds" (MiNAC) has recently been introduced. This term offers greater flexibility, particularly regarding water content tolerance.[4] Whether referred to as NaDES or MiNACs, these novel solvents are reshaping knowledge and processes in natural product extraction. Their exceptional solubilizing power and selectivity have enabled the production of unprecedented ingredients—either through targeted enrichment or through entirely new phytochemical profiles.[5,6] To maintain their sustainability, production processes have been reengineered to eliminate or avoid conventional solvent recovery steps, since these solvents are non-volatile by nature.[7] Selecting the appropriate eutectic solvent for a specific application remains a unique challenge, due to the virtually infinite number of possible compositions. Predictive tools are therefore essential to reduce unnecessary resource consumption. In this context, the Smart Selection Strategy offers a relevant and efficient approach—guiding solvent selection based on the intended end-market. A case study in the cosmetic sector will be presented to illustrate this methodology.[8] Far from being mere extraction media, NaDES and MiNACs function as bioactive extraction matrices or delivery systems with intrinsic properties. They can act as active ingredients themselves—modulating skin or vaginal microbiota,[9,10] enhancing biological activity,[11,12] or even contributing novel textures in cosmetic formulations.[13] Ultimately, these eutectic matrices are not just alternative solvents; they are transformative agents in extraction science, driving continuous innovation and presenting an exciting challenge for R&D teams across disciplines.

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PL3 - Enhancing Drug Delivery with Deep Eutectic Solvent Formulations

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Deep eutectic solvents (DESs) have emerged as highly tunable and sustainable solvent systems with exceptional potential in pharmaceutical formulation and drug delivery. In this lecture, recent advances in the design and application of DESs to overcome major challenges in drug delivery, including poor solubility, low bioavailability, and limited stability of active pharmaceutical ingredients (APIs), will be presented and discussed. Drawing on our group's contributions, focus will be given to therapeutic deep eutectic systems developed for localized and systemic delivery routes, including oral, transdermal, and ocular applications. Case studies involving anti-inflammatory and anticancer agents, as well as the integration of DESs into delivery vehicles, will be presented. Ongoing work with biopharmaceuticals, such as antibodies and nucleic acids, will be finally presented and discussed.

This lecture aims to underscore the transformative role of DESs in formulating safer and more effective drug delivery platforms.

Acknowledgements
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Keynote Lectures

KN1 – Unlocking NADES in environmental chemistry

Andreia S. F. Farinha[a]*, Mariana Rodrigues[a], Lamya Al Fuhaid[a], Joyce Cavalcante[a], Robert Verpoorte[b], Young Hae Choi[b], Geert-Jan Witkamp[a]

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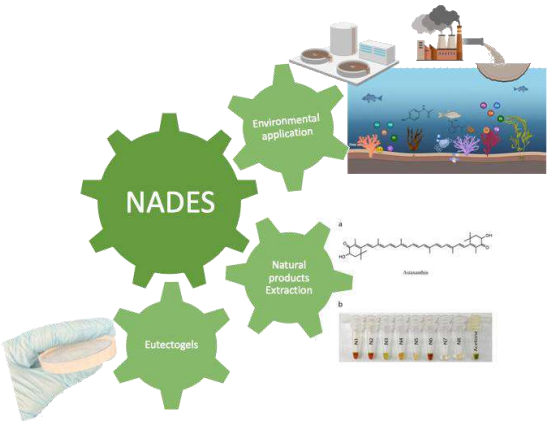
Keywords: NADES, Enviromental samples, natural product extraction, water remediation

Natural Deep Eutectic Solvents (NADES) have emerged as promising green solvents with a broad range of applications owing to their tunable physicochemical properties. Formed by combining naturally occurring compounds such as sugars, organic, and amino acids, NADES exhibit unique features such as exceptional solubility for organic molecules, low volatility, and adjustable viscosity. These versatile solvents find applications in various aspects of environmental chemistry, such as sample preservation, compound solubilization, and environmental remediation [1-3]. Here, we highlight our recent advancements in NADES applications across diverse areas, including water desalination and remediation, trace metal recovery, natural product extraction, and environmental sample characterization. Specifically, we have shown NADES as biofilm solubilization agents, offering a green solution for biofouling in reverse osmosis membranes. NADES have also proven efficient in removing pharmaceutical and personal care products, recovering various trace metals from water, and being green alternative agents for extracting carotenoids from algae and bacteria and characterizing marine samples. These diverse applications underscore the potential of NADES as sustainable and efficient tools for addressing critical environmental challenges.



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KN2 - How to Design Tasty NADES for the Food Industry?

Manuela Panic[a], Marina Cvjetko Bubalo [b], Martina Železnjak[a], Maja Benković [b], Ivana Radojcic Redovniković [b,*]

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Keywords: food industry, natural deep eutectic solvents, sensory analysis, food preservation, plant extract

Natural Deep Eutectic Solvents (NADES) are emerging as sustainable and efficient alternatives to conventional solvents in the food industry, offering advantages such as biodegradability, low toxicity, and tunable physicochemical properties. Their applications range from the extraction of bioactive compounds and food preservation to the valorization of agri-food waste. Despite their great potential, several challenges must be addressed for successful industrial adoption. One major obstacle is regulatory approval, as most NADES lack standardized safety assessments and classification for food applications. Additionally, factors such as viscosity, stability, and recyclability pose challenges for large-scale processing. Beyond technical considerations, an often overlooked but crucial factor is the sensory impact of NADES. Their influence on taste, aroma, color, and texture is critical for consumer acceptance and market integration. Thus, sensory analysis of NADES plays a key role in evaluating food products comprising these solvents, ensuring that such products maintain desirable organoleptic properties while benefiting from enhanced functional or nutritional attributes provided by NADES. This presentation will provide an overview of the latest advancements in NADES applications within the food industry, critically assess existing challenges, and explore strategies for overcoming commercialization barriers. Special emphasis will be placed on the role of sensory analysis in optimizing NADES formulations for food-related applications, ensuring their successful integration into sustainable food production while maintaining high sensory and quality standards.

Acknowledgements

This work was supported by the Croatian Science Foundation (IP-2024-05-9948).

KN3 - Big Data for a Deep Problem: Understanding and Predicting the formation of DES via Machine Learning

Lucas B. Ayres[a], Emmanuel Dike[a], Jorge Barroso[a], Connor Parker[a], Vagner B. dos Santos[a,b] and Carlos D. Garcia[a,*]

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Keywords: Machine learning, antioxidants, food lipids,

The application of deep eutectic solvents (DES) in the pharmaceutical, agricultural, and food industries represents one of the fastest growing fields of green chemistry, as these mixtures can potentially replace traditional organic solvents.[1] These advances are, however, limited by the development of new DES which is today, almost exclusively empirically driven and often derivative from known mixtures. To overcome this limitation, we have developed a series of machine learning approaches, that are able to recognize the patterns in strings that lead to the formation of DES. The simplest approach was adapted from language learning, allowing the use of relatively small datasets and relatively low computational resources and opening the door to the development of multiple novel solvents containing pharmaceuticals.[2] This model has been recently expanded (to an extreme gradient boosting model, eutXG) that is capable of predicting not only the formation but also the melting point (MP) of DES with an average accuracy of 98%.[3] Summarizing these results, this presentation will not only cover the basic concepts behind these models but also provide several examples of their application to address analytical problems.[4-7] More information about the group as well as the list of contributors to this presentation can be found in our web site: scienceweb.clemson.edu/uacl/

Acknowledgements

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KN4 - Asymmetric Organic Synthesis with Chiral-DESs: A Deeper Dive into the Catalytic Properties of Deep Eutectic Solvents

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Keywords: Chiral-DESs; Asymmetric Synthesis; Green Transformations; Homogeneous Catalysis.

The topics in which Deep Eutectic Solvents (DESs) are finding fruitful results is constantly increasing in the literature thanks to their environmentally friendly features as substitutes to common volatile, polluting and toxic organic solvents. However, it is limiting to consider Deep Eutectic Solvents as "only" green liquids because they possess unique structural features and valid catalytic behaviours. DESs formed by acidic, basic or reducing components can act respectively as acid, basic or reducing catalytic liquids in a wide plethora of transformations. Asymmetric catalysis represents one of the most challenging and fascinating catalysis that can be developed by means of small molecules, namely organocatalysts. If one of these molecules can be a DESs component, the organocatalysis can be developed by the chiral resulting liquid itself. This occurs with peculiar and unique mechanisms, different from the ones normally taking place with the organocatalyst itself. In this presentation the asymmetric transformations realised with the use of Chiral-DESs as green active organocatalytic liquids will be shown. Starting from (+)-Camphorsulfonic acid-based DESs, then moving to L-Proline-based DESs and to ammonium pyrrolidine-based DESs, the journey through the mechanisms of organocatalysis made by these intriguing novel liquids will be presented [1-3]. The insights on the catalytic mechanisms of these chiral liquids represent a "deeper than deep" exploration on their structural features and therefore on their effective applications.

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KN5 - CO_2 cycloaddition to propylene oxide using zeolite-Y supported DESs: a combined theoretical and experimental study

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Keywords: Deep eutectic solvents, Zeolite-Y, CO2 cycloaddition, propylene oxide conversion, density functional theory

The process of turning CO2 into useful products may be a more visible way to fight climate change. The cycloaddition of CO2 to propylene oxide presents a sustainable route for synthesizing propylene carbonate, which holds a significant industrial and environmental importance. In this study, a combined theoretical and experimental approach was employed to investigate the cycloaddition of CO2 to propylene oxide catalyzed by deep eutectic solvents (DESs) supported on zeolite-Y. The influence of the DESs with ChCl as hydrogen bond acceptor and urea, ethylene glycol or glycerol as hydrogen bond donors (1:2 molar ratio) were investigated in 100 ml autoclave under the conditions of 110˚C and 16.5 bar CO2 in 7 hours. The solid catalysts were characterized using TGA, XRD, SEM and BET surface area analyser. The product was analysed using GC-FID with a non-polar fused silica capillary column and butanol as internal standard. The computational work was also performed using Density Functional Theory (DFT). The interaction of CO2 with DES molecule were studied considering counterpoise correction method in Gaussian 16 at molecular level. The experimental conversion was the highest (44.2%) for DES having ethylene glycol as hydrogen bond donor as compared to urea and glycerol. The lowest conversion (21%) was found for DES having glycerol as hydrogen bond donor. The similar trend was found for interaction energy by DFT calculations. The interaction energy between CO2 and DES with ethylene glycol was the most negative value (-10.65 kcal/mol) while the least value (-6.09 kcal/mol) was obtained for DES having glycerol as hydrogen bond donor. With an increase in the hydroxy groups in the HBD of DES, the catalytic conversion of propylene oxide decreased. This is attributed to steric hindrance: multiple hydroxy groups create spatial bulk around the propylene oxide, impeding its access to active catalytic sites. This steric bulk limits the ability of the DES-supported catalyst to effectively interact with propylene oxide and CO2, ultimately decreasing the overall reaction rate.

Oral Presentations

OC1 – Fast and Furious: Accelerating openCOSMO-RS with Graph Convolutional Networks

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Keywords: Machine Learning, Sigma Profiles, Activity Coefficients, Artificial Intelligence

The accurate characterization of phase equilibria in mixtures is crucial for the development of novel materials, including deep eutectic solvents (DESs). Phase equilibria behaviour, among many other properties, can be estimated using activity coefficient models such as COSMO-RS [1], or its open-source alternative openCOSMO-RS [2]. This statistical thermodynamic model relies on sigma profiles, which are quantum chemistry descriptors of molecules, to determine pair-wise interactions among mixture components. Although openCOSMO-RS can predict activity coefficients without the need for any experimental data, the generation of sigma profiles through computationally intensive quantum chemistry calculations, which can take several hours for a single compound, remains a major bottleneck of this approach. The objective of this work is to leverage machine learning (ML) to significantly reduce the computational cost associated with openCOSMO-RS. To do so, a comprehensive database of sigma profiles, encompassing over 12,000 different molecules and 700 ions, was constructed using the software package ORCA. This database was used to train a graph convolutional network (GCN), with an initial architecture based on previous work [2] and further optimized here, that uses MMFF atom types as node-level features to boost accuracy and generalizability. This GCN attained coefficients of determination for sigma profiles and structural volumes over 0.96 and 0.99, respectively. Using GCN predicted sigma profiles, the openCOSMO-RS model was reparametrized. This new version of openCOSMO-RS achieved a predictive performance comparable to that of quantum chemistry derived sigma profiles at a fraction of the cost. This allowed for the construction of a full software pipeline, enabling users to input the SMILES of mixture components and obtain their activity coefficients within milliseconds in a personal computer. Finally, examples for DES design were explored as a case study.

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OC2 - On the Limit of Deep Eutectic Solvents and Aqueous Solutions

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Keywords: Deep Eutectic Solvents, Molecular Dynamics and Thermogravimetric Analysis.

The viscosity and polarity of deep eutectic solvents (DES) are particularly important in the extraction of natural compounds, as these characteristics determine the affinity and mass transfer during extraction [1], [2]. Indeed, the addition of water decreases the viscosity and improves the extraction efficiency [3]. However, it has been suggested that there is a limit to the amount of water that can be added without the DES becoming a simple solution of its components [1]. To provide insight into the changes of DES properties upon water addition, an experimental and theoretical study was performed to provide an understanding of DES-water systems at the molecular level. These results will be valuable in understanding the extraction yields of phenolic compounds from plant biomass in DES with varying water content. In this study, two solvents were considered and they were based on choline chloride as hydrogen bond acceptor (HBA) and glycerol and urea as hydrogen bond donors (HBD) in a molar ratio of 1:2 (HBA:HBD), with varying amounts of water, in the range of 25 to 92 mol% water. The mixtures were characterized by FT-IR, TGA, and Kamlet-Taft parameters were measured. Molecular dynamics simulations were performed to gain a molecular-level understanding of the interactions between the DES components. Overall, the macroscopic properties of both DESs were found to correlate with the molecular interactions, which revealed that the optimal water molar ratio to enhance the extraction capabilities of a DES is in the range of 50% to 70% mol of water.

Acknowledgements

This work was financed by Fondecyt project 1231279. Powered@NLHPC: This research was partially supported by the supercomputing infrastructure of the NLHPC (ECM-02).

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OC3 - Advancing Green Extraction Technologies: Computational Design of Recyclable NADES for Bioactive Compound Isolation

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Keywords: Natural Deep Eutectic Solvents (NADES); Bioactive Compounds Extraction; COSMO-RS Computational Modelling; Green Separation Techniques; Thermodynamic Property Analysis

Natural Deep Eutectic Solvents (NADES) have emerged as a promising alternative to traditional volatile and hazardous solvents in the extraction of bioactive compounds for pharmaceutical, medical, and nutritional industries. Conventional extraction methods often involve high energy consumption, substantial economic costs, and potential safety risks. While NADES offer superior efficiency and safety, their practical application hinges on developing effective compound separation strategies to enable solvent recycling and maximize utility. This computational study employs COSMO-RS methodology to investigate the thermodynamical properties of selected Type V NADES previously identified as optimal for bioactive compound extraction. Recognizing the thermal sensitivity of target compounds, which precludes conventional distillation techniques, we systematically explore alternative separation strategies. By comprehensively analyzing solute solubility across various NADES at different temperatures and examining vapor-liquid equilibrium under varied pressure conditions, we evaluate the potential of innovative techniques such as vacuum distillation and controlled precipitation. The research aims to develop a holistic approach to bioactive compound extraction and separation, with a focus on creating a robust, scalable process suitable for future industrial applications. The proposed methodology promises to address current limitations in green solvent technologies, offering a more sustainable and efficient extraction paradigm.

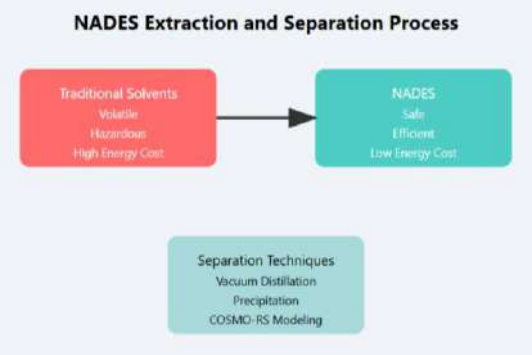

Figure 1. Scheme for the NADES design study performed here for extraction of bioactive molecules.

Acknowledgements: Junta de Castilla y León (Project: NADESforNATURE, Ref. BU047P23); European Union - HORIZON (Project: Convert2Green, Ref. HORIZON-CL4-2022-RESILIENCE-01-Convert2green-GA 101092347).

OC4 - Deep Eutectic Solvent-Based Preparation of High-Purity Protein Pigment, Phycoerythrin from *Porphyridium purpureum*

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Keywords: Deep eutectic solvents, microalgae, cell disruption, extraction, phycoerythrin

Microalgal biomass is a promising renewable feedstock for high-value bioproducts, yet its rigid cell wall poses a challenge for efficient compound extraction. This study presents an ecofriendly and effective approach for extracting B-phycoerythrin (B-PE) from *Porphyridium purpureum* using deep eutectic solvent (DES) as a cell disruption and extraction medium. The solubility of cell wall monomers in 31 DESs was predicted using COSMO-RS, guiding the selection of five glycerol-based DESs for experimental validation. The prediction results generally agreed with the experimental results, while all DESs significantly enhanced B-PE yields compared to water when combined with ultrasound-assisted extraction (UAE). Among them, PGly demonstrated the highest B-PE yield, likely due to its stabilizing effect on the extracted protein despite moderate cell wall dissolution capability. The green nature of the DES-based UAE method was confirmed using the AGREEprep metric. The crude extract obtained from the optimized process was further purified via an aqueous two-phase system (ATPS), two-step ammonium sulfate precipitation (ASP), and ultrafiltration (UF), yielding B-PE with a PE purity comparable to commercial standards. Notably, the ATPS was directly compatible with the DES-based extract, enabling selective removal of coexisting pigment (phycocyanin). This study underscores the potential of DES-based UAE as a highly efficient and eco-friendly strategy for extracting high-purity phycobiliproteins from microalgal biomass, while also demonstrating the predictive power of COSMO-RS for DES selection and thermodynamic modelling [1].

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OC5 - Iodine and CO_2 uptake by Deep Eutectic Solvents

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Keywords: DES, sustainability, uptake, iodine, carbon dioxide

Despite significant progress in energy production from next-generation electrochemical power sources and photovoltaics, nuclear energy still accounts for up to 11% of the world's total electricity demand. However, uranium's use in nuclear power generation results in the release of highly toxic wastes, such as radioactive iodine, primarily ^{129}I and ^{131}I. This highlights the urgent need for effective strategies to sequester and store these contaminants, preventing their release into the environment [1]. Ionic liquids (ILs) have been shown to be effective for this purpose, but their high cost and the difficulty of purifying them after synthesis are major drawbacks. Furthermore, the toxicity of the commonly used imidazolium cations in ILs remains a significant concern. In contrast, deep eutectic solvents (DESs) have garnered considerable attention in recent years due to their simpler synthesis, environmental benignity, and cost-effectiveness [2]. In this study, we present various glycerol-based DESs with exceptional iodine uptake efficiency, outperforming several benchmark porous absorbents. By combining Raman spectroscopy and thermal gravimetric analysis (TGA), we identified the species formed and transformed during the uptake and release of iodine, revealing the role of halogen bonding in these mixtures. Besides Iodine, we also explored some amine-based DES and DES-like mixture to chemically capture CO_2 [3]. Here, the combination of n-butylamine with glycerol or guanidinium hydrochloride allows the CO_2 capture while reducing amine volatilization and thus paving the way for industrial applicability. The capture ability was determined by gravimetric method, while the desorption behavior was monitored through in operando ATR-IR spectroscopy.

Acknowledgements

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OC6 - Green extraction of Pharmaceutical and Personal Care Products from marine sediments using NADES

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Keywords: Marine sediments, NADES, Green extractions.

Pharmaceutical and Personal Care Products (PPCPs) are emerging pollutants increasingly found in aquatic environments; their presence raises serious concerns for human health and marine ecosystems. Marine sediments retain these contaminants by adsorption [1], and several approaches for PPCPs monitoring have been described in the literature [2,3]. However, conventional extraction protocols often employ hazardous organic solvents and require lengthy sample preparation. This study explores the versatile properties of Natural Deep Eutectic Solvents (NADES) in a green and straightforward approach for extracting 18 target PPCPs. Among the tested NADES, choline chloride:glycerol (1:2) demonstrated the highest extraction efficiency, outperforming the conventional benchmarked method for PPCPs extraction from an in-house sediment reference material. When applied to real marine sediments collected from the Red Sea, NADES showed promising results, particularly for the extraction of paracetamol, sulfamethoxazole, carbamazepine, atrazine, and diclofenac.

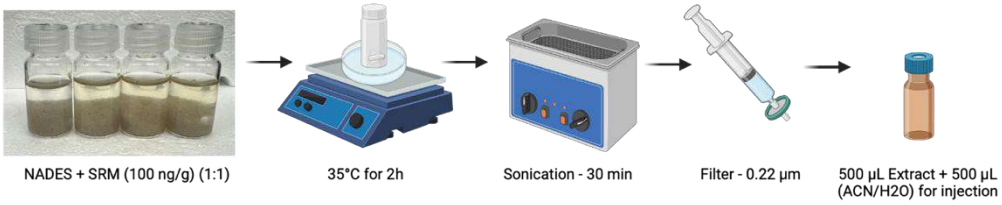

Figure 1: Schematic representation for the extraction of PPCP in marine sediments.

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OC7 - Design of Lignin Derived Hydrophobic Deep Eutectic Mixtures for Sustainable Applications

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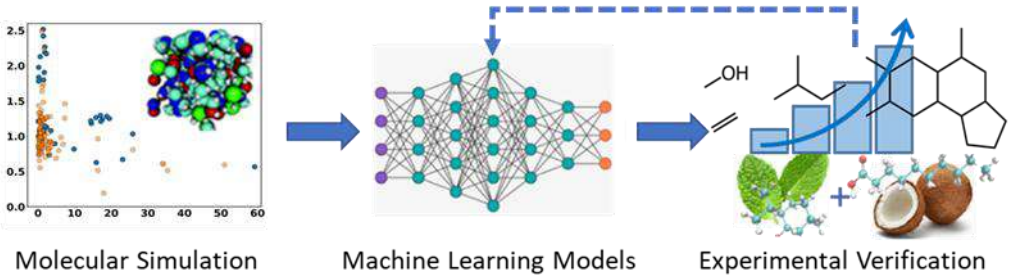
Keywords: Biomass, microplastics, green solvent, spent batteries, pulping

Shifting society's dependence on petroleum-based fuels, chemicals, and materials to biomass derived products is important not only to reduce our carbon footprint but also to increase the robustness of our energy security and economic stability. Leveraging the power of molecular dynamics simulation, meta-analysis, and machine learning (ML) based algorithms, we have developed a simulation-ML-experiment pipeline to explore a large design space of type-V hydrophobic deep eutectic solvents (HDES). One outcome of this design approach is a new class of lignin-derived HDES made from low cost, renewable resources such as plant-based phenolics, terpene, and organic acids. This presentation will share outcomes from our recent research in the new eutectic systems for applications in 1) recycling & recovery of valuable molecules from fermentation broth and integrated fermentation and separation processes; 2) hydrophobic DES based pulping of hardwood and softwood for improved lignin removal and reduced carbon footprint; 3) recycling critical metals from spent lithium-ion batteries; and 4) extraction and detection of micro-, and nano-plastic contaminants from water.



Acknowledgements: Our research is supported by funding sources including US Department of Energy and National Science Foundation (DE-EE0010860, DE-SC0025346, NSF#1929122)

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OC9 - Alternative Green Solvents in Sample Preparation methods for Lead Extraction from Electronic Waste

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Keywords: E-waste, Extraction, Green solvents, FAAS.

Printed circuit boards (PCBs) are essential components in the manufacturing of electronic devices marketed worldwide. They are composed of various materials, including metal alloys and resins, resulting in a complex and heterogeneous composition [1]. The increased use of PCBs over the past decade has generated a significant disposal problem, contributing to the growing generation of electronic waste (E-waste). The metals present in PCBs can be toxic, posing risks of soil and water contamination [2]. Given this context, this study investigated the application of more sustainable alternative solvents in sample preparation methods for lead (Pb) determination in E-waste by flame atomic absorption spectrometry (FAAS). Different alternative solvents, including deep eutectic solvents (DES) and diluted acids, were tested using a conventional extraction method. In addition to the solvent composition and solvent-sample ratio, the extraction time and temperature were optimized by the design of experiments. The DES prepared with choline chloride (ChCl) and oxalic acid (OX) achieved recoveries above 86% prior to optimization steps, followed by DES prepared with formic acid (FA) and acetic acid (AA). After optimizing the experimental conditions, the extraction time and temperature ranged from 60 to 130 min and from 89 to 94 °C, respectively, with stirring at 400 rpm. In the conditions, recoveries ranged from 95% to 106% with DES and from 97% to 101% with diluted nitric acid (10% v v^{-1}). Additionally, the detection limits were below 5.5 mg kg^{-1}, making the method suitable for this application, as high Pb concentration levels were found in the analyzed E-waste. In the greenness assessment of the methods using the AGREEprep metric, scores of 0.68 were obtained for DES-based methods and 0.50 for the HNO_3-based method. The results highlight the potential of DES for metal extraction from E-waste, enabling the development of more efficient and sustainable strategies for lead recovery and mitigating the environmental impacts associated with E-waste disposal.

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OC10 - Sustainable Extraction of Bioactive Compounds from Ginkgo biloba Leaves Using NADES for Cosmetic Applications

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Keywords: Ginkgo Biloba leaves, green extraction, natural deep eutectic systems, bioactive compounds, antioxidant

For centuries, Ginkgo biloba leaves and seeds have played a significant role in traditional Chinese medicine. Ginkgo Biloba leaf extracts have been used to improve cognitive function and memory, enhance circulation, and support respiratory health. These leaves are a rich source of antioxidant compounds, particularly flavonoids and carboxylic acids. The predominant flavonoids include quercetin, kaempferol, and isorhamnetin, mainly found in their glycosylated forms. Additionally, the leaves contain various carboxylic acids, such as shikimic acid, quinic acid, 6-hydroxykynurenic acid, protocatechuic acid, p-hydroxybenzoic acid, and gallic acid. Ethanol and acetone are widely used for extracting bioactive compounds due to their efficiency; however, their application raises environmental and safety concerns, including high flammability and potential health risks. As a sustainable alternative, Natural Deep Eutectic Systems (NADES) have emerged as promising solvents, offering comparable or improved extraction performance while reducing environmental and health hazards. The main objectives of this work were to: evaluate the potential of hydrophilic NADES on the extraction of bioactive compounds from Ginkgo Biloba leaves and their stability over time; identify and quantify the main compounds in selected extracts (using LC/MS-MS); and evaluate the cytotoxicity and the ability to inhibit the formation of reactive oxygen species (ROS) in an immortalized cell line. Three selected NADES significantly enhanced the extraction of phenolic compounds compared to conventional solvents. The extracts demonstrated high antioxidant activity and stability, indicating their potential for cosmetic formulations. In particular, one extract showed low cytotoxicity towards skin cells (HacaT) and potent ROS inhibition at high concentrations. The use of NADES offers a sustainable and efficient approach for extracting bioactive compounds from Ginkgo biloba leaves, promoting their application in cosmetic products. This study highlights the potential of green solvents in developing eco-friendly cosmetic formulations.

Acknowledgements

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OC11 – Path2Green: A New Approach to Evaluating Sustainable Extraction

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Keywords: Sustainability Assessment; Green Extraction; Environmental Impact

We introduce an innovative method to address the growing need for efficient and transparent tools that assess the sustainability of extraction processes. With the rising demand for natural products and the expanding use of biomass, it is essential to ensure that these methods are environmentally friendly. Although extracting natural compounds has historically been viewed as a harmless practice with deep-rooted traditions, modern techniques can have substantial ecological impacts if not carefully managed. To tackle these issues, we have created Path2Green, a unique metric based on 12 newly developed principles specifically designed for green extraction practices. This cutting-edge tool offers a more thorough evaluation than traditional measures by analyzing the environmental effects throughout the entire extraction process—from sourcing biomass to producing the final output. Path2Green takes into account key factors such as resource depletion, energy usage, waste production, and biodiversity conservation, aiming to provide a detailed sustainability assessment. What sets Path2Green apart is its ability to transform complex environmental data into a simple, easy-to-understand metric. This simplification enables industry experts to make informed decisions that encourage greener extraction methods. Moreover, by setting clear sustainability benchmarks, Path2Green drives ongoing innovation and improvement in eco-friendly practices across various industries. Its straightforwardness and accessibility make Path2Green especially valuable in scenarios where comprehensive life cycle assessments are unfeasible due to budget limitations or a lack of expertise. To further assist users, we have also developed a mobile app that facilitates analysis and uses engaging pictograms to display results visually.

Acknowledgements

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OC12 - Natural Low Transition Temperature Mixtures (NaLTTM) as supramolecular solvent of polysaccharides: towards soft materials design and application to plant extracts

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Keywords: NaLTTM, polysaccharides, gelation, plant extracts, stability

Natural Low Transition Temperature Mixtures (NaLTTM) are innovative supramolecular liquids that comply with green chemistry principles. Gattefossé has developed a NaLTTM composed of fructose, glycerol, and water (FGW115) for plant extraction at industrial scale.[1] Like all liquid plant extracts, those obtained with FGW115 have a limited shelf life. To circumvent this issue, we have explored gelation techniques by using different polysaccharides to limit molecular mobility in solution. Firstly, the association mechanism of FGW ternary mixtures was thoroughly examined through a characterization methodology assessing thermal properties (TGA, DSC), rheological properties (viscosity, activation energy), and interactions at molecular-scale (1D ^{1}H, ^{13}C, 2D NOESY NMR). This understanding is a prerequisite to consider interactions with polysaccharides and is pivotal for further industrial applications of FGW ternary solvents.[2] Then, we were interested in the incorporation of polysaccharides into FGW. As an example, the association of k-carrageenan (vegetal polysaccharide) with FGW115 led to fully biosourced thermosensitive physical gels. The thermo-induced gelation was attributed to the formation of aggregated H-bonded helices of polysaccharide chains. These gels exhibited high gel-sol transition temperatures and recoverable viscoelastic properties upon heating/cooling cycles. SAXS analysis evidenced a more extended conformation of polymer chains in FGW, in comparison with water, leading to gels with enhanced mechanical properties, compared to the corresponding hydrogels.[3] Finally, incorporating polysaccharides into supramolecular FGW115 plant extracts demonstrated significant improvements in microbiological stability. Thus, the addition of polysaccharides is a relevant alternative to the use of more conventional preservatives. This approach offers a promising solution for the industrial application of FGW115 biosourced soft materials with tunable rheological properties and high dimensional stability. The potential benefits for cosmetic and pharmaceutical industries are substantial, providing a pathway to more sustainable and efficient products.

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OC13 – From Solvents to Multifunctional Ingredients: Natural Deep Eutectic Solvents for Sustainable Cosmetic Emulsions

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Keywords: Formulation, Physico-chemical properties, Skincare, cosmetics, emulsions

Natural Deep Eutectic Solvents (NaDES) are sustainable solvents derived from natural metabolites like sugars or amino acids, offering biocompatibility and renewability. Their non-toxic and biodegradable nature makes them ideal for green chemistry, positioning NaDES as a promising alternative to traditional solvents while aligning with UN Sustainable Development Goals like Goal3, promoting safer cosmetic formulations.[1] Emulsions are the cornerstone of the cosmetics market, forming the basis for products like moisturizers, sunscreens, and serums by stabilizing immiscible ingredients like oils and water. Consumer demand for clean, sustainable, and high-performing products has driven innovation, with eco-friendly ingredients like NaDES offering new possibilities. This study explores using NaDES as sustainable alternatives in skin-care emulsions, with a focus on their effects on emulsion structure and long-term stability. While most efforts to greenify cosmetic emulsions focus on manufacturing improvements or replacing surfactants, few address the solvents themselves (commonly oils and water). By integrating selected NaDES as core emulsion components, this research examines their multifunctionality, sensory diversity, alignment with bio-based and locally sourced principles. Various NaDES with distinct characteristics were incorporated into emulsions to evaluate their physicochemical and sensory properties, as well as their effectiveness in delivering active molecules. A Design of Experiment (DoE) approach was employed to analyze these systems and correlate their performance with NaDES properties. Key findings, including droplet size and creaming percentage over time (measured via SMLS)[2], identified optimal formulations for efficacy testing. For instance, hydrophobic NaDES in water systems permit to double the retention of retinyl palmitate in RHE compared to conventional oil-in-water emulsions. This research, part of the DES4Skin project, seeks to identify NaDES suitable for skin applications and advance next-generation emulsified systems, contributing to a more sustainable and inclusive global economy.

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OC14 – Polyphenol Formulations in Natural Deep Eutectic Systems

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Keywords: polyphenols, NADES, formulations, solubility, extractability

Polyphenols are a widespread group of secondary plant metabolites and their positive impact on human health has been extensively researched. They play a key role in health maintenance and disease prevention including cardiovascular diseases, cancer, inflammation, diabetes, and immunity support. However, *in vivo* studies on many polyphenols have been disappointing. The main reason is their poor solubility and bioaccessibility. One way to increase polyphenols' extractability, solubility, and bioaccessibility is to use natural deep eutectic solvents (NADES). Obtained formulations could serve as versatile building blocks for preparing various functional materials including hydrogels, nano-emulsions, biofilms, etc. We investigated the solubility of the main food flavonoids (catechin, daidzein, quercetin, naringenin, luteolin, genistein, kaempferol, apigenin, diosmetin, chrysin, and rutin) in choline chloride (ChCl) based natural deep eutectic solvents [1]. NADES systems were formulated with lactic acid, ascorbic acid, urea, sorbitol, and 1,2-propanediol as hydrogen bond donors (HBD). In the case of rutin, the influence of the NADES system on the bioaccessibility of rutin in the *in vitro* digestion process was examined. Catechin demonstrated the highest solubility across all solvent systems, followed by naringenin and quercetin. Among the NADES systems, the blend based on 1,2-propanediol notably enhanced the solubility of quercetin and luteolin to 53.4 mg/mL and 26.9 mg/mL, respectively, surpassing their solubility in conventional solvents. The empirical findings were consistent with theoretical predictions made using the COSMO-RS method. It was also found that rutin solubilization in urea-based system retained rutin for 78.64% in digestive fluids after *in vitro* digestion enhancing its bioaccessibility. Moreover, it was found that certain polyphenol compounds including catechin, quercetin, rutin, naringenin, naringin, resveratrol, chlorogenic acid, rosmarinic acid, gallic acid, and caffeic acid could produce NADES system as HBD after mixing with ChCl. Four NADES systems, comprising catechin, rosmarinic acid, gallic acid, and chlorogenic acid could be diluted with water without affecting the stability of those systems and polyphenol precipitation. Both systems, where the polyphenol is dissolved in NADES or as an integral component of the NADES system, can find application in the food industry, cosmetics, pharmacy, and electrochemistry.

Acknowledgments
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OC15 – Deep Eutectic Solvent for HMF valorization

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Keywords: Deep Eutectic Solvents, HMF, Green Chemistry, Biomass

The pursuit of sustainable and efficient biomass conversion processes is a critical focus in both industrial and academic research. Among key targets, 5-hydroxymethylfurfural (HMF) has emerged as a valuable building block for the production of high-value bio-based chemicals. To enhance reaction sustainability, novel reaction protocols utilizing alternative solvents, specifically mixtures of Hydrogen Bond Donors (HBDs) and Acceptors (HBAs), offer promising pathways. In this study, the chemical stability of HMF in selected DES and their interaction of HMF have been explored using advanced spectroscopic techniques, including multinuclear NMR, FTIR, and Raman spectroscopy. Building on prior investigations into HMF-DES systems, the reactivity of HMF in the most promising DES compositions has been systematically evaluated to obtain its oxidation products (**Figure 1**). Finally, green metrics such as atom economy, solvent recycling, environmental factor and EcoScale have been calculated for the most relevant scenarios.

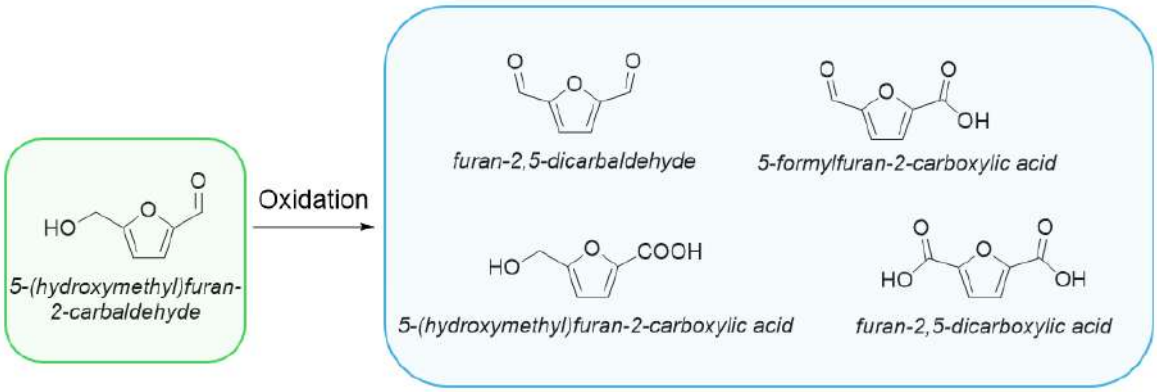

Figure 1: Proposed HMF transformation in DES.

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OC16 - Terpene-based eutectic mixtures for the extraction of molecules from aqueous bio-oil phase

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Keywords: bio-oil, eutectic systems, extraction, acetol, acetic acid, terpenes

The production of biofuels and chemicals from renewable feedstocks, such as lignocellulosic biomass, has gained significant attention in recent research. Bio-oil, which is a biomass derivative and a valuable source of various chemical families, including methoxyphenols, organic acids, and others, is a promising alternative for this purpose. However, the separation of compounds from bio-oil is essential to obtain platform chemicals to replace oil derivatives. In particular, the bio-oil aqueous phase (BAP) has attracted interest for the recovery of value-added chemicals. Also, liquid-liquid extraction (LLE) has been identified as an effective technique for bio-oil fractionation and product recovery. Thus, the first stage of this study focused on evaluating greener solvents, such as bio-based and terpene-based alternatives, for extracting acetic acid and acetol from BAP using both physical and reactive LLE. A comprehensive screening was conducted using COSMO-RS to estimate the distribution coefficient (*Kd*) of each solute in a solvent-water biphasic system. The most promising solvents were further assessed for their environmental, safety, and human health impacts before being experimentally validated through LLE measurements. In the reactive LLE experiments, selected solvents were combined with either trioctylamine (TOA) or tributyl phosphate (TBP) as reactive extractants. The effects of temperature and extractant concentration on *Kd* were analyzed for the most effective solvent-extractant combinations. Among the tested solvents, 2-methyltetrahydrofuran and 2-phenylethanol demonstrated superior performance compared to terpenes. The use of TOA-based extractants significantly enhanced acetic acid extraction, increasing *Kd* by up to 10 times compared to physical LLE, though no improvement was observed for acetol. TBP-based extractants, however, did not show significant enhancements. The second phase of the study aimed to experimentally and theoretically investigate acetol extraction from aqueous systems using terpene-based deep eutectic solvents (DES). After selecting the most suitable candidates, the density and viscosity of binary acetol-solvent mixtures were measured at temperatures ranging from 293.15 to 333.15 K. Furthermore, LLE studies were conducted on acetol-water-terpene solvent mixtures to assess extraction performance. The chosen terpene-based DESs included thymol, eugenol, eucalyptol, and octanoic acid, with pure carvacrol serving as a reference solvent. To further evaluate solvent efficiency, PC-SAFT was applied to calculate acetol *Kd* in solvent-water mixtures. These calculations were used for simulations using Aspen Plus to determine the best solvent alternatives for acetol separation. By integrating experimental and theoretical approaches, this study provides a systematic framework for optimizing separation processes for acetol recovery from bio-oil aqueous phases, reducing reliance on trial-and-error methods and promoting more efficient process development.

OC17 - Mushroom-Derived Extracts for Cosmetics: A Green Approach Using Natural Deep Eutectic Systems

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Keywords: Natural deep eutectic systems; Mushrooms; Extraction; Bioative compounds; Phenolic Compounds

The concern to assure a more sustainable cosmetic industry has been increasing. A possible solution involves adopting sustainable technologies, methodologies, and natural-origin ingredients. Mushrooms, despite being rich in bioactive compounds, remain an underused resource. Their cultivation has minimal environmental impact, requiring less water and energy while producing lower CO_2 emissions compared to traditional crops. The bioactive compounds present in mushrooms, including phenolic compounds, polysaccharides, and vitamins, offer valuable health benefits such as antimicrobial, anti-inflammatory, and antioxidant properties. These compounds are promising natural cosmeceutical ingredients with anti-aging, moisturizing, and brightening effects. However, the extraction of mushroom-derived bioactives relies largely on conventional methods using organic solvents, which are toxic and harmful to both people and the environment. As an eco-friendly alternative, Natural Deep Eutectic Systems (NADES) have emerged as a new class of green solvents. NADES are easy to prepare, biodegradable, non-toxic, and biocompatible, requiring no purification steps while enhancing the stability of natural compounds. Despite being a relatively new technology, NADES show significant potential for extracting bioactives from mushrooms to produce high-value cosmetic extracts. This study focuses on developing bioactive-rich extracts from mushroom species found in Portugal using NADES, which could be incorporated directly into cosmetic topical formulations. The selected mushroom species were analyzed for their bioactive content, health benefits, and cosmetic potential. Various NADES were prepared and characterized, followed by solid-liquid extractions. Comparative analysis revealed that NADES-based extracts outperformed hydroalcoholic extracts, demonstrating superior stabilization of phenolic compounds and validating their role as a sustainable alternative to conventional solvents. The analysis of the extracts confirmed their suitability for topical formulations. When compared to hydroalcoholic extracts, NADES-based extractions yielded better results, demonstrating their ability to stabilize phenolic compounds and act as a viable alternative to conventional solvents.

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OC18 - Extraction of Vitamin E with Deep Eutectic Solvents

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Keywords: Vitamim E; associative extraction; deep eutectic solvent; process intensification

Vitamin E is a classic phenolic compound. Extraction of such compound from natural resources like methylated oil deodorized distillates (MODDs) by traditional solvents and conventional techniques are often inefficient or challenging. To improve the extraction efficiency, deep eutectic solvent (DES) can play strong intensification role as either extractant solvent or intermediate formed by phenolic compound with other media. For extracting natural vitamin E (modeled by α-tocopherol), DESs as a class of emerging media are particularly proposed under mild operating conditions. To select DESs suitable for this task, a rational screening method is presented which covers the thermodynamic evaluation of individual components and component combinations, the assessment of environment, health, and safety (EHS) impacts of components, and the eutectic behavior estimation of component combinations. Based on experimentally reported DESs, individual components as well as random combinations of potential hydrogen bond acceptors and donors are successively prescreened by COSMO-RS predicted thermodynamic proper-ties. Experiments are finally performed with the top-ranked DESs, which well validates the reliability of the screening method and identifies $[P_{4,4,4,4}]$Cl-ethanolamine (2:1) as a suitable DES for the α-tocopherol extraction. Moreover, an innovative intensified vitamin E recovery process from the methylated oil deodorizer distillates (MODDs) is proposed, where vitamin E is in-situ transferred into a intermediate DES with an organic salt. To design the process, $[N_{4,4,4,4}]$Cl is selected as an association solvent which can efficiently form DES with α-tocopherol. Based on the determined phase diagram of the DES freezing points, four phase regions are classified, and the effect of the $[N_{4,4,4,4}]$Cl/tocopherol ratio and temperature on the extraction performance and phase transformation is figured out. Moreover, an intensified association extraction process via in-situ forming DES of α-tocopherol with $[N_{4,4,4,4}]$Cl is designed and validated by experiments. VE products are finally obtained from both model MODD (purity of 99.63 %) and practical MODDs (purity of > 79.18 %), which verifies the excellent extraction efficiency for the proposed recovery method.

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OC19 - Natural Deep Eutectic Solvents for Okara Protein Extraction: *In Silico* Design Study

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Keywords: Soybean proteins, Natural Deep Eutectic Solvents, Multi-scale Modelling, Protein-ligand-solvent interactions, *in silico* Materials Design

A particularly relevant product from the soya food industry is okara (soy pulp, tofu dregs), which is a by-product of soymilk production and is also frequently considered as a waste (Soybean Curd Residue, SCR) (about 14 million metric tons of SCR being worldwide disposed annually). Despite its potential as food product due to the high content of protein (20-40%) present in dried okara, SCR is highly susceptible to putrefaction and its handling is a challenging task, which may lead to environmental problems. Unfortunately, the most common technologies used to extract soybean (okara) proteins affect the protein nutritional characteristics and generates undesired waste alkali acids. In this viewpoint, natural deep eutectic solvents (NADESs) have been recently envisaged for bioactive compound extraction in view of their excellent extraction efficiency, low toxicity, rapid degradation, and low environmental impact. Nonetheless, critical factors determining their extraction performance such as the NADES physico-chemical properties (viscosity, solubility) and safety, or the thermal sensitivity of the proteins; calls for a careful optimization of the operando conditions and the NADES nature. In this context, we have carried out an *in silico* design combining multi-scale modelling simulations, experimental techniques and artificial intelligence (AI) models (Figure 1) to shed light on the main processes involved in the extraction process as a base to enhance their performance. On the one hand, once the most relevant protein-ligand-solvent interactions were identified via classical Molecular Dynamics (MD) simulations, their binding modes and driving forces were further characterized by means of Molecular Docking and Density Functional Theory (DFT)-based analysis. On the other hand, the capability of these NADES to extract soybean proteins from okara residues was tested experimentally, meanwhile assessing the potential risks for their application via 3D cell culture studies. Finally, all collected theoretical and experimental data was gathered to build AI models enable to identify the most important parameters affecting the extraction behaviour of the NADES. Overall, these results evidenced the potential of NADES for soybean extraction by relying on design rules based on accurate structure-property relationships, thus paving their way to their practical industrial application.

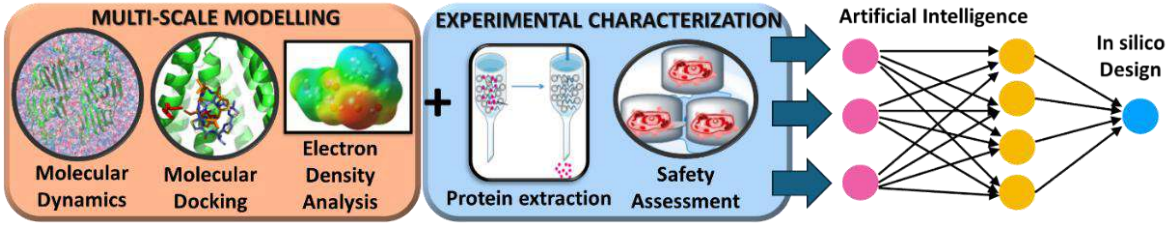

Figure 1. Scheme for the steps involved in the *in silico* NADES design study performed here.

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OC20 - Deep Eutectic Systems as Stabilization Media for Biomolecules: Insights from Case Studies and Computational Design

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Keywords: deep eutectic solvents, biomolecules stabilisation, proteins, biologically active compounds

Deep Eutectic Systems (DES) exhibit remarkable structural flexibility, allowing for precise customization to suit pharmaceutical, cosmetic, and food applications. They have the potential to effectively stabilize biomolecules by enabling higher active ingredient loading, enhancing stability under various storage conditions, and providing intrinsic preservative properties. Additionally, DES-based formulations could improve the bioavailability and permeation of active compounds, thereby increasing their therapeutic and biological efficacy. DES can also be tailored to include compounds with favorable sensory properties, making them highly versatile for practical applications. Here, we will present several case studies where DESs have been employed as stabilization media for various biomolecules. Specifically, we will present our recent research on DES enhancing lysozyme stability under heat and cold shock conditions [1], as well as our findings on the DES ability to stabilize dehydrogenases [2] and their corresponding NAD cofactor [3]. Furthermore, we will demonstrate the successful stabilization of bioactive plant metabolites, either as pure components within DES or as part of a DES-based plant extract [4]. Finally, we will discuss the role of computational approaches in designing optimal DES formulations for biomolecule stabilization, providing insights into the rational design of these innovative solvents.

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OC21 - Separation Processes with Deep Euetctic Solvents and Its Molecular Thermodynamic Applications

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Keywords: deep eutectic solvent, thermodynamics, separation process intensification, molecular mechanism

Separation and reaction processes are two key parts of the modern chemical industry, and the former accounts for most of the energy consumption in the chemical industrial production. Absorption, extraction and distillation are the three most important chemical separation unit operations. In these processes, the choice of separating agent is the first key step. Traditional separating agents are often volatile organic solvents with high boiling points, which lead to inevitable defects such as volatility loss of solvents, secondary pollution caused by product entrainment, low separation efficiency, and high energy consumption for solvent regeneration. In recent years, newly designable green solvents, deep eutectic solvents (DESs) consisting of hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD) as separating agents can avoid the above-mentioned shortcomings of traditional solvents. Similarly, how to choose suitable DESs has become a key issue, the free combination of HBAs and HBDs with various HBA/HBD molar ratios can theoretically produce countless kinds of DES candidates. This requires recourse to powerful molecular thermodynamic models for rapidly large-scale solvent screening to replace time-consuming trial-and-error experimental selection. This work will systematically introduce molecular thermodynamic modeling (such as COSMO-RS, and PC-SAFT models) suitable for complex systems including DESs. Based on these thermodynamic models, we proposed several technologies for chemical separation process, e.g., gas dehydration with ILs, CO_2 capture, volatile organic compounds capture with DESs [1], Li^+ extraction from Mg^{2+}-rich salt lake brines with DESs [2]. Furthermore, these EDS-related separation mechanism at the atomic/molecular level by systematically explored by using quantum chemical (QC) calculations and molecular dynamics (MD) simulations. This can provide a valuable theoretical guidance of the rational molecular design for developing the task-specific DESs.

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OC22 – Theoretical Characterization of Deep Eutectic Solvents as Catalysts: An Indirect Approach to Enhancing Organocatalytic Activity

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Keywords: DES, organocatalysis, Modeling, reaction mechanisms, green chemistry.

Deep eutectic solvents (DESs) have emerged as promising, sustainable alternatives to traditional organic solvents in catalysis, owing to their tunable properties, low toxicity, and environmental friendliness. While DESs have demonstrated potential as reaction media for organocatalytic processes, their direct catalytic activity remains less understood. The role of DESs as potential catalysts themselves is an area of growing interest, but the intricate interactions between the DES components and catalytic systems require a deeper understanding to harness their full potential. This study utilizes Molecular Dynamics Simulations using Machine Learning Interatomic Potentials [1] as an indirect but powerful method to characterize and understand the catalytic behavior of DESs in organocatalytic reactions. We focus here on the catalytic activity of DESs in model Michael additions, where DESs are shown to exhibit catalytic properties via hydrogen-bonding networks and other non-covalent interactions. Calculations provide detailed insights into how these solvents influence reaction pathways, lower activation barriers, and enhance selectivity. Specifically, this works aim to probe the electronic structure of DESs for systems containing L-proline [2] and novel chiral (ammoniummethyl)pyrrolidine-derived hydrogen bond acceptor [3], to compare and understand the influence of DES structure on the catalytic activity. The calculation of radial distribution functions (RDFs) from molecular dynamics trajectories enabled the identification of the strongest hydrogen-bond interactions within the DES, uncovering a significant correlation between the strength and nature of these interactions and the catalytic activity of the DES.

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OC23 - Rational Assessment of Safety and Environmental Impacts of 5-(Hydroxymethyl)furfural + Levulinic Acid Eutectic Solvent: A Computational Approach

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Keywords: Eutectic Solvent, Multiscale Materials Modeling, Toxicological Assesment, Safe and Sustainable by Design, Molecular Initiating Events.

Over the past decade, the field of Deep Eutectic Solvents (DESs) has been significantly developed. These solvents are commonly described as non-toxic, non-volatile and biodegradable. Notably, 20 % of published papers on DES emphasize their low toxicity. However, a deeper analysis reveals that out of 66000 articles, only 100 include toxicological assessment studies. This discrepancy highlights the need for a more cautious use of terms like "non-toxic" and "biocompatible" when describing DESs. Expanding research in toxicological and environmental assessments for DESs is essential to substantiate these claims. Considering the large matrix of possible molecules leading to DESs formation, a systematic, fast and low cost approach is required for the prediction and assessment of DESs safety and sustainability (Safe and Sustainable by Design, SSbD). For this purpose, this research presents a computational approach to assess the toxicological impact of 5-hydroxymethyl furfural (HMF) : levulinic acid (LEV) DES. The concept of Molecular Initiating Event (MIE), which analyze the molecular level interactions between studied molecules (DESs components) and relevant biological targets as key factors for predicting toxicological effects is developed. For this purpose two groups of targets were considered as relevant MIEs: *i*) human proteins and *ii*) model plasma membranes. Therefore, thermodynamic properties predictions employing COSMO and molecular mechanics protein docking considering skin, pulmonary and digestive target proteins were considered. Likewise, quantum mechanics calculations and molecular dynamics simulations were carried out to explore molecular mechanisms and interactions of HMF : LEV DES with model plasma membranes. These results provide novel insights into the toxicological impact of HMF : LEV DES in human health as a case study for a new framework for *in silico* toxicological assessment of DESs, thus providing a potential archetype procedure for future development of SSbD DESs, with suitable environmental and low toxicity profiles.

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OC24 - NADES as Biocompatible Media for Thermally Stable RNA Molecules

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Keywords: RNA, Preservation, Thermal stability, Biocompatibility, Biomedical applications.

The inherently low thermal stability of RNA poses operational, accessibility, and financial challenges for RNA research and RNA-based technologies. Natural deep eutectic solvents (NADES) have been shown to enhance the stability of various macromolecules, including DNA and protein. This study explores NADES as alternative storage media for RNA preservation and evaluates their biocompatibility in human cells. In vitro-transcribed mRNA was stored in various NADES at temperatures ranging from 4-50 °C, and the integrity was assessed by quantifying its translatability, represented by protein-expressing cells. NADES effectively preserved RNA integrity, retaining over 70% of its translatability for at least 28 days at room temperature (21 °C) and 48 hours at 50 °C, in comparison to -80 °C storage. Notably, the preservation efficacy remained unaffected by temperature fluctuations. Furthermore, the selected NADES concentrations maintained ~ 99% cell viability, demonstrating their biocompatibility. These findings establish NADES as efficient, biocompatible RNA storage media, enabling stable storage and transport at ambient and extreme temperatures while withstanding sudden fluctuations. This enhanced stability simplifies and expands the accessibility of RNA-based applications. Additionally, the biocompatibility of NADES supports their potential use in RNA-based biomedical applications.

OC25 - Designing deep eutectic solvents for upcycling spent Lithium-ion battery cathode

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Keywords: deep eutectic solvents; lithium-ion battery cathodes; upcycling

The industrialization of recycling the spent lithium-ion batteries present promising opportunities and challenges. We have designed several strategies for recycle or upcycle spent lithium-ion batteries to value-added materials.[1-5] DESs composed of weak acidic and strong coordinated guanidine hydrochloride + lactic acid,[1] hydroxylamine hydrochloride ($NH_2OH{\cdot}HCl$) + ethylene glycol[2] with acidity, reducibility, and coordination capability, and ternary DESs ChCl:MCl_x:Levulinic acid[3] by synergistic effects were applied for the efficient leaching of cobalt and lithium ions from $LiCoO_2$ (LCO). We further developed a strategy by combination of DES 3,4,5-trihydroxybenzoic acid + ChCl dissolution and a following solvent-induced crystallization for upcycling LCO to cobalt-polyphenol network.[4] When organic building block, Cl^-, and inducing agents concurrently exist in the system, one-step conversion from LCO to MPNPs could be achieved.[4] Finally, we applied machine learning (ML) technique for accelerating the discovery of novel promising DESs systems for cathode leaching.[5] Acidity, coordination, and reducibility were identified as the most important properties for the leaching efficiency and the importance of them were quantified by Shapley additive explanation (SHAP) method. A conditional Generative Adversarial Network (CGAN) model was established for rapidly identifying promising DESs and achieved excellent agreement with experimental results.

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OC26 - Unlocking the Potential of Natural Deep Eutectic Solvents as Tyrosinase Inhibitors

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Keywords: Natural Deep Eutectic Solvents, Mushroom Tyrosinase, Inhibitors

Tyrosinase is a copper-containing enzyme present in mammals, plants, bacteria and fungi and catalyzes oxidation reactions of both monophenolic and diphenolic compounds. Tyrosinase in nature plays a crucial role in melanin biosynthesis and enzymatic browning of fruits and vegetables however, abnormal activity of this enzyme has been associated with problems such as hyperpigmentation.[1] In recent years the interest of the research community is focusing on the discovery of potent tyrosinase inhibitors that could be used in the pharmaceutical, cosmetic and food industry. This study explores the potential of task-specifically designed Natural Deep Eutectic Solvents (NADES) as inhibitors of mushroom tyrosinase. In this context, carboxylic acid-based NADES were synthesized by selecting their components in such a way that they are biocompatible and safe to use for applications in pharmaceutical formulations. The NADES were structurally and physicochemically characterized (pH, viscosity, polarity, water content), while their ability to inhibit mushroom tyrosinase activity was assesed. The results revealed that the NADES containing choline chloride and carboxylic acids as components, show significantly low IC_{50} values from 3.8 to 7.9 μL/mL, rendering the tested NADES as promising tyrosinase inhibitors. Furthermore, the inhibition type (competitive, uncompetitive, non-competitive) of selected NADES was investigated revealing that both the hydrogen bond donor and the hydrogen bond acceptor that participate in the formation of the NADES, affect the inhibition mechanism.

Acknowledgements
Maria-Anna Karadendrou gratefully acknowledges financial support from the Research Committee of N.T.U.A.

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OC27 - Hydrophobic Eutectics and Eutectogels in Water Remediation

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Keywords: hydrophobic eutectics, eutectogels, contaminant extraction

Water is essential for human survival, yet only 40% of surface water bodies currently achieve a "good ecological status," emphasizing the need for effective water pollution monitoring and remediation technologies [1]. Existing approaches for removing industrial contaminants of emerging concern (ICECs) frequently rely on toxic solvents and unsustainable sorbents. This work addresses the issue by developing sustainable extractants based on Hydrophobic Eutectic Solvents (HES) and Hydrophobic EutectoGels (HEG) [2]. Type V HESs, formulated by combining two non-ionic, renewable components, were initially screened, assessing pH, viscosity, density, green metrics and leaching in water. The most effective HESs were tested in liquid-liquid extraction of two contaminants, bisphenol A and diethyl phthalate, and key extraction parameters were systematically optimized to enhance performance. Subsequently, the highest-performing HESs were gelled with the low-molecular-weight gelator dibenzylidene-D-sorbitol (DBS) [3] and utilized in solid-liquid extraction. HEG were characterized by rheological studies to assess their mechanical properties and suitability. In both liquid-liquid and solid-liquid extraction, very good efficiency and low leaching were achieved as measured by UV-Vis and NMR spectroscopy (Figure 1).

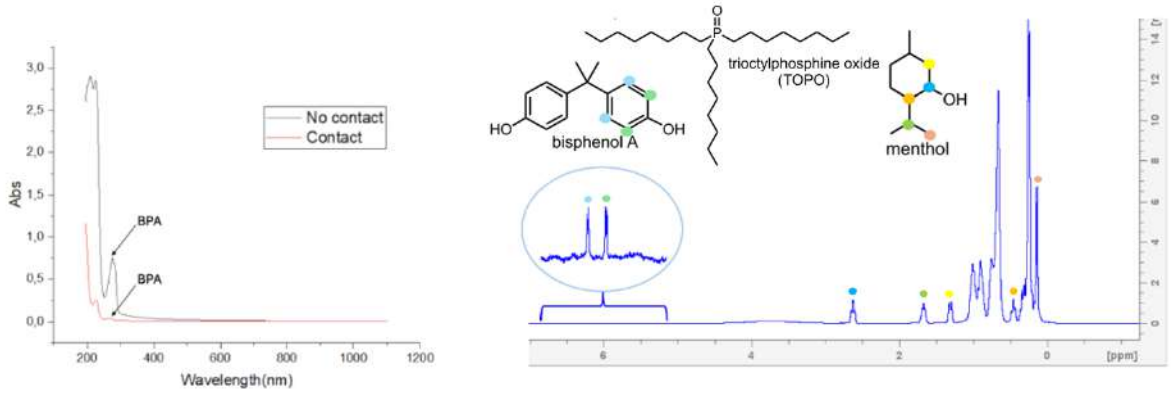

Figure 1: Representative UV-Vis spectra of aqueous phase (left) and ^{1}H NMR spectra of HES phase (right) after extraction of bisphenol A (BPA) with TOPO:Menthol 1:2 HES

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This work has been funded by European Union – Next Generation EU in the framework of the PRIN 2022 PNRR project POSEIDON – P2022J9C3R

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OC28 - Thermodriven Agarose-NADES Eutectogels: A Novel Platform for Controlled and Sustained Drug Delivery

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Keywords: Eutectogels, Natural Deep Eutectic Solvents, Agarose, Drug Delivery

Eutectogels present a versatile platform for drug delivery applications, owing to their unique structural properties and adaptability. This study explores the fabrication of eutectogels using Natural Deep Eutectic Solvents (NADES) in combination with agarose, with an emphasis on their efficacy for controlled drug release. The thermally induced cross-linking of agarose facilitates the formation of a robust three-dimensional network within the gel matrix. Water contact angle (WCA) measurements demonstrated enhanced compatibility with aqueous media in NADES-based eutectogels compared to traditional agarose-water systems. Microstructural analysis via cryo-scanning electron microscopy (cryo-SEM) revealed a well-defined porous network critical for efficient drug transport. Diclofenac, a commonly used nonsteroidal anti-inflammatory drug (NSAID), was selected as a model compound to investigate drug permeation and release through the biopolymer matrix, with Franz diffusion cells employed for permeance studies. Drug release kinetics were quantified using high-performance liquid chromatography coupled to mass spectrometry (LC-MS), confirming the eutectogels' ability to provide controlled and sustained diclofenac release. This study highlights the potential of NADES-based eutectogels, with thermally cross-linked agarose, as promising candidates for advanced drug delivery systems.

OC29 – Development of nanoformulations to encapsulate therapeutic deep eutectic systems for cancer applications

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Keywords: Colorectal Cancer, Nanoformulations, Niosomes, Liposomes and Polymeric Nanoparticles

Cancer remains a major health problem worldwide, with colorectal cancer (CRC) being the third most incident and the second most lethal [1]. Having in consideration this worldwide problematic, therapeutic deep eutectic systems (THEDES) combining terpenes with ibuprofen have arisen as a green alternative that have already been reported as presenting enhanced and selective antiproliferative activity against CRC cells [2]. However, before applying these therapeutics for CRC treatment, there is the need to develop nanoformulations to encapsulate them. Among these nanoformulations, nanoparticles (NPs), such as polymeric NPs, liposomes (LPS) and niosomes, have emerged in the last decades. In this work, poly(lactic-co-glycolic acid) nanoparticles (PLGA-NPs), liposomes and sorbitan monopalmitate-based niosomes were developed using nanoprecipitation method, a microfluidic swirl mixer and thin-film hydration method, respectively. To morphologically characterize the produced NPs, SEM, TEM and dynamic light scattering (DLS) were performed, ATR-FTIR was applied for chemical characterization and HPLC to calculate encapsulation efficiency and evaluate the release profile. Additionally, preliminary cell toxicity assays were performed. The morphological characterization results highlighted that PLGA-NPs were the most homogenous colloidal distribution, LPS were within the size raged needed for cancer applications and niosomes presented the smallest particles, but with a heterogeneous distribution. Having in consideration these results, LPS were the chosen particles for THEDES encapsulation presenting between 10% and 40% of encapsulation efficiency and around 10% of drug release (depending on the THEDES encapsulated). Regarding cell assays, it was possible to observe an antiproliferative effect for all the encapsulated systems. In conclusion, the selection of the right nanoparticles is fundamental for a successful encapsulation of THEDES and for an effective antiproliferative action.

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OC30 - New Bioactive Aryl-Substituted Aurones Via Suzuki-Miyaura Coupling in Natural Deep Eutectic Solvents

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Keywords: Aurones, Suzuki-Miyaura reaction, Deep Eutectic Solvents, Green Chemistry

Deep Eutectic Solvents (DES) are increasingly used as eco-friendly alternatives to conventional solvents. When derived from natural ingredients, the resulting mixtures are called Natural Deep Eutectic Solvents (NADES).[1] The Suzuki-Miyaura reaction, a Pd-catalyzed C-C bond formation between boronic acids and aryl halides, is widely applied in the pharmaceutical industry.[2] Aurones are natural products, which belong to the family of minor flavonoids, and possess a wide array of bioactivities.[1] In the present work, the application of the methodology developed in the Laboratory of Organic Chemistry of NTUA for the Suzuki - Miyaura reaction[2] for the synthesis of new aryl-substituted aurones using task-specifically designed NADES as solvents is studied. The new molecules were obtained in high purity and satisfactory yields, and the NADES were recycled and reused at least up to 3 times (Figure 1).

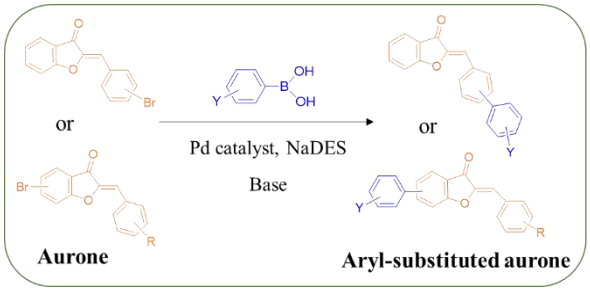

***Figure 1**. Methodology for the synthesis of the selected molecules.*

The new molecules were evaluated *in vitro* for their antioxidant activity through the inhibition of lipid peroxidation of linoleic acid induced by the free radical producer AAPH, as well as for their ability to interact with ctDNA. The majority of the compounds showed satisfactory ability to inhibit lipid peroxidation (up to 90%), while destabilization of the ctDNA double helix was observed, revealing the potential of the new molecules to be exploited as anticancer or antiviral agents.

Acknowledgements

Vasiliki Kakokefalou gratefully acknowledges financial support from the Research Committee of the National Technical University of Athens (scholarship for postgraduate studies).

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OC31 - From chemistry to art: Bringing eutectic mixtures to a new application

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Keywords: Deep eutectic systems; Varnish; Conservation and restoration; Dammar and Mastic resins; Green solvents

Turpentine, white spirit, acetone, toluene, xylene, isopropanol and iso-octane are known as some of the most used organic solvents in the conservation and restoration field. However, what all of them share in common is the high toxicity associated. Restorers, in turn, face a major challenge because despite knowing all the consequences of acute and chronic exposure to these solvents, they are limited in their options for finding alternative green solvents with similar characteristics. From our last work [1], it was observed that eutectic mixtures such as those based on method and fatty acids have the potential to be good substitutes for toxic solvents in the removal of varnish layers from aged paintings. Thus, in this work, the applicability of eutectic systems in conservation and restoration was once again investigated, in particular, the ability of these systems to replace organic solvents such as turpentine, white spirit and isopropanol in the formulation of greener spirit varnishes. This work has consisted of different steps: (1) First, a set of methods was used in the screening and selection of the most potential eutectic mixtures (e.g., FT-IR, polarity, Kamlet-Taft parameters, etc); (2) then the new varnishes were prepared using a similar ratio and method, used typically in organic solvents-based varnishes (dissolving the natural resins dammar and mastic in the alcoholic solvent); (3) finally, the eutectic systems varnishes were compared with organic based ones, in terms of visual aspect, rheological behaviour, drying time and atomic force microscopy (AFM), where it was possible to conclude that in fact they share very similar characteristics. This study has confirmed once again the great potential of eutectic mixtures as a good substitute for toxic solvents in a field so untypical, in this case conservation and restoration.

Acknowledgements
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OC32 - Overcoming the passivation of minerals using ultrasound in Deep Eutectic Solvents

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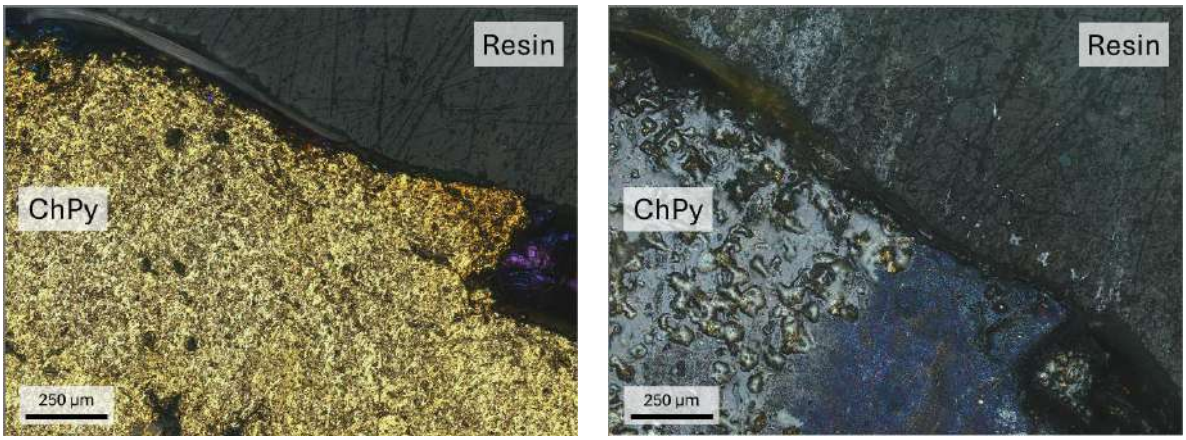
Keywords: ultrasound, deep eutectic solvent, mineral dissolution, alloy

Technology Critical Metals (TCMs) are critical for the global transition to a more sustainable energy infrastructure. Extraction of these metals is often damaging to the environment, due to the pollutant gases produced from pyrometallurgy, or toxic reagents and wastewater from hydrometallurgy. Ionometallurgy, the processing of metals using ionic fluids, could deliver a more sustainable methodology for the extraction of these TCMs from mineral sources. [1] A Deep Eutectic Solvent (DES) formed from a 1:2 molar ratio of choline chloride and ethylene glycol is used in the present work. This solvent has a wider redox potential window than aqueous solvents, as well as a low water environment that minimises the impact of oxide and hydroxide chemistry. This solvent benefits from a high chloride environment, resulting in improved stability of metal ions and complexes in solution. Many TCMs are present in nature as sulphide minerals, which are known to passivate, meaning extraction is slow. [2] Forced convection from ultrasound is hypothesised to sidestep this issue. [3] The rate of extraction for metals from chalcopyrite ($CuFeS_2$) was improved under sonic conditions by a factor of four. Pyrite (FeS_2) was unaffected, potentially due to the fundamental differences in the sulfide bonding, where the redox potential of the sulfide anion of chalcopyrite and the bisulfide pair of pyrite differ significantly. This ionometallurgical approach was applied to the extraction of TCMs from meteorites, looking into the possibility of recovering target metals in-situ using only electrons to regenerate the redox catalyst.



3DM images of chalcopyrite etched before and after etching

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OC33 - Enhanced Antioxidant Properties in Electrospun Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) Films Incorporating Natural Antioxidant Resveratrol Solubilized in Deep Eutectic Solvents for Active and Sustainable Food Packaging

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Keywords: PHBV, DES, resveratrol, electrospinning, active packaging

This study highlights the integration of deep eutectic solvents (DES) to significantly enhance the antioxidant properties of natural antioxidant, resveratrol (Res), within biodegradable poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) films. The use of DES could address a key challenge in utilizing poorly soluble natural antioxidants. Multiple DES formulations were screened to find a composition showing enhanced resveratrol solubility in comparison with common organic solvents. The selected formulation showed 17,400 and 25 times more solubility than in water and dimethyl sulfoxide (DMSO), respectively. This solubilized Res formulation was incorporated into PHBV films, that was produced via electrospinning and subsequent thermal annealing processes, resulting in continuous, non-porous films with improved antioxidant properties. Remarkably, films with DES-solubilized Res exhibited a 30% increase in antioxidant activity and material efficiency compared to those containing same amount of non-solubilized Res. Comprehensive characterizations, including wide-angle X-ray diffraction, optical, mechanical, and barrier property analyses, demonstrated that the incorporation of DES-solubilized Res enhanced the functional performance of PHBV films without compromising their structural integrity. This work sets a new benchmark in active packaging, allowing to increase the efficiency of resveratrol loaded in polymeric films, and consequently observing enhanced active properties and leading to cost reduction of the final product and a shelf-life extension of the food product. Therefore, this study highlights the potential of DES as a potent tool for improving the effectiveness of poorly soluble natural antioxidants, paving the way for the development of innovative solutions in active and sustainable food packaging.

Acknowledgements
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OC34 - Deep Eutectic Solvent-Assisted Electrospinning of Lignin: Towards Sustainable Nanofiber-Based Energy Storage

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Keywords: lignin, electrospinning, urea, lactic acid, energy storage

The development of lignin-based materials is a key step toward advancing green chemistry and reducing environmental impact. However, the processability of lignin remains a major challenge due to its complex structure, variability, and reactivity. This study investigates the potential of a urea-lactic acid-based deep eutectic solvent (ULA-DES) for the dissolution of kraft lignin, enhancing its practical utility in electrospinning applications. Elemental analysis, infrared (IR) spectroscopy, and 2D nuclear magnetic resonance (NMR) spectroscopy confirm a high lignin recovery rate (up to 96.6% at 100°C) and reveal partial esterification of lignin with lactate ions. The effectiveness of ULA-DES in lignin solubilization facilitates the fabrication of lignin-based nanofibers via electrospinning, offering a green alternative for high-performance materials. Furthermore, preliminary electrochemical impedance spectroscopy and galvanostatic charge/discharge measurements indicate that an electric double-layer capacitor (EDLC) incorporating the DES-electrospun lignin membrane as a hydrogel electrolyte demonstrates promising electrochemical properties (specific capacitance = 95 F/g series resistance R = 2.2 Ω, charge transfer resistance RCT = 1.6 Ω). These findings suggest that DES-assisted electrospun lignin membranes have significant potential as sustainable gel electrolyte matrices for energy storage applications, paving the way for environmentally friendly, high-performance supercapacitors.

Acknowledgements

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OC35 - Lessons from DESs to Design Novel Electrolytes for Electrochemical Energy Storage

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Keywords: hydrogen bond mixtures, electrolytes, supercapacitors

With a continuous increase of applications where eutectic mixtures can be used, design of novel mixtures formed by hydrogen bonding and offering “a la carte” properties is becoming a primary objective in many research fields. Herein, we describe the formation of novel mixtures based on double ion salts and different co-solvents. The liquid nature of this novel mixtures not only allowed their use as electrolytes at room temperature but also a significant improvement in the electrochemical stability window, with a widening of the operational voltage.

Acknowledgements

This work was supported by MCIN/AEI/10.13039/501100011033 (TED2021-130372B-C42, TED2021-131812B-I00 and PID2021-123648OB-I00), by “ERDF A way of making Europe” (PID2021-123648OB-I00) and by “European Union Next Generation EU/PRTR” (TED2021-130372B-C42 and TED2021-131812B-I00). L. G.-A. acknowledges the grant PRE2019-090008 funded by MCIN/AEI/10.13039/501100011033 and “ESF Investing in your future”. J. M. V.-L. also thanks C3UPO for HPC support.

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Poster Presentations

P1 – Rational Design of Natural Deep Eutectic Solvents for Efficient PFAS Removal: A Multiscale Computational and Experimental Approach to Water Remediation

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Keywords: Natural Deep Eutectic Solvents, PFAS Extraction, Multiscale Materials Modeling, Water Remediation, Computational Design, Safe and Sustainable by Design.

Per- and polyfluoroalkyl substances (PFAS) represent a critical environmental and public health challenge, with persistent contamination in drinking and wastewaters globally. This research presents a comprehensive multiscale materials modeling approach for designing novel natural deep eutectic solvents (NADES) specifically targeted at PFAS extraction, bridging computational prediction with experimental validation and scalable engineering solutions. The reported methodology integrates COSMOtherm, quantum chemical calculations, molecular dynamics simulations, and machine learning techniques to rationally design NDES with optimized PFAS extraction capabilities. A database with > 3000 PFAS molecules and > 5000 NADES was considered. Additionally, Safety and Sustainability of the considered NADES was predicted via in silico methods for all the possible considered NADES and in vitro experimentally studied for selected solvents. Therefore, interactions between NADES components and PFAS molecules were systematically investigated, considering molecular-level mechanisms, thermodynamic properties, separation efficiencies, as well as Safety and Sustainability by Design. The computational screening was followed by synthesizing and experimentally characterizing the most promising NADES formulations. Experimental validation demonstrated remarkable PFAS removal efficiencies, with selected NADESs achieving up to 99% extraction rates across different water matrices. Scalability studies revealed the potential for practical implementation, with continuous flow extraction experiments validating the computational predictions. The developed NADES show superior performance compared to conventional extraction techniques, offering a green, sustainable approach to addressing PFAS contamination. This research provides a novel computational-experimental framework for designing targeted separation media, with significant implications for water treatment technologies and environmental remediation strategies. The multiscale approach presented herein offers a generalizable methodology for developing tailored solvent systems for challenging environmental pollutants.

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P2 – Extraction of lignin from coconut fiber biomass (*Cocos nucifera*) using ternary eutectic solvents

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Keywords: Lignin; eutectic solvents; pretreatment.

The increase in the use of limited fossil-based resources in the last century has led to various associated environmental problems, and searching for sustainable alternatives and renewable resources is an urgent topic. Among the alternatives, lignin – the largest renewable natural aromatic polymer – present in lignocellulosic biomass has shown to be quite promising and important in producing bio-based chemicals and biofuels [1]. However, only a small amount is currently commercially used, with most being utilized as low-value fuel [2]. In recent years, eutectic solvents have gained considerable attention, especially in biomass pretreatment, due to their advantageous characteristics, particularly their ability to solubilize lignin [3]. Acidic eutectic solvents generally have an excellent delignification capacity due to their ability to provide active protons that break the bonds of the lignin-carbohydrate complexes. However, the conditions typically lead to lignin condensation, complicating its later valorization. Using alcohols as protectors of reaction intermediates is a strategy during the extraction of lignin, preventing the recondensation phenomenon [3]. In this study, ternary eutectic solvents composed of choline chloride (ChCl), carboxylic acids, and alcohols (glycerol or ethylene glycol) were used in the treatment of coconut fiber biomass (*Cocos nucifera*). COSMOtherm was used to predict the phase diagram and molar ratios of 36 eutectic solvents, fixing the molar ratio of ChCl and the alcohols at 1:2 while varying the proportion of acids. Among them, 22 were successfully synthesized and screened for fiber treatment. After treatment, the solid and liquid fractions were separated by centrifugation. The lignin concentration was measured in the liquid samples with UV/VIS at 280 nm as described for Ibrahim et al. [4]. Among the 22 eutectic solvents tested, the most promising were those composed of ChCl:glycerol:lactic acid (1.38±0.11 g/L) and ChCl:ethylene glycol:phenylacetic acid (1.43±0.10 g/L). Compared to the binary eutectic solvents ChCl:ethylene glycol and ChCl:glycerol, all the tested ternary solvents showed higher delignification. Furthermore, the results showed no significant difference in the lignin concentration in the liquid phase between the solvents containing ethylene glycol or glycerol for any of the acids used. These results are preliminary, and further experiments will be conducted to study the effects of the ternary eutectic solvents on biomass treatment.

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P3 - Green Solvents Towards Innovative Osteoarthritis Therapy

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Keywords: Low Transition Temperature Mixtures, Non-steroidal Anti-inflammatory Drugs, Hyaluronic acid, Osteoarthritis

Osteoarthritis (OA) is the most common form of arthritis and a leading cause of disability worldwide, affecting 7% of the population. Current therapies include pain relief with oral uptake of non-steroidal anti-inflammatory drugs (NSAIDs) and intra-articular injections of hyaluronic acid (HA), to restore the lubricant and protective properties of the joint. The administration of both therapies is limited, especially the NSAIDs, given their systemic side-effects. These adverse effects are mostly related to their low solubility in aqueous media, which hinders their bioavailability and efficiency. In this context, why not combine NSAIDs and HA in an intra-articularly delivered formulation, making NSAIDs more readily available for local action while providing a synergetic treatment? Mostly because NSAIDs have poor water solubility, and water is the media used for HA injectables. This explains why no such formulations are yet available to treat osteoarthritis. In the attempt to overcome this limitation, the potential of green solvents was explored: the Low Transition Temperature Mixtures (LTTMs), including but not restricted to Deep Eutectic Systems (DES). In this work, an LTTM-based formulation envisioning the combined intra-articular administration of HA and NSAIDs was explored. From the design of LTTMs and their characterization, a formulation able to increase the solubility of a NSAID was achieved, while simultaneously carrying HA[1]. The developed LTTM+HA+NSAID depicted rheological properties suitable for the proposed approach and proper biocompatibility, *in vitro*[2] and *in vivo*. The *in vivo* evaluation in a post-traumatic osteoarthritic rat model supported reduced inflammation, and the LTTM+HA+NSAID had a positive effect in preventing osteoarthritis progression when compared to HA+NSAID or HA, especially at the level of cartilage (Figure 1) and bone changes.

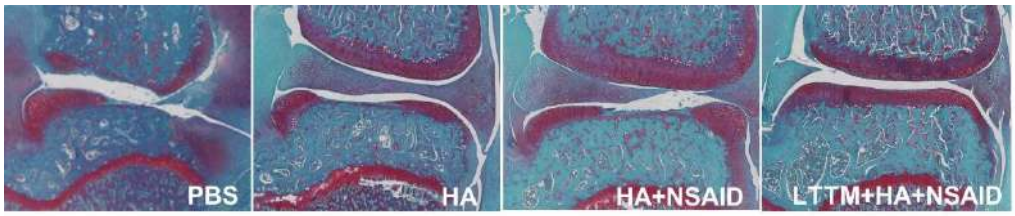

Figure 2 - Histological images of the medial compartment of rat knee joints upon intra-articular injection of PBS (control), HA, HA+NSAID, or LTTM+HA+NSAID. LTTM+HA+NSAID prevented cartilage degradation.

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P4 - Liposome-based Therapeutic Deep Eutectic Systems Encapsulation Using Microfluidic Swirl Mixers for Targeting Colorectal Cancer Cells

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Keywords: Drug delivery systems; Colorectal cancer; Therapeutic deep eutectic systems; Natural occurring molecules; Non-steroidal anti-inflammatory drugs.

Following eutectic systems spotlight due to their remarkable physicochemical properties and biological properties, while being aligned with the green chemistry metrics, the therapeutic potential of eutectics towards colorectal cancer (CRC) was herein explored. CRC is among the most incident and mortal cancers, with conventional therapies being highly invasive or lacking on target specificity, which encompasses poor prognosis and several undesired side effects. The reported promising selective toxicity of therapeutic deep eutectic systems (THEDES), combining a terpene with ibuprofen (Ibu), towards CRC cells, have pushed them forward as potential alternative or complementary therapeutics for CRC [1]–[4]. To leverage THEDES viability as CRC therapeutics, a drug delivery system based on liposomes (LPS) was designed for ensure THEDES accumulation in cancer sites. For that, a microfluidic swirl mixer was used for producing THEDES encapsulated LPS. Nanoparticles with an average size of 200 nm, monodisperse, and negative zeta potential averaging -30 mV were obtained, which foresee a stable monodispersed particle suspension. Furthermore, the obtained THEDES-LPS revealed expected morphology upon electron microscopy observation. The encapsulation efficiency varyed across the different encapsulated THEDES, with a maximum of 40.6% for limonene:Ibu (4:1). Interestingly, the observed release profile was approximately the same among the different THEDES. Finally, it was observed that CRC cells (HT29) proliferative activity was compromised upon THEDES-LPS exposure, which highlights the use of this drug delivery systems as a platform for eutectics anticancer therapeutic application.

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P5 - Could DES work as a sustainable alternative for enzyme growth and stabilization?

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Keywords: DES; Enzymes; Molecular Dynamics; Microorganisms; Biotechnology.

The Biotechnological industry has been improving methodologies over the past decades to maximize procedures and increase profit [1]. One of the major bioproducts produced by this industry are enzymes [2] which are used in a vast number of industries such as pharmaceutical, textile, food industry, and others [3]. The Biotechnological industries obtain enzymes by growing microorganism and extracted them from the medium (extracellular) or from inside the bacterial cell (intracellular). To obtain extracellular enzymes, simple purification processes are applied [4]. On other hand, intracellular enzymes required more step procedures which lead to increase the bioproduct price for the market. Nowadays, cell wall disruption and different purification processes are needed to obtain intracellular enzymes [4]. One downfall of this industry is the lack of a cleaner and less expensive process to obtain intracellular enzymes. This led to the search for new methodologies to decrease the number of steps needed for further downstream processing, and in this perspective, the use of new solvents could be the answer. In recent years, Deep Eutectic Solvents have been explored as solvent or co-solvent for enzyme stabilization, thermostability, and enhanced activity [5], leading to high prospects of the capability of this class of solvents to be used as a sustainable alternative to other solvents. In this work, we explored the capability of three DES, with a water molar ratio variation from 0 to 10, to stabilize enzymes and to work as a co-solvent for bacterial growth and enzyme production. We found that DES can stabilize for a longer period of time the *Bacillus sp.* growth plateau. We followed the enzymatic activity of alpha-amylase and found a similar activity with PBS. We followed through molecular dynamics structural changes on enzyme in the presence of DES and we found three specific amino acids present in the active centre to be highly related with the enzymatic activity.

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P6 - Machine learning boosted eutectic solvent design for CO_2 capture with experimental validation

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Keywords: CO_2 absorption experiment, CO_2 solubility in eutectic solvent, eutectic absorbent design, machine learning, SLE measurement.

Although eutectic solvents (ESs) have garnered significant attention as promising solvents for carbon dioxide (CO_2) capture, systematic studies on discovering novel ESs linking machine learning (ML) and experimental validation are scarce. For the reliable prediction of CO_2-in-ES solubility, ensemble ML modeling based on random forest and extreme gradient boosting with inputs of COSMO-RS derived molecular descriptors is rigorously performed, for which an extensive experimental CO_2-in-ES solubility database of 2438 data points in 162 ESs involving 106 ES systems are collected. With the best-performing model obtained, the CO_2 solubilities of 4735 novel combinations of ES components are first predicted for estimating their potential in CO_2 capture. The top-ranked candidate combinations are subsequently evaluated by examining the environmental health and safety properties of individual components and assessing the potential operating window based on solid–liquid equilibrium (SLE) prediction. Three most promising ES systems are finally retained, which are thoroughly studied by SLE and CO_2 absorption experiments.

Acknowledgements
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P7 - Deep Eutectic Solvent for β-O-4 Bond Cleavage of Lignin

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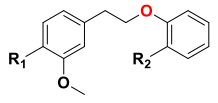
Keywords: Deep Eutectic Solvents, Lignin - Cleavage, Kinetics, Kamlet-Taft Parameters.

Lignin, constituting 15-40% of lignocellulosic biomass dry weight, represents the predominant naturally occurring phenolic biopolymer and a significant by-product of pulping processes [1], [2]. The abundant phenolic moieties within its structure confer notable properties, rendering lignin a viable precursor for value-added derivatives [3]. Nevertheless, its intricate macromolecular architecture presents substantial impediments to environmentally benign fractionation methodologies. Deep eutectic solvents (DES) have demonstrated efficacy as sustainable reaction media for the processing of hydrolyzed lignin, facilitating both solubilization and subsequent structural modification toward lower molecular weight constituents [4]. The selective cleavage of β-O-4 linkages by DES is a promising approach for lignin valorization. This investigation examines the reaction kinetics of β-O-4 ether bond scission in lignin utilizing DES as the reaction medium and sulfuric acid as a selective depolymerization catalyst by means of two lignin model compounds incorporating the β-O-4 ether linkage characteristic of native lignin (Figure 1). The solvent used in this work are describe in figure 2, which were prepared and characterized by FT-IR and ^{1}H-NMR. The kinetic analysis will focuses on elucidating the mechanistic aspects of β-O-4 bond cleavage as influenced by solvent composition. Kamlet-Taft solvatochromic parameters will be employed to quantify solute-solvent interactions.



Modelo **1**: R1= OH, R2= OMe
Modelo **2**: R1= OMe, R2= H

Figure 1: Lignin models.

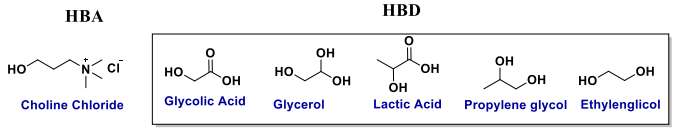


Figure 2: Hidrogen Bond Aceptor (HBA) and Hidrogen Bond Donor (HBD) components of DES.

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P8 - 1,3-Propanediol extraction from aqueous phase using hydrophobic eutectic solvents: Insights from experiments, molecular dynamics, and COSMO-SAC modelling

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Keywords: 1,3-Propanediol, eutectic solvents, Liquid-liquid extraction, molecular dynamics simulation, COSMO-SAC

1,3-Propanediol (1,3-PDO) is a pivotal chemical with diverse industrial applications in polymers, cosmetics, and pharmaceuticals (1). However, current challenges in its downstream processing demand innovative solutions with an emphasis on sustainability (2). This study explores using hydrophobic eutectic solvents to address the critical separation challenges of 1,3-PDO from aqueous systems more efficiently and sustainably (3). Five different eutectic solvents consisting of DL-menthol as hydrogen bond acceptor (HBA) and dodecanoic acid, thymol, and palmitic acid as hydrogen bond donors (HBDs), one eutectic solvent comprising of thymol as HBA and dodecanoic acid as HBD were synthesized and studied for 1,3-PDO extraction from the aqueous solution. All the studied solvents showed excellent results, with distribution coefficient (β) ranging from 20 to 234 and selectivity (S) ranging from 480 to 18000, with DL-menthol: dodecanoic acid (3:1) being the most efficient solvent. Radial distribution function (RDF), spatial distribution function (SDF), and hydrogen bonding analyses performed via molecular dynamics simulation corroborated the experimental findings and highlighted the favorable interactions of the eutectic solvents with 1,3-PDO due to the formation of hydrogen bonds between them. The lower activity coefficient predicted by the COSMO-SAC model indicates strong solute-solvent interaction, facilitating efficient 1,3-PDO extraction. In contrast, higher activity coefficient values for water indicate weaker interactions, emphasizing the effectiveness of eutectic solvents in extracting 1,3-PDO from water.

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P9 - Deep Eutectic Systems as a Sustainable Approach for Extracting Bioactive Compounds from Purslane

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Keywords: purslane; deep eutectic systems; extraction; bioactive compounds

Portulaca oleracea L., commonly known as purslane, is a grassy plant that is distributed in many parts of the world, and it is quite abundant in Portugal.[1] Purslane is a nutritionally rich plant containing various bioactive compounds, including polyphenols, flavonoids, alkaloids, terpenoids, organic acids, vitamins and omega-3 fatty acids, which exhibit antioxidant, anti-inflammatory, and antimicrobial properties. [2] Conventional extraction methods often rely on organic solvents, which can be harmful to the environment and human health. In the literature it has been reported that conventional extractions yield 11.8%, 10.5, 7.4%, depending on the solvent used, water, methanol or ethanol. However, methanol extracts presented higher amounts of phenolic and flavonoid content. [3] In this study, we explore the potential of Deep Eutectic Systems (DES) as a sustainable and efficient alternative for extracting bioactive compounds from purslane. While the use of choline chloride-based DES has previously been reported for the extraction of dopamine from purslane leaves [4], the exploration of DES compositions and its extraction yields remains limited. Here, we expand by evaluating a diverse set of DES formulations, aiming not only to enhance extraction efficiency but also to promote the stabilization of bioactives in order to be part of a final cosmetic formulation. Different DES formulations were evaluated in order to optimize selectivity, and bioactivity of the obtained extracts.

Acknowledgements
This work has received funding from European Union's Horizon 2020 - European Research Council (ERC) - under grant agreement ERC-PoC-ImproVITA-101138403. This work received support through the Associate Laboratory for Green Chemistry (LAQV) and from FCT/MCTES (LA/P/0008/2020 DOI 10.54499/LA/P/0008/2020, UIDP/50006/2020 DOI 10.54499/UIDP/50006/2020 and UIDB/50006/2020 DOI 10.54499/UIDB/50006/2020), through national funds. The work also received support from FCT/MCTES through the contract CEEC 2023.06113.CEECIND and the PhD grant 2024.00705.BD.

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P10 - DES-based leachates containing LCO, NMC or NCA oxides as electrolytes for energy storage and conversion

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Keywords: DES, cathodes of spent batteries, electrolytes, supercapacitors

Nowadays society is increasingly demanding lithium-ion batteries (LIBs). After their useful life, it will be mandatory to recycle the metals found in the spent cathodes to manage the disposal of spent LIBs. Deep eutectic solvents (DES) have been successfully used for the recovery of metals from spent cathodes. Interestingly, little attention has been paid to the recovery of the DES used for metals recovery despite of its relevance. Actually, the process is tedious and time-consuming and, because of the presence of additional solvents and/or reagents, the recovery of the DES is typically unaccomplished. The lack of DES recovery is of utmost importance as the high DES content in the leachate can account for up to 60% of the leachate cost. Our group is lately exploring the direct use of the full leachate (e.g., DES plus recovered metals) as an electrolyte.[1, 2] DESs themselves have commonly used as electrolytes and we have found that the presence of metals indeed produced a significant enhancement of the performance of the original DES as electrolyte. In particular, we have explored the use of the leachates as electrolytes for supercapacitor (SC) cells.

Acknowledgements

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P11 - DES for Efficient Antioxidant Extraction from Halophyte Plants

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Keywords: Halophyte plants; Deep Eutectic Systems; Antioxidant potential; Extraction

Halophyte plants can grow and reproduce in extreme conditions, such as high-drought, light, cold, hot, and salty environments. This is possible due to internal mechanisms of salt tolerance, based on their ability to lead with reactive oxygen species (ROS). It is a potent antioxidant system, that involves not only antioxidant enzymes but also bioactive secondary metabolites [1]. Deep eutectic systems (DES) are a mix of two or more compounds where at least one is a hydrogen bond donor and the other a hydrogen bond acceptor [2]. In this work, the idea is to use DES to extract antioxidant compounds from six different halophyte plants (*Halimione portulacoides*, *Atriplex halimus*, *Inula crithmoides*, *Suaeda vera*, *Salicórnia ramosissima* and *Sarcocornia perenis*). With this intuit three different DES are used (CA: Gly: W (2:1:2), LacA: Glu: W (5:1:1), and Bet: Gly (1:2)) and compared with a traditional solvent (MeOH 70%(v/v)). Suscintly, the results indicate that, Bet: Gly (1:2) is capable of extracting significantly more antioxidant compounds when compared with traditional solvents when the quantification method is ABTS radical scavenger. With respect to the ferric reduction antioxidant power (FRAP) method, the results are not so clear, however in three of the six plants Bet: Gly (1:2) is the best solvent. In response to the DPPH (2,2-diphenyl-1-picrylhydrazyl) antioxidant assay, the top solvents are CA: Gly: W (2:2:2) and Bet: Gly (1:2). In summary, DES can be a good help in making analternative solvents for the extraction of halophyte plants, with a high antioxidant capacity.

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P12 - Assessment on Solubility and Stability of Rifampicin Using Deep Eutectic Solvents: Pursuing Meningo-encephalic Tuberculosis Treatment Improvement

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Keywords: DES, *Micobacterium tuberculosis*, blood-brain barrier, 3D printing

Tuberculosis is a disease caused by *Mycobacterium tuberculosis* and represents a worldwide prevalent disease of great epidemiological importance [1]. The failure of treatments, especially for meningo-encephalic tuberculosis in children under 10 years of age, is influenced by characteristics of one of the most important active pharmaceutical ingredients (API) used in the difficult and long treatment of this disease: its water solubility, permeability to the blood-brain barrier, as well as its palatability, especially important in treatments for the pediatric public [2]. Deep eutectic solvents (DES) have shown significant potential in the development and manufacturing of pharmaceutical products, particularly in enhancing the solubility of active ingredients in water. Studies indicate that DES can increase drug solubility by several orders of magnitude compared to water, as observed for anti-inflammatory and antifungal drugs, thereby improving biocompatibility and consequently enhancing bioavailability [3]. The present work studied the impact of a series of deep eutectic systems (DES) on improving he solubilization of Rifampicin and its stability as a molecule in solution. Three different DES were tested, and Betaine:Ascorbic acid (1:1, 30 wt. % of H_2O) showed the ability to increase Rifampicin solubilization about 4 times fold, when compared with water in different pHs, with enhanced stability. Further steps will assess palatability and formulations' suitability for additive manufacturing (pharmaceutical 3D printing), customized according to individual patient characteristics and needs.

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P13 – Thermodynamic models for physical and thermodynamic properties of Deep Eutectic Solvents: Comprehensive survey two decades after their introduction

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Keywords: Deep Eutectic Solvents; Thermodynamics; modelling; physical properties.

It has been almost two decades since Deep Eutectic Solvents (DESs) were introduced as a novel category of green solvents to the scientific community. In mid-August 2024, a total of 12,730 documents were indexed in the Scopus database on deep eutectic solvents. So, after two decades, it is worthwhile to have an overview of the span of industrial applications for this category of solvents. Are they successfully commercialized yet or still at the research stage in the labs? In addition, it is important to have a survey on the initial research carried out on the fundamentals regarding these green solvents, necessary for any industrial application. This covers knowledge and estimation capabilities of their physical properties. This is the most important fundamental step for investigating any solvent for industrial design and optimization. Therefore, it is vital to have models for estimating a wide range of DES physical properties, from density and viscosity to thermal conductivity and gas solubility. We, at the Des.Solve group, have been working in this field since 2019 to develop different categories of predictive and correlative thermodynamic models, including group and atomic contributions, hybrid machine learning, and semi-empirical models. Our research has led to the development of 20 thermodynamic models for estimating the physical and thermodynamic properties of DEss, covering density, viscosity, surface tension, thermal conductivity, electrical conductivity, heat capacity, refractive index, speed of sound and CO_2, H_2S, and SO_2 solubilities. After five years of research, we would like to share the essence of our achievements with the thermodynamic community, from a bird's eye perspective on physical property investigations on deep eutectic solvents. With this experience, it is possible to highlight the future research paths for physical property estimations, emphasizing the current gaps, which are expected to be filled by researchers for better collaborations of academia and the industries.

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P14 - Innovative approach for the study of Deep Eutectic Systems using thermogravimetric analyses

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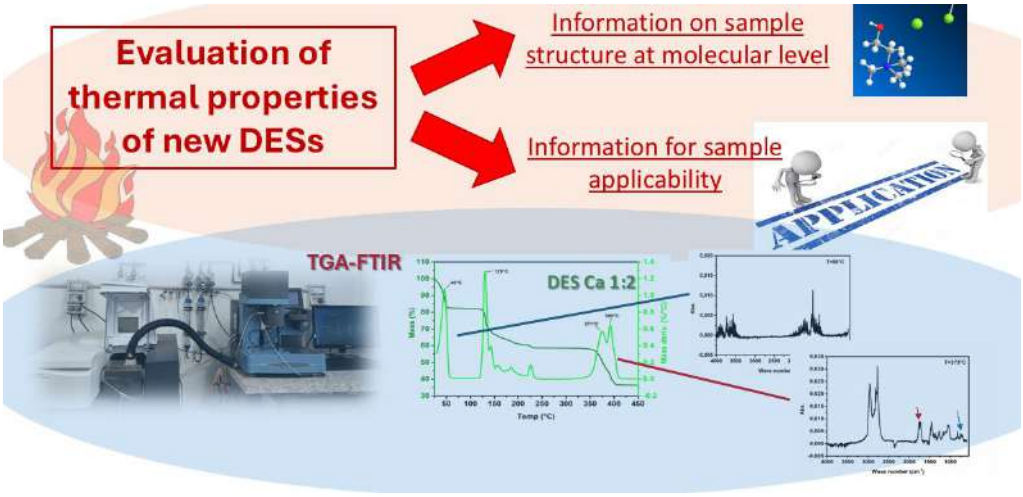
Keywords: thermal stability, type-II DESs, TGA-FTIR, DES nanostructures, modulated TGA.

Deep Eutectic Systems (DESs) are mixtures of two or more compounds with a melting point lower than the one that they would have if the mixture behaved ideally in the liquid phase, following Raoult law [1]. They recently attracted great interest in the industrial and academic fields because they are usually easy to prepare, non-toxic, inexpensive, and have low vapor pressure and flammability. The success that they have experienced in recent periods has led to a proliferation of studies concerning their application, with less investigation of their basic properties. This contribution aims to show the potential of thermogravimetric analysis as a fast and accessible technique for obtaining important basic information on new DESs. This approach may furnish fundamental information both from an applicative point of view (i.e. for the safety assessment of the degradation products and the definition of the optimal temperature range for their usage), and from a microscopic point of view, as thermal profiles could give indirect clues for a deeper understanding of the DES nanostructures [2]. A comparative study on the thermal stability of various type-II DESs (choline chloride with various hydrated metal chlorides) will be presented as an example. Thermogravimetry coupled with FTIR spectroscopy (TGA-FTIR) permitted the identification of thermal degradation products. A comparison among the thermal profiles of DESs and their salt precursors gave indirect information on the involvement of DES components in the hydrogen bond network. Finally, the activation energy of the degradation of the components was evaluated by modulated thermogravimetry.



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P15 - Deep Eutectic Solvents: Properties Induced by Nanometric Confinement

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Keywords: ethaline, neutron diffraction, quasi-elastic neutron scattering, NMR.

Over the past decade, Deep Eutectic Solvents (DESs) have garnered significant attention within the scientific community due to their remarkable functional properties, positioning them as promising alternatives to conventional solvents in green chemistry initiatives[1],[2]. Notably, DESs exhibit unconventional behavior stemming from the formation of nanoscopic domains and dynamic heterogeneity across nanometers scale, attributed to the intricate interplay of ionic and hydrogen bonding interactions among their molecular constituents[3],[4]. Consequently, unravelling the physicochemical intricacies of DESs at the mesoscopic level has emerged as a pivotal pursuit. The interrogation of DES behavior under mesoporous confinement stands as a particularly pertinent endeavour, given the pivotal role of interfaces and nanopores in numerous targeted applications of these solvents. Hence, a pressing question arises regarding the impact of mesoporous confinement on the structure and dynamic (diffusion, rotation and relaxation) heterogeneities inherent within DES systems[5],[6]. The structural and dynamic properties of Ethaline, a deep eutectic solvent (DES) composed of choline chloride and ethylene glycol, were investigated in both bulk and confined states within mesostructured porous silica (SBA-15) using Neutron Diffraction (D16B) and Incoherent Quasielastic Neutron Scattering (QENS) techniques. By combining time-of-flight (IN5B) and backscattering (IN16B) QENS spectrometers that offer complementary energy resolution, a broad dynamical range was covered from the ps to ns timescale.. Additionally, NMR experiments were conducted to explore the long-range translational dynamics of DES, emphasizing the influence of the molar ratio and the measurement lenght and time scales on the observed behavior. This study provides a comprehensive microscopic characterization of Ethaline, examining key parameters such as the elastic incoherent structure factor, diffusion coefficients, residence times, relaxation times, and their temperature dependence.

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P16 - Machine Learning-Guided Solid-Liquid-Equilibrium Prediction and Eutectic Electrolyte Design

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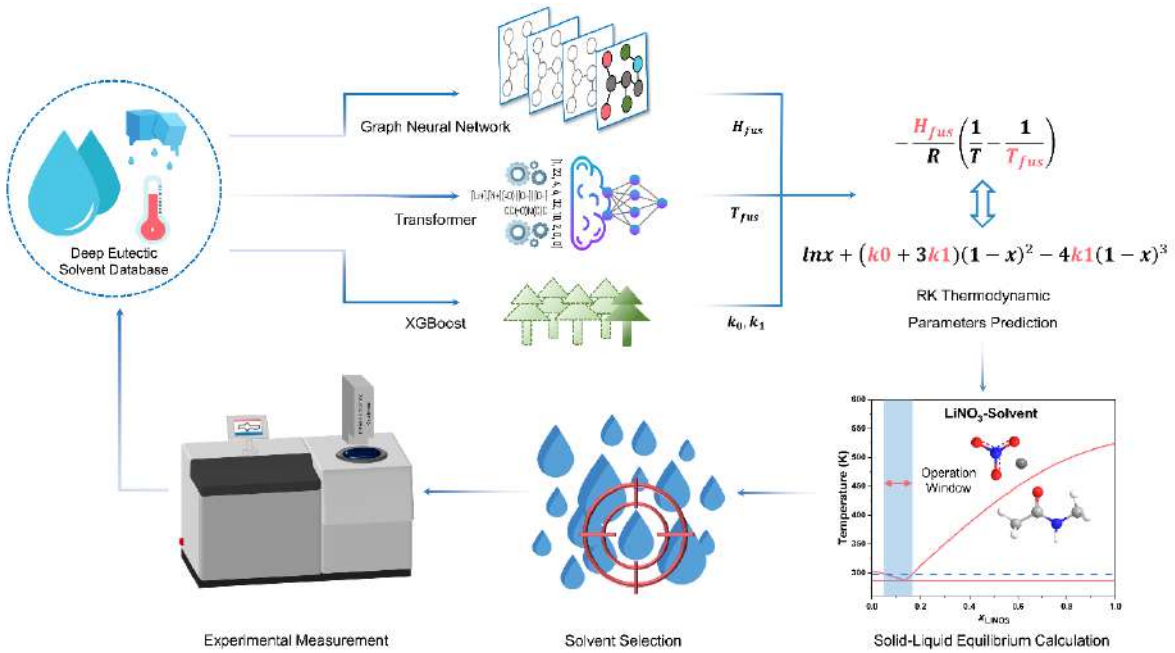
Keywords: Machine Learning; Hybrid Model; Solvent Screening; Eutectic Electrolyte

At the heart of deep eutectic solvents screening and design for a specific process is to judge whether a specific combination of components could meet the requirement of a certain operating temperature. Therefore, predicting solid-liquid equilibrium (SLE) can be very helpful for DES design. Herein, we present a machine learning (ML)-enhanced approach based on Redlich-Kister (RK) theory for accurate SLE prediction and rational solvent design. By applying non-linear ML algorithms for RK parameters prediction, we achieve superior predictive accuracy for complex eutectic behaviors, enabling precise screening of solvents for specific applications. A case study demonstrates the practical utility of this framework, focusing on the solubility of lithium nitrate ($LiNO_3$) for lithium-ion battery electrolytes. Multiple ML models, including XGBoost for RK parameters and deep learning models for fusion properties, were trained to predict the SLE of 10,856 candidate $LiNO_3$-solvent systems. Experimental validation confirmed the effectiveness of the top solvents, with dimethylacetamide emerging as a promising candidate. This work highlights the power of combining traditional thermodynamics with ML, offering a robust pathway for the design of DES and efficient solvent screening in targeted applications.



P17 - Validation and optimization of a suitable protocol using Natural Deep Eutectic Systems as a cryoprotective agent, a sustainable alternative to DMSO, in fibroblast cells

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Keywords: NADES, CPA, Non-toxic alternative to DMSO, Thawing Protocol

Natural Deep eutectic systems (NADES) have potential to be used as cryoprotective agent [1, 2]. This work focuses on the evaluation, validation and optimization of suitable protocol of NADES as non-toxic alternative to the standard cryoprotective agent dimethyl sulfoxide (DMSO). The formulation tested for NADES was prepared according to patent EP3403502A1 [1]. Cell culture, characterization and cryopreservation, was performed in bovine (bSFs,) skin fibroblasts. These cells were isolated, expanded, harvested and resuspended in freezing media (10% NADES or 10% DMSO) and immediately stored at -80°C. One, two and three months after freezing, the cells were thaw and seeded, allowing for their characterization through several tests: cell viability; observation of cell morphology and cell population doubling time determination. Variations of the thawing procedure were also tested to ensure that the protecting properties of NADES were maintained. The results show a considerable increase of viability in the protection granted by the 10% NADES with the new cell thawing protocol, compared to the standard procedure, which hints that indeed NADES can be a viable alternative to DMSO as a cryoprotective agent.

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P18 - Comparative Evaluation of Ionic Liquids and Deep Eutectic Solvents for Enzyme-Based Biopharmaceutical Stabilization

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Keywords: Enzyme, stability, deep eutectic solvents, ionic liquids

Biopharmaceutical stability and activity are critical for biomedical applications, particularly in the development of enzyme-based therapeutics. This work investigates the potential of deep eutectic solvents (DES) and ionic liquids (ILs) as stabilizing agents to address formulation challenges in the biopharmaceutical industry. A comparative study was conducted using these different classes of stabilizers, applied across a range of concentrations, to evaluate their effectiveness in enhancing enzyme stability. The impact of individual components of these stabilizers was also assessed. Structural and functional changes in the enzyme were observed in response to varying hydration levels, with optimal performance identified at a specific concentration. Among the tested stabilizers, ILs exhibited superior performance, demonstrating enhanced molecular interactions, including improved polarity and extended hydrogen bonding with the protein, leading to increased stabilization. In contrast, DES formulations showed lower stabilizing efficiency, with some acting as destabilizers. The most promising IL-based stabilizing agents were further evaluated under different temperature conditions over extended time periods. The best-performing IL formulation significantly enhanced the conformational and colloidal stability of the enzyme, with a notable increase in thermal stability. Additionally, reconstituted enzyme formulations demonstrated prolonged storage potential at refrigerated temperatures, offering possible cost savings and improved therapeutic administration. Moreover, structural integrity and enzymatic function were maintained for a sustained period at room temperature. While stabilization efficiency is dependent on the specific enzyme and experimental conditions, the results presented in this study highlight the superior performance of ILs over DES. These findings underscore the potential of tailored IL-based formulations in extending the stability of enzyme-based biopharmaceuticals, paving the way for improved therapeutic applications.

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P19 – Development and Characterization of Azelaic Acid-Based Systems for Potential Use in Rosacea Treatment

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Keywords: Rosacea, Deep Eutectic Systems, azelaic acid, cytotoxicity, physicochemical study

Rosacea is a chronic inflammatory skin disorder which mainly affects facial skin. It is characterised by persistent erythema, visible blood vessels (telangiectasias), papules, pustules and sometimes thickened skin. It is more common in fair-skinned people and more common in women, although severe cases are more common in men. Mild cases are often treated with azelaic acid, metronidazole or ivermectin. Azelaic acid is used to treat rosacea, acne vulgaris, and melasma. Its growing popularity in cosmetics suggests a promising range of applications. It presents several mechanisms such as antibacterial activity, inhibition keratinization, suppression of melanogenesis, and antioxidant and anti-inflammatory properties [2]. In order to characterise azelaic acid and evaluate its potential as a carrier for other active ingredients, azelaic acid-based systems were developed in this study [3]. These systems consist of azelaic acid and choline bicarbonate in different molar ratios. A physicochemical analysis and a cytotoxicity study using HaCaT cells were carried out to assess the toxicity of the liquid formulations on this human keratinocyte cell line, as these cells predominate in the epidermis. The density measurements showed the expected trend, with an inverse relationship between the density and the temperature. In terms of cytotoxicity, toxicity increased with system concentration and formulations with a higher mole fraction of choline bicarbonate were found to be more toxic than those with a lower fraction. The solubility of other agents used in the treatment of rosacea, such as metronidazole, ivermectin and oxymetazoline, will be investigated in future studies.

Acknowledgements

Alvaro acknowledges the TEVA chair for his grant. Additionally, we appreciate the financial support from Diputación General de Aragón and Fondo Social Europeo "Construyendo Europa desde Aragón" (GreenLife (B58_23R) research group).

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P20 - Deep Eutectic Solvents as Novel Stabilizers for IVT mRNA: A Path Toward Enhanced Biopharmaceutical Formulations

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Keywords: mRNA, stability, deep eutectic solvents

The stability of in vitro transcribed (IVT) mRNA is a key challenge in the development of effective biopharmaceutical formulations, particularly for therapeutic and vaccine applications. Deep eutectic solvents (DES) have emerged as promising alternatives for biomolecule stabilization due to their unique physicochemical properties, including biocompatibility and tunable solvation capabilities. This study explores the potential of DES in enhancing the stability and integrity of IVT mRNA under different environmental conditions. A systematic approach is employed to assess how variations in DES composition and hydration levels influence mRNA structure and degradation kinetics. Key factors such as temperature, storage time, and solvent interactions are considered to understand their impact on the long-term viability of IVT mRNA. Preliminary observations suggest that specific DES formulations may provide a protective effect against hydrolytic and oxidative degradation pathways, thereby contributing to extended mRNA stability. This research aims to shed light on the mechanisms behind DES-mediated stabilization, offering insights into their potential applications in mRNA-based therapeutics. By providing a comparative evaluation of different DES systems, this study contributes to the broader effort of optimizing mRNA formulation strategies, with implications for future vaccine development and gene therapy approaches. The findings from this work will pave the way for further advancements in stabilizing IVT mRNA for biomedical applications.

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P21 - Studying hydrolytic activity of commercial lipases in water/DES media

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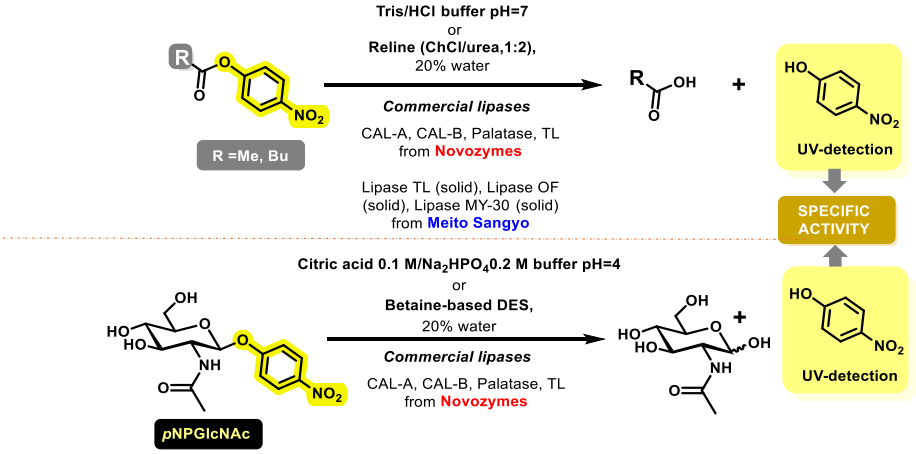
Keywords: Commercial lipases, Promiscous activity, Hydrated DESs, Hydrolytic assay

Lipases (EC 3.1.1.3) are widely used in industry due to their availability, broad substrate specificity, and ability to function in heterogeneous media [1]. Deep Eutectic Solvents (DESs) have emerged as cost-effective, easily prepared media for biocatalysis, with studies showing they can enhance lipase activity and stability [2]. This study compares the enzymatic hydrolysis of *p*-nitrophenyl (*p*NP) containing substrates (2 esters and 1 ether) by commercial lipases in conventional aqueous media and in hydrated DESs (Fig. 1).



While some enzymes showed reduced specific activity in 20%-in-weight hydrated reline DES compared to aqueous media, others displayed increased activity, demonstrating that DESs can enhance certain enzymatic reactions. Interestingly, some lipases showed activity for the hydrolysis of the promiscuous ether-type *p*NPGlcNAc, not previously reported.

Acknowledgements

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P22 - Fractionation of lignocellulosic components by Deep Eutectic Solvents

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Keywords: lignocellulose; separation; lignin, cellulose; solvent

Using lignocellulosic components to prepare materials, energy, and chemicals are negative carbon process. Fractionating lignocellulosic components to lignin, cellulose, and semi-cellulose is a prerequisite for efficiently transforming lignocellulosic components into valuable chemicals or energy. We developed several Deep Eutectic Solvents (DESs) to achieve the above goal[1-5]. At first, we developed deep eutectic solvents with different functional groups[1], and superbase-based DESs[2] for the dissolution of lignins. Then we investigated the dissolution mechanism and concluded that the relationship between lignin solubility and the solvatochromic parameters α, β, and π* varied significantly based on the DESs and the types of lignin. Also, we designed several IL-based DESs using four ILs as the HBAs, and four different HBDs, including thiourea (TU), N-methylthiourea (NMTU), glycerol (Gly), and ethylene glycol (EG) as efficient solvents for xylan[3]. The xylan solubility in DES 1-allyl-3-methylimidazolium chloride plus EG could reach 40.4 wt% at 343.15 K, much higher than that in the corresponding ILs. Furthermore, we designed robust solvent systems by a combination of ionic liquids (ILs), ethanolamine (EA), and organic superbases for the dis- solution of lignocellulose[4]. The EmimOAc/ EA-DBN system showed the best performance, and the solubility values of Populus tomentosa, sugarcane bagasse and Miscanthus giganteus at 90 °C could reach up to 3.8%, 9.5% and 20% (g per 100 g solvent), respectively. Recently, we designed a novel deep eutectic solvent (DES) composed of pyridine hydrochloride, ethylene glycol, and AlCl3 for the pretreatment of lignocellulose[5]. More robust solvents both environmentally benign and cheap are expected for industrial fractionation of lignocellulosic components. Moreover, the dissolution mechanism are far from clarified. Therefore, more efforts must be devoted to this topic for industrialization.

Acknowledgements
This work were supported by the National Natural Science Foundation of China (21873012)

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P23 - Application of Hydrophobic Natural Deep Eutectic Solvent (H-NADES) to remove antibiotics in the primary wastewater

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Keywords: Natural Deep Eutectic Solvent (NADES), antibiotics, wastewater treatment

Wastewater reuse has recently gained significant attention due to the increase scarcity of water resources. However, the presence of pharmaceuticals, even in trace levels, can impact negatively the environment and human health [1]. Given that conventional organic solvents to extract the residual pharmaceuticals, are hazardous, there is a growing demand for green solvents that are environmentally sustainable and less toxic [2]. H-NADES, hydrophobic Natural Deep Eutectic Solvent, has been proposed as an environmentally friendly solution for extracting pharmaceuticals from wastewater [3], due to its biodegradability and lower toxicity. In this study, we will show a systematic study on the use of H-NADES for antibiotic extraction from real wastewater samples. Total six H-NADES using menthol (Men) were prepared, characterized (e.g. stability, viscosity, density, pH and TOC leach for water phase) and evaluated to identify the most effective candidates for application in the extraction of three selected antibiotics, *Ciprofloxacin*, *Tetracycline* and *Sulfamethoxazole* from primary wastewater. Among the several H-NADES used, Men:Decanoic acid and Men:Octanoic acid showed the most promising results, even when ratios H-NADES:wastewater were changed. The extraction efficiency of antibiotics in the real wastewater using Men:Decanoic acid exhibited 95%, 54% and 48% extraction efficiency for CPX, TET and SMZ, respectively. Men:Octanoic exhibited 90%, 49% and 62% extraction efficiency for CPX, TET and SMZ, respectively. The findings of this study demonstrate the high potentiality of H-NADES as a green alternative for pharmaceutical removal in wastewater treatment.

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P24 - Internal Pressure of CO_2 and DES mixtures

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Keywords: Internal pressure, PVT, CO_2 solubility, DES

Deep eutectic solvents (DESs) are promising candidates for CO_2 capture applications. Our earlier investigations revealed significant increases in CO_2 solubility in DESs composed of choline chloride (ChCl) and ethylene glycol (EG) with a 1:2 molar ratio, tetrabutylammonium bromide (TBAB) and EG with a 1:3, and tetrabutylphosphonium bromide (TBPB) and EG with a 1:3 significantly increased from 8 to 10 MPa.[1,2] However, in the range from 10 to 14 MPa,[2] the increase was smaller. Understanding this behavior requires investigating the intermolecular interactions between CO_2 and DES molecules. Internal pressure derived from pressure, temperature, and volume data has been used to analyze such interactions. Previously, the numerator of the second term was calculated using experimental density values at 0.1 MPa, based on the temperature for the calculation conditions. In this study, the numerator of the second term in the previously reported density-correlated equation was modified to incorporate temperature dependence for calculating the internal pressure.

$$\rho_{\mathrm{L}} = \rho_1 x_1^n + \frac{\alpha T^2 + \beta T + \gamma}{1 - C\ln[(aT + b + p)/(aT + b + p^*)]} x_2 + [(cT + d)x_1 + (eT + f)]x_1 x_2 \qquad (1)$$

where, p, T, x, and ρ represent pressure, temperature, mole fraction, and density, respectively. Subscripts 1 and 2 refer to CO_2 and DES, respectively. Fitting parameters include α, β, γ, a, b, C, n, c, d, e, k. ρ_1 in the first term is the CO_2 density obtained using the Span-Wagner equation.[3] Internal pressure was calculated using the modified equation (1).[4] The internal pressure of CO_2 + ChCl:EG (1:2), TBAB:EG (1:3), and TBPB:EG (1:3) mixtures showed a maximum around a CO_2 composition of 0.1 in mole fraction, a minimum in the range of 8–10 MPa, and an increase in the range of 10–14 MPa thereafter. The maximum internal pressure is observed to arise from the uptake of CO_2 into DESs with strong intermolecular forces, leading to an enhancement of interactions within the solution. Conversely, the minimum internal pressure is represented the point where intermolecular interactions are weakest, resulting in a significant increase in CO_2 solubility. Further experimental studies on internal pressure are expected to provide deeper insights into the CO_2 solubility behavior in DESs from the perspective of intermolecular forces. In the future, the development of DESs with enhanced performance in CO_2 separation and capture could be facilitated by this method.

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P25 - Optimized recovery of β-carotene via ternary eutectic mixture

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Keywords: Choline ternary DES, surfactant, β-carotene, extraction, simulation

β-Carotene, a prominent carotenoid widely present in plants, fungi, and algae, is well-known for its diverse biological activities, particularly its antioxidant properties, which offer significant benefits to human health [1]. However, a major challenge in the utilization of β-carotene arises from its typically low concentrations and its occurrence within complex mixtures in fruits and vegetables. Consequently, the development of environmentally sustainable extraction methods that ensure effective recovery of β-carotene while maintaining its bioavailability has emerged as a critical research focus. In this regard, Aqueous Two-Phase Systems (ATPS) and eco-friendly solvents, such as Deep Eutectic Solvents (DES), are in alignment with the principles of green chemistry and demonstrate considerable promise for the recovery of such biomolecules [2]. To address these challenges, this study presents a novel platform for the efficient recovery of β-carotene from aqueous solutions. For the first time, a ternary eutectic mixture comprising Choline Chloride, Urea, and Glycerol in an appropriate molar ratio (ChCl:U:Gly, 1:1:1) is proposed as an extractant to induce phase separation in aqueous solutions of the non-ionic surfactant Triton X-102, thereby facilitating β-carotene recovery [3]. Following the characterization of the ATPS through the delineation of the immiscibility region and correlation of experimental data, optimal conditions were established for maximizing β-carotene recovery from surfactant-aqueous mixtures across varying feed compositions. The results indicated that mixtures with higher concentrations of the DES achieved up to 99% recovery of β-carotene in the surfactant-rich phase. Furthermore, to evaluate the broader applicability of this sustainable approach, a process simulation was performed using SuperPro Designer, underscoring the potential of this innovative methodology.

Acknowledgements
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P26 - NADES/Alginate-Based Beads for Enhanced Curcumin Delivery: A Therapeutic Approach for Intestinal Bowel Diseases

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Keywords: curcumin, alginate beads, natural deep eutectic systems, targeted delivery, IBD

Inflammatory Bowel Disease (IBD) is an autoimmune disease that includes ulcerative colitis and Crohn's disease and affects approximately 5 million people worldwide [1]. Currently, there is no cure for IBD but highly expensive treatments are being used for the management of the disease. Fortunately, nature offers a more sustainable alternative: curcumin. Curcumin is a potent natural anti-inflammatory biomolecule; and therefore, presents the inexpensive alternative for the treatment of IBD [2]. Curcumin is a hydrophobic phenolic compound derived from the rhizomes of the Curcuma longa, which is extensively cultivated in Asia. Traditionally, curcumin has been used for centuries in indigenous medicine to treat common eye infections, bites, burns, acne and other skin diseases as well as wound healing agent [3]. However, curcumin is extremely poorly water soluble and therefore, is poorly bioavailable. Nevertheless, it has been considered, by the Food and Drug Administration, as "generally regarded as safe" (GRAS), even at very high doses. NADES, being known as excellent solvents for hydrophobic molecules are a promising solution for design of a bioavailable formulation [4]. This work aimed to develop a drug delivery system capable of selectively delivering curcumin to the intestinal tract, overcoming the challenges of the gastric environment while simultaneously enhancing its solubility and bioavailability in the intestine. To achieve this, a drug delivery system based on alginate and NADES beads was successfully developed. These beads were fully characterized in terms of size, encapsulation efficiency, water solubility, release profile and cytotoxicity. The results suggest that these beads can deliver curcumin selectively in the intestinal tract, surpassing the gastric tract with minimal release. This work opens a new opportunity for curcumin to be used in the treatment of a highly debilitating condition that is IBD.

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P27 - Natural Deep Eutectic Solvents for Extraction of Stilbenoids from Side-Streams of Wine Production

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Keywords: NADES, COSMO-RS, grapevine roots, stability study of *r*-viniferin

There is significant scientific and commercial interest in developing of sustainable methods for the extraction of secondary plant metabolites, such as polyphenols (including stilbenoids and proanthocyanidins), without the use of organic solvents. The present study focused on the winery residues, which contain significant amounts of extractable antioxidative, cardioprotective and antiproliferative natural products, such as the bioactive stilbenoids *trans*-resveratrol and *r*-viniferin [1]. Developing a sustainable process that utilizes these renewable sources was the main goal of this study. In a preliminary COSMO-RS based in silico-selection of a potential NADES system for the ultrasonic-assisted extraction of *r*-viniferin from grapevine roots, a total of 2080 systems were screened [2,3]. The extraction parameters were then optimized for the most suitable NADES system, consisting of choline chloride (Ch) and 1,2-propanediol (Pdiol). This approach resulted in a 28% higher extraction yield for *r*-viniferin. Compared to a traditional ethanol-water mixture, the NADES extraction process resulted in a 9% higher extraction yield. Analytical studies on the storage stability of *r*-viniferin in NADES systems demonstrated that *r*-viniferin is chemically stable in the Ch/Pdiol system. However, it becomes unstable when stored in a NADES system prepared from fructose (Fru) and lactic acid (LA) (Figure 1). Therefore, an adsorbent material (Amberlite® XAD-16N resin) was utilised, resulting in the effective removal of *r*-viniferin from the NADES mixture, achieving a highly efficient yield of 80%. This application can be used for the solvent-free extraction of stilbenoids from side-streams of wine production and for the subsequent use of these compounds as functional ingredients in dietary supplements, cosmetics, or as phytopharmaceuticals, due to their known bioactivities.

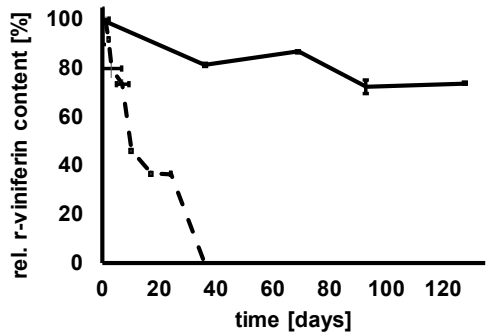

Figure 3. Monitoring the storage stability of r-viniferin in the NADES extract Ch/Pdiol 1/2, 10 wt% H_2O (solid line) and in the acidic NADES extract Fru/LA 1/2, 20 wt% H_2O (dashed line) [4].

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P28 – Improving the Mechanical Properties of Mucin Gels through Natural Deep Eutectic Systems

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Keywords: Natural Deep Eutectic Systems; Eutectogels; Mucins; Rheological properties

Natural deep eutectic systems (NADES) are solvents obtained from the mixture of two or more natural occurring compounds such as sugars, amino acids, organic acids or polyols. When combined on a specific molar ratio the compounds interact with each other through hydrogen bonds, yielding a homogenous mixture with a melting point lower than the original compounds. Over the past decade, NADES have been used for multiple ends, one of them being the preparation of gels, the so called eutectogels. Combining NADES with polymers allows to obtain a supramolecular structure, that in most cases presents better characteristics that the standard materials. Adding NADES to the preparation of biomaterials allows the improvement of mechanical properties, the improvement of stability and the decrease of degradation rates and even the optimization of drug delivery profiles. Mucins are the major nonaqueous component of mucus, which covers the moist epithelium and serves as the first line of defense against microorganisms [1]. Mucus gels can be used to trap viral particles, such as human immunodeficiency virus (HIV), and synthetic mucin gels have been developed to be used for the prophylaxis of individuals exposed to HIV [1]. Despite the developments, their rheological properties can be further improved. With this knowledge we propose the use of NADES to optimize the mechanical properties of mucin-based gels. To select the NADES for this work the main characteristics to be taken in account are bioactivity and affinity with mucins (determined by Hansen Solubility Parameters). The solubility of mucins in NADES/NADES solutions and the possibility to prepare mucin-based gels with NADES will be determined. To characterize the obtained eutectogels swelling and degradation studies will be performed. The rheological, strain-weakening and self-healing properties will also be determined and compared with standard mucin gels.

Acknowledgements
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P29 - How Different from Typical Solvents is Lanthanide Extraction in DES? A Thermodynamic Perspective

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Keywords: Hydrophobic eutectic solvents, lanthanides, metal extraction, calorimetry

The separation of lanthanides is a subject of high interest, being recognized as one of the seven chemical separations that could significantly reduce pollution and energy consumption[1]. Hydrophobic eutectic solvents (HES) offer a promising alternative to traditional organic phases in solvent extraction (SX), offering advantages such as eliminating the need for diluents and preventing the formation of a third phase. However, due to their non-ideal nature, typically being constituted by a highly structured liquid phase and complex intercomponent interactions, the behaviour of these solvents may differ substantially from conventional extraction systems[2]. This study investigates the solvent extraction of lanthanides, focusing on the biphasic transfer of trisnitrato complexes of lanthanides ($M(NO_3)_3$) (aq) with tri-n-octylphosphine oxide (TOPO) as the extractant. In the system under analysis, the TOPO extractant is incorporated in a hydrophobic eutectic solvent together with decanoic acid ($C_{10}OOH$). The partitioning of metal ions between this biphasic liquid system was studied at different temperatures, with the Gibbs free energy and the entropy of extraction (ΔG_{extr} and ΔS_{extr}) being determined from the distribution ratios. The thermochemical signatures associated to the biphasic transfer of $M(NO_3)_3$ were determined using isothermal titration calorimetry. For method validation and to highlight differences in thermodynamic behaviour between hydrophobic eutectic solvents and conventional systems, the results are then compared with a traditional solvent extraction system (described in the literature[3]) in which TOPO is diluted in toluene.

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P30 - NADES as Eco-Friendly Cleaning Agents for Biofouled Membranes in Filtration Systems

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Keywords: biofouling; cleaning in place; nanofiltration; desalination

Biofouling is a major challenge faced by membrane filtration technologies for water production and reuse, necessitating regular cleaning of membrane elements. Conventional clean-in-place (CIP) protocols, involving acid and alkaline cleaning solutions, often fail to fully recover system performance and pose environmental concerns. Hence, there is a strong demand for effective and green CIP solutions. This study evaluates the potential of NADES, which have emerged as eco-friendly alternatives to conventional solvents in various applications, including extraction and dissolution. Previously, NADES composed of betaine, urea, and water (BUW) has been shown to disrupt the biofouling matrix by breaking hydrogen bonds, ionic bonds, and hydrophobic interactions [1,2]. In this study, different dilutions of 1:1:3 BUW NADES stock (molar ratio, 77 wt.% BU) were applied as CIP solutions on biofouled membranes. The physicochemical properties of NADES were tailored by adjusting the water content. For example, the viscosity and density were reduced by a factor 20 and 1.2, respectively, by diluting 1:1:3 BUW to 30% v/v. Hydraulic tests after 1-hour exposure to different BUW dilutions showed that higher concentrations (>50% v/v) significantly increased membrane hydraulic resistance. Conversely, CIP tests in membrane fouling simulators showed that lower BUW concentrations (30% v/v) enabled CIP efficacy equivalent to NaOH without adverse effects on membrane permeability. These results highlight the potential of NADES-based agents as eco-friendly approach in water treatment and desalination. Additionally, it demonstrates the potential of using dilute NADES to dissolve and remove biofouling in membrane filtration systems.

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P31 - The Role of Betaine and Urea Mixtures to Enhance Antibiotics' Water Solubility

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Keywords: ciprofloxacin, metronidazole, tobramycin, deep eutectic solvents

The solubility of drugs is a critical factor influencing their therapeutic efficacy, as it directly impacts bioavailability, absorption, and stability. Many promising pharmaceutical compounds face solubility challenges, limiting their practical applications. Deep eutectic solvents (DES) have emerged as innovative and sustainable media to address these limitations. DES offer remarkable tunability, allowing their components to be tailored to enhance the solubility of poorly water-soluble drugs. Furthermore, DES can improve the chemical stability of sensitive molecules, protect active pharmaceutical ingredients (APIs) from degradation, and provide biocompatible systems for drug delivery [1]. In this work, Betaine (B) and Urea (U) were selected to investigate their solubilization capacity of three antibibiotics: ciprofloxacin (C), metronidazole (M) and tobramycin (T). In this sense, different B:U molar ratios (2:1, 1:1, 1:2) and water contents (30%, 50%, 75% and 100%), as well as B and U aqueous solutions, were studied at temperatures of 25ºC and 37ºC. The supernatants (equilibria of 72 hours) were further analysed by HPLC-DAD (C and M) and HPLC-RI (T). The B:U at 1:1 molar ratio and 30% of water added was the most promising DES for C and M, increasing their water solubility by 10.7- and 2.7-fold, respectively. On the other hand, T was mainly solubilized at higher amounts of water and urea (B:U at 1:2 and 75% of water). The antibacterial potential of the model APIs in DES was object of investigation by determining their respective minimal inhibitory concentration (MIC) against Gram-negative (*E. coli* and *P. aeruginosa*) and Gram-positive (*S. aureus*) bacteria.

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P32 - Assessments of Toxicological Effects and the Influence of Preparation Methods in Mice Administered with Choline Chloride-Urea Deep Eutectic Solvents

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Deep eutectic sovlents (DESs) are neoteric solvents in which the eutectic point is lowered due to hydrogen bonding interactions between two or more compounds. Recently, DESs have garnered attention in various fields, including pharmaceuticals, food, and cosmetics, due to their green, versatile, and tunable biocompatibility, which have contributed to their application in vivo models to enhance therapeutic efficacy. Hence, the safety of DESs is a pivotal consideration. However, when choline chloride and urea at a molar ratio 1:2 (CU), a representative DES, were prepared by heating, side product was formed. Therefore, this study aimed to evaluate the inherent toxicological risks associated with the application of CU in biological models. Furthermore, the metabolic perturbations in mice that received CUs prepared via two different methods - heating, which produced by-product, and freeze-drying, which did not - were compared to investigate the potential toxicity of the commonly adopted heating method. To this end, biological samples such as serum, liver, kidney obtained from mice administered with saline, CU_H, or CU_FD were subjected to non-targeted metabolomics and biochemical assays. For unbiased preprocessing of metabolomics data, the R-based Isotopologue Parameter (IPO), which follow the logic of Design of Experiment (DoE) to automatically optimize parameters for high-throughput data, was employed. Notably, clinical symptoms including dry regurgitation, drooling, swelling, seizure, and gastric damage were observed only in CU_H-treated mice. GC-MS-based examination revealed metabolic alterations not only related to choline chloride and urea metabolism but also those caused by oxidative stress. Oxidative stress was confirmed based on superoxide dismutase (SOD) activity and the ratio of glutathione (GSH) to glutathione disulfide. A comparative analysis of the metabolic profiling of CU_H and CU_FD-treated mice identified metabolic disturbances in ammonia-regulatory, anti-oxidative, nucleotide, and energy metabolic pathways. The differences in the metabolic profiles of mice injected with CU_H and CU_FD, respectively, were presumed to be triggered by side product generated in CU_H. In conclusion, these findings suggest that the induction of oxidative stress may be contemplated when CU is used in biological models and propose that the heating method for CU preparation may precipitate further toxicological consequences.

P33 - Electroactive Polymer-Film Modified Electrodes Prepared in Binary and Ternary Des: Application in Electrochemical Sensors

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Keywords: Binary and ternary DES, Phenazine dyes, Polymer films, Electropolymerization, Electrochemical sensors

Deep Eutectic Solvents (DES) have been used for different applications such as synthesis and electrodeposition of nanomaterials, as dispersion medium for nanoparticles, and preparation of electrochemical sensors, as an alternative to aqueous and non-aqueous solvents, and ionic liquids [1]. Whereas binary DES are formed by the mixing of a single hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD), addition of a second HBD leads to a ternary DES (tDES) that can confer improved properties [2]. DES have been used for preparing electroactive redox polymer films on electrode substrates by electropolymerization [3]. The most common DES for the electropolymerization of phenazine dyes is ethaline (choline chloride and ethylene glycol, molar ratio 1:2) due to its low viscosity, high conductivity, and stability. Electroactive redox polymer films have been used in electrochemical sensors and biosensors due to their electrocatalytic effect on the oxidation of analytes such as carboxylic acids and to their favourable electronic, optical, electrochromic, electroluminescent, and chemo-sensitive properties [3,4]. Phenazines are an important class of dyes that have been employed in the preparation of modified electrodes for electrochemical sensors and biosensors by their electropolymerization in different solvents, most recently in DES [3-5]. The combination, in modified electrodes, of electroactive redox polymer films with nanomaterials such as multiwalled carbon nanotubes (MWCNT), graphene (GN), carbon quantum dots (CQD), and metallic nanoparticles has enhanced the sensitivity and electrocatalytic effects of electrochemical sensors [3,4]. This has been demonstrated in applications involving analytes such as ascorbate, epinephrine, acetaminophen, 5-aminosalicylic acid, dipyrone, and hydroquinone in pharmaceuticals and dermatological creams. Analysis of real samples, such as urine, juice fruits, and commercial medicaments yielded excellent results, indicating that these sensor platforms are promising for future applications in electrochemical sensing.

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P34 - Computational Design of NADES Using COSMO-RS for Ice Control Applications

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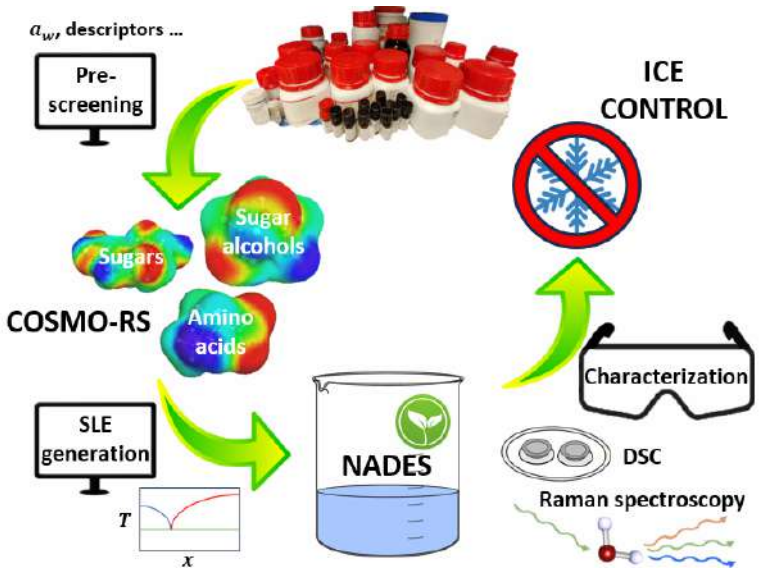
Keywords: NADES, COSMO-RS, Ice control, Low-temperature Raman spectroscopy, DSC

Natural Deep Eutectic Systems (NADES) have shown great promise in sustainable and green chemistry applications due to their low toxicity and ease of preparation. Given the empirical approach of selection of components and the mixing ratios for NADES, we aimed to create a methodology of in-silico pre-screening and eutectic composition prediction to optimize NADES for ice control applications. The water activities of commonly used sugars, sugar alcohols and amino acids were predicted using the conductor-like screening model for real solvents (COSMO-RS) and used as a pre-screening tool to identify potential NADES-forming compounds. Then, binary phase diagrams were generated for mixtures of these compounds using COSMO-RS to find the eutectic point. Experimental characterization of the predicted eutectic compositions for select amino acid-sugar alcohol and sugar-sugar alcohol NADES was performed using differential scanning calorimetry (DSC) and low-temperature Raman spectroscopy. The NADES exhibited significantly reduced enthalpies of fusion and ice crystal formation by over 70% and 50% respectively, compared to pure water, highlighting their anti-icing potential. Lastly, quantum chemical descriptors generated by COSMO-RS were analyzed for the different NADES-forming components to identify new pre-screening parameters such as the hydrogen bond donating moments and propose potential new quantitative structure-property relationship (QSPR) model descriptors.



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P35 - Thermostability of eutectogels

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Keywords: NADES, Eutectogels, NADES content, thermostability

Natural Deep Eutectic Solvents (NADES) have emerged as versatile and sustainable green solvents with a wide range of applications. By combining NADES with natural gelling agents, it is possible to develop natural NADES-based eutectogels, a novel class of materials with tunable properties. The thermostability of these eutectogels can be adjusted by varying the amount of NADES incorporated during their preparation. In this presentation, we explore the preparation and characterization of eutectogels derived from xanthan gum, agar, and agarose, using two NADES systems: betaine:urea:water (BUW) and choline chloride:urea:water (CHClUW). Particular attention was given to the influence of increasing the NADES content on the thermal stability of the gels. Thermogravimetric analysis results (Figure 1) demonstrate the effects of varying BUW quantities on the thermostability of xanthan gum-based eutectogels. These findings highlight the potential of NADES-based eutectogels as sustainable materials with customizable properties for diverse applications.

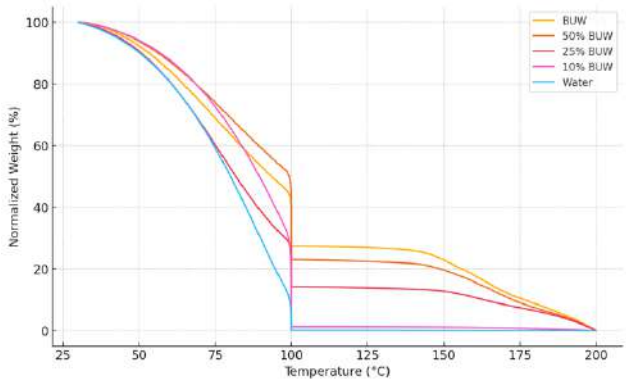

Figure 1: Thermogravimetric analysis results for eutectogels prepared with Xantham Gum (XG) and different quantities of BUW. The ratio of NADES solution to xanthan gum (XG) was maintained at 10:0.15 g/g for all the gels.

P36 - NaCl-Gly deep eutectic electrolyte for stable and high-voltage supercapacitor

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Keywords: DES, electrolyte, sustainability, supercapacitor, energy

In recent years, deep eutectic solvents (DESs) [1] have joined ionic liquids (ILs) as alternative electrolytes in several applications [2], among which their use as electrolytes is of particular interest owing to their low volatility, low flammability and good electrochemical stability [3]. Differently from other electrolytes, such as ILs and those based on volatile organic compounds, these mixtures can be easily prepared without stringent conditions, hence reducing their production cost [4]. Notwithstanding their remarkable features, it is crucial to investigate the correlation between structure and properties further to harness the potential of these electrolytes as eco-friendly alternatives to traditional organic ones and ILs. Herein, we propose a sustainable electrolyte based on NaCl and glycerol. By means of an in-depth multi-technique investigation, including Raman and FTIR spectroscopy, of the formulated electrolytes, we point out the effect of the structuring of the system on the transport and electrochemical properties. The 1:10 molar ratio mixture proves to be a DES, showing good performances when implemented in a supercapacitor, with an high operating voltage of 2.6 V and a capacitance retention of 96% after 1000 cycles. These findings highlight the potential of glycerol-based DESs as alternative electrolytes for sustainable electrochemical energy storage applications.

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P37 - Selective Capture of Hydrofluorocarbons Using Deep Eutectic Solvents

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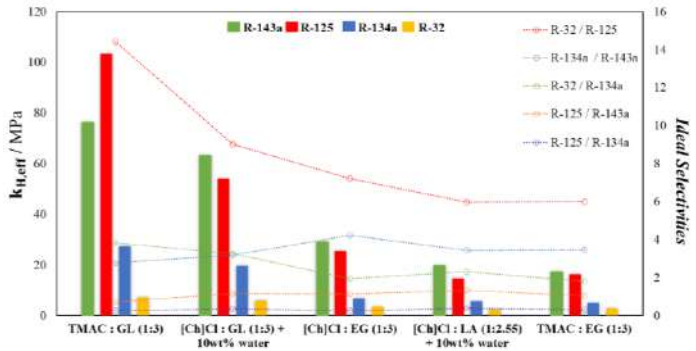
Keywords: Hydrofluorocarbons, refrigeration, soft-SAFT, solubility, competitive selectivity

The widespread use of hydrofluorocarbons (HFCs) in refrigeration presents significant environmental challenges due to their high global warming potential. Efficient separation and recovery of these gases can reduce environmental impact and improve resource utilization. This study explores the use of Deep Eutectic Solvents (DESs) based on choline chloride ([Ch]Cl) and tetramethylammonium chloride (TMAC) as eco-friendly alternatives for selective HFC separation and recovery. The solubility of four common HFCs (R-125, R-134a, R-32, and R-143a) was investigated experimentally at 300.15 K and low pressure, complemented by thermodynamic modeling using the soft-SAFT equation of state. The study provides key insights into density, viscosity, enthalpy and entropy of dissolution, effective Henry's constants ($k_{H,eff}$), and ideal selectivities ($\alpha_{i/j}$). Calculated $k_{H,eff}$ and $\alpha_{i/j}$ for the studied DESs are shown in Fig. 1. Generally, the solubility trend across the DESs was observed as R-32 > R-134a > R-125 ≈ R-143a. Among the studied DESs, TMAC:EG (1:3) exhibits the highest absorption capacity, while TMAC:GL (1:3) and [Ch]Cl:GL (1:3) + 10 wt% water show promising selectivity for separating F-gas mixtures, particularly those containing R-32. The competitive selectivity of DESs for refrigerant blend separation at different pressures is also predicted. Despite relatively low absorption rates, DESs containing TMAC:GL (1:3) and [Ch]Cl:GL (1:3) + 10wt% exhibit promising selectivity for separating F-gas mixtures, especially those containing R-32, which is particularly relevant for recovering compounds from commercial blends such as R410A and R407F. These findings highlight the potential of DESs for recovering key components from commercial refrigerant blends, enabling more sustainable refrigeration practices. Furthermore, this study emphasizes the role of molecular modeling as a powerful predictive tool for guiding the optimization of separation processes.



Calculated effective Henry's constants ($k_{H,eff}$) for HFCs (bars graph, left axis) and ideal selectivity ($\alpha_{i/j}$, symbols and lines, right axis) in TMAC:GL (1:3), [Ch]Cl:GL (1:3) + 10%wt water, [Ch]Cl:EG (1:3), [Ch]CL:LA (1:2.55) + 10wt% water and TMAC:EG (1:3) at 300.15.

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P38 - Elucidating the dynamics behaviour of PFASs at the water and hydrophobic low-melting mixture solvents interphase

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Keywords: Per-and polyfluoroalkyl substances (PFAS) extraction; Water; Hydrophobic low-melting mixture solvents (LoMMSs); Interphase Diffusion; Molecular dynamics (MD) simulations.

In this work, we studied the interphase dynamics of hydrophobic low-melting mixture solvents (LoMMSs) for the advanced remediation of per- and polyfluoroalkyl substances (PFASs) in wastewater systems by using classical molecular dynamics (MD) simulations. We showed the interaction between widely prevalent PFAS-specifically perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) and an innovative LoMMS composed of cineole (CIN) and linoleic acid (LNA) at equimolar ratios. Our investigations reveal that the interphase diffusion of PFASs through the LoMMS is a multi-stage process involving diffusion, interface sorption, and subsequent migration into the bulk aqueous phase. The simulations underscore a robust affinity between the PFASs molecules and the LoMMS, with the displacement of PFASs from the water interface marked by the formation of complex hydrogen-bonded networks. This intricate interplay results in a significant reorganization of water molecules, leading to potential clustering at the interface and compression of the fluid phase. These findings not only substantiate the efficacy of LoMMSs in PFASs extraction but also highlight the need to account for competitive interactions at the water interface, which could impede the absorption kinetics. By providing a detailed molecular-level narrative of the interphase capture phenomena, this study paves the way for designing efficient, low-toxicity LoMMS-based systems for the targeted removal of PFASs from contaminated water sources.

Acknowledgements
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P39 - Optimization of Protein Extraction from *Tenebrio molitor* Powder With Eutectic Solvents

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Keywords: insect powder, alternative solvents, response surface methodology, sustainability, foods

The global demand for sustainable, high-quality protein sources has intensified the search for alternatives to traditional animal- and plant-based options. Insects present nutritional, environmental, and economic benefits, being a promising solution for the extraction of high-value biomolecules such as proteins, with potential application in the food industry [1]. Most studies, however, rely on the use of conventional solvents, raising environmental concerns. In this sense, deep eutectic solvents (DES) have emerged as sustainable and efficient alternatives, with remarkable performance regarding biomolecules extraction, standing out as biocompatible and low environmental impact solutions when correctly designed [2]. The present work looks for biocompatible material-based DES for application in the extraction of proteins from *Tenebrio molitor*. Among the various starting materials screened, two solvents, choline chloride:urea and choline chloride:levulinic acid, both at 1:2 molar ratio and 90% w/w water, were the most promising. Further optimization, using response surface methodology, included the study of key parameters such as time, temperature, and volume of solvent. Then, with a view toward potential industrial application, the protein-enriched extracts were subsequently subjected to precipitation techniques.

Acknowledgements

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P40 - Sustainable Valorization of Olive Leaves: From Waste to Health

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Keywords: Olive Leaves, Phenolic Compounds, Hydroxytyrosol, Oleuropein

Agro-industrial byproducts are rich in bioactive compounds with health benefits, that can be extracted and formulated into food and pharmaceutical ingredients, resulting in sustainable waste processing and the development of novel plant-based products [1]. *Olea europaea L.* leaves are rich in phenolic compounds, especially oleuropein (OL) and hydroxytyrosol (HT) [2]. In this study, we investigated the extraction of phenolic compounds from olive leaves using Natural Deep Eutectic Solvents (NaDES). We evaluated the extraction efficiency of different NaDES assisted by ultrasound (USAE) and microwave (MAE). The results demonstrated that the total phenolic content (TPC) obtained with NaDES was comparable to that achieved using a conventional solid-liquid extraction with methanol (MeOH). Notably, MAE exhibited approximately twice the efficiency of USAE in extracting HT, while also significantly reducing the processing time (15 min vs. 120 min). Regarding OL extraction, the efficiency varied depending on the NaDES used: some solvents performed better with MAE, while others favoured USAE. Furthermore, chemical analyses confirmed the antioxidant capacity of the extracts, and their bioactivity was assessed through antioxidant, anti-inflammatory, and anticancer cellular assays. In conclusion, MAE proved to be an efficient and sustainable method for extracting phenolic compounds from olive leaves using NaDES, yielding bioactive-rich extracts with potential health benefits.

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P41 - DES/EtOH Solvent Systems for Improved Curcumin Solubility, Extraction, and Encapsulation

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Keywords: Deep eutectic solvents, curcumin, solubility, extraction, encapsulation.

Curcumin is widely recognized for its therapeutic potential; however, its clinical efficacy is hindered by its poor aqueous solubility, which severely limits its bioavailability. Developing an eco-friendly and cost-effective solvent system for curcumin dissolution and processing is crucial for biomedical and pharmaceutical applications [1]. Among alternative solvent systems, deep eutectic solvents (DESs) have emerged as promising candidates [2, 3]. In this study, several DES compositions were screened to determine their curcumin solubility. The highest solubility was observed in a DES composed of choline chloride (CC) and 1,2-propanediol (PD) at a 1:2 molar ratio. To further enhance the solvent system's efficiency, ethanol (EtOH) and water were introduced as co-solvents. Physicochemical properties (viscosity, density, and refractive index) of prepared solvent systems were measured and their structures were characterized via FTIR analysis. The DES/EtOH co-solvent system with 1:2:2 was found to have the highest curcumin solubility of 27 mg/mL, determined with HPLC. The DES/EtOH system was then utilized separately as an extraction and encapsulation platform. Microwave-assisted and ultrasound-assisted extraction processes were used to extract curcuminoids. For *in vitro* release studies, saturated DES/EtOH curcumin solutions were encapsulated in alginate-chitosan hydrogel beads. The release tests conducted in simulated gastrointestinal fluids demonstrated that the encapsulated system maintained pH-responsive release behavior, with peak release observed in the simulated colonic fluid. These findings highlight the potential of DES-based solvent platforms as effective alternatives for curcumin extraction and controlled-release applications.

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P42 - New Approaches to Lignocellulose Delignification: Combining Alkaline Deep Eutectic Solvents and Oxygen

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Keywords: alkaline deep eutectic solvents, delignification, pulp, oxygen

Delignification, a key process in the processing of lignocellulosic materials, focuses on the efficient removal of lignin, thereby improving the accessibility of cellulose for further processing. Research confirms that deep eutectic solvents (DESs) have excellent delignification effects on various types of lignocellulose, especially on unbleached pulp [1]. Most commonly used DESs have a pH lower than 7. Previous studies suggest that alkaline DESs increase the solubility of lignin and improve its degradation, which reduces the need for aggressive chemicals and lowers the environmental impact of the process [2]. Many pulp mills use so-called oxygen delignification prior to the bleaching process in order to reduce chlorinated organic compounds in the wastewater. Modifying conventional oxygen delignification, where the residual lignin content would decrease by more than 50%, would reduce the consumption of bleaching chemicals and improve the environmental aspects of the process. Oxygen is a weak oxidizing agent in its normal state, making it ineffective in delignification. Its oxidative power can be enhanced by increased temperature and an alkaline environment. The most important factor in oxygen delignification is the introduction of gaseous oxygen in contact with the fibers under alkaline conditions. This study explores the optimal conditions (alkaline DESs type, temperature, oxygen pressure) that lead to maximum delignification efficiency of hardwood kraft pulp. It also evaluates the effect of oxygen on improving the selectivity of the process, which is crucial for minimizing the loss of valuable biomolecules such as cellulose.

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P43 - Isolation of Extractive Compounds from Biological Waste of the Wood-Processing Industry Using Deep Eutectic Solvents

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Keywords: DES, extraction, bark, wood processing industry

The forest of the European Union represents a rich source of renewable biomass. Nearly half of the renewable resources used for energy production come from forests. A significant amount of harvested wood, approximately 17 %, is utilized in paper industry and 12 % of wood is used to produce wood-based boards [1]. In both industry sectors, debarking is a necessary step preceding the processing of the wood. Bark constitutes approximately 5 – 25 % of the tree´s total weight, depending on the tree species [2]. Therefore, the bark represents a substantial fraction of the generated biomass waste. This biological waste is subsequently used as energy source during wood processing. However, numerous studies have demonstrated that tree bark contains phenolic compounds, such as flavonoids, stilbenes and tannins, which exhibit various health-promoting properties. The primary biological activity of these substances include antioxidant, antibacterial, and antifungal effects, moreover their neuroprotective, cardioprotective and anticancer properties have also been documented [3]. Therefore, the aim of our study is to optimize extraction conditions for the isolation of value-added compounds using by deep eutectic solvents (DES) as potential selective reagents for the valorisation of bark as a waste product of the wood-processing industry.

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P44 - Properties of Paper Made of Pulp Modified with DES-like Mixtures

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Keywords: modification of pulp; mechanical properties; optical properties; DES-like mixtures

Deep eutectic solvent-like mixtures (DES-like mixtures) represent an innovative use of green alternatives for a variety of applications, for example as a replacement of conventional chemicals in lignocellulosic industry. DES-like mixtures effectively remove lignin and reduce need to use harmful chemicals during pulp production. They can also be used to modify cellulose, improving their surface properties for better bonding and fiber flexibility [1,2,3]. The aim of this work was to characterize pulp and paper sheets made from pulp that was delignified by using DES-like mixtures in different ratios, as a replacement for conventional chemical delignification. Suspensions of pulps were grinded and then tested for parameters such as Shopper-Riegler degree, water retention value, zeta potential. The mechanical and optical properties were then measured on the produced paper sheets. Using a DES-like mixtures to delignify the pulp, we observe modifications of the fibers and changes compared to the original sample. Achieved results are comparable to the ones using conventional delignification techniques.

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P45 - Sustainable extraction of lycopene from tomato waste using hydrophilic eutectic solvents

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Keywords: Green solvent; hydrophilic deep eutectic solvents; carotenoids; tomato.

Lycopene, an antioxidant carotenoid, has a unique acyclic structure that makes it lipophilic and soluble in organic solvents. The extraction step is crucial in obtaining bioactive compounds from natural sources, with the organic solvent technique being the most widely used. However, more sustainable alternatives are being developed to replace these solvents. One example is deep eutectic solvents, which are less toxic and more environmentally friendly. This study proposes using green solvents to extract lycopene from tomato processing waste. Different hydrophilic deep eutectic solvents (DESs) based on organic acids and alcohol and polyalcohols in various molar ratios (7 DESs) were prepared and tested as hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD). The DESs were ready with the following parameters: molar ratio of the eutectic mixture (moles HBA: mol HBD), temperature of 80°C, time of 30 minutes, and homogenization at 1000 rpm [1]. The subsequent extraction was performed under the following conditions: solvent/sample ratio of 1000µl/100mg, extraction temperature of 45°C, and extraction time of 120 minutes. The carotenoids extraction yield (µg/g) was the evaluated response. Carotenoid yield (µg/g) was determined by spectrophotometry according to Rodriguez-Amaya [2]. The highest yields (283.48, 251.39, and 214.49 µg/g) were obtained with acetic acid: cinnamyl alcohol, acetic acid: glycerol, and hexanoic acid: cinnamyl alcohol DESs. These results highlight the potential of hydrophilic eutectic solvents as a sustainable approach to recovering bioactive compounds from tomato by-products. Furthermore, their partially nonpolar character increases solubilization, mass transfer, and extraction efficiency, making them promising for separating lipophilic compounds [3].

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P46 - Advancing Green Extraction Technologies: Computational Design of Recyclable NADES for Bioactive Compound Isolation

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Keywords: Natural Deep Eutectic Solvents (NADES); Bioactive Compounds Extraction; COSMO-RS Computational Modeling; Green Separation Techniques; Thermodynamic Property Analysis

Natural Deep Eutectic Solvents (NADES) have emerged as a promising alternative to traditional volatile and hazardous solvents in the extraction of bioactive compounds for pharmaceutical, medical, and nutritional industries. Conventional extraction methods often involve high energy consumption, substantial economic costs, and potential safety risks. While NADES offer superior efficiency and safety, their practical application hinges on developing effective compound separation strategies to enable solvent recycling and maximize utility. This computational study employs COSMO-RS methodology to investigate the thermodynamical properties of selected Type V NADES previously identified as optimal for bioactive compound extraction. Recognizing the thermal sensitivity of target compounds, which precludes conventional distillation techniques, we systematically explore alternative separation strategies. By comprehensively analyzing solute solubility across various NADES at different temperatures and examining vapor-liquid equilibrium under varied pressure conditions, we evaluate the potential of innovative techniques such as vacuum distillation and controlled precipitation. The research aims to develop a holistic approach to bioactive compound extraction and separation, with a focus on creating a robust, scalable process suitable for future industrial applications. The proposed methodology promises to address current limitations in green solvent technologies, offering a more sustainable and efficient extraction paradigm.

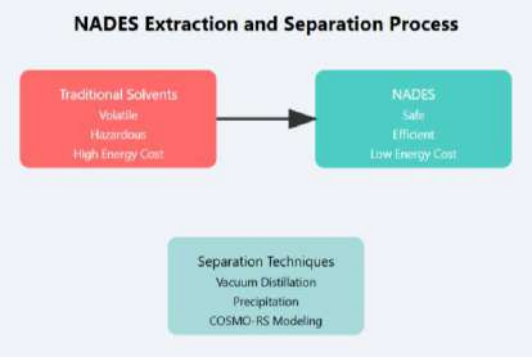

Figure 1. Scheme for the NADES design study performed here for extraction of bioactive molecules.

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P47 - Integrated Extraction and Clarification of mRNA from Yeast Using Ionic Liquids

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Keywords: Ionic liquids, mRNA, aqueous biphasic systems; clarification

Messenger RNA (mRNA)-based vaccines exhibit enhanced safety and efficacy profiles, representing nowadays a promising approach for the prevention and treatment of a wide range of infectious and non-communicable diseases [1]. The current manufacturing process of mRNA involves *in vitro* transcription (IVT), presenting considerable challenges due to its high cost and complexity. With these issues in mind, this work aims the development of efficient and cost-effective strategies for mRNA extraction from yeast cells. To this end, ionic liquids (ILs) are proposed due to their ability to disrupt yeast cells, acting as well as adjuvants in the formulation of aqueous biphasic systems (ABS) for mRNA clarification. mRNA encoding for luciferase was biosynthesized resorting to a yeast strain developed within the scope of the EIC-Pathfinder Yscript project (www.yscript.eu). Bio-based ILs comprising anions of different alkyl chain lengths were synthesized and investigated. The results showcase ILs ability to disrupt yeast cells, evidenced by agarose gel electrophoresis and *in vitro* translation assays. Afterward, the IL extracted samples were applied in polyethylene glycol 8000 g/mol (PEG 8000) and dextran 70000 ABS envisaging to purify the target mRNA. Results show that RNA is preferentially partitioned to the dextran-rich phase, with ILs presenting a positive impact on the purification performance. RNA was obtained with high integrity and A260/A280 nm ratio from spectrometric measurements was approximately 2.0, typically accepted for pure RNA formulations. Ongoing work focuses on the determination of the obtained purification factors and in the optimization of ABS compositions to remove unwanted contaminants. Overall, the results from this work demonstrate the potential of IL-based strategies toward the development of efficient and cost-effective strategies for integrated extraction-clarification of mRNA bioproduced from yeast.

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P48 - Navigating the Design Space of Deep Eutectic Solvents with Stochastic Machine Learning

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Keywords: Artificial Intelligence, Gaussian Processes, Lubricants, Green Chemistry

Deep eutectic solvents (DESs), binary liquid mixtures noted for their strong intermolecular interactions, have emerged as promising green alternatives to traditional organic solvents. The design of these novel solvents is complex, as their properties do not simply reflect the weighted average of their precursors. Incorporating low molecular weight compounds, such as water, to reduce viscosity or modulate other properties is a common practice. This leads to an overly complex and extensive DES design space, where the number, chemical nature, and relative composition of precursors must be carefully tuned. Machine learning (ML), with its innate ability to correlate variables, presents a promising alternative to trial-and-error approaches in the design of DESs. While most ML models require an exceedingly large number of data points to be properly trained, stochastic ML based on Gaussian processes (GPs) can fully capture the properties of organic and inorganic compounds with small and scarce datasets (common in the DES literature), using sigma profiles as molecular descriptors [1]. In this work, GPs were used to fit and predict several physicochemical properties of DESs, namely density, viscosity, and melting temperature. Experimental data was collected from the literature, including over 400 unique DES combinations and more than 4000 independent data points, covering most common families of organic compounds. Each dataset was carefully split into training, validation, and testing sets to determine the optimal GP architecture and hyperparameters for each physicochemical property. Coefficients of determination exceeding 0.95 were achieved for all studied properties, including viscosity, which spanned values over eight orders of magnitude, and melting temperature, which encompassed a range of nearly 700 K. Using the trained GP models, new DES-based lubricants were designed by exploring the sigma profile space of DESs. The GPs suggested novel combinations of precursors not present in the original database to achieve desired viscosities and melting temperatures. These novel DESs were experimentally prepared and characterized for the first time in this work. Viscosity and tribological properties were also measured, which surpassed common standards in the literature for low and high operational temperatures, effectively leading to DES formulations suitable for lubricant applications. Overall, this work highlights the efficacy of stochastic machine learning in navigating the vast DES chemical space and its potential to streamline solvent discovery while promoting sustainable chemical practices.

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P49 - Design of effective nucleic acids separation methodologies using ionic liquids and three-phase partitioning approaches

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Keywords: Ionic liquids, aqueous biphasic systems; three-phase partitioning; separation; nucleic acids

RNA-based biopharmaceuticals represent nowadays a versatile and effective class of medicinal drugs highly effective for the prevention and treatment of several human diseases. However, the therapeutic efficiency of RNA is impacted by its highly labile nature and intrinsic low stability, the multitude of contaminants in cell lysates sharing similar chemical and structural features with RNA, and the complexity/cost of current purification strategies. In this context, amino-acid-based ILs (AA-ILs) may play a significant role in overcoming the described bottlenecks, arising as more sustainable and effective platforms for purifying RNA. This is achieved by exploiting the high versatility of amino acids, in the creation of more biocompatible ILs, as well as due to their ability to establish specific affinity interactions with RNA bases. This work focuses on developing efficient and cost-effective RNA purification platforms from real biological matrices resorting to the use of three-phase partitioning (TPP) strategies based on AA-ILs-based aqueous biphasic systems (IL-based ABS). A new set of AA-ILs was designed and synthesized comprising different combinations of amino acids as cations and/or anions of ILs. Extraction studies were then performed with complex samples. Herein, ABS formed by polypropylene glycol 400 g/mol and the ILs argininium chloride, cholinium L-phenylalaninate, cholinium DL-aspartate stand out as the most promising ones, allowing the selective precipitation of the impurities, and thus fitting within the TPP concept. Overall, these strategies allow to take a step forward in obtaining high-quality RNA molecules with potential use as biotherapeutics.

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P50 – Natural Deep Eutectic Solvents as Crucial Components for the Preparation of Nanostructured Lipid Carriers

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Keywords: Natural Deep Eutectic Solvents, Nanostructured Lipid Carriers, Curcumin

Nanostructured Lipid Carriers (NLCs) have emerged as a new generation of lipid nanoparticles, which are employed as encapsulation matrices and drug delivery vehicles for bioactive substances. NLCs combine solid lipids and liquid lipids (oils) in their structure, leading to enhanced properties for drug delivery applications.[1] The aim of the present study is the development and optimization of a greener methodology for the preparation of NLCs and, subsequently, the encapsulation of natural products, using task-specifically designed Natural Deep Eutectic Solvents (NADESs) as an indispensable part of the NLC structure. The use of NADESs for the preparation of NLCs is an innovative and advantageous approach, since these solvents act both as a solvent for the compound to be encapsulated and as the liquid lipid for the construction of the NLCs.[2] In this context, a series of NADESs were synthesized and characterized, and their ability to play the role of the liquid lipid for the formation of blank NLCs was investigated. The NLCs were evaluated for their size, z-potential and polydispersity index as well as their stability in aqueous dispersion. The combination of components that produced NLCs with the optimum characteristics was chosen as the matrix for the encapsulation of the natural product curcumin. The curcumin-loaded NLCs showed significant antioxidant activity *in vitro* (DPPH free radical scavenging ability and lipid peroxidation inhibitory activity).

Acknowledgements
Financial support from the Research Committee of National Technical University of Athens is gratefully acknowledged (PhD scholarship for Kyriaki Safari).

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P51 - Revealing the Nature of Eutectic Solvents: A Synergy Between DSC and Lock-Free DOSY NMR

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Keywords: DOSY NMR, thermodynamics, COSMO-RS

To properly classify a mixture as a NaDES, rigorous experimental characterization, including the establishment of its solid/liquid phase diagram, is essential to confirm a true eutectic point. Without this, labeling a mixture as NaDES risks oversimplification or misrepresentation. Over the past decade, the scientific community has criticized the overuse of the NaDES term, leading to the development of alternative labels such as Low Transition Temperature Mixtures (LTTMs) and Mixtures of Natural Compounds (MiNaCs).[1–4]. In this study, we sought to resolve these terminological and scientific ambiguities by implementing an innovative multi-technique characterization approach. Specifically, we combined viscosity measurements, differential scanning calorimetry (DSC), and an original lock-free DOSY NMR strategy. This approach was applied to two binary mixtures: octanoic acid paired with menthol and octanoic acid combined with 1,3-propanediol. These experimental analyses were complemented by SLE (Solid-Liquid Equilibrium) simulations using COSMO-RS, providing a theoretical framework for the interpretation of the observed behavior. The results of our multi-technique approach highlight the importance of comprehensive characterization in the study of eutectic solvents. By integrating DSC, DOSY NMR, and theoretical modeling, we were able to uncover critical differences between NaDES and other solvent types. These findings are essential for advancing the design and application of sustainable solvents in green chemistry, ensuring that claims of eco-friendliness and functionality are backed by robust experimental evidence. In addition, this study supports the adoption of the MiNaC nomenclature as a flexible and inclusive term for mixtures of natural metabolites, especially in cases where the presence of a eutectic point or glass transition cannot be conclusively demonstrated.

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P52 - Mechanochemical Fractionation of biomass

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Keywords: deep eutectic solvents, ball milling, lignocellulose, biorefinery.

The efficient fractionation of lignocellulosic biomass is crucial for advancing sustainable biorefinery processes [1]. This study explores the synergistic effect of deep eutectic solvents (DES) and ball milling in the fractionation of Eucalyptus biomass and apple tree pruning. Different types of DES (acidic, alkaline, and neutral) are evaluated under optimized experimental conditions, including speed, number of balls and processing time. The composition of obtained fractions was determined using standard analysis techniques [2].

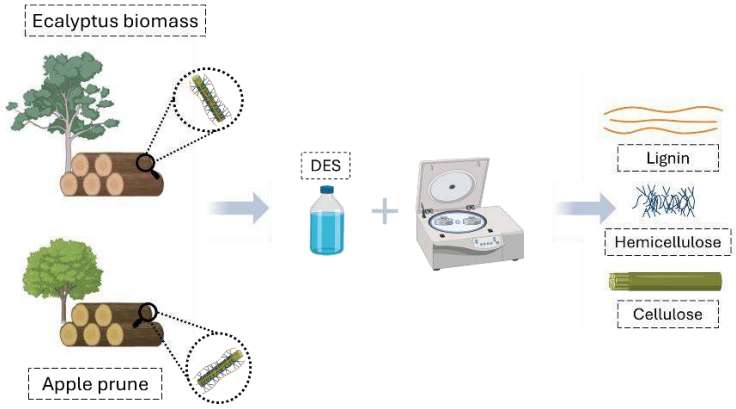

Figure 4. Schematic representation of biomass fractionation process.

The results demonstrate that the combined approach enhances fractionation efficiency, reduces processing time, and improves selectivity, offering a more sustainable alternative to conventional methods. This study provides valuable insights into biomass valorization strategies, guiding the selection of efficient pretreatment methods for industrial applications.

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P53 - Protein Stability Under Heat Stress: Exploring Osmolyte-Based Deep Eutectic Solvents as Protective Agents

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Keywords: Osmolyte-based deep eutectic solvents, protein stabilization, lysozyme, heat stress, biocompatibility

Proteins are prone to denaturation under extreme environmental conditions, such as heat stress, which limits their stability and functionality in various applications. This study explores the potential of osmolyte-based deep eutectic solvents (DESs) as biocompatible and robust stabilizing media for proteins under heat stress. Using lysozyme as a model protein, we tested a variety of DESs composed of natural osmolytes (TMAO, betaine, and sarcosine) and hydrogen bond donors like glycerol. The DESs were exposed to heat shock at 80 °C, and the stability of lysozyme was evaluated through activity assays, aggregation tests, and spectroscopic methods (FT-IR and circular dichroism). Results show that osmolyte-based DESs can significantly enhance the thermal stability of lysozyme, with the best results observed using sarcosine- and betaine-based DESs in combination with glycerol. These formulations were able to preserve lysozyme activity and prevent aggregation even at high protein concentrations (up to 200 mg mL^{-1}). The stabilizing effects are attributed to the synergistic interactions between the osmolytes and glycerol, which help maintain the protein's native conformation under stress conditions. Importantly, the osmolyte-based DESs did not show any cytotoxic effects in human cell lines (Caco-2, HaCaT, and HeLa), confirming their biocompatibility. This research highlights the potential of osmolyte-based DESs as a versatile, non-toxic stabilizing medium, offering new opportunities for protein applications in biotechnology and medicine, particularly in environments involving high temperatures or other destabilizing factors.

Acknowledgements

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P54 - Exploring the Rheology and Cytotoxicity of Betaine-Based Deep Eutectic Systems: A Step Towards Safe, Sustainable Solutions

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Keywords: Deep Eutectic Systems, betaine, rheology, cytotoxicity

Deep eutectic systems (DES) have emerged as promising alternatives to conventional solvents due to their environmental friendliness, ease of preparation and tunable physicochemical properties [1]. In recent years, there has been a significant increase in the use of amino acids and their derivatives, particularly betaine, for the formation of DES because they are sustainably sourced and are considered to have a low toxicity profile [2]. Among them, betaine-based DES combined with different polyols have already been employed in applications such as the extraction of proteins, carbon dioxide absorption or as non-aqueous media for enzymatic reactions [3,4]. While these systems are generally considered non-toxic, a thorough evaluation of their cytotoxic effects is essential to confirm their safety for biomedical and industrial applications. In this study, we investigated the rheological behaviour of nine betaine:ethylene glycol and betaine:glycerol DES at different ratios. In addition, cytotoxicity was assessed in HeLa and HaCaT cells to determine their potential biological impact. The rheological study showed that the viscosity of these systems is temperature dependent. Cytotoxicity analysis revealed a concentration-dependent effect, showing high levels of cell viability in the two cell lines used up to a concentration of 10000 mg/L. Considering these values, all the systems prepared could be classified as low cytotoxic. These results emphasise the need for a comprehensive physicochemical and biological characterisation of DES before their implementation in sensitive applications.

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P55 – Activation and Stability of Laccase in Deep Eutectic Solvents

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Keywords: Deep eutectic solvents, enzyme activity, green solvents, laccase, molecular docking

The research on alternative solvents and co-solvents is a relevant aspect when envisioning the improvement of biocatalytic reactions. Among these solvents and co-solvents, deep eutectic solvents (DES) may be considered as customizable new reaction media for biocatalysis. Accordingly, in this work, sixteen DES aqueous solutions, as well as of the individual DES components at the same conditions have been investigated in laccase catalyzed reactions. Cholinium- and betaine-based DES formed with polyols at different molar ratio and concentrations were evaluated. The results reported show that in presence of most DES the laccase activity is preserved and, with a particular DES, enhanced up to 200% [1]. Molecular docking studies demonstrated that while most DES components establish hydrogen-bonds with the enzyme amino acids, those that establish stronger interactions with the enzyme (expressed by absolute values of docking affinity energies) lead to an enhanced laccase activity. Finally, the laccase stability was evaluated in additional tests under extreme storage temperatures (60 ºC and -80 ºC). Although no significant protection to high temperatures was afforded by DES, an enhanced laccase activity when stored at low temperatures was found, at least up to 20 days [1]. The present work demonstrates that the type of DES, molar ratio and concentration are fundamental issues to improve laccase oxidation reactions. These results suggest that by choosing DES appropriately they can act as remarkable solvents or co-solvents to improve biocatalysis performance.

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P56 – Tailoring Deep Eutectic Solvents for Improved Starch Solubility and Sustainable Extraction

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Keywords: starch, deep eutectic solvents, Hansen solubility parameters, waste valorisation, circular economy

The transition from fossil fuels to renewable energy sources is a key environmental challenge, driving the need for sustainable resource utilisation. Biomass, especially starch-rich sources, holds great potential for industrial applications. However, conventional starch extraction is hampered by different structural properties and solubility, resulting in low yields. Potato peels, which are often discarded as waste, are an abundant but underutilised starch source that offers an opportunity for valorisation. This study focuses on overcoming the solubility limitations of starch using deep eutectic solvents (DES), which provide a tunable and sustainable alternative to conventional solvents. Through the careful selection of hydrogen bond acceptors (HBAs) and hydrogen bond donors (HBDs) — preferably food grade and derived from biomass - DES can be customised to improve the dissolution of starch. The application of Hansen solubility parameters (HSP) provides a predictive framework for optimising solvent polarity and improving solute affinity. Furthermore, a systematic investigation of dissolution kinetics and temperature profiles enables a deeper understanding of the solubility behaviour of starch in DES. The most effective DES formulations will be applied to starch extraction from potato peels, resulting in a double benefit: The environmental impact of waste disposal is reduced and at the same time a renewable resource is used for industrial applications. This research improves the fundamental understanding of the solubility of starch in DES and promotes the development of sustainable biorefinery strategies.

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P57 - Innovative Deep Eutectic Solvent Systems for Enhanced Biocatalytic Lignin Conversion

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Keywords: lignin valorization, lignin depolymerization, deep eutectic solvents, fungal biocatalyst, green chemistry

Lignin, a complex aromatic polymer found in lignocellulosic biomass, has significant potential for conversion into high-value bio-based products, offering a sustainable alternative to fossil feedstocks. However, the effective valorization of lignin from natural and technical sources remains a challenge due to its highly complex and recalcitrant structure. Depolymerization is one of the valorization methods for lignin, which can be achieved by electrochemical, thermochemical, or biological processes [1]. White rot fungi have developed mechanisms for degradation and modification of lignin by extracellular oxidative enzymes. In addition, white rot fungi have high metabolic capabilities to convert the small aromatic compounds released from lignin into intermediates or end products [2]. Complementarily, deep eutectic solvents, which are considered chemically green solvents due to their low volatility, stability, sustainability, biodegradability, and ease of preparation, have emerged as effective agents for enhancing lignin solubility and improving the activity of ligninolytic enzymes, offering a dual-function approach to lignin processing [3]. This study aims at the conversion of lignin into monomers and oligomers using a fungal biocatalyst system in conjunction with DES to enhance the solubility of lignin and promote the activity of key enzymes required for its depolymerization. Combined, the potential of DES and fungal biocatalysis form a sustainable and cost-effective way to unlock the value of lignin, contributing to circular economy solutions and the lessening of dependence on fossil resources. Lignin and lignin-derived monomers will be characterized using NMR spectroscopy, SEC and FTIR to gain insights into structure and composition. Kinetic modeling will also be used to optimize industrial applications and process efficiency.

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P58 - Sustainable and cost-effective strategies for single-step monoclonal antibody purification

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Keywords: sustainability, purification, aqueous biphasic systems, monoclonal antibodies

During the past decades, significant advances have been achieved in the biopharmaceutical arena, including the production of monoclonal antibodies (mAbs). These biological products, which are more complex and labile than conventional chemical drugs, are more difficult to produce, purify, and preserve, resulting in high costs and extremely time consuming. Indeed, biopharmaceuticals are generally 12x more expensive than chemical drugs due to their manufacturing process, encompassing the mAbs production towards specific cell cultures (upstream) and various subsequent stages (downstream), such as clarification, capture, viral inactivation, polishing steps, virus removal, and enrichment/conditioning for preservation. The need for cost-effective and sustainable downstream processing of mAbs is driving the development of single-step, biocompatible continuous purification strategies. Ionic liquids (ILs) offer a promising solution due to their remarkable chemical structure diversity. This allows for precise tailoring of their biological, chemical, and physical properties in order to target and link mAbs, facilitating their efficient purification. This study investigated the capture and purification of mAbs from real serum-free and serum-containing Chinese Hamster Ovary (CHO) cell culture supernatants, using IL-based aqueous biphasic systems (ABS). In this context, ABS composed of polyethylene glycol (PEG) and dextran were considered, using ILs as adjuvants, namely 1-butyl-3-methylimidazolium bromide ([C4mim]Br) and cholinium acetate ([Ch][Ac]). Under optimal conditions, recovery yields of 81.5% and 85.4%, and purity levels of 69.3% and 92.4% were attained for serum-containing supernatants (with anti-interleukin-8, anti-IL-8) and serum-free supernatants (with anti-hepatitis C virus, anti-HCV), respectively. Sodium dodecyl sulfate–polyacrylamide gel electrophoresis (SDS-PAGE) protocol confirmed the integrity and protein profile from each ABS phase, and the mAbs activity maintenance was confirmed by colorimetric activity evaluated using enzyme-linked immunosorbent assay (ELISA). In conclusion, this study showed promising evidences for the remarkable applicability of ILs in the downstream processing of mAbs, by enabling a simpler, cost-effective, and time-saving single-step purification strategy, that will ultimately impact/improve the accessibility of current mAbs-based therapies.

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P59 - Assessment on Solubility and Stability of Rifampicin Using Deep Eutectic Solvents: Pursuing Meningo-encephalic Tuberculosis Treatment Improvement

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Keywords: DES, *Micobacterium tuberculosis*, blood-brain barrier, 3D printing

Tuberculosis is a disease caused by *Mycobacterium tuberculosis* and represents a worldwide prevalent disease of great epidemiological importance [1]. The failure of treatments, especially for meningo-encephalic tuberculosis in children under 10 years of age, is influenced by characteristics of one of the most important active pharmaceutical ingredients (API) used in the difficult and long treatment of this disease: its water solubility, permeability to the blood-brain barrier, as well as its palatability, especially important in treatments for the pediatric public [2]. Deep eutectic solvents (DES) have shown significant potential in the development and manufacturing of pharmaceutical products, particularly in enhancing the solubility of active ingredients in water. Studies indicate that DES can increase drug solubility by several orders of magnitude compared to water, as observed for anti-inflammatory and antifungal drugs, thereby improving biocompatibility and consequently enhancing bioavailability [3]. The present work studied the impact of a series of deep eutectic systems (DES) on improving he solubilization of Rifampicin and its stability as a molecule in solution. Three different DES were tested, and Betaine:Ascorbic acid (1:1, 30 wt. % of H_2O) showed the ability to increase Rifampicin solubilization about 4 times fold, when compared with water in different pHs, with enhanced stability. Further steps will assess palatability and formulations' suitability for additive manufacturing (pharmaceutical 3D printing), customized according to individual patient characteristics and needs.

Acknowledgements

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P60 - Structural Dynamics of Novel Surfactant-Based Deep Eutectic Solvents: A Combined Fluorescence Dynamics and Molecular Dynamics Study

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Keywords: Surfactant-based DESs, fluorescence and simulation studies, micellar type structure, polar/nonpolar domains dynamics, microheterogeneity.

Hexafluoroisopropanol (HFIP)-based deep eutectic solvents (DESs) are newly explored, high-density DESs [1],[2]. In this report, we investigated the structure and dynamics of a special type of HFIP-based DESs, where one of the components is a surfactant, specifically alkyltrimethylammonium bromide (decyl, dodecyl, tetradecyl), using temperature-dependent steady-state and time-resolved fluorescence measurements with a hydrophilic and a hydrophobic solvatochromic solutes {Coumarin 343 (C343) and Coumarin 153 (C153)}. The key observation we made is that these DESs exhibit domain formation with varying polarities, where C153 and C343 distinctly sense different domains of polarity. The excitation wavelength-dependent emission frequency shifts for C153 and C343 are ~ 127-325 cm^{-1} and ~ 60-157 cm^{-1}, respectively, indicating that these DESs exhibit mild spatial heterogeneity with respect to these solutes. The detected dynamic Stokes shift is ~1112-1381 cm^{-1} for C153, while for C343, it is approximately 2.5 times smaller, with significantly larger undetected dynamics. Using C153, solvation dynamics is ~ 1.4 times slower than that of C343, whereas the reverse is true for rotational dynamics. Furthermore, decoupling of solvation and rotational dynamics from viscosity indicates the presence of dynamic heterogeneity in these DESs. These observations are further supported by simulation snapshots, radial distribution functions (RDFs), and computed X-ray scattering structure functions (S(q)). Simulation snapshots and RDFs clearly show that HFIP primarily interacts with the head group of the surfactant, while the tail alkyl chains aggregate to form a micelle-like structure. A few additional RDFs show that C153 is closer to the aggregated tail alkyl region, while C343 is closer to HFIP and the head group of the surfactants. Therefore, the observed experimental time scales reflect the dynamical behavior of the hydrophilic and hydrophobic domains present in the micelle-like structure of these DESs. The microscopic arrangement is significantly influenced by the length of the surfactant cation alkyl chain, which, in turn, affects the structure and dynamics of these DESs.

Acknowledgments
We thank SNIoE for its research facilities and the Shiv Nadar Foundation for funding.

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P61 - Improving Nutrient Accessibility from *Tetraselmis chuii* via Deep Eutectic Solvent-Assisted Cell Wall Disruption

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Keywords: microalgae, *Tetraselmis chuii*, nutrients, deep eutectic solvents, extraction

The search for sustainable food sources is becoming more and more urgent due to the growing global population, projected to reach 9.8 billion by 2050.[1,2] Microalgae represent a promising alternative source of nutrients, thanks to their fast growth rate, high biomass production, minimal arable land requirments, and the ability to grow in different environments while also capturing CO_2.[2] *Tetraselmis chuii* is a microalgal species approved for food applications recognized for its high nutritional value. However, its broader use remains limited due to its thick and complex cell wall, which hinders the nutrient release during digestion.[1] This study aims to enhance the availability of nutritional constituents from *T. chuii* by applying deep eutectic solvents (DESs) in combination with ultrasound-assisted extraction (UAE) and high-pressure homogenization (HPH) as cell wall disruption techniques. Among the solvents tested, a DES composed of betaine:sorbitol:water in a 3:1:10 molar ratio showed promising potential for protein recovery and was selected for further optimization. For the NADES-UAE process, key parameters were varied, including extraction time (10–60 minutes), ultrasound pulse mode (5s on/5s off - 5s on/15s off), and the number of freeze-thaw cycles applied prior to extraction (0–2). Additionally, NADES-HPH was evaluated by varying pressure (100–1200 bar), the number of homogenization cycles (1–3), and the DES:water ratio (1:4-1:20). Extracts obtained through both methods were analyzed for protein, phenolic, chlorophyll, and carotenoid content. Preliminary observations suggest that HPH pressure was the most influential factor in NADES-HPH process, with a significant increase in protein yield observed at higher pressures. Extracts obtained under optimized conditions will be assessed for *in vitro* digestibility to evaluate nutrient bioaccessibility. These findings highlight the potential of combining NADES with physical disruption techniques as an efficient strategy to improve nutrient release from microalgal biomass.

Acknowledgements: This work received support and help from program CEEC IND5ed (https://doi.org/10.54499/2022.04909.CEECIND/CP1725/CT0014).

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P62 - Extraction of Phenolic Compounds from Aqueous Solution using Deep Eutectic Solvents: Experiment and DFT Calculations

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Keywords: Deep Eutectic Solvent, Phenolic Compounds, Wastewater Treatment, Density Functional Theory, Solvation Energy

Phenolic compounds (PCs) such as phenol, o-cresol, and resorcinol are persistent contaminants in wastewater owing to their toxicity and capacity for bioaccumulation. This leads to a serious threat to human health and the environment. Effective techniques are thus essential to lessen the adverse effects of these compounds. Currently, the use of Deep Eutectic Solvent (DES) has gained immense interest to be an efficient and environmentally benign extractant for the removal of these pollutants [1], [2]. This study investigates the extraction of PCs from their aqueous solution using hydrophobic DES prepared from choline chloride and caprylic acid (1:3 molar ratio). The compositions of extracted and raffinate were measured using spectroscopic analysis to evaluate the experimental extraction efficiencies. In contrast, Density Functional Theory (DFT) simulations have been used to compute the solvation energy of phenolic compounds in water at the molecular level. DES exhibited the highest extraction efficiency for O-Cresol (87.92%), followed by phenol (78.68%) and resorcinol (73.77%). This was also verified by DFT calculations, where a similar trend of solvation energy is obtained. Resorcinol exhibited the most solvation energy (-6.65 kcal/mol), followed by phenol (-5.99 kcal/mol) and o-cresol (-4.04 kcal/mol), suggesting that their -OH groups provided more significant interactions with water and increased their water solubility. The presence of a methyl group in O-cresol improves hydrophobic contacts with the DES and thus it has weaker hydrogen bonding with water. This enables the transfer of o-cresol to the organic phase and contributes to its improved extraction. On the other hand, Resorcinol has two hydroxyl groups (-OH) and a stronger hydrogen bond with water, resulting in a poorer extraction efficiency. This study comprehensively explains DES-based extraction mechanisms for phenolic pollutants, bridging experimental and theoretical perspectives to enhance wastewater treatment strategies.

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P63 – DE(S)-bugging chitin: A systematic thermodynamic approach to valorisation of black soldier flies

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Keywords: black soldier flies, chitin, solid-liquid equilibrium, SAFT EoS

Black soldier flies (BSFs) are currently excelling globally as mini-livestock. Of interest are the larvae of this insect which can be reared on low-quality organic waste to produce a fat- and protein-rich larval mass to be used for livestock feed supplementation. Chitin, a biopolymer that complexes with proteins to form the larval exoskeletons, is currently an underutilised by-product of BSF farming, of which totals 8-24% of the product biomass. Application of this biocompatible polymer in the pharmaceutical and biomedical fields remain largely untapped due to its limited solubility in most organic solvents. Solvents such as dimethyacetamide/lithium chloride and ionic liquids have shown varied success at solubilising chitin. The toxicity of the individual components, however, renders products ineffective for biological applications. Deep eutectic solvents (DESs) are an emerging class of solvent with readily biodegradable, biocompatable, inexpensive, and widely available constituents, making for an attractive alternative. Emerging research indicates effective dissolution of crustacean chitin in several (D)ESs, but with limited characterization of BSF chitin and no current literature quantifying its solubility, there is need to verify its feasibility. Typical investigations of DES efficacy for a solute of interest involve a largely empirical approach; DESs (seldom varied from the eutectic composition) are tested at discrete solvent/solute ratios and temperatures. These methods, however, limit the relevance of the data to a solute-specific niche, and leave unexplored the compositional tunability for which DESs are touted. Thermodynamic modelling offers a tool to capture the behaviour of DESs from laboriously collected data. These models can then be used to efficiently explore the impact of compositional and conditional changes, and for preliminary screening for different target solutes. The mechanistic hydrogen bond donor/acceptor pairs of DESs makes the statistical associating fluid theory (SAFT) equation of state (EoS) an apt choice for modeling. The explicit consideration of molecular interactions in the SAFT EoS also offers the opportunity to better understand the complex formation of these DESs. In this study, solid-liquid equilibrium (SLE) data for two DES systems were collected by differential scanning calorimetry. Performance of the two DESs for chitin dissolution are evaluated, with temperature and DES composition as independent variables, with motive to demonstrate the potency of non-eutectic DESs. The SAFT EoS is then fit to both the SLE and solubility data, with the quality of fit quantified using the absolute average deviation. Supplementing these findings with SLE modelling results offer insight into the mechanisms that govern DESs, and supply the groundwork for exploring future application.

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With special thanks to Dr. Loots and the Department of Chemistry and Polymer Science at Stellenbosch University for provision of the differential scanning calorimeter and invaluable assistance.

P64 - Down the rabbit hole: HMF as component of new eutectic systems

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Keywords: Eutectic Solvents, Low Melting Mixtures, HMF, Green Chemistry, Biomass

The use of renewable sources for chemical processes is one of the principles of Green Chemistry [1]. From this perspective, the valorization of biomass as sources of platform chemical for organic synthesis is the object of intense research worldwide. Furan-based aromatic compounds are a particularly important class of molecules, and one notable example is 5-hydroxymethyl furfural (HMF) [2,3], which the US Department of Energy designates as a platform chemical due to its capability of acting as a precursor for high value-added bio-based molecules. In this study, we introduce a novel low melting mixture [4] formed by combining 5-hydroxymethyl furfural (HMF) and levulinic acid (LA), which offers potential for sustainable extraction processes and biomass valorization.

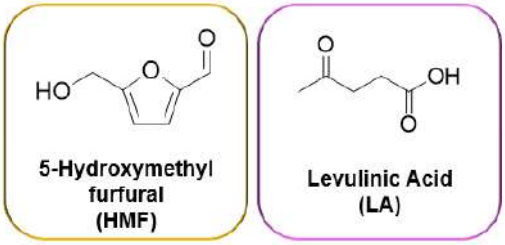

Figure 1. Structural representation of 5-hydroxy methyl furfural and levulinic acid

We present a comprehensive physicochemical characterization of this mixture based on NMR spectroscopy, rheology and COSMO-RS models, which exhibits unique properties, with changes in molecular diffusion and viscosity that suggest the formation of a strong hydrogen-bond network between HMF and LA.

Acknowledgements
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P65 – Investigations on the behaviour of Amphiphilic Block copolymers and Surfactants in Deep Eutectic Solvents (NADES)

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Keywords: Self-assembly, Amphiphilic copolymers

Natural deep eutectic solvents (NADES) are a novel class of polar solvents that has the potential to become a non-toxic and cheap alternative to conventional organic solvents and ionic liquids. Amphiphilic self-assembly is very a well-established phenomenon for solutions of surfactants or amphiphilic polymers in water, allowing to functionalize them.[1] Structure formation by surfactants in DES has been studied to some extent [2], but the solubility of polymers and in particular self-assembly of amphiphilic polymers is a topic that has been addressed to a very limited extent.[3] In this study, we designed custom block copolymers guided by extensive solubility assessments of various homopolymers. Notably, polyacrylamide-b-poly(N-isopropylacrylamide) (PAm-PNiPAm), with PAm as the soluble segment, demonstrates excellent solubility in our NADES Reline. The resulting copolymer exhibits enhanced viscosity and shear-thinning in Reline, which can be tuned by adjusting block lengths, offering a means to control NADES properties(Fig. 1). The systems were studied comprehensively by rheology and with respect to the their mesoscopic structure by small angle neutron scattering (SANS). Furthermore, substituting the insoluble block with poly(dimethylacrylamide) (PDMAm) imparts thermoresponsive behavior, broadening potential applications, particularly for drug delivery systems.

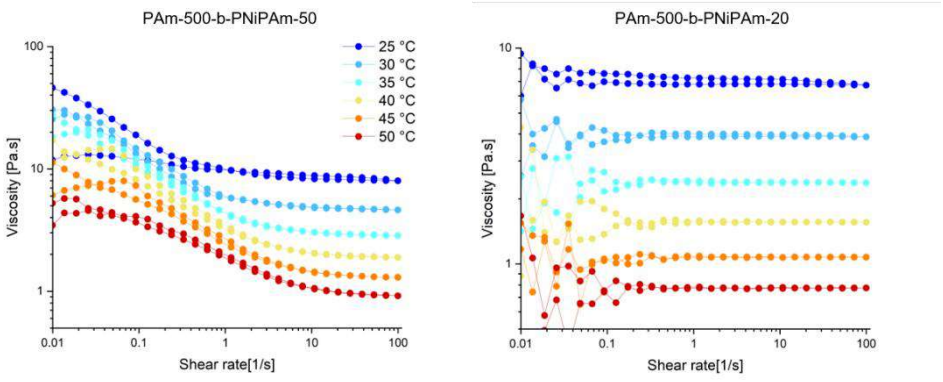

Fig1. Viscosity as a function of shear rate at various temperatures in the range of 25-50 °C for 5 wt% solutions of polymer in Reline (1% water[w/w]) for left) PAm-500-b-PNiPAm-50; right) PAm-500-b-PNiPAm-20.

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P66 - Sustainable multi-product three-phase partitioning for seaweed biorefinery using recyclable deep eutectic solvents

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Keywords: Extraction, multi-product biorefinery, DES recycling

In this study, a multi-product seaweed biorefinery was developed through three phase partitioning (TPP), using a recyclable and natural deep eutectic solvent (Figure 1). Alginate and pigments were effectively recovered from brown seaweed *Saccharina latissima* within one system operating under mild conditions. Nine different biosafe, hydrophobic deep eutectic solvents (DES) based on fatty acids were applied together with an ammonium sulphate salt solution for extractions. Results indicated that extraction with DES and salt solution caused a significant increase in alginate extraction yield (11.5% alginate per g DW) compared to only extracting with the aqueous salt solution (0.98% alginate per g DW). Furthermore, pigments could be extracted simultaneously within the DES phase during alginate extraction. The results indicate that DES can be applied as an extraction aid, assisting in alginate release from the algal cell wall, while also extracting valuable pigments directly. The best-performing DES was selected for subsequent optimization experiments using green extraction conditions. By extracting at a low temperature (35 °C) for only 10 minutes, 20.9% of alginate per DW could be obtained. In addition, the DES could be recycled successfully for at least seven extraction cycles while accumulating pigments in the DES fraction. Subsequent to recycling, recovery of pigments from the DES could potentially be obtained through changing the pH of the DES, thereby regenerating the solvent (Figure 1). This proposed method provides an efficient, mild and sustainable way of extracting various bioactive compounds from brown seaweed using sustainable DES.

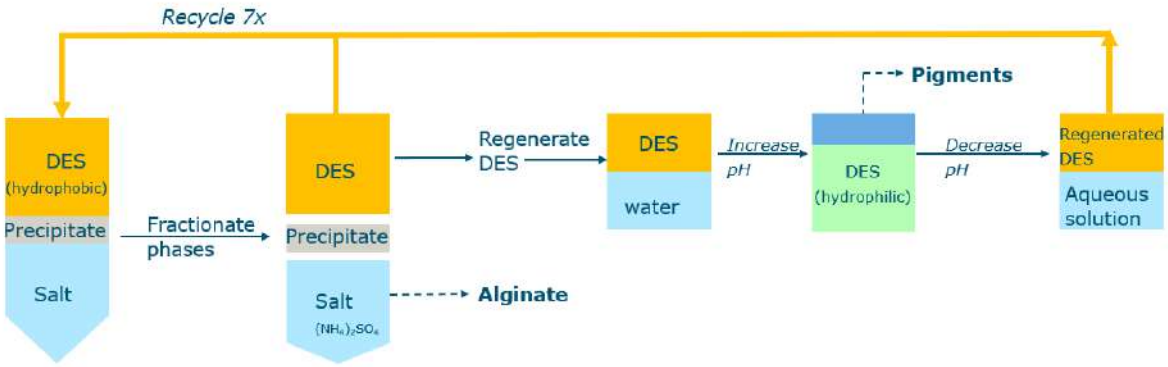

Figure 5. General overview of multi-product seaweed biorefinery with three-phase partitioning using recyclable deep eutectic solvents.

P67 - Assessing the Effect of Deep Eutectic Solvents on α-Chymotrypsin Thermal Stability and Activity

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Keywords: Protein unfolding, Thermal stability, Solvation, Preferential Hydration

The protein's ability to form intricate structures is captivating as it involves biophysical, structural, and catalytic properties. A crucial aspect of protein structural stability consists in describing the forces governing the biomolecular interactions in liquid environments, which are essential for maintaining a protein molecule in its specific rigid conformation. Optimizing the liquid reaction phase holds significant potential for enhancing the efficiency of biocatalytic processes since it determines reaction equilibrium and kinetics. This study investigates the influence of the addition of Deep Eutectic Solvents (DES) on the stability and activity of α-chymotrypsin (α-CT) , a proteolytic enzyme with applications in food, pharmaceutical and wastewater industries. DES composed of choline chloride or betaine mixed with glycerol or sorbitol, were added in the reaction phase at various concentrations. Experimental techniques, including kinetic and fluorometry, assessed the α-CT enzymatic activity, thermal stability, and unfolding reversibility. Several thermodynamic parameters were recovered from the unfolding curves as shown in Figure 1, in order to discriminate the positive effects on enzyme stability qualitatively. Atomistic molecular dynamics simulations were also conducted to assess the interactions and provide molecular-level insights between α-CT and the solvent. The results showed that among all studied mixtures, adding choline chloride + sorbitol improved thermal stability up to 18 °C and reaction kinetic efficiency up to two-fold upon adding choline chloride + glycerol. Notably, the choline chloride + sorbitol system exhibited the most substantial stabilization effect, attributed to the surface preferential accumulation of sorbitol, as corroborated by the computational analyses. Molecular dynamics simulations revealed that DES reduced the structure flexibility of α-CT, leading to an enhanced stability of the active site region. This stabilizing effect is facilitated by the water exclusion phenomenon, which arises due to the interactions between the α-CT surface and the DES that were analyzed using minimum-distance distribution functions and Kirkwood-buff integrals. This work highlights the potential of tailoring the liquid reaction phase of α-CT catalyzed reaction using neoteric solvents such as DES to enhance α-CT performance and stability in industrial applications.

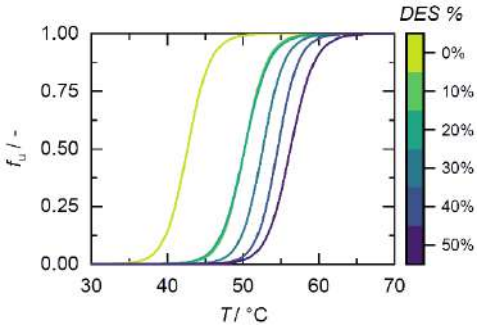

Figure 6: Unfolded fraction sigmoidal curves for α-CT in choline chloride+sorbitol at several concentrations

Acknowledgements

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P68 - Bioactives Compounds Extraction Using NaDES and Conventional Solvents of Three Medicinal Plants (*Psidium Guajava, Buddleja Scordioides* and *Quercus Convallata*)

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Keywords: *Psidium guajava*, *Buddleja scordioides*, *Quercus convallata*, Natural Deep Eutectic Solvents, total phenolic content; total terpenoids content

For the isolation of bioactive compounds from medicinal plants (*Psidium guajava, Buddleja scordioides, Quercus convallata*) neoteric solvents were investigated as Natural Deep Eutectic Solvents (NaDES) (ChCl:glycerol 1:2, ChCl:ethylenglycol 1:1, ChCl:glucose 1:1, ChCl:citric acid 1:1, and ChCl:malic acid 1:1, all systems with 30% water) and compared with conventional solvents (ethyl acetate, acetone, methanol, ethanol, ethanol 70%, ethanol 40%, and water). A 1:10 solid:liquid ratio and fixed conditions were used for ultrasound-assisted extraction. Total phenolic content (TPC, gallic acid equivalents, GAE) and total terpenoid content (TTC, *ρ*-cymene equivalents, PCE) were determined. Results showed that the highest TTC value for *Q. convallata* were ethanol 40% (386 ± 6.68 µg PCE/mL) vs NaDES system ChCl:Cit (500 ± 5.23 µg PCE/mL). For *P. guajava*, were ethyl acetate (309 ± 5.19 µg PCE/mL) vs NaDES ChCl:Mal (578 ± 11.30 µg PCE/mL). Finally, in *B. scordioides* the best output was methanol (147 ± 3.85 µg PCE/mL) vs NaDES system ChCl:Cit (270 ± 0.56 µg PCE/mL). With respect to TCP in *Q. convallata* the highest extraction outputs were ethanol 40% (7.171 ± 0.187 mg GAE/g) vs NaDES ChCl:Mal (6.109 ± 0.020 mg GAE/g). For *P. guajava* the highest were ethanol 40% (7.296 ± 0.204 mg GAE/g) vs NaDES ChCl:Ethyl (7.255 ± 0.430 mg GAE/g). Finally, in *B. scordioides* the highest values were ethanol 70% (2.246 ± 0.075 mg GAE/g) vs NaDES ChCl:Mal (3.073 ± 0.153 mg GAE/g). The extraction yields of bioactive compounds such as phenolics and terpenes depends largely on the extraction conditions, the solvent media, and the structure of targeted compounds. Under these conditions the NaDES have shown a better extraction efficiency of terpenes compared to conventional solvents in the three plant matrices. While in the extraction of phenolics, they were better only in *B. scordioides.*

P69 - Deep eutectic solvent as a green and selective alternative to extract gum from *Acacia* stems

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Keywords: gum arabic, deep eutectic solvents, predictive tools, wastes valorization.

Gum Arabic (GA) is a heteroglycan biopolymer exuded from the stems of acacia trees and used as thickening agent, emulsifier and at drug delivery systems due to its structural and self-aggregation particularities. *Acacia mearnsii* (black wattle) is widely used in Brazil by the tannin and cellulose industries, where gum is obtained as a byproduct from the tannin extraction, especially by the high hydrophilicity of both molecules [1]. In order to design a more selective extraction process and obtain natural compounds, Deep Eutectic Solvents (DESs) stand out as a green and sustainable option in a class of emerging solvents. In this context, the aim is to study the use of DESs as a more selective extraction method for the biopolymer exuded from black wattle, through the GA computational representation and use of predictive tools to investigate the best solvent. Therefore, the neutral monosaccharides format and uronic acids were applied as precursors to the polysaccharide that constitutes the GA. The selected approach for the computational simulation was quantum molecular mechanics, using density functional theory (DFT), the exchange and correlation interactions approximation were performed by the functional BP86 with the def2-TZVP basis set, and the software used to perform these computations was TmoleX16. The solubility estimation of the molecule in aqueous solutions was modelled by COSMO-RS in the COSMOTherm software at 25°C. The results were compared with the values found in the literature for GA to validate the computational representation. DESs were selected based on studies of their use in degumming process and development of biosourced materials combining DES with gum [2]. DESs were represented by the electroneutral mixture approach, using the molecules available in the software database. The results denote the value of computational tools to work with complex natural products representing experimental time and costs reduction in a process project. Furthermore, the results help to consolidate DESs as a green and efficient alternative to extract biocompounds from plant matrices.

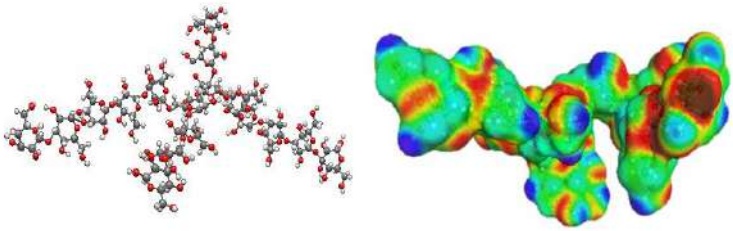

Figure 1. GA baseline structure.

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P70 – Phenolic compounds ultrasound-assisted deep eutectic solvent extraction from black wattle: predictive screening and optimization

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Keywords: green process, deep eutectic solvents, phenolics, extraction optimization, wastes valorization.

Deep Eutectic Solvents (DESs) are a class of emerging solvents used in extraction processes to obtain natural compounds from different plant matrices with a green and sustainable appeal. *Acacia mearnsii* (black wattle) is used by the tannin and cellulose industries, where Brazil stands out as one of the world's largest producers. Its flowers are considered a byproduct of the acaciculture production chain and can be a source of phenolic compounds [1]. In this context, this study aims to develop an extraction process using DESs to obtain bioactive compounds from black wattle flowers, through the selection of the best solvent using predictive tools, and optimal extraction conditions. An initial scan to select the best DES among 15 solvents was performed using the relative solubility screening of gallic acid, carried out in the COSMOTherm software. Predictive screening represents experimental time and costs reduction. DES were represented by the electroneutral mixture approach [2], using the molecules available in the software database. For gallic acid molecule, TmoleX16 software was used to perform energetic optimization and σ-profile creation, using the density functional theory (DFT), BP86 function and triple-zeta valence of polarization (def-TZVP) basis set. The 3 best DESs were selected and prepared through the heating and stirring method at 60 ºC. Regarding the plant matrix, black wattle flowers solid wastes from steam distillation extraction were used, adopting a sequential extraction approach. The material was dried in an oven at 40 °C for 24 h, with a resulting humidity of 2.37 ± 0.69%. Experimental screening was then performed with selected DESs, water and ethanol, using the results of total phenolic content (TPC) analysis of the extracts obtained as a selection criteria. Ultrasound-assisted extraction (UAE) was used at 40 ºC, 30 min, solid-liquid (S/L) ratio 1:20 (m/m), where the DES formed by lactic acid, glycine and water (3:1:3) presented the best results, confirmed by the statistical analysis with Tukey's test performed. Subsequently, the optimal extraction conditions were evaluated according to the Box–Behnken experimental design, with the TPC results as the response and time (20-60 min), temperature (20-60 ºC) and S/L ratio (10-30) as variables. The best parameters were found to be 38 min, 60 ºC and S/L ratio 1:22. The results obtained help to implement computational and predictive tools associated with natural products and to consolidate the combination of DES with UAE as a green and efficient alternative for obtaining compounds with bioactivity from plant matrices.

Acknowledgements: This study was financed in part by FAPERGS and CNPq.

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P71 – Lipid extraction from *Chlorella vulgaris* using biocompatible deep eutectic solvents and microwaves pretreatment

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Keywords: Deep Eutectic Solvents, Extraction, Microwaves, Lipids

Growing awareness of health and environmental issues is diving interest in natural products that benefit both. However, excessive agricultural production threatens sustainability. Urgent action is needed to reduce emissions and ensure resource sustainability for adequate food supply. Bioactive compounds, such as lipids, from marine sources, exhibit various beneficial properties and find applications in food, medicine and beyond. Regular consumption of polyunsaturated fatty acids (PUFAs) has been shown to significantly reduce the risk of heart disease, neurotic disorders, asthma, depression, and inflammation. Although the lipid content present in microalgae is lower than in fish, their high content of unsaturated fatty acids and the numerous advantages of cultivating microalgae, allow them to be considered as a potential source of marine lipids. However, current lipid extraction is a process with high energy consumption, contaminant, and sometimes the extraction yields are unsatisfactory, acting as a significant barrier to large-scale microalgae production for commercial purposes. In the present study, lipid components sourced from *Chlorella vulgaris* (*C. vulgaris*) will be extracted using a microwave-assisted and deep eutectic solvents (DESs) extraction approach. Using less harmful solvents is crucial to avoid disposal costs, legal obligations, and regulatory issues. "Green solvents," including DESs, have emerged as alternatives. DESs have been shown to form hydrogen bonds with biopolymers such as cellulose, which are present in the cell walls of microalgae. Cellulose microfibrils are bound by hydrogen bonds, which are broken in the presence of DESs, allowing for more efficient lipid extraction. Combining microwave-assisted extraction with DESs can bring several advantages, such as higher yield, reduced extraction time, and consequently, reduced energy consumption. This study evaluated the effectiveness of biocompatible DESs and microwaves, both individually and in combination, for extracting lipids from *C. vulgaris* for food applications. Various DESs, formulated in 1:1 and 1:2 ratios using choline chloride and carboxylic acids (e.g., acetic acid, oxalic acid, succinic acid, and adipic acid), were prepared to be further tested alongside microwave-assisted pre-treatment of the microalgae. A DES composed of two carboxylic acids, decanoic acid and hexanoic acid, was also prepared. Prior to this study, a series of optimization procedures had been conducted to determine the most suitable conditions for the MW pre-treatment process. This involved maintaining a temperature of 60°C and a power of 750 W for a duration of 5 minutes. In the initial experiments using the DES choline:acetic acid at a 1:2 ratio, with an algae:DES ratio of 1:20 (w/w), approximately 14% of lipid compounds were extracted during the pre-treatment phase, while approximately 5% remained extractable in the pre-treated algae. These first results indicate that the prepared DESs could serve as promising, cost-effective, biodegradable, and non-toxic solvents for the pre-treatment of algal biomass in lipid extraction.

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P72 – Natural Deep Eutectic Solvents (NADES) as a Sustainable Solution for Grape Seed Phenolic Extraction

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Keywords: Natural Deep Eutectic Solvents, extraction, selectivity, physicochemical properties, phenolic compounds

Natural deep eutectic solvents (NADES) have emerged as an eco-friendly alternative for extracting bioactives, avoiding the use of flammable organic solvents such as ethanol, and extreme temperatures and pH conditions. NADES depend on intermolecular interactions between hydrogen bonding donors (HBD) such as, sugars or alcohols, and hydrogen bonding acceptors (HBA) such as, quaternary amines to form eutectic mixtures. The number of hydrogen bonds and strength of intermolecular interactions will have an impact on the physicochemical properties of the NADES [1]. Therefore, the type and composition of NADES as well as the water composition, will have an effect on these properties and these in turn will impact on the extraction efficiency and selectivity of different bioactives. The aim of this work was to examine how changing the physicochemical properties of the various NADES, such as polarity, pH, and viscosity, influence the extraction efficiency and selectivity of phenolic compounds and then compare with to the reference hydroalcoholic extraction. Additionally, the effect of these physicochemical properties on the bioactivity (antioxidant and anticholinergic) of the extracts was also analysed. This research focused on choline chloride-based NADES combined with malic acid, urea or 1,2- propanediol at different water compositions. The efficiency of extraction was assessed by the total polyphenols, phenolics profile and proanthocyanidins, and selectivity was determined in relation to total sugars. Additionally, antioxidant and neuroprotective activity were determined in all extracts. The extraction yields and selectivity of phenolic compounds showed significant variation depending on the type of NADES used. This work revealed that the most promising NADES are those composed of malic acid and 1,2- propanediol, with a water content of 50%.

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P73- Extraction of Phenolic Compounds in Prosopis laevigata with Conventional Solvent and Deep Eutectic Solvent: Identification of the Main Flavan-3-ols

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Keywords: *Prosopis laevigata*, wood and bark, Flavan-3-ols, Natural Deep Eutectic Solvents

Prosopis laevigata (mesquite) is one of the 40 species of the genus *Prosopis*. It grows in arid lands of Mexico, and is used in traditional medicine, as food (the pods) and as fuel (firewood). In *Prosopis* spp., flavan-3-ol as catechin, epicatechin, gallocatechin have been identified [1,2]. For *P. juliflora* heartwood a large amount of (-)-mesquitol has been extracted and isolated by acetone extraction [3]. In this research, dry and ground material from the woody part of mesquite was used. Extract (CSE- conventional solvent extraction) was obtained by maceration with 70% aqueous ethanol followed by liquid-liquid partition with ethyl acetate. Extract DES (Deep Eutectic solvent) was obtained using choline chloride:glycerol 1:2, ratio 1/10 plant/solvent, sonication at 50°C for 10 min. Water (10 mL) was added and L-L partition with ethyl was done. Both ethyl acetate extracts were analyzed by UHPLC/MS. The report of compounds in the chromatograms showed a total of 32 compounds in CSE sample, and 19 compounds with DES extraction. In DES chromatogram a better signals resolution is observed. Three important signs stand out in both samples, with [m/z] negative mode of 289.077. This mass corresponds to flavan-3-ol, also called catechin group. According to reported by [3], and by the retention time sequence, the compounds may correspond to (+)-catechin, (-)-mesquitol and (-)-epicatechin. With the intensity value in the spectrogram, the relative percentage of each compound was calculated. In DES 31.1% corresponds to catechin, 31.7% mesquitol, 12.9% epicatechin. In CSE 10.2% catechin, 15.5% mesquitol, 1.9% epicatechin. Mesquitol is the compound with the highest concentration in the two extracts. This flavonoid had not been reported in *P. laevigata*. Other common compounds in both extracts are rhamnetin, hispidulin and quercetin derivatives. In DES eriodictyol, taxifolin and apigenin glucoside were identified, however, in DES quercetin, rutin and eriocitrin were identified. These had already been reported for the species with a conventional ethanol extraction70 [2]. Extraction system Deep Eutectic Solvent was selective for the extraction of flavan-3-ol group in mesquite.

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P74 - Pebax® Membranes Functionalized with Non-volatile Solvents for Gas Separation

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Keywords: Deep Eutetic Solvents, Ionic Liquids, Mixed-Matrix Membranes and Gas Separation.

Over recent decades, greenhouse gas (GHG) emissions have risen, leading to an increase in their atmospheric concentrations and amplifying the natural greenhouse effect. This has resulted in adverse impacts on Earth's ecosystems and climate. The annual GHG emissions are approximately 50 billion tons of CO_2 equivalents, comprising 73.7% carbon dioxide (CO_2), 18.9% methane (CH_4), 4.7% nitrous oxide (N_2O), and 2.7% fluorinated gases.[1] Various technologies, including absorption, adsorption, and electrochemical reduction, have been employed to mitigate these pollutants. However traditional abatement technologies face several drawbacks, including high energy demand, low efficacy, solvent toxicity and size requirements.[2] These limitations underscore the need for more efficient and environmentally friendly GHG mitigation approaches. Non-volatile solvents, particularly Ionic Liquids (ILs) and Deep Eutectic Solvents (DES) have emerged as promising alternatives to conventional solvents, due to their attractive properties, including negligible vapor pressure, high thermal stability, and tunable properties.[3] However, the direct implementation of non-volatile solvents in conventional separation units faces obstacles, including the need for large separation units and high energy demands for solvent recovery.[4] To address these challenges, we proposed the development of functionalized polymeric membranes based on Pebax®, incorporating non-volatile solvents. This novel approach aims to optimize the balance between the sorption capacity and selectivity of the solvent with the modularity, compactness, and scalability inherent in membrane technology.

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P75 - Biopolymeric (lignin) membrane using deep eutectic solvent as an alternative green solvent for gas separation

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Keywords: Membrane gas separation, Deep euctectic solvents, Lignin

Air pollution was identified as the second largest mortality risk factor in 2021, and the WHO reports that 99% of the global population is exposed to contaminant levels exceeding guidelines [1]. While atmospheric air pollution is a major concern, indoor air quality is even more critical, as people spend about 90% of their time indoors [2]. Proper ventilation is essential but insufficient to keep pollutant levels within safe limits, highlighting the need for sustainable and efficient air treatment technologies. Conventional techniques such as mechanical/electronic filtration and adsorption, as well as emerging technologies like photocatalytic oxidation and plasma air disinfection, have drawbacks, including high energy consumption and the potential release of harmful byproducts. The use of greener solvents in membrane fabrication has been explored to replace highly toxic solvents. Among sustainable alternatives, deep eutectic solvents (DES) stand out due to their ease of preparation, low toxicity, and compatibility with polymers. However, implementing non-volatile solvents in traditional separation systems remains challenging due to the need for large separation units and high energy demands for solvent recovery [3]. Membrane separation offers advantages such as modularity, scalability, and compactness, allowing formulation adjustments to optimize permeability and selectivity depending on the application. This study combines membranes with sustainable solvents to develop highly selective, compact membranes that operate continuously without regeneration, making them a lower-energy gas separation technology. Polyetherimide (PEI)-supported PEBAX® membranes, enhanced with DES and lignin as additives for air purification, were tested for indoor air treatment. Experiments with CO_2, O_2, and N_2 showed that adding DES reduced membrane selectivity for all gases, facilitating oxygen and nitrogen permeability.

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P76 - Hydrophobic Deep Eutectic Solvents for Advanced Recycling of Spent Nuclear Fuel

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Keywords: Advanced nuclear fuel cycle, hydrophobic DES, actinides and lanthanides co-extraction, hydrometallurgical processes, TOPO, CMPO.

One of the most significant challenges in the nuclear energy field is related to the management of nuclear waste. Within the advanced nuclear fuel cycles under development, a key strategy involves minor actinides (MAn) recovery by selective separation or intermediate co-extraction with lanthanides (Ln) followed by selective MA separation. Current research focuses on addressing this goal through hydrometallurgical processes by exploiting selective extractants dissolved in proper diluents. To the best of authors' knowledge, the application of DESs in this technological field has been only barely investigated [1,2], but they could offer the possibility to overcome some of the critical issues, including economic and environmental sustainability, present in current extraction systems. To this purpose, we report on the extracting properties of four Type V hydrophobic DESs and their potential for extracting An and Ln from spent nuclear fuel surrogate. Some systems utilize tri-n-octylphosphine oxide (TOPO) as hydrogen bond acceptor components of the DES, while others the less common octyl(phenyl)-N,N-diisobutylcarbamoylmethylphosphine oxide (CMPO) (Figure 1).

Figure 1. Structure of the HBA used. Left: TOPO, Right: CMPO

Stability under gamma irradiation and aging of the hydrophobic DESs were evaluated for the first time, demonstrating promising resilience. The tunable extraction properties of DESs through composition adjustments highlight their potential as alternatives to organic solvent for a sustainable nuclear waste management. This study underscores DESs as a fertile area for future research in optimizing extraction processes.

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P77 - Physicochemical and sensory insights into the role of NaDES in cosmetic gels

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Keywords: Sensory properties ; gels ; rheology ; physico-chemistry; cosmetics-

Objectives: Natural Deep Eutectic Solvents (NaDES) are a novel class of solvents derived from biorefinery ingredients, recognized for their eco-friendly extraction properties. Unlike conventional organic solvents, NaDES are non-volatile and remain in the final product alongside extracted molecules. This study aimed to (1) assess the impact of hydrophilic NaDES on the properties of cosmetic gels and (2) determine whether the physicochemical and sensory characteristics of NaDES can predict their suitability for formulation.
Methods: Three widely used hydrophilic NaDES—representing organic acid-based, amino acid-based, and sugarbased families—were analyzed both independently and as additives in a model cosmetic gel (1% and 10% w/w). A blank gel served as a control. Rheological behavior was evaluated through flow and viscoelasticity tests, while thermal properties were assessed via Differential Scanning Calorimetry and Thermogravimetric Analysis.
Additionally, texture analyses of the hydrogels obtained are carried out. An expert panel conducted sensory evaluations to gauge the gels' consumer-perceived qualities. Hypothesis of a modification of the gel's hydrogen bond network following NaDES inclusion was also investigated by NMR and ATR-FTIR spectroscopy.
Results: The introduction of NaDES affected gel properties differently across solvent families. Overall, the gels retained their shear-thinning behavior, with viscosity decreasing as shear rate increased. At low shear rates, viscosity was concentration-dependent, but this effect diminished at high shear rates, relevant for processes like spreading, pumping, or spraying. Thermal analysis complemented rheological findings, highlighting structural differences. Texture analyses revealed that NaDES-containing gels exhibit higher hardness and elasticity. Sensory evaluations identified four key descriptors—odor, visual viscosity, stringiness, and stickiness—as critical for understanding the consumer experience and contextualizing physicochemical data. Molecular exploration of the gels using IR and NMR spectroscopies suggests that the initial hydrogen bond networks in the gel and NaDES undergo changes when mixed.
Conclusion: NaDES hold significant potential as sustainable, bio-based ingredients in cosmetic formulations. However, their incorporation can influence consumer experience, necessitating a comprehensive evaluation of their physicochemical and sensory properties to optimize formulability and performance.

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P78 - Protein Stability in Eutectic Systems: The Role of Eutectogels

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Keywords: deep eutectic solvents, eutectogels, lysozyme, stabilization

Proteins, as complex macromolecules, require a high degree of stability in formulations for biomedical and biotechnological applications. Their delicate structures are highly susceptible to disruption by environmental factors or mechanical stress, leading to denaturation and loss of function. To maintain protein structure and functionality over time, it is essential to create an environment that mimics physiological conditions. Hydrogels offer such an environment by forming a protective layer around proteins, helping preserve their structural integrity and biological activity.

Recently, hydrogels have garnered attention for protein stabilization and controlled protein release due to their favorable properties such as biocompatibility, a porous structure that facilitates enhanced protein transport, and their protective effect against protein denaturation. Hydrogels based on deep eutectic solvents (DESs), known as eutectogels, are particularly promising for protein stabilization due to their non-toxic, biodegradable, and highly modular characteristics. The tunable nature of eutectogels allows for optimization based on specific protein requirements, potentially improving stability in a variety of formulations. Despite their potential, the full scope of applications for eutectogels in protein stabilization remains underexplored.

In our initial findings, we demonstrated the exceptional stabilization properties on lysozyme, an important model protein with antimicrobial activity, in DESs derived from natural osmolytes, under various storage conditions [1]. Building on these results, our current objective is to harness the stabilization properties of DES to develop eutectogels from different eutectic pairs for enhanced protein stabilization. This work aims to open new pathways for utilizing eutectogels in both therapeutic protein preservation and industrial enzyme applications.

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P79 - Natural Deep Eutectic Solvent Pretreatment For Cellulose Extraction From Distiller's Spent Grains

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Keywords: Deep eutectic solvent; Circular economy; Cellulose fibre; Lignocellulosic biomass; Distiller's Spent Grains

Deep Eutectic solvent (DES) is a new class of solvent composed of hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) in a specific molar ratio [1]. Natural Deep eutectic solvents (NADESs) are a class of DES in which the hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) are obtained from natural sources. NADES recently emerged as an environmentally friendly solvent to replace traditional acids and alkalis in lignocellulosic biomass processing due to their non-toxicity and low cost [2]. Distiller Spent grain (DSG), a lignocellulosic by-product of whiskey production, is a rich source of biopolymers, including cellulose, lignin, and hemicellulose [3]. In this study, DES were prepared by mixing each sodium acetate: formic acid and betaine: formic acid in five different molar ratios for each DES. Extractives-free dried distiller spent grain (DDSG) was mixed with the various DES using a biomass solvent ratio 1:10 (w/v) and heated in an autoclave at 100 °C for one hour. After pretreatment, the slurry obtained were separated by centrifugation, and the solid residue was washed with acetone : water mixture (1:1) to remove residual DES. The wet cellulose-rich solid residue was treated with 5% peracetic in an ultrasonic bath at 80°C for 2 hours with centrifugation and the addition of new peracetic acid every 30 minutes until a white purified cellulose fiber is obtained. The purified cellulose fiber was washed with alkaline water followed by deionised water until neutral and freeze-dried to obtain dried, purified cellulose fibre. Advanced analytical techniques such as X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) were used to evaluate the impact of processing conditions on the final quality of the extracted cellulose. Sodium acetate-formic acid shows the best treatment for solid recovery, cellulose retention, purity, and yield. After the pretreatment, the lignin and hemicellulose content decreased, whereas the glucan content in the pretreated biomass increased. NADES showed promising potential as an efficient, green, and environmentally friendly solvent in lignocellulosic biomass processing.

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P80 - Separation of rare earth elements with new hydrophobic deep eutectic solvent based on TOPO

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Keywords: Deep eutectic solvent, rare earth elements, liquid-liquid extraction, phase diagram

The rare earth element (REE) is a metal family composed by the 15 lanthanides, Yttrium and Scandium [1]. Their unique properties make them strategic elements in many everyday objects such as electronic devices, automobiles, medical technologies, space…[2] To date, only 1% of these elements are recycled mainly due to the small quantities involved per devices. With the growth of digitalization, the demand for rare earth is constantly increasing making recycling mandatory [3]. One of the most efficient processes for separating REE from other elements is based on liquid-liquid extractions using highly acidic solvents. The use of such solvents presents significant risks to both the environment and operators [4]. Deep eutectic solvents (DES) propose a promising alternative to conventional extractants. These solvents, composed of a mixture of hydrogen bond donors and acceptors, offer good extraction properties [5]. Spectroscopy study and phase diagrams measurements allow to identify six new deep eutectic solvents based on trioctylphosphine oxide (TOPO). These physico-chemical properties of the news solvents were determined (viscosity, density, thermal stability and hydrophobicity) and their capacity to extract REEs (Yttrium, Lanthanum, Neodymium, Praseodymium and Dysprosium) were evaluated on the synthetized solution. These new extractants achieved extraction efficiencies exceeding 85% for all rare earth elements. The optimal extraction condition was determined by varying experimental conditions such as temperature, organic/aqueous (O/A) ratio and salt concentration. It was found that the complex formed during the extraction depends on the DES and the REE extracted. Finally, the recycling of the DES was tested with the HCl stripping solution. Complete recycling has been achieved and the performance of the solvent remained the same even after four cycles of extraction/recycling.

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P81 - Exploring Novel Solvents for Enhanced Conformational and Colloidal Stability of Antibodies

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Currently, the number of biopharmaceuticals available for clinical use has increased rapidly due to the growing interest of the pharmaceutical industry in these products. Antibodies are one of the best-selling classes on the market, due to their specific action and reduced immunogenicity[1]. Immunoglobulin G (IgG) antibodies have a pivotal role as biopharmaceuticals capable of treating a wide variety of diseases. However, IgG is a protein; hence, it can easily lose stability (forming aggregates) and therapeutic efficiency during its handling, transportation and preservation, which is not desirable from a clinical point of view since they can lead to serious and fatal health effects [2]. To overcome these drawbacks, in this work, deep eutectic solvents (DESs) were investigated to improve the conformational and colloidal stability of IgG, thus opening the door for their use as novel solvents in IgG formulations [3]. A series of DESs was prepared through the combination of cholinium chloride ([Ch]Cl), as a hydrogen-bond acceptor (HBA), and various hydrogen-bond donors (HBD), such as urea, glycerol (Gly) and ethylene glycol (EG). The effect of [Ch]Cl–urea at different molar ratios (1:1, 1:2, 1:3 and 2:1) was also analysed. Conformational stability was checked by thermal fluorescence spectrometry, and it was found that the selected DESs allowed increasing the transition temperature (Tm) of IgG by ca. 4 °C. The observed increase in the conformational stability of IgG in the presence of DESs was in agreement with the results of other spectroscopic studies, including FTIR and Raman spectroscopies. In the presence of DESs, there was a minimum exposed surface of IgG with water molecules, thereby improving its stability. Dynamic light scattering (DLS), size-exclusion high-pressure liquid chromatography (SE-HPLC) and sodium dodecyl-sulphate polyacrylamide gel electrophoresis (SDS-PAGE) techniques were additionally performed to analyse the aggregation rate of IgG, which was found to decrease in the presence of appropriate DESs. Finally, the long-term stability of IgG in the presence of DESs was investigated at room temperature. All the results obtained from the conformational and colloidal studies of IgG demonstrated the outstanding potential of cholinium-based DESs as novel solvents for IgG formulations, with the DESs comprising [Ch]Cl–urea or [Ch]Cl–Gly noted as the most promising candidates. All the described studies were also performed with the DESs' individual components, demonstrating that the DESs (HBD + HDA) are needed to improve the stability of IgG [3].

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