VIII Conference of Pre-doctoral Researchers

Abstract Book

Gerardo Boto & Olga Taravilla (Editors)

Volume VIII, 2024

Universitat de Girona
Escola de Doctorat

Universitat de Girona

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of Pre-Doctoral Researchers
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TABLE OF CONTENTS

PREFACE

It is with great honor that we once again present to the University of Girona community—and, more broadly, to the international academic community—the electronic volume containing the abstracts of the contributions presented at the VIII Conference of Predoctoral Researchers of the University of Girona (UdG). Held from June 17 to 20, 2024, this conference was organized under the auspices of the UdG's School of Doctoral Studies, with the support of the Vice-Rectorate for Research and Knowledge Transfer. The event took place at the Faculty of Law, Montilivi Campus, of the University of Girona. Since its inception in 2017, the Predoctoral Researchers Conference has grown through eight editions, consistently working to enhance the quality and recognition of this academic gathering, both within our university and within the broader scholarly community.

As in previous editions, the organization of this event has been led by a dedicated group of volunteer doctoral students. Their commitment, which has been cultivated and strengthened over the years, has enabled them to mobilize the UdG's doctoral community effectively. As a result, seventy contributions by UdG's doctorands and abroad were presented in accordance with the program. This longstanding academic initiative continues to offer intellectual benefits not only to those doctoral researchers who presented their work orally, but also to the entire predoctoral community at the University of Girona.

It is important to emphasize that the primary objective of the Conference is to provide doctoral students with a platform to present partial results of their research, facilitating the exchange of knowledge and fostering scholarly debate among all researchers in training, including those working on doctoral theses or master's projects at our university. In fact, within the Catalan university system, the UdG is one of the few institutions to host a multidisciplinary Predoctoral Conference that is not limited by specific areas of knowledge or doctoral programs.

During the 8th Conference, doctoral and master's students presented their research both individually and within the framework of roundtables organized around specific Sustainable Development Goals, rather than within narrowly defined disciplinary or scientific boundaries. This approach not only sought to transcend the limitations of specialized fields but also aimed to engage researchers from diverse programs and faculties. It was a priority to align the conference with the core values of the University of Girona, as a community committed to the development and sustainability of the territory it serves and from which it draws.

The challenges of urban sociability, ecological balance, addressing human and environmental pathologies, ensuring equitable healthcare for all citizens, promoting peace and justice, caring life on land and below water, reducing inequalities, fostering respect for marginalized groups, advocating responsible and sustainable production, supporting inclusive education, and preserving cultural heritage through shared memories—all these pressing issues, confronting the uncertainties of the future, can

and must be tackled through doctoral research. Ultimately, the purpose of a doctoral thesis is to offer solutions and pathways for progress that serve society, with research emerging as a form of citizen science that grows in dialogue with the surrounding community and provides innovative, committed responses to global challenges.

This innovative organization of the presentations had an immediate effect: each researcher was afforded the opportunity to engage in discussions about their research outcomes with other leading scholars outside their own research team, project, or PhD program. This demonstrated that oral presentations and dialogues not only contribute broadly to the development of skills in the reasoned and persuasive defense of research proposals, but also specifically aid in the dissemination of research findings to society. In this manner, doctoral students make significant progress toward achieving key milestones within the Open Science paradigm, a conceptual and administrative framework for knowledge communication that is essential in contemporary European societies.

The *VIII Jornades de Investigadores Predoctorales* was organized by a team of eleven volunteer doctoral students from various doctoral programs. This group—Núria Alsina Pla, Carolina Andrade Amaral, Gabriela Adriana Bastida, Lluís Coromina Verdaguer, Samuel Lado Franco, Cinthia Padilla Gallegos, Marta Reales Moreno, Artur Rubinat, Imogen Simpson-Mowday, Olga Taravilla, and Guillem Vila Siles—carried out an exemplary job. They meticulously organized each session and succeeded in bringing predoctoral researchers from other Catalan universities to participate in most of the sessions. Furthermore, they managed each presentation and facilitated the moderation of discussions during all sessions.

As a result, seventy abstracts were submitted, reviewed, and edited. Eigth of these contributions came from predoctoral researchers from other universities, enriching the presentations by UdG doctoral students. This e-book has been compiled and edited by the undersigned, in collaboration with Olga Taravilla, a predoctoral researcher in Human Sciences and Heritage, who has performed an excellent job in the editorial process.

This e-book, as a reflection of the ongoing and evolving landscape of knowledge, affirms the significance of predoctoral research at the University of Girona within both the national and international academic arenas in 2024. Without question, we will continue to focus on the organization and advancement of the IX Conference of Predoctoral Researchers scheduled for 2025. Those of us involved in the production of this e-book are confident that the academic community of the University of Girona has every reason to take pride in this achievement. Nevertheless, we remain aware that there is still room for further enhancement in the quality and innovation of these conferences.

Girona, October 21, 2024

Gerardo Boto Varela

SESSION 1.
SDG2. ZERO HUNGER

DURABILITY ASSESSMENT OF CHICKEN BREASTS WITH MYOPATHIES USING LABORATORY METHODS AND HYPERSPECTRAL IMAGING

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Keywords: Machine learning, quality, shelf-life, spaghetti meat, wooden breast

1. Introduction and objectives

While chicken consumption is rising globally, emerging myopathies – muscle defects that impair quality and consumer acceptance – pose challenges for the industry (Petracci et al. 2019), and the durability of affected chicken breasts remains underexplored. This issue threatens the United Nations' Sustainable Development Goals 2 and 3, related to zero hunger and promoting good health, as it increases food waste and, potentially, spoilage. Hyperspectral imaging (HSI) appears as a promising technology for assessing chicken quality rapidly and non-destructively (Fu and Jinchao 2019). The present study evaluates spoilage of chicken breasts (with/without myopathies) during storage using plate-count methods and HSI.

2. Methodology

Seventy-five chicken carcasses were screened for wooden breast (WB) and spaghetti meat (SM) presence. Subsequently, carcasses were deboned, packaged in pairs using modified atmosphere (30 per cent O_2, 40 per cent CO_2, 30 per cent N_2), and stored at 4.8±0.75ºC in a 12h-light cycle. Over 14 days, balanced groups of 15 pairs of breasts were examined. The right breast was sampled with a sponge to determine counts of aerobic mesophilic bacteria. The left breast was situated on an illuminated moving platform 50 cm from the HSI camara (900 x 1700 pixels, 386–1015 nm at 2 nm interval, Pika L, Resonon INC, Bozeman, USA). Images were imported to Matlab (The MathWorks Inc. 2023), where the average spectrum was extracted from the cranial, central, and caudal regions of the breast. Further analysis, which included principal component analysis (PCA) and support vector machine (SVM) modeling, and was conducted with R software (R Core Team 2022).

3. Results and discussion

Although initial microbial counts were similar, myopathic breasts showed faster increase, reaching +2 log for WB and +1 log for SM on Day 14 compared with normal. Spectral changes were observed both when plotting individual spectra and displaying samples by principal components. On the visible region of the spectra (400–800 nm), the main differences can be

interpreted as changes in the oxidative state of myoglobin (Grau et al. 2011). Spectra from Day 0 were characterized by a higher relative content of deoxymyoglobin, and subsequent samples displayed higher concentrations of oxymyoglobin and metmyoglobin, likely influenced by packaging conditions. On the near-infrared region there were differences on the water absorbance (980 nm), which can be interpreted as an increase in loose water over time (Wold et al. 2017). The SVM model accurately classified samples by days (CV accuracy = 99.35 per cent), although regression on microbial counts had limited success (R^2=0.60, RMSE=1.37).

4. Conclusions

Myopathies have a negative effect on the durability of chicken, and although HSI did not make it possible to predict microbial counts, it does show potential for accurately predicting other durability parameters, offering a non-destructive and efficient approach to assess quality during shelf-life and reduce food waste.

5. Bibliography

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OBTAINING LUPINE (*Lupinus spp.*) PROTEIN ISOLATES: MAXIMIZING PROTEIN RECOVERY AND EXTRACTION OF ANTI-NUTRITIONAL FACTORS

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Keywords: Protein isolate, optimal extraction conditions, anti-nutritional factors, techno-functionality, *Lupinus luteus*.

1. Introduction and objectives

The lupine is a native legume of the Mediterranean region that has a high protein content and low agronomic requirements (Gollnow and Lakes 2014). These characteristics make it an interesting crop with which to address the challenges of food safety and sustainability, through the production of lupine protein isolates (lupine protein isolate: LPI). However, its anti-nutritional factors (ANF) can have a negative impact on the nutritional and techno-functional quality of LPI. This study aimed to model protein extraction and ANF removal depending on the parameters of the LPI production process (thermal treatment assisted by microwave technology, solvent:flour ratio and ethanol concentration) and establish the optimal extraction conditions.

2. Methodology

A central composite design was used to determine the effect of the different variables, with three replications for each treatment. The protein and ANF content of the LPI, including alkaloids, saponins, total phenolic content (TPC) and phytic acid, were analyzed, as was the ANF content of the acid supernatant. The response surface methodology was used to predict the optimal operating conditions. The techno-functional properties of the optimal LPI (solubility, foaming, emulsifying and gelling capacity) were analyzed before and after the enzymatic treatment with phytase.

3. Results and discussion

Microwave heat treatment did not improve protein recovery or content in LPI and did not affect ANF content in protein isolate. The recovery and content of protein and ANF from LPI was influenced by the ethanol concentration and solvent-to-flour ratio, as well as the recovery of ANF in the acid supernatant. The optimal extraction conditions were set at a solvent:flour ratio of 20:1 (mass:mass) and an ethanol percentage of 0 per cent, which resulted in a protein recovery of 54.9 per cent and a protein content of LPI of 86.8 per cent. The content of alkaloids, saponins, phytic acid, and TPC in LPI was 0.21, 0.45, 29.1 and 0.6 mg of each ANF / g LPI,

respectively. Under these conditions, the recovery of alkaloids, saponins and TPC in the acid supernatant was 66 per cent, 52 per cent, and 60 per cent, respectively.

4. Conclusions

In the time and temperature conditions studied, thermal treatments assisted with microwave technology did not provide a significant advantage in obtaining LPI. However, protein recovery and content in LPI were affected by the solvent:flour ratio and the addition of ethanol to the extraction solvent. ANF content in the protein isolate and its recovery in the acidic supernatant were also affected by the solvent:flour ratio and ethanol content.

5. Bibliography

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6. Acknowledgement

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ADVANCING *Arabidopsis* HYDROPONICS FOR ROOT EXUDATES COLLECTION AND INDIRECT STRIGOLACTONES ASSAY VIA *Phelipanche ramosa* GERMINATION

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Keywords: Arabidopsis, hydroponics, strigolactones.

1. Introduction and objectives

Strigolactones (SLs) are groups of molecules derived from carotenoids, recently classified as phytohormones, which are involved in various endogenous processes of plant development. Once exuded from roots into the soil, they regulate plant-rhizosphere interactions. Soil deficiencies in phosphorus and nitrogen trigger the biosynthesis and exudation of SLs (Kapulnik and Koltai 2016; Ravazzolo et al. 2019) to foster beneficial symbiosis with arbuscular mycorrhizal fungi. However, SLs are also known for having the detrimental effect of stimulating seed germination of root parasitic plants.

Building on this knowledge, a hydroponic growth system was developed to collect root exudates from five-week-old *Arabidopsis thaliana* ecotype Columbia plants subjected to diverse nutritional treatments. These exudates were then employed in a bioassay to assess the germination rate of seeds of the parasitic plant *Phelipanche ramosa* (Pouvreau et al. 2013).

2. Hypothesis

Our hypothesis suggests that subjecting plants to nitrogen and phosphorus starvation at varying time intervals stimulates SL exudation. The results indicate that this aprroach is reliabe and applicable in future studies aimed at characterizing the role of SLs in responses to nutritional deficiencies in *Arabidopsis*.

3. Methodology

The hydroponic system comprised two stages: a pre-culture phase aimed at optimizing seed germination and seedling development conditions (two weeks), followed by the culture hydroponic stage, where plants were grown in a complete nutrient solution (three weeks) (Conn et al. 2013). Before the five-week deadline for root exudates collection, plants underwent distinct treatments: either nitrogen or phosphorus starvation for three or seven days, and a positive control without any form of starvation. Exudation was carried out in both 50 and 15 mL of nutrient solution. Nutrient solutions containing root exudates were used for treating parasitic seeds, with germination assessed by counting seeds displaying radicle protrusion through the seed coat using a stereo microscope.

4. Results and discussion

The germination bioassay highlighted that root exudates collected from *Arabidopsis* plants subjected to three-day phosphorus and three-day nitrogen starvation induced a higher germination rate of *P. ramosa* seeds. Moreover, exudates collected in a 15 mL volume were more effective than those collected in a 50 mL volume.

5. Conclusions

The hydroponic system proved effective for studying the exudation of SLs for conducting *P. ramosa* germination bioassay. The growth protocol recommendations considered two variables: the duration of nutritional deficiency and the volume of exudate collected. The most efficient strategy involved combining three-day periods of nutritional deficiency with exudation in 15 mL of nutrient solution.

6. Bibliography

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SESSION 2.
SDG3. GOOD HEALTH AND WELL-BEING

ENCAPSULATION OF CYCLOMETALATED IR(III) COMPLEXES FOR A TARGETED PHOTODYNAMIC THERAPY OF CANCER

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Keywords: Cancer, metallocomplexes, nanoparticles, photodynamic therapy

1. Introduction and objectives

Photodynamic therapy (PDT) is a treatment that utilizes a photosensitizer (PS) to generate cytotoxic oxygen radicals (ROS) after light activation. This approach aims to specifically destroy cancer without affecting healthy cells (Zamora et al. 2018). Additionally, the radicals' encapsulation into nanoparticles (NPs) has been shown to reduce toxicity and enhance accumulation within tumors (Gavas, Quazi, and Karpiński 2021). The present study evaluates the effectiveness of two cyclometalated Ir(III) complexes as PSs (**Ir1** and **Ir2**), along the effect of their encapsulation in polymeric NPs (**NP1** and **NP2**) on their photocytotoxic properties.

2. Hypothesis

These Ir(III) complexes hold great promise as an alternative to conventional chemotherapy. Their encapsulation could enhance tumor accumulation and improve anticancer activity while avoiding toxicity.

3. Methodology

Cytotoxicity of Ir(III) complexes and NPs was determined against prostate (PC3), cervical (HeLa), lung (A549), and breast (MCF-7) cancer cell lines, along with lung fibroblasts (MRC-5) as non-tumoral cells under both dark and blue light irradiation conditions, using two- and three-dimensional cell models and clonogenic assays. Cellular uptake was investigated by mass spectrometry. Intracellular distribution was explored with the phosphorescent complex **Ir1** through confocal microscopy using organelle-specific dyes. Their ability to generate ROS as well as the mitochondrial damage was evaluated by flow cytometry. The effect on cell migration was investigated via wound healing assays. Characterization of cell death mechanism was conducted using Annexin and propidium iodide staining.

4. Results and discussion

Ir1 and **Ir2** demonstrated cytotoxicity against all cell lines under dark conditions, with IC_{50} values of 2–3 μM, which is comparable to that of cisplatin. Importantly, their activity was significantly increased by blue light irradiation, resulting in phototoxicity indices of 31 and 139, respectively, and IC_{50} values in the nanomolar range in A549 cells. Remarkably, **NP1** and **NP2** induced higher cytotoxicity than the free complexes while maintaining the same phototoxicity indices. 3D spheroids and clonogenic assays confirmed the antitumor efficacy of the complexes and NPs. Notably, **Ir1** exhibited rapid internalization into cells and accumulation in mitochondria. Upon photoactivation, complexes and NPs effectively generated ROS, inducing mitochondrial dysfunction and subsequent apoptosis. Additionally, exposure to the complexes significantly inhibited cancer cell migration.

5. Conclusions

Overall, our approach shows promising potential for selective light-controlled cancer treatment. The targeted activity of Ir(III) complexes towards mitochondria offers an alternative mechanism to conventional chemotherapy. Moreover, these complexes can inhibit the dissemination of cancer cells, which is a critical step in preventing metastasis (Scheid, Beadnell, and Welch 2021). Furthermore, the encapsulation of the complexes in nanoparticles further enhanced their antitumoral efficiency.

6. Bibliography

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COMBINATION OF PHOTODYNAMIC THERAPY AND TARGETED DRUG DELIVERY FOR A SELECTIVE CANCER TREATMENT

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Keywords: Bombesin, cancer, metallocomplexes, photodynamic therapy, targeted drug delivery

1. Introduction and objectives

Photodynamic therapy (PDT) consists of the administration of a non-active drug (photosensitizer, PS) which can be locally activated in the tumor with visible light (Agostinis et al. 2011). Moreover, targeted drug delivery (TDD) involves the conjugation of a drug to a carrier molecule to deliver it to a specific tissue (Ashique et al. 2021).

We present a cyclometalated iridium (III) complex (**1**) as a potential PS and its conjugation with different BN3 derivatives as carrier molecules for the selective treatment of prostate cancer (Barrabés et al. 2020). BN3 is a peptide analogous to bombesin, a ligand of the gastrin-releasing peptide receptor (GRPR), which is overexpressed in some tumors (Begum, Moyle, and Toth 2016).

The objectives of the study are to evaluate the photocytotoxic activity of Complex **1** and characterize its mechanism of action, and to establish whether its conjugation to the BN3 derivatives confers selectivity against cancer cells.

2. Hypothesis

Conjugation of Complex **1** to the BN3 derivatives as tumor-targeting ligands may enhance its selectivity and photocytotoxicity in cancer cells overexpressing GRPR.

3. Methodology

We performed cell viability assays to establish the photocytotoxicity of Complex **1** and BN3 conjugates against cancer and non-tumoral cell lines. We also measured the amount of intracellular iridium by ICP-mass spectroscopy to determine the cellular uptake of Complex **1** and the conjugates, and microscopy experiments to establish their intracellular localization. Finally, with a colony formation assay, we evaluated their effect on the capacity of cancer cells to grow and generate new colonies.

4. Results and discussion

Complex **1** displayed a potent cytotoxic activity against different cancer cell lines, which was enhanced by 18.2–25.4 times, depending on the cell line, by light irradiation. Moreover, upon photoactivation it markedly inhibited the clonogenic capacity of cancer cells. Conjugation to the BN3 derivatives significantly reduced its effect on cell viability and photodynamic activity. However, it also resulted in a more selective activity against cancer cells overexpressing GRPR. We also observed differences in the subcellular distribution; while Complex **1** accumulated in the mitochondria, the conjugates appeared to act on the endolysosomal system.

5. Conclusions

Our results demonstrated that Complex **1** is an efficient PS for cancer PDT and that its conjugation to BN3 derivatives as carrier molecules increases its selectivity towards cancer cells. This allows a more selective treatment, with higher accumulation of the drug in the tumors and reduced side effects in healthy tissues.

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ALTERATIONS IN OXIDATIVE PHOSPHORYLATION COMPLEXES IN ARRHYTHMOGENIC CARDIOMYOPATHY USING DESMOSOMAL KO CELL MODEL

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Keywords: Arrhythmogenic cardiomyopathy *(ACM), CRISPR/Cas9, desmosomes, HL1 cell line, oxidative phosphorylation*

1. Introduction and objectives

Arrhythmogenic cardiomyopathy (ACM) is an inherited disease of the cardiac muscle associated with SCD characterized by progressive cardiomyocyte loss and the replacement of the myocardium by fibro-fatty tissue (Corrado, Basso, and Judge 2017). The main genetic causes of ACM are rare variants in desmosomal genes, which represent up to 50 percent of patients (Austin et al. 2019). There is insufficient understanding at the molecular level of the pathophysiological mechanisms that may trigger ACM and determine its progression. Recent studies have proposed a deficit in transcripts encoding for proteins from the electron transport chain, which may be a potential ACM molecular signature in samples from patients carrying mutations in PKP2 (Pérez-Hernández et al. 2022). Our study aims to elucidate whether these proposed mechanisms can be replicated in our ACM edited cell model and determining if they are gene-specific or common in deficiency of desmosomal genes expression.

2. Hypothesis

We hypothesize that deficiency in gene encoding for desmosomal proteins may trigger common mechanisms related to the OXPHOS complexes, which may be a pathomechanism involved in ACM.

3. Methodology

To perform our analysis we used HL-1 edited cell lines for desmosomal genes previously generated by CRISPR/Cas9 (PKP2-KO, DSC2-KO and DSG2-KO) in our group (Vallverdú-Prats, Brugada, and Alcalde 2022). Expression profiling was performed by RNA-seq analysis. To experimentally validate the RNA-seq analysis results, we performed western blot assays using total protein lysate to test protein levels of the five OXPHOS complexes for the three KO

groups. An XFp cell MitoStress Test was performed to test whether these differences have an impact at the functional level.

4. Results and discussion

RNA-seq analysis results showed numerous downregulated pathways related to the electron transport chain, oxidative phosphorylation and ATP synthesis in all desmosomal KO cell lines. Our experimental results showed a significant reduction of the OXPHOS complexes of the mitochondrial respiration chain at the protein level in all KO-tested groups.

At functional level, our preliminary results of MitoStress Test suggest differences in respiration levels, ATP production and spare respiratory capacity between groups; this is consistent with our WB results, as they show a diminished function of OXPHOS complexes in KO groups.

5. Conclusions

Our results support previously published studies describing oxidative phosphorylation as a pathomechanism for PKP2 deficiency and also suggest that these mechanisms may be a common feature for desmosomal mutations in ACM.

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SYNTHESIS OF PSMA-DIRECTED PEPTIDES AS POTENTIAL DRUG CARRIERS TO PROSTATE CANCER CELLS

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Keywords: Prostate cancer, PSMA, solid-phase peptide synthesis, targeted drug delivery

1. Introduction and objectives

Targeted drug delivery is an important way to increase efficiency and reduce the harmful side effects associated with conventional antitumor therapies. In prostate cancer, the prostate-specific membrane antigen (PSMA) has been increasingly used as a target for cancer therapy due to its high expression in prostate tumours and its relation with tumour invasiveness (Wang et al. 2022).

Peptides GRFLTGGTGRLLRIS (**BP602**) and GTIQPYPFSWGY (**GTI**) have been described to exhibit high affinity for PSMA, which led to their specific internalization into LNCaP prostate cancer cells (PSMA-positive) compared to PC-3 cells (PSMA-negative) (Shen et al. 2013; Jin et al. 2016). However, in a recent study conducted by our research group, we observed that **BP602** labeled with 5(6)-carboxyfluorescein (CF) at its N-terminus did not show the expected internalization specificity (Gargallo 2023).

As a continuation of this work, we planned to prepare two **BP602** and two GTI analogues bearing CF at the side chain of a lysine residue added at the N- or the C-terminus (BP602-Lys(CF), Lys(CF)-BP602, GTI-Lys(CF), Lys(CF)-GTI). Their internalization specificity properties will be assessed. Afterwards, a cytotoxic metal complex will be incorporated with the peptides to evaluate the possible specific activity of the resulting metallopeptides against prostate cancer cells.

2. Methodology

The four CF-labelled peptides were synthesized on solid phase through an Fmoc/*t*Bu strategy, purified, analyzed by HPLC, and characterized by mass spectrometry. Flow cytometry will be used to test the internalization efficiency in PSMA-positive cell lines (LNCaP) and PSMA-negative cell lines (PC-3, A549 and MRC5). The cellular localization of the peptides will be determined by confocal microscopy and their internalization mechanism will be studied. Receptor-mediated endocytosis will be analysed by determining peptide internalization at 36ºC, 4ºC, with the addition of dynasore and of an anti-PSMA antibody, using labelled transferrin as a positive control. Macropinocytosis will be evaluated with the addition of cytochalasin, using labelled dextran as a control.

3. Results and discussion

Peptides were obtained in high purities after purification (>99 per cent). Coupling of CF to the side chain of an additional lysine is expected to preserve their specific internalization in PSMA-positive prostate cancer cells, as reported in the literature. The cellular localization and the internalization mechanism of the peptides are also expected to be determined.

4. Conclusions

The peptides are expected to internalize specifically in PSMA-positive prostatic cancer cells. These peptides would be good candidates for targeted drug delivery in prostate cancer treatment. They could also be developed for photodynamic therapy by coupling with a photosensitizer.

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WHO EATS THE PPGPP? ANALYSIS OF THE EUKARYOTIC ENZYME MESH1 ROLE DURING *ESCHERICHIA COLI* PHAGOCYTOSIS

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Keywords: Secondary messenger, ppGpp, MESH1, macrophages, phagocytosis

1. Introduction and objectives

The secondary messenger ppGpp, also known as Guanosine tetraphosphate, is a modified nucleotide crucial for gene expression regulation, found in bacteria, chloroplasts, and a few archaea, in response to environmental stress factors. No synthetases for ppGpp have ever been found in eukaryotic cells. It has been shown that the human cytosolic enzyme MESH1 can hydrolyze bacterial ppGpp, although there is no clear role in immunity against infection. As ppGpp shares chemical similarities with NADPH, the preferred substrate of MESH1 (Ding et al. 2020), it is possible that this feature of MESH1 is only circumstantial. Although the role of ppGpp is well-defined in bacteria, its impact on gene expression in eukaryotic cells remains sparsely documented (Steinchen, Zegarra, and Bange 2020; Pacios et al. 2020), even though it can stop cellular growth (Hesketh et al. 2017).

2. Hypothesis

Our hypothesis is that MESH1 could play a role during bacterial infection by removing the excess ppGpp inside of macrophages during phagocytosis to avoid possible regulatory effects and cellular growth effects.

3. Methodology

In this study, we determined the expression of MESH1 by qPCR during experiments of 24 hours phagocytosis with mouse macrophages (J774) using two different strains of *Escherichia coli,* the commensal strain MG1655 and the Adherent-Invasive *E. coli* LF82 (able to survive inside of macrophages). Mutants that are unable to produce ppGpp were also used for these experiments. By modifying the levels of MESH1 (through overexpression and siRNA silencing) we expected to determine whether the survival rate of our bacterial strains changed.

4. Results and discussion

If MESH1 is important for the process of bacterial phagocytosis, we hope to observe a significant difference in MESH1's expression in response to the presence of ppGpp during *E. coli* infection and/or an effect on the survival of *E. coli* during variations in MESH1's quantity.

Our preliminary results show an increase in the expression levels of MESH-1 after 24 hours in the uninfected control, indicating that MESH1 expression is naturally increased under these conditions. Moreover, the presence of bacteria seems to increase expression of MESH1, even though the absence of ppGpp in both strains seems to reduce the variations found between 0 and 24h, indicating that MESH1 could be more expressed in the presence of ppGpp inside of macrophages.

5. Conclusions

Although MESH-1 has been described as a NADPH phosphatase, our results suggest that its expression also depends on the levels of ppGpp (only be found in bacteria) and MESH1 degrades it during phagocytosis.

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ANALYSIS OF THE BRUGADA SYNDROME-ASSOCIATED HAPLOTYPE AT THE *SCN5A-SCN10A* LOCUS USING NANOPORE SEQUENCING

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Keywords: Brugada Syndrome, haplotype, long-Range PCR, nanopore Sequencing, *SCN5A-SCN10A Locus*

1. Introduction and objectives

Brugada Syndrome (BrS) is a hereditary cardiac disorder that is responsible for 20 per cent of sudden cardiac deaths in patients with normal hearts. The best-known cause of BrS is the presence of genetic variants in the coding regions of the *SCN5A* gene. *SCN5A* encodes $Na_V1.5$, major cardiac pore-forming, α subunit, of the voltage-gated sodium channel, responsible of action potential initiation. The *SCN10A* gene, which encodes a neuronal sodium channel ($Na_v1.8$), has also been associated with BrS (Cerrone et al. 2022). Along with variants of associated proteins, this gene represents 35 per cent of all BrS cases, while the aetiology for the remaining 65 per cent is currently unknown. Our previous case-control study of BrS patients without reported pathogenic variants in *SCN5A* revealed an association with a haplotype (Hap) encompassing seven single nucleotide variants within the *SCN5A-SCN10A* locus. Of these, the most common haplotype in the European population is the so-called Hap1 found in homozygosis in BrS patients, followed by Hap2 and Hap3. However, since 54 per cent of BrS patients are homozygous for Hap1, it was associated with BrS risk, while Hap2 and Hap3 were associated with a protective phenotype. Here, we analyse the haplotype composition at the *SCN5A-SCN10A* locus of BrS patients bearing a pathogenic variant in *SCN5A* using nanopore long-read sequencing, a method that was previously optimized for haplotype analysis (Pinsach-Abuin et al. 2021). As a control, we use DNA from healthy individuals.

2. Hypothesis

The main hypothesis of this study is that control individuals are enriched for the protective Hap2 and Hap3 haplotypes. We address it using nanopore sequencing, which we propose could be a rapid diagnostics method for BrS.

3. Methodology

Our sample group consists of DNA from healthy individuals. A 13 kb DNA fragment from these was amplified using long-range PCR. Subsequently, library preparation was performed, followed by nanopore sequencing and bioinformatics analysis.

4. Results and discussion

We expected that the most abundant haplotypes found in healthy individuals will correspond to Hap2 and Hap3. Our results should help to define the most common haplotypes in the healthy European population. Our data may also contribute to develop a rapid and simple diagnostic method to assess whether patients carrying a potentially pathogenic genetic variant truly exhibit pathogenic traits.

5. Conclusions

Our results support nanopore long-read sequencing as a rapid method for *SCN5A-SCN10A* haplotype analysis and BrS risk stratification.

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SYNTHESIS OF TETRA-*ORTHO*-METHOXYLATED AZOBENZENES FOR PHOTOSWITCHABLE ANTIMICROBIAL PEPTIDES

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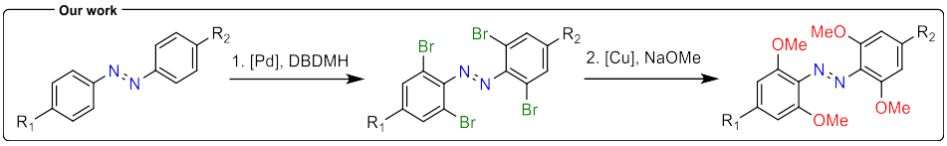
Keywords: Zobenzene functionalization, peptide synthesis, photopharmacology, tetra-ortho-methoxylated azobenzenes, visible-light isomerization.

1. Introduction and objectives

The azobenzene moiety stands as a common photoswitch within the field of photopharmacology. However, its reliance on UV light isomerization limits its in vivo applications. Modifying the azobenzene scaffold with chlorides or methoxys allows a red-shifted isomerization, which enhances tissue penetration (Samanta et al. 2013, 9779). In our laboratory, we reported the first photoswitchable antimicrobial peptides to be fully operated with visible light, which allowed us to control the activity of the compounds with harmless illumination and enabling deactivation by simple exposure to sunlight (Just-Baringo et al., 2021, 12987). Unfortunately, the chlorinated azobenzene presents disadvantages in its application in solid-phase peptide synthesis (SPPS). The tetra-*ortho*-methoxylated counterpart does not present these limitations; however, the syntheses available are limited with low yields or harsh conditions. As such, our group has recently developed a methodology to access the coveted tetra-*ortho*-methoxylated azobenzene scaffold, which presents more robustness than the tetra-*ortho*-chlorinated counterpart in SPPS (Ruiz-Soriano et al. 2023).

2. Hypothesis

Taking advantage of the already reported synthesis of the tetra-*ortho*-brominated azobenzene, we envisioned the following two-step synthesis of the tetra-*ortho*-methoxylated azobenzene through bromide substitution (Scheme 1).



Scheme 1: Synthesis of tetra-*ortho*-methoxylated azobenzene.

3. Methodology

The azobenzene moieties were synthesized via oxidative dimerization or Baeyer-Mills reaction. The bromination reaction was optimized starting from the conditions reported (Liu et al. 2019, 1715). The copper-catalysed methoxylation was developed from precedents in the literature.

4. Results and discussion

The Pd-catalysed bromination was optimized to allow a much broader scope of substrates, including substrates with benzylic positions. The Cu-catalysed methoxylation was developed and applied to produce a wide range of tetra-*ortho*-methoxylated azobenzenes with moderate to excellent yields. Comparative analyses highlight its superior robustness over its chlorinated counterpart, showcasing its potential for SPPS applications.

5. Conclusions

We have developed a two-step methodology to access the elusive tetra-*ortho*-methoxylated azobenzenes, which is tolerant to various functional groups and in good yield. This new methodology allows us to access visible-light-operated peptides using the well-established protocols of SPPS in a more efficient and versatile manner.

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ULTRATHIN POLYMERIC PLATFORM FOR DRUG-ELUTING STENT: A PROOF OF CONCEPT

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Keywords: Additive manufacturing, bioresorbable stent, medical device, stereolithography

1. Introduction and objectives

One of the leading causes of morbidity and mortality worldwide is coronary artery disease, a condition characterized by the narrowing of the artery due to plaque deposits (Scafa Udriște et al. 2021). Drug-eluting stents (DES) consist of a metal core or base and a polymer with drug coating. DES still presents some associated problems, such as biofilm formation, infection, and migration, all of which are related to the cellular response (Marei, Ahmetaj-Shala, and Triggle 2022).

The present work aims to produce an ultrathin permanent polymeric platform for a new generation of polymeric drug-eluting stents (PDES) and compare the cellular response obtained with the novel resins with the traditional stainless steel (SS316L) and polycaprolactone (PCL) to determine whether these polymers could address this challenge. A novel method of tubular 3D micro-stereolithography (ST3DT) was used.

2. Methodology

The novel system is based on vat polymerization technology with a tubular bed. Four different resins were processed and compared with PCL and SS316L. The samples fabricated with the ST3DT were measured, then sterilized in autoclave, and finally, cells were seeded onto them to study the cell viability, adhesion and proliferation.

3. Results and discussion

The results indicate the cell viability of the resins. In this first validation, resins C and SG showed better results than PCL and SS316L. The results of cell adhesion at 24h pointed out that the cells adhere sufficiently to the scaffolds fabricated by vat polymerization but with slight variability, due to rugosity and porosity. After 72h of incubation, all materials exhibited higher cell proliferation than PCL, the reference material. However, cell proliferation occurred on both the outer and inner surfaces only in the PCL tubes. The ST3DT method has shown

great stability being able to manufacture replicas with almost 100 per cent likeness below the 70 µm of strut width.

4. Conclusions

The findings from the assays of cell viability and proliferation, coupled with the successful fabrication of stent struts below 70 µm using the Surgical Guide resin and the ST3DT method, suggest that this resin holds promise as a suitable candidate for the foundation of a PDES. Furthermore, there is an evident need to develop alternative resins with enhanced safety and efficacy, minimizing residues that could potentially enter the cardiovascular system.
The biocompatibility challenges experienced with certain commercial resins highlight the importance of proper printing and postprocessing techniques and the evaluation methods after printing.

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INVESTIGATING THE ROLE OF TYPE II TOXIN-ANTITOXIN SYSTEMS IN ADHERENT-INVASIVE *E. COLI* LF82

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Keywords: Adherent-invasive *Escherichia coli*, Crohn's disease, toxin-antitoxin Systems

1. Introduction and objectives

Adherent invasive *E. coli* (AIEC) pathotype has been related to Crohn's disease etiopathogenesis. AIEC can adhere to and invade intestinal epithelial cells, and can survive and replicate within macrophages. The bacterial factors associated with the intracellular persistence in intestinal epithelial cells need to be elucidated. Toxin-antitoxin (TA) systems are small genetic elements, widely distributed in bacteria, that are involved in different physiological functions such as biofilm formation, persister cell formation, stress response and stabilization of mobile genetic elements (Sonika et al. 2023). Although one study did describe the diversity of TA systems in AIEC, functional studies about the role that TA systems play in AIEC are missing (Bustamante and Vidal 2020). The present work aims to investigate whether type II TA systems may be involved in AIEC pathophysiology.

2. Methodology

We selected six type-II TA systems (*mazEF-1, hipA-2/xre-3, ccdAB-1, relE-1/yiaG-1, parE-1/ higA-1,and parE-3/yiaG-2*) and obtained deletion mutants in AIEC LF82 strain (Datsenko and Wanner 2000). The impact of the mutations was evaluated by comparing the adhesion and invasion abilities of wild type and mutant strains using gentamicin-protection assays on Intestine-407 cells, and by determining the biofilm formation capacity *in vitro*.

3. Results and discussion

A decrease in the invasion indices was observed for *mazEF-1, hipA-2/xre-3 and relE-1/yiaG-1* mutants (45 per cent reduction for *mazEF-1*, 43 per cent for *hipA-2/xre-3* and 42 per cent for *relE-1/yiaG-1*; p value <0.05), although no reduction in adhesion was observed. On the other hand, no reduction in biofilm formation was observed for any deletion mutant.

Although the toxins that influenced the invasion ability differ in structure, MazF and RelE share the same molecular activity. We did not observe an effect on AIEC LF82, but several

studies have indicated that *mazEF*, *hipAB* and *relBE* are involved in biofilm formation and persistence (Sonika et al. 2023).

4. Conclusions

This is a preliminary study investigating the role of type II TA systems in AIEC LF82 that need to be complemented with additional phenotypic analyses. However, we conclude that TA systems *mazEF-1, hipA-2/xre-3 and relE-1/yiaG-1* may be related to the intracellular survival of AIEC in intestinal epithelial cells. Subsequent studies to assess macrophage intracellular survival and persistence are of interest to elucidate the role of these TA systems in AIEC pathogenicity, as well as the molecular mechanism related to greater invasion and intracellular replication.

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INVOLVEMENT OF VOLTAGE-DEPENDENT ANION CHANNEL 2 IN MITOCHONDRIA REGULATION DURING PIG SPERM PRESERVATION

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Keywords: liquid preservation, mitochondria, sperm, pig, VDAC2

1. Introduction and objectives

Sperm storage is crucial for pig breeding to obtain good fertility outcomes (Yeste 2017). Accordingly, exploring the role of proteins involved in maintaining sperm quality during liquid preservation at 15–20 ºC is highly relevant. Voltage-dependent anion channels (VDACs) have been described in pig sperm mitochondria, regulating ion flow between cytosol and mitochondria (Villinger et al. 2010). Previous studies have reported that VDAC2 is implicated in motility and fertilization, as well as in the release of pro-apoptotic factors from sperm mitochondria (Kwon et al. 2013). The present work sought to determine the role of VDAC2 on liquid storage of pig sperm at 17 ºC through its inhibition with TRO19622.

2. Methodology

Semen samples (N=7) were incubated with different concentrations of TRO19622 (0, 5 and 50 µM). At days 0, 4 and 10, a flow cytometer was used to evaluate viability (SYBR-14/PI), membrane lipid disorder (M540/Yo-Pro-1), acrosome integrity (PNA/PI), mitochondrial activity (JC-1/[LIVE/DEAD]), superoxide levels (HE/Yo-Pro-1), total ROS levels (H_2DCFDA/PI) and Ca^{2+} levels (Fluo4-AM/PI). Data were analysed through a linear mixed model, setting the level of significance at $P \leq 0.05$.

3. Results

Flow cytometry analyses revealed that VDAC2 is essential for sperm maintenance during liquid storage, as the highest concentration of TRO19622 led to a decrease in sperm viability at days 4 and 10. This effect was accompanied by a dose-dependent increase in intracellular Ca^{2+} levels, suggesting that inhibition of VDAC2 might lead to an accumulation of Ca^{2+} in sperm, which is known to potentially trigger the activation of cell death pathways (Keshtgar and Ghani 2022). Moreover, mitochondrial activity and ROS levels decreased at day 4 of storage after incubation with the inhibitor. Considering that ion flow is essential for maintaining mitochondrial membrane potential, blockage of VDAC2 could alter the cytosol-mitochondria ion flow, impairing mitochondrial activity. As both Ca^{2+} and mitochondrial activity are known to play a key role in regulating sperm motility (Sampson et al. 2001), the inhibition of VDAC2 is suggested to have an influence on this parameter.

4. Conclusions

In conclusion, our study showed that VDAC2 plays a crucial role in regulating sperm mitochondrial function during liquid storage of pig semen at 17 ºC. High TRO19622 concentrations caused detrimental effects on sperm viability, whereas a dose-dependent effect was observed on the different mitochondria-related parameters. Therefore, proper regulation of sperm mitochondrial activity is revealed to be crucial for semen preservation.

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PREDICTION OF IMMUNOGENICITY AND CONSTRUCTION OF DNA VACCINES OF *KLEBSIELLA PNEUMONIAE VIRULENCE* FACTORS

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Keywords: Antibiotic-resistant bacteria, DNA vaccine, immune simulation, *Klebsiella pneumoniae*.

1. Introduction and objectives

The World Health Organization (WHO) considers *Klebsiella pneumoniae* to be a pathogen of critical priority (Gonzalez-Ferrer et al. 2021, 3). Of special concern is the raise in infections and the emergence of multidrug-resistant strains (Martin and Bachman 2018, 5), which limits the therapeutic options available. Active immunization is a promising strategy to mitigate the severity and mortality associated with these infections. We hypothesize that a DNA vaccine against *K. pneumoniae* can reduce mortality and/or morbidity associated with its infection. The aim of this study is to use *in silico* methods to predict the immune response profile of vaccination based on several virulence factors of *K. pneumoniae*, and to construct plasmids encoding these protein antigens and validate their expression *in vitro*.

2. Methodology

Eight candidate proteins (four porins, three siderophores and a fimbrial subunit) were selected for the study. Firstly, an *in silico* prediction of the immune response profile was obtained using the C-IMMSIM server (Castiglione n.d., February). Data from IgM, IgG, B cell, T-helper (Th) cells, dendritic cells, macrophages, IL-2 and IFN-γ levels were collected. The antigen coding sequences of Por3 and Sid3 were independently cloned into pVAX1 (Thermo Fisher Scientific). Constructs were confirmed by PCR and Sanger sequencing. *In vitro* antigen expression was analysed by transfection of HEK293 eukaryotic cells and RT-qPCR using gene GAPDH as reference.

3. Results and discussion

Regarding the *in silico* simulation, the dendritic active cell counts ranged from 20-25 cells/mm^3, while macrophage counts ranged from 110-125 cells/mm^3. In terms of the humoral response, IgM and IgG levels fluctuated between 1.7x10^5 and 2.5x10^5, respectively, while B cell levels ranged from 750–810 cells/mm^3. Th cell counts ranged between 8.9x10^3 and 1.1x10^4 cells/mm^3. IL-2 levels were within the range of 4.9x10^5–8.9x10^5 ng/mL, and IFN-γ levels ranged from 4.8x10^5–5.5x10^5 ng/mL.

Four clones for Por3 and six clones for Sid3 were successfully confirmed via PCR, and two clones for each vaccine candidate were confirmed by Sanger sequencing. Both vaccine constructs were obtained, yielding a concentration above 3200 ng/µL. Expression in eukaryotic HEK293 cells was confirmed for both constructs, with levels of $2^{-\Delta ct}$ ranging between 1.7–17.

4. Conclusions

The eight candidate proteins of *K. pneumoniae* showed a suitable immunogenic profile, confirming their role as antigens. DNA vaccines based on Por3 and Sid3 have been successfully obtained and expressed in eukaryotic cells. Future steps will address the production process of the vaccines and verify the *in vivo* results.

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INTERVENTION FOR SOCIAL ANXIETY IN INDIVIDUALS WITH AUTISM AND INTELLECTUAL DISABILITY USING IMMERSIVE VIRTUAL REALITY: EFFECTS ON COGNITION, MENTAL HEALTH AND BRAIN FUNCTION

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Keywords: Autism, intellectual disability, immersive virtual reality, brain connectivity, social anxiety

1. Introduction and objectives

Social anxiety co-occurs with approximately 40 per cent of individuals diagnosed with autism spectrum disorder (ASD) and intellectual developmental disorder (IDD) (Johnco and Storch 2015, p. 52). Cognitive-behavioural therapy (CBT) has traditionally been employed as the primary treatment modality for social anxiety (Rosen, Connell, and Kerns 2016, p. 43; Moskowitz et al. 2013, p. 34). Recent advancements in technology, such as immersive virtual reality (IVR), provide novel avenues to augment and customize interventions for the ASD and IDD demographics, resulting in modified cognitive-behavioural therapy (CBT-M). This study aims to evaluate the effectiveness of integrating IVR with CBT-M for treating social anxiety in individuals with ASD and IDD from neuropsychological, psychiatric and neuroanatomical perspectives, focusing particularly on the response of relevant brain regions to the intervention (Sato and Uono 2019, p. 21; Yarger, Nordahl, and Redcay 2021, p. 917). The present study assesses the efficacy of combining IVR with CBT-M in treating social anxiety among individuals with ASD and IDD.

2. Methodology

The next phase of the study will recruit 60 participants from the Specialized Service in Mental Health and Intellectual Disability (SESM-DI) at Parc Hospitalari Martí i Julià (Girona). Evaluations will include neuropsychological assessments, psychiatric evaluations, and neuroimaging analyses, both before and after the intervention. Neuroimaging will utilize functional magnetic resonance imaging (fMRI) to investigate baseline connectivity and brain activation during tasks associated with social anxiety, employing both resting-state and emotional facial recognition tasks using echo-planar imaging (EPI) sequences. The 12-week CBT-M intervention will be structured into two phases: the initial six weeks will focus on psycho education, self-regulation strategies, cognitive restructuring, gradual exposure, and systematic desensitization; this will be followed by six weeks of group therapy.

We conducted a pilot phase study with 28 participants. This phase included neuropsychological and psychological assessment and a CBT-M + ERVI intervention during 12 weeks. The results of this phase are presented in the present work.

3. Results and discussion

In the pilot phase, the intervention demonstrated significant clinical and statistical reductions in social anxiety symptoms, improvements in perceived self-esteem, emotional well-being, interpersonal relationships, personal development, and self-determination. Subsequent phases aim to further validate these outcomes and elucidate the intervention's effects on brain connectivity. The pilot study supports the efficacy of CBT-M in an IVR setting for treating social anxiety in individuals with ASD and IDD. Future work will expand the sample size and enhance the evaluation parameters to confirm and extend these preliminary findings.

4. Conclusions

The preliminary outcomes of the pilot phase endorse the feasibility of this intervention, combining CBT-M and IVR to address social anxiety in individuals with ASD and IDD. The forthcoming phase seeks to substantiate these findings and explore the mechanisms involved, focusing particularly on brain connectivity. This research is poised to substantially contribute to developing more effective treatments that enhance the emotional well-being and overall quality of life for this population.

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CHARACTERIZATION OF REG1B GLYCOSYLATION AS A POTENTIAL PANCREACTIC CANCER BIOMARKER

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Keywords: Pancreatic cancer, biomarkers, glycosylation, REG1B

1. Introduction and objectives

Although pancreatic cancer (PaC) is not a common form of cancer, it has a poor prognosis and, consequently, high lethality (Siegel et al. 2024, 22). There is currently no reliable diagnostic biomarker to detect the disease in early stages, when there are no symptoms. Thus, there is a need to identify new diagnostic biomarkers for early-stage tumours to reduce PaC lethality.

Glycosylation is a posttranslational modification that is altered by the oncogenic process, which makes it a potential source for developing new biomarkers (Munkley 2019, 2570). On the other hand, REG1 is a glycoprotein found in the exocrine pancreas that promotes the regeneration of pancreatic islets. Elevated serum levels are observed in PaC patients compared to healthy individuals, which is why REG1 proteins have been proposed as biomarkers (Chen et al. 2019, 7). Hence, the main objective of this study is to characterize the glycosylation pattern of REG1B to assess its potential as a biomarker for PaC.

2. Methodology

A recombinant REG1B standard, produced in human embryonic kidney cells (HEK293) was been analysed at both the glycoprotein and glycopeptide levels by MALDI-Tof MS. To simplify peak assignment, the glycoprotein was also evaluated after several glycosidases' digestion (NAN1, ABS and BKF). REG1B glycopeptides were obtained after a short trypsin digestion, followed by HILIC purification. These glycopeptides were also digested with glycosidases and further concentrated and desalted using C18 micropipette tips before MS analysis. Finally, REG1B was analysed by western blot with lectins (SNA, MAA, AAL, UEA, PNA, VVL and WGA) and anti-carbohydrate antibodies (F57/27 and 49H.8) to validate the glycoforms assigned by MS.

3. Results and discussion

Following the analysis of the glycoprotein and glycopeptides using MALDI-Tof MS, over 20 distinct glycoforms were identified, with the predominant variant featuring the di-sialyl T antigen (NAcHex + Hex + 2 Neu5Ac), alongside the non-glycosylated protein/peptide. In addition, western blot analyses with various lectins have confirmed the presence of the carbohydrate determinants assigned from the MS results.

4. Conclusions

For the first time, the carbohydrate moiety of a recombinant REG1B standard produced on human cells has been characterized, revealing over 20 distinct glycoforms. These results highlight the main REG1B carbohydrate variants to focus on following studies involving serum-derived REG1B, which will be performed to evaluate the potential of REG1B glycoforms as biomarkers to discriminate PaC patients from healthy individuals.

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MOLECULAR INTERACTION BETWEEN THE ANIONIC EXCHANGER AE3 AND THE CARDIAC POTASSIUM CHANNELS hERG AND Kv7.1

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Keywords: AE3, hereditary channelopathy, hERG, Kv7.1, short QT syndrome

1. Introduction and objectives

There is a growing body of evidence supporting the notion that ion channels can form complexes in the plasma membrane with solute transporters. This novel molecular interaction could be of crucial physiological relevance in the context of cardiac channelopathies. For instance, the gene *SLC4A3*, which encodes the AE3 bicarbonate-chloride exchanger protein, has been recently recognized as a major gene for short QT syndrome (SQTS) (Christiansen et al. 2023). SQTS is a rare hereditary channelopathy associated with a high risk of syncope, ventricular fibrillation and sudden death. This syndrome, characterized by a QT/QTc interval shorter than 330 ms, has been associated with mutations in the two primary potassium channels responsible for the repolarizing phase of the cardiac action potential: the hERG and the Kv7.1 channels (encoded by the *KCNH2* and *KCNQ1* genes respectively) (Hancox et al. 2023). Gain-of-function variants in either channel may lead to a shortened cardiac action potential and a reduction in the ventricular refractory period, triggering SQTS (Cordeiro et al. 2005; Adeniran et al. 2017). The purpose of the present study is to investigate the potential molecular interaction between the anionic exchanger AE3 and the potassium channels Kv7.1 and hERG in heterologous expression models.

2. Methodology

HEK 293T cells were co-transfected with equimolar amounts of the vector encoding AE3 wild type, along with the vector encoding hERG or Kv7.1 and minK (encoded by *KCNE1*). Physical interaction between the AE3 and hERG and Kv7.1 channels was determined by immunoprecipitation and western blot.

3. Results and discussion

Co-transfection experiments have determined the physical interaction between the AE3 transporter and the hERG and the Kv7.1 potassium channels.

Macromolecular complexes between ion channels and transporters, referred to as "chansporter" complexes, represent a novel paradigm in cell signalling (Abbott 2017). In native heart tissue, the novel chansporter complex described here may provide the physical basis for the role of SLC4A3 mutations in SQTS. This is particularly relevant since both the hERG and Kv7.1 channels are known to be tightly regulated by changes in pH, and AE3 is perhaps the most abundant exchanger in the heart, as it governs the bidirectional flow of bicarbonate and chloride anions critical to pH dynamics.

4. Conclusions

Our results suggest that mutations in AE3 may cause modifications in intracellular or extracellular pH in the vicinity of the potassium channels responsible for the cardiac repolarization. This, in turn, may cause a gain of function of these channels, shortening the duration of the cardiac action potential and causing SQTS.

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EFFECT OF A SOLUBLE VARIANT OF APOPTIN ON OVARIAN CANCER CELLS

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Keywords: Apoptin, antitumor drug, ovarian cancer, recombinant protein production

1. Introduction and objectives

Among the various forms of cancer, ovarian cancer has a particularly high mortality rate and one of the worst prognosis (Coburn et al. 2017, 2451). Currently, treatment is based on classical chemotherapy or surgery and this has led to a notable decrease in the quality of life of the affected women. In addition, the high heterogeneity that ovarian cancer presents often drives tumour treatment failure (Akter et al. 2022, 650). This problem gives rise to the need to develop new treatments and strategies to overcome this problem.

In this study, we have assessed the potential cytotoxic activity of Apoptin, a protein from leukaemia chicken virus that induces apoptosis in a selective way in different types of cancer cells (Malla et al. 2020, 524) but we found that its use is hampered by its low solubility. We have previously developed a truncated soluble Apoptin variant that is as effective as Apoptin in different cancer cell lines (Ruiz-Martínez et al. 2017, 260). In the present study we tested its effectiveness against ovarian cancer cells.

2. Methodology

Protein production was carried out by *Escherichia coli* Rosetta (DE3) previously transformed with pET28a ApopΔLeu. Apoptin was purified with a methodology consisting of cell lysis, solubilization of inclusion bodies, affinity chromatography, protein refolding and size exclusion chromatography. The integrity of purified Apoptin was checked by matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF). Apoptin cytotoxicity against different ovarian cancer cell lines was measured with a CellTiter-Blue® cell viability assay where half-maximal inhibitory concentration (IC_{50}) was determined.

3. Results and discussion

Apoptin was successfully produced and obtained in its pure form and MALDI-TOF analysis confirmed its identity. Analysis of the cytotoxicity of Apoptin in different ovarian tumour cell lines was carried out and their IC50 values were compared to those previously obtained in other cancer models.

4. Conclusions

Our results show that the truncated Apoptin variant can be an interesting candidate for the treatment of ovarian cancer. 3D cell culture studies are a possibility as the next step in this research.

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LEGAL CONSEQUENCES OF DIVING-RELATED FATALITIES

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Keywords: Court, diving, fatalities, legislation

1. Introduction and objectives

Diving is one of the most popular underwater activities on the Girona coast (Casadesús 2019). Although it is currently considered a safe practice, new cases of deaths related to such activity are reported every year (Shreeves 2018). According to Spanish legislation, every diving-related fatality occurred requires a police investigation and the opening of a judicial file in the territorially competent court (Casadesús 2021).

Accidental deaths are generally the most common form (Denoble 2008). As a result, the criminal procedure will be frequently archived but even in these cases, public or civil liability can be claimed. It could be also that the fatality occurred while the deceased was working, which sometimes leads to investigation in labour or military court.

The aim of the present study is to analyse all diving-related deaths in Girona (North-eastern Catalonian littoral) between 2009 and 2020 and to provide additional information about their legal consequences.

2. Methodology

According to Regulation 1/2005 regarding accessory aspects of judicial proceedings, we have grouped all the cases by investigating court and made a formal request for data regarding the type of procedure, status and completion of each judicial file. We also reviewed the databases of Forensic Pathology Services of the Institute of Legal Medicine and Forensic Sciences of Catalonia, analysed police reports and forensic autopsy reports, and examined the diving equipment.

3. Results and discussion

A total of 45 cases of diving-related fatalities were documented. All occurred during leisure time, meaning there are no labour or military fatalities. To date, we do not have any data about the criminal investigation status. However, we hope that the data obtained will enable us to identify equipment failures or non-compliance with safety standards that could lead to

criminal and/or civil liabilities in court and to discuss common legal issues associated with diving fatalities.

4. Conclusions

The vast majority of diving fatalities can be attributed to human error. If divers made better decisions, a significant number of fatalities and their associated costs could be avoided every year.

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DECISION-MAKING ON EMERGENCY FOSTER CARE

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Keywords: Decision-making, emergency foster care, children's rights, children's well-being, social educators

1. Introduction and objectives

Children entering the protection system are in vulnerable situations, having often experienced trauma and inequalities, and the decision-making processes to ensure the best interests of children are very complex. These processes involve many factors that need to be considered and it is important to explore some aspects of the care system that tend to remain hidden. Professionals must make decisions that consider stability and permanency as key factors for children's well-being (Cameron et al. 2022; Jackson et al. 2022). The present study assesses the practice and policy regarding emergency foster care delving further into understanding the decision-making that impacts the length of time a child spends in emergency foster care, the transition process to a new home, and the support requirements voiced by those involved in these placements.

2. Methodology

We used a qualitative methodology, involving five focus groups and two interviews, with a total of 24 participants. We conducted a content analysis, contrasting the key themes that emerged from the participants and aligning them with the research objectives through a process of coding and categorization, using the Atlas.ti package.

3. Results and discussion

The analysis showed that emergency foster care often lasts more than six months, in breach of the time limits established by the child protection law. Foster families felt that the transition process to a new placement (for example, another foster family, an adoptive family or the return to the family of origin) was satisfactory when both families perceived it as being carried out flexibly and with consideration of the child's circumstances. The results also indicate that if the connection with the emergency family and children is severed after the emergency placement ends, children may feel abandoned.

4. Conclusions

These findings underscore the importance of enhancing the evaluation of these cases to ensure that placement in emergency foster care is the most appropriate solution. Professionals must

assess whether it is necessary for the child to be placed with an emergency foster family or whether he/she can be sent to a more stable placement, with particular emphasis on reducing the length of time spent in emergency care. Finally, it is essential to make decision-making processes more flexible, adapt to each child and always take them into account and place their needs at the core of the process.

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EVALUATION OF THE COMPREHENSIVE CARE MODEL FOCUSED ON PEOPLE WITH COMPLEX AND ADVANCED CHRONIC DISEASES, ATTENDED IN PRIMARY CARE IN THE BAIX EMPORDA REGION

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Keywords: Advanced chronic diseases, complex chronic diseases, evaluation, person-centred care, primary care

1. Introduction and objectives

The care of people with complex chronic diseases (CCD) and advanced chronic diseases (ACD) is an important challenge for the health system, due to the difficulty in managing their care, their environment and the use of services. The COVID-19 pandemic has transformed the care model in primary care, with a negative impact on the quality standards of care for chronic disease (Caparrós et al. 2022). It is necessary to apply individualized plans and new strategies.

Person-centred care (PCC) places the person and their environment at the centre of health objectives (Mezzich et al. 2016). Primary care is the level of care that can best offer it, due to its longitudinality and home care (Morilla et al. 2015).

The aim is to evaluate the model of comprehensive and person-centred care for people with CCD and ACD treated in primary care of the Baix Empordà region.

2. Hypothesis

The implementation of a PCC model in people with CCD and ACD increases their clinical and psychological stability, improves their satisfaction and quality of life, and should reduce the economic impact.

3. Methodology

The project will be presented in the four Health Care Centres (HCCs). The population of CCD/ ACD attended by the specific chronicity team will be identified. Sociodemographic and clinical data will be collected, as well as health care indicators. These last indicators will be compared to evaluate the extra resource of care for complex chronicity implemented in the HCC of Palafrugell and Palamós, but not in the Torroella de Montgrí and La Bisbal d'Empordà.

The satisfaction of the population treated and the health professionals of the HCC of Palafrugell and Palamós will be evaluated by means of a survey.

Health professionals from the four HCCs using PCC will be trained and then assessed comparing the extent to which they integrate it into their clinical practice, using the ACPAPS questionnaire (Pascual et al.,2023).

4. Results and discussion

We expect that offering an extra resource in the care of people with complex and advanced diseases from primary care will improve comprehensive and person-centred care, contributing to the reduction of the economic impact of diseases. Evaluating whether health professionals integrate PCC into their clinical practice will improve care.

5. Conclusions

It is necessary to evaluate whether new strategies offer added value to CDP care to evaluate the PCC to detect relationship problems with individuals, and evaluate whether or not certain circumstances influence the level of care.

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JOSEP PASCUAL I PRATS (1854-1931): PRÀCTICA PROFESSIONAL I ACTIVITAT CULTURAL DEL METGE GIRONÍ

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Paraules clau: biografia, Girona, historiografia de la medicina, Josep Pascual i Prats, segles XIX-XX

1. Introducció i objectius

Josep Pascual i Prats, metge de l'Hospital Provincial de Santa Caterina de Girona des de 1885, fou un personatge clau en el Sindicado Médico i en el Colegio de Médicos de la província de Girona (Coromina, en premsa; Julià 1994). A més, impulsà una temptativa de repertori de la bibliografia mèdica d'àmbit espanyol, l'*Index Medicus Hispanus* (1904-1906) (Olagüe, Menéndez, i Pulgar 1990). En les biografies sobre aquesta figura es destaca eminentment la seva tasca professional (Julià 1994). Ara bé, quin fou el seu rol en les activitats culturals de la Girona de tombant del segle XIX al XX?, ambdós vessants tingueren vasos comunicants? L'objectiu rau en el fet de confeccionar una aproximació biogràfica per tal de ponderar el quefer com a facultatiu i, simultàniament, el seu rol en el món cultural gironí.

2. Metodologia

En el marc del «retorn del subjecte» a les ciències humanes, depurat de tot rastre hagiogràfic, és implementat el mètode biogràfic, d'acord amb els principis de la historiografia sociocultural (Coromina, en premsa). Es pensa històricament Pascual posant especial èmfasi no només als aspectes socioprofessionals del personatge, sinó que també als culturals. Els documents han estat recollits a l'Arxiu Històric de Girona, l'Archivo Histórico Nacional, la Biblioteca del Col·legi Oficial de Metges de Girona i l'Arxiu Municipal de Girona.

3. Discussió

Les semblances sobre el galè en ressaltaren essencialment la seva dimensió professional (Julià 1994). La hispanista francesa Isabelle Renaudet posà l'accent en la seva dedicació professional, com a «maître d'œuvre» del projecte associatiu a les terres gironines (Renaudet 2012, 395). No obstant això, la historiadora també subratllà la seva funció com a «erudit local»: col·laborador de la *Revista de Gerona*, vicepresident de l'Asociación Literaria de Gerona (1901) i un dels fundadors del Museu Provincial d'Antiguitats y Belles Arts (Renaudet 2012, 395). En la mateixa línia, fou un assistent assidu al Teatre Municipal, bibliotecari del Casino Gerundense

i acadèmic corresponent de la Real Academia de la Historia (1918) (Coromina, en premsa). Així mateix, les fonts d'informació el descriuen com un «bibliófilo consumado» (Pascual 1966).

4. Conclusions

Un dels professionals de la salut més destacats de la Catalunya contemporània és el metge gironí Josep Pascual. La labor com a facultatiu convisqué i es retroalimentà amb els seus interessos culturals i, de resultes d'això, palesem el seu rol proactiu en algunes de les principals institucions culturals gironines de les acaballes del vuit-cents i les primeries del nou-cents (Coromina, en premsa).

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EL DESENVOLUPAMENT DEL MERCAT LABORAL PER A INFERMERES A CATALUNYA A PRINCIPIS DE SEGLE XX

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Paraules clau: Catalunya, infermeria, mercats laborals, professionalització femenina, segle XX.

1. Introducció i objectius

La professionalització femenina es va produir en un context eminentment urbà en el qual es va ampliar el destí laboral tradicional per les dones: el servei domèstic o el treball de l'agulla. En el primer terç del segle XX, les feines de bibliotecàries, secretàries, arxiveres, infermeres, van ser fonamentals en el desenvolupament del sector serveis. A part de la introducció i l'estat de la qüestió que reunirà les principals aportacions en el camp d'història de la infermeria (Domínguez, Carmen 1981; Siles, José 1996) i la historiografia d'altres professions femenines com les mestres, universitàries, metgesses, enginyeres, secretàries, arxiveres (Anderson, Gregory 1988; Porter, Susie 2018; Otero-Carvajal, Luis Enrique i Rodríguez-Martín, Nuria 2022); la tesi constarà de dos grans apartats. En primer lloc, estudiarem la formació de les infermeres. En segon lloc, analitzarem l'aparició d'aquest mercat laboral en clíniques privades i hospitals públics de la capital catalana.

2. Metodologia

La metodologia es basarà en la consulta bibliografia, no només des de la història de la infermeria sinó també la historiografia social del treball, la historiografia urbana i amb perspectiva de gènere. A partir d'aquí, la investigació es durà a terme gràcies a la consulta de fonts primàries i fonts secundàries dels principals arxius de referència com: l'Arxiu Històric de la Universitat de Barcelona, l'Arxiu Històric de la Ciutat de Barcelona, l'Arxiu Municipal Contemporani de Barcelona, l'Arxiu de la Diputació de Barcelona, l'Arxiu Històric de la Caixa de Pensions de Barcelona, l'Arxiu Nacional de Catalunya, l'Arxiu de l'Hospital de Sant Pau i de la Santa Creu, l'Arxiu de la Creu Roja de Madrid, etc. Paral·lelament, també serà fonamental la consulta de premsa d'època als dipòsits digitals com ARCA, Biblioteca Virtual de Premsa Històrica o l'Hemeroteca Digital de la Biblioteca Nacional d'Espanya.

3. Discussió

La intenció és poder dialogar amb els debats generals de la historiografia sobre el treball femení, la disminució de la nupcialitat, l'emancipació de les dones, la seva participació política, les relacions de gènere, etc.

Amb aquesta recerca pretenem contribuir a la història social i del treball de Catalunya tot responent a preguntes fonamentals com el *perquè* es va professionalitzar a les infermeres, *qui* eren, *on* treballaven, *a quins* llocs treballaven.

4. Conclusions

Conèixer aquesta agenda professionalitzadora ens permetrà veure si aquesta professionalització ha devaluat les tradicions artesanals d'aquest ofici o si ha estat un vehicle de mobilitat socioeconòmica ascendent en l'assumpció d'un estatus social respectat.

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SESSION 3.
SDG4. QUALITY EDUCATION

POTENTIAL FOR ARTS-BASED RESEARCH TO INTEGRATE TEACHING KNOWLEDGE

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Keywords: A/r/tography, arts-based teaching methodology, knowledge integration, pre-service training

1. Introduction and objectives

This research focuses on the author's practice as an academic in pre-service training of visual arts teachers in Chile at the Universidad Metropolitana de Ciencias de la Educación (UMCE). Specifically, in the Didactic Integration Workshop, this research aims to facilitate the connection and articulation of knowledge previously acquired from other subjects of the degree, as well as the incorporation of new knowledge relevant to the performance of the visual arts teaching profession in Chile. The research seeks to improve a methodology that started in the previous year (Figure 1) to promote knowledge integration and amplify this comprehension in a contemporary artistic-pedagogical way. The main objective is to vindicate the importance of visual arts education and its specific didactics as a space for the construction of situated knowledge and its potential for integrating teaching knowledge.

2. Methodology

This is arts-based research (ABR) that focuses on the field of education from the perspective of a/r/tography. In this framework, teaching, research and art are deeply connected (Rubio 2021; Irwin 2013). The framework includes an artistic installation of the author as an aesthetic provocation that articulates the formative actions of interpreting, creating, disseminating art and its mediation in the Didactic Integration Workshop. Photography, video, semi-structured dialogue, cartography and bibliographic review are also included. This project is open to reconfiguration in the process.

3. Discussion

Thomas Lehmann's work is an important source of knowledge integration in pre-service teacher education (Lehmann 2020; 2018). The present research expects to broaden the international perspectives by adding a Chilean study, which is developed through a dissimilar methodology and in a different pedagogical career than Lehmann's publications and compilations. The arts-based teaching methodology and A/r/tography do not expect to build a generalisable type of knowledge; instead, they seek to construct a situated knowledge in which the context and the personal experiences of the participants are essential (Rubio 2021; Irwin 2013).

Figure 1. Francisca Maureira, 2023, *Didactic Integration Workshop 2023*, digital photograph. Shared by Francisca Maureira, workshop assistant.

4. Conclusions

Fostering integration of knowledge in the initial formation of visual arts teachers in an artistic and contextualized pedagogical way is a contemporary proposal. It is understood as a process open to configuration. In this case, the experiences of knowledge integration are also content for the students of the Didactic Integration Workshop and learning for the researcher, who is also an artist and teacher of the course.

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INFLUENCE OF LINGUISTIC DOMINANCE ON VISUAL PERSPECTIVE-TAKING

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Keywords: Linguistic dominance, social cognition, visual perspective-taking

1. Introduction and objectives

Visual perspective-taking (VPT) is the capacity to represent and make judgments about another person's point of view and is a crucial skill in human social interaction. Children acquire VPT around the age of four, when self-perspective and other-perspective differ, but an effortful cognitive process is required to overcome the situation, and even adults make mistakes (Surtees, Butterfill, and Apperly 2012). In situations where perspectives are incongruent, errors may be influenced by certain characteristics of the VPT task, such as time pressure or alternating perspectives. However, the impact of language on these situations has not yet been studied.

Our results can be affected by whether tasks are performed in our dominant language or in a foreign language. The language used to administer tasks can impact decision-making (Costa et al. 2019), memory (Beato and Arndt 2021), and emotional reactions (Dylman and Bjärtå 2019). This is because using a foreign language can create emotional distance, leading to more logical decision-making and less susceptibility to emotional stimuli. Therefore, the present study aims to investigate whether the language used during task administration affects performance on a VPT task and whether this effect differs as a function of subjects' linguistic dominance of the administration language.

2. Methodology

Seventy children aged between nine and 10 took part in the study (data collection still ongoing). They were randomly assigned to one of the two conditions (English or Catalan group). All were Catalan-dominant and, depending on the group, they performed the task in English (foreign language) or in Catalan (dominant language). The two groups are comparable in terms of empathy, inhibition and working memory.

3. Results and discussion

Results are not yet available as data collection is ongoing. Three possible scenarios are being assessed: (1) the Catalan group would perform better on the task due to greater linguistic dominance and therefore less emotional distance, which would facilitate the adoption of the

other's perspective; (2) the English group would perform better due to less linguistic dominance and greater emotional distance which would result in less influence of the other's perspective; (3) the absence of significant differences between the groups might suggest that there is no impact of the language of administration on the VPT.

4. Conclusions

Our interest in the effect of linguistic dominance arises from its broad relevance. With millions of multilingual individuals worldwide, it is crucial to comprehend how language affects our ability to perceive others' perspectives.

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THE ROMANISATION OF THE IBERIAN CULTS IN INDIGÈCIA

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Keywords: Iberian world, indigècia, *interpretatio,* romanization, religion

1. Introduction and objectives

This paper approaches the study of religion in the Iberian world, focusing on the northeast area of Catalonia, which corresponds to the zone called *Indigècia*. It will analyse the different sacred spaces located in this region, taking archaeological aspects into special account.

The aim is to analyse how Romanization affected Iberian cults, traced through the modification of religious buildings and the archaeological remains they may have left behind. The process of adoption of Roman divinities by the conquered peoples, known as *interpretation*, is still under-researched in the *Indigècia* area (Nolla, Palahí, Vivo 2010). The present paper attempts to provide more data on this subject and, ideally, to draw new conclusions.

2. Hypothesis

This master's thesis is concerned with the effect of Roman presence on the Iberian populations at a religious level; in other words, how *interpretatio* took place in the *Indigècia* area. There is little written documentation on the Iberian world, so archaeology is the main source of information, but this too is often insufficient (Belarte, Sanmartí 1997). That is why the phenomenon of *interpretatio* in Indigècia is little known, and this is the situation that I would like to address and change in this paper.

3. Methodology

I will survey Iberian religion and elaborate a state of the question through secondary literature. However, in order to investigate Roman *interpretation*, I will use archaeological sources. Bearing in mind that written sources are insufficient to understand the Iberian world, archaeology is the main source of knowledge, especially for studying a topic such as religion and its evolution, which was not commonly addressed by ancient authors. Therefore, it is necessary to refer to excavation reports and archaeological interventions and to make an interpretation or reinterpretation based on the parameters that interest us.

4. Results and discussion

This paper is expected to obtain results that, even though not revolutionary, will contribute to understand better *interpretatio* as a whole in the *Indigècia* area.

5. Conclusions

Interpretatio is little-known phenomenon in the area of *Indigècia*, especially because of the lack of research that addresses this topic as a whole, taking into account different archaeological sites, evidences and the whole area of *Indigècia*. That is why I will address this subject in this thesis and try to shed light into it, to improve our understanding of the Iberian world.

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LA BASÍLICA PALEOCRISTIANA D'ES FORNÀS DE TORELLÓ (MENORCA). REVISIÓ I NOVES INTERPRETACIONS DEL JACIMENT DES DE LA PERSPECTIVA DE L'ARQUEOLOGIA I LA HISTÒRIA DE L'ART

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Paraules clau: arqueologia, basílica Paleocristiana, Fornàs de Torelló, Menorca

1. Introducció i objectius

La Basílica d'Es Fornàs de Torelló (Menorca) va ser descoberta per l'arqueòloga Maria Lluïsa Serra l'any 1957. És un edifici datat de mitjans del segle V i del segle VI, que conserva una nau única amb una capçalera quadrada, espais annexos d'interpretació problemàtica, paviment de mosaic i la base de l'altar principal. Des dels treballs de Serra la historiografia no ha prestat cap atenció al jaciment com a conjunt. Partint d'aquestes premisses, aquest treball de final de màster té com a objectiu principal fer una revisió general del jaciment de manera crítica des de perspectives interdisciplinàries dins dels àmbits de l'arqueologia i la història de l'art.

2. Hipòtesi

La hipòtesi que es va plantejar, després d'haver revisat la documentació escrita i gràfica, és que la suma d'una excavació precipitada i una restauració interpretativa posterior han fossilitzat interpretacions en la historiografia que molt possiblement són errònies.

3. Metodologia

La metodologia que s'ha seguit es basa, en primer lloc, en una recerca bibliogràfica per definir els antecedents dels quals parteix aquest treball. En segon lloc, en la consulta de les fonts primàries, com són el mateix jaciment, els diaris de camp inèdits de l'excavació i les fotografies del transcurs d'aquesta. Per últim,-la presa de mesures i fotografies per a l'anàlisi de l'objecte d'estudi amb la finalitat d'elaborar un projecte fotogramètric del jaciment.

4. Resultats i discussió

La discussió que es presenta és la revisió de les afirmacions que s'han fet al voltant de la basílica de Torelló, ja que es varen fer a partir d'una restitució i restauració interpretativa que ha donat lloc a confusions. Ha estat necessària una revisió de les fonts primàries (material

gràfic i escrit) molt minuciosa per tal de reconstruir els fets i poder obtenir conclusions més objectives gràcies als nous recursos que estan a l'abast.

5. Conclusions

Aquest treball encara està en una fase en la qual no es poden extreure unes conclusions concretes. El que sí que es manifesta és que el resultat obtingut de l'excavació del jaciment és fruit d'uns treballs fets en base a una metodologia que vista des dels paràmetres actuals necessita una revisió crítica i que els nous recursos disponibles en l'actualitat permeten extreure nous resultats i hipòtesis interpretatives del conjunt.

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TEIXIDORS I SASTRES DE CASSÀ DE LA SELVA A LA SEGONA MEITAT DEL SEGLE XVIII: UNA APROXIMACIÓ A PARTIR DEL *OFICIO DE HIPOTECAS* DE GIRONA

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Paraules clau: teixidors, sastres, Cassà de la Selva, segle XVIII, protoindústria.

1. Introducció i objectius

Aquest estudi és la continuació d'una avaluació preliminar de la informació continguda en els registres de *l'Oficio de Hipotecas* de Girona (OHG), relativa a teixidors i sastres. Els nombrosos documents localitzats han requerit acotar l'estudi a la vila de Cassà de la Selva.

L'objectiu principal és avaluar la presència de teixidors i sastres a Cassà de la Selva, les seves possibles nissagues i comportaments socials durant la segona meitat del segle XVIII.

2. Hipòtesi

L'estudi previ i la poca informació sobre teixidors i sastres al corregiment de Girona planteja preguntes com: Quants teixidors i sastres hi havia a Cassà de la Selva? Quin parentiu tenien? A quin estrat social pertanyien? Produïen per la seva àrea d'influència, o hi havia algun tipus de protoindústria? Tenien relació amb Barcelona o altres centres de comerç?

3. Metodologia

S'analitzaran els registres de l'*OHG* mitjançant la plataforma *Transkribus* que permetran aproximar el nombre de teixidors i sastres de Cassà de la Selva a finals del s. XVIII i la seva identitat. Complementarem aquesta informació amb les dates de naixement, matrimoni i defunció extretes dels llibres parroquials disponibles al portal del *Family Search*.

4. Resultats i discussió.

Aquest és el primer estudi sobre teixidors de lli i sastres del corregiment de Girona. Els pocs estudis que hi ha sobre la producció de teixits en època protoindustrial, s'han centrat en els de llana a la Catalunya central (Torras 2019), al cànem a Alacant (Hansen, 2015) i la indústria de la llana i del cotó a Besalú (Serramontmany, 2015, 194).

En els registres de l'OHG entre 1768 i 1792 apareixen 85 teixidors de lli i 38 sastres residents a Cassà. És rellevant que tots els teixidors ho són de lli i que el número és prou elevat per preguntar-se qui era el destinatari de la seva producció. L'anàlisi dels capítols matrimonials

també indica que no hi ha una relació familiar directa entre els dos grups tot i que formarien part dels estrats més humils, especialment els teixidors.

5. Conclusions

L'OHG i els llibres parroquials ens ha permès confirmar que a finals del segle XVIII a Cassà hi havia un nombre significatiu de teixidors de lli i sastres. Hem pogut localitzar nissagues i definir el seu estrat social que, especialment en el cas dels teixidors, era humil. Els documents consultats no expliquen la pràctica de l'ofici, el mercat de matèries primeres o els mercats de destinació, fet que ens obre la porta a noves cerques.

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SESSION 4.
SDG5. GENDER EQUALITY

LA CONSTRUCCIÓ D'UNA MEMÒRIA INDIVIDUAL A *QUAN ÉREM REFUGIATS* (1975), DE TERESA PÀMIES

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Paraules clau: literatura del jo, memòria, *Quan érem refugiats* (1975), història, Teresa Pàmies.

1. Introducció i objectius

La ponència té com a objectiu mostrar els resultats que s'han obtingut durant el primer any de la recerca. Concretament, s'exposarà l'anàlisi de *Quan érem refugiats* (1975), de Teresa Pàmies, narració escrita en primera persona del singular en què l'autora, essent també la narradora i la protagonista, expressa la seva vivència dels primers dies del seu exili.

2. Metodologia

La metodologia d'anàlisi ha sigut bibliogràfica. Per estudiar els models narratius i els recursos estilístics que l'autora utilitza a *Quan érem refugiats* (1975), s'han utilitzat els treballs d'experts en la literatura del jo o literatura autobiogràfica, els més importants dels quals es troben citats a la present bibliografia. Tot i això, en un futur, es preveu fer ús dels mètodes d'anàlisi historiogràfica, fonamentalment el treball d'arxiu.

3. Resultats i discussió

A partir de l'anàlisi de *Quan érem refugiats* (1975), de Pàmies s'ha pogut constatar que l'obra que pertany a "la literatura del jo", presenta una relació problemàtica amb els vincles entre l'escriptura i la realitat, la ficció i la no-ficció, el passat i el present, o la memòria i l'oblit. És així perquè, l'autora opta per diversos recursos literaris per posar de manifest que l'obra té una referència a la realitat o, dit d'una altra manera, que és no-ficció. El primer recurs és la coincidència de nom entre l'autora que signa l'obra, la narradora i la protagonista. És el pacte autobiogràfic de Lejeune entre l'autor i el lector en què el primer promet al segon que explicarà la veritat i, el segon li atorga la seva confiança absoluta. El segon recurs és la introducció de retalls de premsa barcelonina del moment, així com dades històriques i noms propis, els quals serveixen per reforçar el pacte autobiogràfic, ja que, el lector, fàcilment interpreta que hi ha una correspondència amb la realitat.

Ara bé, el vincle transparent entre escriptura i realitat que apropa el relat al camp de la no-ficció passa a ser qüestionat quan s'analitzen altres factors que són inherents a la literatura del jo, com ara el temps i la memòria, els quals podrien semblar més propis de la ficció. Tots ells s'han analitzat a partir de les tesis de Ricoeur. Per una banda, el factor temporal fa trontollar la qüestió, ja que resulta evident que hi ha una diferència temporal entre els fets viscuts i els fets narrats, perquè els fets narrats són sempre posteriors als fets viscuts; i això fa replantejar que fets viscuts i fets narrats no siguin estrictament sinònims. Per altra banda, junt amb el factor temporal hi ha el paper de la memòria, lligada amb el record i l'oblit. S'observa que Pàmies no narra el fet, sinó el record del fet, que és allò que té a la ment i que és subjectiu.

4. Conclusions

En conclusió, es pot afirmar que, per totes aquestes característiques, Quan érem refugiats no es pot definir estrictament com a obra de ficció ni com a obra de no-ficció, sinó justament en la frontera entre aquests dos camps. És una obra narrada en primera persona en la qual hi ha una clara pretensió de correspondència verídica entre els fets de l'exili i l'escriptura d'aquests fets, però, al mateix temps, la distància temporal entre el moment viscut i el moment d'escriure fa impossible que aquesta correspondència sigui mai completa. Aquestes característiques s'observen perfectament en els diferents elements comentats de l'obra i són uns trets inherents a la literatura del jo, de la qual *Quan érem refugiats* n'és una mostra de primer ordre.

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CHALLENGES TO IMPROVE THE PSYCHOLOGICAL ATTENTION OF VIOLENCE AGAINST WOMEN

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Keywords: Feminism, gender studies, qualitative research, psychosocial intervention, violence against women

1. Introduction and objectives

The results presented here are part of a feminist psychosocial study in which we explore the variety of ways in which psychological knowledge and the gender perspective are combined and the resulting effects in professional practice in violence against women. The gender perspective is key in psychological intervention to prevent the effects of individualization of relational or social discomfort, especially in the field of male violence (Cabruja 2017; Ferrer-Pérez and Bosch-Fiol 2019); therefore, one of our specific objectives is to identify the difficulties recognized by the professionals themselves in specialized public services to incorporate the gender perspective into their work. We consider that, to improve the professional approach to gender-based violence, it is important to count with, among other agents, the contributions of front-line professionals.

2. Methodology

We combined feminist methodology (Mendía et al. 2014) and qualitative methodology in social psychology (Parker 2005). We conducted semi-structured interviews with professionals from different public services specialized in male violence in Catalonia, with different degrees of professional experience and professional training. The data obtained from the interviews were analysed following different procedures. Here, we present part of the results obtained from a thematic content analysis (Terry et al. 2017), which has allowed us to identify the difficulties recognized by the professionals themselves to improve their professional practice.

3. Results and discussion

We highlight four difficulties recognized by the professionals who participated in the study: (1) lack of gender perspective in professional training, (2) gender-blind practices by other professionals working in non-specialized public services, (3) precariousness of services and lack of resources, and (4) patriarchal sociopolitical context.

4. Conclusions

Based on these results, we propose the following challenges to improve the incorporation of the gender perspective in the professional practice in violence against women: to incorporate the gender perspective transversally in professional training, to detect and eradicate institutional violence, to increase public investment in specialized services, and to improve prevention and social awareness of male violence.

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HOMICIDIS MÚLTIPLES. LA MIRADA CINEMATOGRÀFICA SOBRE LA VIOLÈNCIA EXTREMA ESTATUNIDENCA (1989-2023)

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Paraules clau: cinema, cultura violenta, EUA, homicidi múltiple, post-guerra Freda

1. Introducció

El fenomen social i criminal dels homicidis múltiples (quatre víctimes mortals, o més, per cada cas) és una plaga que els EUA arrosseguen des de la seva fundació. Les pel·lícules sobre aquest fenomen poden oferir la visió que tenen els cineastes sobre aquest drama nacional, que trobaria les arrels en la cultura violenta i imperialista dels EUA. Es pretén saber fins a quin punt hi ha semblances i diferències entre allò que percep la societat, els cineastes, o els acadèmics sobre el fenomen. S'estudiarà, específicament, la mirada de les pel·lícules realitzades a partir de 1989, any en què va caure el Mur de Berlín, doncs es pretén veure com s'interpreten els homicidis múltiples estatunidencs en un món post-Guerra Freda. Els films analitzats tractaran els dos tipus d'homicidis múltiples: assassinats en sèrie i assassinats massius; però també episodis de tipologia més abstracta amb elements dels dos primers models.

2. Metodologia

L'autor del treball pretén visionar tres cops les pel·lícules: una primera vegada, sense prendre apunts per tal de fer-se una idea del que la filmació pot aportar; una segona vegada, prenent apunts, fixant-se en tants detalls com sigui possible; i una tercera vegada, per acabar de copsar elements que puguin haver passat per alt anteriorment.

3. Resultats i discussió

Alguns films reflecteixen molt bé la problemàtica i alguns no. Les pel·lícules de directors com Scorsese i els germans Coen són molt encertades, però les pel·lícules d'acció s'allunyen de la realitat social en benefici de l'entreteniment. En general, els films dels anys noranta són més realistes que els del segle XXI. Això és el que hom pot extreure quan analitza detingudament el discurs polític/ideològic, moral i, en alguns casos, pictòric, dels films, sigui de forma explícita o implícita.

4. Conclusions

Mentre que els films dels anys noranta es caracteritzen per ser una etapa buida de contingut ideològic, en la qual l'homicidi múltiple passa a ser un element més d'una societat que no pot optar a superar-se, a partir del segle XXI trobem un cinema més crític amb el sistema, que assenyala els factors que fan possible aquesta violència, emfatitzant la possibilitat de superar-los. La crítica al sistema no és només al model post-Guerra Freda, sinó que també fa una revisió del passat, fixant-se en episodis històrics com la Conquesta de l'Oest o la Crisi de 1973, cosa que demostraria la connivència entre la brutalitat extrema i el capitalisme més voraç.

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LEGAL AND SOCIAL PROHIBITION OF ABORTION IN CHILE: A PROPOSAL FOR STUDY AND AWARENESS

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Keywords: Sexual and reproductive rights, sexual trajectories, social representations

1. Introduction

The prohibition of abortion, besides inhibiting women from discussing it and having adequate support when experiencing it, generates a phenomenon in which hegemonic discourses (political, medical, legal and religious) contribute more to a dichotomization of positions than to a sensitization and openness to the variety of discourses of its direct protagonists: women (Green 2021).

The case of Chile is interesting, considering that between 1989 and 2017 it was one of the five countries in the world where abortion was considered illegal under all circumstances (Salas, Zegers and Figueroa 2016).

Based on the need to explore the diversity of experiences of women who abort in contexts of prohibition, this study aims to understand their social representations of abortion, based on the following research questions:

— What has the experience of aborting been like for women in prohibition contexts?
— What social representations about abortion do women have after experiencing it?
— What kinds of tensions and conflicts coexist in the experience of women who have aborted?
— What transformations of social representations of abortion occur after the experience?

2. Hypothesis

1. The legal penalization of abortion is considered a particular type of structural and gender violence (Segato 2021) that harms all women, but mainly poor and young women; in other words, it is intersectional violence.
2. The legalization of abortion contributes to the reduction of risks (physical and judicial) associated with abortion, but not necessarily to the reduction of risks related to social penalization.
3. Social penalization includes stigmatization, a high probability of experiencing the abortion experience in solitude, and experiencing varied feelings that have little chance of being shared with others.

3. Methodology

Based on critical social psychology, and specifically on the procedural approach of the theory of social representations (Moscovici 1969; Banch 1994), a qualitative and situated research will be carried out.

4. Discussion and conclusions

Considering I am in early phase of the investigation, this presentation aims to develop:

1. Share the most significant aspects of the theory of social representations that make it an appropriate theoretical and methodological tool for the study of a phenomenon of abortion in prohibition contexts.

2. Make visible and reflect on the importance of the dissemination of situated qualitative research with a gender perspective as a tool for social and political awareness.

I consider that situated research from a gender and intersectional perspective will promote awareness among the teams involved in support services.

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SESSION 5.
SDG6. CLEAN WATER AND SANITATION

EXPLORING SUSTAINABLE ALTERNATIVES FOR THE PREPARATION OF POLYMER INCLUSION MEMBRANES FOR METALS REMOVAL

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Keywords: Arsenic, cadmium, copper, polymer inclusion membranes, sustainability

1. Introduction and objectives

To enhance the sustainability of polymer inclusion membranes (PIMs), a shift towards utilizing more eco-friendly alternatives is mandatory.

Phthalates have been extensively used as plasticizers to improve mechanical and transport characteristics. However, growing concerns over their health and environmental impacts have prompted exploration of alternative options such as butyl stearate (BTS) for the manufacture of PIMs (Alcalde et al. 2024).

This study evaluates possible alternatives in PIM components to produce sustainable membranes, and also the possibility of producing PIMs while reducing the amount of reagents.

2. Hypothesis

The incorporation of eco-friendly materials and reducing reagent usage during membrane preparation will lead to the development of environmentally sustainable PIMs that are capable of removing toxic elements.

3. Methodology

PIMs were prepared by the solvent casting method. PIMs consisting of 50 per cent CTA/PVC/ 50 per cent Aliquat 336, 29 per cent CTA/ 27 per cent Aliquat 336/ 44 per cent NPOE, and 40 per cent CTA/ 30 per cent D2EHPA/ 30 TBP were investigated for the removal of As (Güell et al. 2011), Cd (Pont, Salvadó, and Fontàs 2008), and Cu, respectively, from aqueous samples. Experiments were conducted using a special device designed to contact the membrane with both the feed phase and the receiving phase, being 0.1M NaCl for As, ultrapure water for Cd, and 0.1 M HNO_3 for Cu. The use of eco-friendly polymers like poly(caprolactone) (PCL) and methacrylate derivatives, and the plasticizer BTS will be investigated.

4. Results and discussion

PIMs prepared with a reduced amount of reagents were successfully fabricated and tested for the removal of As and Cu. Two different amounts have been investigated, with a total mass of 0.4 g and 0.2 g, respectively. The findings indicated that using only half of the reagents resulted in successful membranes with no changes in the removal efficiency.

In the case of Cd, a successful PIM was prepared using half the amount of reagents compared to (Pont, Salvadó, and Fontàs 2008). Moreover, the membrane's reusability for Cd removal was demonstrated, with a consistent removal efficiency of approximately 46 per cent, indicating a sustainable approach to water treatment.

5. Conclusions

New PIMs prepared using reduced reagent amounts are capable of maintaining the removal of toxic metals efficiency. The demonstrated reusability of membranes for Cd removal underscores the sustainability of this approach to water treatment.

6. Bibliography

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WATER ACCESS IN THE AMAZON RIVER BASIN: REALITIES AND FUTURE CHALLENGES

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Keywords: Amazon River basin, barriers, water access

1. Introduction and objectives

The Amazon River basin, which covers an area of more than 6,000,000 km², produces about 20 per cent of the world's freshwater discharge and contains the greatest freshwater on Earth (Jézéquel et al. 2020). Ironically, access to potable water is limited in cities and rural Amazonian communities. While the reasons for this may vary according to location and socioeconomic conditions, the causes need to be investigated. Anthropogenic activities such as urbanization, deforestation and pollution, and population growth have caused the degradation of aquatic ecosystems and the alteration of the hydrological cycle (Martins et al. 2017; Posada-Marín and Salazar 2022). Meanwhile, climate change is generating stronger and more frequent droughts and floods in Amazonian cities (Ruiz-Vásquez et al. 2020).

The aim of the present study is to present the realities and future challenges of water access in the Amazon River Basin through a literature review.

2. Methodology

For this study, I propose to conduct a literature review of databases, government reports and information available on the web on water access in the Amazon River basin.

3. Results and discussion

The unavailability of drinking water may be due to geographical, environmental, technological, economic, and political barriers. Recently, however, two additional barriers have emerged – anthropogenic activities and climate change – that have the potential to continue to affect access to water in the Amazon River Basin.

The expected results are to determine the possible causes of the lack of access to water in the cities and rural communities of the Amazon River basin.

4. Conclusions

Water is an essential resource for human activities, ecosystems, and life in the Amazon River Basin. The lack of access to water in the Amazon could be due to the combination of barriers and characteristics of the area.

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SESSION 6.
SDG8. DECENT WORK AND ECONOMIC GROWTH

THE INSTITUTIONALIZATION OF EVALUATION AT THE LOCAL LEVEL BASED ON MULTILEVEL SOCIAL POLICIES

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Keywords: Evaluation, multilevel policy, local government, institutionalization, social policy

1. Introduction and objectives

Although there is no single mechanism that leads to the institutionalization of evaluation, the literature points to multilevel policies as one of the factors that can favour it, both in state and regional governments. The aim of the thesis is to study the potential of multilevel policies to favour the institutionalization of evaluation in local governments. It will focus on the social policy program contract of the Department of Social Rights of the Generalitat.

2. Hypothesis

The main hypothesis is that multilevel policies between local and regional governments are a favourable space for the institutionalization of evaluation. This implies that:

— The obligation to evaluate policies at the higher level encourages the evaluation of the policy at the local level.
— The resources that are put in place at the local level to evaluate the policy at a higher level facilitate the evaluation at the local level.
— Evaluation training linked to multilevel policies provides resources to evaluate at the local level.
— The local levels find a similar evaluation community that helps them increase their training.

As a result, the culture of evaluation is increased at the local level and evaluation is institutionalized.

3. Methodology

The research is carried out in two phases. The first phase comprises a general description of the programme contract, the local–regional government relationship and how the evaluation is conducted. This phase is carried out based on a qualitative methodology of interviews and documentary review. In the second phase, a case study will be conducted of several territories that participate in the programme contract files.

4. Results and discussion

In local government, participation in a multilevel policy in which an evaluation is proposed and means are put in place to carry it out should favour the institutionalization of the evaluation. This will be not only because of the obligation, but also because resources are provided from the regional government, such as evaluation training or the existence of a community of evaluation professionals. However, other determinants may work for or against the institutionalization of evaluation, as changes take place in the core programme or intervention department guidelines.

5. Conclusions

I expect to conclude that the multi-level policies between local and regional governments are a good tool with which to achieve local institutionalization of evaluation. Nevertheless, there is no unique way because, depending on the characteristics of the policy and the size of local government, among other factors, multi-level policy may favour or discourage evaluation at the local level.

SENSITIVITY IN TRANSITION: AN IN-DEPTH QUALITATIVE STUDY OF EXPATRIATED HIGHLY SENSITIVE MOTHERS

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Keywords: Adjustment, expatriation, motherhood, qualitative, sensory processing sensitivity

1. Introduction and objectives

The 2022 Interactive World Migration report by the International Organization for Migration (IOM) revealed that the number of global international migrants reached 281 million in 2020, having risen steadily over five decades due to increased global mobility.

Expatriation, living and working abroad present psychological, social and cultural challenges. Expatriate mothers confront additional hurdles in parenting within foreign cultures (Lopez-Zafra et al. 2019), managing childcare amidst language barriers and limited support networks (Saneka and de Witt 2019).

The COVID-19 context exacerbated challenges for expatriate mothers (Al-Thani 2021). While individual differences in reactions to overseas postings have been recognized (Smith and Fear 2014), sensory processing sensitivity (SPS) remains unexplored in expatriate motherhood.

SPS is marked by heightened sensitivity to stimuli and emotional responsiveness, affects human functioning and is a temperament trait that still needs further research in contexts such as expatriation. Highly sensitive people (HSPs) may react intensely to experiences, as per the Differential Susceptibility Model (Belsky and Pluess 2009).

Matrescence, which encompasses women's transition to motherhood, also remains underexplored in expatriation (McLeish et al. 2020). Therefore, the present exploratory study aims to analyse the transition to motherhood narrated by expatriate women with high scores in SPS.

2. Hypothesis

The gives visibility to motherhood in an expatriate context, especially for highly sensitive individuals.

3. Methodology

This qualitative study, grounded in Gadamer's hermeneutic philosophy, delves into interpretation and understanding in human experiences, particularly in text interpretation.

4. Results and discussion

The discourse analysis using Atlas.ti revealed key themes in the experiences of highly sensitive expatriate mothers. They faced heightened stress due to the uncertainties of expatriate life, exacerbated by gender inequalities and legal restrictions in some host countries. Despite challenges, support networks played a crucial role in mitigating stress. This underscores the need for targeted interventions to support expatriate mothers' well-being and resilience.

5. Conclusions

This study highlights the difficulties that highly sensitive expatriate mothers encounter and the ways of coping that seem to be influenced by the presence of this trait. This research sheds light on expatriate motherhood and the importance of closely examining possible variables that could promote the well-being of mothers in diverse cultural contexts.

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BENEFICIS ECLESIÀSTICS I SISTEMA CREDITICI A LA CATALUNYA D'ANTIC RÈGIM

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Universitat de Girona

Paraules clau: beneficis eclesiàstics, censals, crèdit, dotalicis, personat

1. Introducció i objectius

Els beneficis eclesiàstics eren una entitat jurídica que a través de les fundacions perpètues, obtenien una renda les quals eren cedides vitalíciament a clergues o sacerdots titulars d'un càrrec eclesiàstic que havien de complir unes determinades funcions de culte o pastoral. Els beneficis eclesiàstics eren una entitat jurídica que a través de les fundacions perpètues, obtenien una renda les quals eren cedides vitalíciament a clergues o sacerdots titulars d'un càrrec eclesiàstic que havien de complir unes determinades funcions de culte o pastoral .

Els beneficis complien una triple utilitat. Es va establir un lligam entre els beneficis i el crèdit a través dels censals.

— Constatar la importància clau de les misses de difunts des de: fundacions d'oficis i aniversaris fins a la constitució de beneficis /capellanies i causes pies.

— Estudiar l'articulació de les misses de difunts amb la institució del censal com a mecanisme d'extracció i de redistribució d'excedent**.**

— Analitzar els diferents sistemes de nomenaments dels beneficis i el complement indispensable: les causes pies.

— Estudiar les diferents maneres de nomenaments de beneficis i l'impacte econòmic que se'n deriva**.**

2. Metodologia

La lectura dels llibres ressenyats i d'altres buidatges de:
— Cens d'Aranda i Floridablanca.
— General i municipis dels corregiments de Girona, Talarn i Aran).
— Llibres mestres de censals, de comptes, de registres de rendes cobrades anualment i els pagaments realitzats als capellans. Extrets dels arxius corresponents.

3. Discussió

Els historiadors Salazar i Ferrer, van en una línia bastant semblant tot i que en un context diferent. J.M. Marquès fa una descripció molt clara de les diferents classes de beneficis, en concret i se centri en la figura del personat.

La meva aportació a la recerca aniria en funció de l'anàlisi i conclusions del sistema creditici, sent Girona, com a concreció i exemple i estès al Pallars i l'Aran. Per altra banda, consistiria en una aportació a nivell en l'àmbit cartogràfic.

4. Conclusions

Anirien projectades entorn de possibilitats ofertes per diverses fonts treballades per a l'estudi del paper de les institucions eclesiàstiques en el sistema creditici català.

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SESSION 7.
SDG9. *INDUSTRY, INNOVATION AND INFRASTRUCTURE*

PHOTOCATALYTIC OER ON SEMICONDUCTORS: MECHANISTIC INSIGHTS FROM DFT

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Keywords: Excited states in solids, OER mechanism, photocatalytic oxidations, pin-polarized DFT

1. Introduction and objectives

Heterogeneous photocatalysis has the potential to replace fossil fuels by clean and renewable H_2 fuel generated from solar energy, water and a cheap semiconductor- (SC) based photocatalysis (PC). The oxygen evolution reaction (OER) that occurs on the photoanode is the limiting step and predetermines the photocatalytic efficiency. Industrial utilization of photocatalysis is constrained by completely unclear composition-activity relationships. Our aim is to uncover the PC mechanism and the role of solid surfaces using quantum chemistry tools. Depending on the material and its physico-chemical properties, the mechanism of the water oxidation could be different. In this work we choose the experimentally studied and well-characterized set of vanadates, focusing on $BiVO_4$ as the most promising material (Yan et al. 2017, 114).

$$2\ H_2O \longrightarrow 4\ H^+ + 4\ e^- + O_2 \qquad \text{(OER)}$$

2. Methodology

Photon adsorption on the SC with the energy greater than band gap leads to the electron excitation from the valence to conduction band. This fact forces us to calculate highly expensive TD-DFT to compute the excited state. Contrary to this, our approach is based on switching the multiplicity to simulate excited states; for example, we used Triplet multiplicity to describe the first excited state. The relative error of using this method is less than 0.1 eV. We utilized periodic boundary condition calculations using VASP 5.4 code at PBE and HSE06 levels of theory to calculate intermediates and transition states. To examine the surface for the hydrophilicity, we performed preliminary simulations using molecular dynamics.

3. Results and discussion

Molecular dynamics simulation confirmed the hydrophilicity of the surface with an adsorption centre on the Bi atom and a distance of 2.4 Å (**A**, Figure 1). The complete OER consists of three proton-coupled electron Ttransfers (PCET) and requires three photons, which generates hole-electron pair, each increasing the multiplicity (**B**, **C**, **F**). At the same time, hydrogen reduction

leads to the h-e recombination (**D**). We successfully determined energy barriers utilizing a nudged elastic band approach, where the proton transfers to active oxygen atoms on the surface. Our findings revealed that, despite the theoretical expectation of four PCETs, in practice, only three photons are required to drive the reaction, which was observed in experiments (Mesa et al. 2020, 12).

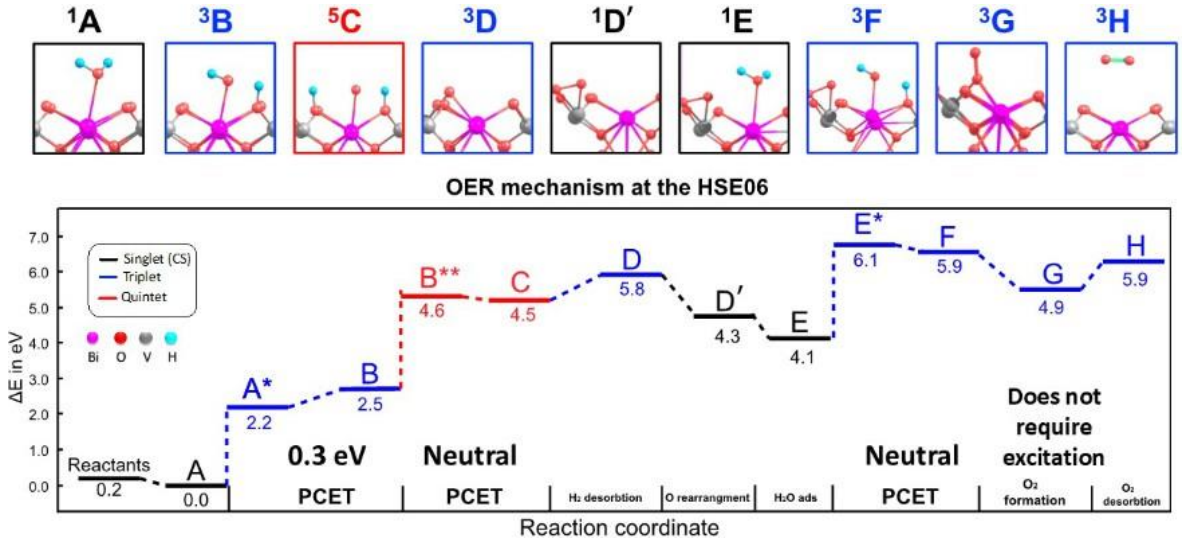

Figure 1. Oxygen evolution reaction mechanism on $BiVO_4$. Own elaboration.

4. Conclusions

Our insights into the OER mechanism revealed experimental findings that diverge from theoretical expectations. These insights propel advancements in photocatalysis, facilitating the development of more efficient and practical catalysts for sustainable energy production.

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REACTIVITY COMPARISON OF *SYN* AND *ANTI* OXO-IRON COMPLEXES OF TMC

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Keywords: DFT, hydrogen atom transfer, non-heme iron-oxo complexes, oxygen atom transfer, topological isomers

1. Introduction and objectives

Oxo-iron (IV) species play a fundamental role as intermediates in oxidation processes. Over the past few decades, extensive efforts have been made to characterize synthetic nonheme oxo-iron (IV) complexes, serving as analogs of nonheme iron oxygenases. The revelation of the crystal structure of anti-[FeIV(O)(TMC)(CH3CN)]2+ (TMC = Me4cyclam) was embarked upon two decades ago (Rohde et al. 2003). Substantial focus has been directed towards hydrogen-atom transfer (HAT) reactions (Morimoto et al. 2018). Nevertheless, scarce attention has been devoted to oxygen-atom transfer (OAT) reactions, despite the observation of olefin epoxidation in selected nonheme iron enzymes. In the present work, we have investigated the HAT and OAT by the anti and syn-isomers of [FeIV(O)(TMC)(CH3CN)]2+.

2. Methodology

All DFT calculations were performed with the Amsterdam Density Functional (ADF), and QUILD programs. Geometries optimization, energies of all possible spin states, gradients, Hessians (for vibrational frequencies), and UV-vi s spectra were calculated using B97-D3, (Grimme 2006), including solvation effects through the COSMO.

3. Results and discussion

Our DFT calculations indicate that the higher reactivity of TMC-*syn* could be partially explained by the higher accessibility of its Fe=O unit. Further, examination of the transition states for the OAT reactions shows that more factors are involved in the higher reactivity of TMC-*syn*. In the case of OAT (2-electron process) with TMC-*syn*, the Fe=O unit moves out of the plane defined by the equatorial nitrogen atoms of TMC and the axial CH_3CN dissociates from the Fe=O unit of TMC-*syn* in the transition state during OAT reactions, while it stays

bound within TMC-*anti*. Moreover, the acceptor orbital is found at lower energy with high-spin *S=2* than in *S=1*, which shows that high spin is favoured. These two effects allow us to propose a rationale for the outcome of the orientation of the Fe=O unit within the TMC ligand (*anti* or *syn*) on reactivity. HAT reactions are one-electron processes, which only involve the lower-lying d_{xy}(ß) orbital, and acetonitrile dissociation has only a limited effect on lowering of the orbital energy. Therefore, MeCN dissociation is limited, with relatively small effects on reaction rates for HAT (~1.3-3 times).

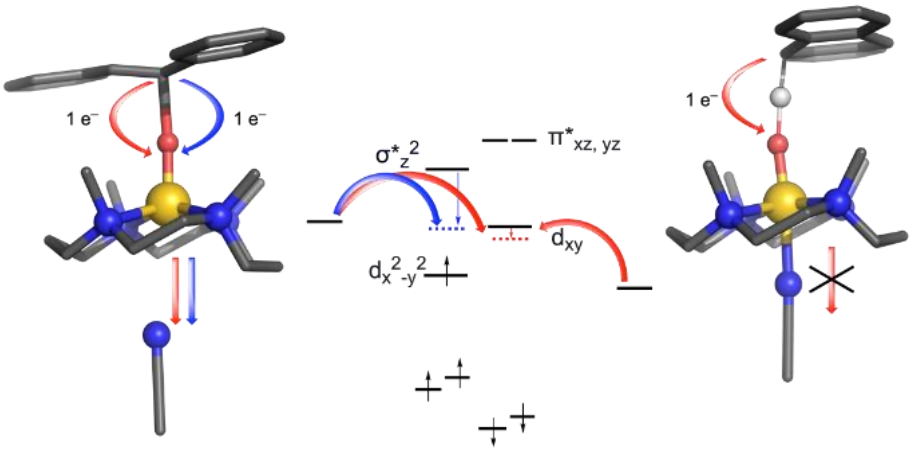

Figure 1. Rationalizing the different outcomes for the axial CH_3CN of TMC-*syn* (1-e HAT reaction with DHA (left) 2-e OAT reaction with *trans*-stilbene (right)

5. Conclusions

Our findings reveal remarkably high OAT rates for PhSMe oxidation (~850 times) by TMC-*syn* in comparison to its anti-counterpart. Only syn complex is capable of olefin epoxidation. Hence, ligand topology emerges as a pivotal factor influencing reactivity.

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THE ROLE OF PROTEIN CONFORMATIONAL DYNAMICS AND ELECTROSTATICS IN CONTROLLING THE CHEMOSELECTIVITY OF O- VS. N-METHYLTRANSFERASES

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Keywords: Computational modelling of biochemical systems, enzymes, molecular dynamics simulations, site-directed mutagenesis

1. Introduction and objectives

Traditional methylation methods in the chemical industry rely on toxic reagents, which has prompted research into eco-friendly strategies like enzymes. *S*-adenosylmethionine (SAM)-dependent methyltransferases (MTs) catalyse most methyl additions in living organisms. They are an ancient family of enzymes that has expanded and diverged over millions of years (Abdelraheem et al. 2022).

Ruta graveolens L. anthranilate nitrogen MT (*Rg*ANMT) and *Prunus persica* caffeate oxygen MT (*Pp*CaOMT) exhibit strong resemblances in sequence and structure due to their shared evolutionary lineage (Rohde et al. 2008), even though they show different chemoselectivity: *Rg*ANMT methylates nitrogen, while *Pp*CaOMT targets oxygen. Their biocatalytic mechanism is described by an S_N2 type of reaction; the substrate's reactive group is first recognized by a histidine, which facilitates the subsequent nucleophilic attack on SAM's methyl group.

When testing multiple variants from the exchange of three evolutionary non-conserved active site residues, our experimental collaborators observed a change in chemoselectivity. Through computational modelling, we aim to rationalize how chemoselectivity is controlled in O- versus N-MTs.

2. Methodology

We ran molecular dynamics (MD) simulations at the holo state for wild type *Rg*ANMT and *Pp*CaOMT, and the variants: 4N (*Rg*ANMT C272D N298E), 4O (*Pp*CaOMT D284C E311N), and 6N (*Rg*ANMT N298E R324Q). For each system, the resulting trajectories were processed with the principal component analysis technique to retrieve the most representative conformations. On each conformation, we employed the APBS software to analyse the active site electrostatic environment.

3. Results and discussion

By monitoring the distance between the catalytic histidine and SAM's methyl group along the obtained MD trajectories, kernel density estimate (KDE) plots showed substantial differences between the two wild type systems. *Pp*CaOMT's KDE plot disclosed two peaks, which we associated to open and closed conformations, whereas *Rg*ANMT's KDE plot depicted a single peak around the open conformation. These observations align to the different acid-base requirements for the N- or O-methylation. Contrary to their wild type, the *Rg*ANMT variants explored distances representative of the closed conformation, whereas the *Pp*CaOMT mutant shifted towards the open conformation.

The electrostatic analysis revealed a slight positively charged region within the active site of *Rg*ANMT and 4O. Conversely, we found a negatively-charged region around the catalytic histidine in *Pp*CaOMT, 4N, and 6N, which interacts directly with the positively charged SAM cofactor. These results suggest that the closed conformation is stabilized through electrostatic interactions.

4. Conclusions

Mutating only a few non-conserved active site residues changed the local electrostatic environment and subsequent conformational control, which directly impacted the enzyme's chemoselectivity. These findings help in the understanding of SAM-MTs and their rational design.

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COMPUTATIONAL EVALUATION OF HG3 KEMP ELIMINASES

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Keywords: Computational enzyme design, conformational dynamics, kemp elimination, molecular dynamics simulations

1. Introduction and objectives

Enzymes adopt multiple conformations in solution, facilitating adaptation to new functions (Tokuriki and Tawfik 2009). This flexibility contrasts with traits of efficiency and specificity, which are attributed to well-preorganized active site pockets. We computationally investigated HG3 series variants' evolutionary trajectory, evaluating hydrogen bonding and interactions, elucidating the role of Gln50 and Cys84 in oxyanion stabilization.

2. Hypothesis

Accurate elucidation of enzyme conformational dynamics through long-timescale MD simulations, coupled with correlation-based tools, will enable us to understand how active site and distal mutations introduced with experimental directed evolution achieve the high enhancements of catalytic activity. This knowledge will facilitate the computational design of more challenging enzymatic activities.

3. Methodology

Microsecond timescale MD simulations (2000 ns x 3 replicas) on HG series variants (HG3, HG3.7, and HG3.17) with transition state analogue 6NT, using AMBER 20 with amber99 force field (ff19SB).

4. Results and discussion

The high catalytic efficiency of HG3.17 has been evaluated by multiple experimental and computational techniques over the years (Blomberg et al. 2013; Otten et al. 2020). Despite the role of some of the suggested key mutations, namely Lys50Gln and Met84Cys, being unclear, evaluation was prompted via microsecond MD simulations. PCA analysis revealed conformational changes. We found that PC0 (x-axis) mostly describes a cis-to-trans isomerization of the peptide

bond of Gly83 and the mutation Met/Cys84 contained in the beta strand 3, whereas PC1 (y-axis) corresponds to reorganizations of the sidechain of Trp44 and Trp88.

5. Conclusions

The evaluation of the conformational dynamics of three Kemp eliminase variants within the HG3-to-HG3.17 evolutionary progression has revealed important differences in the flexibility, network of interactions and water content within the active site pockets.

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ELECTRON CORRELATION DIAGNOSTICS: A TOOL TO OPTIMIZE COMPUTATIONAL CHEMISTRY CALCULATIONS

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Keywords: Electron correlation, machine learning, quantum chemistry

1. Introduction and objectives

Quantum chemistry uses the laws of quantum mechanics to offer a theoretical explanation of the structure, properties and reactivity of a molecule. It makes it possible to understand a given chemical problem without the need to conduct an experiment, saving reactants and laboratory time. Unfortunately, we do not know how to solve quantum mechanical equations when more than one electron is involved, so none of the existing simulation methods is exact and we have to deal with the balance between their accuracy and computational cost. Density functional approximations (DFAs) are the most popular methods among the computational chemistry community. The problem with these methods, however, is that they fail to describe the part of the electron–electron interactions (known as nondynamic electron correlation). Such interactions are not universal, but appear in some systems that are difficult to detect a priori, leading to inaccurate predictions for these cases. In response, our objective is to introduce a nondynamic correlation diagnostic to detect the systems where a DFA calculation might not be accurate.

2. Methodology

Our approach leverages extensive datasets and machine learning computational techniques (specifically, support vector machine models) to develop a DFA-based diagnostic tool tailored for evaluating nondynamic electron correlation within molecules. As reference, we utilise a nondynamic correlation indicator used in a previous work (Ramos-Córdoba and Matito 2017; Ramos-Córdoba, Salvador and Matito 2016; Xu et al. 2024) tailored for wavefunction theory-(WFT) based methods, and employ a SVM model to learn which molecules can be labelled as containing nondynamical correlation, based on a quantity easily obtained from a DFA based calculation (the so-called Kohn-Sham orbital energies).

3. Results and discussion

Our diagnostic tool demonstrates robust performance, effectively distinguishing reliable results (molecules without the presence of nondynamic correlation) from those requiring

further scrutiny (molecules where nondynamic correlation is present and require larger computational effort). The agreement between WFT-based nondynamic correlation diagnostics (computationally more expensive than DFA-based methods) and our DFA based model reaches up to 98 per cent in an extensive dataset of 3165 molecules, which demonstrates the validity of detecting nondynamic electron correlation from a DFA calculation.

4. Conclusions

Our work addresses a crucial aspect of quantum chemistry by providing a practical solution for evaluating DFA-based computational results. With our method, researchers can confidently assess the accuracy of their computational findings, thus enhancing the validity of subsequent experimental investigations and optimising the computational time required for massive calculations in large datasets.

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PREDICTION OF ELECTRICAL DEMAND: THE CHALLENGE TO MANAGE FLEXIBILITY

Alex Segura

Universitat de Girona

Keywords: Demand forecasting, demand response, electricity systems, energy flexibility

1. Introduction and objectives

The increasing use of renewable energy sources, combined with increasing electricity demand, has highlighted the importance of energy flexibility management in electrical grids (Guchhait, Rekha, and Sarkar 2023). Energy flexibility is the ability for the grid operator to manage variations in demand or generation, which is essential in ensuring the stability and efficiency of the grid (Hussain, Lai, and Eicker 2023).

The objective of this paper is to investigate the performance of electricity forecasts in dealing with variations in demand and generation, evaluate the impact of these forecasts on the flexibility of the grid, and discuss the implications of using forecasts to manage energy flexibility.

2. Methodology

Accuracy of generation and demand forecasts is the cornerstone for the flexibility management since traded flexibility is measured as a variation from these forecasts. Thus, the main objectives include definition of requirements for forecasting algorithms, performance assessment of existing forecasting algorithms and adaptation of these algorithms to model and estimate flexibility from metering data (Li et al. 2021).

3. Results and discussion

The results of the study show that accurate electrical forecasts are important to manage energy flexibility because they allow grid operators to anticipate variations in demand and generation. The results ranged from 60 per cent to 95 per cent accuracy depending on the circumstances of the case study. On one hand, in cases with lower demand and irregular consumption patterns, such as household demand, the model achieved lower level of accuracy. On the other hand, in cases with higher demand and more stable consumption patterns, such as large industries or aggregations of customers, the model achieved higher level of accuracy (for example, Figure 1).

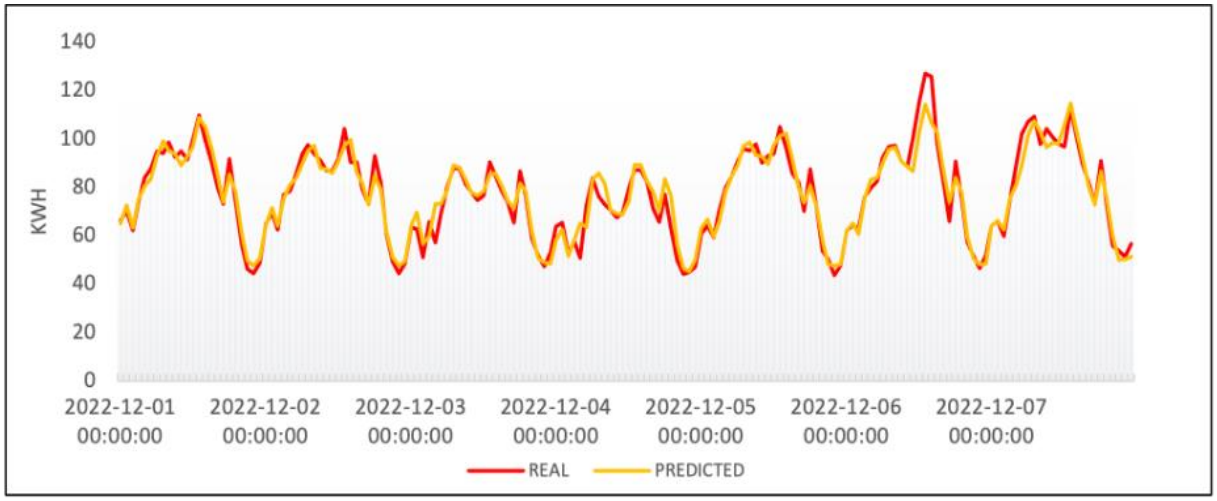

Figure 1. One week demand: Real vs Predicted

This study emphasizes how electricity forecasts can be used to optimize energy flexibility to reduce grid operation costs. Grid operators can use forecasting techniques to maximize the use of renewable energy and improve stability of the electrical grid. Furthermore, electricity forecasting helps demand response programmes by allowing users to adjust their energy consumption patterns in response to price signals and grid conditions, raising total grid flexibility.

4. Conclusions

Effective management of energy flexibility via electricity forecasting is essential for guaranteeing future reliability and sustainability of the grid. Grid operators can optimize resource allocation, improve grid stability, and support the incorporation of renewable energy sources by precisely forecasting variations in demand and generation. Continued advances in forecasting methodology will help grid operators adjust to the raising use of renewable energy sources and face the demands of a fast-changing climate.

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TOOL FOR PREDICTING MICROBIAL INACTIVATION DURING RADIOFREQUENCY HEATING

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Keywords: Decision support system, dielectric heating, food safety, inactivation kinetics, thermal processing

1. Introduction and objectives

Radiofrequency (RF) is a thermal processing technology that uses electromagnetic waves (frequency 1–300 MHz) for heating. RF technology offers significant benefits for large-scale food processing due to its ability to heat food materials more rapidly and evenly than traditional heating methods (Abea et al., 2023). RF is a potential alternative to conventional pasteurization and sterilization processes due to its higher energy efficiency and lower use of water.

2. Hypothesis

The purpose of this study was to develop a user-friendly decision support system prototype for assessing the inactivation of the relevant pathogenic bacteria using the predicted temperature profile of RF treatment.

3. Methodology

Physical properties (specific heat, density, dielectric constant and loss factor) were determined experimentally for a vegetable and fish pure (as model mixed food). For other food matrices, an extensive literature search was conducted. A simple one-dimensional model was applied, which assumes that the product and the electrodes are infinite slabs and the temperature profile is uniform across the sample volume (Abea et al. 2023). Since this microbial inactivation can also occur during the heating and cooling stages, the accumulated lethality and the number of log reductions were calculated for several relevant foodborne pathogens (with inactivation kinetics parameters from van Asselt and Zwietering (2006) using the predicted temperature profile.

4. Results and discussion

Physical properties of 75 distinct food matrices and inactivation parameters for 20 different microorganisms were obtained from the extensive literature search. The result of combining these two models, along with the databases, constituted the basis of a decision support system (DSS) tool (MS Excel). The simulations allowed determining the conditions (voltage, processing time, distance between electrodes, etc.) of the RF treatments for pasteurization and sterilization using the relevant reference pathogens selected. For example, for the pasteurization of the vegetable and fish puree, 15 min RF treatment achieved 6 log reduction of non-proteolytic *Clostridium botulinum*. On the other hand, 19.6 min were needed to sterilize the product (12 log reduction of proteolytic *C. botulinum*).

5. Conclusions

The tool can be used by food producers to design RF processes to inactivate microorganisms of concern, and to promote the use of this technology for having better energy efficiency and a more sustainable use of water resources, while complying with food safety standards.

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CELLULOSE NANOFIBERS AS VERSATILE ADDITIVES IN PAPERMAKING

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Keywords: Biobased additives, cationic cellulose nanofibers, papermaking

1. Introduction and objectives

Cellulose nanofibers (CNFs) are strong candidates in papermaking, namely anionic CNFs for improving paper strength and cationic CNFs to replace polymers employed as retention and drainage aids, such as cationic polyacrylamides (Aguado et al. 2017; Trache et al. 2020). Beyond promoting retention, these polyelectrolytes help in dewatering operations and are intended to obtain good sheet formation; however, they come from petroleum. This work proposes the production of CNFs and their application in papermaking of virgin pulp, constituting a sustainable-by-design alternative to commercial polyacrylamides. Their influences in papermaking and the characteristics of these papers were investigated.

2. Methodology

Anionic and cationic CNFs were produced from bleached kraft eucalyptus pulp (BKEP). For anionic CNFs (e_CNF), the pulp was subjected to an enzymatic treatment. Two different types of cationic CNFs (CCNFs) were produced, differing if the BKEP was treated or not in a mechanical refiner. In both cases, the pulps were mercerized and reacted with (3-Chloro-2-hydroxypropyl) trimethylammonium chloride. After treatment, pulps were subjected to a high-pressure homogenizer to generate the CNFs.

Paper was produced using BKEP. The e_CNFs were added at a 3 wt.%. Concentrations of 0.05, 0.10 and 0.25 wt.% of CCNFs were tested. The papers were characterized in terms of their breaking length (BL).

3. Results and discussion

The CCNF obtained after mechanical refining presented an anionic demand of 2000 μeq/g and a yield of nanofibrillation of >95 per cent, while for the unrefined fibre, the demand and the yield accounted for 1014 μeq/g and 30 per cent, respectively.

All paper compositions with e_CNF and CCNFs presented higher mechanical performance than the paper produced solely with BKEP. The best result was achieved with 0.25 per cent of the CCNF produced with the refined pulp, where an increase of 126 per cent of the BL was

attained. This value was higher than the BL achieved with the commercial polyacrylamide used during testing, which presented a 97 per cent increase in respect to neat paper.

4. Conclusions

It was possible to develop CCNFs with different surface charges and distinct characteristics based on the employment of a refinement treatment. These CCNFs, in conjunction with e_CNFs, drastically enhanced the mechanical properties of paper. The values obtained are comparable to or even higher than the commercial polyacrylamide, especially considering that amounts similar to the ones used in industry were applied. These results highlight the potential use of solely cellulose-based additives in the papermaking sector, contributing to a more sustainable process.

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SILVER NANOPARTICLE INCORPORATED CELLULOSE NANOFIBERS FOR SUSTAINABLE FOOD PACKAGING APPLICATION

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Keywords: Cellulose nanofiber (CNF), enzymatic hydrolysis, food packaging, silver nanoparticle (Ag NP), TEMPO mediated oxidation.

1. Introduction and objectives

The food packaging industry relies on single-use plastics, which poses significant environmental threats due to microplastic degradation (Dey et al. 2021). Paper emerges as an alternative, pending resolution of its barrier limitations (Mujtaba et al. 2022). This study focuses on developing eco-friendly food packaging to extend the shelf life of food. Coating paper with polyvinyl alcohol (PVA), alginate, and silver nanoparticle incorporated cellulose nanofibers (CNFs) enhance barrier and antimicrobial properties. Coated paper shows antibacterial activity against *Escherichia coli* and *Bacillus subtilis* due to Ag NPs. It also exhibits improved air and water vapor resistance compared to uncoated paper. Grease resistance rises to a KIT value of 9 post-coating. Overall, coated paper can be used as an active food packaging material.

2. Methodology

Ag NPs were synthesized using green reagents. Cellulose nanofibers (CNF) were derived from bleached kraft eucalyptus pulp (BKEP) via TEMPO-mediated oxidation and enzymatic hydrolysis. Ag NPs were incorporated into CNF via blending and in-situ synthesis methods. The liner is coated with a layer of PVA, alginate and Ag NP incorporated CNF. Ag NPs size and stability were measured using dynamic light scattering (DLS) experiment and surface resonance methodology. XRD analysis confirmed Ag (0) formation, while UV-Vis spectroscopy revealed the Ag NP formation through surface plasmon resonance (SPR) bands. CNF's cationic demand was determined using Mutek PCD. Antibacterial activity was tested against *B. subtilis* and *E. coli*. Air permeability was evaluated using Gurley and grease resistance was determined with a castor oil, heptane, and toluene mixture.

3. Results and discussion

The formation of Ag NPs was confirmed by SPR band around 400–500 nm range by the UV-Vis spectroscopy. Using DLS, the size of the NPs was found to be 8 nm and 54 nm. The thickness and the grammage of the coated papers were found to be similar, indicating that the applied coating was homogeneous. The value of water vapor transmission rate and air permeability decreased showing its improved resistance when compared with the uncoated papers. The value of grease resistance increased from a value of 1 to 9 after coating it with the formulation. The coated paper showed antibacterial activity against both bacteria.

4. Conclusions

The coated paper showed improved barrier properties and antimicrobial activity compared to the uncoated paper. Thus, the synthesized formulation can be used to enhance the limitation of paper and can be used as a sustainable and environmentally friendly food packaging material.

5. Bibliography

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SESSION 8.
SDG10. REDUCED INEQUALITIES

IMPACT OF THE COVID-19 PANDEMIC ON THE CATALONIAN POPULATION'S HEALTH, VULNERABILITY AND SOCIAL INQUALITIES

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Keywords: Bayesian, COVID-19, health, spatiotemporal

1. Introduction and objectives

The COVID-19 pandemic extended existing social inequalities. Difficulties in access to health care during the pandemic had effects on disease diagnosing and monitoring, leading to a worsened health status, especially among vulnerable populations.

The available research on the topic focuses on ecological studies, some with methodological shortcomings implying uncertainty on the validity of the findings (Barceló 2021). Epidemiological designs based on longitudinal data of individuals are needed to provide robust findings alongside appropriate methodological tools.

The main objectives of the present study are to characterize the socioeconomic inequalities during the pandemic and its effect on the health of the population, especially the most vulnerable, and to implement spatiotemporal modelling algorithms in real-world data (RWD) of high volume.

2. Methodology

A retrospective, observational cohort study was conducted, including routinely collected data from January 2015 to June 2021 for all individuals in the information system SIDIAP, the largest public primary care database in Catalonia covering >80 per cent of the population, a database of which a content report has been documented (Recalde 2022). Key clinical markers were selected for the study. We performed univariate repeated measurements analysis on individuals who had at least one assessment of each marker in both the pre-pandemic (January 2015 to March 2020) and pandemic periods and focused on those diagnosed with type 2 diabetes mellitus (T2D), high blood pressure (HBP), and heart failure (HF).

A Bayesian approach using INLA's spatiotemporal modelling algorithm (Rue 2009) implementing space-time non-separability COVID-19 spread was applied. Non-separability has been an often-omitted assumption about COVID-19 spreading and impact in the spatiotemporal community.

3. Results and discussion

Our analysis finds clinical markers that deteriorated during the pandemic, particularly in cardiometabolic factors of vulnerable population. This underscores the importance of continuous primary care for individuals with chronic conditions.

4. Conclusions

Preliminary findings uphold the hypothesis of impacts in diseases like coronary risk and diabetes as a distinctive result from social status during the pandemic. A broad overview of social and risk factor must be considered to address health prevention and care.

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YOUTH VOICES IN COMMUNITY PARTICIPATION

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Keywords: Community, participation, public policy, social change, youth

1. Introduction and objectives

The aim of my PhD is to explore the meanings and implications surrounding young people's community involvement and how their active participation can lead to transformative social change. My first article addresses young people's perceptions of their own engagement and the community concept, with the goal of offering suggestions to enhance community engagement based on their voices.

Youth seems to be more of a process than a state itself, as young people act as standby citizens rather than full citizens (Bečević and Andersson 2022). Ord et al. (2022) highlighted how practices and policies related to youth work and youth participation do not take the meanings and feelings of youth into account. In that case, it is no wonder that youth participation is becoming more informal, spontaneous and sporadic, increasingly separate from institutions, and growing with and next to the virtual world and social media (Ballesté et al. 2021).

2. Methodology

For the study, we employed qualitative methods in two communities in Catalonia: a small town with 5,000 inhabitants and a neighbourhood in a larger city with 100,000 inhabitants. Data were collected from over 40 young individuals through interviews, life stories and focus groups.

3. Results and Discussion

The results and discussion highlight three main themes. Firstly, many young people feel a loss of belonging to their communities in the last years due to a dismantling of community networks, which has to feelings of insecurity and detachment in public spaces. The lack of recognition among those who live in the same community generates distrust among its members (De Marinis 2010).

Secondly, young people express feeling ignored, criminalized and stigmatized by adults in an adult-centric society (Duarte 2012) they neither like nor trust. Their participation can be seen as a demand for a more inclusive and balanced space.

Lastly, although young people view participation positively, it is often tied to personal and social circumstances. Consequently, inequalities persist regarding how these people engage,

reflecting broader societal disparities. Policies addressing the transition to adulthood must consider these inequalities.

4. Conclusions

Reclaiming public spaces is crucial for community building and fostering connections among people. Political institutions must reflect on and adapt their practices to regain people's trust in democracies. Young people demand not only improved social and material conditions but also understanding and recognition of their perspectives.

5. Bibliography

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DEMOCRATIC HEALTH IN THE 18 CAPITALS OF SPAIN'S AUTONOMOUS COMMUNITIES

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Keywords: Capitals, citizenship, democracy, participation

1. Introduction and objectives

The economic, social and political crisis of 2008 was an abyss and a disregard. Citizens were supposed to be present in public decision-making. This is exactly what ended up happening.

In the Spanish context, public administrations, especially city councils, are going to have to adapt to the new era of digital citizen participation. And the capitals of the autonomous communities will be no exception.

The general objective of this study is to analyse the situation of participatory democracy in the 18 capitals of the autonomous communities of Spain, from 2016 to 2023, through a sampling process. The specific aims of the process are twofold: to study tripartite participatory processes based on the three most common means of citizen participation, and to identify new possible methodologies to reduce weaknesses.

2. Methodology

To achieve the study's objective, the main source of research is the spaces for citizen participation (mostly platforms). Given resource and time limitations, we want to carry out a more detailed analysis of the municipalities that meet the following three criteria: having a citizen platform, an active digital space for participation, homogenisation of the platforms, and having carried out more than 10 participatory processes. For the eight municipalities that meet these criteria, we intend to conduct an analysis of a more detailed participatory sample using the following items: the lack of transparency, the low incidence of citizenship, and the low rate of participation. Also, in order to compare the obtained results, we plan to conduct interviews with representatives of each of these eight municipalities responsible for citizen participation.

3. Results and discussion

There is currently no shared definition of the participatory process. For example, Brugué (2017) considered that deliberation holds the key, while García and Jiménez (2018) argued that the objective is to expand opportunities for citizens to influence public decision-making.

For the present paper, participatory processes are considered to be a mechanism for involving citizens, both with deliberative and/or direct democracy, in order to incorporate their voice in public decision-making. This thesis is based on this theoretical definition. This thesis is at an early stage. However, it is expected that once the three aforementioned weaknesses have been identified, city councils will have implemented public policies to minimize them.

4. Conclusions

Capitals have done a lot of work on citizen participation issues, but there is still work to be done to maintain and improve collective intelligence.

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URBAN ENVIRONMENT AND HEALTH: DETERMINANTS IN SELF-PERCEIVED HEALTH ON A MEDIUM-SIZED CITY

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Keywords: Health, inequality, mixed methods, sociology, urban health

1. Introduction and objectives

The main objective was to explore the factors that determine the inequality in self-perceived health among different districts. The secondary objectives were to investigate the significance of urban typology in health-related issues and the perception and effect of the current situation on diverse population groups.

2. Methodology

The study employed mixed methods (Creswell and Plano 2011), utilizing grounded theory for the qualitative analysis (Oktay, 2012). It aims to understand how urban environments influence residents' health perceptions. The quantitative part aims to understand the urban environment. The following dimensions were considered: (1) Patient saturation (WHO 2015); (2) socioeconomic indicators; (3) health indicators (data obtained from the regional health service were analysed to obtain insights into healthcare utilization patterns); (4) built environment and urban indicators.

3. Results and discussion

In terms of gender factors, females tend to describe their health as worse than their male counterparts. Regarding age factors, youth showed a noticeably worse approach to their self-perceived health, with one-third claiming to have been involved self-harm.

The environmental impact can be divided into three categories. First, regarding physical health, there was an increased risk of chronic diseases (cardiovascular diseases, diabetes) due to limited physical activity opportunities. Regarding mental health, we found elevated stress levels due to the absence of nature-based stress reduction, and also higher rates of mental health disorders (anxiety) without access to green spaces. Finally, the social consequences included reduced social interaction and community engagement, as well as a decreased sense of belonging.

The urban environment is critical in self-perceived health. Gender has a significant effect on the matter. Young respondents show greater concern for current issues (Sallis et al. 2009). They also show more negative viewpoints and higher rates of mental health issues and worse self-perceived health than older individuals.

5. Conclusions

The alarming decline in youth mental health necessitates immediate action. Implementing preventive policies, promoting education and awareness, and establishing accessible support services are critical steps. Improving urban settings and offering better infrastructure will help to ease the current situation. By addressing the current crisis, we can contribute to a brighter and healthier future for young individuals and society as a whole.

6. Bibliography

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SESSION 9.
SDG12. RESPONSIBLE CONSUMPTION AND PRODUCTION

SELECTIVE TRANSITION-METAL-CATALIZED CYCLIZATION REACTIONS INVOLVING 1,6-ALLENYNES

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Keywords: 1,6-allenynes, cascade reaction, cyclization, diels-Alder cycloaddition, rhodium

1. Introduction and objectives

Transition-metal-catalysed cyclizations have garnered significant attention in contemporary synthetic organic chemistry due to their ability to facilitate the simultaneous formation of multiple bonds and/or stereogenic centres in a single step, achieving perfect atom economy (Tanaka 2013). The versatility offered by incorporating allenes in these processes resulting from their unique unsaturation pattern opens up a broad spectrum of opportunities for generating novel cyclic compounds (Pla-Quintana, Roglans et al. 2016; Pla-Quintana, Roglans et al. 2022; Bellemin-Laponnaz, Roglans et al. 2023). In this project, our focus is on investigating the rhodium-catalysed cyclization cascade reaction involving 1,6-allenynes and maleimide derivatives to afford polycyclic *N*-based heterocycles in a straightforward and efficient manner.

2. Hypothesis

We anticipate that by controlling the transition-metal catalytic system, the reaction conditions used and the structure of the starting polytopic unsaturated compounds, exceptional selectivity in cyclisation transformations will be achieved.

3. Methodology

Starting materials that are not commercially available were synthesized and fully characterized by the usual spectroscopic techniques (IR, NMR, MS). Catalytic reactions were optimized by testing different rhodium catalysts, additives, solvents, and temperatures.

4. Results and discussion

Firstly, different 1,6-allenynes and maleimides derivatives were synthesized following an intensive literature review to find the optimal synthetic pathways to achieve them. In order to study the Rh-catalysed cyclization reaction of 1,6-allenynes **1** and maleimides **2** (Scheme 1), different catalytic systems were used, taking into account that the operative pathway is greatly influenced by the coordination ability and the steric parameters of the catalyst as well as the reactive unsaturations. Therefore, 1,6-allenynes **1** react with maleimide derivatives **2** using $[Rh(COD)Cl]_2$ and bis[(2-diphenylphosphino)phenyl] ether (DPEphos) as a catalytic system in *o*-dichlorobenzene (*o*-DCB) at 150 ºC to afford polycyclic derivatives **3** in good yields (Scheme

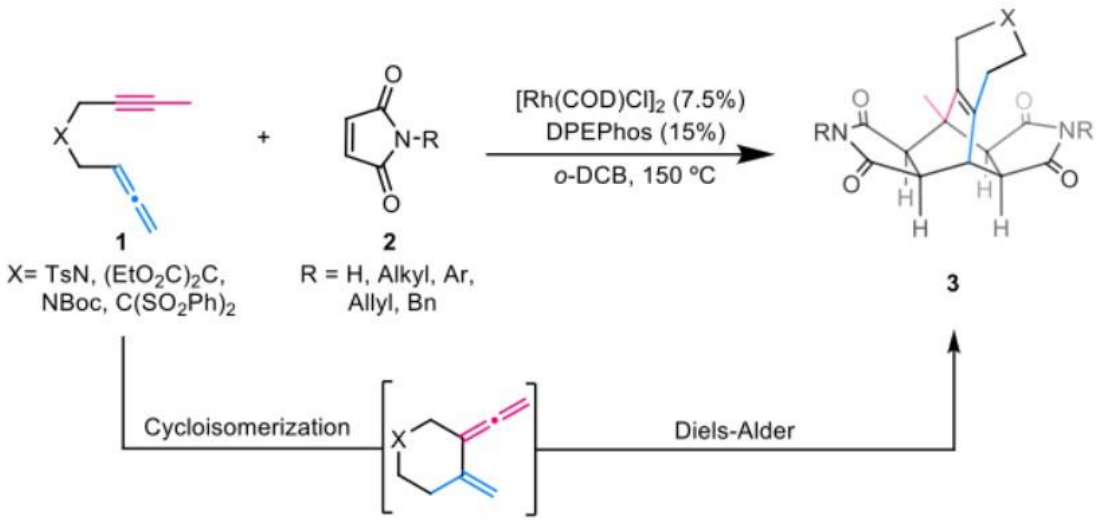

Figure 1. Reaction between maleimide and allenyne derivatives

1). After determining the most favourable conditions for this process, the scope was studied varying not only the dienophile nature (maleimide derivatives), but also the allenyne motif.

Furthermore, experimental mechanistic studies were conducted to gain insights into the reaction and formulate a catalytic cycle for the new cyclization cascade reaction, which encompasses a Rh-catalyzed cycloisomerization of 1,6-allenynes and two consecutive Diels-Alder cycloaddition.

5. Conclusions

We have developed a new method to synthesize polycyclic derivatives **3** via a cascade reaction of Rh-catalyzed cycloisomerization followed by a Diels-Alder process. This transition metal-catalyzed cascade reaction provides a versatile and step-economical approach to the synthesis of bicyclo[2.2.2]oct-7-ene derivatives.

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EFFECT OF LPS-BINDING PEPTIDES ON BACTERICIDAL ACTIVITY AGAINST *Xylella fastidiosa*

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Keywords: Bactericidal activity, functional peptides, LPS-peptide neutralization, *Xylella fastidiosa*

1. Introduction and objectives

Xylella fastidiosa, a xylem-limited gram-negative plant pathogen, causes various diseases in economically important plants. Since it was detected in Italy in 2013, *X. fastidiosa* has spread across Europe (Baker et al. 2015). Effective strategies to regulate both the disease and its causative agent are needed because the only viable options are the eradication of infected material and vector management (Food and Agriculture Organization of the United Nations 2019). Given the relevance of vulnerable crops in the Iberian Peninsula, finding new control methods is imperative.

Antimicrobial peptides (AMPs) are promising candidates for this task due to their bactericidal activity and biofilm inhibition against *X. fastidiosa* (Moll et al. 2021). AMPs can also neutralize lipopolysaccharides (LPS) present in bacterial membranes, a key virulence factor of this bacterium (Skovbakke and Franzyk 2017).

The present study was centred on the development of a method to identify AMPs able to bind to LPS of *X. fastidiosa*. Several AMPs were identified and a relationship was found between LPS neutralization and bactericidal activity against *X. fastidiosa*.

2. Methodology

Peptides were synthesized on solid phase, using a Fmoc/*t*Bu strategy, purified, analysed by HPLC, and characterized by ESI-MS. LPS were extracted from *X. fastidiosa* and evaluated by electrophoresis in Tricine gel. LPS-peptide neutralization assays were tuned up and performed with the commercial Pierce Chromogenic Endotoxin Quant Kit with LPS extracted from *X. fastidiosa* and *E. coli*. Bactericidal activity of peptides was assessed by contact test coupled with v-qPCR. Their hemolysis and effect on tobacco leaves were also analysed.

3. Results and discussion

The capacity of peptides to bind LPS from *E. coli* was first tested using a commercially available kit. Then, LPS from *X. fastidiosa* was extracted and used in this assay. Similar results were obtained from both experiments. Later, the LPS-binding capacity of peptides was determined using the commercial kit. A dose-response assay was carried out with peptides with a higher bactericidal activity. A linear correlation was observed between bactericidal activity and LPS interaction.

4. Conclusions

A method to find peptides that bind LPS of *X. fastidiosa* has been developed and a relationship between bactericidal activity and LPS-peptide interaction has been observed.

5. Bibliography

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PEPTIDES AS A TOOL TO REDUCE THE MOTILITY OF THE PLANT PATHOGENIC BACTERIUM *XYLELLA FASTIDIOSA*

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Keywords: Motility, peptides, pili IV, twitching, *Xylella fastidiosa*

1. Introduction and objectives

Xylella fastidiosa (Xf) is a gram-negative plant pathogenic bacterium that has a wide range of hosts worldwide, including important Mediterranean agricultural crops, such as almond, grapevine, olive, and citrus, making it an important concern in Europe. Xf is a xylem-limited bacterium transmitted by insect vectors (Moll et al. 2021). Its virulence depends on its capacity to form biofilm, which causes the obstruction of the plant vessels, and on its motility, which allows the movement between and within the xylem vessels. Xf lacks flagella, but it has type IV pili, which by their extension, surface attachment and retraction allow the twitching motility of Xf throughout the plant (D'attoma et al. 2020).

The main objective of this research is to identify peptides that are able to affect the motility of Xf.

2. Hypothesis

Previously studies have found that calcium or BSA affect the motility of Xf. Therefore, the hypothesis of this research is that peptides could also affect the motility of this bacterium.

3. Methodology

A total of 17 peptides were selected to assess their effect on the motility of Xf. Their bactericidal activity against Xf was evaluated using the viability-quantitative PCR (v-qPCR) method (Baró et al. 2020) to avoid its interference in the motility experiment.

Motility experiments consisted of spotting Xf in modified Perwinkle Wilt (PW) media (1 per cent agar, no BSA), and water or the peptide was included. Plates were incubated for four days and colony fringe, indicative of twitching motility, was measured in an inverted microscope. First, the motility of six Xf strains was determined and the strain with the largest fringe was then used for peptide screening.

4. Results and discussion

Peptide concentration for the motility assay was set at 12.5 uM. We considered that, at this concentration, the bactericidal activity of the peptide would not interfere in the motility experiment. The strain Temecula L was selected for peptide screening since it was the one that showed the largest fringe and optimal incubation time was set to three days. Out of the 17 tested peptides, four showed a great effect on Temecula L's motility. Their mechanism of action will be elucidated in the future.

5. Conclusions

In conclusion, this study has made it possible to set the conditions to determine the effect of peptides on the motility of Xf. Four peptides have been found to affect motility and will be studied in detail in the future.

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7. Acknowledgements

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NANOFIBER BOOST: ENHANCING CELLULOSE ACETATE MEMBRANE PERFORMANCE

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Keywords: Cellulose acetate, cellulose nanofiber, lectrospinning, membranes, Oxalic acid

1. Introduction and objectives

Membranes play a crucial role in various industries, such as water treatment, energy production, and biomedical applications (Abdellah Ali et al. 2020). The current focus in membrane development is on utilizing biobased polymers to enhance performance for environmentally friendly solutions, improved efficiency, and superior product quality. This research focuses on employing cellulose acetate (CA) as the main component for membrane development. Strengthening involves the incorporation of cellulose nanofibers (CNF) produced through oxalic acid pretreatment (Oxalic-CNF). The uniqueness lies in integrating Oxalic-CNFs into electrospun membranes, boosting mechanical strength for high-load applications and enhancing functionalization capabilities.

2. Methodology

CA membranes with Oxalic-CNFs loadings ranging from 0 to 18 wt% were obtained by electrospinning using a ternary solvent system and thoroughly characterized to determine their physical properties and rheological behaviour. The structural and morphological properties of the membranes reinforced with Oxalic-CNFs were characterized using SEM (scanning electron microscopy). Thermoplastic behaviour of the membranes was confirmed by printing a mould on the film via hot compression, and mechanical properties were also evaluated. The presence of Oxalic-CNFs was verified by Fourier transform infrared spectroscopy (FTIR) and fluorescence.

3. Results and discussion

Oxalic-CNFs were successfully integrated into cellulose acetate membranes, resulting in significant enhancements in mechanical strength. This improvement involved substituting a portion of the ternary solvent system with an Oxalic-CNF solution. Across concentrations

ranging from 0.2 to 6 wt%, the addition of Oxalic-CNF led to a remarkable 383 per cent increase in tensile strength, attributed to a higher content fostering increased inter-fibre bonds and surface area. Oxalic-CNFs exhibited uniform distribution, promoting molecular-level contact during drying, effectively filling pores for improved interfacial compatibility. FTIR spectra confirmed the presence of Oxalic-CNFs, while exposure to UV light revealed a red colour, indicating a chemical reaction with $EuCl_3$ and demonstrating their incorporation into CA membranes.

4. Conclusions

This study makes a significant contribution to the field of high-tech materials by introducing Oxalic-CNFs into AC membranes. These Oxalic-CNFs not only improve mechanical properties but also offer accessible carboxylate groups. The findings highlight the potential of functionalizing these Oxalic-CNFs, transforming them into an attractive system with numerous potential applications. Furthermore, the membranes' immersion in $EuCl_3$ solution, and subsequent observation under ultraviolet light revealing the appearance of a red colour, indicates the accessibility of Oxalic-CNFs, catalysing the opportunity to functionalize these membranes and provide them with unique characteristics.

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MECHANISM OF ACTION OF ANTIMICROBIAL PEPTIDE BP100

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Keywords: Antimicrobial peptides, bacterial membranes, carpet mechanism, molecular dynamics, *Xylella fastidiosa*

1. Introduction and objectives

Despite significant advances in agricultural technology, global hunger remains a pressing concern, extenuated by the emergence of plant pathogens such as *Xylella fastidiosa*. First detected in Europe in 2013 (Trkulja et al. 2022), this bacterium has spread rapidly and is a serious threat to Mediterranean crops. Existing control measures have limitations and it is necessary to develop efficient strategies (Moll et al. 2021). Antimicrobial peptides are providing promising results. In particular, **BP100** has shown remarkable activity against *X. fastidiosa*, disrupting bacterial motility while causing minimal damage to the plant (Badosa et al. 2007 and Moll, L. Unpublished data). **BP100** acts through a carpet-like mechanism, where peptide binding to the outer monolayer surface induces membrane permeabilization and subsequent cell membrane rupture (Strandberg et al. 2023). The present study aims to elucidate the mechanism of action of **BP100** on membrane models of *X. fastidiosa* by atomistic molecular dynamic (MD) simulations.

2. Hypothesis

It has been hypothesized that **BP100** affects *X. fastidiosa* by disrupting bacterial membrane integrity through a carpet mechanism, leading to membrane permeabilization and subsequent cell membrane rupture.

3. Methodology

Model membranes were constructed using the Membrane Builder function of Charmm-gui, generating both pure-lipid anionic and zwitterionic membranes, as well as mixed-lipid membranes resembling those found in *X. fastidiosa*. MD simulations of the BP100-membrane systems were performed using Amber under constant pressure conditions at 323,15 K. Each MD simulation spanned 1 microsecond. Output data were analysed using Suave to assess the peptide's impact on membrane parameters such as area per lipid, bilayer thickness, surface curvature angle, and partial density profile of chemical groups. Additionally, Gaussian

molecular dynamics simulations were employed to accelerate conformational sampling of biomolecules by applying a boost potential to smooth the system's potential energy surface, thus enabling a more comprehensive analysis of the peptide's effects.

4. Results and discussion

The results showed that the peptide initially interacts with the membrane through electrostatic interactions. The peptide then flips and inserts its hydrophobic residues into the membrane, causing its destabilization. To clarify the specific mechanisms and its implications for membrane function, further analysis and simulations are being performed and will be discussed.

5. Conclusions

This research reveals molecular insights into the potential of the antimicrobial peptide **BP100** to control *X. fastidiosa*. Further investigations are necessary to fully understand the implications of these interactions and optimize peptide-based solutions for sustainable agricultural practices.

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SESSION 10.
SDG13. CLIMATE ACTION

ANALYSING A *CLOSTRIDIUM CARBOXIDIVORANS* AND *C. ACETOBUTYLICUM* CO-CULTURE: FROM ACID AND ALCOHOL PRODUCTION TO GENE EXPRESSION

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Keywords: *Clostridium* spp., co-cultures, Fermentation, gene expression, quantitative PCR

1. Introduction and objectives

Implementing synthetic co-cultures of *Clostridium* with different physiological properties has emerged as a solution to improve production rates and expand the product spectrum compared to single cultures, mainly to produce solvents from lignocellulosic feedstock or from CO_2/H_2 (Cui et al. 2021, 914–926). In this study, we investigated the performance of a co-culture comprising Clostridium carboxidivorans and Clostridium acetobutylicum grown on glucose as the sole carbon source, with the aim of producing acids and alcohols by monitoring the growth of both species, their production capacities, and the expression levels of some genes of interest.

2. Methodology

Fermentation was performed in a 5 L bioreactor with 2.5 L of working volume at a constant pH of 5.8. A synthetic medium amended with 5 g/L of glucose was used. The two species were inoculated at a 10 per cent (v/v), maintaining similar proportions. Co-culture fermentation was run in triplicate, and growth (OD_{600} and DNA extraction for quantitative PCR) and productions (acids, alcohols, gases) were monitored. Besides, total RNA was extracted to analyse gene expression using reverse transcriptase quantitative PCR (RT-qPCR) with newly designed primer pairs.

3. Results and discussion

Co-culture of *C. acetobutylicum* and *C. carboxidivorans* showed a high acetate, butyrate, and ethanol production (3, 0.8 and 0.5 g/L, respectively). Both species grew rapidly during the first 24 hours and occurred concomitantly to glucose depletion. After this initial growth, *C. carboxidivorans* continued growing due to its ability to uptake CO_2 as a carbon source. This could be confirmed after gene expression analysis since a high expression of *CODH/acs* gene

(carbon monoxide dehydrogenase/acetyl-CoA synthase) was observed. This gene is involved in the conversion of CO_2 into acetyl-CoA and is found exclusively in *C. carboxidovorans*. Genes leading to the acid production (*ack* and *buk*) were highly expressed during the exponential phase, whereas alcohol production genes (*adhE* and *bdh*) were expressed after 24 hours of growth for both species, indicating that cells shifted into solventogenesis at the early stationary phase.

4. Conclusions

When co-cultured, *C. carboxidivorans* and *C. acetobutylicum* grew rapidly in an acidogenesis phase. The involvement of both species in the production of acetate and butyrate was corroborated by the elevated *ack* and *buk* gene expression. On the other hand, *adhE* and *bdh* related to solvent production were overexpressed after 24 hours of inoculation. The two species seem to act similarly during the experiment, suggesting that no clear co-metabolic relationship between them could be established at the analysed conditions.

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TOWARDS THE PREPARATION OF BIOINSPIRED IRON(IV)-OXO COMPLEXES

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Keywords: Bioinspired chemistry, inorganic chemistry, iron, metal-oxo, oxidation

1. Introduction and objectives

High-valent iron-oxo species are the key intermediates in biological oxidation reactions and intense research has been conducted to mimic these natural transformations. Taurine dioxygenase, for instance, catalyses the hydroxylation of an alkyl C–H bond mediated by a high-valent iron(IV)-oxo compound (Barr 2003, 7497). This species presents a S=2 spin state, which is difficult to achieve through small-molecule model systems. One strategy to reproduce the high spin state of this species is the design of ligands that enforce a trigonal bipyramidal geometry of the iron centre, but just a few examples have been reported (Bigi 2012, 1536; Bominaar 2003, 3622). Considering this, the goal of this project is to generate iron(IV)-oxo species with a spin state S=2 using new TPA-derived ligands containing sterically encumbered substituted isoquinolines that should favour trigonal bipyramidal geometries.

2. Methodology

The preparation and handling of O_2 and H_2O sensitive compounds is done in a N_2 drybox. To characterize the different species, NMR, HRMS and X-ray are used. UV–vis spectroscopy is performed at low temperature to monitor the high-valent species formation.

3. Results and discussion

The designed ligands contain different substituents in the isoquinolines in order to add more steric hindrance into the iron(II) complex. For now, two complexes have been synthesized (Figure 1): [Fe(^{iPr,ISOQ}TPA)(OTf)]$^+$ (**1**) and [Fe(^{CF3,ISOQ}TPA)(OTf)$_2$] (**2**). Compound **2** adopts an octahedral structure, while **1** presents the desired trigonal bipyramidal geometry as ascertained by X-ray crystallography. These compounds have been further characterized by paramagnetic ^{1}H-NMR and mass spectrometry. Finally, some reactivity tests have been carried out. To do so, the experiments have been done in acetonitrile at -40 ºC and the formation of either iron(IV)-oxo or iron(III)-hydroperoxo species has been monitored by UV-Vis spectroscopy. Nevertheless, even though the goal is to generate iron (IV)-oxo species with an

S=2 spin state, for now the iron(IV)-oxo compounds obtained present a S=1 spin state according to their absorption spectra.

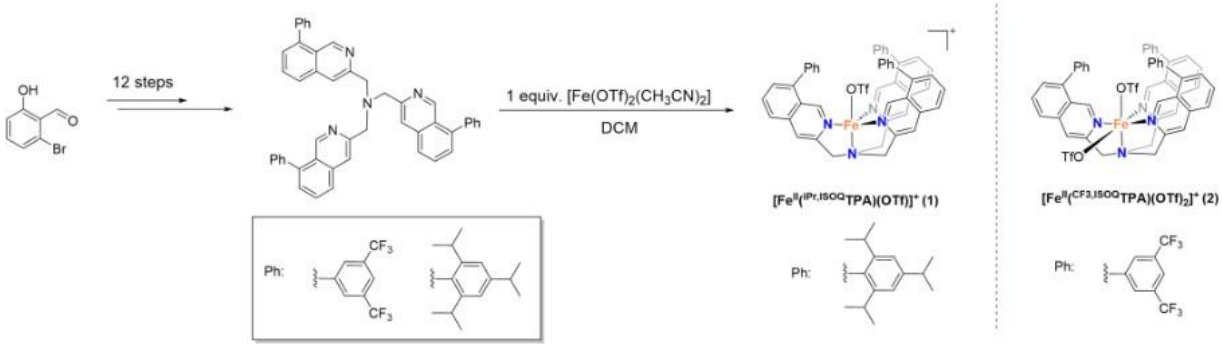

Figure 1. Synthesis of the ^{R,ISOQ}TPA ligands and preparation of $[Fe^{II}(^{iPr,ISOQ}TPA)(OTf)]^+$ (**1**) and $[Fe^{II}(^{CF3,ISOQ}TPA)(OTf)_2]$ (**2**) complexes.

4. Conclusions

In this project, we target the synthesis of different sterically congested ligands to prepare the corresponding iron(II) compounds with a trigonal bipyramidal geometry. For now, two of these complexes have been prepared. Nevertheless, the synthesized iron(IV)-oxo compounds are not S=2 but S=1. New versions of the ligands are currently being prepared to add more steric hindrance to the system to afford the desired S=2 complexes.

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REGIOSELECTIVE BIS-FUNCTIONALIZATION OF FULLERENES BY DIELS-ALDER REACTION VIA SUPRAMOLECULAR MASK STRATEGY

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Keywords: Diels-Alder cycloaddition, fullerenes, supramolecular nanocapsules,

1. Introduction and objectives

Fullerenes are carbon molecules with a spherical-like shape. As such, their functionalization is not regio-controlled and renders mixtures of regioisomers that are not amenable for applications (Fuertes-Espinosa 2020). In this regard, only easily accessible mono-functionalized fullerenes are used as electron transport layers in solar cells devices. Pure regioisomers of poly-adducts are envisioned as good alternative to boost the efficiency of SC. For this reason, the main objective of the present work is the regioselective functionalization of fullerenes by means of the Diels-Alder reaction using a supramolecular nanocapsule as a mask (Pujals 2022).

2. Methodology

The synthesis of bis-adducts has been achieved by the Diels-Alder reaction using a nanocapsule as a mask. The tetragonal prismatic supramolecular nanocapsule has been synthesized according to reported procedures and characterized by NMR and HRMS (García-Simón 2014). The functionalization of the encapsulated fullerenes has been monitored by HRMS. Finally, the products have been characterized by UV-Vis and NMR spectroscopy.

3. Results and discussion

The Diels-Alder reaction was studied over the encapsulated fullerenes within a nanocapsule, using two different dienes to compare the differences on the regioselectivity effected by difference in size. When anthracene was used as the diene, the *equatorial* bis-C_{60}-An_2 (100 per cent regio-purity) and the *12 o'clock* bis-C_{70}-An_2 (91 per cent regio-purity) were obtained. The controls experiments suggest that the nanocapsule protects the bis-adducts from the retro-Diels-Alder, as in the non-templated reaction is promotes the formation of the mono-adduct. Moreover, the nanocapsule effects on the regioselectivity, enhancing the formation of one of the possible regio-isomers. In the case of pentacene, the *trans-1* bis-C_{60}-Pn_2 (78 per cent regio-purity) and the *5 o'clock* bis-C_{70}-Pn_2 (96 per cent regio-purity) were obtained. Compared to the non-templated functionalization, it is observed that the mask enhances the stability of the bis-adducts and prevents the retro-Diels-Alder. Moreover, the nanocapsule increases the

regioselectivity of the reaction. The difference between the dienes was studied by MD Simulations. As the pentacene is larger, the remote aromatic rings clash with the porphyrins of the nanocapsule, restricting the mobility of the addend and the orientation of the second addend to react. FMO study also agrees with the regioselectivity observed.

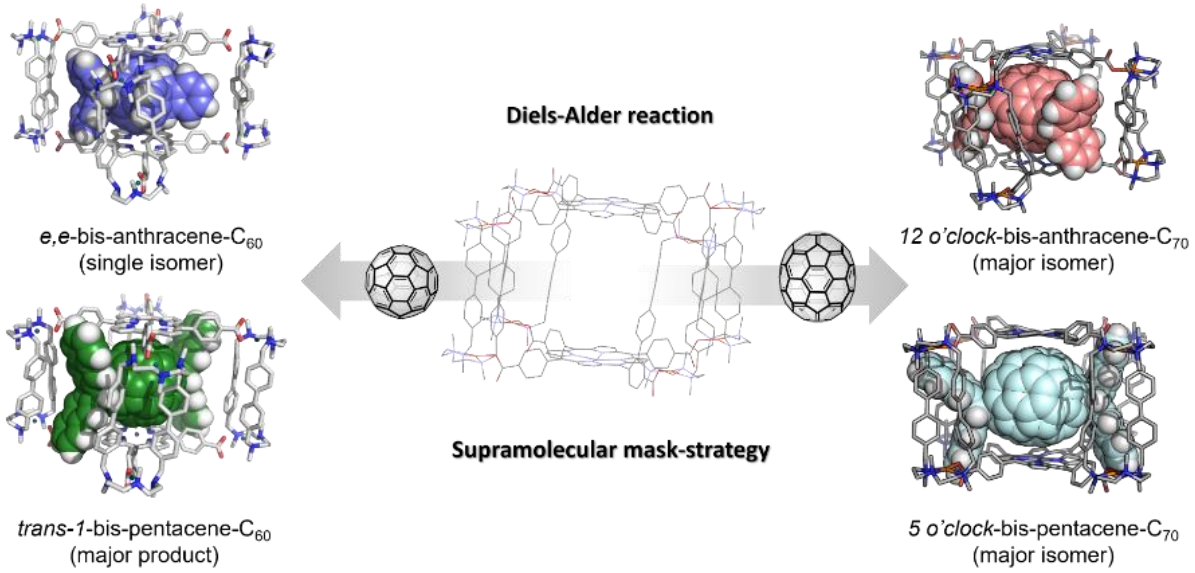

Figure 1. Structure of the products obtained with the Diels-Alder reaction.

4. Conclusions

This work demonstrates that supramolecular nanocapsules can be used as masks to control the chemo- and regio-selectivity in the Diels-Alder functionalization of fullerenes. Moreover, by changing the length of the acene, the regio-selectivity can be tuned.

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MANAGEMENT OF THE BOX TREE MOTH PEST IN EXPERIMENTAL PLOTS

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Keywords: *Buxus sempervirens*, *Cydalima perspectalis*, experimental plots, invasive species, plant ecology.

1. Introduction and objectives

The boxwood (*Buxus sempervirens*) is a dominant species in several shrublands and forest habitats in the mountainous region of Catalonia. This plant is currently under serious threat due to the impact of the box tree moth (*Cydalima perspectalis*) (Figure 1) pest. This lepidoptera is an invasive species of Asian origin that only feeds on the leaves of the boxwood and even on the bark, causing severe damage that can end in the death of the individuals (Nacambo *et al.*, 2014). Control treatments of this pest are necessary since the impact of the box tree moth affects large areas of boxwood in the territory.

Figure 1. Adult box tree moth.

2. Hypothesis

The working hypothesis of the treatments applied to the experimental plots is that *Bacillus thuringiensis* is the most effective control method, and the mass capture is less effective. The *Trichogramma* spp. have low effectiveness under stable conditions, so no better results are expected in the environment.

3. Methodology

The University of Girona is carrying out a study on experimental plots in Osona to analyse the effectiveness of the main control methods. The treatments are the application of *Bacillus thuringiensis* and mass capture with sex pheromones as a claim, while combining the use of genus *Trichogramma* parasitoids.

4. Results and discussion

The results of the monitoring carried out show the effectiveness of the treatment with *B. thuringiensis*, which protects the spring growth of boxwood by reducing defoliation, even though it is a phytosanitary that can affect other lepidopterans. On the other hand, the mass capture treatment is insufficient for boxwood preservation and the application of the parasitoids is not effective in reducing damage. The study also analyses the effects of the plague on the floristic community of box formations, where it has been observed that when the presence of boxwood damage is high, the richness and abundance of plants is higher. This is because the affected boxwoods exert less competition over the rest of the community species.

6. Conclusions

This study highlights the importance of implementing an adaptative management, taking into consideration the limitations and impacts of different treatments on the ecosystem. Pheromone treatments can be used as a preventive tool to manage the pest, while treatment with *B. thuringiensis* should be restricted to regional scenarios of severe boxwood damage. By combining these two approaches, it can be developed a more effective and sustainable management strategy for this pest.

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SESSION 11.
SDG14. LIFE BELOW WATER

PEPTAIBOLS WITH ACTIVITY AGAINST *Xylella fastidiosa*

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Keywords: Antimicrobial peptides, peptaibols, plant pathogens, solid-phase synthesis, *Xyllela fastidiosa*

1. Introduction

The considerable damage inflicted globally by *Xylella fastidiosa* has prompted the urgent exploration of innovative control strategies. Antimicrobial peptides (AMPs) are a promising alternative to current pesticides because they are active against a wide range of pathogens and have a low risk of developing resistance (Badosa 2022).

Peptaibols are a family of AMPs that have attracted considerable interest (Caracciolo 2023). Based on the results obtained from a collection of peptaibols derived from trichogin GA IV, in the present study we designed new peptaibols incorporating an acetyl, a butanoyl or an octanoyl group at the N-terminus and/or a D-amino acid. We also studied the influence on the biological activity of replacing the aminoisobutyric residues with a valine.

This study also focused on the design of peptaibols derived from the lead AMP **BP100**. This peptide exhibits high activity against *X. fastidiosa* while being low toxic. We envisaged that the introduction of an aminoisobutyric residue and/or a leucinol at the C-terminus would enhance the biological activity of **BP100**.

All these compounds are being screened for their antibacterial activity against *X. fastidiosa* and for their hemolysis and phytotoxicity.

2. Methodology

Peptaibols were synthesized on solid phase following a standard Fmoc/*t*Bu strategy, analysed by HPLC and characterized by mass spectrometry. Their antibacterial activity against *X. fastidiosa*, hemolysis and phytotoxicity are being screened following the previously described methodology (Moll 2021).

3. Results and discussion

Twenty-six peptaibols were synthesized on solid phase and obtained in high purities (>99 per cent). They included 17 trichogin GA IV analogs and nine derivatives of **BP100**. The synthesis of these peptaibols and their biological activity will be presented and discussed.

4. Conclusions

In summary, 26 peptaibols derived from trichogin GA IV and **BP100** were synthesized. It is expected to identify compounds with activity against *X. fastidiosa* and low toxicity.

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'COMMON OR GARDEN GROUND': HISTORICAL AGRO-SILVO-PASTORAL LAND MANAGEMENT IN THE EASTERN PYRENEES

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Keywords: Abandonment, agro-silvo-pastoral, common land, terraces, wood-pasture

1. Introduction and objectives

The research objectives are to assess any impacts of the French–Spanish frontier imposed on Catalonia in the Upper Muga Valley by the 1659 Treaty on its landscape historical ecology. Terraces and wood pasture are envisaged as examples of adaptable risk mitigation pertaining to UN Sustainable Development Goal 15: *Protect, restore and promote sustainable use of terrestrial ecosystems, sustainably manage forests, combat desertification, and halt and reverse land degradation and halt biodiversity loss.*

2. Hypothesis

Historic Catalan upland agro-silvo-pastoral landscape management systems demonstrate elements of 'sustainable' land use strategies invested in social and landesque capital. Critical evaluation of these models demonstrates local resilience in marginal landscapes whose fiscal value was quantifiably low but qualitatively significant, informing our adaptions to the challenges of climate-changes during the current 'Anthropocene'.

3. Methodology

The methodology derives from Historical Ecology (Szabó 2015) using a multi-disciplinary approach (Grove, Alfred Thomas and Rackham 2001; Stagno 2019; Watkins 2004).

4. Results and discussion

The combined data suggest that commons comprised fixed sites and extensive rights. Common types of land included *devesa*, perhaps for transhumance, plus wood-pasture and lands, converted, or already enclosed, for subsistence cultivation (emphasising cereals within the *Emprius*) in Costoja. Common lands were possibly divided during the French Revolution (1789) and in Spanish Catalonia during the Desamortización of Mendizábal (1837). However, archival data alone is fragmentary, ideally interpreted in tandem with fieldwork and

toponymic analysis. The first Costoja cadastre of 1837 and land register of 1838 describe multiple plots of land for cultivation, mixed wood pasture and rough pasture within the *Emprius* whose terraces are visible today. Either these terraces were already extant when the land was communally managed by the village *Consul*, or they were constructed once privatized. The parcels of terraced lands may have further transitioned to individual private property as concepts of ownership altered, with new French laws regarding property rights in 1860 (Vivier 2013, 243).

5. Conclusions

By the 21st century, the process of terrace and agro-silvo-pastoral landscape abandonment was complete. The carefully, seasonally, managed communal wood pasture and community grazing in Costoja, transitioned to some patches of municipal forested plots, managed by the state. The terraces within the previous *Emprius*, are abundant ecosystem service providers; their lack of management impacts upon local biodiversity, erosion, and fire control, whilst the previous agro-ecology is lost as rough pastures recede with little active managed grazing. The abandoned landscape provides critical comprehension of the significance of land tenure and role of communality to conservation. Some 17th to 19th century archival data, replete with disputes and details, demonstrate the care requisite to manage upland Mediterranean ecosystems.

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LA GESTIÓ DE RESIDUS EN ÈPOCA ROMANA: L'EXEMPLE DE MAS POC (UE2007), UN ABOCADOR BAIX IMPERIAL

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Paraules clau: Abocador, època romana, escombrera, intervenció arqueològica, residus.

1. Introducció i objectius

El present treball pretén estudiar les restes del jaciment arqueològic anomenat Mas Poc, situat a la Pera (Baix Empordà). En aquest estudi es tractarà la Unitat Estratigràfica 2007, que és el primer nivell de farciment de la fossa FS1.

L'estudi estarà dividit en tres parts ben diferenciades, la primera consistirà en un estat de la qüestió del que se sap del jaciment. La segona, establirà unes bases teòriques per a l'anàlisi del material arqueològic. I la tercera, la més innovadora, mirarà d'aportar una metodologia de treball per a l'estudi del tractament de residus en època romana.

2. Hipòtesi

La hipòtesi principal del present treball és constatar que els romans no abocaven els residus o deixalles de forma aleatòria. Amb l'estudi del registre arqueològic d'una escombrera, en aquest cas de cronologia baix imperial, es pretén copsar els plantejaments que les societats romanes tenien a l'hora de gestionar els residus que generaven.

3. Metodologia

La metodologia que s'emprarà en el present treball és molt diversa. En un primer moment es recorreran a fonts escrites, on poder buscar antecedents i contextos similars al jaciment estudiat. En segon lloc, s'anirà al Servei d'Atenció als Museus on està dipositat tot el material del jaciment Mas Poc, per tal de classificar, individualitzar, dibuixar i fotografiar tot aquell registre arqueològic. En tercer lloc, es procedirà a digitalitzar tots aquells dibuixos de materials en làmines per tal d'estudiar-los i descriure'ls. I, finalment, un cop estigui recopilada tota la informació, i tinguem la totalitat del registre estudiat (ceràmica, ferro, fauna, vidre, bronze~~,~~ i plom) es procediria a caracteritzar les restes arqueològiques.

4. Resultats i discussió

En el present treball es preveu fer una aproximació fidedigna al material arqueològic procedent de la UE2007. Amb la individualització del registre arqueològic es precisarà en la descripció i tipificació dels objectes per tal d'establir dinàmiques de consum i gestió en època romana. La discussió que sorgirà d'aquest estudi és si realment les societats d'antany es

plantejaven quan, com i què llençaven en els abocadors, o bé si aquestes escombreres es farcien de forma aleatòria, de fet Remolà (2000, 107) ja argumenta que les escombraries del passat ens poden donar respostes a aspectes fonamentals de les societats d'antany.

5. Conclusions

Un cop contrastades les dades, sobre la gestió de residus en època romana, es procedirà a cloure el treball mirant de discriminar els tipus de plantejaments utilitzats per al seu abocament. Per altra banda, es pretendrà establir una metodologia de treball que pugui ser usada en estudis posteriors que tractin contextos semblants.

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SESSION 12.
SDG16. PEACE, JUSTICE AND STRONG INSTITUTIONS

THE RELATIONSHIPS BETWEEN POLITICAL PARTIES AND INTEREST GROUPS: THE CASE OF CIUTADANS PEL CANVI AS A PSC'S COLLATERAL ORGANIZATION

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Keywords: Ciutadans pel Canvi, collective political actors, interest groups, institutionalization, political parties

1. Introduction and objectives

The line that separates and differentiates collective political actors is increasingly thin and blurred. The insufficiency of political parties as elements capable of channelling and transmitting new social demands means that new forms of hybrid political intervention proliferate more frequently as intermediaries between institutions and citizens (Heaney 2010). This can be done by using outsider strategies, as employed by interest groups, or by cooperating with political parties through the establishment of coalitions (Lisi 2018). *Ciutadans pel Canvi* was born in 1999 as a political experiment that proposed a new form of political intervention far from the hierarchical organizational systems of political parties, calling into question the role of parties as exclusive tools of civic mobilization. This interest group aspired to become an alternative capable of expanding the civic presence in the Catalan political sphere, as a complement to the traditional political representation exercised by political parties, introducing new social interests into the Catalan political agenda that would substantially increase the quality of democracy. To carry out its original purposes, it established an electoral coalition with the PSC (socialist party of Catalonia), but their particular relationship ended up not being institutionalized because it followed a strategy divergent from that of the party (Verge 2012), causing the dissolution of the group.

2. Methodology

The main methodology used has been the case study, and the technique to infer causality has been process tracing, the applicability of which is especially recommended for case studies.

3. Discussion

One of the main issues of discussion in the doctoral thesis has revolved around the institutionalization of the interest group as a political actor and its particular relationship with the PSC. Ideology alone is not a sufficient condition to establish and maintain organizational links between political groups and parties. Everything seems to indicate that the exchange of organizational resources can better explain the institutionalization of the links between both organizations and, consequently, the institutionalization of the group.

4. Conclusions

Firstly, having different strategies between parties and groups to establish links can lead to the non-institutionalization of the relationship. Secondly, although ideology is a determining factor in the organizational relationship between groups and parties, ideology alone does not consolidate the relationship. Thirdly, the type and amount of resources explains in a better way than ideology the strength of the links between both organizations particularly, and between parties and interest groups in general.

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LA IMATGE DE L'*ECCLESIA* EN ELS MOSAICS DEL SEGLE XII A ROMA COM A ELEMENT DE PROPAGANDA DE L'AUTORITAT PAPAL

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Keywords: *Ecclesia*, mosaics, reforma gregoriana, Roma (segle XII), *Sponsa Christi*.

1. Introducció i objectius

A partir de la Reforma gregoriana es concreta a Roma la conceptualització figurativa de la iconografia del gran tema ideològic del moment: l'*Ecclesia*. Al segle XII, destaquen el mosaic de San Clemente, en què l'Església es representa com a vinya del Senyor, i el de Santa Maria in Trastevere, on l'*Ecclesia* és Maria, com a *Sponsa Christi*, segons les exegesis coetànies del *Càntic dels Càntics*. Són els dos casos que analitzaré com a instrument de propaganda papal i em fixaré les seves particularitats respecte als mosaics bizantins.

2. Metodologia

Per tal de reconstruir els orígens iconogràfics de l'*Ecclesia* a Roma, he compilat les imatges d'aquest motiu en manuscrits, tabletes, relleus o pintures murals. Com a fonts escrites, he utilitzat el *Liber Pontificalis*, on consten les obres promogudes pel papat i els textos bíblics, sobretot el *Càntic dels càntics*. He plantejat l'anàlisi comparativa dels mosaics romans i bizantins a partir dels elements iconogràfics i materials (tessel·les, intersticis o colors).

3. Resultats i Discussió

La meva intenció és defensar la originalitat iconogràfica dels mosaics de Roma que els allunya de l'art bizantí. En quest sentit, el meu treball se situa en la línia de James (2017), que qüestiona la "superioritat" dels mosaics bizantins, sobretot quan no hi ha proves concloents sobre la procedència dels seus artífexs, i també han estat imprescindibles el treball de Labatt (2019) i l'estudi de referència d'Andaloro i Romano (2018), que donen valor a Roma com a centre de producció. A més a més, al segle XII l'art va ser emprat per tal que l'*auctoritas* papal esdevingués també *potestas*. Sobre l'elaboració d'instruments discursius en la dimensió visual han estat essencials l'obra de Tourbet, *Un'arte orientata. Riforma gregoriana e iconografia* (2001) i els capítols de Kessler i Riccioni en el volum *Roma e la Riforma gregoriana. Tradizioni e innovazioni artistiche* (2007).

4. Conclusions

Un cop analitzada la iconografia de l'*Ecclesia* és possible afirmar que el papat la utilitza com a element de propaganda a partir de la Reforma gregoriana. Pel que fa a la relació amb models bizantins, la preeminència de la iconografia de l'*Ecclesia* a Occident per representar el triomf del poder papal és indubtable, ja que a Orient la màxima autoritat és imperial. Atesa la relació intermitent entre Roma i Bizanci, m'inclino a pensar que en l'àmbit musiu es van influir mútuament, encara que Roma destaca per l'originalitat iconogràfica, potser perquè no estava subjecta a la fidelitat al prototip que caracteritza els mosaics bizantins.

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ENTRE CATALANISMES. ELS FELIÇOS ANYS VINT DEL CUPLET CATALÀ

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Paraules clau: Catalunya, cuplet, espectacle, música, política

1. Introducció i objectius

El cuplet català té la seva l'efervescència el 1920 i moltes cupletistes —catalanes o no— van portar als escenaris i gravar un repertori bilingüe. La popularització del cuplet va ser un fenomen de curta durada, en cinc anys s'havia esgotat i altres ritmes —polítics i musicals— envaïen l'escena. Quines són les causes del naixement i el declivi del cuplet català?

2. Metodologia

La metodologia utilitzada és la recopilació i anàlisi de les fonts primàries i secundàries sobre el cuplet català i el seu context històric.

3. Resultats i discussió

Poal i Aregall (1919) situa la popularització del cuplet amb «La Ginestaire» de Costa i Deu, interpretada per Amalia d'Isaura l'any 1918, ignora —a propòsit o no— a Raquel Meller, qui va incloure al seu repertori «La font del Xirineu» de Rossend Llurba el 1917. D'aquest fet se'n fa ressò *El Mundo* (Varó 1917, 1). És el cuplet català, com preconitza la premsa, una aposta de La Lliga?

L'article de Varó s'adscriu i explica la crisi política de 1917, entre vagues generals i les accions de La Lliga Regionalista. Entre el catalanisme i el fet que la Lliga acceptés formar part del govern central. Els esdeveniments de 1917 detonaren en el fracàs i tornada a Catalunya de Cambó el 1919 i, segons Sobrequés (1997), el partit va dedicar els seus esforços a expandir el catalanisme.

Barcelona n'és el bressol, però el fenomen es va estendre per tot el país. Es produí un enfrontament entre els catalanistes a favor i en contra del cuplet català, i els diaris n'anaven plens. Pilar Alonso representarà l'època daurada del cuplet i serà considerada la creadora i difusora. De fet, la seva retirada, l'any 1925, va ser llegida com el punt de declivi del cuplet.

4. Conclusions

El naixement i difusió del cuplet no va estar està exempt de les apropiacions partidistes i ideològiques, com es llegeix a l'article de 1917, i serà també, segons Llurba, un motiu del seu final, perquè «el cuplet català va ensorrar-se quan volgué ser tendenciós» (Tomás 1935, 5). Joaquim Molas (1980) situa la fi del cuplet en la rivalitat simbòlica entre el cuplet i la sardana. La dictadura de Primo de Rivera, segons l'autor, va decantar la balança cap a la sardana com símbol de Catalunya i va ajudar a la decadència del cuplet català. Després d'un llarg silenci amb el franquisme, reviurà amb Guillermina Mota i la Nova Cançó, com una reivindicació política del passat.

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6. Agraïments

Aquesta investigació ha estat possible gràcies a l'ajut de recerca de la UdG amb la col·laboració del Banco Santander.

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