Universitat de Girona
Escola de Doctorat

VII Conference of Pre-doctoral Researchers

Abstract Book

Gerardo Boto & Alejandro Piñel (Editors)

Volume VII, 2023

University of Girona

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of Pre-Doctoral Researchers
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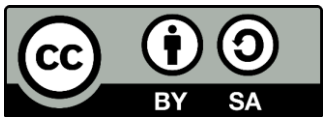

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PREFACE

It is a very pleasing responsibility to provide the University of Girona community once again, firstly, and the international academic community, secondly, with the electronic book containing the abstracts of the contributions presented at the VII Conference of Predoctoral Researchers of the University of Girona (UdG). These conferences, held between June 12 and 15, 2023, were developed under the auspices of the Doctoral School of the UdG, with the support and collaboration of the Vice-Rectorate for Research and Knowledge Transfer. The academic meeting took place at the Faculty of Law (Montilivi Campus) of the University of Girona. These Predoctoral Researchers Conferences began to be held between June 6 and 9, 2017. Throughout seven editions, the organization has sought to improve the quality and recognition of these meetings inside and outside our university.

As in previous editions, a committed group of volunteer doctoral students have led the organization of this event. They, exercising a diligent attitude that has been consolidated and strengthened over the years, have managed to mobilize the doctoral community of the UdG. As a result, it has been achieved, according to the program, that a hundred contributions were presented. Once again, this academic initiative sustained over time has provided intellectual benefits not only to the researchers who have orally presented the progress of their doctoral research, but also to the entire predoctoral community of the UdG. It should be made explicit that the main objective of the Conference is to provide doctoral students with a space for the presentation of the partial results of their research, for the exchange of knowledge and debate among all researchers in training who are doing their doctoral thesis or master's degree at our university. In fact, in the Catalan university landscape, the UdG is one of the few universities that has a multidisciplinary Predoctoral Conference, and not limited by areas of knowledge or doctoral programs.

During the VII Conference, doctoral and master's students presented their theses individually and within the framework of the thematic topics, which sometimes corresponded to the profiles of some doctoral or master's programs and sometimes went beyond these contours and involved researchers from different programs and faculties. This organization of the presentations had an immediate consequence: each researcher had the opportunity to discuss the results of his or her research with other high-level researchers, outside his or herresearch team, project, and doctoral program. It was demonstrated, therefore, that oral communication contributes, in a generic way, to developing skills of justified and persuasive defense of the contents of a research proposal, and in a specific way, to disseminating the results of such research to society.

In this way, doctoral students progress in the achievement of milestones in the Open Science paradigm, a conceptual and administrative framework of knowledge communication required by current European societies.

The VII Jornadas de Investigadores Predoctorales was organized by twelve volunteer doctoral students from different doctoral programs. This team (Alba Ceballos-Escalera, Meritxell Romans Casas, Alejandro Piñel Bordallo, Olga Taravilla Baquero, Fidanka Vasileva, Carolina Rea Gómez, Artur Rubinat Lacuesta, Jonathan Andres Graciano Uribe, Mireia Cots Melero, Lluis Alejandro Moll Dos Santos, Gerard Riesco i Llach and Helena Giramé Rizzo) did an impeccable job. They organized each of the sessions and managed to convene predoctoral researchers from other Catalan universities for most of them. In addition, they managed each intervention and oversaw moderating the debates of each of the sixteen sessions.

As a result, the abstracts of one hundred and two papers have been received, reviewed, and edited. Thirteen of them correspond to predoctoral researchers from other universities, who have added their contributions to those of the UdG doctoral students. This e-book has been edited by the undersigned and the predoctoral researcher in Human Sciences and Heritage, Alejandro Piñel Bordallo, who has done an excellent job.

This mapping of knowledge in construction and progress that is this e-book confirms the relevance of predoctoral research at the UdG in the national and international university landscape in 2023. Undoubtedly, we will address the organization and development of the VIII Conference of Predoctoral Researchers planned for 2024. All of us who have contributed to the realization of this e-book are convinced that the academic community of the University of Girona can feel justifiably proud of it, although we are aware that there is an opportunity to progress in the quality and innovation of these conferences.

Girona, October 22, 2023

Gerardo Boto Varela

SESSION 1.

ORGANISMS ECOLOGY AND COMPOUND PRODUCTION

MONITORING *C. ACETOBUTYLICUM, C. CARBOXIDIVORANS* AND *C. CELLULOVORANS* IN CLOSTRIDIAL CONSORTIA BY QUANTITATIVE PCR

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Keywords: alcohol production, bacterial fermentation, *Clostridium* spp., co-cultures, TaqMan probes

1. Introduction

Fermentative processes using *Clostridium* species to produce butanol and other added-value compounds from biomass gained renewed interest in the biotechnological industry as an alternative to fossil fuel. Coculturing different *Clostridium* species has emerged as an alternative to increase production rates and expand product spectrum (Moon *et al.,* 2016; Pinto *et al.,* 2021). Since cocultures usually lack a natural ecological equilibrium, their perfect functioning mainly depends on the stability and fitness of each species, therefore specific monitoring of members in the consortia is crucial.

2. Hypothesis

The aim of this work was to design a multiplex qPCR with species-specific probes targeting three *Clostridium* species. *Clostridium* species were combined in different consortia and the method tested experimentally. Cocultures were implemented to achieve significant benefits in alcohol production from sugar (glucose and cellobiose) fermentation.

3. Methodology

A triplex qPCR methodology using three species-specific TaqMan probes targeting the 16S rRNA gene of *C. acetobutylicum, C. carboxidivorans* and *C. cellulovorans* was evaluated. The method was optimized to target the *Clostridium* spp. independently when growing in three defined consortia, namely two cocultures – *C. acetobutylicum* and *C. cellulovorans* (consortium-1), *C. acetobutylicum* and *C. carboxidivorans* (consortium-2) – and a triplet consortium with all three *Clostridium* species. The qPCR assay was optimized with DNA samples prepared by mixing DNA extracts (mimicking different proportions), and application confirmed with real clostridial fermentation experiments.

4. Results and discussion

With the designed triplex qPCR, we could quantify all three *Clostridium* strains with good reaction efficiencies (~99%), with no cross-reactions. Quantitative ranges varied from 10^2 to 10^7 cells/mL in all probes, being slightly less accurate for *C. carboxidivorans*. Growth of the three species was correlated with product profiles obtained during fermentation. Higher alcohol productions were obtained when combining *C. carboxidivorans* and *C. acetobutylicum*, and further improved when cocultured with *C. cellulovorans* in consortium-3, which achieved the highest butanol (0.6 g/L) concentration and the highest alcohol-to-acid ratio among all consortia.

5. Conclusions

The designed triplex qPCR methodology could be used to specifically quantify *C. acetobutylicum, C. carboxidivorans* and *C. cellulovorans* in cocultures, pointing out its potential as a methodology to study the growth of *Clostridium* species in bioreactor samples aiming for alcohol production from sugar fermentation.

6. Bibliography

Moon, H.G., Jand, Y.S., Cho, C., Lee, J., Binkley, R., Lee, S.Y. (2016). One hundred years of clostridial butanol fermentation, *FEMS Microbiology Letters*, *363*(3), 1-15. https://doi.org/10.1093/femsle/fnw001.

Pinto, T., Flores-Alsina, X., Gernaey, K.V., Junicke, H. (2021). Alone or together? A review on pure and mixed microbial cultures for butanol production. *Renewable and Sustainable Energy Reviews, 147*, 1-13. https://doi.org/10.1016/j.rser.2021.111244.

7. Acknowledgements

Authors acknowledge funding from the Spanish Government (ref. PCI2019-111932-2). L.F.-P. is grateful for the grant from the Catalan Government (2021 FISDU00132). S.P. is a Serra Hunter Fellow (UdG-AG-575) and acknowledges the funding from the ICREA Academia award.

BUTYRIC ACID AND BUTANOL PRODUCTION FROM CO_2 IN LOW-GAP MES CELLS

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Keywords: bioelectrochemistry, butyric acid, carbon utilization, Megasphaera, microbial electrosynthesis

1. Introduction

To reach economic feasibility, the power demand of microbial electrosynthesis (MES) must be reduced by designing dells with low ohmic resistances, and industrially valuable products such as butyric acid and butanol must be targeted (Pinto et al., 2021). We aimed to achieve selective butyric acid production from CO_2 with low electricity demand by using a low-gap electro-cell and investigated the operational conditions for a further upgrade to butanol.

2. Methodology

Two commercial ElectroCell systems were set up and operated in galvanostatic mode. The cells were inoculated with a mixed culture. The first EC (EC-1) was operated at current densities ranging from 0.3 to 3.0 mA cm^{-2}. Subsequently, a second EC (EC-2) was inoculated with the effluent of EC-1 and directly set at 1.5 mA cm^{-2}. CO_2 was the only carbon source. Optical density (OD), pH and hydrogen partial pressures (pH_2) together with the microbial community were analyzed.

3. Results and discussion

The highest butyric acid production rate was 14.5 g m^{-2} d^{-1}, reached at 1.5 mA cm^{-2} by EC-1. EC-2 reached a similar butyric acid production rate with 82% lower lag phase and a selectivity up to 78%. The low ohmic resistance of the cell (15.7 mΩ·m^2) resulted in a power demand of 34.6 kWh kg^{-1} of butyric acid (Figure 1). After butyric acid accumulation, CO_2 supply was stopped and high hydrogen partial pressure (pH_2> 1.7 atm) was maintained. Such conditions, along with low pH (<4.8), favored solventogenic butanol production, with 2.2 g m^{-2} d^{-1} production rate and a conversion of 28%. The bacterial community was dominated by *Megasphaera* sp a well-known chain elongating microorganism.

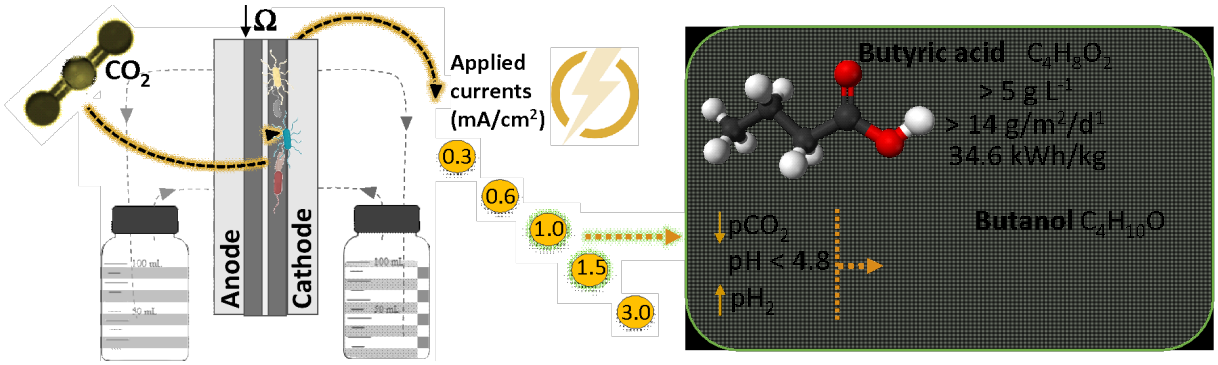

Figure 1. Summary of the process and the most relevant results obtained.

4. Conclusions

Alternating periods of high pCO_2 and pH_2 promoted a selective butyric acid formation, up to 78%, from CO_2 in low-gap, electrically efficient MES cells. Butanol can be effectively produced by interrupting CO_2 supply after butyric acid accumulation.

5. Bibliography

Pinto, T., Flores-Alsina, X., Gernaey, K.V., Junicke, H. (2021). Alone or together? A review on pure and mixed microbial cultures for butanol production. *Renew. Sustain. Energy Rev.* (147), 111244. https://doi.org/10.1016/j.rser.2021.111244.

EXPLORING CATALAN AND FRENCH *Salmonella* spp. GENOMES FROM DRY FERMENTED SAUSAGES

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Keywords: Accessory genome analyses, cgMLST and wgMLST analyses, dry fermented sausages (DFS), *Salmonella*, whole genome sequencing (WGS)

1. Introduction

The second most reported foodborne zoonosis in humans in the European Union (EU) is salmonellosis. In the EU, the health care, social and economic costs due to Non-Typhoidal *Salmonella* cases are estimated to be as high as €3 billion a year and "meat and meat products" are the major sources of human infection (EFSA and ECDC, 2022). During 2020-2022, dry fermented sausages (DFS) were responsible for 17 *Salmonella* alerts of which seven were in France and one in Spain (European Commission, 2023). Five alerts out 17 were linked to "fuet", a sausage whose main producers in the EU are in Catalonia.

2. Hypothesis

In this framework, the genomic diversity of 173 *Salmonella* spp. isolated in Catalonia and France from 1997 to 2022 from DFS, pork and pig carcasses (as DFS row materials) were analysed to investigate their phylogenetic relationships and possible transmission paths.

3. Methodology

The *Salmonella* spp. isolates were sequenced by Illumina technology. Phylogenomic analyses were computed on either SNPs or alleles (*i.e.*, cgMLST and wgMLST) by SNIPPY and SeqSphere+, respectively. Trees were visualised through the interactive Tree Of Life (iTOL). Accessory genome was analysed by VFDB, BacMet and ResFinder databases.

4. Results and discussion

The 173 *Salmonella* spp. genome panel included ten different serovars (i.e., *S.* Typhimurium, its monophasic variant *S.* 1,4,[5],12:i:-, *S.* Derby, *S.* Infantis, *S.* Kedougou, *S.* Rissen, *S.* Wien, *S.* Worthington, *S.* Goettingen, and *S.* London) and twelve MLST profiles. *S.* 1,4,[5],12:i:-, *S.* Derby and *S.* Rissen were the most prevalent. The prevalence of these serovars was matrix-

dependent with *S.* 1,4,[5],12:i:- being the most frequently isolated in the DFS. The cgMSLT and wgMLST analyses showed ten different clusters with *S.* Typhimurium and *S.* 1,4,[5],12:i:- sharing the same cluster and two clusters for the polyphyletic *S.* Derby. *S.* 1,4,[5],12:i:- isolates coming from different matrices, sampling dates and regions were grouped together showing a possible contamination along the DFS production chain. Accessory genome analysis showed antimicrobial resistance genes, virulence factors and resistance genes to heavy metals and biocides, which could explain the higher prevalence of some serovars at the end of the DFS production chain.

5. Conclusions

Genome analyses revealed that close related clones of *S.* 1,4,[5],12: i:-, *S.* Derby and *S.* Rissen are circulating through Spain and France pig and pork sectors. Moreover, our results allowed identifying a regional clonality within Catalonia *Salmonella* strains isolated from DFS and the source of contamination for DFS food producers.

6. Bibliography

European Commission (2023). *RASFF - food and feed safety alerts*. Retrieved from https://ec.europa.eu/food/safety/rasff_en.

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GENETIC DIVERSITY OF CATALAN CHUB (*SQUALIUS LAIETANUS*) POPULATIONS

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Keywords: conservation genetics, mitochondrial markers, population genetics, species hybridization, *Squalius laietanus*

1. Introduction

The Catalan chub, *Squalius laietanus* (Doadrio, 2007) is a freshwater fish found in Catalan rivers from the Ebro River to the French border, and in the Tech, TetMassana and Agly basins, in France. Phylogenetic studies with both mitochondrial (cytochrome oxydase c, *COI*, and cytochrome b, *cytb*) and nuclear markers (subunit 1 of the recombination-activating gene, *RAG1*, and ribosomal protein, *S7*) relate this species with *Squalius orpheus*, present in Greece and Türkiye, and distinguish it from the European chub (*S.cephalus*) and the endemic species of the *Squalius* genus in the Iberian Peninsula (Perea et al., 2010). However, nuclear markers suggest hybridization between *S. laietanus* and *S. cephalus* in the Agly and Tech rivers (Rose et al., 2020).

2. Hypothesis

The aim of this study is to check the genetic integrity of the Catalan chub populations in the Catalan basins, and to determine if the hybridization reported in France also occurs in these basins south of the Pyrenees mountains. This hypothesis will be assessed by genotyping chub specimens from Catalan river basins using mitochondrial and nuclear markers already available from the literature, or new ones designed in this work.

3. Methodology

Specimens of chub have been caught in sections of Catalan rivers in 2021 and 2022. Chub specimens will be characterized by sequencing a fragment of the COI gene, common for barcoding in fish species (Ward et al., 2005). COI sequencing was chosen over cytochrome b because COI amplification produces a shorter PCR product that is easier to sequence.
To detect hybrids between *S. laietanus* and *S. cephalus*, the sequencing of the nuclear RAG1 gene will be used, as done in French populations, but results should be confirmed by additional markers.

4. Results and discussion

Results from two sampled locations in the Muga River (31 chub specimens) using, the mitochondrial marker COI detected only *S. laietanus* haplotypes at Albanyà, but some *S. cephalus* ones where present in Cabanes. Future analyses with the RAG1 gene will inform on the presence of hybrids or the coexistence of both species without admixture.

5. Conclusions

Based on mitochondrial markers, apparently native Catalan chub populations may be present in the Catalan basins, but the coexistence with *S. cephalus* may be threatening the genetic integrity of these populations. Hybridization between the two species should be confirmed by future nuclear genotyping.

6. Bibliography

Doadrio, I., Kottelat, M., & de Sostoa, A. (2007). Squalius laietanus, a new species of cyprinid fish from north-eastern Spain and southern France (Teleostei: Cyprinidae). *Ichthyological Exploration of Freshwaters*, *18*(3), 247–256.

Perea, S., Böhme, M., Zupančič, P., Freyhof, J., Šanda, R., Özulu, M., Abdoli, A., & Doadrio, I. (2010). Phylogenetic relationships and biogeographical patterns in Circum-Mediterranean subfamily Leuciscinae (Teleostei, Cyprinidae) inferred from both mitochondrial and nuclear data. *BMC Evolutionary Biology*, *10*(1). https://doi.org/10.1186/1471-2148-10-265.

Rose, M., Dettaï, A., Lefèbvre, S., Blanc, L., Poulet, N., Baudier, O., Hautecoeur, M., & Denys, G. (2020). *Upstream as a sanctuary for the French populations of catalan chub Squalius laietanus (Teleostei , Leuciscidae) threatened by the allochtonous European chub S. cephalus*. [Poster presentation] VII Congreso Ibérico de Ictiología (SIBIC) Conference 2020, Santiago de Compostela, Spain. https://borea.mnhn.fr/fr/upstream-sanctuary-french-populations-catalan-chub-squalius-laietanus-teleostei-leuciscidae.

Ward, R. D., Zemlak, T. S., Innes, B. H., Last, P. R., & Hebert, P. D. (2005). DNA barcoding Australia's fish species. *Philosophical transactions of the Royal Society of London. Series B, Biological sciences*, *360*(1462), 1847–1857. https://doi.org/10.1098/rstb.2005.1716.

THE EFFECT OF BIOFILM FORMATION STRATEGIES ON METHANOGENIC ACTIVITY AND RESILIENCE TO OXYGEN INTRUSION

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Keywords: biofilm, complex microbial communities, electrochemistry, methanogenesis, oxygen exposure

1. Introduction

Methanogens have gained great biotechnological interest since they are able to use carbon dioxide (CO_2) and convert it into energy-containing methane (CH_4) (Buan, 2018; Nevin et al., 2011). One strategy to exploit their ability is the use of bioelectrochemical systems (BES), but this presents limitations such as biofilm formation on the cathode surface and the sensitivity of methanogens towards oxygen (O_2) intrusions. So, we aimed to analyse the conversion of CO_2 into CH_4 with three enriched methanogenic communities formed by conventional (organic and inorganic media) and electro-assisted procedures, and their recovery after transient O_2 intrusions.

2. Methodology

Methanogenic enrichments were obtained from three different sources (paddy field, hollow tree pond and anaerobic sludge) and maintained in both heterotrophic and autotrophic conditions. Conventional and electro-assisted strategies were used to ensure biofilm formation on conductive surfaces (electrodes). The former consisted of the growth of methanogenic enrichments directly in contact with the electrodes. The latter were done using a bioelectrochemical system (BES) reactor, which consisted of three-neck bottles with two chambers (anode and cathode) separated by a cation exchange membrane. Carbon rods were used as sacrificial anodes and independently connected pieces of carbon felt were used as cathodes. Bioelectrochemical systems were controlled by a potentiostat and operated at -0.8V *vs*. SHE (Standard hydrogen electrode). Methane production rates were calculated in each condition to check for its resilience to O_2 intrusion. Also, microbial community composition and biofilm formation were analysed by 16S rRNA sequencing and qPCR, respectively.

3. Results and discussion

Methane production rates in heterotrophic and autotrophic conditions were statistically compared resulting in non-significant differences. Therefore, methanogens maintain the rates at which they can produce CH_4, independently of the presence or absence of organic matter. Methane production rates were lower after O_2 intrusion in four of the nine tested conditions. In all conditions, methane production rates recovered after re-establishing anaerobic conditions. Electro-assisted enrichments presented higher methanogenic activities and showed higher resilience to O_2 intrusions. The composition of the methanogenic community and the presence of potential O_2 scavengers in biofilms could explain the observed differences in microbial activities.

4. Conclusions

This study supports the role of O_2 scavengers and their potential benefit in the use of bio-cathodes in BES. Our findings demonstrate that the use of heterotrophic or autotrophic conditions do not affect methanogens production and biofilm enrichment strategies are viable and can be engineered to mitigate the harmful effects of O_2.

5. Bibliography

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SESSION 2.

AGRICULTURE FOOD, BIOTECHNOLOGY AND NUTRITION

SUBSTITUTION OF ALLERGENIC COMPOUNDS IN THE FORMULATION OF PORK LIVER MOUSSE

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[1] *Universitat de Girona*

Keywords: Allergenic compounds, mousse, pork liver, protein extract, techno-functional properties

1. Introduction

Pork liver stands out for its richness in proteins of high biological value, mineral elements and vitamins (Feliu-Alsina and Saguer, 2023). However, hard texture and strong flavour make it an unappetizing product, which translates into low direct consumption. This has led to its use as bulking agent or to obtain bioactive composts and/or techno-functional ingredients. It has been shown that under suitable pH conditions it is possible to obtain liver protein extracts with good surface properties, particularly to form and stabilise foams, which makes them good candidates to replace some of the allergenic ingredients in the formulation of some food products such as liver mousse (Feliu-Alsina and Saguer, 2022). In a mousse the lipid fraction comes mainly from butter and the foaming agent from egg albumen. Replacing them with lard/pork fat and protein liver extract, respectively, is a strategy to avoid possible allergenic or intolerant-generating compounds present in the dairy/egg products.

2. Methodology

Pork liver mousse was made following a non-industrial recipe. First, pork liver extract replaced part of the pork liver and egg albumen. Then, the substitution of butter by pork lard and pork fat in different proportions was tested and analysed. The best formulation was chosen to test the use of manioc starch (5, 6 and 7%) to improve the texture of the mousse.

3. Results and discussion

Twenty percent of the pork liver and all the egg albumen were substituted by pork liver protein extract. A 60:40 proportion of lard to pork fat in substitution of butter gave similar characteristics to the original mousse, with a better texture than the original. However, the pork fat made the resulting mousse smell like pork, prompting partial replacement with manioc starch. A formulation with 7% of manioc starch resolved the pork odour and gave texture results similar to the analogue with pork fat but with a lower amount of lipids.

4. Conclusions

The pork liver extract obtained at pH 4.5 makes it possible to reduce the amount of fresh liver in the formulation of mousse and to eliminate egg albumen. Using a mixture of lard and pork fat (60:40), it is possible to eliminate the butter indicated in the original formulation. However, the smell is unpleasant. Replacing part of the pork fat with a 7% starch solution eliminates undesirable odours and reduces the amount of fat in the mousse, although its texture could be improved by using other hydrocolloids with thickening properties.

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DEVELOPMENT OF A BENEFICIAL MICROBIAL CONSORTIA WITH PLANT BIOSTIMULANT EFFECT

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Keywords: bacteria, microbial consortia, plant biostimulant, sustainable agriculture

1. Introduction

A biostimulant is defined as any substance or microorganism which is able to enhance the efficiency of the plant nutrient uptake without providing nutrients directly and the plant's tolerance against abiotic stresses and to improve the crop quality and its nutritional content (du Jardin, 2015). Some bacteria have shown to be beneficial for the plant because they can participate in biogeochemical cycles, nutritional supply, plant nutrient uptake, plant defense, stress tolerance and growth regulation. This is a result of their capacity to fix atmospheric nitrogen, producing iron chelating siderophores or specific enzymes and their ability to solubilize phosphates and synthetize phytohormones, among others.

The use of microbial consortia, which consist of an association of two or more beneficial microorganisms that work synergically in a complex system, could be a potential tool to develop new crop-customized products for sustainable agriculture (Seenivasagan & Babalola, 2021). The aim of this study is the isolation and characterization of bacteria to develop a microbial consortia with plant beneficial activity that can be applied as biostimulant in agriculture.

2. Methodology

First, an exhaustive investigation about microbial species with relevant attributes to develop microbial consortia with biostimulant activity was carried out. Afterwards, different types of crops (soil, rhizosphere, and roots) were sampled to isolate the microorganisms with selective and differential medium. The isolates were glycerinated and stored. From the isolated bacteria, different biochemical and molecular tests were carried out to identify and characterize them for relevant attributes as biostimulants.

At the same time, some previously characterized strains from the collection of the Centre for Innovation and Development in Plant Health (CIDSAV) were selected as candidates in the

development of the microbial consortia. Finally, some synthetic microbial consortia will be designed and tested.

3. Results and discussion

This study expected to isolate a set of microorganisms with suitable characteristics to be used in the development of a microbial consortia with plant biostimulant activity.

Some of the isolated microorganisms are expected to present interesting characteristics such as being able to fix atmospheric nitrogen, to produce iron chelating siderophores and specific enzymes, to solubilize phosphates, or to synthetize phytohormones. After the design of different synthetic consortia, the compatibility between the isolates will be a key attribute in the selection.

4. Conclusions

The approach used in this study has led us to design and select a putative synthetic microbial consortia with potential as a plant biostimulant product.

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CHARACTERIZATION OF DIFFERENT LUPINE VARIETIES TO OBTAIN PROTEIN ISOLATES FOR FOOD APPLICATIONS

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Keywords: anti-nutritional factors, food security, *Lupinus* spp., protein content, sustainability

1. Introduction

The loss of natural resources, climate change, and global food insecurity are three of our biggest challenges. With the growing demand for protein, there is a need to identify plant-based sources that are nutritious and sustainable. Lupine is a legume native to the Mediterranean region with a high protein content. Due to its nutritional profile and potential to reduce Europe's reliance on soy (Gollnow & Lakes, 2014), it is an interesting area of research. The objective of this study is to characterize the seeds of various *Lupinus sp*. and identify those with the greatest potential from both a nutritional and technological point of view.

2. Methodology

To identify and select *Lupinus sp*. varieties with superior nutritional and technological interest, three cultivars of *Lupinus albus*, three of *Lupinus luteus,* and two of *Lupinus angustifolius* were characterized. This included the analysis of the proximate composition, fatty acid composition, and the content of different antinutritional factors (alkaloids, phenolic compounds, phytic acid, and saponins).

3. Results and discussion

The protein content of the different varieties of *Lupinus spp*. studied was between 38-44% DM which is close to that of soybean (Stone et al., 2019). From those, *Lupinus albus* var. Celina was the cultivar with a higher protein content (44.27%).

The fat content of the different varieties of *Lupinus spp*. studied ranged from 5.5 – 9.9% DM. Compared to soybean, *Lupinus spp*. had significantly lower fat content (Stone et al., 2019). *Lupinus luteus* var. Acos and var. Tremosilla had the lowest fat content among those studied.

Lupinus luteus var. Acos and var. Tremosilla also showed the highest protein:fat ratio. This ratio may serve as an indicator for selecting the most suitable cultivar to obtain a protein isolate in terms of protein yield, sustainability, and technological procedure convenience.

The content of antinutritional factors in the flours of the different lupine varieties were as follows: alkaloids (0.731-0.004%), saponins (4.25-2.67%), total phenolic compounds (0.32-0.16%) and phytic acid (1.39-0.74%).

4. Conclusions

L. luteus var. Acos and var. Tremosilla were the cultivars that exhibited the highest protein:fat ratio. Nevertheless, it is essential to consider the remarkable concentration of antinutritional factors present in these cultivars, which may impact food quality and safety. The levels of these compounds must be minimized during the technological processing, to ensure the production of safe and high-quality food products.

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STUDY OF THE CO-OCCURRENCE OF BREAST MYOPATHIES IN BROILERS

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Keywords: meat quality, poultry, spaghetti meat, white striping, wooden breast

1. Introduction

The rising incidence of white stripping (WS), wooden breast (WB) and spaghetti meat (SM) myopathies in poultry is concerning for the sector, causing substantial product devaluation and economic losses. The cause of these three myopathies seems to be related, and breasts affected by multiple myopathies at the same time are documented (Barbut, 2019; Che et al., 2022). Nevertheless, the association between these myopathies has not been statistically evaluated. The present work has studied the co-occurrence of the three most important myopathies in commercial broilers.

2. Methodology

A total of 240 chicken carcasses were selected in a commercial slaughterhouse for the presence of breast myopathies (60 WS, WB, SM and control). Carcasses were than analysed to confirm the myopathy and evaluate its severity according to Kuttappan et al. (2016) and Petracci et al. (2019). The independence between the presence and severity of myopathies was evaluated using a chi-squared test and their correlation using Kendall's rank.

3. Results and discussion

Among the affected breasts, 54.8% presented more than one myopathy, 39.7% presented two and 15.1% three. Che et al. (2022) also observed a high percentage of co-occurrence: 55.5% with two and 28.1% with three myopathies. Breasts with WB alone occurred less than expected assuming independence (2.91% vs. 3.86%). On the other hand, myopathies presenting only severe SM occurred more than expected (5.00% vs. 2.97%). A chi-squared test showed a dependency between WB and WS ($p<0.001$) and no relationship between SM and WB or between SM and WS ($p>0.05$). Kendall's correlation rank between WB and WS was 0.24 ($p<0.01$), confirming the relationship between these myopathies and supporting the theory that they are manifestations of the same underlying disease (Sihvo et al., 2017).

4. Conclusions

The results show an association between WB and WS, supporting a common pathogeny. However, the lack of relationship between SM and the other myopathies indicates a certain independence between them. These findings will be useful to detect and classify meat affected with myopathies at the commercial level, making it more appropriate to jointly characterize WB and WS and individually approach SM. Nevertheless, the high co-occurrence between the three myopathies is important and must be considered.

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DEVELOPMENT OF EFFECTIVE NUTRITION INFORMATION COMMUNICATION SYSTEMS

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Keywords: consumer behaviour; food labelling; nutrition information; Spanish population

1. Introduction

Information provided by food labels is sometimes difficult for consumers to understand (Giró-Candanedo et al., 2022). Therefore, it is important to know the factors in consumers' use of nutritional information. The aim of this work was to study the factors that influence the use and/or reading of nutrition information, and to develop new and more effective systems to inform consumers about the nutritional composition of products.

2. Methodology

The study was organized into different sequential stages. The objective of the **first stage** was to assess consumers' perceptions and beliefs about food nutrition labels and how frequently they read them. To do so, a questionnaire was used and an ethnographic study was carried out. The objective of the **second stage** was to develop more effective communication systems to stimulate the reading of food labels and improve consumers' understanding of this information. To that end, creativity sessions and focus groups were carried out. In the **third stage** of the study, an evaluation was conducted on the three communication systems that showed the most promise for success. The objective of this final stage was to maximize the effectiveness of the transmitted messages and validate the developed communication systems. To do that, a semiotic analysis of the communication systems was carried out. The communication systems were validated by means of personal interviews that included a combination of implicit and explicit measurements. All participants recruited in this work were involved in food purchasing within their households.

3. Results and discussion

Results of the **first stage** showed that dietary patterns, nutrition knowledge and sociodemographic characteristics strongly influence label reading. In the **second stage** of the study, more than 100 ideas of new communication systems were generated in creativity

sessions. Results obtained from the focus groups showed that, in general, the ideas were described as "*Visual*" and "*Easy to understand*". Results obtained in the semiotic analysis (**third sage**) showed that more graphic communication systems were better understood in terms of nutritional information and that they provided more nutritional information about the product. Results obtained in the validation test showed that visual attention and the cognitive rated required for information processing were different between the different systems explored.

4. Conclusions

Nutritional information communication systems containing colours, percentages and the name of the nutrient seems to favour the understanding of the nutritional properties of foods.

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EVALUATION OF THE TECHNOLOGICAL AND NUTRITIONAL SUITABILITY OF UNDERUTILIZED EUROPEAN CROPS FOR THE DEVELOPMENT OF NEW PLANT-BASED BEVERAGES AS MILK SUBSTITUTES

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Keywords: Digestible Indispensable Amino Acids Score (DIAAS), enzymatic liquefaction, plant-based beverages, underutilized crops.

1. Introduction

Plant-based beverages are used as dairy milk alternatives. However, only some soy-based beverages can be considered as alternatives in terms of protein content. When we consider Digestible Indispensable Amino Acid Score (DIAAS), soy-based beverages have lower values than milk (Singhal et al., 2017; Walsh & Gunn, 2020). Considering DIAAS when developing new vegetable drinks can result in drinks with nutritional values comparable to milk. This study aims to design and optimize the process to produce vegetable drinks from six underutilized European crops and evaluate the combination to achieve best DIAAS values. These crops are buckwheat, fava bean, hull-less barley, lupin, oat, and triticale.

2. Hypothesis / problem

The main hypothesis is that there exists a blend of underutilized crops, suitable for developing plant-based beverages with a high-quality organoleptic profile and a protein quality similar to milk. Furthermore, the production method permits the efficient production of the plant-based drink.

3. Methodology

The production process of plant-based beverages was based on preliminary experiments. We established a fixed ratio of flour solids and water to form a slurry with 30% total solids and selected the appropriate enzymes and their dosage according to manufacturer's specifications. Plant based beverages were optimized following a response surface design (RSD) using liquefaction time and temperature as factors, and drink yield, drink total solids and drink viscosity as response variables.

4. Expected results and discussion

Two different production processes were designed, one for cereals and buckwheat and another for leguminous crops. For the first group, the liquefaction temperature ranged from 50ºC to 90ºC, and liquefaction time from 15 to 90 minutes. For the second group, liquefaction temperature ranged from 40ºC to 60ºC, and liquefaction time from 15 to 90 minutes. Measuring drink yield, drink total solids and drink viscosity, we expected to determine an optimized range of liquefaction time and temperature for each crop. To achieve the optimized process, we are going to model the effect of liquefaction time and temperature on the measured parameters. These models will be used to generate response surface contour maps. Finally, DIAAS values for each beverage will be calculated using data from bibliography, and the best blend to achieve better DIAAS values will be identified and produced.

5. Conclusions

We expect to successfully produce different plant-based beverages with attractive organoleptic profiles. In addition, we will be able to design a blend that achieves DIAAS values similar to milk.

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COMMUNICATING FOOD SUSTAINABILITY TO CONSUMERS: EXPLORING THE USE OF IMPLICIT APPROACHES TO ASSESS INSTITUTIONAL CAMPAIGNS

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Keywords: communication, future, implicit methods, sustainability

1. Introduction

Consumers' increasing reflectivity in their food decisions has broadened their understanding of sustainability. There is a growing need to provide relevant information to citizens that enable food choices that match their values and beliefs.

2. Problem

How consumers perceive messages promoting the change to more sustainable consumption is an issue often neglected when studying changes in attitudes, preferences and choices around food. To gain a deeper understanding of consumer motivations and expectations the combination of explicit methods (self-reported measures, i.e., questionnaires) and implicit methods (sensor-based measures, i.e., neuro-physiological indicators) can help capture the complete food experience. This includes pre-consumption experiences (de Wijk & Noldus, 2021) such as consumer's exposure to institutional campaigns.

3. Methodology

This exploratory study examines the electrodermal and neuronal responses from individuals (n=25) exposed to a video stimulus of an institutional campaign promoting aquaculture. Apart from general information, the video included sequences about the positive outcomes of aquaculture focusing on environmental sustainability and biodiversity, animal welfare and social impact, as well as aquaculture's commitment to the future of the planet and local communities.

Additionally, consumers' motivations were rated using explicit measures as the Single-item Food Choice Questionnaire (FCQ) (Onwezen et al., 2019), Spanish versions of the

Prosocialness Scale for Adults (Martínez-Pampliega et al., 2018) and the New Environmental Paradigm Scale (Vozmediano et al., 2005).

4. Results and discussion

Mean frontal alpha asymmetry, the difference between right and left alpha activity over frontal regions of the brain, identified the sequence with references to the future of the planet and local communities as the one that elicited more negative affect, followed by social impact, animal welfare, and environmental sustainability and biodiversity. General information about aquaculture had the less negative affect. Differences varied with age. Younger adults had more adverse responses, especially when the video referred to the future and social dimensions of aquaculture. Arousal levels, measured as skin conductance response peaks per minute, were distributed evenly across all video sequences.

When evaluated explicitly, pro-environmental and prosocial values were predominant among participants. Environmental issues, animal welfare and social justice were judged as more important than price, convenience, familiarity, mood or weight control. Explicit measures showed no significant differences for age group or gender.

5. Conclusions

Implicit methods can be extremely useful when assessing the evidence-based effectivity of sustainability communication aiming to improve campaigns supporting informed consumer decision making.

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SESSION 3.
BIOACTIVE PEPTIDES

STRUCTURAL ELUCIDATION OF PEPTIDE CONJUGATES AND STUDY OF THEIR INTERACTION WITH LIPID MEMBRANES

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Keywords: antimicrobial peptide, bacterial membrane, molecular dynamics, NMR, secondary structure

1. Introduction

Antimicrobial and plant defence elicitor peptides have gained a lot of interest in recent decades as novel tools to combat plant diseases. Recently, our group has developed a library of peptide conjugates that are both antibacterial and capable of inducing plant defence mechanisms. (Oliveras, 2022). The mechanism of action of these peptides is determined by their physicochemical properties such as the net positive charge, the amphipathicity and the secondary structure.

In this work, we selected a set of six peptide conjugates, including highly and poorly active sequences and with a range of hemolysis. The aim was to relate the biological activity with their structure and the way they interact with lipid membranes. In particular, the secondary structure of these conjugates was elucidated by nuclear magnetic resonance (NMR) and molecular dynamics (MD).

2. Methodology

Elucidation of the secondary structure was carried out by NMR in presence of 30% CF_3CD_2OD (TFE-d_3) as well as in anionic SDS-d_{25} and zwitterionic DPC-d_{38} micelles. It was predicted by the Chemical Shift Index based on the ^{1}H, ^{13}C and ^{15}N chemical shifts and confirmed by NOESY and TOCSY correlations (Hafsa, 2015). Several replicas of 500 ns of accelerated MD simulations were performed for selected peptide conjugates.

3. Results and discussion

Peptide conjugates were synthesised by incorporating an antimicrobial peptide at the N- or C-terminus of a plant defence elicitor peptide. They were tested *in vitro* against different plant pathogenic bacteria, and their hemolytic activity was also assessed. These peptide conjugates were characterized by NMR in presence of TFE-d_3, SDS-d_{25} and DPC-d_{38} to mimic bacterial membranes. Moreover, the addition of paramagnetic probes determined the residues involved in the interaction with the micelles. The results agreed with those observed by MD simulations.

In the case of the most active conjugates, the antimicrobial fragment folded into an α-helix, whereas the elicitor moiety remained unstructured as a random coil. In addition, they have low hydrophobic moment and a moderate charge. In contrast, the sequences with the worst biological activity profile were completely structured as an α-helix and they have significantly higher hydrophobicity and charge.

4. Conclusions

This study points out the significance of a moderate amphipathic character and a positive charge for an optimal interaction of peptide conjugates with bacterial membranes. This knowledge will allow us to rationally design new peptides with a better biological profile.

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SYNTHESIS OF PEPTAIBOLS AS POTENTIAL CANDIDATES AGAINST *Xylella fastidiosa*

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

1. Introduction

The Mediterranean agricultural system is threatened by the spread of phytopathogens and the difficulty to combat them. Among bacterial phytopathogens, the Gram-negative *Xyllela fastidiosa* is of particular interest because it is responsible for severe diseases, such as the olive quick decline syndrome that has caused huge economic losses in Europe. Antimicrobial peptides are considered good candidates for plant disease control, being excellent alternatives to pesticides (Badosa, 2022).

In this study, we focused our attention on peptaibols because they have been described as exhibiting antimicrobial activity against several plant pathogens, especially against Gram-positive bacteria, filamentous and yeast-like fungi. We have selected peptaibols trichogin GA IV (Caracciolo, 2023) and trichokonin VI (Li, 2014) and designed new derivatives. On the other hand, we also considered 1036, with high activity against *X. fastidiosa* (Moll, 2021), as a parent peptide to design peptaibol-type analogs. 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, analyzed 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-nine peptaibols were synthesized on solid phase and obtained in high purities (>99%). They included trichogin GA IV, trichokonin VI, 13 trichogin GA IV analogs, 1 trichokonin VI analog and 13 derivatives of 1036. The synthesis of these peptaibols and their biological activity will be presented and discussed.

4. Conclusions

In summary, 29 peptaibols derived from trichogin GA IV, trichokonin VI and 1036 were synthesized. It is expected to identify compounds with activity against *X. fastidiosa* and low toxicity.

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PEPTIDES WITH *IN VITRO* ANTIBACTERIAL ACTIVITY AGAINST THE PLANT PATHOGENIC BACTERIUM *Xylella fastidiosa*

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Keywords: Antimicrobial peptides, plant pathogens, solid-phase synthesis, v-qPCR, *Xylella fastidiosa*

1. Introduction

Xylella fastidiosa is a bacterial plant pathogen that has emerged as one of the main threats to agricultural crops. It is responsible for severe, economically important plant diseases. This Gram-negative bacterium colonizes the xylem of host plants and is transmitted by xylem-sap-feeding insects (Purcell, 2013). A wide range of treatments to fight these diseases are being examined. They address the bacterium, the infected plant, or the vector. However, up to now, no effective treatment has been found. In this context, antimicrobial peptides (AMPs) have emerged as potential candidates to control this bacterium (Liang et al., 2020). In this study, 23 peptides were selected and assessed for their antibacterial activity against *X. fastidiosa* subsp. *fastidiosa* (*Xff*) IVIA 5387.2, as well as, for their hemolysis and phytotoxicity.

2. Methodology

Peptides were synthesized on solid phase using a standard Fmoc/*t*Bu strategy, purified by reverse phase column chromatography, lyophilized, analyzed by HPLC and characterized by mass spectrometry.

The *in vitro* bactericidal activity against *Xff* was determined by a contact test combined with a viable-quantitative PCR (v-qPCR). Three biological replicates of the corresponding peptide dilution were mixed with the *Xff* suspension and were incubated for 3 h at room temperature. Each sample was treated with PMAxx, incubated in the dark at room temperature for 8 min with manual shaking, followed by photoactivation during 15 min. Afterwards, DNA was extracted and analyzed with a TaqMan-based qPCR assay based on the 16S rRNA sequence (Baró et al., 2020).

Phytotoxicity of peptides was evaluated in *Nicotiana tabacum* by infiltrating them into the mesophile of leaves. Results were determined by measuring the lesion diameter. The hemolytic activity of peptides was assessed by analyzing the hemoglobin release from erythrocyte suspensions of horse blood.

3. Results

Peptides were obtained in excellent HPLC purities (>90% after purification) and were characterized by mass spectrometry. Their antibacterial activity is being tested against *Xff* 5387.2 using a contact test coupled with v-qPCR in officially authorized laboratories under biosafety level II+. Furthermore, the toxicity of the peptides is being assessed against erythrocytes and tobacco leaves.

4. Conclusions

The peptides were successfully synthesized manually on solid phase and purified by reverse phase column chromatography. Their identity was confirmed by mass spectrometry. It is expected that this study will provide peptides with bactericidal activity against *Xff*, low hemolysis and phytotoxicity. These peptides would be good candidates for the development of new agents to control plant diseases.

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PEPTIDES AS PLANT DEFENSE ELICITORS ON ALMONDS (*Prunus dulcis)*

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Keywords: flg22, peptides, plant defense elicitors, plant immune response, *Prunus dulcis*

1. Introduction

Prunus dulcis is an economically important crop worldwide, and Spain was the second largest producer of almonds in 2021 (FAO, 2021). This crop can be affected by quarantine diseases resulting in severe economic losses (Baró et al., 2021). Moreover, since Europe is migrating to more sustainable agricultural practices by reducing the use of conventional chemical pesticides (directive 2009/128/EC), there is a need to find eco-friendly alternatives.

Peptides can be promising candidates due to their low environmental impact and their potential to be plant defense elicitors inducing a priming state (Malik et al., 2020). Priming allows a defense response upon infection, which could prevent the development of diseases. An example of plant defense elicitor is a fragment of flagellin, **flg22** (Felix et al., 1999).

2. Hypothesis

We hypothesize that **flg22** could elicit a defense response in *P. dulcis* because it has been described as a defense elicitor in other plant models. If so, a screening platform will be developed to identify new peptides as plant defense elicitors.

3. Methodology

F**lg22-NH$_2$** was applied by spray and endotherapy on *P. dulcis* plants and the effect on the transcriptome was analyzed through RNA-sequencing at 6 and 24 h post treatment (hpt). Differently expressed genes (DEGs) related to defense responses were selected and validated by RT-qPCR. In addition, the effect of the three methods of peptide application (spray, endotherapy and infiltration) and of sampling time (1, 3, 6 and 12 hpt) on the expression of these genes was assessed by RT-qPCR. Finally, a total of 25 peptides were tested to determine their plant defense elicitor activity in *P. dulcis* by RT-qPCR using **flg22-NH$_2$** as reference.

4. Results and discussion

After RNA-seq data analysis, a total of 98 DEGs related to defenses were identified at 6 hpt, confirming that **flg22-NH₂** is a plant defense elicitor in *P. dulcis*. Fifteen DEGs were selected as marker genes related to plant defenses and their expression levels were evaluated through RT-qPCR. These results correlated with the RNA-seq analysis. Application of peptides by endotherapy produced the overexpression of the highest number of genes, most of them being overexpressed after 6 hpt. Twenty-five peptides were tested. Results led to the classification of peptides into 5 groups. Remarkably, one of them (5 peptides) caused a stronger defense response than **flg22-NH₂**.

5. Conclusions

A screening platform to identify plant defense elicitors was set up in *P. dulcis*. This resulted in the identification of five peptides with a stronger defense response elicitation than **flg22-NH₂**.

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Nicotiana benthamiana AS A MODEL PLANT TO STUDY THE PATHOGENICITY AND CONTROL METHODS OF X*ylella fastidiosa*

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Keywords: model plant, *Nicotiana benthamiana, Xylella fastidiosa*

1. Introduction

Xylella fastidiosa is a plant pathogenic bacterium that has been among the most threatening in agriculture worldwide in recent years, causing significant yield losses in a large amount of economically important crops of the Mediterranean region (like olive, almond, vine, and citrus) (Almeida et al., 2019). Finding a model plant host for *Xylella fastidiosa* and an infection method that mimics reality as closely as possible is essential to study the disease and potential control methods because woody host plants have a slow development of the disease and the appearance of symptoms can take several months (Saponari et al., 2017). One such method is the endotherapy system, which enables the inoculation of a predetermined concentration of *X. fastidiosa* cells directly on the vessels of plants (Baró et al., 2021). *X. fastidiosa* has been studied using a variety of plant models, like *Catharanthus roseus*, *Medicago sativia*, *A. thaliana*, and *Nicotiana tabacum,* but some limitations have been found, like limitations in the systemic colonization, delays in the appearance of the symptoms or difficulties with the reproducibility of assays (Baró et al., 2022).

2. Methodology

Nicotiana benthamiana plants infection was performed with a high precision microinjector. Three inoculations of 10 µL each were done in a section of 3 cm at around 15 cm above the substrate level (Baró et al., 2021). To determine the movement of the pathogen, 16 cm of material was sampled above the inoculation points (upward 1 and 2 zones, 8 cm each zone) and 8 cm below (downward zone). A viability-qPCR was performed to analyse the levels of *X. fastidiosa* in the sap, and a TaqMan-based qPCR was used to quantify the total number of remaining cells in the stem.

3. Results and discussion

The population dynamics of *X. fastidiosa* in inoculated *Nicotiana benthamiana* plants showed similarities with those observed in woody host plants (such as almonds) in a shorter time. Symptoms related to the infection were observed a few weeks after the infection. In the same way, when studies were carried out testing the efficacy of different compounds against *X. fastidiosa*, the results were similar to those obtained with the wooden plants. Also, it shows good reproducibility in the results obtained between the different assays.

4. Conclusions

Nicotiana benthamiana plants offer benefits over previously used plant models for studying *Xylella fastidiosa* dynamics in plants, evaluating the effectiveness of various chemicals against *X. fastidiosa*, and other studies as a step before field assays.

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ANTIMICROBIAL PEPTIDES AS POTENTIAL DEFENCE ELICITORS IN THE MODEL PLANT *Nicotiana benthamiana*

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Keywords: Antimicrobial peptides, defence elicitors, *Nicotiana benthamiana*, plant pathogens, solid-phase synthesis

1. Introduction

Fastidious plant pathogens, such as *Xylella fastidiosa*, affect a wide range of hosts and cause severe diseases that result in huge economical losses in agricultural crops (EFSA 2018, Moll et al. 2022). For this reason, there is increasing interest to find sustainable and effective solutions to fight these pathogens. A promising strategy is the use of antimicrobial peptides (AMPs), which are known to display antibacterial and antifungal activity against plant pathogens (Oliveras et al. 2022). AMPs can also act as plant defence elicitors, being useful in preventive treatments (Malik et al. 2020).

Based on the above, in the present work we planned to study the capacity to trigger plant defence responses in *Nicotiana benthamiana* of peptides **flg22, 1036, BP100, BP178, HPAG-23, FV7** and **RJK2**. A previous optimization study to determine the best conditions for the peptide treatments was required.

2. Methodology

Peptides were synthesized manually by a solid-phase protocol following an Fmoc/*t*Bu strategy. They were purified by reverse phase column chromatography, lyophilized, analysed by HPLC, and characterized by mass spectrometry. The optimization study was performed using **BP178**. Expression of 11 genes with RT-qPCR was determined at 6 and 24 h after peptide treatment. Peptide application consisted of 1 or 3 shots each time. Leaf samples were collected and frozen in liquid nitrogen. Then, RNA was extracted and stored at -80ºC until RT-qPCR was performed. Optimized conditions of assay were used to analyse the other peptides.

3. Results and discussion

Peptides were obtained in high purities (> 90%). According to previous studies in *Prunus dulcis*, a similar gene expression is expected at 6 and 24 h after peptide application. Furthermore, as with BP178 peptide, it is also expected that some of the seven peptides studied (**flg22, 1036, BP100, BP178, HPAG-23, FV7, RJK2**) will act as elicitor peptides inducing the expression of defence and stress-related genes in *N. benthamiana*.

4. Conclusions

AMPs are a promising solution to fight against plant pathogens. The peptides used in this work were successfully synthesized in high purities. Best plant defence elicitor peptides could be considered good candidates to be used in preventive treatments to control plant diseases.

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SESSION 4.
FOOD TECHNOLOGY

EFFECT OF EXTRUSION CONDITIONS ON THE PHYSICOCHEMICAL AND SENSORY CHARACTERISTICS OF HIGH-MOISTURE MEAT ANALOGUES FROM PEA PROTEIN ISOLATE

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Keywords: alternative proteins, high moisture extrusion, meat analogues, sensory, texture

1. Introduction

Development of high-moisture extrudates (HME) with meat-like texture is gaining interest in the plant-based food sector. However, HME characteristics are highly influenced by process conditions. The aim of this study was to evaluate the effect of extrusion process parameters on the texture and moisture content of HME obtained from pea protein isolate and to define optimal extrusion conditions to achieve meat-like textures. Sensory texture profile of two selected HME was compared to chicken meat and a commercial soy-based meat analogue.

2. Methodology

HME were elaborated using pea protein isolate and a laboratory-scale twin-screw extruder, following a response surface design (RSD) varying three factors: barrel temperature (T), screw speed (SS) and ratio of water feed rate to solid feed rate (WFR/PFR). Cooked chicken breast and a commercial soy-based meat analogue were also evaluated. Moisture content and shear textural properties were measured. Sensory texture profile of two selected HME was compared to cooked chicken and commercial samples. RSD results were analysed using JMP 16 software. ANOVA and Tukey tests were performed using XLSTAT v2020.1 1.

3. Results and discussion

Moisture content and shear test parameters of HME samples were significantly affected ($p<0.05$) by WFR/PFR ratio and barrel T. Figure 1 shows the effect of WFR/PFR ratio and barrel T on predicted shear parameters. Texture of cooked chicken (striped areas in Figure 1) can only be achieved for all textural parameters simultaneously by applying T between 145-165ºC and WFR/PFR ratio between 1.4 and 1.2 (darker areas in Figure 1).

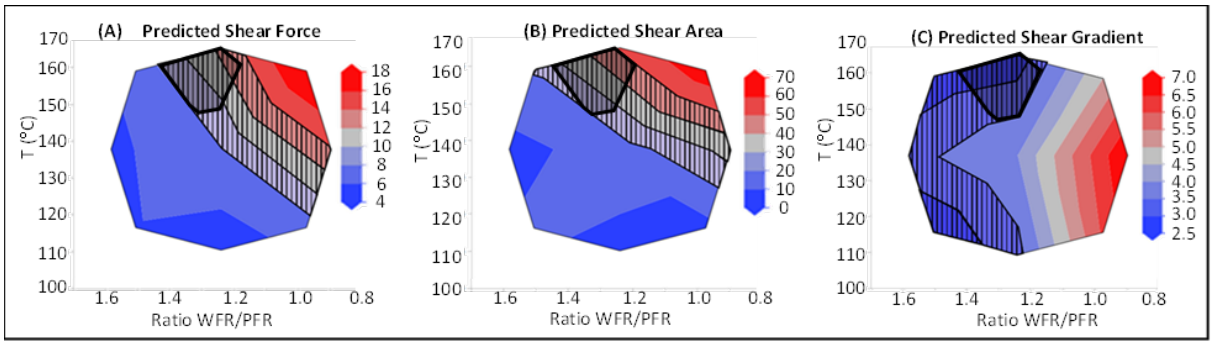

Figure 1. Contour plots fitted to shear force (A), area (B) and gradient (C) as a function of WFR/PFR ratio and T. Striped areas ▨ correspond to chicken breast values for each parameter (reference), and darker areas ▭ indicate common reference areas for all parameters.

The sensory texture profile of two selected samples elaborated at [T, SS, WFR/PFR]: [165ºC, 650 rpm, 1.2] and [159ºC, 456 rpm, 1.0] was more similar to cooked chicken than the commercial soy-based sample. However, gumminess and moisture perception were significantly higher than both cooked chicken and the commercial product. These attributes could be improved by adding oil (Wang et al., 2022) and/or applying a seasoning process after the extrusion.

4. Conclusions

Extrusion process parameters have a significant effect on the characteristics of the product and textures similar to cooked chicken breast can be achieved. Future studies on new formulations and application of further processes to reduce dryness and gumminess are needed.

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6. Acknowledgements

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MODELING OF RADIOFREQUENCY HEATING OF PACKED LIQUID FOODS MOVING ON A CONVEYOR BELT

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Keywords: computer simulation, dielectric heating, heating rate, radiofrequency, tomato

1. Introduction

Radiofrequency (RF) technology has the potential to provide higher heating efficiency, while requiring less water and energy input than indirect tunnel pasteurization. Radiofrequency heating of liquid foods has not been extensively studied, especially in the case of in-package pasteurization (Jiao et al., 2018). The objective of this work was to develop and validate a predictive finite-element model for RF heating of packed fluid foods on a conveyor belt.

2. Methodology

A staggered through-field RF applicator equipped with a conveyor belt was used. Voltage across the electrode was estimated from stationary experiments using NaCl solutions and fitted to regression equations to simulate heating of mixtures of tomato puree, oil, and salt of varying dielectric and thermal properties, at two nominal voltages (3000 V and 5000 V) and electrode gaps (8.14 cm and 8.64 cm). The model was evaluated using the relative error of the volume average temperature during the heating process. Thermal images were obtained to analyze the temperature distribution.

3. Results and discussion

The experimental results for volume average temperatures showed good agreement with the outcome of the simulation (relative error: 3.83 %). Temperature profiles (Fig. 1) indicate a concentration of heat at the bottom and edges of the bottle, although natural convection and the shape of the container helped mitigate heat localization (Huang et al., 2018). It was determined that while simple models could accurately predict volume average temperatures, incorporating convectively enhanced conductivity was necessary to obtain accurate

temperature distributions. The heating rate was found to decrease with an increase in salt concentration due to a reduction in electric field intensity within the sample (Llave et al., 2015).

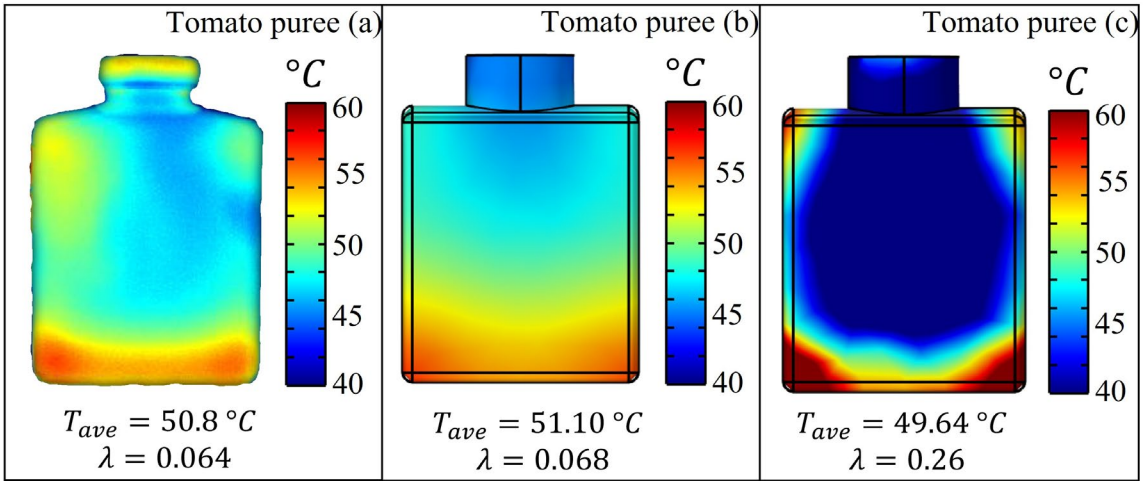

Figure 1. Experimental (a) temperature distribution of a tomato puree sample after RF treatment (5000 V, 8.4 cm gap) and finite-element models with (b) and without (c) convectively enhanced conductivity.

4. Conclusions

Results shows the potential for packed liquid foods to overcome temperature non-uniformities observed during dielectric heating of solid matrices. Further work is needed to evaluate the feasibility of RF in-package pasteurization processes with regard to microbial and sensory quality, as well as the effect of different container types.

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HOW HIGH PRESSURE PROCESSING CAN ASSURE THE FOOD SAFETY OF BABY FRUIT PUREE

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Keywords: baby food, *Escherichia coli*, high pressure processing, inactivation kinetics, predictive modelling

1. Introduction

High pressure processing (HPP) is a non-thermal food preservation technology in which food is submitted to elevated pressure (100-600MPa) for few minutes to reduce the number of microorganisms and to prolong the shelf life of food products, while preserving freshness (Podolak et al., 2020). There are several predictive models for HPP inactivation of pathogens for animal-based food products but none of them has been developed for fruit puree intended for infants (EFSA BIOHAZ PANEL, 2022).

The aim of this study was to quantitatively characterize the effect of HPP on the inactivation of *Escherichia coli* on two types of fruit puree (apple and banana), showing different acidity.

2. Methodology

Apple (pH 3.6) and banana puree (pH 4.2) were independently inoculated with E. coli CECT5947 (non-toxigenic serotype O157:H7) and CTC1029 strains at 7 log cfu/g and treated at different pressures (300-600MPa) and holding times (up to 10 min). The effect of a 24h-acid exposure before HPP was also evaluated. The best fitting primary model to the log reduction data was determined by GinaFit Tool. The one-step global fitting procedure was applied to estimate the parameters of the secondary Bigelow-type model.

3. Results and discussion

The inactivation by HPP was product (acidity) and strain dependent. After 2 min at 400 MPa, the CECT5947 was reduced by 3.21 and 0.55 log units in apple and banana puree, respectively, while higher inactivation was observed for the CTC1029 strain with 5.91 (apple) and 0.65 (banana) log reductions. The range of inactivation at 500MPa (0-10 min) in banana puree were 0.69 to 4.48 log reductions (CECT5947) and 0.06 log reductions to not detected log units (CTC1029), while in apple a total inactivation was achieved after 2 min. Interestingly, acid exposure before HPP provided certain cross-protection in CTC1029, showing less inactivation

compared with the samples pressurised immediately after inoculation. A log-linear inactivation trend was preceded by a shoulder shape in banana puree at 400-600 MPa, while a tail was observed in apple puree at 300-500 MPa.

4. Conclusions

The mathematical models can be used by baby food producers as a decision support tool to define HPP process criteria for puree meeting *E. coli* food safety standards.

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MODELLING OF SALT UPTAKE FOR SALT CONTENT STANDARDIZATION IN DRY-CURED HAM

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Keywords: dry-cured ham, non-invasive technologies, predictive models, process optimization, product standardization

1. Introduction

Salt content standardization in dry-cured ham production is complex as many factors influence salt uptake. These factors are related to the green ham characteristics and to some process parameters. Non-destructive technologies have demonstrated their feasibility to characterize hams in terms of weight, fat, and salt content (Schivazappa et al., 2017). New tools developed using data obtained from these technologies might help to standardize the salt content. The aim of this work was to study and model the salt uptake as a function of salting time and green ham characteristics (i.e., weight and fat content) using different types of hams and salting procedures and applying data obtained from non-invasive technologies. The use of these models to improve the current green ham classification systems and to select the optimal salting time to standardize the salt content of the production was also assessed.

2. Methodology

Two different types of green hams (lean and fatty hams), each one subjected to a different salting procedure (pile salted in two steps and pile salted in one step, respectively), were used in two independent experiments to evaluate and model the salt uptake during the salting process. Weight and fat content of 489 lean hams (experiment 1) and 426 fatty hams (experiment 2) were determined using a magnetic induction scanner (Ham Inspector™, Lenz, Barcelona) and divided into four different categories according to their weight and fat content. Then, the hams were pile salted at 3 ± 2 ºC into containers for 8, 11, 14 and 17 days. After each salting time, the hams were scanned again using the same scanner to determine global salt content. Salt uptake was modelled using different statistical methods. Different hypothetical scenarios, based on different combinations of green ham classification systems and salting times, were evaluated to know the best ones to reduce salt uptake variability during production.

3. Results and discussion

Salt content increased with salting time, showing an asymptotic behavior which was lower in fatty hams. In both experiments, the best models to predict the salt uptake were those obtained using multivariate linear regression, which include salting time, weight, and fat content as independent variables (Table 1).

Table 1. Salt uptake (%) predictive models obtained using different statistical methods for experiment 1 and 2.

Model Description	Variables	Equation	R_P^2	RMSEP
Experiment 1				
OLR	ST	SALT = 1.868+0.072*ST	0.336	0.343
MLR	ST, W	SALT = 6.984-0.398*W+0.069*ST	0.704	0.230
MLR	ST, W, F	SALT = 6.012-0.252*W-0.070*F+0.068*ST	0.858	0.161
Experiment 2				
OLR	ST	SALT = 1.434+0.049*ST	0.368	0.228
MLR	ST, W	SALT = 4.188-0.208*W+0.051*ST	0.501	0.204
MLR	ST, W, F	SALT = 5.025-0.193*W-0.039*F+0.054*ST	0.610	0.180

ST: salting time (in days); W: ham weight (kg); F: ham fat content (%). OLR: ordinary linear regression; MLR: multivariate linear regression.

A classification system based on the categorization of hams according to the estimated salting time leads to the lowest salt content variability, allowing a more individualized salting procedure and a more adjusted target salt content.

4. Conclusions

Salt predictive models might be a useful tool for the dry-cured ham industry to predict the needed salting time to achieve a target salt content and to reduce salt content variability. Besides, these models could also be used to simulate different process modifications that can provide reliable information without the time-consuming and costly trial and error tests.

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MORPHOLOGICAL AND FIRMNESS CHARACTERISTICS OF CROSSED IBERIAN AND PURE DUROC PIG BELLIES

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Keywords: breed, computed tomography, fat, pork, quality

1. Introduction

Belly is an important cut of pig carcasses and its morphological, compositional and mechanical characteristics influence processing and consumer acceptability. Belly characteristics depend on several intrinsic and extrinsic factors such as genetics, sex, feeding or post-mortem conditions. The Iberian pure or crossbreeds are well known for their great tendency to accumulate fat and to produce high quality products and a similar case is true for Duroc breed pigs (Font-i-Furnols et al., 2012). The objective of this study was to compare the morphological and firmness traits of bellies from Iberian x Duroc crossbreed and Duroc pure breed pigs.

2. Methodology

A total of 24 bellies were obtained from carcasses of 50% Iberian×Duroc (IB×DU, n=12) and 100% Duroc (DU, n=12) castrated pigs. After removing the bones, bellies were scanned with the computed tomography GE HiSpeed ZX/i (145 mA, 140 kV, 10 mm-thick, 512x512 matrix) to obtain the fat content considered as the volume between HU-200 and HU-20 following the methodology used by Romvári et al. (2005). The length and the width of the bellies were recorded. The thickness was also measured in the central point of each edge. Then, the skin was tensed in the same points and the final height was measured. The difference between the starting and final height was calculated to determine the firmness in terms of fat and skin separation. Moreover, the firmness was determined using the flop distance and angle using the bar-suspension method (Thiel-Cooper et al., 2001). Variance analysis was performed with SAS software (version 9.4), considering genetics as the fixed effect.

3. Results and discussion

The fat content was higher ($P<0.001$) in IB×DU bellies compared with DU bellies, confirming the tendency of Iberian pigs to accumulate more fat (Nieto et al., 2002). IB×DU bellies were

shorter (P<0.001) and thicker (P<0.10) compared to DU bellies, while their width was not significantly different. These findings may be relevant for industries producing sliced belly products since IB×DU bellies will produce less slices, but these will be thicker and fatter. The firmness measured in terms of fat and skin separation was higher in IB×DU bellies compared to DU bellies (P<0.10). Likewise, IB×DU bellies had higher firmness scores, determined as the flop distance and angle, than DU bellies (P<0.05).

4. Conclusions

The present study shows a great variation of the belly characteristics between IB×DU and DU pigs. The differences reported could be considered by industries to satisfy specific demands of each market.

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SESSION 5.
HEALTH AND SPORT

EVALUATION OF AN EDUCATIONAL INTERVENTION FORPRIMARY CARE NURSES IN THE IMPROVEMENT OF DIAGNOSIS, TREATMENT AND REGISTRATION IN THE CLINICAL HISTORY OF PEOPLE WITH VENOUS LEG ULCER: A RESEARCH PROJECT

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Keywords: chronic venous insufficiency, complex wound, educational intervention, nursing, venous leg ulcer

1. Introduction

The epidemiological data in the bibliography show important variations that are explained by registration in different databases and the variability between the codes of the International Classification of Diseases (Marinelo & Verdú, 2018). At the same time, other methodological problems in the studies, such as the lack of detection and correct identification of cases, could compromise the prevalence (Torra et al., 2004).

According to the *Asociación Española de Enfermería Vascular y Heridas* (2017), vascular ulcers have a prevalence of between 0.10 and 0.30%, with an incidence from 3 to 5 new cases per 1000 people per year. At the same time, they are injuries with high chronicity and recurrence. According to the same association, up to 40-50% remain active from 6 months to a year and approximately 10% will reach 5 years of evolution.

Of the total number of vascular ulcers, venous ulcers (VU) represent between 75 and 80%, with an estimated prevalence of between 0.5 and 0.8% and between 3 and 5% from the age of 65 (Marinelo& Verdú, 2018). A study based on real-world data (RWD) using the SIDIAP database determined a prevalence of 0.21% from age 50 for UV, increasing to 0.40% from age 60 and 1.90% from the age of 80, and an incidence of 0.23 per 1000 inhabitants/year (Homs et al., 2021).

According to Loureiro et al. (2014), the skill, knowledge, and attitudes of nurses affect their ability to assess a wound and treat associated problems, making the use of traditions and subjective information too common in dealing with the wounds they treat.

2. Hypothesis

The intervention will improve nursing skills in preventing, diagnosing, treating, and registering in the clinical history of people with lower extremity venous insufficiency.

3.Methodology

The study includes two main methodologies. The first one is descriptive, with a cross-sectional

design, where we will describe the prevalence and incidence of venous ulcers in leg and the main differential diagnoses before (2019-2022) and after (2024) the intervention. Within this phase, a still-to-be-determined number of clinical historieswill be reviewed to determine if they have recorded variables identified as relevant such as the assessment of skin changes, pulses, or treatment in the care of people with venous ulcers before and after the intervention.
The second part of the study is structured with a quasi-experimental study design without a control group,prospective, through an educational intervention prepared according to experts' recommendations and the needs detected focused on the workplace. This intervention will be evaluated with a self-administered theoretical part, evaluating knowledge with a test, and a practical part, using a simulated patient to evaluate skills.

4.Results and discussion

We expect to see an increase in the competence of nurses in assessment and treatment of this problem, increasing diagnostic labels and improving registration during assessment and follow-up.

5. Conclusions

Conclusions will be presented once the research project has been implemented.

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TIME SAVING INTERVENTION IN YOUTH BASKETBALL PLAYERS: ARE WE APPLYING THE APPROPRIATE TRAINING STIMULUS AT EVERY DEVELOPMENTAL STAGE?

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Keywords: Academy, elite, performance, sport, training, young

1. Introduction

Considering the physical demands of basketball combined with the reality of limited practice times in basketball clubs as well as the complex changes happening during maturation (Stojanovic et al., 2018), it is essential to create the best training environment for youth basketball players' development but also optimizing the maximum practice time possible (DiFiori et al., 2018). Consequently, the aim of this study will be to assess the improvements on basketball-specific physical capacities (endurance, strength, speed, and agility) considering chronological and maturational age after the implementation of a time-saving (30min) intervention based on neuromuscular power training and repeated sprint training, without modifying the normal practice conditions.

2. Methodology

A group of 62 youth male basketball players from 6 different age categories (U-13 to U-18) were recruited to participate in a 30-min weekly intervention for 8 weeks. Groups were created and participants were randomly allocated to an endurance group or a neuromuscular power group. The endurance group performed a repeated sprint training (RST) including 2 sets of RST with 6x10s sprints with 20s active recovery between repetitions and 6min with an active half-court shooting drill (Buchheit & Laursen, 2013). The neuromuscular power group performed a neuromuscular power intervention with explosive strength and power through super set method (Miranda et al., 2020). VO_{2max}, CMJ, 20m sprint test, V-cut and T-test were assessed pre- and post-implementation to evaluate changes promoted by the intervention

considering chronological and maturational age. Maturational age was calculated using estimated peak height velocity (PHV) (Moore et al., 2015).

3. Results and discussion

Significant positive changes ($p<0.001$) with moderate to large effect sizes were evident after the intervention in all assessments. Those changes were not significantly related to the specific intervention performed. Furthermore, results revealed specific changes associated to maturational age.

4. Conclusions

All physical capacities (endurance, strength, speed, and agility) improved after the intervention. Therefore, the current study demonstrates that a time saving (30min) intervention, using 12% of the total practice time, is able to induce positive changes in the most relevant physical capacities in basketball. However, specific training stimulus will be necessary to achieve the desired adaptations at every maturational stage. Power stimulus with high coordination demanding actions should be applied pre-PHV and the application of a progressive and persistent metabolic and mechanical training stimulus in post-PHV players for strength, speed, and agility development.

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PERCEPTIONS AND NEEDS OF THE USERS DURING THE TREATMENT IN SCHEDULED SESSIONS AT THE MULTIPLACE HYPERBARIC CHAMBER OF THE HOSPITAL DE PALAMÓS: PRELIMINARY RESULTS

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Keywords: Clinical Nursing Research, Hyperbaric Oxygenation, Needs Assessment, Nursing Care, Qualitative Research

1. Introduction

Hyperbaric oxygen therapy (HBO) promotes angiogenesis and healing, increases the activity of fibroblasts, reduces edema, and improves the person's antimicrobial defense. Treatments have numerous indications such as decompression sickness, acute CO poisoning, necrotizing soft tissue infections, acute compartment syndrome, arterial insufficiency, radionecrosis, and gas embolism (Desola, 2009; Monteagudo et al., 2013). Users breathe oxygen through masks tied to their heads or through transparent hoods (bells) that cover the entire head. In all situations, professionals breathe ambient air from the hyperbaric chamber for most of the treatment and are present to protect patients from the risks of barotrauma and oxygen toxicity, and to reassure or relieve any anxiety that patients may express during the treatment session (Leifer, 2001).

2. Hypothesis

The main objective of this study was to explore the perceptions and needs of users during the treatment in scheduled sessions in the multi-place hyperbaric chamber of the Palamós Hospital.

3. Methodology

A qualitative study of phenomenological design was carried out through in-depth interviews with patients who had undergone scheduled treatment in the hyperbaric chamber. Data were analyzed with the NVIVO program. Categories were established based on levels of meaning in patients' experiences.

4. Results and discussion

Four women and eight men with an average age of 64 and 71.5 years, respectively, participated. Three thematic areas include the main and secondary categories. First, the thematic area of *Biopsychosocial lived experiences* includes four main categories: symptomatology, basic pathology, sensations, and benefits derived from hyperbaric chamber treatment. Second, the area of *Experiences lived through interpersonal relationships* includes relationships with health personnel, information received, and the role of the companion. Third, the area that explains *Lived experiences related to health structures* includes the main categories hyperbaric chamber, hospital infrastructure, and structural improvements.

5. Conclusions

Several factors influence the experiences of people treated with the hyperbaric chamber: the appearance of symptoms and the benefits they get from the hyperbaric treatment; the concern they show about their underlying pathology; and how the experience is influenced by the assistance received from the healthcare staff.

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RELATIONSHIP BETWEEN THE FORMAT OF CLINICAL QUESTIONS, QUALITY OF EVIDENCE AND NUMBER OF RECOMMENDATIONS

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Keywords: Attention deficit hyperactivity disorder, clinical question, heterogeneity, imprecision, interventions

1. Introduction

Clinical practice guidelines (CPGs) are important tools for determining the best treatment for disorders such as attention deficit hyperactivity disorder (ADHD) (*Woolf et al., 1999*). However, the quality of the scientific evidence and the number of therapeutic recommendations in CPGs depend on the format of the clinical questions used to generate them. There are limited data on how the quality of scientific evidence is affected by the heterogeneity and precision of the results obtained from different clinical question formats.

2. Hypothesis

Compared to a narrower clinical question, a broader question is associated with a decrease in quality of evidence with respect to heterogeneity, but an increase in quality of evidence in terms of the precision of results and an increase in the number of therapeutic recommendations.

3. Methodology

A descriptive study of 23 *in silico* patients was conducted. The data source consisted of the simulated patients used to validate APPRAISE-RS/TDApp (*López et al., 2023*). The independent variable was the degree of concreteness of the clinical question, establishing three levels based on drug and dose (L1), drugs only (L2), and enantiomers (L3). The dependent variables included the consistency and precision of the results (I^2 statistic and width 95% confidence interval, respectively), the quality of evidence and the strength of recommendations (lost points due to heterogeneity and imprecision, overall risk of bias) using GRADE methodology (*Sanabria et al., 2015*), the number of analyzed studies, recommendations in favor, and patients with any recommendation in favor. Measures of central tendency (mean,

median) and dispersion (minimum, maximum), along with proportions (in dichotomous variables) and goodness of fit to normality tests (Kolmogorov-Smirnov and Shapiro-Wilk) were applied for statistical analysis.

4. Results and discussion

Regarding simulated patients, 52.17% were male, 82.61% were underage and 52,17% suffered from comorbidities. As the clinical question broadened and moved up in level, the values of the dependent variables tended to increase, although some values stabilized ("lost points due to heterogeneity", "overall risk of bias") or decreased ("patients with any recommendation in favor", "95% CI width"). A sensitivity analysis was also performed, limiting the intervention to methylphenidate derivatives, and consistent results were obtained.

5. Conclusions

As the narrowness of the clinical question decreases, heterogeneity rises, but imprecision does not diminish. Furthermore, the number of recommended drugs increases.

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AN INTEGRATED NEUROMUSCULAR TRAINING PROGRAM APPLIED DURING PHYSICAL EDUCATION CLASSES INCREASES SALIVARY ADIPONECTIN CONCENTRATION IN HEALTHY SCHOOL-AGED CHILDREN

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Keywords: adiponectin, children, endurance, integrated neuromuscular training, physical education class

1. Introduction

Adiponectin protects cardiovascular health through its vasodilator, anti-apoptotic, and anti-inflammatory activities (Shibata et al., 2017). Adiponectin increases after acute and chronic physical exercise (Becic et al., 2018). Integrated neuromuscular training (INT) is a physical exercise program that improves physical fitness (PF) and health (Zhao et al., 2021).

Our objectives are: 1) to investigate whether baseline salivary HMW (sHMW)-adiponectin relates to body composition and PF; 2) to assess if an INT can induce changes in sHMW-adiponectin, body composition, and PF; and 3) to identify if changes in body composition and PF induced by the INT program are associated to post-INT-sHMW-adiponectin concentration.

2. Methodology

A total of 90 children (44 boys and 46 girls; 7.4±0.3 years) were recruited in primary schools in Girona, and randomly allocated to control or intervention groups (N=45).

The intervention consisted of a 3-month-INT program, as a warmup activity at the beginning of each PE class, twice/week. Children from the control group had traditional physical education (PE) classes during these three months.

Body mass, height, and body mass index (BMI) were measured. Fat mass and fat-free mass were assessed by means of bioelectrical impedance. To assess sHMW-adiponectin, a sandwich enzyme-linked immunosorbent assay was carried out (CSB-E13400h; Gentaur, Belgium). PF: endurance and handgrip strength were assessed by an 800 m run and hand

dynamometry, respectively. All measurements were performed at baseline and after three months.

3. Results

Children with higher baseline sHMW-adiponectin have lower BMI SDS (p=0.007) and fat mass (p=0.037), and better endurance (p=0.017) in comparison to the children with lower baseline sHMW-adiponectin. The INT program increased sHMW-adiponectin concentration, decreased BMI and fat mass, and improved endurance and handgrip strength in the intervention group (0.4% to 37%; p=0.043 to p=0.007). Finally, the change in endurance was associated with the post-INT-sHMW-adiponectin concentration, explaining 34% of its variance (Beta=-0.335, p=0.022).

4. Conclusions

Higher baseline sHMW-adipoenctin levels are related to a better body composition profile and better endurance in healthy school-aged children. Furthermore, an INT program applied during PE classes can simultaneously enhance the secretion of sHMW-adiponectin and improve endurance, suggesting a possible cardio-protective effect of the INT in children through these mechanisms.

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EFFECTIVENESS OF THE APPLICATION OF A NURSING INTERVENTION PROGRAM IN THE MANAGEMENT OF CHILD PAIN IN THE SURGICAL PROCESS OF CHILDREN WHO ARE GOING TO BE CIRCUMCISED: PRELIMINARY RESULTS

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Keywords: Ambulatory Surgical Procedures; Circumcision, Male; Pain; Preoperative Care

1. Introduction

Any surgical intervention on a child involves a high level of stress for the family. Circumcision is a painful intervention and there are various types of interventions for adequate pain management (Simpson 2006; Labban et al. 2021). There are various non-pharmacological strategies, which are used as distraction to reduce pain in children: body and verbal contact with their parents, sucrose, non-nutritive sucking, restraint, distraction, and music therapy (Taddio 2001; León et al. 2016; Vu-Ngoc et al. 2020).

2. Hypothesis / problem

A nursing research program in the surgical process of circumcision reduces pain in children.

3. Methodology

A randomized clinical trial was carried out at the Maresme Polyclinic in Pineda de Mar. The study population consisted of children who were going to be circumcised and their family members. It was randomized by strata based on the day of the intervention. The intervention group underwent a nursing intervention on the characteristics of the surgical intervention and postoperative care, while the control group received the usual information. The FLACC scale (Face, Leg, Activity, Cry, and Consolability), which values the face, the movement of the legs, the activity, when the child cries and if he can be comforted, was used to measure pain in children. Received approval from the Drug Research Ethics Committee (CEIm) of the Maresme Health Consortium (CEIm 03/22).

4. Results and discussion

A total of 314 family members and 192 children participated (98 in the control group and 94 in the intervention group). The mean age of the children was 12.99 months (SD 9.29). In the intervention group, during the circumcision procedure, statistically significant differences were found between the children in the intervention group who had less pain, had more distractions, and less postoperative pain at 24-48 hours than those in the control group (X^2=13.521, p=0.01; X^2=19.238, p =0.001; X^2=6.088, p=0.019, respectively). The 74 (78.6%) parents in the intervention group had fewer problems in caring for the penis at 24-48 hours than the 57 (58.2%) in the control group (X^2=9.770, p=0.008).

5. Conclusions

Preoperative educational intervention is effective in reducing pain in circumcised boys.
The preoperative education of family members allows children to experience less pain and there are fewer problems when performing postoperative penile care 24/48 hours later.

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OPTIMIZATION OF FORENSIC DATA COLLECTION: DATABASE AD HOC

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Keywords: Database, Guidelines, Multidisciplinary investigation

1. Introduction

Diving is a popular and safe practice, but it is not exempt of risk (Shreeves *et al.*, 2018). Different causes and factors involved in deaths have been described (Casadesús *et al.*, 2019; Denoble *et al.*, 2008) and multidisciplinary investigations are essential (Casadesús *et al.*, 2019; Casadesús *et al.*, 2021) to elucidate them. Recently in our country (in 2014), the University of Girona and the Secretary of State for Security have created the Observatory for Diving Accident Fatalities (OMAB, in Spanish), whose aim is to collect data in a standardized manner for the preparation of descriptive studies.

To date, there are no published epidemiological data on mortality in diving in Spain.

2. Methodology

We have used MySQL as a relational database management system to design an easy-to-manipulate and scalable database. All diving deaths recorded on the coast of Spain between 2009 and 2020 will be analyzed. Police technical and medical-forensic data will be collected following a practical standardized work guide. Subsequently, all data will be properly stored so that they will be accessible and usable in a short or long term.

3. Results

The structure of a relational and scalable database has been defined. Multiple tables have been created to include all known data and in its best format. The design also intends to be flexible enough so that not only the data gathered in this study can be stored in it. This means that

introducing new data that has not been yet considered requires minimal effort and redesigning of the database.

4. Conclusions

A standard work procedure has been defined. Once the collection has finished, data will be entered in the database. This tool allows cured data to be stored and easily accessible, avoiding redundancies and facilitating their subsequent reading and interpretation.

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SESSION 6.

MOLECULAR BIOLOGY AND BIOMEDICINE

PHYSICAL ACTIVITY AND VITAMIN D SUPPLEMENTATION EFFECTS IN PATIENTS WITH TYPE 2 DIABETES

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Keywords: Resistance training - Vitamin D - Type 2 diabetes - Insulin resistance

1. Introduction

Type 2 diabetes (T2D) is a chronic disease that occurs when the pancreas does not produce enough insulin or when the body cannot effectively use the insulin it produces (Lu et al., 2018). Low blood vitamin D (25-hydroxyvitamin D) levels have emerged as a risk factor for T2D, and vitamin D supplementation has been hypothesized as a potential intervention to lower diabetes risk (Pittas et al., 2007; Strasser and Pesta, 2013)

The effect of aerobic and resistance training together with vitamin D supplementation variables on insulin resistance and physical and haematological parameters might be studied. Since resistance training has a positive effect on diabetes and exercise has been one of the ways to treat obesity and diabetes (WHO, 2021), it is expected that this study can provide a useful solution to treat or ameliorate obesity and diabetes.

2. Hypothesis

We hypothesize that vitamin D supplementation and resistance added to aerobic exercise will improve clinical aspects of T2D patients.

3. Methodology

A double-blind randomized clinical trial will be developed including forty individuals of both sexes (<40 years old) with fasting blood glucose >126 mg / dL, and glycosylated haemoglobin (HbA1c) <9%. Patients will be selected and later randomly assigned to four groups of 10 patients: 1) Training-Vitamin D, 2) Training-placebo, 3) Vitamin D and 4) placebo. A

sarcoplasm stimulating training system will be applied. The program will consist of three sessions/week for 16 weeks; and it is designed in three 5-week periods. Fitness tests, analysis of insulin resistance, lipid profile and other blood biomarkers will be obtained. Subjects in the Training-Vitamin D Group and the Vitamin D Group will use oral capsules containing 16,000 international units of Vitamin D (Calcifediol, FAES FARMA), once a month during the duration of the study. Previously, the physical activity level will have been obtained through the International Physical Activity Questionnaire (IPAQ). The subjective perception of well-being will be measured through the Psychological Well-Being Index. During the study we will follow the recommendations of the Spanish Society for Diabetes. Nutritional education programs will be designed to provide all participants. A 14-item questionnaire designed to assess adherence to the traditional Mediterranean diet will be administered.

4. Results

It is expected that 16 weeks of exercise and vitamin D supplementation improves the insulin resistance and lipid profile individuals with T2D.

5. Conclusions

We expect that vitamin D supplement and resistance added to aerobic exercise will improve clinical aspects of T2D patients.

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MOLECULAR MECHANISMS OF ARRHYTHMOGENIC CARDIOMYOPATHY

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Keywords: arrhythmogenic cardiomyopathy, desmosomes, DNA damage, HL1, oxidative phosphorylation

1. Introduction

Arrhythmogenic cardiomyopathy (ACM) is an inherited disease characterized by cardiomyocyte loss and the replacement of the myocardium by fibro-fatty tissue which can lead to sudden cardiac death. The main genetic causes of ACM are desmosome genes (PKP2, DSP, DSG2, DSC2, and JUP), representing up to 50% of the total cases (Austin et al., 2019). At the molecular level, we lack sufficient understanding of the pathophysiological mechanism that may trigger ACM and determine disease progression. Recent studies have proposed new potential ACM molecular signatures such as DNA damage and a deficit in transcripts coding for proteins in the electron transport chain in samples from patients with ACM with mutations in PKP2 (Pérez-Hernández et al., 2022). Our study aims to replicate these results in an HL1 edited cell model deficient for PKP2 and to elucidate whether these mechanisms are also triggered in deficiency of DSC2 and DSG2 or are PKP2 specific.

2. Methodology

To elucidate the molecular mechanisms involved in the pathogenesis of the disease, CRISPR edited HL1 cell lines for desmosomal genes were generated (PKP2-KO, DSC2-KO, and DSG2-KO). Expression profiling was performed by RNA-analysis. Preliminary results pointed out that oxidative phosphorylation and DNA damage was potentially involved.

To experimentally validate these results, we preformed the following two-step analysis: 1) To analyze DNA damage, a commercial kit was used to extract DNA from cells, and we performed the assay using a colorimetric kit to measure the apurinic and apyrimidinic sites. 2) For the oxidative phosphorylation analysis, we tested protein levels of the five oxidative

phosphorylation (OXPHOS) complexes for the PKP2-KO, DSC2-KO and DSG2-KO by western blot.

3. Results and discussion

In the DNA damage assay no significative differences were found, although it seems to be a tendency of increased AP sites in the knockout groups tested.

For the oxidative phosphorylation (OXPHOS) complexes, our results showed that complexes of the mitochondrial respiratory chain are significantly reduced at the protein level in all PKP2-KO, DSC2-KO, and DSG2-KO, except for the complex I (band 5) in the DSG2 vs WT (figure 1).

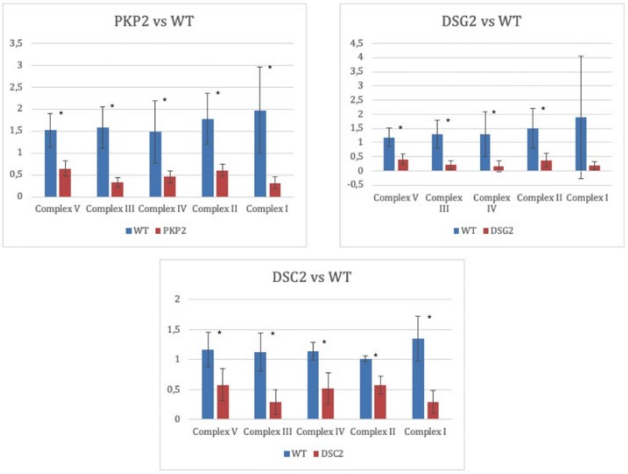

Figure 1. Expression of the 5 OXPHOS complexes. Comparison between knockouts and wild types. * p<0.05

4. Conclusions

Our results support the previously published studies describing DNA damage and oxidative phosphorylation as pathomechanisms for PKP2 mutations. Our results also suggest that these mechanisms could be a common feature for desmosomal mutations in ACM. More studies would be needed to confirm these results.

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SALIVARY CARDIAC-ENRICHED FHL2-INTERACTING PROTEIN (CEFIP) IS ASSOCIATED WITH HIGHER DIASTOLIC TO SYSTOLIC BLOOD PRESSURE RATIO, SEDENTARY TIME, AND PHYSICAL ACTIVITY IN HEALTHY SCHOOL-AGED CHILDREN

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Keywords: cardiac muscle, cardiovascular markers, CEFIP, children, physical fitness, skeletal muscle

1. Introduction

Cardiac-enriched FHL2-interacting protein (CEFIP) is a novel cardiac z-disc-derived protein with a cardiac and skeletal muscle–specific expression profile (Dierck et al., 2017). CEFIP is related to cardiomyocyte hypertrophy by means of modulating calcineurin signaling (Dierck et al., 2017). Cardiomyocyte hypertrophy has been inversely related to physical activity (Wisløff et al., 2002).

Our objectives are: 1) to explore if CEFIP can be detected and quantified in salvia in healthy school-aged children; and 2) to explore the associations of salivary CEFIP with cardiovascular markers, physical activity, and sedentary time in apparently healthy school-aged children.

2. Methodology

The study population consisted of 72 children (24 boys and 48 girls; 7.6±0.3 years) recruited in primary schools in Girona.

Body mass, height, and body mass index (BMI) were measured, and then age- and sex-adjusted standard deviation scores were calculated using regional normative data (Carrascosa-Lezcano et al., 2008). Blood pressure (systolic and diastolic) was measured by means of an electronic oscillometer and the diastolic-to-systolic blood pressure ratio was calculated.

Saliva samples were collected in the morning and stored at -20ºC following the manufacturer's protocol. A sandwich enzyme-linked immunosorbent assay was carried out to assess salivary CEFIP (abx506878; Abbexa, United Kingdom).

Physical activity and sedentary time were measured by means of triaxial Actigraph GT3X accelerometer (Actigraph, Pensacola, FL, USA) that children were instructed to wear for 24h during 7 conssecutive days.

3. Results

CEFIP was easily detected and measured in all saliva samples (0.6±0.2 pg/ml). CEFIP was positively associated with the diastolic-to-systolic blood pressure ratio (r=0.305, p=0.010) and sedentary time (r=0.317, p=0.012), and negatively associated with physical activity (r=-0.350, p=0.002). The associations with the diastolic-to-systolic blood pressure ratio (Beta=0.349, p=0.004) and sedentary time (Beta=0.354, p=0.009) remained significant after adjustment for potential confounding variables such as age, sex and BMI in linear regression analyses.

4. Conclusions

CEFIP can be easily assessed in saliva as a promising biomarker associated with cardiovascular health in school-aged children. Interestingly, a higher diastolic-to-systolic blood pressure ratio and more sedentary time were related to higher salivary CEFIP concentration in these children.

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DOSIMETRIC COMPARISON OF HEART SUBSTRUCTURES BETWEEN FREE BREATHING AND DEEP INSPIRATION BREATH HOLD FOR LEFT-SIDED BREAST CANCER RADIATION THERAPY

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Keywords: Breast cancer, Deep inspiration breath hold, Heart substructures, Hybrid volumetric modulated arc therapy, Radiotherapy

1. Introduction

Nowadays, radiotherapy increases cure rates in breast cancer. However, cardiac exposure in left-sided tumours might increase cardiotoxicity. Deep inspiration breath hold (DIBH) allows the planning target volumes (PTV) of the heart to be separated. Advanced dosimetric techniques such as volumetric modulated arc therapy (VMAT) or hybrid volumetric modulated arc therapy (H-VMAT) reduce heart doses. Duane et al. (2017) describes the methods to delineate the heart substructures in radiotherapy CT planning. The relationships between doses to different heart substructures and subsequent injury of these structures have not yet been investigated. The aim of this study is to compare dosimetric parameters of heart substructures and PTVs between free breathing (FB) and DIBH using two different plans, one in 3DCRT and the other in H-VMAT for both breathing techniques.

2. Methodology

Thirty-seven left breast cancer patients described in a previous essay (Romera-Martínez, 2020) were included. Six heart substructures were delineated following guidelines (Duane, 2017): whole heart, left ventricle, left main coronary artery (LMCA), left anterior descending coronary artery (LADCA), circumflex coronary artery (Cx) and right coronary artery (RCA). For each patient, four dosimetric plans were generated: two using 3DCRT field-in-field plans, and the other two combining 3DCRT with two half-arcs (H-VMAT) for each breathing technique. The heart substructures were evaluated using the following dosimetric parameters: D_{mean}, V25(%), and V30(cm^3) of the whole heart; D_{mean} and V5(%) of the left ventricle, LMCA, LADCA, Cx and RCA. For PTVs, D98%, D2%, D50% and V95% or V90% were obtained,

depending on the PTV. Data were summarized as median (percentile 25, percentile 75). A Friedman Test with Benjamini-Hochberg adjustment was used to determine the significance difference of four techniques with Bonferroni correction to adjust for multiple comparisons. A p-value less than 0.05 was considered statistically significant and multiple comparisons tests were considered one-sided.

3. Results and discussion

The Friedman Test showed significance differences between all four techniques for the dosimetric parameters studied except RCA V5(%) and D50(%) PTV2.

For all but one heart substructures, 3DCRT in DIBH showed statistically significant lower doses than H-VMAT DIBH and FB, according to a previous study (Vikström, 2018). In terms of PTVs, when H-VMAT was used, D98% is increased and D2% is decreased than the use of 3DCRT in both breathing techniques.

4. Conclusions

As compared to other techniques, 3DCRT in DIBH provides the lower heart substructure dosimetric parameters for all six heart substructures except for Cx and V25 whole heart.

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INHIBITION OF CANCER STEM-LIKE CELLS BY CURCUMIN DERIVATIVES IN TNBC CELLS

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Keywords: Breast Cancer, Curcumin, Cancer Stem Cells, TNBC

1. Introduction

Triple negative breast cancer (TNBC) accounts for 15% of all breast cancer cases and is characterized by a lack of therapeutic targets (Siegel *et al.,* 2022). Although the response to chemotherapy is positive, most patients experience rapid disease progression, resulting in relapses and metastases (Vagia *et al.,* 2020). Hence, new therapies for TNBC are required. Cancer stem cells are a subgroup of tumor cells that are responsible for cancer initiation, development, recurrence, and metastasis. These cells exhibit distinct features, such as self-renewal or resistance to anticancer treatments (O'Conor *et al.,* 2018). The anticancer effects of curcumin, a polyphenol extracted from turmeric (*Curcuma longa*), have been demonstrated against breast cancer cells and the cancer stem cell population. Moreover, the use of synthetic derivatives has been suggested to overcome the low bioavailability of curcumin in humans and increase cytotoxicity specifically towards cancer cells (Park *et al.,* 2013). Therefore, the main aim of this study was to evaluate the effects of three curcumin derivatives on TNBC and cancer stem-like cells.

2. Methodology

The MDA-MB-231 TNBC cell line was selected for the experiments. Half-maximal inhibitory concentration (IC_{50}) was calculated using the MTT assay, the mammosphere formation index (MFI_n) was assessed by the mammosphere formation assay, and the induction of apoptosis was analyzed by western blotting.

3. Results and discussion

The new compounds (TL4, TL5 and TL6) showed a relevant decrease in IC_{50} value compared to curcumin, with an IC_{50} of 17.36 μM, as this value was reduced by more than 70%. In addition, all synthetic derivatives showed three times higher MFI_n than curcumin, with a MFI_n of 15.89 %. This indicates a clear effect against the stem-like cancer population.

However, activation of apoptosis was only observed when TNBC cells were treated with curcumin.

4. Conclusions

Treatment with curcumin derivatives emerges as a promising therapeutic strategy for TNBC because of their capacity to reduce the cancer stem-like population, which is directly related to resistance to chemotherapy.

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IRON METABOLISM DYSREGULATION IN HUNTINGTON'S DISEASE IS NOT EXCLUSIVE TO THE STRIATUM

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Keywords: Huntington's disease, Striatum, Hippocampus, Iron, Transferrin Receptor

1. Introduction

Huntington's disease (HD) is a neurodegenerative disorder caused by a mutation in the huntingtin (HTT) gene. Affected individuals show a combination of motor, cognitive and psychiatric symptoms that worsen over time (Labbadia & Morimoto, 2013). The degeneration of the striatum, a subcortical structure involved in movement control, is the main reason behind the motor impairment, while cortical and hippocampal atrophy explain the cognitive symptoms. An accumulation of iron has been observed in the basal ganglia of HD brains, suggesting it may play a role in neuronal degeneration (Bartzokis et al., 1999; Chen et al., 2013). Although the metabolism of iron is controlled by several different proteins, little data exists about their role in HD.

2. Hypothesis

Our hypothesis is that there is a region-specific iron dysregulation in response to different degrees of iron accumulation.

3. Methodology

Transferrin receptor (TfR), iron-responsive binding protein 2 (IRP2), ferroportin (FPn) and hepcidin and glutathione peroxidase 4 (GPx4) levels were assessed by Western blot in the striatum and hippocampus of R6/1 mice, an HD mouse model, at different ages.

Iron accumulation was measured in the hippocampus and striatum of 12-week-old mice using Perl's and Turnbull's stains, which stain for ferric (+3) and ferrous (+2) iron, respectively.

4. Results and discussion

TfR was found to be downregulated in striatum from 12 weeks of age and in all tested ages in hippocampus when compared to WT. IRP2 was found to be downregulated at 8 and 16 weeks

in the striatum but not in the hippocampus. GPx4 variations were found in both regions, although with different patterns. No differences were observed in FPn nor in hepcidin.

Our results indicate that iron metabolism is dysregulated in all HD phases and is not exclusive to the striatum, the most affected area. In addition, TfR reduction seems to be the more consistent dysregulation and happens earlier in the hippocampus than in the striatum. Further studies need to be carried out to elucidate the molecular mechanism that leads to iron accumulation specifically in the basal ganglia.

5. Conclusions

Iron metabolism is dysregulated in all HD phases and is not exclusive to the striatum.

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SESSION 7.

EDUCATION PSYCHOLOGY AND HEALTH

PRACTICES AND MEANINGS IN CHEMSEX

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Keywords: autoethnography, critical chemsex studies.

1. Introduction

Chemsex has been mainly defined as the use of substances to enhance and extend sexual encounters among men who have sex with men. It is a phenomenon that emerged at the beginning of this century in big cities of the global gay circuit in conjunction with new psychostimulant drugs and geolocation-based sexual encounter applications. In these past two decades, studies have focused especially on the positive correlation between the phenomenon and seroconversion to +HIV and/or +Hepatitis, along with the study of problematic drug use.

The knowledge generated until now has barely analyzed three central aspects of the experience: Viagra use, masculinity, and pleasure. This dominant knowledge has focused on risk in sexual practices and transmission of sexually transmitted infections. This research aims to complement and problematize this hegemonic knowledge. To do so, the object of study is the researcher's experience in some chemsex encounters, his participation as a collaborator in workshops for people involved in sexualized drug use, and the analysis of the theater play "El Ge".

2. Methodology

This paper presents the results and conclusions of the analysis of the researcher's experience. For this purpose, autoethnography (Adams, Holman and Elli, 2015) was used as a research methodology and critical chemsex studies (Møller and Hakim, 2021) as a theoretical framework. Part of the field notebook carried to seven meetings in Barcelona between December 2021 and March 2022 is analyzed.

3. Conclusions

The field notebook notes were contextualized in a social and cultural framework to analyze notions and conceptions in the hegemonic discourse of chemsex studies.The first of these is risk. This notion is problematized in terms of its management and administration to establish that psycho-biomedical studies place drugs as the causal agent of risk practices and stigmatize the administration of risk in non-heterosexual bodies. The second is linked to the

notion of better sex used in these studies, establishing experimentation as an alternative. The third is integrally related to body aesthetics generated by the use ofViagra and cathinones. It is established that in some chemsex contexts a masculinized aesthetics would predominate, generating a striated body in which the practices are accommodated.

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WHAT FACTORS INFLUENCE THE DECISION-MAKING PROCESSES IN NON-KINSHIP FOSTER CARE?

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Keywords: child welfare, child protection system, decision-making processes, non-kin foster care, social work

1. Introduction

Decision-making in family foster care is a very complex process, both for the nature of the issues to be decided and for the positive or negative implications that it can have on the lives of the children, foster parents and families of origin (Rafeedie et al., 2019). Focusing the research on decision-making goes to the core of the protection system.

2. Hypothesis

This communication aims to analyse the factors that influence professional decision-making regarding foster care in Catalonia (Spain). It takes into account the three services that are involved throughout the process, as well as the coincidences and discrepancies regarding the importance they attribute to the different factors related to the decision-making process.

3. Methodology

Using a questionnaire to collect quantitative and qualitative data, we analysed 90 cases of children in foster care, all assessed by the three teams involved: the protection teams that assess the situation of the family of origin, the services that monitor the foster carers, and the central services of the regional administration. We also assessed 57 professionals from 28 teams on general aspects of decision-making.

4. Results

The results highlight how the young age of the child and the low likelihood of family reunification have an important influence when it comes to making proposals for family foster care (Figure 1).

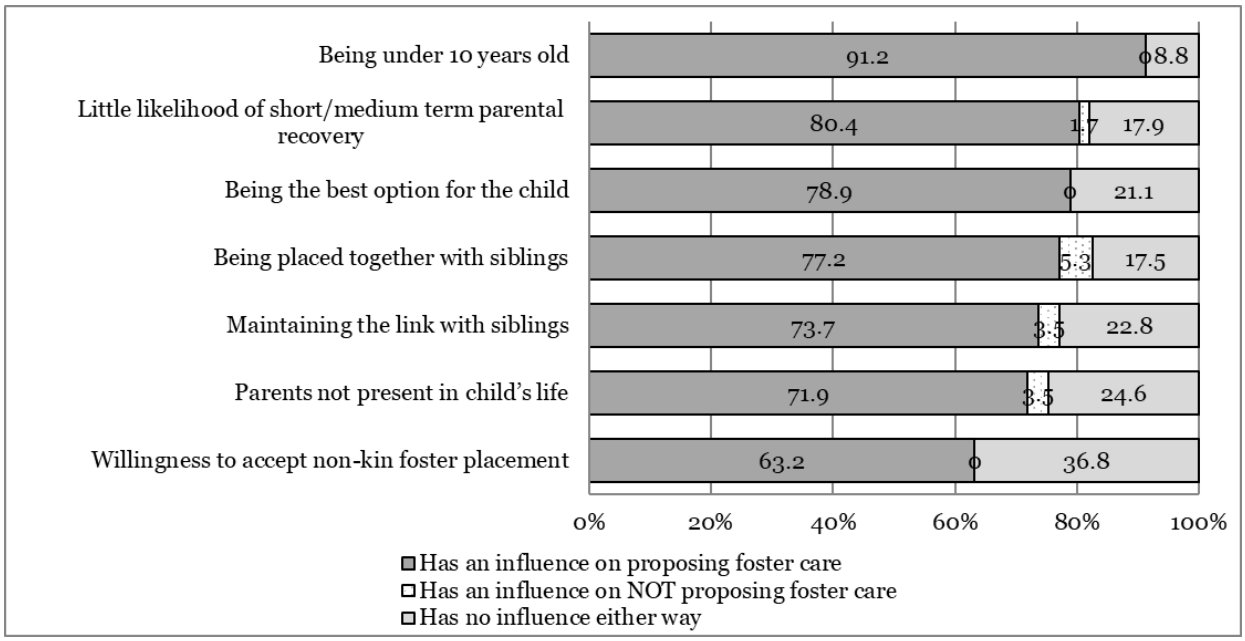

Figure 1. Factors influencing the proposal for foster care (general responses from child protection teams).

5. Discussion

The results open the debate on the place that foster care currently has within the protection system. In general, there is a strong coincidence among the tree teams in the weighting of most of the factors but there are also some discrepancies, such as on the participation of the child in the decision-making process. It is necessary to reflect on the factors of well-being and the breakdown of foster care, to improve professional practices and childhood policies (Llosada-Gistau et al., 2017).

6. Conclusions

Professionals must be aware of the importance of establishing and agreeing on objectives when working with the families - both foster families and families of origin - and above all with the children, promoting teamwork among the teams and between the teams and the children.

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CBT4CBT WEB-BASED ADD-ON TREATMENT FOR COCAINE USE DISORDER: PRELIMINARY RESULTS OF A RANDOMIZED CONTROLLED TRIAL

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Keywords: Cocaine use disorder, outcomes, psychotherapy, randomized clinical trial, web-based treatment

1. Introduction

Cocaine use disorder (CUD) is characterized by high dropout and relapse rates, thus, there is a great and increasing need to improve CUD treatments (World Health Organization & United Nations Office on Drugs and Crime, 2020). Clinical evidence-based guidelines suggest psychological approaches as first line treatments, especially contingency management (CM) and cognitive-behavioral therapy (CBT) (Kampman, 2019). Regarding different mental health conditions, implementation of web-based treatments can optimize current face-to-face interventions, however, web-based interventions in CUD are still limited. CBT4CBT is a CBT web-based treatment for substance use disorders with a positive impact on face-to face treatments, as reported by studies conducted in the US (Carroll et al., 2008, 2009). This study aims to evaluate whether adding a web-based CBT (i.e., CBT4CBT) to standard CUD treatment improves treatment outcomes in a Spanish sample of 52 patients with severe CUD.

2. Hypothesis

Based on previous research, we hypothesize that by adding CBT4CBT to treatment as usual (TAU) in our clinical population treatment outcomes will be substantially improved in both preliminary and secondary measures (i.e., (a) treatment retention and relapse and (b) reduced psychopathological symptoms and craving, improved emotion regulation).

3. Methodology

All participants who met selection criteria for this open-label, randomized controlled trial (RCT) were allocated to TAU (n=27) or to TAU+CBT4CBT (n=25) after impatient treatment. They all received an individualized psychological intervention during hospitalization for cocaine

detoxification. There were six time-point assessments: at beginning of inpatient treatment, at the end of inpatient treatment and before starting day care and outpatient treatment, at the end of the 8-week CBT4CBT/TAU treatment and at 1, 3 and 6 months post treatment.

4. Results and discussion

Analyses show significant pre-post treatment differences in addiction severity (t=3.67; *p*=.003), SCL-90-R global severity index (GSI) (t=3.6; *p*=.007), UPPS-P negative urgency (t=2.7; *p*=.021), UPPS-P positive urgency (t=2.5; *p*=.030) and UPPS-P lack of perseverance (t=-2.31; *p*=.040) within the CBT4CBT group. Within the TAU group pre-post treatment differences are in addiction severity (t=3.43; *p*=.004) and SCL-90-R GSI (t=3.1; *p*=.013). There are no differences between groups in the described variables at post treatment, yet there are more dropouts in the TAU than in the TAU+ CBT4CBT group.

5. Conclusions

Preliminary results point towards a reduction in addiction severity and global psychopathology severity in both groups. Although a larger sample is needed to identify significant differences between the groups, more dropouts are observed in TAU than in TAU+ CBT4CBT.

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SOCIAL ADAPTATION OF CHILDREN AND YOUTH FROM FORCED MIGRANT FAMILIES OF UKRAINE

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Keywords: family role change, family sociogram, "new migrant" group, "old migrant" group, personal narratives

1. Introduction

This study investigates the effect of forced migration from Ukraine on schoolchildren and their mothers. Three main topics of our research are:

- Family role changes in the Ukrainian forced migrant families.

- Interaction and mutual influence regarding "new migrants" from Ukraine, who have just settled in Catalonia and have not had time to integrate and adapt to the new society, and "old migrants" from Russia, who have been living in Catalonia for some time and have managed to integrate and adapt to the new society.

- Nature, main indicators and dynamics of the adaptive process of children and youth from forced migrant families of Ukraine.

2. Hypotheses

One of our hypotheses is that there is a strong correlation between family structure change and family role change in conditions of forced migration from Ukraine due to the war. Contrary to the classical view of the negative connotations of such changes, we argue that a positive scenario is possible. Another hypothesis states that there is serious conflict between Ukrainian and Russian groups of migrants at school.

3. Methodology

We use a mixed-method approach (*quantitative* and *qualitative methods*) and *descriptive and interpretive research designs* because of the level of detail and the in-depth treatment of our topic. It consists of the following tools: *personal narratives*, *interviews* and *family sociogram*. Previous research studies show that forced migrants make sense of their lives by personal narratives representing different experiences, including changing roles in the family after forced migration (Czarniawska 2004, Hiitola 2021, Winkler 2022). Scholars have suggested family

sociograms to study interpersonal family relationships (Eidemiller 2002b, Andreyko 2020). They can visualise the relationships among certain members of the family, in our case between mothers and children. They can also visualise ties with the external environment, such as education services, leisure time activities or friends.

4. Results and discussion

We hope to confirm or refute our hypotheses.

5. Conclusions

We are planning to explore the potential implications of our research for sociology, psychology and pedagogy. Theoretical and empirical data of our study can be useful in developing new areas of educational and social policy in the context of schoolchildren of forced migrant families from Ukraine. Our results might have implications that challenge scientific beliefs and create a basis for future research in these areas.

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BREAKING MYTHS ABOUT THE INABILITY TO CARE IN MOTHERS WITH A MENTAL HEALTH DIAGNOSIS: PHYSICAL CONTACT, AFFECTION AND ACTION FOR SURVIVAL

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Keywords: cares, empowerment, feminism, maternal-filial bond, mental health

1. Introduction

Some of the contemporary research about mother-child bonds focuses on problematic aspects when there are mental health diagnoses in the mothers (Cazurro, 2022). From an intersectional feminist perspective, social constructionism and critical psychology, elements are provided to analyse these approaches by changing the focus despite recognizing their impact, incorporating critiques of ethnocentrism, androcentrism and the psychologism of some theories (Roselló, Cabruja and Salvador, 2019).

For example, as demonstrated by the work of Valerie Walkerdine (1992), "working-class women become objects of surveillance regarding their capacity as mothers, [...] not only are their practices controlled, but their insufficiency or imperfection is considered the cause of a wide range of social problems, such as crime, delinquency, etc. That is, oppression as a basis for understanding the position of working-class women has disappeared from the agenda (if it was ever on it) and has been replaced by the perception of these women (they are only mothers) as the psychopathological cause of the threat to the bourgeois political order as such" (1992:137).

Hence, part of the research results of doctoral thesis, focuses on exploring and systematizing controversial aspects of mother-child stories to problematize, resignify and heal them.

2. Methodology

The research is being conducted using a feminist qualitative methodology. A case analysis is developed from biographical and autobiographical documents, and the methods of narrative analysis (Biglia and Bonet, 2009) and discourse analysis (Burman and Parker, 2016), following the dialogical processes of problematization and interpretative positions. The corpus is formed by eight documents that meet criteria set in relation to the conditions of homogeneity and heterogeneity of the sample. For this communication specifically, we have used:

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3. Results and discussion

From the selected narratives analysed we highlight four situations: 1) Physical contact as a restorer of the feeling of abandonment and with a positive effect for both mother and daughter, when there is no story. We refer to the ideas of physical and relational disconnection attributed to episodes of depression. Specifically, a medical indication/action of body contact offers an emotional relationship/release response and modification of the idea of care. 2) Deep knowledge of psychological distress enables comfort support and containment of sadness and fear. We see affection and care of the mother towards the daughter, but also a possible greater autonomy of the daughter. 3) The need for economic survival as a trigger for the depressive episode/state. Faced with a need for sustainable economic life, there is a way out of apathy to be able to go to work and take care of the daughters. 4) Performing hyperactive care tasks is combined with episodes of rest that mark a dilemmatic experience for care functions (burden or force).

4. Conclusions

As evidenced, it seems essential to contribute to the detailing of aspects and capacities arising from contact with psychological discomfort and to dehegemonize some of the linear interpretations in relation to the dilemmas of care work.

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THE INFLUENCE OF EMOTIONS: EXPLORING THE IMPACT OF NEGATIVE EMOTIONAL STATES ON LEVEL 2 VISUAL PERSPECTIVE TAKING

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Keywords: Emotional induction, Inhibition, Negative emotion, Theory of mind, Visual perspective-taking

1. Introduction

Visual perspective taking (VPT) is a component of theory of mind (ToM) that involves representing and making judgements about another person's point of view. Its first level (L-1) corresponds to the understanding of different perspectives and its second level (L-2) relates to the comprehension of another's viewpoint. (Flavell et al., 1981). ToM can be influenced by our emotional state, especially by a negative emotional state (Himchi et al., 2015). Perspective-taking ability can also be affected by emotions. This leads us to wonder if a basic process such as visual perspective taking is also affected by a person's emotional state. Bukowski and Samson (2016) found that certain negative valence emotions such as anger, guilt or shame influence our level 1 VPT ability. Hence, negative valence emotions could also affect level 2 VPT. This study aims to observe how sadness, a negative valence and low arousal emotion, can affect level 2 VPT ability. At the same time, in situations where self-perspective and other-perspective differ, individuals need to engage in an effortful cognitive process to overcome the interference of their own perspective (Samson et al., 2010). Therefore, in these situations, there is an egocentricbias that results in slower and less accurate judgments of others' perspective while inhibiting our own. In some conditions, such as negative emotional states, this bias is more prominent (Yip & Schweitzer, 2019) increasing the chances of making errors when adopting another perspective. The aim of this study is to investigate how level 2 VPT can be modulated by emotional state. To this end, the perspective to be adopted by the subject (self or other), the congruence between the perspectives (congruent or incongruent), and the emotional state of the participants will be manipulated.

2. Methodology

Fifty-five healthy young adults studying at the University of Girona participated in the study (M = 20.7; SD = 2.3; data collection still ongoing). They were randomly assigned to one of the two conditions (negative and neutral emotional state).

Their emotional state was induced through short videos and was evaluated before and after the induction. Then they performed a level 2 VPT task presented with the E-Prime software.

3. Results and discussion

Our first results showed an egocentric tendency, in line with previous experiments (Bukowski and Samson, 2016). Participants performed better when they responded from their own perspective than when they adopted another point of view (92.6% vs. 74.2%; p <0,01). This egocentric bias suggests that individuals tend to prioritise their own perspective when participating in perspective-taking tasks (Bukowski and Samson, 2014; Himichi et al., 2015) irrespective of their emotional state (negative or neutral). In this case, an emotional state does not determine self-focus errors more than a neutral emotional state.

When participants were subject to a negative induction, they tended to commit more errors (respectively, 18.8% vs. 14.1%; p =0,01). Consistent with Bukowski and Samson (2016), this finding suggests that visual perspective-taking performance is impaired by a negative emotion, such as sadness.

4. Conclusions

In conclusion, these preliminary results extend our knowledge of the link between emotions and perspective-taking processes.

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SESSION 8.

BIOTECHNOLOGY AND BIOMEDICINE

BIOINFORMATIC ANALYSIS AND CONSTRUCTION OF DNA VACCINE CANDIDATES AGAINST *KLEBSIELLA PNEUMONIAE* INFECTION

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Keywords: antibiotic resistant bacteria, DNA vaccine, *Klebsiella pneumoniae*

1. Introduction

Klebsiella pneumoniae is among the pathogens of critical concern identified by the WHO (Gonzalez-Ferrer et al., 2021). During the last three decades, the number of infections caused by this species has increased and strains resistant to multiple antibiotics have appeared, which represents a major public health problem (Martin & Bachman, 2018). The development of vaccines is a promising therapeutic strategy to prevent infections by this microorganism.

2. Hypothesis and aim

We hypothesise that a DNA vaccine against *K. pneumoniae* can reduce mortality and/or morbidity associated with its infection. This study aims to construct plasmids encoding different *K. pneumoniae* proteins to be used as DNA vaccines and confirm antigens expression *in vitro*.

3. Methodology

K. pneumoniae proteins to be used as candidate antigens in vaccine development were rationally selected. These proteins were bioinformatically analysed to predict immunogenicity and B- and T-cell epitopes using the VaxiJen 2.0, ABCpred and ProPred-I servers, respectively. Antigen sequences were adapted for expression in human cells, fused to immunostimulatory elements and independently cloned into pVAX1 (Thermo Fisher Scientific). Constructs were confirmed by PCR and Sanger sequencing. *In vitro* expression of antigens is being verified by transfection of HEK-293 eukaryotic cells and RT-PCR.

4. Results and discussion

Eight proteins were selected as potential antigens, including 2 specific porins, 3 siderophores, 2 outer membrane proteins (OMP) and a fimbrial subunit. Immunogenic capacity scores ranged from 0.60 to 0.78. The antigens with the most immunogenic capacity were a siderophore, a porin and the fimbrial subunit. B-cell epitopes were predicted for all antigens with a score range of 0.95–0.51. Although the sequence with the most predicted B epitopes corresponded to a siderophore, the antigens with the most B epitopes relative to size were an OMP and the fimbrial subunit. Regarding T-cell epitopes, siderophores were the antigens with a higher number of epitopes and the highest score. Of the 8 potential antigens identified, 6 have been successfully cloned into pVAX1 to date. At present, expression in HEK-293 eukaryotic cells has been confirmed for 2 of them.

5. Conclusions

The siderophores are the best vaccine candidates according to the outcomes of the bioinformatic analysis including immunogenicity score, and number of B- and T-cell epitopes. Future studies will address the *in vivo* confirmation of this vaccine candidate's immunogenicity, after assessing *in vitro* expression of the antigenic proteins by transfection in HEK-293 eukaryotic cells and RT-PCR.

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EFFECT ON THE STERILIZATION PROCESSES IN POLYVINYL ALCOHOL HYDROGELS

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Keywords: Hydrogels, Polyvinyl alcohol, Sterilization processes

1. Introduction

Small-diameter synthetic vascular prostheses present severe complications due to their high thrombotic incidence in the first moments after implantation (Wan et al. 2002). For this reason, 3D bioprinted models of prostheses with cellular content are being developed to minimize the immune response.

One of the most used techniques in bioprinting is the direct ink writing of hydrogels. Hydrogels are a good container for cells due to their capacity to encapsulate water as well as nutrients, growth factors, etc. (Fedorovich et al. 2007). Increasingly, polyvinyl alcohol (PVA) is used because, besides having biodegradation and biocompatibility properties, it has improved mechanical properties compared to other natural-based hydrogels (Lin et al. 2018), all of which resemble a cartilage or an artery when they are in contact with an aqueous medium.

2. Methodology

To assess the viability of HFL1 mouse fibroblasts in contact with PVA hydrogels, the effect of sterilization methods on the film properties were analyzed. This work proposes the possibility of sterilizing 28% (w/v) PVA hydrogels with distilled water using UV light, ethanol, and autoclave individually and in combination. The sterilization with ethanol was compared along with their cooperation with UV sterilization. In addition, to include the fibroblasts within the hydrogel itself, the option of autoclaving the hydrogel was also evaluated. Consequently, samples that did not present any type of contamination were tested. Degradation and mechanical properties were evaluated.

3. Results and discussion

All three processes are expected to be capable of sterilizing hydrogels for cell culture. First, UV, ethanol sterilization will be performed for various times to determine the time required to remove all contaminations from the hydrogel. Then combined sterilizations will be performed to see if the interaction of these two methods can lead to more efficient sterilization. Finally, it

is expected that the degradation will slow down as the mechanical properties increase with autoclaving and as the hydrogel increases its cross-linking and thus its crystallinity. However, no significant changes are expected with UV sterilized hydrogel and ethanol.

4. Conclusions

This work aims to find methods to sterilize PVA hydrogel for the 3D culture of mouse fibroblasts. In addition, it could be a promising starting point to create a material that can be 3D printed in tubular form for the creation of vascular prostheses.

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RELEVANCE OF VOLTAGE-DEPENDENT ANION CHANNELS FOR THE REGULATION OF SPERM LIFESPAN AND CAPACITATION

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Keywords: calcium, capacitation, motility, sperm, voltage-dependent anion channels

1. Introduction

Sperm capacitation is the process through which sperm acquire the ability to fertilize oocytes. This process relies on calcium influx, which drives sperm hyperactivation and the posterior acrosome reaction (Breitbart, 2002). Part of this calcium is stored in the mitochondria, involving voltage-dependent anion channels (VDACs) that reside in their inner membranes (Triphan et al., 2007). A previous study reported that inhibition of VDACs with 4, 4'-diisothiocyanatostilbene-2, 2'-disulfonic acid disodium salt (DIDS), a blocking molecule for anionic channels, leads to a decrease in sperm capacitation in mice (Kwon et al., 2013). The present work sought to determine if DIDS also impairs the response of pig sperm to *in vitro* capacitation and progesterone-induced acrosome exocytosis.

2. Methodology

Sperm were incubated in capacitation medium (TCM) and two concentrations of DIDS (5 and 50 µM) for 120 min at 38.5°C and 5% CO_2. A negative control, consisting of non-capacitation medium (TBM) was included. Sperm viability, membrane lipid disorder, mitochondrial activity, acrosome integrity, and intracellular levels of superoxides, total reactive oxygen species, and calcium were determined by flow cytometry, and motility was analyzed using a computer assisted sperm analysis (CASA) system. Assessments were performed after 0, 60, 70 and 120 min of incubation, adding progesterone after 60 min to induce the acrosome reaction.

3. Results and discussion

Incubation with 50 µM DIDS decreased the percentage of progressively motile sperm, which was concomitant with a decrease in intracellular calcium levels compared to TCM. Unexpectedly, although 50 µM DIDS reduced the percentage of viable sperm, it increased the

percentage of viable sperm with high membrane lipid disorder, which would correspond to sperm that initiate, albeit fail to complete, the capacitation process. These results differ from those reported in pigs, where the blocking of VDAC-2 channels with TRO19622 inhibited capacitation (Martínez-Abad et al., 2017). This would indicate that DIDS inhibit other channels than VDAC-2, which would also be involved in the regulation of capacitation. Moreover, the decrease in sperm motility and viability, and of calcium levels, suggests that the channels inhibited by DIDS are implicated in the maintenance of sperm survival, which is consistent with the results reported in mice (Kwon et al., 2013).

4. Conclusions

Our results suggest that incubation with DIDS alters, but does not completely abolish, the ability of pig sperm to elicit capacitation. In addition, the channels inhibited by DIDS appear to be involved in the regulation of sperm lifespan, motility, and calcium homeostasis.

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SPERM-RICH FRACTIONS EXHIBIT GREATER CHROMATIN PROTAMINATION AND CONDENSATION

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Keywords: chromatin, condensation, DNA damage, ejaculate fractions, pig, protamination

1. Introduction

Sperm chromatin integrity, protamination and condensation play an essential role during fertilization and embryo development (Selvam et al., 2021; Ribas-Maynou et al., 2023). In mammals, ejaculates are emitted in two fractions, the sperm-rich fraction (SRF) and the post sperm-rich fraction (PSRF), which exhibit different sperm concentration, volume, and seminal plasma composition (Rodríguez-Martínez et al., 2009). Sperm quality is known to differ between fractions, but whether this is also the case of sperm chromatin condensation and DNA integrity has not been investigated. The current study aims to address whether sperm chromatin condensation and integrity differs between fractions.

2. Methodology

Ejaculates from eight boars were collected separating three fractions: the first 10 mL of the SRF (10-SRF), the remaining volume of the SRF and the PSRF. Samples were incubated for 0, 6 and 24 h at 37ºC with the corresponding fraction of (SP) and stored at -80ºC until analysis of sperm chromatin protamination (chromomycin A3 test, CMA_3), sperm chromatin condensation (dibromobimane test, DBB), double-stranded DNA fragmentation (neutral comet assay) and global DNA damage (alkaline comet assay).

3. Results and discussion

Results for CMA_3, DBB, neutral comet and alkaline comet assays are presented in *Figure 1*. Sperm from the 10-SRF showed statistically higher protamination compared to SRF and PSRF at 0 h (P = 0.003 and P= 0.006) and after 6 h of incubation (P = 0.022 and P = 0.002). This finding suggests that the sperm from the 10-SRF exhibit the best quality traits. Besides, the sperm from the SRF showed a higher chromatin condensation than the PSRF at 0 h (P = 0.034) and after 24 h of incubation (P = 0.003); this higher condensation protects the most important regions of the sperm genome from genotoxic damage. In addition, there was a

decrease of chromatin condensation in the sperm from the PSRF after 24 h of incubation (P = 0.007), which would suggest an in vitro degradation of this chromatin. The similar incidence of DNA breaks reported between fractions at 0 h (P > 0.05) indicates that no differences in the reproductive success should be observed if they were used for fertilization after ejaculate collection. Increased fragmentation was nevertheless found at the 10-SRF compared to the PSRF after 6 h and 24 h of incubation (P < 0.01), revealing the negative impact of seminal plasma on sperm DNA integrity after an extended incubation.

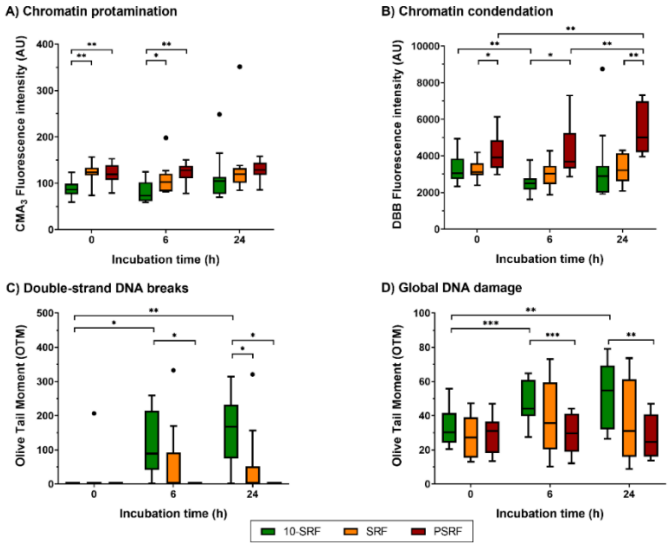

Figure 1. Box-whisker plot showing the effects of incubating ejaculate fractions with seminal plasma after 0 h, 6 h and 24 h at 37ºC on sperm chromatin protamination (A), sperm chromatin condensation (B), double-stranded DNA breaks (C) and global DNA damage (D). The boxes enclose the 25th and 75th percentiles, the whiskers extend to the minimum and maximum values, and the line indicates the median. Outlier values are represented with a dot. Statistically significant differences are shown as * ($P \leq 0.05$), ** ($P \leq 0.01$) and *** ($P \leq 0.001$).

4. Conclusions

While the sperm from 10-SRF and SRF exhibit better chromatin quality in terms of protamination and condensation, fractions are similar in their sperm DNA integrity.

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EVALUATION OF MITOCHONDRIAL FUNCTION IN SKIN FIBROBLASTS AS A BIOMARKER FOR THE EFFICACY OF TWO PHYSICAL ACTIVITY PROGRAMS IN PARKINSON'S DISEASE PATIENTES

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Keywords: Biomarker, Exercise Therapy, Mitochondrial Diseases, Neuroprotection, Parkinson's Disease

1. Introduction

Parkinson's disease (PD) is a disorder characterized by the progressive degeneration of dopaminergic neurons resulting in dopamine deficiency in the striatum (Erbach, 2013). Mitochondrial dysfunction and oxidative stress are associated with PD and are intrinsic factors related to its pathogenesis. Physical activity (PA) increases cognitive ability in older adults, attenuating motor deficits, increasing new neuron formation, ameliorating neurological impairments, and impeding age-related neuronal loss (Carvalho et al., 2015). In addition, skin fibroblasts have been identified as surrogate indicators of pathogenic processes correlating with clinical measures (Yoo et al., 2019; Deus et al., 2020). The present study aims to compare the effects of two different PA programs in PD patients analyzing relevant clinical aspects and the impact on mitochondrial function in patients' skin fibroblasts, used here as biomarker for metabolism improvement and disease progression.

2. Methodology

Patients with early-stage PD (stage I to III, according to the modified Hoehn-Yahr classification; n=24) will be recruited and randomized into three matched groups. The effects of two different PA programs will be compared. The first group (n=8) will perform basic physical training (BPT) based on strength and resistance. A second group (n=8) will perform BPT combined with functional exercises (BPTFE), including exercises aimed to stimulate the specific sensorimotor pathways that are most affected in PD (proprioception-balance-coordination) together with cognitive and motor training. A third group will serve as the control (sedentary group; Sed). Subjects will perform 3 sessions per week for 16 weeks. Motor

function, quality of life, sleep quality, cognitive aspects, and humor will be evaluated before and after intervention. A metabolic characterization of skin fibroblast will be performed by respirometry using the Seahorse XFe96, and by measuring ATP levels and mitochondria-related transcripts and proteins to determine the bioenergetic cellular deficits and characterize the metabolic remodeling induced by the exercise programs.

3. Results

We predict that the application of the BPT and BPTFE programs will ameliorate relevant clinical aspects of the disease by improving systemic mitochondrial function, restoring mitochondrial metabolism, gene expression patterns, and ultimately, translating into mitochondrial neuroprotective effects.

4. Conclusions

The comparison of BPT and BPTFE PA programs will provide insights into the degree of amelioration in several relevant aspects of PD, including motor function, quality of life, quality of sleep, cognitive aspects, humor, and mitochondrial function. Such changes can have a positive clinical impact and PD skin fibroblasts may be used as a biomarker for PD diagnosis and disease progression assessment.

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SESSION 9.
SYNTESIS AND CATHALYSIS

INDOLIZINE SYNTHESIS FROM COPPER CARBENES: A PREDICTIVE CATALYSIS APPROACH

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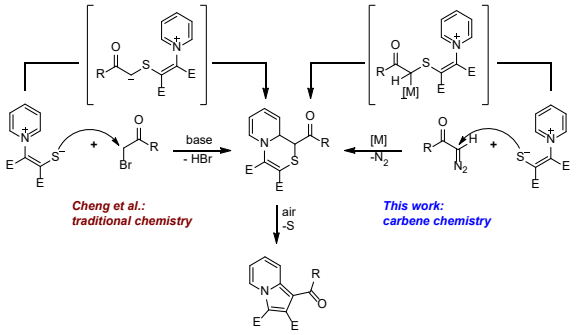
Keywords: carbene, copper, DFT, indolizine, predictive catalysis

1. Introduction

The indolizine motif, found at the core of important pharmaceuticals, shows very relevant biological activities and photophysical properties to the molecules that contain it, which has prompted the development of multiple synthetic methodologies towards this motif. Pyridinium 1,4-zwitterionic thiolates are a class of zwitterions applied in thermal annulations in recent years. The main advantage of using synthons with rich reactivity is that they are air-stable, odorless, and easy to handle.

2. Hypothesis

Drawing inspiration from the (3+2) annulation toward indolizines, we decided to evaluate if carbene chemistry could be a viable alternative to traditional chemistry in the (5+1) annulation of pyridinium 1,4-zwitterionic thiolates described by Cheng et al. (2020) and shown in Scheme 1.



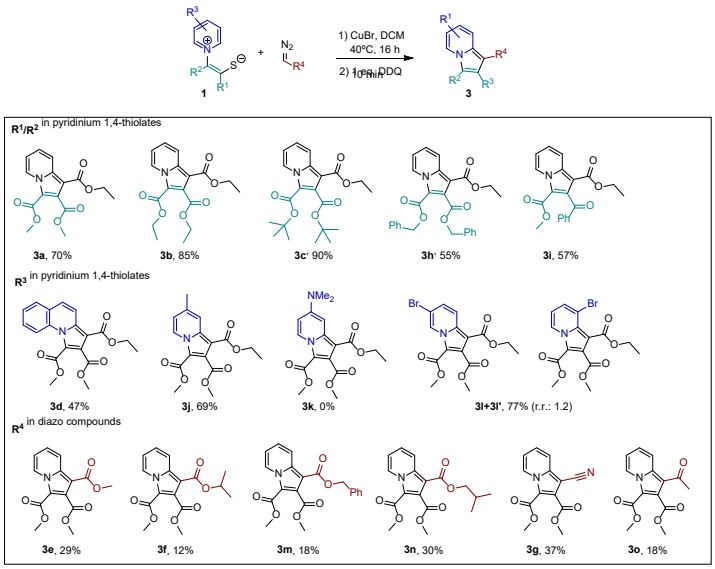
Scheme 1. Traditional vs carbene approach to the (5+1) annulation of pyridinium 1,4-zwitterionic thiolates.

3. Methodology

Density functional theory (DFT) calculations to unveil the reaction mechanism were performed at the B3LYP-D3(SMD)/Def2TZVP//B3LYP-D3/Def2SVP level of theory. Experimentally, the synthesis of indolizine scaffolds was carried out under nitrogen atmosphere. The obtained products were characterized by means of ^{1}H-NMR, ^{13}C-NMR and ESI-MS.

4. Results and discussion

The computed mechanism for the synthesis of indolizines is thermodynamically favorable, and the highest activation energy has a kinetic cost of 20.7 kcal/mol (Monreal-Corona, 2023). The scope was explored using CuBr and DCM at 40°C for 16h, followed by treatment with DDQ. As shown in Scheme 2, the reaction tolerated substituents in both the pyridinium and diazo species.



Scheme 2. Scope of the reaction.

5. Conclusions

Predictive catalysis is applied to the reaction of pyridinium 1,4-zwitterionic thiolates with a copper carbene. Theoretical calculations were first performed to determine the suitability of the annulation reaction and then the scope of the reaction was assessed with yields up to 90%.

6. Bibliography

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REGIOSELECTIVE ACCESS TO ORTHOGONAL DIELS-ALDER C_{60} ADDUCTS AND TRIS-HETEROADDUCTS VIA SUPRAMOLECULAR MASK STRATEGY

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

1. Introduction

Pure-isomer poly-functionalized fullerenes are highly desired because of their unique physico-chemical properties. Nevertheless, their synthesis is hampered by the lack of regioselectivity during functionalization of pristine fullerenes. Thus, complicated mixtures of different regioisomers and carbon-based nanostructures are obtained when they are produced, and they must be purified by tedious, expensive and time-consuming techniques. To address this shortcoming, supramolecular nanocapsules to recognize fullerenes in their inner cavities have been used to increase the levels of regioselectivity of this kind of reaction (Fuertes-Espinosa et al., 2020).

2. Hypothesis

Prismatic tetragonal nanocapsules will be used as supramolecular masks (Fuertes-Espinosa et al., 2020) to bis-functionalize C_{60} fullerenes by means of Diels-Alder (DA) and Bingel-Hirsch reactions to overcome the lack of regioselectivity (Pujals et al., 2022).

3. Methodology

The synthesis and characterization of nanocapsules have been performed following the procedures reported in Reference 2 (Fuertes-Espinosa et al., 2020).
The functionalization of fullerenes has been carried out by templated DA reaction using two different acenes (anthracene and pentacene) to explore the different regioselectivity leads by steric control. The obtained products were characterized by different spectroscopic techniques.
Heteroadducts have been synthetized combining DA and Bingel-Hirsch reactions.
The computational study has been carried out by molecular dynamics simulations and frontier molecular orbital analysis.

4. Results and discussion

The functionalization of C_{60} fullerene using anthracene as the acene of the templated DA reaction led to a single regioisomer, which presented two anthracene moieties at a 90° angle.

On the other hand, when pentacene was used, the DA reaction gave a completely different regioisomer (two pentacene moieties placed at a 180º angle).
Computational modelling showed that mono-An-C_{60} can freely rotate inside the nanocapsule: it can be positioned either horizontally or vertically with respect to the porphyrin subunits of the nanocapsule and can visit the four gates of the nanocapsule. In contrast, mono-Pn-C_{60} was fixed in a single gate and always in a vertical orientation, which dramatically restricted the attack of the second pentacene.
Finally, equatorial heteroadducts could be synthetized by combining DA and Bingel-Hirsh reaction in great levels of regioselectivity.

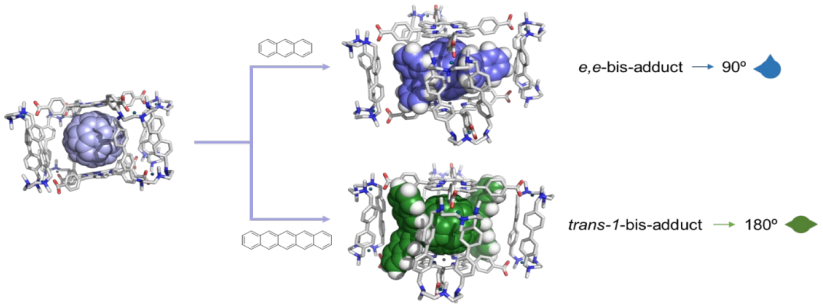

Figure 1. Schematic representation of both host-guest complexes obtained by means of Diels-Alder reaction sharply directed by supramolecular-mask nanocapsule strategy.

5. Conclusions

Tetragonal prismatic nanocapsules have been used as a supramolecular mask strategy to functionalize C_{60} fullerenes by means of Diels-Alder reaction in a sharp and orthogonal regioselective manner by simply enlarging the acene molecule (anthracene vs pentacene). The differences between both reaction systems have been explained by computational modelling. Finally, different equatorial heteroadducts have been successfully formed combining Diels-Alder with Bingel-Hirsh reaction.

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REGIO-SELECTIVE BIS-FUNCTIONALIZATION OF FULLERENE C_{70} VIA SUPRAMOLECULAR MASKS

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Keywords: fullerene, mask strategy, nanocapsule, regioselective functionalization

1. Introduction

Isomer-pure poly-functionalized fullerenes are required to boost the development of fullerene chemistry in any field, specifically in solar cell design (Umeyama, 2019). Developing new synthetic strategies capable of restricting the regioisomer formation is a challenge, especially for C_{70}, less abundant than C_{60}, and with 8 distinct bonds at which mono-functionalization may occur, leading to a complicated mixture of multiple adducts when functionalized.

2. Methodology

In this work, the regio-selective synthesis of bis-C_{70}-adducts has been achieved through Bingel cyclopropanation using supramolecular nanocapsules as masks. A tetragonal prismatic nanocapsule and a three-shell Matryoshka-like complex have been synthetized and characterized by HR-MS. The functionalization using bromo-malonates has been monitored by HR-MS and the products have been identified through the characteristic UV-Vis spectra and by ^{1}H NMR.

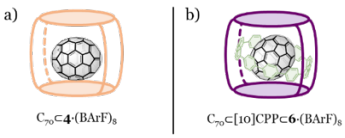

Figure 1. Representation of the supramolecular mask strategies used:
a) C_{70} encapsulated in the tetragonal prismatic nanocapsule (**4**·(BArF)$_8$)
b) The three-shell Matryoshka-like complex with the C_{70} complexated with a [10]CPP ring inside of the tetragonal prismatic nanocapsule. (**6**·(BArF)$_8$).

3. Results and discussion

A comprehensive study about the bis-functionalization of fullerene C_{70} has been performed, starting from the functionalization of bare C_{70} with four different bromo-malonates. In this case, a complicated mixture of poly-adducts is obtained and the ratio between the three possible regio-isomers of the bis-adducts has been calculated showing a preference for the 2 o'clock regio-isomer. To restrict the regio-selectivity, the C_{70} has been encapsulated in a tetragonal prismatic nanocapsule (Fuertes-Espinosa, 2020). Using this mask strategy, we

could find the conditions to obtain just the bis-adducts with a ratio between the 3 possible regio-isomers which switch the preference to the 5 o'clock regio-isomer. Lastly, using the three-shell Matryoshka-like complex (Ubasart, 2021), we could control the chemo-selectivity obtaining just the bis-adduct and, strikingly, in the case of the dibenzyl bromo malonate, a single pure regio-isomer (2 o'clock) of the Bingel bis-adduct of C_{70} is obtained achieving a 100% regioselectivity.

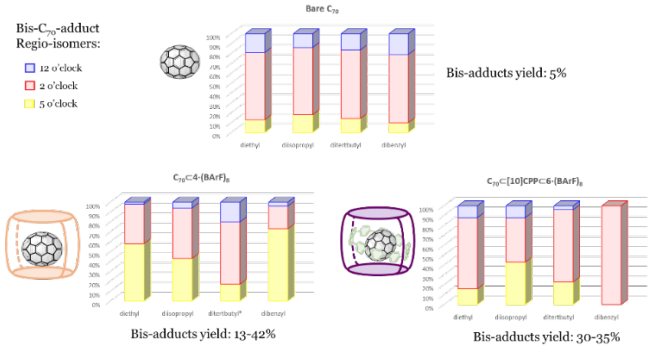

Figure 2. Summary of the results obtained in the bis-functionalization of fullerene C_{70} with the four different bromomalonates (diethyl-, diisopropyl-, ditertbutyl and dibenzyl- bromomalonate) on bare C_{70}, $C_{70}\subset$**4**·$(BArF)_8$ and $C_{70}\subset$[10]CPP$\subset$**6**·$(BArF)_8$

4. Conclusions

This work demonstrates that the supramolecular mask strategy can be a powerful tool to obtain chemo- and regio-selectivity in the functionalization of C_{70}. By changing the type of mask or the type of addend, the regio-selectivity can be tuned. This strategy could be useful for the challenging synthesis of isomer pure C_{70} adducts for important electronics and solar cell applications.

5. Bibliography

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SYNTHESIS OF CYCLIC SULFAMATES BY RHODIUM-CATALYSED NITRENE/ALKYNE METATHESIS

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Keywords: cascade reaction, cyclic sulfamates, nitrene/alkyne metathesis (NAM), rhodium

1. Introduction

Species containing cyclic sulfamates are present in natural products and are widely used in the pharmaceutical industry. As a result, the construction of these derivatives has been extensively studied during recent decades and has attracted the attention of the scientific community (Saeidian, 2015). One straightforward way to construct these heterocycles is via a nitrogen transfer through an intramolecular nitrene/alkyne metathesis (NAM) generating an α-imino carbene intermediate that can be intercepted and/or terminated by various carbene reactions (Hong, 2022; Ren, 2022). In this master's project we will study the intramolecular rhodium-catalysed nitrene/alkyne metathesis of alkyne sulfamates to afford cyclic sulfamate derivatives in a straightforward and efficient way.

2. Methodology

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

3. Results and discussion

To study the NAM process, several starting materials containing a sulfamate and an alkyne will be prepared. A search of the literature will be undertaken to find the best synthetic pathways to synthetize them. Once the starting sulfamates have been prepared and fully characterized, they will be converted into the nitrene intermediate after catalytic oxidation in the presence of $Rh_2(esp)_2$ and bisacetoxyiodobenzene ($PhI(OAc)_2$) as the oxidant. An intramolecular nitrene/alkyne metathesis from the nitrene intermediate will be performed and subsequently an α-imino carbene intermediate will be generated that can be intercepted to provide a modular method for the construction of complex cyclic sulfamates.

Once the best catalytic reaction conditions have been found, the scope of the process will be studied. Additionally, DFT studies will be performed to understand the mechanistic insights of the reaction and to propose a catalytic cycle for the NAM cascade reaction.

4. Conclusions

New cyclic sulfamates will be synthetized via a nitrene/alkyne metathesis cascade reaction under rhodium catalysis. The new catalytic process will be optimized, and the scope of the reaction will be studied. Insights regarding the mechanism of the reaction will be obtained through DFT calculations.

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DEAROMATIZATIVE SYN-DIHYDROXYLATION OF ARENES

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Keywords: arenes, catalysis, iron, naphthalenes, oxidation

1. Introduction

The abundance of arenes in nature makes them very interesting substrates in organic synthesis. Through their oxidative dearomatization reactions, they can be easily converted into very elaborated molecules, containing multiple stereogenic centers with potential biological interest.

In nature, heme and non-heme iron oxygenases can oxidize arenes disrupting their aromaticity while using mild conditions. On one hand, monooxygenases can produce the epoxides of arenes, and on the other hand, Rieske Dioxygenases can perform the syn-dihydroxylation of alkenes and arenes (Boyd and Sheldrake, 1998). The most studied enzyme within this family is naphthalene-1,2-dioxigenase (NDO) which can realize enantioselectively the syn-dihydroxylation of naphthalene.

2. Hypothesis /Problem

Even though enzymes can perform those reactions with good yields and excellent enantioselectivities, due to the complexity of those reactions very little is currently known about their realization using artificial systems.

3. Methodology

In literature we can find an example that imitate the behavior of those dioxygenases. It consists in an iron catalyst that can perform the same reaction of the NDO enzyme, unfortunately, the yield obtained for the product is very low and cannot be used for synthesis (Feng et al., 2008).

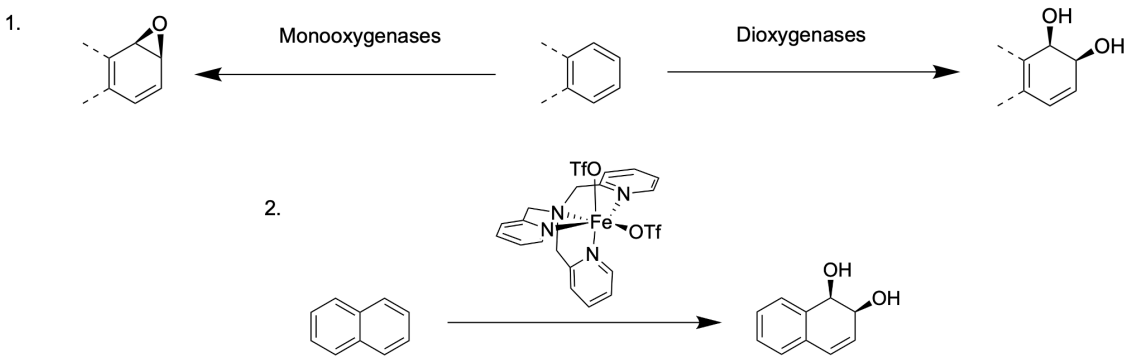

Figure 1

4. Results and discussion

Taking this into account, in this work we want to use transition metal-based catalysts to perform oxidative dearomatization reactions using naphthalene as a model substrate and hydrogen peroxide as oxidant. We want to break the aromaticity while generating different stereogenic centers through the oxidation. Our main objective is to achieve yields that can be used for synthesis.

5. Conclusions

In this work we mimicked the reactivity of naphthalene dioxygenase enzyme using a bioinspired iron catalyst.

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METAL OXIDES TOWARDS THE FIXATION OF CO2 WITH EPOXIDES: FROM HOMOGENEOUS TO HETEROGENEOUS CATALYSIS

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Keywords: CO2 fixation, epoxides, heterogeneous, homogeneous, metal oxides

1. Introduction

Among various CO_2 fixation reactions, cycloaddition with epoxides to produce five-membered cyclic carbonates represents one of the most attractive, straightforward, and green protocols (Monfared et al., 2019). The cyclic organic carbonates produced show promising industrial applications such as an intermediate for polycarbonate and dimethyl carbonate, a solvent in lithium-ion batteries, paint, personal care, and cosmetic products (Kulal et al., 2019).

In the last few years, numerous catalytic systems have been developed that could effectively catalyze the cycloaddition of epoxides with atmospheric CO_2 under solvent-free conditions. This process is sought to be inexpensive and efficient, and the catalytic systems that are active under mild conditions of temperature and pressure must also be recoverable. In detail, Natongchai et al. (2022) reported the use of group I and II metal halides as catalysts for the crucial cycloaddition reaction of CO_2 to epoxides (Figure 1).

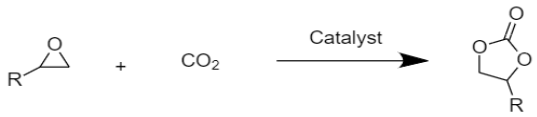

Figure 1. Cycloaddition reaction of an epoxide with CO2 for the formation of a cyclic carbonate.

2. Methodology

For homogeneous calculations, the mechanism was studied in gas phase at the BP86-D3/ Def2SVP~SDD level, where the SDD pseudopotential approximation is used for iodide and heavy metals. Next, single-point energy calculations were carried out at the B3LYP-D3/Def2TZVP~SDD level of theory, this time considering the explicit solvent effects by SMD using the epoxide itself as the solvent.

For heterogeneous calculations, four-layered surfaces of SnO_2 (0 1 1) with a tetragonal crystalline structure and hexagonal ZnO (1 0 1) were built and optimized. After an H coverage

analysis, adsorption of the epoxide was studied on each surface, as was the desorption of the product. These calculations were performed using water as the solvent.

3. Results and discussion

The calculations of the homogeneous systems (each optimized step of the process, as well as the transition states) allow us to better understand the reaction mechanism, and especially the role that hydrogen atoms on the metal oxides plays in it.

For heterogeneous calculations, the main results are the coverage study, adsorption and desorption energies, and frequencies of the systems.

4. Conclusions

The mechanism of CO2 cycloaddition with epoxides to produce five-membered cyclic carbonates has been studied and compared to preexisting experimental data. Several transition states have been proposed in the homogeneous catalytic cycle. Heterogeneous calculations have allowed us to better understand the adsorption and desorption processes.

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EXPLORING THE STABILIZATION OF ALUMINIUM COMPLEXES BY AN AMINOPHOSPHINE BOROHYDRIDE MOTIF

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Keywords: aluminium, aminophosphines, borohydrides, main group

1. Introduction

The fixation of small molecules such as CO2 and H2 is of paramount importance given the widespread demand for inexpensive feedstock to construct multicarbon compounds (organic bulk chemicals, fuels) and to store energy or new materials (Inventory of U.S. Greenhouse Gas Emissions and Sinks: 1990-2018, 2021). In this sense, the chemistry of main group elements has gained significant interest in the recent years. This is a consequence of landmark investigations showcasing the potential of p-block species mimicking the transition metal behaviour (Melen, 2019).

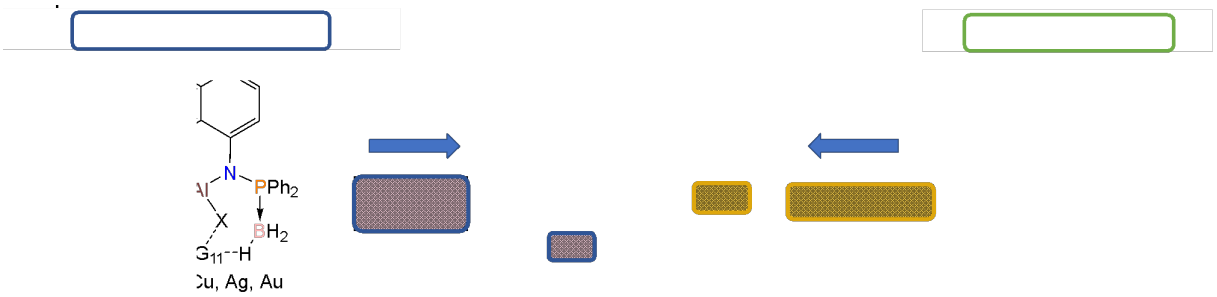
Within group 13 of the periodic table, aluminium is a promising exponent and the most abundant metallic element and the third most common element found in Earth's crust. (Wedepohl, 1995) However, to do such activation, aluminium needs to be tuned either by reduction to access low-valent states or polarization with transition metals (Hicks, 2021). In this work, we synthesise the building blocks for such small activation by investigating the potential of phosphine borohydrides as substituents to provide stabilization for bimetallic compounds and as protecting groups to isolate low-valent aluminium compounds.

2. Methodology

All manipulations were carried out under argon atmosphere (Argon 5.0) using Schlenk line techniques or glovebox.

3. Results and discussion

We synthesise the unknown ligand N^1,N^8-Bis(borane-diphenylphosphino)-1,8-naphthalenediamine and the halide, hydride precursors to explore the low-valent and bimetallic chemistry of aluminium. Up to now, different group 13 (aluminium) compounds have been synthesised and all the compounds were fully characterized by spectroscopic techniques. Furthermore, investigation of the reduction of the aluminium halides show promising results.



Scheme 1: Retrosynthetic picture of the targeted bimetallic and low-valent aluminium compounds.

4. Conclusions

The stabilisation of bimetallic compounds by phosphine borohydride compounds has not been explored in main group chemistry. This work opens the possibility to explore this field with elements other than aluminium.

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HEURISTICS AND SERENDIPITY IN SYNTHETIC METHODOLOGIES

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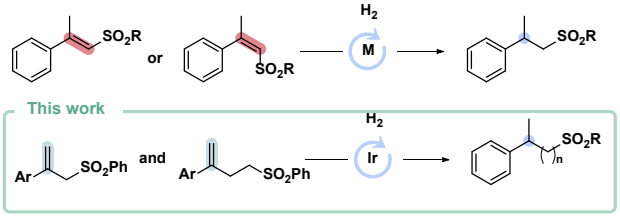
Keywords: allylic sulfones, asymmetric hydrogenation, natural products

1. Introduction

The synthesis of chiral sulfones has been widely used mainly due to the versatility of this functional group (Liu et al., 2016; Trost & Kalnmals, 2019). Regarding asymmetric and catalytic transformations, several groups have been synthetized and vinyl sulfones have been hydrogenated by using ruthenium, rhodium, or iridium complexes (Li et al., 2020; Yan et al., 2019; Peters et al., 2014).



Scheme 1. Asymmetric synthesis of sulfones.

2. Hypothesis

Most reported substrates were internal alkenes (2-aryl-2-methyl vinyl sulfones), which often encounter *E*/*Z* selectivity issues in their preparation steps and may be hard to separate.

3. Methodology

To overcome this issue, the group has been working on the asymmetric hydrogenation of terminal olefins, allylic amines, phthalimides, and homoallylic alcohols (Cabré et al., 2019, 2020). Taking this issue into account, the development of novel methodologies to prepare these unsaturated sulfones is therefore needed.

4. Results and discussion

On the one hand, the synthesis of terminal allylic sulfones was performed through a novel one-pot, three-component Pd-catalyzed Suzuki-Miyaura/Allylic coupling reaction. These tandem

reactions allow the regioselective formation of a wide range of substrates in a single step. On the other hand, homoallylic sulfones were prepared by an improved opening of oxetanes, a novel application for a super Lewis acid.

5. Conclusions

In the present communication, the implementation of a heuristic approach and a serendipitous outcome will describe the course of these two projects.

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SESSION 10.
WATER TREATMENT

MEMBRANE TECHNOLOGY DEVELOPMENT FOR VOLATILE FATTY ACID CONCENTRATION AND PURIFICATION

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Keywords: Forward osmosis, reverse osmosis, VFA, VFA concentration, VFA purification

1. Introduction

Volatile fatty acids (VFAs), such as acetic, propionic, butyric, and valeric acids, are organic compounds that have recently gained interest due to their utility for industrial processes such as pharmaceutical, food, and plastic and bioplastic products. But VFA concentration in the effluent limits the PHA production. For this, different membrane technologies have been tested, and nanofiltration (NF), reverse osmosis (RO), and forward osmosis (FO) appeared to be the best options to achieve higher VFA concentrations and, in some cases, separate them from the initial mixture (Blandin et al., 2020; Domingos et al., 2020).

2. Methodology

NF, RO, and FO membranes were tested under synthetic and real effluent at lab-scale to characterize and assess the capability to concentrate and separate a VFA mix at 3 g/L. For FO, two membranes were used (Toray flat sheet membrane and Aquaporin hollow fiber module) and were tested at 70 g/L of NaCl. NF and RO flat sheet membranes were tested in a pressurized pilot plant at 15 bars using a 0.014 m^2 membrane cell.

3. Results and discussion

During high pH experiments, FO membranes achieved high VFA concentrations, 25 g/L for Toray membranes and 50 g/L for Aquaporin modules (Figure 1). According to VFA analysis, both membranes had more than 95% VFA recovery. The RO flat sheet membrane also resulted in VFA concentration as the membrane had a rejection rate higher than 90%. For nanofiltration, NF 90 (smaller pore size) achieved higher acid rejection than NF 270. These results could be related to the pore size difference between NF 90 and NF 270. Low pH experiments showed a significant loss of VFA recovery/rejection, related to VFA disassociation changes. At high pH, most VFA are negatively charged, which causes an electrostatic repulsion effect with the negatively charged polyamide membrane. But with lower pH, there is no electrostatic repulsion, reducing the VFA rejection to steric effects, where high pore size membranes were the least effective (Pervez et al., 2022).

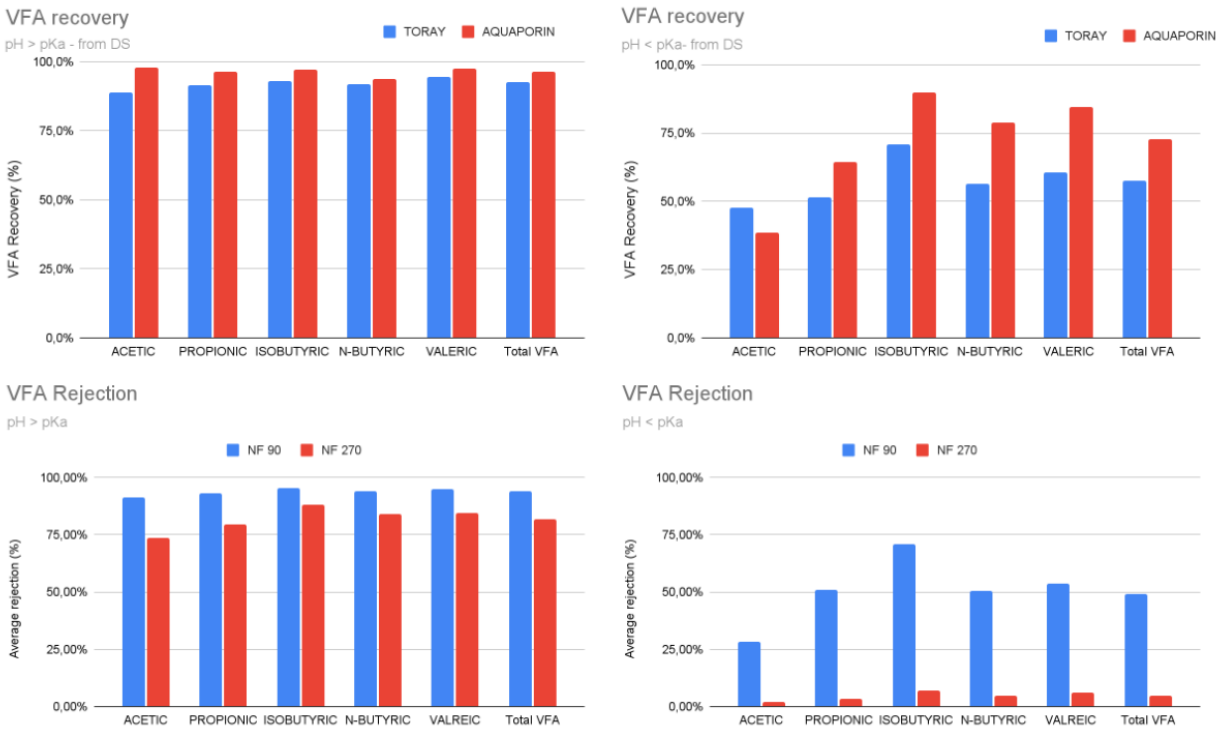

Figure 1. Volatile fatty acid recovery for FO membranes during high pH (upper left) and low pH (upper right) experiments, and volatile fatty acid rejection for NF membranes for high pH (lower left) and low pH (lower right).

4. Conclusions

FO, RO, and NF membranes proved to be capable of concentrating VFAs at a high pH but at lower pH, VFA recoveries and rejections decreased significantly. These phenomena would allow VFAs to be separated from the rest of the mixture, depending on molecular size and weight. In conclusion, membrane technologies have demonstrated to be capable of both concentrating and separating VFAs from an initial mixed broth depending on the operational parameters.

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GRAVITY-DRIVEN RECYCLED MEMBRANE SYSTEM FOR AN URBAN WASTEWATER TREATMENT PLANT

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Keywords: gravity-driven, membrane recycling, nanofiltration, reverse osmosis, ultrafiltration

1. Introduction

Ultrafiltration (UF) and nanofiltration (NF) membranes are used in gravity-driven membrane (GDM) systems. Generally, they produce clean water (permeate) by using water height pressure difference between the feed tank and the permeate. As Pronk et al. (2019) reported, flat sheet or hollow fiber microfiltration and UF membranes are the most common configuration used for drinking water production in developing countries.

This work validates the use of end-of-life reverse osmosis (RO) membranes, converted into UF or NF in a GMD system to treat the secondary effluent of an urban wastewater treatment facility in Quart (Girona, Spain). To assess water quality according to RD1620/2007, water analysis of the feed and permeate were carried out.

2. Methodology

End-of-life RO modules were converted into UF or NF with chlorine according to the standard protocol explained by García-Pacheco et al. (2015). Then, the modules were introduced into an advance membrane housing design as reported by García-Pacheco et al. (2021). The membranes filtered in intermittent mode including cycles of filtration (between 23h and 72h), followed by a relaxation (10 min) and flushing (5 min), for one month. The permeability (taking at least 20L of water/day) was evaluated before and after flushing and normalized at 20ºC.

3. Results and discussion

Figure 1 shows the results of the permeability obtained for a recycled UF membrane before applying the relaxation and flushing sequence (orange dots) and after it (blue dots).

The initial permeability decreased by 61% in the first week even though relaxation and flushing were performed every day. Then, the system was not able to filter during 24h because the membrane was fouled. Therefore, the permeate tubing section was decreased, and permeability remained more constant.

In all cases, the permeability was higher after applying relaxation and flushing than the permeability measured after 24h filtration, suggesting that relaxation and flushing could be a good practice to prevent fouling.

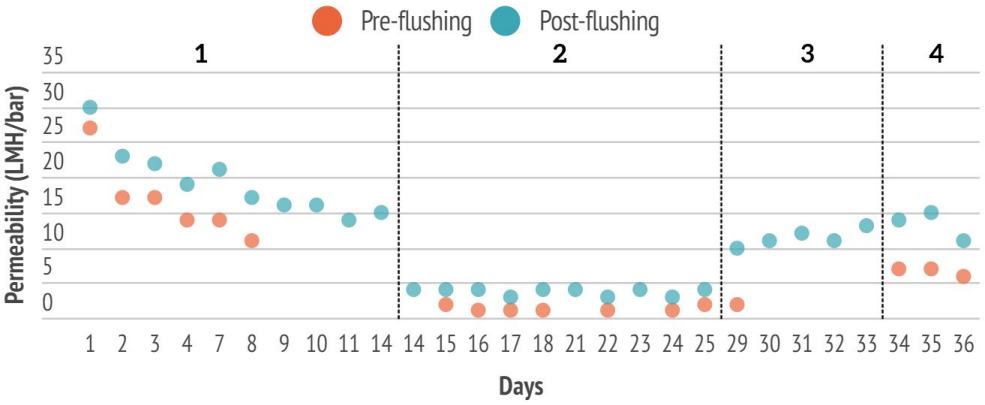

Figure 1. Permeability of UF membrane filtering by gravity-driven conditions. Cycle 1: the permeate t has an internal diameter of 8mm, Cycle 2: internal diameter of 3mm, Cycle 3: internal diameter of 6mm, Cycle 4**:** internal diameter of 6mm and water column 15cm taller.

Additionally, the system was able to reduce 3-5 LRV (*E. coli* and coliforms) and SS were below detection limit.

4. Conclusions

A single end-of-life RO membrane module converted into UF or NF can produce almost between 280 L/d and 50 L/d, respectively, and meet the quality standard defined in RD1620/2007. The values obtained for water analysis, like a 3-5 LRV reduction, demonstrate that the system could potentially be implemented in isolated areas and has a great potential for urban wastewater tertiary treatment.

5. Bibliography

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INITIAL EVALUATION OF RETROFITTING AN EXISTING REVERSE OSMOSIS DESALINATION PLANT TO COMBINE WATER REUSE AND DESALINATION: A DESIGN STUDY

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Keywords: Desalination, Forward osmosis, Reverse osmosis, Software design, Water reuse

1. Introduction

Global warming affects the water cycle and results in recurring events like water scarcity and drought, which highlights the need to identify alternative water sources through desalination and water reuse (Hochstrat, 2010). The alternative to thermal desalination processes are membrane-based desalination technologies, and reverse osmosis (RO) is currently the leading one. By combining water reuse and desalination, forward osmosis (FO) will take advantage of free osmotic energy of seawater to decrease RO energy needs while assuring safe water production (Blandin, 2015). The FO-RO integration should reduce energy consumption with the dilution of the feed seawater stream or possibly an increase in water production (Teusner, 2016).

2. Hypothesis

The key challenge is to evaluate if an existing desalination plant can be upgraded to an FO-RO hybrid system to produce safe water for reuse with much lower energy consumption compared to stand-alone RO desalination.

3. Methodology

The approach was to use LewaPlus (Lanxess) water treatment design package for simulation work. As a reference, a baseline desalination plant (with 35 g/l feed salinity) was modelled with a feed flow of 4,000 m^3/h to produce 1,800 m^3/h of permeate in which overall plant recovery was 45% and there were 2,934 membrane elements. The same plant design was simulated with varying salinity in the feed. The dilution of seawater in FO-RO hybrid systems is done with FO permeate. The percentages of FO permeate used in achieving 5, 10, 20 g/l feed dilutions are 85.5, 75.5 and 43, respectively. The impact of feed dilution on energy consumption, potential design limitations, and permeate water quality was evaluated for several feed salinities. The LewaPlus design software allows modelling of these dilutions and reveals the errors and warnings present, if any, in the given design configuration.

4. Results and discussion

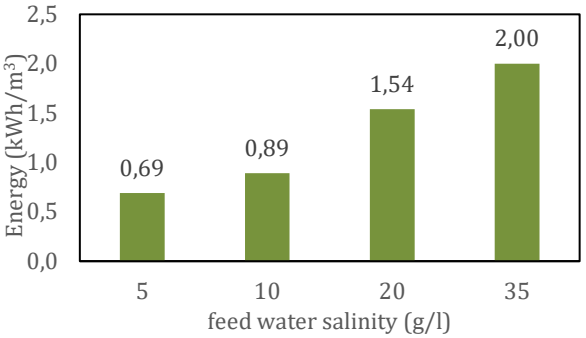

Figure 1. Energy consumption with varying feed salinities

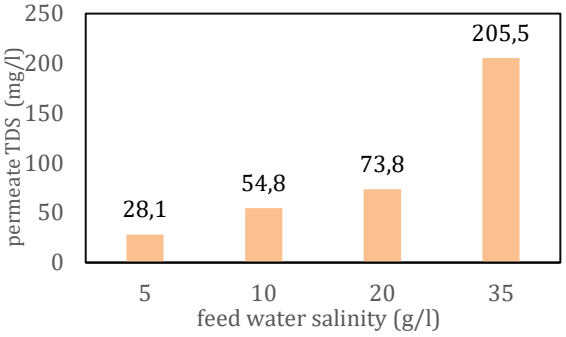

Figure 2. Permeate TDS with varying feed salinities

With a feed flow of 4000 m^3/h, the simulation results from LewaPlus states that there is decrease in energy consumption with dilution in feed water salinity (Figure 1). The dilutions at 5 and 10 g/l in the feed reduced the power consumption by 65.5% and 55.5% respectively. Also, the total dissolved salt content (TDS) in the permeate stream has been reduced with the decrease in feed salinity (Figure 2).

5. Conclusions

The simulation study shows that creating a hybrid FO-RO plant can be made possible by retrofitting an existing desalination plant to produce the desired permeate quantity. The entire configuration is beneficial in lowering energy needs as well as combining water reuse and desalination, which cannot be overlooked.

6. Bibliography

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RECOVERY OF K-RICH STRUVITE FROM THE WASTE SLUDGE PRODUCED IN A BIOLOGICAL NITROGEN REMOVAL UNIT TREATING SWINE MANURE

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Keywords: EDTA, K,Na-struvite, nutrient recovery, oxalic acid, waste sludge.

1. Introduction

A large amount of swine manure highly loaded with nitrogen (N), phosphorus (P) and potassium (K) is produced by the intensive pig farming industry. Under the circular economy framework, innovative procedures for the recovery of P and K as K-struvite (MPP, $MgKPO_4 \cdot 6H_2O$) are of high interest. The waste sludge from a nitrification – denitrification (NDN) bioreactor contains P that can be mobilised by acidification (Company et al., 2022). Unfortunately, calcium (Ca^{2+}) will also be mobilised. The crystallisation of K-struvite is disfavoured by high levels of Ca^{2+} due to the formation of calcium phosphates (Ca-P). Thus, the development of new procedures to prevent the interference of Ca^{2+} during K-struvite formation are needed (Srinivasan et al., 2014). This study aims to investigate the recovery of K-rich struvite from the waste sludge of a NDN bioreactor treating swine manure.

2. Methodology

Waste sludge was collected from a NDN treatment plant on a pig farm in Osona (Spain) (Figure 1). The sludge had a total Mg/K/P molar ratio of 0.7/1.2/1 (1292 ±8 mg P/L). Sulphuric acid (H_2SO_4), ethylenediaminetetraacetic acid (EDTA) and oxalic acid solutions were used as acidifying agents. NaOH was used to increase the pH for crystallization purposes.

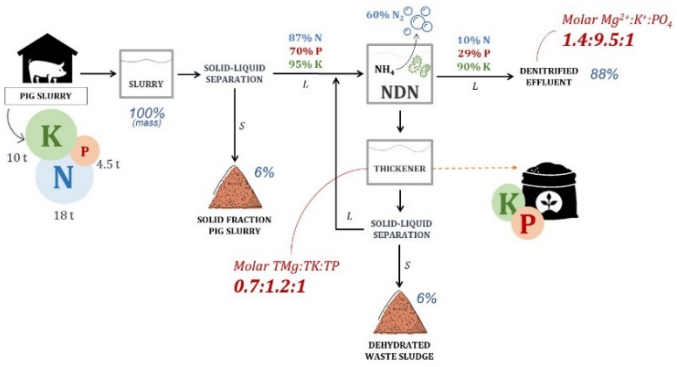

Figure 1. Flow chart of a swine manure treatment plant by nitrification-denitrification (NDN).

3. Results and discussion

As shown in Figure 2, by adding the acidic agent (H_2SO_4, EDTA or oxalic acid) according to a targeted pH (values from 6 to 4), significant amounts of PO_4^{3-}, Mg^{2+} and, Ca^{2+} were released. In each test, the lower the pH considered, the higher the solubilisation achieved.

The concentration of K^+ remained almost invariable during the acidification test because this element was already soluble. By adding oxalic acid, any increase in the concentration of Ca^{2+} was observed (Figure 3) due to the formation of calcium oxalate (insoluble). Contrarily, by adding EDTA, an increase in Ca^{2+} concentration was observed (Figure 2) because of the formation of the sequestering complex Ca-EDTA (soluble).

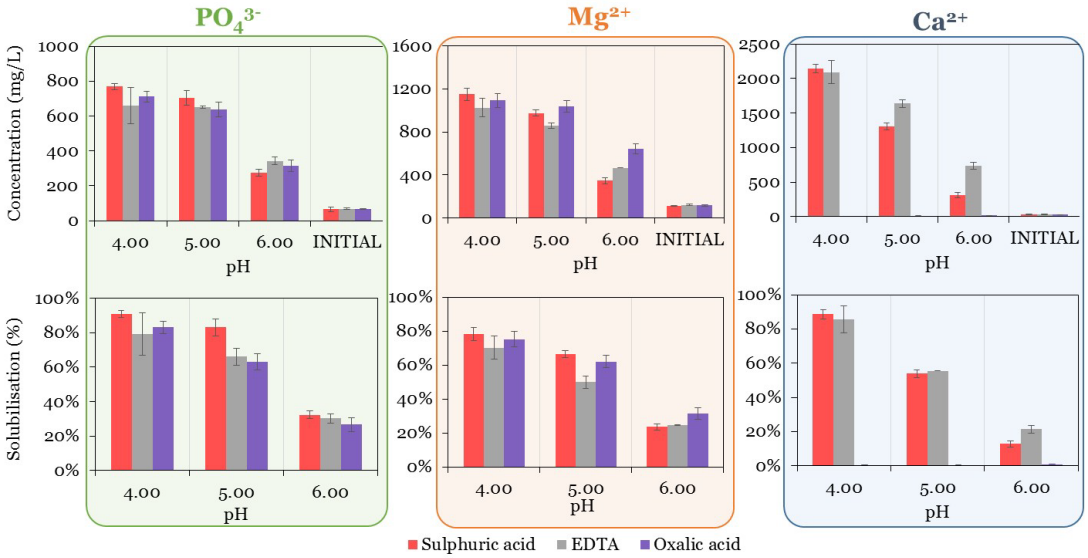

Figure 2. Ion concentrations (top) and solubilisation efficiencies (bottom) for phosphorus (green), magnesium (orange), and calcium (blue) due to the addition of H_2SO_4 (pink), EDTA (grey) and oxalic acid (purple) according to the targeted pH-value.

The analysis of the precipitates formed after raising the pH of the waste sludge using oxalic acid confirmed the presence of K,Na-struvite ($Mg_2KNa(PO_4)_2{\cdot}14H_2O$) with a composition between 10% and 17% for P and 7% to 8% for K.

4. Conclusions

This work has proved the feasibility of the simultaneous recovery of P and K from the waste sludge produced in a NDN system treating swine manure. The use of a Ca-sequestering agent is necessary to prevent the formation of Ca-P compounds. A valuable, multi-nutrient product was recovered. Nevertheless, further work is needed to reduce the presence of Na^+ in the recovered precipitate.

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DEVELOPMENT AND OPTIMIZATION OF A MEMBRANE PHOTOBIOREACTOR FOR THE RECOVERY OF RESOURCES (NUTRIENTS AND WATER)

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Keywords: membrane, microalgae, photobioreactor, recovery, wastewater.

1. Introduction

In the conventional approach to wastewater treatment, urban wastewater is considered waste and must be treated to avoid negative impacts on the environment. But it could be approached by a resource recovery factory (RRF), where anaerobic digestion coupled with a membrane process allows for the extraction of purified water with little remaining COD. The implementation of microalgae is of key interest and a perfect complement to the anaerobic process, since the remaining nutrients allow for the growth of the microalgae which can then be used as fertilizers, phytostimulants, or biofuels (Song et al., 2018). In fact, microalgae-based wastewater treatment is considered more effective in removing pollutants that cause eutrophication in water bodies (Bilad et al., 2014; Castro-Muñoz & García-Depraect, 2021).

The use of forward osmosis and microfiltration membranes is the key factor that will allow the extraction of very high-purity water while concentrating more than 20 times the number of microalgae inside the bioreactor and with only a slight propensity for fouling.

2. Methodology

The reactor design (8L) will be evaluated with two types of submerged membranes (MF and FO), with aeration and without aeration (as a membrane cleaning system) coupled to the microalgae system *(Chlorella vulgaris)*, and the possibility of integrating membrane systems to typical raceway ponds to obtain a low-cost system adapted to wastewater treatment. In this phase, different experiments will be carried out to find out how the operational parameters can affect the operation of the photobioreactor (light, pH, CO_2, contact time, fouling of the membranes, etc.).

3. Results and discussion

The findings of the concentration achieved during microalgae filtration using a submerged membrane system are presented in Figure 1. The results demonstrate that the most favorable

approach, yielding optimal concentration, involves the use of forward osmosis membranes with the addition of air.

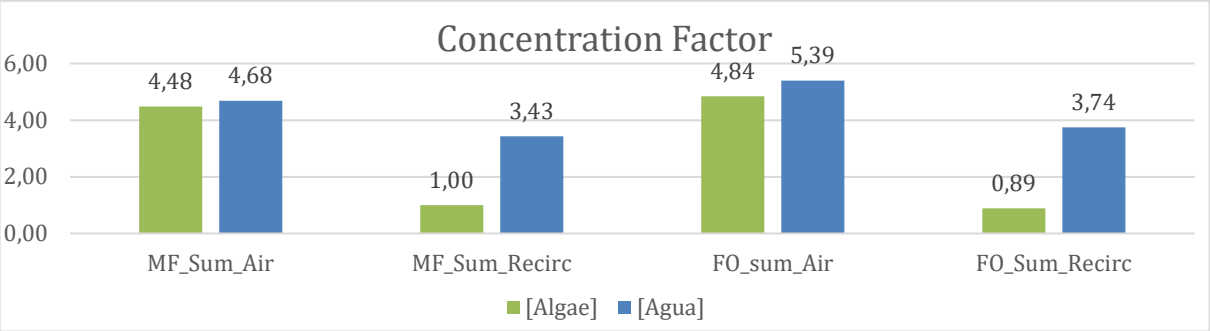

Figure 1. Assessment between the concentration factors of the following systems: submerged microfiltration membrane with air (1), submerged microfiltration membrane with recirculation (2), submerged forward osmosis membrane with air (3), and submerged forward osmosis membrane with air (4).

Subsequent steps in this research will involve exploring alternative configurations of the membrane (forward osmosis and microfiltration) in crossflow mode while manipulating the presence of air and spacer elements.

4. Conclusions

The present work will show that the concentration of microalgae with maximum efficiency can be possible using integrated forward osmosis membranes in bioreactor systems and will optimize the concentration efficiency of microalgae in raceway ponds.

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POLYMERIC FILMS MODIFIED WITH DEEP EUTECTIC SOLVENTS FOR ORGANOPHOSPHORUS PESTICIDE EXTRACTION FROM WATER SAMPLES

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Chemistry Department, University of Girona

Keywords: DES, functionalized membranes, organic pollutant, plasticizers, TFME

1. Introduction

The monitoring of different organic and inorganic pollutants in waters is mandatory to control the levels of environmental contamination in water bodies. For that reason, the development of new materials based on functionalized polymeric films is important. In this work, films modified with deep eutectic solvent (DES) (Carner, 2020) have been prepared and put in contact with water samples following the principles of thin-film microextraction (TFME) (Bruheim, 2003). The target pollutants in our study are organophosphorus pesticides (OPPs): ethoprophos, parathion-methyl, fenchlorphos, chlorpyrifos, protrophios and azinphos-methyl.

2. Hypothesis

The new type of polymeric films, avoiding the use of plasticizers, can be used in TFME to extract different organic pollutants.

3. Methodology

The films have been prepared by the solving casting method, with cellulose triacetate (CTA) as the polymer and modified with DES made of dodecanoic acid/lidocaine and camphor/menthol (Ribeiro, 2015). They have been characterized using infrared spectroscopy (FT-IR). For the microextraction experiments a predetermined volume of 0.01 mol L^{-1} NaCl solution containing the target pollutants (OPPs) has been used and placed into contact with the solution with a piece of film (1x2cm or 2x2cm) for a fixed period of time. One mL ethyl acetate has been used for the elution. The extraction efficiency has been evaluated using SPME. For chromatographic separation of the contaminants, a GC-MS (Agilent) was used (Merlo, 2021).

4. Results and discussion

The new films CTA/DES (Figure 1) have been satisfactorily produced and characterized. The extraction efficiency for the OPP compounds, using the film pieces, after 6 hours of extraction has been quantitative for most of the compounds analysed. (20 mL solution fortified at

50 ugL^{-1}) in a rotative agitation (Figure 2). Elution has been achieved with ethyl acetate as the solvent with good results.

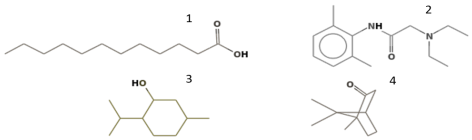

Figure 1. Chemical structure of the DES components (1) Dodecanoic Acid, (2) Lidocaine, (3) Menthol, (4) Camphor.

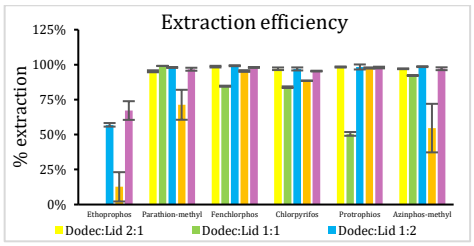

Figure 2. Extraction efficiency for five types of DES. Membrane composition: CTA (70%) /DES (30%) (n=3)

For the TFME configuration using the DES (dodecanoic acid:lidocaine (2:1))/CTA film, a calibration curve has been obtained placing the film suspended in a vial and immersed in the solution for one hour (S-TFME). Good correlation has been found in the working range from 1 to 130 ugL^{-1}.

5. Conclusions

The film made of DES (dodecanoic acid:lidocaine (2:1)) and CTA can be used for the TFME of organophosphorus pesticides. Validation of the method and application to different water samples is under investigation.

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ASSESSING POLLUTANT INTERACTIONS IN WATER WITH POLYMER INCLUSION MEMBRANES (PIMs) FOR DIVALENT METAL IONS

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Keywords: Metal complexation, metal pollution, microplastics, polymer inclusion membrane (PIM)

1. Introduction

Once in the aquatic environment, metals can interact with other components such as organic matter or ions to form different chemical species. Since free ions are the most relevant species when determining the bioavailability and toxicity of metals, it is important to have techniques able to perform speciation studies.

In this study, a simple and affordable tool based on a polymer inclusion membrane (PIM) is presented to measure divalent metal ions in water samples and to assess possible interactions with other pollutants.

2. Hypothesis

The main hypothesis of this study is that it is possible to use PIMs to determine metal complexation in aqueous media.

3. Methodology

The PIM is made of a polymer (cellulose triacetate, CTA), an extractant (di-(2-ethylhexyl) phosphoric acid, D2EHPA) and a plasticizer (tributyl phosphate, TBP). The membrane acts as a semipermeable barrier, which allows the selective permeation of divalent metal ions due to the presence of D2EHPA. A typical feed solution consisted of 0.05 M KNO_3 pH=6 while a 0.5 M HNO_3 solution was used as a receiving phase. Samples were analysed using a microwave plasma – atomic emission spectroscopy instrument (MP-AES).

4. Results and discussion

The performance of a designed PIM was investigated and found to be effective in transporting Cu, Zn, and Ni. Various parameters were investigated, including the impact of metal concentrations and the addition of other pollutants to metal solutions. When the complexing agent EDTA was introduced to the feed solution, the measured free metal decreased because

of the formation of metal-EDTA complexes, as observed in experiments using a PIM made of CTA, D2EHPA and the plasticizer NPOE (Alcalde et al., 2021). In addition, experiments were conducted with mixtures of metals and different types of microplastics, such as polyvinyl chloride (PVC) and polyethylene terephthalate (PET), which demonstrated that high levels of microplastics could adversely affect metal transport through the PIM. This suggests that microplastics have a strong affinity for metals and can contribute to the spread of heavy metal pollution. Furthermore, ongoing experiments are exploring the interaction between metals and various organic compounds, such as antibiotics.

5. Conclusions

A PIM consisting of 40% CTA, 30% D2EHPA and 30% TBP can be used efficiently for multielemental speciation studies and as a tool to improve our understanding of how pollutants interact in water, which is essential for developing effective strategies to manage and mitigate the impacts of heavy metal pollution.

6. Bibliography

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SESSION 11.

COMPUTATIONAL DYNAMICS: ASTRODYNAMICS, FLUID DYNAMICS AND MOLECULAR DYNAMICS

MACHINE LEARNING APPROACHES TO SOLVING CLASSICAL ASTRODYNAMICS PROBLEMS

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[1] *University of Girona*

Keywords: astrodynamics, celestial mechanics, Poincaré sections, proximal policy optimization, reinforcement learning

1. Introduction

The main goal of this master's thesis is to explore the utility of machine learning techniques applied to solving two classical problems in astrodynamics and celestial mechanics: the *spacecraft attitude control problem* and the *computing a Poincaré map of a dynamical system*.

2. Methodology

The spacecraft attitude control problem consists of determining the sequence of movements that allow a spacecraft to reach a desired orientation and angular velocity (Canuto et al., 2018). We built a control agent (consisting of a neural network) and a simulation environment that emulates the behavior of a satellite when a torque is applied. Using the *proximal policy optimization* algorithm (Schulman et al., 2017), and by interacting with the simulation, the agent learns an optimal attitude control policy.

The second focus of this thesis is the study of the dynamics around a periodic orbit of a dynamical system using a Poincaré map that assigns to any initial point the intersection of its trajectory with a suitable section, such that a periodic orbit is a fixed point on the map (Arnol'd, 1992). We will begin by generating a dataset of the Poincaré map of a variation of the two-body problem. A neural network regressor will be trained using this dataset, with the goal of approximating the intersection of new initial conditions not seen in the training data.

3. Results and discussion

Results obtained during the first part of the thesis are similar to other recent related works (Elkins et al., 2020) and show that our control agent is capable of stabilizing the attitude and angular velocity of a microsatellite (1-20Kg) with an absolute error $\leq 10^{-3}$ in both orientation (radians) and angular velocity (rad/s), starting from an arbitrary orientation and a maximum angular velocity of ±4.5 rad/s in all axis. Future experiments will be concerned with

improving the precision and obtaining a general controller capable of working with a wide range of inertia matrix configurations.

Regarding the second part of this thesis, we expect that the experiments done in the following months will allow us to train a regressor capable of simulating a Poincaré map, with an absolute error < 10^{-6}.

4. Conclusions

Since we find ourselves in the early stages of our research, more work is needed to reach a conclusion on whether artificial intelligence techniques are suited to solve the problems presented in this thesis.

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USE OF HYDRODINAMIC MODELLING TOOLS FOR THE OPTIMIZATION OF WASTEWATER TREATMENT PLANTS

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Keywords: Hydrodynamics, modelling, oxidation ditch, wastewater treatment.

1. Introduction

Optimizing WWTP operation is crucial to meet environmental goals and lower costs. WWTP modelling has been progressively applied over the last decades, proving to be an adequate tool for process assessment and optimization (Rehman, 2016). Computational fluid dynamics (CFD) is increasingly used for the solution of complex fluid flow problems in WWTPs, since it can provide a very accurate prediction of the fluid hydrodynamics (Höhne& Mamedov, 2020). The integration of CFD-ASM models enables the quantification of biological interactions among phases (solid-liquid-gas) that occur in the activated sludge reactor, making it possible to simultaneously predict the hydrodynamics of the process and its impact on the bioprocesses that occur in it.

2. Hypothesis

Most frequently used WWTP simulators do not consider the hydrodynamics of the system, assuming homogeneity on fluid mixing and oxygen distribution throughout the reactor (Rehman, 2016). CFD-ASM models show that these conditions vary within the reactor, interfering in the biokinetic processes that occur.
Thus, considering these variations, this CFD-ASM integrated model will provide a detailed prediction of the water and oxygen flows within the system, coupled with the biokinetic reactions that take place. This way, various operating scenarios will be tested to optimize the process in terms of energy and reagents saving, while maintaining the required effluent quality.

3. Methodology

The case study is carried out in the WWTP of La Almunia (Zaragoza). The treatment configuration consists of two oxidation ditches, with a unitary volume of 3,000 m^3, and two clarifiers.
The models were developed using the Ansys software package, Space Claim® for geometry design, and Ansys Fluent® for the meshing and solution of simulations.
The ASM1 biokinetic model will be coupled to the hydrodynamic model, and the results of the integration will be validated with real data obtained from the WWTP, to propose optimization scenarios from this initial model.

4. Results and discussion

First hydrodynamic results of the process are presented in Figure 1. They show some areas with very low velocity and reverse flow, which can potentially cause dead zones or heterogeneity in the distribution of oxygen, both causes of performance reduction.

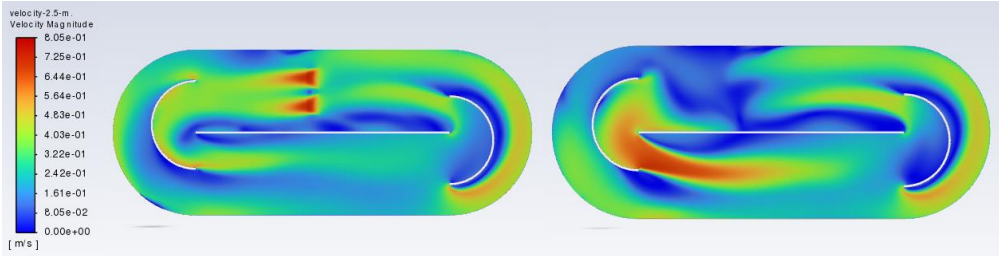

Figure 1. Top view of velocity contours of a) 2.5 m. height and b) top free surface

In future works, it is expected to couple the ASM1 model to this one, to confirm the heterogeneity hypothesis and establish which are the most affected areas by the flow behavior. This whole study will help in planning the best optimization scenarios for this process.

5. Conclusions

CFD hydrodynamic models have proven to be a very accurate tool to identify heterogeneities in the fluid flow in areas of the reactor where homogeneous behavior is assumed. Further developments in the model are needed to prove spatial distribution heterogeneities of biokinetic parameters.

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STUDY OF MICRO-IRRIGATION PRESSURE SAND FILTERS USING NUMERICAL SIMULATION

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Keywords: CFD, drip irrigation, head loss, sand filters

1. Introduction

Computational fluid dynamics (CFD) was used in simulations of a laboratory filter to analyze the results obtained with different equations of head losses in porous media. Simulations were compared with experimental data at different superficial velocities obtained from previous studies, including two packed bed heights.

2. Methodology

Experimental data used in the present study was obtained in (Bové et al., 2015), who analyzed how different types of granular media modified the pressure drop of a filter. This study analyzes silica sand (SS) with grain size range of 0.63mm-0.75 mm, porosity (ε) of 0.42, equivalent diameter (D_{eq}) of 0.72, and sphericity coefficient (ψ) of 0.89. The experiment was carried out with a scaled filter from the commercial sand filter as described by (Arbat et al., 2013). The scaled filter had an inner diameter of 200 mm and a length of 750 mm. A 10 mm-thick, inner plate was welded 133 mm above the bottom of the filter to fit the underdrain element (nozzle) and to support the sand. Above this plate, the filtration media was placed up to a height of 317 mm.

The numerical model was developed with ANSYS-Fluent. This commercial software has successfully been applied in the analysis of pressurized porous media filters for drip irrigation. Turbulence effects were considered in water only regions by adopting the shear-stress tensor (SST) $k - \omega$ model, in which k was the turbulent kinetic energy and ω the turbulent specific dissipation rate. Finally, the coupled numerical algorithm was applied to solve the continuity and momentum equations. Second-order schemes were chosen for all the spatial discretization terms. The absolute value of the residuals was fixed to 10^{-5} for all variables.

3. Results and discussion

The pressure losses across the different values of superficial velocities for a Silica Sand (SS1) are shown in Figure 1. Total filter pressure drop considered not only head losses in the packed bed but also in the packed bed but water-only regions. Simulation in CFD of Δp_f for different values of superficial velocities confirmed that both Darcy and Kozeny-Carman expressions underestimated the pressure drop in the granular region at high velocities.

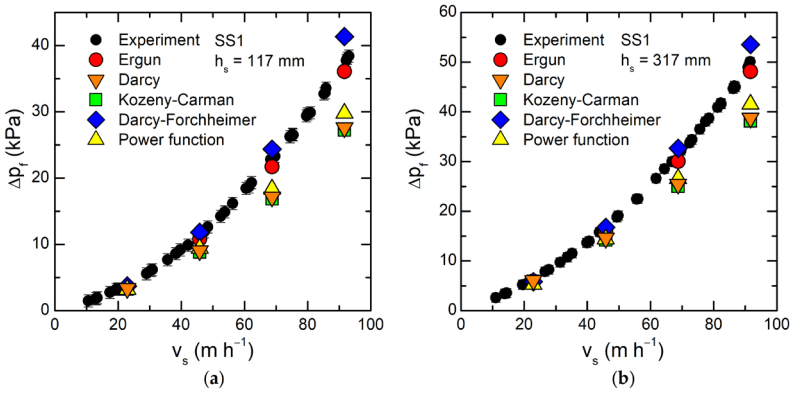

Figure 1. Filter pressure drop as a function of the superficial velocity experimentally observed and simulated with different equations.

4. Conclusions

We carried out CFD simulations of a pressurized granular bed filter with a commercial underdrain unit with the finest discretization found in the literature. Results were compared with experimental data obtained at different superficial velocities for a porous media (silica sand) and two different heights of the granular bed.

Total pressure drop results when applying all the previous porous media equations were very similar and fell within the experimental uncertainty of this superficial velocity range at least up to 38.3 m/h for both heights.

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PARAMETRIZATION OF OLIGOMER MALEIC ANHYDRIDE: A THEORETICAL STUDY FOR IMPROVISED SIMULATIONS

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Keywords: general AMBER force field, molecular dynamics, MP2, oligomer maleic anhydride

1. Introduction

Molecular dynamics (MD) are widely used in chemistry to study the dynamic behavior of organic molecules. However, the accuracy of these simulations relies heavily on the force field parameters used. Commonly used force fields such as the general AMBER force field (GAFF) (Wang et al., 2004) utilize fixed parameters for non-bonded interactions, leading to possible inaccuracies during simulations. In this work, we present a new approach to assign starting non-bonded parameters for oligomer maleic anhydrides (OMAhs) (Zhou et al., 2017) using GAFF, resulting in improved accuracy for MD.

2. Hypothesis

Our main hypothesis is to parametrize OMAhs (to identify the most stable conformer) for further simulation studies.

3. Methodology

We will be using methods like MP2 and GAFF. Also, we will link the quantum mechanical component to couple Gaussian with AMBER.

4. Results and discussion

Firstly, we started with the preliminary study of OMAhs (Mol.wt~1060). We have optimized the charges and coordinates, and then calculated both MP2 (second-order Møller-Plesset perturbation) and GAFF energies for the stacked monomers (lateral stacking in the +Z-direction). Then, the variables from the Lennard-Jones potential (Figure 1), i.e, 'σ' and '$\in$' were investigated thoroughly by performing variations causing changes in the displacement and depth of the curve, respectively. This directly improves the free energy values. These parameters explain the non-bonded or van der Waals interactions (vdWs), as required in the

simulation studies. After this, we also analyzed for different orientation changes (in 3D space), which occur with change in the angles (ranging from 0° to -360°, respectively). Taking these results, in all combinations of monomer strands, we identified the least energy state (global minima) for the best conformer.

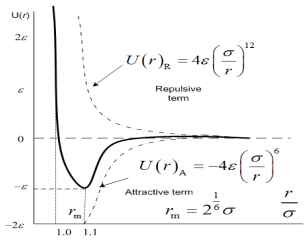

Figure 1. Lennard-Jones potential curve (Maghfiroh et al., 2020)

5. Conclusions

In summary, we have successfully optimized the starting parameters for oligomer maleic anhydrides (OMAhs), using internal coordinate constraints to improve the accuracy of non-bonded parameters for MD. Our approach involved optimizing the charges and coordinates for the monomer and oligomer, and then calculating MP2 and GAFF energy values for various combinations and orientations. By comparing these results, we have identified the most stable conformer for OMAhs. Finally, this approach overcomes the problem of using fixed parameters for the initial structure of molecules and ultimately leads to more reliable simulation studies in the future.

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MOVING TOWARDS NEW STRATEGIES IN DRUG DESIGN: EXPLORING THE POTENTIAL OF FRAGMENT DISSOLVED MOLECULAR DYNAMICS

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Keywords: Fragment-based drug discovery (FBDD), fragment-dissolved molecular dynamics (fdMD), Gaussian accelerated molecular dynamics (GaMD), Markov state models (MSM)

1. Introduction

During the last decades, the significant surge in the application of fragment-based drug discovery (FBDD) to identify novel drug candidates has led to a breakthrough in the development of new computational strategies. It is in this framework that fragment-dissolved molecular dynamics (fdMD), a relatively new and semi-automatic approach, was conceived. Based on molecular dynamics (MD) simulations with multiple copies of the same ligand, the methodology aims to increase the conformational sampling and identify the most favourable binding sites (BS) for small fragments exhibiting strong interactions with the target protein (Privat et al., 2021). However, some scenarios of the fdMD methodology can still be improved. For example, reducing the computational effort and the occurrence of false positives in the identification of the optimal binding sites or taking advantage of recurrent association/dissociation events that may be one of the main drawbacks in fdMD for small ligands presenting weak binding affinities. To mitigate their impact, several sampling techniques have been considered.

2. Hypothesis

The hypothesis of this study focuses on two main ideas. First, the use of Gaussian accelerated molecular dynamics (GaMD) (Miao et al., 2015) as a major improvement in the rapid and unambiguous prediction of the most favourable binding modes. Second, the introduction of Markov state models (MSM) (Linker et al., 2019) as a further step in the fdMD analysis and a good strategy in BS identification and affinities prediction for fragments exhibiting recursive binding and unbinding processes.

3. Methodology

For the present work, two main methodologies have been selected: GaMD, to boost the system's potential energy to lower energetic barriers and enhance the exploration of the system, and kinetic MSM, to study long time-scale processes taking place during the simulation.

4. Results and discussion

Overall, the use of fdGaMD as an alternative to conventional fdMD has resulted in a significant improvement in the computational effort needed to clearly predict the most favourable binding site of the studied systems. Additionally, the implementation of MSM as a further step into the fdMD workflow has turned out to be a great alternative, producing reliable results for trajectories in which many binding and unbinding processes occur.

5. Conclusions

In conclusion, introducing enhanced techniques to fdMD has resulted in an accurate BS identification and prediction of the corresponding kinetic constants. Ongoing research efforts are now focused on the exploration of additional applications and techniques.

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SESSION 12.

COMPUTACIONAL AND THEORETICAL CHEMISTRY

BOTTOM-UP APPROACH TO UNDERSTAND EUMELANIN OLIGOMERIZATION FROM 5,6-DIHYDROXY INDOLE

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Keywords: dihydroxy indole, eumelanin, oligomerization

1. Introduction

Eumelanin is a naturally occurring biomaterial with functions such as pigmentation of the skin and hair and photoprotection (X. Wang et al., 2023). In 1927, it was proposed that 5,6-dihydroxy indole (DHI) would be the final monomer in the oxidative polymerization process to form eumelanin (Raper, 1927). But despite a long history of study, we don't know the structure of eumelanin at an atomic scale, owing to its heterogeneity and poor solubility. Therefore, we propose to simulate a eumelanin model using a bottom-up approach that can represent real eumelanin properties such as broadband absorption. Considering the vast structural diversity of the eumelanin dimers (J. Wang & Blancafort, 2021), it is crucial to understand the preferentially formed dimers. For this purpose, we have determined the elementary steps of the eumelanin oligomerization mechanism starting from DHI and eventually leading to the formation of thermodynamically favored dimers. Scientists have observed that dimers formed from DHI in the catechol oxidation state do not show the optical and electronic properties of eumelanin (Corradoini et al., 1986), while the presence of oxidized units in the dimers gives them eumelanin-like properties (J. Wang & Blancafort, 2021). Apart from the reactions of DHI in the catechol oxidation state, we have also studied the initialization and dimer formation from the conjugate base of DHI (DHI^-). This work will provide insight into the mechanism of eumelanin dimer formation, enabling a better understanding of the photoprotective nature.

2. Methodology

To build representative DHI models, we have established the elemental steps of oxidative coupling and oxidation mechanisms. The energy profile of these reactions has been mapped out using the M062X density functional.

3. Results and discussion

The initialization reaction with the possible options of hydrogen abstraction and e^- transfer and DHI deprotonation with molecular oxygen were studied. The energy barrier for hydrogen abstraction of DHI by molecular oxygen was quite high to produce the semiquinone (SQ). From the work done so far, we have understood that DHI^- produces SQ with much less barrier through e^- transfer and hydrogen abstraction. Further, we have studied coupling reactions involving DHI^-, DHI, SQ, and other oxidized units that form in the initialization reaction.

4. Conclusions

The eumelanin oligomerization has been studied using a bottom-up approach. The initialization reactions of oxidative polymerization have been explored. The SQ formation from DHI^- is much more favorable than from DHI. Furthermore, the products formed from this initialization reaction and other substrates are considered for coupling reactions producing the dimers.

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GENERATION OF THEORETICAL DHICA MELANIN MODELS FOR THE SIMULATION OF OPTICAL SPECTRA

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Keywords: DFT, eumelanin, hydrogen atom transfer, monomer, optical properties

1. Introduction

Eumelanin is the predominant type of melanin in human pigment. It is considered a beneficial biomaterial that provides protection from UV light due to its distinctive optical properties, broad monotonic absorption of UV-vis light, and strong nonradiative relaxation of absorbed photons. Those arguments justify the increasing interest in eumelanin, especially in material sciences (D'Ischia et al., 2020). However, eumelanin also exhibits an ability to generate reactive oxygen species under UV irradiation (Korytowski et al., 1987).

It is important to determine the complex structure of eumelanin and its structural organization to understand its different photobiological aspects. Eumelanin has a hierarchically assembled particle structure composed of stacked layers of oligomers derived from two key monomers, 5,6-dihydroxyindole (DHI) and 5,6-dihydroxyindole-2-carboxylic acid (DHICA), that undergo either oxidation or oxidative coupling to form oligomers (Ju et al., 2016). The structure of these oligomers is unknown because many different reactions can occur and several connectivity possibilities exist between monomers.

2. Hypothesis

Our hypothesis is that Density Functional Theory (DFT) calculations (along with machine learning algorithms) could help us build representative realistic melanin models starting from DHICA monomers on a theoretical basis and then analyze their use for simulations of the optical properties of larger melanin oligomers.

3. Methodology

Computational calculations have been made using the M06-2X/6-311G(d,p) level of theory, with water as implicit solvent. To analyse the interactions between the systems and the solvent molecules in a better way, water has also been considered explicitly.

4. Results and discussion

DHICA monomers can participate in three different types of reactions: hydrogen atom transfer reactions caused by aerial exposure, electron transfer reactions, and dimerization reactions (see Figure 1). All the regiochemical possibilities for these reactions have been analyzed, such as abstracting different hydrogen atoms or performing the dimerization with different connectivity between the two fragments of the dimers.

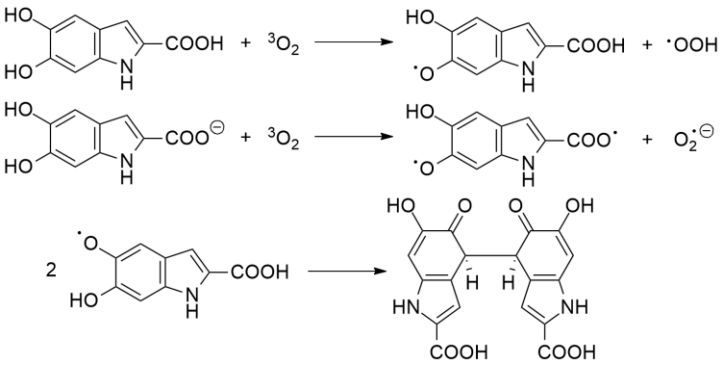

Figure 1. Examples of the three studied reaction types for the DHICA monomers.

5. Conclusions

The reactivity of eumelanin at the monomer level has been revealed by means of DFT calculations. Knowing the reaction pathway of the monomers will give us a better picture to address a subsequent study of larger DHICA oligomers.

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SIMULATION OF ELECTRONIC EXCITATION IN BIOMEDICAL SYSTEMS: PHOTOPHYSICAL PROPERTIES OF PORPHYRIN DERIVATIVES

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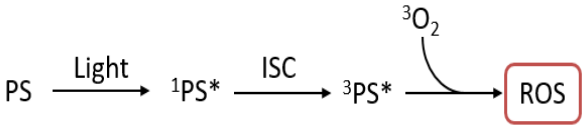
Keywords: computational chemistry, gadolinium, photodynamic therapy, photophysics, yttrium.

1. Introduction

Photodynamic therapy (PDT) can provide selective cytotoxic activity towards tumours in a minimally invasive way. It consists of the excitation of the photosensitizer (PS) to its first excited state using light. Then, there is a change in the multiplicity from the singlet to the triplet through intersystem crossing (ISC). Finally, there is an energy transfer between the PS and a molecule of oxygen in its ground state ($^3O_2$), which results in the generation of reactive oxygen species (ROS) (Agostinis et al., 2011) (Scheme 1). Gd and Y complexes are interesting because they combine photosensitization and their use as contrast agents, since Gd is MRI active (Sigel et al., 2021).



Scheme 1. General mechanism of PDT.

2. Hypothesis / problem

We want to see if the photophysical properties of the porphyrins are retained in the complexes regarding the ligands or the metal centre and if the ISC from the singlet to the triplet is efficient.

3. Methodology

To study these properties computationally, we use DFT (density functional theory) and TD-DFT (time-dependent density functional theory) with the different structures for the absorption/emission spectra and CASPT2 to calculate the spin-orbit coupling (SOC) to measure the ISC.

4. Results and discussion

For the absorption, the complexes showed almost no variation between each other and they are very similar to the experimental values. However, although there are more differences in the emission energies, they are still quite alike. Regarding the energy gap between the triplet and the ground state of the complexes, we observe that all the complexes would transfer enough energy to the molecule of oxygen to excite it to its singlet state (0.98 eV).

For the ISC, we obtain higher couplings in the Gd complexes, but the energy difference between the singlet and the triplet states are quite similar regarding the metal or the ligand.

5. Conclusions

The objective of this work is to know if our complexes were good candidates for PDT. To do so, we study the abs/em spectra of the complexes to see if the photophysical properties of the porphyrin are retained and measure the ISC from the singlet to the triplet.

The results showed that the energies of the complexes for the absorption and the emission are very similar in all the compounds, which means that the photophysical properties of the porphyrin are preserved.

However, for the ISC, the Gd complexes presented higher SOC than the Y ones probably due to the heavy atom effect (Kou et al., 2023)

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GRAPHITIC CARBON-NITRIDE MOLECULES FOR ELECTRONIC DEVICES

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Keywords: aromaticity, electrical conductivity, gCN surface, graphitic carbon nitride, single molecule electronics

1. Introduction

Creating functional nanoscale devices using single molecules as active electronic components is the ultimate goal of the interdisciplinary field of molecular electronics. Besides their potential to meet the ever-increasing miniaturization of electronics, molecular electronics opens up possible functionalities beyond silicon-based technologies.

Through the conceptual chemical perspective, descriptors and protocols can be developed to achieve the rationalization and understanding of molecular conductance, allowing the prediction and design of efficient nanoscale devices. As an example, Stuyver, Alonso and co-workers found a large dependence of the transmission spectra depending on the connectivity to the gold electrodes. They proposed a set of qualitative selection rules to predict the presence of constructive and destructive quantum interference around the Fermi level for Hückel and Möbius cyclic polyenes at the Hückel level of theory.

Two-dimensional (2D) graphitic carbon nitride is recognized as a relatively wide, accessible and inexpensive band-gap semiconductor with excellent electronic properties for multiple applications in the field of photocatalysis. Besides synthesis, the unique electronic behaviour of its molecular derivatives makes them promising candidates in novel molecular junctions.

2. Hypothesis

Do cyanide-graphene based single molecular junctions enable efficient electronic transmission? Can prediction rules be applied with prediction purposes?

3. Methodology

This is an in-silico project, within the nonequilibrium Green's function and DFT (NEGF-DFT) method, as implemented in the Artaios code. The molecular junction is constructed by the addition of thiolphenylethynyl linkers with sulphur atoms as actors, required to achieve proper

linking of the organic moiety between the gold contacts. This system is optimized via DFT. Next, the junction is formed by including two 9-unit gold clusters (FCC-hollow-Au9) on both ends, and single-point DFT calculations at the B3LYP/LanL2DZ level of theory are performed in order to obtain overlap and Hamiltonian matrices. The previous outputs are finally used for the NEGF calculations, yielding to the transmission spectra and local transmission plots.

4. Results and discussion

Preliminary results show the systems have good transmission levels under specific connections. The selection rules described for hydrocarbon-only systems showed to be not that straightforward to apply. The broken hole-electron symmetry introduced by the heteroatom makes the counting rule fail in many cases, making it not as reliable as in the pure carbon chains. The orbitals also get affected, so the HOMO and LUMO orbitals may not be the only main contributions of the Green's Function.

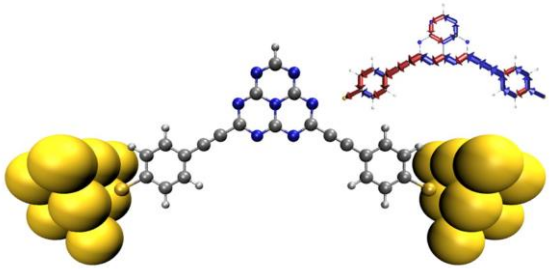

Figure 1. Molecular junctions of graphitic carbon nitride molecule using sulphur-based linkers.

5. Conclusions

While it is true that heteroatoms may help to develop more specialized and versatile junctions, they also introduce additional complexity on the system, making some unexpected contributions appear on their operation. More research on this relatively young field will accelerate the scope of application of these single-molecule electronics.

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DOES SERIAL FEMTOSECOND CRYSTALLOGRAPHY DEPICT STATE-SPECIFIC CATALYTIC INTERMEDIATES OF THE OXYGEN-EVOLVING COMPLEX?

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Keywords: manganese, oxidation, photosynthesis

1. Introduction

Manganese ions in the oxidation states +III and +IV are constituents of one of the most important enzymes of Earth's biosphere, the photosystem II (PSI), which catalyzes the light-driven oxidation of water into dioxygen. The Mn4CaO5 cluster at the oxygen-evolving complex (OEC) of PSII cycles through five intermediates states S_i (i=0-4) (Kok et al., 1970). In this work we address the question of whether the serial femtosecond crystallography combined with the X-ray free-electron laser source (SFX-SFEL) models depict the correct Mn oxidation states and adequately capture structural changes at the OEC.

2. Methodology

We use a comprehensive array of methods, ranging from structure-based analysis to evaluation of electronic structure. Among others, we employ an effective oxidation state analysis (EOS) applied for the first time to the OEC (Ramos-Cordoba et al., 2015). EOS analysis relies on Mayer's spin-resolved effective fragment orbitals (EFOs) and their occupations. The EFOs are sorted by decreasing occupation number and the electrons are assigned to the most occupied EFOs until the total number of electrons is reached, thus obtaining an effective configuration of the atoms/ligands within the molecule. The OS of each fragment considered is then obtained by subtraction from the corresponding nuclear charges. The difference in occupation (R%) from the last occupied (LO) and first unoccupied (FU) EFOs in the EOS procedure reflects the uncertainty on the overall OS's assignment and can be used as a criterion to detect problematic structural models of Mn clusters:

$$R(\%) = 100\min(1,\max(0,\lambda_{LO} - \lambda_{FU} + 1/2))$$

3. Results and discussion

We examined the 1F structures with the charge and spin multiplicity that correspond to the S_2 state, as well as to the S_1 and S_0 states, to examine the possibility that the samples can be reduced.

Table 1. R(%) values for the EOS calculated.

	1F								QM
	6JLK-A	**6JLK-B**	**7CJJ-A**	**7CJJ-B**	**6DHF-A**	**6DHF-B**	**6W1P-A**	**6W1P-B**	S_2
S_0 (III, IV, III, III)	**81.1**	70.8	**79.9**	**77.7**	**84.5**	**83.5**	72.7	**79.0**	<50[b]
S_1 (III, IV, IV, III)	61.0	**75.0**	64.7	71.2	69.7	64.4	**80.5**	66.9	50.2
S_2 (III, IV, IV, IV)	51.7	58.0	56.5	58.4	66.3	64.6	68.4	71.5	**78.4**

For all 1F structures, significantly higher R(%) values are obtained when the total charge and spin multiplicity of the S_1 and S_0 states are used instead of the S_2 state.

4. Conclusions

All 1F models considered here are over-reduced. The results quantify limitations in state-specific interpretations of current SFX-XFEL models of the OEC.

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HOW THE CHALCOGEN ATOM SIZE DICTATES THE HYDROGEN-BONDING CAPABILITY OF AMIDES

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Keywords: amides, chalcogens, density functional theory, H-bonding, quantum chemistry

1. Introduction

The formation of hydrogen bonds between amides is one of the central interactions underlying the formation and stability of biosupramolecular systems, such as proteins and nucleic acids. Inspired by these ubiquitous interactions, the development of novel (bio)molecular systems and materials relying on amide hydrogen-bonding with controllable stabilities and reactivities represents an active field in chemistry (Olivo et al., 2021). It has been found that thio- and selenoamides can give rise to stronger hydrogen-bond interactions than carboxamides, despite the lower electronegativity of the heavier chalcogen (*i.e.*, Group 16) atoms S and Se compared to O (Figure 1). This counterintuitive phenomenon has been experimentally explored in the field of hydrogen-bond-donor organocatalysis (Jakab et al., 2012), as well as in supramolecular chemistry (Berrocal et al., 2019), but a sound explanation was lacking for a long time.

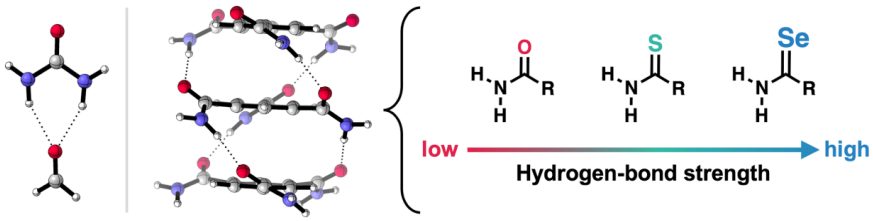

Figure 1. Changing O in the amide bond for the larger chalcogens (S or Se) enhances the amide hydrogen-bond strength in various supramolecular systems.

2. Methodology

Quantum chemical computations in this work are based on density functional theory (DFT) and are performed with the Amsterdam Density Functional (ADF) program at the ZORA-BLYP-D3(BJ)/TZ2P level of theory using COSMO to simulate solvation.

3. Results and discussion

In this paper, I will demonstrate how the steric size of the chalcogen atom in the amide bond dictates the hydrogen-bonding capability of amides. First, by showing that the amino (NH_2) groups in thio- and selenoamides are more positively charged than in carboxamides, and thus better hydrogen-bond donors (Nieuwland & Fonseca Guerra, 2022). Our quantum chemical analyses reveal that this originates from a larger flow of electrons from the N(H_2) lone pair

towards the low-energy $\pi^*_{C=S}$ and $\pi^*_{C=Se}$ orbitals than to the high-energy $\pi^*_{C=O}$ orbital. The energetic lowering of the $\pi^*_{C=X}$ orbital for the heavier chalcogens is due to the decreased overlap between the carbon 2*p* and chalcogen n*p* atomic orbitals, a consequence of the longer equilibrium C=X distance caused by the larger steric Pauli repulsion between the two bonded atoms. Thus, not the electronegativity, but the effective steric size of the chalcogen atoms determines the amide's hydrogen-bond donor capability. Finally, I will demonstrate how the larger size of the heavier chalcogens atoms not only affects the amide hydrogen-bond interaction strength, but also distorts the geometry of amide supramolecular building blocks thereby enhancing their ability to form intermolecular hydrogen bonds (Nieuwland et al., 2023).

4. Conclusions

The hydrogen-bonding capability of amides is dictated by the steric size of the chalcogen atom in the amide bond.

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DESIGNING TRYPTOPHAN SYNTHASES FOR STAND-ALONE FUNCTIONALITY

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Keywords: tryptophan synthase, allostery, molecular dynamics, conformational landscape, shortest path map

1. Introduction

Many enzyme complexes are allosterically regulated by a protein partner making them inefficient as a stand-alone catalyst. However, the use of stand-alone protein units is desirable for industrial applications. Tryptophan synthase (TrpS) is a heterodimeric enzyme complex, forming an αββα arrangement. The α-subunit (TrpA) catalyses the IGP-retroaldol cleavage into G3P and indole. In Nature, it already exists a blueprint for a stand-alone TrpA protein named BX1 from Zea Mays (ZmBX1). ZmTrpA and ZmBX1 share the ubiquitously encountered $(\beta\alpha)_8$-barrel fold and show a high sequence identity of 63.3%. However, ZmBX1 exhibits high stand-alone activity whereas ZmTrpA is a poor catalyst in the absence of TrpB. Similarly, TrpA from the Last Universal Common Ancestor (LBCA) depends on LBCA TrpB for enhanced activity (sequence identity of 45.1% with ZmBX1). Remarkably, ZmBX1, ZmTrpA and LBCA TrpA have two loop regions that are known to be important for the allostery and catalytic activity of TrpA: loop6 (residues 174-189 for ZmBX1) and loop2 (residues 56-76). These loop regions interact with β-subunit in the wild-type dimer (Axe *et al.*, 2015; Dunn, 2012). We recently generated ZmTrpA variants with moderate stand-alone activity by replacing loop6 of ZmTrpA with the corresponding loop of ZmBX1 into (Schupfner, Busch, Wysocki, & Sterner, 2019).

2. Methodology

Herein, we use Molecular Dynamics (MD) simulations and correlation-based tools in *apo* and IGP-bound states to rationalize the differences between systems and design new variants. Thus, we aim to generate new LBCA TrpA variants with stand-alone functionality and also to elucidate the changes on the allosteric regulation between both subunits through TrpS evolution. This is done by computationally reconstructing the conformational landscapes associated with different key features (i.e. loop6 closure distance, catalytic distance…), and applying the correlation-based tool SPM (Romero-Rivera, Garcia-Borràs, & Osuna, 2017) to design new stand-alone TrpA variants. The

most promising enzymes are experimentally validated in Prof. Sterner laboratories (Univ. Regensburg, GER).

3. Results and discussion

By computationally reconstructing the conformational landscapes, the low stand-alone activity of LBCA TrpA could be explained as a consequence of a non-productive loop6 closure and IGP binding. After applying the SPM tool, we detected those conformationally relevant positions of zmBX1 and LBCA. Using this methodology, we could design a new rationally evolved LBCA TrpA variant that reach a 6.6-fold increase in k_{cat} (experimentally validated in Prof. Sterner laboratories).

4. Conclusions

Our study identifies a new variant with a remarkable k_{cat} fold increase compared to the native enzyme (LBCA TrpA). In spite of this achieved improvement, we believe that we can boost the activity even higher.

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LOOKING FOR ECHOES OF THE PAST: RECONVERTING AN HYDROXYNITRILE LYASE TO AN ARYLESTERASE

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Keywords: enzyme design, catalysis, molecular dynamics, esterase, hydroxynitrile lyase

1. Introduction

Enzymes are biodegradable catalysts that can operate under mild conditions (i.e. low temperatures and pressures). The proper arrangement of the active site residues leads to a decrease in the activation barriers of the catalytic reaction. Thus, enzymes are considered superb catalysts. Hevea brasiliensis hydroxynitrile lyase (*Hb*HNL) and salicylic acid-binding protein 2 (SABP2) are two enzymes from the α/β-hydrolase fold superfamily that evolved from the same esterase ancestor. Even though they share the same Nucleophile-His-Acid catalytic triad and high structural similarity, they only have a 45% of sequence identity. *Hb*HNL catalyzes the cleavage of hydroxynitriles and SABP2 the ester hydrolysis. To identify the most important amino acids involved in each reaction, Prof. Kazlauskas and coworkers made a set of variants in which they substitute the active site amino acids of *Hb*HNL into the corresponding SABP2 residues. Although an increase in esterase (EST) activity and a decrease in hydroxynitrile lyase activity (HNL) were expected, pure EST activity was not reached by any *Hb*HNL variant (*Hb*HNL-EST) (Nedrud *et al.*, 2014).

2. Methodology

Herein, we develop a specific protocol to identify the most relevant active site amino acids located at the first and second shells to regenerate the esterase activity. In this work, we use molecular dynamics (MD) simulations to explore the conformational space of the different intermediates along the esterase reaction coordinate. For the identification of hot-spot residues, we take advantage of correlation-based tools (e.g. Shortest Path Map) (Romero-Rivera, Garcia-Borràs, & Osuna, 2017). After the *in-silico* test of our rational designed variants, they were experimentally validated by our collaborators from Prof. Kazlauskas' laboratory (Univ. Minnesota, US). The expertise

acquired thanks to this synergy allows us to go even further in the catalytic improvement of the rational design procedure.

3. Results

The information gained from the MD simulations highlights how active site dynamics play an essential role in the different reaction steps. However, 2nd shell mutations located in the protein surface have a crucial impact on the activity improvement. Consequently, the design of a new variant with a k_{cat} fold increase of 698 in esterase activity compared to the HbHNL-EST was achieved. Interestingly, our best variant outperforms by a fold increase of 2 the SABP2 enzyme.

4. Conclusions

In this work, we identify the most relevant residues involved in the improvement of esterase activity in *Hb*HNL-EST variants. In addition, we obtained a rationally designed variant that surpasses in esterase activity the previously described *Hb*HNL-EST variant and the SABP2 esterase enzyme.

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SESSION 13.

SOCIETY, PUBLIC POLICY AND FEMINISM

DISCURSIVE ANALYSIS IN THE PROCESS OF ENACTING LAWS REGULATING VIOLENCE AGAINST WOMEN

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Keywords: discourse, law, feminism, women, legislation, violence

1. Introduction

Violence against women in Mexico, such as the femicides in Ciudad Juarez, in the state of Chihuahua, (1993-1999), was a social event that mobilized society and the government to take various actions aimed at resolving this situation. In 2004, a legislative process was initiated to address the determination that violence against women is structural, due to the patriarchal organization of society. In 2007, the first law on the subject was issued to comply with the international commitment to address the problem of violence against women and girls. Undoubtedly, the General Law on Women's Access to a Life Free of Violence has been a step forward in terms of prevention. However, violent deaths against women and girls have increased in the country. Currently Mexico registers an average of 10.6 women victims of violent deaths per day (IMUJERES Report, 2020).

Our interest is to understand the ways in which violence against women can be reflected in legal texts that attempt to contribute to finding solutions. We assume that those who draft the laws are not exempt from a heteropatriarchal symbolic imaginary and that, therefore, their worldviews are projected in the laws. We wonder to what extent this heteropatriarchal and androcentric imaginary in the discourse filters into the discourse produced by laws for the protection of women or laws dealing with violence against women, and what meanings or representations legislators give to violence against women.

2. Methodology

The method employed is qualitative and articulates three critical perspectives that focus on three complementary aspects: the use of language by the producers of the discourse, the critical legal perspective and feminist analysis. The corpus, consisting of two bills presented in 2004 and in 2006, is analyzed from a critical interactional perspective (Bolívar, 2007) in which linguistic analysis based on functional systemic linguistics and the multidisciplinary analysis of critical discourse studies converge. In this analysis, linguistic data provide support for interpretations that can be made with contributions from other disciplines, such as law (Ruiz, 2001), and are complemented by the feminist perspective (Haraway, 1995; Cabruja, 1995; Segato, 2016).

3. Results and discussion

A first analysis was based on the explanation of the lexicon and grammar in the texts, which made it possible to identify the actors involved in the production of meanings, their roles and actions, their representations and messages, as well as the assessment and dynamics of change in the discourses observed in the two bills analyzed.

The data obtained served as a basis for studying the discourse at the ideological level and its different representations of violence and "women", as well as the meanings that those responsible for drafting the initiatives construct: the protection of "women" and the defense of "women's" rights.

4. Conclusions

The study observes that this process of discursive construction shows a dominant discourse, in this case patriarchal, and a discourse of resistance whose effects influence and affect the General Law on Women's Access to a Life Free of Violence. We identified some representative metaphors of each discourse that deserve to be studied in a second phase of analysis to observe the transfer of meaning and metaphorical representation of a patriarchal imaginary to a law that aims to solve the problem of violence against women.

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CONTRIBUTIONS OF THE GENDER PERSPECTIVE TO THE PROFESSIONAL PRACTICE OF PSYCHOLOGY IN VIOLENCE AGAINST WOMEN

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

1. Introduction

The gender perspective is widely recognized as a quality standard essential to professional fields addressing violence against women. Although it encompasses a wide diversity of theoretical concepts that can even be contradictory to each other, we can affirm that a gender perspective guarantees better professional practice by avoiding the revictimization of women, since it allows the origin of violence to be located in the social context, challenging the individualistic explanations that psychology has generally reproduced (Cabruja, 2017; García, 2019). In this qualitative study, we take a critical psychosocial (Ibáñez and Íñiguez, 1997) and feminist (Haraway, 1995) approach to identify the variety of ways in which the gender perspective and feminist contributions are incorporated into the professional approach to address violence against women and its effects.

2. Methodology

We present part of the results of the material obtained from semi-structured individual interviews with professionals working in public services focused on violence against women in Catalonia. Following the theoretical sampling procedure, we interviewed 12 professionals from different services and territories, and with different degrees of professional experience and training in gender perspective. For the data analysis, we used the thematic analysis method (Terry et al., 2017), with the support of the Atlas.ti computer program.

3. Results and discussion

First preliminary results:

Professionals identify gender perspective with interdisciplinary theoretical resources that locate the origin of violence against women in the social, political, and cultural context. Therefore, professional practice avoids the re-victimization implied by reductionist explanations that hold women individually responsible for their own situation.

Participants also state that incorporating the gender perspective promotes the detection of "gender blindness" in other professionals' practice, representing an opportunity to improve networking.

4. Conclusions

Although the incorporation of the gender perspective in the professional practice of psychology is not free of dilemmas and tensions, we can affirm that it has a positive impact on the recovery process of victims and improves both professional practice and networking.

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FACTORS THAT AFFECT THE QUALITY OF THE PUBLIC ADMINISTRATION: CASE STUDY OF THE ECUADORIAN PUBLIC ADMINISTRATION IN 2021

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Keywords: corruption, internal control, public politics, quality, risk

1. Introduction

Public policies provide states with administrative, operational and financial strategies aimed at achieving efficiency and effectiveness (Miao, Newman, Schwarz, & Cooper, 2018); that is, to offer a public service of quality and with compassion. However, when there is no adequate internal control, risk management or information security, external factors arise that were not subject to provision or contingency in the procedural action. This is not only true of organizations, but of an entire territory and can lead to social convulsion because of public management vulnerabilities (Grimmelikhuijsen, Jilke, Olsen, & Tummers, 2017). This is particularly the case in this investigation of the Ecuadorian public administration.

2. Hypothesis

Ecuador through the Government Plan oriented to the Plan for the Creation of Opportunities 2021-2025 and the United Nations' 2030 Agenda for Sustainable Development. This document was related to the socioeconomic evaluation of the effects of the pandemic caused by COVID-19, and the national territorial strategy and model. However, the Ecuadorian situational reality in the analysed sample reveals facts incompatible with the precepts described above, which led us to ask ourselves: Do current state policies in Ecuador lead to quality in the public administration? From this question arose the two research hypotheses. H1: The Ecuadorian Government Plan has increased and guaranteed quality management in public finances. H2: The Ecuadorian government plan has strengthened public ethics, increased transparency and continued the fight against corruption. In addition, the general objective is established: To analyse the factors that affect the quality of the public administration in Ecuador. The specific objectives are to determine the efficiency and effectiveness in the management of public finances in the year 2021 and to determine the level of compliance of the public administration with respect to transparent information.

3. Methodology

Qualitative research - descriptive and quantitative analytical (Hernández, Fernández, & Baptista, 2014). The hypotheses were analysed by means of logistic regression through the R language, (Navarrete & Chávez, 2019; Hennink & Kaiser, 2022).

4. Results

The publications disseminated during from 2016 to 2022 focused on scientific developments to guarantee a public service of quality and with compassion.

5. Conclusions

This investigation identified the main factors leading to problems in the Ecuadorian public administration, and proposes implementation of ICSRMIS to mitigate the impact of the economic, social, comprehensive security, ecological and institutional transition crisis in Ecuador.

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THE COVID-19 PANDEMIC'S IMPACT ON CATALONIA'S SOCIAL VULNERABILITY: THE SPATIOTEMPORAL CASE

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Keywords: Bayesian, spatiotemporal, health, COVID-19, vulnerability, integrated nested Laplace approximation

1. Introduction

The COVID-19 pandemic deepened existing social inequalities. Difficulties in access to health care during the pandemic had effects on disease diagnosis and monitoring, leading to a poor health status, especially in the vulnerable population.

Available research on the topic focuses on ecologic studies, some with methodological shortcomings, implying uncertainty about the validity of the findings, as analyzed by Barceló (2021). Epidemiological designs based on longitudinal data of individuals alongside appropriate methodological tools are needed to provide robust findings.

The main objectives are to characterize the socioeconomic inequalities during the pandemic and their effect on the health of the population, especially the most vulnerable, and to apply spatiotemporal modeling algorithms to real-world data (RWD) of high volume.

2. Methodology

Data is provided by the Catalan Health Institute (ICS) via the Information System for Research in Primary Care (SIDIAP) from 2015 to 2022, database of which a content report was produced by Recalde *et al.* (2022). It contains curated data on the population registered with the public health system. The data include demographic information, diagnoses, drug prescriptions, and consultations at primary care facilities.

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

3. Results and discussion

Expected results from the analysis are spatial and temporal parameters that describe and help to understand how social context behaviors during the pandemic impacted the health status of the Catalan population.

4. Conclusions

Preliminary findings uphold the hypothesis of pandemic impacts on other conditions like coronary heart disease and diabetes as distinctive results of social status. With the development of the research, these findings are expected to be measured and confirmed.

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HOMONATIONATIONALISM IN CATALONIA

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Keywords: Feminist epistemologies, homonationalism, LGBTI+.

1. Introduction

Homonationalism is a term coined by Jasbir Puar (2017) that refers to the way how, in the Global North, some LGBTIQ+ discourses have been co-opted with nationalist positions. Discursive formations in the Global North are moving towards the exceptionalist notion view that accepting LGBTIQ+ people is a yardstick for democracy (Haritaworn et al., 2008) in a territory. Homonationalism has become an indicator that countries that are openly LGBTIQ+ phobic are, hence, backward and uncivilised -and, evidently, those countries are all in the Global South. Even though the lives of LGBTIQ+ people in the Global North are not necessarily improving, certain LGBTIQ+ discourses reinforce colonial conceptions of progress. It is in this sense that Jasbir Puar locates homonationalism as a facet of Modernity.

This doctoral research interrogates LGBTIQ+ inclusion in Catalonia through the lens of homonationalism. It is an exploratory and descriptive work based on fieldwork with 14 LGBTIQ+ activists working across Catalonia.

2. Hypothesis

Because of the epistemological stance of this doctoral dissertation, there is no formulated hypothesis, as that would not be coherent methodologically.

3. Methodology

This doctoral research uses the Narrative Production Methodology (Balasch & Montenegro, 2003), one of the methodological explorations of feminist epistemologies. This methodology consists of the co-creation of texts, or Narratives, between participant and researcher. To create a Narrative, the researcher interviews the participant. The content of the interview is then transformed into an essay-like text and shared with the participant. The participant is free to change anything they like from the text -including adding, modifying, and eliminating content, and the researcher can use these changes to ask additional questions, if necessary. The Narrative is finished once the participant feels that it portrays all they want to portray. Once the researcher has all the necessary Narratives, they are not treated as mere sources of

information, but rather they are regarded as theoretical texts and put in conversation with the theoretical documents that informed the researcher's theoretical framework.
For the present doctoral research, the researcher in training has elaborated 14 Narratives with LGBTIQ+ activists. The participant activists carry out their activity in different parts of Catalonia, specifically in the provinces of Girona, Barcelona, and Lleida.

4. Results and discussion

The research has not yet reached the Results phase, which is why only the expected results will be discussed in this presentation. The study expects to track the way the LGBTIQ+ liberation movement and discourses in Catalonia are embedded in the structure of homonationalism. The main expected result of this doctoral dissertation is to describe how homonationalism is deployed in Catalonia.

5. Conclusions

The research has yet to arrive to the final phase, where conclusions will be drawn. Conclusions in this PhD dissertation will be directly informed by the analysis of Narratives within the theoretical framework of homonationalism. Because of this, this doctoral dissertation aims to contribute to the growing discussions about homonationalism.

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FAMILY AND EMPLOYMENT: A NEVER-ENDING CONFLICT?

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Keywords: care, employment, gender equality, social policy, women

1. Introduction

My research investigates how European social policy addresses the family-employment tensions experienced by women with childcare responsibilities. The aim is to contribute to the debate about the relevance of recognizing the social and economic value of care for the design of social policy.

Women are one of the groups most exposed to poverty and social exclusion due to the gender-biased environment that still characterizes our society. Their vulnerable position is generally linked to the unequal distribution of unpaid care work between men and women and to women's disadvantaged position in the labour market (Lewis & Giullari, 2005). In fact, albeit in recent decades there has been a general change in traditional gender and family roles, care continues to be a feminised activity (Huppatz & Craig, 2022). This situation also influences the way women approach employment: Crompton (2006), for example, highlights that flexible and part-time jobs are often "concentrated" among women with childcare responsibilities. These are considered a "win-win combination" to reconcile family and employment (p.7), but may also entail low wages, poor working conditions and high time consumption. These considerations are confirmed by the data collected by Eurostat in recent years: in 2019 the gender pay gap was 14% - about 24% of it related to the overrepresentation of women in lower-paid sectors - and in 2020 the gender employment gap was 11% (EAPN, 2022). The pandemic has confirmed women as mainly responsible for caregiving with the added burden of home schooling and permanent childcare in the same physical space as paid work (Huppatz & Craig, 2022). Furthermore, many working mothers have ended up poorer and more impacted due to their "concentration in poorer, more precarious jobs and sectors" (EAPN, 2021, p.31).

2. Methodological Plan

The research will be developed to answer the following question:

How does the social policy design address family-employment tensions?

To this end, I will provide a multilevel analysis of family-employment tensions, moving from the institutional to the policy level, and finally focusing on the experience of individuals. This strategy will allow me to analyse the topic from different perspectives in accordance with the level of involvement of the actors. In three different articles, I will address different puzzles. Table 1 better explains the overall strategy.

***Table 1**. General conceptual scheme of the research*

LEVEL	DOMAIN	GENERAL CONTENTS	OBJECTIVE	RESEARCH QUESTION	TERRAIN
MACRO LEVEL	Institutional domain (Conceptualization of the institutional evolution regarding family and employment)	The development of the Welfare State and the institutionalization of the current relationship between employment, care provision, and social protection	Not applicable	Not applicable	EU general development with a focus on the 7 countries part of the Euroship project of IGOP (Estonia, Germany, Hungary, Italy, Norway, Spain, and UK)
MESO LEVEL	Policy domain (Analysis of specific policies that may influence the way women cope with their employment and childcare responsibilities)	Fostering work-life balance for precarious workers: culture and social protection systems in a comparative perspective (paper 1)	Observing how the intersection between WLB policies, social protection, and labour market regulations support precarious workers to combine work, family, and personal life.	To what extent do WLB realities and entitlements improve the opportunities to make meaningful choices for workers at the intersection of various dimensions of inequality?	Specific focus on the 7 countries part of the Euroship project of IGOP (Estonia, Germany, Hungary, Italy, Norway, Spain, and UK)
		Care and Minimum Income Policies: Between Social Rights and Social Monetary Benefits (Policy analysis - paper 2)	Analysing to what extent minimum income schemes could constitute an opportunity structure for women with childcare responsibilities to exit poverty or social exclusion.	To what extent are unpaid care work and care responsibilities incorporated in the conditionality design of European minimum income policies?	4 EU countries belonging to different welfare regimes (chosen among the 7 which are part of Euroship: Hungary, Norway, Spain, and UK?)
MICRO LEVEL	Domain of individuals (Concrete case of family-employment conflict of a particularly vulnerable group)	Time-money conflict of lone mothers in Spain: a case study (paper 3)	(1) understanding to what extent the family-employment tensions experienced by lone mothers may "deform" the way they respond to particular situations; (2) observing the implications of policies and laws on their quality of life and freedom of choice.	To what extent does the time-income conflict experienced by lone mothers affect their freedom of choice regarding the reconciliation of their work and care responsibilities?	Only Spain

3. Conclusions

Analysing the family and employment tensions experienced by women with childcare responsibilities is crucial in current times. In fact, as Arlie Hochschild highlighted back in 1989, focusing only on employment is seeing half of the problem. Introducing the concept of care, instead, is crucial to reflect whether equal participation in employment is enough for gender equality. That is especially important considering the current strategy promoted by the European Social Policy Agenda, which considers employment to be the best solution to poverty, social exclusion and gender inequality. Care policies continue to be relevant, but there is also a need to address care from a broader perspective of social policy. The terrain of the research will be European Social Policy because in Europe we find some of the most advanced welfare states in the world as well as multiple approaches to social policy.

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IS CLIMATE CHANGE THE PROBLEM? A FEMINIST ANALYSIS OF CLIMATE CHANGE DISCOURSES IN SPAIN AND CATALONIA

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Keywords: climate change, feminist perspective, WPR approach

1. Introduction

Is it possible to reverse climate change? How will it affect our futures? Are we still on time to reverse this situation? Those questions have been asked by scientists and policy makers and in society for quite some years. And while this year marks the 50th anniversary of the report on the limits of growth (Meadows et al., 1972), there is not a clear or simple answer. What if we are not asking the right questions? It is necessary that we, as a society, start to recognize the power relations embedded in our daily interactions with other humans and non-humans, if we hope to survive as a civilization.

The way in which climate change is framed and represented reveals a gap in the interface between policy and research regarding how to apply a feminist perspective in policy-making in general, and in climate change policy-making specifically.

We propose to look at climate change from a different perspective in order to find different solutions to these multiple crises. We see climate change as not the problem itself, but rather as the consequence of a failed system that has misunderstood the materialism in which we are all immersed and that we have exploited incessantly. To do this, we apply a feminist perspective to the national (Spain) and regional (Catalonia) climate change policy discourses to identify what can be done differently and to try to build some guidelines for policy-making and apply them in the future.

2. Methodology

This research uses a qualitative approach following the top-down policy analysis methodology developed by Carol Bacchi (2009): What is the problem represented to be? (WPR). This methodology insists that how "problems" are framed discursively affects their understanding, and that these understandings are central in the development of strategies to address the

problems (Bacchi & Eveline, 2010). This methodology allows us to address and examine how public policy problems are constructed and represented, through a series of questions:

1. What is the problem represented to be?
2. What assumptions underlie this representation?
3. How did this representation come about? What is its context?
4. What is left without problematizing? What are the silences? What could be thought of differently?
5. What effects does this representation have?
6. How/where has this representation been produced/disseminated/defended and/or questioned/replaced?

3. Results and discussion

What we have found is that the climate change policy discourse in Spain and Catalonia represents climate change as a biophysical problem of increasing concentrations of greenhouse gases (GHG). The policy offers the opportunity for modernization and progress but at the same time it is a threat to energy security, economic security, in short, a threat to national security, and it is also an accelerant of the vulnerabilities that already exist in our country. The alternative discourse represents climate change not as the problem but as the visible consequence of a failed, patriarchal, and colonial system that will only be fixed from a perspective of climate justice. What we see now is the tip of the iceberg. Climate change forces us to rethink the productive (and reproductive) model and we must approach it by putting the sustainability of life as the central axis of transformation, to live a life that deserves to be lived.

4. Conclusions

From a feminist perspective, there is an urgent need to include other knowledges in the creation of climate change discourses for public policy development as well as in the implementation of those policies. Exercises such as citizen assemblies might be a good opportunity, despite the constraints.

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SESSION 14.

ARCHITECTURE, URBANISM AND HERITAGE

WALKING THE LINE: SOCIO-GEOGRAPHICAL CONNECTIONS ON ANCIENT PATHS IN THE EASTERN CATALAN UPLANDS

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Keywords: agro-silvo-pastoralism, heritage, landscapes, paths, social-relations

1. Introduction

The environment is the 'locale' where agency occurs (Evans, 2003:28). Action, time, and space conflate producing places ontologically. Externally, these are landscapes: "the world as it is known to those who dwell therein, who inhabit its places and journey along the paths connecting them" (Ingold 2000). High Muga Valley paths formed through agro-silvo-pastoralism linking some terraced plots. Today they are affected by roads and declining agro-silvo-pastoralism, putting their heritage at risk, and many ancient paths have disappeared. Yet, historically, people maintained their social relations along mid-range, ancient, sometimes paved, particularly transverse, cross-border paths. One was apparently a 'royal road' linking the Vallespir to Olot (Roque, 1987) like the 'Camí Ral' (Olot-Vic). Paths were the internet of the epoch, along which information, people, plants, animals, and concepts spread.

2. Methodology

Comparing path remains with archives and cartography suggests ethno-historical evidence for connections between people from the Alta Garrotxa and High Vallespir.

3. Preliminary results

Seventeenth-century archives suggest close social relationships between the people of Costoja (Vallespir) and the Alta Garrotxa, especially along ridgelines. In addition, close intra-relationships existed among Vallespir highlanders who arguably developed similar upland economies (Serralonga to Costoja) in the 16th-18th centuries (Peytavi Deixona, 2010). For example, some early Costoja church records from 1667 to 1677 contain 203 baptisms involving 406 godparents, of which 86 (21.18%) dwelt in either the Alta Garrotxa or Alt Empordà. Costoja recorded 110 weddings between 1654 and 1681; 28 brides and grooms were from either the Alta Garrotxa or the Alt Empordà (12.72%). Many of the marriages (34 couples) were between members of the Costoja parish, presumably travelling along the highland paths (Costoja church records).

Figure 1. Examples of 'lost' partially paved paths.

4. Conclusions

Paved stone paths suggest status and antiquity - investment as landesque capital maintained through social capital. Agency linked people through seasonality, transhumance, charcoal production, common lands (Evans, 2003). Walking these lines was integrated in ontological understanding, incorporated internally, and affected the landscape. Paths were tread through agro-silvo-pastoral 'taskscapes' (Ingold 2000), entwining temporality shared lifeways, resilient mobility, and rites of passage, and perhaps these agencies altered with imposed national borders. With systemic abandonment many paved paths slipped into decay although some have been maintained through festivals, outdoor recreation, or hunting. Thus, landscape is perceptually alive through paths. Movement 'a peu' is entrenched and connects the high landscapes and its peoples (Puigmal & Duran 1981) across trans-frontier paths that, when walked, invert the border into an *axis mundi,* linking spirits of place, time, people and locales together; we could do more to conserve these heritage paths.

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DISCRIMINATORY HOUSING

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Keywords: habitability, inclusive architecture, interculturality, North African architecture, social housing

1. Introduction

The work focuses on the study of private space and proposes to analyse how the spatial and architectural configuration of domestic interiors can condition and even exclude people from diverse cultural backgrounds.

Since the late 19th century, the modernization process has promoted a broad rationalization of society, extending to all areas, and affecting both the institutional public sphere and the private domain of life and family organization. With this modernizing purpose, a certain family model based on a nuclear family was promoted through various political means, conditioning social behaviours considered acceptable and desirable for the modern productive society. These values have been reflected over the years in our way of living in our homes, imposed through different habitability regulations like Catalan decree law 141/2012 promoted by various public institutions. This homogenizing process excluded any consideration of alternative ways of inhabiting domestic space that did not respond to the normalizing model, as well as other family forms and other cohabitation rituals (Casals Tres, 2013). Anything that did not fit into the corpus of behaviours and universal models was ignored. This is the case of immigrant social groups.

2. Results and discussion

This strict application of the law and regulations has rigidified the housing model and, consequently, is following a distribution standard that favours certain common ideas considered the appropriate way to solve housing issues. This thinking, apart from limiting the range of housing typologies, reduces the capacity to adequately respond to other lifestyles present in our society today (Monteys, 2006). It translates into a loss of identity and, often, of richness when this factor is not taken into consideration and an attempt is made to "conquer" these forms of domesticity through the standardization of housing. This loss of identity generates diverse types of conflicts that can lead to dogmatisms. An example of this is the religious fundamentalism emerged in recent decades, a symptom of this lack of identity and cultural whitewashing that the North African community suffers (Stefano, 2003).

3. Conclusions

This work proposes the redefinition of habitability based on the study of different domestic orders in other cultural realities. It is the task of architects to develop projects that provide solutions to users' needs and to promote debate about a housing model that can be inclusive and diverse.

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DESIGN THE CAPITAL, IMAGINE THE NATION: TRADITIONS, MODELS AND THEORIES IN TENSION FOR THE ARTISTIC TEACHING OF ARCHITECTURE AT THE UNIVERSITY OF BUENOS AIRES, 1878-1931

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Keywords: architectural training, École des Beaux-Arts, history of design, theory of architecture, University of Buenos Aires

1. Introduction

At the end of the 19th century, architectural training at *Facultad de Ciencias Exactas, Físicas y Naturales-Universidad de Buenos Aires* (FCEFN-UBA) adopted an artistic orientation to place architecture in the sphere of fine arts. This artistic dimension would allow architects to intervene in the cultural debate about the proposed character of the architecture in the Argentine capital and the main regions of the nation (Liernur, 2001). The incorporation into the FCEFN-UBA of artists and architects trained in major European academies and especially in the French education system dominated by the Parisian École de Beaux-Arts implied an appropriation of theories and teaching models into Argentine architectural culture in the context of the polytechnic profile developed throughout the 19th century at the FCEFN-UBA (Aliata & Gentile, 2022).

2. Hypothesis / problem

Artistic teaching of architecture at FCEFN-UBA was implemented at a crossroads of international traditions – mostly French, but also Italian, Belgian, and Spanish – that operated in the context of a polytechnic tradition of the university system. This meant a conflictive appropriation of a global reference of teaching model at that time, the Parisian École des Beaux-Arts, and of a series of theories, practices, and pedagogical instruments implemented around the institution (Epron, 1997; Lucan, 2009; Lambert & Thibault, 2012). Trained under this teaching system were professors of the UBA, who as relevant members of professional societies led discussions about architecture, and heads of the leading architectural firms in Buenos Aires, who designed emblematic buildings across the country. These professors and professionals established architectural training that articulated discipline and professionalism, theory and practice.

3. Methodology

The research is based on the compilation and analysis of textual and graphical documentary sources in public and private archives in Argentina, France, Italy, and Spain. In addition, critical bibliography on the history, theory, and criticism of architectural teaching of the 19th and 20th centuries will be analyzed.

4. Results and discussion

This research provides new analytical perspectives to build a broader cartography of the international circulation of architectural training models in the 19th century, restores the importance of objects, books, treatises and magazines, as well as relevant institutions and societies in architectural education that have been ignored in the historiography of the period, and provides new interpretations of those parts of the canon of architectural history.

5. Conclusions

This research aims to provide new analytical perspectives for a more rigorous understanding of the transatlantic circulation and correspondences of architectural education models at the beginning of the 20th century and the impact on the institutionalization of architectural training in Argentina.

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URBAN/RURAL GREEN INFRASTRUCTURE: METHOD BASED ON THE CONTRIBUTION OF NATURE AND GOOD LIVING. THE CASE OF CUENCA – ECUADOR

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Keywords: contribution of nature, green infrastructure, landscape ecology, territorial planning

1. Introduction

The growth of urban agglomerations is a phenomenon that, although globally accepted, admits nuances and particular considerations depending on the local context. This is the case of Latin America and specifically Cuenca, Ecuador, where the urbanization process, especially in the 20th century, occupied the land in a chaotic and expansive way, generating social and environmental conflicts. This expansive growth puts the natural ecosystem at risk. The objective of this research is to value natural ecosystems. The methodology consists of three phases: identification, assessment, and prospecting. The most important results revolve around understanding the city and the territory as parts of the same system and proposes three strategies: conservation, regeneration, and potential spaces, articulated in the urban/rural green infrastructure (Benedict & McMahon, 2002). This concept emphasizes the importance of open land and open space as interconnected parts of the same system that have to be managed and protected for the ecological benefits they provide (Swyngedouw, 1996).

2. Hypothesis

The starting hypothesis is that the urban/rural green infrastructure (URGi), structured through the contributions of nature and good living, can shape the urban form and contain the expansive growth of the city, conserving nature and improving people's quality of life.

3. Methodology

URGi presents the following phases. 3.1 IDENTIFICATION: the case of Cuenca, Ecuador. This section has two aspects, an intentional reading based on land uses and a supervised classification based on the ecology of the landscape. 3.2 ASSESSMENT: contributions of nature and good living. This phase proposes a matrix validated by experts that contains the predominant land uses in the planning of the last eighty years in the city of Cuenca (Y axis), and nature's contributions to people organized into three categories: provision, regulation, and social-cultural services detailed in 28 subcategories (X axis). 3.3 PROSPECTION: URGi. This section structures a URGi through three strategies – conservation, regeneration, and potential

spaces – as part of the same system that must be managed and protected for the ecological benefits it provides (Toledo, 2013).

4. Results and discussion

The supervised classification, in addition to identifying spaces with ecological value, allows us to establish the "hubs" (matrix of each one of the parishes) that structure the green infrastructure (Forman, 1995). These “core” spaces determined through landscape ecology are basically páramo (3), forest (7) and agricultural land (11), and are a fundamental part of the social-cultural fabric of the canton. Although, there are embedded subcategories within these large tesserae, they are beyond the scope of this research, which focuses on their fit into current land use and the contributions they provide to people.

5. Conclusions

This new methodological approach places nature at the center for a better harmonization between urban growth and environmental values, by establishing protection, regeneration, and potential spaces, articulated through environmental corridors, forming a URGi, capable of conserving nature and improving people's quality of life (Tzoulas et al., 2007).

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ANALYSIS AND MODELING SPATIOTEMPORAL EVENTS IN COMPLEX SPATIAL REGIONS

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Keywords: Barrier model, Integrated nested Laplace approximation, Spatiotemporal modeling, Stochastic partial differential equations, Whittle-Matérn fields

1. Introduction

Spatial statistics is traditionally based on stationary models like Matérn fields (Lindgren et al., 2011). However, applying stationary models to complex spatial regions having physical barriers like islands or coastal areas can result in inappropriate smoothing of such regions (Bakka et al., 2018). Additionally, in many environmental applications such as stream systems or urban road networks, it is essential to define statistical models in linear networks.

2. Hypothesis

This research thesis explores the benefits and limitations of integrated nested Laplace approximations (INLA) along with the traditional stochastic partial differential equations (SPDE) for Bayesian spatiotemporal modeling (Lindgren & Rue, 2015). The study focuses on complex distributed spatial regions with physical barriers, as well as linear networks like urban road networks. The initial approach involved utilizing explicit network triangulation and barrier model techniques to explore and analyze the occurrences of traffic accidents on urban road networks. We proposed the novel concept of spatial triangulation restricted to linear networks. But complex boundary regions create fictitious spatial structures resulting in artificial spatial dependencies (Krainski et al., 2018). To avoid this, we applied an alternative computational strategy to design nonstationary barrier models in linear networks. But in both cases, boundaries lie within the spatial domain of interest, preventing the high boundary effects from being reduced. An alternative to Euclidean distance is to define the model using non-Euclidean metric on graph structures. In this case, it is challenging to find flexible classes of functions that are positive definite to formulate Gaussian fields on compact metric graphs, very recent special type of spatial data structure (Bolin et al., 2022).

3. Methodology

Utilizing the recent concept by Bolin et al. (2022), a novel category of Gaussian processes has been applied on compact metric graphs. The Whittle-Matérn fields employed in this approach are defined through a fractional SPDE on a metric graph. The proposed fields are a

natural extension of Gaussian fields with Matérn covariance functions on Euclidean domains to non-Euclidean metric graph settings (Bolin et al., 2022).

4. Results and discussion

A ten-year period (2010-2019) of daily traffic-accident records from Barcelona, Spain has been used to evaluate the three models referred to above. While comparing model performance using evaluation metrics, we observed that the proposed fractional SPDE on the metric graph model outperformed network triangulation and barrier models.

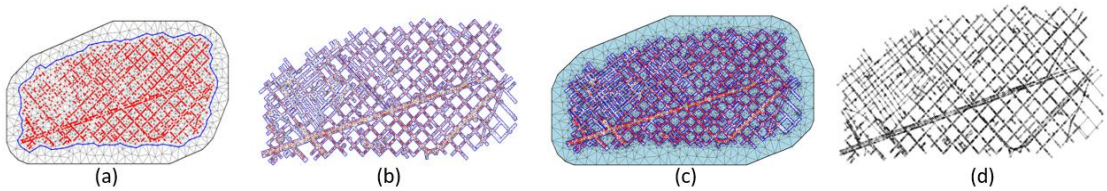

Figure 1. SPDE triangulation for (a) entire region, (b) only road network, (c) barrier model and (d) graph data structure for road network

5. Conclusions

Due to this flexibility, this methodology can be applied to a wide range of environmental issues and specifically to linear networks such as spatio-temporal modeling of water contamination in stream networks or modeling air quality or accidents on urban road networks.

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BARCELONA CATHEDRAL AND ITS PRESBYTERY SPACE (CA. 1298-1390): CONFIGURATION, FUNCTIONALITY AND PERCEPTION

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Keywords: architecture, Barcelona, cathedral, gothic, liturgy.

1. Introduction

In the period between ca. 1298 and 1390, on the architectural and liturgical base of a previous Romanesque cathedral consecrated in 1058, a new church was planned and built for the episcopal headquarters of Barcelona to replace the previous building, largely unknown to this day due to the paucity of material, documentary and liturgical evidence that has been preserved (Boto & Sureda, 2021).

2. Hypothesis

The presbytery of the new cathedral, the focal point of liturgical life, was articulated, on the one hand, from an architectural perspective on two planes: a vertical one (crypt and main presbytery) and a horizontal one (radial chapels and the choir) and, on the other hand, from a functional, symbolic and cultic point of view with decorative and liturgical elements (Borau 2003; Carrero, 2014).

Based on these hypotheses, the aim of this thesis is to investigate the process of adaptation, transformation and materialisation of the new Gothic cathedral complex from ca. 1298 onwards. The study perspective addresses, in a tangential way, the analysis of the continent (building), the content (liturgical and decorative artefacts that give meaning and occupy the space) and the way in which these are presented and perceived by the spectator who experiences the ensemble multisensorially.

3. Methodology

The methodology used covers different areas due to the interdisciplinary nature of the project. Bibliographical analysis and compilation; architectural and material study (taking measurements, photographs and study of planimetries); documentary work in the *Arxiu de la Catedral de Barcelona* to search and transcribe original documents; and other methodological aspects, such as spatial experimentation *in situ* of sensorial and intangible elements like sound, light, etc.

4. Results and discussion

In the new Gothic cathedral, new cults, devotions and liturgical modes were combined with those inherited from the previous building, in an architectural space modulated and equipped in response to the functional needs and social concerns and realities of those individuals (religious and lay) who inhabited and experienced the cathedral space.

5. Conclusions

This thesis, which is still being written, aims to contribute an interdisciplinary vision to the study of the Barcelona Cathedral, focusing on the configuration and use of its presbytery during the 13th and 14th centuries, and to create a study methodology, in line with current historiographical trends, applicable to other cathedrals in Spain and Europe.

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MATERIAL AND POWER IN MEDIEVAL ÁVILA'S BUILT ENVIRONMENT

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Keywords: Ávila, material, materiality, medieval, stone

1. Introduction

At the close of the eleventh century, Ávila emerged as a strategic city at the foothills of the Guadarrama mountains as part of the centuries-long effort to expand Christian territory south into al-Andalus, which historians later came to refer to as the Reconquest or *Reconquista*. It was a period of immense social, political, and economic upheaval that flooded the city with new settlers and ushered in a substantial building boom in the twelfth and thirteenth centuries. Within the span of a century, Ávila became home to over two dozen parish churches, a small handful of monasteries or convents, a Gothic cathedral, city walls, a bishop's palace, and an alcázar.

The following presentation draws from my broader dissertation project to discuss the construction materials that make up medieval Ávila's preserved architectural heritage, most of which date from the mid-twelfth to the late-thirteenth century. Curiously, the materials are asymmetrically distributed across monuments: *spolia* dot the towering walls built in granite and bedrock; the red and white marbled *piedra sangrante*, or "bleeding stone," makes up the cathedral's sanctuary; and, with the exception of a single brick aberration, the city's parish churches combine hard and soft granites in particular ways. More curiously, these materials rarely overlap — *spolia* is lacking in church architecture while *piedra sangrante* appears almost exclusively in an episcopal context. By focusing on materials, my project takes a fresh look at traditional frontier themes through the lens of materiality — expressions of power, socio-cultural conflicts in a plural society, and architectural language at the meeting point of politically opposed communities.

2. Conclusions

I demonstrate how careful and purposeful utilization of materials, especially different types of stone, reinforced complex social divisions, upheld structures of authority, and communicated difference and unity in the medieval city. In particular, I argue that, on the whole, specific materials were favored and privileged for specific building types — city walls, parish churches, and cathedral all employed distinct materials. Each monument type was associated with a different social group, and their materials became markers of those specific groups. In this

way, materials helped communicate the identity of each authoritative power in medieval Ávila while building a perduring monumental landscape on newly conquered land for the Crown of Castile.

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SESSION 15.
HUMANITIES

PHILOSOPHY IN THE NATIONAL CONSTRUCTION OF CATALONIA. STUDY OF NATIONALIST HISTORIOGRAPHY OF PHILOSOPHY

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Keywords: nationalism, historiography or philosophy, national philosophy, history of philosophy in Catalonia

1. Introduction

Nationalism uses cultural sources, such as history and literature for the construction of national identities (Núñez Seixas, 1998; Smith, 2009). But has the history of philosophy also played such a role? During the 19th and 20th centuries, there were numerous debates about which could be considered the "national philosophy" of a given territory (Crépon, 1989, 1996). In Catalonia, coinciding with the apparition of Catalan nationalism, some intellectuals went back to medieval philosophers such as Ramon Llull or Ramon Sibiuda and discussed who represented the so-called "Catalan spirit" (Bilbeny, 1985).

2. Hypothesis

Nationalism uses, among others, the history of philosophy as symbolic material for the construction of the national collective identity. The thesis shall aim to answer: (1) How and why does nationalism use the history of philosophy? (Gracia, 1992; Rorty, 1984) (2) Which argumentative strategy lies behind the discourse on national histories of philosophy? (Worms, 2001) (3) Is this a past phenomenon, restricted to the rise of nationalist movements, or does it persist today? Finally, (4) do the specificities of the Catalan example constitute an exception or can they be used as a study case?

3. Methodology

The identification and study of cases of national philosophy around the world offer empirical material to analyse their origin, persistence, logic, and political use. The cases of Germany (Courtine, 2001; Klaute, 2013) France (Worms, 2001), Poland (Mróz, 2016), Romania ((Blaga, 1943; Crépon, 1989), China (Thoraval, 1994; Van den Stock, 2021), Indonesia (Makin, 2016), and Basque Country (de Alzo, 1934) are diverse but significant, and shall prove useful for understanding the phenomenon formally and for analysing the specificities of the Catalan debate.

In order to understand the Catalan case, the study of the most significant authors (and many others) who studied Catalan philosophers between 1892 and 1931 is crucial: Josep Torras i Bages (1981), Frederic Clascar (1896), Salvador Bové (1896, 1902), Josep Pou i Batlle (1907), Francesc Pujols (2012) and Tomàs Carreras i Artau (1931).

4. Results

By proposing a particular interpretation of their philosophical heritage, nationalist philosophers deduce a so-called essential "philosophical character" of their nation, that is not only descriptive but has performative consequences on politics (Worms, 2001). This manoeuvre had particular importance in countries with pollical conflicts such as war, colonialism, or the existence of ethnic minorities (Crépon, 1996; Duddy, 2002). The uses and study of Catalan history of philosophy develop in parallel to the history of Catalan nationalism and its struggles for political autonomy. Their thorough study shows that they can be understood as a paradigmatic example of this strategy.

5. Conclusion

National philosophy is a political alliance between the historiography of philosophy and nationalism. Nationalists base their discourse on the prestige of philosophers of their territory to construct, legitimize or reinforce their collective identity. Therefore, the study of this phenomenon could be called "nationalist historiography of philosophy" and must be studied as a field comprised between cultural studies and political philosophy.

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ELS OBLIDATS D'ETOBON

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Keywords: Aurora Bertrana, Catalan writer, 20th century Catalan literature, post-war literature, Second World War

1. Introduction

Els oblidats d'Étobon analyse two narratives that are part of Aurora Bertrana's post-war narrative cycle of and. In addition, they have not received attention from researchers. These two stories complete the narrative cycle with the novels *Tres presoners* (1957) and *Entre dos silencis* (1958). The narratives in question are the short story *Un pomell de violes*, published in the volume *Vocació de viure* (1956), which also contains short stories by Alfred Vilaplana and Agustí Esclasans, and *La madrecita de los cerdos*, an unpublished manuscript from Bertrana's archive. I intend to analyse the texts while also adding them to the post-war narrative cycle and discussing their place in the storyline. In addition, I aim to know if there is a name to call this cycle and to identify it.

2. Hypothesis

There is a bibliographic gap in the biography of Aurora Bertrana after her return from exile in 1949, partly intended by the author and partly due to lack of research. For this reason, one of my aims is to start filling this gap and offer, from the start, a critical study of some novels from this period that have not been researched, in this case *La madrecita de los cerdos* and *Un pomell de violes*.

3. Methodology

My research has two well-define stages, which require different methodologies. The first one consists of reading the unpublished manuscript in Bertrana's archive at the University of Girona and analysing the author's correspondence to find information about why some manuscripts are published and others are not. The second stage involves bibliographical research on the publication of *Tres presoners* and *Entre dos silencis* as well as on Bertrana's biography.

4. Conclusions

While my research is still at an initial stage, I believe it can be an interesting contribution to an under-researched period in Bertrana's evolution as a writer. Both the published nature of one of the texts and the fact that they form a cycle with two better-known pieces ensures the relevance of the results. Since my research involves an unpublished manuscript, I am also considering a revision of the text and a critical edition.

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HATE AND FLAMES: REVOLUTIONARY REPRESSION IN GIRONA DURING THE SPANISH CIVIL WAR

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Keywords: Anticlerical repression, Girona, political violence, revolutionary repression, Spanish Civil War

1. Introduction

On 18 July 1936, the Spanish Civil War began. During the war, repression was carried out by both sides. Between 200,000 and 300,000 people died as a result of this repression. Of these, 50,000 were killed by the Republican side. Of these, 800 were killed in the province of Girona. That is the subject of our research. In our province there is no research beyond the numbets of the dead, and that is the hole we are trying to fill.

2. Hypothesis

Our aim is to answer questions about the revolutionary repression in the province of Girona: where, when, who, how, what, and why. These questions we are raising have not been answered. There are some local studies, but nothing more. Based on authors who have dealt with this question in other places, we believe that this phenomenon can be explained by power relations and conflicts in a context of power, by political culture, by the global context, and by local relations.

3. Results and discussion

Among the victims were a large number of priests and monks, the most affected group, and, albeit in smaller numbers, members of the military and right-wing militants. As for the when, we're seeing that most of the victims were killed in the first months of the war. As to how, in the first months the violence was commited by the revolutionary committees. As for where, the areas with the most deaths are close to the French border. Most of the killers were members of the local committees. As to the why, the power structure due to the war, the disintegration of the Republican state and the revolutionary political culture can explain the violence. Discussion can focus on who the killers were, on the phenomenon of outsiders, on certain myths that still persist, such as the fact that anarchists are seen as the main culprits, the theory that places where left and right were more evenly matched had more violence, the reason for

so many clergy deaths, or whether the Gramscian concept of hegemony can be used to explain the phenomenon.

4. Conclusions

In the end, this research wants to understand revolutionary violence in our province. Our aim is to understand why this happened and why in this way. With this, we hope to be a little closer to understanding what happened in our civil war.

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VICTIMS OF THE *EINBAHNSTRASSE:* CROSSED DIALOGUES IN THE MARKING OF TIME AND THE WRITING OF HISTORY BETWEEN W. BENJAMIN AND J. HEJDUK

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Keywords: John Hejduk, Memory, Time, Victims, Walter Benjamin

1. Introduction

This paper studies the influences of Walter Benjamin's philosophical discourse on the architectural work of John Hejduk, focusing on the representation of time, the writing of history and the concept of progress.

The aim of the paper is to identify in John Hejduk's work the projectual mechanisms that would give way to the other writing of history that Benjamin claimed.

2. Problem

In their works, both authors question the definition of history and describe it as a story that unfolds in open time, in a time that is neither chronological nor finite. They understand history as a living thing, incorporating present and past events in a process of interaction with memory.

The paper aims to describe the architectural strategies used by John Hejduk to address the relationship between time, history and architecture, analysing a design process that began with the *Diamond Houses* and culminated in *Victims*.

3. Methodology

Hejduk uses different methods of expression in his works. The research in primary and secondary sources, as well as the thematic analysis of some of his projects, allows us to establish a theoretical framework to observe how Hejduk works with the marking of time and the representation of history, placing them in relation to the thought of Walter Benjamin.

4. Results and discussion

Through the analysis of Hejduk's works, we can observe how the architect's work is imbued with Benjamin's philosophy. In *Victims*, the architecture is constituted as a catalyst for the legibility of memory, time and oblivion. The project articulates a process of representing the history of the place and of constructing a discourse and practices alternative to those of epic memory that officialise the monument and the memorial.

Hejduk conceives time in relation to space and linked to movement, in a plastic and cyclical process, not exempt from reflection on the discipline itself. This conception begins in his first projects, where he explores the architectural, geometric and formal resources that will allow him to explore the temporal dimension of an architecture that seeks to encompass both the representation of space and time, masked in geometric forms and layers saturated with opacities.

5. Conclusions

On the basis of Benjamin's premise that in order to change the world it is necessary to change the notion of time and update the history, the architect establishes the mechanisms to give way to an alternative future temporality, which unmasks the idea of progress and lays the foundations of a pessimistic utopia that he elaborates in later projects.

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CÈSAR MARTINELL AND THE CATALAN BAROQUE ALTARPIECE: HIS CONTRIBUTION AS AN ART HISTORIAN, COLLECTOR AND RESTORER

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Keywords: altarpiece, Baroque, Catalonia, Cèsar Martinell

1. Introduction

Cèsar Martinell's commitment to the Catalan baroque altarpiece was consistent throughout his career, and his success was mainly due to the publication of *Arquitectura i escultura barroques a Catalunya*. However, besides being an art historian, Martinell approached the subject from the perspectives of an art collector and a restorer. The objective of this presentation is to show these three different ways Martinell approached Catalan baroque altarpieces and how all three still play an essential role in the present study of the subject.

2. Results and discussion

One of Cèsar Martinell's first works as an art historian was *Llibre de notes de Lluís Bonifàs i Massó, escultor de Valls* (Martinell 1917). Since then, his historiographic production was constant and progressively acquired a more academic tone. In his main work, *Arquitectura i escultura barroques a Catalunya* (Martinell 1959-1963), the author designed a studio pattern for the baroque altarpiece, concerned about its formal and typological evolution throughout the 17th and 18th centuries. These three volumes show a solid formation in the subject and his ideology about baroque art (Company 2001). As a collector, Martinell acquired around a hundred altarpiece designs, now held at *MNAC* (Bassegoda 1989). The stylistic analysis of the drawings, all of which are high quality designs, reveal a solid number of altarpieces from the end of the 18th century, one of the least known periods of altarpiece history in Catalonia. As an architect, Martinell directed the restoration of some altarpieces after the Spanish Civil War (Mignorance 1998, Martinell 1952). The *Col·legi d'Arquitectes de Catalunya* preserves the documentation of several projects, revealing different approaches: while the main altarpiece of Igualada was restored following pictures of the original work, the ones of Sant Antoni (Mignorance 1999) and the Sacred Family, both in Igualada, were completely redesigned by Martinell by following his own ideas from baroque aesthetics.

3. Conclusions

The analysis of Cèsar Martinell's contributions to the study of the baroque altarpiece shows an exemplary approach due to its multidisciplinary condition. His works as an art historian,

despite their age, are still the starting point of every study on the subject. His wide collection of designs allows us to understand the evolution of the baroque altarpiece by filling some gaps of our history. And as a restorer, Martinell shows an approach to the world of the altarpiece from a less common - and overlooked - perspective, where we can sometimes find his most creative proposals.

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EVALUATING THE CONSERVATION EDUCATION PROGRAMME OF THE FUNDACIÓ MONA: IMPACT ON KNOWLEDGE AND ATTITUDES TOWARDS PRIMATE WELFARE AND CONSERVATION

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Keywords: attitudes, environmental education, Fundació MONA, knowledge, primates

1. Introduction

Education and raising awareness should be one of the primary roles of the institutions that work in biodiversity conservation. The Fundació MONA (MONA) is a primate sanctuary that provides housing for chimpanzees (*Pan troglodytes)* and Barbary macaques (*Macaca sylvanus*), who were victims of illegal wildlife trade. The main objective of the Fundació MONA is to give these primates a place where they can live and be rehabilitated in the best possible natural and social conditions.

2. Hypothesis

MONA (Fundació MONA, 2022) has a conservation education programme, whose main goal is to provide participants with knowledge and promote attitudes and behaviour in favour of the conservation of primates. This study aims to evaluate the effectiveness of this programme using the knowledge and attitudes that participants have before and after been exposed to the programme (Feliu et al., 2023).

3. Methodology

For the data collection we developed two different questionnaires, which were answered by 1221 participants between January 2019 and December of 2020. One focused on knowledge of primate species and the other on the attitudes towards primate welfare and conservation. A control group and an experimental group were established. The control group answered the questionnaire before participating in the educational programme, and the experimental group answered afterwards. We apply a between-subjects design, so each participant belonged to only to one group. The groups were selected randomly. With this, we wanted to avoid participants being affected by exposure to the same questions twice (Clayton, 2017; Bowie et al., 2020).

For the analysis, first we computed a questionnaire score, based on the proportion of pro-conservation responses. Next we analysed the effects of the predictors on the questionnaire score using a linear model (Baayen, 2008) run with Imer function in R. Finally, we ran a comparison using the function emmeans and adjusted by the Bonferroni method, to see the differences inside each predictor that had significance influence on the questionnaire score.

4. Conclusions

Results showed that in both cases the experimental group had significantly better results on the questionnaires than the control group. This confirms that the educational activities carried out at MONA had a positive impact on the knowledge and attitudes towards primate conservation and welfare of the people that took part in the activities. With this, we can assure that MONA is accomplishing the goal of its conservation programme.

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SESSION 16.
ART AND SOCIETY

THE CREATION OF AN INEQUAL FUTURE: SOCIOECONOMIC CONDITIONS, HUMAN DEVELOPEMENT AND PREDISPOSITION TO CREATE

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Keywords: creativity, human alienation, human liberation, human practices, socioeconomic inequality

1. Introduction

This thesis aims to shed light on the black box that lies between the socioeconomic conditions of people and the eventual exercise of creativity. I define predisposition to create *as: all the human practices during the life trajectory of a person that, free from alienation, lead this person to create (to make and/or think new things) with social impact (the creation reaches beyond the neighborhood).* I first review relevant theory on what creativity is about and its main general dimensions. I also review human development theory in relation to creativity and Marxist perspectives on human development in relation to creativity. From these three main theories, I derive my definition and the human practices that seems to matter most for the development of creativity.

2. Hypothesis

Socioeconomic conditions have an influence on the human practices that make up the predisposition to create. Better socioeconomic conditions lead to better physical and mental condition, more political participation, higher educational levels, more cultural and artistic participation, more and better free time, more critical thinking, and therefore more freedom, and from that, a greater chance of ending up creating new things or ideas with social impact.

3. Methodology

I use explanatory sequential mixed methodology. First, I do statistical analysis (correlations and regressions) and, second, I analyze the content of 25 semi-structured interviews. Statistical analysis will help to test in general terms the relationships between socioeconomic condition and predisposition to create related indicators, with data from all the districts of Barcelona. The qualitative analysis will help to better understand the complexity of the predisposition-to-create phenomenon.

4. Results and discussion

Statistics: it seems that socioeconomic related indicators are positively correlated with satisfaction with life, high political participation, high education level, high cultural activity, satisfaction with leisure time, and high critical thinking. However, I observe differences in the intensity of the correlations. It is worth mentioning the positive correlations between, for example, socioeconomic condition and variables such as people that work in the creative sector. Interviews: I have only been able to conduct make some of them. But it seems that the creative people interviewed, have a middle-high socioeconomic level. Some of them add new (or refute some) dimensions on what matters to end up creating.

5. Conclusions

Provisionally, I can confirm that socioeconomic conditions are related to the main indicators of predisposition to create. People of middle to higher classes seem to be less alienated in all aspects of life. They express more critical thinking, more cultural activity, more inclination to entrepreneurship, etc. What is still unclear is if some of the proposed indicators of predisposition to create can be changed for others. Furthermore, if "the future is unequally created," this can have consequences for democracy.

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CONSTRUCTING A COLLECTIVE MEMORY THROUGH TERESA PÀMIES' EXILE LITERATURE

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Keywords: exile, collective memory, history, literature, Teresa Pàmies

1. Introduction

One of the most fascinating debates taking place at humanities faculties around the world is the link between arts and humanities. Numerous theorists have assumed the challenge of defining the different disciplines, providing solid arguments in support of an interdisciplinary approach. In effect, Teresa' Pàmies work, as memorialistic literature written in the first person whereby Pàmies is at once author, narrative voice and main character, can be situated in the middle of this debate. On one hand, Pàmies' work is literature because it is a literary work; on the other hand, it belongs to history because it narrates a lived experience about historical facts. Therefore, acknowledging the interdisciplinary character of Teresa' Pàmies work, the doctoral thesis will not only have an interdisciplinary approach, but it will also establish a link between literature and history. In other words, through the analysis of Pàmies' literary work, literature and history will come closer together.

2. Expected results

My aim is to test that Pàmies' exile literature contributes to the construction of a collective memory that builds on our understanding of the history of Catalonia in the 20th century. In other words, the link between historical witnesses, literature and the processes of building a collective memory can test that there is a link between witness and the construction of collective memories of traumatic processes. More precisely, in the case of the Spanish Civil War and exile, in the context of a considerable gap in studies on women, the figure of Teresa Pàmies is fundamental to understanding the complex construction of a communist and militant memory.

3. Conclusions

Despite the fact that Pàmies is a recognized figure in the institutional field, as evidenced by the recognition she received in 1985 with when awarded the Sant Jordi Cross from the Government of Catalonia or when awarded the *Honor de les Lletres Catalanes* from Omnium in 2001, she is not recognized in either the publishing world or in the political and social world. It seems

that Pàmies was part of a group of great Catalan writers who belong to the intellectual and political debate of the transition to democracy, but, unfortunately, time has forgotten them. Thus, my doctoral thesis highlights Pàmies as a literary figure and, at the same time, gives her a reference status that helps to understand the clandestine struggle from exile.

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THE FILMIC-FLUID BODY: MENSTRUAL ESTHETICS IN BARBARA HAMMER'S FILMS (1968-2015)

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Keywords: Barbara Hammer, menstruation, biopolitics, Film Studies, Critical Menstruation Studies

1. Introduction

Barbara Hammer was an American filmmaker of experimental and documental cinema. She was a pioneer in representing lesbian pleasure and desire on screen and was a key figure in the New Queer Cinema movement and the feminist cinema of the 1970s. Besides this, her filmography revindicates her as a pioneer of menstrual body representation in cinema history.

2. Hypothesis

Barbara Hammer is a pioneer in creating a menstrual esthetic in the cinema. Her film *Menses* (1974) establishes a new way of representing menstruation on screen, from the subjectivity and pleasure of the menstrual body. This film establishes a menstrual esthetic that is transferred and recognized in the rest of Hammer's cinematographic work.

3. Methodology

This research follows a methodology that combines film studies and critical menstruation studies from an analysis of the visual esthetics of film representations that show menstruation, primarily following the theories of Bee Hughes (2020) on the concept of "menstrual performing" in visual art applied to moving images of cinema. The study sample comprises all of Barbara Hammer's filmography (more than 80 movies): from her first film in 1968 to her last in 2015.

4. Results

The menstrual esthetic in Hammer's films is recognized, on the one hand, from its representation within the frame (image-body), with the explicit evidence of sexual and menstrual fluids within the image. On the other hand, it is recognized from the boundaries of the frame, with dripping, stains, and splashes on the celluloid or video. Hammer herself theorizes this under the "screen-body" concept: the camera is the body itself. Thus, Hammer

films are evidence of a fluid body through corporeal materiality over the images, making the separation between the filmed body (image) and the film body (screen) indivisible.

5. Conclusions

This menstrual esthetic visualizes corporalities traditionally reduced to oppression and invisibility on screen. Therefore, this esthetic questions the hegemonic and patriarchal audiovisual language based on an optical vision to present a sensory, material, and haptic cinema, directly associated with a queer gaze on the images, which refers to the rest of the senses and the bodily physicality of the spectators. Thus, Hammer's films manifest a fluid body politics, a sample of physical, carnal, sexual, menstrual, and material identity. Her films present a collective identity showing multiple fluids and menstrual bodily experiences in motion.

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WOMEN'S PERFORMANCES ON THE MUSIC'S CIRCUIT IN CATALONIA (1900-1950)

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Keywords: Catalonia, Performance, 20th century, Women musicians

1. Introduction

This presentation focuses on the study of women who, in small groups or alone, performed in theatres, halls, cinemas, and cafés between 1900 and 1950 in the Catalan counties of Girona, Lleida, and Tarragona. The social and political changes between 1900 and 1950 have their origin in the fall of the *Ancien Régime* and the Industrial Revolution in the 19th century. The new political and economic system, liberalism, facilitated the strengthening of the bourgeoisie and the birth of a new social class, the proletariat. These changes were essential to the organization of recreational societies and the business network that generated a stage circuit in which women had a significant presence in the Catalan territory.

3. Methodology

The methodology used for this study is a compilation and analysis of articles from five specialized magazines. Each of the magazines specializes in a specific music circuit. The analysis of the documentation leads to a deeper understanding of the different areas of professionalization of women in the world of music. Documentary sources: Arte y cinematografía (1923-1935), edited in Barcelona; Eco Artístico (1909-1923), edited in Madrid; Revista de varietés (1914), edited in Madrid; Ritmo (1929-1950), edited in Madrid; Scherzando (1906-1935), edited in Girona.

3. Results and discussion

Analysis of the documentary sources reveals a considerable presence of women, especially those who toured the counties alone, both vocalists and concert performers (Fig. 1).

Among the 600 women documented, 496 are vocalists touring alone. In Scherzando magazine, the presence of women pianists is noteworthy; they outnumber women vocalists. (Fig. 2).

From the quantitative analysis of performances in the counties of Catalonia, the most significant results (Fig. 3) are the differences we found between the number of performances per province and the number of localities programming performances.

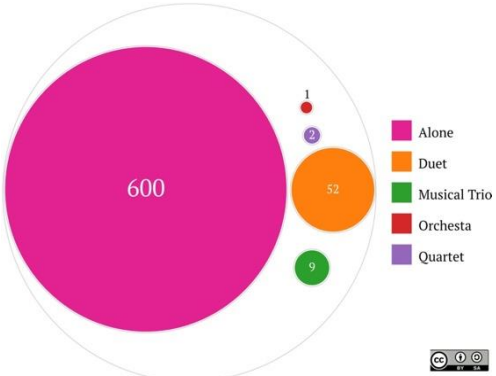

Figure 1. Women's musical groups. Own elaboration

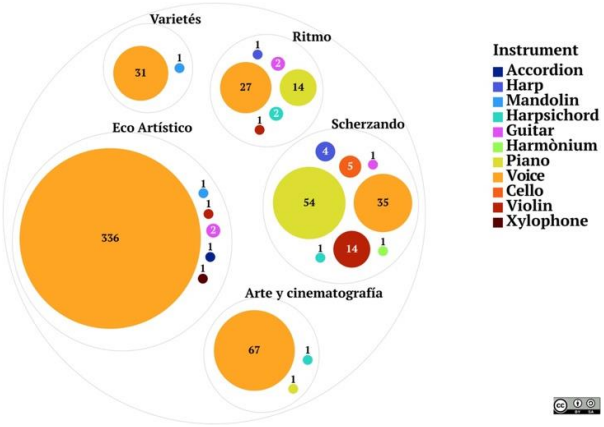

Figure 2. Performances in Catalan counties by magazines and instruments. Own elaboration

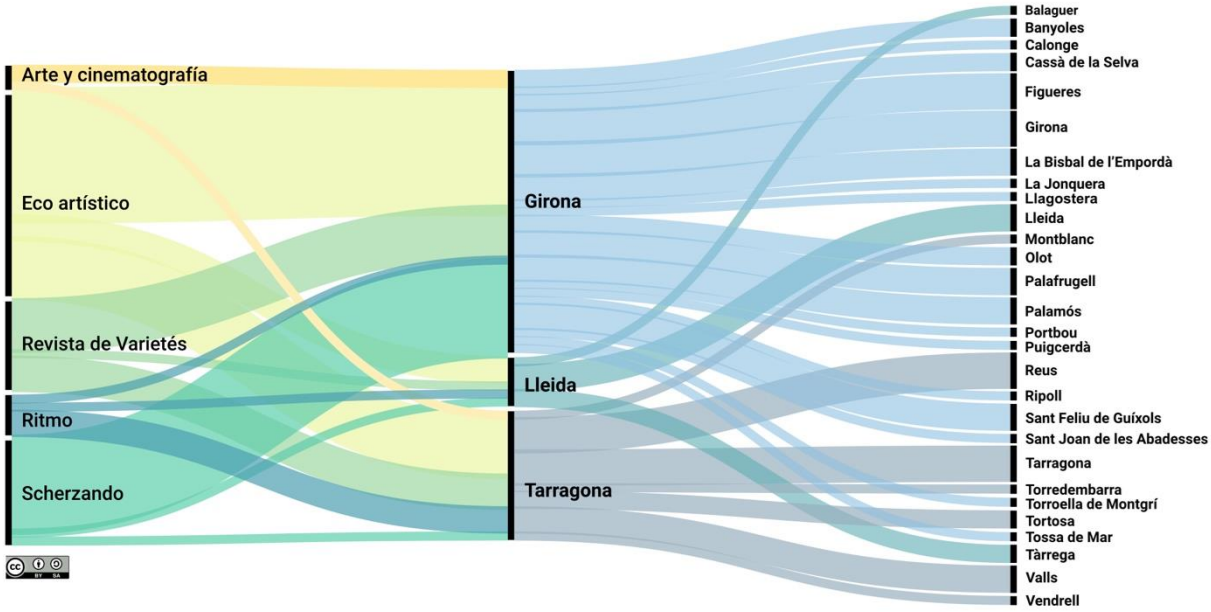

Figure 3. Performances in Catalan counties by magazines and towns. Own elaboration

4. Conclusions

The city with the most performances is Lleida, but as a region it is the one with the fewest cities with actions documented. The city of Girona has fewer performances, but the number of municipalities hosting performances is much higher, reaching seventeen. This fact leads us to conclude that a more detailed study is needed to investigate the reasons for the multiplication of performance spaces in the towns of the Girona.

FEMINISMS AND IBERIAN DIFFERENCE: SOME NOTES FOR A TOOLBOX OF OUR OWN

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Keywords: contemporary art, feminist art, Iberian feminism, cultural studies

1. Introduction

In 2014, Itziar Ziga published *Malditas: una estirpe transfeminista*; the first words of the essay are a declaration of intentions: "I am not Betty Friedan's daughter" (9). With these words, the Basque author joins the denunciation, initiated in 1981 by bell hooks, about what they both consider to be a kidnaping of feminism by a few white, heterosexual, high-social class activists and theorists, located in a very specific geographic context and production of thought, the Global North. Although the critique of the two authors is framed in what is known as the crisis of the political subject of feminism and its political agenda, the formula they use allows us to introduce the foundational premise of our proposal: the need to construct a history and theory of feminism and feminist art from a *glocal* perspective; that is to say, to begin by analyzing the specificities of each context, and from there to think about how this local specificity interrelates with the globalized scene. Or, to express it in another way, thinking in a very concrete way about our local context, which allows us to think about the Iberian difference.

2. Results and discussion

By linking the Foucaultian image of a toolbox, to express the utility of critical thinking, and that of Virginia Woolf's in *A Room of One's Own* (1929 [1977]), we will present some concepts to work towards a history, theory, and methodology of what Maria Aurèlia Capmany named *Iberian feminisms* (1970). From there, we will analyze the specificities and similarities of the process of consciousness-raising among Iberian women during the late-dictatorship era, as well as the production, reception, and circulation of the main feminist texts and ideas of the time.

3.Conclusion

We will end up demonstrating, along with Aurora Morcillo (2012) that, until today, "The Anglo-Saxon paradigm has corseted our analysis" (53), and that a truly social and human science

pronounced from feminism requires, always, starting by "reevaluating what the term feminism means" (Íbidem).

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GAY VISUAL CULTURE IN POST-FRANCO CATALONIA (1975-1984)

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Keywords: homosexuality, post-Franco, repression, underground, visual culture

1. Introduction

The representations of homosexuals in the decade immediately following the death of the dictator Franco show a type of masculinity that is almost a carbon copy of hegemonic heterosexual masculinity. Comic books, movies, and certain entertainment magazines show this type of masculinity in a very clear way. This study will show, put in context, and link these samples of masculinity, relating them to the models that followed immediately afterwards.

2. Hypothesis

The fear of appearing too effeminate determined the behavior of many gays during the post-Franco period. This behavior is the result of a sexist and homophobic heritage, the trajectory of which can be traced throughout the dictatorship. Homosexual representations in cinema and general visual media (magazines, television, ephemera) were forbidden and limited to marginal circuits. The end of the dictatorship and, consequently, censorship, brought a more permissive attitude for this type of representations. Nevertheless, homosexuals still felt not comfortable to come out of the closet and speak out about their homosexuality, because Catalan and Spanish society still carried a deeply homophobic legacy.

3. Methodology

Different methodologies will be followed. First, a search of images and articles from different magazines and comics (Party, Ploma, El Rrollo) will be made in the archive of the Armand de Fluvià Documentation Centre. The critical analysis of the discourse will help us to explain the creation of the bibliography and this information, so that we can analyze the power relations and ideologies behind these images and understand how they contribute to the social construction of identities and relationships. Interviews are planned with people involved in the cultural environment of Catalonia at the time, such as Luis Escribano, from the cinematographic collective Els 5QKs.

Finally, we expect that, during the research, other visual materials will appear, whether artistic or not, which are particularly interesting to analyze the premises mentioned above.

4. Conclusions

Party magazine was a clear example of how to visually represent a masculinity that did not clash with the status quo, but at the same time was sufficiently suggestive for the homosexual public. There were some other manifestations, so critical of masculinity, that have not been completely studied, as is the case of the cinematographic collective Els 5QKs. Their productions can be cataloged as underground cinema and, like other magazines such as Ploma, they also highlight the masculinities of the Franco regime to subvert them in a variety of ways.

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