

 Universitat de Girona
Escola de Doctorat

VI Conference of Pre-doctoral Researchers Abstract Book

Gerardo Boto & Laia Vicens (Editors)

Volume VI, 2022



University of Girona

**VI Conference
of Pre-Doctoral Researchers
Abstract Book**

Gerardo Boto & Laia Vicens (*Editors*)

Volume VI, 2022

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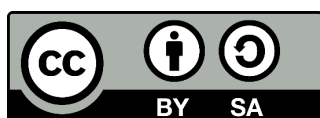
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Edita:

Escola de Doctorat. Servei de Publicacions de la UdG.

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Primera edició: novembre 2022

ISBN: 978-84-8458-634-0

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PREFACE

The document before the reader's eyes is an electronic book containing the abstracts of the contributions presented at the VI Conference of Predoctoral Researchers of the University of Girona (UdG), held between 30 May and 2 June 2022 under the auspices of the School of Doctoral Studies of the UdG with the collaboration of the Vice-Rectorate for Research and Knowledge Transfer. These conferences were held in classroom format and took place at the Faculty of Business and Economic Sciences (Montilivi Campus) of the University of Girona. Essentially, they are a continuation of the I Conference of Predoctoral Researchers, held between 6 and 9 June 2017.

Throughout these years, the predoctoral researchers themselves and a selected group of volunteers have led and made a consolidated effort to organize this event. This sustained academic initiative has brought intellectual benefits not only for the researchers who have orally presented the progress of their doctoral research, but also for the entire predoctoral community of the UdG. In fact, the aim of the conferences is to provide a space for training, the exchange of knowledge, the dissemination of research and debate among all the researchers in training who are working on their doctoral or master's thesis at our University.

During the VI Conference, in addition to informative sessions and workshops on job placement, doctoral and master's degree students presented their thesis individually and within the framework of the corresponding doctoral or master's programme. As a result, each presenter had the opportunity to discuss the results of their research with colleagues and with senior researchers. It has been shown that oral communication contributes, in a generic way, to develop skills of justified and persuasive defence of the contents of a research proposal, and in a specific way, to disseminate to society the results of this research. The latter is a basic requirement of Open Science, the paradigm of knowledge communication required by the European societies of today.

The VI Conference of Predoctoral Researchers was organised by eight volunteer doctoral students from different doctoral programmes. This team did an impeccable job: scheduling the sessions, convening fifteen predoctoral researchers from other Catalan universities, managing the details of each intervention and being responsible for moderating the debates of each of the fifteen sessions.

As a result, the abstracts of eighty-seven papers have been received, reviewed and edited. Thirteen of them correspond to predoctoral researchers from Barcelona universities, who have added their contributions to those of the UdG doctoral students. This e-book has been edited by the undersigned and the pre-doctoral researcher in Chemistry, Laia Vicens. I would like to express my gratitude for her extraordinary work.

All of us who have contributed to the completion of this e-book are convinced that the academic community of the University of Girona can feel justifiably proud of it. This mapping of knowledge in construction and progress confirms the relevance of predoctoral research at the UdG on the national and international university landscape in the year 2022. It is therefore a stimulating prognosis for the organisation and development of the VII Conference of Predoctoral Researchers scheduled for 2023.

Girona, 11 November 2022

Gerardo Boto

SESSION I. ART, HERITAGE AND CULTURE

GENESIS OF 'CARTES D'ITÀLIA' (1955) BY JOSEP PLA: A HISTORY OF A FASCINATION

David Portillo de Barrio

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Keywords: Josep Pla, Italy, travel literature, *Cartes d'Itàlia*, literary reworking

1. Introduction

One of the most characteristic aspects of Josep Pla is the admiration he always felt for Italy. The first contact the writer had with Italian culture was in Barcelona (Gavagnin, 2011). Not until 1922 was he able to travel to Italy for the first time. According to Garolera (1998), the best example of this connection can be found in *Cartes d'Itàlia* (Pla, 1955), a collection of travel chronicles he wrote, mostly during that first stay in Italy. The reappearance of Pla's chronicles was the result of a process of reworking (Quintana Trias, 2020). Thus, the study of this genesis, initiated by Arqués (2002), is interesting as a way to understand the literary evolution of Josep Pla and his vision of Italy.

2. Hypothesis

The hypothesis proposed in this work lies in showing that *Cartes d'Itàlia* by Josep Pla is not a book that came out of nowhere in the mid-1950s. Rather, it is the result of selecting and rewriting that took the author more than thirty years.

3. Methodology

Research in newspaper archives indicates that the original articles were published in *La Veu de Catalunya* and *La Publicitat*. Subsequently, Pla retrieved them throughout his literary and journalistic until their inclusion in *Cartes d'Itàlia*. A comparison of the variations proposed by Arqués (2002) will demonstrate most important changes the author made to the texts.

4. Results

The methodology used has made it possible to discern two groups of travel chronicles: those newly created and those that have gone through a process of reworking. The study shows that only eight are newly created and that they are influenced by the travel guides of the time. The rest are the result of subjecting the original articles to different processes of transformation, including addition, deletion and synonym variation.

5. Conclusion

These results make it clear that *Cartes d'Itàlia* by Josep Pla is a statement of intent arising from the writer's admiration for Italy. In addition, tracing the origins of the chronicles that make up the book and studying of the processes of literary reworking used by the author delve deeper into the study of Josep Pla's methods of literary creation.

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THE JOURNALISM OF PRUDENCI BERTRANA

Judit Pujol Prat

University of Girona

Keywords: Prudenci Bertrana, journalism, Girona, Barcelona, intellectual

1. Introduction

Prudenci Bertrana Comte (1867-1941) was a painter, a writer, and a journalist. This paper summarizes the doctoral dissertation whose thesis aims to undertake an extensive historical, literary, and documentary study of the journalistic production of Prudenci Bertrana. Although studies on Bertrana as a painter or as a writer are not numerous, they are even scarcer when it comes to examining his role as a journalist (Granell, 2003; Roig, 1955; Tasis, 1966; Triadú, 1967). Several academic articles have pointed out that Bertrana was a journalist by necessity — to support his family (Castellanos, 1991, 1992; Lanao, 1989). Also mentioned are his theatrical reviews and the sections he published in various relevant newspapers, such as *La Publicidad* or *La Veu de Catalunya*, as well as many of the publications he directed or collaborated on (Rufí i Pagès, 2017). However, there are no exhaustive studies on Bertrana's journalism. As a result, there is a bibliographic gap and the purpose of this thesis is to fill it. Bertrana's journalistic production has been separated into two stages in this thesis: his beginnings as a journalist in Girona, and his most prolific period in Barcelona (Fabre, 1985; Jerez Columbié, 2019; Portell, 1989). The thesis attempts to highlight some significant moments, such as the chronicles published during the First World War, to focus on the literary style and underlying themes that often emerge in his narrative work, and to give his writings the attention and consideration they deserve.

2. Results

Tracing Bertrana's journalistic career has led to a proposed hypothesis: Prudenci Bertrana was not the rural, uncivil, and anti-intellectual artist he wanted us to believe. Behind the image of a barbarian, which he intentionally projected, was an intellectual who cared about society and the events of his time, and this was reflected in the pages of the newspapers and magazines with which he collaborated. What is more intellectual than an intellectual who claims to be anti-intellectual?

3. Conclusion

Even though journalism was not a vocation for Bertrana, it was obviously very fertile ground that has left us thousands of journalistic texts in which the writer, the journalist, and the painter are merged. In addition, many of his values, ideals, and attitudes towards life are found throughout his articles.

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ADOLF FARGNOLI: CABINETMAKER, CERAMIST AND POET (1890-1952)

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Keywords: Adolf Fargnoli, Noucentism, cabinetmaking, pottery, Girona

1. Introduction

Fargnoli is the name of a well-known Italian family in Girona. Even though Valentí Fargnoli – the eldest of five brothers – is more widely recognised for his work in the field of photography, Adolf Fargnoli, known as the “Fargnoli of the Chests”, is the focus of this project. Although Adolf devoted himself to handcrafts such as carpentry and ceramics, he always presented himself as an artist, using the technique of pyrography to mark his pieces with poems that gave them unique and particular names. Close to Masó’s circle (Catllar, 2006; Panyella, 2014; Tarrús & Comadira, 1996), Fargnoli was part of the group of artists from Girona linked to *Noucentisme* (Aragó, Falgàs, Faxedas, Pujol, & Rabaseda, 2013; Fontbona & Miralles, 1985; Oliveras, Bover, Sais, Comadira, & Marcó, 1993; Peran *et al.*, 1994). He exhibited pieces in cities such as Barcelona, Madrid, Paris, and Buenos Aires (Montmany, Navarro, Tort, & Fontbona, 1999). Despite having achieved a name in the artistic sphere, time has made Adolf Fargnoli an almost forgotten artist (Vila, 2014).

2. Hypothesis

The starting point of this research project is the monograph dedicated to the Fargnoli brothers (Valentí and Adolf) by Suquet & Vélez i Vicente (1997). This monograph presents a review of the lives and the art of the two brothers. In Adolf’s case, this survey is completed with a catalogue that includes 39 signed pieces and a chronological list of exhibitions in which he participated. While Pilar Vélez’s study provides a very solid foundation from which to start, I would like to delve deeper into Fargnoli’s life and work. My main purpose is to study Fargnoli’s footprint at Can Marcó – the Quart pottery factory – using any documentation found there, and to catalogue and attribute pieces to the artist. This perspective could become the strength of my research project because historiography has not delved too deeply into Fargnoli’s ceramic production, focusing solely on his wooden chests.

3. Methodology

I intend to locate and analyse primary sources related to Adolf Fargnoli (work, correspondence, exhibitions, photographs, etc.) and secondary sources (articles, books, etc.). I will visit the factory of Can Marcó, where Fargnoli learned the art of pottery in his early years (Bover, Casademont, & Negre, 1990), and I will visit the Masó Foundation to understand the circle of artists related to Rafael Masó. I will browse websites such as ARCA, Regira, SGDAP or the Hemeroteca Digital de la BNE. I will also review the preserved material related to Fargnoli in

the Historical Archive of Girona as well as the Vicens Vives and Carles Rahola collections. Finally, I will delve into the bibliography from which I start.

4. Results

An initial review of the bibliographic sources and an interview with the director of the Masó Foundation demonstrated that historiography has not continued to explore the figure of Adolf Fargnoli. However, the visit to the factory of Can Marcó revealed a large number of moulds and pottery objects, leading to the conclusion that Fargnoli's hands produced pieces that remain uncatalogued to this day. My goal, or my priority, is the attribution of these pieces in order to discover a part of Fargnoli's trajectory that has not been studied.

5. Conclusion

I hope this perspective will enrich not only studies of Fargnoli's work, but also place greater focus on the important yet understudied discipline of pottery.

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THE SPANISH SEX WARS? A THEORETICAL AND VISUAL APPROACH TO REPRESENTATIONS OF SEXUALITY IN LATE-FRANCOISM SPANISH ART

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Keywords: feminism, visual studies, art, sexuality, Spanish art

1. Introduction

One of the main topics of the historiography of feminism and feminist art is whether it is desirable, even possible, to (re)present female sexuality from a feminist point of view. In post-May 1968 Spain, this question channelled the anxieties and concerns of a group of feminists, who understood women's vindication of sexuality in terms of collaboration with the patriarchal system. In the North American case, the debate was framed in terms that were soon known as the *sex wars*.

2. Methodology

We will base our analysis on a critical study of the paradigmatic positions in the debate (Dworkin, 1998; Llamas & Vila, 1997; Vance, 1989; Weeks, 2017) as well as on the interpretation of it by the Spanish sociologist Raquel Osborne (1993).

3. Results and discussion

Taking this dilemma as a starting point, we will analyse the discourses and artistic practices around sexuality produced in the Spanish state between the sixties and the late eighties. We will focus our arguments on two main theses. The first is that sexuality has always been a central topic in Spanish feminism and proto-feminism, even before the dictator's death and the introduction of the sexual wars debate at the beginning of the 1980s. Although here the importance and virulence of the debates were also noticeable, the second thesis concerns the substantial differences between the ways the debate developed in our context as compared to the North American experience. The most obvious of these is the generalized predominance of the pro-sex position, which is due to various factors. They are the central role of lesbian activists in leading the debate, the discrediting of the anti-sex position – then highly questioned due to the alliance with conservative forces – and the strong commitment against censorship that characterized the anti-Franco movement (Llamas & Vila, 1997; Uría Ríos, 2009).

4. Conclusion

Throughout our proposal, we will defend the argument that artistic and feminist representations of sexuality play a central role in social transformation. To prove this, we will develop the concept of *gender technologies*, which conceives gender as a conjunct of discourses and representations (De Lauretis, 1987). Furthermore, we will try to show that this role is even more important in a context like ours, where the women were subjugated by both the

patriarchal and the dictatorial systems. Finally, we will claim the importance of thinking of feminisms in the plural, to be able to attend to the specificities of otherness-feminist experiences like ours, which are not Anglo-Saxon.

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TOURISM AS A PROMOTER OF SAFEGUARDING CULTURAL HERITAGE IN UNESCO'S CREATIVE CITIES OF GASTRONOMY

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Keywords: cultural tourism, gastronomy, intangible heritage, creative cities network, UNESCO

1. Introduction

The Creative Cities Network (UCCN) of the United Nations Educational, Scientific and Cultural Organization (UNESCO) was created in 2004 to promote the culture of creativity in seven areas of creative industry (crafts and popular art, design, cinema, gastronomy, literature, media and music). This research focuses on 48 cities in the field of gastronomy. These 48 cities, from 32 countries, make up a very varied gastronomic landscape. They include Burgos and Dénia (Spain), Jeonju (South Korea), Zahle (Lebanon), and Florianopolis (Brazil), just to mention a few (Ferreira, 2017).

According to López-Guzmán & Sánchez Cañizares (2012), gastronomic tourism is one of the great endeavours to promote or consolidate tourist destinations. These authors point out that accessing knowledge related to the gastronomic culture of a certain place is an increasingly strong motivation for travellers. Gastronomic tourism, considered a segment of cultural tourism, is understood by the European Association for Tourism and Education for Leisure (ATLAS) as "the movement of persons to cultural attractions away from their normal place of residence, with the intention to gather new information and experiences to satisfy their cultural needs" (Richards, 1996).

Martos Molina (2016) emphasizes that gastronomy is an intangible heritage of great relevance to humanity, along with other cultural manifestations, such as language, crafts and popular art, rites, customs and traditions. For UNESCO, intangible heritage instils in humanity a feeling of identity and continuity, a concept that encompasses "the uses, representations, expressions, knowledge and techniques, together with the instruments, objects, artifacts and cultural spaces that communities, groups or individuals recognize as part of their cultural heritage" (UNESCO, 2003).

6. Methodology

The research is being developed using a qualitative and exploratory methodology (Flick, 2004), in addition to bibliographic analysis and other relevant documents to support the study and interpretation of data. The bibliographic review will allow us to focus on the current state of the subject in the academic field, the adoption of inherent concepts, the conceptual interrelation and connection points, and the theoretical support for the definition of the creative cities (Florida, 2004; Landry, 2008) that will be part of the study. Along this

methodological line, semi-structured interviews (DiCicco-Bloom & Crabtree, 2006) will also contribute to the study the perspective of the local actors involved in the management of gastronomic tourism in the sphere of the UCCN.

7. Results

We expect this research to highlight the role played by tourism and its contributions to the safeguarding of gastronomic heritage, for example, initiatives that make the visitor aware of the intangible heritage expressed through local gastronomy. Finally, we intend to publicize the initiatives implemented to expand their effects on the preservation of gastronomic cultural heritage in other tourist destinations, not only in those cities that already make up the UCCN, but in others that can benefit from the experience and knowledge already developed.

8. Conclusion

In this context, identifying what role tourism has played and what it can contribute to enhance the gastronomic cultural heritage of UCCN cities should contribute to safeguarding said heritage, even in other tourist destinations.

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DIGITAL IMAGE ESTHETICS: EARLY CINEMA'S VIRTUAL WORLDS' PERSISTENCE IN THE FILMS OF DAVID LYNCH

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Keywords: early cinema, virtual, esthetics, digital, visual culture

1. Introduction

Digital technology development has transformed our relationship with pictures. In recent years, we have witnessed the intensification of a process of virtualization that "affects not only information and communication, but also bodies, economic functioning, collective frameworks of sensitivity or the exercise of intelligence" (Lévy, 1999). This phenomenon has also reconfigured the cinematographic image, modifying its links with issues such as reality (Quintana, 2011) or time (Sánchez, 2013). However, in this process of dematerialization "while the film disappears, the cinema persists" (Rodowick, 2007).

2. Hypothesis

Cinema persists as the ultimate element of the moving image. The so-called "digital cinema" (Manovich, 2016) underlines the convergence between a new medium and a pre-existing language, where becoming virtual is accompanied by the updating of the image and its problems. Early cinema's virtual worlds appear as the imprint that stands firm against films' disappearance. The link with the forms of the past is essential to understand those of the present.

3. Methodology

To undertake this research, I propose a comparative analysis between American filmmaker David Lynch's films, whose work embodies the transition from analogical to digital, and films from early cinema. This theoretical approach arises from concepts such as "Primitive Mode of Representation" (Burch, 1995), "intensified continuity" (Bordwell, 2002) or "blinking" (Gunning, 2017), with the aim of verifying its permanence.

4. Results and discussion

The application of these parameters and the study of their correspondence offers, as a main result, the possibility of addressing the permanence of primitive features in the contemporary (Agamben, 2011) and its implications. In other words, it allows us to establish a dialogue with tradition, to inscribe digital representation within a broader visual historiography framework and to propose a critical reading of images.



Figure 1. A still from *La Sortie de l'Usine Lumière à Lyon* (Lumière, 1895) and a frame from *Twin Peaks, The Return* (Showtime, 2017)

5. Conclusion

From the tension between cinematographic forms' past and present, one can deduce not only a figurative actualization, which amplifies the problems related to representation, but also the emergence of a renewed visual regime and a new model of spectator. In conclusion, digital esthetics is presented as the symptom of a deeper change, comparable to the one that led to the birth of the cinematograph in the 19th century: that of the gaze.

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STUDY OF THE STABLE PROGRAMS OF PERFORMING ARTS IN GIRONA COUNTIES

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Keywords: performing arts, cultural program, theatre, stage equipment, performing arts companies

1. Introduction

Each theater ensemble, through subjective criteria, chooses its own programming, but why do they choose one play over another? There are studies on the expansion audiences (Bacquelaine Vidal de Llobatera, 2017; Baraut, 2017), the *Generalitat de Catalunya* publishes statistics annually answering general questions about the sector (Generalitat de Catalunya; BCF Consultors, 2020), and the performing arts companies publish results of their current state of affairs (Deutscher Bühnenverein, 2005). However, none reports objectively on the reasoning behind these programming decisions or on how they affect those involved.

2. Hypothesis

This research study analyzes the performing arts programs of the Girona region (Coca & Nogué, 2016). It is an objective report that reflects the shortcomings and needs of the sector. At the same time, it highlights the lack of studies on the subject to promote the implementation of new management models.

3. Methodology

This study is divided into four areas: performing arts companies, management direction at the main municipal facilities, distribution networks, and public financial support. Through the analysis of data and direct surveys within the sector, the objective is to make a diagnosis that does not currently exist in the Girona region and to develop a plan of action for improvement (Bonet & Schargorodsky, 2011, 2016; Carreño Morales, 2014; Colomer, 2017; Heras, 2013; Pérez Martín, 2006).

4. Results

Preliminary results indicate that the lack of studies and objective criteria in the performing arts programming causes job instability in the performing arts companies and artists in particular, in addition to not helping to create audience attendance habits.

5. Conclusions

The aim is to present good practices guide that will serve as a reference for the performing arts sector to make changes in their programming methods and thus promote the region's cultural health.

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THE PRODUCTION AND CONSUMPTION SYSTEM OF PIGMENTS AT LES COVES DEL FEM SITE (ULLDEMOLINS, PRIORAT-TARRAGONA)

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Keywords: pigments, Neolithic, operational chain, Les Coves del Fem, Priorat

1. Introduction

Recent archaeological interventions in the Neolithic site of Les Coves del Fem (Ulldemolins, Priorat-Tarragona), a rock shelter annex to the Montsant River presenting evidence of human occupation dating from the sixth millennium BC, have revealed a series of engraved boulders and other materials with traces of pigment (ochre) at the oldest level of the Cardial Neolithic (Palomo *et al.*, 2018). The technomorphological characteristics and state of conservation of the materials allow assimilation of the register with anthropic activity related to the process of production of prehistoric pigments (Bofill, Chondrou, Palomo, Procopiou, & Valamotti, 2017).

2. Hypothesis

The macrolithic materials engraved with traces of pigment (ochre), made up mostly of schist boulders, have a morphology, evidence of use and state of conservation that allow identification and classification of these materials as querns, handstone and mortars, thought to be tools, and archaeological ochres, considered transformable matter. The joint presence of these materials in stratigraphy allows us to identify an activity related to the production and manufacture of prehistoric pigments developed at the site. At the same time, the diversity of materials, technomorphological characteristics and traces of use evoke processes involved in the Operational Chain, namely: supply, processing, storage, and use.

3. Methodology

In the methodology for this project, different lines of research have been coordinated. After the macroscopic and microscopic observation of the archaeological record, the typological identification and classification is done, paying attention to the morphology of the piece, the presence of pigment, and the marks of use. Based on these criteria, a taxonomic corpus of analysis has been prepared for the identification, classification, and registration of the material. The analysis takes into consideration the typometric attributes, the technomorphological configuration, techno-functionality, the decoration, and the different shades of colouring matter and their classification according to a digital colorimetry system

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The methodology is completed with chemical analyses, whose main objective is to identify the mineralogical composition of the pigments. The techniques used are Raman spectroscopy, Scanning Electron Microscopy (SREM) and microanalysis and X-Ray Diffraction (XRD).

Based on the results obtained from these analyses, the experimental study proposed for this project will be developed.

4. Results and discussion

In quantitative terms, the record is composed of more than eighty materials related to the production of prehistoric pigments. The techno-functional classification of the lithic materials allows them to be denominated and distinguished as "tools", "decorative supports" (those pieces with evidence of decoration) or "contact pieces" (materials with traces of ochre not related to pigment processing). The technomorphological diversity and state of preservation of the record offers the possibility of observing issues such as functionality (and multifunctionality and/or reuse), gestures, and configuration of pieces.

5. Conclusions

We can observe an extensive archaeological record that evidences the existence of a prehistoric anthropic activity directly related to the manufacture of pigments. This place makes Les Coves del Fem as a site of relevance within the modest map of relevant sites to produce mineral pigments chronologically located in NE Spain.

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SESSION II. PEPTIDES, PROTEINS AND ENZYMES

PRUNUS PERSICA PLANT ENDOGENOUS PEPTIDES PpPEP1 AND PpPEP2 CAUSE PTI-LIKE TRANSCRIPTOME REPROGRAMMING IN PEACH AND ENHANCE RESISTANCE TO XANTHOMONAS ARBORICOLA PV. PRUNI

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Keywords: plant elicitor peptide (Pep), plant defense, Prunus, RNA sequencing, differential network analysis

1. Introduction

Rosaceae species are economically highly relevant crops (Christenhusz & Byng, 2016). However, their cultivation systems are constrained by pests, compromising crop production and causing significant economic losses. The bacterial canker of stone fruits caused by the bacterial pathogen *Xanthomonas arboricola* pv. *pruni* (Xap) is a common and severe disease of *Prunus* spp. spread worldwide with relevant economic impact (Stefani, 2010). Its management on peaches is based on prophylactic measures and preventive copper treatments (Morales, Moragrega, Montesinos, & Llorente, 2018), which may cause resistances and environmental pollution. Thus, there is a critical need to develop sustainable strategies to control Xap.

Plants respond to invading pathogens through signaling mechanisms, a component of which are plant elicitor peptides (Peps). Peps trigger and amplify the innate immunity of plants (Albert, 2013; Tang *et al.*, 2015). Their exogenous application activates defense mechanisms and reduces the symptoms of pathogen infection in various pathosystems (Huffaker *et al.*, 2013). We have previously identified the Rosaceae Peps and showed, in an *ex vivo* system, that their topical application efficiently enhances resistance to Xap (Ruiz, Nadal, Foix, *et al.*, 2018; Ruiz, Nadal, Montesinos, & Pla, 2018).

2. Methodology

We performed *in vivo* assays to demonstrate the effectiveness of *Prunus persica* peptides PpPep1 and PpPep2 in protecting peach plants from Xap. Additionally, we used deep sequencing to characterize the transcriptomic response of peach plants to preventive treatment with PpPep1 and PpPep2.

3. Results and discussion

PpPep1 and PpPep2 reduced the symptoms of a Xap massive infection up to 40%. The two peptides induced highly similar massive transcriptomic reprogramming in the plant. One hour, 1 day and 2 days after peptide application there were changes in expression in up to 8% of peach genes. We visualized the transcriptomic dynamics in a background knowledge network and detected the minor variations between plant responses to PpPep1 and PpPep2, which might explain their slightly different protective effects. By designing a *P. persica* Pep background-knowledge network, comparison of our data and previously published immune response datasets was possible.

4. Conclusions

Topical application of *P. persica* Peps mimics the PTI natural response and protects plants against massive Xap infection. This makes them good candidates for deployment of natural, targeted and environmental-friendly strategies to enhance resistance in *Prunus* species and prevent important biotic diseases.

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PEPTIDES WITH ANTIBACTERIAL OR LPS-TARGETING ACTIVITIES WITH POTENTIAL APPLICATION TO CONTROL PLANT DISEASES

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Keywords: plant pathogens, solid-phase synthesis, antibacterial peptides, LPS-interaction, toxicity

1. Introduction

Plant pathogens cause serious diseases in plants, resulting in severe damage in economically important crops (Agrios, 2005). Chemical compounds, such as copper derivatives and antibiotics, have been employed to control these diseases, but their use raises environmental and ethical concerns (Oliveras, 2020). In this context, peptides with antimicrobial activity or the ability to interfere with pathogen's virulence factors, such as lipopolysaccharides (LPS), are being studied as an alternative to conventional pesticides (Datta *et al.*, 2015).

Our research is mainly focused on developing peptides as agents to control the plant diseases caused by the Gram-negative bacteria *Xylella fastidiosa*, *Xanthomonas axonopodis* pv. vesicatoria, *Erwinia amylovora*, *Pseudomonas syringae* pv. *syringae* and *Pseudomonas syringae* pv. *actinidiae* (Moll *et al.*, 2021; Montesinos *et al.*, 2021; Oliveras, 2020). In particular, this work is centred on studying the application of peptides **BP214**, **Lf(28-34)**, **LBP-14**, **BPI(84-99)**, and **YW12D** to control these diseases antibacterially and/or through interaction with LPS (Kim, Jang, Kim, & Cho, 2016; Oddo *et al.*, 2016; Zhang *et al.*, 2019) (Kim *et al.*, 2016; Oddo *et al.*, 2015; Zhang *et al.*, 2019).

2. Methodology

Peptides were synthesized on solid phase following an Fmoc/*t*Bu strategy, purified, analysed by HPLC and characterized by mass spectrometry. The *in vitro* antibacterial activity was determined from the minimum inhibitory concentration or from a viability test with qPCR. Haemolysis was evaluated by analysing the haemoglobin release from erythrocytes and phytotoxicity was measured by infiltrating peptides in tobacco leaves.

3. Results

Peptides **BP214**, **Lf(28-34)**, **LBP-14**, **BPI(84-99)** and **YW12D** were successfully synthesized and obtained with HPLC purities >96% after purification, and were characterized by mass spectrometry. Their antibacterial activity is being evaluated against the above plant pathogenic bacteria. In addition, their interaction with LPS is being assayed. This assay

involves the extraction of LPS from *Escherichia coli* and, afterwards, the evaluation of the peptide/LPS interaction. Moreover, the toxicity of these peptides is being studied by determining their haemolysis and phytotoxicity.

4. Conclusions

The solid-phase synthesis of the above peptides was successful, and they were obtained in excellent purities after purification. Characterization by mass spectrometry confirmed their identity. It is expected that this study will provide peptides with antibacterial activity and/or with LPS interaction properties, and with low toxicity. These peptides would be good candidates to be further developed as agents to control plant diseases.

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THE ROLE OF A LIPID TRANSFER PROTEIN IN PHELLEM SUBERIZATION

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Keywords: suberin, Lipid Transfer Protein, phellem, periderm, secondary growth

1. Introduction

During plant secondary growth, the phellem becomes the protective tissue of stems and roots. The protective function of phellem is attributed, in part, to suberin, an insoluble lipid polyester deposited in the inner face of the primary cell walls as a secondary layer (Serra, Mähönen, Hetherington, & Ragni, 2022). The suberin fatty acyl precursors are synthesized in plastids and further modified in the endoplasmic reticulum. Once synthesized, the precursors need to pass through the plasma membrane to reach the apoplast, where they polymerize (Beisson, Li-Beisson, & Pollard, 2012).

Lipid Transport Proteins (LTPs) have been identified as suberin precursor transporters in the apoplast (Deeken *et al.*, 2016; Lee & Suh, 2018). However, reverse genetics on LTPs shows a mild effect on suberization, suggesting that other LTPs may also be functional in such tissues.

In previous phellem transcriptomic works, we identified a LTP candidate highly upregulated in phellem of *Quercus suber* (Boher *et al.*, 2018; Soler *et al.*, 2007) and *Solanum tuberosum* (Soler, Serra, Fluch, Molinas, & Figueras, 2011).

2. Methodology

The characterization of the LTP candidate in phellem suberization was carried out in *Arabidopsis thaliana* by reverse genetics. We first identified the *Arabidopsis thaliana* LTP ortholog by phylogenetic analysis. Arabidopsis transcriptomic datasets were used to confirm the LTP involvement in suberization. We finally selected two Arabidopsis LTP loss-of-function mutants (*ltp*) and studied the suberin distribution and composition using specific dyes and suberin depolymerization analyses, respectively.

3. Results and discussion

We identified a specific Arabidopsis LTP as the orthologous of potato and cork oak previously identified and we confirmed its high and specific expression in Arabidopsis phellem. LTP also showed expression in endodermis, a suberized tissue present in the younger part of the roots that still have not completely progressed to the secondary development.

Specific suberin staining of roots of *ltp* mutants did not show any significant difference in the phellem suberization, nor in the endodermis. A more detailed analysis of suberin monomeric composition of phellem tissue displayed a significant but mild change in the abundance of particular suberin monomers in *ltp* when compared to the wild type. The changes were in

agreement with previous characterizations of different LTPs involved in suberization (Deeken *et al.*, 2016).

4. Conclusion

Despite the strong upregulation of the LTP gene in suberized tissues, no major changes were observed in the phellem when the LTP was knocked out. This suggests that other members of the LTP family may have a redundant function in phellem suberization. Further research is needed to clarify the role of LTP proteins in the suberization process.

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RATIONAL DESIGN OF A P450-BASED ENZYMATIC PLATFORM FOR THE REGIOSELECTIVE HYDROXYLATION OF DECANOIC ACID

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Keywords: directed evolution, enzymatic catalysis, hydroxylation, P450, molecular dynamics

1. Introduction

Cytochrome P450s are a super-family of haem-dependent enzymes that exhibit high reactivity on the oxidation of organic compounds. Selective hydroxylation of aliphatic C-H bonds present in fatty acids is of high interest in biocatalysis due to the synthetic application of these challenging chemical reactions. Among P450 enzymes, CYP116B46 from *T. Thermophilus* (P450-TT) is interesting due to its thermostability, self-sufficiency and wide reactivity, also including hydroxylation (Tavanti, Porter, Sabatini, Turner, & Flitsch, 2018). The hydroxylation of decanoic acid (DA) by the P450-TT enzyme was recently investigated, indicating that the oxidation reaction mainly produces (S)-5-hydroxydecanoic acid with high regio- and stereoselectivity (Manning *et al.*, 2019). This compound is a precursor of (S)- δ -decalactone, which is of high interest due to its fragrance.

2. Hypothesis

To gain access to other potentially attractive products, it was envisioned that protein engineering could switch the selectivity of the oxidation reaction towards other C-H bonds on the DA aliphatic chain.

3. Methodology

To gain a deep understanding of the binding poses of decanoic acid in the P450-TT active site, docking calculations followed by molecular dynamics (MD) simulations were carried out to analyse how the substrate can explore catalytically relevant poses to perform catalysis.

Site-saturation mutagenesis experiments were performed in a 96-well plate with an *E. Coli* expression system to obtain new P450-TT variants with enhanced activities or new regioselectivities for DA hydroxylation.

4. Results and discussion

Consequently, a first round of experimental mutagenesis followed by computational modelling based on molecular dynamics (MD) simulations were carried out to characterize the catalytically relevant binding poses of DA in P450-TT. Based on the acquired understanding on the factors controlling the selectivity of the reaction, site-saturation mutagenesis on

computationally selected residues was performed in the laboratory to obtain new P450-TT variants that gave access to new regioselectivities and increased activities for the hydroxylation of DA. Further MD simulations on the evolved P450-TT variants reveal how these mutations modify DA binding poses in the active site and thus lead to new regioselectivities for the hydroxylation of this substrate.

5. Conclusions

This study shows how the combination of wet-lab experiments and in-silico modelling enables the rational design of an enzymatic platform based on P450-TT, which allows controlling and switching the regioselectivity of this reaction towards other C-H positions along the aliphatic chain.

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SIMULATION OF ENZYME REACTIONS IN GLYCOSIDE HYDROLASES

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Keywords: human milk oligosaccharides, lacto-N-biosidase, glycosidases, quantum mechanics / molecular mechanics, metadynamics

1. Introduction

Carbohydrates are the most abundant biomolecules on Earth. They are relevant for many biological functions, such as structural organization, energy storage or molecular recognition, and adopt a vast array of structures (Ardèvol & Rovira, 2015). Studying the enzymatic mechanisms of the so-called carbohydrate active enzymes (CAZymes) provides insight into the catalytic processes that carbohydrates undergo and is of interest for many applications from drug design to the cosmetic and food industries. To characterize the catalytic mechanism and the substrate conformational changes, we start from X-ray structures and use molecular dynamics, QM/MM MD, to describe the chemically active area of the enzyme, and metadynamics (Laio & Parrinello, 2002) to accelerate sampling and model the reaction.

Bifidobacterium bifidum lacto-*N*-biosidase (LnbB) is an enzyme that degrades human milk oligosaccharides in the gut of breast-fed infants and has secondary synthetic activity (Wada *et al.*, 2008). Starting from available crystal structures (Ito *et al.*, 2013), we computed its catalytic mechanism using QM(DFT)/MM methods coupled with metadynamics. The results agreed with the predicted two-step, substrate-assisted mechanism.

2. Methodology

For simulating the reaction mechanism of LnbB, we started from an available crystal structure solved in 2013 (Ito *et al.*, 2013), with PDB code 4JAW. After treating it with force field, classical MD to relax the structure, we selected the chemically active area (the atoms implicated in the predicted mechanism) and proceeded with the QM/MM treatment. Next, we chose degrees of freedom to bias the simulation using the metadynamics scheme.

3. Results

We unveiled the molecular mechanism of LnbB, which matched the predicted substrate-assisted mechanism using the previously identified Asp320 and Glu321 as catalytic residues, with both reaction steps (with free energy barriers) in agreement with kinetic assays (~15 kcal/mol the first and rate-limiting step). Notably, the simulations demonstrated that a histidine residue (His263) at the active site changes interactions along the reaction path, switching between both catalytic residues, acting as a pK_a modulator that favours catalysis. We

characterized the reaction intermediate as most likely in the oxazolinium ion rather than the neutral oxazoline, which showed a smaller population. We show the conformational itinerary of the substrate: ($^1S_3/^1,4B \rightarrow [^4E]^\ddagger \rightarrow ^4C_1/^4H_5$ and $^4C_1/^4H_5 \rightarrow [^4E/^4H_5]^\ddagger \rightarrow ^1,4B$) (Cuxart *et al.*, 2022).

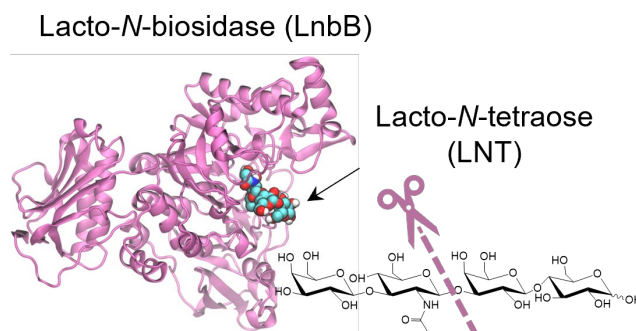


Figure 1. Lacto-*N*-biosidase degrades type I HMOs, the ones that contain a core of lacto-*N*-tetraose.

4. Conclusions

We used QM/MM MD coupled with metadynamics to uncover the reaction mechanism of LnbB and characterize the most relevant states. The substrate-assisted mechanism takes place with the modulation of a nearby histidine residue. The insights from this project open a door towards protein engineering of LnbB and exploitation of its synthetic activity to produce high added-value oligosaccharides.

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SESSION III. ELECTROCHEMISTRY AND COMPUTATIONAL CHEMISTRY

UNDERSTANDING THE ELECTRONIC STRUCTURE OF EXCITED-STATE AROMATIC SYSTEMS AND MACROCYCLES

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Keywords: aromaticity, computational chemistry, electronic delocalization, hydrocarbons

1. Introduction

Aromaticity is widely employed to predict and rationalize the electronic structure of molecules and reaction mechanisms. This concept is associated with cyclic molecular systems displaying the effects of cyclic electron delocalization, which results in enhanced thermodynamic stability, large magnetic anisotropies and abnormal chemical shifts, among other properties. A way to predict aromaticity is by using Hückel's $4n+2$ rule, and Baird's analogous $4n$ rule for low-lying singlet and triplet states. These rules state that annulenes with $4n+2$ ($4n$, for excited states) π -electrons are aromatic, whereas $4n$ ($4n+2$) π -electron systems are antiaromatic (Baird, 1972; Scheibe, 1938). The capacity to anticipate properties of the system can help design new molecules with complex structural and excited-state natures (Rosenberg, Dahlstrand, Kilså, & Ottosson, 2014).

2. Hypothesis

Applying different methodologies to well-known systems, as well as to new ones, as suggested in this work, will contribute to the field by determining whether the general rules known for groundstate aromaticity can also be applied to excited states and macrocyclic systems. The existence of (anti)aromaticity effects in the low-lying excited states will be supported by means of structural and reactivity studies of several systems.

3. Methodology

We mainly used (time-dependent) density functional theory methods for the modeling of our systems. Then, we computed aromaticity indicators like nucleus-independent chemical shift (NICS), fluctuation index (FLU), multicenter indices (I_{ring} , MCI, AV_{min}), among others, as well as atomic charges and spin densities. We performed all the calculations with Gaussian, AIMAll, ESI and EDDB programs.

4. Results

Here we present a further step towards understanding excited-state (anti)aromaticity and macrocyclic aromaticity. Our results are based on different projects with different aims. First, we explored the effect of structural changes and proposed ways to increase the Hückel or Baird

aromatic character of quinoidal compounds (Figure 1a). Second, we studied the aromatic circuits in porphyrinoids (Figure 1b), (Sub)phthalocyanine. Finally, we explored nanographene and another class of macromolecules formed by porphyrin and linker units known as nanorings (Figure 1c) (Escayola, Callís, Poater, & Solà, 2019; Escayola *et al.*, 2021). In the first studies, we found that the formation of a diradical located at the exocyclic substituents favors Hückel aromaticity even in the excited states and it is rather difficult to form Baird aromatic species, resulting from charge-transfer excited states. In the second and third studies, we observed that the macromolecules present many circuits with delocalized electrons and, in some cases, the values obtained are too low to be considered aromatic.

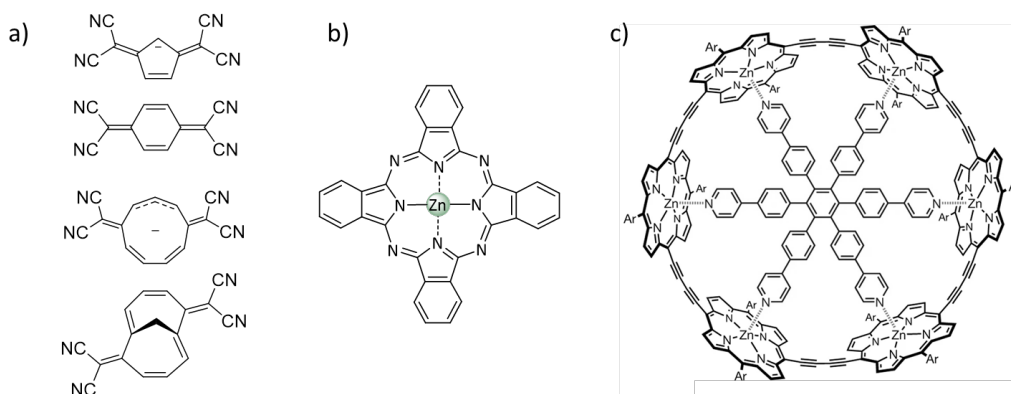


Figure 1. Representation of a) quinoidal compounds, b) Phthalocyanine, c) c-P6-T6 nanorings.

5. Conclusions

A proper understanding of aromaticity is needed to make correct interpretations of the experiments, as only then can the excited-state aromaticity concept be developed into a useful tool for the design of high-performance organic electronic devices.

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COMPUTATIONAL ANALYSIS OF 1,3 -DIPOLAR REACTIONS INSIDE CARBON NANOTUBES

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Keywords: carbon nanotube, ONIOM, 1,3-dipolar, selectivity, confinement

1. Introduction

Nature developed enzymes to recognize specific substrates and transform them inside well-defined pockets that ensure product selectivity and enhancement of reaction rates. To mimic nature, various nanoreactors have been used or designed to control, by encapsulation of guest molecules, kinetics and thermodynamics of chemical transformations. Recently, the effect of encapsulating a metal-free 1,3-dipolar cycloaddition reaction in narrow carbon nanotubes (CNTs) was investigated by (Miners *et al.*, 2019).

2. Methodology

All the electronic structure calculations have been carried out by the Gaussian16 software package using the ONIOM method. Geometry optimizations were performed by quantum mechanics, at the B97-D3/6-311+G** level of theory, while CNTs were described using molecular mechanics (MM) with the UFF force field. In detail, electrostatic embedding was considered and the partial atomic charges in the MM region were computed using the Qeq formalism. Solvent effect was also taken into account, optimizing again all the critical points with the polarizable continuum model (PCM) and using benzene as the solvent.

3. Results

The reaction of benzyl azides with various substituted acetylenes, chosen for their different steric and electronic properties, was studied (Figure 1).

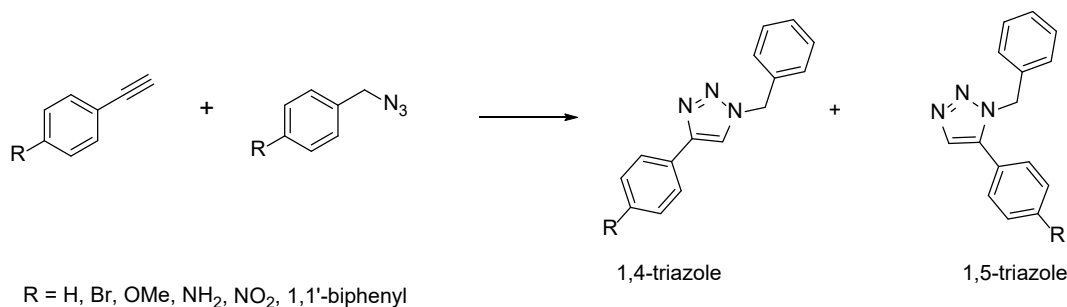


Figure 1. 1,3-dipolar cycloaddition reactions analyzed in this study

The reaction mechanism was unveiled, and then it was tested inside CNTs with different diameters (Table 1). We found that the reaction becomes catalyzed if confined inside CNTs. In addition, the formation of the more linear 1,4-triazole results were favored inside CNTs, specially for the narrowest ones.

Table 1. Relative Gibbs energies of the cycloaddition between benzyl azide and phenylacetylene (in kcal/mol), without CNT and inside (8,8) and (10,10) CNTs at 353.15K.

CNT	$\Delta G^\ddagger_{1,4\text{-triazole}}$	$\Delta G_{1,4\text{-triazole}}$	$\Delta G^\ddagger_{1,5\text{-triazole}}$	$\Delta G_{1,5\text{-triazole}}$
-	23.0	-47.2	20.4	-49.9
(8,8)	22.1	-49.5	24.6	-41.2
(10,10)	27.2	-43.6	31.3	-38.1

4. Conclusions

A 1,3-dipolar cycloaddition between benzyl azide and different substituted acetylenes was studied, and then inside different CNTs through computational methodologies. We found that confining the reactive system inside CNTs can enhance the reaction regioselectivity and, depending on a combination of steric and electronic effects, on the CNT diameters.

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EXPLORING THE FLUXIONAL BEHAVIOUR OF BIOINSPIRED ARTIFICIAL RECEPTORS WITH MD SIMULATIONS

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Keywords: cavitands, supramolecular chemistry, computational chemistry, molecular dynamics, bioinspired receptors

1. Introduction

The driving force that confers enzymes their remarkable catalytic performance is closely linked to the dynamism of the proteinogenic structure. Ligand recognition, size/shape-selectivity, and product release are just a few examples of how important the dynamics are for these systems. Analogously, some bioinspired artificial receptors also show fluxional behaviour, and its understanding is key for applications in catalysis (Raynal, Ballester, Vidal-Ferran, & van Leeuwen, 2014).

2. Hypothesis

Given the established parallelisms of bioinspired receptors with enzymes, we resort to Molecular Dynamics (MD) simulations –the method of choice for computationally modelling enzymatic catalysis– to reconstruct in detail the binding and exchange dynamics of supramolecular systems. MD simulations have rarely been used on artificial hosts, and the few examples found in the literature were limited to the *ps-ns* timescale (Longhi, Fabris, Zonta, & Fornili, 2006).

3. Methodology

The geometries of the starting points for conventional MD (cMD) simulations were optimized at the semiempirical level using Gaussian09. Then, the system was parameterized with known *Force Fields* and charge calculation methods within AMBER16. The parameterized system was immersed in a CHCl₃ box, minimized for solvent rearrangement, gradually heated to 300K, and finally equilibrated to reach P_{atm} . After these steps, the system was ready to run a cMD simulation.

For accelerated MD (aMD) simulations, the starting points were generated from the final step of a short conventional MD simulation. Different dihedral, total, and dual boosts were tested to sample the high-energy barrier processes. The energy barrier of these processes was recalculated using the PyReweighting toolkit (Miao *et al.*, 2014).

4. Results

A multi-timescale strategy for exploring the fluxional behaviour of an experimentally well-studied prototypical cavitand (**1**, Figure 1a) (Rudkevich, Hilmersson, & Rebek, 1997) –a receptor obtained by covalently bridging the phenolic moieties of resorcin[4]arenes with aromatic spacers– has been modelled, exploiting cMD and aMD techniques (with more than 60 μ s of simulations).

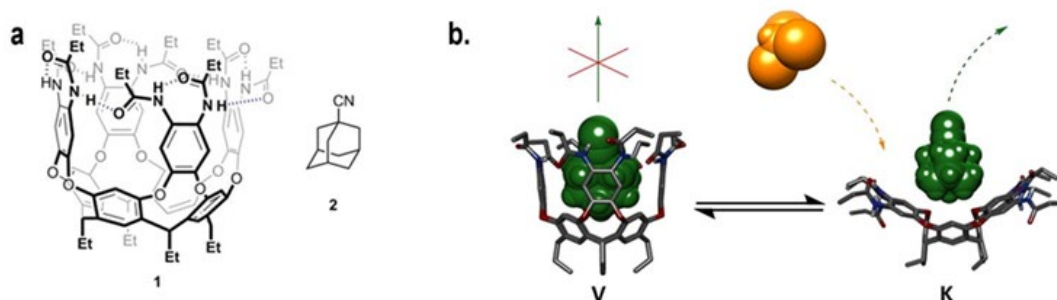


Figure 1. a) Structure of the cavitand (**1**) and guest (**2**) used in this study. b) Equilibrium between the closed (V) and open (K) conformers, where the guest exchange takes place, connected through an (un)folding process.

Green: 1-adamantanenitrile (**2**); orange: chloroform

5. Conclusion

Overall, our results constitute the first comprehensive computational characterization of the complex dynamic features of cavitand receptors, and a leap towards the rational design of synthetic host-guest systems (López-Coll, Álvarez-Yebra, Feixas, & Lledó, 2021).

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BIO-ELECTRO CO₂ RECYCLING TO ETHANOL

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Keywords: biocatalysis, carbon dioxide, solventogenesis, electrochemistry, biofuels

1. Introduction

The increase in carbon dioxide (CO₂) emissions is a challenging problem facing the world. Microbial electrochemical technology (MET) is a promising platform for the bio-electro recycling of CO₂ into carbon-neutral chemical building blocks and fuels (Blasco-Gómez *et al.*, 2019; Dessì *et al.*, 2021; Romans-Casas, Blasco-Gómez, Colprim, Balaguer, & Puig, 2021).

Until now, MET studies have obtained high concentrations of acetic acid, but other compounds, such as ethanol, are preferred for their market value. This alcohol can be used as a drop-in fuel or as an electron donor for subsequent reactions in more valuable compounds. In spite of this, ethanol production from CO₂ has hardly been investigated.

2. Hypothesis

The present work proposes to study the features of the bio-electrochemical production of ethanol from CO₂ as the sole carbon source. Special attention will be given to enhance its accumulation and utilization.

3. Methodology

Two 330 mL MET cells were assembled and set up as a three-electrode configuration and operated in batch mode and at -0.8 V *vs.* Standard hydrogen electrode (SHE). The systems were operated for 60 days. Liquid- and gas-phase samples were taken to monitor the CO₂ conversion into short chain fatty acids and alcohols production. The changes over time of pH, optical density (OD) and hydrogen partial pressures (pH₂) received special attention. The microbial community was analysed.

4. Results and discussion

Figure 1 shows the concentrations of each carbon-neutral compound produced from CO₂, current density, pH and OD during the whole experiment in both cells (S1 and S2). Both cells required some start-up time to acquire the suitable working conditions to trigger solventogenesis reactions to produce ethanol. Finally, acetic acid (HAc) concentration surpassed 11 g L⁻¹ in both reactors and the maximum production rate achieved was 39.12 g m⁻² d⁻¹. The highest ethanol concentration achieved was 5.28 g L⁻¹ with a peak production rate of 10.95 g m⁻² d⁻¹ which is 4-fold higher than the maximum previously reported (Srikanth *et al.*, 2018). The coulombic efficiencies surpassed 80 % in both cells indicating the current was

driven to the targeted products. Microbial community analyses unraveled the dominance of *Clostridium autoethanogenum* and *Clostridium ljungdahlii*.

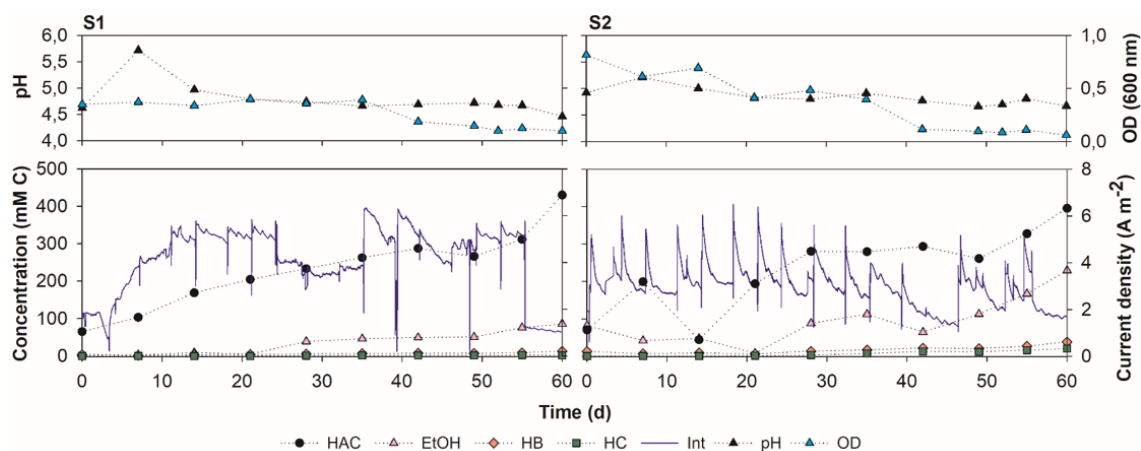


Figure 1. Cells conducted during the experiment. Concentrations of acetic acid (HAc, black circles), ethanol (EtOH, pink triangles), butyric acid (HB, orange rhombus), caproic acid (HC, green squares) are presented together with intensity demand (Int, blue solid line), pH, and optical density (black and blue triangles).

5. Conclusions

This study demonstrates for the first time the continuous and substantial bioelectrochemical CO₂ recycling into ethanol. The present work opens new technology horizons and pave the ground for its future implementation.

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ENGINEERED MICROBIAL BIOSENSORS FOR ENVIRONMENTAL MONITORING

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Keywords: environmental monitoring, microbial biosensors, heavy metals

1. Introduction

Ionic silver is known to be an effective antimicrobial agent widely used in the cleaning and medical industries (Randall, Gupta, Jackson, Busse, & O'Neill, 2015; Silver, 2003), however, there are several concerns regarding the release of silver pollutants into the environment (Gorsuch & Klaine, 1998). Presented here are two engineered bacterial biosensors for the detection and quantification of silver. The biosensors were shown to detect silver ions released from silver nanoparticles, and have the potential to become a method for monitoring ion release rates of different nanoparticles. Interestingly, the close homology of the silver resistance and copper resistance genes allowed for the biosensor to also be responsive to copper ions, implying that copper ions activate silver resistance.

2. Hypothesis

Further development of this biosensor could lead to commercial applications for environmental monitoring.

3. Methodology

Biosensing plasmids were constructed by fusing a mutGFP gene with silver regulated promoters from the *sil operon*. Two biosensing plasmids were made, pRADEK.1 and pRADEK.2, corresponding to two different silver dependent promoters found on the *sil operon*. These constructs were then transformed into *E. coli* J53(pMG101) (Randall *et al.*, 2015) to create the bacterial biosensor. Methods are further described by Martinez, Heil, & Charles (2019).

4. Results and discussion

Correlation between GFP signal and silver ion concentration makes it possible to quantify silver ions within a sample. The biosensor's ability to correlate silver ions and GFP within a select range proposes a possible method for approximating the amount of silver ions within a sample. It was shown that the composition of the sample in which the biosensor is cultivated in can affect the detection range and standard curve due to various halides which affect the availability of silver ions. If a silver ion standard curve is made with each sample that needs quantification, this can yield a better approximation. In addition, since the correlations between silver and GFP are linear, it is possible to give a relative proportion of silver ion concentration between two samples.

The biosensor was responsive to copper sulfide and exhibited an upward correlation trend with GFP and copper concentration similar to silver. This proposes that silver regulated GFP production via the *silRS* two-component system can also act as a mechanism for detecting copper(II) ions assuming the presence of a copper resistance gene. More interestingly, though, this result provides novel insight into the close homology of the copper and silver resistance mechanisms. Bioinformatic analysis of the two mechanisms *sil* and *cus* have confirmed many genetic similarities between various proteins. *Rensing et al.* found the silver ions activate the promoter regions found in the *cop* copper resistance mechanism (Rensing, Fan, Sharma, Mitra, & Rosen, 2000). The findings from this study prove the reverse; copper(II) ions can activate the promoter regions of the *sil* operon since an increase in GFP production was seen in pRADEK.1 and pRADEK.2 which contain the two silver regulated promoters found in the *sil* operon. No result was seen when the biosensor was tested with zinc salts at any concentration tested.

5. Conclusions

For long term environmental monitoring applications, plasmid based engineering methods are not suitable as it does not account for factors such as copy number and plasmid loss. Further work can look into integrating the *sil* operon and plasmid vectors pRADEK.1 and pRADEK.2 into the chromosome of *E. coli J53*. By doing this, plasmid loss does not need to be accounted for, and thus the use of selection antibiotics are not needed. This may result in a larger detection range since the bacteria does not need to express resistance to ampicillin and kanamycin as needed in this study to maintain the plasmid vector.

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SESSION IV. GENETICS AND BIOMEDICINE

MANGANESE AND MAGNESIUM IONS INDUCE DNA DAMAGE *IN VITRO* IN FULLY CONDENSED PIG SPERM

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Keywords: sperm, male infertility, DNA damage, sperm quality, pig

1. Introduction

Sperm DNA fragmentation has been reported to be one of the main factors affecting male fertility (Zeqiraj *et al.*, 2018). Previously, it has been shown that the integrity of sperm DNA is reduced after incubation with $MnCl_2$ with and without $CaCl_2$, producing double strand DNA breaks through a mechanism called sperm chromatin fragmentation (SCF), which may rely on the activity of topoisomerases or DNases (Shaman, Prisztoka, & Ward, 2006; Yamauchi, Shaman, & Ward, 2007).

Since this mechanism has only been described in mouse spermatozoa, we aim to elucidate whether it is also present in the pig by assessing: i) the dose and incubation time response to sperm DNA fragmentation; and ii) the effect of Mn^{2+} and Mg^{2+} concentration and incubation time on sperm physiology.

2. Methodology

Ejaculates were collected from different boars and prepared as commercial seminal doses. To assess the induction of DNA breaks, Comet assay and pulsed-field gel electrophoresis (PFGE) analysis were performed to permeabilized and non-permeabilized samples. Ejaculate samples were treated with $MnCl_2$ and $MgCl_2$ in a concentration range between 0.1 mM to 50 mM (concentration dependent) and from 2 to 60 min (time dependent) at 37 °C. Flow cytometry and CASA were used to determine the impact of all treatments on sperm physiology, motility, and viability.

3. Results and discussion

Comet and PFGE analyses revealed an active role of Mn^{2+} , causing DNA breaks, whose impact varied between concentrations and incubation times ($P < 0.0001$). However, a minor effect of Mg^{2+} on DNA integrity was observed. Results with both ions showed no difference between permeabilized and non-permeabilized sperm, supporting the involvement of an intracellular mechanism. With regard to sperm physiology, the influence of Mn^{2+} was found to be dose-dependent, as viability, progressive motility, and total motility notably decreased at high concentrations (5, 10 and 50 mM). Otherwise, no time-response dependence was observed in Mn^{2+} treatments since sperm physiology strongly decreased after only 2 min of incubation.

Finally, Mg^{2+} affected viability and progressive and total motility when working at high ion concentrations (10 and 50 mM).

4. Conclusion

This study demonstrated that Mn^{2+} ions are capable of causing sperm DNA breaks in fully condensed and non-permeabilized sperm, following a dose-dependent response. The same incubations caused detrimental consequences to sperm physiology, because viability and motility were significantly affected. Alternatively, Mg^{2+} showed a smaller impact on DNA fragmentation and, consequently, on sperm physiology. These results support that the SCF mechanism may be induced in pigs, triggering a specific intracellular pathway.

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INTRACRANIAL SELF-STIMULATION INCREASES SERUM LEVELS OF miRNA-181c IN A RAT MODEL OF ALZHEIMER'S DISEASE

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Keywords: Alzheimer, miRNA, serum levels, self-stimulation, rat model

1. Introduction

Deep brain stimulation (DBS) is being evaluated as a treatment for Alzheimer's disease (AD) (Suthana & Fried, 2014). However, a target for stimulation and the underlying molecular mechanism must be established. Intracranial self-stimulation (ICSS) applied to the medial forebrain bundle (MFB) is a rewarding type of DBS with facilitating effects on learning and memory (García-Brito, Morgado-Bernal, Biosca-Simon, & Segura-Torres, 2017; Ruiz-Medina, Morgado-Bernal, Redolar-Ripoll, Aldavert-Vera, & Segura-Torres, 2008). It modulates the expression of specific miRNAs, which show altered circulating levels in AD patients and postulated as potential biomarkers of AD progression (Puig-Parnau *et al.*, 2020; Salta & De Strooper, 2017).

2. Objective

In this context, we analysed the effects of MFB-ICSS on serum expression of eleven AD related miRNA in a sporadic rodent AD model.

3. Methodology

Rats were implanted with an electrode at the MFB and bilaterally injected with 2 mg/Kg of stz or citrate buffer into the ventricles. The ICSS treatment consisted of 5 sessions of 45 minutes, administered immediately after each of the 5 sessions of acquisition of the Morris water maze (1 session daily, 2 trials each), carried out on days 33 to 37 after the STZ infusion. The levels of miRNAs were quantified by qRT-PCR in serum samples obtained immediately after the last ICSS or Sham session.

4. Results

Serum levels of miR-181c were significantly decreased in STZ rats, which also showed increased latencies in the 3rd and 5th acquisition sessions and in the mean distance to the target during the first 60 seconds (Dmt60) in the retention test, at 40 days post-stz compared to control rats. Because of ICSS-MFB treatment, AD rats showed significant lower latencies in

the 3rd and 5th acquisition sessions compared to non-treated AD rats. Serum levels of miRNA-181c on ICSS-MFB-treated AD rats were similar to control rats. A negative correlation was observed between miR-181c levels and A5 and Dmt60 parameters. No significant differences were observed in serum expression of the other analysed miRNAs.

5. Conclusions

Our results indicate that ICSS-MFB restores the miRNA-181c serum levels in AD condition and monitoring it could serve as a measure of effectiveness of DBS treatments to fight AD cognitive deficits.

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TRANSFERRIN RECEPTOR IS DOWNREGULATED IN THE STRIATUM OF HUNTINGTON'S DISEASE: ASSOCIATION WITH IRON ACCUMULATION

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Keywords: Huntington's disease (HD), striatum, iron, iron-responsive element-binding protein 2, transferrin receptor

1. Introduction

Huntington's disease (HD) is a neurodegenerative disorder caused by a mutation in the huntingtin (HTT) gene leading to the expression of mutant HTT (mHTT) protein. People suffering from HD show motor discoordination, mostly due to striatal degeneration. It has been suggested that iron accumulation participates in neuronal degeneration (Labbadia & Morimoto, 2013). Neurons acquire iron mainly through the transferrin receptor (TfR) and the divalent metal transporter 1 (DMT1). These two proteins are upregulated by the iron-responsive element-binding protein 2 (IRP2) (Ke & Qian, 2007). In human HD, iron accumulation has been reported in striatum (Bartzokis, Cummings, Perlman, Hance, & Mintz, 1999), as well as a dysregulation of iron metabolism in the late phases of HD in R6/2 mouse model (Muller & Leavitt, 2014). However, the dysregulation of iron homeostasis in the progression and development of HD and its association with mHTT-mediated degeneration is unknown.

2. Hypothesis

Our hypothesis is that iron homeostasis is dysregulated in the HD striatum and plays a role in striatal degeneration.

3. Methodology

TfR, DMT1 and IRP2 levels were assessed by Western blot in the striatum of R6/1 mice, a HD mouse model, at different stages of the disease and in STHdh cells, a cellular HD model. To reproduce the accumulation of iron in the striatum, ferric ammonium citrate (FAC) at 2.5 and 10 mM was added to STHdhQ7 cells (wild-type cells) and STHdhQ111 (HD cells) during 24 hours. Then, a cell survival assay and analysis of TfR, DMT1 and IRP2 levels were performed.

4. Results

The analysis of R6/1 striatum revealed a significant and sustained decrease of TfR from the onset of disease. We also observed a reduction of IRP2 and DMT1, but only in a presymptomatic phase and in the onset of disease. The addition of FAC induced cell death to both STHdh cells. Interestingly, HD cells are more sensitive to FAC-mediated cell death. Additionally, the presence of FAC in STHdh cells promoted a reduction of TfR and IRP2, without changes in DMT1 at both concentrations.

5. Discussion

Our results indicate that iron homeostasis dysregulation is present in all HD phases. In addition, TfR reduction seems to be the more consistent dysregulation. In STHdh cells the accumulation of iron reduced TfR probably by IRP2 degradation, as IRP2 levels are drastically reduced. Accordingly, it has been described that iron accumulation induces IRP2 degradation.

6. Conclusions

We conclude that iron homeostasis is dysregulated in the striatum of HD, suggesting its role in the degeneration of striatal neurons.

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STUDY OF LEVELS AND ACTIVITY OF PROTEIN TYROSINE PHOSPHATASE 1B IN HUNTINGTON'S DISEASE MODELS

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Keywords: Huntington's disease, mutant huntingtin, protein tyrosine phosphatase 1B, striatum, phosphatase

1. Introduction

Huntington's disease (HD) is a hereditary neurodegenerative disorder caused by a mutation in the huntingtin (HTT) gene (Labbadia & Morimoto, 2013). The characteristic symptom of HD is motor discoordination, mainly due to the specific degeneration of medium spiny neurons (MSNs) in striatum (Wheeler *et al.*, 2000). The MSNs' degeneration is due to the dysregulation of molecular mechanisms mediated by the expression of mutant HTT (mHTT) leading to synaptic plasticity deficits and neuronal death (Wheeler *et al.*, 2000). Therefore, it is crucial to study proteins involved in synaptic plasticity and neuronal survival to propose therapeutic targets. Protein tyrosine phosphatase 1B (PTP1B) is a phosphatase expressed within the central nervous system (Vieira, Lyra e Silva, Ferreira, & De Felice, 2017) and, in neuroinflammation, it is activated acting as a negative regulator of neuronal plasticity and survival (Feng *et al.*, 2020). Additionally, studies in neurodegenerative disease models showed that PTP1B levels are altered, and its inhibition exerts a neuroprotective effect (Feng, Chen, Chan, & Chen, 2020; Ricke *et al.*, 2020). However, its role in HD has not yet been investigated. Our aim is to characterize the levels and activity of PTP1B in HD models.

2. Methodology

We used striatal samples from R6/1 mice, HD mice expressing the exon-1 mHTT at different ages, representing different phases of the disease. Wild-type littermate animals were used as the control group. We also used the STHdh cell line, an immortalized striatal knock-in cells stably expressing full-length wild-type HTT (STHdh^{Q7/Q7}; control cells) or full-length mHTT (STHdh^{Q111/Q111}; mutant cells). Cells were cultured in serum and non-serum conditions. Then, we studied the protein levels of PTP1B by Western blot and activity of PTP1B by a colorimetric assay.

3. Results

We observed a reduction of total PTP1B levels in the R6/1 mice at presymptomatic phases. In addition, we also detected a decrease of the proteolytic PTP1B band at presymptomatic phases. In STHdh cells, no differences were observed in PTP1B levels in mutant cells compared to

control cells, in serum and serum starved conditions. The study of PTP1B activity could reveal changes in PTP1B activity without changes in protein levels.

4. Discussion

A reduction of PTP1B is associated with the presymptomatic phases suggesting that the inhibition of PTP1B blocks the apparition of motor symptoms. In addition, the expression of mHTT could alter PTP1B activity. Differences in the phosphorylation of PTP1B substrates need to be characterized.

5. Conclusions

The levels and activity of PTP1B could be altered in HD.

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SYNTHETIC ANALOGUES OF PITUITARY ADENYLATE CYCLASE-ACTIVATING POLYPEPTIDE (PACAP) IMPROVE MOTOR DEFICITS IN R6/1 MOUSE MODEL OF HUNTINGTON'S DISEASE

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Keywords: Huntington's disease (HD), striatum, pituitary adenylate cyclase-activating polypeptide (PACAP), analogues, PAC1 receptor (PAC1R), neurodegenerative diseases

1. Introduction

Huntington's disease (HD) is a neurodegenerative disorder caused by the expression of the mutant huntingtin (mHtt) protein. Motor dysfunction is the most characteristic symptom of HD and it is associated with the progressive degeneration of striatum (Vonsattel & DiFiglia, 1998). Pituitary adenylate cyclase-activating polypeptide (PACAP) is a multifunctional peptide that acts through three receptors named PAC1R, VPAC1R, and VPAC2R (Vaudry *et al.*, 2009). Recently, we found that intranasal administration of PACAP improves motor symptoms in HD mice enhancing PAC1R signaling (Solés-Tarrés *et al.*, 2022).

2. Problem

Therapeutic use of PACAP is hindered because of its poor metabolic stability and because the activation of VPAC receptors is associated with peripheral side effects (Warren *et al.*, 1992). Therefore, we studied the therapeutic potential of two PACAP analogues showing better biostability and different affinity for PACAP receptors: Acetyl-[Ala15, Ala20] PACAP-38-propylamide displaying more selectivity for PAC1R, and Ac- [Phe(pI)6, Nle17]PACAP(1-38) showing lower affinity for VPAC receptors.

3. Methodology

We administered 30µg/Kg of PACAP analogues to 18-week-old R6/1 transgenic mice intranasally for 12 days and we evaluated motor function using rotarod and balance beam tests. Then, we analysed the effect of PACAP analogues on striatal PAC1R protein levels by western blot and striatal volume based on Nissl staining. Finally, we studied DARPP-32+ neuronal population and the presence of mHtt aggregates by immunofluorescence.

4. Results

The administration of PACAP-analogues improves motor function of R6/1 mice in rotarod and balance beam tests. In the brain, treated mice showed no changes in PAC1R protein levels and no significant improvement in striatal volume. However, we found a significant increase in the size of DARPP-32+ neurons. Importantly, only mice treated with Acetyl-[Ala15, Ala20] PACAP-38-propylamide showed an increase in the number of DARPP-32+ neurons and a decrease in mHtt aggregates.

5. Conclusions

Both PACAP-analogues tested in this study improve motor deficits of R6/1 HD mice, with the Acetyl-[Ala15, Ala20] PACAP-38-propylamide being the most efficient in protecting the striatum from mHtt toxicity.

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MUTATIONAL FOOTPRINTS ARISING FROM CHEMOTHERAPY DUE TO INTERPLAY BETWEEN DNA DAMAGE AND REPAIR

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Keywords: DNA damage, repair, chemotherapy, alkylation, nucleotide-resolution map

1. Introduction

Cytotoxicity due to DNA damage caused by alkylating agents is a mechanism commonly employed in routine chemotherapy. Concomitantly, these drugs impose a high mutagenic burden on repair-deficient cancer cells by generating a disproportionate balance between DNA damage and repair. Sites that go undetected by repair proteins could further accelerate genomic instability, making it imperative to identify such potentially mutagenic regions. In addition, it would also shed light on the interdependence of mutagenesis and repair levels with epigenetic factors like chromatin architecture or transcriptional levels, providing a comprehensive view of the evolution, progression, and in some cases, relapse of tumors by identifying common drivers of positive selection. In this project, we propose to build a nucleotide resolution map throughout the entire genome of two types of DNA damage generated by mutagenic agents in different experimental models.

2. Objectives

To do so, our main objectives include:

- (1) Creation of damage maps in human and yeast cells at different time points to study the dynamics of repair at damaged lesions.
- (2) Computational study of the influence of chromatin features on differential repair for various types of damage, giving insight into mutagenesis.
- (3) Comparison of the observed mutation profiles with the actual distribution of mutations found in human tumors.

3. Methodology

In the project, we study damage by alkylating agents with a panel of seven drugs, and test them in parallel on both human and yeast genomes for reference. Monofunctional alkylators include: methyl methanesulfonate (MMS); ethyl methanesulfonate (EMS); methyl nitrosourea (MNU), now replaced with N-methyl N'-Nitro N-nitrosoguanidine (MNNG); dacarbazine; and temozolomide. The bifunctional alkylators are carmustine and cyclophosphamide. The first stage of the study involves optimization of drug concentrations and incubation periods for both yeast cells and human immortalized RPE-1 h-TERT cells. These optimal conditions are then

used for generating damage libraries, using a custom protocol (adapted from Mao, Wyrick, Roberts, & Smerdon, 2017) for post-sequencing detection of damaged sites. Once we have damage maps of instantaneous damage, we will follow up with chasing repair dynamics by generating multiple maps at both early and late time points to study the evolution of damage over time. Finally, all this information will be merged to identify sites of mutagenesis and profile mutation signatures for each treatment.

4. Results

We have been able to generate maps of methylation damage, mostly in guanines and adenines using MMS, and of ethylation damage using EMS, in RPE-1 cells. These are depicted below in Fig. 1 as higher enrichment of G's and A's as these two bases are the most likely to get alkylated, and the damage can be identified and excised using the *ycaQ* and EndoIV glycosylase-endonuclease complex. With TMZ, we were able to follow a time-course of recovery at four different time-points, i.e. 0h, 2h, 4h and 16h. The damage seems to fade at the latest time point of 16h, which is along the line of expectation.

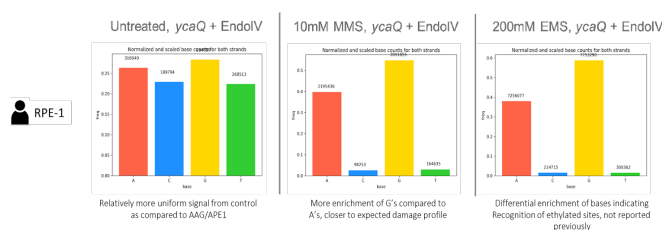


Figure 1. Plots depicting frequency of each nucleotide base in control, MMS-treated, and EMS-treated samples.

5. Conclusions

From the results, it is evident that our protocol for damage capture allows efficient detection of the same. We can progress with the same technique to pursue our objectives, which will help in generating information about the interplay between DNA damage and repair to understand mutagenesis and its associated processes.

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SESSION V. HEALTH

PRACTICE GUIDELINES FOR DIVING-RELATED FATALITIES: MULTIDISCIPLINARY, EXPERIENCE-BASED INVESTIGATION

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Keywords: diving, multidisciplinary investigation, guidelines, police reports, cause of death

1. Introduction

Diving is a safe practice and cases of deaths are uncommon (Shreeves, Buzzacott, Hornsby, & Caney, 2018). Drowning is the most common cause of death (Buzzacott, 2018; Edmonds & Caruso, 2014) but others have been described, such as natural disease processes, trauma, gas poisoning (Casadesús & Aguirre, 2011) or those secondary to the biophysical foundations that govern the hyperbaric environment (arterial gas embolism and decompression sickness) (Denoble, Caruso, Dear, Pieper, & Vann, 2008). Multidisciplinary investigation is essential for elucidating the cause of death (Casadesús *et al.*, 2019; Casadesús *et al.*, 2021). To date, there are no published practical guidelines to investigate diving-related fatalities in Spain.

The aim of this work is to provide a practical guideline that would include the collection of technical-police and medical-forensic data. These data are necessary to carry out a complete analysis of each case (Robert & Teather, 2013) and to avoid overdiagnoses of deaths by drowning.

2. Methodology

The police technical and the forensic autopsy reports of diving deaths recorded on the coast of Girona (Spain) between January 2009 and May 2020 were analysed. Police technical reports were recorded before the autopsies. They consisted of preliminary data about the testing of the diving equipment, the diving plan, the emergency and evacuation plans, and the decedents' dive profiles. Data analyses related to autopsy results, together with macroscopic findings, histopathological analyses, and toxicological results, were also analysed.

3. Results

An easy-to-use guide has been written to direct the collection of data that are essential to successfully investigating fatalities due to diving accidents. It consists of two well-differentiated blocks, indicating the order of application through a decision tree algorithm. The first one refers to all the technical-police aspects of the accident that must be known, referring to diving equipment and dive profiles. The second block consists of the medical-forensic aspects (including both external and internal examinations).

It is important to choose a sequence of the most appropriate autopsy techniques and complementary tests, such as the determination of diatoms, strontium, or carboxyhemoglobin, and to correctly identify all events related to the accident, including the cause of death.

4. Conclusions

This guide provides a standard work procedure that systematizes the research and the autopsy and sampling techniques used by the different professionals involved. Consequently, it makes possible to identify risk factors or unsafe behaviours about which to develop prevention measures.

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POST-COVID-19 PATIENTS SHOW INCREASED ENDOTHELIAL PROGENITOR CELL PRODUCTION

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Keywords: COVID-19, endothelial progenitor cell, endothelial damage, embolism, biomarker

1. Introduction

SARS-CoV-2, the cause of COVID-19, has generated a global emergency. SARS-CoV-2 targets the endothelium (Pesaresi *et al.*, 2020), generating endothelial dysfunction and an unbalanced vascular homeostasis, a key step in the development of cardiovascular complications including coagulopathies and thromboembolisms (Wichmann *et al.*, 2020). The number of endothelial progenitor cells (EPCs) acts as an indicator of vascular damage (Sen, McDonald, Coates, & Bonder, 2011). However, its role in SARS-CoV-2 is unknown.

2. Hypothesis

Increased production of EPCs 3-months after SARS-CoV-2 infection would indicate the presence of vascular sequelae in these patients. The aim of this study is to quantify the number of EPCs and assess for the first time if there is a significant increase after SARS-CoV-2 infection. An evaluation will indicate whether there are differences in the number of EPCs in post-COVID-19 patients who have suffered an acute pulmonary embolism (PE) and those that did not. Moreover, the study will determine whether this increase correlates with any of the clinical parameters studied.

3. Methodology

Sixty-three subjects were recruited in the study, including 32 subjects 3-months after overcoming COVID-19 and 31 healthy controls. Of these 32 COVID-19 patients, 14 had suffered PE. EPCs were obtained from mononuclear cells isolated from peripheral blood, cultured in specific media and conditions. The appearance, the number of colonies and the days of appearance were quantified.

4. Results

The results show a significant increase in the appearance of EPCs in patients 3-months after COVID-19 compared to the healthy controls. However, there were no differences in the number of EPCs in COVID-19 patients depending on whether or not PE was detected. Patients with a high number of EPCs showed higher levels of haemoglobin at the time of EPC isolation and

lower levels of PaO₂ at admission, but they did not show a relationship with any other parameter studied.

5. Conclusions

The results obtained confirm the presence of vascular sequelae in post-COVID-19 patients, with an abnormal increase in the number of EPCs in blood circulation.

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ASSOCIATION BETWEEN SOCIO-ECONOMIC FACTORS AND VACCINATION COVERAGE AGAINST MEASLES, MUMPS, AND RUBELLA IN 8-YEAR-OLD CHILDREN IN CATALONIA: AN ECOLOGICAL STUDY

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Keywords: child, ecological study, measles-mumps-rubella vaccine, primary health care, vaccination

1. Introduction

In Catalonia, vaccination coverage with two doses of measles-mumps-rubella (MMR) vaccine is around 93% (MSCBS, 2020). Different factors may explain this non-optimal vaccination coverage (<95%), among which socio-economic factors stand out (Moscrop, Ziebland, Bloch, & Iraola, 2020).

2. Methodology

Information from an ecological study of the total provider units (PUs), of which data were available in the Information System of Primary Care Services (SISAP), was merged with information from the Catalan Agency for Quality and Health Assessment (AQuAS). Aggregate information was included by PU on the number of doses of the MMR vaccine administered (first and second doses) and two different socio-economic indicators: the AQuAS socio-economic index (higher score=worse socio-economic status) and the MEDEA deprivation index of urban PUs (AQuAS, 2017; Domínguez-Berjón *et al.*, 2008). Vaccine coverage grouped by PU and health region in served and assigned populations was estimated. The association between the different study variables and vaccination coverage was investigated using bivariate analyses.

3. Results

Three hundred (80%) PUs were analysed out of 375 available in the SISAP registers. Of the PUs, 82.3% were managed by the Catalan Health Institute (ICS) and 62.7% were urban. The mean socio-economic index was 47.5 (standard deviation, 15.2). According to MEDEA deprivation index, 20.0% of the urban PUs were in a very unfavourable socio-economic situation. Statistically significant differences were observed in the mean percentage of vaccination coverage of the assigned population between the nine health regions (maximum coverage, 82.1% and minimum 73.9%). The mean percentage of vaccination coverage was higher in PUs with a ratio of served to assigned population above 85%. This percentage, in the assigned population, was higher in rural compared to urban PUs (Borràs, Domínguez, Oviedo, Batalla, & Salleras, 2008). The socioeconomic index showed a low positive association with vaccination coverage of the served population ($r=0.335$) and a moderate association with the

assigned population ($r=0.508$). Higher average coverage was observed in urban PUs where the socioeconomic status was more unfavourable. As for the percentage of PUs with optimal vaccination coverage, in the served population, it was 29.6% and in the assigned population, it was 1.3%. The PUs with optimal vaccination coverage in the served population had a higher index of socioeconomic deprivation than the PUs with non-optimal coverage. Of the urban PUs with optimal vaccination coverage, 55.0% were in the fourth quartile (lowest socio-economic status) of the MEDEA deprivation index.

4. Conclusion

Vaccination coverage with the MMR vaccine varies between health regions. Unfavourable socio-economic factors are associated with higher vaccination coverage rates (Bryden, Browne, Rockloff, & Unsworth, 2019). These findings have important implications for understanding how socio-economic inequalities may affect vaccination coverage with the MMR vaccine and for the development of future studies (Arat, Burström, Östberg, & Hjern, 2019; Arat, Norredam, *et al.*, 2019).

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A TREATMENT WITH OLIVE LEAF EXTRACT AND ASSESSMENT OF HEALTHY LIFESTYLE REDUCES MILD HYPERTENSION

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Keywords: mild blood pressure, olive leaf extract, antihypertensive treatment

1. Introduction

The olive leaf tisane has been taken to improve blood pressure and, in the last 30 years, it has been investigated as a medicine (HMPC, 2017; Cherif *et al.*, 1996; Ismail, Norhayati, & Mohamad, 2021; Perrinjaquet-Moccetti *et al.*, 2008; Susalit *et al.*, 2011). This clinical trial investigates its antihypertensive effect in a mild hypertension and low cardiovascular risk population (Williams *et al.*, 2018). It has been placed in a compact capsule (Munin & Edwards-Lévy, 2011) to avoid bitterness and to assure a blind clinical trial.

2. Objective

Compare the arterial blood pressure before and after treatment with extract in powder of commercialized olive leaf extract or placebo.

3. Methodology

Mild hypertension was confirmed with a battery blood pressure measure. To reinforce the diagnosis of mild hypertension, WatchBP3 monitors were used. Every participant was given a graphic sheet to reminisce about a healthy lifestyle.

Design: experimental double blind randomized crossed-over assay (n 24) in mild hypertensive adults with low cardiovascular risk and without treatment.

The participants took a daily dose of 1000 mg of a powder extract of 20% of oleuropein or a placebo in an opaque capsule of methylcellulose for the first month. During the second month, they did not receive any treatment. In the third month, they took the extract if they had taken the placebo, and vice versa.

The effectiveness was controlled with four ambulatory blood pressure measurements (ABPM) before and after the first and third months. They had three blood tests.

4. Results

At the end of the study, the best control of blood pressure was in diurnal ABPM of the group extract: 65.2% of the participants had blood pressure $\leq 135/85$ mmHg. The diastolic difference in mmHg of the ABPM 24 hours ($\leq 130/80$) was significant in both groups (p-value=0.046; 0.037 placebo and extract, respectively). In the group extract, 69.6 % had a diastolic blood pressure < 80 mmHg.

The daytime diastolic ABPM was 3.22 mmHg lower in the group extract than the group placebo, yet the differences were not significant. Of the participants, he 78.3 % controlled the diastolic blood pressure < 85 mmHg at the end of study.

In a comparison at the beginning and end of the trial of the extract and placebo groups, the blood tests did not show significant changes.

5. Conclusion

The olive leaf extract as a food supplement reduces significantly the diastolic ABPM 24 hours and, together with lifestyle intervention, reduces mild blood pressure, is digested well in capsule, and does not alter the values of the blood tests.

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EPICARDIAL FAT, INTERVENTRICULAR SEPTAL AND LEFT VENTRICULAR POSTERIOR WALL THICKNESSES ARE ASSOCIATED WITH CARDIOMETABOLIC RISK MARKERS AND PHYSICALLY ACTIVE BEHAVIOR IN SCHOOL-AGED CHILDREN

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Keywords: epicardial fat, interventricular septal thickness, left ventricular posterior wall thickness, physically active behavior, sedentary behavior

1. Introduction

Epicardial fat (EF), interventricular septal (IVST) and left ventricular posterior wall (LVPWT) thicknesses are markers of cardiovascular risk and potential therapeutic targets to improve cardiovascular health (Ansaldi, Montecucco, Sahebkar, Dallegri, & Carbone, 2019; Gupta *et al.*, 2010).

Sedentary behavior (hours/metabolic equivalents (METs) of sitting + listening to music + reading + studying) is associated with cardiometabolic risk, while physically active behavior (hours/METs of playing alone + playing with others + physical activity) is associated with cardiometabolic health (Carter, Hartman, Holder, Thijssen, & Hopkins, 2017; Nystoriak & Bhatnagar, 2018).

Our objective is to study the associations of EF, IVST and LVPWT with physical (in)activity, body composition, cardiovascular and metabolic parameters in apparently healthy school-age children.

2. Methodology

A total of 156 children (70 girls and 86 boys; 8.9±1.8 years; -1<BMI SDS<1) recruited in primary health centers in Girona (Northeastern Spain) were studied.

EF, visceral fat (VF), IVST, LVPWT and carotid intima media thickness (cIMT) were measured by high-definition ultrasound. BMI, waist circumference (WC) and fat mass (FM) were assessed. Fasting blood was used to measure serum lipids, tryglicerides, HOMA-IR, C-reactive protein, and high molecular weight (HMW) adiponectin. Children's parents answered the Physical Activity Questionnaire (enKid study) to assess physical (in)activity as hours and METs.

3. Results

EF is positively associated with BMI, WC, FM, VF, cIMT, C-reactive protein (all $p < 0.001$) and HOMA-IR ($p = 0.006$), while it is negatively associated with HMW adiponectin ($p = 0.006$). IVST and LVPWT are positively associated with BMI, FM, cIMT and triglycerides ($p < 0.001$), while they are negatively associated with HMW adiponectin ($p < 0.001$).

EF, IVST and LVPWT are positively associated with hours/METs of sedentary behavior, while negatively associated with hours/METs of physically active behavior ($p < 0.05$ to $p < 0.001$). However, IVST and LVPWT are positively associated with hours/METs of organized sports activities, i.e. practising a sport ($p = 0.001$).

4. Conclusions

Higher EF, IVST and LVPWT are associated with cardiometabolic risk markers in 9- year-old children. Furthermore, physically active behavior may induce beneficial effects on cardiometabolic health by remodeling the cardiac structure in these children.

Being part of an organized sports activity may induce higher IVST and LVPWT as a physiological adaptation to the training specificity of the particular sport, rather than as a morbid change.

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STUDY OF IODINE STATUS IN ADOLESCENTS THROUGH FOOD INTAKE AND URINARY IODINE ANALYSIS

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Keywords: iodine, adolescents, daily iodine intake, urinary iodine, iodized salt

1. Introduction

Iodine deficit is the cause of an avoidable mental retardation and remains a public health problem. Salt iodization and dairy consumption are the most efficient measures of prevention for the population (Vila *et al.*, 2020). Changes in lifestyle and eating habits during adolescence can affect the main dietary sources of iodine (Serra-Majem *et al.*, 2002). One of the main sources of iodine is dairy, and its consumption is especially low in teenage girls, which suggests there could be a population at risk (Chacón *et al.*, 2015; Soriguer *et al.*, 2012). Our aim is to determine the median urinary concentration of iodine and to estimate its daily intake in an adolescent population.

2. Hypothesis

The median urinary iodine concentration (UIC) in adolescent population will be lower than that one observed within the infant population. Daily iodine intake will be below the optimal nutritional requirements for the group aged between 15 and 17 years old.

3. Methodology

A cross-sectional descriptive study with 480 adolescents from 15 to 17 years old who attend public education centers in Blanes. Descriptive univariate analysis will be carried out. The association between the UIC and the iodine intake will be analyzed together with the covariates by means of a bivariate analysis and a logistic regression.

4. Results

Preventing iodine deficiency in the pregnant population is a health priority, as iodine participates in the synthesis of thyroid hormones necessary for the proper neuronal development of the baby (Donnay, Arena, Lucas, Velasco, & Ares, 2014). During adolescence, it is critical to ensure that iodine levels are sufficient before the onset of the reproductive stage. Adequate levels of iodine in children and adolescents will also prevent the onset of goiter and thyroid dysfunction in the adult population.

5. Conclusions

A preventive intervention aimed at promoting the health of women of childbearing potential could be an effective focus for improving preconception health.

Investing in adolescent health has a threefold benefit: their health now, their health in the future, and the health of the next generation.

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THE EFFECT CONCURRENT AEROBIC AND RESISTANCE TRAINING AND VITAMIN D SUPPLEMENTATION ON LIPID PROFILE 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 either when the pancreas does not produce enough insulin or when the body cannot effectively use the insulin it produces (WHO, 2021). Low blood 25-hydroxyvitamin D (25[OH]D) level has emerged as a risk factor for T2D, and vitamin D supplementation has been hypothesized as a potential intervention to lower diabetes risk (Lu *et al.*, 2018; Pittas, Lau, Hu, & Dawson-Hughes, 2007).

In this study, the effect of resistance training and vitamin D supplementation on the insulin resistance in patients with T2D is investigated and the effect of each of the training and supplementation variables are compared separately and together. Since resistance training has a positive effect on diabetes and exercise has been one of the ways to treat obesity and diabetes (Strasser & Pesta, 2013), the results of this study can provide a useful solution to treat or ameliorate obesity and diabetes.

2. Hypothesis

We hypothesize that vitamin D supplement 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 (50-70 years) with fasting blood glucose >126 mg/dL, and glycosylated haemoglobin (HbA1c) <9%. Patients will be selected and later randomly assigned to four groups 1) Training-vitamin D (n=10), 2) Training-placebo (n=10), 3) Vitamin D (n=10) and 4) Placebo (n=10). A

sarcoplasmic stimulating training system will be used. The programme will consist of 3 sessions/week for 15 weeks; and it is designed in 3 five-week periods. Fitness tests, as well as analysis of insulin resistance, lipid profile, and other blood biomarkers will be obtained. Subjects in the vitamin D and resistance training group, and the vitamin D group will use oral capsules containing 5,000 international units of vitamin D every two weeks for four months.

4. Results

It is expected that 15 weeks of exercise and vitamin D supplementation could affect the insulin resistance and lipid profile individuals with T2D, and vitamin D supplementation can improve triglycerides, blood cholesterol, and the ratio of HDL to LDL. Study limitations include "dropout" or losses for several causes, as the study will be voluntary, and participants may refuse to continue. When calculating the sample size, an expected dropout rate of 20% will be assumed.

5. Conclusions

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

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SESSION VI. CHEMISTRY

ALKYLATION OF BENZOYL HYDRAZINES: ACCESS TO MONO- OR DI-SUBSTITUTED COMPOUNDS

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Keywords: borrowing hydrogen, ruthenium complex, catalysis, alkylation, multicomponent

1. Introduction

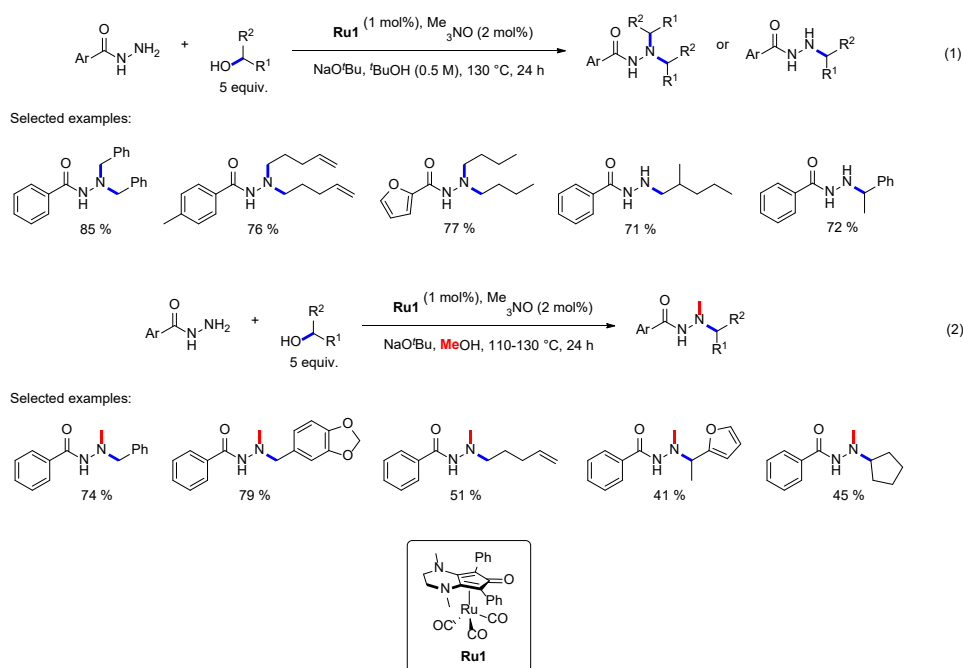
N, N acyl hydrazides are a class of compounds often encountered in chemical industries. While *N*-alkylation of nitrogen compounds, such as reductive amination via the borrowing hydrogen strategy, is well studied and developed, few examples describe alkylation of hydrazine derivatives (Thiyagarajan & Gunanathan, 2019; Yang *et al.*, 2017). Following our ongoing interest in the borrowing hydrogen strategy, we decided to study this reaction.

2. Methodology

Experimentally, the diaminocyclopentadienone iron tricarbonyl complex had previously shown its efficiency for various alkylation reactions. Unfortunately, only the analogous ruthenium complex **Ru1** provided interesting results. We decided to explore in detail this alkylation reaction, with various benzoyl hydrazines and alcohols. Density Functional Theory (DFT) calculations were performed at the Mo6/cc-pVTZ~sdd(PCM)//BP86/SVP~sdd level of theory using *t*-BuOH as a solvent.

3. Results and discussion

A wide range of primary and secondary alcohols were introduced in this reaction affording mono- and dialkylated acyl hydrazides in moderate to good yields (Joly, Bettoni, Gaillard, Poater, & Renaud, 2021; Scheme 1, (1)). In addition, DFT calculations and the %V_{Bur} of the DFT-optimized alcohols provided mechanistic insights and allowed us to explain the selectivity. Mono- versus dialkylation selectivity can now be anticipated with this catalytic system as it depends on the steric parameters of the alcohol. Next, we focused our research on the synthesis of non-symmetric dialkylated acyl hydrazides involving two different alcohols (Bettoni *et al.*, 2021; Scheme 1, (2)). The success of each reaction relies on the difference of reactivity between the two alcohols. Indeed, dehydrogenation of methanol is the most energy-demanding oxidation step compared to other alcohols. Deuterium experiments confirmed that both alcohols are involved in the borrowing hydrogen process. DFT calculations show that the formation of the cross-dialkylation product cannot be perfectly explained neither structurally nor electronically, but might be dependent of the physical state of the aldehyde or ketone intermediate (gas vs. liquid) at the reaction temperature.



Scheme 1. Mono- or dialkylation of benzoyl hydrazines catalysed by Ru1.

4. Conclusions

Our research disclosed a first phosphine-free ruthenium complex-catalysed mono-alkylation, dialkylation and cross-dialkylation of acyl hydrazide using alcohols as pro-electrophiles. We tested various benzylic, cyclic and aliphatic primary and secondary alcohols. The first cross-dialkylation of hydrazides in one pot was catalysed by the ruthenium complex **Ru1**. DFT calculations clearly explained the observed selectivity favouring the mono- or the dialkylation with the calculation of the %V_{Bur}. They also confirmed that methanol was the more reactive as a pro-electrophile, favouring the formation of the dimethylated product.

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LINKING DOM FRACTIONS AND THMFP IN DRINKING WATER BY AN ENHANCED HPSEC-DAD-DOC ANALYTICAL APPROACH

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Keywords: drinking water, disinfection by-products (DBPs), HPSEC-DAD-DOC, THMFP, multiple linear regression (MLR)

1. Introduction

Dissolved Organic Matter (DOM) is considered one of the main precursors of DBPs in drinking waters. Understanding its physical and chemical characteristics to improve treatment processes is of paramount importance. Size exclusion chromatography with organic carbon and UV254 Detection (LC-OCD) method, developed by Huber, Balz, Abert, & Pronk (2011), provides qualitative information about DOM composition useful to bridge the gap between techniques with high compound identification potential (i.e. MS detection-based) and those with high mass balancing potential (i.e. bulk DOC). However, the impact of molecular weight (MW) fractions from LC-OCD on DBP formation has only recently been evaluated (Carra *et al.*, 2021).

2. Hypothesis

This work aims to evaluate possible correlations between the different MW DOM fractions obtained by a modified LC-OCD separation method and the gains achieved by improving resolution and exploiting the simultaneous spectroscopic measurements at multiple wavelengths by detecting hyphenated high performance size exclusion chromatography with diode array and dissolved organic carbon (HPSEC-DAD-DOC).

3. Methodology

Water samples (21) were collected in three drinking water treatment plants (DWTPs) located in NE Spain (Llobregat, Ter and Cardener). Trihalomethane formation potentials (THMFPs) for trichloromethane, bromodichloromethane, dibromochloromethane, and tribromomethane were determined following standard procedures. DOM fractionation was determined by HPSEC-DAD-DOC and the results were contrasted with the LC-OCD separation carried out by Het Water Laboratorium (Netherlands). Acquired chromatographic signals were processed with OriginLab software to perform deconvolutions and spectroscopic calculations. Multiple linear regression (MLR) models were adjusted and simplified (Rstudio) to correlate THMFP among DOM fractions.

4. Results and discussion

Fractionated parameters presented better correlations among THM congeners than bulk 254 nm and DOC measurements. Additionally, improvements in the chromatographic separation method led to better models to explain the relationship between THMs and the DOM fractions in a majority of congeners. High values of R^2_{adj} reject that goodness of fit because of the high number of predictors (7 MW fractions).

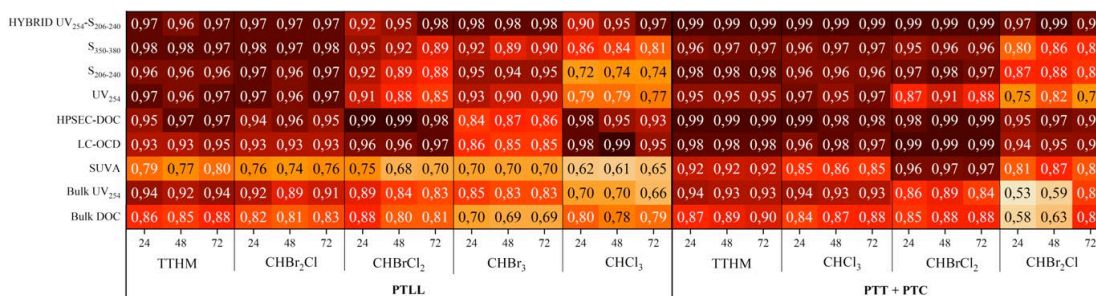


Figure 1. Adjusted R^2 coefficient heatmaps of the MLR models fitting DOC and spectroscopic parameters after fractionation, and bulk DOC and absorbance at 254 nm for brominated samples (Llobregat DWTP (PTLL) left) and low brominated samples (Ter (PTT) and Cardener (PTC), right). *LC-OCD measurements did not include samples from the Cardener DWTP. On the x-axis, species are shown according to their prevalence.

Moreover, spectroscopic-based models also presented good correlations (high R^2_{adj} values), especially with the total THMs, which could become a helpful tool to simplify the necessary setup and establish a smoother analytical routine.

5. Conclusions

In view of the results, separation through HPSEC-DAD-DOC could provide useful information, especially regarding spectroscopic approaches, to link different DOM fractions as main THM precursors. That could be of major interest for the optimization of treatment processes in DWTPs.

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A DFT STUDY OF THE N₂O FUNCTIONALIZATION FOR THE PREPARATION OF TRIAZOLOPYRIDINE AND TRIAZOLOQUINOLINE SCAFFOLDS

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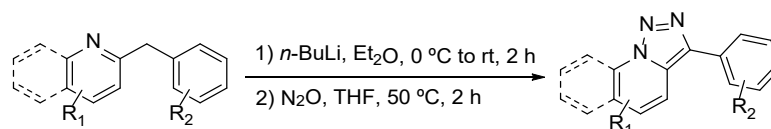
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Keywords: DFT, nitrous oxide, diazo, triazolopyridines, triazoloquinolines, prediction

1. Introduction

Nitrous oxide is a well-known reagent used in synthetic chemistry, mainly due to its oxidant properties (V. Leont'ev, A. Fomicheva, V. Proskurnina, & S. Zefirov, 2001), which enable it transfer an oxygen atom to the desired product (Severin, 2015), but it can also be a nitrogen donor. It was not until the last decade that N₂O was used for the first time as a nitrogen-atom donor for the preparation of organic nitrogen-containing molecules under efficient synthetic procedures.

Landman, Fadaei-Tirani & Severin (2021) reported the functionalization of nitrous oxide for the synthesis of triazolopyridines and triazoloquinolines, which are useful building blocks for heterocycle synthesis. The reaction was performed in two steps (Scheme 1).



Scheme 1. Experimental reaction conditions for the functionalization of nitrous oxide.

2. Hypothesis

We thought that density functional theory (DFT) calculations on the experimental results could help to understand how the functionalization of N₂O for the preparation of triazolopyridine and triazoloquinoline scaffolds work and to improve the experimental performance of such a transformation.

3. Methodology

The mechanism was unveiled at the B₃LYP-D₃(SMD)/Def2SVP level of theory using tetrahydrofuran as a solvent. For better accuracy, single-point energy calculations were carried out at the B₃LYP-D₃/Def2TZVP level of theory, again considering the explicit solvent effects by SMD. The rate-determining step of the reaction was studied in detail to find correlations.

4. Results and discussion

The reaction profile starts with the lithiation of the initial 2-(phenylmethyl)pyridine, followed by the nucleophilic attack from the metalated species to the terminal nitrogen atom of nitrous oxide. Then, a hydrogen transfer and the generation of LiOH takes place, as the rate

determining step (rds) of the reaction, giving rise to the diazo species that can cyclize to form the final triazolopyridine or triazoloquinoline scaffold (see Figure 1). A direct correlation is identified when the yield of the experimental scope is plotted against the computed activation barrier.

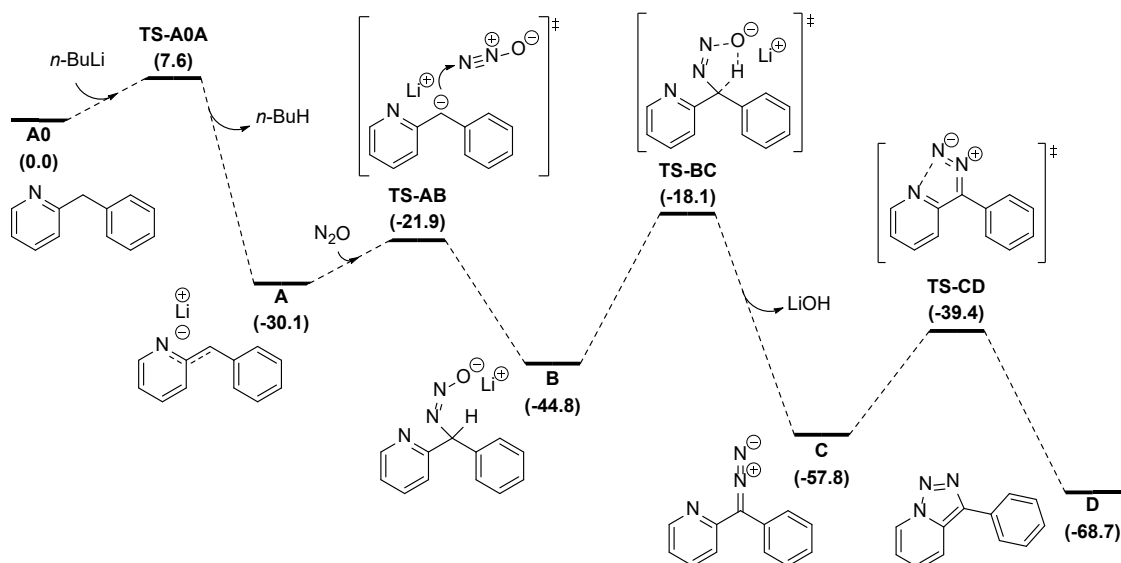


Figure 1. Full reaction mechanism (relative Gibbs energies in kcal/mol)

When the methods are computationally applied to the synthesis of triazolopyrazine, triazolopyridazine, triazolopyridimidine and triazolotriazine scaffolds, lower energy barriers for the rds are observed, indicating the feasibility of their preparation.

5. Conclusion

The mechanism of the functionalization of N_2O for the synthesis of triazolopyridine and triazoloquinoline scaffolds has been unveiled by means of DFT calculations. We also predicted the feasibility of the preparation of a wide variety of nitrogen-containing heterocycles as well as sulphur and oxygen-containing diazo species.

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A VERSATILE AND COMMERCIALY AVAILABLE IRON CATALYST ACTIVE IN CARBENE TRANSFER REACTIONS

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Keywords: iron, carbene, transfer, commercial, synthesis

1. Introduction

The development of C-H functionalization reactions catalyzed by non-precious metals is an important aim for gaining sustainability in chemical synthesis. In 1992, Hossain reported the first example of carbene transfer reactions using iron as a catalyst, $[\text{CpFe}(\text{CO})_2(\text{THF})]\text{BF}_4$ (Seitz, Saha, & Hossain, 1993). With this as a starting point, over the past decades iron has exhibited promising results in this field (Damiano, Sonzini, & Gallo, 2020).

We have recently described a synergy between an iron catalyst, $[\text{Fe}(\text{Fpda})(\text{THF})]_2$, and a lithium aluminate salt, $\text{Li}[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]$, which activates azoesters under mild conditions, promoting both intramolecular and intermolecular functionalization of strong $\text{Csp}_3\text{-H}$ bonds *via* carbene insertion (Hernán-Gómez, Rodríguez, Parella, & Costas, 2019; Rodríguez, Font, Nadal-Moradell, Hernán-Gómez, & Costas, 2020).

2. Problem

Despite the great reactivity shown by $[\text{Fe}(\text{Fpda})(\text{THF})]_2$ on the activation of $\text{Csp}_3\text{-H}$ bonds, it presents some drawbacks for it to be synthetically appealing. Two of the most critical are: (1) its extreme sensitivity to air and moisture, which make it difficult to prepare and store, and (2) the generation of considerable amounts of “hydride shift” side products.

3. Methodology

We aim to achieve carbene transfer reactions using commercially available iron catalysts as well as diazo compounds as carbenes precursors. All the chemistry is performed under strict inert atmosphere due to the air and moisture sensitivity of the system.

4. Results and discussion

During our research, we have been able to identify a much simpler and manageable catalyst, $[\text{Fe}(\text{acac})_3]$, which exhibits superior performance. Of important to note is that $[\text{Fe}(\text{acac})_3]$ is commercially available, cheap and air/moisture stable.

$[\text{Fe}(\text{acac})_3]$ has shown excellent selectivity, practically avoiding the formation of “hydride shift”, and being able to be operative with only a 5% of $\text{Li}[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]$, a five-fold reduction when compared to our previous system.

On top of that, $[\text{Fe}(\text{acac})_3]$ has proven to be a versatile catalyst achieving good yields in intermolecular C-H insertion and cyclopropanation reactions, and it is also able to access to Buchner ring expansion products generating cycloheptatriene derivatives.

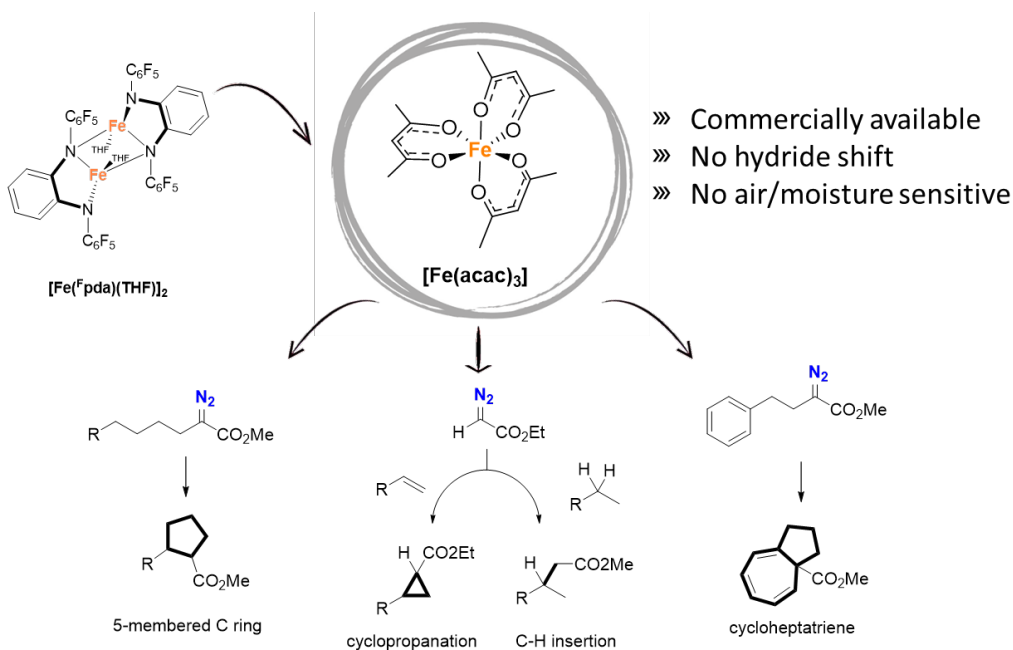


Figure 1. Versatility of $[\text{Fe}(\text{acac})_3]$ as a catalyst

5. Conclusion

In conclusion, the superior catalytic performance and versatility of $[\text{Fe}(\text{acac})_3]$, together with its commercial accessibility, make this complex stand out as a powerful synthetic tool in the field of carbene transfer reactions.

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NICKEL-CATALYZED C_{sp2}-OME FUNCTIONALIZATION FOR CHEMOSELECTIVE AROMATIC HOMOLOGATION EN ROUTE TO NANOGRAPHENES

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Keywords: Ni-catalyzed, C_{sp2}-O activation, aromatic homologation, directing group, nanographene

1. Introduction

Metal-catalysed cross-coupling transformations have revolutionized organic chemistry, representing some of the most fundamental platforms to form C-C and C-heteroatom bonds. The classic reaction is based on the use of organometallic species and prefunctionalized substrates such as organic halides as electrophiles (Arun Kumar *et al.*, 2016). Activation of C_{sp2}-O bonds of aryl ethers by transition metals is much more difficult than the activation of aryl halides, thus their use as electrophilic counterparts in cross-coupling protocols is much more limited. Among all the transition metals, Ni-catalysed C_{sp2}-OR activation has become the methodology of choice to cleave these strong bonds (Tobisu & Chatani, 2015). Recently, the QBIS-CAT group reported a nickel-catalysed C_{sp2}-F functionalization with internal alkynes to form either alkyne monoannulation or aromatic homologation products in a chemodivergent manner using 8-aminoquinoline as directing group (Capdevila *et al.*, 2019). This strong bond C_{sp2}-F activation set the stage to attempt an analogous methodology to activate C_{sp2}-OMe.

2. Methodology

Preparation and handling of air-sensitive reagents were carried out in a N₂ glovebox.

Substrates have been synthesized following reported procedures, and all products have been purified by chromatography column and characterized by 1D and 2D NMR.

3. Results and discussion

First, we focused on the selective functionalization of C_{sp2}-OMe bond over C-H bonds using internal alkynes with a similar methodology as for the C_{sp2}-F substrates recently reported by the group. We screened different directing groups: 8-aminoquinoline, 2-pyridylisopropylamine, and 2-pyridylmethylamine at the *ortho* position with respect to the C_{sp2}-OMe bond. We could only achieve the selective functionalization using the 8-aminoquinoline as directing group. At this point, we optimized the conditions of the reaction. We observed that we could selectively form the aromatic homologation product adding two equivalents of LiOTf and we could change the chemoselectivity of the monoannulation with

the addition of PPh_3 . Interestingly, the 1,2,3,4-tetraphenylnaphthalene unit in the homologation could undergo a DDQ oxidative coupling to synthesize nanographene-like compounds.

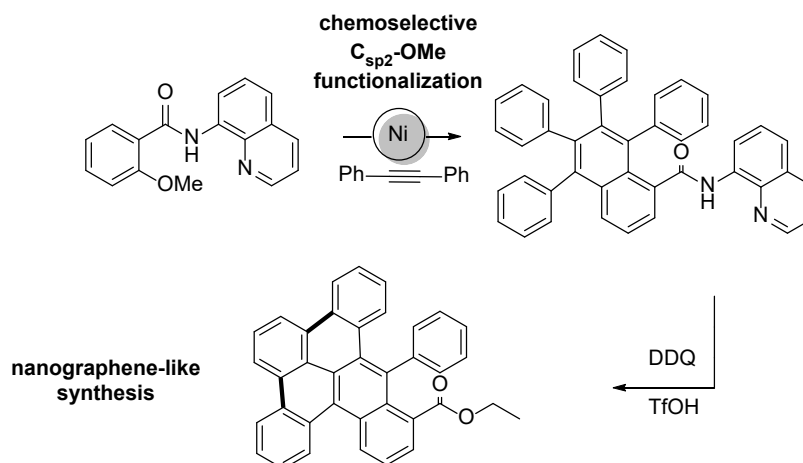


Figure 1. Ni(o)-catalysed methodology to achieve the $\text{C}_{\text{sp}^2}\text{-OMe}$ functionalization and the diversification towards nanographene-like synthesis.

4. Conclusions

In summary, we have developed a Ni-catalysed selective functionalization of $\text{C}_{\text{sp}^2}\text{-OMe}$ substrates bearing bidentate directing groups (DG), using diphenylacetylene as a non-activated coupling partner to render the corresponding aromatic homologation product and the alkyne monoannulation product in variable proportions (Capdevila, Sala, Ackermann, & Ribas, 2022). Furthermore, we have demonstrated that aromatic homologation products are valid precursors towards bottom-up nanographene-like synthesis.

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EVALUATION OF ELECTRONIC ASPECTS AND HAT MECHANISM IN NICKEL-HYPOCHLORITE SPECIES

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Keywords: nickel, ligands, electronic effects, reaction mechanisms, oxidations

1. Introduction

Oxidations of inert C-H bonds catalysed by transition metals are important reactions in synthetic chemistry. High-valent metal-oxygen species are often involved in these reactions as key reactive intermediates, thus making their study essential. Oxidations through high-valent M-O species are inspired in natural metalloenzymes commonly based on Fe (Meunier, de Visser, & Shaik, 2004), although enzymes based on less common metals, like Ni, can also form these reactive species (Barondeau, Kassmann, Bruns, Tainer, & Getzoff, 2004).

Despite many examples of well-defined high-valent Ni-O species reported in the literature, most of them show poor reactivity. In 2015, our group reported the synthesis of a Ni^{II} complex bearing a bis-amidate N-based macrocyclic ligand, **1^H**, which is an excellent platform to support high-valent Ni-O reactive species, like **2^H** (Corona *et al.*, 2015) and **3^H** (Corona *et al.*, 2016) (Figure 1). Especially interesting is **3^H**, which shows very high reaction rates in hydrogen (HAT) and oxygen atom transfer (OAT) reactions compared to other Ni-based systems.

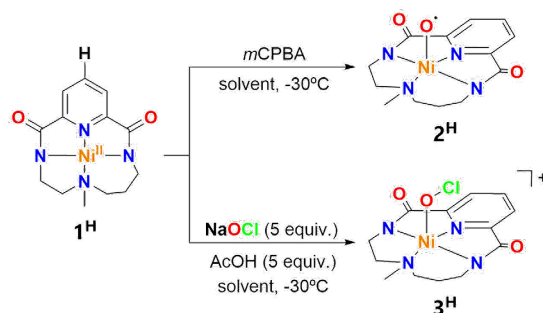


Figure 1. Generation of **2^H** and **3^H** upon reaction of **1^H** with *meta*-chloroperbenzoic acid (*m*CPBA) and sodium hypochlorite (NaOCl), respectively.

2. Methodology

Two new electronically tuned complexes, **1^{OMe}** and **1^{CF3}**, were synthesized according to modified reported procedures, and characterized by NMR and UV-Vis spectroscopy. Generation and reactivity of the nickel-hypochlorite species **3^H**, **3^{OMe}** and **3^{CF3}** were monitored by UV-Vis spectroscopy at -30°C. Stability of Ni-OCl species was evaluated recording the self-decay experiments. Reaction of Ni-OCl species with organic substrates followed pseudo-first order kinetics, thus making possible the calculation of the observed rate constants (k_{obs}) and reaction constants (k) for each studied reaction with the spectroscopic data obtained.

3. Results and discussion

Generation of the reactive species **3^H**, **3^{OMe}** and **3^{CF3}** was successfully achieved (Figure 2), and relative stability was studied by calculating the half-life time ($t_{1/2}$) for each species. Reactivity of these Ni-OCl intermediates was tested with 1,4-cyclohexadiene (HAT) and 1-octene (OAT)

(Figure 2). According to the results, **3^{CF3}** is the most reactive and unstable Ni-OCl species studied. Furthermore, **3^{OMe}** is slightly more stable than **3^H**, although no remarkable differences among them were found in terms of reactivity.

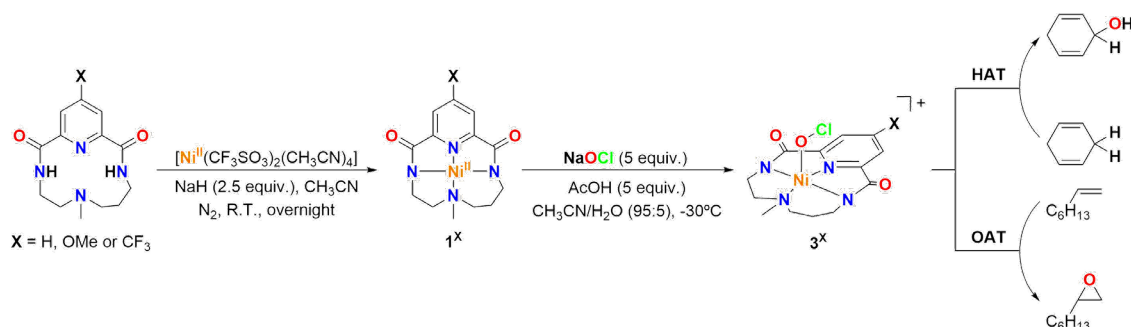


Figure 2. Synthesis of electronically tuned complexes, **1^X**. Generation of **3^X** upon reaction of **1^X** with NaOCl. Reactivity of **3^X** with organic substrates in HAT and OAT.

4. Conclusions

The addition of an EWG to **1^H** resulted in the formation of a more unstable and reactive Ni-OCl species, **3^{CF3}**. Nonetheless, the addition of an EDG did not represent a significant change neither in the stability of the reactivity of **3^{OMe}** compared to **3^H**.

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GOLD(I) SUPRAMOLECULAR ASSEMBLIES TO ACHIEVE PHOSPHORESCENCE EMISSION

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Keywords: gold(I), luminescence, phosphorescence, supramolecular, photophysical

1. Introduction

Luminescent materials (Lima & Rodríguez, 2011; Pinto, Svahn, Lima, & Rodríguez, 2017; Pujadas & Rodríguez, 2020) are known to absorb light and then emit it because of different pathways followed by their excitons. One mechanism can provide phosphorescence emission, which is very useful in several fields (He & Yam, 2011; Nielsen, 2016), such as materials (e.g. OLEDs, sensing) or biology (e.g. anticarcinogenic therapy).

This emission is not easy to achieve because thermal deactivation or oxygen quenching can prevent it. Nevertheless, scientists have focused on its promotion since it is a more efficient emission than fluorescence. That is because the excitons formed when the molecule is excited recombine themselves and 75% of them end up in the triplet state, which is the one responsible for phosphorescence emission. Therefore, avoiding the loss of these excitons will efficiently obtain luminescent material.

2. Methodology

The population of the triplet state can be harvested by promoting the intersystem crossing process, which allows the transition of the excitons from the singlet excited state to the triplet excited state. This transition is forbidden, but thanks to the introduction of a heavy atom such as gold, it can be induced.

Different strategies can be used to prevent the relaxation of the triplet excitons by non-radiative pathways.

In order to prevent thermal deactivation, the compounds can be immobilized in thin films to reduce the vibrational loss of energy. In addition, oxygen quenching can be overcome by saturating the atmosphere with nitrogen gas, which does not quench the T₁ excitons.

3. Results

During this project, different strategies have been tested to overcome the drawbacks mentioned previously. The inclusion of gold(I) compounds in organic matrixes (Figure 1) has been used (de Aquino, Caparrós, Aullón, *et al.*, 2021; de Aquino, Caparrós, Truong, *et al.*, 2021), so the vibrations that promote non-emissive relaxation decays can be prevented or reduced. Another method uses liquid nitrogen to decrease the temperature, so the vibrations do not occur in a significant way. On the other hand, oxygen quenching can be overcome by saturating the atmosphere with nitrogen or argon.

As can be seen, multiple strategies can be followed in order to promote this desired phosphorescence emission.

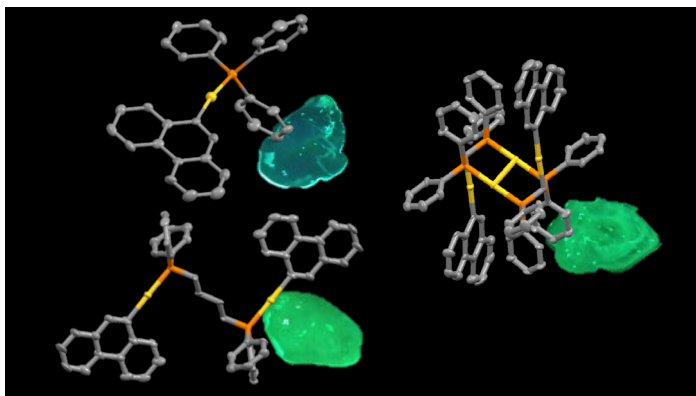


Figure 1. Gold(I) derivatives immobilized in organic matrixes.

4. Conclusions

Phosphorescence emission can be achieved by several methods. In our work, we use heavy atoms in the chemical structure of the molecules. We study in detail each system and choose the most suitable strategy to improve this type of emission.

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SESSION VII. ARCHITECTURE AND CONSTRUCTION

THE TEMPLES OF THE SOUTHERN AREA OF EMPÚRIES' NEAPOLIS

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Keywords: temple, ritual, worship, Empúries, ancient Greek world

1. Introduction

The study of the southern area of the Greek city of Empúries has led to establishing a series of phases that reflect its chronological evolution resulting from the various reforms carried out there. In addition, architectural, sculptural and epigraphic elements gathered and documented in the sector throughout the excavations help understand it as a whole.

2. Hypothesis

In the Greek city of Empúries the sanctuaries are located in a specific space, which, far from being random, is the result of a plan designed by those who shaped the urban planning of the city: the southern area has a sacred connotation.

Considering that the sector had been in use for a long period, it was adapted according to the needs of the times and gave rise to several changes and renewals, following the will of the society and the urban solutions of the moment.

The cults associated with the area refer to deities related to medicine and healing, evidenced, for example, by sculptural findings or a series of anatomical votive offerings documented in the area.

3. Methodology

The study of documentation from the excavations carried out in the southern area has led to the creation of a database that brings together the most significant sculptural, architectural and epigraphic materials of the sector. Introducing the documentation coordinates of some of the materials into a geographic information system (GIS) and visualizing their location have revealed some areas with a high density of materials, allowing scholars to make hypotheses of various sorts.

4. Results

A historical sequence has been proposed, showing the structures built in each century. Thus, a suburban sanctuary was built in the 5th century BC (Sanmartí i Grego, Castanyer i Masoliver, & Tremoleda i Trilla, 1992). A new defensive enclosure went up in the 4th century BC (Sanmartí i Grego, Castanyer i Masoliver, & Tremoleda i Trilla, 1988) with a temple and an altar inside. New walls were built in the 2nd century BC (Sanmartí i Grego, Castanyer i Masoliver, & Tremoleda i Trilla, 1990) as well as a porticoed square (implying a great renovation). Finally,

new temples were erected and remodelling took place between the 1st century BC and the imperial period (Sanmartí i Grego *et al.*, 1990).



Figure 1. Southern area of the Greek city of Empúries

5. Conclusion

Although the research is not completed, the part that has been carried out so far seems to confirm the hypotheses raised: the southern sector was the sacred area, and, despite experiencing remodelling, over time it maintained a cult character, associated with health deities.

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ARCHITECTURE AND MEMORY: THE (RE) PRESENTATION OF THE PLACE

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Keywords: architecture, place, collective memory, representation, narration

1. Introduction

The relationship between architecture and memory is very close (Huyssen, 2003) because memory always tries to locate, to find the place of something that has happened in the past (Halbwachs, 2004). This means that it works with space-time co-ordinates and social recognition, as it is with architecture (Muntañola Thornberg, 1973, 2006). Losing memory is not losing the ability to record anything (Freud, 1917; Ricoeur, 2000b), but losing the ability to place things in a physical space-time and refer to what they mean socially (Huyssen, 2012; Lynch, 1960).

Therefore, the second part of the title refers to (re)presenting places. We will take the socio-physical definition of place to approach the notion of place based on the definitions of Khôra by Plato and Derrida (Derrida, 1989), Aristotle's Topos, Rossi's Locus (Rossi, 1972) and Norber-Schultz's Genius Loci (Norberg-Schulz, 1979), among others.

2. Methodology

Our understanding of representation is threefold: as the act of crossing history and fiction, as the action of re-presenting, and as a project of the future. The places are the spaces that make possible collective communication; thus, they are spaces of memory and narration (Bajtín, 1982, 1989). We will argue that memory is a source of representation and exploration of place and a reflection on the individual and collective present and past (Nietzsche, 1974). We will also analyse, through architectural projects, how the relationship between narrated time and constructed space occurs (Ricoeur, 1983, 2000a, 2000b).

The projects of architects such as Sverre Fehn (Norberg-Schulz & Postiglione, 1997), John Hedjuk (Hejduk, 1998) and Dimitri Pikionis, among others, allow us to explore the past. We will delve into figures such as *the ghost*, the trace or *the invisible*; into poetics created from *homo rhythm*, *significant opposition* or *the continuous flow of history*; and into the sense of actions such as *specialising time*, *erasing / forgetting* or *reviving a myth*.

3. Results

The analysis of the meaningful reading and interpretation made by the inhabitants of a place will allow us to grasp the meaning of these concepts and will enable us to study the relationships, parallels and interactions between the two types of (re) presentations, those of architects and those of inhabitants.

4. Conclusion

The research will examine the identity between the autonomy of the built object and the social and individual representation of architecture, and will introduce time and otherness as design factors. In this way, through *Architecture and Memory: the (Re) presentation of the Place*, we will understand architecture as the place where the two vectors intersect, the spatial – between the self and the others – and the temporal –between the past, present and future.

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LE DÔME, THE NEW GENERATION RESEARCH CENTRE IN CAEN: A CASE STUDY OF RESILIENT ARCHITECTURE

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Keywords: resilient architecture, freespace, spatial indeterminacy, change of use, sustainable development

1. Introduction

The New Generation Research Centre, known as Le Dôme, was part of the regeneration plan of a former industrial area on the Caen peninsula in France. The project, designed by the Parisian architectural firm Bruther in 2015, is a compact building extended vertically that reinterprets the structural system of a hangar to achieve the maximum open plan and to provide overlapping platforms (Cecilia & Levene, 2018; Dorval-Bory, 2015). Le Dôme consists of three double-height storeys, each with different configurations of independent mezzanines (Ursprung, Rojas, de Vylder & Bruther, 2017). The main bulk rises from the ground, offering a large double-height, covered public square, and presents a variety of autonomous, overlapped *freespaces* up to the roof, which act as artificial urban grounds by emphasizing the horizontal plane. *Freespace* (Farrell & McNamara, 2017) enables the evolution and persistence of Le Dôme and the change of uses over time.

2. Methodology

Le Dôme serves as a case study to theorize resilient architecture within a grounded theory methodological framework. Data was collected for this case study through a methodological triangulation: interviews, observation notes and secondary research. The architectural firm Bruther and three inhabitants of Le Dôme were interviewed in 2021, using semi-structured interviews.

3. Results and discussion

Thanks to the *freespace* planning, Le Dôme's architectural system has the resilient properties of persistence, adaptation and transformation. *Freespace* is an indeterminate space due to its excess of space and its redundancy of components, which facilitates the evolution and change of uses of space over time according to the needs of the inhabitants. Bruther was proactive, adjusting to the available budget through the *bricolage* technique and the overlap of layers, in order to offer the maximum intelligibility and operability of the *freespaces* for the future appropriation of the inhabitants.

4. Conclusions

Le Dôme has generated a resilient architectural system. As a dynamic device, its resilient system consists of three dimensions: social, spatial and temporal. The inhabitants of Le Dôme can adapt and transform the *freespaces* to accommodate an open and changing programme. Their proactivity creates a self-organised system based on the overlapped *freespaces*. The evolutionary potential of Le Dôme's *freespaces*, their flexibility and the ease of replacing their layers autonomously can lead to the sustainable development of the building, since they contribute to reducing the probability of its long-term obsolescence and to confronting unpredictable or uncertain circumstances.



Figure 1. Exterior view of Le Dôme. Freespaces overlapped

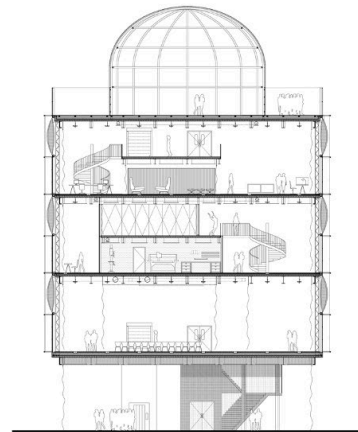


Figure 2. Cross section of Le Dôme, 2015

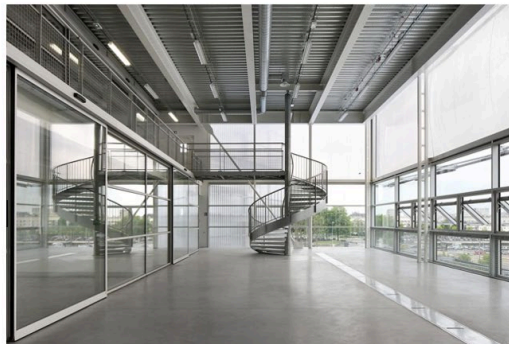


Figure 3. Freespace of the second floor, 2015



Figure 4. Intermediate *freespace* of the rooftop, 2015

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RE-INHABITING FROM THE ROOFS: INTERSECTIONS BETWEEN THE INHERITED CITY AND WHAT INTERVENTION PROJECTS DO. ROOFTOPS AND THE CITY OF BARCELONA

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Keywords: liveable rooftops, re-inhabit, operational methodology, atlas, Barcelona

1. Introduction

Nowadays most cities are overcrowded and the available urban spaces are insufficient to meet the needs of a growing urban population (Lefebvre, 2013). Therefore, instead of increasing the surface area of cities, it is time to think about making cities above the cities (Borja, 2010; Rudofsky, 1964). That means reusing unused spaces, such as most rooftops. Expanding cities from the rooftops could be a solution, adding new naturalized and community open spaces onto existing buildings (Sim, 2019).

Today's rooftop architecture has to learn from the past (Calvino, 1983). The vernacular and modern Mediterranean architecture are significant because they continue to provide new conceptions of rooftops as outdoor space to live in (Llorente, 2014; Portas, 1969; Venturi & Scott Brown, 2004). Their exploration will highlight the links between the habitability of rooftops (Delgado, Juan, & Pinarelli, 2012) and the urban environment.

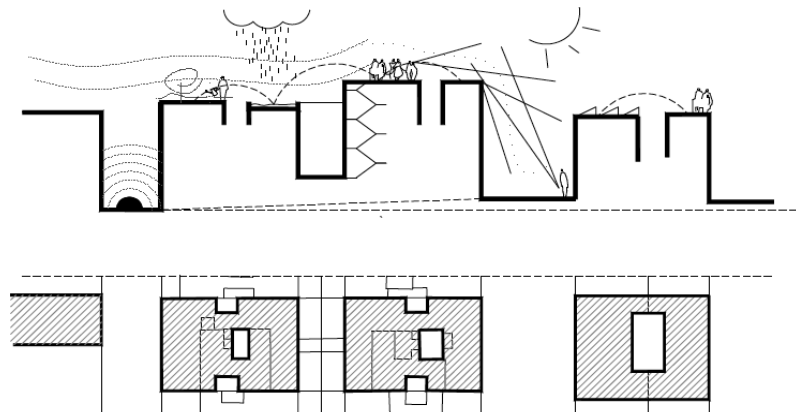


Figure 1. Diagram of parameters that define the roofs. Own elaboration.

2. Hypothesis

Rooftops are the last frontier in our overcrowded cities. Most of them remain underused and unloved, but they hold great potential as engines of sustainable urban development and therefore need to be reconsidered in the urban city contexts. The research question asks how important rooftop architecture could be in solving urban, economic, social and environmental issues.

3. Methodology

The research methods of the thesis unfold in three stages that complement each other. First, a review of the roof as a living space in Mediterranean architecture and more specifically in the urban development of Barcelona (Maas, van Rijs, & de Vries, 2021). This stage will be important, taking a more general view, discussing fundamental issues from rooftops, and establishing the basis of the research through a bibliographic review. The second stage will analyse all the information found and propose an operational methodology (analytical and design) for reusing rooftops (Gehl & Svarre, 2013). Finally, the methodology will be applied to the study of Barcelona through fieldwork on real cases.

4. Results

The main result will be a rooftop reuse atlas. The atlas will try to be a realistic and sometimes visionary approach to define how rooftops can be redesigned to become multi-layered in-between spaces of contemporary cities. This will be relevant to establish the basis for the urban development of rooftop landscapes.

5. Conclusion

There are three important conclusions. First, the relevance of the culture of inhabiting roofs in Mediterranean architecture and the ways of intervening in Barcelona today. Second, the need to propose an operational methodology for reusing rooftop spaces in any context. Finally, the main conclusion is the great potential of rooftops in sustainable urban development.

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DEFINING PARAMETERS OF VENTILATED FACADES AND THEIR INFLUENCE ON ENERGY PERFORMANCE

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Keywords: ventilated facades, air cavity, energy performance

1. Introduction

In the current climate emergency, any strategy or system that can reduce environmental impacts must be assessed. Ventilated façades can make progress in this direction by avoiding the overheating of sunny enclosures, thereby reducing the cooling demand (Sánchez, Giancola, Blanco, Soutullo, & Suárez, 2020; Soto Francés *et al.*, 2013). Architects lack the tools to know how design decisions (cavity width, joint height, outer sheet material, etc.) influence the energy performance of ventilated façades (Balter, Pardal, Paricio, & Ganem, 2019). The aim of this work is to develop a method for estimating that influence.

2. Methodology

An algorithm considering the defining parameters is developed and validated with data taken from real buildings. Once validated and applied, it can provide design guidelines for ventilated façades.

3. Results

Energy performance. There are four energy flows involved in energy performance: shortwave solar radiation, longwave infrared radiation, conduction, and convection. Additionally, material flow must be considered: air entering through the joints and moving along the cavity under the influence of the stack effect and wind pressure (Ibañez-Puy, Vidaurre-Arbizu, Sacristán-Fernández, & Martín-Gómez, 2017; Marinosci, Strachan, Semprini, & Morini, 2011). Any parameter affecting any of these flows will affect the overall performance.

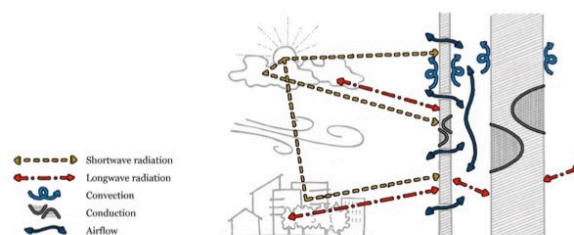


Figure 1. Energy and material flows in the ventilated façade.

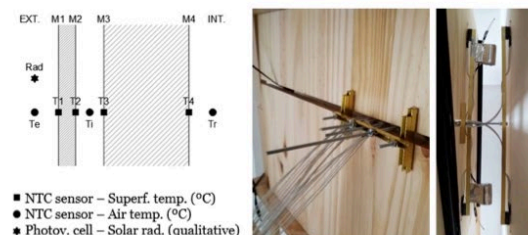


Figure 2. Diagram of measured temperatures and image of the clamp installed in a mock-up.

Algorithm development. The transient algorithm calculates the flows and the evolution of temperature on each surface; it also calculates the air circulation through electrical analogy (Soto Francés *et al.*, 2013). Once the whole daily cycle is complete, the algorithm displays the desired data, which can be used to draw conclusions.

Data measurement. The study of the air movement in the cavity is not for the movement itself, but rather its energy effect. To validate the algorithm, we need data over several days, from different points of the façade. Temperatures are measured with small sensors, without significantly affecting the performance of the measured facade. A clamp developed for this purpose attaches the sensors without dismantling or damaging the façade. Recent comparisons provide relatively good numerical correlations, as shown in the graphs below. This validates the algorithm.

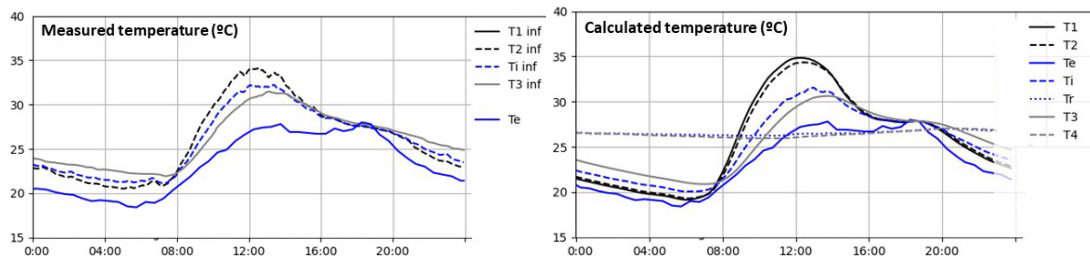


Figure 3. Measured and calculated temperatures in one of the studied cases: Omega UPC 23/06/2019.

4. Conclusions

The results obtained show that the proposed algorithm, once validated, can provide guidelines for the energetic design of the ventilated facade.

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SESSION VIII. ENVIRONMENT

COMPOSITIONAL AND BAYESIAN INFERENCE ANALYSIS OF THE CONCENTRATIONS OF AIR POLLUTANTS IN CATALONIA, SPAIN

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Keywords: compositional data, integrated nested Laplace approximation, air pollution, air pollutant, T-spaces

1. Introduction

According to the European Environmental Information and Observation Network (EIONET), the air pollutants that most affect health are coarse particles (PM₁₀), nitrogen dioxide (NO₂), ozone (O₃), carbon monoxide (CO), and sulphur dioxide (SO₂) ((EIONET), 2020; Sicard, Agathokleous, De Marco, Paoletti, & Calatayud, 2021).

Many countries have networks of pollutant monitoring stations, but they do not normally cover the whole territory. Therefore, to conduct a spatial and temporal study, it is necessary to use air pollution predictions in places without monitoring stations and at different times.

2. Methodology

The research was conducted as an observational, quantitative, retrospective, and longitudinal study. It took place in Catalonia, Spain from 2009 to 2019 and was based on the information concerning air pollutants that had been collected by 94 monitoring stations located throughout Catalonia (n = 10,081 records).

In our research, we combine two new approaches. To account for time, space, and covariates, Bayesian inference is used with integrated nested Laplace approximation (INLA) (Lindgren & Rue, 2015; Rue, Martino, & Chopin, 2009; Rue *et al.*, 2017). And compositional data (CoDa) analyse the relative concentrations of chemicals by means of balances (Pawlowsky-Glahn, Egozcue, & Tolosana-Delgado, 2015; Sánchez-Balseca & Pérez-Foguet, 2020) while total contamination is analysed by means of T-spaces (Pawlowsky-Glahn, Egozcue, & Lovell, 2014).

3. Results

Among all the pairs of air pollutants studied, the one with the most variability is that formed by O₃ and NO₂. This variance explains how high concentrations of O₃ are associated to low concentrations of NO₂ and vice-versa.

The balance of SO₂ over the remaining pollutants comes second in explained variance. This could be due to the strong presence of SO₂ in industrial and non-urban areas. On the other hand, it shows that other pollutants are higher in areas with dense road traffic.

The use of the INLA method in this study to predict the pollutant balances and the total temporality during 2019 confirms that the highest accuracy occurs in NO₂ with respect to O₃, and the worst in the balance between SO₂ and PM₁₀, NO₂, O₃ and CO.

4. Conclusions

The use of the CoDa method to analyse air pollution allows a better understanding of the data because it shows trade-offs between air pollutants in addition to overall pollution. The balances and the total become variables in the spatio-temporal analysis and along with the application of the INLA method make effective predictions about air pollution.

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EVALUATING THE EFFECTS OF LANDSCAPE CHANGE THROUGH THE DRYSTONE TERRACES IN THE HIGH MUGA VALLEY: TRANS-FRONTIER ENVIRONMENTAL AND PATRIMONIAL PERSPECTIVE

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Keywords: drystone-terrace abandonment, landesque capital, ecosystem services, biocultural heritage

1. Introduction

My thesis investigates drystone terrace bio-cultural heritage in the High Muga Valley (HMV), presenting a synopsis from the Northern Catalan sector.

2. Hypothesis

Terracing use, tenure, abandonment, regeneration, and perception are contingent upon the social order. Terraces are landesque capital and biocultural heritage. Ecosystem services depend on management and conditions. Ecological degradation mirrors social degradation. Rewilding and biocultural conservation must be integrated with human requirements to provide local food solutions, which presents a challenge for abandoned terraces. Terrace construction was initially environmentally destructive (Vera, 2002), and their social context varied over millennia. Terraces might therefore symbolise poverty, exploitation, hard labour, and degraded social conditions. They can provide sympathetic landforms as well as functional and biodiverse refuges, by retaining soils, controlling water, and enhancing moisture for crops (Montgomery, 2012). Farmland abandonment is extensive in the Mediterranean uplands: its drivers, tipping points, effects, and management are debated (Vila Subirós *et al.*, 2016). Interest in terrace ecosystem services is growing and 80% of previous farmland is revegetating (Khorchani, Nadal-Romero, Lasanta, & Tague, 2021). Traditional ecological knowledge and ancient, cross-border cultural meanings of cultivars and husbandry are lost (Puigmal & Duran, 1981; Vilar, 2019).

3. Methodology

I use historical ecological methods (Crumley, Lennartsson, & Westin, 2018) to identify and categorise archival, toponymical, cartographical research, and original ethno-historical interviews, comparing cross-border terraced land trajectories.

4. Results

Initial results show terrace diversity: classification, historic land use, land tenure, abandonment, land cover, current use, meaning. Now there are no cereal or sown forages produced. Some lands are horticultural, pastoral, and recreational, but many are abandoned. They are categorised as: 1. central village gardens; 2. peripheral village; 3. in previous common Lands, “Els Emprius”; and 4. associated with a ‘mas’. Few clues reveal the biography of terraced land use. Some 19th century sources refer to terraces for rye and other cereals (Cabanas, 2011), and oral traditions recall legumes, vegetables, potatoes, fruits, grazing, and apiculture.

5. Conclusion

By terracing, people optimised soils - with access to manures. The poorest lacked traction animals and worked sub-optimal strips by ‘foot’ with low yields. Terracing here was an inequitable ‘land-bank’, complementary to pastoralism and forestry. Most people left seeking industrialised lifestyles by the 1980’s. Terrace types were unequal, but the past teaches us that adaptive knowledge must be transferred to test ancient and new cultivars with rainwater capture, mulching, and no-till technologies. We cannot justify ecological destruction by clearing marginal lands for farming during a global food crisis, and we could restore selected terraces through equitable rural regeneration (<https://resilience.earth/project/femgarrotxa>).

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WATER REUSE FOR IRRIGATION: HOW TO PERFORM HAZARD CHARACTERIZATION FOR HUMAN EXPOSURE TO PHARMACEUTICALS ACCUMULATED IN FOOD CROPS

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Keywords: food, human health risk assessment, pharmaceuticals, reference value, water reuse

1. Introduction

To counter the growing natural water stress, the European Union's 'Circular Economy Strategy' drives the development of measures to promote water reuse and nutrient recovery. Careful consideration of the necessary safety requirements for water reuse and its application to irrigate crops for human consumption is required. The current water reuse regulation (European Union, 2020) restricts quality of reclaimed water using a set of standard parameters but includes organic micropollutants like pharmaceuticals (PhACs) in a list of potential hazards for future restrictions, if a human health risk assessment (HHRA) proves the concern is justified (EU 2020/741, annex II, section (B), point 6). The limited number of studies on the exposure to pharmaceuticals (including antibiotics) accumulated in food crops irrigated with reclaimed water use highly variable terminology and approaches for the hazard and risk characterization, which makes the identification of a preferred approach more difficult.

2. Methodology

Human health risk assessment (HHRA) approaches described in guidance documents of organizations like the EFSA, the EPA, and the WHO/FAO, as well as those applied in the literature were reviewed to prioritize the application of different hazard characterization approaches for PHaCs (including antibiotics) with different toxicological behaviour.

3. Results

HHRA estimates the probability of chronic adverse health effects in humans from daily exposure to chemical contaminants in environmental contaminated media over the course of their lives. The assessment consists of four main assessment stages (Figure 1).

During hazard characterization the threshold level (reference value) of exposure that is not expected to cause an adverse health effect, is calculated. The method to be applied contains the highest level of variability and uncertainty in the risk assessment. Guideline documents prioritize the calculation based on extensive toxicological experimental data (e.g., no or low-

observed-adverse-effect level (NOAEL/LOAEL) and benchmark dose lower confidence limit (BMD/BMDL)). However, it may be unfeasible to conduct extensive toxicological studies for the rising number of contaminants of concern detected in the environment. Consequently, most studies in the literature apply an estimation of the reference value based on the lowest therapeutic dose (LTD) (Christou, Karaolia, Hapeshi, Michael, & Fatta-Kassinos, 2017) and/or the in-silico modelling of a threshold of toxicological concern (TTC) based on compound's chemical structure (Liu, Liang, Liu, Zhao, & Han, 2020).

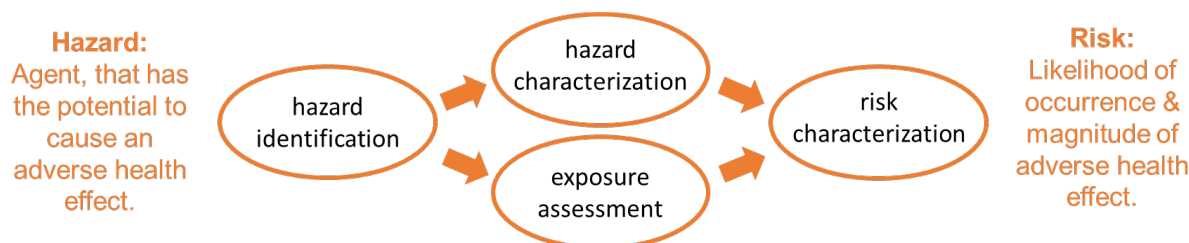


Figure 1. General HHRA scheme

4. Conclusions

A combination of the lowest therapeutic dose approach (applying (Snyder, Stanford, Bruce, Pleus, & Drewes, 2010) default safety factors) and the TTC approach (Kroes *et al.*, 2004) has been found to generate sufficiently conservative reference values for all the compared compound groups with different toxicological behaviour.

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ANALYSIS OF AFRICAN DUST INTRUSION AS AEROSOLS MODIFYING SOLAR RADIATION IN GIRONA (NORTHWEST IBERIAN PENINSULA)

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Keywords: aerosol, solar radiation, African dust, Iberian Peninsula

1. Introduction

Atmospheric aerosol loading constitutes one of the planetary boundaries, due to its effects on the global energy budget and consequently on climate and population at the regional level (Forster *et al.*, 2021). Aerosols can influence radiation directly by scattering and absorbing incoming radiation and indirectly by cloud-aerosol interactions. In the Iberian Peninsula, African dust intrusions are among the most relevant phenomena related to atmospheric aerosols (Querol *et al.*, 2010).

2. Hypothesis

This work aims to compile the episodes of African dust intrusion that have affected Girona in past years. Simultaneously, it will show how these episodes have affected the incident solar radiation.

3. Methodology

Information is collected about intrusion events that have affected Girona during a certain period (2009-2020) using a data base from the Spanish Ministry for Ecological Transition and the Demographic Challenge, as it has been recording these episodes for years due to the potential effects of particulate matter on human health. Treatment of surface radiation data is available at the UdG's Research Group in Environmental Physics for the selected intrusion episodes. Data collected with pyranometers reveals both global and diffuse irradiance (Calbó, González, & Sanchez-Lorenzo, 2017).

4. Results

With all the days during which there have been intrusions in the northeastern area of the Peninsula, different analyses have been carried out.

At first glance, we can see two different groups (Figure 1, left). The first one (2009-2014), where the average number of days with intrusion is around 50 days/year, and the second one (2015-2020), where there are 65 days/year. Statistical analyses will be carried out to see if this is significant. However, the number of events does not show any clear trend. On average over the entire time series (2009-2020), we have obtained a total of 58 intrusion days and 17 events per year.

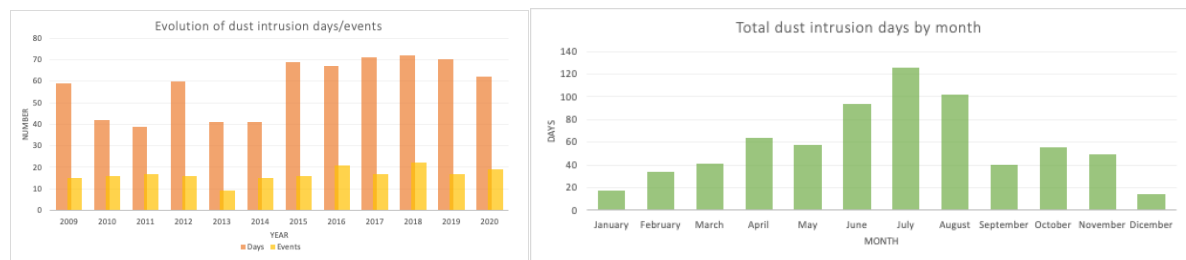


Figure 1. Left: Evolution of dust intrusions days/events in northeast Iberian Peninsula (2009-2020). Right: Summary of intrusion days by month for all the time series (2009-2020)

The months with the most intrusions are between June and August, with July having the most frequent ones (Figure 1, right). This is related to air mass formation processes in Africa, which are more frequent and intense in summer. Finally, Figure 2 shows an example of a 3-day intrusion where beam radiation decreases and diffuse increase.

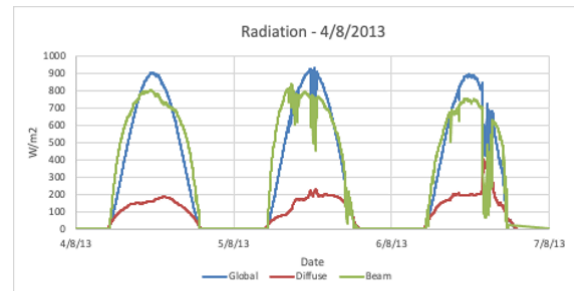


Figure 2. Global, diffuse and beam radiation (W/m²) from the Research Group in Environmental Physics' pyranometer (4-6/8/2013).

5. Conclusion

Figure 2 evidences that, for the date where we have recorded intrusion, there is effect on the type of radiation. However, since statistical analysis has not been carried out yet, we cannot state major conclusions.

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THE ANTARCTIC AS A SENTINEL OF GLOBAL POLLUTION

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Keywords: persistent organic pollutants, amplification, snow, sea-surface microlayer, Antarctica

1. Introduction

Persistent organic pollutants (POPs) have long lifetimes in the environment, accumulate in biota, and have the potential to reach remote regions such as the open oceans and Antarctica (Cai *et al.*, 2012; Casal, González-Gaya, *et al.*, 2017). Oceanic currents are thought to play an important role in the transport of POPs at regional and global scales. However, the Antarctic Circumpolar Current acts as a barrier, encircling the Antarctic and resulting in a weak north-south exchange of seawater (SW), and restricting the marine transport of POPs to this region. Nonetheless, despite its geographical isolation, some legacy POPs and some emerging contaminants are able to reach Antarctica. Polychlorinated biphenyls (PCBs) and organochlorine pesticides (OCPs) have often been studied as model compounds to understand atmospheric transport and deposition, accumulation in organisms, and biogeochemical cycling of POPs in polar regions and at the global scale. However, an increasing number of emerging POPs, such as organophosphate esters (OPEs) and poly- and perfluoroalkyl substances (PFAS), have been identified in Antarctica and the mechanisms driving their accumulation in different matrices are yet not fully understood.

2. Objectives

The goal of this study was to determine the presence and the dynamics of a wide range of both “legacy” and emerging POPs at coastal Antarctica. Specific objectives were to evaluate the relative importance of the atmosphere-land-water exchanges as the entry of POPs into Antarctic coastal waters, focusing on the role of snow deposition and melting as input of POPs there, and the sea surface microlayer (SML) amplifying the concentrations of PFAS in surface waters (SW) in ocean.

3. Methodology

Air, snow, the fugacity in soils and snow, SW, the SML and plankton were sampled in three sampling campaigns at Livingston and Deception Islands (South Shetlands, Antarctica), and analysed for PCBs, OCPs, polycyclic aromatic hydrocarbons (PAHs), PFAS and OPEs.

4. Results and discussion

Coastal SW mirrored the pollutant profile in snow⁴, consistent with the amplification of concentrations in snow and the snowpack releasing POPs to SW during the austral summer. The influence of snowpack and glacier inputs was further evidenced by the correlation between net volatilization fluxes of semi-volatile POPs and SW salinity. In addition, there was an amplification of PFAS in the SML and aerosols, supporting the role of sea-spray aerosol as a vector for long-range atmospheric transport of PFAS (Casas *et al.*, 2020). These results further indicate that the amplification of concentrations in snow and the SML contribute to the generalized occurrence in Antarctica of legacy and emerging organic pollutants with a wide range of physical chemical properties, and confirms the role of the polar regions as sentinels of global pollution.

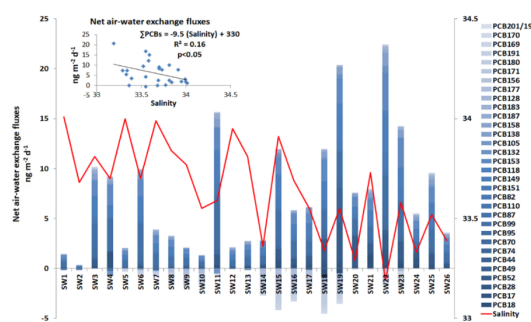


Figure 1. Net diffusive SW-air fluxes ($\text{ng}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$) of PCBs, and correlation between fluxes and salinity (Casal *et al.*, 2019)

5. Conclusions

These results indicate that the amplification of concentrations of pollutants in snow and the SML contribute to the generalized occurrence of legacy and emerging organic pollutants with a wide range of physical chemical properties in Antarctica. The measured amplification of concentrations in marine aerosols supports the role of SSA as a relevant vector for long-range atmospheric transport of PFAS. Our study in coastal Antarctica contributes to a better understanding of the role of polar regions as sentinels of global pollution.

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SESSION IX. SUSTAINABILITY AND SOCIAL CHANGE

REALITIES AND MYTHS OF YOUTH PARTICIPATION IN THE COMMUNITY

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Keywords: participation, youth, community, youth organizations, social change

1. Introduction

The current socioeconomic framework of precariousness and instability is generating effects on young people and, therefore, on their participation forms (Ballesté Isern & Feixa Pàmpols, 2019; Ferrer-Fons, 2020; García-Albacete & Lorente, 2019; Mora, 2020), which we cannot ignore. In addition, the structures and channels of youth participation are reproduced, largely, from the adult perspective, which lead to certain forms of participation that do not take into account the interests and needs of youth (Francés García, 2008). In fact, the different ways in which the young people participate in their environment are not appreciated and even ignored (Claret, 2014; Trilla, 2011).

2. Methodology

If we understand participation as the implication in actions or projects collectively with the capacity to influence one's own environment (Corbella Molina, Trull Oliva, Rodrigo-Moriche, & Úcar Martínez, 2021), young people have recently been participating and adapting to new times and new needs. Precisely because of this, it is important to know the opinion of young people and youth organizations regarding their own way of participating to guide the challenges and goals and to favour their participation in the community.

3. Results

Among the results that the thesis would like to obtain are the perspectives and interpretations of youth about *participation* and *community* as concepts. It also aims to reflect on which scenarios and imaginaries of community participation are being constructed. Through a case analysis of different organizations and youth movements, it aims to identify how the dynamics of participation display these perceptions and scenarios.

Ultimately, the intersection of this knowledge of perceived and actual reality can provide elements of contrast to elaborate new proposals for youth and community. Evaluations of youth participation, as well the spaces, processes, and moments in which they are made, should be possible. These are the challenges that will contribute to social change.

4. Conclusion

We ask young people about their participation and involvement in the community without knowing what they want and what they need. We should allow them enough space to rethink and reimagine new scenarios, moments, and processes of youth participation.

Participation in the social, political, cultural, and community affairs has always been an element of life in society, and can even be an indicator of democratic health and social citizenship that can contribute to transforming society and meeting current social needs (Font Redolad, 2014; Hart, 2009; Morales Morales & Rebollo Izquierdo, 2014; Morán & Benedicto, 2003)

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COMMUNITY MEDIATION AND VULNERABILITY. CHALLENGES AND LESSONS FROM A CASE STUDY IN OLOT (LA GARROTXA)

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Keywords: community mediation, vulnerability, social capital, participation, social policies

1. Introduction

The local sphere has recently become not only an increasingly relevant space for citizen participation but also a space for covering the needs of people (Blanco & Gomà, 2016). Sennet (2019) points out that, in the face of these circumstances, we must explore the skills needed to produce more sustainable environments, which promote diversity and relationships.

2. Hypothesis

With this research, we want to explore community mediation from the perspective of vulnerability and to attempt to confirm two hypotheses:

- (1) When the organization of communities is strengthened, this makes them more responsive to solving problems, which contributes to a decrease in vulnerability.
- (2) When communities are not organized, community mediation can become useful to articulate processes of transformation and to reinforce cohesion.

3. Methodology

For the case study, we focus on the interventions carried out in three groups of buildings from three different neighbourhoods in Olot where 394 families live. The empirical research uses a qualitative approach. A life story will be created for each of these buildings based on the actions carried out by the service, including more than 500 interviews, 40 neighbourhood meetings, community interventions such as painting buildings, clean-ups, neighbourhood activities and volunteer projects, and training sessions and conversation spaces among neighbours to exchange knowledge and experiences.

4. Results

With this empirical approach, we aimed to show how, in some cases, interventions have increased social capital and generated learning and actions in a self-organized way, promoting learning spaces and allowing the empowerment of people. However, the interventions have not led to a reduction in vulnerability and we detected difficulties in solving structural problems that could change people's living conditions and, at the same time, we have seen a need to promote interventions more continuously.

5. Conclusion

The analysed case shows the importance of connections among communities to take advantage of community capital, and highlights how community intervention can contribute to meet social needs and respond to the growing vulnerability in our societies by giving prominence to individuals and groups that are more and more involved in the transformation of their neighbourhoods (Rebollo, 2012).

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PROMOTING YOUTH COMMUNITY PARTICIPATION AS A BASIC STRATEGY FOR SOCIAL TRANSFORMATION

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Keywords: youth participation, community, empowerment, youth workers, social transformation

1. Introduction

The thesis proposal is part of the Industrial Doctorate Plan (DI) promoted by the *Generalitat de Catalunya*, in collaboration with public and private universities. The project links one of the *Liberi* research group's lines with work developed by the Catalan Youth Agency (ACJ) on community youth participation to provide useful knowledge for developing new youth policies. On one hand, the ACJ team wants to analyse the youth workers' role in community youth participation. On the other, the university group is working on the concept of youth empowerment, which could be conceptualized, among other ways, through community participation (Soler Masó, Trull Oliva, & Jiménez-Morales, 2018). In this interaction, the thesis aims to analyse the contribution of youth workers to youth empowerment through their community participation.

2. Hypothesis

The methodological approach used by youth workers can promote community youth participation as a privileged space for empowerment and as a basic strategy for social and community transformation.

3. Methodology

The thesis combines three papers. The first one focuses on knowing how socio-educational projects affect youth community participation. The second aims to review, with five youth worker focus groups, how they understand and develop youth community participation. The last paper tries to understand which spaces, moments and processes facilitate youth community participation using a mixed approach: nine life stories of youths and quantitative analysis of the results of the Youth Survey of Catalonia 2022.

4. Results

Socio-educational projects, with youth empowerment as a main goal, do not sufficiently encourage youth participation in their community. Consequently, the contribution of youth professionals as facilitators of youth community participation will be analysed, reviewed both from a professional perspective and from the voices of youths themselves.

5. Conclusion

The research aims to delve deeper into the youth policies debate and, specifically, to make known the role of youth workers in the strengthening of the community through their support for youth leadership and participation. We understand that social transformation will happen through community participation (Checkoway, 2009), which depends on youth leadership being developed (Benedicto & Morán, 2002; Francés García, 2008).

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PROFILE OF GIRONA ENVIRONMENTAL ACTIVISTS

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Keywords: territorial conflict, NIMBY, environmentalist collective, environmental activist

1. Introduction

The research aims to create a socio-demographic profile of environmental activists in the Girona region. More specifically, it aims to analyse the strengths, weaknesses, and challenges of different environmental groups (Castells, 1986, 2012; Chihu, 2006; Díez García & Betancor Nuez, 2019; Iborra, Martí, & Gomà Carmona, 2002) and the assessment of these political actors (Meyer & Gamson, 1999) in the face of possible energy transition scenarios.

2. Hypothesis

The research question asks whether the territory is in a moment of weakness with regard to the respective environmental groups and the explanatory hypothesis is that there is a lack of generational change in these movements. The research will attempt to verify two other hypotheses. The first is whether environmental activists in the Girona counties are mostly people who were not born or raised in the Girona counties. The second is whether a significant portion of environmental activists responds to the NIMBY phenomenon, as they have a second home in the Girona region and the protection of the landscape of their home drives them to mobilize.

One additional objective throughout the research consists of providing a cartographic representation of a node network locating the different environmental activist members of the environmental groups. A second objective involves mapping the interconnections between the groups to visualize the degree of cooperation and interaction between them (della Porta, 2013a, 2013b; McCammon, 2013). And a third objective is the elaboration of a report on the evaluation by environmental activists of the different scenarios of energy transition.

3. Methodology

The research methodology is diverse. First, as part of larger research projects such as *Paisatges Salvats*, the first stage of work consists of gathering a documentary collection of the various files already prepared by each of the environmental groups present in the counties of Girona.

In addition, conducting in-depth interviews with the different leaders of the largest environmental groups (one per region) [qualitative research] as well as surveying all activists [quantitative research] has been proposed. Having the contacts of the environmental groups thanks to the documentary archive of *Paisatges Salvats* means that they will have been informed of the research project and of the interest of different environmental actors in obtaining these data in order to identify the challenges facing the movement and be able to mitigate them more efficiently. The various groups, once contacted by the people behind *Paisatges Salvats*, will have sent this survey to their active members.

4. Results and discussion

The results show an evident lack of generational renewal but a high degree of cooperation between the different environmental entities. The results also indicate that the environmental movement is largely nourished by people from outside the counties of Girona. The environmental entities must discover why they are not able to incorporate new members. Environmental awareness in the population is high, but this has not translated into organized activity.

5. Conclusions

In conclusion, the territory is interconnected, cooperating as a community faced with environmental struggles, but with a great problem to solve: the lack of people to continue the half-century of work already carried out.

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INFLUENCE OF SMART CITIES' SUSTAINABLE TOURISM ACTIONS ON THE TOURIST SELECTION PROCESS: THE CASE OF BARCELONA

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Keywords: sustainability, tourism planning, tourism policy, tourist behaviour, destination branding

1. Introduction

The development of more sustainable tourist destinations depends largely on the strategies adopted by destination managers, which, depending on the actions carried out, make them valuable elements for the destination, residents, and visitors, while having an impact on its image and boosting its competitive advantage (WTO, 1994; Gunn & Var, 2002; Rivas García & Magadán Díaz, 2008). This paper aims to explore the influence of sustainable tourism actions undertaken by tourism boards in smart destinations on the tourist's process of selecting destinations. For this, we study the case of Barcelona as a smart destination model (López de Ávila Muñoz & García Sánchez, 2015) that integrates sustainability into its tourism policy.

2. Methodology

We will establish the sustainable tourism actions (Imbert-Bouchard Ribera, 2021) that the tourism board uses to plan and manage Barcelona as a destination, analysing the evolution of specific tourism plans and their progress towards sustainability (Crespi-Vallbona, 2020; Domínguez Pérez & Crespi-Vallbona, 2021). We will also study Barcelona's latest strategic tourism plans, dating from 2015 and 2020 (*Ajuntament de Barcelona*, 2009, 2016), which include specific sustainability-related actions around which the planning and management of the destination are currently centred. This will subsequently be used to build a solid state of affairs on which to focus the research.

Later, we will study the influence of these actions and their promotion of brand image, examining what influence they have on the tourist's process of selecting destinations. Finally, we will define the level of suitability of the different variables studied.

We will then create key performance indicators (KPIs) of sustainable tourism used by the Barcelona Tourism Board, which will be evaluated with Likert or Osgood scales. In addition to conducting a survey and contrasting the results with the tourist's perception, we will obtain real post-check-in results with which to make correlations.

3. Results

Urban tourism destinations that integrate sustainability policies into their management and planning are currently tackling fresh challenges by designing a new smart city model.

4. Conclusion

The managers of such destinations need to modify their management and planning strategies to integrate new variables. This requires in a need to know the degree of influence of their actions on the end recipient, thereby allowing them to create appropriate planning, management, and communication proposals for the consumer of this type of smart destinations.

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HOW DO WE SHAPE A SUSTAINABLE SOCIETY? FROM INTERGOVERNMENTAL PLANS TO THE ROLE OF CONSUMERS

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Keywords: sustainability, society, planning, consumers, capitalism

1. Introduction

Global society faces severe sustainability challenges at all three levels of the triple bottom line (TBL): environmental, social and economic. At a public level, such challenges are recognised and tackled through a top-down approach from intergovernmental to regional and local plans (Mensah, 2019; Michelsen, Adomßent, Martens, & von Hauff, 2016).

2. Problem

Current implementation of TBL-based planning on sustainability focuses strongly on the economic pillar, which upsets the triple equilibrium of the TBL and compromises the efficacy of plans on the environmental and social pillars. In addition, a lack of clarity in the field of sustainability science and around its concepts challenges reflections on public planning (Glavič & Lukman, 2007).

3. Methodology

First, the author carried out a literature review on sustainability science. Complementary to that, the author reviewed public planning for sustainability in the EU since the 1970s and made an extensive analysis of the European Green Deal as a masterplan for a sustainable Europe in 2050. On top of the above-mentioned, the author undertook a philosophical reflection on the role of society and the economy, based on the works of leading writers in the field. All these methods are part of the author's PhD research on sustainability quantification since fall 2019.

4. Results and discussion

Results of the literature review suggest that sustainability can be understood by society as its capacity to endure over time, and that the TBL is an approach that suggests a triple equilibrium among the basic pillars – economic, social and environmental. Other concepts such as sustainable development and the circular economy (Geissdoerfer, Savaget, Bocken, & Hultink, 2017), which are gaining momentum within the field of sustainability science, are explored and defined from a critical point of view.

Results of the review on policies and of the analysis on the European Green Deal (Siddi, 2020) suggest that the plan is not a masterplan for a sustainable Europe in 2050 mainly due to criticism on the actual sustainability of its guidelines, which favour economic growth over

sustainability. These results encourage the author to think about an approach towards sustainability other than a top-down one; here, the role of consumers as the base of a bottom-up approach for a sustainability transition is presented. To enable the empowerment of consumers, the challenges addressed should include the attitude-behaviour gap or clear information and, equally, the role of disinformation.

Results of the philosophical review on society and the economy suggest that society's main role is to satisfy the human needs of its individuals, for which the economy should not be considered as a pillar of society. Instead, the author suggests a more appropriate consideration as a means towards achieving the goal of sustainability, which would be based only on the environmental and social pillars.

5. Conclusions

Results of this work suggest the need to move from TBL-based sustainability towards a stronger vision of sustainability, focused on the environmental and social pillars (Hereu-Morales & Valderrama, 2022). Also, bottom-up approaches towards sustainability transitions need to be enabled.

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SESSION X. MATERIALS APPLIED TO SCIENCE

INFLUENCE OF PSEUDO-DUCTILITY ON THE NOMINAL STRENGTH OF NOTCHED SPECIMENS

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Keywords: pseudo-ductility, translaminar toughness, nominal strength, stress concentration factor, numerical analysis

1. Introduction

Nominal strength (σ_N) – the ratio of peak load to net section area – of notched quasi-brittle materials like composites and concrete tends to two extremes (Maimí, González, Gascons, & Ripoll, 2013) depending on the relative size of the failure process zone to the specimen width (l_{FPZ}/W). If the failure process zone is relatively small in relation to specimen width ($l_{FPZ} \ll W$), the σ_N tends to the failure strength; on the other hand, if the $l_{FPZ} \gg W$ the specimen tends to the elastic limit (σ_f/K_t), where K_t is the stress concentration factor. Plasticity reduces the stress concentration factor by re-distributing the stresses around the notches, as does pseudo-ductility in extension. But plasticity is absent in composite materials. To improve the notched performance of composite materials, pseudo-ductility is actively pursued. Although, the K_t reduction in pseudo-ductile materials has been demonstrated for limited specimen sizes (Czél *et al.*, 2018; Fotouhi, Jalalvand, & Wisnom, 2018), strength over specimen sizes ranging from very small to very large – size-effect behaviour – are necessary for a comprehensive understanding of the influence of pseudo-ductility. The size effect law proposed by Bažant to determine the nominal strength is obtained by asymptotically matching these two limits (Bažant & Planas, 1998). Thus, we intend to obtain size-effect by conducting numerical parametric studies with different pseudo-ductile materials to elucidate its influence.

2. Methodology

We use an idealised material model representing the quasi-isotropic pseudo-ductile material, which we implemented as a user-material in the finite element (FE) tool (Abaqus). FE models containing typical notches like centre-crack, elliptical hole, and open hole of different sizes (Figure 1), ranging from 0.2mm to 160mm, were developed to determine the size-effect behaviour using the nominal strengths. To determine the limits, however, stress concentration factors of the corresponding pseudo-ductile material are required. By re-purposing some of the nominal strength models, the K_t is determined for the parametric material cases considered. We included a linear elastic case to validate the FE models.

3. Results and discussion

The nominal strengths obtained for the linear elastic models of all the notches (ε_{d1}) agree well with the size effect law (Figure 2), validating the developed FE models. In general, the pseudo-ductile material (ε_{d4}) recovers higher nominal strengths than the linear elastic counterparts.

Furthermore, nominal strengths from the FE models agree well with the elastic strength limit that we obtained using the K_t from the second set of FE models.

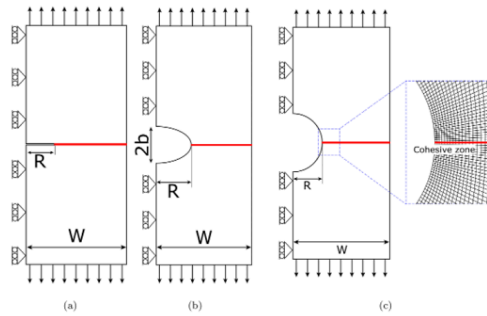


Figure 1. FE elements to determine nominal strengths containing centre-crack (a), elliptical-hole (b) and open-hole (c). The red line indicates the cohesive elements, where the crack is expected to grow.

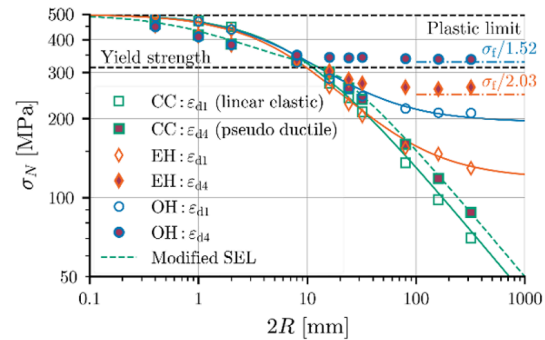


Figure 2. Size-effect behaviour of the pseudo-ductile material. The two nominal strength extremes of notched specimens are plastic limit and elastic limit (dash-dotted line), with σ_f/K_t .

4. Conclusion

The results obtained illustrate that pseudo-ductility can be highly beneficial (for large specimens) to recover more strength by reducing the stress concentration factor. However, it affects the nominal strength negatively for smaller specimens below a critical specimen size. In that same region, the nominal strengths are independent of the notch shape.

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FUNCTIONALIZATION OF FULLERENES BY CYCLIZATION REACTIONS

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Keywords: cyclization, rhodium, catalysis, fullerene, cycloisomerization

1. Introduction

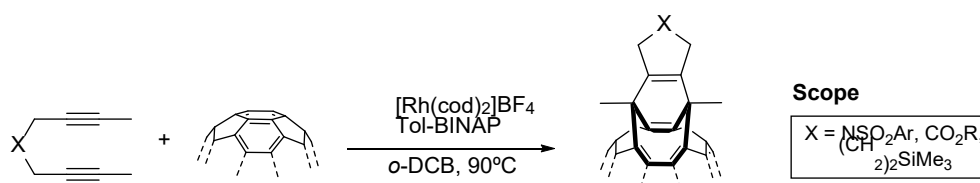
Fullerenes are spherical allotropes of carbon with remarkable electronic and physicochemical properties that make them excellent compounds for use in a variety of fields, such as biomedicine or photovoltaics devices (Castro, Garcia, Zavala, & Echegoyen, 2017; Collavini & Delgado, 2018). However, to be useful molecules, they must be chemically functionalized. Nowadays, synthetic chemists have developed many methodologies to functionalize fullerenes. The [6,6] bonds, which are the double bonds between the six-membered rings, can participate in numerous chemical reactions. The most well-known reactions for their functionalization are cyclopropanations and 1,3-dipolar cycloadditions (Montellano López, Mateo-Alonso, & Prato, 2011). Our research is based on the development of efficient new strategies using transition metal catalysis to functionalize fullerenes and aim to explore potential applications of these derivatives in different fields, such as photovoltaic devices.

2. Methodology

All non-commercial starting materials were synthesized and characterized. Transition metal catalysed cyclization reactions were optimized to improve the efficiency of the process and the synthesized products were completely characterized. We then evaluated the scope of the reaction as well as the electrochemical behavior of the fullerene derivatives. All the reactions were studied by DFT calculations with the aim of identifying the most favourable reaction mechanism.

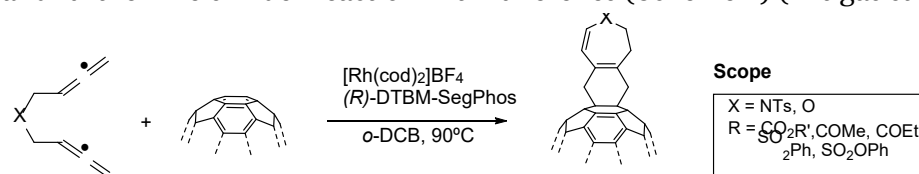
3. Results and discussion

We have developed the synthesis of open-cage fullerene derivatives through a cascade process triggered by the Rh-catalysed [2+2+2] cycloaddition of diynes and C₆₀ and followed by fullerene-cage opening. This innovative process is carried out in a single step reaction, in catalytic conditions and without photochemical activation (Scheme 1) (Artigas, Pla-Quintana, Lledó, Roglans, & Solà, 2018).



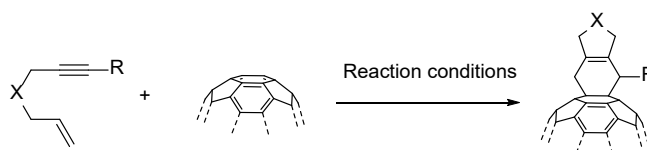
Scheme 1. [2+2+2] cycloaddition catalysed by Rh(I) between C₆₀ and diynes

Furthermore, we have reported a synthetic methodology and step-economical approach to prepare fused dihydroazepine derivatives of C₆₀ and C₇₀ by a cascade process composed of the *in situ* generation of the 1,3-diene by a selective Rh(I)-catalysed cycloisomerization of 1,5-bisallenenes and further Diels-Alder reaction with fullerenes (Scheme 2) (Artigas *et al.*, 2021).



Scheme 2. Rh(I)-catalysed cycloaddition reaction between 1,5-bisallenenes with C₆₀/C₇₀.

We have also involved 1,6-enynes in the cyclization with fullerenes. Optimization, the scope of the reaction and DFT mechanistic studies are currently ongoing (Scheme 3).



Scheme 3. Rh(I)-catalyzed cycloaddition reaction between 1,6-enynes with C₆₀.

4. Conclusion

We have developed new efficient methodologies based on transition metal catalysis for the functionalization of fullerenes involving different unsaturations. Moreover, we tested the electrochemical behaviour of the synthesised fullerene derivatives for their application in perovskite solar cells.

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THREE-DIMENSIONAL HYDROPHOBIC SCAFFOLDS FOR *IN VITRO* TUMOROID CULTURE

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Keywords: breast cancer, tumoroids, partial hydrophobic, scaffolds, personalized medicine

1. Introduction

The second leading cause of death among women in the USA and Europe is breast cancer, and triple-negative breast cancer (TNBC) is the most aggressive subtype (Dent *et al.*, 2007), because it lacks an overexpression of the hormonal and epidermal growth factor (HER2) receptors. One theory suggests that cancer stem cells (CSCs), a subpopulation of cancer cells with stemness properties within the tumours, may be responsible for drug resistance and relapses among patients (Li, Kong, Ahmad, Bao, & Sarkar, 2013). Unlike conventional three-dimensional (3D) platforms or scaffolds, 3D organoids maintain the physiological and genetic conditions of the cells used (Takahashi, 2019), and could be the best alternative method to study diseases like breast cancer. Even now, the beginning of the tumoral process remains unknown. Specific hydrophobicity of the materials appears to be crucial to regulate cell adhesion (Ayala *et al.*, 2011). This work aims to develop partial-hydrophobic scaffolds to assess tumour-like cell aggregates or tumoroid formation.

2. Methodology

Scaffolds of polycaprolactone (PCL) and polylactic-co-glycolic acid (PLGA) were used as controls in experiments with scaffolds of methoxy polyethylene glycol-poly(lactic acid) (mPEG-PLA) and PLGA. Fibre diameter and pore area were measured using scanning electron microscopy. With fluorescence microscopy, we observed the cellular deposition at 2, 4, 6, and 8 days, using 4,6-diamidino-2-phenylindole (DAPI) staining. All the images were processed with ImageJ software. The MDA-MB-231 cell line was used for the experiments.

3. Results

Only mPEG-PLA/PLGA scaffolds were capable of forming cell aggregates, specifically, at 6 and 8 days, which might suggest the presence of tumoroids on the samples. PCL/PLGA scaffolds only have dispersed cells on their surfaces, without proper organization.

4. Discussion

As stated earlier, the hydrophobicity of materials plays a vital role in cell adhesion. The hydrophilicity of mPEG modulates the hydrophobicity of the other materials, which could explain the presence of tumoroids only in the mPEG-PLA/PLGA scaffolds (Girard *et al.*, 2013).

5. Conclusions

Partial-hydrophobic materials, like the co-polymer of mPEG-PLA, are essential for the development of 3D platforms to study the tumoral process due to their ability to induce the formation of tumoroids. In the future, these platforms might be used for drug development and screening, in the context of personalized medicine of cancer.

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THE INFLUENCE OF SOLVENT ON POLYCAPROLACTONE FIBERS AFFECTING THE BEHAVIOR OF LUNG CANCER CELLS

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Keywords: electrospinning, 3D cell culture, lung cancer, polycaprolactone, solvent

1. Introduction

Lung cancer is the leading cause of cancer-related mortality in both genders (Bray *et al.*, 2018). Despite the development of various targeted therapies in recent years, several mechanisms of resistance to the treatment have been described (Tan & Tan, 2022).

The extracellular matrix (ECM) provides a physical support where cells organize, interact and grow. Consequently, polystyrene surfaces modify cell behavior, apical-basal polarity, and oxygen and nutrient distribution (Boucherit, Gorvel, & Olive, 2020). Thus, different 3D cell culture systems have been developed to mimic physiological conditions (Hu *et al.*, 2017).

The electrospinning technique allows the manufacture of nanofibers and the definition of their morphology (Braghirolli, Steffens, & Pranke, 2014). Few researchers have related the effect of manufacturing parameters on cell behavior (Feng *et al.*, 2015; Heath, Lannutti, & Cooper, 2010). Additionally, no literature was found on how the solvent may alter fiber morphology and, thereby cell behavior of lung cancer cells.

Therefore, the main objective of this work was to explore the impact of five solvent solutions on PCL nanofibers and connect it directly to the influence on cell morphology and viability of lung cancer cells.

2. Methodology

Five PCL solutions (15% w/v) were prepared using the following solvents: acetic acid (AA), acetic acid-formic acid (AA-FA) (3:1, v/v), acetone (Ace), chloroform-ethanol (Chl-EthOH) (7:3, v/v) and chloroform-dichloromethane (Chl-DCM) (7:3, v/v). Scaffolds were manufactured with an electrospinning apparatus using a stainless steel 24G needle emitter. PCL structures were characterized by dynamic mechanical analysis and protein adsorption assay. The microarchitecture was also observed by scanning electron microscopy. NCI-H1975 cells were seeded into PCL scaffolds for 3 and 6 days. Nuclear and cytoplasmic circularity and cell viability was assessed by confocal laser scanning microscopy and MTT assay, respectively.

3. Results

Ace, Chl-EtOH, and Chl-DCM scaffolds showed thicker fibers and higher porosity and pore area than the other PCL scaffolds (AA and AA-FA structures). The stiffness and protein adsorption of Ace, Chl-EtOH and Chl-DCM meshes was also greater than the other PCL scaffolds. Furthermore, cells cultured on Ace, Chl-EtOH and Chl-DCM structures exhibited more elongated nuclei and cytoplasm and a higher cell viability than cells seeded on AA and AA-FA meshes.

4. Conclusions

The solvent used to prepare the solution for the electrospinning process has a great influence on fiber morphology and, as a result, on cell behavior of lung cancer cells. Consequently, its use should be considered.

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INNOVATIVE SYSTEM FOR ELECTROSPRAY COATING OF POLYMERIC CARDIOVASCULAR STENTS

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Keywords: electrospray, cardiovascular stent, coating

1. Introduction

The purpose of a cardiovascular stent is to support the artery just after hyperplasia. After the operation, a stent, usually made of metal, is inserted and remains inside the body. That is why the revolution in cardiovascular stents towards bioresorbable materials is more and more promising. Usually cardiovascular stents are coated with antiproliferative drugs to prevent neointimal hyperplasia, such as everolimus (Sorrentino *et al.*, 2017). This study proposes the coating of polymeric stents with electrospray (ES) techniques. This coating can potentially be loaded with antiproliferative drugs. Therefore, the study presents the construction of a system coupled to the electrospinning machine to coat polymeric cardiovascular stents.

2. Methodology

Poly-L-lactic acid (PLLA) stents were obtained by cylindrical printing onto a rotating mandrel (Chausse *et al.*, 2021). A solution of a PLCL copolymer (PLC 9538, Purac) was synthesized in chloroform at 0.6% w/v. The 3D-printed stents were mounted onto a grounded collector mandrel (Figure 1).

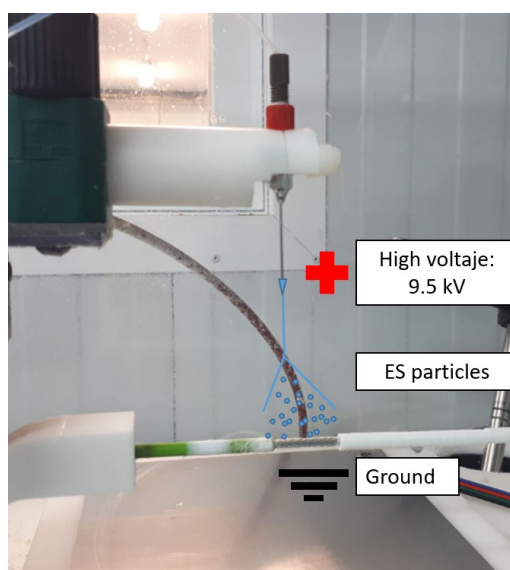


Figure 2. Schematic diagram of the electrospray system

This setup was employed to coat the stents with ES particles. The ES parameters used during the process are presented in Table 1.

Table 1. Range of parameters analysed in the ES process for stent coating

	Range	Sample interval
Flow (mL/h)	1.75 -3.75	0.25
Distance from nozzle to collector (mm)	112 -152	10
Speed (rpm)	10 - 50	10

A polynomial regression model was calculated to fit the experimental data, eliminating the non-influential parameters ($p > 0.05$) and providing the effect of these parameters on the final weight of the coating.

3. Results and discussion

PLLA stents were successfully coated by ES, obtaining a homogenous PLCL layer. The data showed a proportional relationship between the distance from the nozzle to the collector and the weight of the coating. No differences were observed for the rotational speed. However, the standard deviation was reduced at 30 rpm. Finally, the flow had a slight inverse tendency to the weight. This occurred because the same voltage was set for all conditions. The energy to evaporate the solvent was the same. Therefore, the only differences were in the accumulation of material in the Taylor cone, which was removed at the end of the experiment.

4. Conclusions

This research presents a proof of concept of the possibility to coat polymeric stents with ES technologies and demonstrates the impact of the printing parameters on the result.

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MULTIWALLED CARBON NANOTUBES EMBEDDED IN A POLYMERIC MATRIX AS NEW MATERIALS FOR TFME FOR ORGANIC POLLUTANT EXTRACTION

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Keywords: carbon nanotubes, organic pollutant, functionalized membranes, TFME

1. Introduction

For the monitoring of organic pollutants in waters, the development of new samplers based on functionalized polymeric membranes is of interest (Almeida, Cattrall, & Kolev, 2012). The materials investigated are polymeric films modified with multiwalled carbon nanotubes (MWCNTs) that are used for pollutant extraction in thin-film microextraction (TFME) techniques (Bruheim, Liu, & Pawliszyn, 2003). The studied pollutants are chlorpyrifos (CPS), atrazine (ATZ), and two emerging contaminants, musk tonalide (AHTN) and triclosan (TCS) (Merlo, Profumo, Fontàs, & Anticó, 2022). The compounds are retained in the film, then eluted, and finally analysed by GC-MS.

2. Hypothesis

MWCNTs polymeric films, avoiding the use of plasticizers, can be used in TFME to extract organic pollutants.

3. Methodology

The films are made with cellulose triacetate (CTA) as the polymer and modified with MWCNTs. For comparison, films with plasticizer (dibutyl sebacate, DBS) are prepared. The films are characterized using infrared spectroscopy (FT-IR) and scanning electronic microscopy (SEM). For the microextraction experiments, 10 mL 0.01 mol L⁻¹ NaCl containing the target pollutants is contact with a piece of film (1cm x 2cm) for 1 hour. The elution step is carried out with 1 mL ethyl acetate. For chromatographic separation, a GC-MS (DSQ, Thermo Scientific) was used.

4. Results and discussion

Homogenous films are satisfactorily prepared using CTA and MWCNTs (90%:10%) (Figure 1). The slow evaporation of the solvent is crucial to prevent the aggregation of MWCNTs.



Figure 1. Polymeric matrix with MWCNTs embedded

The films with MWCNTs present similar effectiveness as with DBS for the microextraction (Figure 2).

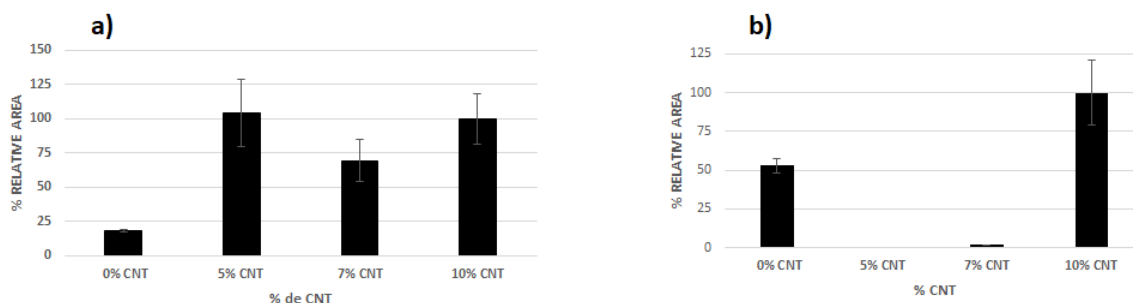


Figure 2. Effect of the presence of MWCNTs on the extraction ability: a) CPS; b) TCS.

5. Conclusion

The CPS and AHTN results with CTA-MWCNTs films using TFME are promising. For ATZ and TCS, further investigation is required.

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HOW DO THEY DO IT? BIOINKS EDITION

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Keywords: bioinks, 3D printing, rheological properties, substance of human origin

1. Introduction

The demand for organ replacement is increasing. Consequently, new strategies are emerging to solve this problem, such as tissue regeneration and 3D bioprinting (Agarwal *et al.*, 2020). These techniques can be a solution to generate new tissues and organs (Ciampi *et al.*, 2019; Ren *et al.*, 2016). For this reason, it is necessary to develop materials that can be processed using 3D printing and can mimic the cell microenvironment (bioinks). Substances of human origin (SoHO) are materials extracted directly from a human patient (Chen & Liu, 2016), thereby ensuring the biocompatibility and cell cues needed to regenerate the tissues. The capability to transform SoHO materials into bioinks opens a wide field of applications for the replacement of organs and tissues.

2. Problem

The main problem in the development of bioinks is that the proposed material must satisfy both printability and biocompatibility. However, addressing one factor usually goes against the other. To solve this problem a methodology that considers both factors must be considered.

3. Methodology

First, materials need to be tested to determine cytotoxicity. Afterwards, a rheological evaluation to check whether the bioink has the appropriate rheological properties, such as shear thinning and shape retention, is required to predict printability. Then, it is important to quantify the resolution of printed structures to evaluate printability of the material. If the resolution is suitable for the application in question and a scaffold is formed, the next step is to check its degradation, mechanical properties, and swelling, and to determine the porous size. The last step is to combine the material with cells and print them to achieve 3D cell encapsulation.

4. Results and discussion

It has been possible to develop gelatine-based bioinks using the methodology presented.

Cytotoxicity assay. Indirect and direct cytotoxicity assays show that materials reduce cell viability (Figure 1a), but they are not cytotoxic; therefore, they can be used to develop bioinks.

Rheological properties. Most gelatine-based bioinks do not display good rheological properties for 3D printing (Figure 1b). For this reason, bioink formulation optimization is needed before printing.

3D printability. After formulation optimization, and resolution quantification, GelMA and GelMA-collagen formulation exhibit good printability (Figure 1c).

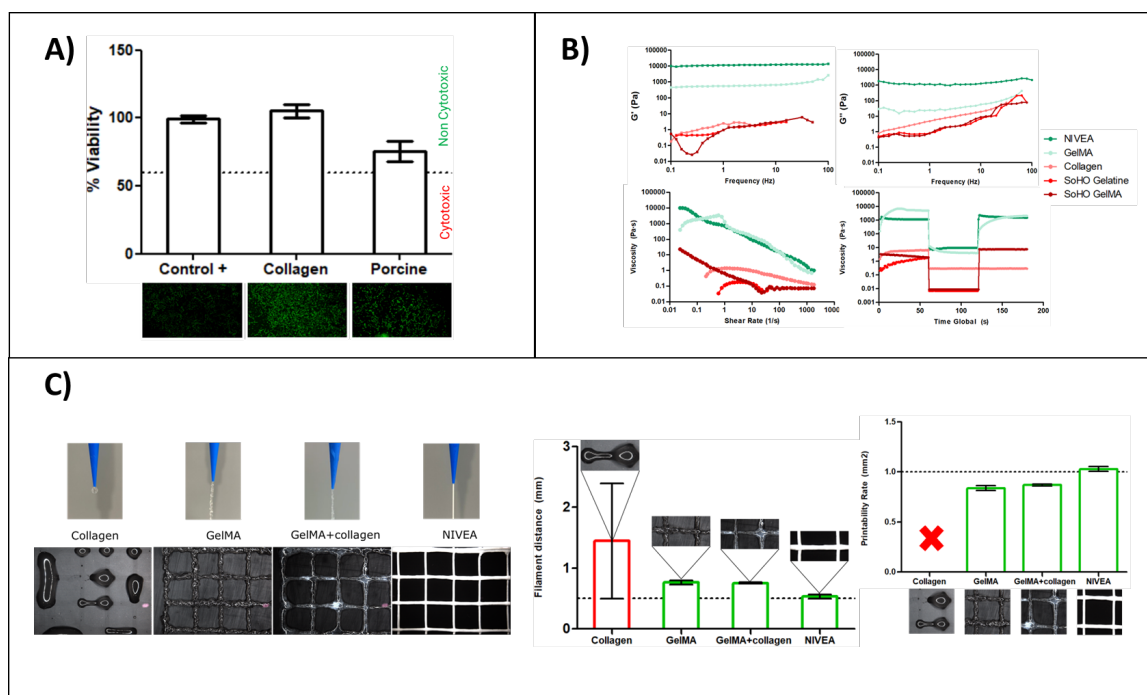


Figure 1. Methodology for the development of a gelatine-based bioink. A) Cytotoxicity assay. B) Rheological evaluation and C) 3D printability

5. Conclusions

First, as shown in the results, the methodology presented is a good strategy to follow to create a new bioink. Second, the development of GelMA and GelMA-collagen SoHO bioink is achieved by formulating these materials and demonstrating their 3D printability.

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SESSION XI. NEW TECHNOLOGIES

SOFTWARE APPLICATIONS AT THE SERVICE OF ARCHAEOLOGY: A GIS FOR EMPÚRIES

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Keywords: archaeology, archaeological site, Empúries, GIS, AutoCAD

1. Introduction

The informatization of archaeological data has turned out to be of the utmost importance in the administration of cultural heritage. Using detailed knowledge of the archaeological reality creates new opportunities for the scientific community in research, intervention, fruition and assessment (Maratini, 2011).

2. Hypothesis

The aim of this study was to create a specific GIS for the management of the archaeological site of Empúries. Specifically, it proposed an information system characterized by a relational database composed of alphanumeric data (descriptive), identification records and multimedia documentation, related to a georeferenced cartography. In addition, it intended to catalogue a complete set of data, so that the Empúries team could work independently from the data entry, and to ensure the access to information in a wider catchment area.

3. Methodology

An innovative map of the Empúries archaeological site was created in AutoCAD and the DWG file has been used as a GIS cartographic base and configured according to specific coordinates of the area.

The need to query the database by relying on spatial and descriptive attributes has made it essential to realize a structure based on principles of uniformity and founded on criteria of recognized scientific validity. For that purpose, a closed code list was arranged according to an established format, through a drop-down menu. That is to say, the query offers the opportunity to produce a wide range of reports and thematic cartography according to research, dissemination and preservation needs.

This work has necessitated careful bibliographic research, characterized by documents published, modern and historical cartography, historical sources, archival documents and historical and artistic data.

4. Results

The analysis of the entire epigraphic *corpus* brought together all the inscriptions found in Empúries, but preserved in various Spanish locations, and provided information about its political-administrative and urban structure, as well as its economic-cultural history.

The cataloguing of epigraphical documentation was positioned using specific and unprecedented symbology. This has made it possible to identify 23 epigraphs whose traces had been lost: for 16 of them information was found to allow their retrieval (Fabre, Mayer, & Rodà, 1991).

Specifically, the *Archaeology Museum of Catalonia* (MAC) of Empúries has activated the procedure for identifying and retrieving of the epigraph, which was discovered during this research in the hands of a private citizen of L'Escala.

5. Conclusion

The initial results have confirmed the validity of GIS as an aid for safeguarding and enhancing the archaeological site of Empúries.

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CO-CREATION AND HERITAGE EXPERIENCES WITH AUGMENTED REALITY

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University of Girona

Keywords: nomad museology, augmented reality, co-creation, cultural heritage, user experience

1. Introduction

“Motiv-ARCHE” is an application created with the aim of developing a new tool for disseminating cultural and natural heritage (González Vargas, Fabregat, Carrillo-Ramos, & Jové, 2021), from a multidisciplinary and updated approach. It aims to make it easier for wealth managers to create content and educational resources, and to become a tool for communication and interaction with users (Colomer, 2020), through the co-creation of content (Nisi, Dionisio, Barreto, & Nunes, 2018). It accomplishes all this using immersive technologies, such as augmented reality, adapted to the preferences, needs and characteristics of visitors to cultural and natural heritage sites (Badalotti, De Biase, & Greenaway, 2011; Fanini, Ferdani, Demetrescu, Berto, & d’Annibale, 2021; Grevtsova, 2013; Imbert-Bouchard Ribera, Llonch Molina, Martín Piñol, & Osàcar Marzal, 2013).

2. Hypothesis

This work aims to study the experiences users have when using Motiv-ARCHE and to improve user experience in the processes of co-creation and use of content for education and dissemination of this heritage content with interactive and immersive features.

3. Methodology

The research will use qualitative methodology that obtains information from case studies, participant observations, interviews, questionnaires, focus groups, etc. The qualitative methodology is divided into three phases (Hernández Sampieri, Fernández Collado, & Baptista Lucio, 2014): the initial phase, the implementation phase, and the validation and analysis phase.

4. Results

The results will be the final evaluation of technological resources developed and their application by museums and users (Roussou & Katifori, 2018), especially in terms of improving the experience. We will use four criteria to measure these parameters, which will be defined in questionnaires (González Vargas, Fabregat, Carrillo-Ramos, & Jové, 2020).

5. Conclusion

The results obtained will be analysed to find out what this application should look like and how the co-created content should be. The benefits of using ICT in learning and sharing the heritage in a different way will also be analysed.

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DIGITAL TECHNOLOGIES' ADOPTION IN EUROPEAN MANUFACTURING COMPANIES – FROM ANTECEDENTS TO IMPACT

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Keywords: digital technologies, sustainability, manufacturing

1. Introduction

The proposed research aims to study the relation between digital technologies in the context of Industry 4.0, sustainable performance, circular economy, their impact on business model elements such as value proposition, and other aspects of competitive advantage and organizational development.

Adopters of digital technologies in European manufacturing companies will be studied, determining their characteristics, the barriers/drivers they perceive in the adoption of digital technologies, and the impact that digital technologies generate on their sustainability performance and business model innovations.

The rapid development and implementation of digitalization in manufacturing has an enormous impact on the environment. Although the adoption of information technology in the monitoring of manufacturing systems has the potential to increase overall sustainability performance (Demartini, Evans, & Tonelli, 2019), it is still unclear whether digitalization of applications in manufacturing has positive or negative environmental impacts (Chen, Despeisse, & Johansson, 2020).

The proposed digital technologies for the thesis are big data analytics, artificial intelligence, and additive manufacturing (3D printing). The proposed project will be a compendium of publications dealing with the specified aspects of digital technologies (Figure 1).

2. Methodology

For each of the lines of research and their corresponding objectives, a deep revision of the literature is necessary to justify the existing gap there and its relevance as a topic of study, and to set consistent theoretical backgrounds or models for each research question. European Manufacturing Survey data will be used to provide empirical evidence to the research questions.

3. Results and discussion

Results will be presented in the form of descriptive and regression analyses for the studied relations. The hypothesis on the relation between selected variables will be evaluated and the effect of selected variables as mediators will be presented.

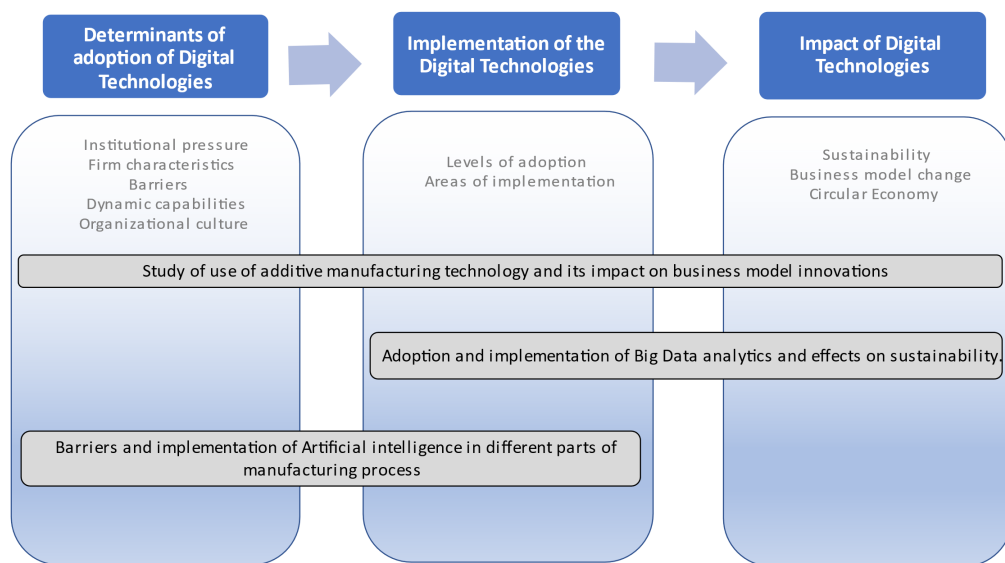


Figure 1. Proposed scheme of the project

4. Conclusion

The proposed study will generate new and in-depth knowledge on the relation between selected digital technologies and their effects on selected performance. This research aims to contribute to the emerging body of knowledge combining latest technologies with green manufacturing. It also contributes to a better understanding of the determinants of digital technologies' configurations conducive to product innovation. Further, suggestions about the digital and green transition will be formulated.

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COLLISION DETECTION AND AVOIDANCE FOR UNDERWATER VEHICLES USING OMNIDIRECTIONAL VISION

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Keywords: visual SLAM, omnidirectional multi-camera systems, collision risk assessment, risk map, ROVs

1. Introduction

For many decades, the study of marine habitats has been carried out in environments that are inaccessible or dangerous for direct human intervention. Thus, the development of underwater robots such as remotely operated vehicles (ROVs) and autonomous underwater vehicles (AUVs) plays an important role, and high accuracy navigation, planning and mapping in these systems plays a vital role.

In the last few years, omnidirectional cameras have received increasing interest, as their wide field of view is very convenient for visual SLAM and mapping tasks. They enable a comprehensive 3D reconstruction of the surroundings and can extend the pilot's spatial awareness and reduce common orientation problems during missions, especially in cluttered environments where pilots need to ensure robot's safety. As such, the envisioned system is intended to generate warnings when an ROV pilot reaches a position of high collision risk and to override human inputs sent to the vehicle control.

2. Methodology

A visual-based system for early collision detection was developed, using an omnidirectional multi-camera sensor as the only information input. The proposed framework uses motion information estimated from a SLAM package to produce dense point cloud maps of the environment, which are used to calculate the associated risks for each of the points. The system can provide two outputs: (1) a resulting repulsion force that moves the robot away from a potential collision; and (2) an omnidirectional risk map.

3. Results

The system capabilities were assessed in real time using a simulated environment on the Stonefish simulator (Cieřlak, 2019) and by integrating the system into real AUV performing tests on a controlled environment. The tests showed that the system can correctly detect when an obstacle becomes a danger to the robot. Dangerous zones appear when the robot comes close to an obstacle and the path of motion is not changed. They also showed that whenever the repulsion force becomes greater than a set value, an auxiliary control system uses this as input and takes control of the robot to perform evasive manoeuvres.

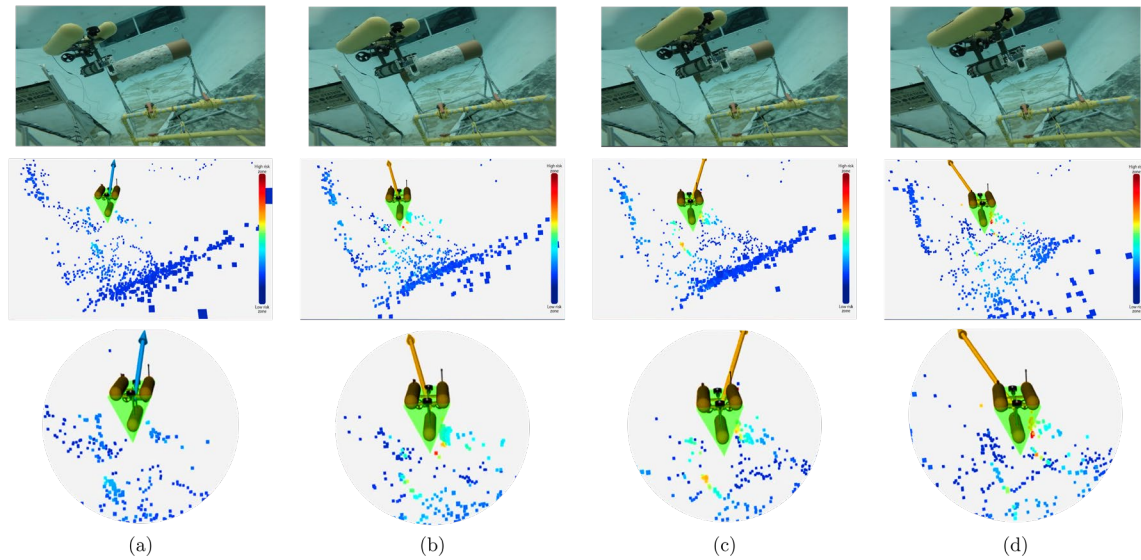


Figure 1. Test scenario where the Girona 1000 was controlled to pass through a narrow passage created by the set obstacles. The images from (a) to (d) show a sequence of frames with their respective point cloud representation, and the risk calculated for each obstacle. Frames (c) and (d) depict medium danger zones (yellow areas) where the Girona has gotten too close to a wall of the pipe, and the force points out of this area.

4. Conclusion

This work shows the implementation of a visual-based early collision detection system. The system can correctly detect when an obstacle becomes a danger to the robot and generate warning signals accordingly. To the best of our knowledge, no system with the presented capabilities has been implemented and tested for ROV applications, and this work constitutes a first achievement in this direction.

5. Bibliography

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INTELLIGENT ANALYTICAL TOOL TO IMPROVE GAS TURBINE PERFORMANCE

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Keywords: artificial intelligence, machine learning, condition assessment, gas turbine

1. Introduction

The way decisions are made in the industry nowadays is changing thanks to increasing data availability (Lei *et al.*, 2020) and the development of intelligent tools for condition and fault assessment (Cheng *et al.*, 2021). The main purpose of this data analytics process is to improve the performance of systems, to make them more reliable, available at all times, and safer (Daily & Peterson, 2017).

The main goal of this study is to develop an analytical tool based on machine learning techniques following the autoencoder architecture to assess the condition of an industrial gas turbine using real plant data.

2. Methodology

An autoencoder is defined by an architecture, usually in the form of artificial neural networks, which is trained to copy its inputs to its outputs (Goodfellow, Bengio, & Courville, 2016). Its structure is based on two neural networks: an encoder and a decoder network. The encoder G is defined as an encoding function $z = G(x)$, where x is the model input and z is a set of latent variables. The decoder F is defined to reconstruct the encoded signal, $x' = F(z)$, where x' is the reconstructed input signals. The parameter sets of both networks are simultaneously learned by minimizing the loss $e = d(x, x')$ according to some distance metric (Jia, Lei, Lin, Zhou, & Lu, 2016).

3. Results and discussion

The main result of the present study is a machine learning-based analytical tool that is able to assess several significant factors of industrial gas turbines (Figure 1).

First, a drift is captured between the model output and real plant values showing a significant deviation in gas turbine performance. This deviation is due to major maintenance, indeed a change in the machine core (Figure 1A). Then, the drift is further analysed by using a signal decomposition technique, where the trend, seasonality, and residuals are obtained, as shown in Figure 1B. The perturbations detected in both trend and residuals are properly mapped as gas turbine faults.

To visualize the encoding results of the autoencoder properly, the u-map technique is used. The structure of the data is transformed while preserving the distance between points. This leads to an advanced visualization of data, where the ghost-based shape shown in Figure 1C

corresponds to the drift shown before. Finally, Figure 1D shows long-term performance of gas turbines with major maintenance service, presented in different colours. The robustness of the tool is verified by having similar behaviours in short-term and long-term performance.

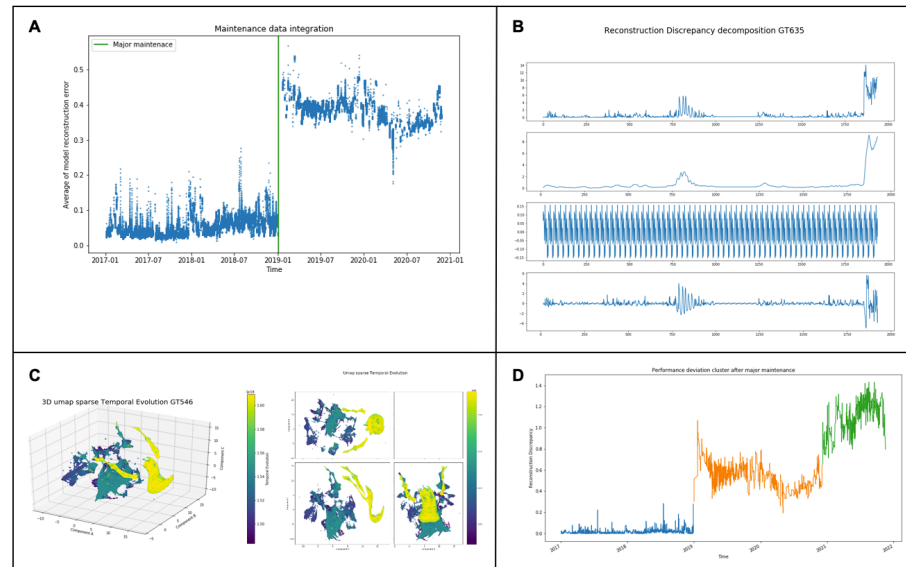


Figure 1. Main results obtained. A) Drift detection in gas turbine performance because of a major maintenance. B) Detection of gas turbine faults in drift decomposition. C) Advanced drift visualization using U-map technique. D) Advanced drift visualization using U-map technique.

4. Conclusions

The goal of this study is to develop a machine learning tool to assess gas turbine performance. As shown in the results, the tool is able to evaluate several important factors of its behaviour, for instance how it works after major maintenance or how a fault affects its performance. It is also able to give advanced visualization to understand the internal data structure properly.

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SESSION XII. SOCIETY AND QUALITY OF LIFE

EFFECTIVENESS OF THE APPLICATION OF A NURSING INTERVENTION PROGRAMME IN THE MANAGEMENT OF PARENTAL ANXIETY AND INFANT PAIN IN THE SURGICAL PROCESS OF CHILDREN TO BE CIRCUMCISED

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Keywords: anxiety, child preschool, circumcision, male, pain

1. Introduction

Entering the hospital and waiting for surgery is a very stressful time for people. According to some studies, surgical interventions in children generate concerns in family members related to many issues. These include anaesthesia, fear of being harmed, penile injury, excessive pain, the death of their children, and not being able to contain their own anxiety. Therefore, they may have difficulties in assuming an active role in caring for their children (Ayenew, Endalew, Agegnehu, & Bizuneh, 2020; Mavhu *et al.*, 2016; Moerman, van Dam, Muller, & Oosting, 1996)

For these reasons, we propose the development and implementation of an action programme for the reduction of children's pain and of anxiety in parents in the Muslim population residing in Spain.

2. Hypothesis

A nursing intervention programme in the surgical process of circumcision decreases the degree of anxiety of family members and reduces infant pain.

3. Methodology

A randomized clinical trial will be carried out at the Policlínica Maresme, located in Pineda de Mar, on the relatives/guardians and children aged 0-3 years who are going to undergo circumcision.

The intervention group of the children's relatives/guardians will undergo an educational programme related to the circumcision process. The control group will receive the usual intervention of the centre. It has been estimated that 157 subjects are needed in each group, estimating a loss to follow-up of 10%.

Among other variables, the preoperative anxiety level of the parents will be measured using the Hamilton scale (Rangel Ávila, Haro Haro, & García Méndez, 2012). Intraoperatively, children's pain will be measured using the FLACC scale (Merkel, Voepel-Lewis, Shayevitz, & Malviya, 1996). Subsequently, a postoperative telephone follow-up will take place during the 2

and 10 days following the intervention, to assess aspects related to the clinical evolution of the surrounded children and the resolution of any doubts that the caregivers may have.

The confidentiality of the study participants will be guaranteed. The research project has been approved by the Comit   d'  tica d'Investigaci   Cl  nica amb Medicaments de l'Hospital de Matar   with code CEIm 03/22.

4. Results

Data collection will start in June 2022.

5. Conclusions

Results are expected in June 2023.

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QUALITY OF LIFE, OPTIMISM, AND RESILIENCE IN WOMEN WITH BREAST CANCER

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Keywords: optimism, resilience, quality of life, breast cancer

1. Introduction

Bravo-Doddoli and Sánchez-Aragón (2021) estimate that by 2030, the number of cases of cancer will reach 23.6 million globally, endangering not only the physical health but also the quality of life of those that develop it (Gómez-Villaroya *et al.*, 2021). In the face of this, scientific research has focused on providing evidence regarding psychological modulators (optimism, resilience) that promote the maintenance of quality of life in the chronically ill, where optimism and resilience have been associated with a lower vulnerability to health issues (Mera & Ortiz, 2012).

Previous studies (Cuesta-Guzmán, Sánchez-Villegas, & Bahamón, 2020; Guil *et al.*, 2016) have observed a positive correlation between resilience and quality of life in women with breast cancer, finding that women who show higher levels of resilience are able to take advantage of the positive aspects they can extract from the disease. Similarly, Pastells Pujol and Font Guieras (2014) have concluded that optimism is a predictor of quality of life preservation in women with breast cancer.

The overall objective of the research is to analyze the relationship between quality of life, optimism and resilience in women diagnosed with breast cancer.

2. Methodology

This is a quantitative, non-experimental, exploratory, descriptive cross-sectional study. The population will be composed of Chilean women, aged 18-49 years, who are diagnosed with breast cancer and are health controlled and/or receiving outpatient treatment in the city of Coquimbo, Chile. A convenience sampling method will be used, and all data collection will be carried out virtually, where the participants will complete the instruments as part of a series of questions included in a Google Form.

3. Results

This study aims to provide evidence of the relationship between quality of life, optimism, and resilience in women diagnosed with breast cancer so that the scientific evidence provided can help create interventions to promote resilience and optimism in this population, helping them to preserve their quality of life.

4. Conclusion

It is expected that this study will reveal that the findings are similar to what has been published in other countries where optimism and resilience are shown to be good predictors of health, well-being and adjustment in the face of stressful situations.

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DISCOVERING SOCIAL REALITY RELATED TO PERSONAL APTITUDES AND HEALTH: QUALITATIVE STUDY BASED ON FOCUS GROUPS

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Keywords: personal aptitudes, health perception, quality of life, health-oriented behaviours, focus groups.

1. Introduction

Individual aptitudes play an important role in the ability to adopt health-promoting behaviours and to respond appropriately to adverse situations, which can be related to harmful health outcomes and physical and mental health problems (Christensen *et al.*, 2002; Laaksonen, Prättälä, & Karisto, 2001). For this reason, one of the points on which the Ottawa charter is based is the promotion of a public policy that favours the development of personal aptitudes (WHO, 1986). This personal development should be aimed at providing information, health education and perfecting the essential skills for life (Lalonde, 1974).

This study will help to obtain relevant information to identify and understand if personal aptitudes related to behaviours influence the lifestyle, physical health, mental health, quality of life and current health status of the Spanish population. Personal aptitudes are characteristics of each individual, including social and economic environments, among other contextual determinants, that can have an impact on health. This monograph aims to explore the opinions and experiences of the population about the relationship between personal aptitudes and their perception of current behaviours, quality and health status. Participants' responses will address the main topics under study: activation, current health status, personality traits, health perception, quality of life, health habits and health literacy.

2. Methodology

The sample group is the focus of the qualitative research from a phenomenological perspective, with participants from primary care centres throughout Spain, who will be between 35 and 74 years old. The research forms part of a larger study, DESVELA. To analyse the content of the interviews, it is necessary to record the sessions. The video and audio, and the data collection process will be analysed later through the triangulation of analysis.

3. Results

It is hoped that the results of this study will help to understand health behaviours and provide sufficient and relevant information that can be applied in health care promotion campaigns. In addition, it can contribute to the dissemination of data for health improvement through

publications in scientific journals, presentations at academic meetings, workshops or local and national media.

4. Conclusion

Hopefully, the results of this study will help to understand health behaviours and provide sufficient and relevant information that can be applied in health care promotion campaigns, as well as contribute to the dissemination of data for health improvement through publications in scientific journals, presentations at academic meetings, workshops or local and national media.

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SYSTEMATIC LITERATURE REVIEW OF THE PERSPECTIVES OF WOMEN WITH INTELLECTUAL DISABILITIES WITH REGARD TO THEIR SOCIO-AFFECTIVE RELATIONSHIPS

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Keywords: intellectual disability, women, socio-affective relationships, inclusion, gender

1. Introduction

The relationships of people with intellectual disabilities are a major cultural taboo (Huaiquián Billeke, Arriagada Vega, Betanzo Briones, Inostroza Soto, & Llanquitruf Paillán, 2018), resulting in the scarcity of literature on the subject (Dixon & Robb, 2015). This lack of study and understanding of their sexuality makes them more vulnerable to abuse as a group (Ballan & Freyer, 2012). Additionally, the perspective of women in this collective on their affective-sexual lives has been mostly ignored in studies (Hoorn, 2015). That is why it is imperative to analyse the intersection between socio-affective relationships and people with intellectual disabilities from the point of view of women with intellectual disabilities.

2. Methodology

A systematic literature review that selected keywords and conducted searches in twelve databases yielded 116,463 articles. After we read the titles and abstracts, we selected 227 articles for further analysis. Then, after we read these articles in depth and applied the exclusion criteria, we chose 11 investigations for the final analysis. After making the final selection, we proceeded with the thematic analysis of the documentation and the subsequent extraction of results.

3. Results

The findings revealed that women are interested in discussing their socio-affective relationships and sharing their perspectives and experiences on topics such as abuse, the LGBTIQ+ community, relationships, and contraception.

4. Conclusion

This study lays the groundwork for future research to identify and establish support, as well as to provide adequate information and training for women with learning disabilities. It also emphasizes the importance of professionals listening to the voices and experiences of these women to ensure adequate social and educational accompaniment.

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CHALLENGES OF THE FUTURE: A PERSPECTIVE FROM THE HUMANITIES

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Keywords: future, humanities, climate change, education, culture

1. Introduction

According to the latest IPCC (Intergovernmental Panel on Climate Change) report (04/2022), half of the world's population is highly vulnerable to the climate emergency, and these consequences are a violation of several of the articles present in the Declaration of Human Rights (UN, 1948). The experts point to society as mainly responsible for this global problem (Shiva, 2015).

Given the seriousness of the matter, it is desirable to look for possible ways to face this present and future challenge. Education, for example, is a very valuable way to teach a culture of peace and non-violence, and encourage tolerance and respect (Spindler, 1987). Several authors comment that we cannot change the world or improve it if we forget to educate adequately future generations (Puleo, 2016). Consequently, it is necessary to merge education and the environment, within the social ecosystem. For this to be perpetuated, it is necessary to approximate what is needed to maintain living ecosystems, and vice versa. Therefore, we need to move forward in a culture of self-restraint (Riechmann, 2012) in order to mitigate the damage caused by this planetary socioecological crisis.

2. Objectives

This research aims to investigate two key points in environmental education among adolescents: (1) the knowledge that students have about the climate emergency in relation to their way of life and (2) the environmental awareness of these subjects. The second point is required to identify the starting point when introducing an effective communication of this ecosocial problem.

3. Methodology

The sample selected for this research consists of 100 students aged between 15 and 17 from a school in Barcelona (Spain). They were tested on previous knowledge: a questionnaire about environmental awareness and two focus groups.

4. Results and discussion

The results respond to both quantitative and qualitative variables. We have extracted the following data: only 5% of the sample knows the concepts ecofeminism, decrease or interdependence; less than 40% have been trained in sustainability by the teaching staff; and

only 20% know the serious consequences of the climate emergency and its direct relationship to our consumption patterns.

5. Conclusions

From the qualitative results extracted, we can see that the communication of the ecological problem from a socio-humanistic perspective helps students to be part of the change through their habits and to understand better its causes and consequences.

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SESSION XIII. HISTORY AND ART HISTORY

LA PROSA DE JOAN VINYOLI

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Keywords: Joan Vinyoli, literatura catalana contemporània, narrativa, obra inèdita, anàlisi textual

1. Introducció

Sovint s'ha retret a Joan Vinyoli que no escrivís prosa. Tanmateix, (Macià, 2001) recuperà algunes narracions primerenques que Vinyoli va publicar a la revista *Iuventus* i n'hi afegí una d'inèdita, i (Solà, 2019) esmentà altres intents de l'autor d'adoptar aquest gènere literari (Genette, 1987; Todorov, 1996).

Aquest buit aparent en l'obra de Vinyoli, tingut en compte només en els dos treballs esmentats, fa encara més excepcional la troballa d'una setantena de proses inèdites a l'Arxiu Comarcal de la Selva.

2. Hipòtesi

Com molts altres escriptors, Vinyoli va experimentar amb la prosa durant la seva joventut i, més endavant, va decidir abandonar-la i centrar-se en la poesia. Malgrat alguns indicis que s'havia plantejat de publicar alguns contes, sembla que finalment ho va descartar. A través de l'anàlisi dels relats inèdits que hem localitzat esperem trobar pistes que ens permetin apropar-nos a les raons que el van dur a allunyar-se de la prosa i descobrir si aquest tempteig amb la narrativa va tenir cap repercussió amb la poesia que va publicar.

3. Metodologia

Pretenem estudiar i editar les narracions que es conserven al Fons Joan Vinyoli (ACSE). Les transcriurem adaptant l'ortografia a la normativa actual però amb el màxim respecte pel text original. La datació dels documents i la consulta dels llibres que formaven part de la biblioteca de Vinyoli ens permetran contextualitzar-les i, probablement, identificar-ne algunes influències. Això es complementarà amb les referències que Vinyoli pugui fer d'aquests relats a les cartes del període 1930-1969.

4. Resultats

Hem pogut localitzar una setantena de contes (alguns d'acabats i d'altres fragmentaris), proses assagístiques i proses biogràfiques escrits majoritàriament entre 1930 i 1960 i inèdits. Un cop datades i ordenades podem delimitar-ne els temes, elements simbòlics... del món literari de Vinyoli i elaborar una hipòtesi de treball.

5. Conclusió

Aquestes proses inèdites són una nova via d'investigació de la figura de Joan Vinyoli: la d'un Vinyoli narrador que, a banda de beure de Hölderlin i Rilke, estava atent a les noves veus del panorama literari català i, en l'època en què es publicà *Cita de narradors* (Sarsanedas, de Pedrolo, Espinàs, Capmany, & Perucho, 1958), es demanava quines possibilitats expressives tenia la narrativa breu en contrast amb la lírica. Segurament podem situar aquestes preguntes de Vinyoli en una polèmica més àmplia sobre la situació de la literatura catalana de postguerra (de Riquer, Comas, & Molas, 1972).

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JACINT MORATÓ AND THE PARADIGM SHIFT IN THE STRUCTURE OF THE 18th CENTURY ALTARPIECE: RESEARCH AND WAYS OF ANALYSIS

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Keywords: Jacint Morató, altarpiece, 18th century, Baroque, Catalonia

1. Introduction

Over the years, historiography has been concerned with determining models and typologies in the evolution of the Baroque altarpiece in Catalonia. In this sense, one of the figures that stands out is the sculptor Jacint Morató, author of altarpieces such as that of Igualada or of Santa Clara de Vic. These works, appreciated by many authors for their typological novelty, became referents for a large part of the Catalan altarpieces of the 18th century. A focus on the bibliography, as a state of the art, reveals the importance given to this sculptor and his proposals.

2. Results

Cèsar Martinell highlighted the Igualada altarpiece as a turning point in the Catalan Baroque (Martinell, 1959), especially in terms of its classicism and academicism. This view was supported and defended by Aurora Pérez. She insisted in several publications that Jacint Morató had played key role in creating a new altarpiece model based on those of Igualada and Santa Clara de Vic (Pérez Santamaria, 1988, 1994, 2000). Authors such as Carles Dorico and Joan Bosch questioned this pre-eminence traditionally accorded to Morató. They debated the attribution to the sculptor of the altarpiece of Santa Clara and indicated that Pere Costa took part in both this work and the new type of altarpiece that emerged in the 18th century (Bosch Ballbona, 2014; Dorico i Alujas, 1997, 1999). At the same time, Bosch discussed the inappropriate vocabulary used by some authors to refer to Morató's work, calling it inaccurate and historically anachronic (Bosch Ballbona, 2006, 2007). Recent historiography has dealt with the study of the original design of the altarpiece of Igualada (Avellí, 2006; Miralpeix, 2021), which led to the discovery that Joan Roig was its author (Fernández i Bermúdez & Asturiol i Castelló, 2010).

3. Conclusion

Having analysed both the bibliography and the sculptor's work, we can argue that Jacint Morató's innovations were crucial. The architecture of his works became significant, with a preference for classical columns, a reduction of ornamentation, and a progressive unity of the whole ensemble. However, his proposals needed to be pursued and refined by other artists, such as Pere Costa. Furthermore, some of the arguments used to defend Morató's authority, in particular the attribution of the altarpiece of Santa Clara de Vic, do not seem to be entirely

solid, as part of the historiography has shown. This leads us to rethink the work of Jacint Morató and the scope of his groundbreaking formulas.

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THE DISAPPEARANCE OF LARGE CARNIVORES IN THE IBERIAN PENINSULA

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Keywords: Iberian Peninsula, large carnivores, experimentation, plistocene

1. Introduction

This work will deal with the disappearance of large Palaeolithic carnivores in the Iberian Peninsula (Baquedano Pérez, & Rosell Foxà, 2010). This group consists of cave lions (*Panthera spelaea*), leopards (*Panthera pardus*), cave bears (*Ursus spelaeus*), and hyenas (*Crocota crocuta spelaea*). In addition, the work will explain how and when these large carnivores arrived in the Iberian Peninsula.

2. Hypothesis

The working hypotheses are as follows: Was their disappearance due to genetic isolation? Was it due to climate change in the late Pleistocene and early Holocene? Was it due to food competition with other carnivores and humans? Did humans cause their disappearance?

3. Methodology

After all possible bibliographic sources are collected and thoroughly analysed (Blasco Sancho, 1995; Davis & Estévez, 1989; Estévez, 1979; García García, 2003; Kurtén, 1995; Maroto, Ramió, & Galobart, 2002; Nagel, Hilsberg, Benesch, & Scholz, 2003; Sanchis, 2015; Sanchis *et al.*, 2015; Stanton *et al.*, 2020), a critical synthesis will be made.

4. Results

Provisional results indicate a significant decrease in the four large carnivores in the Early Upper Palaeolithic, although some evidence of their presence exists from the end of the same period. Perhaps survival in the Cantabrian was greater than in the Mediterranean.

5. Conclusion

Neither human involvement (modern humans appear in the Upper Palaeolithic) nor environmental factors can be ruled out.

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BETWEEN COERCION AND COORDINATION. THE CORRESPONDENCE OF THE BARCELONA BOARD OF TRADE AS A SOURCE FOR TRACKING SOCIAL CHANGE (1760-1847)

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Keywords: industrialization, guilds, social change, social conflict, economic institutions

1. Introduction

The Barcelona Board of Trade was set up in 1758 and, throughout the following eighty years, it increasingly asserted its authority to regulate guilds, received countless petitions from both artisans and the budding entrepreneurial class, and served as a link between state institutions and economic agents. As a result, until its abolition in 1847, the Board generated copious correspondence, which has not yet been systematically analysed. Copies of all outgoing letters were entered into 51 books, comprising 22,693 pages, from 1760 until 1847, alongside more than 20,000 incoming letters, dating from 1806 onwards.

2. Hypothesis

This study is concerned with two opposing interpretations of the role that guilds and other institutions played during the late 18th century. On the one hand, some proponents of institutional economics and social capital theory have argued that guilds contributed to a stable social environment that encouraged economic growth (Epstein & Prak, 2008; Simon i Tarrés, 2021; Zanden, De Moor, & Lucassen, 2008). On the other hand, historians such as G. Barnosell (1999) or J. Torras Elias (2018) give a more contentious account of the industrialization process, tracing the origins of the 19th-century working class back to the internecine and external conflicts of guilds. Insomuch as the Barcelona Board of Trade handled numerous industrial and guild-related administrative disputes from all over Catalonia, a systematic analysis of its correspondence should allow us to quantify the amount of conflict over time and assess how state institutions dealt with new social agents and economic structures during this period.

3. Methodology

This study employs a research design drawing from both qualitative and quantitative approaches. The language used in letters, as well as techniques derived from content analysis, may allow in-depth case studies. At the same time, its homogeneity and continuity over time should allow parametric tests, such as variance and correlation analysis.

4. Results

A large number (531) of outgoing letters pertaining to three sample groups from 1770, 1789 and 1801 have been examined so far. The percentage of letters addressing guild ordinances or regulations decreased, from over 50% in 1770 to just 20% thirty years later. However, the share of such letters mentioning conflicts increased from 38% to 71%.

5. Conclusion

The nature of conflicts also shifts noticeably, from regulation enforcement to shielding independent producers from guilds. Covariance between different types of letters should be tested further through correlation analysis of incoming and outgoing correspondence.

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THE «ANTIGUA FARMACIA ESTEVA DE LLIVIA» AS A PHARMACEUTICAL «*LIEU DE MÉMOIRE*» OF THE 20th CENTURY

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Keywords: *Lieu de mémoire* [place of memory], Llívia, 20th century, pharmaceutical historiography, museology

1. Introduction

The cornerstone of the Municipal Museum of Llívia, inaugurated in 1981, lies in the «antigua Farmacia Esteva de Llívia». There have been two myths surrounding the pharmacy. On the one hand, the myth of origins. In other words, the *tópos koinós* that the establishment dates from the early 15th century and was the oldest in Europe (a dissertation refuted by González (1974)). On the other hand, the Esteva's family property over the apothecary. It has not been documented that it was run by them since its foundation, but that the relationship began in the first half of the 18th century (Bosom, 1984).

2. Hypothesis

This case study investigates the creation and the socio-cultural processes of a certain narrative appropriation that has occurred in a pharmaceutical place of memory during the 20th century and over its elongated shadow. In particular, the hypothesis that the mythologized account, transmitted by the museum of Llívia from the 1980s and disseminated by the specialist and generalist (inter)national press, was not born *ex nihilo* when it was musealized. Rather, the myth's formulation began when the pharmaceutical establishment was active, at least in the early decades of the 20th century.

3. Methodology

Museology is a transdisciplinary field cultivated by sociology, anthropology, historiography or art historiography (for example, Bourdieu & Darbel, 1969; Géal, 2005; Iniesta, 1994; Portús, 2018). Some studies have focused on medical and pharmaceutical museology *stricto sensu* (Cid, 2007; Pelayo, 2014; Zarzoso, 2005). Applying the logic of socio-cultural historiographic principles (Coromina, 2020, 2021), to deconstruct the *lieu de mémoire*, the mythologized narrative, the socio-cultural appropriation processes and the promoting agents, documentary research —bibliographic, epistolary, newspaper, photographic and oral— has been carried out in different institutions, notably the Municipal Museum of Llívia.

4. Results

The embryogenic obsession, promoted by Antonio Esteva, was documentarily displayed during the first decades and was consolidated in the second half of the century, encouraged by the

museum's curator, and socialized by the press. In the 1980s and 1990s, the museum was very crowded, with a further downward trend. However, the commonplace of origin is still present in people connected with the museum and among scholars.

5. Conclusion

Before its musealization, the *Llivienc*a pharmacy was a place of memory, the result of two mythologized narratives that evolved during the 20th century. In a parallel way, despite scientific research, *topoi* are stubborn.

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THE EUROPEAN AND NON-EUROPEAN CAPITALS OF CULTURE. REPRESENTATIONS AND URBAN IMAGINARIES

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Keywords: cultural capital, representations, urban imaginaries

1. Introduction

Cultural capital, frequently associated with the creative and cultural economy, is also a sociological notion that refers to the interaction between cultural and social structures (Bourdieu, 1983). In cultural history (Roche, 2000), the concept has been systematized in relation to cities of relevance in certain fields of symbolic production (literature, music, theater, painting, etc.), such as Paris, New York, London, and Rome (Zukin, 1995). For the purpose of this communication, we will refer to a very distinct dimension of the phenomenon: the generic denomination “Capital of Culture”, which we understand as an instrument of urban regeneration, a political tool, and a city branding process. Nevertheless, in empirical reality, the different edges overlap.

Thinking of the city as a space for multiple sociabilities (Simmel, 1903; Wirth, 1938) and a condensation of symbols and signs (Barthes, 1990) implies, inexorably, addressing the underlying relationships between objectified cultural capital, symbolic capital and the different expressions of spatiality (Castoriadis, 1975; Pintos, 2014).

The European Capital of Culture (ECC, 1985), a pioneer of an epistemic frame and rationality that conceives culture as a resource for regional integration and urban development, has hatched a myriad of similar manifestations around the world. We have witnessed the confirmation of a pattern of the capital of culture. The Ibero-American (1991), Arab (1996) and American (1997) capitals of culture belong to the first generation of this kind of initiative.

2. Hypothesis

- (1) The European and non-European Capitals of Culture sustain the narrative of a modern, global city, associating the creative, the smart, and the cultural in a strategy of repositioning cities on the international scene, to the detriment of the traditional or popular cultural city.
- (2) The instituting imaginary of the “capital of culture” accounts for the referent behind certain public policies of the city.

3. Methodology

The methodology used will be a systematic analysis of documentation (resolutions, calls, evaluation reports and press articles) and critical and qualitative content analysis.

4. Results and discussion

Cultural capitals function as devices for repositioning cities, influencing the conditions for the production of social representation, and providing socio-cognitive contents and practices for their conformation/transformation.

The media's action (the narratives of the cultural capital) and the political discourses (modernization, shared identities or social cohesion) impact the perception of the city in two directions: inwards (inhabitants themselves) and outwards (visitors, tourists, national and international audiences).

5. Conclusions

The social imaginaries mobilized by the cultural capital – focused on the potentialities of the cities as a global modern space – confront the territorial imaginaries anchored in history and traditional practices. The “capitals of culture” become spaces of conflict, negotiation and consensus between the different narratives, discourses and instituted and instituting urban imaginaries.

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SESSION XIV. EDUCATION

ART THINKING AS EXPERIMENTATION IN EDUCATIONAL INNOVATION. SOCIO-EDUCATIONAL IMPACT ON GREEK SOCIETY: ANALYSIS, IMPLEMENTATION, AND EVALUATION AS A CHALLENGE TO ENHANCE THE SOCIETY OF TOMORROW

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Keywords: art thinking, a/r/tography, innovation, artistic education, citizen

1. Introduction

Art thinking is an educational innovation that uses the arts as a backbone to study, analyze and enable solutions for the different fields and actors involved in education. This broad field of action ranges from the creation of educational strategies (curriculum), through the study of the actors involved to the formal and structural analysis of teaching spaces. Since it is a wide spectrum of research, this doctoral thesis has focused on the theoretical-practical field of artistic education, which means that it is restricted to the field of the curriculum. Maria Acaso López-Bosch has stated it well:

“I think that today we must vindicate the teaching of the arts and visual culture as an area related to knowledge, with the intellect, with mental processes and not only with manuals, with teaching to see and do with the head and with the hands and not only teach to do with the hands” (Acaso, 2009).

According to the ideas of Tim Ingold, we cannot understand human activity and its relationship with the environment as something mechanical; it is about promoting and developing creativity, group work, critical judgment and empathy as tools to develop knowledge and enhance human capabilities.

Through the construction and production of alternative dynamics, we attempt to position the participant as the central axis that generates knowledge. It is about encouraging the citizen as a civic and democratic being involved in a society that is capable of individually and collectively creating its own body of knowledge (Acaso & Megías, 2017).

2. Methodology

This research is framed within the methodologies in art-based research. More specifically it is shaped in a/r/tography “as a research methodology that reveals the three interconnected identities of the ‘artist, researcher and teacher’, as that person who, in its teaching action, is able to develop a creative practice with their students through experimental processes in artistic research” (Mesías-Lema, 2018).

3. Results

This first investigation has resulted in the articulation of educational activities of an artistic nature. They are put into practice in formal and informal spaces and are based on games, cartography and the use of digital devices as an educational method.

4. Conclusions

These educational proposals intertwine archaeology, anthropology and contemporary art to generate new ways of exploring human relationships and the environment in which we live.

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ADAPTATION TO SPANISH AND VALIDATION OF A QUESTIONNAIRE TO MEASURE TEACHER PERCEPTIONS OF STEAM

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Keywords: teachers, questionnaire, instrument, validation, STEAM

1. Introduction

The STEAM educational approach has gained relevance due to its realism and inclusion, which favour "responding to the challenges of the real problems of daily life within a globalized and changing society" (Santillán-Aguirre, Jaramillo-Moyano, Santos-Poveda, & Cadena-Vaca, 2020). However, prior to implementing such an innovation in educational establishments, it is necessary to consider teachers' preparation and their perceptions about the proposal. In this scenario, it is proposed to translate into Spanish and validate the Kindergarten Teachers' Attitudes toward and Confidence for Integrated STEM Education instrument (Tao, 2019), in order to explore the perceptions of Chilean teachers related to STEAM education for designing a teacher training course on this approach.

2. Methodology

After translation into Spanish, the instrument was validated by experts in translation and the STEAM disciplines. Subsequently, it was applied to a sample of 31 teachers and, due to the adaptation process, statistically processed to verify its validity and reliability.

3. Results

The translated instrument consisted of four items focused on attitudes towards STEM education, and six items focused on confidence to teach STEM. However, the analysis of the validity and reliability of the instrument yielded an extra dimension. A review of the base instrument of the adaptation indicated that the first two items corresponded to the familiarity category. This new category is consistent with indications in the original instrument and with Cronbach's Alpha measure.

4. Discussion

In this study, an instrument has been adapted to the Spanish language and validated to characterize the perceptions of Chilean teachers regarding the STEAM approach. A statistical analysis ascertained to what extent the instrument maintained its reliability; Cronbach's alpha was between 0.828 and 0.921. These results affirm that the instrument is viable for use in this context.

5. Conclusions

The validation results show an adequate variance, thereby validating the reliability of the instrument. Likewise, since it is a brief questionnaire, it allows a rapid application and analysis of the results. Based on the above, the adaptation of the Attitudes toward and Confidence for Integrated STEM Education to the Spanish culture and language is proposed as a reliable instrument to expand the study of the perceptions of Chilean teachers regarding the STEAM approach.

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A MISMATCH BETWEEN TEACHERS' BELIEFS AND ACTUAL PRACTICES RELATED TO STEAM EDUCATION

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Keywords: STEAM education, teacher training, STEAM training, perceptions, predispositions

1. Introduction

A bibliometric analysis on the Web of Science concluded *teacher training* is a recent trend in research related to STEAM education (interdisciplinarity among science, technology, engineering, arts/humanities and mathematics) (Marín-Marín, Moreno-Guerrero, Dúo-Terrón, & López-Belmonte, 2021). While teachers' beliefs about STEAM are not completely understood (Kim & Lee, 2018), models like the realistic-reflective model argue that those beliefs should be considered in teacher training (Rodrigues-Silva & Alsina, 2021). Accordingly, we sought to explore teachers' beliefs and actual practices related to STEAM Education.

2. Methodology

The research takes a quantitative approach, in which 14 teachers answered a Likert questionnaire (scale 1 to 5) that evaluated 18 educational approaches related to active learning, such as problem-, project-, and inquiry-based learning. We ran multiple Wilcoxon signed-rank tests, using the threshold of 5%, to verify differences regarding four dimensions: knowledge (K), usage (U), willingness to use (W), and appropriateness to STEAM (A). Since multiple tests may lead to “p-hacking”, we avoided specific evaluations.

3. Results

In Table 1, we present the total of significant and non-significant Wilcoxon results regarding the four dimensions.

Table 1. Total of significant and non-significant differences in educational approaches regarding knowledge (K), usage (U), willingness to use (W) and appropriateness to STEAM (A).

Wilcoxon results	Knowledge (K) versus usage (U)	Knowledge (K) versus appropriateness to STEAM (A)	Usage (U) versus appropriateness to STEAM (A)	Willingness to use (W) versus appropriateness to STEAM (A)
Significant	13 (K>U)	1 (K>A)	-	1 (W>A)
	-	14 (K<A)	16 (U<A)	2 (W<A)
Non-significant	5	3	2	15

The results indicate an evident difference between teachers' knowledge and usage of educational approaches; teachers know more of them than they use (13 out of 18). We also observe a mismatch between knowledge and usage versus appropriateness to STEAM. Teachers indicate the approaches are appropriate to STEAM but they have lower knowledge (14 out of 18) or lower experience of usage (16 out of 18). On the other hand, willingness to use versus appropriateness to STEAM had most approaches with a non-significant difference (15 from 18).

4. Conclusions

We concluded there is a mismatch between what teachers know, use, and consider appropriate to STEAM. Interestingly, there is accordance between their willingness to use and appropriateness to STEAM. In a teacher-training programme, we may account for openness towards STEAM, but also cognitive conflicts involving theory and practice. Therefore, we should account for training programmes that address those incongruences, such as the realistic-reflective model.

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OPPORTUNITIES TO DEVELOP ALGEBRAIC THINKING IN EARLY CHILDHOOD TEXTBOOKS

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Keywords: early algebra, mathematical tasks, textbooks, early childhood education

1. Introduction

The incorporation of algebra as a block of content from the first years of schooling responds to a proposal for curricular innovation known as early algebra. This new trend proposes teaching this block of content during early childhood education (Alsina, 2019; Kaput, Carraher, & Blanton, 2007).

Contemporary early childhood education curricula have not remained oblivious to this innovation and have assumed the importance of content linked to early algebra, incorporating knowledge of an algebraic nature progressively from this stage of school (Pincheira & Alsina, 2021).

2. Problem

The curricular transformation of early algebra to its current state requires teachers who are able to meet the pursued objectives and conduct their teaching effectively, by selecting and implementing mathematical tasks based on the contents set out in the curricular guidelines.

In accordance with this point of view, teachers must pay attention to the tasks proposed in textbooks, since they constitute an element of support in classroom instruction. In addition, the knowledge promoted by mathematics textbooks is closely linked to students' learning opportunities (Stylianides, 2009).

Based on this, in this study we ask what opportunities textbooks offer to develop algebraic thinking in early childhood education.

To answer this question, we assume the characterization of the mathematical knowledge involved in solving tasks that promote the development of early algebraic thinking in early childhood education proposed by Pincheira & Alsina (2021).

3. Methodology

The study presents a qualitative methodology of a descriptive nature (Hernández, Fernández, & Baptista, 2014). A sample of eight Chilean textbooks for early childhood education (4 to 6 years of age) was selected and examined using the content analysis technique, and classifying the mathematical tasks on early algebra, in accordance with the characterization of early algebra for early childhood education (Pincheira & Alsina, 2021).

4. Results

The results show the highest concentration of tasks establishing relationships based on attribute recognition (79%). Far behind are seriation tasks based on repetition patterns (20%). Finally, the presence of tasks related to the description of qualitative and quantitative changes is practically nonexistent (1%).

5. Conclusion

The textbooks analysed do not provide the necessary tools for children in early childhood education to deepen and develop early algebraic thinking. The textbooks need to incorporate a variety of tasks that focus on working with patterns and describing change.

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ANALYSIS OF THE PRESENCE OF PATTERNED TASKS IN EARLY CHILDHOOD EDUCATION TEXTBOOKS

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Keywords: early algebra, patterns, mathematical tasks, textbooks, early childhood education

1. Introduction

Several studies highlight that early mathematical skills can be an indicator of academic success at later stages (Wijns, Verschaffel, De Smedt, & Torbeyns, 2021). Some authors such as Mulligan, Oslington, & English (2020) and Wijns, Torbeyns, De Smedt, & Verschaffel (2019), have indicated that knowledge of patterns and their structure positively influences early mathematical development. From this perspective, the exploration of patterns can be a springboard to promote essential mathematical skills, such as generalisation (Cetina-Vázquez & Cabañas-Sánchez, 2022).

2. Problem

Taking into account the approaches of Alsina's Mathematics Teaching Itineraries Approach (Alsina, 2020), teaching concludes in graphic and symbolic contexts where the representation and formalisation of mathematical knowledge is worked on, mainly through textbooks and/or activity books. However, (Wijns *et al.*, 2019) note that it remains to be studied whether the patterned activities proposed in these resources optimally exploit their full potential. We formulate the following research question: How is the teaching of patterns with 3-6 year olds approached through textbooks? From this question, we derive the following objective: To demonstrate the presence of tasks with patterns in textbooks for early childhood education when this content is formalised with children aged 3, 4 and 5 years old.

3. Methodology

Our study adopted an exploratory-descriptive qualitative approach (Hernández Sampieri, Fernández Collado, & Baptista Lucio, 2014) to analyse how patterns are taught using graphic resources, and to assess the formalisation process carried out by 3- to 6-year-old children through textbooks. The technique used to conduct and facilitate our research is content analysis.

4. Results

The results obtained show that, in general, pattern-teaching tasks are present in the five publishing projects that make up our sample. However, of the 850 tasks analysed, only 9.8% correspond to patterns. From this perspective, it is evident that in the textbooks analysed, the average presence of proposals with patterns is 2.8 tasks for 3-year-olds (minimum range 1 and

maximum range 6); 6.6 for 4-year-olds (minimum range 2 and maximum range 18); and 7.2 for 5-year-olds (minimum range 2 and maximum range 21).

5. Conclusion

These data affirm that some editorial projects deal with the teaching of patterns in a limited way. As a result, teachers must have access to data that allows them to critically analyse textbook tasks and implement proposals that offer children the opportunity to recognise, represent and generalise patterns.

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SESSION XV. LAW AND ADMINISTRATION

THE CYCLE OF CONTINUOUS IMPROVEMENT AND ISO INTERNATIONAL STANDARDS AS A BASIS FOR MITIGATION OF ADMINISTRATIVE AND FINANCIAL INFRACTIONS IN THE PUBLIC ADMINISTRATION: ECUADORIAN PUBLIC MANAGEMENT CASE STUDY

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Keywords: management, internal control, risk, security, corruption

1. Introduction

According to ISO internationally recognized standards, quality public management infers the integration of existing management systems in organizations. These standards analyze, evaluate and manage the probable risks that may arise due to procedural action or omission, to mitigate them and to implement the four actions that make up the continuous improvement cycle (Calso Morales & Pardo Álvarez, 2018; Gómez Fernández & Fernández Rivero, 2018).

2. Problem

Ecuadorian public management currently suffers a structural crisis due to non-existent or deficient systems of internal control, risk management and information security (SCIGRSI, in Spanish). It has been vulnerable to non-observances, breaches and crimes of corruption as a result of precarious action in its formal structure and technical and behavioral characteristics (Deming, 1989). This situation leads to the following question. Would greater internal control decrease administrative infractions in Ecuadorian public management? This inversely proportional relationship leads to the formulation of two hypotheses; (1) The integration of the continuous improvement cycle and ISO international standards increases the efficiency of organizational internal control and (2) It is possible to reduce administrative and financial infractions by increasing SCIGRSI. In addition to these hypotheses, we can establish a general objective of this study: Analyze the level of incidence of the four actions of the continuous improvement cycle supported by ISO international standards for quality public management. The specific objectives are 1.1 Determine the impact of administrative infractions due to the absence of SCIGRSI in the public procedural action and 1.2 Analyze the procedural consequences of the lack of implementation of the continuous improvement cycle – plan-do-verify-act – supported by ISO international standards in Ecuadorian public management.

3. Methodology

Initially, the methods used were qualitative (descriptive) and quantitative (analytical) (Hernández Sampieri, Fernández Collado, & Baptista Lucio, 2014) based on the result of 1,504

general data and 10,528 specific data from subsequent government control in Ecuador. The hypotheses were analyzed using the R Language (Navarrete & Chávez Pullas, 2019).

4. Results

The disclosure of the actions carried out from 2016 to 2021 focused on scientific development aimed at restructuring public management.

5. Conclusions

The organizational transformation based on comprehensive internal control systems sustain the economic, social, political and technological development of a country. However, they must be complemented by real legislation focused on a situational diagnosis of society based on the cycle of continuous improvement and ISO international recognition standards in administrative and financial processes.

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PUBLIC ADMINISTRATION AND THE SUMAK KAWSAY

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Keywords: public administration, sumak kawsay, plurinational state, legal pluralism, administrative law

1. Introduction

The configuration and structure of public administration is designed under the European criterion and tradition (Poesche, 2020) of Administrative Procedural Law (Trayter Jiménez, 2017). However, the situation is different in plurinational states such as Ecuador (constituent assembly), in which indigenous nationalities (Acosta, 2013) proclaim customary law with atypical authority systems and allow the emergence of legal pluralism.

Undoubtedly, the law as a structure (Bobbio, 2013) is the result of agreement among the inhabitants, who have aligned their aspirations towards a collective legal good. Therefore, the public administration, under the premise of Eurocentric law, pursues the achievement of the collective good and the administrative protection of people's rights. Ecuador, as well as other Latin American countries with large indigenous populations, have proclaimed republican models of government and plurinationality. This means that several indigenous nations, each different from the others and having its own identity, language, culture, law, customs and other characteristics, come together and form the state.

2. Hypothesis

The following hypothesis is formulated due to identification of the existence of customary law, typical of each nationality: the public administration does not comply with the principle of efficiency in plurinational states. In other words, the common interest, considered generically as the core of the vision of the public administration, does not apply in the indigenous worldview.

The general objective of this work is to analyze the degree of adaptation of public administrations and their management in multinational states. This includes two specific objectives: to determine the degree of efficiency of public administrations in guaranteeing indigenous collective rights; and to analyze the result of the control exams carried out on public administrations in indigenous councils, in which regulatory compliance is evaluated (González-Ortiz de Zárate, Alonso García, & Berrocal Berrocal, 2017).

3. Methodology

The research methodology is qualitative (descriptive) and analytical (quantitative) (Hernández Sampieri, Fernández Collado, & Baptista Lucio, 2014). The hypotheses have been tested using the R Language (Molina, Mulero, Nueda, & Pascual, 2014).

4. Results

The incorporation of indigenous nationalities, made up of inhabitants plus the population that defines itself as indigenous, requires that their freedoms be guaranteed by public administrations unable to recognize the diversity and multiplicity of legal orientations.

5. Conclusion

The incorporation of indigenous nationalities, made up of inhabitants plus the population that defines itself as indigenous, requires that their freedoms be guaranteed by public administrations unable to recognize the diversity and multiplicity of legal orientations.

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TAXATION OF TELEWORK

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Keywords: taxation, telework, residence, public spending, income

1. Introduction

This thesis analyses teleworking from the perspective of financial and tax law. First, it will examine the different modalities and characteristics, as well as its legal-labour treatment at different levels: international, European and domestic (Calderón Carrero, 1997; Ushakova, 2015). Second, it deals with the issue of tax residence. This concept is important to be able to identify where the service is provided and also how it can be proven to the tax authorities (or how this should be done). Subsequently, it also deals with questions related to public expenditure, i.e. what implications teleworking has and will have for the funding of public services. Finally, there will be a comparative law study and conclusions.

2. Hypothesis

In the aftermath of the health crisis, teleworking emerged as an alternative to maintain employment and economic activity. This means that certain taxation principles and rules need to be reconsidered. In the digital age, intangible assets have to be valued appropriately (Pérez Agulla, 2020). Above all, such assets must be located so that they are taxed in the right place (Ubero Truyo & Toribio Bernárdez, 2019). Therefore, the thesis will examine the concept of residence, i.e. the displacement produced without informing tax authorities. In addition, it will examine how teleworking will affect the distribution of public expenses and how the operations carried out through teleworking are taxed, paying particular attention to goods in kind.

3. Methodology

The methodology used in the thesis will be, first, to structure the research correctly into a table of contents with the most relevant questions, several chapters and conclusions. Second, it will conduct a bibliographic search of the most essential authors on the subject, together with supporting jurisprudential and normative research. This will establish a solid argument in each part of the research.

4. Results and discussion

It is too early to obtain significant results. However, it is true that a number of problems in the tax area can be identified with the advent of telework: the difficulties for tax authorities to locate teleworkers; imbalances in public spending as a result of commuting not being reported to the authorities; and the complex tax treatment of certain income from teleworking.

5. Conclusion

The conclusion we can draw for the moment is the need to establish a solid and modern body of law that is capable of accommodating new ways of providing services, i.e. adapting the legal world to new technologies. The need to resolve the problems raised will be the subject of this thesis.

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THE PROTECTION OF VICTIMS OF TRAFFICKING IN THE INTERNATIONAL LEGAL SYSTEM AND ITS APPLICATION AT THE EUROPEAN REGIONAL LEVEL: A PROPOSAL FOR THE STATUS OF VICTIMS

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Keywords: International Law, Human Rights, human trafficking, victims, protection

1. Introduction

Trafficking in human beings, one of the most harmful criminal activities in terms of victims' integrity and dignity, violates fundamental human rights protected by the international order. Through the 2011/36/EU Directive (Villacampa Estiarte, 2011), the European Union established a framework for fighting trafficking from a threefold perspective, known as the 3P paradigm: protection of victims, prosecution of criminals, and prevention of the phenomenon. From the perspective of International Human Rights Law (Gallagher, 2011), this research will focus solely on the protection of the victims of human trafficking.

Beyond the provisions of this specific legal instrument, General Principles emanating from International Human Rights Law are of great importance, yet often forgotten (Jordana Santiago, 2020). They need to be taken into consideration in the protection of trafficked persons, as they can offer valuable protection to them, particularly to the most vulnerable groups, for instance, women, refugees and children (Milano, 2020).

This study seeks to determine to what extent these general principles can be used to improve the current European framework dealing with human trafficking (Haverkamp, Herlin-Karnell, & Lernerstedt, 2019). Once they have been analysed, it will propose a European Directive that, inspired by the international framework, protects victims adequately and can be adapted to their needs.

2. Hypothesis

Is the current European framework sufficient to protect the Human Rights of trafficked persons or is an improvement of the current regulation needed?

3. Methodology

The main methodology used to carry out this doctoral thesis is research into the wide variety of instruments offered by the United Nations, the Council of Europe, and the European Union, as well as extensive research conducted at the academic level. Furthermore, I have been accepted for a research stay in the prestigious ICMPD (International Centre for Migration Policy Development), which works closely with the EU on trafficking issues. There, I will be able to collaborate with the best specialists in the field.

4. Results and discussion

During this first year and a half of research, some issues for review have been identified: (1) residence permits for third-country national victims, (2) victim identification systems, (3) vulnerable groups, and (4) cooperation between different European actors.

5. Conclusion

Many aspects of the Directive need to be improved to provide a system that truly protects victims. International Human Rights Law can play a key role in inspiring the proposal.

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THE EUROPEAN UNION AND CONSTITUTIONAL IDENTITY

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Keywords: European Union, ECJ, democracy, constitution, constitutional identity

1. Introduction

The Court of Justice of the European Union (ECJ) has changed over time. Until now, the Court had been reluctant to develop a clear face-to-face with Article 4(2) of the Treaty on European Union (TEU) due to the fear that a more precise definition would increase conflicts with national (constitutional) courts in Member States (MS). With the 'twin-decisions', the ECJ has explicitly used European identity to place a limit on the scope of operation and application of the different constitutional identities.

2. Methodology

Study and analysis of the constitutional documents of the EU and MSs and the relevant case law and jurisprudence of the ECJ and European constitutional courts (Case C-156/21, Case C-157/21, Case C-391/20, Case C-430/21).

3. Results

The ECJ's recent 'twin-decisions' on the rule of law conditionality mechanism introduced, de facto, the concept of 'European Constitutional Identity' (Faraguna & Drinóczi, 2022). Its scope is still unexplored, but with potentially profound effects for the EU.

This paradigm shift has three consequences: 1) the ECJ proceduralized the use of Art. 4(2) TEU through the preliminary reference procedure by national (constitutional) courts (Bonelli, 2022); 2) the identity claims should not be used in such a way that turn into a violation of the European constitutional identity (Faraguna & Bartole, 2022); and 3) the possibility to define substantive constraints to the Treaty that amend power based on Art. 2 TEU (Faraguna & Bartole, 2022).

4. Discussion

I intend to develop this perspective outside the rule of law issue, focusing on another value enshrined in Article 2 and specified in Title II (TEU), namely the 'principle of democracy' (Lenaerts, 2013).

This principle is part of the European identity itself, but without any precise development (Fromage & De Witte, 2021). The political genesis of the rule of law conditionality mechanism demonstrates to what degree democratic principles have only been structurally downgraded in the European treaties, but have been further restricted by the European institutions. Moreover, no ECJ jurisprudence could explain how it can be a legally binding obligation for the MS.

The unresolved question of the principle of democracy at the European level is the basis of two problems:

- (1) The "*Europa-Streit*", which is a dispute over what the EU is: 'an advanced species of the genus international law' or a 'sui generis political community', different from both the *Bundesstat* and the *Staatenbund*.
- (2) This burning issue is addressed by the *Bundesverfassungsgericht* (BVerfG) with its famous decisions. They highlight that the EU is in democratic terms a derivative of the MS and see it as an international organization whose further democratization/constitutionalization would damage national democracies.

5. Conclusions

The principle of democracy will be the next great European challenge in two ways: (1) what democracy is for the EU and (2) what the relationship will be between European democracy and national democracies.

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