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Abstract Book

Miquel Solà, PhD (Editor)

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Miquel Solà, PhD *(Editor)*

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PREFACE

The First Conference of Pre-doctoral Researchers of the University of Girona (UdG) was organized in 2017 by the School of doctoral studies of the UdG and the UdG.doc association, in collaboration with the Offices of the Vice-rector for research and of the Vice-rector for students. This year, 10 volunteer PhD students have organized the Fifth Conference of Pre-doctoral Researchers of the UdG.

The main aim of these Conferences is to offer a forum of training, knowledge exchange, research dissemination, and debate among doctoral students of our University. These Conferences offer PhD students the opportunity to present his/her research in the form of oral communications and to discuss the results of their research with peers. Ability to communicate research to peers and to society is in an important soft skill for the future professional careers of PhD students. In addition, these Conferences contain informative sessions and workshops on topics relevant to researchers in training like labor insertion, diversity, equity and inclusion, open science, etc.

The Fifth Conference of Pre-doctoral Researchers of the UdG was held from 14th to 17th June 2021 at the Faculty of Law. For the first time, we had more than 100 oral communications from PhD and master students. Like in the past Conference, attendance to the Fifth Conference of Pre-doctoral Researchers of the UdG was restricted following the recommendations given by Office of Occupational Health of the UdG to ensure adequate protection of the safety and health of participants. All talks, conferences, and workshops were broadcasted through streaming. Moreover, some PhD students decided to deliver their oral communications by video-conference. It was not easy to combine talks that were delivered in-person with those that were given by video-conference or to allow questions from PhD students attending the talks from their houses. I want to express my deepest gratitude to the 10 enthusiastic PhD students that took part in the organization of this Fifth Conference. They did an excellent job as organizers and chairpersons of the different sessions! Without their involvement, the Conferences of Pre-doctoral Researchers of the UdG would not be possible!

This book contains the abstracts of the 101 talks given by the participants in the Fifth Conference of Pre-doctoral Researchers of the UdG. They are organized in thirteen sections corresponding to the different sessions in which the conference was divided. This collection of abstracts represents a good summary of the research that is being carried out nowadays in our University. We hope you enjoy reading the book and we look forward to meeting you in the next Sixth Conference of Pre-doctoral Researchers of the UdG.

Girona, 4th October 2021
Miquel Solà

SESSION I. PEPTIDES, PROTEINS AND ENZYMES

CHARACTERIZATION OF ALDOSE REDUCTASE B1 IN PIG SEMINAL PLASMA AND REPRODUCTIVE TISSUES

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1. Introduction

Aldose Reductase B1 (AKR1B1) is a seminal plasma (SP)-protein that has been positively related with *in vivo* fertility outcomes in pigs (Pérez-Patiño *et al.*, 2018). Thus, the aim of the present study was to characterize the synthesis of AKR1B1 alongside the boar reproductive tract. To this end, the specific objectives were: i) to evaluate the concentration of SP-AKR1B1 in boar ejaculate-fractions (which include the first 10 mL of the sperm rich fraction (SRF-P1), the rest of the SRF (SRF-P2), and post-SRF (PSRF)); ii) to describe the immunohistochemical localization of AKR1B1 in boar reproductive tissues.

2. Methodology

A total of seven ejaculates were collected in separate fractions (SRF-P1, SRF-P2, PSRF) from seven Artificial insemination (AI)-boars. Ejaculates fractions were centrifuged (1500 ×g for 10 min twice) to obtain SP-samples, which were stored at -80ºC until AKR1B1 concentration was measured using a porcine-specific quantitative Enzyme-Linked Immunosorbent Assay. Tissue samples from the reproductive tract (testis, epididymis, prostate, seminal vesicles and bulbourethral grands) were obtained from three AI-boars slaughtered for replacement reasons. For immunoblotting analysis, protein samples obtained from each tissue were incubated with an anti-AKR1B1 primary antibody. Immunohistochemical analysis was performed with tissue sections from paraffin-embedded samples.

3. Results

Concentration of SP-AKR1B1 differed ($P < 0.05$) between ejaculate fractions; whereas it was lower in SRF-P1 (458.2 ± 116.33 ng/mL) than in PSRF (1342.4 ± 116.33 ng/mL) and SRF-P2 (1105.0 ± 229.80 ng/mL), no differences between SRF-P2 and PSRF were found. The immunoblotting assay revealed the presence of AKR1B1 in the testis, caput, corpus and cauda of the epididymis, seminal vesicles, and prostate. AKR1B1 monomeric (36 kDa) and dimeric (~80 kDa) forms were detected in all tissues assessed, except the prostate, which only exhibited the monomeric form. Immunohistochemical analysis demonstrated the presence of AKR1B1 in testis Leydig cells cytosol, basal and principal cells of the epididymis, and in the glandular epithelial cells of prostate and seminal vesicles.

4. Conclusions

This study demonstrated, for the first time in pigs, that AKR1B1 is expressed in the testis, epididymis, and accessory sex glands, except in bulbourethral glands. In addition, this study also found the highest concentration of SP-AKR1B1 in PSRF, which suggests that seminal vesicles could be one of the major contributors of this SP-protein to the entire ejaculate. Moreover, AKR1B1 higher expression in PSRF indicates that this protein could play its active role in the female reproductive tract rather than in sperm.

Keywords: *Aldose Reductase 1 B1, seminal plasma, ejaculate fractions, sperm quality, pig*

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ELUCIDATION OF THE SECONDARY STRUCTURE OF ANTIMICROBIAL LIPOPEPTIDES BY NMR

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6. Introduction

Antimicrobial peptides are considered a good alternative to traditional pesticides to prevent plant diseases caused by bacteria. Their mechanism of action involves their interaction with the bacterial membrane, followed by their insertion into the phospholipid bilayer. Among other parameters, the hydrophobicity, the charge, and the secondary structure of peptides play an important role in this process.

In this work, NMR experiments were used to analyse the structure of lipoundecapeptides previously described in our group (Oliveras *et al.*, 2018). In particular, we investigated the effect on the secondary structure of incorporating an acyl group and/or a D-amino acid in the sequence of the parent undecapeptides. The influence of the secondary structure on their antibacterial activity was also analysed.

7. Hypothesis

It was postulated that the presence of a fatty acid chain and/or a D-amino acid in our lipopeptides confers them with a secondary structure that favours the antibacterial activity.

8. Methodology

Lipopeptides were synthetized on solid-phase following a standard Fmoc/*t*Bu strategy and screened for their antimicrobial activity. They were fully characterized by ^{1}H, ^{13}C and ^{15}N NMR (Manzini *et al.*, 2014), and their secondary structure was elucidated using the *Chemical Shift Index 3.0* webserver (Hafsa, Arndt, & Wishart, 2015) and compared with the non-acylated peptides.

9. Results and discussion

Results showed that all the studied peptides are completely unstructured in water and they adopt a secondary structure in the presence of 30% 2,2,2-trifluoroethanol-d_3 (TFE). Based on the NOESY and TOCSY correlations, the amino acid sequences were completely assigned, and it was deduced that they adopt a secondary structure. In comparison with their non-acylated counterparts, results suggest that the presence of an acyl group has no effect on the formation of the secondary structure, but it notably increases the biological activity. Moreover, it was determined that although the incorporation of a D-amino acid distorts the structure blocking the formation of the secondary structure, it decreases the hemolysis compared to their L-amino acid analogues (Güell *et al.*, 2011).

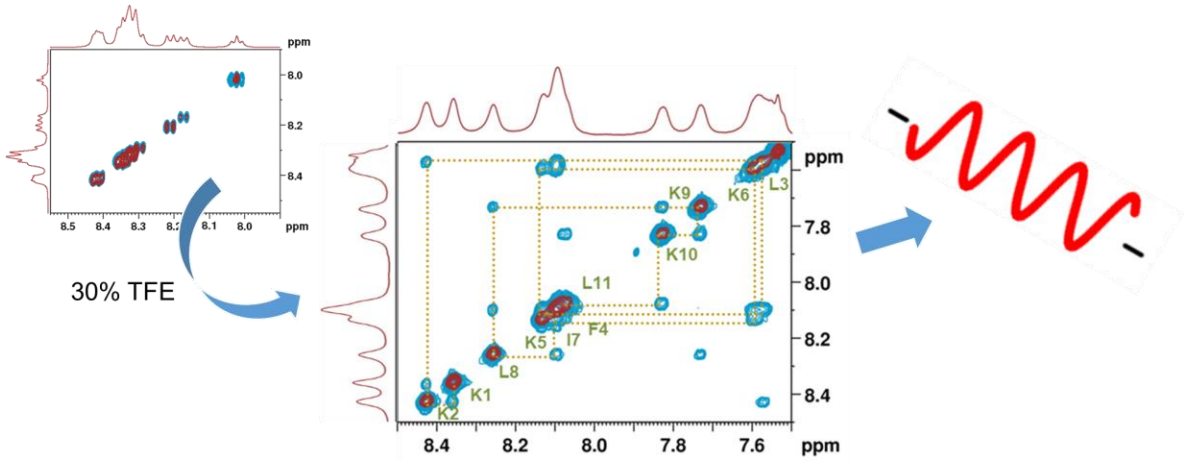

Figure 1. ^{1}H-^{1}H NOESY spectra of unstructured and structured lipopeptide **BP389** in the HN-HN amide region. The addition of TFE induces the formation of an α-helix.

10. Conclusions

It was concluded that while the incorporation of an acyl chain into the sequence of our undecapeptides does not lead to any significant change of their α-helix conformation, the replacement of an L-amino acid with its D-isomer disrupts the secondary structure. Interestingly, the latter modification provides low hemolytic lipopeptides. This knowledge will allow us to design new peptides with a better biological profile.

Keywords: *lipopeptide, antimicrobial, NMR, secondary structure, D-amino acid*

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DESIGN OF A SCREENING PLATFORM FOR ELICITOR PEPTIDES IN *Prunus dulcis*

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1. Introduction

Xylella fastidiosa is a quarantine plant pathogen that affects a variety of hosts of economic relevance, such as grapevine (*Vitis vinifera),* olive *(Olea europaea)* and almond (*Prunus dulcis)* trees (Rapicavoli, Ingel, Blanco-Ulate, Cantu, & Roper, 2018). Nowadays, the preventive methods used in Europe to control *X. fastidiosa* include the eradication of the infected plants and the use of pathogen-free plant material. Unfortunately, once the plant is infected, there are no effective treatments available. Peptides have emerged as promising candidates, because they can act as plant defence elicitors (Ruiz *et al.*, 2018). For instance, peptide **flg22** has been described as an elicitor in *Arabidopsis* (Chinchilla, Bauer, Regenass, Boller, & Felix, 2006). Detection of plant defence induction could be performed using the RT-qPCR technique for transcriptomic analysis. In this work, **flg22** was used to set up an RT-qPCR platform suitable for testing potential elicitor peptides.

2. Hypothesis

Described as a defence elicitor in other plant models, it was assumed that **flg22** was also a defence elicitor in *P. dulcis*. **Flg22** was used to identify and select genes related to defence pathways using an RNA-Seq transcriptome analysis. These were used as markers to develop a screening platform to identify synthetic peptides as defence elicitors in *P. dulcis* through RT-qPCR.

3. Methodology

Plants of *P. dulcis* were treated with **flg22** and samples of leaves were collected at 6 h and 24 h after treatment. Afterwards, RNA was extracted from leaves and the quality of the extraction was assessed. RNA-Seq transcriptome analysis was performed to identify genes related to the defence elicitor capacity of **flg22** as well as to select candidates to be used as marker genes for defence activation.

4. Results and discussion

The obtained data from RNA-Seq demonstrated that **flg22** is a defence elicitor peptide in *P. dulcis*, since several defence related genes were overexpressed. It was also found that **flg22** treatment for 6 h induced a more enriched and powerful overexpression than the treatment for 24 h. The analysis of this data allowed the selection of twenty-one genes to be used as markers in the screening platform for the defence induction in *P. dulcis*.

5. Conclusions

RNA-Seq is a high precision technique for the identification and selection of a set of defence related genes, overexpressed after **flg22** treatment in *P. dulcis*. These results are being applied to set up and validate an RT-qPCR screening platform that will be used to test other potential elicitor peptides.

Keywords: *Xylella fastidiosa, plant defence, elicitor peptide, RNA-Seq Prunus dulcis*

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EXPLORING THE FUNCTIONAL ROLE OF AQUAPORINS IN MAMMALIAN SPERM CAPACITATION

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1. Introduction

Aquaporins (AQP) are a family of proteins involved in transmembrane transport of water and small solutes. In mammalian sperm, they have a key role in osmoregulation and sperm motility activation (Chen & Duan, 2011). Sperm achieve fertilizing ability during capacitation, which is triggered by pH and extracellular ion gradients within the female reproductive tract. The aim of this study was to elucidate the functional relevance of different AQPs during mammalian sperm capacitation, using the pig as a model.

2. Methodology

A total 16 boar ejaculates were used, and samples were split into different subfractions: the control and the treatments with AQP inhibitors ($CuSO_4$; $HgCl_2$; and silver sulfadiazine, AgSDZ). *In vitro* sperm capacitation and acrosome reaction were performed, and function parameters were assessed after 0, 120, 240, 250 and 300 min of incubation. Sperm motility was evaluated through a computer-assisted sperm analysis system; viability, acrosome integrity, membrane lipid disorder, mitochondrial membrane potential (MMP), and intracellular levels of calcium, peroxides and superoxides were assessed through flow cytometry. Levels of tyrosine phosphorylation were evaluated through immunoblotting.

3. Results

Samples treated with $CuSO_4$ showed increased levels of peroxides compared to the control. In the presence of $HgCl_2$, MMP was lower than in the control after triggering the acrosome reaction, and membrane lipid disorder was higher from 120 min until the end of incubation. In the presence of AgSDZ, motility parameters were lower after 120 and 240 min of incubation; MMP was lower and tyrosine phosphorylation levels were higher than in the control after triggering the acrosome reaction.

4. Discussion

The effects of $CuSO_4$, a specific inhibitor of AQP3 (Zelenina, Tritto, Bondar, Zelenin, & Aperia, 2004), evidence that this AQP does not have a key role during sperm capacitation, since none of the key capacitation-related parameters were altered. The presence of $HgCl_2$, an inhibitor of all AQPs except for AQP7 (Hirano *et al.*, 2010; Ishibashi *et al.*, 1998), seemed to increase membrane fusogenicity, but the sperm ability to undergo the acrosome reaction was unaltered. The effects observed in the presence of AgSDZ, an unspecific inhibitor of AQPs (Niemietz &

Tyerman, 2002), could be attributed either to AQP7 inhibition or to an absence of functional AQPs that could compensate their function.

5. Conclusions

Despite different AQPs being relevant for sperm function, sperm capacitation seems to be exclusively altered when all AQPs are inhibited, which suggests that when some AQPs are blocked, other functional AQPs are able to compensate their function.

Keywords: *aquaporins, mammalian, capacitation, sperm*

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METABOLITE PROFILING OF SEMINAL PLASMA UNCOVERS *in vivo* FERTILITY BIOMARKERS IN PIGS

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1. Introduction

The -omics approaches allow in-depth exploration of potential biomarkers for infertility. In this realm, metabolomics, which includes the study of low molecular weight metabolites, is a promising technology in expansion that has already been used in humans (Mumcu, Karaer, Dogan, & Tuncay, 2020) and cattle (Kumar, Kroetsch, Blondin, & Anzar, 2015) to investigate seminal plasma (SP). In spite of this, studies profiling pig SP and aimed at identifying *in vivo* fertility biomarkers are yet to be conducted. Thus, the aim of the present study was to explore the putative relationship between SP-metabolites and *in vivo* fertility outcomes (farrowing rate (FR) and litter size (LS)) in pigs.

2. Methodology

A total of 32 entire ejaculates were collected from eight artificial insemination (AI)-boars (three ejaculates per boar). From these boars, FR and LS deviations were calculated following the model described by Broekhuijse, Feitsma, & Gadella (2012). Immediately after collection, ejaculates were centrifuged to harvest SP samples, which were stored (−80 °C) for subsequent metabolomic analysis. For SP processing, samples were thawed on ice and centrifuged through Amicon® Ultra Centrifugal Filters (14,000 g at 4 °C for 90 min) for proteins and cell debris removal. A total of 500 µL were then mixed with 100 µL of PBS containing 10% D2O with 0.33% of DSS. Samples were analysed using Bruker 600-MHz AVANCE III nuclear magnetic resonance (NMR) spectrometer.

3. Results

The ^{1}H-NMR (noesygppr1d) profile allowed the identification and quantification of 24 metabolites in pig SP samples. sPLS-DA analysis for both FR and LS allowed the identification of two different groups. Next, ROC curve analysis showed several putative biomarkers for both *in vivo* fertility indicators: i) lactate (area under the curve (AUC) = 0.76) and formate (AUC = 0.69) were found to be biomarkers for FR; and ii) carnitine (AUC = 0.861), hypotaurine (AUC

= 0.826), sn-glycero-3-phosphocholine (AUC = 0.833) and glucose (AUC = 0.764) were found to be LS predictors.

4. Conclusions

This is the first report exhaustively analysing the relationship between SP-metabolites and FR and LS in the pig. Moreover, the evaluation of these metabolites opens up the possibility of: i) better ejaculate selection prior to elaborate AI-doses, and ii) exogenous supplementation of semen extenders to improve *in vivo* fertility outcomes.

Keywords: *metabolite, seminal plasma, pig fertility, biomarkers*

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GLUTATHIONE S-TRANSFERASE Mu3 IS A BIOMARKER OF *in vitro* FERTILIZATION IN PIGS

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1. Introduction

Previous studies of our research group established glutathione S-transferase Mu 3 (GSTM3) as a predictor of sperm cryotolerance and quality (Llavanera *et al.*, 2020). Furthermore, investigations of Kwon *et al.* (2015) suggested GSTM3 as a biomarker of *in vivo* fertility through artificial insemination in pigs. Consequently, the present study sought to explore the potential role of GSTM3 as a predictor tool of in vitro fertilization (IVF) rates, as this could maximise the efficiency and profitability of assisted reproduction techniques in pigs.

2. Methodology

In this regard, seven pig ejaculates were initially evaluated through CASA and flow cytometry to assess sperm motility, viability and intracellular calcium levels. Moreover, GSTM3 was quantified through immunoblotting analysis followed by a band-pattern quantification and α-tubulin normalisation. Following this, all ejaculates were subjected to IVF using standard procedures. Briefly, pig oocytes were retrieved from pre-pubertal ovaries and *in vitro* matured for two days at 38.5ºC and 5% CO_2. One thousand sperm per oocyte were co-incubated for 5h and subsequently *in vitro* cultured for two days, when cleavage rates were calculated. Finally, Pearson correlation coefficients between relative GSTM3 levels, sperm quality parameters at day 0, and IVF rates at day 2 were calculated.

3. Results and discussion

As expected, total sperm motility (R=0.86; $P<0.05$) and the percentage of viable sperm with high intracellular calcium levels (R=0.93; $P<0.05$), but not viability ($P>0.05$), at day 0 were positively correlated with IVF rates at day 2. Regarding GSTM3 levels, immunoblotting analysis showed a double-band pattern of ~25 and ~28 kDa. The relative levels of the ~28 kDa-band of GSTM3 at day 0 showed significant correlations with IVF rates at day 2 (R=0.88; $P<0.05$). However, the ~25 kDa-band did not show significant correlations ($P>0.05$).

4. Conclusions

Levels of the ~28 kDa-band of GSTM3, but not the ~25 kDa-band, at day 0 are highly correlated with IVF rates at day 2, showing similar predictive value than conventional sperm quality parameters. While these results are preliminary, the relative content of GSTM3 in sperm should be considered as a quality biomarker for IVF, since it could be able to predict IVF rates at day 2. This could ultimately improve IVF success.

Keywords: *biomarker, GSTM3, in vitro fertility, sperm*

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

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1. Introduction

Enzymes are excellent catalysts capable of increasing the chemical reaction rates many orders of magnitude. This rate acceleration is achieved by decreasing activation barriers, making reaction possible at lower temperature and pressures. Hevea brasiliensis hydroxynitrile lyase (HbHNL) and salicylic acid binding protein 2 (SABP2) are two enzymes evolved from the same esterase ancestor. They share 45% amino acid sequence identity and the same Ser-His-Asp catalytic triad. However, they catalyse different reactions. HbHNL catalyses the cleavage of hydroxynitriles and SABP2 has esterase activity. To understand the differences between the catalytic activity of both enzymes, Kazlauskas and coworkers made a set of variants by substituting active site HbHNL amino acids into the corresponding SABP2 residues. Although an increase of esterase (EST) activity and decrease of hydroxynitrile lyase activity (HNL) were expected, pure EST activity was not reached by any HbHNL variant (HbHNL-EST) (Nedrud *et al.*, 2014).

2. Methodology

In this work, we focus on the identification of the missing first and second shell active site amino acids required to convert the most active HbHNL-EST variant to reach a complete esterase activity. For the identification of these positions, we use correlation-based tools (e.g. Shortest Path Map) (Romero-Rivera, Garcia-Borràs, & Osuna, 2017). The corresponding HNL variants with presumed EST activity improvements were in-silico tested with molecular dynamics (MD) simulations in both the *apo* state (i.e. without ligand) and with the tetrahedral intermediate involved in the rate-limiting step of the reaction. Finally, our collaborators from the lab of Prof. Kazlauskas (Univ. Minnesota, US) experimentally validated our rationally designed variants.

3. Results

The previous methodology and the synergy with our experimental collaborators allowed us to reach a fold increase in kcat/KM up to 239 with our rationally evolved variant, thus outperforming the SABP2 enzyme by a fold increase of 2.

4. Conclusions

Our study identifies a new variant with significant fold increase in esterase activity compared to the HbHNL-EST variant of the previous work. Even though we were able to achieve an impressive fold increase in EST activity, we believe that we can boost the EST activity even higher.

Keywords: *enzyme design, catalysis, molecular dynamics, esterease, hydroxynitrile lyase*

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SESSION II. ART AND CULTURE

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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1. Introduction

The world we live in today is engulfed by the world of images. Images have become a fundamental characteristic of our daily culture without any literacy in it.

Given this situation, the Art Thinking methodology has emerged in recent years, based on artistic and visual strategies. It starts from the premise that art is not only a generator of manual capacities but also creates and produces knowledge. Using, promoting, and developing artistic abilities such as group work, creativity, empathy, social inclusion and resorting to contemporary art as an integrating element, all these are intended to develop a new way of thinking in students, enhancing creative and critical skills to train them in this new society; all these are intended to improve education to improve society. This "is an integrative and multidisciplinary approach" (Guillén, 2017).

2. Hypothesis

The central objective of this research is to apply the Art Thinking methodology in three educational projects related to art and heritage, which are being carried out in the subject of plastic arts. It is intended to answer the question: Is Art Thinking an educational innovation that provides and promotes in students the intrinsic capacities of art and therefore enables knowledge? Does it allow shared learning, create experiences, and promote the establishment of links between art and society?

3. Methodology

This research is methodologically based on A/r/tography as an Art-Based Research modality. It unifies the purposes of the research and is coherent with the researcher who generates it, since it combines the artistic, educational and research aspects. As Viadel points out, "it becomes the meeting area between the qualitative methodological innovations of the human and social sciences, and the community, participatory and social tendencies of contemporary art, such as "Artivism" (Viadel & Roldán, 2019).

The research has been carried out in Greece because it is the place of residence of the researcher and because she is currently in a critical situation about artistic education. It is being carried out in four Public Centers (secondary education) and in non-formal centers (Momus,

Experimental Center of the Arts, Thessaloniki, and Ecomuseum of the Prehistoric Lakeside Settlement of Dispilio).

4. Conclusions

Through the study, assessment, and application of this research, it is intended to establish, on the one hand, the value of this methodology as educational innovation at an artistic level. On the other hand, re-situate art education in two approaches: firstly, as a damping system for encoded information through visual language, of which we are producer-consumers and of which we are not. We make a reflection and a critical use of it. Secondly, this research serves to help re-locate art as a primary subject in the educational system.

Keywords: *art thinking, A/r/tography, innovation, artistic education, society*

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EDUCATIONAL THEATRE FOR STEAM EDUCATION

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1. Introduction

Educational theatre is a tool for learning content in an integrated manner with behavioural change potential (Falk & Dierking, 2012). STEAM Education is an interdisciplinary approach of Science, Technology, Engineering, Arts (and humanities) and Mathematics for deep and engaged learning, enhancing students' creativity and problem-solving skills (Hardiman & JohnBull, 2019).

2. Problem

Engineering courses commonly have the discipline Science, Technology and Society (STS) that should directly promote education in humanities, but is largely reported for its failure in capturing students' interest. One reason is that STS seems unrelated to the other disciplines (Cech, 2013). The study aims end the culture of disengagement through ET as STEAM Education activity in terms of accomplishing interdisciplinarity, fostering abilities and STEAM literacy (Zollman, 2012).

3. Methodology

Eleven undergraduate students volunteered in theatrical laboratories: actor preparation, scenario conception, writing and presenting a play about Mechanical Engineering (Figure 1). The research is qualitative: Collaboratively written script and transcribed semi-structured interviews were analysed through multiple comparisons in grounded theory. There were induced categories that were organized in the contextual model for ET of Falk and Dierking (2012): physical, socio-cultural and personal contexts.

Figure 1. Actors wrapped in aluminium foils representing robots

4. Results and discussion

As a result, the categories induced from the play script match with the interviews analyses, supporting that the play represent students' ideas. In the interviews students demonstrated owner sentiment towards the play; they valued development of speaking in public, collaborative and creative skills. They valued development of speaking in public, collaborative and creative skills. Engineering was portrayed in an interdisciplinary approach in other STEAM areas – mainly the engineers' role in society and ethical dilemmas, and mathematical elements.

5. Conclusions

ET is a good substitution for, or a complement to, the discipline of STS in terms of STEAM literacy and abilities, engagement and affect domain.

Keywords: *drama activity, educational engineering theatre, STEAM education, mechanical engineering, higher education*

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THE CARNIVAL IN MATARÓ AT THE END OF THE 19th CENTURY: A STUDY OF THE CULTURAL LIFE OF THE WORKING CLASS

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1. Introduction

In the middle of the 19th century, as in all the western societies that underwent the Industrial Revolution, the proletariat, linked with class-consciousness and the labour movement, was born in Mataró. In this city, in particular, the labor movement was strong enough to generate alternatives, such as the example of the cooperative projects that formed a network of production and consumption that lasted until the Civil War. This historical subject is sufficiently relevant to study it from different perspectives.

2. Results

In this study, we want to ask what the more or less homogeneous role of the Mataro working class was in the cultural field of the city. Working class manifests some kind of particular cultural formulas, with subaltern character, within what we understand as popular culture. We want to identify the cultural spaces and manifestations that were generated in Mataró and value their grade of autonomy or particularity and the relations that were established with the hegemonic culture in order to determinate if we can include them in the paradigm shift that is being experienced around the occidental world. We focus on the carnival festivity as an example that links working class with tradition and religion and we put them in relation to the perspective of the social and cultural elite of the city.

3. Conclusions

A series of chronicles, press releases and personal opinions have been collected that help us to trace the development of the festivity through the last decades of the 19th century and the way in which the different cultural agents were related. In this study, the theorizing that authors made about the question of popular culture is also important. We have looked at some theories of 19th century contemporaries and put them in relation with the personal opinions that we obtained from the documentary sources and then analysed from our theoretical framework. The Mataró carnival at the end of 19th century involved masked dances in casinos and athenaeums, anti-monarchical parades, charity parades and gypsy dances, among other elements that make up a diverse map that welcomes all social classes by opposition and by relationship.

Keywords: *popular culture, working-class culture, carnival, Mataró*

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PILAR AYMERICH. A 50-YEAR PHOTOGRAPHIC CAREER

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1. Introduction

Pilar Aymerich (Barcelona, 1943), began her career as a photographer in the late 1960s, becoming one of the leading photojournalists in capturing, from the street, the turbulent years of the end of the Franco regime and the Spanish transition in Catalonia. Already from the beginning, she developed her side as a portraitist, creating images full of complicity that offer a glimpse of the connection between the photographer and her portraits. Furthermore, a large part of her photographic collection is dedicated to theatre photography, as a result of her time as a student at the Adrià Gual School of Dramatic Art. She is a reference figure in the history of Catalan photography and her work is valued as a documentary and artistic testimony. However, there is no monographic study of her work, a gap that we consider necessary to fill both because of the quality of her images and the collective memory that they constitute.

2. Results

The large theoretical basis of our research comprises readings focused on the photography genre, as well as a bibliography which allows us to address the issue from a perspective far removed from the official male and heterosexual discourse of Art History (Aliaga & Mayayo, 2013). One of the most methodologically relevant aspects is the study of her photographic archive, which Pilar donated to the National Archive of Catalonia (ANC) in 2011. This large collection is accompanied by the author's documentary archive, kept by herself in her apartment. It consists of 14 folders with reviews that she has been collecting since 1977 and which address her work. Finally, another part of the documentary archive comprises a number of reports by Aymerich in the magazines where she has been collaborating over the years.

3. Conclusions

The figure of Pilar Aymerich serves us to review the photographic discourse of an entire period and shed more light on the generation of photojournalists of the seventies, which is often blurred in the midst of a confrontation between the previous generation, labelled neorealist, and the next one, represented by photographers following more experimental trends. Ultimately, the main goal is to contribute, within the history of Catalan photography, with the first monographic study of Pilar Aymerich, where readers can meet the photographer described, in words of her friend Montserrat Roig «as a half-witch and a little bit cat» (Aymerich, Moix, & Roig, 1978).

Keywords: *photography, Spanish transition, Franco regime, feminism, theater*

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LYRICS FROM BOTH SIDES OF THE PYRENEES: URGELL, FOIX AND THE TROUBADOURS (12th-13th C.)

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1. Introduction

Traditional historiography has tended to study the diffusion and roots of troubadour culture in Catalonia from a rather monarchic-centric point of view, without paying too much attention to the role played by the different noble dynasties and their respective courts. A seminal example of this line of research is Milà i Fontanals (1861). I started reviewing this approach in my final degree project (TFG) (Vera, 2020) by studying the specific case of the Urgell lineage, and I determined that a total of twenty-three poems may be related to it, mainly through the mention of one of the three women of the lineage who held political power. From the joint reading of the poetic compositions associated with this dynasty, I was able to study some crucial events for the county of Urgell from a different perspective and to highlight the poetic patronage carried out by the family.

2. Methodology

Following the same objectives, in the present study I will compile (by means of the digital corpus COM) all the troubadour poems that might have links with the house of Foix –closely related to that of Urgell–, in order to analyse them in their historical context (starting with the earliest works about the counts of Foix, such as Baudon de Mony 1896, and using Cabré 2013 as a reference for troubadour activity in Catalonia). Additionally, I will review some poems related to the dynasty of Urgell that need to be included in my TFG corpus and compare both families regarding their contact with the troubadours. Lastly, I will compile a preliminary list of the poems related to all the Catalan lineages.

3. Results

This methodology, implemented first on my TFG, will allow me to assess the presence of the Foix lineage in troubadour poetry and to highlight their eventual patronage. This new approach gives me substantially different interpretative tools to those of the editors of these troubadours' lyrics, as their rather global perspective sometimes prevented them from paying enough attention to a single Catalan toponym or character.

4. Conclusions

The results of my TFG clearly prove the need to carry out more extensive research to assess the actual participation of all the Catalan noble houses in the diffusion of troubadour culture in Catalonia. The present work will become an important milestone that will allow me to contrast the results of the comparative analysis of the activity of the two lineages.

Keywords: *troubadours, Catalan nobility, Crown of Aragon, Urgell, Foix*

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EFFECT OF A MUSIC-BASED RHYTHMIC AUDITORY STIMULATION ON GAIT AND BALANCE IN SUBACUTE STROKE

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1. Introduction

Global stroke statistics from (Thrift *et al.*, 2016) shows that gait and balance impairments are common after a stroke. Music rhythm can modulate motor performance and become effective for motor control through auditory-motor integration pathways in the brain (Thaut, 2008).

2. Hypothesis

The hypothesis of the study was that a music-based rhythmic auditory stimulation (RAS) in combination with conventional physiotherapy in a subacute stroke produces more gains in gait parameters and walking ability, compared with conventional physiotherapy alone.

3. Methodology

This historical controlled trial included 55 patients who had suffered a stroke within the three weeks prior to enrolment. Patients from 2018 (n = 27) were assigned as the historical control group whereas 2019 patients (n = 28) received music-based RAS three times a week. Both groups received 11 hours of conventional physiotherapy per week during hospitalization. Primary outcomes were gait and balance parameters (Tinetti test and gait speed) and walking ability (Functional Ambulation Category scale). Secondary outcomes were trunk control, assistive devices, functional independence (Functional Independence Measure, Barthel index).

4. Results

Outcomes clearly improved in the two groups, but no between-group differences were identified for gait and balance parameters nor for secondary outcomes. Significant between-group differences were observed in the Functional Ambulation Category: the intervention group showed greater improvement (p = 0.002) than the control group. At patient discharge, 9 (33.3%) subjects in the control group could walk indoors, 7 (25.9%) could walk outdoors independently and 17 (63%) could walk without any assistive device; in the intervention group 15 (53.5%) could walk indoors, 5 (17.9%) could walk outdoors independently and 23 (82.1%) could walk without any assistive device.

5. Discussion

Compared with conventional physiotherapy alone, our results suggest that the walking ability of subacute stroke patients might be improved with music-based RAS combined with conventional physiotherapy, but this treatment is not more effective than conventional

physiotherapy in obtaining gait and balance parameter gains, agreeing with Van Criekinge *et al*, 2019. A possible explanation might be related not only with the sample size, but also to the lack of reliability and sensitivity of the measures and scales used (Ghai & Ghai, 2019). Only a little research exists about walking outcomes related to the quality of walking as the walking ability (walk indoors, outdoors, climb stairs) and the use of walking assistive devices (Fujii, Sugawara, Ishikawa, & Fujiwara, 2020).

6. Conclusions

Music-based RAS as an additional rehabilitation improves walking ability in a subacute stroke. But is there any applicability in community-dwelling when patients go home? Future research in long-term effects of a music-based RAS is needed.

Keywords: *music-based rhythmic auditory stimulation, musical therapy, walking ability, physiotherapy, stroke rehabilitation*

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CITIES, MAPS, PUBLIC ART

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1. Introduction

Maps can help us better understand the –not so obvious- shared space of our cities. Public life is diverse and hosts multiple activities, needs, and experiences within the city streets. Mapping and analysing the overlay of these layers can help shine some light and knowledge on this complex intertwined universe that is the public space. In this sense, the advances in cities' shared open data and the analysis of the urban space with GIS technology are fundamental to define our new understanding of the shared built environment. With this new understanding come more informed urban planning decisions and in consequence a better and richer relationship between people and our shared public space.

Public Art can help us better understand the –not so obvious- shared space. Filmmakers, painters, photographers, and artists generally, have been analysing the relationship between people and their built surroundings for years. This artist's insight has been actively participating and constructing our collective imagery of cities and the experience of public space. "Public Art" is an art that inscribes itself directly in the public space. In that sense, not only does public art give us a historic retrospective of the understanding of our shared space, but it also offers multiple solutions to the question of how people interact with the built townscape.

2. Methodology

A comparative analysis methodology has been employed between the most accessible and searchable open data platforms. With this methodology some indicators have been outlined that help understand how Public Art is represented to the general public.

3. Results and discussion

As we want to have a deeper knowledge of the hidden entanglements of our cities, mapping and public art present themselves as two highly interesting tools for further insight into how we live and experience our shared space. But, are we using these two instruments efficiently together? "We measure what we care about" (Gehl, 1987). Within this newly available data, not all topics have the same representation, and cities prioritize what they think is more relevant.

The presence of public art within the main global data-sharing platforms have been analysed through the selection and consultation of 10 open data web portals. The proportion of datasets obtained in each platform using the input "art" is diverse: 5 platforms present less than 0.5% of their datasets when searched with the input "art", 3 platforms present between the 2 and 5% of their datasets, and two platforms present 10% and nearly 30% of their datasets when searched with the same input.

4. Conclusions

The differences between the search engine workability makes comparisons between the open data portals and a reliable interpretation of the results difficult.

However, the representation of city art on global data-sharing platforms seems considerably small. Further analysis is needed to reach a definitive conclusion about the presence of art within the mapped cities.

Keywords: *urbanism, public space, public art, mapping, open data*

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SESSION III. ENVIRONMENT, CLIMATE CHANGE AND SUSTAINABILITY

DEVELOPMENT AND OPTIMIZATION OF A QUANTITATIVE ANALYSIS OF MAIN ODORANTS CAUSING OFF FLAVOURS IN CORK STOPPERS USING HS-SPME GC-MS/MS

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1. Introduction

Natural cork stoppers have been used for many years in wine industry for bottling wines because they have a positive impact on bottle-aging given that they contribute to the bouquet of the wine. Nevertheless, cork taint, the term used to describe the effect of different volatile compounds which negatively influence the wine's sensory properties (Prat, Bañeras, & Anticó, 2008) is a problem in the wine industry, although it is not, as often mistakenly thought, always caused by the cork stoppers. For this reason, the cork industry needs simple and sensitive methods to check the materials throughout the different stages of production. Hence, monitoring these compounds in both the raw cork and the cork stoppers are important quality-control steps to be taken before sending either product to the market.

2. Hypothesis

Cork taint is commonly associated with a dusty, mouldy and earthy aroma. Some compounds that are most reported as being responsible for the musty-earthy off-flavour in wine with cork stoppers are namely, chloroanisoles (2,4,6-Trichloroanisole (TCA), 2,3,4,6-Tetrachloroanisole (TeCA), 2,4,6-Tribromoanisole (TBA), Pentachloroanisole (PCA)), some pyrazines such as 2-Isopropyl-3-methoxypyrazine (IPMP), 2-Methoxy-3,5-dimethylpyrazine (MDMP) and 2-Isobutyl-3-methoxypyrazine (IBMP), geosmin (GSM), 2-Methylisoborneol (2MIB) and guaiacol (GUAI) (Chatonnet, Bonnet, Boutou, & Labadie, 2004; Franc, David, & de Revel, 2009; Simpson, 1990). The perception threshold of these compounds in water or wine is mainly at ng L^{-1}, for this reason, highly selective and sensitive analytical techniques are required for their unequivocal determination and identification.

3. Methodology

The analysis was performed using headspace solid-phase microextraction (HS-SPME) coupled with gas chromatography tandem mass spectrometry (GC–MS/MS). In addition, the influence of the fibre coating used, the extraction times and temperatures, the sodium chloride additions and desorption temperatures were investigated.

4. Results

The optimal HS-SPME conditions established were divinylbenzene / carboxenpolydimethylsiloxane / polydimethylsiloxane (DVB/CAR/PDMS) fibres, a 50ºC extraction temperature, 60 min extraction time, an ionic strength of 3 g sodium chloride and a 290°C desorption temperature. The method showed a good linearity (R2 ≥ 0.994) within the tested range (from 0.1 to 50 ng L−1) for all the compounds. Using TCA-d10 and MIB-d3 as internal standards the precision, expressed as repeatability and reproducibility RSD, was < 10% in both. Limits of quantifications (LOQs) are below the sensory threshold levels for such compounds in water and wine. Good recoveries were obtained for cork macerates (from 100.4 to 126 %).

5. Conclusions

A rapid, accurate, sensitive method for the analysis of trace concentrations of 10 off-flavours in cork stoppers has been developed and validated.

Keywords: *cork stoppers, earthy-musty compounds, headspace solid phase microextraction (HS-SPME), GC-Triple quadrupole MS*

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CLAIMS TO THE STONES: THE HISTORICAL ECOLOGY OF THE DRYSTONE TERRACES IN THE UPPER MUGA VALLEY

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1. Introduction

Abandoned drystone terraces are common Mediterranean upland features epitomising biocultural heritage. Historical ecology demonstrates they created viable agricultural habitats. Terrace 'traditional' pasts idealistically represent sustainable lifeways, yet rural people were eviscerated - terraces are not symbols of self-sufficiency but of property. They were maintained only as *landesque capital* where social relations made it worthwhile: renewed intermarriage between tenants facilitated a regenerative relationship, rationalising the investment now mostly dislocated. *Landesque capital* relies on imagined renewal: artistry of drystone walling is an emotional connection to landscapes through which 'Nature' and biocultural heritage transmute. Once lost it is problematic to recover without an economic shift in approach to land as property. Those that hold the land, hold the power.

2. Problem

My thesis investigates drystone terraces belonging to the communities divided by the Treaty of the Pyrenees (1659) in the Upper Muga Valley into French and Spanish Catalunya. I investigate if national territoriality effected the historic land-use and tenure of the drystone terraces. Did landless families find ways of 'retaining' land and solidifying terrace *landesque capital,* and artistry, through continued intermarriage as tenants? Has the frontier led to the evolution of different socio-ecological drystone terrace conditions?

3. Methodology

My thesis is multi-methodological, employing social agency theories (Evans, 2003), entwining archives, cartography, archaeology, ecological surveys and oral memory. I catalogue the terraces probing for uses, assessing typology, altitude, aspect and species and examine how the terraces were and are perceived. Searching for similarities or differences in abandonment drivers: evaluating the effects the frontier has had on terraced land tenure and management.

4. Results

Terrace typology reveals multiple origins, uses, meanings, historical socio-ecologies: adaptability to socio-geographical terrain. Oral memories recall recourse to some like a 'scattered land bank' during times of need, others are mysterious, not marked cartographically. Evidence suggests that currently used terraces are private; that completely 'abandoned' land represents ancient farmland whose socio-economic system collapsed by the Mid-20th Century,

some replaced by neo-ruralist pastoralism in the 1980s which now has almost ceased; previously rented gardens and land with absentee landowners.

Figure 1. My "landed" son who will inherit my terraces in the Upper Muga Valley

5. Conclusions

Rural development is hybrid in the Mediterranean (Font, 2021). This is a response to our current disorientation, potential chaos, migration, rapid climate change (Latour, 2018). During 'The Anthropocene' we return to terraces, their resilience, diversity, hybridity, flexibility, 'ecosystem services', potential renewal: however, their historical ecology isn't applicable if we cannot keep apace, and if territorialised, terraced land remains in the private hands of the new green elite (which perhaps I represent!), how can the landless benefit? (Estes, 2021).

Keywords: *abandoned, drystone terraces, biocultural heritage, historical ecology, climate change*

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GLOMALIN CARBON IN SOIL AGGREGATES FROM DIFFERENT SOIL TYPE AND USE OF GIRONA IN THE CONTEXT OF CLIMATE CHANGE MITIGATION

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1. Introduction

Soil organic carbon (SOC) has been gaining attention in carbon sequestration studies because it may provide the largest store of terrestrial carbon and play an important role in climate change mitigation (Emran, Gispert, & Pardini, 2012; Lal, 2008). Recently, the identification of the glycoprotein glomalin produced by fungi at the end of their lifetime has provided new insight on stable SOC and aggregate stability (WSA) (Rillig, 2004). Glomalin may represent 2% to 30% of soil organic carbon and may last in soil for decades.

2. Methodology

Soils (from forest, meadows and rapeseed cultivation) in Fornells de La Selva, Canet d'Adri and Brunyola have been sampled at 4 depths (0-5, 5-10, 10-15, 15-20 cm) in order to explore the organic layer. Glomalin, glomalin carbon and aggregate stability have been analysed according to established methods (Emran *et al.*, 2012). Glomalin was extracted from soil with 50 mM trisodium citrate in autoclave at 121°C for 1h and then measured by spectrophotometer at 595 nm. Glomalin carbon was determined in glomalin extracts by the dichromate oxidation method. Aggregate stability was carried out by calculating the remaining mass of soil after 60 cycles of immersion-emersion of aggregates in water for a duration of 3 min each.

3. Results and discussion

The WSA values measured in the 0.25-2 mm aggregate fraction for the three soil uses and all depths were noticeably lower (20-50%) in cultivated soils of all sites which corroborated the lower values of glomalin and glomalin carbon. The highest values of glomalin were found in Canet D'Adri soil in the 0.25-2 mm fraction at 0-5 cm depth and decreased with depth. Glomalin was lower in the 2-5.6 mm fraction. Research on soil aggregate stability have indicated that the reduction of soil organic components may affect coarser aggregates which are generally detached into smaller aggregates where they can be better protected (Castellano, Mueller, Olk, Sawyer, & Six, 2015; Gispert, Pardini, Emran, Doni, & Masciandaro, 2018). Significant correlation was found among WSA and glomalin and glomalin carbon especially in the volcanic soil of Canet d'Adri, independently of the use.

4. Conclusions

WSA, glomalin and glomalin carbon indicate a descending order Fornells de La Selva-Brunyola-Canet d'Adri showing forest and pasture soils contain higher levels of glomalin with respect to the cultivated soil.

Keywords: *soil type, soil use, glomalin, glomalin carbon, aggregate stability*

5. Bibliography

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CHARACTERIZATION OF *Verticillium sp.* ISOLATES CAUSING VERTICILLIUM WILT AND MORTALITY OF *Ailanthus altissima* IN CATALONIA

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1. Introduction

Ailanthus altissima (Mill.) Swingle is a fast-growing tree that has become established worldwide. The species is regulated as an Invasive Alien Species in the European Union, so efforts are being made to find biocontrol agents.

Verticillium sp. has been reported as the causal agent of wilt and mortality of ailanthus in USA and Central Europe (Brooks, Snyder, Bush, Salom, & Baudoin, 2019; Maschek & Halmschlager, 2015; Schall & Davis, 2009). Ailanthus trees showing wilt symptoms were observed in forest ecosystems in Catalonia. Native *Verticillium sp.* isolates might be used in biocontrol of ailanthus in the Mediterranean Basin.

2. Hypothesis

The aim of this study was to recover and characterize *Verticillium sp.* isolates from diseased *Ailanthus altissima* trees in Catalonia.

3. Methodology

Verticillium sp. isolates were obtained from six ailanthus populations in forest ecosystems in Catalonia. Three trees showing verticillium wilt symptoms were sampled per area. Symptomatic and asymptomatic branch samples were collected for fungal isolation.

Samples were disinfected, placed onto PDA plates and incubated at 22.5ºC and 12 h light photoperiod for 7 to 10 days. After isolation, morphological characterization was carried out. Colonies resembling *Verticillium spp.* were grown on WA-p and PDA for species identification (Inderbitzin *et al.*, 2011; Inderbitzin, Davis, Bostock, & Subbarao, 2013).

DNA sequencing using primer pair ITS1-F and ITS4 was done for a preliminary molecular characterization of isolates (Inderbitzin *et al.*, 2013).

4. Results

Eighty-four isolates were preliminarily identified as *Verticillium* spp. based on morphology. Most isolates (77%) were classified as *V. dahliae*, 13% as *V. albo-atrum* and 10% were assigned to *V. alfalfae/nonalfalfae*.

Concerning the molecular characterization based on the ITS sequence, most isolates had identical or near identical sequences. BLAST analysis of ITS sequences gave 100% to 90% homology to *V. dahliae*, *V.albo-atrum* or *V.nonalfalfae* sequences in GenBank.

5. Discussion

The study recognized the previously described species of *Verticillium* causing verticillium wilt of ailanthus in USA and Central Europe*; V. dahliae* and *V. nonalfalfae*. Results suggest that both species may play a role in this disease of ailanthus in Catalonia.

6. Conclusions

Verticillium dahliae and *Verticillium nonalfalfae* seem to be associated to ailanthus wilt disease in Catalonia. Further studies on the pathogenicity on ailanthus, host-range and effects on non-target species of these isolates are needed to evaluate their potential in biological control of ailanthus in the Mediterranean Basin.

Keywords: *Ailanthus altissima, biological control, fungi, invasive tree, Verticillium sp.*

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SPECIES DISTRIBUTION MODELS: A GOOD TOOL TO EVALUATE THE EFFECTS OF HYDROLOGICAL ALTERATION ON FRESHWATER FISH

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1. Introduction

Understanding the climatic, topographic and anthropogenic factors that drive species distribution has challenged ecologists for a long time, and it is essential to implement appropriate management measures. This is especially relevant in freshwater ecosystems, which are among the most diverse but, at the same time, most threatened ecosystems globally (Albert *et al.*, 2021). Fresh waters are threatened by manifold interacting factors such as pollution, habitat fragmentation and destruction through land use changes and damming, climate change and invasive alien species (Albert *et al.* 2021). Thus, our objectives are to assess the importance of different environmental variables in shaping the distribution of inland fish, and to evaluate the role of hydrological alteration.

2. Methodology

We computed species distribution models for 68 inland fish species present in the Iberian Peninsula (51 native and 17 alien). We used the BIOMOD computational framework, as implemented in the R-package 'biomod2' (Thuiller, Georges, Engler, & Breiner, 2019), and we used four different algorithms: generalized linear models (GLM), boosted regression trees (BRT), random forests (RF), and Maxent. We computed variable importance for each species-specific ensemble model to determine the most influential environmental factors. Finally, to explore the importance of specific environmental variables in determining the distribution of different traits of freshwater fish, variable importance obtained from our models were subjected to a redundancy analysis.

3. Results and discussion

We found that topographic and climatic variables (e.g. basin, distance to the sea, temperature) were generally more important than anthropogenic factors (e.g. hydrological alteration) in explaining inland fish distributions. However, we found significant differences in the importance of variables explaining the distribution of native and alien species (Figure 1). For instance, river basin was most important for primary native and many alien species with restricted distributions. Mean temperature and damming had positive effects on the distribution of alien species but were less important for native fishes. Hydrological alteration caused by dams was associated with phytophilic, water-column, warm-water alien fishes introduced from more hydrologically stable habitats. For example, hydrological alteration was positively related with the occurrence of several alien species like *Silurus glanis*, *Esox lucius*, *Scardinius erythrophthalmus*, *Sander lucioperca* and *Ictalurus punctatus*.

4. Conclusions

Our results show that species distribution models are a good tool to evaluate the effects of hydrological alteration on inland fish, and reveal that the effects of hydrological alteration on fish distribution differed between native and alien species, favouring the occurrence of phytophilic, water-column, warm-water alien fishes.

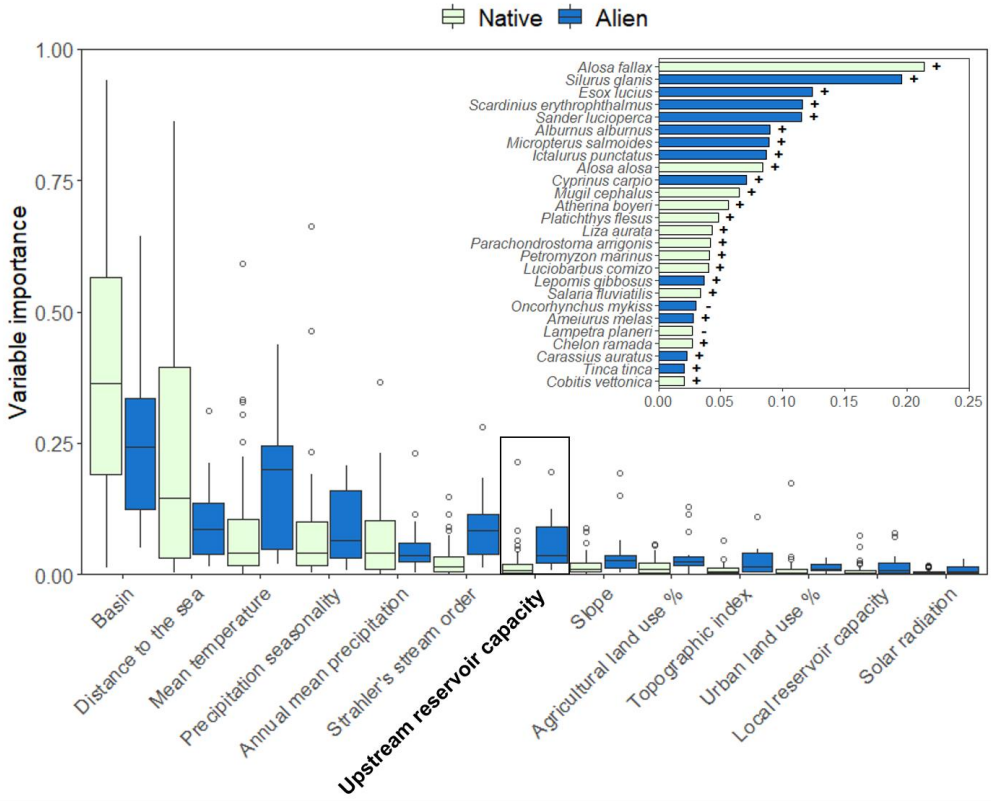

Figure 1. Importance of the different predictor variables used in the SDMs across alien and native species. Boxes correspond to the 25th and 75th percentiles; lines inside a box show the median; whiskers extend to the last observation within 1.5 times the interquartile range from the quartiles and outliers are indicated by empty circles. The bar plot in the right corner shows the variable importance of upstream reservoir capacity (i.e. an indicator of hydrological alteration) for the 25 species for which the predictor was most important. Signs next to the bars indicate whether hydrological alteration was positively or negatively associated with the probability of presence of a species.

Keywords: Inland fish, species distribution models, trait-based approaches, alien species, Iberian Peninsula

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LA BORDA, A CASE OF RESILIENT ARCHITECTURE

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1. Introduction

The housing cooperative La Borda is a non-speculative pilot project built in 2018 within the Can Batlló site, an old industrial complex transformed into a social and mixed facility in Barcelona. The Lacol architects' activism and the neighbourhood group's proactivity of the Can Batlló community allowed its promotion on a plot granted for 75 years by the Barcelona City Council. The La Borda community is diverse, participative and self-organised in relation to its spaces (Girbés-Peco, Foraster, Mara, & Morlà-Folch, 2020). Slack spaces (Schneider & Till, 2007; Till, 2009) of the dwelling units and *freespaces* (Farrell & McNamara, 2017) of the community spaces support the evolution of the building and change of use over time.

2. Hypothesis

The hypothesis aims to demonstrate that La Borda, as a case of resilient architecture, is capable of creating a dynamic architectural system to promote sustainable economic, social and environmental development of its community and the city of Barcelona.

3. Methodology

La Borda serves as a case study to theorize about resilient architecture within a grounded theory methodological framework. The data collection methods for this case study were conducted through data triangulation: interviews, observation notes and secondary research. The Lacol architects cooperative and three inhabitants of La Borda were interviewed using semi-structured interviews during 2020.

4. Results and discussion

La Borda, in its spatial dimension, has the resilient properties of persistence, adaptation and transformation. The inhabitants are able to extend or shrink their dwelling units according to their needs by means of slack space, an indeterminate, flexible, empty space. They adopt a sliding scale of rent depending on the appropriation of slack spaces in each basic housing module. The community is free to decide any use in its *freespaces*, an extra, intermediate, democratic space. La Borda has created an interconnection between three stakeholders: Lacol architects, its community and Barcelona City Council.

5. Conclusions

La Borda is a case of resilient architecture as it has been able to create a dynamic architectural system. This dynamic system is formed of three interdependent dimensions: social, spatial and temporal. The La Borda community can adapt and transform its slack spaces and *freespaces* to change uses according to their conditions. This proactive community creates a self-

organised and self-managed horizontal system based on spatial indeterminacy. La Borda is an example of sustainable development for dwellings and cities.

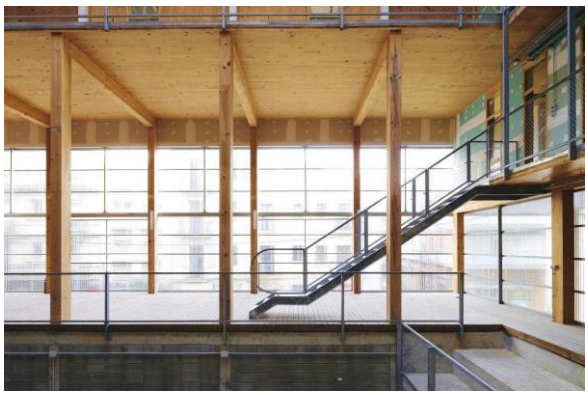

Figure 2. Community *freespace* without activity, 2018

Figure 2. Community meal in its *freespace*, 2019

Figure 3. Slack spaces with the basic housing modules

Figure 4. Transformation of an apartment, 2019

Keywords: resilient architecture, proactive community, slack space, freespace, sustainable development

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WHEN DOES *S. aureus* BECOME A RELEVANT RISK IN DRY-CURED HAM? - THE COMBINED EFFECT OF TEMPERATURE, a_w AND PACKAGING

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1. Introduction

The potential risk associated with *Staphylococcus aureus* growth in sliced dry-cured ham (DCH) is controlled by key hurdles such as water activity (a_w), pH and temperature. As halotolerant bacteria, *S. aureus* is able to grow over more adverse conditions than other pathogens, 0.83 being the minimum a_w (ANSES, 2011). According to available predictive models for *S. aureus*, the physico-chemical characteristics of commercialized DCH are associated with a probability of growth higher than 90% at temperature above 15ºC. In this framework, the main objective of the study was to experimentally quantify the behaviour of *S. aureus* as a function of storage temperature and a_w for different packaging conditions.

2. Methodology

Selected DCH with different a_w (0.861-0.925) were sliced, packaged under aerobic, modified atmosphere (MAP, 80:20% N2:CO2) or vacuum and stored at different temperatures (2 - 25 ºC) up to 1 year. Samples were inoculated (at 2 – 6 log CFU/g, depending on the conditions) with a cocktail of 3 strains of *S. aureus* (CECT4466, CECT976 and CTC1008). The pathogen was enumerated and temperature, pH and a_w were monitored along the storage. The Logistic growth model and the Weibull model were fitted to data to estimate the primary kinetic parameters for the pathogen growth and inactivation, respectively. The influence of a_w and storage temperature on the kinetic parameters was quantified through polynomial models. Finally, secondary polynomial models were integrated into the primary model to obtain a global model for the behaviour of *S. aureus* in DCH along the storage as a function of a_w and temperature for each packaging.

3. Results and discussion

Under aerobic conditions, growth was observed only for DCH with the highest a_w, increasing up to 2.7 and 4.54 $\log_{10}$ units in 1.7 and 4.7 days at 20 and 25 ºC, respectively. Vacuum and MAP packaging compromised the pathogen viability in all DCH regardless a_w and storage temperature. Under conditions not supporting growth, the delta parameter (δ, time for the first $\log_{10}$ reduction) was only statistically dependent on the storage temperature, while the shape parameter could be fixed to a common value for all conditions in each packaging type. DCH's a_w did not significantly affect *S. aureus* inactivation kinetics, which could be attributed to the halotolerance of this microorganism.

4. Conclusions

The mathematical models developed can be used by the DCH producers to assess the risk associated with *S. aureus* on their products and take decisions on the suitability to commercialize them without refrigeration.

Keywords: dry-cured ham, Staphylococcus aureus, shelf-stable food, predictive microbiology, microbial inactivation

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VALORISATION OF PIG'S LIVER BY OBTAINING PROTEIN EXTRACTS UNDER DIFFERENT pH CONDITIONS

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1. Introduction

Offal, which can be defined as nonmeat edible parts obtained during animal slaughtering, are present in many dishes of traditional regional cuisine all around the world because of both their nutritional richness and the organoleptic characteristics (Babicz *et al.*, 2018). However, their consumption in Western countries has drastically decreased in the last decades due to changes in consumer preferences. In the current context, their valorisation might no longer be an option to become an obligation due to the increase in animal source protein demand that is expected to be coming in the near future (Corrado, Ardente, Sala, & Saouter, 2017; Seong *et al.*, 2014).

2. Hypothesis

Offal can be use as food ingredients in the formulation of different food products due to their nutritional characteristics, but their potential must also be borne in mind from the point of view of techno functionality (Toldrá, Aristoy, Mora, & Reig, 2012). The aim of the current study is to determine the potential of porcine liver as source of techno-functional ingredients.

3. Methodology

A gradient experimental design was applied in order to study the effect of pH of extraction buffer on protein recovery from porcine liver, physicochemical properties of the obtained extracts, the SDS-PAGE profile under reduction conditions and the techno-functional properties. Ten pH levels were considered (from 4.0 to 8.5, each half pH unit), without replicates. Three livers from healthy adult pigs were obtained from a local abattoir for each sampling. Colour is measured in the CIELAB space; chemical composition was analysed according to standard methods; and emulsifying and foaming properties were determined according to Pearce, K.N. & Kinsella, J.E. (1978). All parameters were analysed at least in duplicate.

4. Results and discussion

Protein extraction yield was strongly dependent on pH buffer, being maximum at pH = 6.5 and minimal at pH ≤ 4.5; under these last conditions, the lowest supernatant volume was recovered and with a lowest protein content. However, foaming properties were maximal at these pHs conditions, while a lineal positive relationship was evidenced between emulsifying properties and buffer pH. The differences in the protein profiles of supernatants obtained using different adjusted pH buffers, could be of great help to explain this behaviour.

5. Conclusions

Liver protein extraction conditions should be adjusted depending on the final application of liver fractions.

Keywords: *pig, liver, pH buffer, techno-functional properties, physicochemical properties*

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SESSION IV. LAW, SECURITY, POLITICS AND GENDER PERSPECTIVE

PSYCHOLOGICAL INFLEXIBILITY AND PERCEIVED PERSONAL COMPETENCE AS PREDICTORS OF THE GRADE POINT AVERAGE IN UNIVERSITY STUDENTS IN ECUADOR

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1. Introduction

The Grade Point Average (GPA) is considered a reflection of academic achievement and the fulfilment of pedagogical goals (Alhadabi & Karpinski, 2020). Several studies claim that non-cognitive factors can influence GPA (Han, Farruggia, & Solomon, 2020).

Psychological inflexibility "*refers to patterns of behaviour in which actions are rigidly guided by internal experiences (i.e., thoughts, feelings, and urges), rather than personal values or direct contingencies*" (Levin et al., 2016).

Perceived Personal Competence "*refers to one's self-perceived ability to interact effectively with one's environment*" (Smith, Dobbins, & Wallston, 1991).

The research aims to analyze whether Psychological Inflexibility and Perceived Personal Competence contribute to the GPA of university students, in a sample from Ecuador.

2. Methodology

The sample involved 6107 undergraduate students from an Ecuadorian university, with an average age of 22.45 years old. Women made up 52.5% of the participants.

We used the Spanish version of the Acceptance and Action Questionnaire-II (AAQ-II) by Ruiz, Langer Herrera, Luciano, Cangas, & Beltrán (2013) and the Spanish version of the Wallston Perceived Personal Competence Scale (PCS) by Fernández Castro, Álvarez, Blasco, Doval, & Sanz (1998)

Statistical analysis was carried out through the Multiple Linear Regression. We used SPSS v24 software.

3. Results and discussion

Perceived Personal Competence contributed significantly to the linear regression model that predicts the GPA, $r^2 = 0.060$, [$F(2.6104) = 194.57$; $p = 0.000$]; on the other hand, Psychological Inflexibility did not contribute to the model, nor did it moderate the relationship between perceived personal competence and GPA ($p = 0.372$).

4. Conclusions

Perceived Personal Competence contributed positively to the GPA, in a sample of university students from Ecuador. However, Psychological Inflexibility did not influence the results of the study.

Therefore, it is concluded that the interventions aimed at improving the GPA should focus on strengthening the Perception of Personal Competencies.

Keywords: *psychological inflexibility, perceived personal competence, grade point average (GPA), university students, psychological evaluation*

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THE BODY IN BRAZILIAN PUBLIC PLACES: A STUDY IN TWO SQUARES IN BELO HORIZONTE - MINAS GERAIS, THROUGH AN EDUCATIONAL APPROACH

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University of Girona

1. Introduction

This research aims to analyze how the Raul Soares and Liberdade squares, in the city of Belo Horizonte - Brazil, are shown through their different bodies, especially thanks to the practices they produce from the perspective of non-formal education.

2. Hypothesis

The square is a social space that is kept alive by human manifestations and through the interventions of its users (Freire, 1996) which create codes in the city.

3. Methodology

The methods used were documentary and bibliographical analysis, influenced by ethnographic action carried out in the two areas over two and a half years. These two squares were chosen as the object of study because they are close to each other in territorial realities, approximately two kilometres apart, and yet they manifest themselves in their use in ways that differ from each other in terms of their processes of maintenance, meaning and representation for the citizens.

4. Results

Among the findings, what stands out is the fact that the square, in the city, is maintained through the creation and recreation of the codes generated by its diverse users, producing learning processes among its members and in the social development of this public place. Among these figures are the people who have the power of public management of the places; those who, not having this power, use the squares for leisure; the workers in the most diverse possibilities of offering services; the tourists who drive the economic machinery of the area; the marginal actors, invisible in part because of the diverse policies applied in the city, and, finally, the citizens in general, who, with their routines, complete the square with a mixture of possibilities for existing and resisting in it.

5. Conclusions

Using knowledge formation, we move away from understanding this learning from prescribed curricula (Faria, 2017), considered as schooled, and we see that the communication of people in the squares relates to the movements of adaptation and resistance of these curricula, which (re)configure them in contemporary times, and that the public and private apparatus integrates the movements of these places. It also emphasizes the actions that these bodies

reproduce in these places with respect to work, violence and sexuality (Langarita, 2015). The aim is to discuss the historical, cultural and social perspectives of these public squares and how the relations between the body and the appropriation of space by members of the city are processed in them.

Keywords: *square, body, public space, non-formal education*

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TORT LIABILITY FOR VIOLATIONS OF THE OUTER SPACE TREATY

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1. Introduction

The current intensification of human activities in outer space, with commercial actors undertaking a prominent role once reserved to countries, brings together the potential for harmful results. Yet, the current law on outer space does not clearly address private activities.

2. Problem

What are the rules that govern the liability of private actors for their activities in outer space?

3. Methodology

This study is part of broader research on the liability of corporations for violations of international law. To that effect, we will compile, systematize, analyse, and compare the statutory framework, case law and literature in the world's major legal traditions (common law, civil law, Asian systems). Proposals for improved efficiency will be made.

4. Results and discussion

The Outer Space Treaty of 1967 ("OST") sets universally accepted standards of conduct for human activity in outer space and celestial bodies ("OS/CB"), representing the global consensus with respect to what is right and wrong when operating in OS/CB. However, the OST regulates prima facie, the conduct of countries and intergovernmental organizations. In principle, non-state actors are not bound to act in conformity with these rules.

We contend that the rules set in the OST permeate certain "traditional/nominate" torts so that their breach may give rise to a civil action in domestic courts. In American law, three torts may provide redress for conduct in violation of the OST: (1) an action under the Alien Tort Statute; (2) negligence per se; and (3) public nuisance.

The types of conduct addressed include, among others, interference with lawful space activities, placing mega-constellations, private appropriation of celestial bodies and waste of space resources, failure to assist distressed astronauts, or release of debris or biological material into OS/CB.

5. Conclusions

First, the international liability regime established in the OST and Liability Convention is not the sole remedy available for conduct in violation of the OST. Second, traditional torts may provide redress albeit in limited circumstances. In the U.S., the most promising avenues are ATS causes of action, negligence per se and public nuisance. Third, a specific and comprehensive regulation of tort liability of commercial actors operating in OS/CB is desirable

for a number of reasons: to provide redress, avoid impunity, create certainty for investors, or avoid diplomatic friction. The solution may be the codification of new nominate torts such as tortious interference with space freedoms, waste of space resources, or harmful contamination of OS/CB.

Keywords: *space torts, outer space treaty, alien tort statute, public nuisance, negligence per se*

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ILLICIT PROOF. GENERAL TOPICS ABOUT CONCEPT AND CONSEQUENCES

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1. Introduction

Illicit evidence or illicit proof and the basis for admission or exclusion is at the heart of my investigation. This is an issue that has been much debated in doctrine and legal practice, but it remains a problem with diverse solutions and issues to be re-thought. In this thesis I try to standardize the criteria of application of this institution and systematize the fundamentals that explain its admission or exclusion, avoiding that the exclusion is always thought.

Despite being an institution that is conceptually built from its consequences, I think there is much to contribute if we focus on the clarification part of the concept with its main elements. This will allow the concept of consequences to be separated, and perhaps the application of the unlawful evidence in judicial practice can be made clearer.

2. Problem

Illicit evidence is generally studied from exclusion as one of its effects.

3. Methodology

Based on the problem raised, an investigation is structured to study the illicit evidence in the judicial process considering first a conceptual analysis, which helps to clarify the elements that make up this. Secondly, to deepen the context in which wrongdoing takes place and, finally, the analysis of the consequences or effects that lead to it. With this methodology, what we are trying to show is that the unlawful evidence does not necessarily become linked to the exclusion of evidence.

4. Results

Currently, the main discussions on the subject focus on determining the legal consequences to apply when unlawful evidence occurs. However, controversies about subjects who incur wrongdoing, when the wrongdoing takes place, whether it applies only to criminal law or may also extend to other branches of law.

Every time we think of unlawful evidence, the first thing that comes to mind is the exclusion of it; where in practice there are other alternatives to solve the crime committed, and if it is relevant and reliable evidence, it can be saved as important evidentiary material in a case in order to achieve justice. Exclusion (as noted above) is the legal consequence that is commonly spoken of not only in doctrine but also in jurisprudence. However, this is only one of the possible legal consequences that can be used when illicit proof occurs; there are others such as the so-called “alternative remedies”, which are also applied in judicial practice to a lesser extent.

Those other legal consequences - or alternative remedies - are a) the imposition of criminal sanctions, b) disciplinary sanctions, c) civil claims for damages for illegal activity. This topic has been discussed for some time, but I would say that these debates have been oriented above all from the point of view that they are alternatives to the exclusion rule, and not as independent issues, that is, as consequences also derived from the occurrence of an illegal act.

Perhaps an analysis of the legal consequences derived from the illicit evidence from a different approach could contribute something interesting to what has already been worked on in this regard. I mean to account for all the legal consequences that may derive from illicit proof, placing first the type of wrongdoing that occurred, and then assessing what has to happen with said proof, that is, is it extracted or not; and within what is to be understood as the extraction or admission of that evidence in the trial, then also analyze whether other complementary actions can be applied apart from that. In this context, it is important to deepen the study that reflects the ideas discussed in theory and doctrine, while seeing their impact on judicial practice. All of which will allow a determination of the trends that are taking place, and from there, determine the best solution alternatives.

5. Conclusions

This study aims to deepen the subject of illicit proof, not only from the theoretical-dogmatic perspective, but should also shed new light, from legal epistemology to different debates and possible solutions. The methodology of a joint analysis can help in clarifying topics like these.

The points to be clarified start from the expression or term to be used when we talk about illicit proof, until the analysis of the subjects that incur it, its consequences, and foundations. Also, a study is needed that explores examples of judicial practice, hence assessing the trends that are occurring in the theory on the subject in question. Finally, when it comes to the issue of illicit proof, it is important that we know what we are talking about and the range of options that must be applied once it happens.

Keywords: *illicit proof, fairness, process, justice, reliability*

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THE INTERNET, FAR-RIGHT POLITICAL PARTIES AND DEMOCRACY: THE USE OF HATE SPEECH AGAINST GENDER THEORY IN SPAIN

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1. Introduction

The last years we have seen a rise of far-right wing parties across Europe. Spain has its own far right-wing party (Vox) as the third major political force in parliament. The internet and specifically social media platforms are one of the important channels to reproduce their discourse and ideas. One of the crucial points in their dialogue is the attacks on what they call "ideology of gender".

2. Hypothesis and problem

Individuals and gender-sensitive social groups are calling for this online discourse to be stopped, accusing them of inciting hatred by causing these people personal and social harm.

The aim of this research is analyse why the discourse of Vox through social media platforms against the theories of gender can be interpreted as hate speech, why the lack of regulation can undermine our democracy and whether the law is efficient in regulating or preventing such online acts.

3. Methodology

The methodology of the research is based on a literature and legal review.

Firstly, an analysis of the literature on the grounds of hate, hate speech and internet, and far-right political parties in Spain.

Secondly, analysis of the legislation on hate speech and internet, political freedom, and freedom of expression, at national, European, and international level and the most important legal cases in Europe and Spain.

Thirdly, the monitoring of five of the most-followed Twitter accounts of the Vox political party in Spain (far-right party with a political representation in congress) over the years 2019 and 2020.

4. Results

(1) The tension between hate speech and Freedom of Expression and Political Ideas in our legal system.
(2) Analyze how the actual law regulates, prevents, or stops these kinds of acts on the internet.

(3) The importance of the internet and the regulation of the platforms, regarding the transnational conflict between overseas enterprises and the states of the European Union, especially in Spain.
(4) The problems with information from the internet (fake news and hate news).

5. Conclusions

How the online anti-gender hate speech has been used by far-right political parties in Spain as a weapon of social domination among different social groups and how this erodes our democracy. This includes a set of legal and non-legal proposals to prevent and deal with hate speech by political parties at national level and to propose which type of legal and public policy Spain can implement to protect our democracies and human rights.

Keywords: *far-fight, social networks, democracy, anti-gender, hate speech*

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THE CONTINUITY OF CATALAN AND SPANISH NATIONALISM THROUGH PARLIAMENTARY POLITICAL SPEECH

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1. Introduction

According to Hobsbawm (2018) and Gellner (1998), nationalism is considered an ideology related to capitalism and political liberalism. The ideology promotes the creation of the Nation State, a political conception that organizes social life. One of the characteristics of the Nation State is language as a bond between the inhabitants of the territory. As a result, political discourse becomes a tool to spread nationalism.

2. Hypothesis

The research is based on the idea that nationalism has evolved and has become a part of society and discourse, both in the media and political. Its presence can be difficult to perceive but it appears throughout history. For this reason, the main goal of this research is to demonstrate lines of continuity in the Catalan and Spanish parliamentary political speeches.

3. Methodology

The methodology used is Critical Discourse Analysis (CDA) as defended by Ruth Wodak (2003). There are two reasons for this choice of discipline. On one hand, to enable a historical context approach. On the other hand, to perform an analysis of arguments and language used in two different periods of Spanish and Catalan history: Spanish Constitutional debates in 1978 and Catalan Statute debates in 2005 and 2006. Then it can be determined if a continuity of nationalism exists in the analysed discourses.

4. Results

In the current state of the art, the recurrent use of some kind of arguments can be demonstrated to support or reject concepts such as national unity and self-determination. For example, the use of causal or transitivity arguments. In addition, the use of metaphors (Lakoff and Johnson, ed. 2020) is an essential element of the argumentation. This indicates a continuity in the Catalan and Spanish nationalist political discourse.

5. Conclusions

In conclusion, nationalism as an ideology has a continuity that can be identified through political discourse. Research demonstrated that in Catalan and Spanish nationalism there is continuity through the parliamentary political speeches analysed. Therefore, according to Billig (2006), discourse is essential to perpetrate nationalist ideology.

Keywords: *nationalism, Spanish nationalism, Catalan nationalism, critical discourse analysis, political discourse*

6. Bibliography

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THE FEMINISATION OF THE CHILEAN STUDENT MOVEMENT

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1. Introduction

The Chilean student movement has always raised social demands for access and the right to education. From the resistance to and confrontation with the military dictatorship brought on by the "University Reform of 1968" through the Confederation of Students of Chile, it reached its maximum expression with the cycle of protests beginning in 2011 demanding *free quality public education* (Donoso Díaz, 2016).

However, in May 2018, women within the student organizations denounced the fact that beyond the historical and visible gains in education through reforms and new laws, gender and feminism demands had not been addressed by educational establishments or by the leadership of the student movement: Sexual harassment, macho treatment and abuse by teachers and other students.

2. Hypotheses

The hypotheses of the investigation are:

(1) Women's demands within the student movement generate hostilities, tensions, and divisions within it.
(2) The pressure of women participants in the Chilean student movement produces a change of direction and with it a reinvention of the social movement, which is redefined from that moment on.

The research questions arise: How has the Chilean student movement been reconfigured and feminized after the irruption of women within it?

3. Methodology

As for the methodological scope of this study, it will be approached from a qualitative approach, the basis of which is the search for exploration and investigation of a case study (Quinn Patton, 2002), in this specific case, within the feminist incubation within the Chilean student movement and with a feminist perspective (Martínez *et al.*, 2014). The information will be obtained through primary and secondary sources of information. As for the primary sources, interviews and auto-ethnography (Calva, 2019). The analysis of minutes of assemblies of feminist groups will also be used.

Interviews will be conducted with women who have lived through the student mobilization process of May 2018, in the main cities of Chile (Santiago, Valparaiso and Concepción). The selection of informants will be based on a sample of criteria (Paredes P & Valenzuela Fuentes, 2020). For this research, the informants will: (1) be women who participate in the student movement and/or its organizations (2) have been part of the May 2018 phenomenon 3) be

defined as feminists. The number of interviewees will be limited by the criterion of information saturation.

4. Results

By way of preliminary findings, we can point out that the feminist movement is the promoter and catalyst of a phenomenon of deconstruction of Chilean society, which ranges from the domestic to the cultural and the political. Social movements have feminised themselves and are feminist according to their internal definition of who they are and where they want to go.

5. Conclusions

The feminist student movement is considered the window of opportunity for women and feminism to establish and define transcendental political processes such as the current constituent process, which is a pioneer in terms of parity.

Keywords: *social movements, feminism, feminization, student movement*

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DIVING-RELATED DEATHS IN SPAIN 2009-2020

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1. Introduction

Diving is one of the most popular underwater activities on the Spanish coast (Casadesús *et al.*, 2018). Although today it is considered a safe practice (Shreeves, Buzzacott, Hornsby, & Caney, 2018), new cases of deaths related to such activity are described every year. Drowning is the main cause of death, but others are observed, such as decompression illness and natural pathology (Casadesús *et al.*, 2019; Denoble, Caruso, Dear, Pieper, & Vann, 2009). Epidemiological data on mortality in diving in Spain does not exist (Casadesús *et al.*, 2021).

The aim of this study is to collect the data referring to all the diving-related deaths between 2009 and 2020 in Spain and to describe the technical characteristics and the causes of death using a multidisciplinary investigation.

2. Methodology

The Observatory for Diving Accidents Fatalities (OMAB, in Spanish) was established in 2014 by the University of Girona and the Secretary of State for Security. We have conducted a retrospective collection of technical data from the police diving team. All the final autopsy reports of each analyzed case were accessible in accordance with Regulation 1/2005 regarding accessory aspects of judicial proceedings. We have analyzed data from January 2009 to December 2020 from the Girona coast to evaluate our efficacy in this type of observation and improve these registers. We have performed multivariable statistical analysis (frequency table, SPSS statistical package, version 25.0, IBM, Armonk).

3. Results

A total of 33 cases with self-contained underwater breathing apparatus (scuba) have been documented through the OMAB (preliminary results): most fatalities were males (24 divers) aged between 50 and 69 years of age (24 divers), although the most prevalent range was between 55 and 65 years of age (16 divers). The most common identified triggers included exertion, panic, buoyancy problems and disorientation. The main factors identified as disabling agents were rapid ascent, a cardiac incident, panic and entrapment. Asphyxia, lung over expansion, and myocardial ischemia were the most frequent disabling injuries. Finally, drowning represented the main cause of death (18 divers), followed by arterial gas embolism (10 divers) and natural causes or internal diseases (5 divers).

4. Conclusions

The work of the OMAB will allow the collection of technical-police and medical-forensic data in a regulated and standardized manner for the preparation of descriptive studies of diving fatalities in Spain. Protocols must be developed to highlight the risk factors and we expect that the data provided can help to avoid unsafe behaviour and prevent future diving accidents.

Keywords: *diving, police reports, autopsy, causes of death, multidisciplinary investigation*

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SESSION V. INTELLIGENCE AND ATTENTION TO DIVERSITY

VALIDATION OF A QUESTIONNAIRE TO EVALUATE VOCATIONAL TRAINING PROGRAMS ADDRESSED TO PEOPLE WITH INTELLECTUAL DISABILITIES

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1. Introduction

People with intellectual disabilities have few options to participate in vocational training programs once they have completed compulsory secondary education (Pallisera, Vilà, & Fullana, 2014). Except for some programs, most young people with intellectual disabilities must be trained through programs offered by foundations and organizations in the tertiary social sector. These courses, which are carried out in non-formal areas, do not allow accreditation of the achievement of professional skills (Pallisera *et al.*, 2018).

The European EQUALvet project is funded through the Erasmus+ call in which the Diversity Research Group from the University of Girona, the Mas Xirgu Foundation and other associates from Greece, Portugal and Belgium participate as partners. It aims to develop a proposal for professional training in the specialities of kitchen, gardening and cleaning assistants and test a system of certification of the skills achieved. The final master's thesis (TFM) presented is placed in the context of this project and aims to develop a questionnaire to assess these training programs by participants, and to be accessible and adapted to people with intellectual disabilities.

2. Methodology

To achieve this, a validation process is carried out with people with intellectual disabilities that participate in the professional training course for gardening assistants effectuated by the Mas Xirgu Foundation. To undertake the validation, a pilot test of the questionnaire was performed on a group of 6 participants. Once applied, the participants were interviewed to assess its format and understand what improvement proposals could be made to make it more accessible. This way not only was an accessible resource created by the participation of people with intellectual disabilities but also these people were given the opportunity to make their opinion present in the evaluation of the training programs.

3. Results

The communication presents the process followed to make this validation, the results obtained from the interviews, as well as the new improved version of the questionnaire, which will then be applied to all participants in the three different training programs offered by the EQUALvet project partners.

4. Conclusions

Once the validation process was made, it was concluded that the original questionnaire could consider some changes to be more accessible for people with intellectual disabilities.

Keywords: *intellectual disability, work inclusion, vocational training, inclusion, cognitive accessibility*

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PERCEPTIONS OF UNIVERSITY STUDENTS FROM AN INCLUSIVE PILOT PROPOSAL FOR PEOPLE WITH INTELLECTUAL DISABILITIES (ID)

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1. Introduction

One of the key factors for inclusion is building a positive culture around diversity and being able to understand its needs (Gunnþórsdóttir, 2014). For this reason, it is considered important that university students can learn about disability and understand the differences by living directly with them (De Luna, 2004). It is essential that future professionals from socio-educational fields are committed to inclusion, so in their training, they must have opportunities that allow them to experiment and understand diversity from their own experience.

With the aim of facilitating and implementing inclusive education for young people with ID at the University of Girona (UdG), a pilot proposal called "Participation Inclusive Project" (PRINPAR) was developed through a training course that lasted 5 months during the 2018-2019 school year. The participants in the project were 16 trainers, 20 university students and 14 young people with ID. In this sense, the objective of the research was to investigate and analyse the perceptions regarding inclusive education of the university students who participated in the project.

2. Methodology

The research was developed from a qualitative perspective, through an initial and a final interview with 20 university students (aged 18-44) pursuing degrees in: Social Education, Social Work, Infant Education and the double degree in Infant and Primary Education. The transcription of the individual interviews preceded the thematic content analysis, using the Atlas.ti 9 software, looking for similarities, coincidences and differences through the coding process (Braun & Clarke, 2016).

3. Results

University students believe that their perception of inclusive education has changed considerably. Although their theoretical knowledge has not changed much, they claim to have debunked some misconceptions regarding disability and inclusion. They consider that access to the educational context should be guaranteed without distinction or exclusion due to people's cognitive level so that they can benefit from the same learning opportunities as others.

4. Conclusions

Inclusion does not only mean allowing people with disabilities access to education but, when possible, eliminating or minimizing difficulties or barriers that may limit the participation of

people with disabilities (Booth & Ainscow, 2000). Having this type of experience, in addition to being recognized by students as something enriching (Lundell, Higbee, & Arendale, 2005), has allowed the generation of changes in negative factors that can hinder inclusion, such as prejudices and attitudes from university students towards disability.

Keywords: *inclusive education, misperceptions, university, university students, intellectual disabilities*

5. Bibliography

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SOCIALLY WITHDRAWN YOUTHS: THE IMPORTANCE OF EDUCATIONAL CONTEXTS IN THE SPREAD OF THE HIKIKOMORI PHENOMENON

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1. Introduction

The term Hikikomori (social withdrawal) refers to those young people who choose to retire to their bedroom, avoiding any form of sociality and commitment (Saito, 2013). It appeared in the late 1970s in Japan, and then spread to many Asian and Western countries. Among the many factors that characterize this complex phenomenon, school refusal appears as a significant element.

2. Hypothesis

The starting hypothesis considers school as a non-negligible factor in favouring the choice of social withdrawal in young people. The study intends to explore how scientific research has investigated the relationship between school and hikikomori.

3. Methodology

A literature review has been carried out which included 69 articles, published in peer reviewed journals, with the aim of answering the following questions: (a) to which scientific field do the journals that published the articles belong? (b) what theoretical model have the researchers followed? (c) how does the relationship between hikikomori and school become explicit?

4. Results and discussion

The analysis of the publications examined showed that most of the journals are of the medical-psychiatric type (59%), 9% are psychology journals and only 32% are of the socio-cultural area. Five thematic areas were identified in relation to how the role of the school was addressed in the selected studies: school refusal as a contributing cause or symptom; bullying and rejection by peers; organization of the school system; relationship between school transformations, society and the labour market; school as a recovery area. The review found that scientific research on the subject still suffers from a medicalizing paradigm and that the space reserved by research for schools and its transformations in advanced capitalist societies (Furlong, 2008) is still marginal.

5. Conclusions

The results, on the one hand confirm the centrality of the school in relation to social withdrawal, on the other they highlight a lack of depth that allows us to consider this field of investigation as a terrain to be explored.

Keywords: *hikikomori, social withdrawal, school refusal, education, young*

6. Bibliography

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ASSESSMENT OF AN INCLUSIVE RESEARCH EXPERIENCE BASED ON THE PERSPECTIVE OF THE PARTICIPANTS: THE ADVISORY COUNCIL OF THE DIVERSITY RESEARCH GROUP

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1. Introduction

The concept of inclusive research summarizes the impulse to incorporate people with intellectual disabilities in designing and conducting research on issues that concern them, learning about them, reaching and representing their experiences and valuing different ways of learning. The main objective of the study presented in this communication is to know the assessment made by a group of people with intellectual disabilities, who are part of the Advisory Council of the Diversity Research Group of the University of Girona, about their experience in inclusive research. This council advises and collaborates with academic researchers in the development of research on topics of interest to them.

2. Methodology

To develop this research, a qualitative approach was used. Participants were 5 people (4 women and 1 man) between 28 and 60 years old, with intellectual disabilities and members of the Advisory Council of the Research Group on Diversity. A semi-structured interview was applied. Information was collected on objectives, contents, dynamization of the sessions, satisfaction with participation, lessons learned, feelings generated with facilitators and colleagues, among others. Each participant signed an informed consent document. The interviews were audio recorded and transcribed. A thematic content analysis was performed to analyze data obtained.

3. Results

According to the results, the advisors valued positively the experience of being part of the research process because it allows them to learn new things, express their opinions about various life issues, feel fulfilled and at ease in a group where they feel they were listened to and respected.

4. Conclusions

The assessment made by the participants is essential in order to have a global understanding of the research carried out in an inclusive manner and to make suggestions for improvement (Flood, Bennett, Melsome, & Northway, 2013). The results turn out to be compatible with some studies that, among other things, highlight the contribution of inclusive research in fostering a sense of belonging to a group (Nind & Vinha, 2014), building friendship bonds

(Flood *et al.*, 2013) or being empowered (Di Lorito, Bosco, Birt, & Hassiotis, 2018; March, Steingold, Justice, & Mitchell, 1997).

Keywords: *inclusive research, intellectual disabilities, assessment, advisors, advisory board*

5. Bibliography

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VIEWS OF YOUNG PEOPLE WITH DOWN SYNDROME ABOUT THE SUPPORT OFFERED BY THEIR BROTHERS AND SISTERS

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1. Introduction

Historically, research on the role of siblings of those with intellectual disability (ID) has been carried out from different perspectives, helping to create reference models such as those by Meyer & Vadasy (1996) which suggest support activities for the family.

These approaches demonstrate the lack of perspective of people with ID. In this field of study, scientific developments are limited (Stoneman, 2005) and even more so in those referring to Down Syndrome (DS). However, those that exist are beginning to acclaim new approaches which include the voices of the protagonists (Meltzer & Kramer, 2016), the recognition and analysis of each case, the distinctive features of each relationship between siblings (Cuskelly, 2016) and the help of participative activities in the research of people with ID.

This communication presents the first results of research that aim to know, in first person, the opinions of young people with Down syndrome about the role their siblings without disabilities play in building their supportive relationships (Fernández Peña, 2015). Thus identifying the factors that assist in these positive relationships they have.

2. Methodology

This is qualitative research which as a starting point contains accounts in the form of interviews and visual support with 7 young people with Down syndrome between the ages of 12 and 18.

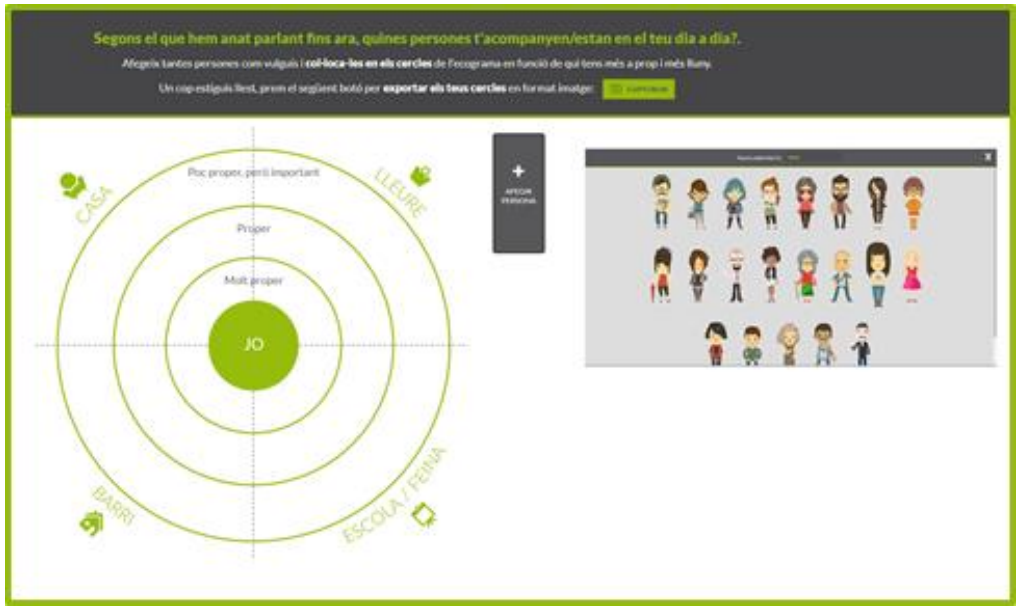

Figure 1. Sample of visual and multimedia support applied in the interviews (https://www.sindromeup.cat/cercles-confianca/)

The methodological design includes inclusive activities carried out through the participation of an advisory committee made up of people with ID.

3. Results

Although each family situation must be taken into account individually, this study helps to reach the perception first hand of sibling support for young people with DS.

The results are orientated to the analysis of topics such as the activities and hobbies they share, the evaluation between each brother or sister, the position of siblings in the social network of the young person with DS, supportive exchanges that occur between them.

4. Conclusions

Studies in this knowledge area show a lack of perspective of people with disabilities. This fact has outlined new opportunities for research such as addressing this topic from inclusive angles, including opinions of those with ID in order to understand their experiences and the experiences of siblings with and without DS. It is considered that people with DS may need more support than the rest to participate with satisfaction in daily life. Knowing these needs from the perspective of perceived support is the study's contribution to those that already exist.

Keywords: *Support, Down syndrome, Siblings, Intellectual disability*

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ASSESSING MATHEMATICALLY GIFTED STUDENTS: AN EXPLORATORY STUDY

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1. Introduction

Research in mathematics education contributes significantly to understanding the factors involved in the mathematics teaching-learning process. However, studies focused on the assessment of learning are still scarce, especially those related to the assessment of mathematical competence. Niss (2003) conceptualizes mathematical competence as the ability to understand, judge, do and use mathematics in a variety of intra- and extra-mathematical contexts and situations, in which mathematics plays an important role. Furthermore, Azcárate Goded & Cardeñoso Domingo (2012) state that mathematical competence is achieved when mathematical knowledge is applied spontaneously in various situations, coming from other fields of knowledge and everyday life.

Regarding mathematical talent, some authors (de Guzmán, 2004; Freiman, 2006) consider that mathematically talented students generally ask questions that go beyond a mathematical task, look for patterns and relationships, build mathematical links and structures, produce original and profound ideas, pay attention to details, develop efficient strategies, think critically and persist in achieving goals.

2. Hypothesis

What knowledge do teachers have to evaluate the mathematical competence of mathematically talented students?

3. Methodology

Our study is framed in the interpretative paradigm with a mixed methodological design. In order to investigate the teachers' knowledge in evaluating the mathematical competence of mathematically talented students, a questionnaire was designed with open, closed and semi-closed questions and subsequently validated by expert judgment. The participants were 32 active teachers selected by non-probabilistic convenience sampling.

4. Results

The data obtained were analysed using Microsoft Excel 2019 and Atlas.ti V8. They reveal a lack of knowledge from the teaching staff in aspects related to the assessment of mathematical competence of mathematically talented students. Specifically, it is found that 70.31% of participants do not clearly distinguish between assessment means, techniques and instruments. One of the probable reasons is that expressed by Hamodi, López Pastor, & López Pastor (2015), who state that there is some confusion in the use of terminology related to the learning assessment.

5. Conclusions

Considering the knowledge gaps detected in our study, one of the key aspects to improve the assessment processes of mathematically talented students, is to incorporate topics that address conceptual aspects related to assessment in the initial and continuous training of teachers. In addition, teachers should be provided with various activities that allow them to use different techniques and instruments to assess the learning of these students.

Keywords: mathematical talent, mathematical competence, assessment of mathematical competence, initial and in-service teacher training.

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SESSION VI. CHEMISTRY

SELECTIVE ENCAPSULATION OF CORONENE IN A SELF-FOLDING CAVITAND

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7. Introduction

Supramolecular chemistry is one of the most promising approaches for the mimicry of biological systems. Imitating enzymes, for instance, is particularly desirable because of their ability to dramatically accelerate the rate of chemical reactions. This is only possible because of the unique properties of their active sites, which provides a confined space isolated from bulk solution, a flexible structure capable to adapt to the substrate, and the ability to orientate the substrate into a reactive conformation (Ringe & Petsko, 2008). The development of a synthetic system combining all these features is a challenging objective. Cavitands, synthetic receptors with a well-defined confined space, constitute excellent candidates to reproduce the properties of enzymatic active sites (Raynal, Ballester, Vidal-Ferran, & van Leeuwen, 2014).

8. Methodology

We have focused on calix[5]arene scaffolds, a family of wide and flexible macrocycles. We have synthesized a cavitand in a bottom-up fashion, through well-established organic transformations. We then tested the encapsulation of different polycyclic aromatic hydrocarbons (PAHs). The unique dynamic properties of this system have been thoroughly studied by nuclear magnetic resonance (NMR) spectroscopy and molecular dynamics (MD) simulations.

9. Results

The cavitand presents a semi-permanent cavity stabilized by an intramolecular network of hydrogen bonds (Figure 1). It binds coronene selectively over smaller polycyclic aromatic hydrocarbons (PAHs). The host features a network of hydrogen bonds that is essential for the binding process because it provides stabilization and also enough flexibility to adapt to the guest's shape. This adaptable behaviour is illustrated with the binding of *N*,*N*'-dimethylnaphthalenediimide (MeNDI), a guest of smaller size and different shape that is bound due to the complementarity between the electron-rich and electron-deficient π surfaces of the cavity and MeNDI respectively (Lozano, Álvarez-Yebra, López-Coll, & Lledó, 2019).

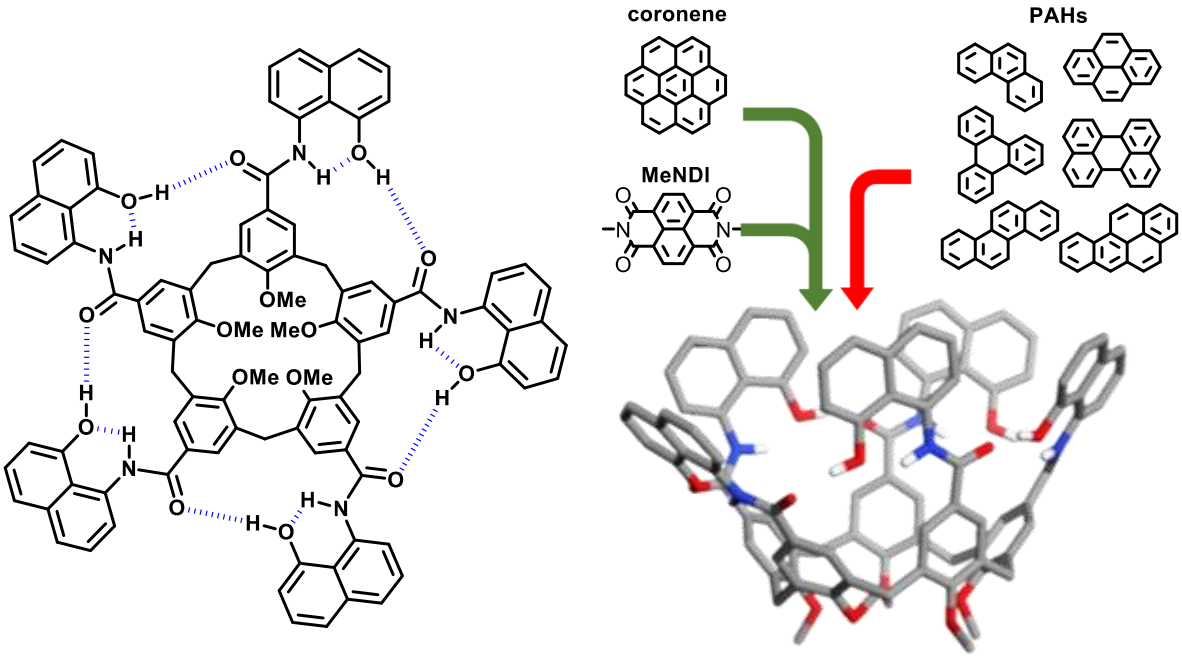

Figure 1. Self-folding cavitand structure (left). DFT-optimized structure (B3LYP/6-31(d)/GD3BJ) and PAHs binding possibilities (right).

10. Conclusions

In conclusion, we have developed a new flexible self-folding receptor based on calix[5]arene that is able to bind coronene and MeNDI.

Keywords: *supramolecular, chemistry, cavitand, calixarene, PAHs*

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A PREDICTIVE JOURNEY TOWARDS TRANS-THIOAMIDES/AMIDES

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[2] *Dipartimento di Chimica e Biologia, Università di Salerno, Via Ponte don Melillo, 84084, Fisciano, Italy*

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1. Introduction

Itai, Toriumi, Saito, Kagechika, & Shudo (1992) demonstrated the cis-preference of the amide bond in N-methylbenzanilides. Although acyclic amides strongly prefer trans conformation around the N–C(O) bond, their N-methylated counterparts undergo a conformational switch arising from avoidance of unfavourable steric interactions while retaining substantial double bond character of the amide bond through nN→ π*C=O conjugation. This led to a switch from trans to cis conformation just by playing with the substituents next to the amide. Amides are important since they participate in medicinal chemistry, biochemistry, molecular recognition, organic synthesis, conformation relays, and synthetic switches.

In this work, we study, with Density Functional Theory (DFT) calculations, the mechanism of the cis-trans isomerization of thioamides or amides (see Figure 1), previously synthesized by (Zhang *et al.*, 2020), to obtain hints of the higher preference for the cis conformation.

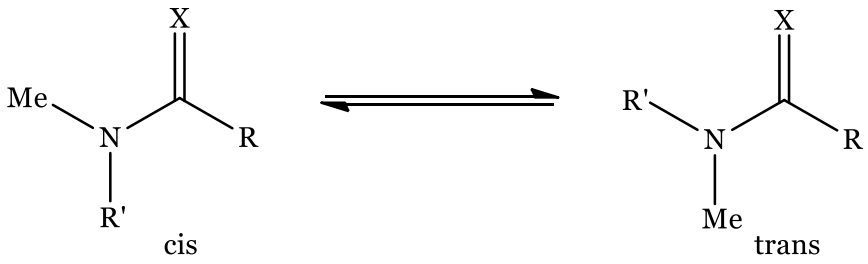

Figure 1. Cis-trnas equilibrium of C=X bond studied in this work.

2. Methodology

All DFT calculations were performed with the Gaussian16 at the B3LYP-D3/6-311++G(d,p) level. Solvent effects were included in the geometry optimizations with the Solvation Model based on Density using toluene as solvent.

3. Results

A set of thioamides and amides, chosen for their different electronic properties and their steric hindrance, was analysed.

The increase of steric hindrance (R=t-Bu, R'=t-Bu) leads to the desired major stability for the trans isomer. On the other hand, the electronic effects were also tested and only the electro-

donating capacity of the methoxy ligand (R=OMe, R'=Ph) is able to favour the trans isomer for the amide, whereas it still does not favour the thioamide counterpart. Mixing steric and electronic factors at the same time (R=C(CF_3)$_3$ and R' = Ph) shows us that both effects are important. The cis conformer remains only slightly more stable because of the electro-withdrawing character of substituents including fluor atoms, that destabilize the trans isomer.

4. Conclusions

The cis-trans isomerization of amide/thioamides bond is studied through computational methodologies. Steric and electronic effects were tested and they result in playing a key role in determining cis-trans preference. No doubt the steric element is distorting and predominates when two large groups collide in cis.

Keywords: *amide, thioamide, DFT, cis-trans isomerization*

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COMPUTATIONAL STUDY OF AMBIMODAL REACTIONS

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1. Introduction

A chemical reaction is considered ambimodal when it presents a post-transition state bifurcation in its potential energy surface (PES) that gives rise to multiple products, all of them without passing through any other barrier (Ess *et al.*, 2008). This type of reaction is present in many biological reactions of interest, as well as in multiple organic and organometallic reactions. Ambimodal reactions can be detected, computationally by means of molecular dynamics techniques. Nowadays, the methods that have been proposed to rigorously determine the presence of bifurcations in the PES from a static point of view, are very expensive. For this reason, it is interesting to design a new tool that allows us to detect ambimodal reactions in an easy and efficient way.

2. Methodology

Throughout the research, two types of methods have been used: static and dynamic density functional calculations.

All the electronic structure calculations have been carried out in the Gaussian16 software package by using the ωB97XD density functional, and spanning the molecular orbitals into the Def2SVP basis set. All the stationary points of the potential energy surface have been characterized through a vibrational harmonic frequency calculation.

3. Results and discussion

In this study, a [3,3]-sigmatropic rearrangement described by Villar López, Faza, & Silva López (2017), which can form two products from the same transition state has been *in silico* analyzed (Figure 1).

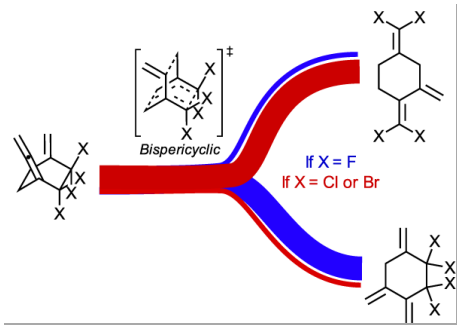

Figure 2. [3,3] Sigmatropic rearrangement featuring a bispericyclic transition state. X=F in this study.

Several tools to evaluate the outcome of the reaction after the bispericiclic transition state have been tested, and a protocol to determine whether the reaction is ambimodal has been set up,

consisting of geometrical optimizations in subspaces of the 3N-6 PES. Subsequently, dynamics simulations have been carried out to validate the results obtained with the static calculations. Then, a second reaction consisting of a [6+4] cycloaddition between tropone and dimethylfulvene described by Yu *et al.* (2017) has been studied.

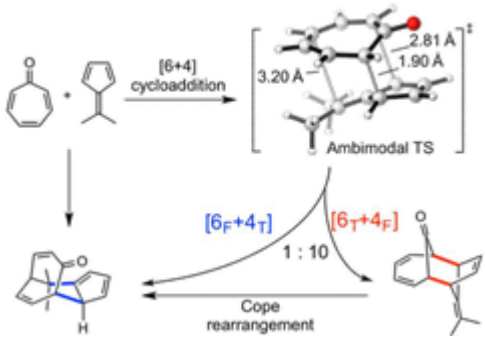

Figure 3. Ambimodal [6+4] cycloadditions between tropone and dimethylfulvene.

Such reactions have been analyzed with the strategy devised in the previous reaction. Finally, the effects of the substituents on the fulvene on the bispericiclic transition state has been explored.

4. Conclusions

A fast and simple protocol based on static calculations was elaborated, in order to know whether a reaction is ambimodal or not. Furthermore, to verify the process, a homologous but non-ambimodal reaction was characterized. Finally, by using molecular dynamics, the proposed method was validated.

Keywords: *Density Functional Theory, post-transition state bifurcations, organic chemistry, reactivity, dynamics*

5. Bibliography

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GUIDELINES FOR TUNING THE EXCITED STATE HÜCKEL-BAIRD HYBRID AROMATIC CHARACTER OF PRO-AROMATIC QUINOIDAL COMPOUNDS

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1. Introduction

The excited state aromatic character of TMTQ, a quinoidal compound with a central 1,6-methano[10]annulene and two 5-diacyanomethyl-thiophene units, is controversial as it can be described as Hückel and/or Baird aromatic. The T_1 state was earlier characterized as Hückel-Baird hybrid (Jorner *et al.*, 2016), but recently it was claimed that S_1 is a Baird aromatic compound as a result of a double charge transfer upon excitation (Kim *et al.*, 2019).

2. Hypothesis

Similarly to what was found for TMTQ in T_1, the aromaticity of S_1 state can also be mainly attributed to the Hückel resonant form (Figure 1).

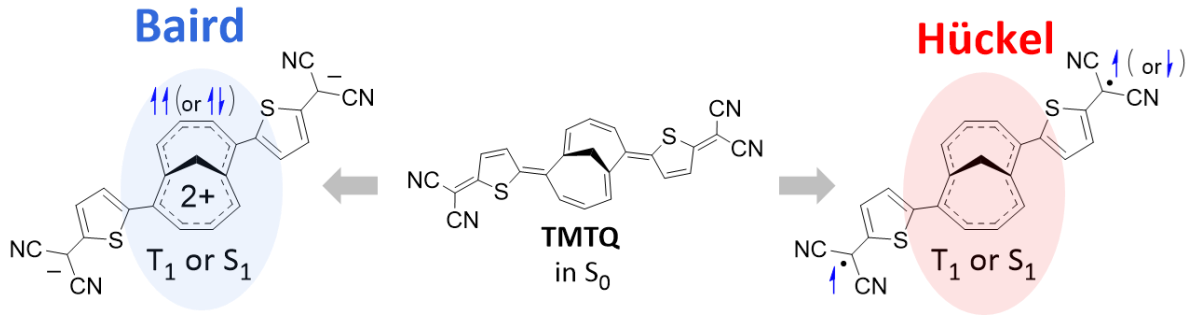

Figure 1. Hückel- and Baird-aromatic resonance structures of TMTQ in T_1 and S_1 excited states.

3. Methodology

(Time-dependent) density functional theory methods were used, specifically B3LYP/6-311+G(d,p). Then aromaticity indicators like nucleus independent chemical shift (NICS) and fluctuation index (FLU) among others were computed, as well as atomic charges and spin densities. All the calculations were performed with Gaussian 16 rev. A.03/B.01, AIMAll and ESI programs.

4. Results and discussion

Our results showed that the interpretation by D. Kim and coworkers[2] needs to be revised because the low-lying excitations of symmetrically substituted conjugated rings including TMTQ hold a very weak charge transfer character. We also found that the high Baird character of the central ring is achieved only with anionic and small conjugated central rings with electron donating groups as substituents and small exocyclic groups with electron withdrawing substituents (Escayola *et al.*, 2021).

5. Conclusions

Our study aims to warn about the need to make correct interpretations of the experiments in this area of research, as only then can the excited state aromaticity concept be developed into a useful tool for the design of high-performance organic electronic devices.

Keywords: *aromaticity, excited state, quinoidal compounds, rational design, computational chemistry*

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RATIONALIZING THE BEHAVIOUR OF PADDLEWHEEL TRANSITION METAL CATALYSTS

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1. Introduction

Rhodium paddlewheel complexes are extremely useful catalysts for transformations involving carbenes. Computational (Nakamura, Yoshikai, & Yamanaka, 2002) and inhibition kinetic studies (Pirrung, Liu, & Morehead, 2002) of the rhodium-catalyzed carbene reactions show that the active [Rh_2] catalyst uses only one of its two coordination sites at a time for carbene binding.

Since rhodium is a very expensive metal, formation of a heterobimetallic unit by replacing one of the rhodium atoms with less expensive metal is an appealing alternative (Collins, van Gastel, Neese, & Fürstner, 2018). [BiRh] heterobimetallic carboxylate paddlewheel complexes have been shown to be excellent catalysts in carbene mediated reactions (Collins, Auris, Goddard, & Fürstner, 2019).

2. Hypothesis

The interactions between the 4d orbitals of rhodium and the 6p orbitals of bismuth may result in weaker π-back-bonding interactions for bismuth-rhodium carbene complexes in comparison with the dirhodium carbene complexes. The different reactivity of the two catalysts may be due to this different electronic effect. Therefore, our aim is to determine the electrophilicity of the carbene complex in bimetallic cores.

3. Methodology

All the geometry optimizations were performed using the PW91PW91 exchange-correlation functional in combination with the triple zeta valence polarization basis set (def2tzvp). The description of the bond to quantify the electron donation from the ligand to the metal and the metal to the ligand were carried out with the *effective oxidation state* (EOS) analysis.

4. Results

The nitrogen extrusion takes place driven by the back-donation from the Rh $4d_{xz}$ orbital to the C-N σ*-orbital and our EOS analysis shows that the [Rh_2] catalyst is more π-donor than the [BiRh]. Higher activation barriers were calculated for this step carbene formation in the case of bismuth-rhodium catalysis (BiRh:28.2 kcal/mol, Rh_2: 10.6 kcal/mol), in accordance with our previous description.

The second step is a nucleophilic attack of the alkane into the carbene carbon atom. In this case, the attack is more favourable in the [BiRh] catalyst due to the lower π-donation from the rhodium atom to the carbene in comparison with the [Rh_2]. The energy barriers are consistent

with this behaviour (BiRh:13.2 kcal/mol, Rh_2:22.5 kcal/mol). The same analysis was performed in 25 different paddlewheel complexes revealing that the π-donation of the metal atom describes the energy barriers very well.

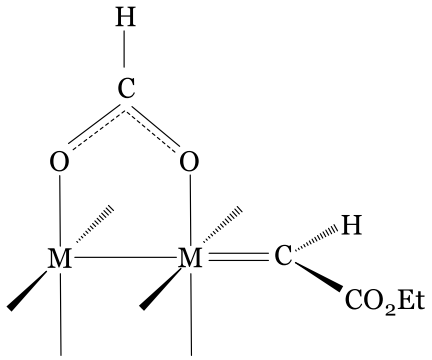

Figure 4. Bimetallic carbene complex $M_2(O_2CH)_4C(H)(COOEt)$ where we modify the core (M_2) to form 25 different paddlewheel carbene complexes.

5. Conclusions

The comparison of reactivity in homo- and heterobimetallic complexes shows that the distal metal centre plays an important role in controlling the electrophilicity of the carbene. The divergent reactivity of the paddlewheel complexes can be explained by the π-donation of the metal atom to the carbene.

Keywords: *catalyst, rhodium, carbene, electrophilicity*

6. Bibliography

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REMOTE AMINO ACID RECOGNITION ENABLES EFFECTIVE HYDROGEN PEROXIDE ACTIVATION AT A MANGANESE OXIDATION CATALYST

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1. Introduction

The selective oxidation of organic substrates via activation of O_2 or peroxides is commonly performed in nature by metalloenzymes. The first coordination sphere around the metal center present in the active site has an important influence in its reactivity; but an exquisite control of the secondary coordination sphere has a great impact in defining high selectivities. In particular, the presence of an acidic moiety in close proximity to the metal facilitates the O-O cleavage step that generates the oxidizing high valent metal-oxo species (Costas, Mehn, Jensen, & Que, 2004).

During the last decades, synthetic chemists tried to mimic the structure and activity of these enzymes. The main approach consists of the use of tetradentate N-based ligands that resembles the first coordination sphere of metalloenzymes (Sun & Sun, 2019). These complexes are able to efficiently activate H_2O_2 and found to proceed with analogous mechanisms that those operating in metalloenzymes. However, while the latter need only a single acidic function, bioinspired manganese systems need a high excess of carboxylic acid, up to 17,500 equivalents for the metal center (Vicens, Olivo, & Costas, 2020).

2. Hypothesis

Taking inspiration from the mechanism operating in metalloenzymes and the huge effect of the second coordination sphere, it is envisioned that introduction of a single carboxylic acid in close proximity to the metal center of a manganese oxidation catalysts by manipulating the second coordination sphere of the metal center may enable enzyme-like H_2O_2 activation.

Moreover, tuning of the second coordination sphere may substantially affect the catalyst structure, which can be translated into an improvement of the stereoselectivity in oxidation reactions.

3. Methodology

Supramolecular recognition was the chosen strategy to modify the second coordination sphere of the catalyst. A series of C_1-symmetric manganese catalysts bearing one 18-benzo-crown-6-ehter receptor that strongly bind protonated primary amines were designed (Olivo *et al.*, 2017). This receptor would bind a carefully designed α,ω-protonated amino acid, placing the carboxylic acid function in proximity to the metal center (Figure 1).

4. Results and discussion

The designed system was tested in the epoxidation of 1-chloro-3-methylbut-2-ene. Using 1 mol% of Mn catalyst, 1.5 mol% of amino acid **(AA)**, 2 equiv. of H_2O_2 in CH_3CN at -40°C, the reaction proceeds with 65% yield and 67% ee (Figure 1), being this result the highest enantioselectivity reported for this substrate in the literature.

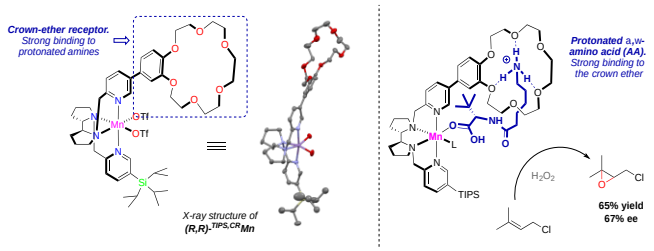

Figure 1. Design of the system and application in the epoxidation of 1-chloro-3-methylbut-2-ene.

Control experiments demonstrated that incorporation of stoichiometric amounts of **AA** in the second coordination sphere of the catalyst via supramolecular recognition is the key to obtain high catalytic activity. Moreover, the binding of the **AA** to the crown ether forms a rigid oxidizing species with a highly defined chiral structure that is needed to obtain high enantioselectivities.

5. Conclusions

An efficient enzyme-like hydrogen peroxide activation at a manganese catalyst is described by locating an amino acid in the second coordination sphere of the metal center. The system is applied in the asymmetric epoxidation of olefins and represents a pioneering example of how supramolecular recognition can be used to efficiently tune the second coordination sphere of bioinspired oxidation catalysts.

Keywords: *supramolecular recognition, oxidation, hydrogen peroxide, amino acids, epoxidation*

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COMPUTATIONAL ASSIGNMENT OF OXIDATION STATES FROM FIRST PRINCIPLES

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1. Introduction

One of the most fundamental chemical concepts is the Oxidation State (OS), which is widely used for rationalization, characterization, categorization and prediction of reactivity of inorganic compounds. Some years ago, a new generic definition of OS was entered into IUPAC's Gold Book, which reads as the atom's charge after ionic approximation of its heteronuclear bonds (Karen, McArdle, & Takats, 2014). For homonuclear bonds, its electrons must be divided equally, independently of the chemical environment.

The OS of an atom (typically a metal) in a molecule is the net (imaginary) charge that results from the application of the ionic approximation to its bonds. Because of that, the partial atomic charge, obtained with one or another population analysis, has been often erroneously seen as a sort of non-integer version of the OS. In recent years, there has been some particular interest in developing computational strategies to extract OS from ab initio calculations.

In 2015, our group introduced a general scheme to derive OS from the analysis of the first-order density matrix, the so-called Effective Oxidation States (EOS) analysis (Ramos-Cordoba, Postils, & Salvador, 2015). Formally, it is applicable to any molecular system (i.e. not restricted to transition metal atoms) independently of its spin distribution (closed- or open-shell), and for any level of theory. Up to now, the EOS analysis has been successfully applied to a considerable number of systems of different nature (Postils, Delgado-Alonso, Luis, & Salvador, 2018), obtaining very consistent results. An alternative for single-determinant methods is to assign OS from the analysis of localized orbitals, such as the Localized Orbitals Bonding Analysis (LOBA) (Thom, Sundstrom, & Head-Gordon, 2009).

2. Methodology

Kohn-Sham Density Functional Theory calculations have been performed to obtain the electronic energies and wave functions of all molecular systems. The fragment OSs have been obtained by means of the LOBA and EOS methods. All calculations have been performed with the Q-Chem and APOST3D software.

3. Results and discussion

In this work we focus on comparing the IUPAC, EOS and LOBA assignments for complexes where elucidating OS is challenging, unveiling that all definitions typically agree for systems with simple ionic bonding and innocent ligands but disagree as the boundary between ionic and covalent bonds is approached, or as the role of ligand non-innocence becomes non-trivial (Gimferrer, Van der Mynsbrugge, Bell, Salvador, & Head-Gordon, 2020). For this reason, we propose an extension to the LOBA algorithm by introducing a function that determines in

which situation the localized orbital electrons should be split between fragments. Furthermore, some intrinsic limitations of the method are unveiled for the carbine systems.

4. Conclusions

With this work, we pinpoint some limitations of EOS and LOBA, opening the door to the development of new improved strategies for OS elucidation, namely by improving the definition of orbital localization procedures for molecular fragments, or going beyond the paradigm of treating all electrons individually.

Keywords: *oxidation states, redox non-innocence, chemical bonding,*

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ELECTRON TRANSFER IN FULLERENE COMPLEXES OF π-CONJUGATED MOLECULAR CROWNS

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1. Introduction

The electron transfer capability of certain fullerene-based inclusion complexes makes them a promising platform for the development of photovoltaic devices. Their photophysical properties can be varied significantly by changing both the inner and outer subunits. Curved nanographenes have attracted much attention due to their significant applications for organic field-effect transistors. Du and co-workers (Huang *et al.*, 2020; Huang *et al.*, 2019) recently reported the synthesis and photophysical properties for a series of π-extended crown-shaped macrocycles bearing conjugated segments of different sizes (Figure 1). We have performed the computational study of photoinduced electron transfer processes in these complexes with the inclusion of C_{60} fullerene.

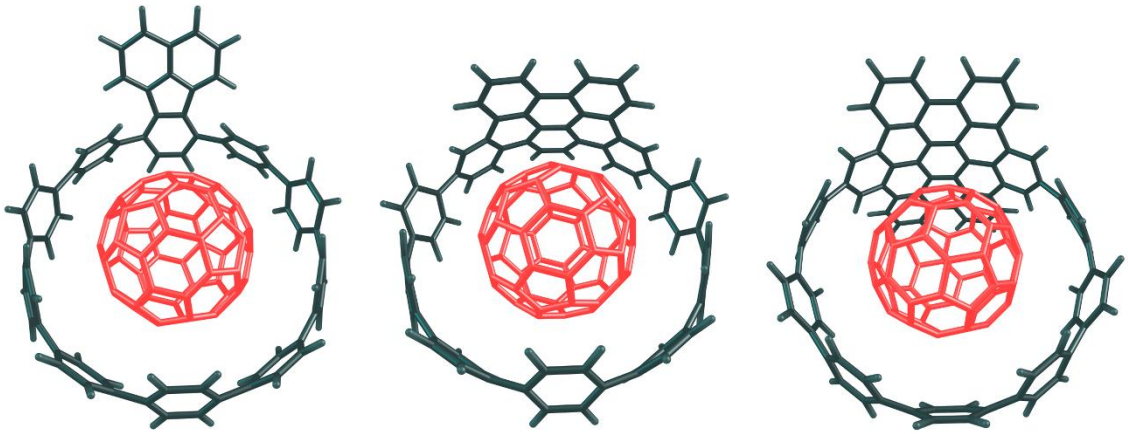

Figure 1. Fullerene encapsulated π-conjugated molecular crowns studied

2. Methodology

Geometry optimizations were carried out using the B3LYP-D3(BJ)/def2-SVP level of theory. Excited states were calculated by TD-DFT using the CAM-B3LYP functional and the def2-SVP basis set. The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes was carried out in terms of transition density. The COSMO-like model with dichloromethane as the solvent was applied to estimate the effect of polar environment on electronic excitations.

3. Results

To estimate the stability of the complexes, the interaction energy (ΔE_{int}) between π-extended crown-shaped macrocycles and fullerene were computed. To get more insight, we performed the energy decomposition analysis of the ΔE_{int} proposed by Morokuma (Morokuma, 1971). Among the total binding forces, the dispersion term is dominant with a contribution of about 60%. Later come the electrostatic and orbital interactions, respectively. The NCI and QTAIM analysis performed for studied systems provided the access to the interaction topology between fragments. The host (crowns) and guest (C_{60}) molecule contributions to the excited state electronic density were analyzed for the lowest 50 excited states of each complex. For the complexes of interest, the locally excited states and charge-transfer states were detected. The rates of electron transfer were calculated using the semi-classical Jortner approach.

4. Conclusions

In conclusion, photoinduced charge separation in a series of C_{60} fullerene encapsulated π-conjugated molecular crowns complexes has been studied in detail using the TD-DFT approach. In these inclusion complex fast photoinduced electron transfer has been revealed. The charge-separated states with the electron transfer from the crown to the C_{60} unit can be efficiently populated through the decay of the locally excited states and occurs in sub-nanosecond time scale.

Keywords: *fullerenes, photoinduced electron transfer, nanographene/fullerene heterojunctions, non-covalent interactions.*

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INTERMOLECULAR CARBENE TRAPPING

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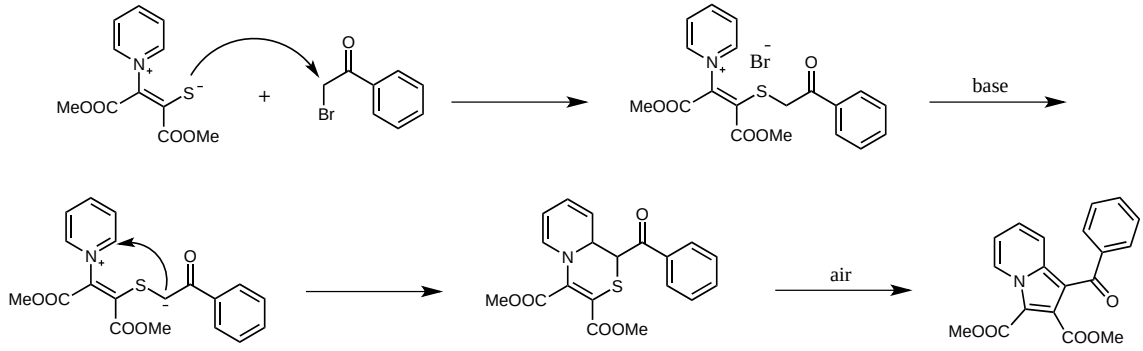
1. Introduction

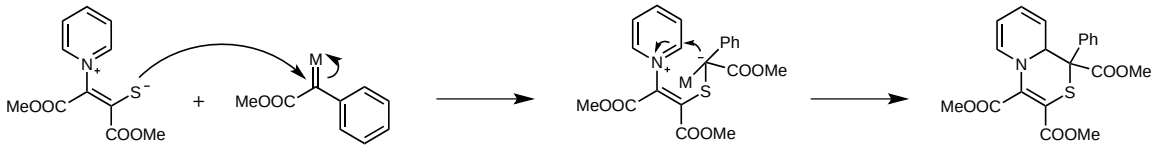
We became involved in the intermolecular trapping of carbenes as part of a research program focused on transition metal-catalyzed reactions involving carbenes (Torres & Pla-Quintana, 2016). A collection of publications from Cheng's group reporting on the rich reactivity of pyridinium 1,4-thiolates (Cheng, Bao, *et al.*, 2020; Cheng *et al.*, 2019; Cheng, Zhang, *et al.*, 2020; Zhai *et al.*, 2020) drew our attention. One of the reactions consists of a formal [5+1] cyclization of the zwitterionic pyridinium thiolate and α-functionalized bromoalkanes, in which the dihydropyridothiazine product formed slowly oxidizes when kept in air to an indolizine (Scheme 1) (Cheng, Zhang, *et al.*, 2020).



Scheme 1. Mechanism of a formal [5+1] cyclization of the zwitterionic pyridinium thiolate and an α-functionalized bromoalkane.

2. Hypothesis

We thought that a similar reactivity could be obtained by the reaction of the zwitterionic pyridinium thiolate with a metalcarbene, through an initial formation of an ylide, followed by an intramolecular nucleophilic attack onto the pyridinium cation (Scheme 2). Furthermore, by using disubstituted carbenes, the oxidation of the dihydropyridothiazine formed would not be possible.



Scheme 2. Mechanism of the reaction of the zwitterionic pyridinium thiolate and a metalcarbene

3. Methodology

Experimentally, the synthesis of dihydropyridothiazine scaffolds was carried out under oxygen and nitrogen atmospheres and employing a wide number of Cu(I) salts as catalysts. The products obtained were analyzed by means of NMR and ESI-MS.

DFT calculations at the B3LYP-D3/Def2SVP(smd) were carried out to unveil the reaction mechanism, as well.

4. Results

Initial attempts showed that copper can be used as a catalyst, and a blank reaction showed no reactivity at all without a copper catalyst. Moreover, the reaction was determined to work better under nitrogen atmosphere. Formation of dihydropyridothiazine scaffold was confirmed by spectroscopic and spectrometric techniques, and no hint of oxidation to the indolizine was detected upon standing in air.

We then experimentally optimized the process reported in Scheme 3 including the study of the stereoselectivity and evaluation of the scope of the reaction. Moreover, we theoretically confirmed that the reaction takes places through the pathway proposed in Scheme 2, and then assisted the optimization of the catalytic system, as well as predicted the effect of substituents on the pyridinium ring.

5. Conclusions

The reaction conditions to prepare dihydropyridothiazine scaffolds in a stereoselectively manner were optimized, as well as the reaction mechanism by DFT calculations being unveiled.

Keywords: *carbene, trapping, cyclization, dihydropyridothiazine, copper*

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SYNTHESIS OF HIGHLY FUNCTIONALIZED 1*H*-ISOINDOLES VIA A Rh(II)-CATALYZED CASCADE REACTION INVOLVING CARBENE ALKYNE/METATHESIS AND NITRILES

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1. Introduction

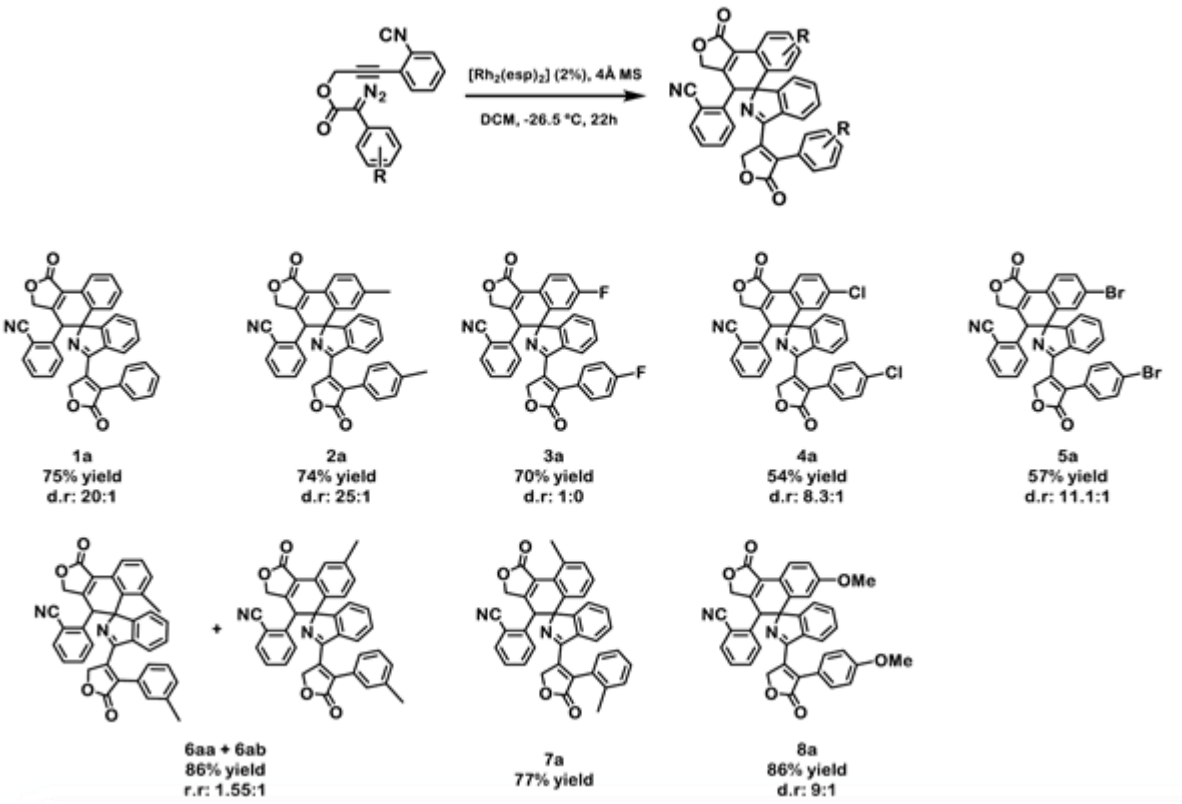
Carbene/alkyne metathesis (CAM) cascade reactions have become one of the most powerful tools for the synthesis of polycyclic molecules through multibond formation in a single reaction step (Pei, Zhang, Qian, & Xu, 2018; Torres & Pla-Quintana, 2016). In continuation of our ongoing research using carbene reactions with various insaturations for terminating the cascade reaction, we wish to report a CAM tandem process terminated by reaction with a nitrile for the synthesis of highly functionalized 1*H*-isoindoles.

2. Methodology

Firstly, the diazo compounds that served as the precursors of the metal carbene were prepared. The reaction conditions were then optimized to achieve the best results. Finally, the substrate scope of the transformation was tested by modifying the aryl ring next to the diazo moiety. All the products obtained were characterized by means of spectroscopic and spectrometric techniques.

3. Results and discussion

The best results were obtained when $Rh_2(esp)_2$ was used with dichloromethane as the solvent, at -26,5°C for 22h. As shown in Scheme 1, the reaction tolerated substituents in the *ortho*, *meta* and *para* positions. The yields were affected by the electronics of the substituents in the *para* position of the aryl, with the more electrondonating ones being those obtained in higher yields (up to 86% in the case of **8a**). *Meta* substituents gave rise to two distinct products (**6aa + 6ab)** with low regioselectivity (1,5:1), albeit with a combined high yield (86%). A methyl group could also be tolerated in the *ortho* position with a 77% yield (**7a**).



Scheme 1. Substrate scope of the reaction

4. Conclusions

We have developed a CAM cascade process in which five new bonds and four new rings are formed in just one reaction step for the preparation of highly substituted 1*H*-isoindoles. The reaction proceeds with a high yield and high diasteroselectivity, and tolerates several substituents in the aryl group.

Keywords: *carbene/alkyne metathesis, carbene, cascade reaction, isoindole*

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SESSION VII. MATERIALS SICENCE

EFFECT OF POLYETHER-POLYSILOXANE BOND ON SILICONE SURFACTANTS

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1. Introduction

Non-ionic silicone surfactants are a particular case of surface-active agent where permethylated siloxane hydrophobic chain (polydimethylsiloxane, PDMS) is coupled to one or different non-ionic groups based on polyethylenoxide (pEO) and polypropyleneoxide (pPO). These groups are commonly known as polyethers or polyglicols (Hill, 2002).

Some unique properties are related to its structure. The hydrophobic group is silicone, so they are able to lower surface tension to 20 dyn/cm while hydrocarbon surfactants achieve a minimum surface tension of 30 dyn/cm. This important feature gives the ability to be surface active in both aqueous and non-aqueous media (Hill, 1999).

There are two synthetic pathways for preparing polyether-polysiloxane copolymers from silicone hydrides and different polyethers.

The first is to use the well-known hydrosilylation reaction, where a silicon-hydride precursor reacts with an allylic polyether and a carbon-silicon (C-Si) bond is obtained. The reaction usually uses platinum catalysts. The most common are Speier's catalyst (H_2PtCl_6) and Karstedt's catalyst (Hofmann, Vlatković, & Wiesbrock, 2017; Putzien, Nuyken, & Kühn, 2010).

The second consists of the dehydrogenative silylation reaction, where a silicon-hydride precursor reacts with a polyether with terminal hydroxyl group and a silicon-oxygen-carbon (Si-O-C) bond is obtained with hydrogen gas release. It has been recently described that the formation of silyl ethers can be achieved using $B(C_6F_5)_3$ as a catalyst (Oestreich, Hermeke, & Mohr, 2015).

2. Problem

Our goal is to synthesise and characterize the two different products that can be obtained from silicon hydride and polyether (Scheme 1). In addition, it will be evaluating the products in a model system regarding its wetting, de-foaming and anti-foaming properties.

3. Methodology

Product **1** and **2** have been prepared from commercially available heptamethyltrisiloxane and allyl alcohol polyether of 210 g/mol molecular weight. Product **1** was obtained from the general procedure for hydrosilylation reaction and product **2** was obtained through a new synthetic route, developed in Concentrol, for dehydrogenative silylation reaction using a low-cost catalyst as an alternative to the usage of $B(C_6F_5)_3$.

The two products were well-characterized using ^{1}H-NMR and ^{29}Si-NMR. In addition, they were tested as additives in acrylic system where the wetting, de-foaming and anti-foaming properties had been analysed.

4. Results

Product **1** and **2** have been obtained through the two different synthetic routes described in scheme 1. ^{29}Si-NMR has proven to be a powerful tool to confirm the obtention of the Si-O-C new bond formation between the polysiloxane and the polyether, thanks to a characteristic signal for the silicon atom attached to the polyether.

Product **1** has better properties as wetting agent than product **2**. However, product **2** has great de-foaming and anti-foaming performance compared with product **1**. We hypothesize that these differences cannot only be attributed to how the polyether is bonded to the siloxane, and that the terminal group probably plays an important role, which will be a matter of study in further works.

5. Conclusions

The synthesis and characterization of product **1** and **2** have been successfully achieved with good selectivity and conversions.

From the same starting reagents, two structures can be obtained with completely different properties only by adjusting the way of bonding the polyether to the polysiloxane.

Keywords: *silicone surfactants, hydrosilylation, dehydrogenative silylation, ^{29}Si-NMR*

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ORIGIN-INDEPENDENT ENERGY-BASED DECOMPOSITION OF (NON)LINEAR OPTICAL PROPERTIES

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1. Introduction

Nonlinear optical properties (NLOP) are of interest both for technological applications (materials with large values, for these properties are commonly used in optical communication technology) as well as theoretical applications (e.g., calculation of dispersion coefficients). Historically, there has been great interest in decomposing these properties (e.g., the molecular polarizability, α), into contributions of individual atoms or functional groups (Laidig & Bader, 1990). Transferable group polarizabilities would give insight about the value of the NLOP, and also allow for their prediction.

The problem that arises with such decompositions is that the atomic contributions obtained from the straightforward decomposition of the NLOP are origin-dependent, meaning that when the origin of the coordinates changes, the contributions also change.

2. Methodology

These properties (P) can be defined as derivatives of the electric field-dependent energy:

$$P = -\left.\frac{{}^{n}E(F)}{F^{n}}\right|_{F=0} \tag{1}$$

Looking at the expression for this energy (Eq. 2), we explored the possibility of ignoring the second energy term (Eq. 3, where one can observe how this term explicitly introduces the dependence on the r coordinate), avoiding the origin-dependence while still being able to recover the entirety of the property (Eq. 4).

$$E(F) = \langle \_(F)\left|H^{(0)} - \hat{\_}F\right|\_(F)\rangle = E^{(0)}(F) - \hat{\_}(F)F \tag{2}$$

$$\hat{\_} = \sum_i q_i r_i \tag{3}$$

$$P = \frac{1}{n-1}\left.\frac{{}^{n}E^{(0)}(F)}{F^{n}}\right|_{F=0} \tag{4}$$

This is based only on the mathematical expressions of the properties, without any assumptions or approximations (Montilla, Luis, & Salvador, 2021).

3. Results

The obtained atomic/group contributions had the expected properties (all positive, adding up to the total value...), but they differed noticeably from those obtained with previous methodologies (Keith, 2007), which allowed us to perform several comparisons based on different indicators.

We have used calculated atomic contributions to predict the polarizability of 16 amino acids, obtaining relative errors ranging from 0.01% to 4%.

Furthermore, our methodology can be used to plot polarizability densities in the 3D space.

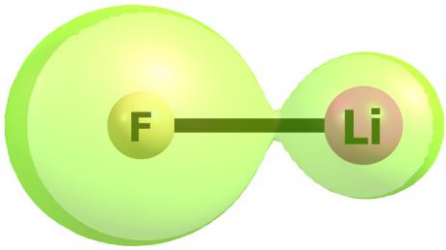

Figure 5. Polarizability density for FLi (Shown: isosurface for a chosen, relevant value); unpublished results.

4. Conclusions

We present here the first genuinely origin-independent decomposition of nonlinear optical properties. The atomic/group contributions obtained are very reasonable, and have proved to be useful for the prediction of properties of other molecules. Interestingly, these contributions can be very different from those obtained by other methodologies, and several analyses suggest that ours is better for describing the actual physics behind the system.

Keywords: *nonlinear optical properties, decomposition, origin-independent, real-space analysis*

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PREDICTION OF OPTICAL PROPERTIES THROUGH DOUBLE-HYBRID DENSITY FUNCTIONAL THEORY

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1. Introduction

The study and rationalization of the nonlinear optical properties (NLOP) of materials such as the static (hyper)polarizabilities are very helpful in the design of new functional optoelectronic materials (Autschbach & Srebro, 2014). Density functional theory (DFT) is a cheap methodology to compute NLOPs, however only tuned range-separated functionals display moderate accuracy for the calculation of this type of properties, and still the errors depend on the family of molecules studied (Besalú-Sala, Sitkiewicz, Salvador, Matito, & Luis, 2020). We have developed a new double-hybrid density functional approximation to generalize the accuracy of DFT methods for all molecules.

2. Methodology

All the electronic structure calculations have been computed by using the Gaussian16 package. The NLOP properties have been computed numerically making use of the central-field derivative procedure, and the systematic error appearing due to the truncation of the Taylor series has been minimized through the Romberg iteration formula. The training set contains 56 molecules presenting large first and second hyperpolarizabilities, while the test set contains 60 molecules bearing different NLO features. Reference values have been obtained at CCSD(T) level from the work of Besalú-Sala *et al.*, 2020.

3. Results and discussion

Compared with most of the state-of-the-art functionals including the range-separated hybrids LC-BLYP, CAM-B3LYP and the T_{α}-LC-BLYP, which was designed specifically to compute NLOPs, our novel functional approximation called LC-B2KPLYP is able to reduce by 17-25 percentual points the error respect to the CCSD(T) reference on several NLOPs such the 1st or the 2nd hyperpolarizabilities for both the training and the test set. Furthermore, LC-B2KPLYP is the only functional able to outperform CCSD on NLOP calculations nowadays, which is an indicator of the high accuracy achieved. 2D maps scanning the amount of MP2 correlation and exact exchange added in the functional will serve as explanation and justification for the final definition of the parameters of the functional, minimizing the relative error respect to CCSD(T).

4. Conclusions

Our novel functional LC-B2KPLYP is able to predict NLOPs with high accuracy, even outperforming the CCSD wave-function method. By using LC-B2KPLYP, new promising building blocks for high-valuable optical devices are expected to be discovered in the near future.

Keywords: *optical properties, density functional theory, computational chemistry*

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DEVELOPMENT OF ANALYTICAL AND COMPUTATIONAL METHODS TO PREDICT THE MECHANICAL BEHAVIOUR OF THERMOPLASTIC-BASED COMPOSITE MATERIALS

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1. Introduction

Nowadays, there is a growing interest in the use of thermoplastic-based composite materials in the aeronautical industry owing to their ability to be recycled and the reduction of manufacturing costs in contrast to thermosets-based composite materials. The use of this type of materials in aeronautical complex structures requires foundational airworthiness certification. This implies extensive experimental test campaigns to understand their mechanical response.

To reduce the size of the test campaigns, efficient and reliable numerical tools are required. The aim of this thesis is to develop and validate a robust constitutive model to predict the inelastic deformation and fracture of thermoplastic-based composite material at the meso-scale. The thesis is part of the private project VITAL co-financed by AIRBUS and Clean Sky 2 Joint Undertaking under the European Union's Horizon 2020 research and innovation program under Grant Agreement Number 864723. In addition, this work has received funding from the Catalan Government, through Grant 2019FI_B_01117.

2. Methodology

The thesis is divided in four main tasks:

(1) An extensive state-of-the-art literature review of the current constitutive models to reproduce the mechanical behaviour of thermoplastic-based composite material and their experimental evidences.
(2) Development of the constitutive model.
(3) An experimental test campaign to characterise the material and to validate the developed constitutive model.
(4) Modification of the constitutive model based on the experimental evidences found in the previous task and its validation.

3. Results and discussion

Currently, the constitutive model has been developed and implemented in a user Fortran subroutine to be used in a Finite Element (FE) commercial software. In addition, the specimens of the experimental test campaign have started being manufactured. Therefore, the model will be validated with the experimental data in the next few months.

The next step will deal with different level testing of the thermoplastic-based composite material. After that, the constitutive model will be calibrated, and it could be modified depending on the conclusions from the experimental data. Finally, the constitutive model will be validated by comparing the experimental data with those obtained by performing the same virtual tests.

The numerical results presented in this section have been compared with the experimental data obtained by (Koerber *et al.*, 2018), see Fig. 1. The authors carried out quasi-static compressive off-axis tests on a thermoset-based composite material. Good predictions were obtained with the constitutive model developed in the non-linear region, therefore, it can be concluded that the model can capture the plastic behaviour for different orientation angles and loading states.

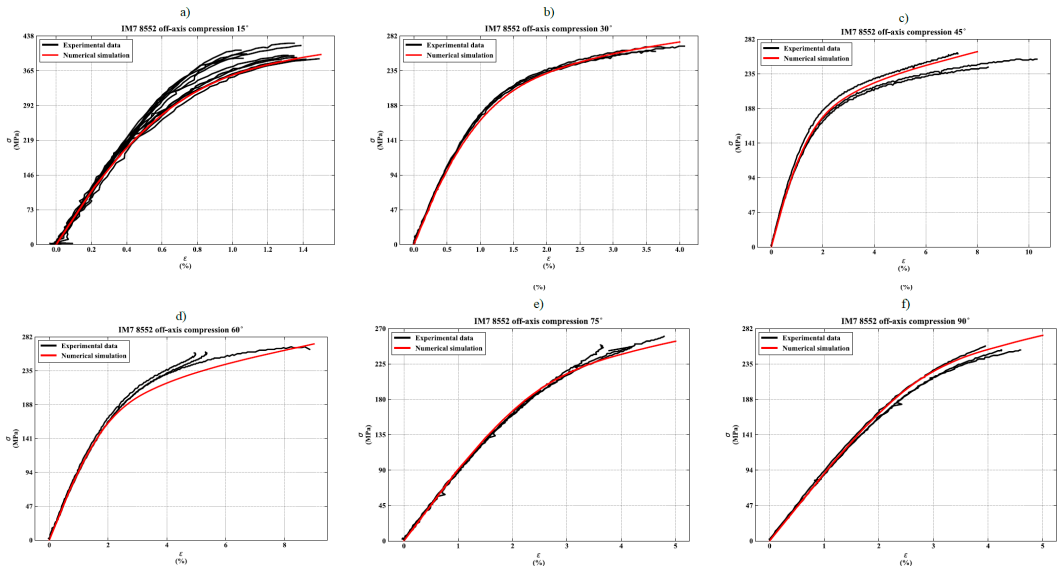

Figure 1. Stress vs. strain curves obtained from the off-axis compression tests and the FE model with an orientation of: a) 15◦, b) 30◦, c) 45◦, d) 60◦, e) 75◦ and f) 90◦.

4. Conclusions

A constitutive model to predict the inelastic deformation and the fracture of a transversely isotropic material has been developed. The model can be calibrated using standard laboratory tests. The material model combines elastic, plastic and damage behaviour for any direction governed by the matrix, and elastic and damage behaviour in the fibre direction. The model is implemented in a user material subroutine to be used with FE commercial software. Experimental data from compressive off-axis tests were compared with those obtained from the FE model with good predictions.

Keywords: *constitutive model, thermoplastic-based composite materials, damage, plasticity*

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NUMERICAL MODELLING AND EXPERIMENTAL BEHAVIOUR OF DELAMINATION AND ADHESIVE JOINTS UNDER DYNAMIC LOADING

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1. Introduction

Aerospace structures are subjected to a variety of dynamic loading cases. Impact is one of the most concerning cases due to its possible disastrous consequences. Therefore, it is crucial to understand how the composite materials employed in the aerospace sector behave under dynamic loadings. However, the methods to characterize and model the dynamic behaviour of composites are still under development and often limited to academic research levels, without any type of standardization. The aim of this investigation is to address a methodology (including innovative tests, measurements, and analysis methods) to properly characterize the dynamic interlaminar behaviour of composite structures subjected to dynamic loadings. The principal task will be to update and modify the current interlaminar constitutive models for modelling interface failure for any propagation mode under dynamic loading. Accordingly, the investigation will also deal with the design of dynamic experimental test setups, including associated data reduction methods. This investigation is in the framework of the European BEDYN project (reference number 886519) of the Clean Sky programme.

2. Methodology

The quasi-static models previously developed in AMADE will be taken as the base line and they will be adapted to include dynamic effects. After that, the developed models will be implemented and calibrated by means of Abaqus/Explicit subroutines. Both alternatives of interface modelling will be analysed: cohesive elements and cohesive interactions. The material model will be based on an experimental test campaign. The suitable test setup, and data reduction methods for each mode of propagation will be defined. Then, the test clamping systems will be manufactured according to the proposed design. Finally, the models will be validated. The validation must be done by using conventional shell finite elements since this modelling strategy offers an equilibrium between precision and computational time, which is of significant interest for industrial applications. The first level of validation will be to simulate the crack propagation characterization tests. Then, more complex demonstrators such as three-point bending tests or filled holed tension tests will be simulated and compared to the experimental data.

3. Results

We expect to achieve enough data to correctly design the test set up and specimens to dynamically characterize the composite material and then validate this model by means of more complex demonstrators.

3. Results

We expect to achieve enough data to correctly design the test set up and specimens to dynamically characterize the composite material and then validate this model by means of more complex demonstrators.

4. Conclusions

A new methodology will be developed to correctly characterize composite materials under dynamic loadings. These tools will improve the design of aeronautic components, making more efficient structures and reducing CO_2 emissions; responding to an industrial and social necessity.

Keywords: *composite material, dynamic load, interlaminar behavior, cohesive element, crack propagation*

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HIGH CONCENTRATED SILK BASED BIOINK FOR 3D PRINTING – DESIGN PARAMETERS

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1. Introduction

Silk fibroin has been successfully used in biomedical applications such as wound healing, cell culture and tissue engineering (Vepari & Kaplan, 2007). Sponges, gels, fibres, tubes, microspheres or films based on silk fibroin have been fabricated (Rockwood *et al.*, 2011). These applications undergo complex fabrication processes to construct specific devices. However, alternative methods can be used to manufacture silk fibroin-based applications, such as 3D printing (Rodriguez *et al.*, 2018). Nevertheless, although some researchers have conducted the freeform printing of concentrated silk fibroin, this method has not yet been fully explored. In this abstract, an innovative method based on thermal crosslinking is proposed. The morphology, molecular structure and mechanical properties of the 3D printed silk fibroin, and thus the potential behaviour of medical devices printed with this technology have been described. Furthermore, four different post-treatment techniques were evaluated on these features.

2. Methodology

Silk fibroin was prepared at 5-7 wt % and concentrated to 35 -40 wt % as described in the Rockwood *et al.* protocol (Rockwood *et al.*, 2011). A homemade bioink printer was used to fabricate test-pieces for mechanical trial. The ultimate tensile strength (UTS), the elastic modulus (E) and the strain at failure ($\varepsilon_{failure}$) were calculated from stress-strain data for the four post-treatment techniques. The effect of the printing parameters, such as the printing speed, the nozzle temperature, the needle gauge and the ink flow were assessed with a DOE model. Fourier transform infrared (FTIR) spectra was obtained using a spectrometer in the spectral region of 4000–350 cm-1, to determine the molecular structure of the printed material. The morphological structure was visualized with the stereoscopic microscope. The morphologic characteristics were quantified with image processing tools.

3. Results and discussion

The mathematical model from the DOE data provides predictions of the UTS, E and $\varepsilon_{failure}$ for the different independent variables. It shows that finer lines were achieved with the interaction of high velocities and low flows, which reported higher UTS, E and Young modulus, $\varepsilon_{failure}$ and strain at break. Moreover, the post-treatment that showed the highest mechanical properties was the methanol treatment, although the material became very brittle. The water-annealed treated materials reported the most ductile results and showed the best compromise between flexibility and mechanical properties, in the tested post-treatments.

4. Conclusions

This work provides design parameters to develop silk-based applications via free forming that require specific mechanical properties, morphology or molecular structure.

Keywords: *silk, freeform, medical device*

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IMPROVEMENT OF TRANSLAMINAR FRACTURE TOUGHNESS OF COMPOSITE MATERIALS THROUGH PSEUDO-DUCTILITY

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1. Introduction

Composite materials are notable for their high strength-to-weight ratio, but the inherent quasi-brittle nature of its constituents prevents the material's optimal use. Translaminar fracture of composite materials is defined as the crack breaking all the plies in a laminate, and toughness is the inherent material resistance against the fracture. Fracture toughness in an elastic-plastic material is dominated by the crack tip plasticity leading to steady-state (state variable is nearly constant) toughness that increases several times the initiation toughness. However, the plasticity is practically absent in composite materials, so the toughness contribution is mainly from the resistance to separation (matrix cracking, fibre bridging and pull-out). Therefore, several research groups try to confer "ductile" behaviour to laminated composites to achieve increased notched strengths and more damage-tolerant designs. Several approaches have been demonstrated to achieve pseudo-ductility (Czél & Wisnom, 2013). Most of them are based on combining low-strain materials (e.g. carbon fibre) with high-strain materials (e.g. glass fibre) either at a ply level or laminate level (Wu, Fuller, Longana, & Wisnom, 2018).

2. Methodology

The objective of the current study is to numerically determine the influence of the parameters associated with describing pseudo-ductility on the translaminar toughness and notched strengths. Developed Finite Element (FE) models use continuum mechanics based on homogenised linear elastic-plastic material behaviour, while the separation behaviour beyond the damage initiation is modelled by the cohesive law. Systematic investigation of non-dimensional material parameters and their influence was studied with Compact Tension (CT) specimens, followed by the notched strengths with Open-Hole (OH) and Centre-Crack (CC) specimens.

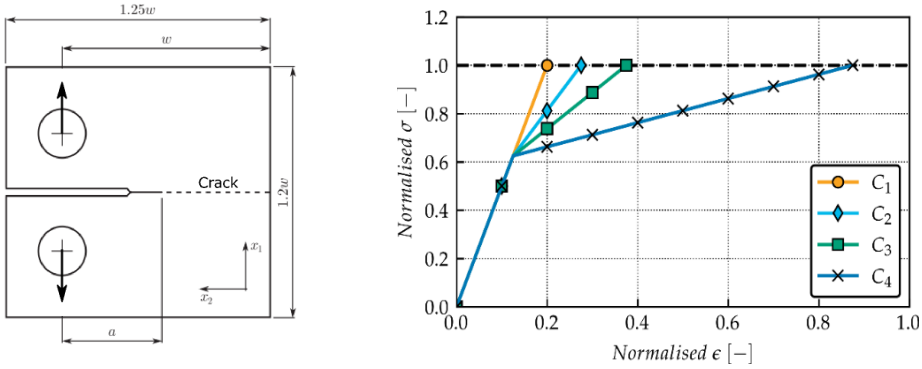

Figure 1. (a) CT specimen geometry. (b) Different forms of pseudo-ductile material behaviour considered

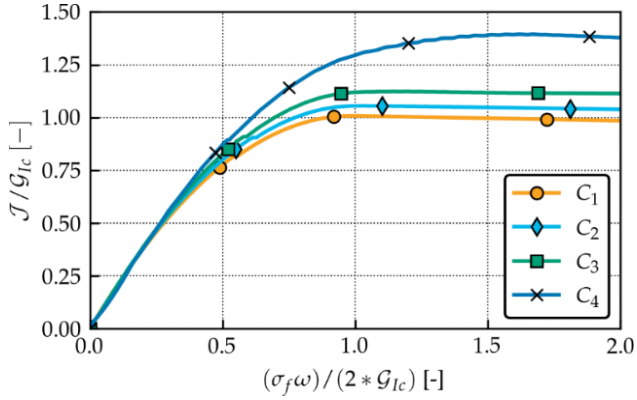

Figure 2. Observed normalized fracture toughness

3. Results and discussion

Results obtained illustrate,

(1) The improvement of pseudo-ductility on fracture toughness of CT specimens is illustrated in Figure 2, where the effect of pseudo-ductility (a) in the fracture toughness (b) is presented.

(2) The reduction of notch sensitivity factor on the nominal strength of OH and CC specimens (Maimí, González, Gascons, & Ripoll, 2013).

4. Conclusions

From the comprehensive numerical analysis carried out, we can highlight with certainty that incorporating pseudo-ductile behaviour will offer improvements in initiation toughness. Moreover, we can also recover more of the lost strengths due to the holes and cracks in open-hole and centre-cracked specimens.

Keywords: *composites, translaminar toughness, pseudo-ductility, numerical analysis*

5. Bibliography

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SESSION VIII. BIOMEDICINE AND HEALTH

FABRICATION OF ELECTROSPUN THREE-DIMENSIONAL SCAFFOLDS FOR TRIPLE-NEGATIVE BREAST CANCER STEM CELLS EXPANSION AND CHARACTERIZATION

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1. Introduction

Breast cancer stem cells (BCSCs) represent a small tumor subpopulation which displays tumorigenesis and resistance to chemotherapy, anchorage-independent growth capacity forming spheres, and an enlarged activity of the aldehyde dehydrogenase (ALDH) enzyme (Matsui *et al.*, 2008). BCSC niche is, therefore, related to tumor initiation and relapse. This fact gains importance in some specific cancer types with a high recurrence rate, such as the triple-negative breast cancer (TNBC) (Dent *et al.*, 2007). Additionally, TNBC is characterized by the absence of any known breast cancer molecular biomarkers amplification. The elevated relapse rate and the lack of a targeted therapy highlight the need to find new therapeutic options for TNBC.

2. Hypothesis

Targeting BCSCs may represent a novel approach for TNBC, but their study is hindered by the fact that standard two-dimensional (2D) culture induces their differentiation, converting them to non-stem cancer cells (Vergani, Grattarola, & Nicolini, 2004). Nanofibrous scaffolds have emerged as an alternative option for three-dimensional (3D) culture mimicking the extracellular matrix. Scaffolds are composed of a network of polymeric filaments where cells adopt an elongated morphology. Previous studies demonstrated that 3D culture expanded BCSCs population compared with monolayer culture. Therefore, scaffold fabrication and 3D culture of TNBC cells are proposed to study BCSC subset.

3. Methodology

Polycaprolactone (PCL) scaffolds were fabricated with an electrospinning apparatus and characterized through scanning electron microscopy (SEM) and a dynamic mechanical analysis (DMA). Two TNBC cell models (MDA-MB-231 and MDA-MB-468) were cultured on PCL scaffolds and monolayer. Cell morphology and proliferation were analyzed by fluorescence microscopy and MTT assay, respectively. A possible enrichment in stem features was verified through chemoresistance and mammosphere-forming assays, ALDH activity quantification, and stemness-related markers expression analysis. Finally, fatty acid synthase (FASN) activity was determined, and the impact of its pharmacological inhibition was studied.

4. Results and discussion

PCL scaffolds have been proven to provide a softer 3D network compared with standard 2D supports. When cultured in scaffolds, TNBC cells displayed an extended cytoplasm in contrast with the round and flat size on 2D culture. Scaffold culture led to a BCSC subpopulation enrichment in TNBC cells, resulting in higher mammosphere-forming capacity, ALDH activity, stemness-related genes expression, and chemoresistance. To the best of our knowledge, we are the first to define a FASN hyperactivation in stemness-enriched TNBC cells cultured on 3D structures. Interestingly, FASN inhibition overcame BCSC enrichment achieved in 3D culture in terms of mammosphere-forming capacity, suggesting the possibility to inhibit FASN to treat the cancer stem-like cells.

5. Conclusions

Collectively, PCL scaffolds represent a potent tool to expand the BCSC niche in TNBC by providing resemblance to a physiological structure. Nanofiber meshes may facilitate research in the cancer stem-like cells field, since novel biomarkers and treatments need to be developed. FASN deserves further investigation to elucidate its potential as a novel biomarker for BCSCs-enriched TNBC samples, specially within 3D surroundings.

Keywords: *triple negative breast cancer, breast cancer stem cells, electrospinning, three-dimensional cell culture, fatty acid synthase*

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ENRICHMENT OF CANCER STEM CELL POPULATION USING POLYCAPROLACTONE ELECTROSPUN SCAFFOLDS IN LUNG ADENOCARCINOMA

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1. Introduction

Lung cancer is the leading cause of cancer-related death worldwide. About 40% of patients are diagnosed as lung adenocarcinoma. The discovery of activating mutations in the epidermal growth factor receptor (EGFRm) allowed the development of targeted therapies, for instance gefitinib or osimertinib (Forsythe *et al.*, 2020). Nevertheless, a better understanding of this disease is needed due to the acquisition of resistance of most patients to the treatment.

Cancer stem cells (CSCs) are a tumor-initiating subpopulation that shows self-renewal and pluripotency capacities. CSC niche represents a small proportion within tumor and it is responsible for drug resistance, tumor recurrence and metastasis (Nassar & Blanpain, 2016). However, traditional two-dimensional (2D) cell culture causes their differentiation, barring their study in vitro.

Different three-dimensional (3D) models have been reported (e.g., spheroids or hydrogels) to mimic the tumor microenvironment (Tapias *et al.*, 2015). Nanofibers manufactured through electrospinning technique are similar to the extracellular matrix structure. Polycaprolactone (PCL) is a synthetic polymer suitable for biomedical purposes due to its low melting temperature, biocompatibility, and malleability (Cipitria, Skelton, Dargaville, Dalton, & Hutmacher, 2011). Previously, we demonstrated that electrospun (ES)-PCL scaffolds were useful for 3D culturing lung adenocarcinoma cell models. Therefore, the main aim of this study is the evaluation of ES-PCL scaffolds' suitability for culturing lung CSCs (LCSCs).

2. Methodology

PCL was dissolved (10 and 15% w/v) in acetone and scaffolds were fabricated using an electrospinning apparatus using a stainless steel 18G needle emitter at fixed voltage 9 and 7 kV, for 10% and 15% respectively, and a flow rate of 6 ml/h. Sensitive (PC9) and gefitinib- and osimertinib-resistant (PC9-GR3) cell models were seeded into scaffolds for 3 and 6 days.

Resistance to osimertinib was tested through MTT assay and different genes and proteins related to LCSCs were evaluated by quantitative reverse transcription polymerase chain reaction (RT-qPCR) and Western blot.

3. Results

EGFRm lung adenocarcinoma cultured on both 10% and 15% ES-PCL scaffolds exhibited more drug resistance compared to 2D. Additionally, different genes and proteins related to LCSCs, such as Vimentin and Sox2, were upregulated on 3D culture compared to monolayer confirming the enrichment of this malignant population in PC9 and PC9-GR3.

4. Conclusions

ES-PCL scaffolds create a suitable microenvironment for culturing LCSCs in sensitive and gefitinib- and osimertinib-resistant EGFRm lung adenocarcinoma. Consequently, cells seeded on these 3D meshes will enable the study of LCSC niche to develop new targeted therapies and identify new biomarkers.

Keywords: *electrospinning, EGFRm, lung adenocarcinoma, 3D cell culture, polycaprolactone, cancer stem cells*

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POLYPHENOLIC-RELATED COMPOUNDS TARGETING TRIPLE-NEGATIVE BREAST CANCER CELLS

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1. Introduction

Breast cancer (BC) represents the highest incident carcinoma in women. Triple-Negative Breast Cancer (TNBC) represents approximately 20% of all BCs and is characterized by the lack of any known pharmacological target such as expression of estrogen and progesterone receptors or HER2 oncogene expression/amplification. Therefore, available targeted therapies to treat other BC subtypes are useless in TNBC, leaving cytotoxic chemotherapy as the sole treatment option. Additionally, TNBC presents a high recurrence after chemotherapy, which is associated with poor survival. One of the main causes of therapy failure is the presence within tumors of a small population of cells with stem cell properties (Cancer Stem Cells or CSCs) that have metastatic and evasion capacities and resistance to current therapies. For this reason, there is an unmet need to develop new agents targeting this cell population (Giró-Perafita *et al.*, 2019).

Natural polyphenolic compounds have emerged as potential anticancer candidates for their safety and multitarget intrinsic features. Some of them have been shown to directly or indirectly act on self-renewal and survival pathways of CSCs. Among them, epigallocatechin-3-gallate (EGCG), the most abundant catechin in green tea and curcumin (extracted from the plant *Curcuma longa*), have proven efficacy in targeting breast CSCs (Kakarala *et al.*, 2010; Kim *et al.*, 2006; Zhou *et al.*, 2015). However, the therapeutic use of natural compounds as antitumor agents is limited due to their low efficacy and relative instability under physiological conditions (Turrado *et al.*, 2012).

Therefore, the main aim of this work has been the synthesis of polyphenols derived from EGCG and curcumin and the evaluation of their cytotoxic activity in TNBC cells.

2. Methodology

Different polyphenolic compounds have been synthetized using conventional organic synthetic techniques. They have been purified by column chromatography and have been characterized by nuclear magnetic resonance (NMR) and mass spectrometry. On the other hand, their cytotoxic activity has been evaluated by determining the half minimal concentration (IC_{50}) using the MTT colorimetric proliferation assay.

3. Results

The synthesis and purification of the polyphenolic compounds have been successfully achieved with a high percentage of purity. The new synthetized compounds showed better cytotoxicity against MDA-MB-231 TNBC cells in comparison to their parental dietary compounds.

4. Conclusions

The improvement of the properties such as efficacy of natural compounds through the design of synthetic derivatives is a promising strategy for the development of targeted therapies against TNBC.

Keywords: *triple negative breast cancer, cancer stem cells, EGCG, curcumin, organic synthesis*

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TRANSFERRIN RECEPTOR LEVELS IN RESPONSE TO IRON OVERLOAD IN THE STRIATUM AND DESCRIPTION OF AN IRON TOXICITY MODEL

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1. Introduction

Huntington's disease (HD) is a neurodegenerative disorder caused by a mutation in the gene that codes for the huntingtin protein (HTT). Said mutation results in a faulty protein that hinders normal cellular function and leads to neurodegeneration and, ultimately, cell death in striatum, cerebral cortex and hippocampus (Labbadia & Morimoto, 2013). As in other neurodegenerative disorders, iron metabolism is dysregulated in HD (Muller & Leavitt, 2014) and an iron accumulation in the basal ganglia has been described (Bartzokis, Cummings, Perlman, Hance, & Mintz, 1999). However, its role in the HD physiopathology is poorly investigated. Our aim in this work is to characterize the expression of the main proteins involved in iron metabolism in HD and to develop an *in vitro* iron toxicity model that mimics the striatum iron overload reported in HD.

2. Methodology

Transferrin receptor (TfR) levels in mouse model R6/1 striatum were assessed by Western Blot at different ages representing different HD phases. To develop the *in vitro* iron toxicity model, striatal derived cell line expressing full-length mutated HTT, STHdh$^{Q111/Q111}$, and it's wild-type counterpart, STHdh$^{Q7/Q7}$, were incubated with different concentrations of Ferric Ammonium Citrate (FAC). Cell viability was assessed via MTT assay after 24 hours.

3. Results

TfR expression was found to be decreased in the striatum in all tested ages: 8, 12, 16, 20 and 30 weeks. FAC was able to induce cell death at different rates and different concentrations starting at 0.5 mM. STHdh$^{Q111/Q111}$ cells were found to be more sensitive to iron overload in comparison to STHdh$^{Q7/Q7}$.

4. Conclusions

TfR is decreased in R6/1 mice striatum tissue. The decrease is not as severe in the disease's early stage. Striatal cells expressing mutant HTT are more sensitive to FAC-mediated cell death than striatal cells expressing wild-type HTT. Differences in protein expression in FAC iron toxicity model need to be characterized.

Keywords: *Huntington's disease, Iron metabolism, Iron regulatory proteins, Transferrin receptor, Striatum iron accumulation.*

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SPECIFIC AND COMMON MOLECULAR ALTERATIONS IN KNOCK OUTS OF 3 DESMOSOMAL GENES IN HL1 CELL MODEL OF ARRHYTHMOGENIC CARDIOMYOPHATHY

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1. Introduction

Arrhythmogenic Cardiomyophathy (ACM) is a rare inherited disease characterized by the progressive replacement of the myocardium by fibrofatty tissue. Worldwide prevalence of ACM is ranging from 1:1000 to 1:5000 (Corrado, Basso, & Judge Daniel, 2017), and it is responsible for around 20% of all cases of sudden cardiac death (SCD) among people under 35 years of age (Ye, Delmar, Lundby, & Olesen, 2019). The main genetic causes of ACM are mutations in desmosomal genes, especially in PKP2 (Basso, Pilichou, Bauce, Corrado, & Thiene, 2018). It is known that mutations in those genes could alter important molecular functions such as calcium homeostasis (Cerrone *et al.*, 2017), and they also could cause important structural and electrical alterations such as fibrosis, adipogenesis, inflammation and arrhythmogenesis (Austin *et al.*, 2019). We lack better understanding of those pathophysiological mechanisms and their relationship with the causal gene.

2. Hypothesis

ACM pathomechanism is a combination of gene-specific expression and disease molecular hallmarks. This study aims to elucidate molecular pathways triggered by genetic defects in three of the main genes in ACM and determine common and gene-specific molecular features.

3. Methodology

Cardiac HL-1 cell line was edited by CRISPR/Cas9 to generate Knock Outs (KO) of three of the most frequent causal genes in ACM: PKP2, DSG2 and DSC2. Expression levels of ACM-related genes were tested by RT-PCR: desmosome, calcium handling and connexome related genes. Changes in the total amount of protein were checked by western blot using total protein lysate. Moreover, calcium transients were performed on *PKP2* clones.

4. Results

HL1 KO-PKP2 showed downregulation of *SCN5A, CX43, RyR2, Atp2a2, Slc8a1, Casq2, ANK2, DSC2 DSG2* and *DSP*. Functionally, calcium transients showed significant differences in Half Width and Rise and Decay Time of the 10mM peak of caffeine. HL1 KO-DSG2 showed a downregulation of *ANK2*, *DSC2, CX43* and *PG*. HL1 KO-DSC2 clones presented a downregulation of *CASQ2* and *ANK2*.

5. Conclusions

Results suggest that pathophysiological mechanisms of ACM are partially depending on the causal gene. Loss of function of PKP2 and DSC2 may be related to a dysregulation of calcium homeostasis and loss of function of DSG2 may cause alterations in connexome genes expression related to electrical dysfunction. Moreover, the absence of ANK2 expression in all HL1 cell lines has been revealed as a common molecular hallmark of ACM.

Keywords: *arrhythmogenic cardiomyophathy (ACM), desmosomal genes, HL1 cell line, CRISPR/Cas9, Knock Out (KO)*

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THE ROLE OF LIPID LEVELS IN THE INCIDENCE OF CORONARY AND CEREBROVASCULAR DISEASES IN A LOW CORONARY RISK POPULATION

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1. Introduction

Abnormal lipid levels, including high levels of low-density lipoprotein cholesterol (LDL-c) and triglycerides (TG), and low levels of high-density lipoprotein cholesterol (HDL-c), are modifiable risk factors for coronary heart disease (CHD) and ischemic stroke (IS) (Ference *et al.*, 2017; Piepoli *et al.*, 2016). However, it is not well understood how these associations differ between sex and age groups. We aimed to analyse the association between LDL-c, TG and HDL-c and CHD and IS events in a low coronary risk population.

2. Methodology

We performed a retrospective cohort study with information from the System for Research in Primary Care (SIDIAP), a database that contains pseudo-anonymised records of 5.7 million people registered in primary care centres throughout Catalonia. We calculated the incidences and hazard ratios (HR) for CHD and IS associated with a 1 mmol/L increase in lipid levels. We stratified all the analyses by age groups: 35-44; 45-54; 55-64; 65-74; 75-84; ≥85 and sex.

3. Results

The cohort included 364,308 participants (mean age 67 years; 60.3% women; median follow-up 6.8 years). There were 10,273 CHD events (5,296 in men and 4,977 in women) and 13,103 IS events (5,640 in men and 7,463 in women). Each mmol/L increase in LDL-c, TG and HDL-c was associated with an increase of 21% (HR 1.21, 95% CI 1.18-1.24), an increase of 12% (HR 1.12, 95% CI 1.08-1.16), and a decrease of 40% (HR 0.60, 95% CI 0.56-0.64) in the CHD risk, respectively. The associations between lipid levels and the hazard of CHD diminished progressively with age; thus, young people showed a higher hazard than the elderly. Only LDL-c levels presented differences by sex: men were at higher CHD risk than women across all age groups.

Each mmol/L increase in TG and HDL-c was associated with an increase of 8% (HR 1.08, 95% CI 1.05-1.12) and a decrease of 9% (HR 0.91, 95% CI 0.87-0.96) in the IS risk, respectively. The association between TG and HDL-c and IS risk was stronger in the young than in the elderly; HDL-c levels showed such association only in women.

4. Conclusions

CHD risk increased in young participants (35-45 years) with high LDL-c and TG levels and decreased with high HDL-c levels. For IS risk, high TG and HDL-c levels might increase and decrease risk, respectively. However, most of these associations lost significance at 75-84 and >85 years. We suggest efforts to reduce lipid levels in young and middle-aged people to prevent cardiovascular diseases.

Keywords: *cholesterol HDL, cholesterol LDL, triglycerides, coronary heart disease, ischemic stroke*

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A SYNTHETIC ANALOGUE OF PITUITARY ADENYLATE CYCLASE-ACTIVATING POLYPEPTIDE (PACAP) IMPROVES MOTOR DEFICITS IN R6/1 MOUSE MODEL OF HUNTINGTON'S DISEASE: ROLE OF PAC1 RECEPTOR

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1. Introduction

Huntington's disease (HD) is a neurodegenerative disorder caused by the expression of the mutant huntingtin (mHtt). Motor dysfunction is the most characteristic symptom of HD and it is associated to the progressive degeneration of striatum (Vonsattel & Difiglia, 1998). It has been proposed that an increase in CREB-binding protein (CBP) and brain-derived neurotrophic factor (BDNF) expression could prevent motor discoordination, as the reduction of both proteins are involved in the HD striatal loss. 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 intranasal administration of PACAP improves motor symptoms in HD mice by a recovery of PAC1R (Solés-Tarrés, Cabezas-Llobet, J., Vaudry, & Xifró, 2021). Unfortunately, therapeutic use of PACAP is hindered because of its poor metabolic stability and because the activation of VPAC2R is associated with peripheral side effects (Warren *et al.*, 1992). Therefore, the use of PACAP analogues showing more selectivity for PAC1R and VPAC1R and better biostability has been proposed.

2. Problem

It is required to determine through which receptor PACAP exerts beneficial effects in HD and investigate PACAP analogues in HD models.

3. Methodology

To uncover the contribution of PACAP receptors we used the full-length mHtt striatal STHdhQ111/Q111 cellular model. We compare the neuroprotective effect of PACAP to Vasoactive Intestinal Peptide (VIP), which interacts with VPAC1R and VPAC2R, but not with

PAC1R. To study PACAP analogues effects in HD we used transgenic R6/1 mice. We administrated intranasally for 12 days the Ac-[Phe(pI)6, Nle17]PACAP(1-27), a synthetic PACAP analogue displaying lower affinity for VPAC receptors and showing greater biostability (Lamine *et al.*, 2016). Then, we evaluated motor function using Rotarod and Balance Beam tests and we studied some proteins expression by Western Blot.

4. Results and discussion

In STHdhQ111/Q111 cells, we found VIP treatment inhibits apoptosis preventing caspase-3 activation, but it cannot enhance the expression of the pro-survival and neurotrophic genes c-fos, egr1 and BDNF, as PACAP treatment does. These results show VPAC receptors can protect from mHtt toxicity, but only PAC1R allows a potent activation of pro-survival and neurotrophic signaling. In R6/1 mice, we observed that PACAP-analogue improves motor function without promoting PAC1R expression but raising CBP and BDNF protein levels in the striatum. These results suggest PACAP-analogue improves motor deficits by promoting a local neurotrophic activity in HD striatum.

5. Conclusions

PAC1R-related signaling activation offers neuroprotection against mHtt neurotoxicity and stimulates a neurotrophic effect. Moreover, the synthetic analogue Ac- [Phe(pI)6, Nle17]PACAP(1-27) reduces motor deficits in R6/1 HD mice.

Keywords: *Huntington's disease (HD), striatum, Pituitary Adenylate Cyclase-Activating Polypeptide (PACAP), PAC1 receptor (PAC1R), Brain Derived Neurotrophic Factor (BDNF)*

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SESSION IX. EDUCATION AND LEARNING

MATHEMATICAL TASKS PROPOSED IN TEXTBOOKS TO PROMOTE THE TEACHING OF EARLY ALGEBRA IN PRIMARY EDUCATION

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1. Introduction

The incorporation of algebraic knowledge from primary school levels has been established as an alternative curricular change under the guidelines of the early algebra approach, whose purpose is to promote the development of algebraic thinking from the first levels of schooling and to facilitate a better understanding of mathematics (Cai & Knuth, 2011). Primary Education mathematics curricula in countries such as the United States, Australia, Singapore and Chile, among others, have integrated this knowledge as an additional content standard (Pincheira & Alsina, 2021).

2. Problem

The introduction of early algebra in Primary Education curricula directly challenges teachers to develop teaching practices that consider the relevant selection of mathematical tasks that systematically promote the teaching of this content block.

In this context, it is necessary to pay attention to the tasks proposed in textbooks, since teachers support and guide their teaching practice by relying mostly on this resource (Shield & Dole, 2013).

Based on this, in this study we ask ourselves: What mathematical tasks do Chilean textbooks of Primary Education promote to teach early algebra?

To answer this question, we will use the perspective of Demosthenous and Stylianides (2014) who propose an analytical framework to determine the mathematical tasks related to early algebra, considering three categories of tasks: situated arithmetic relations, rule-based relations and known-unknown relations.

3. Methodology

The study presents a qualitative methodology of a descriptive nature (Hernández, Fernández, & Baptista, 2014). A sample of eight Chilean textbooks of Primary Education (1st to 6th grade) was selected and examined under the technique of content analysis through the classification of mathematical tasks on early algebra, according to the categories proposed by Demosthenous & Stylianides (2014).

4. Results

The results show a higher concentration of rule-based relationship tasks, with 44.7%. This was followed by known-unknown relations tasks, with 34.1%. Finally, a lower presence of situated arithmetic relations tasks is observed, with 21.2%.

5. Conclusions

The study highlights the need to enrich the type of mathematical tasks for teaching early algebra. To this end, it is recommended that teachers should favour the progressive incorporation of early algebraic tasks as school levels advance in Primary Education.

Keywords: *early algebra, mathematical tasks, textbooks, Primary Education*

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RELATIONSHIP BETWEEN EMOTIONAL INTELLIGENCE, EXECUTIVE FUNCTIONS AND ACADEMIC ACHIEVEMENT

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1. Introduction

Educational researchers are continually in search of predictors to academic success. In the last years, Emotional Intelligence (EI) and Executive Functions (EF) have arisen as two of the components that play a significant role in learning and academic achievement. EI is defined as a set of socio-emotional competencies that allow us to recognize and express our own feelings and those of others, regulate our emotions and cope with the daily demands of our environment (Bar-On & Parker, 2000). People with a higher EI are able to generate a mood that allows them to do better in challenging cognitive tasks, resulting, in turn, in better academic performance (Schutte *et al.*, 2001). On the other hand, the main EF (working memory, cognitive flexibility and inhibition) also demonstrated to have a close association with school grades (Blair & Razza, 2007). However, only limited research has explored these relationships in depth and has looked for the specific subcomponents that are more correlated with achievement. Similarly, much less is known about whether there are differential associations with achievement in language or mathematics.

2. Hypotheses

The present study aims to take a close look at the relationships between Emotional Intelligence and Executive Functions with children's academic achievement in school. Its main objective is to go deeper into these relationships by identifying the specific components of EI and EF that are more related to school competencies. Additionally we also want to discover whether there are differences in these associations depending on the subject.

3. Methodology

One hundred and eighty students from 8 to 11 years old from two primary schools in the province of Girona (Spain) participated in this study (M = 9.67 years, SD = 1.03): 95 boys (52.8%) and 85 girls (47.2%). From this sample, 88 were in 3rd grade (M = 8.68 years, SD = .28) and 92 in 5th grade (M = 10.65 years, SD = .31).

All children participated in three sessions. The first one included the assessment of EI with the Spanish version of BarOn inventory (Bar-On & Parker, 2000). The second session was devoted to evaluating linguistic and mathematic competencies with a set of school tests; and the last session covered the evaluation of EF. For this last one, we used the Inhibition subtest of NEPSY-II (Korkman, Kirk, & Kemps, 2014), the Digit Span task of WISC-V (Wechsler, Raiford, & Holdnack, 2015) and the Wisconsin Card Sorting Test (Heaton, Chelune, Talley, Kay, & Curtiss, 2001).

4. Results

The analyses show statistically significant correlations between some components of EI and EF and school grades. Focusing on EI, Adaptability emerged as the most important predictor for both of the competencies analyzed, together with the Interpersonal component of EI for maths. Students with high adaptability scores are good at finding solutions for the problems they face, the difficulties they experience and the things they do not understand in the classroom, and this is what could help them to perform better in the academic setting. Regarding EF, all of the scores were positively correlated with the performance on both subjects, with the magnitude of the association being higher in maths than in language. Focusing on the EF subcomponents, Inhibition stood out as the most important predictor for both competencies, followed by cognitive flexibility. Inhibition could be important to focus on the task inhibiting off-goal information. In general, EF have demonstrated to have a stronger impact when predicting school achievement than EI.

5. Conclusions

Our findings provide substantial support for a positive link between academic competencies on the one side, and emotional intelligence and executive functions on the other side. In practical terms, the data suggest the need to consider emotional competencies and executive functions when trying to foster the academic success of the students. By making teachers increasingly aware of the role that EI and EF play in academic development, as well as within specific academic domains and subjects, they would be able to implement more meaningful educational experiences for children.

Keywords: *emotional intelligence, executive functions, academic achievement, school competencies, children*

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THE DIDACTIC AND MATHEMATICIAL KNOWLEDGE OF NURSERY SCHOOL PROFESSIONALS: (RE)THINKING THE SPACES AND MATERIALS OF THE SCHOOL TO BOOST THE DEVELOPMENT OF THE MATHEMATICAL THINKING IN THE EARLY AGES (0-3)

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1. Introduction

The three first years of life are of great importance for the development of infants and toddlers (0-3) because they are the bases for all learnings that are to come, being a big opportunity, unique and decisive, in their development (World Health Organization & UNICEF, 2018). From this point of view, the professionals of the Nursery School have a key role to facilitate the scaffolding and environments of rich, quality and stimulating learning.

2. Hypothesis

Numerous investigations exist that inquire and try to answer the aspects linked to the knowledge of Nursery School professionals. In this sense, there exists the need for trained professionals conscious of the importance of offering educational contexts of quality in mathematics from early ages (Alsina, 2015; Clements & Sarama, 2015; among others). Based on this need, this study analyzes the mathematical knowledge of Nursery School professionals (0-3 years) to facilitate the development of intuitive mathematics, through the design of the spaces and materials.

3. Methodology

By using a mixed method of investigation (Fàbregues, 2015), an almost-experimental study (Pre-Post) (Creswell, 2009) has been designed, in which, before and after of a training activity to improve the didactic and mathematical knowledge of the professionals, the didactic and mathematical knowledge of the 28 professionals of the Municipal Network of Nursery Schools of Vic-EBMV (Catalonia, Spain) has been analyzed beginning with groups of discussion, questionnaires and photography and video documentation.

4. Results and discussion

Synthetically, the main results show significant changes in mathematical knowledge before and after the training and, consequently, in the design of the spaces and materials with mathematical sense, as is collected in the following tables 1 and 2.

Table 1 shows us how, only a 17.9% of professionals knew the informal mathematics according to the 0-3 cycle before the training, whereas, after the training, they were known by 89.9%.

Table 1. Knowledge of the professionals in relation with the informal mathematics in the Childish School

			Post		Total
			Yes	No	
Pre	Yes	N % Vertical	5 17.9%	0 0%	5 17.9%
	No	N % Vertical	20 71.4%	3 10.7%	23 82.1%
Total		N % Vertical	25 89.3%	3 10.7%	28 100.0%

Table 2 shows us, in global terms, how we can find significant differences in the statistic results between the first and the second questionnaire, the first having an average of 1.3 and the second one, 3.5.

Table 2. Number of contents designed around the learning of mathematics in the Nursery School

	N	Min.	Pct 25	Average	Median	Pct 75	Máx.	Standard Deviation
Pre	28	0	0	1.3	1	2	4	1.2
Post	28	1	2	3.5	3	5	8	1.8

p-value = 0,000 Calculated by means of T-Student for samples mated with a level of confidence of 95%

5. Conclusions

It is concluded that if the professionals are not aware of the importance of the mathematical knowledge and how they can facilitate it through the proposals of exploration, manipulation and gamification, hardly could they plan and manage activities that would facilitate the development of the mathematical thinking in children. In this sense, it is necessary and indispensable an initial and continuous training that guarantees that the professionals of the Nursery School have the necessary didactic and mathematical knowledge to design rich spaces of quality from a mathematical point of view.

Keywords: *teachers' mathematical knowledge, intuitive mathematics, mathematics teaching, spaces and materials, Early Childhood Education*

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ACADEMIC WRITING: THE ASSESSMENT PROCESS CARRIED OUT IN INITIAL ACADEMIC LITERACY SUBJECTS TAUGHT IN UNDERGRADUATE DEGREES IN THE AREA OF HEALTH AND SOCIAL SCIENCES BELONGING TO TRADITIONAL CHILEAN UNIVERSITIES THAT ARE PART OF THE COUNCIL OF RECTORS OF VALPARAÍSO (CRUV)

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1. Introduction

In higher education, Academic Literacy (AA) is recognized as one of the characteristics of the quality of teaching and learning process. Thus, it has become an objective "where writing becomes a learning tool" (Guzmán-Simón & García-Jiménez, 2015). In recent years, Chilean universities have integrated AA subjects in several, promoting the concepts of written production and particular textual genres of each discipline. Regarding writing, there are diverse studies on: the need and objective of establishing university programs; the identity that is assumed through written discourse; the importance of writing as a human activity that permeates all domains of knowledge; the types of academic texts that disclose a technical domain; the management of the linguistic and discursive characteristics of the texts that convey knowledge of the specialties. Carlino (2013) proposes that the vision of academic writing should underline the teaching processes that preserve the meaning of the practices involved. The assessment process is one of these practices, which arises as a regular and mandatory action. "Recently, assessment as an issue has reached an evident prominence until it has become one of the central aspects of pedagogical discussions, reflections and debates. The reason? ... few tasks provoke so many doubts and contradictions to teachers, such as those related to assessment and the actions or decisions associated to it" (González & Pérez, 2004). This instance "uses a great variety of instruments that act as mediators or external aids" (Camps & Ribas, 1998) that respond to teachers and particular circumstances.

2. Methodology

In the context of AA subjects taught in undergraduate degrees of Health and Social Science area in traditional Chilean universities that are part of the Council of Rectors of Valparaíso (CRUV), this research proposes the following objectives:

(1) Understand the formative and summative assessment practices on text production.

(2) Analyze similarities and differences of perception that academics and students have regarding the assessment process applied to written production.

(3) Associate formative and summative assessment practices on text production from the students' and teachers' perception.

The study will be carried out considering a mixed approach; quantitative and qualitative techniques, methods, concepts, or language are linked in a single investigation. The combination allows a greater understanding of the object of study and opportunities to analyze various problems, since "... they represent a set of systematic, empirical and critical research processes and involve the collection and analysis of quantitative and qualitative data" (Hernández, Fernández, & Baptista, 2014).

3. Results

As a result of the pandemic that has affected the world since 2019, this research's results have been delayed, even though and the research itself is still under development.

4. Conclusions

It is expected to corroborate hypotheses based on the results obtained:

(1) The descriptive ones refer to the diverse modalities and approaches of the formative and summative assessment practices stipulated in subject programs.

(2) The ones related to relationship between formative and summative assessment criteria reflected in the instruments used.

(3) And the quantitative ones that will allow identification of statistically significant differences between the perceptions of students and teachers about the assessment process.

Keywords: *academic literacy (AA), written production, evaluation*

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THE ACQUISITION OF SPANISH DP

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1. Introduction

The general aim of this dissertation is to examine the Spanish Determiner Phrase (DP) of adults who have Arabic as a mother tongue and English as a second language. According to the Typological Primacy Model (Rothman & Halloran, 2013), from the two languages that constitute the prior linguistic knowledge of the L3 learner, the one that has a similar structure is the one that will influence the acquisition process. The research focuses on: (1) gender agreement, (2) the use of the article or possessive in structures of inalienable possession, and (3) the presence or absence of the article in generic structures.

2. Hypothesis

In the acquisition of gender agreement, the ending of the transparent word will facilitate the acquisition of gender, masculine will be the default gender, L1 will have an active role in acquiring the values of DP in gender agreement, as we will find transfer of L1 or L2 in inalienable possession and in the generic constructions.

3. Methodology

We carry out three types of experimental tasks, acceptability judgments, filling in the blanks, and forced choice. We obtained perception and production data from a total of 80 participants: 60 L1 Arabic speakers with three varying levels of Spanish proficiency and 20 L1 Spanish speakers.

4. Results

The results of the experiments show, firstly, evidence in favour of partial transfer of the L1. Secondly, the statistical analysis shows that the L2 does not play a relevant role in the acquisition of the L3. Thirdly, masculine gender is not the default gender of the interlanguage. Fourthly, feminine transparent nouns are easier to learn, perhaps due to the morpho-phonetic similarities between Spanish and Arabic.

5. Conclusions

This study supported the view that L1 Arabic was the source of morphosyntactic (non)-facilitative transfer in the L3, not only at the initial stages but also at advanced stages. Thus, the L1 transfer scenario provided a more viable account of the L3 performance than the L2 Status Factor. Our L3 learners did not resort (unconsciously) to transfer from L2 English, despite the implication of three potential factors, i.e., language genetic proximity, structural similarity, and psychotypological relation between L2 English and L3 Spanish.

Keywords: *interlanguage, L3 acquisition, L1Transer, Typological Primacy Model*

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DIDACTIC SUPPORT MODEL FROM GENDER PEDAGOGY TO THE TEACHING-LEARNING PROCESS OF THE DEGREE WORK AND ORAL DEFENSE EXAMINATION IN THE ENGINEERING AREA

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1. Introduction

The Final Degree Project (TFG) and oral defence are two academic discursive genres that link university education and job performance. Both are considered key in the training trajectory, as they generate the professional and communication skills necessary for the insertion of the future professional in the corresponding practice community. They also constitute a challenge for the engineers' training process, so the teaching-learning process of the capstone project must consider a series of academic, professional, and motivational variables that will confirm the mastery of the complex skills that make the student a civil engineer.

2. Hypotheses

In this sense, firstly this research aims to learn about the teaching-learning process of the degree work and oral defence exam in one of the Civil Engineering majors programmes at two Chilean universities, and secondly, consolidate a didactic coaching model adapted to the training process' needs for both teachers and students (Flower & Hayes, 1981), disciplinary and academic writing (Bazerman, 2005; Navarro, 2014; Parodi, 2010) and gender-based pedagogy (Venegas, Núñez, Zamora, & Santana, 2015).

3. Methodology

The proposed methodology belongs to the paradigm of applied research and action research. The instruments used to meet the objectives are, mainly, semi-structured interviews, satisfaction questionnaires, analysis of drafts and calculation of writing quality indices. As a result, it is expected to characterize the writing process of the TFG and the oral defence exam of an engineering major. It will also establish a didactic proposal aimed at overcoming the difficulties and critical nodes identified, that is, a comprehensive methodology of collaborative work that contributes to the fulfillment of the graduate profile of each discipline.

The methodology belongs to the paradigm of applied research and action research. The study is carried out during the 2020-21 academic years in two programmes of Chemical Civil Engineering from two public universities in Chile. The phases of the research plan are: 1) theoretical inquiry, 2) diagnosis for the survey of the TFG genre and defence examination, 3) design of a didactic proposal adapted to the practice community, 4) evaluation. The instruments established to meet the objectives set are, mainly, semi-structured interviews, satisfaction questionnaires, analysis of drafts and calculation of writing quality indices. The research is in its second phase.

4. Results

Therefore, these are expected to characterize the writing process of the TFG and the oral defence exam of a specialty in the engineering area, as well as establish a didactic proposal aimed at overcoming the difficulties and critical issues identified, that is, a comprehensive methodological collaborative work that contributes to fulfilling the graduate profile of each discipline.

5. Conclusions

This research highlights the importance of having didactic materials in place for the engineering classroom that promote the accreditation of knowledge and the construction of professional identity.

Keywords: *coaching, gender-based approach, teaching, learning, writing*

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SCIENCE TEACHERS' PERCEPTIONS OF EMOTIONS DURING PRACTICE: AN ANALYSIS OF NOVICES AND EXPERTS' TEACHING DIARIES

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1. Introduction

This study looks at the emotional response of science teachers during their practice. We are especially interested in the early career science teachers' experiences, which have been identified as highly formative in terms of emotions (Bellocchi, 2019).

2. Methodology

We have collected and analysed teaching diaries from two academic years, six years apart (2012 and 2018). Each period we looked at an early career teacher as well as an experienced teacher. It is important to highlight that the expert teacher in 2018 was the novice in 2012.

All three teachers implemented, in different class groups, the same instructional sequence with slight changes between 2012 and 2018. This sequence comprised 20 sessions across 15 weeks, and after each lesson the teachers were asked to complete a diary entry explaining and reflecting upon what happened in class, including the development of the tasks.

We conducted a textual analysis of the diaries identifying implicit or explicit references to teachers' own emotions and students' ones, as noticed by teachers (Chan, Xu, Cooper, Berry, & van Driel, 2021). All identified emotions have been related to the description of concurrent classroom events.

Dimensions	Examples of quotations (diary date)	Emotions
Teachers' emotions	"The class today was a real disaster" (26/03/2012) "I'm so excited that I speak very fast" (12/03/2012)	Frustration Excitement
Emotional events	"13 students attended [...] it's so easy to work" (20/03/2012) "Explanation of Moon-Earth attraction" (20/03/2012)	---------- ----------
Students' emotions described by teachers on their teaching diaries	"They get bored" (26/03/2012) "They were impressed" (30/05/2012) "They were scared of the exam" (04/06/2012)	Boredom Awe Fear
"Potential for emotions"	"I don't insult anyone and he does not have to have that attitude with me" (05/03/2012) "The questions generate a lot of comments and it keeps them engaged all the time" (20/03/2012)	Respect Interest

Figure 1. Representative data obtained

3. Results

Classroom management and noticing students' negative emotions are related to the expression of disappointing emotions in the diaries for early career teachers much more than for more experienced, who express them less explicitly in their diaries. However, as the module progresses, early career teachers' diaries tend to reduce reference to emotions. These changes are also evident in the longitudinal comparison of the teacher who completed the diaries again after six years.

4. Conclusions

The analysis suggests that teachers' awareness of students' emotions is related with a lesser prominence of expressed emotions, which might be connected to a better understanding of the emotions' role in the students' learning process.

Keywords: *teachers' emotions, teaching diaries, novice/expert*

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SESSION X. PSYCHOLOGICAL PROCESSES AND MENTAL HEALTH

PHYLOGENETICALLY ACQUIRED COOPERATIVE AND COMPETITIVE COGNITIVE CAPABILITIES AND THEIR INFLUENCE ON THE DIFFERENT TYPES OF PERSONALITY DEPENDING ON THE DEVELOPMENT CONTEXTS

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1. Introduction

Current theories propose that personality is made up of different levels constructed over time: phylogenetic, ontogenetic, and narrative (McAdams & Pals, 2006). Here we present a study on the relationship between the most basic phylogenetic level and the first level of development, personality traits.

Throughout evolution, human sociocognitive abilities have co-evolved in conjunction with the competitive socio-evolutionary ecological niches and subsequently the cooperative socio-evolutionary niches of our hunter-gatherer ancestors (Moll & Tomasello, 2007). Human personality is formed from this phylogenetic inheritance of sociocognitive abilities in coevolution with ecological niches built over evolutionary time and ontogenetic niches that the person experiences from birth. Personality traits would be the result of this phylogenetic inheritance adapted to group relationships and lifelong experiences (Narvaez *et al.*, 2013; Packer & Cole, 2019)

2. Hypothesis

The hypothesis raised in relation to personality is that there are innate predispositions to both cooperation and competitiveness, resulting from the legacy of competitive and cooperative ecological niches. These predispositions will develop into a more or less cooperative or competitive personality depending on the micro niches that develop in the interrelationships with group members, which will give rise to personality traits (Figueredo & King, 2001), family beliefs, and the dominant culture of the group. The main objective of the work we present is to analyze whether competitive / cooperative behaviours are reflected in the personality traits assessed through the Big Five Questionnaire (BFQ).

3. Methodology

Participants: 360 individuals, 308 women and 49 men, aged between 21 and 73 who have been mothers or fathers. Data collection was done through social media. All participants completed an online protocol that included four different questionnaires: competitive / cooperative behaviour, personality traits (BFQ) morality, and parenting styles. Preliminary results related to the first two variables are presented here.

4. Results

The results show positive and negative correlations between competitive and cooperative behaviours with BFQ subdimensions.

5. Conclusions

In conclusion, we find a significant association between the personality traits of individuals and their more competitive or cooperative behaviour. These results will be discussed in the June presentation.

Keywords: social contexts of development, sociocognitive Niche, socioevolutionary Niche, competitive personality traits, cooperative personality traits

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THE DARK CONSTELLATION OF PERSONALITY AND MECHANISMS OF MORAL DISENGAGEMENT IN OFFENDERS

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1. Introduction

The analysis of dysfunctional personality traits associated with criminal behaviour is becoming increasingly important (Paulhus, 2014). In the present work, we focus on those socially aversive traits that integrate the Dark Triad of personality (Paulhus & Williams, 2002) consisting of Machiavellian, narcissistic and psychopathic personality. More recently, sadistic personality has been added to this dark constellation, deriving to the currently named Dark Tetrad of personality (Chabrol, Melioli, Van Leeuwen, Rodgers, & Goutaudier, 2015).

In prison population research, one of the most important and necessary aspects is to understand which psychological processes underlie antisocial behaviour. In this respect, it is essential to refer to the self-regulation mechanisms of thoughts and actions derived from the evaluation of one's own behaviour, which are based on one's own values and moral norms. However, in this process it is worth mentioning that some cognitive and psychosocial strategies exist that allow us to selectively disconnect from moral self-regulation. These strategies are known as mechanisms of Moral Disengagement (Bandura, Barbaranelli, Caprara, & Pastorelli, 1996).

This study aims to analyse the association between the personality patterns that configure the Dark Constellation and the mechanisms of Moral Disengagement.

2. Methodology

Participants were 62 offenders (30% female) located at three different prisons in Catalonia and convicted of a wide variety of crimes. The mean age of the sample was 40 (SD=10.64).

All the participants volunteered for the study and provided informed consent to the procedures approved by the Justice Ministry of *Generalitat de Catalunya*. They were interviewed individually in the penal institution.

Psychopathic personality was assessed using The Self-Report Psychopathy Scale (SRP-III; Paulhlus, Neumann, & Hare, in press), the Dark Triad of personality with the Short Dark Triad (Paulhus, 2014), and the mechanisms of Moral Disengagement were assessed using the Mechanisms of Moral Disengagement Scale (MMDS; Bandura *et al.*, 1996).

3. Results

Significant associations were found between the different facets of psychopathy and the eight mechanisms of Moral Disengagement. Dehumanization was the mechanism with the strongest associations with all the facets of this dysfunctional personality pattern.

In addition, we found positive associations with the Machiavellian and the aggressive-sadistic personality, as well as with the narcissistic personality, but in relation to different mechanisms compared to the other dark personalities.

4. Conclusions

In conclusion, these results indicate that these cognitive processes of reasoning and moral justification may act as underlying variables between these dark and maladaptive personality traits and antisocial behaviour and furthermore, that these cognitive patterns of reasoning may help in the justification of aggressive-sadistic and antisocial behaviours in the prison population.

Keywords: *Dark Constellation, psychopathy, Moral Disengagement, offenders*

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QUALITY OF LIFE OF PEOPLE AFFECTED BY CHRONIC LUMBAR PAIN AND THE ASSOCIATED FACTORS

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1. Introduction

The experience of chronic low back pain has a major impact on the quality of life of those affected, making it difficult for them to carry out their basic daily activities.

2. Problem

The overall aim was to study the perceived quality of life of people affected by chronic low back pain and associated factors, according to sex.

3. Methodology

Longitudinal, observational and prospective design was carried out in the pain unit of the Doctor Josep Trueta University Hospital in Girona on people with chronic low back pain with a follow-up of three months.

4. Results

129 people participated (58.1% women) who presented chronic low back pain under follow-up at the Doctor Josep Trueta Hospital in Girona. The mean age was 62.56 years (SD 15.29). The mean pain intensity scores were of moderate severity (6.42 points) with a slight improvement in scores during follow-up (6.17 points). The most significant therapeutic intervention to reduce the intensity of pain was lumbar epidural blocks.

People showed a negative perception of health in relation to quality of life with low scores for both constructs, both in the baseline state (health index of 0.444 and perception of health status of 38.76 points) and in the follow-up (health index of 0.447 and perception of health status of 40.43 points). Participants reported severe functional limitation scores (50.79 points). The active coping strategies of participants decreased during the study (21.28 to 15.6 points), and a significant increase was observed in passive strategies (23.6 to 30.21 points) and in catastrophizing (13.98 to 14.56). Total resilience scores were slightly better at baseline (27.50 points) compared to follow-up (26.67 points). Significantly worse results were observed in the perception of health, the state of health, the intensity of pain and the effects on the basic activities of daily life in women. A direct relationship between resilience and quality of life ($\beta = 0.199$; $p = 0.01$) and an inverse relationship were observed in the intensity of mean pain ($\beta = -0.304$; $p < 0.001$) and passive strategies ($\beta = -0.256$; $p = 0.002$) with quality of life.

5. Conclusions

The chronification of low back pain makes it difficult for people to adapt to life at a biopsychosocial level. More than half of the study participants have manifested a mean score in the intensity of pain of moderate severity with multiple effects on activities of daily life, with a negative perception of health in relation to quality of life and health status, and significantly so in women. People with higher levels of resilience and more active coping strategies showed a significantly better perception of perceived health and health status in general.

Keywords: *chronic low back pain, health-related quality of life, functional performance, coping strategies, catastrophism and resilience*

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THE STUDY OF MATERNAL-FILIAL RELATIONSHIPS: TENSIONS BETWEEN MOTHERS AND DAUGHTERS IN THE DISCOMFORT OF GENDER INEQUALITY

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1. Introduction

The thesis is based on research on the maternal-filial bond, in order to problematize the relationships between mothers and daughters from an intersectional feminist perspective, socio-constructionist theory and critical psychology.

The central objectives of the study are: first, to explore and give a new meaning of the tensions that specifically affect people who occupy the position of women-mothers with mental health symptoms or diagnosis and their daughters; and second, the de-psychopathologisation of women-mothers and the feminine, when relating the personal discomforts and experiences with the socio-political and cultural contexts marked by the patriarchal and capitalist system and by the 'psi' sciences.

2. Methodology

The research is being carried out with qualitative methodology. Specifically, the data collection techniques used are the documentary technique, the biographical technique and the case study technique. The corpus consists of a selection of biographical and autobiographical publications that meet the appropriate criteria. And the methods of analysis are discourse analysis and narrative analysis. In this way, triangulation is also used as a criterion of validity and reliability of the research process.

3. Results

From the first analysis of the corpus that makes up the sample, we detected situations where women-mothers express –with actions, words, feelings, etc.– psychological discomfort, in such a way that (as we will illustrate with quotations):

(1) A distance is generated with "the mystique of femininity / motherhood", as these expressions do not fit with the stereotypes and gender roles assigned to normative femininity.
(2) There is an impact on daughters from accountability / blaming / temporary imprinting.

However, as Walkerdine (1992), Martin (2001), Ussher (2011) and Cabruja (2017) especially point out, such expressions should be contemplated more as possible strategies of resistance or having to do with the difficulty of sustaining oneself, at the intersection of gender inequalities in which each woman-mother finds herself, and less as psychopathologies, which

are assigned –socially or medically–, by attributing to the woman-mother a damaged or errant "biological feminine essence".

4. Conclusions

These first results are relevant in showing that the present thesis can produce a gender impact, insofar as it can generate effects that bring a benefit in terms of gender equity:

Making visible some expressions of women-mothers' discomforts, which have been psychopathologised as if they were personality issues ("bad woman-mother"), when they are truly the cause of gender inequality conditions, is a way to be able to understand, transform and heal these maternal-filial relationships, enabling mothers and daughters to stop assuming and perpetuating patterns of pain throughout their lives.

Keywords: *maternal-filial bond, motherhood, women mental health, feminism, de-psychopathologisation*

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SESSION XI. WATER SCIENCES

FIXED-BED COLUMN DYNAMIC ADSORPTION OF HEAVY METAL IONS FROM AQUEOUS SOLUTIONS USING PINE CONES

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1. Introduction

Lignocellulosic agricultural residues, containing pectin, lignin, hemicellulose and cellulose, have suitable characteristics and structural compounds to adsorb heavy metal ions on their surface binding sites through interaction with the chemical functional groups (e.g. hydroxyl and carboxyl groups). These materials are becoming alternative adsorbents to activated carbon as they are available in large quantities, cheap, environmentally friendly, and efficient (Lakshmipathy & Sarada, 2015). The lignocellulosic nature of the pine cone shell, an agricultural waste largely produced in the Mediterranean area, makes this material an efficient biosorbent for Pb(II), Cd(II) and Cu(II) with maximum adsorption capacities at pH 5.5 of 100.01, 78.73, and 33.55 mg g^{-1}, respectively, whereas for Cr(VI) a maximum adsorption capacity of 57.36 mg g^{-1} was obtained at pH 2 (Amar, Walha, & Salvadó, 2021). In order to treat large volumes of effluents, fixed and fluidized bed columns are used. Several studies have been performed to investigate metal adsorption using fixed bed columns (Kaur, Singh, Khare, Cameotra, & Ali, 2013). The good results in terms of adsorption capacity obtained using pine cones as a biosorbent in the batch experiments encourage us to study dynamic adsorption in a column in order to progress towards industrial applications. Hence, the main objectives of the present study are to evaluate the ability of pine cones to adsorb Pb(II) in a fixed-bed column, and the capacity of this biosorbent to separate metal ions such as Pb(II), Cu(II) and Cr(VI) from a multi-metal aqueous solution, and Cu(II), Cr(VI) and Ni(II) from a simulated electroplating industry effluent.

2. Methodology

The adsorption capacity of the biosorbent has been investigated by performing dynamic experiments and the effect of flow rate. Inlet metal concentration and bed height on the removal of Pb(II) has been studied. The breakthrough curve for the adsorption of Pb(II) was determined by Adams-Bohart, Thomas and Yoon-Nelson models. The capacity of pine cones to adsorb and separate Cu(II), Cd(II) and Pb(II) in a fixed bed column has been investigated at different initial metal concentrations. Additionally, the competition of other divalent metal ions such as Ca(II) and the elution of the adsorbed metal ions have also studied. The removal and separation of Cu(II), Cr(VI) and Ni(II) from a simulated electroplating wastewater have been investigated.

3. Results

The results show that the experimental data of Pb(II) fit the Thomas model with an determination coefficient $R^2 > 0.96$, with the best results, 56.6 mg of Pb(II) g^{-1}, being obtained at a flow rate of 2.2 mL min^{-1} and 1 cm of bed height (1 cm). Cd(II) has the lowest breakthrough and exhaustion times followed by Cu(II) and Pb(II), allowing the separation of the three metal ions at initial concentrations of 25 mg L^{-1}. Ca(II) is not adsorbed by milled pine cone when the other metal ions are present and the adsorption of Cu(II), Cd(II) and Pb(II) is not affected by Ca(II). In simulated electroplating industry effluent (pH 4.4), the removal percentage of Cu(II), Ni(II) and Cr(VI) by pine cone in a fixed-bed column are 99%, 98% and 73% at a flow rate of 2.2 mL min^{-1} and a bed height of 2 cm. The desorption percentage using a 1.0 M HCl was higher in the case of Cr(VI) with 52.6% in comparison with Cu(II) and Ni(II) that were of 33.9% and 17.16%, respectively.

4. Conclusions

Pine cone biomass has been demonstrated to be an efficient adsorbent for the continuous removal of Pb(II) from aqueous solutions in a fixed-bed column at laboratory scale. The effects of various operation parameters such as flow rate, initial metal concentration and height of packed-bed on the adsorption process have been reported. Selective separation and removal of Pb(II), Cu(II) and Cd(II) was achieved indicating the absence of competition between them in the tested conditions and that pine cone is able to treat multi-metal effluents. Cu (II) and Ni (II) are the most efficiently removed metal ions, 98%, from a simulated electroplating industry effluent whereas for Cr (VI) the removal percentage was of 79%.

Keywords: *fixed bed column, pine cone, adsorption*

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AN ANALYSIS METHOD FOR DETERMINING THM AND HAA IN WATER SAMPLES

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1. Introduction

Trihalomethanes (THMs) and haloacetic acids (HAAs) are two most common classes of disinfection by-products (DBPs) that are present in treated water (Cardador, Fernández-Salguero, & Gallego, 2015). Studies suggest that consumption of drinking water with high concentrations of these compounds increases risks of bladder, kidney, stomach and pancreatic cancers in humans and animals. Therefore, exposure to such compounds should be minimized (Dos Santos, Martendal, & Carasek, 2011).
These common DBPs will be quantified by a combined technique to determine the amount of DBPs present in tap water from Girona.

2. Hypothesis

Develop a method to analyze both THM and HAA compounds using a single HS-SPME-GC-MS methodology for water samples at the same time.

3. Methodology

This analysis is carried out using a gas chromatographic system from Agilent 7890B with an automatized injection module RSI 85 PAL system (HS-SPME unit is also included with the injection system). To optimize this method, several parameters from GC and HS-SPME, will be studied and tested. A certificated standard mix has been used and Fluorobenzene as an internal standard. All analyses were performed using the Agilent MassHunter Quantitative Data Analysis software. Each parameter was optimized to ensure the largest peak area of the compounds of interest.

4. Results

The evaluation of parameters was performed to optimize as the effect of ionic strength with NaCl and NaSO4 (2, 10, 12 and 20% w / v), the extraction temperature by HS-SPME (25, 30, 35 and 37 ° C) and the extraction time (10, 20 and 30 min. With the results obtained, the selected parameters are 10% Na SO4, 20 minutes of extraction time and 30 ° C as the optimal extraction temperature. The last step was the analysis of the time and temperature of thermal desorption (200, 225 and 250 ° C) and time (2, 3 and 4 minutes), selecting 225 and 3 minutes for the desorption stage.

Then the validation of the proposed methodology and its application was performed.

5. Conclusions

A rigorous procedure was performed to analyze the results obtained with the best signal chromatograms using the commercial house data analysis software to obtain a joint method of analysis.

Keywords: *THMs, HAAs, water, HS extraction, GC*

6. Bibliography

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DEVELOPMENT OF FUZZY LOGIC SYSTEM FOR CONTROLLING OZONE DOSING RATE IN A DRINKING WATER TREATMENT PLANT

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1. Introduction

Drinking water treatment plants (DWTPs) must ensure that all customers receive high-quality water. The removal of numerous compounds present in surface waters is necessary to meet regulated quality parameters. The presence of natural organic matter (NOM) is the main cause for trihalomethane (THM) formation upon final chlorination (Camel & Bermond, 1998). The ozonation is one of the unit operations to ensure high NOM removal and is used in early stages in the water treatment process removing mineral compounds, colour, turbidity, suspended solids, and unpleasant taste and odors (Camel & Bermond, 1998).

In order to monitor the efficiency of ozonation, various quality parameters are used: Oxidation Reduction Potential (ORP), Total Organic Carbon (TOC), or ultraviolet 254 nm (UV254) are widely used to calculate the impact of ozone on NOM composition. As the correlation between data from *ozonation processes and water quality parameters is not well-defined, ozonation requires to be optimized to ensure not only the organic water compounds removal but also to avoid an overdose, which ultimately results in high costs and in the formation of ozonation by-products*. Based on this, there are several AI techniques, such as Fuzzy Logic (FL) systems. FL systems are efficient modelling techniques for consolidating process engineering knowledge, which is acquired through experiencing and observing a system's operation (Godo, 2020). FL covers a broad range of decision-making-related topics and is based on the goal of simulating human reasoning in order to interpret real-world data on a scale ranging from true to false. The use of FL in drinking water production is an opportunity to minimize its derived costs. The aim of this study is to develop a FL system for controlling the dose of ozone in a DWTP.

2. Methodology

The DWTP for the town of Figueres extracts water from the Darnius-Boadella reservoir. At Figueres DWTP, ozonation is the first step in the water treatment train (Figure 1).

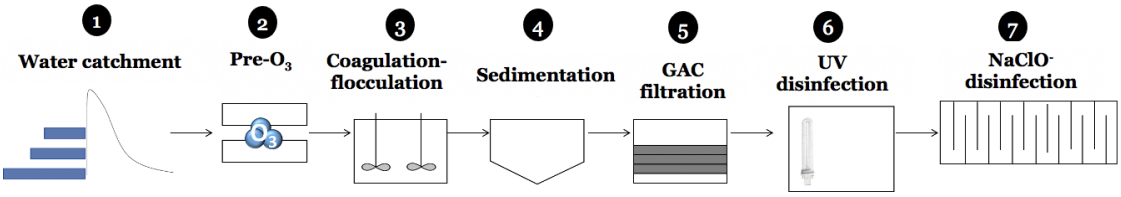

Figure 6. Figueres DWTP scheme.

To develop the system, three steps are involved: i) Data (on-line and off-line) and knowledge acquisition, ii) Data analysis (MATLAB) and iii) Model selection (FL system). The main parts of FL system are: i) Fuzzification of input variables, ii) Fuzzy inference rules, and iii) Defuzzification of output variables (Godo-Pla *et al.*, 2021).

3. Results and discussion

According to the data, three separate databases were created: DWTP online sensors, DWTP laboratory analyses and another resulting from the specific analyses performed for this study. Table 1 shows the characteristics of these databases.

During ozonation, ozone modifies the organic load of raw water. ORP was previously designed as the control variable for determining the ozone dosage since ORP is directly related with the oxidative capability of water, but later it was pointed out that residual ozone also affects the ORP values, which led to the selection of a better and more suitable control variable. TOC and UV_{254} parameters are directly correlated with the amount of OM in water, motivating their use hereinafter as control parameters. The results show that ozonation leads to a decrease in UV_{254} by 25% due to the loss of aromaticity. Upon ozonation, TOC is often reduced, but TOC experienced a slight rise in some cases during this study. This behaviour was attributed to the transformation of high molecular weight humic and fulvic materials into lower molecular weight materials.

Table 1. Characteristics of ozone unit stage in Figueres DWTP

Parameter	Units	Average
Database (1) from online sensors		
pH	-	7.82 ± 0.28
Turbidity	NTU	2 .52 ±1.42
Flow	$m^3 \cdot s^{-1}$	0,14±0.01
ORP pre	mV	610 ± 63
ORP post	mV	499 ± 62
Ozone dosing rate	ppm	1.33 ± 0.2
Database (2) from DWTP laboratory analysis		
Temperature	°C	13.53 ± 4.19
UV 254 nm pre	cm^{-1}	0.08 ± 0.01
UV 254 nm post	cm^{-1}	0.06 ± 0.01
ORP pre	mV	320 ± 38
ORP post	mV	310 ± 32
Database (3) from specific analysis		
TOC pre	ppm	3.47 ± 0.78
TOC post	ppm	3.55 ± 1.23

FL system was used, and membership functions were input to the Mamdani-type fuzzy inference system (Mamdani, 1977) to find out the ozone dosing rate based on expert knowledge. The input variables for this method were influent temperature and absorbance at 254 nm. Fuzzy inference rules are shown in Table 2.

Table 2. Scheme of fuzzy inference rules.

		Absorbance 254 nm		
		Low (0.05-0.1)	***Medium (0.1-0.15)***	***High (0.15-0.20)***
TEMP	***Low (6-14 ºC)***	Min	Low	Medium
	Medium (14-20 ºC)	Low	Medium	High
	High (20-22 ºC)	Medium	High	Max

4. Conclusions

Data processing and analysis has shown the behaviour of different parameters. Anomaly values for certain parameters should be explored further. A FL model that predicts the dose of ozone in a primary disinfection of a DWTP was developed based on the temperature and the absorbance of 254 nm of feedwater. The model will be validated in a closed loop and will be implemented into an EDSS for automated decision-making in Figueres DWTP.

Keywords: *drinking water treatment plant, ozone, NOM, fuzzy logic, modelling*

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ELECTROCHEMICAL DISINFECTION OF E. COLI WITH REDUCED GRAPHENE OXIDE FOAM ELECTRODES

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1. Introduction

Electrochemical treatment is a promising and emerging method of (waste)water disinfection, which has the advantage of not requiring any chemical addition to operate. In electrochemical disinfection processes, the production of oxidants (disinfectants) may occur directly by water discharge (i.e., hydroxyl radicals, ozone), dissolved species (i.e., active chlorine or hydrogen peroxide via oxygen reduction), or anode dissolution (i.e., ferrate) (Palmas *et al.*, 2018). When chlorine is present in water, the active species can enhance the disinfection capacity, but this has the drawback of generating toxic disinfection by-products (DBPs).

2. Methodology

A one pass electrochemical reactor is used for the disinfection of *E. Coli*. The electrodes used were mineral wool containing Reduced Graphene Oxide, which was reduced using Boric Acid (BRGO) and Urea (NRGO) respectively. Stainless steel was used as a current collector. The buffer used was PB 10 mM and the flowrate 5 mL/min. The plate count method was used for the determination of the *E. Coli* inactivation.

3. Results and discussion

In this study, we examined the disinfection ability of graphene sponge electrodes for the removal of *E. Coli*, in the absence of chlorine species in a one pass mode. Three and 4.5 log removal were achieved when Boron and Nitrogen doped RGO anode were used, consecutively (Figure 1). To examine the energy efficiency, experiments with pulsed current application were conducted, achieving up to 4.5 log removal with the NRGO anode. Graphene foam electrodes were prepared using a simple, low-cost method. The main advantage of the prepared graphene sponges is that they did not produce any chlorine, chlorate or perchlorate, which is one of the main limitations in electrooxidation of chloride-containing water.

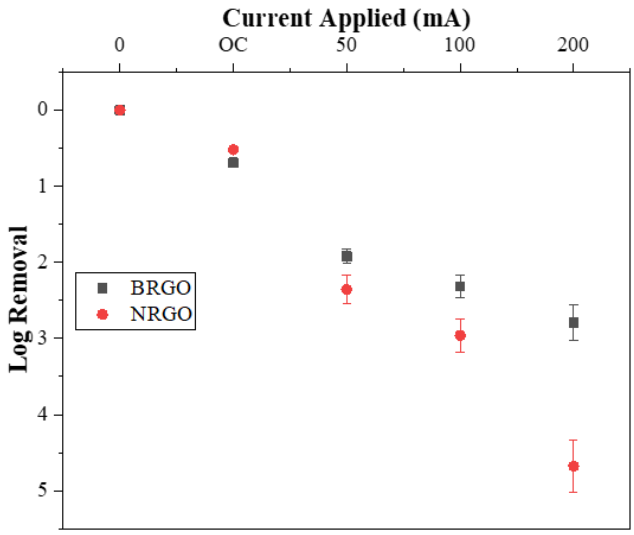

Figure 1. Electrochemical inactivation of E. Coli using Boron and Nitrogen Doped RGO sponge anodes at different applied currents

4. Conclusions

The developed electrode materials are extremely promising as they can provide successful disinfection without forming toxic DBPs, thus opening the door for future electrochemical water treatment applications.

Keywords: *disinfection, electrochemistry, E. Coli, sponge electrodes, RGO*

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SPATIAL AND TEMPORAL FLOW INTERMITTENCY PATTERNS IN A MEDITERRANEAN BASIN: PRESENT AND FUTURE

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1. Introduction

Non-perennial rivers and streams are ubiquitous globally, especially in semi-arid and arid landscapes (Acuña *et al.*, 2014). Nonetheless, despite their prevalence worldwide, non-perennial systems have been under-represented in the hydrology research, and our understanding of their hydrology is minimal compared to perennial systems (Leigh, Boersma, Galatowitsch, Milner, & Stubbington, 2019; Shanafield, Bourke, Zimmer, & Costigan, 2021). Predicting the availability of freshwater resources is essential, especially in the Mediterranean area, where most of the agricultural systems depend on precipitation and irrigation (Pulighe *et al.*, 2020). The modelling of these dynamic systems remains a challenge. Most of the existing models focus on continuously flowing rivers, without addressing some relevant characteristics of these systems such as the spatial and temporal intermittency patterns (Jensen, McGuire, McLaughlin, & Scott, 2019).

2. Methodology

In our study, we implemented a watershed-scale hydrological model on a Mediterranean intermittent basin, using the Soil and Water Assessment Tool (SWAT+) program. The model was calibrated and validated using data from two gauging stations located at the mainstem (20 years), and 14 stage recorders dispersed across the river network (18 months). Simulation results and observed flow intermittency patterns were analysed. Furthermore, we also simulated climate change scenarios and compared the flow intermittency patterns with the current ones.

3. Results

Preliminary results indicate that longer duration of non-flow periods may be expected under climate change conditions. Theses affecting most of the streams network turning into ephemeral and a few and isolated stretches remaining as permanent.

4. Conclusions

This study indicates that the constructed hydrological model reliably represented the spatiotemporal variability of the flow regime in non-perennial systems. This study also establishes a quantitative framework to assess the possible impact of climate change in

Mediterranean basins. Finally, the analysis of the spatial and temporal flow intermittency patterns in the Mediterranean basins is an indispensable factor in its appropriate management, especially under climate change conditions.

Keywords: *non-perennial rivers, hydrological modelling, SWAT+, climate change, flow patterns*

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POLYMER INCLUSION MEMBRANE AS A SENSOR FOR FREE COPPER AND ZINC IN NATURAL WATERS

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1. Introduction

The development of analytical techniques for the measurement of free metal species is of paramount importance for predicting metal bioavailability and toxicity. Polymer inclusion membranes (PIMs) containing a selective carrier have been studied for this purpose where the metal flux through the membrane is related to the free metal ion and labile complexes (Vera, Fontàs, Galceran, Serra, & Anticó, 2018). Hence, we present in this work the use of PIMs for zinc and copper speciation studies in water samples.

2. Methodology

The PIM used for our purpose was made out of cellulose triacetate (CTA, 50% w/w) as base polymer, di-(2-ethylhexyl) phosphoric acid (D2EHPA, 50% w/w) as carrier, and nitrophenyl octyl ether (NPOE, 10% w/w) as plasticizer. A designed device (Figure 1) reported by García-Rodríguez *et al.* (Garcia-Rodríguez et al., 2016) was used with the PIM placed at the bottom opening. The acceptor phase was 0.01 M HNO_3 (5 mL). The device was immersed in the donor solution (100 mL) which contained Zn and/or Cu under stirring conditions. After a certain time, the device was removed from the solution and the acceptor phase was taken for analysis.

3. Results

The influence of metal concentration and contact time have been evaluated in a solution containing the two metal ions in both individual and competitive experiments. It was found that the presence of different ligands in the donor solution, such as ethylenediaminetetraacetic acid (EDTA) or humic acid (HA), influenced the metal accumulated in the acceptor phase due to the formation of non-labile metal complexes in the donor solution (Figure 1). Finally, the sensor has been deployed at different points of a river rich in Zn, due to the drainage from an abandoned mine, where different accumulation rates were found.

4. Conclusions

In conclusion, it has been demonstrated that the PIM device can be envisaged as an efficient sensor to study the speciation of Cu and Zn.

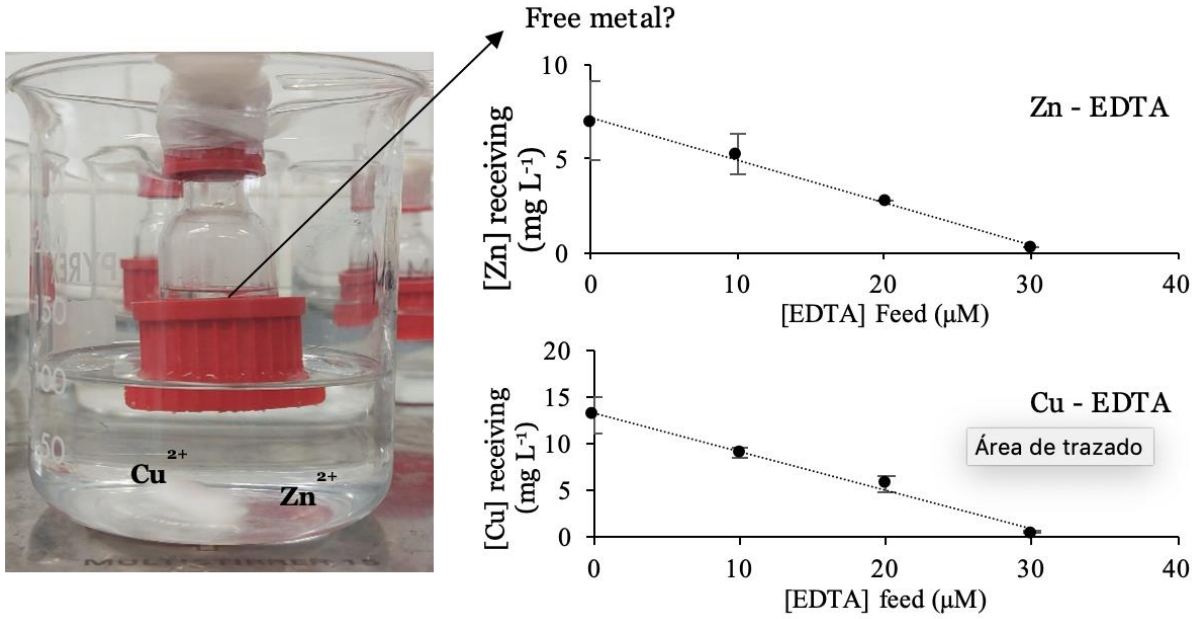

Figure 1. The designed device used in this work and the results of the influence of EDTA ligand in Cu and Zn.

Keywords: *polymer inclusion membrane, metal bioavailability, zinc, copper, di-(2-ethylhexyl) phosphoric acid*

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INTEGRATION OF BIOLOGICAL TREATMENT OF SWINE MANURE WITH PHOSPHORUS AND POTASSIUM RECOVERY AS K-STRUVITE

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1. Introduction

A large amount of swine manure highly loaded with nitrogen (N), phosphorus (P) and potassium (K) is produced by the intensive pig farming industry in some areas of Catalonia. The unavailability of agricultural land near the farm may make manure treatment necessary before discharge to prevent water and soil pollution. Nitrification-denitrification (NDN) is usually applied for biological N removal (Giner Santonja *et al.*, 2017) and the fulfilment of legal criteria. However, under the circular economy framework, following the biological step, innovative procedures for the recovery of P and K as the phosphate salt K-struvite ($MgKPO_4 \cdot 6H_2O$) are of high interest.

The sludge purged from the NDN bioreactor (Figure 1) has higher concentration of P than the liquid effluent, which can be mobilised by acidification. Unfortunately, calcium (Ca) will be also mobilised. The crystallisation of K-struvite is inhibited by high levels of Ca due to the formation of Ca-P compounds, and thus, the development of new procedures for preventing the interference of Ca during K-struvite formation are needed. Some options to investigate are the addition of a chelating agent (Zhang, Bowers, Harrison, & Chen, 2010) or the use of nanoparticles consisting of layered double hydroxides (LDHs) to adsorb soluble orthophosphate (Mandel *et al.*, 2013). This study aims to investigate K-struvite production as a new biofertilizer (11.6% P and 14.6% K, % as weight) from the NDN liquid effluent taking advantage of the solubilisation of P from the thickened sludge.

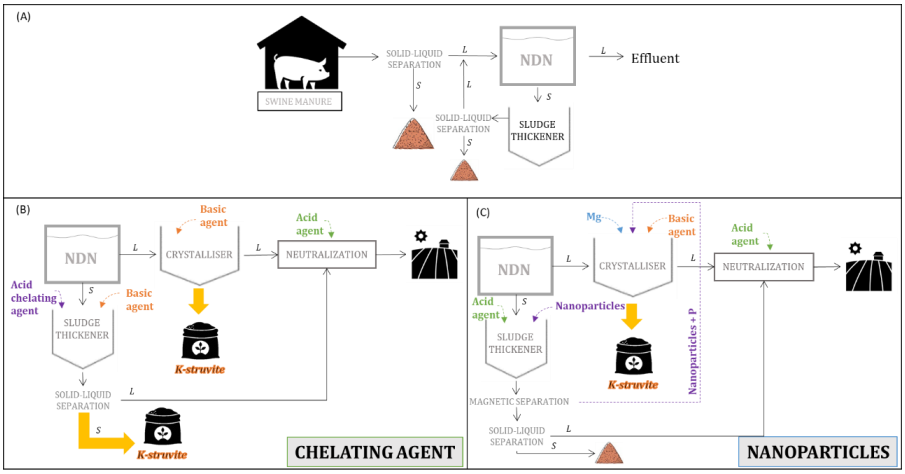

Figure 1. Flow chart of the swine manure treatment plant in Osona (A). Recovery of K-struvite using a chelating agent (B) or LDH nanoparticles (C).

2. Methodology

The NDN treatment plant under study was located in a pig farm from Osona. The liquid effluent had as soluble Mg/K/P molar ratio 1.4/9.9/1.0 (130 mg PO_4-P/L). The thickened sludge had as total Mg/K/P molar ratio 0.7/0.9/1.0 (1420 mg TP/L). Tests with the chelating agent and the LDH nanoparticles were conducted in 1 L glass beakers mixed at 150 rpm, lasting 60 min. To modify the pH, NaOH and H_2SO_4 were used as needed. $MgCl_2$ was dosed as the magnesium source when required.

3. Results and discussion

Final pH during the acidification step highly influences P and Ca mobilization. A final neutralization step should be considered before water discharge. Recovery of K-struvite from the NDN liquid effluent was shown as feasible although it is limited by the lack of P (29% P and 17% K from manure were estimated as recoverable). The use of the thickened sludge as an additional source of P will help to increase the recovery efficiency. Two different processes were studied for this purpose, consisting on (1) direct recovery of K-struvite from the sludge using a Ca chelating agent or (2) selective capture of phosphate using LDH nanoparticles, and their subsequent use as an internal source of P when treating the liquid effluent. If all the P that could be mobilized resulted in the formation of K-struvite, then, recoveries of up to 70% P and 41% K could be feasible. A cost assessment at the farm scale is necessary to elucidate final interest of the alternatives proposed.

4. Conclusions

By considering the thickened sludge as an internal source of P the process of recovering K-struvite after NDN can be significantly improved.

Keywords: *magnesium-potassium-phosphate, biofertilizer, circular economy, swine manure, thickened sludge*

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BIO-ELECTRO CO_2 RECYCLING PLATFORM: FROM SPENT CO_2 GASES TO COMMODITY CHEMICALS

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1. Introduction

Over the years, carbon dioxide (CO_2) emissions have been rising despite green EU policies, society efforts and strategies to decrease them. Microbial Electrochemical Technology (MET) is an emerging research field with feasible and yielding productions of short organic compounds (C2 compounds) from carbon dioxide contributing to the creation of a decarbonized economy. Despite this, further elongated compounds (i.e. C4) are more desirable due to their higher value.

2. Hypothesis

The present work assessed the alliance of MET and fermentation in a two-step process for the electro-bioconversion of CO_2 into elongated chemical building blocks.

3. Methodology

The electro bio-reduction of CO2 into acetic acid and ethanol (EtOH:HAc) at a 1-to-1 ratio was linked to a subsequent elongation step to produce C4 and C6 compounds. Key conditions aiming to steer each stage and maximize production rates were assessed. Effects of (i) pH, (ii) hydrogen partial pressure and (iii) dissolved CO_2 were evaluated in the first step. The impact of (i) pH, (ii) ethanol-to-acetate ratio and (iii) feeding gas regimes on the production of elongates compounds (such as C_4 and C_6) were analysed in the second step.

4. Results and discussion

Figure 1 summarizes the performances of both steps. An EtOH:HAc ratio over 1:1 was reached in the MET step. This allowed a subsequent chain elongation process. The fermentation step got up to C_6 compounds at pH 7 with H2 supply, achieving yields higher than 80%. Furthermore, outcomes unravelled that low ethanol-to-acetate ratios (1:1) favoured butyrate and caproate compounds production; whereas higher ratios (3:1) enhanced the selective production of caproate, agreeing with the suggestions of Raes, Jourdin, Buisman, & Strik (2017).

The overall process showed a carbon conversion efficiency of 38% the CO_2 transformation being the limiting step. 1 m^3 of CO_2 (normal conditions) captured resulted firstly in the production of 0.90 kg C_{C2} and then, 0.75 kg $C_{C4\text{-}C6}$ are finally acquired.

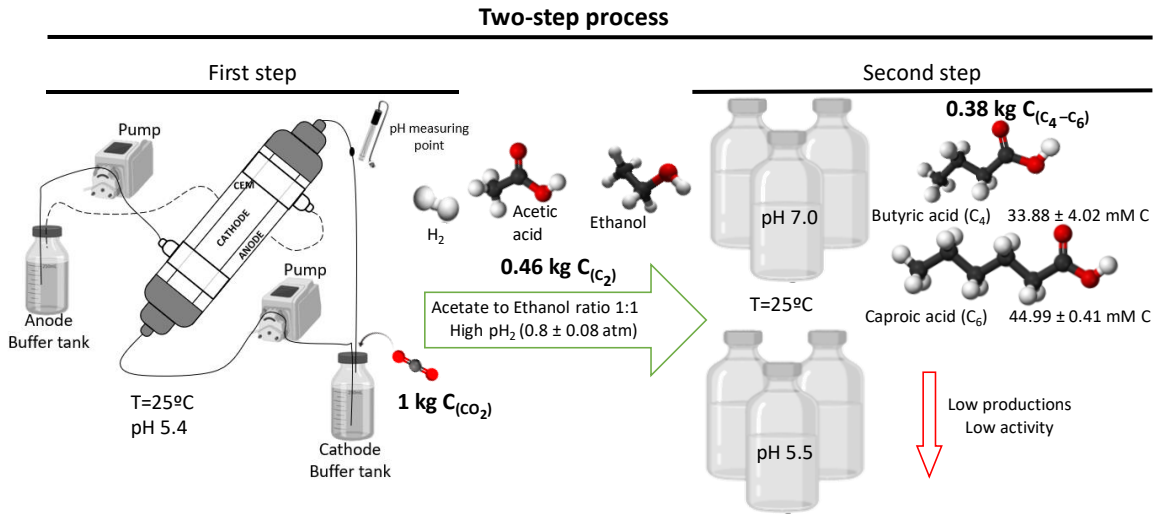

Figure 1. Schematic representation of the proposed bio-electro CO_2 recycling platform, its stages and carbon conversion efficiencies.

5. Conclusions

The present study proposes a bio-electro CO2 recycling platform to produce elongated compounds from CO_2. These results pave the way for future studies on the selective production of more reduced commodity chemicals from carbon dioxide and electricity.

Keywords: *bio-conversion, CO_2 valorization, chain elongation, electrochemistry, gas fermentation*

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SESSION XII. MOBILITY, IMMIGRATION AND HISTORY

TRADE, TRANSPORT AND REDISTRIBUTION NETWORKS BETWEEN THE FIRST CENTURY BC AND FIRST CENTURY AD FROM THE STUDY OF PASCUAL I AMPHORAE

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1. Introduction

The Underwater Archaeological Charter of Catalonia houses massive storage of archaeological material, which reveals the heavy commercial traffic in Roman times – a matter that remains to further explored. This work aims to develop a study of the Pascual I amphorae, a part of this unpublished material, to learn more about trade, transport, and redistribution networks in the first century BC and first century AD at the northern end of the Mediterranean strip of the Iberian Peninsula. This study is set within a four-year research project (2018 to 2021) of the Underwater Archaeology Centre of Catalonia (CASC).

2. Hypothesis

The hypothesis raised in this work is that the Pascual I amphorae were manufactured in the *Conventus Tarraconensis* and were distributed with cabotage routes along the northern strip of the western Mediterranean.

3. Methodology

This research will be performed in the facilities of the Underwater Archaeology Center of Catalonia. Initially, the Pascual I pieces and amphorae will be cleaned, studied and drawn. At the same time, an exhaustive study of all the existing documentation in the Underwater Archaeological Charter of Catalonia will be carried out to know all the surveys and excavations that have been accomplished in the archaeological sites where the Pascual I amphorae have been located in recent years.

From the study of the previously available material, a second study of the possible marks or stamps found on the artefacts will associate them with the different ceramic production centers identified in order to determine the origin of the object of study. Finally, from all the information obtained, the master's thesis will be written.

4.Results

The initial amphorae study will determine whether the relics are Pascual I or Pascual I B, and finally, if the newly discovered modality Pascual I Parva can be found in the sample.

Secondly, the study will allow us to fathom out the possible relationship between the stamps or marks of the Pascual I amphorae and the *figlinae* of the northeast area of the Catalan coast.

This will help us conclude which production centers in the area had the highest manufacturing index.

Finally, it will be possible to delimit the maritime trade routes where Pascual I amphorae were most used and detect whether these were cabotage routes or not.

4. Conclusions

With the preliminary studies, we will be able to delimit the maritime trade routes and thus have a global vision of the economic activity of the area of the northern end of the Mediterranean strip of the Iberian Peninsula between the 1st century BC and 1st century AC.

Keywords: *wreck, Amphorae Pascual I, trade, transport, redistribution network*

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FISHERMEN AND FISHING IN THE 15th AND 16th CENTURY REGION OF *LA SELVA*

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1. Introduction

Catalan fishing history is a rather understudied subject. There are not many papers, chapters or monographs that have produced in-depth research into medieval fishermen and their activities. Apart from some 16th and 17th century-focused studies (Garrido, 2012; Garrido & Alegret, 2006), there are few of them regarding the Middle Ages (Riera i Melis, 2009). Thus, this research is an attempt to shed light on the general study of this activity in a two-hundred year period, focused on a specific region of North-West Catalonia.

The choosing of this particular period and geographical context responds to a willingness to concentrate on a multilevel approach: Firstly, the study of the techniques, material and human resources of fishing. Secondly, the organisation of the collective, either in labour or social aspects. Thirdly, social and economic interactions, the subsequent hierarchisation of fishermen and their relationship with the rest of the rural community. Lastly, feudal impact on the activity and the people around it.

2. Results

At this point of the research, it can be asserted that fishing was a dynamic activity that empowered some coastal towns such as Blanes. This town experienced, however, a radical economic change towards the wool market. Such phenomenon shows that fishing could also be an attractive temporary activity and not only a subsistence option. Fishing as a main economic action can also be understood through individual case studies of rather important fishing skippers.

Regarding collective hierarchisation, not only do we appreciate a generic economic difference between skippers and regular fishermen, but we also can transport this into specific categories to reaffirm these aspects. One of these areas is the study of complementary agricultural activities and investment in land (Ginot Julià, 2020).

The relationship with feudal lords contributes to the understanding of this activity as key in coastal domains. The analysis of tithes and other exactions over fishing and fish is important here.

3. Conclusions

There is still work to be done, but the main threads of the research are already drawn. Fishing implied the participation of several people and was one of the main driving forces of coastal towns. Fishermen developed strategies of organisation and legislation in consonance with the seigneurial power. They also participated in other activities such as commerce and agriculture, which transformed them into a complex and diverse collective. In addition, the dynamics of

feudal exaction evolved during the Middle Ages to consolidate one of the main incomes of coastal seigneuries.

Keywords: *fishing, fishermen, rural history, La Selva (Girona), social history*

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CONSTRUCTION TRADES IN THE SECOND HALF OF THE 18th CENTURY: AN ANALYSIS THROUGH THE *REGISTRE D'HIPOTEQUES*

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University of Girona

1. Introduction

This paper use a significant new primary source material called l'Ofici *d'Hipoteques* to examine the building craftsmen in the second decade of the eighteen century in Girona and the surrounding area. In terms of historical setting, the vast majority of literature has viewed the period as a time of economic, demographic and urbanistic growth. Despite this, we have no evidence about how this prosperity affected the local brick makers, carpenters, builders, master builders and master carpenters. For this reason, using the data gathered from the books of the registry deeds automatically transcribed through a project lead by the *Centre de Recerca d'Història Rural,* we would like to elaborate a prosopography of the constructors and determinate their geography. In addition, provide a first study of the buying and selling trades to analyze their share in the land market and, in particular, present a preliminary step for their economic taxonomy.

2. Results

This has an implication for our understanding of the construction workers' socioeconomic profile during the pre-industrial period. All the evidence shows that construction workers, following the narratives about the pre-industrial development, worked and lived all over the northern Catalan region. A useful indication is that they lived in both the largest cities and in small towns, proving their implication in the economic and urbanistic growth.

3. Conclusions

This has implications for our understanding of how liberation of the trade and guilds affected the distribution of these workers and benefited them by making it possible to work in a larger area.

Keywords: *Girona region, building craftsmen, Ofici d'Hipoteques, 18th century*

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DOWRIES AND GOODS IN A RURAL SOCIETY DURING THE SECOND HALF OF THE 18th CENTURY: THE REGION OF "LA SELVA"

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University of Girona

1. Introduction

The present communication aims to illustrate the evolution of consumption patterns, in relation to the purchasing power, of families from the region of "la Selva" in the second half of the 18th century. To carry out this comparison, the presence of certain goods in households, associated to a certain grade of comfort, luxury and/or new consumption patterns, have been evaluated. Then, when comparing these results with the dowries paid to the brides as an indicator of socioeconomic family status (R. Congost, 2010), we have been able to assess whether wealth played a determining role on consumption patterns or, on the other hand, some factors such as traditions, tastes, fashion, or proximity to diffusion centres should have been considered as well.

2. Methodology

Two notarial sources have been used to perform this study: marriage contracts for the dowries and after death inventories for goods., A database of 819 marriages and 305 inventories from three chronological periods: 1750-1755, 1775-1780 and 1800-1805 has been collected.

3. Results and discussion

As it is shown in Table 1, the highest dowries are paid by the *pagesos* (landowners) occupational group, doubling and even tripling those satisfied by *treballadors de la terra* (land workers). Noteworthy, non-agricultural families stand in an intermediate position. By contrast, regarding the consumption of certain goods associated to new and modern habits, such as napkins and forks (Table 2), they are more commonly found in artisans and merchants' houses in the period of 1750-1755. However, at the beginning of the 19th century this trend reversed. Accordingly, chocolate pots, as indicator of the consumption of an exotic and colonial product like cocoa, serve as a good example of this phenomenon. By way of illustration, between 1750 and 1755, chocolate pots are only found in non-agricultural households, soon starting to appear in the richest "masos" (farmhouses) and, finally, arriving to nearly one third of them by 1800-1805.

Table 1. Median dowries (in *lliures barcelonines*) paid, according to bride's father occupation group.

	1750-1755	1775-1780	1800-1805
pagesos	100	100	150
treballadors de la terra	50	60	50

non-agricultural (artisans & merchants)	73	100	100

Table 2. Percentage of after death inventories with certain goods according to bride's father occupation group (P = *pagesos*, T = *treballadors de la terra*, NA = non-agricultural (artisans & merchants).

	1750-1755			1775-1780			1800-1805		
	P	*T*	*NA*	*P*	*T*	*NA*	*P*	*T*	*NA*
sheets	75%	68%	83%	95%	80%	100%	93%	92%	78%
napkins	66%	32%	63%	74%	37%	75%	72%	56%	52%
spoons	69%	32%	69%	87%	37%	85%	86%	71%	65%
forks	19%	0%	31%	71%	20%	80%	79%	52%	61%
chocolate pots	0%	0%	14%	16%	0%	25%	34%	8%	22%
gold & silver	34%	4%	31%	14%	6%	14%	17%	3%	15%

4. Conclusions

The evidence from this study suggests that marriage and goods markets have some common characteristics, inasmuch as the poorest families (*treballadors*) are those having access to a smaller range of items. On the other hand, it seems that non-agricultural households, who usually live in the towns, are more permeable to new consumption patterns in comparison with those who live in the countryside (*pagesos*), regardless of whether they have a greater purchasing power.

Keywords: *18th century, La Selva, social history, dowries, goods consumption*

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THE IMMIGRATION IMPACT ON SANT HILARI SACALM (1900-1980)

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1. Introduction

Until the second half of the 20th century, Sant Hilari Sacalm had principally a farming and forestry economy. The number of inhabitants, except during the Spanish Civil War, was around 2700 people. Since the 1950s, the development of the turnery industry drove social-economic and demographic changes. It attracted labour from nearby locations. While the secondary sector was growing, in number and volume of production, it required more working men. An immigration to Catalonia was necessary to fulfil this requirement. Mass arrivals during the 1960s were the solution, and an escape from the misery of rural Spain. It led to the creation of migration corridors from three villages from Andalusia: Écija (Sevilla), Alhama (Granada) and, above all, Priego de Córdoba (Córdoba).

From oral sources and the municipal register, the purpose of this study is to analyze why this immigration was necessary, how the corridors were formed, where they were produced and how migrants were included in the labour local market. Moreover, we want to investigate how the arrival of Andalusian people had an impact on the rhythm of the population growth produced in Sant Hilari Sacalm since the beginning of the twentieth century.

2. Results

Oral sources have produced two remarkable results. Firstly, the difficulty of entrepreneurs to find local workers for a growing industry between 1965 and 1980. Secondly, the active role of the Guardia Civil in the creation of the migratory corridors between the three Andalusian villages mentioned and Sant Hilari Sacalm.

3. Conclusions

The number of inhabitants in the village of Sant Hilari Sacalm was stagnant, from the beginning of the 20th century until the 1960s, with 2700 inhabitants. It followed the model of mountain villages: first an ageing population and then a depopulation. The change in this trend was due to the development of woodturning and burned wood articles to fabricate auxiliary furniture and decorative elements that were exported to Europe, the United States and other countries such as Japan.

This development required a volume of labour that the local population was unable to provide. It was necessary to seek labour outside the region.

This led to the formation of migratory corridors between Priego de Cordoba, Écija and Alhama. Entrepreneurs prospected for newcomers, however, we must not detract from the role played by the Guardia Civil as an interface between Sant Hilari and these places. They informed their family and friends of the lack of manpower in the area.

Industrialization and consequently, immigration, ended the trend of an ageing population, and resulted in an increase in population.

Keywords: *immigration, Sant Hilari Sacalm, 20th Century*

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FACILITATING TRANSFORMATIVE EXPERIENCES IN MUSEUMS THAT DEAL WITH THE "DIFFICULT KNOWLEDGE" OF IMMIGRATION

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1. Introduction

Museums have long since been regarded as institutions of learning and education, and certain types of museums even go further to declare a strategic aim of fostering action. However, more research is needed, on how immigration museums can provide not just educational experiences, but transformational ones. Several authors have examined elements or strategies that can contribute or detract from a museum's transformative potential. The focus on triggering lasting behavioural or attitudinal change within visitors represents a highly valuable asset at a time when the global community requires "immediate actions to counter the negative impacts of global trends such as climate change and increases in intolerance and extremism" (Soulard, McGehee, & Knollenberg, 2020). When it comes to curating "difficult knowledge", such as historical and contemporary immigration narratives, Simon (2011) suggests that the real challenge is provoking "sustained attention, concern, and corrective action rather than a few days' sensation that is soon forgotten" (p. 206).

Based on existing literature, it is clear that spurring action and transformation in a museum context is challenging, yet necessary. The purpose of my research is to capture museums' perspective, particularly museums that specialize in difficult knowledge of immigration, and how they provide transformational experiences to their visitors. Therefore, my two-part research question is as follows: How do immigration museums perceive their role in facilitating transformative experiences for their visitors, and what curatorial approaches do they use to facilitate transformation?

2. Methodology

Semi-structured qualitative interviews were conducted with curatorial staff from 15 different immigration-related museums around the world. Due to the broad and exploratory nature of the research, the data was analysed using a hybrid approach, employing both deductive and inductive coding techniques.

3. Results and discussion

The findings from this study illuminate the various perspectives that immigration-related museums hold regarding their role in providing transformative experiences, as well as the strategies they use in exhibit design to provide those experiences. A number of challenges were also uncovered which highlight the ways that museums are often constrained from facilitating transformation within their visitors. The results are further interpreted using transformational learning theory (Mezirow, 1991), the principles of hot interpretation (Ballantyne, Packer, & Bond, 2012), and an identity exploration design framework (Kaplan, Sinai, & Flum, 2014).

4. Conclusions

This thesis contributes to a broader understanding of the role that museums can play in fostering a more tolerant society. The effectiveness of the strategies uncovered in this study can be further tested through visitor evaluation.

Keywords: *immigration, museums, transformation, difficult knowledge, exhibit design*

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CO-LIVING EXPERIENCES FROM DIGITAL NOMADS AND REMOTE WORKERS LEADING TO RURAL DEVELOPMENT: THE CASE OF SPAIN

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1. Introduction

In our modern and ever-changing world, the tourism industry is continuously adapting to new trends and emergent markets. Experts and entrepreneurs in this field must ongoingly take into account many shifting factors that determine the direction of their analysis and decision-making. Therefore, this study focuses on understanding what is perhaps one of the most salient factors, as of late, of our global economy: the worldwide trend of attracting digital nomads and other remote workers to far-off destinations. Unlike remote workers who can work online, digital nomads are known for "roaming" freely with an alternative lifestyle while working and traveling (Müller, 2016). International attention is growing to satisfy these market demands with innovative spaces, such as co-living sites. Co-living is a significantly advantageous alternative that provides a balance between work, home, and social needs by offering co-working areas, high-speed internet, accommodation, and like-minded communities (Lee *et al.*, 2019), however, co-living and its impact on rural areas have been scarcely studied.

Essentially, the study seeks to investigate the fusion and mutual viability of three trends: digital nomadism, co-living, and rural development. The study's objective is twofold: to understand if co-living experiences in rural areas satisfy the needs of digital nomads and remote workers, and to identify whether having satisfying co-living experiences can promote rural development. In this way, the study will explore the three aforementioned trends by analyzing digital nomads and remote worker co-living experiences in Spain with the following research question: *How can digital nomads and remote workers' co-living experiences promote rural development?*

2. Methodology

To accomplish the aims of the study, 18 semi-structured interviews were conducted with digital nomads and other remote workers found in Facebook and Instagram online communities from Spain. The main reason for using online communities is that digital nomads use them to communicate about destinations, taxes, living conditions, social meetings, and other relevant topics (Lee *et al.*, 2019). Co-living hosts were also interviewed as they significantly contribute to the social integration of their guests by organizing community-building events and networking opportunities (von Zumbusch & Lalicic, 2020). Content analysis was utilized to connect main categories to the theory of sense of place and placemaking.

3. Results

The study elaborates on how co-living can be pivotal for attracting these new markets to rural areas that have been mostly neglected in Spain. Main findings include co-living practices

between users, interactions with the local community, barriers and opportunities for rural development, such as a standalone interest in rural tourism. Study participants demonstrated an interest in escaping urban overcrowding, reconnecting with nature, and exploring local cultures, which is convenient for developing projects, as rural areas have the socio-economic opportunity to offer immersive tourism experiences (The World Tourism Organization, 2020; Vaishar & Šťastná, 2020).

4. Conclusions

By understanding these workers' sense of place, the study provides practical knowledge for entrepreneurs and rural communities who want to establish co-living sites and tourism projects that promote sustainability in rural regions.

Keywords: *rural development, co-living, digital nomads, remote workers, sustainable tourism*

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LIFESTYLE MOBILITIES AND COVID-19: IMPLICATIONS AND IMAGINED FUTURES

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6. Introduction

In the last decades, time-space compression, development of telecommunications and globalization lead to exponential growth of spatial mobility (Sheller & Urry, 2006). Sheller & Urry (2006) maintain that mobilities are now shaping every aspect of our lives, indicating the need for a mobility turn in social sciences. Under the emergent ¨new mobilities paradigm¨, the concept of lifestyle mobilities are conceptualized as voluntary mobility practices, of a variable duration, with or without any significant 'home base(s)', that are primarily driven by search of alternative lifestyles and aspirations to increase quality of life (Åkerlund & Sandberg, 2015; Cohen, Duncan, & Thulemark, 2015).

7. Hypothesis

COVID-19 pandemic has drastically changed the reality of the lifestyle movers. This research aims to answer the following question:

What are the implications of COVID-19 pandemic on lifestyle mobilities?

The implications here are understood in a wide sense and divided into themes based on studied relevant literature. The themes include sustainability, economic and political regimes within which the lifestyle movers operate, fear of travel due to COVID-19.

8. Methodology

Under the constructivist paradigm, this research uses qualitative methods as a tool. Instead of using the localizing strategies of conventional ethnography, it intends to gain a holistic understanding of the experiences of lifestyle movers. It therefore does not focus on a specific geographical area. The method used for collecting data are semi-structured in-depth interviews. The method used for analysing the data is thematic analysis.

9. Results

So far, the research has revealed that COVID-19 did affect lifestyle movers on multiple levels. Drawn from the interviews that have been done so far (only 4), respondents generally expressed that they started appreciating spending time amidst nature and with their close friends more than they did previously. They all plan to continue their mobile lifestyles, and are trying to sustain these through valid reasons for travel (study or work). Respondents from non-EU countries currently residing in the EU expressed their concern in regards to the economic crisis that might follow the pandemic and decrease their chances of staying in Europe.

10. Conclusions

The research has not come to its conclusions yet, since most of the data is still to be collected and analysed.

Keywords: *lifestyle mobilities, COVID-19*

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ANALYSIS OF THE PSYCHOLOGICAL IMPACT OF COVID-19 ON FEMALE HOTEL WORKERS: A CASE STUDY OF CRETE

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1. Introduction

COVID-19 is an unprecedented crisis which had devastating effects on the accommodation sector. The Greek economy, which is heavily dependent on tourism, is expected to suffer a significant blow. Crete is one of the most popular destinations in Greece, which receives a large number of international visitors during the summer months. Emerging evidence on the impact of COVID-19 suggests that women's economic and productive lives will be disproportionately affected, with the economic impacts lingering for many years to come even after the end of the pandemic (Nanthini & Nair, 2020). Women earn less, hold jobs that are more insecure and lack advancement opportunities (Nanthini & Nair, 2020). Additionally, women still have the greatest share of household and caring responsibilities, which amidst the COVID-19 crisis have increased their burden of unpaid work (Nanthini & Nair, 2020). Economic crises have been associated with increased suicide rates (Barr, Taylor-Robinson, Scott-Samuel, McKee, & Stuckler, 2012), and insecure employment and unemployment with decrease in psychological wellbeing (Flint, Bartley, Shelton, & Sacker, 2013). Furthermore, COVID-19 has led to an increase in domestic violence rates (Nanthini & Nair, 2020). All these factors put additional pressure on women, compromising their mental well-being (Nanthini & Nair, 2020). Consequently, the research question that my thesis aims to address is the following: How has COVID-19 affected the mental well-being of female workers in the accommodation industry in Crete?

2. Methodology

Due to the novelty of my research topic, my thesis is exploratory. My data collection method is in-depth semi-structured interviews with low-level female employees in the hotel industry and I will analyze the data using the method of content analysis.

3. Results

At the time this abstract was being written, I was still in the process of collecting data. Consequently, I am not able to present any results yet.

4. Conclusions

The aim of my thesis will be to investigate the psychological impact of COVID-19 on low-level female employees in the accommodation industry in Crete. There is no doubt that COVID-19 had crippling effects on the accommodation industry and islands like Crete that are dependent

on tourism will be hard hit. Furthermore, the ongoing pandemic will take its toll on women's livelihoods and mental well-being.

Keywords: *COVID-19, accommodation sector, women, Crete*

5. Bibliography

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THE RENT REDEMPTION, A PROVINCIAL APPROACH: GIRONA (1836-1854)

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1. Introduction

The studies of the ecclesiastical confiscation and the liberal reform still presents some gaps if we take in mind the few works that have studied the process of rent redemption. The rent was steeped in the crowd of properties confiscated by the church. In addition, a large part of this rent was really a credit instrument generated by the church. The fixation for the auctions of the goods confiscated, in the majority works of the second part of the 20th century with interpretative analyses, places an important aspect to understand the totality of the process. Juan Ramón Diaz Espinosa, between 1986 and 1993, was one of the first to insist on the little attention that had been given to rent redemption in the majority studies of the ecclesiastical confiscation. Years later, some studies have proliferated whch have helped to create some interpretative bases for future and more ambitious research.

2. Results

The hypothesis of present work is the little intention of the renters to redeem their rent, in spite of the efforts of the liberal state to do so. It defends the idea that the conditions of redemption, with the possibility of making the cost from titles of debt cheaper, was not beneficial or accessible for the majority of the population tied to rent. This problem, added to the difficulties of the liberal state to manage the volume of confiscated rents, could have propitiated that a large majority of rents were not redeemed. Also, it tries to see if the credit rents of the church were the majority in the group of ecclesiastic rents, so, as defended by the majority of authors, the church was the hegemonic institution of credit until the late 19th century. It tries to address the issue and confirm or refute the hypotheses from the analysis of the redemption deeds from tax authority's notary of Girona region.

3. Conclusions

From the volume of censuses redeemed, the territorial distribution and the real price paid in contrast to the price of capitalization, the study tries to give an answer to the possibilities or intention to redeem between the population. Finally, the differentiation between the typology of the rents, as well as their localization, has shown the importance of the credit in the set of rents and the regional differentiation in the same province of Girona.

Keywords: *Rent redemption, Girona province, ecclesiastical confiscations, liberal reform, credit instruments*

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SESSION XIII. INNOVATION AND TECHNOLOGY

DIGITALLY DEPRIVED CHILDREN IN EUROPE

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1. Introduction

The outbreak of the COVID-19 pandemic has completely changed the need for internet connection and technological devices among the whole population, but especially so among school-aged children. Nowadays, having a computer connected to the internet makes the difference between being able to keep up with their education and falling badly behind. This paper provides a detailed account of who the digitally deprived children in Europe are.

2. Methodology

We use data from the European Union Statistics on Income and Living Conditions. A child is defined as digitally deprived if s/he lives in a household that cannot afford to have a computer and/or lives with adults that cannot afford an internet connection. Importantly, and to our knowledge, this is the only data set that records *enforced lack* (Mack & Lansley, 1985; Marlier, Atkinson, Cantillon, & Nolan, 2007).

3. Results and discussion

We find that 5.3% of school-aged children in Europe are digitally deprived –the differences across countries being substantially large. While in Northern and Continental Europe the percentages of digitally deprived children are low, in the Mediterranean countries and in Eastern Europe the prevalence is higher.

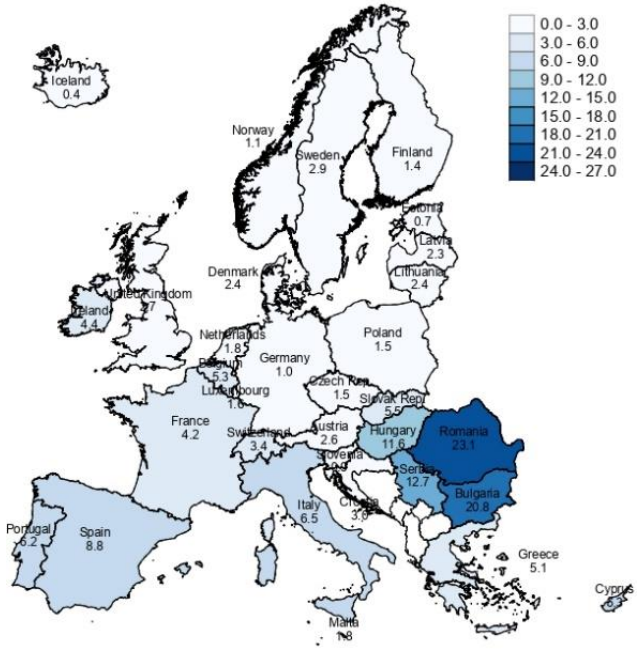

Figure 1. Percentage of digitally deprived school-aged children (6-16), Europe, 2019

Regarding the socioeconomic characteristics of digitally deprived children in Europe, we consider six vulnerable groups: (i) living in a lone parent household; (ii) living in a poor household; (iii) living in severe material deprivation; (iv) from immigrant origin; (v) living with low educated parents and (vi) living in a large family. We find that the digital deprivation affects particularly children in severe material deprivation, that cohabit with low educated parents and in poverty. However, the heterogeneity of characteristics that describe a digitally deprived child is large across country clusters.

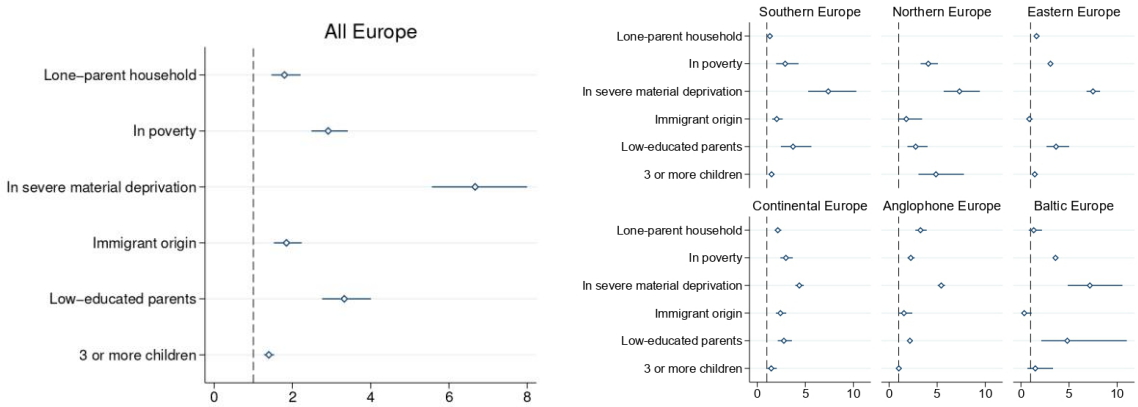

Figure 2. Probability of being digitally deprived, by socio-economic characteristics in school-aged children (6-16 years), Europe and European country clusters, 2015-2019

4. Conclusions and policy recommendations

Finally, we argue that digital deprivation should be considered as part of the definition of material deprivation used by the European Commission to monitor the progress of European societies.

Keywords: *digital deprivation, computer, internet connection, vulnerable children, EU-SILC*

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STUDY ON THE REALIZATION AND DEVELOPMENT OF THE PROJECT "PECT COSTA BRAVA I PIRINEU DE GIRONA: NATURA, CULTURA I INTEL·LIGÈNCIA EN XARXA" WITH MOTIVI-ARCHE APPLICATION

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1. Introduction

This final master's degree project aims to study the use of the application "Motiv-ARCHE" in the PECT project Costa Brava and Pyrenees of Girona: Nature, Culture, and Intelligence network, which was created to develop a new tool for disseminating cultural and natural heritage, from a multidisciplinary and current perspective, with the use of new technologies. The Motiv-ARCHE is an application that seeks to increase students' motivation in issues related to cultural heritage through the use of augmented reality and the creation of heritage routes and itineraries with up-to-date and interactive content for all levels.

The name of the application "Motiv-ARCHE" is born precisely from the description of its objectives. "Motiv" refers to motivation, "AR" because it uses Augmented Reality (AR), "CH" because it focuses on teaching on issues related to cultural heritage (Cultural Heritage - CH), and "E" because it is for education.

This application aims to make it easier for heritage managers to create content and educational resources and become a tool for communication and interaction with users through the content co-creation space. Using immersive technologies, such as Augmented Reality, can be adapted to visitors' preferences, needs, and characteristics of Cultural and Natural Heritage.

2. Hypothesis

The use of mobile applications and augmented reality for renewing methods of disseminating cultural heritage and its pedagogy. Approaches to reach out to the younger generations.

3. Methodology

In the TFM (Master's Thesis), I propose the analysis and study of cultural itineraries through the application in two towns on the Costa Brava, Cadaqués (in the Natural Park of Cape de Creus) and Tossa de Mar.

The study will focus on the analysis of five aspects: 1) the platform developed; 2) the acceptance of the same by the users (heritage experts and end-users); 3) the co-creation process; 4) the quality of the co-created content; and 5) aspects related to the motivation (attention, relevance, confidence, and satisfaction) of the users of the application.

4. Results

The results of the Master's Thesis will focus on analyzing the benefits of using new technologies such as augmented reality, videos, and 3D models to educate and disseminate heritage compared to traditional ones.

5. Conclusions

The conclusions will be based on the results of the analysis of the application of the Motiv-ARCHE app.

Keywords: *Heritage & AR, cultural tourism, augmented reality (AR), Motiv-ARCHE, cultural itineraries*

6. Bibliography

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SCOPE OF LIABILITY ON MACHINE LEARNING METHODOLOGIES: A DESIGNER'S APPROACH

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1. Introduction

Artificial Intelligence is a broad concept that defines the way computers are replicating the human brain (Turing, 1950). It influences every aspect of modern life; innovation emerges from specialized circles. Due to the drastic reduction of digitalization costs, private actors are fiercely competing for data and the best tools to process it. Machine learning methodologies are essential in this goal; they provide competitive advantages that are hard to replicate for those attached to the industrial age. Data mining provides valuable information for anticipating the market, acquiring competitors, and/or optimizing products. As AI machines are based on algorithms that, even after the product is sold, capture and process the required data from the Internet, producers are both obliged and interested in controlling this traffic. It flows either from users, third parties, machines, or other interconnected systems. However, what damages can they cause?

2. Problem

Liability allocation is one of the most relevant market aspects when considering AI systems' complex structures and synergies, not only because they are frequently misunderstood due to the fact that they operate on black boxes (Bathaee, 2018), but because sometimes it is impossible to foresee or control the machine's output. According to Tort Law, civil liability is fault-based; meaning, that the tortfeasor acted wrongfully. In some cases, strict liability emerges when the defendant created a risk: defective product regime is one of those.

Europe has a long tradition of considering products as material things. Services and systems are not part of that regime, so legislators must take action quickly, but IT is moving fast. Information economy specifics generate multiple issues. When considering some aspects such as opacity or foreseeability of ML methodologies, who must be liable when damage was caused by a product or service based on Machine Learning methodologies? The answer has several economic and market implications for those who use or design AI systems. One of the key aspects to assess in this research is the implication of programmer's conduct when designing AI-based systems. Legislators are aiming to impose strict liability to suppliers. In this scenario, courts must have objective factors to consider when judging a party's responsibility. Legislators, SMCs and innovators should also know their role implications. In Torts, the «scope of liability» concept represents that answer. Based on The European Principles of Tort Law — PETL — (European Group on Tort Law, 2008) and IT specifics, the Ph.D. thesis objective is to identify that, or those objective factors, that could determine designer´s liability on ML structuration process.

3. Methodology

This is qualitative research developed on a grounded theory methodology (Strauss & Corbin, 1997). The process to formulate a theory on ML torts liability starts with a six-step procedure: key topic determination, literature skim, literature analysis (coding), concept description, topic construction and writing (Machi & McEvoy, 2016). The first chapter will describe the state of knowledge in AI systems and Tort's relationship. Chapters 2, 3, 4 & 5 will analyze key concepts regarding Torts and IT. Chapters 6 and 7 will develop arguments in order to support the objective theory about ML designing process. The goal is to identify new relationships around already developed concepts and themes on the topic, due to the fact that many technical and juridical factors are already accepted in each field as traditional concepts (post-positivism paradigm).

4. Results and discussion

The researcher has identified critical facts to be assessed in future legislative proposals that should help to maintain a balance between victims' rights and innovation:

a) IT services and products are different because of the remote control that the producer/designer has over it. End User License or confidential agreements are mandatory and there is a commercial interest in maintaining this control. Therefore the duty to prevent damages could also be imposed on the Data manager; b) In absence of AI systems regulation, ethics and industry sector norms play a fundamental role. Designers complied duty to prevent harm could justify an exoneration. Transparency, portability or security are DGPR obligations that should also be part of this analysis; c) Resilient and neutral norms on IT applications must avoid hypes and should be grounded on Tort Law fundamentals. Sector novelty and growing expertise are the source of a whole new field on damages, therefore, millennials Tort's logic and novel Machine Learning procedures, could ground new theories that serves the EU's digital market intentions.

5. Conclusions

Technological applications should be designed according to a well-known framework in order to keep a balance between innovation and a safe market implementation.

Keywords: *AI liability, Digital Market, Defective Products Liability, IT damages*

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TECH STARTUP'S ROLE FOR SUSTAINABLE DEVELOPMENT WITHIN THE SERVICE INDUSTRY JOB TRANSFORMATION

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7. Introduction

Intelligent Automation is transforming the service ecosystem by helping service providers solve business problems and enhance current practices with processes that do not necessarily involve human interference. Therefore, there is public concern about human displacement and the eradication of jobs (Institute of Electrical and Electronics Engineers, 2019; The World Tourism Organization, 2020). This phenomenon will have an impact on all the spheres of the service sector's sustainable development (Nishant, Kennedy, & Corbett, 2020). Existing literature covers the overall societal impact of AI; however, a lack of research where intelligent automation, job transformation, entrepreneurship, and the service sector's sustainable development converge has been identified. Therefore, the present master's thesis aims to fill this gap and contribute theoretical and practical recommendations.

8. Hypothesis

The focus is on the Tech startups that create Intelligent Automation products that could replace human tasks in the service industry, such as AI chatbots and self-service robots. These startups have multiple guidelines available for the ethical application of AI. Nevertheless, these are just persuasion instruments. Research has shown that having more robust AI and driving profit is often more important than acting ethically (Hagendorff, 2020). Thus, the aim is to understand what Tech startups' responsibilities are and the main barriers and advantages they encounter. The first research question is 'What is Tech startups' role in contributing to sustainable development in the service sector job transformation?' The second research question is 'How might Tech startups fulfil their role in contributing to the sustainable development of the service sector job transformation?'

9. Methodology

I designed a research project following the constructivist paradigm. Since there are two research questions, I considered them as two stages. Stage one is based on 12 semi-structured interviews with policymakers to understand Tech startups' role within sustainable development in the service sector. Then, stage two will entail 12 semi-structured interviews with Tech startup members to understand their perspective. Each of the 24 interviews had a duration of between 30 and 60 minutes. After every interview, the information was transcribed and analyzed using the inductive coding approach to identify patterns, determine categories, analyze and interpret them in-depth. Then, I used theory triangulation to increase credibility, using multiple theoretical perspectives to interpret the data.

10. Results

The results show that Tech startups' role is to be aware of their products' socio-economic impact. Moreover, they should offer decent work, which implies designing products that create meaningful tasks for humans. Additionally, ethics should be applied through their managerial practices. Lastly, business models need to be innovative to help to mitigate the negative impact of job transformation. However, these companies present knowledge, time, and resource constraints that limit their capacities of contributing to sustainable development.

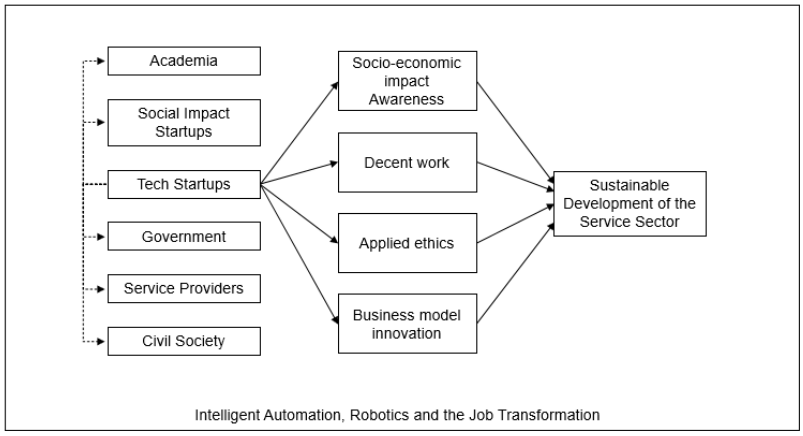

Figure 7. Intelligent Automation, Robotics and the Job Transformations

11. Discussion

Indeed, having more robust AI and driving profit is more relevant than acting ethically (Hagendorff, 2020). Thus, Tech startups might fulfil their role in contributing to the sustainable development of the service sector job transformation by collaborating with other actors of the service ecosystem, finding ways to progress with technological innovation without creating inequalities amidst unsustainable development.

12. Conclusions

Tech startups have multiple roles for contributing to the sustainable development of the service sector job transformation. However, their resources limit their capacities for this. Collaboration with other actors of the service ecosystem might be a way to overcome these constraints.

Keywords: *Artificial Intelligence, Intelligent Automation, Service Sector, sustainable Development, Human-Machine cooperation*

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CONSEQUENCES OF TECHNOSTRESS AND ITS IMPACT ON THE QUALITY OF ORGANIZATIONAL MANAGEMENT

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[3] *University of Valencia*

1. Introduction

The doctrine that supports an adequate organizational management based on internal control, risk management and information security, described in this thesis, reveals that the most representative risk is techno-stress (Cuervo Carabel, Orviz Martínez, Arce García, & Fernández Suárez, 2018; Mendoza Zamora, García Ponce, Delgado Chávez, & Barreiro Cedeño, 2018; Sabadell i Bosch & García González-Castro, 2015) and its types: anxiety, fatigue and addiction as a consequence of applying Information and Communication Technology (ICT) in the development of procedural action by human talent linked to organizations.

2. Hypothesis

Therefore, the question arises: Does reducing techno-stress increase quality in management? From which an inversely proportional relationship is projected between: higher quality in management, lower techno-stress. In this regard, the following hypotheses arise: H1: It is possible to increase the productive capacity of Human Talent if techno-stress is decreased, H2: The types of techno-stress: techno-anxiety, techno-fatigue, and techno-addiction can decrease if ICT training is increased. In addition, a general objective is established: Determine the correlation between the techno-stress index of human talent and quality in organizational management and specific objectives: (1) Determine the level of impact of techno-stress on the productive capacity of Human Talent; (2) Evaluate the competences related to the use and application of ICT on human talent in the organization; (3) Analyze the behavior of Human Talent after the ICT training provided in organizational policies.

3. Methodology

This action research contributes to change and improvement in management from reengineering in procedural action (Alarcón Espinosa & Torres Paredes, 2017; Vega de la Cruz, Lao León, & Nieves Julbe, 2017). To mitigate techno-stress as a representative risk, empirical and positivist research was undertaken, supported by qualitative and quantitative techniques to obtain information, from the observation and analysis of focus groups; as well as scientific bibliography.

4. Results and discussion

Concomitant to the research carried out between 2016 and 2020, the study contributes to scientific development from various perspectives: on the one hand, the analysis of variables

that affect management, where Human Talent stands out as the manager and responsible for different adverse events that put the organization at risk, as a result of phenomena such as techno-stress due to the use of ICT.

5. Conclusions

The practical proposal provides a SCIGRSI strategic measurement model (SCIGRSI refers to the proposal of a strategic measurement model based on internal control, risk management and information security) to manage risks, including techno-stress in order to establish structured control maps and mitigation plans.

6. Results

The results obtained during the research have been disseminated through publications of books, scientific articles and papers, in national and international events, which has generated important academic and scientific debates.

Keywords: *internal control, risk management, information security, techno-stress, management*

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HUMANIST BUSINESS CULTURE AS THE CENTER OF A STRATEGIC MODEL THAT GENERATES NETWORK CONNECTED VALUE: CULTEX MODEL

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1. Introduction

The new global "lifestyle" requires competitiveness in countries and companies. Ecuador is no exception within this complex context. For the IMF (International Monetary Fund), it is one of the nations that has grown the least in the region (0.5% in 2019 and -9.5% in 2020), with an inadequate employment of 37.9% in 2019 and extreme poverty according to UNICEF which went from 10.9% in 2019 to 19.3% in 2020. (Forum, 2018) places Ecuador in 86th place out of 140 countries measured (90 in 2019) with a score of 55.8 points out of 100 in competitiveness. For this, three pillars are analyzed: (1) Technological adoption: information and communication technologies; (2) Quantity and quality of innovation: and (3) Business dynamism: management supported by a solid organizational culture. The fundamental element to consider within this "operating system" that constitutes the organizational culture are people. If people are the center of a humanistic organizational culture, beliefs and values are related to the deepest motivations that move individuals to act (Dilts, 2004).

2. Hypothesis

Future business strategy is determined by the proper design of a humanistic organizational culture.

3. Methodology

The quantitative - qualitative method is used, which (Bernal, 2006) defines as "a method based on the different ways of seeing social reality, in the way of knowing it scientifically and in the use of methodological tools that are used to analyze it". With 34 questions addressed to organizations with revenues between $5 and $50 million USD, 276 responses were obtained on organizational culture, strategy and project execution; the margin of error is less than 6%. The data were processed with statistical methods such as factor analysis that "summarizes the information to describe it more easily" (De la Garza, Morales, & González, 2013). The study was complemented with interviews.

4. Results and discussion

(Kofman, 2008) suggests that "the bad news is that changing an organizational culture is difficult; it can only be reformulated by new behaviors". (Walsh, 2019) mentions that "culture is the true operating system that requires identifying and nurturing the right set of principles". The results are indicated in the infographic (Figure 1):

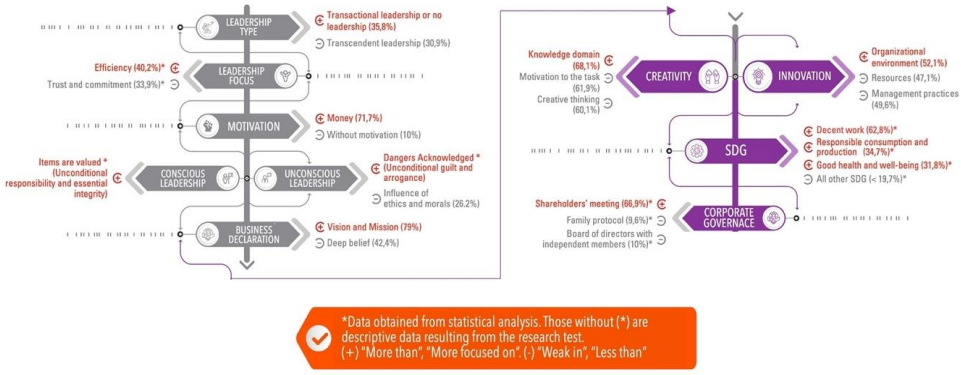

Figure 1. Results of the research on Organizational Culture.

The model used in organizations in Ecuador has a "carrot and stick" orientation towards leadership, extrinsic motivation (money), less influence of ethics, moderate incorporation of innovation, limited knowledge of SDG and little interest in formalizing Corporate Governance; that is, a focus on efficiency.

5. Conclusions

The design of a person-centered culture should contain the following elements: (1) Conscious leadership; (2) Deep belief; (3) Cultural drivers; and (4) Corporate Governance. The scheme is as follows:

Figure 2. Proposed Business Culture Elements.

The balance of the elements allows sustaining a strategic model with future choices, a fundamental part of the CulteX Model (culture, strategy and growth).

Keywords: transformation, competitiveness, CulteX Model, humanism, strategy.

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THE DIFFUSION OF BLOCKCHAIN IN TOURISM

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7. Introduction

Blockchain adoption in tourism lags behind when compared to other industries (Valeri & Baggio, 2020). Currently, its adoption is limited to innovators and early adopters in tourism. Blockchain is a decentralised ledger system that stores blocks of data on a peer-to-peer network. With its inherent traits such as transparency, security, and trustworthiness, it is well-established that blockchain can be used in different business operations. Blockchain can reduce operational cost and improve efficiency by eliminating intermediaries (Attaran & Gunasekaran, 2019; Önder & Treiblmaier, 2018). This study aims to explore the implications of blockchain, the current state of the art and to discover the challenges and barriers for broader blockchain diffusion in tourism. It applies the diffusion of innovation theory by Rogers as a conceptual framework. The five attributes such as relative advantage, compatibility, complexity, trialability and observability have an impact on facilitating broader diffusion of a technology (Dibra, 2015; Rogers, 2003). The research question *"How can blockchain contribute to the tourism ecosystem?"* and a sub question: "What are the challenges and barriers for blockchain adoption in tourism?" are explored.

8. Methodology

To explore the phenomenon, 10 semi-structured interviews with the founders and executives were conducted. All the respondents are from enterprises in the tourism (and related) industry that implemented blockchain in their business operations. Respondents were recruited using a combination of purposive and snowball sampling methods. The responses were analysed using thematic analysis.

9. Results

The results suggest that blockchain diffusion is limited in tourism since many enterprises do not yet perceive it as business value to their strategic plans. For potential blockchain adopters, the successful cases of blockchain use in tourism are still limited, specifically, the observability is constrained to a few successful examples. In the current blockchain landscape, scalability is still a challenge since blockchain is not compatible with existing legacy systems. The findings depict that the challenges in blockchain diffusion are due to perceived benefits, compatibility, observability, users' knowledge, and other market barriers.

10. Conclusions

Blockchain contributes to the tourism ecosystem by enhancing efficiency, reliability, and trustworthiness. The main implications are in distribution system, smart contracts, loyalty programs, reviews, and identity management etc. Companies implementing blockchain in their reservation system to reduce overdependence on intermediaries have proven

success. Some respondents aim to have a completely decentralised tourism ecosystem which seems to be futuristic for now. Yet the advancement in the blockchain is growing exponentially.

Keywords: *blockchain, diffusion of innovation, tourism innovation*

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ELECTRICITY LOAD PROFILING USING MACHINE LEARNING

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1. Introduction

This research will present the methods used to obtain a precise stratification of typical consumption profiles from the energy measurements using machine learning methods and spatial analysis.

2. Hypothesis

It is relevant for utilities companies to know in detail and with an appropriate periodicity the consumption profiles of their customers. Smart Meters (SM) open the door to an immense amount of data and analysis due to the frequent and accurate consumer information. However, this rich source of information makes conventional methods unable to address the voluminous and fast-paced generation of data.
Hsiao (2015) and Zhou, Yang, & Shen (2017) use clustering techniques with SM measurements to forecast energy consumption. Also, Li, Ji, & Xuehui (2016), Tascikaraoglu & Sanandaji (2016) and Xu, Meng, Katramatos, & Yoo (2016) make use of spatial analysis to load forecasting. This research has encouraged us to use machine-learning techniques combined with spatial analysis to generate more efficient and accurate load profiles in study zones.

The objective of this work is to identify the typical behaviour profile of electricity power users over a certain period of time, based on data gathered from SM.

3. Methodology

First, we deploy a classification methodology to cluster the load-profile time series according to their monthly characteristic behaviours using the Dynamic Time Warping measure. Next, we perform a temporal and spatially constrained clustering technique to extract electricity load profiles in geographic zones (Figure 1).

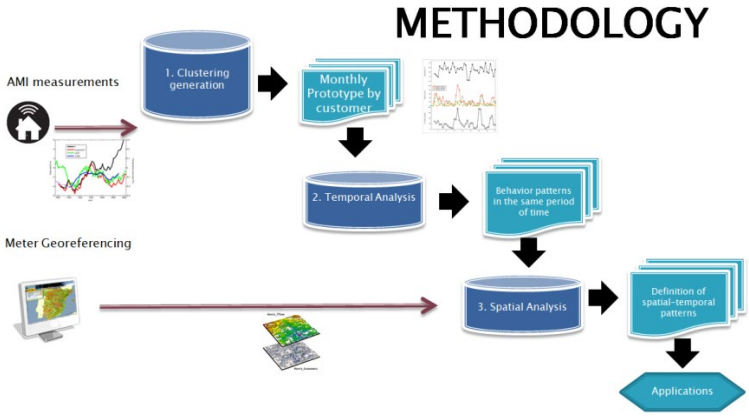

Figure 1. Methodology for defining consumption profiles using ML.

4. Results and discussion

The temporal analysis of measurements gathered by SMs revealed two typical monthly profiles of the consumption. The case of Ecuador revealed a hidden fact that the power profile does not change significantly due to weather variability, but differences may exist during holiday periods. The spatial analysis aims to define geographical zones where all the meters have the same behaviour in the same time period.

The accurate knowledge from the user consumption profile represents a valuable asset that will produce benefits for the utilities companies. From a commercial perspective, the presented methodology allows prioritizing zones in consumer awareness campaigns, whereas from a technical perspective it allows better planning of maintenance activities and a more accurate estimation of future demand. Factors that are useful for network planning.

5. Conclusions

In this study, we have presented a methodology that can generate the electricity load profile in nearby zones. Joining ML methods and spatial analysis allows consumption behaviour profiles to be defined in specific geographic zones with leading to an improvement in the forecast of energy consumption.

Keywords: *clustering, smart meter, machine learning, load profiles, spatial analysis*

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