

IV Conference of Pre-doctoral Researchers Abstract Book

Miquel Solà, PhD (Editor)



IV Conference of Pre-Doctoral Researchers Abstract Book

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Volume IV, 2020

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CONTENT

PREFACE	13
SESSION I: POLLUTANTS IN WATER: DETECTION AND	
PURIFICATION	15
A POLYMER INCLUSION MEMBRANE (PIM) FOR THE REMOVAL OF FLUORIDE FROM NATURAL WATERS	
Berta Alcalde, Clàudia Fontàs, Enriqueta Anticó	17
DEGRADATION OF PERSISTENT ORGANIC POLLUTANTS AND THE SIMULTANEOUS REGENERATION OF GRANULAR ACTIVATED CARBON IN A $_3\mathrm{D}$ ELECTROCHEMICAL REACTOR	
Giannis-Florjan Norra, Jelena Radjenovic	19
PHARMACEUTICAL ACTIVE COMPOUNDS AND THEIR TRANSFORMATION PRODUCTS: A HIDDEN THREAT?	
Marc Castaño-Trias, Lucia Gusmaroli, Sara Rodríguez-Mozaz, Gianluigi Buttiglieri	21
FERTILIZER-DRAWN FORWARD OSMOSIS FOR SUSTAINABLE WATER REUSE IN TOURISTIC MEDITERRANEAN REGIONS	
Esther Mendoza, Gaetan Blandin, Joaquim Comas, Gianluigi Buttiglieri	23
BIOCATHODES AS AN $\mathit{IN-SITU}$ HYDROGEN EVOLVING PLATFORM	
Elisabet Perona-Vico, Laura Feliu-Paradeda, Sebastià Puig, Lluis Bañeras	25
EVALUATION OF TWO BIOSORBENTS, OLIVE STONES AND PINE CONE, FOR THE REMOVAL OF TOXIC METALS FROM AQUEOUS EFFLUENTS	
Marwa Ben Amar, Victoria Salvadó, Khaled Walha	27
SESSION II: TOURISM AND CULTURE	29
TERRITORIAL APPROACH TO THE RELATIONSHIP OF STUDENTS TO	
LOCAL HERITAGE AND INVOLVEMENT OF EDUCATION STAKEHOLDERS: AN EXPERIENCE IN VILLEFRANCHE SUR SAÔNE 69-FRANCE	
Hermínia Andreu i Aparicio, Dolors Vidal i Casellas	31
THE ROLE OF A HOST DESTINATION IN THE CONSTRUCTION OF IDENTITY THROUGH INTERNATIONAL STUDENT MOBILITY	
Karla Quintero, Konstantina Zerva	35

STUDY: THREE SOLAR ECLIPSES OF SPAIN IN 2026/27/28	Ľ
Mohammad Soltanolkotabi	37
BIOCULTURAL HERITAGE, THE ROLE OF INDIGENOUS WOMEN IN THE SAFEGUARD OF THE ANDEAN FOOD HERITAGE: THE CASE OF IMBABURA- ECUADOR	
Sonia Arellano Guerrón, Dolors Vidal Casellas, Silvia Aulet Serralonga	39
THE "VOICES" OF RAMON VINYES, THE "CATALAN SAGE" IN THE CARIBBEAN MAGIC REALISM OF COLOMBIA	
Xavier Colomer-Ribot	41
THE SUBTRACTION-IMAGE: REDUCTION AND STILLNESS IN CONTEMPORARY CINEMA	
David Ferragut	45
SESSION III: METAL COMPLEXES, SUPRAMOLECULAR	
CHEMISTRY AND PEPTIDES	··· 47
A THREE-SHELL SUPRAMOLECULAR MATRYOSHKA ENABLES THE	
SYMMETRY-MISMATCHED CHEMO- AND REGIOSELECTIVE BIS-FUNCTIONA-LIZATION OF C ₆₀	
Ernest Ubasart, Youzhi Xu, Carles Fuertes, Cristina Garcia-Simón, Laura	
Gómez, Harald Maid, Judit Juanhuix, Felipe Gándara, Inhar Imaz, Daniel	
Maspoch, Max von Delius, Xavi Ribas	49
METALLACARBORANES AS PHOTOREDOX CATALYSTS IN WATER	
Isabel Guerrero, Zsolt Kelemen, Clara Viñas, Isabel Romero, Frances Teixidor	51
PEPTIDE CONJUGATES WITH ACTIVITY AGAINST PLANT PATHOGENS	
Pau Caravaca-Fuentes, Jesús Francés, Esther Badosa, Marta Planas, Lidia Feliu, Emilio Montesinos, Anna Bonaterra	53
Rh-CATALYSED CYCLIZATION REACTIONS INVOLVING 1,5-BISALLENES	S
Jordi Vila, Anna Pla-Quintana, Anna Roglans	55
NEW CYTOTOXIC IRON-BASED COMPLEXES AS POTENTIAL	
ANTI-TUMOUR AGENTS	
Marlon Bravo, Meritxell Albertí, Oriol Martínez, María Alonso, Anaís Marsal, Maria Isabel Romero, Montse Rodríguez, Piet Van Leeuwen, Antoni Benito, Maria Vilanova, Jessica Castro	
SITE- AND STEREO-SELECTIVE C-H HYDROXYLATION WITH BIOLOGICALLY INSPIRED OXIDATION CATALYSTS	07
Andrea Palone, Michela Milan, Massimo Bietti, Miquel Costas	59

S	SESSION IV: A BRUSHSTROKE ON THE UdG MASTER'S	61
	UNIÓN PATRIÓTICA IN BARCELONA (1924-1930): ORGANIZATION AND NATIONAL PERSPECTIVE OF ITS INTELLECTUALS	
	Pau Font Masdeu	63
	ART CONSUMPTION IN THE FIRST HALF OF THE 18TH CETURY BASED ON POST-MORTEM INVENTORIES FROM GIRONA	
	Anna Nadal Tenllado	65
	THE IMPORTANCE OF 'KM 0' PRODUCTS IN RESTAURANTS LINKED TO COOKING GROUPS: CASE OF THE PROVINCE OF GIRONA	
	Denis Alvarado Vanegas	67
	MARRIAGE CONTRACTS FROM VIC: A SOURCE FOR THE STUDY OF THE STANDARDS OF LIVING IN THE LATE MIDDLE AGES	
	Juli Moreno Peré	71
	ATTIC RED-FIGURE POTTERY FROM THE IBERIAN VILLAGE OF SANT SEBASTIÀ DE LA GUARDA: AN ICONOGRAPHIC ANALYSIS	
	Marta Prieto i Bayé	75
	ANTIMICROBIAL PEPTIDES AGAINST <i>Xylella fastidiosa</i> : SYNTHESIS AND EVALUATION OF <i>IN VITRO</i> ACTIVITY	
	Jan Atienza, Lluís Moll, Esther Badosa, Marta Planas, Lidia Feliu, Emilio Montesinos and Anna Bonaterra	79
	CONFRATERNITIES IN EARLY MODERN CATALONIA: SOURCES & APPROACHES	
	Francisco Valhondo Domínguez	81
	COMPARISON OF PLA AND PCL ELECTROSPUN SCAFFOLDS FOR THREE- DIMENSIONAL CULTURE OF NON-SMALL CELL LUNG CANCER	
	Nil Naval Ruiz, Emma Polonio-Alcalá, Joaquim Ciurana, Teresa Puig	83
	EVALUATION OF EPOXIDE HYDROLASE CONFORMATIONAL DYNAMICS	
	Cristina Duran, Guillem Casadevall, Eila Serrano-Hervás, Sílvia Osuna	87
	RESOURCES FOR THE DEFENCE OF THE RIGHT TO STAND AS A CANDIDATE IN ELECTIONS TO THE EUROPEAN PARLIAMENT	
	Santiago-Francisco Rodríguez Ríos	89
	<i>EL GENIO DE LA LIBERTAD</i> (1837): AN UNKNOWN TEXT BY RAMON XAUDARÓ	
	Pere Gibert i Geli	91
	STUDY AND DESIGN OF SYN -DIHYDROXYLATION CATALYSTS WITH STERIC MAPS	
	Najoua Choukairi, Albert Poater and Miquel Costas	93

THE SODIUM CHANNEL $\beta 2$ SUBUNIT LOCALIZES TO LIPID RAFTS	
Montse Colomo, Èric Cortada, Ramon Brugada, Marcel Vergés	95
THE MEDICAL-PHARMACEUTICAL <i>LIEUX DE MÉMOIRE</i> IN CONTEMPORARY CATALONIA (c. 1890-1936): OBITUARIES AND BIOGRAPHIES AS ANALYTICAL LABORATORIES IN THE CREATION OF PROFESSIONAL IDENTITIES	
Lluís Coromina Verdaguer	97
SESSION V: GENETICS AND ANIMAL HEALTH	99
SEMINAL FACTORS TRIGGER NETOSIS IN MAMMALIAN FEMALE POLYMORPHONUCLEAR CELLS	
Yentel Mateo-Otero, Fabiola Zambrano, Jaime Catalán, Marc Yeste, Jordi Miró and Beatriz Fernandez-Fuertes	101
GENETIC DIVERSITY AND TEMPORAL STABILITY OF <i>Aristeus antennatus</i> SPAWNING FEMALE'S GROUNDS ALONG THE SPANISH MEDITERRANEA COAST DURING TWO CONSECUTIVE SUMMER SEASONS 2016-2017	N
Melania Agulló, José-Luis García-Marín, Sandra Heras, Laia Planella, Manuel Vera, Alba Abras, María Inés Roldán	103
EXPLORING GLUTATHIONE S-TRANSFERASE MU 3 (GSTM3) AS A QUALIT BIOMARKER OF MAMMALIAN SPERM PRESERVATION	ſΥ
Marc Llavanera, Ariadna Delgado-Bermúdez, Yentel Mateo-Otero, Sandra Recuero, Isabel Barranco, Sergi Bonet, Marc Yeste	105
IDENTIFYING THE FUNCTIONAL ROLE OF AQUAPORINS IN MAMMALIAN SPERM CRYOPRESERVATION	1
Ariadna Delgado-Bermúdez, Marc Llavanera, Jaime Catalán, Sergi Bonet, Jordi Miró, Marc Yeste	
SESSION VI: WELL-BEING AND MENTAL HEALTH AT DIFFERENT STAGES OF LIFE	109
INCIDENCE OF AGING IN PEOPLE WITH INTELLECTUAL DISABILITIES IN THEIR WORK ENVIRONMENT AND THEIR QUALITY OF LIFE	
Hèctor Valenzuela	111
EFFECTS OF A PSYCHOEDUCATIONAL INTERVENTION PROGRAMME ON THE SEXUAL AND AFFECTIVE ATTITUDES OF PEOPLE WITH INTELLECTUAL DISABILITIES WHO ATTEND AN OCCUPATIONAL THERAPY SERVICE	
Jordi Fernandez Suriñach	113

THE WELL-BEING OF CHILDREN WITH EDUCATIONAL NEEDS: LEARNING FROM THEIR SCHOOL-BASED PERSPECTIVES	
Mari Corominas	. 115
PHYSICAL EXERCISE PROGRAMME TO IMPROVE THE HEALTH-RELATED QUALITY OF LIFE OF STROKE SURVIVORS	
Míriam Barra, Bernat Carles Serdà, Arantza del Valle, Montserrat Grau	. 117
EVALUATION OF LOW-DOSE INTRAVENTRICULAR INFUSION OF AMYLOID BETA IN A RAT MODEL TO TEST LONG-TERM TREATMENTS FOR EARLY ALZHEIMER'S DISEASE	
Irene Puig-Parnau, Soleil Garcia-Brito, Laia Vila, Laura Aldavert-Vera, Elisabet Kádár, Pilar Segura-Torres, Gemma Huguet	. 119
SESSION VII: DATA ANALYSIS, COMPUTATIONAL METHODS AND MACHINE-LEARNING TECHNIQUES AS TOOLS FO SCIENTIFIC RESEARCH	121
MARKOV STATE MODELS TO IDENTIFY HIDDEN CONFORMATIONAL META-STABLE STATES IMPORTANT FOR CATALYTIC ACTIVITY	
Christian Curado-Carballada, Ferran Feixas, Javier Iglesias-Fernández, Sílvia Osuna.	. 121
ANALYZING THE KEY FACTORS THAT EXPLAIN SWIMMING PERFORMANCE VARIABILITY IN FRESHWATER FISH	
Carlos Cano-Barbacil, Johannes Radinger, María Argudo, Francesc Rubio-Gracia, Anna Vila-Gispert, Emili García-Berthou	. 125
DIAMONDS ARE A CHEMIST'S BEST FRIEND	
Frederico F. Martins, Lawrence Que Jr., Marcel Swart	. 127
UNRAVELLING THE MILLISECOND ALLOSTERIC ACTIVATION OF IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE (IGPS) BY MEANS OF MOLECULAR DYNAMICS SIMULATIONS	
Carla Calvó-Tusell, Miguel A. Maria-Solano, Ferran Feixas, Sílvia Osuna	. 129
MONTE CARLO METHODS FOR BOLSTERING THE CONFIDENCE IN INDICATIVE CLUSTERING OF SCARCE MORBIDITY SETTINGS	
Enrique Y. Bitchatchi	. 131
RATIONALIZING THE REGIOSELECTIVITY CONTROL OF DECANOIC ACID HYDROXYLATION BY P450-TT ENZYME USING MOLECULAR DYNAMICS SIMULATIONS	
Jordi Soler, Marc Garcia-Borràs, Sílvia Osuna	. 133
APPLICATION OF ADVANCED ALGORITHMS FOR THE PREDICTION	

Mireia Plà-Castellana, Oriol Gutierrez, Jordi Raich-Montiu, Wolfgang Gernjak	135
MACHINE LEARNING ALGORITHMS AS A CLINICAL TOOL TO DIFFERENTIATE LYMPHOPROLIFERATIVE DISORDERS	
Javier Nieto-Moragas [,] Anna Marull, Orlando Jiménez, Raul Benitez, Francisco Reina, Maite Serrando	. 137
SESSION VIII: MONA FOUNDATION	139
ENVIRONMENTAL ENRICHMENT IN A SOCIAL SETTING: ASSESSING THE USE OF A NOVEL FOOD MAZE IN SANCTUARY-HOUSED CHIMPANZEES	Ξ
Maria Padrell, Maria Pau Córdoba, Federica Amici, Miquel Llorente	. 141
CHOOSE YOUR EDGE: THE POTENTIAL BENEFITS OF MULTIPLEX ANALYSIS IN CHIMPANZEES' SOCIAL NETWORKS	
Dietmar Crailsheim, Toni Romani, Miquel Llorente, Elfriede Kalcher-Sommersguter	. 143
SESSION IX: BIOMEDIC RESEARCH: CANCER AND HEART	
DISEASE	145
THE SODIUM CHANNEL BETA2 SUBUNIT RELIES ON CHOLESTEROL TO REMAIN AT THE TOP OF THE CELL	
Eric Cortada, Robert Serradesanferm, Montse Colomo, Irene Pulido, Ramon Brugada, Marcel Vergés	. 147
THREE-DIMENSIONAL CULTURE USING POLYCAPROLACTONE ELECTROSPUN SCAFFOLDS WITH NON-SMALL CELL LUNG CANCER MODELS	
Emma Polonio-Alcalá, Sònia Palomeras, Santiago Ruiz-Martínez, Joaquim Ciurana, Teresa Puig	. 149
PREMATURE TERMINATION CODON IN <i>PLAKOPHILIN2</i> (<i>PKP2</i>) CAUSES A DOWNREGULATION OF DESMOSOMAL AND CALCIUM HANDLING GENES IN AN HL1 CELL MODEL OF ARRHYTHMOGENIC CARDIOMYOPATHY	
	151
Marta Vallverdú-Prats, Mireia Alcalde, Ramon Brugada PATTERNS AND FACTORS ASOCIATED WITH INCIDENCE AND	. 151
SURVIVAL OF CHRONIC LYMPHOCYTIC LEUKAEMIA IN GIRONA (SPAIN) 2008–2015: A POPULATION-BASED STUDY	l
Alicia Villavicencio, Rafael Marcos-Gragera, Marta Solans, Marc Saez	153

p.G357S_RYR2 USING PATIENT-SPECIFIC INDUCED PLURIPOTENT STEM CELL-DERIVED CARDIOMYOCYTES (iPS-CM)	
David Carreras, Rebecca Martínez-Moreno, Elisabet Selga, Ramon Brugada, Fabiana S. Scornik, Guillermo J. Pérez	155
CHARACTERIZATION OF MESOTHELIN GLYCOSYLATION: ADVANCING TOWARDS A NOVEL PANCREATIC CANCER BIOMARKER	
Adrià Duran, Pedro E. Guerrero, María José Ferri, Rafael de Llorens, Radka Saldova, Esther Llop, Rosa Peracaula	157
SESSION X: EDUCATION	159
THE PERCEPTION OF THE FAMILY REGARDING THE MEASURE FOR COURT-ORDERED LIVING IN EDUCATIONAL GROUPS IN CATALONIA	
Carme Trull Oliva	161
PEDAGOGIGAL CONTRIBUTIONS OF HOMESCHOOLING	
Maria Bellmunt i Borràs	163
CHARACTERIZATION OF EARLY ALGEBRA IN EARLY CHILDHOOD AND PRIMARY EDUCATION	
Nataly Pincheira Hauck, Ángel Alsina	165
COLLABORATIVE INTERVENTION IN DEVELOPMENTAL LANGUAGE DISORDER (DLD)	
Claudio Bahamonde Godoy	167
AN APPROACH TO VULNERABILITY AND POVERTY CHRONIFICATION: DISCOVERING NEW REALITIES FROM A CASE STUDY	
Eduard Carrera, Quim Brugué	169
PSYCHOLOGICAL WELLBEING OF UNACCOMPANIED MIGRANT YOUTHS IN THE TRANSITION TO ADULTHOOD: THE ROLE OF YOUTH MENTORING IN BARCELONA	
Xavier Alarcon, Magdalena Bobowik, Oscar Prieto Flores	171
RELATIONSHIP BETWEEN EMOTIONAL INTELLIGENCE, ACADEMIC ACHIEVEMENT AND SOCIAL SKILLS	
Georgina Perpiñà Martí, Elisabet Serrat Sellabona, Francesc Sidera Caballero	173
PERSONAL SUPPORT NETWORKS OF YOUNG PEOPLE WITH INTELLECTUAL DISABILITIES: A RESEARCH PR OJECT BASED ON SOCIAL NETWORKS ANALYSIS	
Ana Rey Freire	175

SESSION XI: CLIMATE CHANGE, ECOSYSTEM MODIFICATION AND SUSTAINABILITY	177
ENVIRONMENTAL SUSTAINABILITY IN THE TEMPORARY EXHIBITIONS OF ART MUSEUMS	
Anna Alcubierre Roca	179
WATER RESOURCES MANAGEMENT DURING DISRUPTIVE EVENTS: AN INTEGRATED PERSPECTIVE	
Iban Ortuzar, Ana Serrano, Àngels Xabaida	181
THE ROLE OF HYDROLOGICAL ALTERATION AND SEASONALITY IN THE ECOLOGICAL STRUCTURE OF A METAL POLLUTED PYRENEAN STREAM	
Alejandro López, Helena Guasch, Romero Roig, Iara Jiménez, Anna Vila	183
PHARMACEUTICAL POLLUTION IN A THREATENED COASTAL LAGOON IN S.E. SPAIN	
Jose M. Castaño-Ortiz, Rubén Gil-Solsona, Víctor M. León, Damià Barceló, Sara Rodríguez-Mozaz	185
CABLE FACTORY, A CASE OF RESILIENT ARCHITECTURE	
Fèlix Breton	187
ECOLOGICAL COEXISTENCE OF SPANISH TOOTHCARP (Aphanius iberus) AND INVASIVE EASTERN MOSQUITOFISH (Gambusia holbrooki) IN A SALINITY GRADIENT	
Andrés Fernández-Vilar, Lluís Zamora Hernández and Emili García-Berthou	189
SESSION XII: CRIME, VIOLENCE AND GENDER PERSPECTIVE	191
FRAUD REPORTING IN THE INTERNET ERA: DETERMINANTS AND MOTIVES	
Steven Kemp	193
THE SPACES OF VIOLENCE IN VÍCTOR CATALÀ'S SHORT STORIES	
Carla Riera Roca	195
THE FEMINISATION OF THE CHILEAN STUDENT MOVEMENT	
Natalie Sofía Rojas Vilches	199
CONSCIENTIOUS OBJECTION TO ABORTION	
Alba Lupiáñez Mateu	203

THE INTERNET, FAR-RIGHT POLITICAL PARTIES AND DEMOCRACY: THE USE OF HATE SPEECH AGAINST GENDER THEORY IN SPAIN	
Adrián Alberto Pascale	205
THE TRANSVERSAL EFFECTS OF CULTURALLY MOTIVATED CRIMES ON CRIMINAL LAW THEORY	
Isaac Pratdesava Gonzalez	209
THEY UNDERSTAND THE EMOTIONS: A STUDY OF EMOTIONAL INTELLIGENCE AND PSYCHOPATHIC PERSONALITY TRAITS IN INCARCERATED OFFENDERS	
Glòria Brugués, Beatriz Caparrós	211

PREFACE

The First Conference of Pre-doctoral Researchers of the University of Girona (UdG) was held from 6th to 9th June 2017. It was organized 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. During the Conference, doctoral students of the UdG presented his/her research in the form of oral communications. The abstracts of the conference were collected in an electronic Book of Abstracts. After this First Conference, three more have followed with the same type of organization.

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 to PhD students the opportunity to present and discuss the results of their research with peers. Ability to communicate research to peers and to society is 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, mindfulness, gender equality, research communication, etc.

This year the Fourth Conference of Pre-doctoral Researchers of the UdG was organized by 10 volunteer PhD students that did an excellent work in difficult conditions. The Conference, held from 13th to 16th July 2020 at the Faculty of Medicine and Nursery, was the first in-person activity that was offered at the UdG after the first lockdown. Recommendations given by Office of Occupational Health of the UdG were fully followed to ensure adequate protection of the safety and health of participants. 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 Fourth Conference. They did a great job as organizers and chairpersons of the different sessions!

This book contains the abstracts of the 78 talks given by the participants in the Fourth Conference of Pre-doctoral Researchers of the UdG. They are organized in twelve sections corresponding to the different sessions in which the conference was divided (for instance, one of the sections specifically collects communications from master's students). 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 Fifth Conference of Pre-doctoral students of the UdG.

Miquel Solà Girona, 11th November 2020

SESSION I: POLLUTANTS IN WATER: DETECTION AND PURIFICATION

A POLYMER INCLUSION MEMBRANE (PIM) FOR THE REMOVAL OF FLUORIDE FROM NATURAL WATERS

Berta Alcalde, Clàudia Fontàs, Enriqueta Anticó Chemistry Department, University of Girona

1. Introduction

Many people are exposed to excessive amounts of fluoride through contaminated drinking water coming from natural geological sources. Fluoride intake in low concentrations has beneficial effects for both bones and teeth, making them denser and harder. Nonetheless, in prolonged exposure at high concentrations, fluoride can cause dental and skeletal fluorosis. [1] The World Health Organization (WHO) [2] has prescribed 1.5 mg·L·1 as the maximum permissible limit of fluoride in drinking water. However, the concentration of fluoride in natural waters can exceed this value and, therefore, there is a need for simple and efficient techniques to remove this anion.

In this study, we present the use of a polymer inclusion membrane (PIM) to remove fluoride from natural waters. In PIMs, [3] a suitable extractant is immobilized within the chains of a polymer, such as polyvinyl chloride (PVC) or cellulose triacetate (CTA). The polymer provides the membrane with mechanical strength whereas the carrier is the responsible for the extraction. In general, PIMs are easy to prepare, possess good mechanical properties (e.g. strength and flexibility), and are versatile in terms of the target chemical species they can extract.

2. Methodology

The commercial ionic liquid (IL) Aliquat 336 (trioctylmethylammonium chloride) has been used as the carrier for PIM and CTA as the polymer. The effect of the addition of other components to the membrane such as plasticizers (dibutyl sebacate or 1-(2-nitrophenoxy)octane) or the solvating agent tributyl phosphate (TBP) has been investigated. For that, both synthetic solutions of F-(from 10 to 200 mg L⁻¹) and spiked natural waters were used as a feed phase, whereas a 1 M NaCl solution was used as stripping phase.

3. Results

It was found that the best PIM composition was CTA (30%, wt), Aliquat 336 (50%, wt), and TBP (20%, wt), which allowed the quantitative removal of fluoride for the different water types tested. It was observed that the presence of other ions present in water samples affects the kinetics of the fluoride transport, but the PIM was able to remove the anion from naturally occurring fluoride in water. Moreover, the reuse of the PIM was also investigated, and it was found that after 5 cycles of 24 h each, the fluoride removal efficiency only decreased by 11%.

4. Conclusion

In conclusion, it has been demonstrated that a PIM system can be conceived as an efficient and economical solution to remove fluoride from natural waters.

Acknowledgements

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Keywords: Polymer inclusion membranes; Fluoride; Removal; Natural water

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DEGRADATION OF PERSISTENT ORGANIC POLLUTANTS AND THE SIMULTANEOUS REGENERATION OF GRANULAR ACTIVATED CARBON IN A 3D ELECTROCHEMICAL REACTOR

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1. Introduction

Granular activated carbon (GAC) is widely used for the treatment of wastewater as an adsorber, due to its high surface area, porosity, high removal efficiency and adsorption kinetics. The drawback of adsorption is that the pollutants are just removed from the water and not degraded, which causes the saturation of GAC and thus it cannot be reused. Saturated GAC is usually disposed of in landfills, thus causing a serious environmental impact. [1] Besides, the continuous replacement of GAC with fresh GAC is not financially viable. Despite its proven potential, the development of the electrochemical regeneration technology progresses slowly. The two main regenerative processes include the enhanced desorption from the GAC surface (either because of the changes in pH, the ionized species or the electrodesorption) and electrochemical degradation of the desorbed contaminants, either by the main electrodes or the polarized granules. [2] When GAC is placed between two main electrodes, it gets polarized due to its high conductivity and functions as a third electrode converting a 2D electrochemical system into a 3D one, where there is a synergy between GAC adsorption and 2D electrochemical oxidation, because of electrosorption and degradation of pollutants on the surface of GAC. Giannis-Florjan Norra1,2, Jelena Radjenovic2,3

2. Methodology

In this study, GAC that was previously saturated with wastewater, is used as the bed material in a 3D electrochemical oxidation reactor to treat secondary effluent and simultaneously demonstrate its regeneration as a bed material. GAC was placed between the anode and the cathode while not being direct contact with either. In order to investigate the regeneration capacity of GAC, the removal rates of a group of persistent contaminants were calculated, during various consecutive runs in a 3D electrochemical system that had BDD as an anode and stainless steel as cathode. The contaminants were spiked in a certain concentration every time in the secondary effluent that was treated.

3. Results

From Figure 1 it can be observed that there is synergy between adsorption and 2D electrochemical oxidation, which increases after 11 runs, proving that GAC regeneration is happening.

As seen in Figure 2, removals from 80 to almost 90% of iopromide are achieved during the different runs of the reactor.

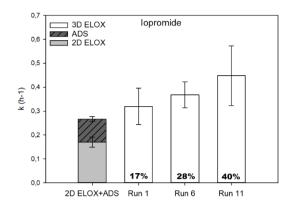


Figure 1: Apparent removal kinetic rate constants and synergies for iopromide degradation over 11 runs. 3D ELOX refers to the 3D electrochemical experiment, ADS refers to the open circuit experiment and 2D ELOX to the electrochemical experiment without GAC.

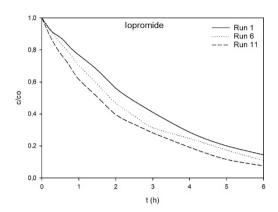


Figure 2: Comparison of iopromide removal between runs 1, 6 and 11, where c/co is the ratio of the actual concentration to the initial concentration of iopromide (time 0)

4. Conclusion

These results are very promising, since in situ regeneration of GAC was achieved, while persistent contaminants were degraded to a high extent in real secondary effluent.

Keywords: Electrochemistry, 3D, Regeneration, GAC, Persistent Contaminants

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PHARMACEUTICAL ACTIVE COMPOUNDS AND THEIR TRANSFORMATION PRODUCTS: A HIDDEN THREAT?

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1. Introduction

Organic pollutants released into the environment in effluents from wastewater treatment plants (WWPTs) can persist, bioaccumulate through the food web, and pose a risk to human health and the environment. The sensitivity of analytical methods has greatly improved in recent years allowing the detection of more contaminants, including the what are known as emerging contaminants. There are many different classes of micropollutants with pharmaceuticals (PhACs), including one of the most important ones, antibiotics. These compounds are not always completely removed in WWTPs and therefore, they have been detected in the aquatic environment worldwide (rivers, seas)^[1] and may pose a risk for the aquatic biota. Pharmaceuticals have actually been detected in aquatic organisms such as mussels^[2] and fish^[3] exposed to contaminated water. In addition, plants (including those intended for human consumption) irrigated by regenerated water can bioaccumulate these compounds (e.g. lettuce, celery).^[4]

Moreover, "transformation products" (TPs) can be formed from parent compounds by means of biological and chemico-physical reactions in WWTPs and/or in the environment and in many cases, they are not detected as they are not targeted in analytical methods. Currently, one of the main challenges in environmental chemistry is the development of strategies to analyse them and study their presence and fate in the environment.

2. Methodology

A comprehensive literature review and prioritization exercise was performed and 65 pharmaceuticals (containing 15 TPs) were selected for monitoring. A tailored analytical method was developed by means of a Waters Acquity Ultra-PerformanceTM liquid chromatograph system coupled to a 5500 QTRAP hybrid triple quadrupole-linear ion trap mass spectrometer (Applied Biosystems, Foster City, CA, USA) with a turbo ion spray source. This method was applied to analyse water samples from Greek islands in different matrices (WWTP influent, river water, sea water), to be compared with similar samples from Catalonia.

3. Results

The sum of all the detected PhACs and TPs concentrations (left) and the fraction of TPs over the total (right) are reported in Figure 1. TPs were present in all selected matrices. Influent wastewater had the highest concentration of TPs. Nonetheless, their concentration compared to non-transformation products is much lower in this matrix than in rivers and seas.

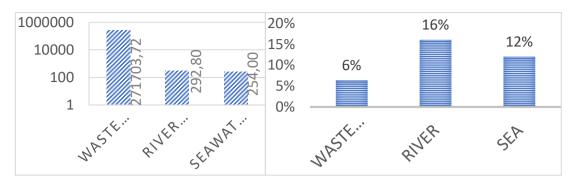


Figure 1. Sum of PhACs and TPs for each matrix: influent wastewater, river and sea (log scale) (left)

Fraction of TPs over total amount (right)

4. Conclusions

A tailored method to detect and quantify both pharmaceuticals and TPs has been developed. TPs were detected in all matrices, with higher relative abundance in rivers and seas compared to wastewater. New methods are required to also study their presence in food and biota that can be exposed to them through contaminated water.

Keywords: Organic micropollutants, Transformation Products, Monitoring, Wastewater

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FERTILIZER-DRAWN FORWARD OSMOSIS FOR SUSTAINABLE WATER REUSE IN TOURISTIC MEDITERRANEAN REGIONS

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1. Introduction

Touristic cities of the Mediterranean region face challenges related to the intense use of fresh water and its scarcity in the area. Thus, the reuse of reclaimed wastewater may represent an important source of water and nutrients.

In forward osmosis (FO), a concentrated solution (draw) is diluted by a less concentrated solution (feed) thanks to a dense semipermeable membrane. FO is driven by the difference in osmotic pressures between feed and draw, avoiding the need for hydraulic pressure. Although FO presents high rejection and low fouling propensity, reverse solute fluxes lead to the loss of solutes from draw to feed. In fertilizer-drawn forward osmosis (FDFO), osmotic dilution of the fertilizer draw solution occurs and is applied in plant irrigation, as it contains essential nutrients for plant growth.

This study aimed to evaluate the potential of FDFO to dilute reclaimed water with a fertilizer solution in order to reach a proper nutrient ratio (NPK: nitrogen, phosphorous, potassium) to nourish hydroponic systems with edible plants.

2. Methodology

Commercial hollow fibre membrane modules (HFFO2, 2.3 m^2 , Aquaporin) were used at the FO lab scale system. The draw solution contained different concentrations (Table 1) of KNO₃ and (NH₄)₂HPO₄ (DAP), commonly used fertilizers worldwide. [4] DI water was used as feed solution. Initial volumes were 2 L for draw and 60 L for feed solutions. The water flux crossing the membrane (J_w , from feed to draw) was determined by mass increase of the draw solution. Ion concentrations were analysed by ion chromatography.

3. Results

Water fluxes and nutrient losses from draw to feed were diverse throughout the tests (Table 1). Higher water fluxes were found in tests with a higher initial salt concentration, because of the higher osmotic pressure difference between feed and draw.^[5] Cations (ammonium and potassium), with equivalent size and charge, had very similar reverse fluxes (Table 1). In the case of anions, while nitrate presented the highest losses, phosphate, the biggest ion with three negative charges, had minimal losses.

Concentrations close to the targeted ones (i.e. N: 120mg/L; P: 60mg/L and K: 200mg/L) were reached with some ratios (Figure 1), although not for all elements within the same test.

Conversely, with other studies, where the final draw solution needs to be further diluted to be used in irrigation purposes, this configuration could lead to direct application.

Table 1. Water flux and nutrient loss of FO tests					350 .			
Test	init concentr draw so (N	ation in	Jw (L.m-	% nutrient loss from draw to feed (reverse salt diffusion)			300 250	
	KNO₃	DAP	2.h-1)	K⁺	N- NH ₄ ⁺	N- NO ₃ -	P- PO ₄ ³⁻	100
MIX 0	0.05	0.050	5.7	17	17	41	2	50
MIX 1	0.10	0.050	6.6	20	22	35	1	
MIX 2	0.08	0.030	4.0	24	24	37	0	mxo mx2 mix2 mix3 mixa mixs
MIX 3	0.20	0.050	2.6	24	24	33	1	≥ P
MIX 4	0.10	0.025	5.6	27	30	36	2	····· N-target —— P-target — — K-target
MIX 5	0.15	0.025	6.9	30	27	30	1	Figure 1. NPK final and target concentrations for FO tests

4. Conclusion

These preliminary results show the potential of FDFO as a promising technology for sustainable water reuse, since this configuration could reach a proper NPK ratio for direct application of the solution in hydroponic system.

Keywords: forward osmosis; fertigation; water reuse

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BIOCATHODES AS AN *IN-SITU* HYDROGEN EVOLVING PLATFORM

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1. Introduction

Microbial electrosynthesis (MES) is understood as the usage of electricity and CO₂ as the only energy and carbon sources for biosynthesis. This technology is conducted in bioelectrochemical systems (BES) and takes advantage of a reduced number of microorganisms able to capture electrons^[1] and convert them into soluble (energy containing) compounds. Hydrogen (H₂) acts as the key intermediate element to transform electrical current into final products since it can mediate several biological processes.^[2,3] Thus, improving H₂ evolution efficiency via integration of proper microbial catalysts conducting such function is a desirable platform, since biocathodes have been proved to be self-regenerating, inexpensive and non-susceptible to corrosion.^[4]

2. Hypothesis

The aim of this study is to evaluate ten bacterial strains (including *Rhodobacter*, *Rhosopseudomonas*, *Rhodocyclus*, *Desulfovibrio* and *Sporomusa*) as H₂-evolving candidates using a comparable methodology to assess their use in stable biocathodes.

3. Methodology

Bioreactors were composed by H-type cells with two chambers, anodic and cathodic, separated by a cationic exchange membrane. Biocathodes basically consisted of carbon cloth electrodes poised at -o.8 V *vs.* standard hydrogen electrode (SHE) in which monospecific biofilms were formed. H₂ evolution was monitored on line using a microsensor directly placed into the cathodic liquid phase close to the electrode.

4. Results

Despite showing some electroactivity, H_2 evolution rates did not increase significantly for most strains compared to abiotic conditions. The most relevant performance was shown by *Desulfovibrio paquesii* DSM16681 with an 8-fold increase compared to abiotic conditions (45.6 \pm 18.8 μ M·min⁻¹ and, 5.5 \pm 0.6 μ M·min⁻¹, respectively).

5. Conclusions

The presented results indicate that, although most of the microorganisms tested were able to respond to electrons, a direct translation of energy into evolving hydrogen was not obtained for all of them. More data is still needed to understand biotic H₂ production in cathodes and evaluate their use in increasing electron-to-chemical conversion rates.

Acknowledgements

This study received funding from the European Union Horizon 2020 research and innovation programme under grant agreement No 760431.

Keywords: electroactive bacteria, electrochemistry, electro-microbiology, hydrogen, pure cultures

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EVALUATION OF TWO BIOSORBENTS, OLIVE STONES AND PINE CONE, FOR THE REMOVAL OF TOXIC METALS FROM AQUEOUS EFFLUENTS

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- ² University of Sfax/Laboratory of Material Sciences and Environment, Faculty of Sciences of Sfax.

1. Introduction

The discharge of metal-containing aqueous effluents from plating, pigment mining, electroplating, tanning and other industries is the main contributor to metal pollution which is of environmental concern due to the toxicity and non-biodegradability of most of the metal ions [1]. Among the different technologies that are applied for the removal of toxic metal ions, adsorption is deemed as being one of the most effectively techniques. In the search for highly efficient, eco-friendly and economic adsorbents, agricultural are residues such as fava beans [2], bark [3], maize stalk [4], milled olive stone [5]. Cellulosic agricultural waste materials have been successfully used as non-conventional cost-effective adsorbents for removing metal ions due to the presence of functional groups such as acetamido, alcoholic, carbonyl, phenolic, amido, amino, sulphydryl groups etc., which have high affinity for heavy metal ions. Hence, olive stones, pine cones are selected as promising biosorbents for the removal of toxic metals Cd(II), Cu(II), Pb(II) and Cr (VI) from effluent wastewaters.

2. Methodology

The physico-chemical properties of OS and PC have been characterized by scanning electron microscopy, surface elemental analysis, BET surface area analysis, and Fourier infrared spectrophotometry. The adsorption capacity of both biosorbents has been investigated by performing batch experiments and the effects of different parameters such as pH, contact time, amount of adsorbent and initial metal concentration on the removal of heavy metals have also been studied. The equilibrium data was analysed by the Langmuir, Freundlich and Temkin isotherm models and the kinetics of the adsorption processes have been evaluated by the application of pseudo-first-order and pseudo-second-order kinetic equations.

3. Results

The efficiency of milled pine cone in removing trace concentration levels of Pb(II), Cu(II), and Cd(II) has been demonstrated as resulting in capacities of 119.04 mg g⁻¹, 50 mg g⁻¹, and 33.55 mg g⁻¹ at pH 5.5 respectively which are higher than those reported for milled olive stone which were 0.581, 0.557 and 0.3 mg g⁻¹, for lead, copper and cadmium, respectively, whereas chromium gave a maximum capacity of 2.345 mg g⁻¹ and 68.03 mg g⁻¹ at pH 2 for milled olive stone and pine

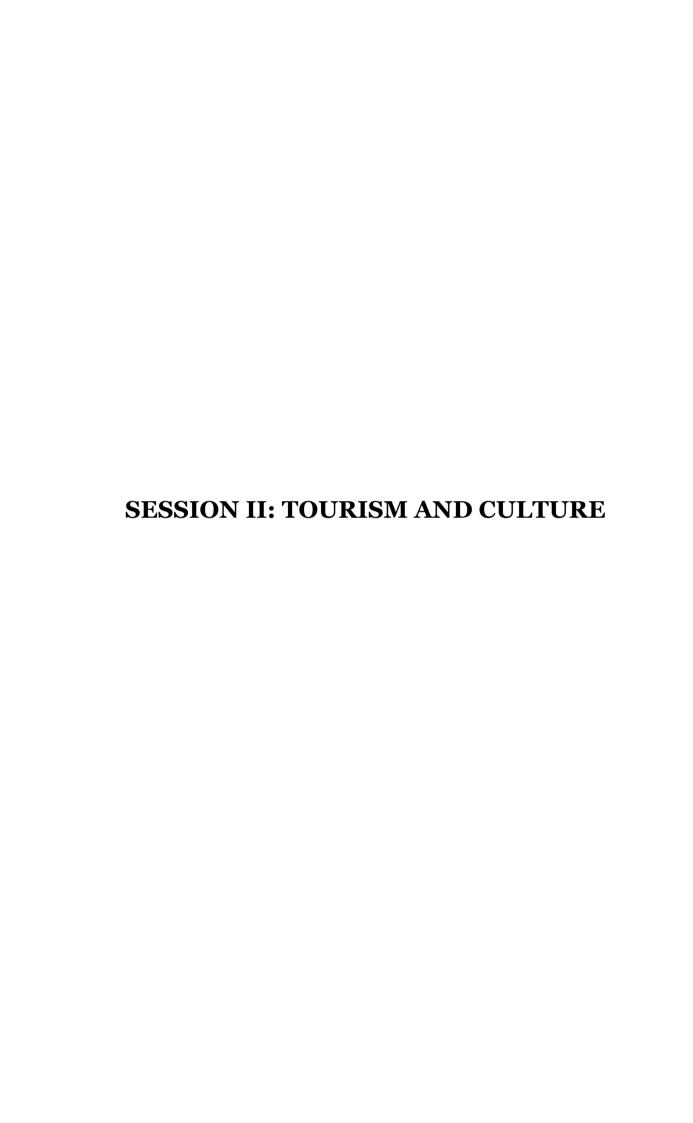
cone respectively. Equilibrium data shows a good agreement with the Langmuir model for Cu(II), Cd(II) and Pb(II), respectively, whereas for Cr(VI), the Temkin model provided the best fit. In the case of pine cone, Pb(II) followed Freundlich, Cu(II) followed the Langmuir model, and Langmuir-Freundlich was the best model for Cd(II) and Cr(VI). The kinetic data fitted well into the pseudo-second-order model for both biosorbents. Moreover, competitive experiments using multi-metal solutions were performed and proved the absence of competition between Pb(II), Cu(II) and Cd(II) on the adsorbent sites at low metal concentration levels (1-10 mg L⁻¹) whereas in the case of pine cone, the sorption capacities of metals decreased to 6.8% (30% reduction) for C(III), and 9.8% (15% reduction) for Cd(II), respectively.

4. Conclusion

The results showed that both biosorbents can be used for the removal of toxic metals from aqueous solutions. Milled pine cone has been demonstrated to be more efficient than olive stone in the removal of Pb (II), Cu (II), Cd (II) and Cr (VI). However, the maximum adsorption capacities for these ions differ depending on the experimental conditions used (initial metal concentrations, dosage of adsorbent and pH). Moreover, the capacity of pine cone to adsorb Cr (VI) is higher than that of milled olive stone.

Keywords: Adsorption, Kinetic, Isotherm, Olive stone, Pine cone

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TERRITORIAL APPROACH TO THE RELATIONSHIP OF STUDENTS TO LOCAL HERITAGE AND INVOLVEMENT OF EDUCATION STAKEHOLDERS: AN EXPERIENCE IN VILLEFRANCHE SUR SAÔNE 69-FRANCE

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1. Introduction

Tourism and its development are said to create regional synergy effects, generating social and cultural benefits in destinations. At the same time, the scale of this phenomenon means that it is able to generate economic growth, making tourism a key factor in regional development policy (Giaoutzi, 2017). Realizing these regional development impacts through tourism is often problematic because of the uneven distribution of impacts in space, among stakeholders, and between economic, ecological and socio-cultural domains.

Tourism is not a concept used very frequently in education. This is because "sightseeing" is associated with leisure, and with pleasure, while education is associated with objectives, compulsory activities and the education system.

Establishing policy frameworks and a culture of collaboration between tourism and non-tourism actors is essential and, practically speaking, often easier said than done.

2. Hypothesis

Teenagers' heritage education in Villefranche sur Saône (69 France) is very poor¹ so their ability to change the interpretation and knowledge level of their own cultural heritage is mostly non-existent, as it is among residents and tourists.

Through innovative action using the young students as actors, public and private tourism agents are urged to create a cultural and industrial heritage tourist route in the village, to be exploited as a tourist product for visitors, residents and at the same time used as a heritage educational tool for other students.

This initiative will exponentially increase knowledge about the heritage of the region among the young people, the residents and potential tourists.

3. Problem

The aim of this study is to better understand the role of cultural tourism development innovation practices in the development of regions, including rural, peripheral and urban areas, by knowing the influence of an educational tourist project on the teenagers' level of knowledge about the heritage of the surrounding region. It also aims to develop a methodology which will become a

¹ See the official education programmes for all the students between 16-18 yrs. in <u>"BAC Général, BAC Technologique or BAC Professionnel"</u> from the French Ministry of Education.

tool to be used in any other region with the objective of developing the heritage education of the young residents.

4. Methodology

Analysis of the GAP between cultural and heritage tourism management and promotion and the youngest residents' (16-18yrs.) perceptions and participation in the development of tourism, through an ad-hoc study about the evolution of the level their knowledge about the surrounding heritage.

Starting with an experimental study which introduces an intervention and studying the effects through an initial reconnaissance survey and research measures including survey questions, interview questions, or constructed situations directly related to the research questions.

Using the method of randomized controlled trial (RCT), the eligible students are randomly assigned to one of two groups. The chosen class of 19 students which is going to develop the project receives the intervention, while the 2 control groups, 79 other students in the same secondary school and 15 teachers, receive nothing. The main goal is to study what happens to people in each group. Any difference in outcomes will then be linked to the intervention.

5. Results and discussion

Originality/value

Overall, the study highlights the discrepancies in the educational national programme in France, the extent of the students' heritage knowledge and the co-creative tourism experience in relation to previous studies on younger students (Barthes, 2017).

Research limitations/implications

This study has some limitations. First, it is highly site-specific and based on a convenience sample, rendering the findings non-generalizable to either the destination under investigation or any other tourism destination. Further studies should be conducted in other medium-sized French cities in order to generalize the significance of these findings. Although the chosen school can be considered a good sample, the fact that the survey was only carried out in a technical college could have excluded students without learning difficulties from a general secondary school from participating in the study. In addition, the study did not consider public educational institutions. In the future, preparing the survey into more accurate content and interviewing an equal sample of all educational establishment types might be useful.

6. Conclusions

In evolution.

Note: this study was carried out before the COVID-19 outbreak so the results of the perception of heritage are what they are. The instruments to improve the enhancement of heritage will be made according to the most innovative methods and systems developed in full COVID-19 and post COVID-19 era. That is why only the first part of the study has started and all the final conclusions will be delayed until "the new normality" is established, obviously also adapting the project to the post COVID-19 new tourism destination management paradigm.²

https://www.researchgate.net/post/The_after_COVID-19_crisis_new_tourism_destination_

Keywords: Innovation, Governance, Education, Policy and planning, Regional Tourism Development, Residents' perceptions, Participation, Cultural, Heritage, Tourism, Regional Development, Destination Management

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management_	_paradigm	

THE ROLE OF A HOST DESTINATION IN THE CONSTRUCTION OF IDENTITY THROUGH INTERNATIONAL STUDENT MOBILITY

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1. Introduction

Tertiary education has become progressively 'internationalized'; that is, students are increasingly willing to move to another country to obtain post school education. While the consideration of mobility in international education in terms of academic development has been a traditional focus, further research has indicated that non-academic considerations such as personal development and growth have emerged to be important factors shaping international student mobility. Host destinations offer students seeking transformation through mobility a range of interactions with the socio-physical environment and tourism experiences capable of influencing identity. Since tourism and travelling are strongly associated with students' mobility, and it is well documented that these two concepts are related to identity issues such as "finding yourself", "self-development" and "self-actualization, a research gap exists in the academic literature when exploring students' identity-related motivations for studying abroad and their connection to the host destination through their daily adaptation and their experiences as tourists. Through the perspective of academic tourism, this study introduces an analysis of the role of a host destination as a place for students to undergo identity transformation encompassing the international student mobility experience.

2. Methodology

For this exploratory qualitative investigation, twenty-eight in-depth semi-structured interviews were performed on international students of different nationalities who had finished a tourism master's degree programme at the University of Girona.

3. Results

This investigation reveals the ability of a host destination to establish strong sentimental and emotional attachment with international students when it provides a) the context to become home; b) change and opportunities; and c) a place for memorable tourism experiences.

4. Conclusion

By demonstrating the transformative potential of a destination in international student mobility, this research suggests the importance of generating positive place experiences to enhance students' intention to re-visit, recommend and promote tourism encounters among future visitors.

Keywords: Identity, place experiences, student mobility, tourism

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ECLIPSE CHASING AND SUSTAINABLE TOURISM DEVELOPMENT. CASE STUDY: THREE SOLAR ECLIPSES OF SPAIN IN 2026/27/28

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1. Introduction

The sky has always been inspiring for humankind. Man has always observed the sky to explore the universe and understand its scientific laws. In the world of astronomy, a total solar eclipse is one of nature's most spectacular shows. A solar eclipse can be a great pretext to promote tourism in a scientific way and eclipse chasing is form of astrotourism that promotes sustainable tourism development. This research is a pioneering work to demonstrate a rare opportunity for Spain to host one of the greatest eclipse-chasing events in history, in 2026, 2027 and 2028. This work aims to study the upcoming phenomena and to start an early comprehensive plan to organize these events. The thesis studies the role of this rare opportunity to promote tourism in Spain based on planning, education and awareness.

2. Hypothesis

The rare opportunity of Spain to observe three solar eclipses in 2026, 2027 and 2028 plays an important role to develop creative ideas in the Spanish tourism industry through eclipse chasing based on scientific, educational, cultural and natural capacities.

3. Results

The early weather forecast models predict clear skies for these great events and the research shows that a large number of travellers will come to Spain primarily to observe the solar eclipses. The author shows that Spain can become the focal point of eclipse chasing in the whole world. The research highlights the potential of growing astrotourism in Spain to support the project. Moreover, a great number of the biosphere reserves of Spain within the eclipse path as well as the roads to Santiago provide a unique situation to host eclipse observers (Soltanolkotabi, 2017).

4. Discussion

The Covid-19 health crisis in early 2020 definitely makes us reconsider many upcoming projects in the tourism industry especially those in the near future. Fortunately, the first eclipse will take place six years after this global pandemic. It does not necessarily mean that this crisis will not overshadow this project but, on the one hand we hope that life will return to normal years before

the first event and on the other, we expect to overcome the possible obstacles by early planning in order to achieve the goals of this research.

5. Conclusion

These events will dominate Spain before, during and after the eclipse days. Early, thorough planning will offer great opportunities to Spain. In fact, early planning for the Spanish eclipses will have a major cultural and educational impact.

Keywords: Eclipse chasing, early planning, Spain, astrotourism, solar eclipse

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BIOCULTURAL HERITAGE, THE ROLE OF INDIGENOUS WOMEN IN THE SAFEGUARD OF THE ANDEAN FOOD HERITAGE: THE CASE OF IMBABURA - ECUADOR

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Introduction

UNESCO in April 2019 declared Imbabura - Ecuador as a World Geopark; soon after, the Cotacachi canton of this same province received the name of "Magical Town". The remarkable geological heritage together with the living culture of the indigenous communities of the Imbabura province has been the key to these achievements.

Objectives and research question

From a qualitative approach, the following research question is posed: Will the study and documentation of ancestral knowledge contribute to highlighting the role of indigenous women as custodians of the intangible heritage of the Imbabura World Geopark? The study proposes to develop specific objectives through which to seek, identify, classify, inventory and document good agro-ecological, cultural and social practices. It is a non-experimental and cross-sectional qualitative study, where the field work was carried out in 2017, 2018, 2019 and 2020 in the province of Imbabura. Data collection was carried out through the method of gathering information on oral testimonies; the observation technique was used and in-depth interviews were applied.

Results

The development of this used research: socializing good gastronomic practices applied in indigenous communities and their resilience against COVID-19, these millennial peoples did not suffer shortages during the confinement by the coronavirus, the management of the concept of family farm (small plot of land), will provide them with food permanently. Actions in favor of food sovereignty could be compiled. Its agro-ecological fairs are well known, one of the most important is the Andean native seed fair (Muyu Raymi), an annual meeting that attracts national and foreign visitors. Describe new ways of behaving in tourism enterprises in the face of the coronavirus pandemic, rural communities were better adapted to the change and acceptance of biosecurity protocols required in the post-Covid-19 century. Value Slow Food's proposal as a diversified offer of local products and an ally of gastronomic tourism.

Conclusion

Intangible heritage is liable to disappear if it is not adequately supported; In the Imbabura World Geopark there are several indigenous communities, where tourism-women-knowledge synergies have been created, which translates into a cultural dynamic that contributes significantly to improving the quality of life of its inhabitants, generating opportunities for transformation to the territory in A potential non-crowded emerging destination, ideal for the practice of tourism from an ethno-cultural perspective.

Keywords: Cultural tourism, indigenous women, ancestral gastronomy, intangible heritage, seeds.

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THE "VOICES" OF RAMON VINYES, THE "CATALAN SAGE", IN THE CARIBBEAN MAGIC REALISM OF COLOMBIA

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1. Introduction

This research links the sources that originated in Colombian Caribbean Magic Realism with the postulates that Ramon Vinyes shared with Barranquilla's group. We highlight the main aesthetic and literary concerns that unite Alfonso Fuenmayor, Germán Vargas and Álvaro Cepeda Samudio. These constitute the essential lines of the literary youth of Gabriel García Márquez, which culminate in his great work One Hundred Years of Solitude. We situate the narrative of Ramon Vinyes and Gabriel García Márquez in the coordinates and the themes that are developed within the group. This was an environment where the emergence of the figure of Ramon Vinyes, originally from Berga (Barcelona), was fundamental and his role as teacher of all of them, as a mentor, together with José Félix Fuenmayor, led to the appearance of Magic Realism in Colombia with *Premacondismo*. We work with the sources, some written and others oral, in which the testimonies, evaluations and conclusions that allow me to carry out this investigation are collected. The significance of the circumstances that surrounded the transfer of Vinyes to Colombia is evident. Also, we analyse the narrative of Javier Auqué Lara who, with his novel Los muertos tienen sed, cultivated the sub-genre of the banana novel, which already announces stylistic forms of the first Magic Realism in the Colombian Caribbean. Therefore, we concluded that the arrival of the "Catalan sage" in Barranquilla was essential for the emergence of Magic Realism in the Caribbean and its transmission to the rest of Latin America.



En 1950, Ramón Vinyes decide regresar definitivamente a Berga. Tiene un brazo sobre los hombros de Alfonso Fuenmayor, que a su vez está al lado de Gabo. Germán Vargas está de pie entre otros dos.

Figure 1. https://escoincarceller.files.wordpress.com/2013/08/ramon-vinyes-22.jpg

2. Results

Ramon Vinyes realized in Barranquilla that the path of tellurism had already run its course and that it was necessary to look for other aesthetic paths for the literary expression of America. This is Vinyes' *premacondismo*: how "the Catalan sage" transmitted his theories of new literatures to his disciples in the Barranquilla Group, some of whom he had already brought from Catalonia, from Europe, applied to the modernization of the Colombian novel in particular and Latin American novel in general. He introduced them by reading authors that we can already call classic, and who were the springs from which all the writers of these generations of the first half of the

twentieth century drank. They are mainly Alejo Carpentier and Miguel Ángel Asturias, and also Jorge Luis Borges, Pablo Neruda, Julio Cortázar and Felisberto Hernández. And others such as Franz Kafka, Massimo Bontempelli, Hugo von Hofmannsthal and Friedrich Nietzsche; Gustave Flaubert, Honoré de Balzac and Stendhal; Albert Camus and Jean-Paul Sartre; Charles Dickens, Virginia Woolf and James Joyce; Fyodor Dostoevsky and Leo Tolstoy; and William Faulkner, Ernest Hemingway, Herman Melville, William Saroyan, John Dos Pasos, John Steinbeck, Erskine Caldwell, and Aldous Huxley; some in versions translated or with a prologue by Borges himself and his friends and almost always edited by the publishing houses Losada and Sudamericana.

3. Conclusions

The "Catalan sage" represented for Gabriel García Márquez much more than a literary and/or cultural orientation and his mastery. Especially for what it means going back to the origins, to the classics, updated, modern, or postmodern already. This was one of the main legacies for those young Colombians. Ramon Vinyes was the one who recommended that he flee the local village and look for the global, universal village, Macondo. He convinced Gabo and his friends that from Barranquilla one could be literally as modern as from any great city in the world. This is the idea that he spread among his disciples and that produced so many good results, and not only in the Barranquilla Group. This is what made it easier for García Márquez to find what he had been looking for so many years since he began writing the original for La Casa. Ramon Vinyes laid the foundations of Caribbean Magical Realism in Colombia. Gabriel García Márquez witnessed the generational change, the testament of the "Catalan sage", and was able to adapt it to Colombian literature.

Keywords: Ramon Vinyes, the "Catalan sage", Barranquilla's group, Gabriel García Márquez, Javier Auqué Lara.

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THE SUBTRACTION-IMAGE: REDUCTION AND STILLNESS IN CONTEMPORARY CINEMA

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1. Introduction

Throughout the first chapter of *Matter and Memory*, Henri Bergson (2006 [1896]) describes the link between living beings and the world in *three* stages: perception, affection and action. The link begins with the receipt of specific images of objects (first stage), which changes the positioning and the connection living beings have with the world (second stage). With this, living beings immediately modify the objects received (third stage). This same diagram (used as method of analysis) is recovered by Deleuze (1984) in *The Movement-Image*, in which a type of cinematic image is assigned to each stage: perception-image expresses movement; affection-image reveals the transformation of faces and bodies; and action-image follows the characters' processes and outcomes.

2. Results

However, a gesture remains hidden: all images received by living beings are a selection, in other words, only a part (and not the totality) of the images are perceived (Meillassoux, 2018). This coincides with filmmaking, in which some components are chosen over others (Marrati, 2003) – thus selecting frames and time fragments. A logical process based on the reduction of components achieves a minimalist, subtractive image (Fiant, 2013). The subtraction-image is a type of image not mentioned by Deleuze and inferred from Bergon's diagram. This image occupies an empty (and virtual) space in Bergson's diagram in that the stages of perception, affection, and action presuppose subtraction. This paper proposes that if the subtraction-image is detached from the diagram, an image of stillness appears (Jaffe, 2014; Muñoz Fernández, 2017), since the link between living beings and the world is hindered. The stillness allows for connections to be created between the two image systems that Deleuze proposes, which correspond with his two texts on cinema (Rancière, 2018): it is possible to drift from the Movement-Image (related to the actions and narratives of classical cinema) to the Time-Image (related to the unpredictable actions and long takes of modern cinema).

3. Conclusions

This paper illustrates this possibility by analysing *The Turin Horse* (Béla Tarr, 2011), a film built on – and structured around – the gradual elimination of components (images). This removal of

elements leads the characters to a narrative paralysis, perpetually waiting for their own disappearance – and as such, epitomizing the definitive subtractive gesture.

Keywords: movement, image, subtraction, minimalism, cinema

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SESSION III: METAL COMPLEXES, SUPRAMOLECULAR CHEMISTRY AND PEPTIDES

A THREE-SHELL SUPRAMOLECULAR MATRYOSHKA ENABLES THE SYMMETRY-MISMATCHED CHEMO- AND REGIOSELECTIVE BIS-FUNCTIONALIZATION OF C₆₀

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1. Introduction

Functionalized fullerenes exhibit improved solubility and different chemical and physical properties that allow applications in multiple fields, for example in organic solar cells, redox flow batteries or biomedical applications. Since fullerene functionalization lacks regioselectivity against multiple additions of a product, the development of new synthetic strategies capable of restricting the regioisomer formation remains challenging.^[1] Recently our group published a supramolecular mask strategy, which is a useful tool for the regioselective Bingel-Hirsch cyclopropanation of C₆₀ leading to *e,e,e,e*-Tetrakis-adducts.^[2]

2. Hypothesis

The work presented here has taken a step forward, combining an enlarged self-assembled supramolecular nanocapsule, $\mathbf{6} \cdot (BAr^F)_8$, and a cycloparaphenylene ring, [10]CPP, which is a suitable directing group,^[3] to develop a new heteroleptic three-shell Matrioshka, $C_{60} \subset [10]CPP \subset \mathbf{6} \cdot (BAr^F)_8$. The main objective of this work is to develop a new regioselectivity in the Bingel reaction's product, aiming for the formation of one single isomer.

3. Methodology

The synthesis of the supramolecular nanocapsule, $\mathbf{6} \cdot (BAr^F)_8$, is performed by a self-assembly reaction of Zn-porphyrin (2 eq.) with a Pd or Cu-based macrocyclic clip (4 eq.). Then, by a host-guest equilibrium, the $C_{60} \subset [10]$ CPP is added. The whole structure is characterized by HR-ESI-MS and NMR techniques. To undergo the Bingel reaction, NaH (5 eq.), used as the base, and a bromomalonate (5 eq.) are added sequentially and the reaction is stirred for 16 hours under N_2 . Crystallographic data is obtained for the starting three-shell Matrioshka compound as well for the product trapped at the inner shell. The characterization of the realized product, *trans-3-C*₆₀, is performed by UV-Vis, NMR, HPLC.

4. Results and discussion

Control experiments for this newly developed system show that no host-guest assembly is formed unless the three components of the Matrioshka are present, which is an example of a supramolecular key-lock assembly. The synergistic effect of the tetragonal prismatic nanocapsule and the hoop-like [10]CPP molecule severely limit the exposed surface of the C_{60} entrapped and lead to the selective formation of *trans-3* bis-adduct.

5. Conclusions

In conclusion, we have developed a new system based on a three-shell heteroleptic Matryoshka assembly, $C_{60} \subset [10]$ CPP $\subset 6 \cdot (BAr^F)_8$, found to be an effective system to produce solely the *trans-3*- C_{60} regioisomer. This strategy can become a strategy to synthesize very challenging regioisomerically pure fullerene bis-adducts, which in turn may lead to further advances in organic electronics and solar cells.

Keywords: host-guest chemistry, supramolecular Matryoshka, regioselective functionalization of C₆₀, fullerene derivatives, supramolecular mask strategy.

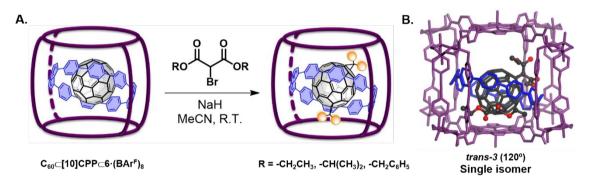


Figure 1. A. Schematic representation of the Bingel reaction inside the three-shell supramolecular Matryoshka. **B.** Crystallographic structure for the trans-3-C₆₀ \subset [10]CPP \subset 6·(BAr^F)₈.

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METALLACARBORANES AS PHOTOREDOX CATALYSTS IN WATER

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1. Introduction

The development of photocatalytic methods for organic transformations is an important challenge in the effort to make a more environmentally friendly world. Solar energy and water are the right alternative energy sources for the development of non-fossil-based fuel. [1] Cobaltabisdicarbollide $[3,3'-Co(1,2-C_2B_9H_{11})_2]$ is the most studied of metallabisdicarbollide due to its properties [2] and water solubility. [3] The interactions in a supramolecular approach seem to be significant in the processes of electron transfer and therefore in the effectiveness of photocatalytic systems. [4]

2. Methodology

The cobaltabisdicarbollide salts were prepared by cationic exchange resin from cesium cobaltabisdicarbollide. We describe the photocatalytic behaviour of cobaltabisdicarbollides (Figure 1) in the oxidation of alcohols in water using $Na_2S_2O_8$ operating under homogeneous conditions by exposure to UV irradiation. Different bases, NEt_3 and K_2CO_3 , are also tested. We planned this research at two levels, under 0.4-1% mol and the other under more dilute conditions, 0.01-0.1% mol of catalyst vs. substrate. The reaction product was quantified and characterized by 1H NMR spectroscopy and by gas chromatography.

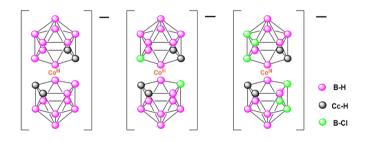


Figure 1. Cobaltabisdicarbollide complexes used in this work

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3. Results and discussion

A concentration of catalyst 0.4 mmol % shows moderate to high yields with selectivity ≥99 % and conversion enhanced by the presence of electron-donating substituents. Increasing acidity produced in the system could be responsible for the moderate yield. Thus, the use of a weak base (Et3N or K2CO3) increases the yield. Hexachloro derivate as a catalyst shows slightly higher activity than dichloro, probably due to the enhanced oxidizing capacity of CoIV as a consequence of the presence of more electron-withdrawing substituents on the metallacarborane. The reduction of the catalyst to 0.1 mol % revealed that primary alcohols were slightly less reactive than secondary ones and the 0.01 mol % catalyst loading shows high efficiency towards aliphatic alcohols.

4. Conclusions

It has been demonstrated that cobaltabisdicarbollides are efficient tunable photoredox catalysts for the oxidation of alcohols in water, through single-electron transfer processes. This behaviour has been possible thanks their high solubility in water, their lack of photoluminescence, their high oxidizing power for the couple $\mathrm{Co^{4+/3^+}}$ and the easy modification of the HOMO-LUMO gap, among other characteristics.

Cobaltabisdicarbollides showed high conversions and selectivity values in the photooxidation of alcohols, with yields near 90-95%, using catalyst loads of 0.4 mol %, in neutral media. By reducing the catalyst load to 0.01 mol %, quantitative conversion of reactants to products was achieved, reaching TON=10000. This value is among the highest turnover number achieved in the alcohol photoredox oxidation performed in homogeneous conditions.

Keywords: carboranes, cobalt, homogeneous catalysis, oxidation, photochemistry

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PEPTIDE CONJUGATES WITH ACTIVITY AGAINST PLANT PATHOGENS

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1. Introduction

Plant diseases caused by pathogenic bacteria are responsible for economic and environmental problems. ^[1] The scarcity of compounds available for their treatment and their negative effects on human health and the environment have prompted the development of new pesticides. Antimicrobial peptides, which display selectivity, biodegradability and difficulty in generating bacterial resistance, seem to be a suitable alternative to control these diseases. ^[2] Some of them have been modified in order to improve their biological properties. The conjugation of peptides with different properties could be an efficient strategy to obtain bioactive sequences. ^[1] Herein we have conjugated the antimicrobial peptide BP16 with the plant resistance elicitor flg15 and evaluated various *in vitro* and *in planta* properties of the resulting conjugates.

2. Methodology

Peptides were synthesised on solid-phase, purified, and analysed by HPLC and mass spectrometry. [3] The *in vitro* antimicrobial activity was determined from the minimum inhibitory concentration, haemolysis was evaluated by analysing the haemoglobin release from erythrocytes and phytotoxicity was measured by infiltrating peptides in tobacco leaves. [3,4] Moreover, 11 genes related to the expression of plant defences were tested from tomato plants by qPCR. [5] *In planta* assays were performed using pear and kiwi plants. [5]

3. Results and discussion

As expected, BP16, but not flg15, showed antibacterial activity against several phytopathogens. The conjugate BP358 (flg15-BP16), which was low haemolytic and phytotoxic, was more active than BP359 (BP16-flg15) and BP16. Thus, BP358 was selected for further assays. Regarding defence gene expression in tomato plants, flg15 overexpressed the majority of genes and BP16 did not cause the expression of any genes. The conjugate BP358 promoted the expression of more genes than a mixture of BP16 and flg15. Concerning the *in planta* assays, BP358 and a mixture of BP16 and flg15 significantly reduced the disease in pear plants compared to BP16 or flg15, with an efficacy similar to kasugamycin. In kiwi plants, BP16 alone did not show any activity while BP358 was effective, but less than the mixture of BP16 and flg15 or kasugamycin. An improvement of defence-related genes expression was not observed.

4. Conclusion

Peptide conjugate BP358 and the mixture of BP16 and flg15 showed improved *in vitro* and *in planta* activities compared with flg15 and BP16 alone. Conjugates may be more practical if peptide

expression in plants is required, but the use of a mixture of the corresponding monomers might be easier and cheaper.

Keywords: antimicrobial peptides, peptide conjugates, fire blight, bacterial canker, induced resistance

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Rh-CATALYSED CYCLIZATION REACTIONS INVOLVING 1,5-BISALLENES

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1. Introduction

Among the more common approaches for the preparation of polycyclic systems, transition-metal catalysed cyclizations of unsaturated compounds stands out as one of the most efficient, generating carbocyclic and heterocyclic scaffolds in a single step with perfect atom economy. [1] Recently, increasing attention has been focused on allenes and bisallenes for such related processes. [2] For the specific case of rhodium-promoted cyclization reactions of 1,5-bisallenes, there are only a few examples involving an external unsaturation. [3] Given these precedents, we envisaged developing a cycloaddition reaction of 1,5-bisallenes with alkenes and alkynes, and rationalising, through computational studies, the mechanism of these transformations.

2. Methodology

The first step of the study entailed the exploration of the reactivity between 1,5-bisallenes and either alkenes or alkynes under rhodium catalysis in different reaction conditions. After an interesting reactivity pattern was found, the obtained products were fully characterised and the reaction conditions optimised to improve both the yield and the selectivity. Then the scope of the process was evaluated. In parallel, DFT studies were carried out to describe a mechanistic pathway that was energetically feasible and to explain the experimental results.

3. Results and Discussion

We have efficiently developed a cascade process involving a Rh-catalysed cycloisomerisation of 1,5-bisallenes leading to a non-isolable intermediate, followed by a regioselective Diels-Alder reaction with alkenes to generate polycyclic heterocycles (Scheme 1).^[4]

Scheme 1. Rh(I)-catalysed cycloaddition reaction of 1,5-bisallenes with alkenes.

On the other hand, when the N-tosyl-tethered 1,5-bisallene was tested with dimethyl acetylenedicarboxylate (DMAD) under rhodium catalysis, the outcome was completely different, providing a cis-3,4-substituted pyrrolidine derivative (Scheme 2).

Scheme 2. Rh(I)-catalysed cycloaddition reaction of 1,5-bisallenes with alkynes.

The mechanism is postulated to be a [2+2+2] cycloaddition reaction between one allene moiety and two molecules of DMAD followed by a cyclisation with the remaining allene. The scope of the reaction as well as DFT mechanistic studies are currently ongoing.

4. Conclusions

A new methodology for the synthesis of azepine and oxapine derivatives from 1,5-bisallenes has been developed. Moreover, a tandem reaction was also successfully developed to generate a family of aromatic bicyclic compounds, involving 1,5-bisallenes and alkynes using rhodium as a catalyst.

Keywords: cycloisomerisation, cycloaddition, bisallene, rhodium, catalysis.

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NEW CYTOTOXIC IRON-BASED COMPLEXES AS POTENTIAL ANTI-TUMOUR AGENTS

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1. Introduction

The exponential development of bioinorganic chemistry over the last three decades has manifested the unique properties that transition metals present for the design of new pharmaceutical drugs. [1-2] As an example, some platinum complexes constitute one of the most successful chemotherapeutic treatments. [3-4] We are interested in the development of new anticancer agents based on ruthenium, copper, iron and other metals, to evaluate their cytotoxic activity and their mechanism of action. [5] This study aimed to analyse the cytotoxicity of new nitrogen-based ligands coordinated with iron in ovarian (OVCAR-8) and lung (NCI-H460) tumour cell lines and in the human colon fibroblasts CCD-18Co. We characterized their mechanism of cytotoxicity by analysing their ability to bind DNA and their ability to produce reactive oxygen species (ROS).

2. Methodology

The analysis of cytotoxicity was performed with the MTT assay. The study of the interaction of the compounds with DNA was performed by analysing the mobility shift in agarose gel electrophoresis. To verify whether the metallic compounds have the capacity of producing ROS flow, cytometric assays were performed together with the H2DCF-DA probe. Cell cycle analysis and studies of apoptosis were also carried out by flow cytometry.

3. Results

All the tested compounds exhibited cytotoxic effects against the tumour cell lines OVCAR-8 and NCI-H460. Among them compound C7 presents a cytotoxicity and selectivity for cancer cells much higher than that shown by both cisplatin and carboplatin. Translocation of phosphatidylserine to the external hemi-membrane showed that the cytotoxicity of this compound is produced through apoptosis. The cell cycle analysis also showed that cell death induced by compound C7 is accompanied by an accumulation of cells in the S phase, concomitant with a decrement of Go/G1 cell cycle phase, compared to untreated growing cells. Moreover, tumour cells treated with C7 showed a clear increase in the levels of ROS in a dose- and time-

dependent manner in OVCAR-8 and NCI-H460 cells. Finally, gel electrophoresis mobility showed that in the presence of H2O2 compound C7 interacts with DNA.

4. Conclusion

Compound C7 displays a remarkable and selective antitumor activity higher than that shown by other metallic compounds such as cisplatin or carboplatin. This compound induces apoptosis and generates ROS species that enable it to interact with DNA. Therefore, compound C7 is a promising drug for cancer treatment.

Keywords: iron compounds, ROS, cell viability, antitumor, DNA interaction

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SITE- AND STEREO-SELECTIVE C-H HYDROXYLATION WITH BIOLOGICALLY INSPIRED OXIDATION CATALYSTS

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1. Introduction

Enantioselective aliphatic C-H bond oxidations remain an unsolved problem in organic synthesis. Reagents that are both chiral and capable of oxidizing inherently strong C-H bonds are rare. [1]

Figure 1. Enantioselective C-H bond Oxidation reaction using bioinspired catalyst

In the case of bioinspired Fe and Mn oxidation catalysts, asymmetric oxidations are envisioned from the use of chiral complexes since the initial HAT (hydrogen atom transfer) is performed by a chiral metal-oxo complex, and the subsequent short-lived carbon centred radical is trapped by hydroxyl transfer before planarization (Figure 1). Furthermore, overoxidation of the first formed secondary alcohol product occurred, leading into ketone. Excellent results have been obtained in my research group for the oxidation of N-cyclohexylpivalamide (S1) in MeCN with hydrogen peroxide catalysed by Mn(TIPSecp), leading a yield of K-3 of 84% with an ee (enantiomeric excess) of 91% (Figure 2a). [2]

Within the framework of selective aliphatic C-H bond functionalization, it was recently shown that by strongly interacting with fluorinated alcohol solvents such as trifluoroethanol (TFE) and 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) via hydrogen bonding, the hydroxyl groups of alcohol substrates undergo strong deactivation of the proximal C-H bonds, providing resistance to overoxidation.^[3]

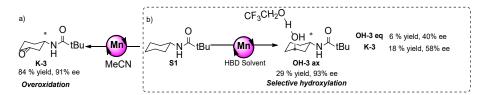


Figure 2. a) Previous work b) Enantioselective C-H Hydroxylation using fluorinated solvents

2. Hypothesis

Building on these initial results, we combined these two concepts with the aim of achieving enantioselective C-H hydroxylation of prochiral methylenes to chiral secondary alcohol (Figure 2b).

3. Methodology

The C-H bond oxidation reaction is carried out in the presence of the catalyst and a carboxylic acid in fluorinated alcohol or acetonitrile, using H_2O_2 as oxidant. Conversions, yields and selectivity are analysed by NMR, mass spectrometry and GC.

4. Results and discussion

Regarding enantioselective aliphatic C-H bond hydroxylation in TFE, with **S1**, we succeeded in obtaining a good ee (93%) and a moderate yield on one of the two hydroxylation products at C-3, **OH-3 ax** (29%). Instead, poor yield and ee were obtained for **OH-3 eq**. The moderate yield of hydroxylated products is due to the partial overoxidation of **K-3** (18%).

5. Conclusion

We have shown that the most reactive C-H bond that gives the highest enantiomeric excess is the axial. The reaction can be extended to other mono-substituted cyclohexanes bearing different substituents, as shown in **Figure 3**, where possible substrates to be investigated are displayed.

Figure 3. Future development for enantioselective aliphatic C-H bond hydroxylations.

Keywords: C-H Oxidation, Bioinspired, Hydrogen peroxide activation, asymmetric, catalysis

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SESSION IV: A BRUSHSTROKE ON THE UdG MASTER'S

UNIÓN PATRIÓTICA IN BARCELONA (1924-1930): ORGANIZATION AND NATIONAL PERSPECTIVE OF ITS INTELLECTUALS

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1. Introduction

This project aims to start research on the official political party in Primo de Rivera's dictatorship, *Unión Patriótica* (UP), through a qualitative analysis of the most remarkable personalities in the city's local party and, to a lesser extent, the province. Taking an analysis perspective of intellectual study, the aim is to define the diversity of political cultures that formed the party. In addition, it is to show which national vision each political culture (or the several leaders) had, for Catalonia and Spain, in comparison to the state party's leadership and intellectuals.

This study will be based on UP press publications – or related publications – and the publications of these personalities in the party, at the local and state levels, with reference to a contemporary bibliography.

The project will have several parts, beginning with a brief statement of the issue and the context. The second part will deal with the deployment of *Unión Patriótica* in Barcelona, emphasizing the party's organization and who the main personalities at its head were, as well as what political career they followed – and what political affinity they had before becoming UP members. The third part will compare the national visions between these leaders and party and government heads.

This is a first step in a wider research project related to a theoretical PhD to study in greater depth the political trajectory of these political cultures, the leaders and what kind of link there was with conservative Catalan sectors, close to *La Lliga* party.

2. Results

At first look, Barcelona's *Unión Patriótica* organization appears to be modern: it had several sections (*youth, workers, culture*) and a hierarchical structure, with Andrés Gassó Vidal as the provincial chief. For other villages and cities, there was a local committee supervized by the provincial chief's delegates. In the city of Barcelona, the party had ten district divisions, each ruling as a local committee with its own board of directors.

Unión Patriótica was a political party that included several political cultures within it. The majority was a monarchic-conservative one, with roots in Catalonia over the previous years. There were also other political cultures such as Carlism and other far-right Spanish nationalists. In nationalist terms, the main difference between monarchist and Carlist and far right members was in the appearance of regionalism: acceptable for the first two (in a non-separatist way) and unacceptable for far-right Spanish nationalists.

Keywords: Primo de Rivera dictatorship, Barcelona, Unión Patriótica, political cultures

ART CONSUMPTION IN THE FIRST HALF OF THE 18TH CETURY BASED ON POST-MORTEM INVENTORIES FROM GIRONA

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1. Introduction

This is a master's degree thesis supervised by Dr Francesc Miralpeix, within the Cultural, Artistic and Political Studies (9th-21st centuries) Research Group led by Dr Joaquim Maria Puigvert. The subject was chosen after realizing that very few studies related to art in domestic spaces in Girona have been written. The chronological choice has been selected in order to fill the documentary void that the first half of the 18th century presents, since traditional historiography generally favoured the second half of the century, and usually extrapolated the results about the late eighteenth century to its entirety.

2. Hypothesis

This thesis aims to establish the evolution of taste and luxury indicators of Girona's local society from 1700 to 1750, drawing on the internal configuration of private art conceived as a reflection of the constant evolution of the owner's taste, fashion, devotion and desire. In order to define artistic consumption patterns and the relationships between the owner and the artistic object, it is necessary to build an intersection of many different methodological points of view. This requires historical, political and religious studies, as well as those of daily life, education and the economy, combined with knowledge of artistic consumption, art markets, collecting, and art history.

3. Methodology

The documentary corpus is based on *post-mortem* inventories from eleven notaries, kept in the Historical Archive of Girona. The data was classified with a Microsoft Access database that relates information about the owner (name, job, social class and home location) to information on the piece of art (type, material, theme, dimensions, location inside the home, its physical condition and price reached if sold at auction).

4. Results

The current studies have shown that the aristocracy had more artworks in their houses than the rest of society; and religious works of art were more prevalent than profane ones. So far, my ongoing study has shown an interesting difference with previous research. All studies to date suggest that there existed a proclivity to place artworks in a "public" room, (e.g. living room) but so far, the data analysed shows that in Girona they used to display their art objects in "private" spaces (e.g. bedrooms). As this is still an ongoing study, its final conclusions will have to wait.

Keywords: Art history; *Post-mortem* inventories; 1700-1750; Girona; Art consumption.

THE IMPORTANCE OF 'KM 0' PRODUCTS IN RESTAURANTS LINKED TO COOKING GROUPS: CASE OF THE PROVINCE OF GIRONA

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1. Introduction

Currently, the different lifestyles and eating patterns of people have generated changes in food trends, prompting a greater demand for healthier products in food and beverage distribution establishments such as restaurants, bars and supermarkets. Therefore, the use of 'km o' products is gaining relevance within the gastronomic world.

'km o' products are linked to a philosophy of life in which ecological values prevail. This new food trend makes people aware of the consumption of healthy products, and promotes sustainable production mechanisms that guarantee the continuity of food resources for future generations. These products are characterized by having a low impact on the environment (since they do not contain chemical elements in their production chain), respecting seasonality and reducing the distance to consumers as much as possible (considered as a radius of 100 km). Therefore, they are healthy local products that keep their organoleptic properties and are a great nutritional resource. Nor should it be forgotten that the commercialization of these products generates benefits for local producers, improving the internal economy of the territory.

2. Methodology

The aim of this research is to define the importance of using 'km o' products in restaurants in the province of Girona. To carry out the research, a qualitative methodology is developed to review scientific documents and seventeen semi-structured interviews with leading people in the restaurant sector (chefs, food journalists, directors of groups, among others). This study seeks to answer the following research questions: How important are 'km o' products to the restaurant groups? What is the possibility of finding 'km o' product distributors in the Girona regions? A menu analysis is also carried out in restaurants that belong to the cooking groups, which have standard online menu. It is important to analyse these establishments since they are an important information and communication link between producers and final consumers.

3. Results and Conclusions

The results of this research will present a current diagnosis of 'km o' products within the catering sector, in addition to the causes and effects produced by the low consumption of these products by society. The analysis developed in this document will allow us to propose a series of strategies that will revalue 'km o' products, highlighting their organoleptic characteristics and the impact that these products generate in the daily life of people and productive sectors.

Keywords: 'Km o' products, Sustainability, Local gastronomy, Kitchen groups.

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MARRIAGE CONTRACTS FROM VIC: A SOURCE FOR THE STUDY OF THE STANDARDS OF LIVING IN THE LATE MIDDLE AGES

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1. Introduction

The study of the standards of living in the late Middle Ages has always been a problematic issue for historians. The absence of major indicators and the commonly localized perspective had led to research that cannot be generalized for all types of society. This is the case of the traditional Catalan historiography, headed by authors like Vicens Vives and Pierre Vilar, who in the midtwentieth century developed a theory about the supposed economic crisis at the end of the medieval age: successive periods of bad harvests and hunger, aggravated by the arrival of the Black Death in 1348, led to a situation of collapse among the servant peasantry. In consequence, this poor community had no other alternative than to fight against their feudal lords, starting with the *remença* revolt and the Catalan Civil War between 1462 and 1472.

Nevertheless, the point of view of this traditional group of researchers was too focused on the area of Barcelona city, and obviated the dynamics of the rural people from the rest of the territory. In order to obtain a larger view of the economic situation of the country, new investigations approaching alternative and local resources revealed that after the direct consequences of the Black Death, there was a boom in the general economy until the 1430s, surpassing that of the era before the epidemic.

According to the previous theory, my hypothesis is that in general, the population of Catalonia had in fact grown economically and demographically between 1370 and 1430, and what is more, it was a period of relative rebalance of the existing social inequality, both within each social class and between different classes. Therefore, my research targets notarial documents, specifically marriage contracts, to reveal the standards of living of the whole population in the region of Vic. These have proven to be useful because they register the monetary amount that is given by one family to the other for the union, called *dot* or *esponsalici*, usually equivalent to the house patrimony. By analysing the entire series of Vic's marriage contracts from the fourteenth century, we can present a whole image of their evolution during the economic growth and decline, and give certain results that could provide insight into the controversial paradigm of the late medieval crisis.

2. Results

My research accomplished analysis of a total of 120 marriage contracts from the region of Vic between 1348 and 1351. These constitute a database with abundant information about the wealth of the families: their jobs, rural or urban residents, what type of possessions they had and who their lords were. Moreover, we can answer questions about the economic patterns or strategic manoeuvres families used at that time by looking closely at these marriages.

3. Conclusions

Marriage contracts are a unique source which can offer a dynamic view of a society over the years, and show the economic transition of the whole population of one area, even though there are internal differences between individual subjects. This research is focused on a period of time when people had struggled through the epidemic of the Black Death and were dealing with the consequences of that terrible event on the population of Vic, measuring the actual impact on their standards of living.

Keywords: Late-middle ages, crisis, Black Death, standards of living, notarial documents, *remença* peasantry.

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ATTIC RED-FIGURE POTTERY FROM THE IBERIAN VILLAGE OF SANT SEBASTIÀ DE LA GUARDA: AN ICONOGRAPHIC ANALYSIS

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1. Introduction

The iconographic study of Attic red-figure pottery from the Sant Sebastià de la Guarda excavation is part of the line of research of the Arqueologia, Prehistòria i Patromoni group (UdG), currently headed by Dr David Vivó, who is also the director of this work. This line of research approaches the study of the past through the material remains found in the course of excavations and archaeological surveys, mostly in the counties around Girona, and has as one of its main objectives the study of material culture in all its aspects.

This research focuses on the iconographic analysis of the Attic red-figure pottery found in silo n°4 of the Sant Sebastià de la Guarda archaeological site (Palafrugell), excavated in 1999. This specific type of pottery imported from Athens was considered a luxury item by the Iberians, whose elites often used it as grave goods or prestigious objects. The study of these archaeological remains can be helpful to deepen the knowledge of these ancient societies, both Iberian and Greek, and also to study the commercial relations they established with each other.

The pieces were located in the SAM (Servei d'Atenció als Museus-Girona), where they were detected, photographed, measured, drawn and described in order to update and complete the records. After that, a piece-by-piece iconographic description of motifs and scenes was performed to attempt to establish chronology, authorship and provenance. Then, similarities were sought with pieces found at other sites on the Iberian Levantine coast and up to Massalia so as to investigate potential commercial routes connecting Athens and Emporion (the nearest Greek settlement in the area).

2. Results

This study attempts to offer another point of view on the Attic red-figure pottery studies. The results so far show that there are pieces of at least two different periods, a great variability in the quality of the ceramics and most of the fragments have stylistic similarities that may indicate only one or few Athenian workshops as departure points for these objects that made a long way through the Mediterranean to reach the "far west" where they were found centuries later.

3. Conclusions

Unfortunately, this research was cut short by the Covid-19 pandemic. In recent months it has been impossible to access the materials to be analysed and this makes it impossible to communicate the results publicly for the moment. Delivery time has been extended, but fieldwork has not yet been completed. This work is unlikely to be defended until December 2020.

Keywords: Iconography, Attic red-figure pottery, Iberia, Greek vases, Sant Sebastià de la Guarda.

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ANTIMICROBIAL PEPTIDES AGAINST Xylella fastidiosa: SYNTHESIS AND EVALUATION OF IN VITRO ACTIVITY

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1. Introduction

Xylella fastidiosa is one of the world's most dangerous plant bacteria, causing a variety of diseases with huge economic impacts on agriculture, public gardens and the environment. *X. fastidiosa* is a gram-negative, rod-shaped (0.25–0.35 \times 0.9–3.5 μ m), non-flagellated bacteria, with twitching motility mediated by type IV pilis, and an optimum growth between 26 and 28°C.^[1,2] It is transmitted exclusively by insects that feed on the sap of the xylem.^[3]

Antibiotics were initially used to fight *X. fastidiosa* with no success. Therefore, other alternatives are being investigated, such as antimicrobial peptides (AMPs).^[4] In this work, two AMPs, which were described as displaying antibacterial and antibiofilm activity against other gram negative bacteria, were selected from the literature. Our aim was to design analogues of both sequences, to synthesize them and to evaluate their antibacterial and antibiofilm activities against *X. fastidiosa*. The two sets of peptides were named **JA1** to **JA3**, and **JB1** to **JB7**, respectively.

2. Methodology

The peptides were synthesized on solid phase, purified and analysed by HPLC and mass spectrometry. *In vitro* antimicrobial activity was determined from a viability test with qPCR and antibiofilm activity was assessed by adapting a method previously described by O'Toole.^[5] The parent peptides were included for comparison purposes.

3. Results and discussion

Most of the peptides showed antibacterial and antibiofilm activity against *X. fastidiosa*. From the first set (**JA1-JA3**), it was observed that peptides with a C-terminal amide group displayed similar activity to those with a C-terminal carboxylic acid group. Moreover, the substitution of a leucine at position 2 with a D-phenylalanine had a negative effect on antibacterial activity.

From the second set, which consisted of lipopeptides **JB1-JB7**, it was concluded that the deletion of a proline caused an increase in antibacterial activity. It was also observed that the incorporation of hydroxylauric acid resulted in an improvement of antibiofilm activity.

4. Conclusions

Since peptides from the first set exhibited similar antibacterial and antibiofilm activities, and taking into account that peptides with a C-terminal carboxylic group are difficult to synthesize, the design of analogues with a C-terminal amide group was preferred.

Regarding the second set, **JB1** to **JB7**, the removal of the proline and the length of the fatty acid had a direct effect on the antibacterial and antibiofilm activity, respectively. A more complete study is needed to analyse all the amino acids of the sequence that are necessary for the activity as well as the length of the fatty acid.

Keywords: antimicrobial peptides, lipopeptides, plant pathogenic bacteria, Xylella fastidiosa

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CONFRATERNITIES IN EARLY MODERN CATALONIA: SOURCES & APPROACHES

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1. Introduction

Since the 1970s, interest in the study of confraternities in the early modern period has increased, perhaps due to the rise of new cultural history. Despite a large number of studies aimed at mere description, and framed in local history, many others have provided a reflection of a scientific nature, in dialogue with other disciplines such as sociology, and with a greater focus on the line of comparative history. These studies were carried out to a large extent in the Catholic tradition territories: France, Spain, and especially Italy.

2. Hypothesis

But in Catalonia, the subject remains largely unexplored, except for contributions from some authors in more general works. This may be due to a lack of interest on the part of historians, but perhaps also to a lack of favourable sources. However, non-catalogued monastic documents have recently been found in the ACA, where there is a lot of documentation referring to the confraternal world.

We propose to study, in the long term (doctoral thesis), the confraternities of early modern Barcelona, with an emphasis on aspects such as the social composition of these associations, how they were financed, or how they could become vehicles for interests outside the strictly religious realm. But in the short term (this final master's thesis), the aim is to make a first sounding based on the confraternities of the city of Girona.

3. Methodology

For this sounding, it has been decided to use the bequests in notarized wills; a type of alternative source that can be used, at least, to complement the most classic sources such as the founding chapters, benefices, censuses, books of accounts or lawsuits.

4. Results

Through the above sources, it is possible guess the socio-professional composition of the city's confraternities and its members over three centuries of the modern era. An exploration of the 18th century confirms a high rate of clergy who made bequests in confraternities, although the highest amounts were bequeathed by the nobility.

5. Conclusions

The number of bequests found during our first sounding has been very low. This leads us to think that the degree of solvency of this source of a notarial nature with regard to the study of confraternities is not very high.

Keywords: confraternities, civic religion, notarized wills, Girona

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COMPARISON OF PLA AND PCL ELECTROSPUN SCAFFOLDS FOR THREE-DIMENSIONAL CULTURE OF NON-SMALL CELL LUNG CANCER

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1. Introduction

Lung cancer is the most diagnosed cancer and the leading cause of cancer death worldwide. Approximately 85% of diagnosed cases correspond to non-small cell lung cancer (NSCLC).^[1] Despite advances in therapies, NSCLC still results in a high percentage of relapses (30-50%).^[2] Traditional *in vitro* cell culture systems do not replicate physiological conditions and tumour environments properly.^[3] To overcome these shortcomings, three-dimensional (3D) structures emerge as a new strategy to study NSCLC. Electrospun (ES) scaffolds can mimic the extracellular matrix (ECM), a fibrous network that enfolds cells and supplies physical structure. ^{4,5} Hence, this study compares two synthetic biopolymers, poly (lactic acid) (PLA) and poly (£-caprolactone) (PCL), using electrospinning technology for 3D NSCLC cell culture.

2. Methodology

PLA was dissolved in chloroform at concentrations of 12 and 15% w/v. A 24G needle emitter with an inner diameter of 0.55 mm was used and a fixed voltage of 9 kV and a flow rate of 2 ml/h were established to manufacture ES-PLA scaffolds. Regarding ES-PCL scaffolds, PCL was dissolved at concentrations of 10 and 15% w/v in acetone. An 18G needle emitter with an inner diameter of 0.80 mm was used and a fixed voltage of 7 kV and a flow rate of 6 ml/h were established to assemble ES-PCL scaffolds. Scaffolds were physically characterized through scanning electron microscopy (SEM). Then, they were seeded with NCI-H1650 and NCI-H1975 cell lines for 3 and 6 days. Cell proliferation on ES-PLA and ES-PCL scaffolds were evaluated by MTT assay.

3. Results

Twelve and fifteen percent ES-PLA scaffolds weighed 6.84 and 8.72 mg and their fibres showed a diameter of 5749.9 and 8309.7 μ m, respectively. On the other hand, 10 and 15% ES-PCL scaffolds weighed 8.74 and 9.06 mg; the fibres measured a diameter of 638.8 and 2727.7 μ m, respectively, and they exhibited non-filamentous structures named beats. NSCLC cells exhibited a higher cell proliferation rate in ES-PLA scaffolds (between 37 and 59% for the NCI-H1650 cells and 29 and 48% for the NCI-H1975 cells) than ES-PCL scaffolds (between 22 and 39% for the NCI-H1650

cells and 4 and 22% for the NCI-H1975 cells). Additionally, cell growth was greater for 3 days (between 22 and 59%) than 6 days (between 4 and 45%) in both cell lines.

4. Conclusions

In summary, ES-PCL and ES-PLA scaffolds could be used for 3D NSCLC cell culture. Although, ES-PLA scaffolds have given a greater proliferation of NSCLC cells, ES-PCL scaffolds have other properties that make them equally interesting.

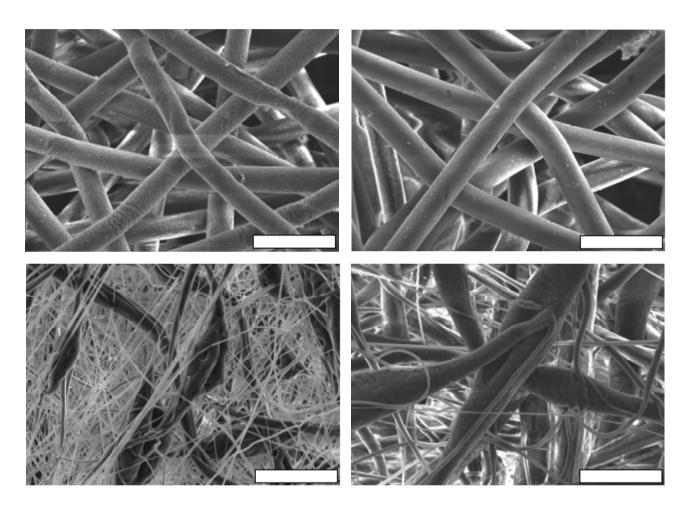


Figure 1. SEM images of 12% PLA (**a**), 15% PLA (**b**) and 10% PCL (**c**), 15% PCL (**d**) meshes. At magnification of x 1500 (Scalebars: 20 μm).

Keywords: non-small cell lung cancer; epidermal growth factor receptor; three-dimensional cell culture; poly(lactid acid); poly (Εε-caprolactone)

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EVALUATION OF EPOXIDE HYDROLASE CONFORMATIONAL DYNAMICS

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1. Introduction

Enzymes sample different thermally accessible conformations that are crucial to their function. These different conformations that exist in dynamic equilibrium are represented in the free energy landscape concept. [1] Any alteration introduced in the enzyme, for example mutations, can induce a redistribution of populations of the conformational states that pre-exist in solution, [2] thus impacting the enzyme catalytic activity. This highlights the important role of enzyme conformational dynamics in enzyme design and evolution.

Epoxide hydrolases (EHs) have shown promising features for preparation of enantiopure epoxides and diols from epoxide racemic mixtures, exhibiting high enantioselectivity that depends on the epoxide substrate structure and its substituents. In particular, *Bacillus megaterium* epoxide hydrolase (BmEH) provides an unusual (R)-selectivity towards phenyl glycidyl ethers (PGE), which is critical for the synthesis of β -blocker drugs.

2. Methodology

We evaluate the conformational dynamics of *Bm*EH through conventional long-timescale molecular dynamics (MD) simulations. We construct the free energy landscape (FEL) of *Bm*EH in the *apo* state and investigate how it is altered by mutations M145A and F128A. To identify which conformational states are relevant for catalysis, we measure active site volume calculations and key geometric parameters to evaluate the pre-organization of the active site in the different conformational states sampled. The optimal arrangement for catalysis of the catalytic residues is taken from quantum mechanics (QM) calculations.^[3]

3. Results

The constructed FELs have unveiled relevant conformational differences between wild-type (WT) and M145A and F128A variants. In all three systems, a conformational state displaying a proper pre-organization of the active site for catalysis is found. Active site volume calculations of these well pre-organized states indicate that mutants have expanded pockets compared to WT. This enlargement happens as a consequence of the introduced mutation, but also due to a conformational change of one catalytic tyrosine with respect to the QM geometry. Previous studies indicated that Tyr144 plays a minor role in activating the epoxide substrate, [3] thus the activity

increase of the variants towards bulkier substrates is explained by the combination of wider active site volumes and proper pre-organization of catalytic residues.

4. Conclusion

Enzyme conformational dynamics linked with other geometric parameters have been crucial to unveiling how the catalytic activity of M145A and F128A mutants towards bulkier epoxide substrates has been increased with respect to the WT. This study suggests that by exploring the ensemble of conformational states of BmEH and evaluating key active site geometric parameters, new variants with high efficiency towards bulky substrates could be rationally designed.

Keywords: Epoxide Hydrolase (EH), Molecular Dynamics (MD) / Free Energy Landscape (FEL), Bulky substrates

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RESOURCES FOR THE DEFENCE OF THE RIGHT TO STAND AS A CANDIDATE IN ELECTIONS TO THE EUROPEAN PARLIAMENT

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1. Introduction

This is the case of two candidates in the elections to the European Parliament who, following their election, were not recognized as MEPs by the Spanish electoral authority because they did not comply with the requirement to abide by the Constitution.

2. Hypothesis

In view of the case presented, which is very topical and bears close resemblance to the so-called "Catalan process", we propose the defence strategy that could best respond to the interests of the Kingdom of Spain Bearing all this in mind, we contemplate the different appeals that could be filed with the Community courts, and if appropriate, with the European Court of Human Rights, and consider the analysis and defence of the non-violation of fundamental rights.

3. Methodology

The scientific method is based on the analysis of norms, jurisprudence and legal literature, with an emphasis on the study of jurisprudence.

4. Results and discussion

Formulated as an initiative to articulate the best procedural strategy for the defence of Spain's interests, well-founded arguments have been put forward to rule out possible appeals.

These are based firstly on Article 8(1) of the Electoral Act,^[3] according to which the electoral procedure is governed, in each Member State, by national provisions.

In this sense, article 224 LOREG^[4] imposes on elected candidates the obligation to promise to or swear to abide by the Constitution. Failure to comply with this requirement will result in the declaration of non-occupancy of seats.

Likewise, having analysed the case law of the Court of Justice of the European Union,^[5] it cannot be ruled out that the European Parliament may adopt any act that contradicts the decision of the Spanish electoral authority.^[6]

^[3] Act concerning the election of the representatives of the European Parliament by direct universal suffrage, annexed to Council Decision 76/787/ECSC, EEC, Euratom of 20 September 1976.

^[2] Ley Orgánica 5/1985, de Régimen Electoral General of 19 June.

^[3] Judgment of the Court (Fourth Chamber), of 30 April 2009, *Donni and Italy v. European parliament* C-393/07 and C-9/08; Judgment of the Court (Grand Chamber), of 12 September 2006, *Kingdom of Spain v. United Kingdom* C-145/04; Judgment of the Court (Second Chamber), of 7 July 2005, *Le Pen v. European Parliament* C-208/03 P.

^[4] This is without prejudice to the implications of the Judgment in Case C-502/19, Junqueras Vies, of 19 December, regarding the moment of acquisition of full M.E.P. status

5. Conclusions

This legal framework, and an effective judicial system before which to challenge the decision of the JEC,^[7] will serve as a basis for claiming the non-violation of any fundamental rights.

Keywords: right to stand for elections, election Law, European Parliament, Court of Justice of the European Union, European Court of Human Rights, Spanish electoral authority

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^[5]Junta Electoral Central as the Spanish electoral authority.

EL GENIO DE LA LIBERTAD (1837): AN UNKNOWN TEXT BY RAMON XAUDARÓ

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1. Introduction

Ramon Xaudaró was a Catalan liberal politician who participated in what became known as the Barcelona *Bullangas* and was executed by firing squad in 1837. In order to contextualize our study of political theory in his book *Bases d'une constitution politique* (Limoges, 1832), we conducted research through digital copies of old newspapers and found various advertisements for the sale of his translation from Italian to Spanish of the work *Las noches romanas en el sepulcro de los Scipiones* (Roman Nights in the Grave of the Scipiones).

Since Xaudaró's translation seemed to be anachronistic (the original Italian was published on 1792), we wanted to see the work, which was difficult because in the catalogues it was attributed to an author named Vandaró (sic). In addition, there was an earlier translation into Spanish: that of Rodríguez de Ledesma, 1821.

2. Methodology

The comparison of the three works (the original Italian and the translations by Xaudaró and Rodríguez de Ledesma) made evident an important difference between them: the chapter entitled *Il parricida* (original Italian) or *El parricida* (Rodríguez de Ledesma) appeared with the title *El Genio de la libertad* (The Genius of Freedom) in the translation by Xaudaró.

3. Results

Lucius Ostius, a character referred to by Plutarch, who considered him the first parricide in the history of Rome, is the central theme of *Il parricida*. Instead, *El Genio de la Libertad* addresses the spectres of the ancient Romans, an elaborate speech on liberty that embarrasses Julius Caesar, who ends up being consoled by Cicero.

4. Conclusion

In conclusion, the sixth chapter of the third night of Roman Nights is not a translation of the Italian, but a new text, drawn from the pen of Xaudaró, that gives us a better understanding of his political thinking.

Keywords: liberalism, Xaudaró, Verri, republic, translation

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STUDY AND DESIGN OF SYN-DIHYDROXYLATION CATALYSTS WITH STERIC MAPS

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1. Introduction

Nowadays, to find out more sustainable processes is a major research topic, especially in chemistry where it is essential to reduce the waste generated, not only for economic reasons, but also for the environment. With the use of catalysts, the products can be obtained with high yields, employing mild conditions and achieving high selectivities.

Unfortunately, the design of good catalysts is a very challenging task, sometimes guided by intuition leading to inefficient catalysts, with the associated waste of time and reagents.

Computational tools can be used in this respect to study how the different ligands perform when combined with the transition-metals. In particular, electronic or steric effects can be used to get better catalysts.

2. Methodology

In this work, steric effects of different iron catalysts for *syn*-dihydroxylation reactions (Figure 1)^[1,2] have been studied through the SambVca2.1 package developed by Cavallo et al.^[3]

Figure 2. a. $[Fe(tpa)(CH_3CN)_2]^{2+}$ b. $[Fe(CH_3CN)_2(5-tips3tpa)]^{2+}$ c. $[Fe(CH_3CN)_2(5-tips2tpa)_2]^{2+}$ d. Syn-dihydroxylation reaction conditions and yield of diol obtained.

As can be seen in Figure 1d, the yield and selectivity of the reaction are higher when [Fe(5-tips3tpa)(CH₃CN)₂]²⁺ is used.^[1]

3. Results and discussion

Firstly, the benchmark was performed using the reported X-Ray structure of [Fe(OTf)₂(5-tips3tpa)].^[1] The best results were obtained with B3LYP functional in combination with Def2SVP basis set at 273K.

Subsequently, the steric maps of the X-Ray structure at 6 Å (Figure 2a) was compared with the one of the computationally optimized structure (Figure 2b) and it was seen that they were very similar, so the optimization can be used as a prediction of new structures without the need of their synthesis in the laboratory. Likewise, the steric maps of the in silico structures [Fe(tpa)(CH₃CN)₂]²⁺ (Figure 2c) and [Fe(5-tips3tpa)(CH₃CN)₂]²⁺ were compared. The bulkiness of triisopropylsilyl (TIPS) groups is very clear, leading us to think that more sterically demanding

ligands increase the catalyst efficiency. However, this might lead to a shortening of the range of substrates, the most sterically hindered ones.

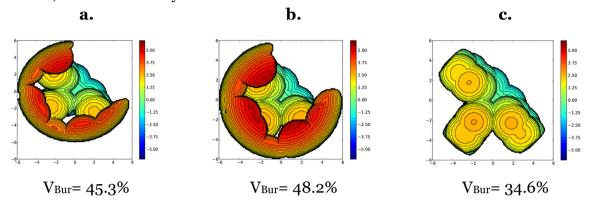


Figure 2. Steric maps of complexes: a. [Fe(OTf)₂(5-tips3tpa)] b. [Fe(5-tips3tpa)(CH₃CN)₂]²⁺ c. [Fe(tpa)(CH₃CN)₂]²⁺

Finally, the steric map of a newly designed complex (Figure 1c) was generated (Figure 3). It is possible to see how the two TIPS give the steric effects required for the reactivity. Moreover, with this new structure, the central pyridine is not occupied, allowing bigger substrates to come close to the metal centre.

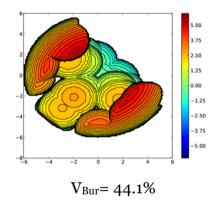


Figure 3. Steric map of complex [Fe(5-tips2tpa)(CH₃CN)₂]²⁺

4. Conclusions

In conclusion, computational methods can help us to study catalytic structures and know how they behave in space without the need of the X-Ray structure, saving us time and being more economically affordable.

Keywords: iron, benchmark, alkenes, hydrogen peroxide, homogeneous catalysis

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THE SODIUM CHANNEL β2 SUBUNIT LOCALIZES TO LIPID RAFTS

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1. Introduction

The $\beta 2$ subunit, an auxiliary transmembrane glycoprotein, modulates localization of the voltage-gated sodium channel on the cardiomyocytes surface. These channels are crucial for cardiomyocyte excitation, which precedes heart contraction in response to an action potential, i.e. a quick succession of changes in voltage across the membrane. The channels are composed of a pore-forming α subunit, Na_V1.5, and several β subunits, such as $\beta 2^{[1][2]}$.

β subunits are cleaved by the membrane-associated enzymes β and γ secretases. Palmitoylation could allow β2 localization in cholesterol-enriched, lipid raft domains, where β-secretase (β-site amyloid precursor protein cleaving enzyme 1, or BACE1) is also located. β2 cleavage by BACE1 releases extracellular and intracellular peptides [3]. It has been shown that the β2 intracellular peptide could regulate sodium channel expression [4]. This exciting finding could imply a whole new mechanism of Nav1.5 regulation by β2.

2. Hypothesis

- 1- Palmitoylation partitions β 2 into lipid rafts, where BACE1 is enriched.
- 2- In MDCK cells, BACE1 cleaves β 2.
- 3- β2 Cys182Ser, lacking its putative palmitoylation site, is less processed by BACE1.

3. Methodology

To determine whether $\beta 2$ localizes to lipid rafts, we expressed $\beta 2$ -YFP (yellow fluorescent protein), wild type (WT) or Cys182Ser, in Madin-Darby canine kidney (MDCK) cells. Then, we isolated detergent-resistant membranes (DRMs) by sucrose density gradient ultracentrifugation, and analysed the samples by western blot (WB).

To assess $\beta 2$ cleavage by BACE1, we cotransfected MDCK and human embryonic kidney (HEK293T) cells with plasmids to co-express BACE1 and $\beta 2$ -YFP, WT, or Cys182Ser. Then, we analysed cleavage of $\beta 2$ by WB.

4. Results

Our experiments demonstrate that WT $\beta 2$ is found at DRMs in MDCK cells, while palmitoylation-deficient Cys182Ser $\beta 2$ is not. This supports our idea that palmitoylation partitions $\beta 2$ into lipid rafts, as DRMs are highly enriched in these.

On the other hand, both in MDCK and HEK293T cells, BACE1 cleaved β 2 WT. However, no significant differences were detected between WT and mutant β 2.

5. Conclusions

In MDCK cells, Cys182 palmitoylation partitions $\beta 2$ into lipid raft-rich DRMs. In addition, $\beta 2$ is substrate of cleavage by BACE1. Although more research is required to validate our third hypothesis, these results will help us understand $\beta 2$ role in cardiac arrhythmia.

Keywords: β2 subunit, BACE1, Na_v1.5, Cys182Ser, palmitoylation

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THE MEDICAL-PHARMACEUTICAL *LIEUX DE MÉMOIRE* IN CONTEMPORARY CATALONIA (c. 1890-1936): OBITUARIES AND BIOGRAPHIES AS ANALYTICAL LABORATORIES IN THE CREATION OF PROFESSIONAL IDENTITIES

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1. Introduction

The French political historian Pierre Nora coined the phrase *lieux de mémoire* (1984-1992), which is used simultaneously in two different ways. On the one hand, as an object of study, it designates every material or immaterial artefact that brings to the present the symbolic values of the «collective memory» of our past; Nora refers to it as: «the political instrumentalization from the past in the present» (vol. I, 1984: XXV). On the other hand, as an analytical methodology, it advocates the deconstruction of the manifested identities in the *lieux*. Stéphane Michonneau (2002) spread the locution and the historiographical current in Catalonia (about the reception in Spain, *vid.*: Coromina, 2019).

2. Hypothesis

This work proposes to refocus the conceptualization from Nora, who refers to national identity, to «other» collective identities. Specifically, the «case study» will explore the fabrication and socio-cultural process of professional identity appropriation (medical-pharmaceutical) that are materialized in two typologies of *lieux de mémoire*, obituaries and biographies, between the end of the nineteenth century and the beginning of the twentieth century in Catalonia. This was a key time for the construction of the professional-corporate praxis because of the debate on memberships (Villacorta, 1989; Puigvert, 2002, 2003).

3. Methodology

In the framework of the «return to the subject» in the social sciences (Burdiel, 2000; Dosse, 2007), following the methodology of sociologist Pierre Bourdieu (1989), and developed by Bridget Fowler (2007), in the style of Joaquim Maria Puigvert (2007), I have researched the obituaries — understood as «urgent biographies»— and their shadow in the biographies tout court, present in the colleges' bulletins, and the specialized press (for example, La Independencia Médica or the Gaceta Médica Catalana), as well as publications promoted in corporate institutions. On the one hand, I have considered the authorship, the relationship with the described person, and the language. On the other hand, I have considered the facultative, namely: the genre, chronological, geographic, social, and family frameworks, as well as academic studies, professional practice, socio-professional recognition, and other activities that they might have done.

4. Results and conclusions

In the junction of memory and oblivion, there are —in the memorial artefacts— similarities and dissimilarities, continuities and discontinuities—sometimes conflicted, sometimes in harmony—between doctor and pharmaceutical interests, between rural and urban areas, and between different provincial capitals, as well as between professional identity and «other» identities of the subject (political, social, religious or related to the genre). It is a spearhead for the historiographies of memory, identities and health, and any subsequent transnational and comparative studies.

Keywords: *Lieux de mémoire*, socio-cultural historiography, professional identities, medical-pharmaceutical historiography, obituaries.

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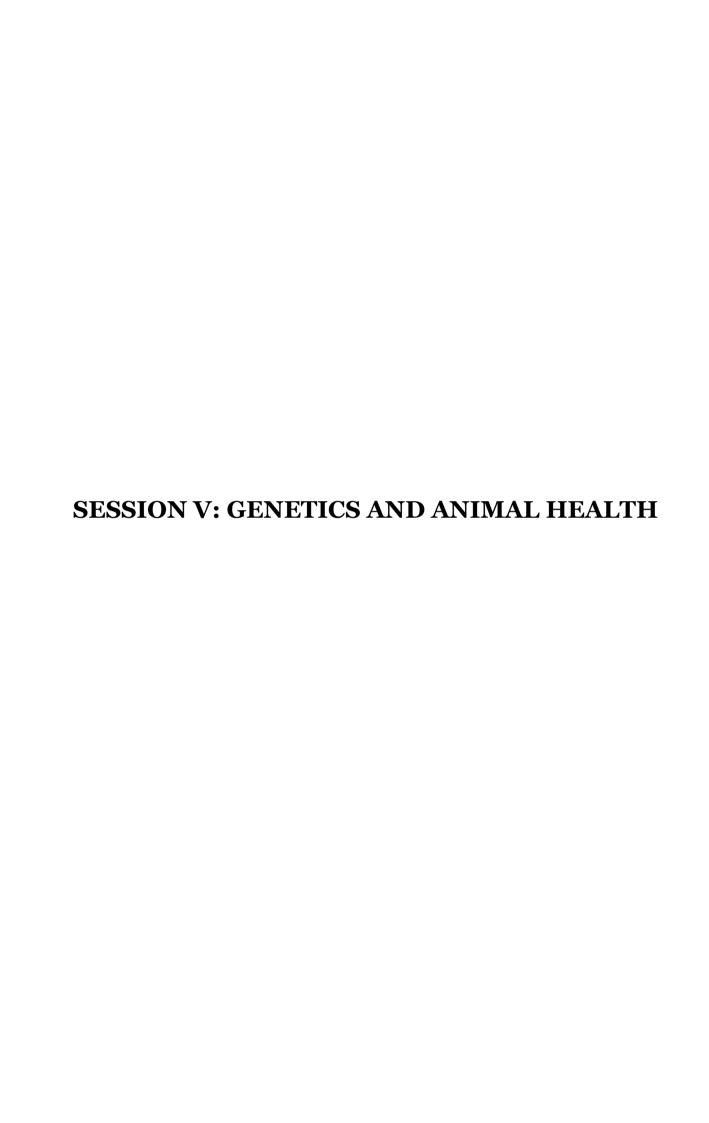
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SEMINAL FACTORS TRIGGER NETOSIS IN MAMMALIAN FEMALE POLYMORPHONUCLEAR CELLS

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1. Introduction

In several species, acute endometritis driven by the recruitment of polymorphonuclear cells (PMNs) occurs in response to semen. Release of DNA from PMNs to form neutrophil extracellular traps (NETs) is stimulated by bull, stallion and human sperm, leading to their entrapment (Fichtner, 2020). While there is no evidence of this phenomenon in donkeys, artificial insemination (AI) with frozen semen leads to poor pregnancy rates (Oliveria, 2016).

2. Hypothesis

We hypothesised that: 1) NETosis in response to semen also occurs in jennies and 2) frozen-thawed (FT) semen induces more NETosis than fresh semen.

3. Methodology

In Experiment 1, PMNs from jennies (n=4) were isolated by centrifugation of blood through a density gradient. After confirming the presence of >90% PMNs by flow cytometry, cells were incubated in the presence or absence (control) of 1:1, 1:2 or 1:5 fresh semen (n=1 jackass). After 2h or 4h incubation, cells were fixed, stained with Sytox, and the percentage of PMNs that underwent NETosis was determined. After determining the optimal conditions, in Experiment 2, PMNs (n=3 jennies) were incubated for 2h in the presence or absence (control) of 1:5 fresh or FT semen (n=3 jackasses), replicating commercial seminal doses used in AI. Finally, to elucidate the factor triggering NETosis, in Experiment 3, PMNs (n=3 jennies) were incubated for 2h with: 25% SP with or without sperm, sperm without SP, or media lacking seminal factors (control).

4. Results

Although NETosis increased in all groups from 2-4h, more PMNs had reacted in the 1:2 and 1:5 groups, compared to the control ($P \le 0.05$; Fig.1). On the other hand, exposure to fresh semen induced higher NETosis than FT semen ($78\pm5.7\%$ vs. $23\pm2.4\%$, respectively; $P \le 0.01$). No differences were observed between the FT group and the control ($23\pm2.4\%$ vs. $31\pm3.7\%$, respectively; P > 0.05; Fig.2). Because fresh semen contains more seminal plasma (SP) than FT, we hypothesised that SP rather than sperm could be responsible for activation of PMNs. NETosis increased in the presence of SP, regardless of the presence or absence of sperm, compared to the control ($77\pm4.9\%$, $84\pm5.1\%$ vs. $15\pm2.8\%$, respectively; $P \le 0.01$; Fig.3). There was no difference in NETosis rate between PMNs incubated with sperm without SP and the control ($22\pm3.7\%$ vs. $14\pm2.8\%$, respectively; P > 0.05).

5. Conclusion

In conclusion: 1) NETosis is both incubation-time- and fresh-semen-concentration-dependent; 2) frozen-thawed semen does not elicit this response; and 3) jenny PMNs react to SP rather than sperm-intrinsic factors. Future experiments will elucidate the role that NETs play in reproductive physiology.

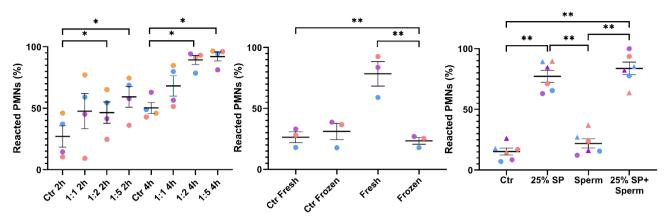


Figure 1. NETosis kinetics depending on the concentration and the time.

Figure 2. NETosis in response to fresh or frozen-thawed.

Figure 3. NETosis in response to seminal plasma and/or fresh sperm.

Acknowledgments

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Keywords: NETosis, sperm, seminal plasma, neutrophils, donkey

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GENETIC DIVERSITY AND TEMPORAL STABILITY OF Aristeus antennatus SPAWNING FEMALE'S GROUNDS ALONG THE SPANISH MEDITERRANEAN COAST DURING TWO CONSECUTIVE SUMMER SEASONS 2016-2017

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1. Introduction

The blue and red shrimp *Aristeus antennatus* (Risso, 1816), a highly abundant marine crustacean on the Spanish Mediterranean coast, is exploited by the deep-water bottom trawl fisheries mostly at depths of between 500 and 800 m.^[1] During the reproductive period, which takes place in late spring and summer,^[2] there are spatiotemporal migrations, forming aggregations on the middle slope. Those aggregations are mainly composed of mature females.^[3]

2. Hypothesis and objectives

The main objectives of this study were to estimate the levels of genetic diversity within the spawning females' grounds, to estimate the genetic divergence among them and to know the degree of temporal genetic stability on the Spanish Mediterranean coast from Gulf of Lions to Cabo de Palos.

3. Methodology

We analysed seven locations corresponding to the main fishing grounds (Port de la Selva, Roses, Palamós, Blanes, Vilanova i la Geltrú, Dénia and Santa Pola) in two consecutive summer seasons (July, 2016 and 2017). We genotyped 12 microsatellite *loci* previously reported in ^[4] in a total of 1343 female individuals of *Aristeus antennatus*, and 11 of them were applied in all the genetic data analyses.

4. Results

The number of alleles detected per *locus* ranged from 2 to 24 with a total mean of 8.96. The mean observed heterozygosity (H_0) for each location varied from 0.427 to 0.491 in 2016 and from 0.464 to 0.492 in 2017, while the mean expected heterozygosity (H_0) varied from 0.613 to 0.643 in 2016

and from 0.628 to 0.644 in 2017. Of a total of 168 comparisons between the observed and the expected genotypic proportions under the Hardy-Weinberg equilibrium, 90 were significant after Bonferroni correction, which caused deviations from the Hardy-Weinberg equilibrium in the fourteen samples analysed. The AMOVA did not show differences among locations in 2016 either ($F_{ST} = 0.00128$, p-value > 0.05) and in 2017 ($F_{ST} = 0.00033$, p-value > 0.05). Likewise, we did not find any significant differentiation between the two temporal replicates ($F_{CT} = 0.00020$, p-value > 0.05).

5. Conclusion

Our study provides the first evidence of a scenario of high genetic connectivity and temporal stability in spawning females' grounds of *A. antennatus* over the large studied area. Consequently, we argue for taking into account the genetic results in the management of this important Mediterranean marine resource.

Acknowledgments

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Keywords: *Aristeus antennatus*, microsatellites, genetic connectivity, temporal stability, management recommendation

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EXPLORING GLUTATHIONE S-TRANSFERASE MU 3 (GSTM3) AS A QUALITY BIOMARKER OF MAMMALIAN SPERM PRESERVATION

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1. Introduction

Glutathione S-transferases are essential detoxifying enzymes involved in cellular protection against oxidative stress. Recent experiments performed in our laboratory showed evidence that GSTs are essential to maintain mammalian sperm motility, mitochondrial activity and plasma membrane stability (Llavanera, 2020). However, while GSTM3 has recently been established as a fertility biomarker of boar sperm (Kwon, 2015), the potential role of GSTM3 as a specific quality biomarker of sperm preservation is yet to be investigated. Consequently, the aim of the present study was to investigate the potential role of sperm GSTM3 as a quality biomarker of liquid-preserved and cryopreserved sperm.

2. Methodology

With this purpose, seven boar ejaculates were extended and liquid-stored at 17°C for 72 h. Sperm motility and viability were evaluated at 0 and 72 h through CASA and flow cytometry. On the other hand, 12 boar ejaculates were cryopreserved. Sperm motility and viability were evaluated in prefrozen and frozen-thawed samples. Subsequently, samples were classified as good freezability ejaculates (GFE) or poor freezability ejaculates (PFE) based on their sperm motility and viability at post-thaw. In each experiment, immunoblotting of sperm GSTM3 was performed, and subsequent pattern quantification was normalised using α -tubulin. Finally, Pearson correlation coefficients between relative GSTM3 content and sperm quality parameters were calculated. In addition, a t-test for independent samples was run to compare pre-frozen GSTM3 content between GFE and PFE sample groups.

3. Results and Discussion

In liquid-stored samples, whereas GSTM3 content at 0 h was not correlated to sperm viability, it was negatively correlated with the percentage of total motile (r=-0.92; p<0.01) and progressively motile spermatozoa (r=-0.91; p<0.01) at 72 h of liquid-storage. Related with this, a relationship between GSTM3 content at 0 h and sperm motility at 72 h was found.

On the other hand, ejaculates classified as GFE showed significantly lower levels of GSTM3 than PFE in both pre-frozen and frozen-thawed samples (p<0.05). These results evidenced that lower levels of sperm GSTM3 in fresh ejaculates are an indicator of higher resilience to preservation procedures, for both liquid-storage and cryopreservation.

4. Conclusions

In conclusion, lower relative levels of sperm GSTM3 in fresh samples are related to higher resilience to preservation procedures and higher sperm quality after both liquid-storage and cryopreservation. Therefore, this study suggests that sperm GSTM3 levels in fresh samples can be used as a quality biomarker for boar sperm preservation methods.

Keywords: Biomarker; Boar; Cryopreservation; GSTM3; Liquid storage

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IDENTIFYING THE FUNCTIONAL ROLE OF AQUAPORINS IN MAMMALIAN SPERM CRYOPRESERVATION

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1. Introduction

Aquaporins (AQP) are a family of transmembrane proteins that ease the transport of water and small solutes, including orthodox AQPs, aquaglyceroporins (GLPs) and superAQPs. The role of AQPs in volume regulation and osmoregulation of sperm cells, and the drastic osmotic stress occurring during cryopreservation explain the relationship between AQP levels and sperm cryotolerance. The aim of this study was to elucidate the functional relevance of different groups of AQPs during mammalian sperm cryopreservation, using two animal models (pigs and horses).

2. Methodology

A total of 27 pools from 42 boar ejaculates and 12 stallion ejaculates were used. After dilution in cryopreservation media, sperm samples were split into different subfractions: the control, and the treatments with different AQP inhibitors (1,3-propanediol, PDO; acetazolamide, AC; and phloretin, PHL). Samples were cryopreserved with a controlled-rate freezer and thawed in a water bath. Sperm quality and function were assessed in fresh samples, and after 30 and 240 min (boar), or after 10 and 120 min (stallion) of thawing. Total (TMOT) and progressive motility (PMOT) were assessed through a computer-assisted sperm analysis system, and flow cytometry analyses were performed to assess viability, acrosome integrity, membrane lipid disorder, mitochondrial membrane potential (MMP), and intracellular levels of calcium, peroxides and superoxides.

3. Results

Stallion spermatozoa treated with PDO presented higher percentages of TMOT, PMOT, spermatozoa with an intact acrosome, and spermatozoa with high levels of calcium than the control (P<0.05). In addition, both boar and stallion PDO-treated samples showed higher viability and MMP, and lower membrane lipid disorder (P<0.05). Boar spermatozoa treated with PDO showed higher levels of peroxides and superoxides than the control (P<0.05).

In contrast, stallion samples treated with PHL showed lower TMOT, PMOT, sperm viability, acrosome integrity, and higher MMP and intracellular calcium levels than the control (P<0.05). In boar samples, these effects were restricted to the highest concentration of PHL (P<0.05). Finally, the effects of AC were neither consistent nor concentration-dependent.

4. Discussion

The effects of PDO suggest that instead of being an AQP inhibitor, it acts as a cryoprotective agent, with more apparent effects on stallion than on boar sperm. While the effects of PHL underpin the

relevance of GLPs for mammalian sperm cryotolerance, those of AC suggest that orthodox AQPs are either absent in boar and stallion sperm or irrelevant during cryopreservation.

5. Conclusion

The inhibition of different groups of AQPs suggests that GLPs are more relevant than orthodox AQPs in mammalian sperm cryopreservation.

Keywords: aguaporins, mammalian, cryopreservation, sperm

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SESSION VI: WELL-BEING AND MENTAL HEALTH AT DIFFERENT STAGES OF LIFE

INCIDENCE OF AGING IN PEOPLE WITH INTELLECTUAL DISABILITIES IN THEIR WORK ENVIRONMENT AND THEIR OUALITY OF LIFE

Hèctor Valenzuela Universitat de Girona

1. Introduction

Social and work inclusion of people with intellectual disabilities (PID) has improved substantially in recent years because they have been guaranteed environments that promote their well-being and quality of life. Nowadays, we are facing a population of PDI with increasing life expectancies and symptoms associated with the aging stage that are more premature than the population without intellectual disability (Del Barrio, 2016).

Unfortunately, the fact of entering an aging stage is synonymous with many PID being forced to leave their work, which in turn leads to a reduction in their quality of life (Brotherton, 2016).

Based on this evidence and the need to provide answers, this doctoral thesis aims to assess the changes that occur in the PIDs in the aging stage in sheltered employment in Catalonia. Based on this evaluation, action plans will be proposed to extend the working life of the group of aged people, based on their quality of life, support needs and adaptation of the person to the job.

2. Methodology

In order to assess the signs of aging and the quality of life in the work environment of the target population, a semi-structured interview has been designed ad hoc, which will be reviewed by experts in the field and subsequently administered as a pilot test to 5 PID working in sheltered employment in order to assess the adequacy and understanding of the interview questions.

To complement the semi-structured interview (once validated), the Personal Outcomes Scale (2014) will be administered to measure the support needs of the people who participate in the study.

3. Results

This paper will focus on the results obtained from the expert analysis of the semi-structured interview: an analysis will provide an appropriate tool to measure aging and quality of life according to Shalock and Verdugo's model.

In a second phase, the pilot test administered to 5 PID will allow the necessary adjustments to administer it to a larger number of people.

4. Conclusions

The results of the pilot test will allow us to administer the interview to a larger number of people to extract information for developing action plans that promote the detection of support needs of PIDs in the aging stage that work in Catalan sheltered employment, and generate a change in

organizational culture in order to adapt workplaces to people's needs and extend their working lives, while increasing their quality of life.

Keywords: Intellectual disability, Sheltered employment, Quality of life measurement, Aging measurement, Personal outcomes

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EFFECTS OF A PSYCHOEDUCATIONAL INTERVENTION PROGRAMME ON THE SEXUAL AND AFFECTIVE ATTITUDES OF PEOPLE WITH INTELLECTUAL DISABILITIES WHO ATTEND AN OCCUPATIONAL THERAPY SERVICE

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1. Introduction

Various studies show that people with intellectual disabilities tend to receive little education in sexual and affective matters from their families or from those in charge of their care. The purpose of many educational approaches was not to arouse sexual need in them, but rather to control their manifestations in a repressive way (Navarro, 2010). Like other studies, they show that those affected wish to have more knowledge and better training to develop their sexuality and affectivity satisfactorily.

2. Methodology

A pre-post quasi-experimental design, with a non-randomized control group, was used. A total of 56 people (32 men and 24 women) with a mean age of 48.86 years (min = 23; max = 78) and a standard deviation of 13.14 participated in the study. Through group techniques and during 10 sessions of 1 hour a week, different topics related to sexuality and affectivity were studied. The data were collected with a hetero-applied questionnaire while questions were primarily answered using a Likert scale. This questionnaire for the data analysis was an adaptation of the EcenSexual-DI psychometric test (McCabe, 1994).

3. Results

The mixed design analysis of variance [ANOVA] (group x time) revealed the participants showed high prior knowledge in topics related to contraceptive methods and sexually transmitted diseases. On the other hand, they demonstrated near total ignorance about masturbation and homosexuality.

Before going through the training programme, the participants also showed negative attitudes regarding masturbation and homosexuality.

Modifications in attitudes related to sexual interaction are obtained in post-training data. The programme produced a notable change in their negatives attitudes towards masturbation, so that their acceptance of it increased. Contrarily, they did not change their initial attitudes, extremely negative, in relation to homosexuality.

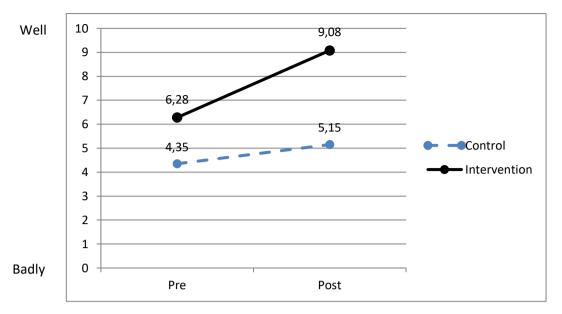


Figure 1. Graphical representation of the average scores in relation to the question "How do you feel when you do these things (masturbation)?" Depending on the group and the moment of evaluation.

This study shows the necessity of educational programmes. Before receiving such training, more than two thirds of the participants said that no one had informed them about sexual matters and showed deficiencies in their knowledge on this subject and an interest in learning more.

The educational programme was successful at significantly increasing their sexual knowledge in a majority of the examined areas and very markedly changing their negative attitudes towards masturbation. Their negative view of homosexuality changed remarkably with the new information, but did not change their attitude towards this sexual option.

Keywords: disability, intellectual, education, programme, attitudes

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THE WELL-BEING OF CHILDREN WITH EDUCATIONAL NEEDS: LEARNING FROM THEIR SCHOOL-BASED PERSPECTIVES

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1. Introduction

At present, there are 65,907 children and adolescents with educational needs due to different disabilities or disorders in the Catalan non-university education system, representing 4.5% of the total students (Catalan Ministry of Education, 2019). What is known about the subjective well-being (SWB) of children with educational needs in schools? The quality of children's school experiences is linked to their SWB, which is explained by environmental factors (peer relationships, teachers' behaviour or parental involvement) and individual differences (academic performance or behavioural engagement) (Andresen, 2014; García-Bacete, 2014; Huebner, 2014). Are the children with educational needs getting the care they need to be as satisfied with their school life as the other students? The objective is to know whether the school-based SWB of children with educational needs is lower than that of the other students.

2. Methodology

The hypothesis is answered through the analysis of the responses given by a probabilistic sample of primary school students from Barcelona city in 2017 (mean age=10.7, analysed sample=3,962) to an adaptation of the Children's Worlds questionnaire. Children self-reported 'having a major visual or auditory difficulty, or some type of malformation (wearing glasses not included)' (3.9%), 'having a learning difficulty (dyslexia, attention deficit or hyperactivity)' (7.8%), and 'having a long-term illness (diabetes, an allergy, asthma, stunted growth or epilepsy)' (14.1%) (Andresen et al., 2020; Barcelona Institute of Childhood and Adolescence, 2019). In the selected indicators of children's SWB, the means of children who perceive learning difficulties and those who do not are compared.

3. Results

The results are shown in Figure 1. The global life satisfaction of children who perceive learning difficulties is already lower than those who do not (-0.41). In the school environment, the greater difference is in student life satisfaction (-1.07), followed by school-based learning satisfaction (-0.49). The difference in classmate satisfaction is at the limit of statistical significance.

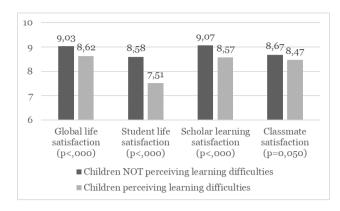


Figure 1. Children's SWB by perceived learning difficulties

Children make very positive evaluations, but those who perceive learning difficulties seem to have reasons to evaluate their life as students and school-based learning more negatively than the others. Although the children self-report the perception of learning difficulties, with the available data, it can be corroborated that the school-related SWB of children with educational needs is lower than that of the other students. It should not be normal or expected: more research based on educational interventions is needed to improve the quality of education from a diversity and inclusion perspective (XTEC, 2020).

Keywords: children's subjective well-being, school environment, educational needs, learning difficulties, Barcelona Children's Worlds

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PHYSICAL EXERCISE PROGRAMME TO IMPROVE THE HEALTH-RELATED QUALITY OF LIFE OF STROKE SURVIVORS

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1. Introduction

The number of people who survive a stroke increases every year. Stroke survivors suffer significant neurological deficits and physical deconditioning that compromise walking ability, activities of daily living (ADL) and, in consequence, the health-related quality of life (HRQOL).^[1,2] The intensity of the stroke rehabilitation sessions is inadequate to induce a cardiovascular training effect. ⁽²⁾ Aerobic exercise after stroke improves certain vascular risk factors, including glucose intolerance, high resting blood pressure and elevated total cholesterol. In addition to the benefits related to the cardiorespiratory system, it provides clinically meaningful health benefits in many physical and psychosocial aspects such as fatigue, execution functioning and memory and depressive symptoms. ^[3] Therefore, adherence to aerobic exercise is important to decrease the risk of recurrence and improves HRQoL.^[2,3] The objective of this study is to evaluate the effect of the physiology of exercise, physical activity and rehabilitation (PEPAR) based on aerobic exercises in stroke survivors to improve their physical condition and their HRQoL.

2. Methodology

The study carried out at the Rehabilitation Service of the Dr Josep Trueta University Hospital in Girona was based on a combination of quantitative and qualitative methodological approaches. This was a prospective and quasi-experimental design with pre-post intervention measures aimed at stroke patients after conventional rehabilitation. The quantitative method focused on the evaluation physical and medical variables and the qualitative method focused on participants' perception of improvement in the context of their everyday life. A total of forty-three participants underwent the PEPAR, consisting of a twelve-week intervention of one-hour sessions two days per week. Quantitative data were collected at three moments: before initiating the intervention; at the end of the intervention programme and; six months after treatment. PEPAR evaluated the progress on physical condition, reduction of cardiovascular risk, HRQoL and measurement of adherence. Qualitative information was generated through in-depth interviews and focus groups with participants and caregivers.

3. Results

PEPAR showed a statistically significant effect in reducing sedentary lifestyle and improving physical condition, HRQoL and adherence to physical exercise. However, six months later, a worsening in the outcome of these variables is observed, although it did not reach the pre-intervention level.

PEPAR is an effective treatment to improve the physical condition of stroke survivors that allows realisation of the ADL with a lower energy cost and improved HRQoL. This study highlights the need to design new strategies in the community environment to increase adherence to physical exercise after completing the PEPAR.

Keywords: Stroke, Physical Exercise Program, Quality of life, Vascular risk factors, Adherence.

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EVALUATION OF LOW-DOSE INTRAVENTRICULAR INFUSION OF AMYLOID BETA IN A RAT MODEL TO TEST LONG-TERM TREATMENTS FOR EARLY ALZHEIMER'S DISEASE

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1. Introduction

Alzheimer's disease (AD) is the most common type of dementia, with no effective therapy. Research on potential treatments for AD is limited by the lack of reliable animal models of sporadic AD. [1] Infusion of amyloid β (A β) oligomers into the brain has been proposed to this aim, but there is a widespread disparity in methodologies, leading to different results.

2. Objectives

In this study, we aimed to assess the suitability of intracerebroventricular (ICV) injection of previously reported well-characterized A β aggregates^[2] to obtain sustained memory disruption similar to that observed in early AD, by characterizing its behavioural and neuropathological features and their stability over time.

3. Methodology

Rats were bilaterally injected (ICV) with oligomeric A β 1-42 (0.677 μ g/rat, AB group) or PBS. Behavioural impairment was analysed at 15-22 days or at 26-33 days by Morris water maze consisting of 5 acquisition sessions (4 trials/daily session) and a retention test after 72 hours. Neurodegeneration was assessed in hippocampus and prefrontal cortex by Nissl staining.

4. Results

AB rats showed increased latencies in 4th and 5th acquisition sessions, and a decrease in time spent in the target quadrant in the retention test, at 22 days. However, for rats sacrificed at 33 days, no differences were found in the acquisition latencies, and only a difference in the mean distance to target in the retention test was observed. Similarly, there was a decrease in the number of neurons in the prelimbic cortex at 22 days, which was recovered at 33 days. In contrast, a decrease in the number of neurons in the CA3 hippocampal subfield was found only at 33 days.

5. Conclusion

These results suggest that A β 1-42 impaired learning dynamics and caused prefrontal neurodegeneration detectable at 22 days, which partially recovered after ten days. However, hippocampal neurodegeneration was detected at a later time. We can conclude that low-dose ICV

injection produces a non-stable model for early AD, rendering it non-suitable to test potential long treatments.

Keywords: Alzheimer's disease, amyloid beta, neurodegeneration, hippocampus, prefrontal cortex

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SESSION VII: DATA ANALYSIS, COMPUTATIONAL METHODS AND MACHINE-LEARNING TECHNIQUES AS TOOLS FOR SCIENTIFIC RESEARCH

MARKOV STATE MODELS TO IDENTIFY HIDDEN CONFORMATIONAL META-STABLE STATES IMPORTANT FOR CATALYTIC ACTIVITY

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1. Introduction

The pharmaceutical industry is in search of new methods for the manufacture of chiral amine building blocks, as approximately 40% of drugs contain at least one chiral amine in their structure. [1] In this regard, monoamine oxidase from *Aspergillus niger* (MAO-N), emerged as a promising biocatalyst for the industrial production of chiral amines when used in combination with a non-selective chemical reductant. [2] MAO-N is a homodimeric enzyme responsible for the oxidation of amines into the corresponding imine. Directed evolution experiments raised an extensive library of variants with different substrate scope and catalytic activities. [3] In this study, we focus on the study of the conformational dynamics of both wild-type and D5 variant, with mutations I246M in the substrate entrance tunnel, N336S near the active site, and M348K/T384N/D385S located at distal positions.

2. Methodology

Molecular dynamics simulation and the dimensionality reduction protocol tICA (time-lagged independent component analysis) were used to identify different conformations in MAO-N. Additionally, we used Markov state models to characterize the kinetics of the transitions between the different conformational meta-stable states as well as their relative populations and the kinetics of the transitions in them. In addition, we use accelerated molecular dynamics to elucidate the potential interplay between the β -hairpin conformational dynamics and catalytic activity in MAO-N wild type and its evolved D₅ variant.

3. Results

Molecular dynamics (MD) simulations reveal the existence of different conformational states of MAO-N, that arise from the motion of an important β-hairpin located at ca. 20 Å far from the active site, displaying *open* and *closed* conformations. The Free Energy Landscape (FEL) reconstruction allows the quantification of the populations of the different meta-stable states by means of MSM, suggesting that along the evolutionary path, the *closed* conformation has been stabilized, increasing the catalytic activity of MAO-N. Finally, the effect of the different conformations in the substrate binding was determined through aMD simulations, revealing a communication path between MAO-N subunits and the importance of the *closed* conformation in the substrate binding process.

4. Conclusions

Our study demonstrates the existence of a delicate communication between both MAO-N subunits that impacts the active site architecture, and thus its catalytic efficiency. In both MAO-N WT and the laboratory evolved D5 variant, the \(\beta\)-hairpin conformation in one of the monomers affects the productive binding of the substrate in the active site of the other subunit. However,

both MAO-N WT and D₅ variants show a quite different behaviour due to the distal mutations introduced experimentally with directed evolution.^[4]

Keywords: Molecular Dynamics, Distal Mutations, Enzyme Catalysis, Substrate Binding, Monoamine Oxidase

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ANALYZING THE KEY FACTORS THAT EXPLAIN SWIMMING PERFORMANCE VARIABILITY IN FRESHWATER FISH

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1. Introduction

Swimming performance is a key feature that mediates fitness and survival of fish and other aquatic animals, playing a crucial role in predator-prey interactions, reproduction, migration and dispersion processes. Swimming performance in fish is traditionally assessed using swim tunnels and the critical swimming speed (U_{crit}) test is the most common and straightforward method to estimate it. The objectives of this study are: i) to compare the role of several predictors (i.e. body length, water temperature, species identity, native status, body shape and form factor) on U_{crit} in a large set of Iberian freshwater fishes, and ii) to test for differences in swimming performance between native and alien species.

2. Methods

We analysed the contribution of the different variables studied in explaining the variation of $U_{\rm crit}$ for inland fishes, using linear models and, for the first time, random forests, which is a machine-learning technique that is frequently used because of its advantages, including computational efficiency on large databases with many correlated predictors, the provision of estimates of variable importance, the ability to impute missing data while maintaining accuracy, and the handling of non-linearities and interactions. [3] We compiled 227 cases for 35 fishes inhabiting the Iberian Peninsula, including 17 alien species widely distributed worldwide.

3. Results

We found that body length is the most important predictor of $U_{\rm crit}$, followed by species identity (Figure 1). By contrast, body shape, the form factor, temperature and native status were less important. The relationship of $U_{\rm crit}$ with body length was highly species-specific and could be described by power functions with significantly different exponents. We also found that taxonomic family is not as good a predictor as species identity because of the high diversity of species with different lifestyles and forms within the same family. Similarly, body shape explained much less variation in $U_{\rm crit}$ than species identity and native and alien species did not show significant differences. Although there was a positive relationship between $U_{\rm crit}$ and temperature, our findings indicated that the latter is not a very important factor affecting swimming abilities of fishes under standard laboratory procedures.

This study provides an overview for further theoretical and empirical studies. The data and models could contribute to the management of Iberian ichthyofauna, to design fish bypasses, to develop barriers for the exclusion of invasive species, to assess the effects of hydrologic alteration or to categorize fish habitat preferences.

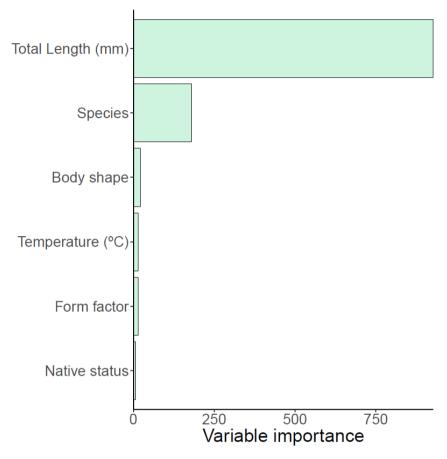


Figure 3. Variable importance of predictors of U_{crit} according to the random forest model. Total percentage of explained variation was 64.3%.

Keywords: U_{crit} , random forests, temperature, alien species, Iberian Peninsula

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DIAMONDS ARE A CHEMIST'S BEST FRIEND

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1. Introduction

Efficient conversion of methane into methanol is crucial to solving the current energy crisis because it would allow for a better utilization of this major feedstock, drastically facilitating its handling and transportation.^[1] This oxidative process is currently carried out by enzymes such as the soluble methane monooxygenase (sMMO).^[2] In an attempt to mimic such activity with greater atom economy and industrial viability, several synthetic models have been produced, mainly consisting of diiron complexes with polydentate ligands containing nitrogen heterocycles.^[3] Compounds with diamond cores have been particularly enlightening in the understanding of biocatalysis.^[4]

Recently, Banerjee and coworkers reported^[5] the first model capable of incorporating O_2 , generating a (μ -1,2-peroxo)diiron(III) adduct (\mathbf{P}) that further transforms into a bis(μ -oxo)diiron(IV) diamond-shaped complex (\mathbf{D}) upon treatment with a Lewis acid. Both have been shown to be key intermediates in the catalytic methane oxidation by sMMO. Although these species are known, the mechanism behind its formation is unclear. Thus, we intend to study and throw light on it in this work.

2. Methodology

To address these issues, we have performed density functional theory (DFT) calculations with the Amsterdam Density Functional (ADF) and QUILD programs. Molecular orbitals were expanded in an uncontracted set of Slater type orbitals of triple-ζ quality with double polarization functions (TZ2P). The frozen core approximation was used to reduce computational demand. Geometry optimization and frequencies were calculated using S12g,^[6] taking into account solvent effects through the Conductor-like Screening Model. While computing Gibbs free energies, small frequencies were raised to 100 cm⁻¹ to compensate for the breakdown of the harmonic oscillator model. Scalar relativistic corrections have been included self-consistently in all calculations by using the zeroth-order regular approximation.

3. Results

Here we present a study on the "heat" that drives the formation of the diamond core from the peroxodiiron(III) pentagonal species and explore the chemical space to probe for relationships between coordination geometry and spectroscopic data. To do so, we employ a density functional theory method that has excelled in the description of open-shell transition-metal complexes.

We have found viable mechanisms for the transformation of **P** to **D** with energy barriers lower than 30 kcal mol⁻¹. The results obtained do not show any correlation between <(Fe-Ô-Fe) and vibrational frequencies or isomer shift/quadrupole splitting. Vibrational frequencies depend instead on the distance between the iron atoms.

We have successfully provided further insight into the workings of biomimetic iron complexes for methane oxidation through the activation of O_2 . This allowed us not only to understand the current synthetic models, but also to provide indications on how to design the next generation of biocatalysts.



Figure 1. Diamond formation through conversion of the pentagonal species.

Keywords: methane oxidation, sMMO, diiron complexes, DFT

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UNRAVELLING THE MILLISECOND ALLOSTERIC ACTIVATION OF IMIDAZOLE GLYCEROL PHOSPHATE SYNTHASE (IGPS) BY MEANS OF MOLECULAR DYNAMICS SIMULATIONS

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1. Introduction

Allostery is an intrinsic property of proteins generally described as the process by which the effect of binding at one site is transmitted to another functional site, allowing for activity regulation. ^[1] Exploring the mechanisms of allosteric regulation is important in understanding biological processes such as enzyme catalysis or cell signalling. Transitions that mediate allosteric processes require the order of microseconds to seconds to take place. Imidazole glycerol phosphate synthase (IGPS) is a heterodimeric enzyme complex widely used as a model to study allosteric regulation in enzyme catalysis. Previous studies based on NMR experiments reported that the allosteric activation of IGPS takes place on the millisecond timescale. ^[2] However, the allosteric activation mechanism of IGPS has not been yet characterized. ^[2,3] Computational methods are used to study allostery, but obtaining enough conformational sampling to completely characterize allosteric events represents a challenge for current simulation techniques. ^[4]

In this work, the goal is to design a computational protocol to characterize step by step the millisecond allosteric activation mechanism of IGPS.

2. Methodology

Molecular dynamics (MD) simulations of IGPS are performed following the subsequent methodology. To describe the system, the Amber force-field (*ff14sb*) for the protein residues, TIP3P parameters to account for explicit water molecules and GAFF parameters for the allosteric effector and substrate are used. Enhanced sampling techniques (accelerated MD and metadynamics) have been used to access microsecond and millisecond timescale motions.

3. Results and discussion

Here, a computational protocol has been designed to completely reconstruct the millisecond allosteric mechanism of IGPS enzyme by means of a combination of simulation techniques.

Conventional molecular dynamics (cMD) simulations revealed nanosecond to microsecond motions that initiate the allosteric signal transmission. With accelerated molecular dynamics (aMD), the microsecond to millisecond allosteric activation of IGPS is reconstructed, including the complete characterization of the active structure (characterized by the formation of an oxyanion hole that stabilizes the reaction intermediate). Then, the substrate binding process is simulated to characterize the reactive complex of the allosterically activated enzyme. Metadynamics simulations are used to estimate the energy barriers of the allosteric transition.

Finally, the allosteric communication pathway is traced through key residues for IGPS function and allostery using correlation-based tools.^[6]

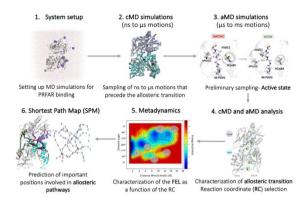


Figure 4. Computational protocol to describe the allosteric mechanism of IGPS.

4. Conclusions

In summary, the activation mechanism of IGPS has been unravelled by applying a computational protocol designed to describe and characterize complex long timescale motions. This protocol can be generalized to study the activation mechanism of other allosterically regulated enzymes or to engineer allosteric enzymes.

Keywords: computational chemistry, molecular dynamics, enzyme catalysis, biochemistry, allostery

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MONTE CARLO METHODS FOR BOLSTERING THE CONFIDENCE IN INDICATIVE CLUSTERING OF SCARCE MORBIDITY SETTINGS

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1. Introduction

In fairness to the discussion on the precautionary principle and unnecessary delay, the European Environmental Agency has since claimed that *paralysis by analysis*, as linked to the downgrading of uncertainty up to inaction, counteracts the tenet of preventing harm to public health.^[1] Avantgarde biostatisticians challenge the featuring of *p values* as an ultimate standard for endorsing positive results in observational research.^[2,3] Government hesitancy and the proposition of likeliness for spurious positive findings are commonplace when infrequent disease clustering arises.^[4] In the realm of clustering of chronic diseases, sequential techniques, integrated and tailored for their timely detection and interpretation, have proved compatible with knowledgeable guidelines and their performance suits the foregoing recommendations.^[5] After double cancer clustering arose in various communities of a province, a workable aid for revisiting robustness came from Monte Carlo iterations over the available results.

2. Methodology

Sequential techniques are applied covering about half the occurrences of myeloid malignancies in Girona province over 15 years, down to municipality level. We then interrogated any presumption of genuine causative clustering by summoning up a-priori intelligence. Focusing on 3 huddle series with 2 concurrent independent categories of myeloid malignancies, which showed in a subset of 5 communities, we aimed at estimating what the empirical anticipation was for such a distribution.

3. Results

The tailored sequential techniques working together thereby detected 10 indicative temporal aggregations encircling 6 communities. Using tests, 8 indicative clusters showed otherwise (5 communities). Physiopathological commonalities corroborated in favour of causal grounds for distinct leukaemias that clustered in the same circumscription. The Monte Carlo mean of the numerical vector conveying a distribution where 3 out of 5 communities presented ≥ 2 clusters amounted to zero, meaning that the 3 twofold malignancy assemblages that had been observed across the local subsets are far-fetched to ascribe to pure chance.

4. Conclusions

The strong indication of double clustering of distinct myeloid leukaemias must be steadfastly addressed. It confers internal validation. At least it does to mechanistic plausibility – given the acknowledged multilevel commonalities between these tumours. At present, the imposed scarce

number of cases per set hinders meaningful quizzing of primary interest variables and thereby they do not lend themselves to further auditing of such plausibility. Here, the Monte Carlo simulation underpins confidence in the findings of our exploratory approach to ascertaining temporal clusters. Negligible turnaround plus outright interpretability ancillaries repay its incorporation in these undertakings for the public health authorities to come across without procrastination.

Keywords: Cuscore test, Temporal clustering, Relative Interval (*RI*); *q-interval*; Precautionary Principle

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RATIONALIZING THE REGIOSELECTIVITY CONTROL OF DECANOIC ACID HYDROXYLATION BY P450-TT ENZYME USING MOLECULAR DYNAMICS SIMULATIONS

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1. Introduction

Cytochromes P450 are a super-family of haem-thiolate enzymes that exhibit large reactivity on the oxidative activation of C-H bonds. Selective hydroxylation of aliphatic chains present in fatty acids is of high interest in biocatalysis due to its industrial applications. Among P450 enzymes, CYP116B46 from *Tepidiphilus thermophilus* (P450-TT) is interesting due to its thermostability, self-sufficiency and broad reactivity, including hydroxylation. [1] Decanoic acid (DA) hydroxylation by P450-TT has been evaluated and results suggest that the oxidation reaction mainly produces (S)-5-hydroxydecanoic acid with high regio- and stereoselectivity. This product is a precursor of (S)-δ-decalactone, which is of high interest due to its fragrance. [2]

In order to switch the regioselectivity of this reaction towards other C-H positions along the aliphatic chain and to access to other potentially attractive products, the Flitsch Lab is engineering P450-TT to obtain new useful regioselectivities. In collaboration with them, we are applying molecular dynamics (MD) simulations to study the conformational dynamics of the wild type P450-TT enzyme. We are interested in understanding how the DA substrate binds in a catalytically competent pose to rationalize the observed activity. The acquired knowledge will be essential to further rational engineering of the enzyme and to proposing new *in silico* mutations to control the regioselectivity of the hydroxylation towards other interesting positions.

2. Methodology

To have a deep understanding of the different conformational states that P450-TT can adopt, up to 11,000ns of MD simulation with the holoenzyme was carried out, and dimensionality reduction techniques (PCA and TICA) were applied.

To characterize which of these conformational states are catalytically competent, docking calculations followed by MD simulations were carried out to analyse whether the substrate can explore catalytic poses to perform catalysis.

3. Results and discussion

The conformational landscape obtained through PCA and TICA suggests P450-TT can explore open and closed structures that might play an important role in substrate binding and catalysis.

Within the different conformational states, a promising catalytically competent conformation was identified. In this conformation, Thr278 and Ser425 side chains can establish persistent polar interactions with the carboxyl group of DA, which allow the DA-C₅ position to explore relatively

short distances with respect to the iron(III)-oxo haem active species, thus allowing regioselective hydroxylation at this position.

4. Conclusion

In this study, the molecular basis for substrate binding in a catalytically active pose towards regioselective C_5 hydroxylation of DA was elucidated. This information is of utmost importance in order to rationally design further enzyme variants with shifted regio- and stereoselectivities.

Keywords: Enzymatic Catalysis, P450, Hydroxylation, Regioselectivity, Molecular Dynamics

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APPLICATION OF ADVANCED ALGORITHMS FOR THE PREDICTION AND IMPROVEMENT OF COAGULANT DOSAGE IN WRPS

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1. Introduction

Defining the optimal coagulation dosage is an important operation that intervenes in flocculation processes in Water Reclamation Plants (WRPs). The capacity of a coagulation system to achieve a good flocculation level depends on influent parameters such as pH, temperature, conductivity, turbidity, etc. An inadequate control of coagulant added during flocculation can result in a higher plant management cost and an unsatisfactory secondary effluent treatment.

WRP on-line monitoring and systematic assessment are necessary to improve daily operational processes. In this work, a model comparison analysis is proposed, using three mathematical methods to select the best technique to predict the coagulation dosage related to real-time water quality.

2. Methodology

For four months, two spectrophotometric probes were installed in a WRP in Catalonia at the inlet of the tertiary system and at the end of the coagulation process. Both probes monitored quality changes of secondary effluent during operation.^[1]

The selected parameters from the inlet spectrophotometer were turbidity, pH, conductivity, flow velocity, UV-visible wavelengths and coagulant dosage added. From the outlet spectrophotometer, selected parameters were turbidity, pH and UV-visible wavelengths.

The chosen mathematical algorithms to compare their behaviour predicting the coagulant dosage were Multiple Linear Regression (MLR), Support Vector Machine (SVM) and Artificial Neural Networks (ANN). [2-4]

3. Results and discussion

Figure 1 shows performance of models in predicting coagulant dosage. Overall results showed a good correspondence between real and predicted values. While MLR showed low to medium correlations ($R^2 = 0.62-0.71$), non-linear regressions SVM and ANN had slightly better results ($R^2 = 0.81-0.84$ and $R^2 = 0.89-0.91$, respectively).

Overall, ANN and SVM provided better predictions than MLR. For small values of coagulant and abrupt slowdown peaks, SVM and ANN algorithms gave an overestimated prediction. Instead, SVM could predict and reproduce the changes slightly better than the ANN model. It was hypothesised that these sudden variations could be related to turbidity changes of the influent.

A good correspondence between real and predicted data was obtained. Specifically, the application of different non-linear models of ANN and SVM were better than linear models of MLR to predict the coagulant dosage in a WRP. The ANN and SVM algorithms could better reproduce the variations in the parameters produced by changes in the influent. This confirms the models used as suitable tools to predict and improve the operation in a WRP.

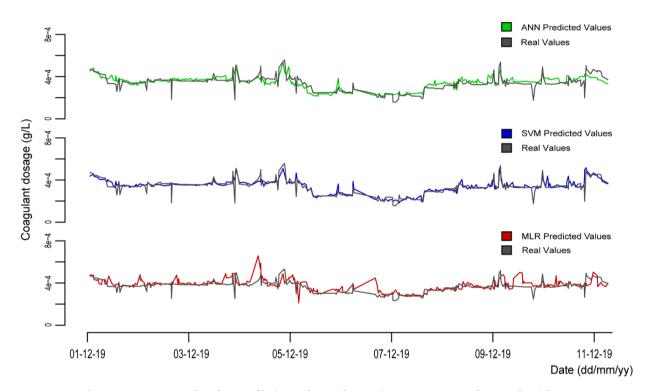


Figure 1. Accuracy of 11-day predictions of coagulant using ANN, SVM and MLR algorithms.

Keywords: Coagulant dosing, on-line monitoring, Water Reclamation Plant, mathematical modelling

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MACHINE LEARNING ALGORITHMS AS A CLINICAL TOOL TO DIFFERENTIATE LYMPHOPROLIFERATIVE DISORDERS

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1. Introduction

Cell population data (CPD) measured by Sysmex XN-series haematology analysers can describe white blood cell (WBC) subpopulations according to their morphology. Machine learning algorithms (MLA) are non parametric methods that can recognize data using a training process. Then, this learning process is evaluated predicting different data cases.

2. Hypothesis

Lymphocytosis is a common disease seen in laboratory medicine and could be a challenging process for non-expert staff to differentiate malignant from infectious pathologies. CPD information can be used by MLA to assist laboratory staff to classify lymphocytes. The aim of this study is to determine how good MLA are at classifying lymphocyte disorders using cell population data obtained from a haematology series analyser to improve diagnosis in the clinical laboratory.

[1,2]

3. Methodology

84 patient samples were included retrospectively and were classified as follows: 33 infectious mononucleosis (IM), 38 chronic lymphocytic leukaemia (CLL) and 13 splenic marginal zone lymphoma (SMZL). 35 subjects were included as a health control group. Cell blood count and cell population data were considered for the prediction analysis. Data was divided randomly in four parts, respecting the proportions of the group. 75% of patients were chosen to train the algorithm and 25% of patients to test the model. Supervised machine learning algorithms (linear support vector machines, decision trees and random forests) were trained with the training cohort and were validated with the testing cohort. R programming language R and the caret package were used to perform the statistical analysis.

4. Results

Support vector machines presented the best accuracy for differentiating haematological pathologies when compared to other algorithms (Table 1). Prediction of testing cohort labels was performed (Table 2). Sensitivity of 100%, 80% and 81% were obtained for CLL, splenic marginal zone lymphoma and infectious mononucleosis, respectively.

Table 1. Accuracy for the training cohort and the testing cohort obtained using different machine learning algorithms

Accuracy	Training cohort	Testing cohort
Support Vector Machines	98%	90.0%
Decision tree	100%	89.0%
Random Forest	98%	86.4%

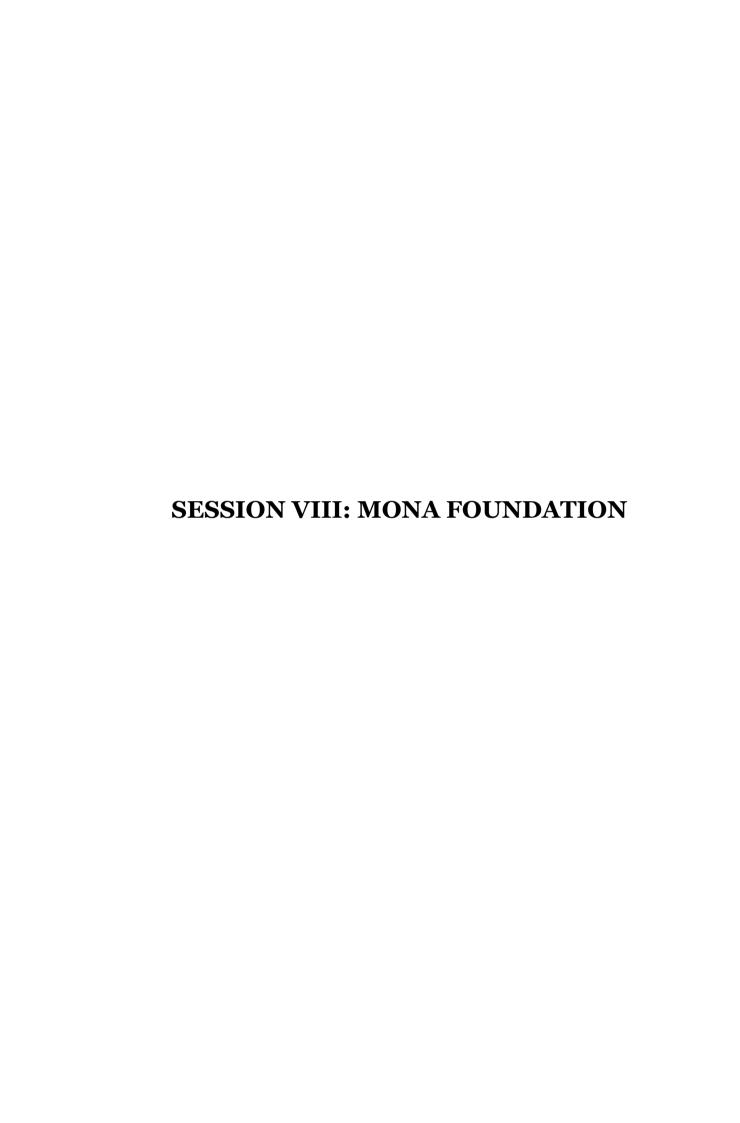
Table 2. Confusion matrix of cases prediction

	Tubic = Communical matrix of cases production				
		Prediction			
		IM	CLL	MEL	HC
Reference	IM	8	0	1	0
	CLL	1	10	1	0
	MEL	0	0	2	0
	HC	0	0	0	7

Machine learning algorithms can be helpful in differentiating different pathologies during diagnosis. Results have shown that morphometric data managed by MLA can be helpful information for laboratory staff. More data is needed to validate this SVM algorithm to prove the power of these models in differentiating between reactive lymphocytosis and malignant lymphoproliferative disorders.

Keywords: machine learning, lymphocytes, malignant, reactive, disorders.

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ENVIRONMENTAL ENRICHMENT IN A SOCIAL SETTING: ASSESSING THE USE OF A NOVEL FOOD MAZE IN SANCTUARY-HOUSED CHIMPANZEES

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1. Introduction

Foraging devices constitute an effective enrichment strategy in non-human primates, providing both cognitive and manipulative stimulation, thus enhancing animal welfare (Dutton et al., 2018). Additionally, when implemented in social settings, they better simulate a natural environment, and therefore constitute more ecologically valid enrichment activities (Cronin et al., 2017). In this study, we evaluated the behavioural effects of a novel enrichment device requiring tool-use in 14 sanctuary chimpanzees (*Pan troglodytes*) housed at Fundació Mona (Girona, Spain).

2. Hypothesis / problem

We predicted that chimpanzees would show interest in the enrichment device, and that this would increase the frequency of species-typical behaviours (e.g. manipulation and tool use), while decreasing the frequency of undesirable behaviours (e.g. inactivity and abnormal behaviours).

3. Methodology

Chimpanzees lived in two groups of equal size, in two separated enclosures containing one enrichment device each. This device was a vertical food maze filled with nuts as rewards, which chimpanzees needed to extract by using tools from their environment (Figure 1). For each group, we monitored behaviour in two conditions: 12 enrichment days (food maze loaded) and 12 control days (food maze empty), randomly distributed over a 2.5-month period. Data was collected using 2-min scan sampling in two daily sessions of 80 minutes each, one in the morning and one in the afternoon.



Figure 5. Enrichment device (food maze) evaluated in this study.

4. Results and discussion

Participation (i.e. the proportion of scans in which subjects interacted with the enrichment) widely varied across individuals (0.22-53.52%) and groups (mean participation: Group 1= 12.14%, Group 2 = 5.71%), being three times higher in the morning than in the afternoon. Only two chimpanzees mastered the task, reliably retrieving the rewards across sessions. The frequency of manipulation and tool use significantly increased in the enrichment days. However, inactivity and abnormal behaviours did not decrease, and unexpectedly, social play decreased. Furthermore, in the group with higher participation (Group 1), locomotion increased on the enrichment days, while agonistic behaviours decreased. In contrast, no significant changes in the frequency of these or other behaviours were observed in Group 2.

5. Conclusions

Overall, the presence of the food maze promoted species-typical behaviours, but it did not reduce the frequency of undesirable behaviours. It should also be noted that participation was unevenly distributed across subjects and groups, suggesting differences in the level of interest and behavioural impact of the enrichment device. Future studies should evaluate enrichment devices during longer periods and take into account individual preferences.

Keywords: behaviour, chimpanzees, cognitive enrichment, tool-use, welfare

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CHOOSE YOUR EDGE: THE POTENTIAL BENEFITS OF MULTIPLEX ANALYSIS IN CHIMPANZEES' SOCIAL NETWORKS

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1. Introduction

Social network analysis based on one interaction type became increasingly popular over recent decades. While mono-layer networks allowed us to gain a deeper understanding of social interactions, the complex interaction patterns of highly social animals such as chimpanzees (*Pan troglodytes*) might require a more realistic framework to draw meaningful conclusions. The recent development of new tools to analyse a vast amount of data from multiple sources enables us to explore multiple interaction types simultaneously by using multiplex networks.

2. Hypothesis

We implemented multiplex analysis with two groups of chimpanzees (N=14) housed at Fundació MONA. We predicted that (1) the multiplex approach could provide meaningful insights even in smaller groups of chimpanzees, (2) different patterns might be found depending on the interaction type (layer), and (3) a multiplex analysis indeed would lead to an increase of information, compared to traditional mono-layer network analysis.

3. Methodology

Using the tools provided by the MuxViz software^[1], we created 4-layered multiplex networks based on the following social interaction types: stationary vicinity (i.e. staying out of an arm's reach but within 5 metres), affiliative behaviour, allogrooming, and passive close proximity (i.e. staying within an arm's reach). We ran interlayer correlations to detect (dis)similarities, conducted a reducibility analysis to evaluate the information gain and redundancies of layers, calculated and ranked the eigenvector centralities/versatilities.

4. Results and discussion

We found the global overlap between all four layers to reach only 18-20% and layer overlap between two layers scored on average 58±9% (Mutamba group) and 56±14% (Bilinga group). However, we found stationary vicinity to be more similar to passive close proximity, and allogrooming to be more similar to affiliative behaviour. In the reducibility analysis, we detected that each layer imparted different and new information and the maximum relative entropy was achieved by maintaining all layers separately. When comparing the eigenvector rankings between all four layers, its aggregate and multiplex state we could not detect any clear tendency.

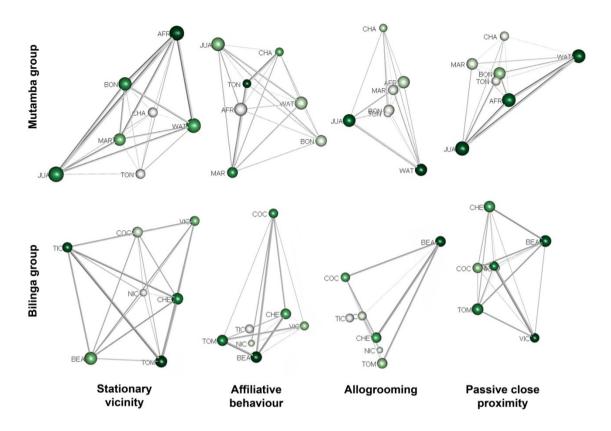


Figure 6. Multiplex networks of two social groups (Mutamba and Bilinga). Each layer represents one of the four different social interaction types. Edge width is proportional to the value of the dyadic interaction weight. Node size is proportional to the eigenvector versatility (uniform scaling in all layers) and node colours depend on the individual's strength centrality per layer.

5. Conclusions

We conclude that the multiplex approach provides interesting insights into the interplay of different types of social interactions and has the potential to give a broader understanding of the complex interactions within a social group compared to traditional mono-layer networks. Our findings show that it is possible to implement the multiplex approach even in small and densely connected groups of chimpanzees, as typically found in captivity.

Keywords: chimpanzees, welfare, multiplex networks, social behaviour, proximity

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SESSION IX: BIOMEDIC RESEARCH: CANCER AND HEART DISEASE

THE SODIUM CHANNEL BETA2 SUBUNIT RELIES ON CHOLESTEROL TO REMAIN AT THE TOP OF THE CELL

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1. Introduction

The sodium channel beta2 subunit (encoded by *SCN2B*) is an important component of the cardiac-voltage gated sodium channel. Beta2 promotes proper membrane localization of the channel's alpha subunit, Nav1.5.^[1,2] The channel is essential for cardiac electrical conduction. Pathogenic mutations in beta2 result in fewer channels at the cell surface, which turn into severe arrhythmias.^[3,4]

2. Hypothesis

Beta2 is a transmembrane protein displaying polarized trafficking in epithelial cells. Specific motifs in beta2 are responsible for its polarized localization and membrane dynamics at the cell surface, namely its putative S-acylation at Cys182 and association to lipid rafts.

3. Methodology

We generated constructs to express beta2 fused to YFP, WT and Cys182Ser, which is unable to be palmitoylated. We then expressed these in polarized Madin-Darby canine kidney (MDCK) cells. We used confocal microscopy, biochemistry and functional assays to determine how palmitoylation and cholesterol association rule beta2 behaviour.

4. Results

Our data showed that beta2 colocalizes with lipid rafts at the apical domain of the plasma membrane. Beta2 permanence at this domain was dependent on association to cholesterol-rich lipid rafts. Upon plasma membrane cholesterol depletion or pharmacological disruption of intracellular cholesterol trafficking, beta2 lost exclusive apical localization. In addition, palmitoylation of its Cys182 partitioned the protein to detergent-resistant membranes. Surprisingly, both lack of palmitoylation and cholesterol depletion reduced beta2 mobility in the plane of the plasma membrane.

5. Conclusion

Beta2 traffics and localizes to the apical domain of polarized cells in a cholesterol-dependent manner. Cys182 palmitoylation partitions the subunit to lipid rafts.

Keywords: Cholesterol, palmitoylation, sodium channel beta2 subunit, lipid raft, polarity

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THREE-DIMENSIONAL CULTURE USING POLYCAPROLACTONE ELECTROSPUN SCAFFOLDS WITH NON-SMALL CELL LUNG CANCER MODELS

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1. Introduction

Cells cultured in monolayer using flat plastic supports do not represent physiological conditions.^[1,2] Researchers have developed different three-dimensional (3D) systems to culture cells providing spatial distribution and allowing different interactions between cell-cell and cell-matrix.^[3] Electrospinning is a technique used to manufacture scaffolds whose fibres are similar to the extracellular matrix.^[4] Polycaprolactone (PCL) is a synthetic polymer suitable for cell culture purposes due to its biocompatibility, resorbability and viscoelasticity.^[5,6]

Lung cancer is the most prevalent cancer and the leading cause of cancer death in the world. Almost 90% of lung cancer cases correspond to non-small cell lung cancer (NSCLC) which is the most common subtype. [7] Epidermal growth factor receptor (EGFR) tyrosine kinases inhibitors (TKIs) are successful therapies which have been developed for those patients who have mutated EGFR genes. Unfortunately, a great number of patients become resistant to EGFR-TKIs. [8] Therefore, further studies are needed to understand this lung cancer subtype and 3D culture could provide trustworthy results, but it is essential to determine a perfect scaffold for culturing these cells. The main aim of this work is the evaluation of electrospun ES-PCL scaffolds to be used for culturing NSCLC cells.

2. Methodology

Two different PCL concentrations (10 and 15% w/v) were dissolved with acetone and scaffolds were manufactured by electrospinning using a 18G needle emitter, a fixed voltage of 7 kV and a flow rate of 6 ml/h. Both 10 and 15% PCL scaffolds were characterized by DSC and TGA methods. The microarchitecture was also analysed by scanning electron microscopy (SEM) and the fibre diameter, surface porosity and pore area were calculated. Sensitive and gefitinib resistant cell models, PC9 and PC9-GR3, were grown into the scaffolds for 3 and 6 days. Cell proliferation was tested by MTT assay and cell morphology was studied by confocal laser scanning microscopy.

3. Results

The results obtained were 15% ES-PCL scaffolds exhibiting higher fibre diameter, larger pore area, and lower surface porosity compared to 10% ES-PCL scaffolds. Nuclear and cytoplasmic elongation factors were higher on cells cultured in scaffolds compared to monolayer in PC9 and PC9-GR3. Cell proliferation rate was higher in 15% ES-PCL scaffolds than 10% ES-PCL scaffolds in both culture times assayed.

4. Conclusions

ES-PCL scaffolds are useful for the 3D culture of sensitive and gefitinib-resistant NSCLC cells. They obtain trustworthy results since cells are surrounded by a suitable environment, similar to the physiological one.

Keywords: electrospinning, non-small cell lung cancer, three-dimensional cell culture

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PREMATURE TERMINATION CODON IN PLAKOPHILIN2 (PKP2) CAUSES A DOWNREGULATION OF DESMOSOMAL AND CALCIUM-HANDLING GENES IN AN HL1 CELL MODEL OF ARRHYTHMOGENIC CARDIOMYOPATHY

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1. Introduction

Arrhythmogenic Cardiomyopathy (ACM) is a rare inherited disease characterized by the progressive replacement of the myocardium by fibrofatty tissue. Worldwide prevalence of ACM ranges from 1:2000 to 1:5000, and it is responsible for around 20% of all cases of sudden cardiac death (SCD) among people under 35 years of age. The main genetic causes of ACM are mutations in desmosomal genes, especially the presence of premature termination codon (PTC) in PKP2. ACM is characterized by high phenotypic variability and low penetrance, and, in some patients, by compound heterozygosity. It is known that mutations in PKP2 may cause a dysregulation of the Wnt/ β -catenin pathway, which could lead to enhanced adipogenesis. These molecular mechanisms are still uncertain, and we lack better understanding of the pathophysiological mechanisms that trigger adipogenesis, electrical disturbances and structural heart disease.

2. Objectives

The main purpose is to study the molecular mechanisms underlying *PKP2* depletion and their functional implications. We aim to study the expression levels of ACM-related genes at RNA and protein levels and the possible impact of the Wnt signaling pathway.

3. Methodology

Cardiac HL-1 cell line was edited by CRISPR/Cas9 to generate a PTC after the 92nd amino acid of *PKP2* in both alleles. Expression levels of ACM-related genes were tested by RT-PCR: desmosomal, calcium-handling and connexome-related genes. Changes in the total amount of protein were checked by western blot of the total protein lysate. To evaluate *PKP2* role on Wnt signaling, a TCF/LEF luciferase reporter assay was performed.

4. Results

HL1 PTC-PKP2 showed downregulation of *SCN5A*, *CX43*, *RyR2*, *Atp2a2*, *Slc8a1* and *Casq2* at the mRNA level, and complete absence of *DSC2* and *ANK2* expression. There were no significant differences in *DSP*, *DSG2*, *PG* and *ANK3* gene expression. Western blot results showed complete absence of PKP2 and ANK2 expression at the protein level. Luciferase assays indicate that there is no significant difference between HL1 WT and PTC-PKP2 clones related with the activity of Wnt signaling pathway.

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5. Conclusions

Results suggest PTC-PKP2 mRNA degradation by nonsense meditated decay system causing a complete absence of *PKP2* at the protein level. PTC-PKP2 causes massive changes at the molecular level on calcium-handling and connexome-related genes. *PKP2* depletion provokes a complete absence of expression of *ANK2* and *DSC2* at mRNA levels, suggesting a role on their transcription regulation.

Keywords: Arrhythmogenic Cardiomyopathy (ACM), Plakophilin 2 (PKP2), HL1 cell line, CRISPR/Cas9, Premature stop codon (PTC)

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PATTERNS AND FACTORS ASOCIATED WITH INCIDENCE AND SURVIVAL OF CHRONIC LYMPHOCYTIC LEUKAEMIA IN GIRONA (SPAIN) 2008–2015: A POPULATION-BASED STUDY

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1. Introduction

Chronic lymphocytic leukaemia (CLL) is a mature B-cell clonal malignancy and represents one of the most common diseases in western countries.^[1,2] CLL presents in adults, at higher rates in males than in females and in whites than in blacks. Median age at diagnosis is 64–70 years.^[1,3] Despite the main advances in treatment, CLL remains incurable.^[4,5] The main objectives of the study are: to estimate the real incidence of CLL and their trends, to describe the characteristics of this disease based on geriatric patterns and to detect differences in survival of this disease by the major prognostic factors (stage at diagnosis time, age of patients). In this study, we analysed chronic lymphocytic leukaemia incidence and its trends, and survival between 2008 and 2015 in Girona.

2. Methodology

Data were extracted from the population-based Girona Cancer Registry. Incidence was analysed in terms of crude rate (CR) and world and European age-standardized rate (ASRw, ASRe). Trends were assessed using the estimated annual percentage of change (EAPC) of the ASRe. We also analysed the observed survival and relative survival at 1, 3 and 5 years.

3. Results

We identified 400 CLL adult cases (>32 years), 43.7% females and 56.2% males. Median age at diagnosis was 72 years. Analysis: For the selected study, crude rate (CR) cancer incidence was 6.73 cases per 100,000 inhabitants/year (7.51 men; 5.93 women). Regarding the ASR, results show an ASRE13 of 7.71 (95% CI 6.97;8.52) and ASRW of 3.33(95% CI 2.98;3.74). A statistically significant decrease in the incidence was found for patients older than 75 years with an EAPC -11.6 (95% IC -13.6;-9.5). In addition, a significant decrease was observed in patients who presented a high intermediate risk Rai index (stages 1, 2, 3 and 4), with an EAPC -14.4 (95% IC -20.9:7.4). Five-year observed and relative survival rates were 67.3 and 85.8%, respectively.

4. Conclusions

We found a decreasing trend in the incidence of elderly patients, as well as in patients with an intermediate-high Rai index. Observed and relative survival rates of CLL are consistent with the age of the patient and the stage at the time of diagnosis, being high in young patients with a Rai index o (low risk).

Keywords: Chronic lymphocytic leukaemia (CLL), Incidence, Survival, Trends.

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FUNCTIONAL CHARACTERITZATION OF CPVT-ASSOCIATED MUTATION p.G357S_RYR2 USING PATIENT-SPECIFIC INDUCED PLURIPOTENT STEM CELL-DERIVED CARDIOMYOCYTES (iPS-CM)

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1. Introduction

Catecholaminergic polymorphic ventricular tachycardia (CPVT) is a severe arrhythmogenic disease characterized by adrenergically-induced ventricular tachycardia associated with sudden cardiac death. A mutation in type-2 ryanodine receptor (RYR2), p.G357S_RYR2, was recently associated with CPVT in a large family from the Canary Islands. We were able to obtain skin biopsies from heterozygous and homozygous donors and further derive iPS-CM from those samples. The aim of this study was to evaluate whether the number of mutated alleles can have an additive effect on RYR2 function.

2. Methodology

We generated iPS-CM using a heparin-based differentiation protocol^[1] followed by glucose starvation and hormonal-maturation treatment using triiodothyronine and dexamethasone.^[2-4] We used cells derived from one heterozygous (HT) and one homozygous (HM) patient, and from a non-carrier healthy donor, used as control (CTRL). Calcium imaging techniques were employed to assess RYR2 caffeine sensitivity in basal and β -adrenergic stress conditions (100nM isoproterenol).

3. Results

Peak amplitude of calcium transients elicited with 10 mM caffeine was similar in both HT and HM cells respect to CTRL cells (in $\Delta F/F_0$: CTRL=2.46±0.10, HT=2.80±0.08, HM=2.57±0.10). In dose-response studies, performed in basal conditions, both HT and HM cells showed a similar caffeine sensitivity that was higher than the one obtained with CTRL cells (K_{dCTRL} =2.53±0.34mM K_{dHT} =1.67±0.19mM and K_{dHM} =1.72±0.10mM). When these experiments were repeated in the presence of isoproterenol, we were able to promote an augmented response in CTRL cells, but no further increase was observed in HT or HM cells (K_{dCTRL} =1.38±0.06mM, K_{dHT} =1.68±0.09mM and K_{dHM} =1.40±0.12mM).

4. Conclusion

Our present results show that both HT and HM cells present a similar gain in function with respect to CTRL, in spite of their different allelic composition. This suggests that for p.G357S_RyR2 one mutated allele is enough to produce a gain in function in RYR2 with no further additive effect.

Key Words: CPVT, iPS-CM, RYR2, calcium imaging, caffeine.

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CHARACTERIZATION OF MESOTHELIN GLYCOSYLATION: ADVANCING TOWARDS A NOVEL PANCREATIC CANCER BIOMARKER

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1. Introduction

Pancreatic cancer (PaC) is the third most common cause of death from cancer, with a 5-year survival rate of just 8%. The finding of novel biomarkers for an earlier diagnosis is mandatory, as most PaC cases are not curable when detected. [1] The majority of cancer biomarkers are glycoproteins, as altered glycosylation is a feature of tumour progression. Therefore, the analysis of glycan epitopes on specific glycoproteins could yield novel biomarkers with increased accuracy. [2] Mesothelin is a candidate glycoprotein for such studies, as it is *neo*-expressed in PaC and other cancers, can be detected in the bloodstream and its glycosylation has not been previously studied.

2. Hypothesis

The analysis of mesothelin glycosylation could help in the development of new biomarkers to discern pancreatic cancer from other tumours and pancreatic benign diseases. Hence, we aimed to evaluate mesothelin expression in PaC cell lines, their conditioned media, tumour pancreatic tissues and non-tumour ones. We also focused on the full characterization of mesothelin glycosylation (both at site occupancy and N-glycan structures) and the development of a methodology to rapidly identify the most promising glycoforms.

3. Methodology

We also collected the conditioned media from the cell lines to assess mesothelin secretion. Mesothelin expression was determined through western blotting on the aforementioned samples, and glycan analyses were conducted on mesothelin immunopurified from the conditioned media. N-glycosylation site occupancy was studied by PNGaseF digestion and mass spectrometry (UPLC-ESI-QTOF). N-glycan structures were sequenced by hydrophilic interaction liquid chromatography (HILIC-UPLC) combined with multiple exoglicosidase digestions, and were also evaluated through western blot on immunopurified mesothelin using specific lectins.

4. Results

All the studied cell lines expressed mesothelin, in higher amounts on the secreted media. In tissues, mesothelin was present in 76.7% (n=30) of PaC patients, while it was only observed in one out of ten control cases. Regarding N-glycosylation, its site occupancy was almost complete. N-glycan sequencing mainly showed complex N-glycan structures with terminal sialic acid. Some glycan determinants (core fucose, branching and bisecting GlcNAc) presented differential

expression on mesothelin for PaC and ovarian cancer. Thus, we established a combined ELISA/ELLA assay to quickly quantify these specific mesothelin glycoforms.

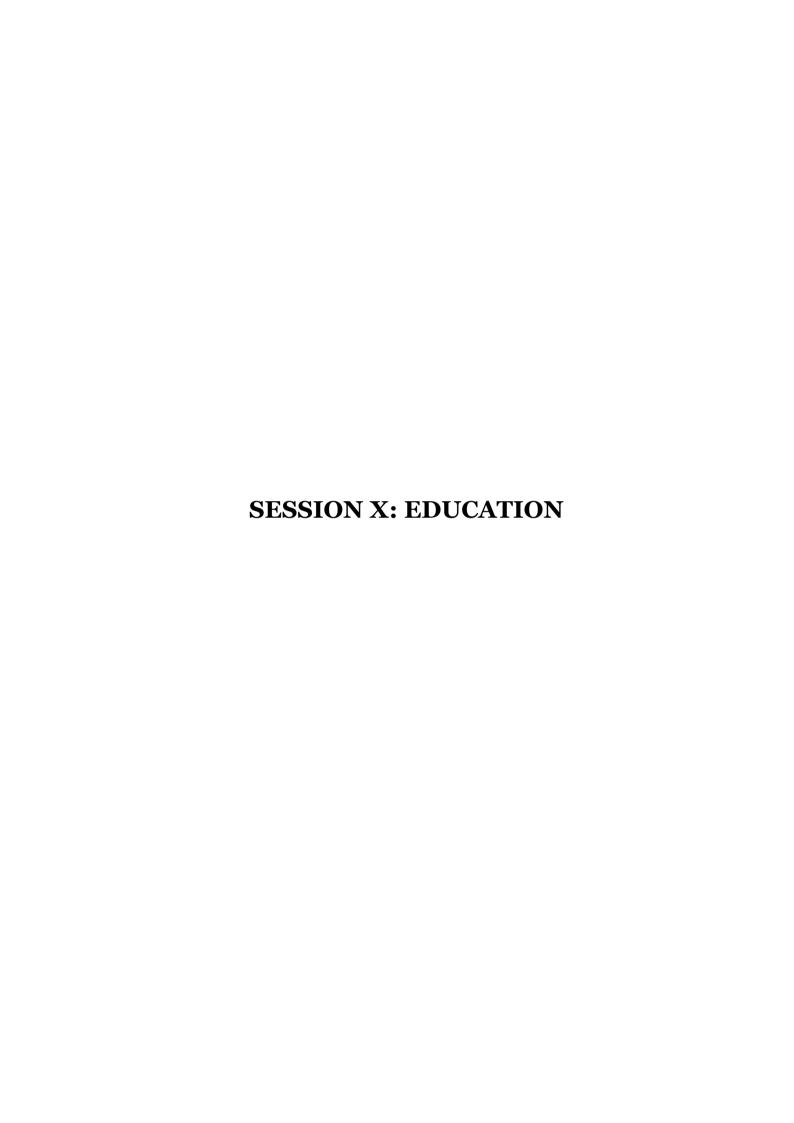
5. Conclusions

Mesothelin is highly secreted from PaC cells. We have described its N-glycan structures and developed an assay to detect specific glycoforms that can be used in serum samples to determine the potential of these glycoforms as biomarkers.

Keywords: pancreatic cancer, biomarkers, glycosylation, glycoproteomics, mesothelin

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THE PERCEPTION OF THE FAMILY REGARDING THE MEASURE FOR COURT-ORDERED LIVING IN EDUCATIONAL GROUPS IN CATALONIA

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1. Introduction

Child-to parent violence is a growing reality at national and international levels which has prompted the Catalan youth justice system to recently create two specialized units called "educational groups" to address crimes of this character (Departament de Justícia, 2018; Ibabe et. al., 2018). The family is the context where this violence is generated, so we aim to gather the perceptions of the family in terms of learning, change and evolution of the young person following the socio-educational action of the judicial measure of cohabiting in educational groups in Catalonia.

2. Hypothesis

The research presented starts from the following hypothesis:

- The family values the stay in the educational group because it believes that it allows the development and consolidation of skills that empower the young person.

3. Methodology

Five semi-structured interviews were conducted with 5 families of young people who have complied with the judicial measure of cohabiting in educational groups in Catalonia, based on the range of dimensions and indicators of youth empowerment from the HEBE Project (Ref.: EDU2017-83249-R)⁸ (Planas *et. al.*, 2016).

Each interview was conducted with a single person in the family after 3-4 months of compliance with the court order. The selection of the interviewee was based on four criteria: predisposition, proximity to the young person before and after their time in the educational group, linguistic accessibility and recommendation by the educational team of the judicial measure.

4. Results

The family positively values the educational group for its proximity, interdisciplinarity and continuous interrelationship during and after the judicial measure. Also, because it establishes daily standards, guidelines and routines that help structure the daily habits of the young person. However, it is believed that these practices have not fully consolidated youth empowerment. Families consider that the person returning home lack skills such as self-esteem, responsibility or

⁸ www.projectehebe.com/en

participation, which do not help to improve family coexistence since they generate fear or tension that disruptive behaviour will reappear.

5. Conclusions

To raise awareness and sensibility for the present and future, as well as strengthen and consolidate empowering capacities and skills, socio-educational strategies should ensure involvement and collaboration of the young person during and after their stay in the educational group. This could be done, for example, through mentoring or project learning.

Acknowledgments

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Keywords: family, youth, empowerment, juvenile justice, child-to-parent violence

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PEDAGOGIGAL CONTRIBUTIONS OF HOMESCHOOLING

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3. Introduction

Nowadays our country is able to provide compulsory education for all children between 6 and 16 years of age. There are some families, however, who choose not to enrol their children in school and to take responsibility for the formal and non-formal education of their children in all skill areas: academic, social, cultural, physical and psychological. This phenomenon, called homeschooling, is little known in our country and is not regulated by education legislation. However, several researchers from the USA (Chatham-Carpenter, 2015; Medlin, 2015; Montgomery, 2015; Kunzman, 2015;) and England, (Rothermel, 2015) – where homeschooling is a recognised right and choice for families – seem to indicate that there are certain advantages to this type of education.

4. Problem

The aim of this thesis is to study the homeschooling phenomenon in Catalonia. On the one hand, we want to understand and analyse the types of families that practice it, and which curriculum, activities, methodologies and resources they follow. On the other hand, we want to analyse the different pedagogical contributions of homeschooling that could improve the process of teaching and learning.

5. Methodology

To answer these questions we used qualitative case study methods to interview 15 families with a structured interview of 57 open-ended questions and completed the research with the analysis of 5 family blogs, where mothers described their experiences using the qualitative data analysis program named Atlas.ti. These families were chosen for their characteristics, looking at three criteria: age, social category and living environment. The interview grid was validated by a group of experts.

With the analysis of blogs we focused on three criteria: the different subjects, the methodology they use and the advantages or disadvantages they have.

6. Results

In general terms:

- -The most popular subjects are maths and language, followed by science and history. And they work from everyday activities.
- -They practice pedagogical conversation, from which they devise projects, excursions and searches on specific topics.
- -They work on artistic expression and use art as an instrument (clay, painting, cardboard).

- -They use play-based methodology, project-based learning, and specific methodologies, including Glenn Doman, Montessori and Waldorf.
- -They also learn about professions, like mechanics, carpentry and plumbing.

7. 5. Conclusion

In conclusion, homeschooling is a focus of research in education, the digital world and the new challenges of modern life that push us to look for alternatives and solutions to the problems and shortcomings of education today. The state of emergency caused by Covid-19 has made it clear that school attendance is not always feasible and flexible educational options and alternatives are needed to handle future scenarios where temporary confinements are part of the survival strategies. Access to new technologies and the information society make a paradigmatic change in society possible. Teachers can counsel and assist parents by organising education platforms and online classes to ensure children's capacity to learn.

Keywords: Homeschooling, unschooling, e-learning, personal education, private education

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CHARACTERIZATION OF EARLY ALGEBRA IN EARLY CHILDHOOD AND PRIMARY EDUCATION

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1. Introduction

A progressive transformation, at the curricular level, has manifested itself during recent decades in various countries, such as the United States, Australia, and Singapore. It incorporates the development of algebraic thinking from the first years of schooling and forms the basis of a recent line of research, early algebra.

Early algebra proposes to include the development of algebraic thinking from levels below primary education (Carpenter, 2003; Davis, 1985; Vergnaud, 1988). This process, called by Kaput (2000) "algebraization" of the curriculum, aims to integrate algebraic thinking throughout all courses. From this perspective, we have been interested in characterizing the mathematical knowledge present in contemporary curricula for the teaching of early algebra.

2. Problem

Over the past few decades, the study of early algebra has undergone a radical change in mathematics curricula as it has been largely incorporated from the early years of schooling. This new proposal, which appears in the standards of the National Council of Teachers of Mathematics of the United States (NCTM, 2000), raises the importance of beginning to develop algebraic thinking from the age of three.

Under this scenario of changes and curricular integration of algebraic thinking, we seek to answer the question: What mathematical knowledge characterizes the teaching of early algebra in the early childhood and primary education curricula?

3. Methodology

The study adopts a qualitative methodology, using the content analysis method (Krippenddorff, 1990) in the curricula of countries advanced in the study of early algebra in early childhood and primary education: United States (NCTM, 2000), Australia (ACARA, 2015), Singapore (MOE, 2012, 2013), and Chile (MINEDUC, 2012, 2018). The categories of analysis have been established based on the coding of presence or absence of curricular content.

4. Results

The results show the knowledge that characterizes early algebra in early childhood education: experimentation with elements from attribute recognition to establish relationships; seriation from repetition patterns: identification, construction, representation; description of qualitative and quantitative changes. The mathematical knowledge that characterizes early algebra in primary education: understanding of different types of relationships and patterns; use of algebraic symbols and mathematical models to represent mathematical situations; understanding of change; use of variables to determine a constant or unknown.

5. Conclusions

The curricula emphasize the importance of working with patterns and relationships as a fundamental pillar in laying the groundwork for the transition of early algebra teaching from the the early childhood to the primary stage.

Keywords: characterization, early algebra, curriculum, early childhood education, primary education.

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COLLABORATIVE INTERVENTION IN DEVELOPMENTAL LANGUAGE DISORDER (DLD)

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1. Introduction

Developmental language disorder (DLD) corresponds to a functional difficulty that creates long-term obstacles to communication and learning (Bishop, 2016; Aguilar-Mediavilla, 2019). It affects 7.4% of the childhood population and is usually diagnosed from the age of 4 (Acosta, 2014). Speech therapists and special education teachers carry out the intervention.

2. Problem

Despite its importance for language development, learning and socialization, the intervention has been one of its less addressed dimensions (Acosta, 2012; Mendoza, 2012). Collaboration between professionals has been identified as one of the main needs (Fernández, 2009; Muntaner, 2019).

3. Methodology

Case study design. A systematic review, interviews and focus groups will be carried out. The sample corresponds to speech therapists and special education teachers. The findings will be analysed using Atlas.ti software.

4. Results and discussion

The systematic review indicates a significant increase in intervention research in the last decade and the prevalent use of the DLD concept in the last three years. Experimental studies focused on specific language aims (semantics and morphosyntax) predominate over literacy and other dimensions. Teacher or family involvement is still minimal.

5. Conclusion

There is a need for more research on literacy aims and other dimensions associated with DLD. Consideration should be given to intra-subject research designs, and observation of medium and long-term effects. It is necessary to undertake studies with samples of young people and adults with DLD. Teacher participation is essential to achieve collaborative intervention dynamics.

Keywords: Developmental language disorder (DLD), Speech therapy, Collaborative intervention, Systematic review.

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AN APPROACH TO VULNERABILITY AND POVERTY CHRONIFICATION: DISCOVERING NEW REALITIES FROM A CASE STUDY

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1. Introduction

The 2008 recession tested the effectiveness of social policies and social services to confront poverty. The responses were preceded by spending cuts and a withdrawal of care guarantee measures. However, we observe that neither vulnerability nor chronicity were part of the usual lexicon in traditional social policies. These policies have been directed at those people in situations of social exclusion and not at those who are at risk of finding themselves in that situation. The former are the users of social services, while the latter are vulnerable citizens who, until now, have never approached these services.

2. Hypothesis

The aim of this research is to contribute empirical references that allow us to contrast the theoretical contributions on the new manifestations of social exclusion and, also, on the difficulties of articulating responses adapted to these new situations.

3. Methodology

Our empirical quantitative and qualitative research focused on social services in la Garrotxa, a region of Girona, based on information from a survey of more than 400 people, 17 in-depth interviews and 3 discussion groups with political actors, technicians from the public administration, third sector social entities and users of social services.

4. Results

After the empirical approach, we observe how vulnerability has increased and diversified, and we found a subgroup of people who appear to have no real possibilities of overcoming their social exclusion situation: people for whom exclusion has become a chronic state.

5. Conclusions

The case analysed allows us not only to have data that demonstrate an increase in social exclusion, but also to observe situations, profiles and trajectories that were unprecedented until a few years ago. Let us recall the phrase of Beck (1998), observing how in the late 20th century the only thing that has really become democratized is the risk of social exclusion. The services we have been traditionally offering must change and take a look at new realities – vulnerability and chronicity –that, therefore, require different responses (Bauman, 1999; Rodríguez, 2016).

Keywords: social exclusion, social services, social policies, poverty

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PSYCHOLOGICAL WELLBEING OF UNACCOMPANIED MIGRANT YOUTHS IN THE TRANSITION TO ADULTHOOD: THE ROLE OF YOUTH MENTORING IN BARCELONA

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1. Introduction

Figures show that, during recent years, the number of unaccompanied immigrant minors arriving to Europe has increased steadily. Once in the new context of reception, they usually have access to protection services for minors. But when they turn 18, they start an uncertain route with a lot of challenges to obtain a viable future because of the lack of institutional and social support. Prior empirical evidence shows that they are exposed to a great variety of environmental stressors, which have an impact on their mental health, depending on the existing public health and social policies (Clayton, 2019; Correa-Velez, 2010). Youth mentoring interventions have a modest but significant effect in improving various youth outcomes across behavioural, emotional, social and academic domains (Raposa, 2019; DuBois, 2002). For this reason, this research examines the effects on psychological and educational outcomes of a mentoring programme with unaccompanied migrant youth who legally became "adults" in the Barcelona Metropolitan Area. This paper is part of the project "Applying mentoring", funded by the Recercaixa grant, focused on knowing which elements and practices can improve the effectiveness and efficiency of social mentoring programs.

2. Methodology

Data in this mixed-methods study was gathered from 44 surveys with mentored (treatment) and non-mentored (control group) youths who recently turned 18, as well as through 30 semi-structured interviews with mentored youth, their adult mentors as well as non-mentored youth. We monitored them for seven months between 2018 and 2019 to see if participation in the mentoring programme was effective in overcoming challenges with regard to their wellbeing and educational trajectories.

3. Results

The mean effect size values have been more positive for youth mentee groups for self-esteem (0.54 vs. 0.16), youth hope (0.45 vs. -0.31), resilience (0.70 vs. -0.14) and educational expectations (0.86 vs. 0.21). Also, we present the qualitative results of what type of social support unaccompanied youth identified from mentors and how these supports helped them to cope with transitioning into adulthood in the new context.

4. Conclusions

We conclude that well-targeted and problem-specific mentoring programmes have a relevant role as a protective factor for unaccompanied migrant youths' mental health. Social and political implications of these outcomes are also discussed, providing information on how interventions can offer effective networks of support for the settlement and social inclusion of unaccompanied immigrant youths.

Keywords: unaccompanied, migrant, youth, wellbeing, mentoring

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RELATIONSHIP BETWEEN EMOTIONAL INTELLIGENCE, ACADEMIC ACHIEVEMENT AND SOCIAL SKILLS

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1. Introduction

In the last decades, emotional intelligence (EI) has received much attention in the field of education. Most studies have shown that EI is an important predictor of children's socio-emotional adjustment at school and academic achievement (Parker, Saklofske, Wood & Collin, 2009). However, the evidence in support of this view comes mainly from studies focusing on college students and late adolescents and very few have centred their attention on children. On the other hand, the construct of social skills (SS) has also emerged as an important factor in school adjustment and has shown a positive correlation with academic achievement (Eisenberg, Valiente & Eggum, 2010).

2. Objectives

The present study examines the relationship between emotional intelligence and social skills 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 SS that are more closely related to the linguistic and mathematic competences and are predictors of their performance.

3. Methodology

One hundred and eighty students from the ages of 8 to 11, 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 $3^{\rm rd}$ grade (M = 8.68 years, SD = .28) and 92 in $5^{\rm th}$ grade (M = 10.65 years, SD = .31).

All children participated in three sessions. The first session included the assessment of EI and SS, with the Spanish versions of the BarOn inventory (Bermejo, 2018) and the SSIS-RS (Gresham, 2008), respectively. The second session was devoted to testing the academic abilities with the EFAI battery (Santamaría, 2005); and finally, the last session covered the assessment of linguistic and mathematic competence with a set of school tests.

4. Results

The analyses show a statistically significant correlation between general EI and SS scores. Regarding academic achievement, the EI components that emerge as the most important predictors of the school competences scores are the adaptability and the interpersonal factors, together with the intrapersonal component for Maths and the interpersonal for Catalan. Focusing on the SS, the factors of communication and cooperation appear to be the ones more related to academic achievement, together with the factor of responsibility for Catalan.

5. Conclusion

Our findings provide substantial support for a positive link between academic competences on the one hand, and emotional intelligence and social skills on the other, which is in line with previous research (Nikooyeh, 2017). In practical terms, the data suggest a need to take into account emotional competences and social skills when trying to foster the academic success of the students.

Keywords: Emotional intelligence; Social skills; Academic achievement; School competences; Children.

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PERSONAL SUPPORT NETWORKS OF YOUNG PEOPLE WITH INTELLECTUAL DISABILITIES: A RESEARCH PROJECT BASED ON SOCIAL NETWORKS ANALYSIS

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1. Introduction

Research highlights the important role that interpersonal relationships have as facilitators or inhibitors of the processes of social inclusion of people with intellectual disabilities, as well as the difficulties that many young people with intellectual disabilities experience in establishing meaningful interpersonal relationships on which their support social networks are based. The aim of this piece of research is to know the characteristics of social support networks of young people with intellectual disabilities during the transition to adulthood, specifically, young people between 13 and 16 years old enrolled in compulsory secondary education and special education.

2. Methodology

The study uses the methodology of personal network analysis (Molina, 2005). Individual interviews were conducted with 27 young people, focused on collecting data on their relationship network from the point of view of each young person, following the *egocentric network model* (McCarty, 2010). Subsequently, with the interview data, a computer questionnaire was completed for each participant. The data analysis provides information about the size of the network, its composition, the kind of relationship or link, the content of the support (emotional, instrumental or informational) and the structure of the network, among others.

3. Results

Preliminary results showed that young people's social networks are mainly made up of schoolmates and family members, and for the most part their relationship environments were the schools and their own homes. In very few cases were relationships carried out in the neighbourhood or in leisure settings, and friendships were usually limited to settings that are implicit in an adolescent's daily activities, such as compulsory schooling. Most of the participants perceived that members of their networks provided support, especially emotional and informational. Most of the young people interviewed considered that it was classmates, whom they often labelled as friends, who provided support.

4. Conclusions

Based on this analysis, proposals are made for action aimed at improving opportunities to build and maintain social networks that can act as natural supports in the life paths of young people with intellectual disabilities and, thus, guarantee the fulfillment of their rights, moving towards their social inclusion.

Keywords: personal support networks, intellectual disabilities, social relationships, education, social inclusion.

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SESSION XI: CLIMATE CHANGE, ECOSYSTEM MODIFICATION AND SUSTAINABILITY

ENVIRONMENTAL SUSTAINABILITY IN THE TEMPORARY EXHIBITIONS OF ART MUSEUMS

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1. Introduction

Within the rich universe of temporary exhibitions, we live in a make-and-undo. Most of the world's museums and cultural centres, and especially art museums, allocate one or more rooms to schedule a series of exhibitions each season, with start and finishing dates. The architecture of these exhibitions is based on the concept of constructing to deconstruct. This ephemeral nature or "expiration" requires giving consideration to the impact of constructing the spaces that host the travelling works of art. Temporary exhibitions that create permanent waste must be avoided. In this summary, we will look at a specific case study, the *Almacén. El lugar de los invisibles* display at the Museo Nacional de Escultura in 2019 (Figure 7) and will examine the concept of sustainability in temporary museum exhibitions.

2. Hypothesis

The main objective of the research is to provide practical recommendations to museum institutions and collaborators, so that they can reduce the environmental impact generated by temporary exhibitions. In this way, we also nurture ourselves, as a society, to relate to a less anthropocentric environment.

3. Methodology

We use an explanatory or relational type of programmatic qualitative methodology, which is intended, based on the results, to be able to make decisions, even in a predictive manner. Different techniques are combined: content analysis by defining the limitations of the theoretical and conceptual framework; observation to know the state of the issue and to know what systems and processes are being used; the case study to implement the evaluation system; and the in-depth interview, including cases, for the experts involved to pass on their experience to us. This is presented in a holistic way, in relation to several linked subjects.

4. Results

In addition to the possible ecological empathy or environmental awareness that every person may have, museum institutions must demonstrate that they are in favour of improving their management and acting responsibly with regard to the ecosystem and society. Precisely, the specifics of having to show highlights some practices where the idea of "compensating" is generalized as a balancing formula, acting for one's own interest without considering the environment and "exhibiting sustainability" in retrospect.

5. Conclusions

The exhibition spaces of art museums, which often have to fight for sustainable construction without evidence of this characteristic – "camouflaged sustainability" – have particularities typical of the sector. In the *Almacén. El lugar de los invisibles* display (Figure 8), respect for the environment is manifest, as it hardly generates waste, the museography uses as a support a material that is reusable and painting from the previous exhibition. In addition, the transport of pieces of art and the construction of custom packing boxes are not necessary.



Figure 9. Almacén. El lugar de los invisibles exhibition in the Museo Nacional de Escultura. Photographs by Anna Alcubierre

Keywords: Museums, Exhibitions, Sustainability, Environmental awareness, Ephemeral spaces, Ecodesign

WATER RESOURCES MANAGEMENT DURING DISRUPTIVE EVENTS: AN INTEGRATED PERSPECTIVE

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1. Introduction

Climate change has already led to an increase in the frequency and magnitude of extreme weather events such as droughts, floods, severe storms and heat waves, (Berbel, 2019), and it is expected that these climate phenomena will increase further once global warming exceeds the 1.5°C threshold (Hoegh-Guldberg, 2018). Droughts will exacerbate water scarcity problems in many regions worldwide, thus fostering further the need for effective water resources management (Kiem, 2013). The scientific literature has addressed the impacts, vulnerability and limitations of adaptation to scarcity. Yet, the traditional and most common approach has been to design partial equilibrium models to improve water management in specific sectors rather than develop models on a macro scale.

2. Hypothesis

Water management strategies need, therefore, to depart from partial equilibrium approaches that concentrate on specific sectors and rely on more comprehensive models that account for the linkages inherent in global supply chains. Failing to incorporate this interconnectedness and the potential inter-regional rippling effects in the modelling framework can lead to suboptimal economic analysis and inefficient policy design. To this end, in this paper we aim to assess the economic impacts of extreme water scarcity events in the economy by combining environmentally-extended multi-regional input-output (EE-MRIO) tables and non-linear programming (NLP) optimization models.

3. Methodology

For the simulation of water scarcity impacts, we employ the non-linear programming (NLP) optimization model recently introduced by Oosterhaven (2016). The microeconomic assumption behind this method is that, right after a hazard event, economic agents (i.e., households, firms and governments) will try to follow and re- build old-established commercial patterns as closely as possible. As far as the data is concerned, we use the third version of the EXIOPOL environmentally-extended (EE) multi-regional input-output (MRIO) dataset (Wood et al. 2015), which provides information on economic linkages among 163 sectors in 48 areas (43 countries and 5 regions of the world) for the year 2011, matched with multiple social and environmental satellite accounts.

4. Conclusions

Early results on virtual water flows and water footprint indicators reveal crucial agricultural subsectors that are highly water intensive. Based on these insights, four simulation scenarios of water-related disruptive events are defined. In the first set of scenarios the production of three specific sub-sectors is ceased due to a severe drought (scenarios 1A-1C). The second scenario assumes that the production of the three subsectors is jointly diminished (scenario

2). In addition, a third scenario is simulated in which production of vegetables for domestic demand is satisfied but their export is cancelled. Finally, scenario 4 represents a global drought where the whole Mediterranean agrifood system is affected.

Keywords: water scarcity, droughts, input-output, disruptive events, non-linear optimization

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THE ROLE OF HYDROLOGICAL ALTERATION AND SEASONALITY IN THE ECOLOGICAL STRUCTURE OF A METAL POLLUTED PYRENEAN STREAM

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1. Introduction

Freshwater ecosystems are biodiversity hotspots which are extremely vulnerable to species loss due to many human-mediated stressors. [1] Despite this, lotic ecosystems are one of the most exploited on the planet and human pressure on them is rising, especially with the construction of dams for the access to clean energies and water supply. [2] Climate change will exacerbate those alterations, especially in the Pyrenees, with an expected increase in temperatures and a decrease in precipitation. [3] We ask ourselves if well-preserved natural spaces can be exploited in a sustainable way while humanity faces a future with rising water and clean energy needs.

2. Methodology

Over a two-year period we studied a well-preserved but dam-impounded headwater stream in the Pyrenees that is affected by metals leaking from an abandoned mine. We used two sampling points at each side of the dam to assess the differences in water physicochemical parameters and in the structure of algal and macroinvertebrate communities between seasons, positions relative to the dam, and between different precipitation regimes for each season.

3. Results & Discussion

We observed a strong role of seasonality in the stream due to changes in precipitation and temperature regimes that drive changes in the ecological community structure. Winter was the most differentiated season, with the highest levels of algal and macroinvertebrate production-related parameters caused by the bloom of the macroalgae *Hydrurus foetidus*. Metals found in the water, especially arsenic, caused a decrease in algal production and bioaccumulated in the biofilms. Flow constriction caused by the dam and the drought situation altered the physicochemical parameters of the water, also affecting the ecosystem structural parameters. This stream presents a bottom-up control of production, so climate change and the presence of the dam are threatening the stability of the structure of this ecosystem.

4. Conclusions

Dams can be a useful resource for humans in this climatic change scenario because they grant access to water resources and clean energy, but their impacts should be individually assessed because headwater streams are key biodiversity areas and disturbance can alter the ecological structure and function of the whole river basin system.

Keywords: freshwater conservation, hydrological alteration, climate change, ecosystem structure.

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PHARMACEUTICAL POLLUTION IN A THREATENED COASTAL LAGOON IN S.E. SPAIN

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1. Introduction

The Mar Menor is one of the largest coastal lagoons in the Mediterranean. Located in S.E. Spain, it represents a heavily impacted ecosystem due to surrounding anthropogenic activities. The discharge of pollutants from urban, agricultural or mining sources is a major threat to the ecological and socio-economic value of the area. Confinement from the open sea makes coastal lagoons especially sensitive to human disturbances and the Mar Menor is no exception. Pharmaceutical residues have received little attention since their widespread detection in the lagoon (2010-2011).^[1] Recently, management actions have been implemented in the area to mitigate the impact of urban pollution. In this scenario, it is important to address the current prevalence of urban pollutants in the lagoon.

2. Methodology

For this purpose, we selected a set of wild aquatic organisms that are relevant, not only to local food webs, but also to human consumption. Specifically, two mollusc (clams and sea snails) and one fish species were sampled in three locations across the Mar Menor in summer and winter. Sampling locations cover areas of differing suspected pollution sources (i.e. urban sites, sewage discharge sites, reference locations). Biota was pooled according to species, location, season and size (n=50), and then freeze-dried, milled and stored at -20°C until analysis. Bead-beating extraction and a clean-up procedure were applied as described by Santos et al. [2] using a 100 mg sample (dw). Extracts were reconstituted to 1 mL methanol:water (2:8) and analysed with a LC-MS/MS method derived from Gros et al. [3]

3. Results

Preliminary results indicate overall very low occurrence and levels of pharmaceuticals in aquatic organisms. These findings would be in accordance with the decreased detection of urban pollutants in Mar Menor waters compared to ten years ago. Altogether, we suggest that improved wastewater management may have reduced the discharge of pharmaceutical residues into the lagoon, as well as their accumulation in mollusc and fish species. These results are relevant to human health given the potential risk of pharmaceutical exposure through seafood. Despite the seemingly good news regarding pharmaceutical pollution, additional pressures remain in the area and are contributing to the on-going deterioration of the Mar Menor ecosystem.

Keywords: pharmaceuticals, wastewater, management, seafood

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CABLE FACTORY, A CASE OF RESILIENT ARCHITECTURE

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1. Introduction

The Cable Factory is a cultural centre produced by time. In 1989, a social and cultural movement called Pro Kaapeli was created, where Pia Ilonen—ILO managing architect—was the negotiating technician, responsible for an alternative to the Helsinki City Council's plan to divide the Cable Factory into three separate parts. During more than 30 years, the Cable Factory has hosted a proactive community committed to the building, with a diversity of activities and independent management. Its evolution of spaces and the change of uses over time by means of raw spaces (a flexible and empty space with indeterminate qualities) is an example of sustainable development for the planning of Helsinki.

2. Hypothesis

The hypothesis aims to demonstrate that the Cable Factory, 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 Helsinki.

3. Methodology

The Cable Factory 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 ILO architectural firm and some inhabitants of the Cable Factory were interviewed using semi-structured interviews during 2020.

4. Results and discussion

The Cable Factory, in its spatial dimension, has the resilient properties of persistence, adaptation and transformation. The inhabitants are able to modify the raw spaces according to their needs by paying a low rent. Once the function or activity is finished, the spaces must be emptied again for future use. The Cable Factory has created an interconnection between architects, its community and Helsinki City Council, who are all committed to the building.

5. Conclusions

The Cable Factory is a resilient piece of architecture for creating a dynamic architectural system—an interdependent system in its social, spatial and temporal dimensions. Its modes of spatial evolution allow the Cable Factory's community to change uses according to their conditions. This dynamic and proactive community creates a self-organised and self-managed bottom-up system based on spatial indeterminacy. The diversity, independence and self-conditionality of its

community give the Cable Factory a sense of place and it is an example of sustainable development for the planning of cities and societies.

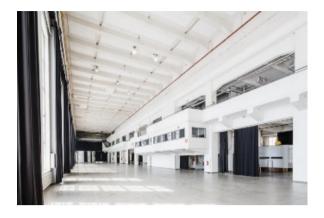


Figure 10. The Sea Cable Hall – Raw Space



Figure 2. Performance in the Sea Cable Hall, 1989



Figure 3. Slush Event in the Sea Cable Hall



Figure 4. Helsinki Design Week in the Sea Cable Hall

Keywords: Resilient architecture, dynamic architectural system, proactive community, spatial indeterminacy, sustainable development

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ECOLOGICAL COEXISTENCE OF SPANISH TOOTHCARP (Aphanius iberus) AND INVASIVE EASTERN MOSQUITOFISH (Gambusia holbrooki) IN A SALINITY GRADIENT

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1. Introduction

The Spanish toothcarp, Aphanius iberus (Valenciennes, 1846), is an endangered species.^[1] This endemic fish has been being displaced by the invasive Eastern mosquitofish, Gambusia holbrooki Girard, 1859, for a century, [2] and salinity appears to play a key role modulating the interaction of these two fish species.^{[3], [4]} Unveiling the underlying mechanisms mediating their coexistence is our final goal, and this study is the first step to assessing a starting field hypothesis. We hypothesized that the relative abundance of the two fish species in La Rubina reserve area (PNAE) is strongly dependent on the salinity gradient (i.e., high salinities would host a greater relative abundance of the more euryhaline endemic species). By contrast, the invasive species would dominate at low salinities. The method to test this hypothesis was to sample fish in 21 sites ranging from coastal marshes to channels and permanent water bodies of the area in February 2020. We used 3 to 6 fyke nets per site to catch fishes, and we recorded the initial and final times of net catching to obtain the effort time in minutes. We logged water conductivity, a surrogate for salinity, of each site. The method guaranteed that a whole salinity gradient, ranging from hypersaline to almost freshwater, was monitored in this study. We calculated the catch per unit effort (CPUE = n / t, where n is the number of fishes captured in a fyke net per unit time t, in minutes) averaged per site, as an estimate of relative abundance. We analysed the relationship of CPUE with conductivity with generalized linear models in the R software environment.

2. Results

A. iberus was significantly more common at higher conductivity sites, whereas *G. holbrooki* did not clearly show such a trend (Figure 1). These results indicate that high conductivity may provide the Spanish toothcarp with an eco-physiological advantage over the invasive species.

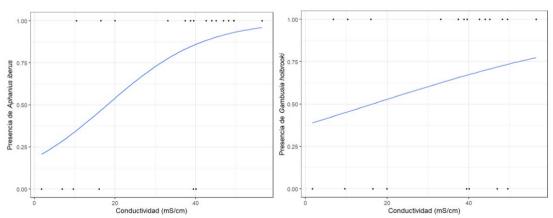


Figure 1. Presence (1) and absence (0) of *Aphanius iberus* (left) and *Gambusia holbrooki* (right) in the 21 sampling sites in relation to water conductivity. The logistic regressions (blue lines) account for 25 and 4 % of the variability, respectively. The model for *A. iberus* is significant (P = 0.011).

Moreover, the catches of the native fish increased significantly as conductivity rose, and the invader displayed an opposite trend (Fig. 2).

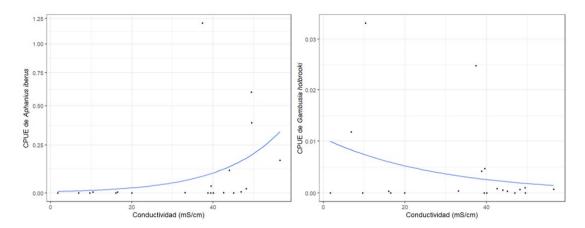


Figure 2. CPUE for *Aphanius iberus* (left) and *Gambusia holbrooki* (right) in the 21 sampling sites in relation to water conductivity. We show the Poisson regressions (generalized linear models, blue lines), which account for 17 and 12 % of the variability, respectively.

3. Conclusions

This study has confirmed that the relative abundance of *A. iberus* and *G. holbrooki* in sympatry is related to the salinity gradient according to our results in specific CPUEs. This finding agrees with previous research on the role of salinity in the life cycles of these species. [5] However, the scope of this paper was limited to test a cornerstone hypothesis in the field; further research must focus on unveiling the underlying physiological mechanism. We recommend maintaining the natural hydrology of the toothcarp coastal habitats to enhance its conservation.

Keywords: conductivity, sympatry, killifish, invasive species

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SESSION XII: CRIME, VIOLENCE AND GENDER PERSPECTIVE

FRAUD REPORTING IN THE INTERNET ERA: DETERMINANTS AND MOTIVES

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1. Introduction

Fraud has been identified as one of the most prevalent property crimes in the Internet era (Kemp, 2020) and underreporting represents one of the most pressing challenges to prevention and policing (Reep-van den Bergh, 2018; Van de Weijer, 2019). Like fraud itself, the issue is not new and therefore traditional findings and approaches designed to foster reporting may also be applicable to online fraud.

2. Methodology

This study performs a series of regression models to analyse data on fraud victims from 2 editions of the representative Catalan Public Security Survey (n = 1177). The aim is to identify and compare socio-demographic, context and crime event determinants of online and offline fraud reporting as well as the reasons for not reporting.

3. Results

The findings show that, surprisingly, online fraud is reported at a higher rate than offline fraud, mainly due to greater odds of being considered a crime by the victim. In general, fraud reporting appears to involve a rational component as financial and non-financial harms and the expected utility of reporting are more relevant to the decision than socio-demographic factors. In addition, the most common reasons for not reporting refer to the opportunity costs of doing so. The demographic predictors of online reporters show only slight differences from their offline counterparts, but more associations are found regarding the reasons for not reporting.

4. Conclusion

The present paper responds to calls for fraud reporting research posed in previous studies (Copes, 2001; Schoepfer, 2009; Van de Weijer, 2019) by analysing and comparing the determinants of fraud reporting and the reasons for non-reporting, including the crime event characteristics. Online and offline reporting were compared; thus, the paper contributes to the 'old wine in new bottles' cybercrime debate (Grabosky, 2001) and, more specifically, by examining the applicability of the scientific literature on crime reporting to fraud and online fraud, it strengthens the evidence base for policies that aim to stimulate reporting for an especially prevalent crime in the digital age.

Keywords: fraud, crime reporting, dark figure, quantitative analysis, crime impact

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THE SPACES OF VIOLENCE IN VÍCTOR CATALÀ'S SHORT STORIES

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1. Introduction

The aim of this study is to analyse the spaces of interpersonal violence and social violence in short stories written by Víctor Català. For the research, *Drames rurals* (the author's first book) is analysed using close reading and various theories regarding both violence and spatial representation in literature. Examples of the former are Rüdiger Safranski's ideas on freedom and control, based on, amongst other things, Friedrich Schelling's personal and universal freedom, and Terry Eagleton's notion of how materialistic conditions explain violence, an idea shared by Jordi Castellanos. Regarding spatial representation, we use approaches such as Robert Tally's spatiality and literary cartography.

We study the points of view from which the mentioned spaces are described, mainly located in a rural environment at the end of the 19th and the beginning of the 20th century. Linguistic elements such as explicit adjectives or the characterization of spaces through literary topics, symbols or recurring images are also examined.

2. Results

The analysis of the texts shows that violence is present in all environments, yet the author qualifies spaces according to different types of violence. Thus, social or collective violence takes place in symbolic spaces of the rural environment such, as the town square, and male and female characters take part in it, although the latter have a significant role. In addition, violence is articulated through physical aggression and also through surveillance. The victims are characters who distinguish themselves from the community. In contrast, interpersonal violence occurs mainly in isolated spaces, such as the field, or in private places, such as the home. In this case, both perpetrators and victims are diverse: there are different ages, conditions and genders. However, Català continues to apply a rule of "difference": victims do not fit with either social norms or the practical logic of the rural world.

3. Conclusions

Social violence occurs mainly in spaces dominated by the "mass": linguistic elements create a contrast between uniformity and individuality, and are usually connected to images of corporality. In contrast, to present interpersonal violence the author uses elements connected to the eyes and the gaze, both literary topics related to intimacy. In those latter spaces, Català presents both the victim's and the aggressor's perspectives.

Nevertheless, there are also connection points between incidences of violence: social norms are fundamental to explain them, and appear explicitly when violence occurs, proving the "difference" of the victim and the importance of control and coercion of personal freedom.

Keywords: Catalan literature, violence, Víctor Català, spatiality, social norms

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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.

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 (Follati, 2018; Lamadrid, 2016; Reyes-Housholder, 2019).

- Denunciations of sexual harassment and abuse by teachers and other students.
- Denunciations of the macho treatment received by male teachers and students both in learning spaces and in student political organizations.
- Absence of feminist lectures.

In view of this situation, two research questions arise: How is the Chilean student movement reconfigured and feminized after the irruption of women within it? What are the political consequences of this feminist shift in the student movement?

The objectives are the following:

- To investigate the practices, actions, beliefs and motivations of women within the Chilean Student Movement.
- To conduct a frame analysis of the women's movement within the student movement.

2. Hypotheses

The hypotheses of the investigation are:

- Women begin to make demands within the student movement that generate hostilities, tensions and divisions within it.
- 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.
- Feminism is used as a politicizing tool within the student movement.

3. Methodology

As for the methodological scope of this study, it will be approached qualitatively, and be based on a case study (Della Porta, 2012), specifically, within the feminist incubation in the Chilean student movement. The information will be obtained through primary and secondary sources. Primary sources include interviews, focus groups and ethnography will be used in discussions and actions. The minutes of assemblies of feminist groups will also be analysed.

Interviews will be conducted with women who have lived through the student protest movement 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 (Ruiz, 2003). 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 and 3) are defined as feminists. The number of interviewees will be delimited by the information saturation criterion.

The focus group will be made up of feminist activists from the student movement with different levels of involvement in it. Feminist academics who are experts in gender violence, young university activists and second wave feminist activists will generate debate about: 1) being a feminist in a cyber world connected to and with the existence of networks of solidarity and feminist containment; 2) the differences between being a feminist today and 20 years ago; 3) the disputes around gender roles in politics and the consequent reaction in men; and 4) the changes of meaning in the spaces of political participation.

4. Results and discussion / Conclusions

Although there is an abundance of academic literature that addresses the phenomenon of student movements and protests, a preliminary review found little research on women's protests and the Chilean feminist movement. The studies of Silvia L. Álvarez and Alexandra B. are fundamental. Navarrete (2019) made a chronology of the feminist movement in Chile, which includes the period 2006-2016 but does not cover the "Third Feminist Wave" that developed in Chile during 2018, therefore, only the embryonic phase of reactivation of women's movements in the country.

The research work of Catherine Reyes and Beatriz Roque (2019) does investigate the year of greatest growth of Chilean feminism (2018) and the third wave, but does not go into the feminist movement but rather focuses on the macro conditions (political, economic and social) that give rise to feminist protests and the contribution that feminist debates make to the strengthening of democracy.

Luna Follegati (2018), on the other hand, has conducted historical research on the organisms of the feminist movement, addressing their role within the "democratic recovery in Chile", characterizing the feminist movement as a space of struggle and internal organization of the same, focusing on the differences between the contested issues of Chilean feminism in the 1990s and a scenario that seeks to expand feminism within consolidated social movements such as the student movement.

Keywords: Social movements, feminism, feminization, student movement, third feminist wave.

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CONSCIENTIOUS OBJECTION TO ABORTION

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1. Introduction

Conscientious objection is a legal institution and a challenge to public law because it confronts fundamental rights like freedom of conscience and ideological and religious freedom to practice abortion.

The aim of the research is to analyse the conscientious objection to abortion in the Spanish law and to compare it with Argentinean, Uruguayan and Chilean laws. It is also important to evaluate jurisprudence context and determine how the juridical culture of each state affects the regulation of conscientious objection to abortion.

In essence, the object of the research is the comparison between the situations in Spain, Argentina, Chile and Uruguay in order to assess the importance of the legal culture of a community in the existence (or not) of conscientious objection as an accepted and regulated legal phenomenon.

2. Methodology

The methodology used in the research is based on an interpretative approach, which seeks to understand how and why the institution of conscientious objection is regulated in different legal systems. The qualitative methodology is focused on the analysis and evaluation of legislation about conscientious objection to abortion in different countries, analysing laws and jurisprudence.

3. Results

The study shows that conscientious objection is a relevant aspect in studies of fundamental rights because it interacts not only with a woman's options to have an abortion but also with ideological and religious freedom. Nowadays, the main problem we are facing is how the legislation can provide both rights without discrimination.

In this context, the study must explain which laws better guarantee the rights of the actors and which will be the better protocol to assure all the rights will be respected. The comparison between the situations in Spain, Argentina, Chile and Uruguay is a way to reveal the importance of the legal culture of a community in the existence of conscientious objection as an accepted and regulated legal phenomenon.

4. Conclusions

This study examines the realities in different legal systems to explain how and why the institution of conscientious objection is regulated. For the moment, the results have been very enriching and interesting but there is much more work to do. On the one hand, Uruguay has a voluntary pregnancy termination law similar to the Spanish one; both countries explicitly regulate conscientious objection to abortion. On the other hand, Chilean and Argentinean laws about abortion are more restrictive and objection is not legislated in a specific law.

Keywords: conscientious objection, abortion practice, freedom of conscience, ideological and religious beliefs, juridical culture.

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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

In recent years we have seen a rise in far right wing parties across Europe. Spain has its own far right wing party (Vox), which is the third major political force in parliament. The internet, and specifically social media platforms, is one of the important channels for reproducing their discourse and ideas. One of the crucial points in their speech is the attacks on what they call "ideology of gender".

2. Problem and Hypothesis

Many, from individuals to 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 to analyse why the discourse of Vox on 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 hate, hate speech and the internet, and far-right political parties in Spain.

Secondly, legislation analysis about hate speech and the internet, political freedom, and freedom of expression, at the national, European, and international levels and the most important case law in Europe and Spain.

Thirdly, the monitoring of five of the highest - in number of followers - Twitter accounts of the Vox political party in Spain in the years 2019 and 2020.

4. Results and discussion

- The tension between hate speech and freedom of expression and political ideas in our legal system.
- Analysis of how the actual law regulates, prevents, or stops these kinds of acts on the internet.

- The importance of the internet and the regulation of the platforms, regarding the transnational conflict between overseas enterprises and European Union States, especially in Spain.

- The problems with the information through internet (fake news and hate news).

5. Conclusions

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 this erodes our democracy. A set of legal and non-legal proposals are made to prevent and deal with hate speech by political parties at the national level and to propose which type of legal and public policy in Spain can be implemented to protect our democracies and human rights.

Keywords: hate speech, gender theories, far-right parties, democracy

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THE TRANSVERSAL EFFECTS OF CULTURALLY MOTIVATED CRIMES ON CRIMINAL LAW THEORY

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1.- Introduction

The majority of states worldwide are multicultural (Carnevali Rodríguez, 2007). Since criminal law is mainly a cultural product, it is strongly influenced by the culture of the main society (Höffe, 2008). Therefore, we find individuals whose cultural norms clash with the legislation of the State they reside in. When this collision takes place, and subjects choose to act according to their cultural backgrounds, the result is the commission of a *culturally motivated crime* (De Maglie, 2012).

2.- Hypothesis

Criminal liability depends greatly on the perpetrator being normally motivated by the legislation they infringed (Mir Puig, 2011). That lack of internalisation and the conflict experienced by the individual modify the criminal liability of the subject from the minority group, making a case for a more lenient or even an absolutory sentence.

3.- Methodology

The methodology followed comprises the search and study of legislation, jurisprudence, and literature relevant to the topic, in order to assess the current situation and provide an innovative solution to it.

4.- Results and discussion

The provisional results show, through the analysis of specific cases, that *common law* systems provide answers such as the *cultural defence* that do not exist in *civil law* systems (Renteln, 2005; Lee, 2007). The need to transpose an institution similar to the *cultural defence* is one of the main focus of discussion, as is the possibility of including it in already existing criminal theory categories or creating an *ad hoc* institution.

5.- Conclusions

Although it is an ongoing project, there seems to be a need to create bilateral mechanisms to further integrate minorities in the main society in the case of immigrated population and, using power sharing mechanisms with national minorities, to avoid conflict or oppression (Kymlicka, 2017). This would allow the laws of the State to better accommodate the diversity of the current society. Transposing the *cultural defence* could improve the overall fairness of the trials, since it would regulate the process of balancing the right to one's own culture, and the purposes of the criminal law.

Keywords: Criminal defence, equality, multiculturalism, social justice, tolerance

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THEY UNDERSTAND THE EMOTIONS: A STUDY OF EMOTIONAL INTELLIGENCE AND PSYCHOPATHIC PERSONALITY TRAITS IN INCARCERATED OFFENDERS

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1. Introduction

Psychopathic personality is characterized by a constellation of interpersonal, affective, lifestyle and behavioural characteristics that manifest in wide-ranging antisocial behaviours (Hare, 2008).

In fact, individuals with psychopathic traits present a number of emotional deficits (Ermer, 2012), abnormalities in emotional processing (Blair et al., 2006) and poor behavioural control (Kiehl, 2006), that may be related to impaired emotional intelligence (EI; Mayer, 2002) and has motivated investigation of the relation between psychopathy and EI.

Previous work on EI has shown that the impulsivity and the antisocial factor of the psychopathic personality were negatively associated with it (Grieve, 2010; Pertrides, 2011; Vidal, 2010; Copestake, 2013).

The present study aims to examine the association between psychopathic personality traits (callous affect, interpersonal manipulation, erratic lifestyle and criminal tendencies) and the four abilities of EI (perceiving emotions, facilitating thought, understanding emotions and managing emotions) in incarcerated offenders.

2. Methodology

Participants were 29 offenders (41.3% female) located at three different prisons in Catalonia and convicted of a wide variety of crimes. The mean age of the sample was 39.3 (range, 26-66 years).

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 – version three (SRP-III; Pauhlus, Hemphilll & Hare, in press) and emotional intelligence was assessed with the Mayer-Salovey-Caruso Emotional Intelligence Test (MSCEIT; Mayer, 2002).

3. Results

First, we found that those participants with the highest scores in psychopathic personality were less competent in EI. Furthermore, the secondary traits of this personality (impulsivity and antisocial behaviour) seem to be negatively associated with EI (-.482), in line with the previous research.

4. Conclusions

In general, the previous data of this study show that psychopathic personality is negatively associated with EI, and more specifically with this experiential area, denoting that those participants with high psychopathic traits are less competent in the ability to perceive, respond and manage emotional information, without their comprehension of this emotion being affected.

Keywords: psychopathy, offenders, emotional intelligence, SRP-III, MSCEIT.

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