TEMES PER A TREBALLS DE FI DE GRAU (TFG)

GRAU EN QUÍMICA
Curs 2025-2026

DEPARTAMENT QUÍMICA ANALÍTICA I APLICADA

1. **Desenvolupament d'un mètode per l'anàlisi d'aminoàcids no proteics tòxics produïts per cianobacteris mitjançant un HPLC(HILIC)-MS/MS d'última generació.**

   Degut a l'increment de les temperatures globals a causa del Canvi Climàtic així com l´ús intensiu de fertilitzants en la indústria agrícola, cada cop és més habitual la presencia de cianobacteris en aigua dolça arreu del món. Algunes espècies de cianobacteris poden generar potents neurotoxines com els aminoàcids no proteics β-metilamino-L-alanina (BMAA), l'àcid 2,4-diaminobutíric (2,4-DAB) o l'aminoetilglicina (AEG), metabòlits altament tòxics relacionats amb malalties neurodegeneratives com l'esclerosi lateral amiotròfica, Parkinson o Alzheimer.

   L'objectiu del projecte és el desenvolupament de un mètode d'injecció directa (evitant preparativa de mostra) per l'anàlisi d'aquestes cianotoxines en matrius aquoses mitjançant HPLC(HILIC)-MS/MS d'última generació. Aquesta línia de recerca s'emmarca dins del projecte ESCCAP (ref. RDI001/24/000010) subvencionat per l'Agència Catalana de l'Aigua.

   Direcció: Dr. Xavier Ortiz Almirall

2. **Ús de vehicles aeris no tripulats (drons) per la monitorització ambiental de cianotoxines en els embassaments de les conques internes de Catalunya.**

   Degut a l'increment de les temperatures globals a causa del Canvi Climàtic així com l´ús intensiu de fertilitzants en la indústria agrícola, cada cop és més habitual la presencia de cianobacteris en aigua dolça arreu del món. Una de les dificultats en la monitorització d'aquests microorganismes és l'elevada heterogeneïtat dels afloraments algals que produeixen en aigua dolça, que a més solen produir-se en localitzacions de difícil accés. Per tal de donar resposta a aquesta doble problemàtica, el present projecte pretén estudiar l'ús de drons aeris com a eina per la presa de mostres d'aigua.

   Amb aquesta finalitat, es visitaran diversos embassaments de les conques internes de Catalunya i s'empraran vehicles aeris no tripulats (drons) per a) detectar afloraments de cianobacteris, b) prendre mostres aquoses de forma remota, i c) analitzar el contingut de cianotoxines de les mostres mitjançant HPLC-MS/MS d'última generació. Aquesta línia de recerca s'emmarca dins del projecte ESCCAP (ref. RDI001/24/000010) subvencionat per l'Agència Catalana de l'Aigua.

   Direcció: Dr. Xavier Ortiz Almirall

3. Comparació de mètodes instrumentals basats en cromatografia de gasos acoblada a espectrometria de masses de triple quadrupol (GC-MS/MS) i d'alta resolució (GC-HRMS) per a l'anàlisi de dioxines i furans polibromats.

Les dibenzo-p-dioxines i furans polibromats (PBDD/Fs) son una família de Contaminants Orgànics Persistents (COPs) emergents que comprenen 210 congèneres. Aquests compostos encara no figuren en la llista de contaminants detallats en el Conveni d'Estocolm i per tant no s'estan monitoritzant de forma sistemàtica al medi ambient. Tot i així, degut a la semblança estructural amb les dibenzo-p-dioxines i furans policlorats (PCDD/Fs) podrien tenir una toxicitat, capacitat de transport, persistència i capacitat per bioacumular-se a través de la xarxa tròfica similar. En aquest sentit, la UE està ja proposant la seva monitorització en emissions atmosfèriques de determinats focus tèrmics a curt/mitjà termini.

L'objectiu del present projecte és comparar el mètode d'anàlisi de PBDD/Fs emprant cromatografia de gasos acoblada a un espectròmetre de masses de triple quadrupol (GC-MS/MS) amb el mètode basat en cromatografia de gasos acoblada a un espectròmetre de masses d'alta resolució de sector magnètic (GC-HRMS), en la seva aplicació a l'anàlisi de mostres d'emissions atmosfèriques.

Direcció: Dr. Jordi Díaz Ferrero i Dr. Xavier Ortiz Almirall

4. Avaluació de diversos adsorbents sòlids per a la fabricació de captadors passius per l'anàlisi de diverses famílies de contaminants en aigües continentals

Degut a diverses fonts antropogèniques com la indústria agrícola, farmacèutica o nuclis urbans, la concentració de contaminants com les cianotoxines, fàrmacs o pfas ha incrementat exponencialment en rius i llacs d'arreu del món els darrers anys, afectant negativament als ecosistemes aquàtics i a la qualitat de l'aigua. Una de les limitacions en l'anàlisi d'aquestes famílies de contaminants en rius i llacs és la baixa reproductibilitat de l'etapa de mostreig, ja que les concentracions poden variar ordres de magnitud en funció del cabal, temperatura o salinitat de l'aigua. Una alternativa a aquests mètodes de mostreig més clàssics (grab sampling) és l'ús de captadors passius (passive sampling), a on un adsorbent sòlid capta els contaminants dissolts en aigua durant llargs períodes d'exposició.

Durant el present projecte, es pretén avaluar diverses classes d'adsorbents sòlids com l'HLB, HP-20, C18 o ambersob en la captació de varies famílies de contaminants mediambientals a escala de laboratori, per acabar emprant-los en rius i llacs de Catalunya. Les anàlisis dels contaminants es duran a terme mitjançant HPLC-MS/MS d'última generació.

Direcció: Dr. Xavier Ortiz Almirall i Dr. Cristian Gómez Canela

5. Caracterització d'enzims mitjançant LC-QTOF

Els biosensors enzimàtics són eines clau en el control de qualitat de diferents sectors industrials. Tanmateix, un dels majors reptes a l'hora de desenvolupar biosensors enzimàtics és poder immobilitzar el major nombre de molècules d'enzim en la seva conformació biològicament activa. A més, en moltes ocasions s'hi afegeix una dificultat extra, ja que molts dels enzims que es comercialitzen sovint contenen impureses com ara pèptids, proteïnes, sals o polímers que afecten la sensibilitat del dispositiu final. Per tant, quan es dissenyen i construeixen nous biosensors enzimàtics, és essencial conèixer i caracteritzar els enzims que s'utilitzaran com a bioreceptors.

En el present treball, es proposa utilitzar la tècnica de cromatografia de líquids acoblada a espectrometria de masses d'alta resolució (LC-HRMS) per caracteritzar diferents dissolucions d'enzim amb diversos graus de puresa, que puguin servir per a la construcció de biosensors electroquímics.

Direcció: Dra. Margalida Artigues Cladera i Dr. Sergi Colominas Fuster

6. Desenvolupament de sensors d'hidrogen per aliatges Pb-Li

El projecte ITER té com a objectiu demostrar la viabilitat d'una reacció de fusió nuclear entre el deuteri i el triti com a futura font d'energia. Atès que el triti és un element que no es troba a la natura, s'ha de generar in situ. Una de les propostes per generar triti és a partir del 6Li, el qual es trobarà en un aliatge fos de Pb-Li en la seva composició eutèctica. En aquest context, es requereix el desenvolupament d'eines capaces de quantificar la concentració dels isòtops d'hidrogen en aquest l'aliatge fos.

L'objectiu d'aquest projecte és el desenvolupament de sensors d'hidrogen utilitzant l'electròlit en estat sòlid $BaCe_{0.6}Zr_{0.3}Y_{0.1}O_{3-\delta}$. Aquests, es podran emprar tant com a sensors amperomètrics com a potenciomètrics en l'aliatge fos. Normalment, en aquests casos, la correlació entre la variable mesurada (intensitat o diferència de potencial) i la concentració d'analit s'estableix mitjançant un procés de calibratge, on s'haurà d'establir tant el rang lineal com la sensibilitat.

Direcció: Dr. Sergi Colominas Fuster i Dr. Jordi Abellà Iglesias

7. Desenvolupament de sensors d'oxigen per aliatges Pb-Li

El projecte ITER té com a objectiu demostrar la viabilitat d'una reacció de fusió nuclear entre el deuteri i el triti com a futura font d'energia. Atès que el triti és un element que no es troba a la natura, s'ha de generar in situ. Una de les propostes per generar triti és a partir del 6Li, el qual es trobarà en un aliatge fos de Pb-Li en la seva composició eutèctica. En aquest context, un dels punts crítics és la presència d'impureses en el metall fos, per exemple l'oxigen.

L'objectiu d'aquest projecte és el desenvolupament de sensors d'oxígen utilitzant l'electròlit en estat sòlid YSZ. Aquests, es podran emprar tant com a sensors amperomètrics com a potenciomètrics en l'aliatge fos. Normalment, en aquests casos, la correlació entre la variable mesurada (intensitat o diferència de potencial) i la concentració d'analit s'estableix mitjançant un procés de calibratge, on s'haurà d'establir tant el rang lineal com la sensibilitat.

Direcció: Dr. Sergi Colominas Fuster i Dr. Jordi Abellà Iglesias

8. Reutilización de productos sintetizados en prácticas de química general: evaluación de pureza y aplicación en nuevas síntesis como estrategia de economía circular en el laboratorio docente

Este Trabajo de Fin de Grado pretende estudiar la viabilidad de reutilizar productos obtenidos por estudiantes en prácticas de química general e inorgánica, evaluando su pureza y aplicabilidad como reactivos en nuevas síntesis. El objetivo es fomentar la economía circular en el laboratorio docente, reducir la generación de residuos y optimizar el uso de recursos. Se estudiará cómo afecta la pureza de dichos productos cuando se utilizan como reactivos de partida para nuevas reacciones, y se diseñarán nuevas prácticas que incorporen estos productos reciclados. El estudio incluirá una comparación entre productos comerciales y reciclados en términos de rendimiento y calidad de los resultados.

Tiene los siguientes objetivos especificos: i) Clasificar y caracterizar los productos almacenados según tipo de compuesto y posible uso; ii) Determinar la pureza de los productos mediante técnicas accesibles en laboratorio docente; iii) Comparar los resultados obtenidos con reactivos reciclados frente a reactivos comerciales; iv) Diseñar y probar nuevas prácticas que incorporen estos productos como reactivos de partida; v) Proponer estrategias para implementar la economía circular en laboratorios de docencia química.

Direcció: Dra. Judith Báguena Polo i Dra. Mª Victoria Codera Pastor

9. Risk Assessment of pharmaceuticals in the rivers of Catalonia

Pharmaceuticals residues are classified as Emerging contaminants (ECs) becoming a huge threat for the population and the environment. Pharmaceuticals administrated at home or in pharmacies are excreted by faeces and urine after consumption, and wastewater treatment plants (WWTPs) are not able to remove all pharmaceuticals residues that eventually will end up in the aquatic media (rivers and sea). For this reason, analytical techniques must be developed and implemented for the monitoring of these ECs. For the last decade, extraction techniques such as solid phase extraction (SPE) have become very popular among scientific community and the injection to standard LC-MS chromatography has been giving good results for the identification and quantification of pharmaceuticals. However, analytical instruments are becoming more and more sensitive and sometimes extraction procedures can be avoided. For

these reasons, direct injection methods are prominent which simply consist of injecting directly the water matrix into LC instruments.

Direct injection shows great advantages. It eliminates the extraction step which is time and cost consuming. Also, no solvents are needed, the total waste is reduced, and human errors are less likely to occur. In this work, a direct injection method was developed for the monitoring of 80 pharmaceuticals in river water using Liquid Chromatography-Tandem Mass Spectrometry (SCIEX Q-TRAP 7500 ®), working in MRM mode and ESI+/- ionization respectively. Quality assurance was performed for all compounds and high sensitivity of the instrument allowed to arrive at very low concentrations (1 ng L-1 for most of the compounds). Furthermore, recoveries and matrix effect were very consistent, and results were obtained with just the injection of 100 µL of river water previously filtered.

Thus, the aim of this study will be to evaluate the presence of different classes of pharmaceuticals in all rivers of Catalonia and to study their risk assessment.

Direcció: Dr. Cristian Gómez Canela

10. Future Data Storage Using Colloidal Memory Technology

Data is being generated at ever-increasing rates with the widespread digital transformation in businesses and society. The continually increasing demand for affordable data storage puts tremendous pressure on storage technologies. New concepts for low-cost, high storage-density memories are urgently needed to keep storage capabilities in line with the growing demand. FastComet is a colloidal memory concept in which colloidal nanoparticles are considered data carriers. The memory consists of a large array of nanocapillaries in which two types of nanoparticles with antagonistic electrophoresis (DEP) properties can be selectively inserted into the capillary by DEP forces. Data can be stored as the specific stacking sequence of the different particle types. During the following two years, we aim to establish a proof-of-concept for colloidal memory.

In this project, we aim to study the DEP properties of antagonistic nanoparticles with the aim to find the best particle combination for high data storage capacity. The student will get valuable experience in material characterization and optical microscopy in the framework of an international consortium with members from Spain, Belgium, and France. Exist the possibility to extend this project with a MSc and/or PhD thesis with short research stays in their laboratories.

Direcció: Dr. Roger Bresolí Obach i Dr. Santiago Nonell Marrugat

11. Metallodrugs in phototherapies. Analysis of drug uptake by cells

Light-based disinfection processes cause the inactivation of bacteria and viruses through mechanisms such as (a) damage to the membrane or envelope, (b) inactivation of essential

enzymes and proteins, and/or (c) oxidative damage to nucleic acids. For this, it is essential that the drugs are internalized by the microorganisms.

In this Bachelor's Thesis, an analytical technique will be developed to quantify the incorporation of metallodrugs into bacteria.

The project will involve learning how to perform bacterial cultures, learning photodynamic therapy, and using state-of-the-art ICP-MS equipment to quantify metals in bacteria. ICP-MS is one of the most sensitive techniques for trace metal quantification. In this project, it will be used to quantify the total metal internalized by the bacteria, and additionally, the new Single Cell-ICP-MS module will be used to obtain information on the metal content at the single-cell level.

Direcció: Dra. Ariadna Verdaguer Ferrer, Dra. Maria Auset Vallejo i Dr. Santi Nonell Marrugat

DEPARTAMENT QUÍMICA ANALÍTICA I APLICADA / DEPARTAMENT ENGINYERIA QUÍMICA I CIÈNCIA DE MATERIALS

12. Identificació i Avaluació del Risc de microplàstics a les Conques Hidrològiques dels Rius de Catalunya

La contaminació per microplàstics als rius de Catalunya s'ha convertit en una preocupació ambiental significativa. Els microplàstics, petites partícules de plàstic de menys de 5 mm, provenen de diverses fonts, com ara productes de consum (cosmètics, tèxtils, pneumàtics) i la descomposició de residus plàstics més grans. Aquests fragments ingressen als ecosistemes aquàtics a través de les aigües residuals, l'escorrentia de les aigües pluvials i els vessaments industrials, persistint en l'entorn a causa de la seva lenta degradació.

Els estudis realitzats en rius catalans com el Llobregat i el Ter han detectat concentracions preocupants de microplàstics, afectant tant la biodiversitat local com la qualitat de l'aigua. La fauna aquàtica, especialment els peixos i invertebrats, pot ingerir aquests plàstics, generant problemes de salut que afecten la cadena alimentària. A més, els microplàstics actuen com a vectors de contaminants químics i poden transportar substàncies tòxiques.

Aquest problema planteja reptes importants per a la gestió de l'aigua a Catalunya i subratlla la necessitat de mesures preventives, com ara millorar el tractament d'aigües residuals, controlar l'ús de plàstics a la indústria i promoure la reducció de residus plàstics a nivell social.

En aquest TFG es planteja identificar i caracteritzar els diferents microplàstics en les aigües de totes les conques hidrogràfiques de Catalunya per tècniques de microscòpia acoblades a IR i RAMAN.

Direcció: Dr. Cristian Gómez Canela i Dra. Núria Agulló Chaler

DEPARTAMENT QUÍMICA ORGÀNICA I FARMACÈUTICA

13. Ruthenium-catalyzed N-O-bond cleavage for the synthesis of aldehydes and primary amides.

The discovery of new chemical methodologies is essential for the advancement of Chemistry, as well as key to obtaining complex products minimizing waste and energy consumption. In particular, catalytic methods that convert easily accessible hydroxylamine derivatives to more valuable functionalities such as primary amides or aldehydes could be very valuable for chemists. In this project we aim to explore the synthesis of both aldehydes and primary amides with affordable ruthenium catalysts. By carrying out this project, the student will gain experience in a synthetic chemistry laboratory as well as knowledge in the fields of Organometallic Chemistry and Homogeneous Catalysis with a focus on the mechanistic aspects of the reactions. Important: The TFG is experimental, therefore 75% of the work will be done in the laboratory.

Direcció: Dr. Andrés Seoane Fernández

14. Palladium-catalyzed synthesis of spirocylobutanes through an amino-functionalization and C-H activation step.

The discovery of new chemical methodologies is essential for the advancement of Chemistry, as well as key to obtaining complex products minimizing waste and energy consumption. In particular, catalytic methods that can easily form C-C bonds leading to cyclic scaffolds are very attractive for synthetic chemists. In this project we aim to explore the synthesis of cyclobutanes from easily available starting materials by means of palladium catalysis. By carrying out this project, the student will gain experience in a synthetic chemistry laboratory as well as knowledge in the fields of Organometallic Chemistry and Homogeneous Catalysis with a focus on the mechanistic aspects of the reactions. Important: The TFG is experimental, therefore 75% of the work will be done in the laboratory.

Direcció: Dr. Andrés Seoane Fernández

15. Preparation of asymmetric liposomes by chemically fueled reversible reactions.

The existence of bilayer asymmetry (i.e. having different lipid composition in the inner and outer leaflet of the lipid bilayer) is a key aspect of biological organisms. Moreover, asymmetric liposomes are being explored as drug delivery systems because of the possibility to tailor their inner layer to the necessities of the payload and their outer layer to the needs of the receiving organism. However, the obtention of these asymmetric liposomes is far from straightforward, thus limiting their possible applications. In this project we aim to use reversible covalent reactions to easily obtain asymmetric liposomes that could be used to build synthetic cells or drug delivery systems. By carrying out this project, the student will gain experience in a synthetic chemistry

laboratory as well as knowledge in the fields of Supramolecular and Systems Chemistry. Important: The TFG is experimental, therefore 75% of the work will be done in the laboratory.

Direcció: Dr. Andrés Seoane Fernández

16. Molecular Design by Scaffold Hopping Strategy Towards the Identification of New Protein Kinase Inhibitors.

Kinases are one of the most important human protein families and are directly or indirectly involved in all cellular biochemical pathways. Since early 2000s, 88 kinase inhibitors have entered in the clinics, representing a remarkable success story in drug development. However, there is still large number of unexplored kinases which have a strong genetic link to disease but poorly biology understood (see https://doi.org/10.1021/acs.jmedchem.1c00980).
Through a systematic computational study, in this project the student will replace the central chemical core of known kinase inhibitors with a variety of other heterocyclic rings, aiming to achieve an improved molecular affinity and selectivity towards the selected target kinase.
Here we are looking for very motivated students to work in the molecular design lab modelling new protein kinase inhibitors. The results could potentially provide a valuable foundation for future Medicinal Chemistry programs in different therapeutic fields.

Direcció: Dr. Roger Estrada Tejedor i Dr. Ricardo A. M. Serafim

17. Development of Covalent Inhibitors for Understudied Protein Kinases.

Although many successful and historical drugs such as aspirin, penicillin and omeprazole act inhibiting covalently their molecular targets, for a long time the design of drugs with a covalent mechanism of action has been avoided by pharmaceutical industries due to concerns about safety and selectivity. However, with the advent of structure-based approaches and the “omics” era, pharma-companies and academic labs have recently revival the design of covalent inhibitors in a rational manner, with outstanding results demonstrated by recent approvals of covalent drugs exemplified by Sotorasib, a mutant-KRASG12C inhibitor, and Nirmatrelvir, a SARS-CoV2 Mpro inhibitor. Protein kinases are among the most important human drug targets, being responsible for regulating cellular cycle and many others crucial physiological events. Overexpression of these proteins implies several diseases, such as different types of cancers. Currently, we have 88 approved drugs as protein kinase inhibitors, however, there is still a substantial fraction of the so-called “kinome” with an unknown biological function, which is an enormous potential source for the developing of new drugs (see https://doi.org/10.1021/acs.jmedchem.1c00980).
Here we are looking for very motivated students to work in a synthetic organic chemistry lab to generate covalent inhibitors for understudied protein kinases.

Direcció: Dr. Ricardo A. M. Serafim

18. Preparació de “linkers” amb aplicacions a l’alliberament controlat de fàrmacs.

En aquest treball es proposa preparar una sèrie de productes de partida per l’obtenció de sistemes d’alliberament de fàrmacs basats en nanopartícules de sílice mesoporosa. Es requereix un excel·lent nivell de Química Orgànica tan teòric com experimental.

Direcció: Dr. David Sánchez García

19. BN-doped arenes: new synthetic tools for main group-based organic optoelectronic materials.

Polycyclic ***A***romatic ***H***ydrocarbons *(PAHs)* have shown wide applications in organic electronics, including organic field-effect transistors *(OFETs)*, organic light-emitting diodes *(OLEDs)*, and organic photovoltaics *(OPVs)*. In this context, the incorporation of main-group heteroatoms into the *PAHs* skeleton is an effective strategy to further modulate their optoelectronic properties. We became fascinated by the so-called sp^2-type B/N isosterism that represents an interesting strategy to incorporate boron-nitrogen units into *PAHs* (see ***Chem. Sci.***, 2024,**15**, 5674-5680). This type of isosterism consists of exchanging a C=C bond by an isoelectronic B=N fragment. This unit usually alters the reactivity patterns and new optoelectronic features. As part of our own efforts in this field, we decided to focus now on the design and synthesis of new BN species in which the B-N unit replaces a Csp^2-Csp^2 single bond. These types of molecules are very promising in this field, since they could provide access to atropoisomeric BN-biaryls without the use of classic synthetic disconnections, such as, the well stablished metal-catalyzed cross-coupling. We are convinced that these basic chemical developments will contribute to expanding the synthetic tools required for realistic progress in the area of organic semiconductors. The student will get valuable experience in advanced molecular manipulation, a fundamental skill for a solid chemist.

Direcció: Dra. Ana Belén Cuenca González i Alexandr Shafir (IQAC-CSIC)

20. Electrochemically assisted C-H functionalization of main group-doped polyaromatic compounds.

Electro-organic synthesis leverages electrons as “traceless” redox reagents, replacing stoichiometric oxidants/reductants to minimize waste and enable milder, safer reaction conditions. Modern electrochemical reactors offer precise control of potential/current, unlocking chemoselective C–H activation and radical pathways that are difficult to access thermally or with photochemistry, while improving heat/mass transfer and reproducibility. Applied to main-group-doped polycyclic aromatics, electrosynthesis enables late-stage, site-selective functionalization without pre-functionalization, directly tuning the potential optoelectronic properties of these privileged structures. The goal of this project is to explore the viability of the C-H functionalization of a series of model main-group doped polyaromatic compounds using electrochemically generated radicals. By carrying out this project, the student will gain experience in a synthetic

chemistry laboratory (preparation, purification and characterization of starting materials) as well as knowledge in the field of Electrochemistry with a focus on the mechanistic aspects of the reactions.

Direcció: Dra. Ana Belén Cuenca González i Dr. Andrés Seoane Fernández (IQAC-CSIC)

21. Don't be jealous, there's enough for both of us! Design of dual inhibitors against key proteins in DLBCL

Diffuse large B cell lymphoma (DLBCL) is the most common form of adult lymphoma. Data gathered in the last decade have identified selective inhibitors for key proteins in DLBCL. This project aims to contribute to the study of structural features of target proteins by means of molecular modeling and structure-based drug design techniques (+info).
Basic linux is recommended but not mandatory.

Direcció: Dr. Roger Estrada Tejedor

22. Synthesis and characterization of new compounds with potential activity against Diffuse large B-cell lymphoma (DLBCL)

Lymphomas are “blood cancers” affecting lymph nodes. Our research group has wide experience in designing and synthesizing new drug candidates in this area of research. Now we are focused on developing new polyamine compounds with a promising activity against different B-cell lymphoma cell lines. This work is focused on synthesize some members of a family compounds with this special characteristic. We are looking for a candidate who likes Medicinal Chemistry, Organic Synthesis and lab work.

Direcció: Dr. Raimon Puig de la Bellacasa Cazorla i Dr. Albert Gibert Bosch

DEPARTAMENT BIOENGINYERIA

23. Synthesis and characterization glyconanoparticles as a new glycovaccines to activate inmune system A

Nanomedicine plays a fundamental role in today's medicine. This new approach of medicine is enabling the development of prophylactic and therapeutic treatments. Advances in the field of combating cancer or infectious diseases position nanomedicine as an effective and highly promising response, although it is still under development. Notably, immunotherapy, which leverages the body's immune system to fight diseases, has benefited significantly from nanomedicine. Nanoparticles can be designed to improve the delivery and efficacy of immunotherapeutic agents, enhancing the immune system's ability to target cancer cells more

precisely. With the emergence of COVID-19 vaccines, the scientific community has focused on developing vaccines based on genetic material to combat various diseases.
We have recently published the design of glyconanoparticles to specifically activate the inmune system presenting the mRNA as antigen and also the galactose moiety to target the nanoparticles to dendritic cells as a key point in terms of effective immunotherapy (Patent 2024, Gónzalez-Rios et al., 2023). Particularly in this project, we desire to synthesize a library of glycopolymers to assay as glyconanoparticles and in cell cultures at IQS and also in vivo at the group of Salome Pinho, Institute for Research and Innovation in Health, Oporto (Portugal).
Methodology: Carbohydrate and PBAE synthesis, nanoparticles characterization, uptake in cell cultures.

Direcció: Dra. Magda Faijes Simona i Dra. Cristina Fornaguera Puigvert

24. Synthesis and characterization glyconanoparticles as a new glycovaccines to activate inmune system B

Nanomedicine plays a fundamental role in today's medicine. This new approach of medicine is enabling the development of prophylactic and therapeutic treatments. Advances in the field of combating cancer or infectious diseases position nanomedicine as an effective and highly promising response, although it is still under development. Notably, immunotherapy, which leverages the body's immune system to fight diseases, has benefited significantly from nanomedicine. Nanoparticles can be designed to improve the delivery and efficacy of immunotherapeutic agents, enhancing the immune system's ability to target cancer cells more precisely. With the emergence of COVID-19 vaccines, the scientific community has focused on developing vaccines based on genetic material to combat various diseases.
We have recently published the design of glyconanoparticles to specifically activate the inmune system presenting the mRNA as antigen and also the galactose moiety to target the nanoparticles to dendritic cells as a key point in terms of effective immunotherapy (Gónzalez-Rios et al., 2023). Particularly in this project, we desire to synthesize the Gal and GlcNAc-glycopolymers to assay as glyconanoparticles and in cell cultures at IQS and also in vivo at the group of Salome Pinho, Institute for Research and Innovation in Health, Oporto (Portugal).
Methodology: Carbohydrate and PBAE synthesis, nanoparticles characterization, uptake in cell cultures.

Direcció: Dra. Magda Faijes Simona i Dra. Cristina Fornaguera Puigvert

DEPARTAMENT BIOENGINYERIA / DEPARTAMENT QUÍMICA ANALÍTICA I APLICADA

25. Developing a uhplc-qtof mass spectrometry protocol for sequencing chitosan oligosaccharides.

Plant pathogenic fungi partially deacetylate their cell wall chitin to be resistant to plant chitinases or deacetylate the released chitooligosaccharides to escape recognition by chitin receptors and evade the plant immune responses. Chitin is a linear polysaccharide of β-1,4-linked N-acetylglucosamine (GlcNAc) monomers, whereas chitosans are highly or fully deacetylated chitin polymers. Depolymerization of chitin results in chitin oligosaccharides (COS) and de-N-acetylation of chitin and COS yield chitosans and partially acetylated chito-oligosaccharides (paCOS), respectively. COS and paCOS have gained recent interest due to their biological activities as antifungals in agriculture for crop protection against fungal pathogens, and as immunostimulants in animals, being target compounds for sustainable and environmentally friendly applications. The Laboratory of Biochemistry is studying the structure and function of chitin deacetylases to produce sequence-defined paCOS: from discovery, cloning and recombinant expression of chitin deacetylases (CDAs) from different microorganisms to their applications as biocatalysts for the production of paCOS. Since different CDAs produce different patterns of deacetylation, our next goal is to determine the fine structure of paCOS to correlate them with their biological activities. In collaboration with the IQS-SCIEX Demo Lab, the aim is to develop analytical methodologies based on mass spectrometry for the characterization of this family of compounds.
Objective: In this project we want to develop a mass spectrometry protocol to characterize the fine structure of oligosaccharides derived from enzymatic treatments of chitin oligosaccharides. The compounds will be isotopically labeled for MS/MS characterization to determine the sugar sequence and functionalization. Preliminary experiments have been conducted with chromogenic labels for structure determination but now we what to include isotopic labelling for quantification of different structures in reaction mixtures.
Methodology: enzymatic reactions, synthetic chemistry for isotopic labeling, structural characterization by MS/MS

Direcció: Dr. Antoni Planas Sauter i Dra. Margalida Artigues Cladera

26. Analysis of the volatile components of coffee samples from Guatemala using gas chromatography-mass spectrometry and its correlation with the type of fermentation carried out in Guatemala and with the cupping value.

Guatemala's economic dynamics are significantly driven by the coffee industry, where numerous small-scale producers play an essential role. Currently, there is a close collaboration between the renowned Rafael Landívar University (Guatemala) and IQS, with the clear objective of enhancing the quality and value of Guatemalan coffee in international markets. In this context, the sensory scores (valor de cata) of the final product are crucial to increase the economic value

of the product. Different fermentations will be carried out with starter cultures in the coffee mills of Guatemala and in this TFG, the aim is to analyze the volatile components using the method developed (López, Murillo et al., in preparation) of solid phase microextraction with headspace and analysis by gas chromatography-mass spectrometry (HS-SPME-GC-MS) and correlate the results obtained with the tasting values previously obtained in Guatemala. This project, rooted in the Service-Learning approach (ApS), stands out for its social impact by contributing to the development and knowledge of the coffee industry, benefiting local communities, and strengthening academic and scientific collaboration between the involved institutions.

Direcció: Dra. Magda Faijes Simona i Dra. Margalida Artigues Cladera

27. Lipidomics analysis of engineered yeast strains for enhacing pool of ceramide, an added-value compound in cosmetics.

Ceramides make up 50% of the intracellular lipids in the human stratum corneum. Together with free fatty acids and cholesterol, they build up the skin barrier whose function is retaining moisture and preventing transepidermal water loss. Out of the twelve different classes of ceramides, phytoceramide is believed to be the most abundant ceramide in the stratum corneum of the skin. A decrease in its concentration has been detected in skin alterations like psoriasis or atopic dermatitis. For this reason, this lipidic compound is present in dermatologic formulations that target skin hydration and the restoration of the epidermal barrier. Ceramides are currently obtained from plants. However, the extraction process is laborious, and the resulting products are structurally different from human ceramides. The need to find a production technique that delivers human-like ceramides arises. The lipid metabolism of Saccharomyces cerevisiae yeast includes that of ceramides and it can be metabolic engineered to direct the metabolism to synthesize phytoceramide.
New engineered yeast strains has been generated to produce ceramide, an important added-value compound in cosmetics. Knock-out of different genes and overexpression of others are key points for the biosynthesis of this compound. In this project, the lipidomics analysis of these strains using advanced UPLC-MS/MS techniques will be applied to see the effect of these genetic modifications on the different ceramide species.

Direcció: Dra. Magda Faijes Simona i Dra. Margalida Artigues Cladera

DEPARTAMENT BIOENGINYERIA / DEPARTAMENT QUÍMICA ORGÀNICA I FARMACÈUTICA

28. Low-dose insulin in dermatological formulations for skin regeneration and wound healing.

This Final Degree Project focuses on the development of a dermocosmetic cream formulation containing low concentrations of insulin, aimed at evaluating its potential regenerative and

wound-healing properties on superficial skin injuries. The study includes the in vitro assessment of insulin efficacy as a healing agent in human dermal fibroblasts (hDF), as well as the design, preparation, and physicochemical characterization of the topical formulation. Additionally, the stability and skin safety of the product will be investigated. This project seeks to provide an innovative approach to the use of bioactive pharmaceutical ingredients in topical products intended for skin repair and regeneration.

Direcció: Dra. Nuria Oliva Jorge i Dr. Carles Bofill Bonet

29. Design of Amisamide-Based Smart Polymers for Targeted Cancer Therapy and Their Integration into Therapeutic Hydrogels.

This Final Degree Project focuses on the synthesis and characterization of functional polymers derived from amisamide, a ligand known for its cancer cell-targeting capability. These polymers will be chemically modified to enhance their biocompatibility and affinity toward specific membrane receptors. Subsequently, they will be incorporated into hydrogel matrices to create hybrid systems capable of localized mRNA delivery. The project combines polymer engineering, biomedical chemistry, and *drug delivery* design with potential applications in oncology.

Direcció: Dra. Cristina Fornaguera Puigvert i Dr. Carles Bofill Bonet

DEPARTAMENT MATEMÀTIQUES I ANALÍTICA DE DADES

30. Aplicació de la Descomposició en valors singulars en l'anàlisi i modelat de dades químiques.

La descomposició en valors singulars (SVD, per les seves sigles en anglès) d'una matriu, real o complexa, és una factorització d'aquesta com a producte de tres matrius: dues d'elles ortogonals i una de diagonal amb valors no negatius a la diagonal. La SVD s'utilitza, entre altres aplicacions, per analitzar grans conjunts de dades i permet reduir la dimensionalitat, filtrar dades sorolloses i extreure patrons. En aquest treball es proposa estudiar les bases teòriques de la SVD, explorar els àmbits de la Química on s'utilitza i analitzar alguna contribució científica en què aquesta metodologia ha estat rellevant.

Direcció: Dra. Teresa Cortadellas Benítez i Dr. Sergi Novell Masot

DEPARTAMENT MATEMÀTIQUES I ANALÍTICA DE DADES / DEPARTAMENT QUÍMICA ANALÍTICA I APLICADA

31. Disseny i avaluació d'un qüestionari en línia sobre coneixements de química.

Identificar les dificultats i avaluar els resultats d'aprenentatge de l'estudiantat és una de les preocupacions habituals dels equips de recerca en didàctica de la química. Per aquest motiu, s'han anat creant diversos qüestionaris centrats en l'avaluació de temes concrets de la química. Es proposem partir de les preguntes creades en aquestes proves conceptuals en l'àmbit de la química, per dissenyar, crear, analitzar i validar un qüestionari conceptual en línia que permeti avaluar les competències específiques en química de qui respon.

Direcció: Dr. Jordi Cuadros Margarit i Dra. Judith Báguena Polo

DEPARTAMENT MATEMÀTIQUES I ANALÍTICA DE DADES / DEPARTAMENT QUÍMICA ORGÀNICA I FARMACÈUTICA

32. Creació d'una unitat didàctica sobre la substància química usant recursos quimioinformàtics.

Quan hom comença a entrar en els sistemes d'identificació computacional de les substàncies química, pren consciència de dues coses: (1) la importància de les representacions informàtiques per a la gestió de la informació química, i (2) la manca de precisió de la terminologia que sovint usem per a parlar-ne. A partir d'aquestes dues reflexions, i de la diversitat de recursos disponibles, el treball se centra en el desenvolupament en obert d'una unitat didàctica a nivell de primer de carrera sobre la substància química que tingui la precisió conceptual que sovint ens manca i usi els recursos quimioinformàtics que tenim a la nostra disposició.

Direcció: Dr. Jordi Cuadros Margarit i Dr. Roger Estrada Tejedor

DEPARTAMENT QUÍMICA ORGÀNICA I FARMACÈUTICA

33. Decoration of a new tricyclic structure with promising antimicrobial activity.

Antibiotic resistance is nowadays a big deal for our society, if we do not generate new antibiotic entities, we risk in a near future to lose our ability to treat common infections.
Our research group has a long experience in synthesis of pyrido[2,3-d]pyrimidines with good activities against different cancer types, such as lung, pancreas, lymphoma,… During one of these projects, we get by serendipity a new tricyclic compound. We believe that this new tricyclic compound can have antimicrobial activity, so we want to decorate this structure with a group that allow a better water solubility. This work is ideal for a candidate who likes Medicinal Chemistry, Organic Synthesis and lab work.

Direcció: Dr. Raimon Puig de la Bellacasa Cazorla

34. Synthesis and characterization of a PROTAC precursor of a new compound with potential activity against aggressive B-Cell Lymphoma (BCL)

PROTACs (proteolysis targeting chimera) are molecular tools that can specifically degrade proteins. A PROTAC is formed by two active domains and a linker which can induce the proteolysis of a target protein. Our research group has extensive experience on the development of new potential compounds with activity against lymphomas by inhibiting key kinases involved in these processes, such as Bruton's tyrosine kinase (BTK) or interleukin-1 receptor-associated kinase 4 (IRAK4). The aim of this project is modifying a previously developed compound by our group with activity against BTK allowing the functionalization with the required linker to form the corresponding PROTAC. This work is perfect for a candidate who likes Organic Synthesis lab work with a clear Medicinal Chemistry application.

Direcció: Dr. Raimon Puig de la Bellacasa Cazorla

DEPARTAMENT QUÍMICA ORGÀNICA I FARMACÈUTICA / DEPARTAMENT ENGINYERIA INDUSTRIAL

35. Development of a Sustainable Solid Perfume

This Final Degree Project focuses on the formulation and design of a solid perfume aligned with the principles of sustainable cosmetics. The work involves the selection and blending of natural, ethically sourced essential oils to create a fragrance, the development of a solid base using biodegradable and skin-safe excipients, and the conception of environmentally responsible packaging made from recyclable or compostable materials. The project follows a holistic and responsible innovation approach, ensuring that every stage -from ingredient sourcing to final presentation - adheres to sustainability, ethical production, and environmental preservation standards.

Direcció: Dr. Carles Bofill Bonet, Dr. Giovanni Gómez Gras i Sr. Luca Caprera

DEPARTAMENT QUÍMICA ORGÀNICA I FARMACÈUTICA / DEPARTAMENT ENGINYERIA QUÍMICA I CIÈNCIA DE MATERIALS

36. Polimorfisme d'APIs i compatibilitat entre principi actiu i excipient, i la seva influència en l'activitat farmacèutica.

Estudiar la influència del potencial polimorfisme de productes (Principis Actius Farmacèutics – API) així com de la interacció entre principi actiu i l'excipient, en l'activitat del medicament. Es faran estudis de solubilitat de les diferents formes, d'estabilitat de les possibles formes cristal·lines i amorfes, ..., tant de productes comercials com de síntesi. És un treball experimental i es treballarà, principalment, amb DSC, TGA i cromatografia

Direcció: Dra. Ana Cuartero Albesa i Dr. Eduard Serra Hosta

DEPARTAMENT ENGINYERIA QUÍMICA I CIÈNCIA DE MATERIALS

37. Design of a polymeric coating to enhance the degradation performance of bioresorbable stents.

Bioresorbable stents offer a transformative approach to treating pediatric aortic coarctation, restoring vessel patency while gradually resorbing to accommodate somatic growth. However, current polymeric scaffolds face critical limitations, including non-uniform degradation, premature loss of mechanical integrity, and suboptimal biological integration. This project proposes the development of a polymeric coating specifically designed to enhance the performance and reliability of bioresorbable stents in dynamic vascular environments.
The primary objective of the coating is to delay the onset of core scaffold degradation until the stent is fully integrated within the aortic wall, thereby ensuring sustained mechanical support during key stages of healing and adaptation. The coating must be biocompatible and undergo uniform surface erosion rather than bulk degradation to achieve a more predictable and stable resorption profile.
Beyond stabilizing degradation, the coating concept presents additional potential benefits that could further improve clinical outcomes. A mildly adhesive surface may enhance stent apposition to the vessel wall and improve mechanical coupling with the pulsatile vasculature, while the coating matrix could also be engineered to enable localized, time-controlled drug delivery. These secondary features would add versatility to the platform, positioning it as a multifunctional solution for next-generation bioresorbable stent technologies.

Direcció: Dr. Jordi Martorell López

38. Synthesis and characterization of intermediates for the synthesis of novel psychedelic compounds with therapeutic potential.

Summary: The past years have seen a resurgence in the study of psychedelic drugs as potential therapeutic tools to treat various psychiatric ailments. While this field of study first bloomed during the 50s and 60s, stringent controls over these drugs brought to a stop this area of research. Nonetheless, a resumption has been taking place during the past two decades, and new research is showing that drugs such as LSD or psilocybin, with the aid of psychotherapy, could potentially help in the treatment of depression, anxiety, end-of-life distress, and addiction.
Furthermore, novel molecules are being developed with less adverse effects, which warrant a deeper examination.
Thus, the main objective of this project is to synthesize a family of building blocks which will be helpful in the making of new psychedelic drugs. These will be later evaluated at the Department of Pharmacology, Toxicology and Therapeutic Chemistry (UB) for their affinity towards the 5-HT2A receptor, responsible for the psychoactive effects of these drugs.

Direcció: Dr. Xavier Berzosa Rodríguez

39. Síntesis y caracterización de oxalatos de metales.

Los complejos oxalatos son compuestos de coordinación en los que el ion oxalato ($C_2O_4^{2-}$) actúa como ligando, formando enlaces con un ion metálico central. Este tipo de complejos es de gran interés en química inorgánica y química de coordinación, ya que el ion oxalato es un ligando

bidentado, lo que significa que puede unirse al metal en dos puntos, generando estructuras más estables y variadas. Debido a esta capacidad de formar enlaces múltiples, los complejos oxalatos son especialmente valiosos en la síntesis de compuestos con estructuras geométricamente interesantes y propiedades específicas, como las propiedades ópticas, magnéticas y catalíticas. La formación de complejos oxalatos es común con una variedad de metales de transición, como el hierro, el cobre y el cobalto, así como con algunos metales alcalinotérreos. Estos complejos pueden prepararse generalmente disolviendo una sal del metal en una solución de ácido oxálico o de uno de sus derivados, lo que permite la coordinación del ion oxalato al metal. Los complejos resultantes tienen aplicaciones tanto en el ámbito de investigación, como en procesos industriales de catálisis, purificación de metales y fabricación de materiales avanzados, y en algunos casos, son estudiados también por su relevancia en procesos biológicos y medioambientales.
Este TFG es experimental y supone trabajar más del 75 % del tiempo en el laboratorio.

Direcció: Dr. Manuel David Abad Roldán

DEPARTAMENT ENGINYERIA QUÍMICA I CIÈNCIA DE MATERIALS / DEPARTAMENT BIOENGINYERIA

40. Adapting OM-PBAE synthesis protocols to Flow Chemistry for the production and characterization of polymeric nanoparticles.

Flow Chemistry is acquiring a key importance in the Fine Chemistry and Specialties industry. It allows, among other advantages, to automate processes, increase quality, minimize safety problems, reduce development times and lower investment in facilities. The focus of this project is to investigate the adaptation of the oligo(β-amino ester) (OM-PBAE) polymer synthesis protocol to continuous flow chemistry, aiming to enhance the efficiency and reproducibility of polymer production. The focus is on synthesizing different types of OM-PBAEs using flow chemistry and subsequently using these polymers to produce polymeric nanoparticles.

Direcció: Dr. Xavier Berzosa Rodríguez i Dra. Marta Guerra Rebollo