

DEPARTAMENT DE QUÍMICA ORGÀNICA

NÚMERO	TEMA	TUTOR(S) ACADÈMIC(S) (si un és d'un altre departament, posa'l entre parèntesi)	TUTOR EXTERN (si escau)
1	Organocatalytic Enantioselective Desymmetrization of bisphenols using isocyanates	Carlos Vila Descals	
2	Benzodiazepines detection for optical methods	Margarita Parra Álvarez	
3	Hybrid MCM-41-Based Materials for Drug Detection	Pau Arroyo Máñez	
4	Design and synthesis of a molecular gate responsive to reductase	Pablo Gaviña Costero	
5	Design and synthesis of a molecular gate responsive to glutathione	Pablo Gaviña Costero	
6	Modification of optical fibers with mesoporous materials	Salvador Gil Grau	
7	Mesoporous materials for drug detection	José Antonio Sáez Cases	
8	Integration of drug sensors on solid surfaces	José Antonio Sáez Cases	
9	Synthesis of derivatives of the mycotoxin citrinin for their application as analytical standards	Daniel López Puertollano	
10	Synthesis of Functionalized Derivatives of Tropane Alkaloids	Antonio Abad Somovilla	
11	Evolution of malaria drugs and the significant role of artemisinin	Juan Francisco Sanz Cervera	
12	Studies towards a new synthetic route of the sex pheromones of the armored scale <i>Aspidiotus nerii</i> (diaspididae) and <i>Delotococcus aberiae</i> .	Ismael Navarro Fuertes	
13	Synthesis of photoactive esters of the 2-sulfoacetic acid for decarboxylative sulfoalkylation reactions	Gonzalo Blay Llinares	
14	New synthetic methodologies with conjugated sulfinyl imines	María Sánchez Roselló / Carlos del Pozo Losada	
15	Sustainable synthesis of pyridinediimine ligands and their catalytically active copper and palladium complexes	Salah-Eddine Stiriba Lakani	
16	Catalytic Atroposelective Desymmetrization of Diaryl Phenols	Jaume Rostoll Berenguer	
17	Study of the intramolecular oxa-Michael reaction in new enantioselective desymmetrization processes	Santiago Díaz Oltra / Marcos Escolano Pérez	
18	Study of unsaturated C-C bond hydroamination through catalyst design	Carmen Ramírez de Arellano Sánchez / Andrea Olmos Vergé	
19	Catalytic synthesis of carbonyl derivatives of industrial interest from raw materials	Andrea Olmos Vergé / Carmen Ramírez de Arellano Sánchez	
20	Cascade cyclization reactions catalyzed by 3d metals	Andrea Olmos Vergé / Carmen Ramírez de Arellano Sánchez	

21	Difunctionalization reactions of unsaturated C-C bonds catalyzed by 3d metals	Carmen Ramírez de Arellano Sánchez / Andrea Olmos Vergé	
22	Synthesis of Nitrogen-Containing Heterocycles via Hydrogen Autotransfer Reactions: A Sustainable Approach	Rafael Ballesteros Garrido / Rafael Ballesteros Campos	
23	Development of Novel Materials for the Capture of Mercury and Cadmium from Aqueous Media	Rafael Ballesteros Garrido / (Roberto Sáez Hernández)	
24	New Catalyst from hidrogels	Rafael Ballesteros Garrido	
25	New Materials from Biopolymers	Rafael Ballesteros Garrido	
26	Formation of Metallic Nanoparticles Using Hydrogel-Derived Materials: Synthesis and Characterization	Rafael Ballesteros Garrido	
27	Enantioselective addition reactions of isocyanides	Alicia Monleón Ventura	
28	Can colouring clothing be environmentally sustainable?	Ana C. Cuñat Romero	
29	How tyres are turning green	Ana C. Cuñat Romero	
30	Synthesis of nanoheterostructures based on upconversion nanoparticles	María González Béjar / Julia Pérez Prieto	
31	Photocatalytic approach for the oxidation of boronic acids using near-infrared light	Jorge Escorihuela Fuentes	
32	Photocatalytic [4 + 2] cycloadditions of N,N-dimethylaniline with maleimides mediated with near-infrared-light	Jorge Escorihuela Fuentes	
33	Photocatalytic Trifluoromethylation of Alkynes	Jorge Escorihuela Fuentes / María González Béjar	
34	Computational study on gold-catalyzed spirocyclization of 3-ene-1,7-diynes	Jorge Escorihuela Fuentes	
35	Synthesis and applications of sulfonyl fluorides	Marc Montesinos Magraner	
36	Anodic Oxidative [4 + 2] Cycloaddition of o-Phenylenediamines with Alkenes	Amparo Sanz Marco	
37	Introducing organocatalysis in undergraduate teaching: design of a practical session for the "Laboratory of Organic Chemistry II"	Amparo Sanz Marco / Jaume Rostoll Berenguer	

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Carlos Vila Descals

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed):

Department: Química Orgànica

TITLE (Mandatory in English)

Organocatalytic Enantioselective Desymmetrization of bisphenols using isocyanates

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Es ben coneguda la importància de la quiralitat de les molècules orgàniques en diferents àrees, que van des de la Biologia a la Ciència dels Materials. Així, el desenvolupament de nous mètodes de síntesis enantioselectiva constitueixen en la actualitat un àrea de intensa investigació. Entre ells, els procediments catalítics (catàlisis asimètrica) resulten especialment atractius ja que permeten minimitzar el consum de quiralitat i disminuir la producció de residus. En este context existeixen molt pocs exemples de la desimetrització de compostos orgànics amb dos anells de fenol per generar compostos quirals de manera enantioselectiva. Així en aquest projecte es planteja com objectiu l'estudi de la desimetrització de compostos amb dos anells de fenol utilitzant isocinats com a electròfils.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

Es seguirà una metodologia similar a la utilitzada pel nostre grup de investigació en altres reaccions enantioselectives organocatalítiques. En concret es durà a terme:

- 1) Síntesis de diferents substrats de partida.
- 2) Identificació de les condicions òptimes de reacció, en lo que fa referencia al rendiment de la reacció i, en especial, a la enantioselectivitat, utilitzant diferents organocatalitzadors.
- 3) Estudi de l'abast i limitacions de la reacció, utilitzant diferents compostos orgànics.
- 4) L'anàlisi dels productes finals de cada reacció es durà a terme segons la metodologia estàndard en síntesis orgànica (mètodes cromatogràfics i espectroscòpics). L'excés enantiomèric per a cadascun dels productes obtinguts es determinarà mitjançant cromatografia líquida d'alta resolució (HPLC) i la configuració absoluta es determinarà per difracció de raigs X de monocristall.

(Department stamp)

VNIVERSITAT DE VALÈNCIA (ò*) Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Margarita Parra Alvarez

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Benzodiazepines detection for optical methods

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Establecer el estado del arte del tema en los últimos 10 años
- Comparar los métodos existentes
- Detectar carencias

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Realizar una revisión bibliográfica de los métodos descritos para la detección óptica de benzodiazepinas tanto en bebidas como en fluidos orales.
- Realizar un estudio comparativo sobre las ventajas e inconvenientes de cada uno
- Detectar cuáles son las carencias existentes y proponer una línea de mejora.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Pau Arroyo Máñez

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Hybrid MCM-41-Based Materials for Drug Detection

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Se dissenyarà y sintetitzarà un sistema basad en nanopàrticulas de sílice mesoporosa que sea capaz de, en presencia del analito para el que será diseñado, producir un cambio de color o fluorescencia. El objetivo principal del sistema es que sea implementado en un soporte sólido del tipo lateral flow. Posteriormente se evaluará su aplicación con muestras reales.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se realizará una búsqueda bibliográfica de los sensores actuales y se analizará la posibilidad de llevar a un sistema que produzca el desplazamiento necesario para liberar la carga de la nanopartícula y revelar el cambio de color.
Se sintetizará la puerta molecular y se caracterizará mediante métodos espectroscópicos. Posteriormente, se cargará la nanopartícula y se cerrarán los poros mediante la puerta molecular diseñada.
Finalmente se evaluará su utilidad mediante métodos de espectroscopía UV-Vis y/o emisión de fluorescencia, así como a simple vista.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Pablo Gaviña Costero

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Design and synthesis of a molecular gate responsive to reductase

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Síntesis de una puerta molecular sensible a reductasas
- Síntesis del material mesoporoso con la puerta molecular
- Estudio de liberación en cultivos celulares

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Revisión bibliográfica

Síntesis de una puerta molecular incorporando un derivado de trialcóxido de silicio para su anclaje sobre sílice y un azo derivado que se reduzca en presencia de azoreductasa.

Caracterización espectroscópica de la puerta molecular y del material mesoporoso mediante las técnicas habituales (^1H y ^{13}C NMR, UV-vis, MS...)

Evaluación de su ruptura en un entorno hipóxico en células

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Pablo Gaviña Costero

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Design and synthesis of a molecular gate responsive to glutathione

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Síntesis de una puerta molecular sensible a glutathione
- Síntesis del material mesoporoso con la puerta molecular
- Estudio de liberación en cultivos celulares

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Revisión bibliográfica

Síntesis de una puerta molecular incorporando un derivado de trialcóxido de silicio para su anclaje sobre sílice.

Caracterización espectroscópica de la puerta molecular y del material mesoporoso mediante las técnicas habituales (^1H y ^{13}C NMR, UV-vis, MS...)

Evaluación de su ruptura en un entorno hipóxico en células



VNIVERSITAT E VALÈNCIA (ò*) Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Salvador Gil Grau

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Modification of optical fibers with mesoporous materials

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Preparation of optical fibers covalently modified with mesoporous materials
- Study of the modulation of the optical signal according to the surface modification

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Synthesis of mesoporous material
- Characterization of the material
- Activation of the optical fiber
- Optimization of the method of covalent bond of the material on the fiber surface
- Determination of the degree of modification of the surface
- Study of the modification of the optical signal

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Jose Antonio Sáez Cases

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Mesoporous materials for drug detection

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Synthesis of silica-based mesoporous nanomaterials functionalised with molecular gates for the detection of different drugs.
Evaluation of the detection capacity of functionalised hybrid nanomaterials on samples.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Synthesis of silica-based mesoporous nanomaterials.
Synthesis of smart molecular gates.
Loading of mesoporous silica nanoparticles with a fluorophore.
Assembly of the molecular gates on the mesoporous nanomaterials.
Evaluation of drug detection with these hybrid nanomaterials
Evaluation of detection limit, selectivity, ...

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Synthesis of derivatives of the mycotoxin citrinin for their application as analytical standards

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Citrinin is a mycotoxin frequently found in various types of cereals, fruits, and dairy products. When ingested, it causes several adverse effects, with its high nephrotoxicity being particularly notable. Immunoassays are commonly used methods for citrinin detection in food samples, which rely on antibodies for mycotoxin recognition. In the research group where this work will be conducted, specific antibodies against citrinin have recently been developed. In order to characterize the specificity of these antibodies, natural metabolites and derivatives of citrinin will be chemically synthesized.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The synthetic strategy to be followed for the preparation of natural derivatives/metabolites citrinin will be based on previously described approaches for the synthesis of the mycotoxin itself, appropriately modified to incorporate the necessary functional groups.

The methodology to achieve this objective will involve the following tasks:

- Targeted literature search.
- Reading and analysis of the most relevant scientific literature.
- Evaluation of the most suitable synthetic methodology to achieve the objective.
- Development of the synthetic sequence using various synthetic techniques, which will include, among others:
 - Carrying out reactions at variable temperatures (from -78°C to +200°C);
 - Working under an inert atmosphere;
 - Monitoring reactions using chromatographic methods (TLC, GC and/or analytical HPLC, etc.) and processing them;
 - Product purification using chromatographic techniques (column chromatography, preparative HPLC, etc.);
 - Structural identification of all products using spectroscopic techniques such as 1D and 2D NMR, mass spectrometry, etc.;
- Discussion of the results obtained.
- Preparation of the final report and public presentation.

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Antonio Abad Somovilla

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Synthesis of Functionalized Derivatives of Tropane Alkaloids

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El presente proyecto tiene como objetivo la preparación por síntesis total de nuevos derivados funcionalizados de alcaloides tropánicos, un grupo de contaminantes naturales de productos alimenticios sobre los que la EFSA ha centrado recientemente su atención, particularmente escopolamina y atropina. Los nuevos derivados sintetizados se utilizarán para el desarrollo de procedimientos inmunoanalíticos que permitan la determinación rápida y económica de estos contaminantes en múltiples muestras.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

La estrategia sintética que se seguirá para la preparación de los nuevos derivados de los alcaloides tropánicos se basará en la modificación estructural apropiada del sistema bicíclico comercial exo-6-hidroxi-3-tropanona para poder incorporar sobre la función hidroxílica un brazo espaciador alifático, funcionalizado en su extremo con un grupo carboxilo para su conjugación a proteínas y enzimas mediante química mediada por carbodiimida.

La metodología que se seguirá para completar este objetivo implicará las siguientes tareas:

- Búsqueda bibliográfica dirigida y análisis de la bibliografía más relevante.
- Análisis de la metodología sintética más adecuada para alcanzar el objetivo.
- Desarrollo de la secuencia sintética utilizando diferentes técnicas sintéticas, purificación de productos por técnicas cromatográficas e identificación estructural de todos los productos por técnicas espectroscópicas.
- Discusión de los resultados alcanzados y elaboración de la memoria correspondiente.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Juan Francisco Sanz Cervera

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Organic Chemistry

TITLE (Mandatory in English)

Evolution of malaria drugs and the significant role of artemisinin

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This TFG aims to study the evolution over the years of the drugs used in the fight against malaria. Additionally, emphasis will be placed on the discovery of artemisinin and related compounds as essential antimalarials nowadays.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The student will gather information through a bibliographic search and develop a paper that includes the most relevant aspects of the objectives stated above, all under the guidance and direction of the TFG supervisor.

VNIVERSITAT VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Ismael Navarro Fuertes

ACADEMIC TUTOR (if needed): _____

EXTERNAL TUTOR (if needed): _____

Department: Organic chemistry

TITLE (Mandatory in English)

Studies towards a new synthetic route of the sex pheromones of the armored scale *Aspidiotus nerii* (diaspididae) and *Delotococcus aberiae*.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

El objetivo del trabajo es explorar síntesis alternativas para obtener la feromona sexual del piojo blanco del limón *Aspidiotus nerii* (diaspididae), y *Delotococcus aberiae* (pseudococcidae) o un intermedio de la mismas. Ambas plagas afectan a cultivos de cítricos, y son terpenos que presentan una estructura de tipo 1,1,2 ciclobutano o ciclopentánica respectivamente. El estudio comprende la optimización de alguna de las etapas de síntesis para mejorar procedimientos que permitan, por un lado, obtener estas feromonas con rendimientos superiores a los actualmente descritos, y por otro, que sean escalables desde el punto de vista de la producción industrial de estas moléculas.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

En el caso de la propuesta de la feromona sexual de *Aspidiotus nerii* y *Delotococcus aberiae*, se propone en el primer caso una síntesis vía la ciclación intramolecular fotoquímica de un 1,6 dieno catalizada por cobre (I) para obtener el esqueleto ciclobutánico requerido, mientras que el segundo, la estrategia de formación de la estructura final se estudiará vía la formación y de un epóxido mediante una sal de sulfonio a partir de una enona pentacíclica y su posterior apertura.

La metodología comprenderá:

- 1) Búsqueda bibliográfica y análisis de la más significativa.
- 2) Propuesta de las metodologías sintéticas más adecuada para alcanzar el objetivo.
- 3) Implementación de la secuencia sintética. Las técnicas a emplear comprenden:
 - i) Desarrollo de reacciones a temperatura variable (-78°C hasta +200°C); ii) Trabajo en atmósfera inerte; iii) Seguimiento de la reacción por métodos cromatográficos (CCF, CG y/o HPLC analítico, etc); iv) Procesado de reacción; v) Purificación de productos por técnicas cromatográficas (CC, HPLC preparativo, etc); v) Identificación estructural de productos y conjugados por técnicas espectroscópicas de RMN y espectrometría de masas.
- 4) Discusión de los resultados alcanzados y elaboración de la memoria para su presentación pública

(Department stamp)

VNIVERSITAT E VALÈNCIA (ò*) Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Gonzalo Blay Llinares

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgànica

TITLE (Mandatory in English)

Synthesis of photoactive esters of the 2-sulfoacetic acid for decarboxylative sulfoalkylation reactions

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Development of a synthetic procedure for the preparation of NHPI esters of 2-fluorosulfonyl acetic acid from 2-sulfoacetic acid.
- Preliminary study of the fluorosulfonylalkylation of alkenes under photoredox or electrochemical conditions

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

To achieve the synthesis of the target NHPI ester, sulfoacetic acid will be transformed into its carboxylic acid chloride and treated with N-hydroxyphthalimide. The resulting NHPI ester will be converted into the corresponding fluorosulfone upon treatment with thionyl chloride and KF. Once prepared, the NHPI ester will be used to achieve the introduction of a fluorosulfonylmethyl group into alkenes via a radical pathway under photochemical or electrochemical conditions. The reaction conditions will be optimized to achieve the highest possible yields and the scope of the reaction will be studied.

The student should acquire skills in the following aspects:

Bibliographic search.

Advanced organic chemistry laboratory techniques.

Chromatographic techniques (thin layer and column chromatography)

Structural analysis (NMR, EM, etc.)

Instrumental analysis (HPLC, GC, etc.)

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Examples in the literature dealing with the use of conjugated sulfinyl imines as conjugated partners in Michael-type reactions are very scarce. The objective is to extend the study of the reactivity of those Michael acceptors with several nucleophiles for the asymmetric synthesis of new heterocyclic scaffolds.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Our research group is working with those substrates for the last five years. Our goal is to extend this study to the use of alfa bromo dicyanoalkenes as nucleophiles, since an intramolecular nucleophilic displacement would allow us to synthesize pyrrolines with simultaneous generation of two chiral centers. The feasibility of this transformation will be evaluated.

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

SALAH-EDDINE STIRIBA LAKANI

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Organic Chemistry

TITLE (Mandatory in English)

Sustainable synthesis of pyridinediimine ligands and their catalytically active copper and palladium complexes

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objectives of this TFG project are as follows:

- i) The mechanochemical preparation and physical characterization of pyridinediimine (PDI) ligands.
- ii) The mechanochemical and physical characterization of their copper(I)/(II) and palladium(II) complexes.
- ii) The study of the catalytic potential of such complexes in the sustainable carbon-carbon and carbon-nitrogen bonds forming reactions in water as solvent.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The above objectives will be addressed through the synthesis of C2-symmetric imino-pyridine ligands under mechanochemical conditions.

Their copper and palladium metal complexes will also be prepared under the same conditions.

The C2-symmetry PDI ligands and their complexes will be characterized by FTR, UV-visible, NMR, mass-spectrometry, photoluminescence and X-ray diffraction on single crystals.

Their catalytic properties will be tested on sustainable fashion of the Suzuki and Heck

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Catalytic Atroposelective Desymmetrization of Diaryl Phenols

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Desenvolupament d'una metodologia per a la generació de quiralitat axial en diaril fenols mitjançant una desimetrització catalítica i enantioselectiva.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se seguirà una metodologia similar a la utilitzada pel nostre grup d'investigació en altres reaccions enantioselectives organocatalítiques. En concret es durà a terme:

- 1) Síntesi de diferents substrats de partida.
- 2) Identificació de les condicions òptimes (catalitzador, dissolvent, temperatura,...) de la desimetrització dels diaril fenols per maximitzar el rendiment de la reacció i, especialment, l'excés enantiomèric.
- 3) Estudi de l'abast i limitacions de la reacció.

Els compostos orgànics obtinguts seran analitzats i caracteritzats mitjançant tècniques espectroscòpiques (ressonància magnètica nuclear, infraroig...) i no espectroscòpiques (espectrometria de masses, difracció de raig X). L'excés enantiomèric serà determinat mitjançant cromatografia líquida d'alta eficàcia (HPLC).

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Study of the intramolecular oxa-Michael reaction in new enantioselective desymmetrization processes

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo principal del trabajo es desarrollar y optimizar un nuevo proceso de desimetrización enantioselectiva para obtener heterociclos oxigenados quirales. Para ello se deberá:

- Diseñar y sintetizar nuevos sustratos de partida capaces de experimentar una reacción de oxa-Michael intramolecular
- Optimizar y comprobar el alcance de la reacción de oxa-Michael intramolecular.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

La metodología principal utilizada en este trabajo para la generación de la quiralidad será la organocatálisis asimétrica, que se basa en el empleo de pequeñas moléculas orgánicas quirales capaces de catalizar con eficacia diversos tipos de reacciones enantioselectivas.

Además durante la realización del trabajo, el alumno deberá familiarizarse con las técnicas y habilidades más comunes en el ámbito de la síntesis orgánica. Entre ellas destacan: el montaje de reacciones en condiciones inertes, la purificación y secado de disolventes y reactivos, la caracterización de compuestos orgánicos mediante RMN y la obtención de los excesos enantioméricos de los productos finales mediante HPLC de fase estacionaria quiral.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Determination of the scope of raw substrates for the catalytic introduction of nitrogen moieties on unsaturated derivatives.
- Design and synthesis of potential electrophilic catalysts of 3d metals for the increase of molecular functionality.
- X-ray crystal structure determination and study of intermediates.
- Study of the catalytic activity in synthesis of azocompounds.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Theoretical/practical introduction to the synthesis of metal complexes in inert conditions (use of Schlenk line and dry box) and crystallization of metallo-organic systems.
- Theoretical and practical initiation to the catalytic processes for hydroamination of unsaturated C-C bonds.
- Theoretical/practical introduction to structural determination using single-crystal X-ray diffraction, including: crystal isolation and treatment, diffractometer handling, use of computer programs for data processing and interaction studies.
- Theoretical/practical initiation to the spectroscopic characterization of the characterized systems.

VNIVERSITAT E VALÈNCIA (ò*) Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Catalytic synthesis of carbonyl derivatives of industrial interest from raw materials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Determination of the scope of raw substrates for the catalytic synthesis of carbonyl derivatives.
- Design and synthesis of potential electrophilic catalysts of 3d metals for the synthesis of carbonyl derivatives.
- X-ray crystal structure determination and study of intermediates.
- Study of the catalytic activity in carbonyl derivative formation processes.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Theoretical/practical introduction to the synthesis of metal complexes in inert conditions (use of Schlenk line and dry box) and crystallization of metallo-organic systems.
- Theoretical and practical initiation to the catalytic processes for carbonyl derivatives preparation.
- Theoretical/practical introduction to structural determination using single-crystal X-ray diffraction, including: crystal isolation and treatment, diffractometer handling, use of computer programs for data processing and interaction studies.
- Theoretical/practical initiation to the spectroscopic characterization of the characterized systems.

VNIVERSITAT E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Determination of the scope of raw substrates for the catalytic cyclization of polyunsaturated derivatives.
- Design and synthesis of potential electrophilic catalysts of 3d metals for the increase of molecular complexity.
- X-ray crystal structure determination and study of intermediates.
- Study of the catalytic activity in heterocycle formation processes.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Theoretical/practical introduction to the synthesis of metal complexes in inert conditions (use of Schlenk line and dry box) and crystallization of metallo-organic systems.
- Theoretical and practical initiation to the catalytic processes for cyclization of polyunsaturated compounds.
- Theoretical/practical introduction to structural determination using single-crystal X-ray diffraction, including: crystal isolation and treatment, diffractometer handling, use of computer programs for data processing and interaction studies.
- Theoretical/practical initiation to the spectroscopic characterization of the characterized systems.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Carmen Ramírez de Arellano Sánchez

ACADEMIC TUTOR 2

Andrea Olmos Vergé

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Organic Chemistry

TITLE (Mandatory in English)

Difunctionalization reactions of unsaturated C-C bonds catalyzed by 3d metals.

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Determination of the scope and preparation of unsaturated substrates for catalytic syntheses of highly functionalized derivatives.
- Design and synthesis of potential electrophilic catalysts of 3d metals for the activation of unsaturated compounds.
- X-ray crystal structure determination and study of intermediates.
- Study of the catalytic activity for a sustainable increase of molecular complexity

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Theoretical and practical initiation to the preparation of unsaturated substrates.
- Theoretical/practical introduction to the synthesis of metal complexes in inert conditions (use of Schlenk line and dry box) and crystallization of metallo-organic systems.
- Theoretical/practical introduction to structural determination using single-crystal X-ray diffraction, including: crystal isolation and treatment, diffractometer handling, use of computer programs for data processing and interaction studies.
- Theoretical/practical initiation to the spectroscopic characterization of the characterized systems.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Synthesis of Nitrogen-Containing Heterocycles via Hydrogen Autotransfer Reactions: A Sustainable Approach

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop sustainable synthetic methodologies for the preparation of nitrogen-containing heterocycles using hydrogen autotransfer and related catalytic reactions, and to evaluate the scope, selectivity, and efficiency of these transformations under mild conditions.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The student will carry out the synthesis of various nitrogen-containing heterocycles through hydrogen autotransfer (borrowing hydrogen) strategies, employing alcohols and amines as starting materials. These reactions will be performed under catalytic conditions, using transition metal complexes or organocatalysts, and monitored over time to optimize parameters such as temperature, reaction time, and catalyst loading. Product identification and purity will be confirmed using techniques such as thin-layer chromatography (TLC), nuclear magnetic resonance spectroscopy (^1H and ^{13}C NMR), and mass spectrometry (MS). The student will also use infrared spectroscopy (IR) and, where applicable, melting point determination to further characterize the compounds. This methodology will allow the student to acquire practical experience in modern synthetic organic chemistry, including reaction design, purification, and advanced structural elucidation. The project will enhance the student

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Ballesteros Garrido

ACADEMIC TUTOR 2 Roberto Saez Hernandez

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica y Química Analítica

TITLE (Mandatory in English)

Development of Novel Materials for the Capture of Mercury and Cadmium from Aqueous Media

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To design, synthesize, and evaluate new adsorbent materials for the efficient removal of mercury (Hg^{2+}) and cadmium (Cd^{2+}) ions from aqueous solutions, and to quantify metal uptake using atomic absorption spectroscopy (AAS).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Novel adsorbent materials will be synthesized, potentially based on functionalized biopolymers, hybrid organic-inorganic matrices, or modified clays. These materials will be characterized in terms of morphology, functional group content, and thermal stability using techniques such as Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM), depending on availability. The adsorption experiments will be carried out by exposing known concentrations of Hg^{2+} and Cd^{2+} solutions to the synthesized materials under controlled pH, time, and temperature conditions. After separation, residual metal concentrations in the supernatants will be quantified using flame or graphite furnace atomic absorption spectroscopy (AAS), allowing for the determination of adsorption capacities and removal efficiencies. This methodology will provide the student with hands-on experience in materials synthesis, analytical chemistry, and environmental applications.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Ballesteros Garrido

ACADEMIC TUTOR 2 Roberto Saez Hernandez

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica y Química Analítica

TITLE (Mandatory in English)

Development of Novel Materials for the Capture of Mercury and Cadmium from Aqueous Media

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To design, synthesize, and evaluate new adsorbent materials for the efficient removal of mercury (Hg^{2+}) and cadmium (Cd^{2+}) ions from aqueous solutions, and to quantify metal uptake using atomic absorption spectroscopy (AAS).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Novel adsorbent materials will be synthesized, potentially based on functionalized biopolymers, hybrid organic-inorganic matrices, or modified clays. These materials will be characterized in terms of morphology, functional group content, and thermal stability using techniques such as Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM), depending on availability. The adsorption experiments will be carried out by exposing known concentrations of Hg^{2+} and Cd^{2+} solutions to the synthesized materials under controlled pH, time, and temperature conditions. After separation, residual metal concentrations in the supernatants will be quantified using flame or graphite furnace atomic absorption spectroscopy (AAS), allowing for the determination of adsorption capacities and removal efficiencies. This methodology will provide the student with hands-on experience in materials synthesis, analytical chemistry, and environmental applications.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Rafael Ballesteros Garrido

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

New Catalyst from hidrogels

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop and characterize novel materials derived from polymers and metal.

To evaluate the catalytic activity of those new materials.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Hydrogels will be prepared by dissolving polyvinyl alcohol (PVA) in water at 80–90°C, followed by the addition of metal sulfate salts. Borax will be added as a crosslinker to form stable hydrogels. After gelation, the samples will be washed, dried, and combusted in air at 400–600°C to obtain the final catalysts. The materials will be characterized by X-ray diffraction (XRD), inductively coupled plasma spectroscopy (ICP), elemental analysis, and Raman spectroscopy.

Catalytic tests will be performed in a high-pressure autoclave under hydrogen atmosphere. Reaction progress (nitrobenzene derivatives reductions) and product analysis will be monitored by nuclear magnetic resonance (NMR) spectroscopy.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Rafael Ballesteros Garrido

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

New Materials from Biopolymers

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop and characterize novel materials derived from biopolymers.

To evaluate the antimicrobial properties of biopolymer-based materials and assess their potential use in applications requiring bacterial.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Biopolymer-based hydrogels will be prepared using conventional synthesis techniques, involving the dissolution of the polymer in aqueous media under controlled temperature and stirring conditions. Once formed, the hydrogels will be loaded with active agents for subsequent release studies. The release profile of these agents will be monitored using UV-Vis spectroscopy to evaluate diffusion behavior over time. Structural and chemical characterization of the materials will be carried out using powder X-ray diffraction (PXRD), inductively coupled plasma optical emission spectrometry (ICP-OES), and ion chromatography. This methodology will not only enable the student to understand the fundamentals of material synthesis and characterization, but also to acquire hands-on experience with advanced instrumental techniques and data interpretation. In doing so, the project will promote the development of critical scientific skills and reinforce the student's training in experimental research within the field of sustainable materials.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Rafael Ballesteros Garrido

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Formation of Metallic Nanoparticles Using Hydrogel-Derived Materials:
Synthesis and Characterization

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To study the synthesis of metallic nanoparticles mediated by hydrogel-derived materials, focusing on controlling particle size, distribution, and stability, and to evaluate their potential applications through comprehensive characterization.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Hydrogel-derived materials will be synthesized following established protocols involving polymer dissolution and crosslinking under controlled conditions. These materials will be employed as templates or stabilizing agents for the in situ reduction and formation of metallic nanoparticles (e.g., zinc, nickel or copper). The formation and properties of the nanoparticles will be monitored using UV-Vis spectroscopy to detect surface plasmon resonance bands characteristic of metallic nanoparticles. Further characterization will include powder X-ray diffraction (PXRD) to determine crystalline phases, transmission electron microscopy (TEM) or scanning electron microscopy (SEM) for morphology and size distribution analysis, and inductively coupled plasma optical emission spectrometry (ICP-OES) for elemental quantification.

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Alicia Monleón Ventura

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Enantioselective addition reactions of isocyanides

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo de este trabajo consiste en el desarrollo de un método catalítico y enantioselectivo de adición de isocianuros a compuestos insaturados y el estudio de las condiciones de reacción para la obtención del correspondiente producto.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Para el estudio de la reacción de adición enantioselectiva, se llevará a cabo:

- Síntesis de los isocianuros y su caracterización mediante RMN, HRMS y punto de fusión (si procede).
- Optimización de las condiciones de reacción entre el isocianuro y el compuesto insaturado seleccionado. Para ello, se evaluarán diferentes catalizadores quirales, disolventes y aditivos, así como la influencia de la temperatura, la concentración y el tiempo de reacción en el rendimiento y la enantioselectividad de la reacción.
- Estudio del alcance y limitaciones de la reacción, aplicando las condiciones óptimas seleccionadas, utilizando compuestos de partida con sustituyentes de diferente naturaleza electrónica y estérica.
- Los productos obtenidos se caracterizarán mediante RMN, HRMS, punto de fusión (si procede), HPLC quiral y polarimetría.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Ana C. Cuñat Romero

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

Can colouring clothing be environmentally sustainable?

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The TFG aims to study the evolution over the years the use of dyes for colouring clothes. With special attention to the use of more sustainable colorants.

El objetivo del trabajo es hacer un estudio evolutivo sobre el uso de colorantes para dar color a los tejidos. Haciendo especial hincapié en el uso de colorantes más sostenibles medioambientalmente.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Tomando como base referencias actualizadas, ampliar la búsqueda sobre el tema indicado.

Desarrollar un informe que recoja los aspectos más relevantes de los objetivos planteados arriba.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Ana C. Cuñat Romero

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgánica

TITLE (Mandatory in English)

How tyres are turning green.

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The TFG aims to study the evolution over the years the materials use for tyres manufacturing

El objetivo del trabajo es hacer un estudio evolutivo sobre los materiales empleados para la fabricación de los neumáticos. Haciendo especial hincapié en una manufactura más sostenible medioambientalmente.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Tomando como base referencias actualizadas, ampliar la búsqueda sobre el tema indicado.

Desarrollar un informe que recoja los aspectos más relevantes de los objetivos planteados arriba.

VNIVERSITAT E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

María González Béjar

ACADEMIC TUTOR 2

Julia Pérez Prieto

EXTERNAL TUTOR (if needed):**DEPARTMENT(S):** Química Orgánica**TITLE (Mandatory in English)**

Synthesis of nanoheterostructures based on upconversion nanoparticles

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)**Main Objective:**

To synthesize nanoheterostructures via cation exchange incorporating upconversion nanoparticles (UCNPs), and to derivatize them with organic ligands and chromophores in order to enhance their optical properties for potential applications in photocatalysis.

Specific Objectives:

- To design, synthesize, and characterize nanoheterostructures based on upconversion nanoparticles (UCNPs).
- To derivatize the synthesized nanostructures with organic ligands and chromophores to tailor their surface chemistry and improve their photocatalytic performance.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project will be carried out in several stages, combining wet-chemical synthesis techniques with advanced characterization methods:

1. Synthesis of upconversion nanoparticles
2. Nanoheterostructure fabrication and derivatization with organic ligands and chromophores
3. Characterization:
 - Transmission Electron Microscopy (TEM): For morphology and size distribution.
 - X-ray Diffraction (XRD): To confirm crystal phase and structural integrity.
 - Fourier Transform Infrared Spectroscopy (FTIR): To analyze surface functional groups.
 - Dynamic Light Scattering (DLS): For hydrodynamic size and colloidal stability.
 - Photoluminescence Spectroscopy: To measure emission spectra and quantum yield.
4. Data Analysis and Interpretation
5. Documentation and Reporting

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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Photocatalytic approach for the oxidation of boronic acids using near-infrared light

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

General Objective: Development and evaluation a photocatalytic method for the oxidation of boronic acids under near-infrared (NIR) light irradiation

Specific Objectives:

Optimization of a photocatalytic system capable of absorbing and utilizing NIR light for the activation of boronic acid oxidation.

Investigation of substrate scope by testing a variety of aromatic and aliphatic boronic acids.

Elucidation of the reaction mechanism

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The study will begin with the selection and preparation of a series of aryl and alkyl boronic acids as model substrates. A range of photocatalysts including commercially available dyes will be evaluated. Reactions will be conducted under NIR light irradiation using LED sources, with control of temperature, solvent, and reaction time. Reaction conditions (photocatalyst loading, solvent, etc) will be optimized to achieve maximum conversion and selectivity. Products will be isolated and characterized using NMR spectroscopy, mass spectrometry, and IR spectroscopy. Mechanistic studies will be performed using radical scavengers, time-resolved spectroscopy, and control experiments in the absence of light or photocatalyst. Finally, the scope and limitations of the method will be assessed by applying the optimized conditions to a diverse set of boronic acid derivatives, evaluating yields, reaction rates, and functional group tolerance.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Jorge Escorihuela Fuentes

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Departamento de Química Orgánica

TITLE (Mandatory in English)

Photocatalytic [4 + 2] cycloadditions of N,N-dimethylaniline with maleimides mediated with near-infrared-light

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop a photocatalytic method for [4 + 2] cycloaddition reactions between N,N-dimethylaniline and maleimides using near-infrared (NIR) light as the activation source.

To explore the scope and limitations of the cycloaddition reaction by varying the maleimide substituents and electron-donating groups on N,N-dimethylaniline.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Phase 1: Literature Review and Planning
Review recent advances in NIR photocatalysis.

Phase 2: Reaction Design and Optimization
To develop a base reaction system and optimize key parameters: photocatalyst loading, solvent, temperature, etc.

Phase 3: Substrate Scope and Mechanistic Studies
To evaluate the reaction scope with different maleimides and N,N-dimethylaniline derivatives.
To investigate the mechanism of the reaction and confirm the nature of intermediates.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop a novel, efficient, and selective photoredox-catalyzed protocol for the trifluoromethylation of terminal and internal alkynes under mild reaction conditions.

To investigate the scope and limitations of the reaction with respect to a variety of alkyne substrates.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project is structured into different stages over a period of 3-4 months, covering the conceptual design, experimental development, mechanistic investigation, and final analysis.

- Photocatalytic trifluoromethylation of alkynes
- Optimization of reaction conditions to establish the optimal conditions for the photocatalytic reaction: solvents, photocatalyst loading, temperature, time, concentration, stoichiometry.
- Perform control experiments (no light, no catalyst, etc.)
- Substrate scope to explore the reaction scope with different alkynes.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Jorge Escorihuela Fuentes

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Departamento de Química Orgánica

TITLE (Mandatory in English)

Computational study on gold-catalyzed spirocyclization of 3-ene-1,7-diynes

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To investigate the reaction mechanism of the gold-catalyzed spirocyclization of 3-ene-1,7-diynes using computational chemistry tools, with particular attention to key intermediates and transition states.

To determine the energetics and activation barriers associated with the different possible reaction pathways, helping to identify the most favorable catalytic cycle.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The computational investigation will be conducted using density functional theory (DFT) with Gaussain 09 to explore the mechanism, energetics, and selectivity of the gold-catalyzed spirocyclization of 3-ene-1,7-diynes.

Initially, a model selection Will be carried out to reduce computational cost while retaining essential reactivity features. Next, geometry optimization and frequency calculations of All stationary points (reactants, intermediates, transition states, and products) will be performed using DFT methods. Frequency calculations will confirm minima (no imaginary frequencies) or transition states (one imaginary frequency) and provide thermochemical corrections. Finally, solvent effects using implicit solvation models (e.g., SMD or PCM) will be applied to simulate experimental conditions.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Marc Montesinos Magraner

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Orgànica

TITLE (Mandatory in English)

Synthesis and applications of sulfonyl fluorides

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Synthesis of sulfonyl fluorides
- Study of their potential as intermediates in organic synthesis

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The student will be trained in:

- Organic synthesis.
- Chromatographic techniques (TLC, column chromatography)
- Structural elucidation (NMR, HRMS).
- Instrumental analysis (chiral HPLC).
- Searching literature.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Búsqueda bibliográfica.
- Técnicas de síntesis orgánica y electroquímica.
- Técnicas cromatográficas (cromatografía de capa fina y de columna)
- Análisis estructural (RMN, EM, etc.)
- Análisis instrumental (HPLC, CG, etc.)

VNIVERSITAT
E VALÈNCIA (ò*) Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Amparo Sanz Marco

ACADEMIC TUTOR 2 Jaume Rostoll Berenguer

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Organic Chemistry

TITLE (Mandatory in English)

Introducing organocatalysis in undergraduate teaching: design of a practical session for the "Laboratory of Organic Chemistry II"

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Identify and select an organocatalytic reaction.
2. Adapt and optimize the reaction.
3. Prepare the laboratory manual.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. A bibliographic search will be carried out to identify organocatalytic reactions suitable for undergraduate teaching laboratories, considering factors such as reaction time, safety, cost, environmental impact, and pedagogical value.
2. The selected reaction will then be optimized by adjusting parameters such as substrates, organocatalyst, solvent, and temperature, so that it can be completed within a laboratory session. The characterization of the potential product (NMR, IR, optical rotation...) will also be studied.
3. Teaching materials will be prepared, including a theoretical introduction, experimental procedure, and pre- and post-lab questions, to guide students through the experiment