



TRABAJOS FIN DE GRADO EN QUÍMICA (CURSO 19/20 – BILINGÜE)
Aprobados por la Comisión de Docencia del Grado en Química en la sesión ordinaria del 4 de octubre de 2019

ÁREA DE QUÍMICA ANALÍTICA

QA01B Determination of potassium in fertilizers

Determinación de potasio en fertilizantes

Fertilizers are chemical compounds applied to promote plant and fruit growth. They are usually applied either through the soil or, by foliar feeding for uptake through leaves. Inorganic fertilizers are composed of simple chemicals and minerals, the major nutrients being nitrogen, phosphorous and potassium. The aim of this project is to develop a method that allows the determination of potassium in different fertilizers.

Supervisor: Jorg Bettmer

QA02B Evaluation of the content of caffeine in tea

Evaluación del contenido en cafeína en infusiones

Tea is one of the most commonly and widely used soft beverage in the household. It acts as a stimulant for central nervous system and skeletal muscles. The principal constituent of tea that is responsible for these effects is caffeine. The objective of this study is to determine the caffeine content in various tea samples.

Supervisor: Jorg Bettmer

QA03B Analysis of ethanol and other alcohols in juices

Análisis de etanol y otros alcoholes en zumos

The determination of different alcohols is relevant to the beverage industry, apparently for liquors, wines, or beers. However, alcohols, especially ethanol, can also be found in juices e.g. due to starting fermentation during storage of the fruits. Selected beverages should be analysed for their potential content of ethanol and other alcohols during this project.

Supervisor: Jorg Bettmer

QA04B Determination of β -carotene in extracts of vegetables

Determinación de β -carotenos en extractos vegetales

β -carotene, a precursor of vitamin A, possesses pronounced radical scavenging properties. It is an orange coloured pigment, which is present in many fruits and vegetables. The aim of this study is to optimize the extraction of β -carotene from selected vegetables and to finally determine its content.

Supervisor: Jorg Bettmer

QA05B Studies on the “protein corona” formed around nanoparticles

Estudio de la corona proteica formada sobre nanopartículas

Once a nanoparticle enters a biological system, it is well known that it is recognized by the organism and a so-called “protein corona” is formed around these exogenic “invaders”. Finally, the “protein corona” defines the identity of the nanoparticles within a biological system, and it is important to understand its role. Therefore, the proposed work aims to study the interaction of selected nanomaterials with the most abundant serum proteins and to identify affinity differences.

Supervisor: Jorg Bettmer



ÁREA DE QUÍMICA FÍSICA

QF01B The particle in a champagne box. Applying variational quantum chemistry.

The particle in a one-dimensional champagne box is a particle subjected to the potential $V=A \sin(\pi x/a)$, where A is a constant and a is the box length. It is one of the best known examples that illustrates the application of approximate methods in quantum chemistry. In this TFG, the student will carry out a thorough analysis of the use of variational methods to solve this problem.

Supervisor: Ángel Martín Pendás

QF02B The particle in a champagne box. Applying perturbative quantum chemistry

The particle in a one-dimensional champagne box is a particle subjected to the potential $V=A \sin(\pi x/a)$, where A is a constant and a is the box length. It is one of the best known examples that illustrates the application of approximate methods in quantum chemistry. In this TFG, the student will carry out a thorough analysis of the use of perturbation methods to solve this problem.

Supervisor: Ángel Martín Pendás

QF03B Wavefunction analysis. The molecular graph.

A molecular graph is usually drawn from a set of ad hoc rules that started with G. N. Lewis. In these recipes, electron counting, chemical intuition, and interatomic distances play a major role. To answer the question, are these two atoms bonded or not? modern quantum mechanical methods use topological methods like the quantum theory of atoms in molecules (QTAIM). An exam of the electron density of a molecular system provides a unique graph which coincides, most times, with chemical intuition. The student will learn the basics of the theory. After getting familiar with it, a number of simple molecules will be computed and analyzed through topological eyes.

Supervisor: Ángel Martín Pendás

QF04B Wavefunction analysis. Electron populations.

The wavefunction of a system contains all the information that can be obtained from a system by performing dynamical measures. In a molecular system, the total number of electrons is fixed, and is input a priori before undertaking a computation of its electronic structure. From the chemical point of view, however, knowledge of the partial charge of atoms or functional groups is important, since they provide information about electrostatic interactions with other molecules or about electrophilic or nucleophilic regions. The methods that divide the total electron population into atomic components are called population analyses. In this work, the student will get familiar with the several methods that have been proposed over the years, and will obtain the atomic charges using the quantum theory of atoms in molecules for a series of toy molecules.

Supervisor: Ángel Martín Pendás

QF05B Basis functions in computational chemistry: Analysis of the second period diatomic fluorides.

To build a wavefunction, computational chemists use one-electron functions called spinorbitals. These are expanded as linear combinations of a set of primitive functions, which is called the



basis set. Usually these primitive functions are gaussian functions for computational reasons. The basis set is known before-hand, and is selected by the user of an electronic structure code. Usually, the larger the basis set, the better the results, and the longer the computation. This means that basis sets have to be carefully selected so that a compromise between computation time and accuracy is met. In this work the student will learn the different set of basis sets found in the literature, and examine the convergence of several properties (the energy, the dipole moment, etc) as the basis set is changed in the second period diatomic fluorides.

Supervisor: Ángel Martín Pendás

ÁREA DE QUÍMICA INORGÁNICA

QI01B Reactivity of Mo(CO)₆. From Mo-Mo multiple bonds formation to ligand substitution reactions.

Reactividad de Mo(CO)₆. Formación de enlaces múltiples Mo-Mo y reacciones de sustitución de ligandos

The Mo(CO)₆ complex is a representative example of group 6 carbonyl complexes. The chemistry of this complex is highly influenced by the low oxidation state of the metallic centre and the lability of the CO ligand. The chemical versatility of this complex leads to a variety of ligand substitution reactions, and the formation of bimetallic complexes having multiple Mo-Mo bonds. In the context of this TFG project, and after a bibliography revision of the Mo(CO)₆ reactivity, student will choose few examples to prepare in the laboratory.

Supervisor: Alejandro Presa Soto

QI02B Synthesis of Nickel(0) derivatives from Ni(II) complexes

Síntesis de complejos de Niquel(0) a partir de complejos de Niquel(II)

Homogeneous nickel catalysis has continued to develop in recent years as a powerful set of tools for the construction of a wide variety of carbon-carbon and carbon-heteroatom bonds. Nickel is a low-cost, versatile, and attractive metal for use in catalytic transformations. In the context of this TFG project, and after a bibliography revision of the topic, student will choose few examples of Ni(0) complexes to prepare in the laboratory from available Ni(II) source.

Supervisor: Alejandro Presa Soto

QI03B Synthesis of manganese carbonyl complexes from Mn₂(CO)₁₀

Síntesis de complejos de manganesos usando Mn₂(CO)₁₀

Transition metals of the fourth row are abundant and cheap compared to those of the fifth and sixth rows. Therefore, by introducing new reactivities with fourth-row metal complexes, it might be possible to replace fifth- and sixth-row metals in some fundamental and important reactions. Catalytic Grignard-type addition of nucleophiles to aldehydes is one such reaction. In the context of this TFG project, and after a bibliography revision of the topic, student will choose few examples of Manganese carbonyl complexes to prepare in the laboratory from Mn₂(CO)₁₀ dimer.

Supervisor: Alejandro Presa Soto

QI04B Synthesis of mono-substituted ferrocenes

Síntesis de ferrocenos monosustituidos

Ferrocene and its derivatives possess a range of useful properties, which led to their applications in catalysis, materials science, and medicine. For instance, one of the key building blocks for incorporation of a ferrocene moiety into target structures is vinylferrocene. Vinylferrocene has been used in organic synthesis in Heck type reactions and Diels-Alder cycloadditions. In the context of this TFG project, and after a bibliography revision of the topic, student will choose few examples of mono-substituted ferrocene derivatives to prepare in the laboratory.



Supervisor: Alejandro Presa Soto

QI05B Square planar dichloropalladium(II) complexes
Complejos plano cuadrados de dicloruro de paladio(II)

Palladium complexes have found wide application as homogeneous catalysts in organic synthesis, and, accordingly, organopalladium complexes have been the subject of many mechanistic studies. In the context of this TFG project, and after a bibliography revision of the topic, student will choose few examples of square planar palladium(II) derivatives to prepare in the laboratory.

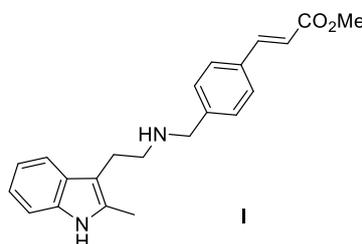
Supervisor: Alejandro Presa Soto

ÁREA DE QUÍMICA ORGÁNICA

QO01B Approximation to the synthesis of the antitumor drug panobinostat.
Preparation of the functionalized triptamine.

Aproximación a la síntesis del fármaco antitumoral Panobinostat:
Preparación de la triptamina funcionalizada.

The objective of the project is the synthesis of the substituted tryptamine **I**, [methyl (E)-3-(4-(((2-(2-methyl-1H-indol-3-yl)ethyl)amino)methyl)phenyl)acrylate], which is a key advanced intermediate in the preparation of the antitumor drug Panobinostat. The student must carry out a bibliographic search to design a proper synthesis of the target molecule from affordable starting materials, perform the synthesis in the laboratory and characterize the product.

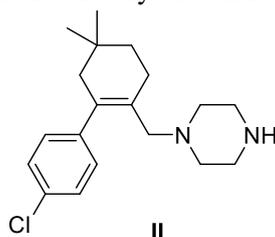


Supervisor: Carlos Valdés

QO02B En route towards the anti leukemia drug Venetoclax: Preparation of the intermediate piperazine.

En ruta hacia el fármaco antileucemia Venetoclax: Preparación de la piperazina intermedia.

The objective of this Project is the preparation of the piperazine **II**, [1-((4'-chloro-5,5-dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)methyl)piperazine], which is an intermediate in the industrial synthesis of the recently approved drug Venetoclax. The student must carry out a bibliographic search to design a proper synthesis of the target molecule from affordable starting materials, perform the synthesis in the laboratory and characterize the product.



Supervisor: Carlos Valdés

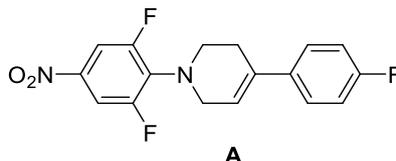
**QO03B Non stabilized diazo alkanes: Synthesis and reactivity of 4-diazo-1,1-dimethylcyclohexane*****Diazoalcanos no estabilizados: Síntesis y reactividad del 4-diazo-1,1-dimetilciclohexano***

Diazo alkanes are highly useful, yet unstable synthetic intermediates. The purpose of this project is to prepare 4-diazo-1,1-dimethylcyclohexane as an example of a non stabilized diazo alkane and subsequently trap the unstable intermediate through a proper C-C bond forming reaction. The student must carry out a bibliographic search to find the most convenient way to generate the diazo alkane from affordable materials and with the equipment available in the practice laboratory, and select a proper C-C bond forming reaction to trap the generated compound. Then, the selected experiments must be performed in the lab and the products characterized.

Supervisor: Carlos Valdés

QO4B 4-Aryltetrahydropyridines in medicinal chemistry. Synthesis of a precursor of the drug Priventasvir***4-Ariltetrahidropiridinas en química médica. Preparación de un precursor del fármaco Priventasvir***

The objective of this Project is the preparation of the tetrahydropyridine **A** (1-(2,6-difluoro-4-nitrophenyl)-4-(4-fluorophenyl)-1,2,3,6-tetrahydropyridine), which is an intermediate in the synthesis of Priventasvir, a new drug against Hepatitis B. The student must carry out a bibliographic search to design a proper synthesis of the target molecule from affordable starting materials, perform the synthesis in the laboratory and characterize the product.



Supervisor: Carlos Valdés

QO5B Multicomponent reactions in the generation of molecular diversity: application of the Ugi reaction in the synthesis of isoquinolines.***Reacciones multicomponentes en la generación de diversidad molecular: aplicación de la reacción de Ugi en la síntesis de isoquinolinas.***

The Ugi reaction is a four component reaction widely used for the generation of molecular diversity. The goal of this project is the preparation of isoquinolines through a synthetic route that will include a proper Ugi reaction followed by a subsequent cyclization step. The student must select a procedure based on the literature that will enable the synthesis of a set of isoquinolines, perform in the lab the synthesis of various derivatives and characterize the products.

Supervisor: Carlos Valdés