

# Resúmenes de la Primera Jornada del Grupo de Catálisis de la Universidad Pedagógica y Tecnológica de Colombia (GC-UPTC)

Conference proceedings of the first meeting on Catalysis of the Pedagogical and Technological University of Colombia

Carlos Cifuentes-Espitia<sup>1</sup>, Jaime Portilla<sup>2</sup> Ximena Aguilera<sup>3</sup>, Laura Barbelli<sup>3</sup>, D. Lick<sup>3</sup>, M. Casella<sup>3</sup>, L. Pizzio<sup>3</sup>, M. Murguía<sup>4</sup>, Eliana Nope<sup>1</sup>, Gabriel Sathicq<sup>1</sup>, G. Romanelli<sup>3</sup>, M. Hernández-Laverde<sup>1</sup>, M.C. Hidalgo<sup>4</sup>, J.A. Navío<sup>4</sup>, Andrés Álvarez<sup>1</sup>, Diana Santos<sup>1</sup>, M.A. Gil<sup>1</sup>, J.S. Hernández<sup>1</sup>, P. Valencia<sup>1</sup>, J.S. Hernández<sup>2</sup>, Daniela Barrera<sup>1</sup>, Cristian Castillo<sup>1</sup>, Valentina Coca<sup>1</sup>, Jhoan Miguel Camargo López<sup>1</sup>, Luna López Rodríguez<sup>1</sup>, Alejandra Rodríguez Montaña<sup>1</sup>, Mauricio Pineda Corredor<sup>1</sup>, Juan Alejandro Pérez Aguilar<sup>5</sup>, Ricardo Benítez Benítez<sup>6</sup>

## Resumen

Se presentan los resúmenes de la primera Jornada de Catálisis de la Universidad Pedagógica y Tecnológica de Colombia. Esta conferencia permitirá en poco tiempo potencializar la apropiación social del conocimiento en esta área de la ciencia a nivel regional, brindando oportunidades para que los participantes expongan sus trabajos, y facilitando la difusión del conocimiento científico en esta área.

**Palabras clave:** Síntesis orgánica, Fotocatálisis, Catálisis heterogénea, Biocatálisis.

## Abstract

The conference proceedings of the first meeting on Catalysis of the Pedagogical and Technological University of Colombia are presented. This conference will be allowed in short time to potentiate the social appropriation of knowledge in this area of science at the regional level, providing opportunities for participants to present their work, and facilitating the dissemination of scientific knowledge.

**Keywords:** Organic synthesis, Photocatalysis, Heterogeneous catalysis, Biocatalysis.

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<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

<sup>2</sup> Bioorganic Compounds Research Group, Department of Chemistry, Universidad de los Andes, Carrera 1 No. 18A-10, Bogotá, Colombia

<sup>3</sup> Centro de Investigación y Desarrollo en Ciencias Aplicadas "Dr. Jorge J. Ronco" (CINDECA-CCT La Plata-CONICET-CIC-PBA), Universidad Nacional de La Plata, Calle 47 No 257, B1900AJK La Plata, Argentina.

<sup>4</sup> Laboratory of Applied Chemistry. Faculty of Biochemistry and Biological Sciences. National University of the Litoral (UNL). Ciudad Universitaria, (3000) Santa Fe, Argentina

<sup>5</sup> Instituto de Ciencia de Materiales de Sevilla (ICMS), Centro Mixto Universidad de Sevilla-CSIC, Américo Vespucio 49, 41092 Sevilla, Spain

<sup>6</sup> Química de Productos Naturales, Universidad del Cauca, Joven Investigador, Maestría en Bioingeniería, Popayán, Colombia.

<sup>6</sup> Química de Productos Naturales, Departamento de Química, Universidad del Cauca, Popayán, Colombia

## 1. Organic synthesis assisted by catalysis

### 1.1. N-Arylation of azoles with arynes produced by o-silylaryl triflates

Carlos Cifuentes-Espitia<sup>1</sup>, Jaime Portilla<sup>2</sup>

<sup>1</sup> *Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

<sup>2</sup> *Bioorganic Compounds Research Group, Department of Chemistry, Universidad de los Andes, Carrera 1 No. 18A-10, Bogota, Colombia*

[carlos.cifuentes@uptc.edu.co](mailto:carlos.cifuentes@uptc.edu.co)

In this work, we describe the time-efficient synthesis of diverse N-arylazoles in good yields and high regioselectivity through a metal-free N-arylation reaction of azoles and o-(trimethylsilyl)aryl triflates under mild reaction conditions. Remarkably, some structures were studied and confirmed by single-crystal X-ray diffraction

### 1.2. Solvent and catalysis-free microwave transesterification of $\beta$ -ketoesters and its application in the production of potential antitumor dihydropyrimidinones (thiones)-fatty acids derivatives

Ximena Aguilera<sup>1</sup>, Laura Barbelli<sup>1</sup>, D. Lick<sup>1</sup>, M. Casella<sup>1</sup>, M. Murguía<sup>2</sup>, L. Pizzio<sup>1</sup>, and G. Romanelli<sup>1</sup>

<sup>1</sup> *Centro de Investigación y Desarrollo en Ciencias Aplicadas “Dr. Jorge J. Ronco” (CINDECA-CCT La Plata-CONICET-CIC-PBA), Universidad Nacional de La Plata, Calle 47 No 257, B1900AJK La Plata, Argentina.*

<sup>2</sup> *Laboratory of Applied Chemistry. Faculty of Biochemistry and Biological Sciences. National University of the Litoral (UNL). Ciudad Universitaria, (3000) Santa Fe, Argentina*

In this work, we report a study of the transesterification reaction of  $\beta$ -ketoesters in solvent-free conditions and in the absence of a catalyst, using microwave radiation. Different alcohols including

fatty alcohols were tested in order to optimize the reaction conditions. Good yields, without formation of secondary products, were observed at 130 °C, in periods of time that did not exceed 3 h, using microwave irradiation. The compounds obtained were used as starting substrates in a Biginelli-type multicomponent synthesis to obtain 3,4-dihydropyrimidin-2(1H)-ones (thiones) C-5 and C-8 long chain ester derivatives, at 80 °C in solvent-free condition using bulk tungstophosphoric as catalyst. Several DHP-derivatives were obtained in about 4 h, with a yield greater than 50%.

### 1.3. Microwave assisted multicomponent synthesis of chromenes with magnetic hydrotalcites as bifunctional catalysts

Eliana Nope<sup>1</sup>, Gabriel Sathicq<sup>1</sup>, G. Romanelli<sup>1</sup>.

<sup>1</sup> *Centro de Investigación y Desarrollo en Ciencias Aplicadas “Dr. Jorge J. Ronco” CINDECA – Facultad de Ciencias Exactas – Universidad Nacional de La Plata, 47 N° 257, La Plata 1900, Argentina.*

[eliana.nope@quimica.unlp.edu.ar](mailto:eliana.nope@quimica.unlp.edu.ar)

Magnetic hydrotalcites (Fe<sub>3</sub>O<sub>4</sub>-LDH) were synthesized as bifunctional catalysts for the microwave-assisted multicomponent synthesis of chromene derivatives under solvent-free conditions. The synthesis of the materials was carried out by the coprecipitation method incorporating divalent metal cations such as Ni<sup>2+</sup> and Co<sup>2+</sup> in LDH-Mg and combining them with Fe<sub>3</sub>O<sub>4</sub> nanoparticles. The characterization results show that the combination with Fe<sub>3</sub>O<sub>4</sub> significantly improves the textural properties of hydrotalcite. This multicomponent protocol allows obtaining chromene derivatives with excellent yields in short reaction times, with high atomic economy and operational simplicity, in addition, the catalytic activity of these materials is maintained without appreciable loss of their properties in five reaction cycles, allowing this protocol sustainable and advantageous compared to conventional methods.

#### 1.4. R-(+)-Limonene diastereoselective epoxidation using dimeric racemic Jacobsen's catalyst and in-situ generated dimethyldioxirane as oxidant agent

Juan A. Rubio Rodríguez<sup>1</sup>

<sup>1</sup>Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[juan.rubio01@uptc.edu.co](mailto:juan.rubio01@uptc.edu.co)

The present work aim to show the results from the diastereoselective epoxidation of R-(+)- limonene using dimeric Jacobsen's catalyst and in-situ generated dimethyldioxirane (DMD) as an oxidizing agent. The optimized reaction conditions yielded values of conversion, diastereomeric excess (d.e) and diastereomeric yield excess (d.e.y) to majority diastereomer (cis-(+)-1,2-limonene oxide) of 96%, 77% and 71.7%, respectively.

#### 1.5. Synthesis of functionalized 2(1H)-pyridones with potential antitumor activity

Diana Hurtado-Rodríguez<sup>1</sup>

<sup>1</sup> Grupo de Catálisis de la UPTC, Escuela de Ciencias Químicas, Universidad Pedagógica y Tecnológica de Colombia, Avenida Central del Norte 39-115, Tunja, Colombia

In this work, we describe the solvent-free three-component synthesis of 2-oxo-1,2-dihydropyridine-3-carbonitrile derivatives in good yields and short reaction times. Some structures were studied and confirmed by single-crystal X-ray diffraction. Importantly, two compounds exert remarkable antitumor activity against MDA-MB-231 breast, OVCAR-4 ovarian, and SF-295 CNS cancer cell lines with %GI in the range of 92–99%.

#### 1.6. Obtaining furfural from xylose by heterogeneous catalysis

Cristian Fernando Gonzalez Supelano<sup>1</sup>

<sup>1</sup> Grupo de Catálisis de la UPTC, Escuela de Ciencias Químicas, Universidad Pedagógica y Tecnológica de Colombia, Avenida Central del Norte 39-115, Tunja, Colombia

The conversion of xylose to furfural was studied by testing different heterogeneous catalysts. The Preyssler heteropolyacid was the most efficient. Under optimal reaction conditions, the xylose was converted to furfural with a 70% yield in a short times using DMSO as a solvent at 170°C. The catalyst showed good catalytic activity after 4 reuses.

#### 1.7. Bibliographic review of the use of residual biomass in South America

Camila Alejandra Rosas Mateus<sup>1</sup>

<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[camila.rosas@uptc.edu.co](mailto:camila.rosas@uptc.edu.co)

The use of residual biomass (BR) will contribute to solving environmental problems, since it is considered an alternative energy source to fossil fuels. For this reason, a bibliographic review of the use of BR in South America was carried out. Brazil, Colombia and Ecuador were the countries with the largest number of BR sources and have also made better use of them.

## 2. Photocatalysis

### 2.1. Self-cleaning photocatalytic surfaces for the elimination of enteric bacteria

M. Hernández-Laverde<sup>1</sup>, M.C. Hidalgo<sup>2</sup>, J.A. Navío<sup>2</sup>.

<sup>1</sup> *Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

<sup>b</sup> *Instituto de Ciencia de Materiales de Sevilla (ICMS), Centro Mixto Universidad de Sevilla-CSIC, Américo Vespucio 49, 41092 Seville, Spain*

[monica.hernandez@uptc.edu.co](mailto:monica.hernandez@uptc.edu.co)

The ingestion of water and food contaminated with pathogenic bacteria are the main cause of foodborne diseases and acute diarrheal disease in developing countries. Photocatalytic surfaces are proposed in this work as alternative for the elimination the E. coli and total coliforms. The photocatalytic materials have been synthesized by sol-gel method, and the substrates to be coated with them by dip-coating technique were glass, marble, and 304 stainless steel.

### 2.2. Photocatalytic degradation of 4-chlorophenol using NiO/TiO<sub>2</sub>-F heterostructured materials

Andrés Álvarez<sup>1</sup>, Diana Santos<sup>1</sup>

*Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

[andres.alvarez03@uptc.edu.co](mailto:andres.alvarez03@uptc.edu.co)

The photocatalytic behavior of NiO/TiO<sub>2</sub>-F heterostructured materials in the degradation of the 4-chlorophenol (4CP) was evaluated. The physicochemical characterization of the materials confirmed the formation of p-n type heterojunctions between the semiconductors, which favored the

effective separation of charge carriers, promoting an increase in photoactivity. In addition, it was shown that a NiO content of 1.0% wt. is optimal for the degradation of 4CP.

### 2.3 AOPS and biological treatment for industrial wastewater

M.A. Gil<sup>1</sup>, J.S. Hernández<sup>1</sup>

<sup>1</sup> *Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

[mariana.gil@uptc.edu.co](mailto:mariana.gil@uptc.edu.co)

In this study photocatalysis by TiO<sub>2</sub> and UV-H<sub>2</sub>O<sub>2</sub> complemented with microbiological treatment, were employed for industrial effluents recovering. The photocatalytic treatment was able to reduce the heavy metals content, and also was obtained 99.7% of enteropathogenic bacteria elimination. In addition, during the microbiological treatment, 42.0% of Total organic Carbon was removed, thus showing a synergistic effect between both treatments.

### 2.4. Heavy metals removal from industrial wastewater by Advanced Oxidation Processes. Case of study: treated wastewater recycling for pastures irrigation

P. Valencia<sup>1</sup>, J.S. Hernández<sup>2</sup>

<sup>1</sup> *Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

[tatiana.valencia@uptc.edu.co](mailto:tatiana.valencia@uptc.edu.co)

Industrial wastewater is involved in the natural water sources pollution, in developing countries. This water is usually employed for crop irrigation

without any previous treatment, which has a negative impact for human and animal health. In order to solve this problem, in this work industrial wastewater was treated by AOPs, thus, photo-fenton and H<sub>2</sub>O<sub>2</sub>/UV-Vis combination shows the best performance as potential treatments for water recovering and employed in crop irrigation.

### 2.5. Evaluation of the photocatalytic reduction of 2,4-dinitrophenol using NiO supported on laminar materials

Daniela Barrera<sup>1</sup>

<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[laura.barrera10@uptc.edu.co](mailto:laura.barrera10@uptc.edu.co)

Nitroaromatic compounds as 2,4-dinitrophenol (2,4-DNP) are one of the most common contaminants that can be found in wastewater effluents from industry. 2,4-DNP is widely used for the manufacture of phytosanitary supplies, dye and in the preservative industry. The photocatalytic reduction of this pollutant is a topic of interest for applications in green chemistry. In the present study, NiO/MgAl materials were synthesized by co-precipitation method and evaluated in the photoreduction of 2,4-DNP employed sodium sulfite as sacrificial agent.

## 3. Biocatalysis

### 3.1. Evaluation of solid state fermentation conditions from postharvest residues using *B. subtilis* and *L. rhamnosus*

Alejandra Rodríguez Montaña<sup>1</sup>

<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[alejandra.rodriguezmontana@uptc.edu.co](mailto:alejandra.rodriguezmontana@uptc.edu.co)

The residual biomass of the corn chaff is generally consumed as fuel for the burners of the mills themselves or wasted in other minor uses. In this work, the use of corn chaff generated as lignocellulosic waste was proposed to develop a food with high nutritional value, quality and easy to digest by animals using solid state fermentation as a biotechnological tool.

### 3.3. Hidrólisis enzimática de tallos residuales de *Cannabis sativa* medicinal para la producción de azúcares reductores.

Juan Alejandro Pérez Aguilar<sup>1</sup>, Ricardo Benítez Benítez<sup>2</sup>

<sup>1</sup> Química de Productos Naturales, Universidad del Cauca, Joven Investigador, Maestría en Bioingeniería, Popayán, Colombia,

<sup>2</sup> Química de Productos Naturales, Departamento de Química, Universidad del Cauca, Popayán, Colombia, [rbenitez@unicauca.edu.co](mailto:rbenitez@unicauca.edu.co).

[alejandp@unicauca.edu.co](mailto:alejandp@unicauca.edu.co).

Se determinó la composición química de tallos residuales de *Cannabis*, se encontró contienen 45,56% de celulosa y 12,08% de hemicelulosa. El

pretratamiento termoquímico con hidróxido de sodio seguido de la hidrólisis con las enzimas Celluclast® 1.5 L y Cellic® CTec3 a 20 UPF/ g de biomasa produce 28,59 mg/mL y 24,94 mg/mL de azúcares reductores respectivamente. El aumento de la carga enzimática no aumentó la producción.

### 3.4. Bioplastics from protein isolates of sweet granadilla seeds (*Passiflora ligularis*)

Mauricio Pineda Corredor<sup>1</sup>

<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[mauricio.pineda@uptc.edu.co](mailto:mauricio.pineda@uptc.edu.co)

This work determined the moisture (35.8%), ash (2.6%), crude fat (20.1%) and crude protein (10.40%) from sweet granadilla seeds. By solubility curve, the isoelectric (pH=2) and solubility (pH=8) points of the proteins contained were obtained. The protein was isolated and its water retention capacity (2.17 mL/g) and fat retention capacity (1.78 mL/g), foaming capacity (37.5%) and emulsifying capacity (38.3%) were obtained. Finally, the method for bioplastics making from proteins was standardized using albumin as a control.

## 4. Heterogeneous catalysis

### 4.1. Nanoparticulate catalytic systems as potential materials for hydrogen production from acetic acid decomposition

Cristian Castillo<sup>1</sup>

<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[cristian.castillo04@uptc.edu.co](mailto:cristian.castillo04@uptc.edu.co)

The present research in development was focused on obtaining and characterize physicochemically (DRX, XPS, Raman, TEM, TPD-NH<sub>3</sub>, N<sub>2</sub>-physisorption and DRIFTS) nanoparticulate bare and supported on Al<sub>2</sub>O<sub>3</sub> catalytic systems based on zerovalent iron (NZVI), which are visualized as potential materials for hydrogen production from acetic acid decomposition as an alternative method with less environmental impact.

### 4.2. Comparison of the catalytic activity of Mg(OH)<sub>2</sub> and MgO materials in the Knoevenagel condensation reaction

Valentina Coca<sup>1</sup>

<sup>1</sup> Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.

[diana.coca01@uptc.edu](mailto:diana.coca01@uptc.edu)

Knoevenagel condensation is one of the more significant reactions to obtain products and intermediates in pharmaceutical and polymer synthesis. In this work, the condensation of 5-hydroxymethylfurfural with malononitrile using MgO and Mg(OH)<sub>2</sub> prepared by co-precipitation and sol-gel methods was studied. The physicochemical properties of the catalysts were



determined to evaluate the behavior of these materials and correlate with their catalytic activity.

can be economic catalysts in catalytic hydrochlorination of diclofenac.

#### **4.3 Production of activated carbons use metal chlorides as activating agents from waste biomass for CO<sub>2</sub> adsorption**

Jhoan Miguel Camargo López<sup>1</sup>

<sup>1</sup> *Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

[jhoan.camargo@uptc.edu.co](mailto:jhoan.camargo@uptc.edu.co)

Carbonaceous materials were obtained from soursop seeds, as the precursor material. The effect of the CaCl<sub>2</sub> and MgCl<sub>2</sub> as activating agents was studied. Surface areas between 200 and 500 m<sup>2</sup>g<sup>-1</sup> were obtained and these values is strongly related with the chemical characteristics associated type of activating agent as heating ramp employed, which causes a distinct affinity with the adsorbate.

#### **4.4. Synthesis of nZVI from cypress pine for possible application in catalytic hydrodechlorination of diclofenac**

Luna López Rodríguez<sup>1</sup>

<sup>1</sup> *Grupo de Catálisis. Universidad Pedagógica y Tecnológica de Colombia UPTC, Avenida Central del Norte, Tunja, Boyacá, Colombia.*

[luna.lopez@uptc.edu.co](mailto:luna.lopez@uptc.edu.co)

In this work, an extract from Cupressus sempervirens leaves was employed as a reducing agent for obtaining zerovalent iron nanoparticles (nZVI). The materials were characterized by distinct techniques as XRD, XPS, and TEM. These materials