

C-1 ELECTRONIC AND MOLECULAR STRUCTURE OF BIS (N-R-SALICYLALDIMINATE) AND BIS (N-R-NAPHTHYLALDIMINATE) CU(II), R=H, Me, Et, n-Pr, Iso-Pr, n-Bu, iso-Bu, sec-Bu, tert-Bu.

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An intriguing feature of many bis-bidentate Schiff bases is that Cu(II) when coordinating adopt a pseudotetrahedral geometry. Here we present calculated Cu(II)-Schiff bases complexes where the nitrogen of the ligands binds to H, Me, Et, nPr, isoPr, nBu, isoBu, sec-Bu and tert-Bu to evaluate the effect of the change of these substituents in both of these systems.

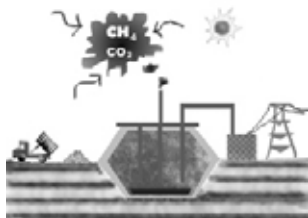
C-2 THE Os-Os INTERACTION IN H₂O₃(CO)₁₀ IS NOT A DOUBLE BOND!

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The H₂O₃(CO)₁₀ possesses a particular chemical behaviour since the electron counting rules assigns 46 valence electrons to the structure. This electron deficiency has been invoked to propose the binding in this cluster is similar to B₂H₆ (4c-2e). However has been suggested the formation of a double metal-metal bond or a metal-metal interaction mediated by the bridging atoms. Here a study of the nature of the bonding in this structure and of its ruthenium analogue, based on an analysis of the electron density is presented, using densities obtained by DFT calculations with the deMon2k code. Also a topological analysis of the s and t dimensionless gradients is presented

C-3 ESTIMACIÓN DE LA PRODUCCIÓN DE METANO EN RELLENO SANITARIO: UNA APROXIMACION DINÁMICA Y FRACTAL. Claudia Aranda De la Teja y Armando

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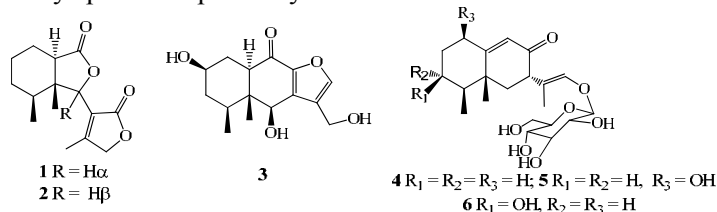


Landfill operation implies waste compaction, and leachate reduction, giving unsaturated flow conditions into a tortuous medium, mostly solid, and unstirring, i.e. a very heterogeneous reaction medium. Traditionally, models to predict methane production consider a total conversion in a homogeneous medium, unsustainable hypothesis in the landfill context. This study presents a model that considers the evolution of the microbiota causing the solid fermentation, and its effect on the kinetic of methane production in a low dimensional medium.

C-4 EREMOPHILANE DERIVATIVES FROM PITTOCAULON VELATUM.

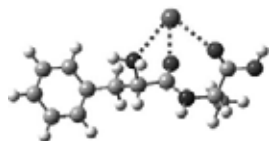
Amira Arciniegas,* Karina González, Ana-L. Pérez-Castorena, Alfonso Romo de Vivar. Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Coyoacán 04510, México, D.F.

Two *seco*- γ,γ -eremophiladiolides (**1,2**), one trihydroxyfuraneremophilane (**3**) and three eremophilane glucosides (**4-6**) were isolated from *Pittocaulon velatum*, together with several known compounds. The structures of these compounds were elucidated by spectroscopic analysis and chemical reactions.



C-5 SYNTHESIS OF SOME L- α -DIPEPTIDE-BISMUTH (III) COMPLEXES AS POTENTIAL ANTIMICROBIAL AGENTS.

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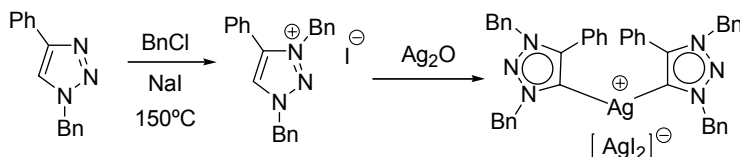


The antibiotic resistance is now a major clinical problem all over the world; more infectious stages are difficult to manage clinically. The antibacterial and antifungal activity of several metal complexes of amino acids, dipeptide and peptides, places them as a good alternative for the development of new antibiotics. However, to date there are no reports of possible antimicrobial activity of dipeptide- Bi (III) complexes. So, in the present work, we synthesized a series of ten L- α -dipeptides and their Bi (III) complexes, to evaluate their antibacterial activity.

C-6 GENERACIÓN DE UNA SAL DE 1,2,3-TRIAZOLONIO POR BENCILACION DIRECTA DE 1,2,3-TRIAZOLES 1-SUSTITUIDOS.

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Se presenta un nuevo procedimiento para la generación de sales de 1,2,3-triazolonio, haciendo reaccionar el 1-bencil-4-fenil-1,2,3-triazol con una mezcla de cloruro de bencilo y yoduro de sodio. La sal de triazolonio formada se hizo reaccionar con óxido de plata para formar un complejo carbénico con posibles aplicaciones en procesos catalíticos.



C-7 PROCEDIMIENTO PARA LA ESPECIACIÓN DE ARSÉNICO EN AGUAS SUBTERRÁNEAS.

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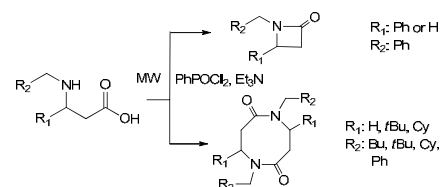
Se presenta la metodología para la separación y cuantificación de las especies del arsénico (III) y (V) utilizando la técnica de cromatografía iónica, la cual se aplicará para la determinación selectiva de las especies del arsénico en muestras de agua subterránea del Municipio de Tezoyuca, Morelos donde se han reportado concentraciones totales de arsénico por arriba de la norma oficial mexicana. La metodología desarrollada utilizó como fase móvil ácido hidroxibenzoico (ajustado a pH de 8.5 con hidróxido de sodio). Se realizó una curva calibración tomando en cuenta los valores por la NOM. (Límite máximo de As 0.025 mg/).

C-8 SYNTHESIS OF CYCLO- β -PEPTIDES USING MICROWAVES.

Luis Gabriel Hernández Vázquez, Jaime Escalante García

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In nature exist less β -amino acids than its α -analogous, while α -amino acids are part of proteins, some β -amino acids are part of construction blocks of natural peptides and antibiotics. In last years, researchers were focused on lineal peptides, leaving cyclo- β -peptides aside. Our research group has been worked with β -amino acids derivatives and now we evaluated the microwaves on β -amino acids to form cyclo- β -peptides.



C-9 DL-FLUOROBENZENAMIDES ANTICONVULSANTS

Hernández M Miguel Angel,¹ Bolaños V Llanet,¹ Jiménez H Marcos,¹ Peralta A Belen,¹ Peralta C Javier,² Meza T Sergio Enrique.¹ Departamentos de Bioquímica¹ y Química Orgánica², Escuela Nacional de Ciencias Biológicas, IPN. DL-HEPA (1), DL-HEPP (2) and DL-HEPB (3) protected mice against seizures induced by pentylenetetrazol, bicuculline, 4-aminopyridine and maximal electroshock. They also protected cats and rats against hippocampal kindling. Furthermore, DL-HEPP protected rats against the γ -aminobutyric acid withdrawal syndrome, a model of focal epilepsy, which shows an extraordinary resistance to the classic antiepileptics. In previous studies, incorporation of fluorine, chlorine or bromine in the phenyl ring of 1, 2 and 3 increased their anticonvulsant activity. It appears that the enhancement of the anticonvulsant activity of compounds 1, 2 and 3 could be related to the presence of a hydrophobic site in their receptor. Accordingly, it may be possible that the incorporation of trifluoromethyl groups in the phenyl ring of 1, 2 and 3 could lead to an increase in their anticonvulsant activity. In this work, we describe the synthesis and anticonvulsant activity of some DL-Fluorobenzenamides.

C-10 STRUCTURAL RELAXATION BEHAVIOR OF AMORPHOUS SOLIDS: EFFECT OF RESIDUAL WATER ON MOLECULAR MOBILITY. Enrique Lemus Fuentes.

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This work contributes to the understanding of the phenomena of phase transition in amorphous materials, obtaining an exact and general relation for the density of vibrational states registered during the glass transition. Moreover, the results indicate that this ansatz is a major improvement with respect to those obtained with Debye's and Einstein's models. The mechanistic understanding of the phenomena of stability in terms of the density of vibrational states has added further value to the use of heat capacity data as a rapid means to characterize the molecular mobility in amorphous solids.

C-11 ALUMINOSILICATE STRUCTURES DESIGNED TO TRAP ORGANIC DYES

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We synthesized via the sol-gel process three amorphous aluminosilicates having the stoichiometry of Zeolites Type A, X, Y, respectively. The aluminosilicate so-called SX, having the chemical composition of Faujasite X, proved to be amorphous in the range 298 K up to 1273 K. The anionic organic dye 1,2-Dihydroxyanthraquinone (Alizarine, AL) was successfully encapsulated in the aluminosilicate matrix SX. On the other hand, 7, α -D-glucopyranosil-9,10-dihydro-3,5,6,8-tetrahydroxy-7-methyl-9,10 dioxanthracene Carboxylic acid (carminic acid, CA) could only be deposited on the matrix surface. The adsorbents and the Dye impregnated matrices were characterized using several techniques: FTIR and diffuse reflectance Spectroscopies, Small Angle X-ray Scattering, nitrogen physisorption and X-ray diffraction (XRD).

C-12 DEVELOPMENT (WITH X-RAY CHARACTERIZATION) OF AMIDES AZAHETEROCYCLE CLOFIBRIC WITH POTENTIAL EFFECT ON METABOLIC SYNDROME. Alaniz Palacios Alfredo,

¹ Tlahuext Hugo, ² Gabriel Navarrete-Vázquez¹

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Hybridization represents an alternative to complex conditions involving more than a physiological alteration. The formation of amides is the ground of this work, the union of two pharmacophore, where the first, which is the constant to whole series, is an agonist PPAR α ; to clinical use (clofibrate), used as clofibric acid and the second is a selective inhibitor of the enzyme 11 β -HSD Type I, in form to 2-amine-6-replaced- benzothiazole. Steglich's synthesis, yielded seven molecules of this project with reaction times of between two and twenty four hours. The results of x-ray diffraction showed the influence of substituents on the bond angle of the carbon atom located between the ether and carbonyl to pharmacophore agonist PPAR α . This implies a different 3-D array, due to the presence of the substituent. In terms bioactivity involves different lengths and different degrees of ligand-receptor interaction.

C-13 *IN SILICO* ASSESSMENT OF ANTIDIABETIC AND ANTI-OBESITY EFFECT OF HYBRID THIAZA-HETEROCYCLES. Vicente Fabian Kuyoc Carrillo, Gabriel Navarrete-Vázquez*. Facultad de Farmacia, Universidad Autónoma del Estado de Morelos, Cuernavaca, Morelos, México.

According to the predictions of the bioactivities calculated with PASS (Prediction of Activity Spectra for Substances), we found that 8 designed thiaza-heterocycles, which are hybrids from glitazone and arylsulfonamides, have good antidiabetic activities and medium antiobesity effects (Table). On the other hand, we found that compounds could have a good oral absorption according to the values of the Lipinski rule. The identification of the metabolic sites with the program Metasite 3.0.4, provides a useful tool in drug design, in order to modify and prevent possible inactivation or changes of its original activity due to phase I biotransformations.

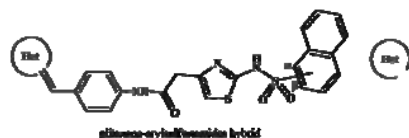
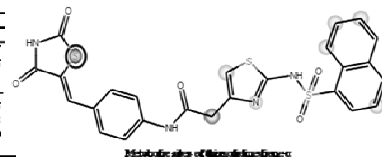


Table 1. Prediction of activities using the PASS program.

Comp	Pos	Het	Antidiabetic		Antiobesity	
			Pa	Pi	Pa	Pi
1	x	Thiazolidine	0.746	0.064	0.431	0.017
2	x	Thiazole	0.052	0.065	0.453	0.015
3	x	Barbituric acid	0.472	0.012	0.324	0.291
4	x	Thiothiazolidine	0.429	0.015	—	—
5	3	Thiazolidine	0.771	0.064	0.453	0.015
6	3	Barbituric acid	0.694	0.065	0.471	0.013
7	3	Barbituric acid	0.511	0.065	0.365	0.039
8	3	Thiothiazolidine	0.477	0.012	—	—

Pa - probability of activity Pi - probability of inactivity



C-14 DESIGN AND *IN SILICO* ASSESSMENT OF 5-NITROINDAZOLE-SARTAN HYBRIDS: POTENTIAL ANGIOTENSIN II AT1 RECEPTOR ANTAGONISTS.

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Using medicinal chemistry criteria, we designed a series of hybrid 5-nitroindazole and sartan compounds, implementing an isosteric replacement in the acid group of sartan (carboxyl, tetrazole and imidazoline). The compounds were prepared from 5-nitroindazole and 4'-bromomethyl-2-biphenylcarbonitrile. Compounds were evaluated *in silico* using PASS software (Prediction of the spectrum of bioactivity substances). Predictions obtained by PASS were found to possess AT1 antagonist activity ($P_a \geq 0.4$ vs $P_i \leq 0.002$), also the compounds exhibited vasorelaxing activity predictions by inhibiting phosphodiesterase 5 enzyme (PDE-5) and antianginal activity. The *in silico* data show that molecules designed with a high probability of showing antagonist activity of angiotensin II receptors, and inhibition of PDE-5.

C-15 ELECTROCHEMICAL IMPEDANCE FOR STUDYING THE CORROSION MECHANISMS OF AN EXPERIMENTAL AlMgZn ALLOY

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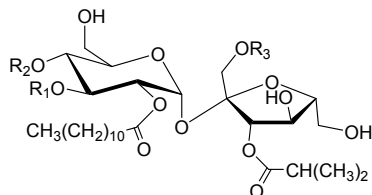
The Electrochemical Impedance (IE) applies to evaluation of the electrochemical behavior of interface electrode electrolyte and is useful for phenomena interpretation of processes like electrocatalysis, corrosion, or coatings behavior on metal substrates. This work focuses on the use of electrochemical impedance for analyzing the corrosion mechanisms of AlMgZn alloy by thermic treatment (aging). The tests were performed in NaCl to 3.5 % to determine possible application as a sacrificial anode.

C-16 ACYLSUCROSES FROM *PHYSALIS SOLANACEUS*.

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Separate chemical studies of fruits, calices and roots of *Physalis solanaceus* afforded three new (**1** - **3**) and one known (**4**) acylsucroses. In addition, other known compounds were isolated and steroidal derivatives of the physalin group were detected.



- 1 $R_1 = (\text{CH}_3)_2\text{CHCH}_2\text{CO}$ $R_2 = R_3 = \text{H}$
- 2 $R_1 = R_2 = (\text{CH}_3)_2\text{CHCH}_2\text{CO}$ $R_3 = \text{H}$
- 3 $R_1 = (\text{CH}_3)_2\text{CHCH}_2\text{CO}$ $R_2 = \text{H}$ $R_3 = (\text{CH}_3)_2\text{CHCO}$
- 4 $R_1 = (\text{CH}_3)_2\text{CHCO}$ $R_2 = R_3 = \text{H}$

C-17 TERPENOIDS AND OTHER CONSTITUENTS FROM *CROTON NIVEUS*, *SAPIUM LATERIFLORUM* AND *S. MACROCARPUM* (EUPHORBIACEAE)

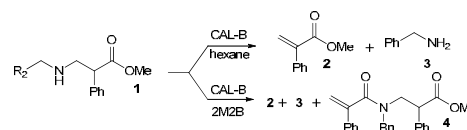
C. Ileana Reyes-Hernández,¹ Paola Bravo,² Marcela Aguiar,² Verónica Rosero,² Blanca M. Reyes,¹ Guillermo Delgado.¹ ¹Instituto de Química, Universidad Nacional Autónoma de México. Circuito Exterior, Ciudad Universitaria. México, D.F. ²Facultad de Ciencias Químicas, Universidad Central del Ecuador, Quito, Ecuador. In continuation with our research seeking bioactive secondary metabolites from species belonging to the Euphorbiaceae family, several known compounds including sitostenone, lupeol, lupenone, vomifoliol, β -sitosterol, and β -sitosteryl β -D-glucopyranoside were isolated from *S. lateriflorum* and *S. macrocarpum*. Cajucarinolide and three rosadien-type diterpenes were characterized from the branches of *C. niveus*. The structures were elucidated by spectroscopic and X-ray analyses, and the absolute configuration of the diterpenes was determined by circular dichroism. The rosadienes displayed moderate cytotoxicity against several human tumor cell lines.

C-18 RETRO-MICHAEL ADDITION (RMA) CATALYZED BY CAL-B

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CaL-B catalyzes the retro-Michael addition (RMA) for β^2 -methyl 3-(benzylamine)-2-phenylpropanoate (**1**) in hexane to obtain its precursors α,β -unsaturated ester (**2**) and benzylamine (**3**). When the reaction was carried out in 2-methyl-2-butanol (2M2B) or with more quantity of enzyme, also was observed the α,β -unsaturated product (**4**).



C-19 CUANTIFICACIÓN DE METANO EN EL TIRADERO TLATEL XOCHITENCO, MUNICIPIO DE CHIMALHUACÁN, ESTADO DE MÉXICO

Efrain Rojas Merino,¹ Ruth Esther Villanueva Estrada,² Pedro Villanueva González,³ Claudia Arango,² Jazmín Rentería Martínez,² Dayan Rodríguez Torres.²

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Se diseñó una cámara para coleccionar el biogas producido en el tiradero Tlatel Xochitenco. La cámara se construyó utilizando placas de acrílico de 5 mm. de espesor, con dimensiones de 30x30x20 cm. Comprende un puerto (válvula) cuya función es permitir la toma de muestra, un termómetro y manómetro para poder medir la velocidad real de las emisiones en el tiradero y así calcular la tasa de crecimiento.

C-20 HIDRODESTILACION ASISTIDA POR MICROONDAS DEL ACEITE ESENCIAL DE *CLINOPODIUM LAEVIGATUM* Y *BACCHARIS HETEROPHYLLA*

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La hidrodestilación es uno de los métodos más usados en la obtención de aceites esenciales a partir de especies vegetales, sin embargo, requiere mucho tiempo, debido a la necesaria ebullición del agua. La energía de microondas, por otra parte, favorece la obtención de compuestos oxigenados y reduce considerablemente el tiempo de calentamiento. Considerando las ventajas de aplicación de la energía de microondas en la hidrodestilación convencional, en este trabajo se utilizó el método de hidrodestilación asistida por microondas para la obtención del aceite esencial de las muestras en estado seco de especies *Clinopodium laevigatum* (poleo) y *Baccharis heterophylla* (chamizo) realizando cinéticas de extracción. La caracterización del aceite esencial se realizó mediante la técnica de GC-MS y se identificaron compuestos de aplicación medicinal y aromática.

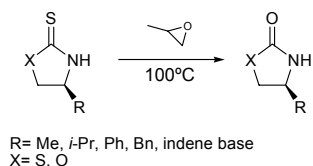
C-21

DESULFURIZATION-OXYGENATION OF 1,3-THIAZOLIDINE-2-THIONES. AN EFFICIENT METHOD FOR THE PREPARATION OF 1,3-THIAZOLIDINE-2-ONES.
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^a Departamento de Química Orgánica, Facultad de Química, Universidad Autónoma del Estado de México. Toluca, México.

^b Medicinal and Natural Products Chemistry, The University of Iowa. USA.

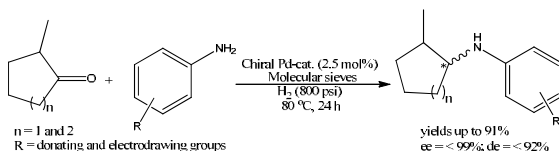
The use of chiral 1,3-thiazolidine-2-thiones and 1,3-oxazolidine-2-thiones for the stereoselective construction of C-C bonds is well documented in the chemical literature. Nevertheless, these chiral auxiliaries give the intramolecular sulfur transfer process in 1,4 addition reactions of *N*-enoyl derivatives. In this work, we report a desulfurization-oxygenation reaction of 1,3-thiazolidine-2-thiones and 1,3-oxazolidine-2-thiones using propylene oxide under thermic conditions. These transformations induced the formation of the desired products in good yields.



C-22 STABLE CHIRAL PALLADIUM COMPLEXES CATALYZED DIRECT ASYMMETRIC REDUCTIVE AMINATION OF SUBSTITUTED CYCLOALKYLKETONES.

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For the first time, stable chiral palladium complexes based on BINAP derivatives, CHIRAPHOS and heterobidentate (phosphine-oxazoline) ligands were used as catalysts for the asymmetric reductive amination reactions of a variety of substituted cycloalkylketones with primary amines to afford the corresponding secondary chiral cycloalkylamines in good yields with high diastereo- and enantio- selectivities.



ESTUDIO DE ADSORCIÓN DE ARSÉNICO Y PLOMO EN BARITA

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La muestra utilizada pertenece al yacimiento de barita en el Estado de Coahuila, Municipio de Múzquiz. La muestra se caracterizó por medio de Difracción de Rayos X y microscopía electrónica de Barrido. Se determinó el pH de carga cero y posteriormente se realizaron los experimentos de adsorción tipo batch utilizando soluciones de As(V), As(III) y Pb(II). La caracterización de la barita mostró que no tenía impurezas significativas y el pH de carga cero calculado fue de 9.8 ± 0.8 . Los resultados mostraron que el Plomo fue la única especie química que se adsorbió sobre la superficie de la barita con un porcentaje de 2.32% en promedio.

C-24

PAHS AND ALKYLATED OF OIL WASTE AND THE ENVIRONMENTAL TOXICOLOGY APPLICATIONS. R. Uribe-Hernández, M. A. Montes de Oca-García, J.A. Zermeño-Eguía Lis, V.E. Martínez-Martínez. Dirección de Seguridad y Medio Ambiente, Instituto Mexicano del Petróleo, México, DF.

Petroleum-derived hydrocarbons continue to persist after many decades in sediments of the tropical wetland. Recent analysis of marsh sediments revealed that residues of degraded oil are present with concentrations of total petroleum hydrocarbons as high as 287.8 mg g⁻¹. Polycyclic aromatic hydrocarbons (PAHs) constitute only a minor fraction of these residues with maximum concentrations of 54.89 µg g⁻¹, but their fate is of interest because of their potential toxicity to organisms. Based on comparison of rates between PAHs unsubstituted and alkylated was possible identify the weathering process biotic and abiotic as well as the source of these compounds, with application for assess the vertical transport of PAHs and the possible damage in the organisms. These compounds are suggested for fingerprinting in studies of environmental pollution and ecotoxicology.

C-25 SINTESIS DE NUEVAS ESPIROPIRROLIDINOCROMANONAS VIA UN PROCESO UGI- POSCONDENSACION

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Se describe la síntesis de heterociclos nitrogenados del tipo espiropirrolidinocromanonas en dos etapas de reacción. La estrategia sintética se basa en el uso de una reacción de multicomponentes tipo Ugi y un proceso de postcondensación vía radicales libres.

