JDD2023 :8-9 Mai 2023

Electrochemical Aptasensor Based on Chitosan-Pectin Nanoparticles for the detection of Ochratoxin A

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Code : 463330 **Commission** : chimie **Poster**:pc1

Mots clés : Chitosan Pectin Nanoparticles, sensor, Ochratoxin A, Aptamer.

Abstract :

As a highly toxic mycotoxin, Ochratoxin A (OTA) presents a major threat to food safety. Produced by fungi of the Aspergillus and Penicillium species, OTA can contaminate a wide range of plant-based foods, including grains, coffee, cocoa, nuts, and dried fruits. The health risks associated with OTA consumption are serious, and can include kidney damage, immune system suppression, and carcinogenic effects. In this regard, an electrochemical sensor has been proposed as a solution for the detection of OTA. The sensor consists of an aptamer immobilized on Chitosan-Pectin Nanoparticles. Electrochemical impedance spectroscopy (EIS) and Cyclic voltammetry (CV) have been used to characterize the properties of the fabricated sensor. This electrochemical aptasensor showed a low limit of detection of 0.35 ng/mL as well as good reproducibility with the relative standard deviation (RSD) of 1.92%. Overall, the proposed sensor holds significant potential for the detection of OTA in food products, which can help to ensure the safety of food products for consumers.

JDD2023 :8-9 Mai 2023

Quantification of the electrophilicity parameter E of a thiophene derivative and structure-reactivity correlations

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Code : 464745 **Commission** : chimie **Poster**:pc2

Mots clés : Electrophilicity, Kinetics, Mayr equation, Correlations, pKa values, σ constants

Abstract :

Kinetics of the reaction of 3,5-dicyanothiophene 1 with a series of secondary cyclic amines (pyrrolidine 2a, piperidine 2b, and morpholine 2c) have been investigated in aqueous solution at 20° C. The second order rate constants have been measured specrophotometrically and then have been employed to determine the electrophilicity E of the thiophene 1 according the Mayr equation log k (20° C) = s(E + N). where E is the electrophilicity parameter, N is the nucleophilicity parameter, and sN is the nucleophile-specific slope parameter. Using this correlation, we successfully evaluated the electrophilicity E value of thiophene 1 in H2O for the first time. Additionally, good linear correlations were found between the bimolecular rate constant k1 and and the pKa values of the secondary cyclic amines 2a-c and the σ constants of the substituents 3 for the

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Synthesis of New Carboheptahelicene Derivatives for Photovoltaic OPV Devices: Combined Experimental, Optical, Electrochemical and DFT-Theoretical Study

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Code : 465590 **Commission** : chimie **Poster**:pc3

Mots clés : π, conjugated helicenes, Photophysical properties, DFT, RDG, ELF.

Abstract :

Abstract: In this work, two new organic carboheptahelicene derivatives, as π-conjugated aromatic-fused systems, were synthesized by a coupling Heck and classical oxidative photocycling method. Optical and electrochemical properties of the studied materials were explored using spectroscopic analyses such as thermogravimetric analysis (TGA), optical absorption (OA), photoluminescence (PL) and cyclic voltammetry (CV). This experimental study is consolidated by theoretical calculation based on the density functional theory (DFT) approach and the time-dependent density functional theory (TD-DFT) at B3LYP, CAM-B3LYP and (B97XD functionals at 6-311G(d,p) basis set. The obtained data provides access to their optoelectronic properties (gap (Eg), stabilization energy (Estab), electron affinity (EA), ionization potential (IP), optoelectronic parameters) and to explore many characteristics: structural parameters, molecular orbitals MOs, molecular electrostatic potential (MEP) and the surface reactivity and evaluate their optoelectronic properties and performance. In addition, several topological analyses, coupled with DFT and TD-DFT, were performed in order to analyze the non-covalent interactions of studied molecules.

Starting from the outstanding properties of pristine carboheptahelicene, our research highlights the molecular design and understanding of the photophysical processes of these carboheptahelicene, providing high-performance as an active layer. All the results demonstrate their potential applications as an excellent organic acceptor in photovoltaic OPV devices.

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Development of Electrochemical Sensor Based on Titanium Dioxide Nanoparticles and Molecular Imprinted Film for Detection of Dopamine Compounds

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Code : 466699 **Commission** : chimie **Poster**:pc4

Mots clés : Dopamine, Sensor, Molecularly imprinted polymers, Differential pulse voltammetry (DPV), Nanoparticule

Abstract :

Dopamine coexists in the serum and extracellular fluid of the central nervous system as a major product of purine metabolism. It plays a key role in the early diagnosis of many human diseases associated with abnormal dopamine levels. Therefore, it is of great importance to explore rapid, simple and accurate methods for the detection of dopamine with high sensitivity and specificity. Here, a new chemical sensor was prepared by electropolymerization using pyrrole-chitosan composites and dopamine as template onto the titanium dioxide nanoparticles-modified glassy carbon electrode surface (GCE). The resulting MIP was characterised by cyclic voltammetry (CV), scanning electron microscopy (SEM), fourier transform infrared spectroscopy (FTIR) and UV-Visible. Throughout the study, various analytical parameters, such as the monomer and the template concentrations, the electrolyte support concentration, the electropolymerization cycles, the pH medium, the incubation time and the scan rate, were optimized. The peak current of dopamine was linear to its concentration in the range of 1x10-6 mol. L-1 to 1x 10-5 mol. L-1 with a good detection limit and high selectivity by differential pulse voltammetry (DPV). The developed imprinted dopamine sensor was successfully used for dopamine determination in real samples with acceptable recovery.

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Chemical profile, antifungal and antibiofilm properties of the aerial parts essential oil of Glycyrrhiza foetida (Desf.) growing in Tunisia

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Code : 467556 **Commission** : chimie **Poster**:pc5

Mots clés : antibiofilm and antifungal activities, G. foetida, essential oils, mass spectrometry, gas chromatography

Abstract :

Fabaceae represents the second family of dietary importance after Poaceae. Food legumes and seeds of certain Fabaceae species constitute a primary source of important oils and edible nutrients associated with human and animal health benefits [1]. Fabaceous species of Glycyrrhiza genus serve commercially as depigmentation agents in cosmetics and as flavoring and sweetening safe agents in food products [2]. The identification of the organic volatiles by GC-FID and GC-MS techniques revealed that sesquiterpene hydrocarbons, dominated by δ-cadinene (13.9%) and (E)-caryophyllene (13.2%), constitute the first major category of G. foetida components. Furthermore, the results of biological revealed a complete inhibition of C. albicans and Microsporum canis growth by the volatile oil at 0.4 and 0.2 mg.mL-1, and allowed noticing that G. foetida essential oil possess a promising role in the control of fungal agents and in inhibiting Candida albicans biofilm development [3].

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Investigations on the non-covalent interactions, drug-likeness, molecular docking and chemical properties of 1,1,4,7,7-pentamethyldiethylenetriammonium trinitrate by density-functional theory

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Code : 467950 **Commission** : chimie **Poster**:pc6

Mots clés : AIM, DFT calculation, MEPS, Molecular docking, RDG.

Abstract :

Non-covalent interaction is believed to play a vital role in stabilizing various complex chemical species. Herein, we have undertaken a theoretical study to understand the nature and extent of non-covalent interaction between organic and inorganic group of 1,1,4,7,7-Pentamethyldiethylenetriammonium trinitrate (abbreviated as PMDT). The quantum chemical study has been carried out using the DFT calculation with B3LYP/6-31++G (d, p) basis set. The non-covalent interactions have been established using different methods such as Atoms-in-Molecules approach (AIM) and the reduced gradient of the density (RDG). By using Natural Bond Orbital (NBO) method intra molecular interactions are studied and the charge transfer energies are explained. The reactivity of the compound is analyzed by using Molecular Electrostatic Potential Surface (MEPS) map. Furthermore, the Frontier molecular orbital's (HOMO-LUMO) was discussed to afford the information about the reactivity of the PMDT molecule. Finally, a molecular docking study is carried out to investigate the antibacterial activities of the studied compound.

JDD2023 :8-9 Mai 2023

Synthesis and Structural identification of the novel Strandberg-type polyoxoselenomolybdate

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Code : 468008 **Commission** : chimie **Poster**:pc7

Mots clés : Hybrid, Strandberg material, Crystal structure, Hydrogen bonds, Hirshfeld surface analysis

Abstract :

A supramolecular assemblies of a novel material built from Strandberg-type selenomolybdate and benzylammonium groups (C7H10N)4[Se2Mo5O21]·4H2O has been prepared by conventional solution process at room temperature. The hybrid compound has been structurally characterized by single-crystal X-ray diffraction methods, scanning electron microscopy (SEM), FT-IR and Raman spectroscopy, also analyzed by Hirshfeld surface approach. Single X-Ray diffraction technique is used to complete structure elucidation which confirm the title compound crystallizes in the triclinic space group P-1 with four asymmetric units per cell (Z = 4). The structural study showed a three-dimensional supramolecular framework obtained by a periodic arrangement of the Strandberg clusters anions [Se2Mo5O21]4-, connected to each other by Benzylammonium counter cations and solvation water molecules through a network of conventional and non-conventional hydrogen bonds. Additionally, the intermolecular interactions which ensure the cohesion between different entities were quantified and analysed by the Hirshfeld surface approach showing different contacts other than hydrogen bonds such as H··· H, C··· C, Se··· O, C··· O and O··· O which lead to the stability of our crystal. Furthermore, FT-IR and Raman spectroscopy were used to explore the modes of vibration of the different functional groups present in the crystallized phase.

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Electrochemical study on the stability of new naphthalene-containing species forming complexes with Cu2+, Pb2+ ,Zn2+, and Cd2+: comparative studies by different techniques.

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Code : 468159 **Commission** : chimie **Poster**:pc8

Mots clés : metal cations, speciation, electrochemical sensing

Abstract :

The formation constants of various M/Naphthalene systems (M =Cu2+, Zn2+, Pb2+, Cd2+) at T =298.15K, by potentiometry, spectrophotometric and voltammetry. The elucidation of the metal (M2+)-naphthalene interactions in aqueous solution highlighted the speciation model for each system, the dependence of formation constants of the complex species on ionic strength and temperature T =298.15K and changes in enthalpy and entropy. For all of these reasons, the aim of the present paper is to define a critical speciation scheme for some M/Naphthalene (M = Cu2+, Pb2+, Zn2+, Cd2+) systems, which is independent from both the adopted experimental conditions and the analytical techniques used to obtain the thermodynamic parameters. To reach this objective, the four M/Naphthalene systems were studied at different ionic strengths and with different analytical techniques, such as potentiometry , spectrophotometric and DP-ASV(differential pulse-anodic stipping voltammetry), and varying any possible experimental condition (reagent stocks, solution concentrations, operators,etc.). The three cited electrochemical techniques give complementary information concerning solution equilibria. Electrochemical responses in the presence of Cd2+ Cu2+, Zn2+ and Pb2+ have been shown to be promising for the electrochemical detection of these metal cations in aqueous environments.

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Holothuria polii and Sargassum vulgare from Tunisian Seashore, sustainable sources of chondroitin sulfates and bioactive polysaccharides for health and well being

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Code : 468267 **Commission** : chimie **Poster**:pc9

Mots clés : Chondroitin sulfates, Fucan, Human dermal fibroblasts, Matrix metalloproteases, Zymography.

Abstract :

Chondroitin sulfates are sulfated glycosaminoglycans that are used in the pharmaceutical, cosmetic, and nutraceutical sectors as pro-regenerative compounds or dietary chondroprotective supplements. Unfortunately, industrial production from bovine or avian sources faces sanitary risks (1). Our study focuses on an unusual alternative source of chondroitin sulfates from Tunisan seashore: Holothuria polii , echinoderms that naturally produce chondroitin sulfates in their coelomic fluids and teguments (2). Thus, our work aims to study some biological activities of chondroitin sulfates extracted from the coelomic fluid (PFH, Polysaccaride Fluid Holothuria) and from the teguments (PHP, Polysaccharides Holothuria polii) and compare the results to a high molecular weight Fucan (Fuc, from the brown algae, Sargassum vulgare) (3). We followed the effects of these polysaccharides on parameters involved in tissue repair: cell proliferation of human dermal fibroblasts in 2D culture and secretion of matrix metalloprotease (MMP) by dermal fibroblasts in 2D culture and by reconstructed connective tissue through zymography. Our aim was to determine if chondroitin sulfates from H.polii have the same properties as those currently produced in the industry. This way, we can determine if they can be regarded as an alternative source of chondroitin sulfate from a more sustainable production with less sanitary risks.

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The Extraction of natural dye using scCO2 technique from Hypericum Triquetrifolium Turra and the Evalution of Dyeing properties

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Code : 468285 **Commission** : chimie **Poster**:pc10

Mots clés : KEYWORDS: CO2 supercritical, Multifiber fabrics, Extraction, Dyeing, Metal Mordents, Affinity

Abstract :

The textile and clothing industry is an important sector however it has a very high impact on the environment. Dyeing fabrics with natural dyes have become an attraction because of its eco-friendly and less threatening disposition towards humankind. In the textile coloration industry, natural dyes play an important role because of the need for replacement synthetic dyes which have a great deal of tension with the environmental issues. The use of natural stuff in textile dyeing is gaining popularity all over the world. Therefore, there is a need for developing better solid-liquid extraction techniques for leaching natural dyes from plant materials for applications in food and cosmetic fields as well as textile industries. In this study, supercritical CO2 extraction techniques such was done to extract natural dyes from Hypericum triquetrifolium Turra. UV-VIS spectrophotometry and gravimetric analysis were performed on each extract. The results indicated a significant improvement in the extraction efficiency of the obtained dyeing stuff due to the use of supercritical CO2. Afterwards, preliminary tests were carried out to investigate the dyeing potential of the obtained extract from the Tunisan speice The Hypericm by different techniques using multifiber fabrics using different mordanting modes.

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Synthesis, Characterization, and DFT Modeling of Optoelectronic Properties of New Hexahelicene Derivatives

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Code : 468536 **Commission** : chimie **Poster**:pc11

Mots clés : Helicene, Screw shaped compounds, Photophysical properties, TD, DFT.

Abstract :

In this work we deal with the synthesis, structural and quantum chemical modeling of new hexahelicene derivative properties. Two new helical compounds denoted 3-brom-[6]helicene (BHH) and 3-bromo-14-methoxy-[6]helicene (BMHH). Herein, the helicene derivatives, exhibiting a non-planar structure, were obtained in moderate heck reaction followed by photocyclodehydrogenation and characterized using analytical, spectroscopic and electrochemical techniques and a complementary quantum-chemical modelling based on DFT method at B3LYP/6-31G(d,p). Electronic structure in their excited and ground electronic states. IR vibrational behavior, stability and optical characteristics have been measured and interpreted by use of DFT and TD-DFT methods. Optoelectronic properties such as HOMO and LUMO energies, IP and EA energies, absorption and emission spectra exciton binding energy values are examined. ESP, RDG, ELF and other characteristic parameters of the organic compounds were studied. The introduction of side groups onto the molecular scaffold of a [6]helicene was reflected in a slight shift of UV–vis absorption and emission spectra maxima when compared to unsubstituted [6]helicene. These kinds of organic compounds are promising materials for organic electronics and the access to all these compounds properties may open the way to many and diverse applications of such compounds, allowing for the exploitation of their remarkable electronic and photophysical properties.

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A novel electrochimical sensor for detemination of Cu(II) based on Chitosan And gC3-N4 modified glassy carbon electrode

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Code : 468707 **Commission** : chimie **Poster**:pc12

Mots clés : Chitosan, g, C3N4, Heavy metal, Cu (II) determination, DPV Measurements, wastewater

Abstract :

Copper(II) is a long-standing environmental pollutant in industrial wastewater. Because of multiple toxicity and gradually accumulation, copper poisoning can cause serious damage to the central nervous system, digestive system, along with reproductive system[1]. Moreover, many brain diseases, such as Alzheimer's, Parkinson's disease, are related to copper [2]. In this work a glassy carbon electrode (GCE) modified with chitosan (CS) and the graphite nitride carbon (g-C3N4) used to determine Cu(II). The electrochemical reponse of the developed sensor was performed using the differential pulse voltammetry technique(DPV). The combination of chitosan and gC3-N4 gives the electrodes good stability, as well as high selectivity and sensivity. various analytical parameters, such as pH value of acetate buffer solution, concentration of Chitosane, and time of agitation, were optimized.

JDD2023 :8-9 Mai 2023

Valorization of agri-food by-products into absorbents used in wastewater treatment.

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Code : 468719 **Commission** : chimie **Poster**:pc13

Mots clés : Valorization of agrifood, Activated carbon, iodine number (QI2), methylene blue number (QMB)

Abstract :

The recovery of food by-products is the transformation of residues or by-products from the food industry with a view to reintroducing them as new products. This transformation presents the iterated thanks to the great availability of its waste,its low costs during the transformation, its biodegradability...One of the agri-food by-products is prickly pear seeds from the essential oil production industry. These seeds are transformed by chemical activation into activated carbon which is a good adsorbent used in wastewater treatment. This chemical activation was done by phosphoric acid H3PO4(85%). Different experiments in summer made using an experimental plan to determine the optimal activated carbon which is then characterized in order to determine the adsorbent power of the activated carbon developed for the retention of certain pollutants... This characterization was made by the iodine number (QI2), the methylene blue index QMB, the pHzch, the surface functions (Boehm method). A concentration of the activating agent H3PO4 at 12.5% associated with a pyrolysis temperature of 800°C and a heating time of 137 min would make it possible to develop the best CA. The results of QI2 obtained under different conditions is 999.64(mg/g) ,8.53 (mg/g.) for the methylene blue number, and 2.5 for pH ZCH

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Complexes diazadiènes: Synthèse et application pour la dégradation des polluants organiques en milieux aqueux

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Code : 468720 **Commission** : chimie **Poster**:pc14

Mots clés : complexes de coordination, colorants, adsorption, génération d'hydrogène

Abstract :

Le rejet de matériaux synthétiques de la chimie industrielle sans traitement approprié peut avoir des conséquences environnementales néfastes. Cela conduit à la contamination de l'eau et de l'air et contribue au problème du réchauffement climatique. Notre objectif s'est concentré sur la synthèse de composés de coordination, ciblant spécifiquement les complexes α-diimines et hexa-ammines du cobalt. Ensuite, nous avons mis ces composés à l'épreuve, en examinant leur réactivité en ce qui concerne deux fonctions clés - l'adsorption du colorant bleu de méthylène et la génération d'hydrogène via l'hydrolyse de NaBH4.

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INSERTION DE LA RÉACTIVITÉ DE 1,3,5-TRINITROBENZÈNE DANS L'ÉCHELLE UNIVERSELLE N DE MAYR

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Code : 468859 **Commission** : chimie **Poster**:pc15

Mots clés : Super, électrophile / nucleophile / Cinétique / σ, complexation / équation de Mayr.

Abstract :

Le présent travail décrit les résultats de l'étude cinétique de la réaction de couplage de 1, 3,5-trinitrobenzène 1 avec divers super-électrophiles (4,6-dinitrobenzofuroxane 2, 6-cyano-4-nitrobenzofuroxane 3 et l'ion benzhydrylium (mfa)2CH+ 4) dans l'acétonitrile à 20 °C. Les diverses corrélations structure-réactivité obtenues lors de cette étude ont permis de montrer la formation d'un σ-complexe. log k (20 °C) = sN (E+ N) (1) Les analyses des constantes de vitesses du second ordre, k, en termes d'équation de Mayr (1) révèlent que les composés 2-4 peuvent être utilisés comme des super-électrophiles de référence pour la détermination des paramètres de nucléophiles N et sN du trinitrobenzène. Comme nous le verrons, le résultat le plus original, est la mise en évidence d'un caractère nucléophile du trinitrobenzène. Notons que le trinitrobenzène est considéré à ce jour comme l'électrophile de référence pour le processus SNAr et σ-complexation (E = -13.19).

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APPROCHE EXPÉRIMENTALE ET THÉORIQUE DE LA RÉACTIVITÉ DES PYRIDINES SUBSTITUÉES

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Code : 468862 **Commission** : chimie **Poster**:pc16

Mots clés : Cinétique, Electrophile, Nucléophile, RMN, Approche de Mayr, Approche de Parr.

Abstract :

Une étude cinétique par spectrophotométrie UV-visible de la réaction de couplage de la 2-méthoxy-3,5-dinitropyridine avec trois amines secondaires cycliques (pyrrolidine, pipéridine et morpholine) a été réalisée dans l'acétonitrile à 20 °C. Les données cinétiques et spectrales ont révélé l'existence d'une seule attaque de l'amine sur la position méthoxylée de la pyridine. Les constantes de vitesse du second ordre ont été utilisées pour évaluer le paramètre d'électrophilie E de la 2-méthoxy-3,5-dinitropyridine selon la relation de Mayr: log k (20 °C) = s (E + N) où N et s sont des paramètres spécifiques au nucléophile. Par ailleurs, une corrélation linéaire satisfaisante entre le paramètre d'électrophilie E selon l'approche de Mayr et l'électrophilie globale ω proposée par Parr, a été obtenue et discuté.

JDD2023 :8-9 Mai 2023

Synthesis and Spectroscopic Characterization of a New (Chloro) Meso-aryl porphyrin complex. Crystal structure of [FeIII(TFPP)Cl]•CH2Cl2•H2O

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Code : 469067 **Commission** : chimie **Poster**:pc17

Mots clés : Fer(III) porphyrin complexes, X, ray molecular structure, UV, visible

Abstract :

Iron (III) metalloporphyrin is widely used as a synthetic model of hemoproteins since these species are very close structurally and electronically to the active sites of many biological macrocycles. The main use of iron (III) porphyrin complexes remains the catalysis in organic chemistry (epoxidation, oxidation, cyclopropanation reactions, formation of pyrrolines, furans.
Etc.) [1]. We have focused on the synthesis, crystal structure, UV-visible, IR, and 1H NMR, of
the (chloro)[(meso-tetra(para-fluorophenyl) porphyrinato] iron (III) dichloromethane mono solvate monohydrate with the formula [FeIII (TFPP)Cl]•CH2Cl2•H2O.
The title compound crystallizes in the monoclinic crystal system (space group C2/c) with the cell parameters: a = 16,0450(3) Å, b =19,3320(3) Å, c = 26,0230(5), β =98,881(7) °, with V =

2875,43 Å3, Z = 8, R1=0.0410, wR2 = 0,0995 and S =1,027.

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Synthesis of new chiral N-carbonylamino acids and Evaluation of their anti-inflammatory activity

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Code : 469101 **Commission** : chimie **Poster**:pc18

Mots clés : : chirality molecule, Amino acids, Urea derivatives, Anti, inflammatory

Abstract :

Synthesis of new chiral N-carbonylamino acids and Evaluation of their anti-inflammatory activity Mehrez S, Absi S, Hamdi A, Kacem Y, Kraiem J Laboratory of chemical, galenic and pharmacological development of drugs, Faculty of Pharmacy of Monastir Abstract We have synthesized a series of new chiral N-carbonylamino acid derivatives containing urea units. In silico studies, showed interesting anti-inflammatory activity. The selected compounds were submitted to the in vivo study of their anti-inflammatory activity. The experimental results are in agreement with the theoretical study. All the prepared molecules were characterized with H1 NMR, C13 NMR and IR spectroscopic methods.

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Development of Schiff base linked 4-hydroxycoumarin: chemosensor for colorimetric detection of metal ions

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Code : 469221 **Commission** : chimie **Poster**:pc19

Mots clés : Chemosensor, hydroxycoumarin, schiff base, imine, fluorescence

Abstract :

The Schiff base ligand's imine functions provide specific binding sites for metal ion detection. Moreover, colorimetric alterations are caused by the charge and energy transfer combination.1 Here, we synthesize imino-hydroxycoumarin a new chemosensor that acts for sensitive and selective detection of metal ions to the optical Schiff bases sensor. The recognition is determined by shift in UV–visible, emission intensity changes in fluorescence and signal changes with the addition of ions to the ligand. The insights into the color changes are described visually and under different wavelengths of light. The results show that, from the studied compounds, CA1 and CA3 present a strong response to copper(II), with ~40-fold and ~50-fold increase in the emission of CA1 and CA3, respectively. Moreover, both compounds present remarkable sensitivity to copper (II), when compared to a broad series of mono- and divalent cations which induce no response from the sensor molecules. As a result, our findings may aid in the development of novel chemosensors for the selective detection of Cu2+ ions. References 1. C. Lochenie, K. Sch¨otz, F. Panzer, H. Kurz, B. Maier, F. Puchtler, S. Agarwal,A.K¨ohler, B. Weber,J. Am. Chem.Soc. 2018, 140 , 700–709.

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Etude cinétique de la réactivité électrophile carbonée des benzothiadiazoles

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Code : 469310 **Commission** : chimie **Poster**:pc20

Mots clés : Cinétique / Approche de Mayr / Addition nucléophilie / Brönsted

Abstract :

Le travail que nous venons de présenter constitue une contribution à la compréhension de la réactivité électrophile carbonée du 2,1,3-benzothiadiazole avec divers nucléophiles à savoir la pyrrolidine, la pipéridine et la morpholine dans le DMSO à 20 °C, en utilisant les techniques spectrophotométriques UV-visible. L'application de la relation log k (20 °C) = s (N + E) à permis de chiffrer et de situer, pour la première fois, la réactivité électrophile du 2,1,3-benzothiadiazole dans l'échelle universelle E introduite par H.Mayr en 1994. Par ailleurs, la corrélation de Brönsted obtenue lors de cette étude a permis de montrer que le degré de transfert de charge du nucléophile vers l'électrophile est approximativement réalisé à 70 % dans l'état de transition (βnuc = 0,67) et qu'il s'agit d'une réaction de σ-complexation.