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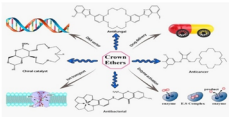
Content Highlights

DOI:10.3390/app12031102

Heterocyclic Crown Ethers with Potential Biological and Pharmacological Properties: From Synthesis to Applications

Authors: Faiz Ullah, Taskin Aman Khan, Jawaria Iltaf, Saleha Anwar, Muhammad Farhan Ali Khan, Muhammad Rizwan Khan, Sami Ullah, Muhammad Fayyaz ur Rehman, Muhammad Mustaqeem, Katarzyna Kotwica-Mojzych and Mariusz Mojzych

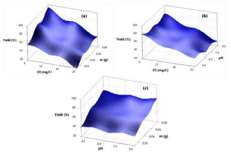


Abstract: Cyclic organic compounds with several ether linkages in their structure are of much concern in our daily life applications. Crown ethers (CEs) are generally heterocyclic and extremely versatile compounds exhibiting higher binding affinity. In recent years, due to their unique structure, crown ethers are widely used in drug delivery, solvent extraction, cosmetics manufacturing, material studies, catalysis, separation, and organic synthesis. Beyond their conventional place in chemistry, this review article summarizes the synthesis, biological, and potential pharmacological activities of CEs. We have emphasized the prospects of CEs as anticancer, anti-inflammatory, antibacterial, and antifungal agents and have explored their amyloid genesis inhibitory activity, electrochemical, and potential metric sensing properties. The central feature of these compounds is their ability to form selective and stable complexes with various organic and inorganic cations. Therefore, CEs can be used in gas chromatography as the stationary phase and are also valuable for cation chromatographic to determine and separate alkali and alkaline-earth cations.

DOI:10.3390/app12157587

Zeolite Waste Characterization and Use as Low-Cost, Ecofriendly, and Sustainable Material for Malachite Green and Methylene Blue Dyes Removal: Box–Behnken Design, Kinetics, and Thermodynamics

Authors: Ali Imessaoudene, Sabrina Cheikh, Jean-Claude Bollinger, Lazhar Belkhiri, Ammar Tiri, Abdelkrim Bouzaza, Atef El Jery, Aymen Assadi, Abdeltif Amrane and Lotfi Mouni

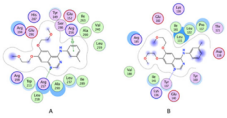


Abstract: This study investigated the potential of 4A zeolite, named4AZW in this work, generated by natural gas dehydration units as solid waste after several treatment cycles, as a low-cost adsorbent to separately remove two cationic dyes, methylene blue (MB) and malachite green (MG), from an aqueous solution within a batch process. The adsorbent material was characterized by N2gas adsorption–desorption, X-ray fluorescence spectrometry, X-ray diffraction, FT-IR spectroscopy, and the determination of its cation exchange capacity and point of zero charge. The influence of key operating parameters, such as the pH, adsorbent dosage, ionic strength, contact time, initial dye concentration, and temperature, was investigated. Three independent variables acting on MB adsorption performance were selected from the Box–Behnken design (BBD) and for process modeling and optimization. An analysis of variance (ANOVA), an F-test, and p-values were used to analyze the main and interaction effects. The experimental data were satisfyingly fitted with quadratic regression with adjusted R^2= 0.9961. The pseudo-second-order kinetic model described the adsorption of the dyes on 4AZW. The equilibrium data were well-fitted by the Langmuir model for each adsorption system (MB-4AZW and MG-4AZW) with maximum adsorption capacity (qmax) values of 9.95 and 45.64 mg/g, respectively, at 25 °C. Thermodynamics studies showed that both adsorption systems are spontaneous and endothermic.

DOI:10.3390/app12073575

Influence of Rutin, Sinapic Acid, and Naringenin on Binding of Tyrosine Kinase Inhibitor Erlotinib to Bovine Serum Albumin Using Analytical Techniques Along with Computational Approach

Authors: Tanveer A. Wani, Ahmed H. Bakhei, Seema Zargar, Arwa Ishaq A. Khayyat and Abdulrahman A. Al-Majed

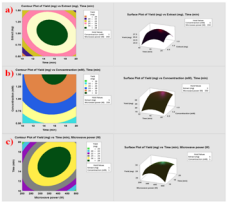


Abstract: Flavonoid-containing food supplements are widely used as antioxidants, and the continuous use of these supplements with other drugs can lead to clinically significant interactions between these and other drugs. The medications in systemic circulation are mainly transported by serum albumin, a major transport protein. This study evaluated the interactions of rutin (RUT), naringenin (NAR), and sinapic acid (SIN) with the most abundant transport protein, bovine serum albumin (BSA), and the anticancer drug, the tyrosine kinase inhibitor Erlotinib (ETB), using various analytical methods. Interaction between multiple types of ligands with the transport proteins and competition between themselves can lead to the bound ETB's displacement from the BSA-binding site, leading to elevated ETB concentrations in the systemic circulation. These elevated drug fractions can lead to adverse events and lower tolerance, and increased resistance to the therapeutic regimen of ETB. The experimental and computational methods, including molecular-docking studies, were used to understand the molecular interactions. The results suggested that the complexes formed were utterly different in the binary and the ternary system. Furthermore, comparing the ternary systems amongst themselves, the spectra differed from each other. They thus inferred that complexes formed between BSA-ETB in the presence of each RUT, NAR, and SIN separately were also different, with the highest value of the reduction in the binding energy in RUT, followed by SIN and then NAR. Thus, we conclude that a competitive binding between the ETB and these flavonoids might influence the ETB pharmacokinetics in cancer patients by increasing ETB tolerance or resistance.

DOI:10.3390/app12031384

Optimization of the Synthesis of Fungus-Mediated Bi-Metallic Ag-Cu Nanoparticles

Authors: Fuad Ameen

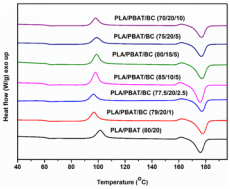


Abstract: Bi-metallic nanoparticles (NPs) have appeared to be more efficient as antimicrobials than mono-metallic NPs. The fungus *Aspergillus terreus*-mediated synthesis of bi-metallic Ag-Cu NPs was optimized using response surface methodology (RSM) to reach the maximum yield of NPs. The optimal conditions were validated using ANOVA. The optimal conditions were 1.5 mM total metal (Ag + Cu) concentration, 1.25 mg fungal biomass, 350 W microwave power, and 15 min reaction time. The structure and shape of the synthesized NPs (mostly 20–30 nm) were characterized using several analytical tools. The biological activities of the synthesized NPs were assessed by studying their antioxidant, antibacterial, and cytotoxic activity in different NP concentrations. A dose-dependent response was observed in each test. Bi-metallic Ag-Cu NPs inhibited three clinically relevant human pathogens: *Klebsiella pneumoniae, Enterobacter cloacae,* and *Pseudomonas aeruginosa. Escherichia coli, Enterococcus faecalis*, and *Staphylococcus aureus* were inhibited less. The DPPH and hydrogen peroxide scavenging activities of the NPs were high, reaching 90% scavenging. Ag-Cu NPs could be studied as antimicrobials in different applications. The optimization procedure using statistical analyses was successful in improving the yield of nanoparticles.

DOI:10.3390/app13020902

Improvement of Electrical and Mechanical Properties of PLA/PBAT Composites Using Coconut Shell Biochar for Antistatic Applications

Authors: Justin George, Daeseung Jung and Debes Bhattacharyya



Abstract: Biochar-based environment-friendly polymer composites are suitable substitutes for conventional non-biodegradable polymer composites. In this work, we developed polylactic acid (PLA)/polybutylene adipate-co-terephthalate (PBAT)/biochar (BC) composites with improved mechanical and electrical properties for antistatic applications. Coconut shell biochar was obtained through the pyrolysis of coconut shell in an inert atmosphere, and characterised using scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD), to investigate the morphology and structural properties. The biochar was converted to powder form, sieved to reduce the particle size (≤30 µm diameters), and melt-mixed with PLA and PBAT to form composites. The composites were extruded to produce 3D printing filaments and, eventually, 3D-printed tensile specimens. The tensile strength and tensile modulus of the 3D-printed PLA/PBAT/BC (79/20/1) composite with 1 wt% of biochar improved by 45% and 18%, respectively, compared to those of PLA/PBAT (80/20). The interfacial interaction between the biochar and polymer matrix was strong, and the biochar particles improved the compatibility of the PLA and PBAT in the composites, improving the tensile strength. Additionally, the electrical resistivity of the composite did reduce with the addition of biochar, and PLA/PBAT/BC (70/20/10) showed the surface resistivity of ~10^{11} Ω/sq, making it a suitable material for antistatic applications.

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