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Electrochemical Sensing of Paracetamol Using Functionalized MWCNTs: Integrating Computational and Experimental Methods

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An electrochemical sensing platform for the detection of paracetamol is proposed in this work. The sensor (Asp-MWCNTs/IL/ITO) is based on Indium Tin Oxide (ITO) electrode loaded with asparagine functionalised Multi Walled Carbon Nanotubes (MWCNTs) and Ionic Liquid (IL). Initially, *in-silico* studies were performed to check the favourable interaction of the drug with the nanocomposite. The potential energy surface of Asp-MWCNTs and paracetamol complexes were explored using density functional theory and single-point energy coupled cluster calculations. The analysis of non-covalent interactions showed hydrogen bonding interactions predominantly stabilising the complex. The interaction process between Asp-MWCNTs and paracetamol is spontaneous due to negative value of binding energy (−0.75 eV). The functionalised MWCNTs were characterised through different techniques. Asp-MWCNTs/IL/ITO electrode showed good sensitivity with a linear range from 20–300 μgL^{-1} and limit of detection of 0.0194 μM for paracetamol in phosphate buffer as supporting electrolyte. The sensor showed excellent repeatability and reproducibility with a relative standard deviation of 1.45% at 60 μgL^{-1} concentration. The chemical functionalization resulted in providing extra stability as it retained 95% of its signal response even after 45 days. The sensor's applicability was tested in real water samples with the help of spiking study which showed good recovery $>$95%."

1. Introduction

Electrochemical sensors are a crucial, diverse analytical platform for detection of various analytes in different settings from industry, environment and biological systems.[1] A thrust area of research has been the incorporation of nanoscience into the development of electrochemical sensors for improving sensitivity, selectivity and stability. Nanomaterials possess high surface-area to volume ratio, improving adsorption, reactive capacity and tunability across the structure, making them more suitable than bulk materials.[2–3] Electrochemical technologies are increasingly being used to monitor environmental, biotechnology, and medicinal matrices, as well as manage industrial operations. Electrochemical sensing challenges include overlapping of oxidation peaks. Modifiers can overcome this obstacle, allowing for sensitive and selective determination of specific species. Chemically modified electrodes are an excellent instrument for assessing several analytes at the trace level using sensitive electroanalytical techniques. Functionalised nanomaterials in analytical systems like electrochemical sensors have shown remarkable potential to detect environmental pollutants.[4–5] Thus revealing their importance as an effective pathway to ensure accurate, real-time monitoring in the face of growing pollution and population pressure. Among various electrochemical techniques, voltammetry have attracted our attention as it provides fast response, speciation of analytes, simultaneous analysis and gives insight about various thermodynamic and kinetic properties of a process.[6–7]

Drug pollution has emerged as a silent yet serious environmental issue.[8–9] In fact, with improved access and use of pharmaceuticals across the globe, there exists a present and well-documented hazard due to their uncontrolled and untreated disposal. Persistence of these pollutants in the environment can pose significant risk to microorganisms and marine life, including progress of antimicrobial resistance which indirectly harms humans.[10]

Paracetamol (N-acetyl-para-aminophenol), first used clinically in 1893, is the world's most commonly used drug. A commonly prescribed antipyretic and analgesic drug, with a proven extensive safety profile, it remains the most popularly consumed over-the-counter drug. Nowadays it is being widely used in COVID-19 as it is effective in reducing fever and pain management such as migraine, backache, chronic pain, muscular pain etc. While it does not have any detrimental side effects when used in regulated amounts, overdosing can lead to toxicity. However, overdose of paracetamol can harm kidney and liver though nephrotoxicity and hepatotoxicity.[11–12]

In this light, efficient determination of paracetamol is vital, and the attempt to do so begins with detection techniques. Over the years, multiple approaches such as spectrophotometry, chemiluminescence, chromatography and electrochemical

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