Abstract No: MP-10

Role of graphene oxide in urease-immobilized biosensor for heavy metals: molecular interaction analysis

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The accumulation of toxic heavy metals like Cu^{2+}, Cd^{2+} and Pb^{2+} is a major health risk in ensuring quality and safe access to drinking water. Due to high toxicity caused by these metal ions there is a conspicuous requirement to quantify them swiftly on site at trace levels. Biosensing mechanisms are proven for potential heavy metal toxicological monitoring in recent years. Graphene-based materials become potential source for such sensing tools. Present blind docking-based investigation reports the candidacy of graphene oxide (GO) for heavy metal biosensing applications. Urease-urea enzyme-mediated biosensor model has been contemporarily investigated to quantify heavy metal contamination levels in pollution monitoring sectors. It is aimed to elucidate binding energies and molecular interactions between GO with urease enzyme and urea with GO to explore the potential of the GO, whether as an enzyme immobilizer or as an active sensing material using blind docking tools and method. Docking results revealed that GO plays a significant role in urease-assisted system. The strongest binding affinity of the stable conformation of urease-GO interaction is -12.4 kcal/mol and primarily dominated by electrostatic interactions. In addition, hydrogen bonding and hydrophobic interactions were also elucidated. Selective amino acids of the chain C of the protein Urease dominate the protein-ligand interactions. The most stable mode showed no root mean square deviation (RMSD) while the least stable one showed higher RMSD values A prospect of direct sensing mode of urea by GO was also studied where urea-GO interaction is solely dominated by conventional hydrogen bonds with a much lower binding affinity of -3.6 kcal/mol at the most stable pose. The relatively small difference between the strongest and the weakest binding affinity values of urea-GO complex indicate that urea binding can take place at possible GO sites with relatively same strength. Overall present in silico studies of GO interactions in the urease-urea heavy metal biosensing system portrait the fitness of GO as a potential biosensor material.

Keywords: Graphene oxide, Heavy metal detection, Urease, Molecular docking, Biosensor