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Investigation of the Host-Guest Complexation Between 4-Sulfocalix[4]Arene and Nedaplatin for Potential use in Drug Delivery

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Macromolecules including macrocyclic species have been reported to have the potential to encapsulate biologically active compounds such as drugs through host-guest complexation to increase their solubility, stability and bioavailability. In this paper an experimental and theoretical investigation of the complexation between nedaplatin, a second generation antineoplastic drug, and p-4-sulfocalix[4]arene, a macromolecule possessing a bipolar amphiphilic structure with good biocompatibility and relatively low haemolytic toxicity is examined. Data from 1H NMR, UV, Job's plot analysis, HPLC and DFT calculations are presented and suggest the formation of a 1:1 complex. The stability constant of the complex was estimated to be 3.6 x 104 M-1 and 2.1 x 104 M-1 which correspond to values of -6.2and -5.9 kcal mol-1, respectively for the free energy of complexation while the interaction free energy is calculated to be-4.9 kcal mol-1. The formed species is shown to be mainly stabilised due hydrogen bonding between the host and the guest not involving endo complexation where nadaplatin penetrates the cavity of the p-4-sulfocalix[4] arene. The low binding constant of the complex will most likely lead to its dissociation in biological media.

Biography:

Dr. Tamer Shoeib is a professor of chemistry at the American University in Cairo. He obtained his chemistry BSc with honors and PhD both from York University (Toronto, Canada). In 2004 he was awarded a prestigious Natural Sciences and Engineering Research Council of Canada post-doctoral fellowship to join the National Research Council of Canada at the Institute for National Measurement Standards. His research interest lie in the areas of analytical chemistry, biophysical chemistry and molecular structure with a keen interest in examining the structure, reactivity, and function of metal-containing bio-molecules, the complexes formed by these interactions and their uses in medicinal and pharmaceutical chemistry.