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Title

Developing a platform to enhance the oral bioavailability of novel pharmacophores via a protein drug delivery system for treatment of cancerous and neurodegenerative diseases”

Authors and affiliations

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Abstract

Nitrosative stress has recently been demonstrated as a crucial causal in the pathogenesis of Parkinson's and Alzheimer's diseases. Specifically, increased levels of NO disrupt the redox activity of protein-disulfide isomerase which leads to aggregation of misfolded proteins. We have demonstrated *in vitro* that polyphenolic phytochemicals, curcumin and 3,5-Bis(2-fluorobenzylidene)-4-piperidone (EF24), can rescue S-nitroso-PDI formation by scavenging NO<sub>x</sub> adducts. In our current research, we will explore the ligand-protein binding of 4 novel pharmacophores (pyridineamine platinum (II) complexes) which exhibit similar anti-cancerous effects. Spectrofluorimetry will determine the binding efficacy of these novel pharmacophores to  $\beta$ -lactoglobulin and human serum albumin. Binding of these novel pharmacophores to the milk protein and human transport protein ensures delivery to the microvilli of the intestine where it can be absorbed and transported directly into the systemic blood system. Based on a theoretical model, we propose a method for extracting the binding constants and corresponding binding site concentrations. According to this model, protein-ligand binding curves are solutions to a given linear second order partial differential equation. This method could be an alternative to the standard method of finding dissociation constants and concentrations using least squares methods. The results from this technique will allow us to guide protein-ligand docking experiments.