In Silico Studies of Fullerene C60 with Zebrafish Proteins Prostacyclin Synthase and S100z Calcium Binding Protein

Abstract

Nanotechnology offers many societal benefits and this have prompted the rapid growth of engineered nanomaterials. Fullerene (C60) due to its unique properties has become an important nanomaterial in biomedical and biotechnological applications. Once in water, Fullerene forms stable suspended aggregates and thus become bioavailable to aquatic biota. The fate and transport of fullerene in the aquatic environment is poorly understood. Little data are available on the molecular interactions of fullerene with native proteins of zebra fish (Danio rerio) which is a universally accepted experimental model. In this study, we made an attempt to assess the binding mode of fullerene with two key zebrafish proteins viz. Prostacyclin synthase (cytochrome P450 8A1) and S-100Z Calcium binding protein using Autodock 4.0. The data indicates that Fullerene potentially binds to the active sites of both the...
proteins and this may induce conformational changes in the native protein structure thereby altering the function, which might have a toxic effect to fish in survival. Further in vivo studies are required to evaluate the toxic impact on the expression and function of above proteins.

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Index Terms

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Autodock 4.0