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Similar to their results, in our study, Delavirdine exhibited favourable interaction with GP 120 protein which was greater than Maraviroc. Therefore, we selected Delavirdine as the standard for GP 120 inhibitors. The binding

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### **Molecular Dynamics Simulations of a Protein Protein Dimer**

Abstract In this article we present two 1000 ps molecular dynamics simulations on the rat -glutathione S-transferase dimeric enzyme in complex with the product 1-(S-glutathionyl)-2,4-dinitrobenzene, in a periodic box with explicit solvent molecules, and investigate the effect of long-range electrostatics models on the structure and dynamics of

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### **The Structure and Dynamics of ACTH 1-10 on the Surface**

ACTH (1-10), an adrenocorticotropin hormone fragment, was studied by molecular dynamics (MD) simulation in the NPT ensemble in an explicit sodium dodecylsulfate (SDS) micelle.

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