Title: Interaction between (E)-3-(3-(2,3-dimethoxyphenyl)acryloyl)-6-hydroxy-2H-chromen-2-one (DAC) with human serum albumin

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Abstract: Human serum albumin (HSA), the major carrier of blood components, is the most abundant plasmaprotein of the globular proteins family with a complete alpha-helical structure. HSA is able to transfer a lot of drugs such as coumarin. Coumarin is found naturally in many plants, which has a low toxic effect to the human body. (E)-3-(3-(2,3-dimethoxyphenyl)acryloyl)-6-hydroxy-2H-chromen-2-one (DAC), as a new derivative of coumarin, has anti-cancer effects comparable with cis-platin and much lower toxicity. This study was focused on the interaction between DAC and HSA as a drug carrier. Fluorescence spectroscopy were carried out in aqueous solutions at two temperatures of 25 and 37 °C and were complemented with molecular docking simulation for molecular details. Spectroscopic analysis of the emission quenching has revealed that the quenching mechanism of DAC is a static quenching mechanism. Using the modified Stern–Volmer equation, the number of binding sites was determined close to 1 at both temperatures of 25 and 37 °C. Since HSA has many potential binding sites, a blind docking was conducted over the protein after dividing it to eight overlapping boxes of equal size. The results were then refined via re-docking with finer grids of interactions. Reasonable agreement was found between computational and experimental results. This study can be useful in rational drug design to have fewer side effects for drugs.

Human serum albumin, Drug binding, Coumarin, Fluorescence

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