Experimental and theoretical studies on interaction of some drugs with human serum albumin

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ABSTRACT
The interaction of 14 anti-inflammatory drugs with human serum albumin (HSA) was studied by fluorescence quenching technique, molecular docking studies, and "quantitative structure activity relationship" (QSAR) method. Binding constants of the drugs obtained by fluorescence quenching method. Molecular docking was used for estimation of binding sites and binding constants of these anti-inflammatory drugs. The results of molecular docking indicated the role of hydrogen binding of the selected drugs in interaction with HSA. Finally, the QSAR model constructed between experimental binding constants of the drugs and theoretical descriptors. Theoretical descriptors were classes of constitutional, geometrical, functional group counts, atom-centered fragments, 2D frequency fingerprints, and molecular properties of DRAGON software [1]. A stepwise multiple linear regression (MLR) was used in the selection of the most relevant descriptors. Finally, a two-parameter model was developed. Descriptors revealed in model were sum of conventional bond orders (SCBO) and presence/absence of N and O at topological distance of 03 (B03 [N-O]). In order to assess the robustness of model, the leave-one out cross validation test was applied. The correlation coefficient of model was 0.95. The value of cross-validation correlation coefficient (Q^2) was found as 0.62, which showed robustness of the model.

Keywords: “Anti-inflammatory drugs”, “Human serum albumin”, “Fluorescence quenching”, “Quantitative structure activity relationship”, “Molecular docking”

References
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