Investigation of interaction between two anti-diabetic drugs and human serum albumin, through molecular docking simulation

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Abstract: Human serum albumin (HSA) is the most abundant protein in the body, which forms about 60-65% of the blood plasma proteins [1]. Many observations indicate an important relevancy between HSA concentration and health [2, 3]. In this study, the interaction between two anti-diabetic drugs (alogliptin and miglitol) with HSA is investigated. Employing molecular docking simulation helped to reveal the energy and site of these interactions. Docking results indicate that the interactions between alogliptin and miglitol with HSA are mainly located in domain IIA. Moreover, the interaction energy between alogliptin and miglitol with HSA is equal to -136.252 kcal/mol and -93.335 kcal/mol, respectively. The interaction between these two drugs to HSA is mainly attributed to the hydrogen bond and steric interactions. On the other hand, tyrosine150, compared to the other amino acids, highly increases the stability of these two drugs when interacts with HSA. The geometrical structure of miglitol and the steric hindrance regarded to the functional group of this compound are responsible for the weak binding of this drug to HSA. As a result, the interaction energy for alogliptin and miglitol explains the low and high necessary dosages of these drugs for diabetic disease, respectively.

Keywords: Human serum albumin (HSA); Molecular docking simulation; Alogliptin, Miglitol

References

[1] G. Zolese, G. Falcioni, E. Bertoli, R. Galeazzi, M. Wozniak, Z. Wypych, E. Gratton, A. Ambrosini, "Steady-state and time resolved fluorescence of albumins interacting with N-oleylethanolamine, a component of the endogenous N-acylethanolamines," J. Proteins: Struct Funct Genet. 40 (2000) 39-48.
[2] T. Peters. Jr, "All about albumin: biochemistry, genetics, and medical applications", 1rd Ed., Academic Press, New York, 1995.
[3] Y. Wang, Sh. Wang, M. Huang, "Structure and Enzymatic Activities of Human Serum Albumin," J. Curr. Pharm. Des. 21 (2015) 1831-1836.