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Pyrethroids and reproductive function: some endocrine disrupting perspectives from molecular simulations

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Abstract

Pyrethroids are widely used insecticides with huge applications for household as well as agricultural purposes and contribute to improved product quality and higher yields. In recent decades, the demand for pyrethroids has increased significantly due to advantages such as broad-spectrum efficacy, high insecticidal potential, and lower pest resistance. However, several studies have suggested that human exposure to pyrethroids leads to reproductive problems. Sex hormone-binding globulin (SHBG) is an important hormone transport protein regulating the availability of steroids at their target site. The aim of our study was to investigate the structural interactions of commonly used pyrethroids, cypermethrin and deltamethrin, with ligand binding pocket of SHBG. Cypermethrin and deltamethrin were docked into the steroid binding pocket of SHBG using Schrodinger's induced fit docking (IFD) followed by molecular dynamics (MD) simulation studies. The resultant SHBG-pyrethroid complexes from IFD experiments were subjected to structural analysis including the molecular interactions followed by binding energy estimation. The analysis revealed that both the ligands were tightly bound in the SHBG pocket with high percentage of commonality among the SHBG residues between the indicated pyrethroid ligands and the SHBG native ligand, dihydrotestosterone (DHT). The estimated binding energy values for cypermethrin were less but close to the values calculated for the SHBG native ligand, DHT. However, the estimated binding energy values for deltamethrin were higher compared to the values calculated for SHBG native ligand, DHT. Furthermore, the MD simulation results also revealed the higher stability of SHBG-deltamethrin than SHBG-cypermethrin complex. To sum up, the results suggested that deltamethrin has a greater capability than cypermethrin to prevent sex steroid hormone from binding to SHBG, even though both pyrethroids have this ability. Consequently, this might hamper the circulatory transport of sex steroid hormones and their availability at the target site, subsequently interfering with reproductive function.

Keywords: Endocrine disruption; pyrethroids; reproductive function; sex hormone binding globulin; structural studies.

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