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Non-specific side effects of the steroidal hormones found in oral contraceptives on lipid membranes

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All commercially available pharmaceutical products must undergo rigorous testing to determine their safety and efficacy, however these drugs interact with our bodies on a cellular level is often unknown. Hormonal oral contraceptives are commonly used by women to prevent pregnancy and treat symptoms, such as acne. While the drug mechanism that causes the desired effect -prevention of ovulation -is well understood, little is known about how the synthetic steroidal hormones interact with human cells. Understanding the non-specific interactions of these molecules with human cells could provide insight into the underlying causes of previously documented side effects and provide a more comprehensive understanding of how oral contraceptives interact with the human body.

In this study, Molecular Dynamics (MD) simulations were used to examine the behaviour of lipid membrane systems when introduced to norethindrone and ethinyl estradiol, two hormones used in oral contraceptives. Simulations containing 10mol% norethindrone, 10mol% ethynyl estradiol, and a 10mol% mix, with a 90mol% 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) membrane were run for 200ns. From this we visualized the location of the hormone molecules in the system, their effect on the membrane, as well as obtained electron density profiles of the system. This was compared to analysis of X-ray diffraction data of analogous experimental systems to see if MD corroborates the experimental results. This will improve our understanding of how oral contraceptives interact with human tissue, and potentially inform a mechanism as to the underlying causes of their side effects.

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