DEVELOPMENT OF BIOCOMPATIBLE DRUG CARRIERS FOR IMPROVED DRUG LOADING AND RELEASE PROFILES

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Extensive research has focused on developing effective and biocompatible drugs and drug-delivery systems. Capsaicin, a natural compound found in hot peppers, has potential therapeutic properties, such as pain relief and anti-inflammatory effects. However, its clinical application is limited by low cellular absorption, chemical instability, poor aqueous solubility, and some side effects, such as skin irritation and burning sensation. Lecithin, a phospholipid with biocompatibility and liposome-forming abilities, can be used in drug delivery systems. Both capsaicin and lecithin exhibit hydrophilic and hydrophobic characteristics, allowing them to self-assemble in aqueous solutions for drug loading and release.

Molecular docking and molecular dynamics, two crucial computational techniques in the fields of computational chemistry and structural biology, are instrumental for scrutinizing molecular interactions, especially in the context of drug discovery and protein-ligand interactions. In this study, we employ these methodologies to investigate the self-assembly behaviour of capsaicin and lecithin in an aqueous environment, revealing strong self-assembly into well-defined, arbitrarily shaped aggregates. The hydrophilic-hydrophobic nature of the materials enables improved drug loading and controlled release. Furthermore, the carrier enhances the physicochemical properties of capsaicin by forming stable complexes through nonbonded interactions. These findings inform the development of new drug delivery systems that utilize the self-assembly properties of amphiphilic molecules to improve the delivery and effectiveness of hydrophobic drugs.

The distance between the hydrophobic groups in capsaicin and lecithin appears to be smaller compared to the hydrophilic groups. The spacing ranges from 0.33 to 0.62 nm and 1.28 to 1.48 nm, respectively, this variation is because of an increased concentration of lecithin monomers, which ranges from 1-8. Increasing the concentration of lecithin has an impact on the rotation angle of capsaicin at the centre, reducing it from 123° to less than 60° and increasing the availability of water surrounding it. Additionally, an increase in lecithin concentration affects the arrangement of atoms attached to it. For example, the distance between the hydrogen of the hydroxyl group and the oxygen of the methoxy group increases from 0.25nm to 0.44nm, allowing more water to interact with capsaicin, thereby enhancing its ability to dissolve in water.

These observations suggest that hydrophobic groups play a crucial role in facilitating the rapid entrapment of capsaicin via hydrophobic forces. As the concentration of lecithin increases, the complex becomes more stable, strengthening the hydrophobic forces that hold capsaicin tightly and reducing its flexibility, which is crucial for effective loading and release.