ABSTRACT

Curcumin is a chemical compound abundantly found in the rhizome of turmeric (Curcuma longa). Over the past eight decades, curcumin has demonstrated a wide range of disease-preventing properties, such as anticancer, antimicrobial, antioxidant, Alzheimer's, Parkinson's, and anti-inflammatory activities. However, curcumin has poor water solubility (11 mg/mL) and low stability, resulting in less than 50% absorption during metabolism. It also undergoes hydrolysis and oxidation in the gastrointestinal environment, leading to poor bioavailability. This is disadvantageous for patients, as much of the drug is excreted in feces before being absorbed. This presents a major challenge in utilizing curcumin as a drug. An innovative approach to this issue involves a drug delivery system that penetrates the skin to reach the bloodstream with minimal side effects. CMC (carboxymethyl cellulose) can enhance solubility stability, is safe for skin application, widely used in healthcare, and capable of delivering drugs to targeted cells. One such transdermal drug delivery development involves a highly selective method using Molecularly Imprinted Polymer (MIP), which includes molecular imprinting to provide high selectivity for the target molecule, high binding capacity, excellent permeability, and tunable release over time, with controlled drug release, supported by classical in silico computations (molecular docking and sequential docking). This study resulted in the synthesis of MIP in the form of a fine yellow powder. MIP with varying compositions yielded the best result at 0.4 grams, with an imprinting factor (IF) of 2.97. Adsorption on MIP followed the Langmuir adsorption isotherm model with values of KL, Qm, and R being 0.012, 9.911, and 0.9997, respectively. The binding capacities of MIP, NIP, and CMC were 1157.88 µg/g, 389.93 µg/g, and 265.25 µg/g, respectively. Desorption and in vitro testing followed the Higuchi model, which indicates that curcumin release is proportional to the square root of time, meaning the release rate increases with time. Computational results confirmed that more negative (more stable) binding free energy indicates stronger interaction between the receptor and ligand. Binding energy can be utilized for drug release: the surface of CMC can strongly bind to curcumin and is assumed to release the drug slowly, serving as a foundation for sustained drug release in a drug delivery system.

Keyword: CMC, MIP, Curcumin, Transdermal, In silico