Nano-Bio Interactions: Curcumin Positioning on Native and Modified Cellulose Fibers

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ABSTRACT

Cellulose nanofibers have attracted much attention because of their high potential for adaptive drug delivery systems. In this study, the binding affinity of curcumin to native, acetylated and methylated 10-monomer fibers was compared using molecular docking methods. Given the stronger interaction of acetylated fibers with curcumin, these fibers are expected to replace less efficient carriers, thereby improving the drug delivery of curcumin.

Keywords: **Curcumin, Cellulose Nanofiber, Molecular Docking, Acetylation, Methylation, Drug Delivery**

1. INTRODUCTION

Curcumin, the most active curcuminoid found in the *Curcuma longa* plant [1], has anti-microbial, antiviral, and antifungal qualities, while also being effective in treating inflammatory diseases, cancers, arthritis, and asthma [2]. Despite its extensive medical applications, this polyphenol molecule's physicochemical instability, rapid systemic elimination, limited permeability, low bioavailability, and low solubility in release media are some of curcumin's drawbacks [3]. Therefore, in order to preserve this compound's unique character, certain delivery mechanisms are necessary [4]. The hydrophilicity, capacity to retain moisture and structural stability of cellulose [5], nanocellulose's unique structure, high surface area, and biological properties—including biodegradability, biocompatibility, fewer side effects, and low toxicity—and its ability to provide continuous or regulated medication release and targeted distribution in the body make it a promising drug delivery vehicle system [6–8]. As interest in cellulose nanofibers has grown recently, studies have been carried out to improve their extraction and uses using techniques such as TEMPO-mediated oxidation, Fourier transform infrared spectroscopy, and enzymatic hydrolysis [9]. Furthermore, due to the importance of the 3D structure in the functionality of this biopolymer, extensive studies have been carried out in this field [9]. Physical and chemical surface modifications of nanocellulose can enhance its processability, broaden its industrial applications, and improve its quality [10]. In this study, the potential of various forms of cellulose in drug delivery of curcumin were investigated using computational biology methods.

2. METHODS

The 3D coordinates of three types of 10-monomer β-cellulose fibers—native, triacetylated, and trimethylated—were generated using Glycam [11]. Then, the interactions between these cellulose fibers and curcumin (retrieved from the PubChem database, CID: 969516) were analyzed using AutoDock 4.2 and AutoDockTools [12]. All dockings included 50 genetic algorithm runs with 25000000 as the maximum energy evaluations. Finally, the best complexes were visualized using PyMOL [13].

3. RESULTS

The results demonstrate that cellulose fibers modified by acetylation and methylation, with binding energies of -6.9 and -4.7 kcal/mol respectively, exhibit stronger interactions with curcumin compared to native fiber with a binding energy of -4.1 kcal/mol. In this visualization, it was observed that, the curcumin is positioned at the end of the native fiber (Figure 1a), but on the other two types of fibers, it is located approximately in the middle of the nanofibers (Figure 1b,c).

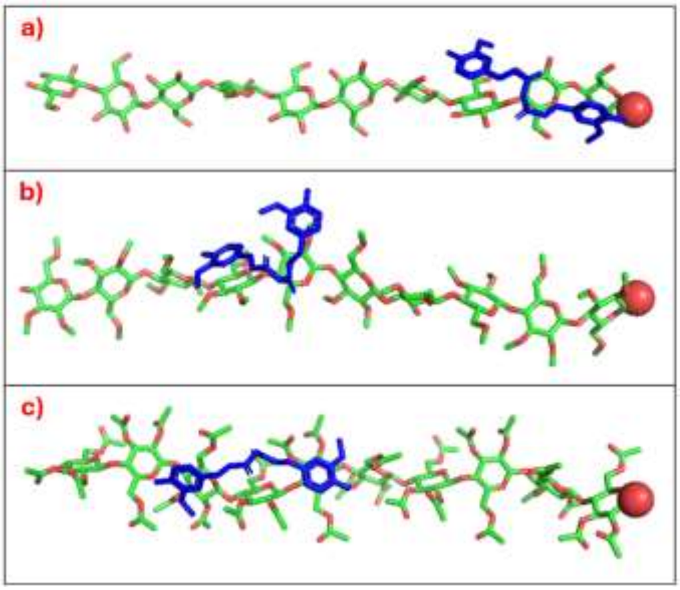

Fig. 1. The selected and reported docking results with the lowest and most optimal binding energies. Molecular docking best poses of curcumin docked on a) native cellulose, cellulose units with modifications of b) methylation, and c) acetylation. In all sections, fibers and curcumin are depicted in green and blue accordingly.

4. DISCUSSION AND CONCLUSIONS

Compared to native cellulose, cellulose derivatives and nanocellulose have better solubility, biocompatibility, tuneability, and functionalization properties, making them more appropriate for the creation of composite materials [5]. Additionally, this analysis indicates that acetylation modifications on cellulose create more potent curcumin delivery options.

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