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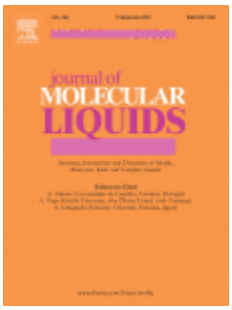

Fabrication, characterization, and application of wound dressing based on PVP/PVA nanofibers containing β-cyclodextrin/curcumin complex: From in silico to in vitro studies

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Abstract

The β-cyclodextrin-curcumin (β-CD-Cur) complex was applied in this study to modify the PVP nanofibers. The complexation of the Cur with β-CD was investigated using density functional theory (DFT) and molecular dynamics modeling. Geometries for all compounds were optimized based on DFT-D. Then, in order to adsorb compounds on the substrate, Monte Carlo calculations were used. The physicochemical properties (morphology, surface functional groups, water absorption, water vapor permeability, solubility, and tensile strength) and biological studies such as biocompatibility, blood compatibility, drug release, and antioxidant tests were performed. The Monte Carlo/Molecular Dynamics calculations strongly affirmed the complexation of Cur with *β*-CD and *β*-CD /Cur over the polymer due to negative energies. The obtained results indicated that the *β*-CD /Cur complex increased the solubility of this compound in an aqueous medium. The amount of drug released reached its maximum in 48 h, which is suitable for wound healing applications. Compared to unmodified nanofibers, the amount of hemolysis decreased significantly, which indicates the favorable effects of introducing the complex and its appropriate blood compatibility for clinical studies. MTT studies showed that modified nanofibers increase cell viability after 24 and 72 h. This increase is directly related to improving the concentration of the complex from 5 to 15%. The current study provides data regarding the interactions between Cur and β-CD and their combination in the polymeric matrix. Moreover, experimental results revealed the promising potential of the fabricated structure as a nanofibrous wound dressing.

The skin is a barrier between the human body and the external environment. It protects the body against exogenous chemical and physical factors, participates in metabolic processes, acts as an absorbent and heat regulator, and is the first line of defense against pathogenic microorganisms, and participates in immunological processes [1]. Physical or thermal damage can cause defects or breaks in the epidermis of the skin or mucous membranes and cause ulcers. Wounds are classified as acute or

Materials

In this study, β-CD, Cur, PVP, and PVA were all supplied from Sigma Aldrich (USA). DMSO and ethanol were both prepared from Merck (Germany). The phosphate-buffered salt was obtained from Shimi-Tajziyeh (Iran).

Complexation of cyclodextrin with curcumin

To synthesize the β-CD/Cur, 250 mg of Cur was dissolved in 10 mL of ethanol. In another vial, 1.4 gr β-CD was dissolved in 30 mL of water, then the Cur solution was added to the β-CD solution dropwise and stirred for 24 h. After the specified time, the final solution was freeze-dried.

Drug loading

For

SEM images

The SEM imaging showed that the fabricated nanofibers were almost identical in diameter ($P < 0.01$). In addition, the results showed that the fabricated nanofibers are nearly uniform, and no spindle-shaped structure was observed (Fig. 2). It was also found that introducing the complex to the nanofibers did not disrupted the structure and morphology of the nanofibers. As it is apparent (red circles), β-CD/Cur complexes are placed in the nanofibers as agglomerates. In addition, with the increase

Conclusion

The results of the present study indicate that the addition of cyclodextrin-curcumin complex to nanofibers did not significantly altered the structure and morphology of the nanofibers. With the increase in the concentration of the β-CD/Cur complex in the nanofibers, the tensile strength decreases. The drug released reached its maximum in 48 h, and 100% of the drug released. This feature is essential for regenerative medicine studies, including burn wounds. The present study showed that the

Availability of data and materials

The datasets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

CRediT authorship contribution statement

Hossein Derakhshankhah: Conceptualization, Supervision. **Rahime Eshaghi Malekshah:** Visualization. **Zhil Izadi:** Investigation. **Mahya Samari:** Investigation. **Mohammad Rezaee:** . **Hadi Samadian:** Conceptualization, Visualization, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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