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Research Article

Spectroscopic, Quantum Chemical, Molecular Docking Studies on Cellulose Acetate: Polyvinylidene Fluoride Blend Polymer Membrane for Wound Healing

S Pushpam, Shamima Hussain, T Joel, T Mathavan, A Milton Franklin Benial*

Department of Physics, N.M.S.S.V.N. College, Nagamalai, Madurai, India

ABSTRACT

Recently, extensive research works are going based on wound healing and drug release materials. In the present work, cellulose acetate: Polyvinylidene fluoride blend polymer film was prepared to access its drug release activity against wound healing. Polymer film was prepared by solution casting technique and DMSO solvent. The optimized sample was determined using different characterization technique for different composition of CA: PVDF. The change in FTIR peaks upon varying the PVDF content in CA: PVDF shows the complexation. This complexation results in the collapse of CA matrix semi crystallinity which is observed from the reduced intensity in the XRD diffraction peaks. The result reveals that the sample is semi crystalline in nature. Nevertheless, the addition of PVDF decrease the semi crystallinity nature that the enhancement of amphorous nature.

Keywords: Cellulose acetate; Polymer film; PVDF; XRD; FT-IR; DFT calculation; Molecular docking

INTRODUCTION

Even as healthcare has seen rapid advancements in recent decades, creating appropriate biomaterials for wound healing remains highly challenging. The healing process involves fibroblast proliferation for wound contraction, followed by matrix deposition to regenerate new vessels and epithelial tissue. Any disruption in this process can lead to healing failure and prolonged recovery. There is an urgent need for biomaterials that can effectively support skin reconstruction. These materials must be biocompatible, bioactive, possess sufficient mechanical strength, and maintain appropriate rates of biodegradation and stability in physiological conditions. Topical drug delivery is important for effective management and treatment of wounds, ensuring patient compliance. However, challenges such as enzymatic degradation and drug permeation through skin barriers remain significant concerns. To address these issues, novel delivery techniques like scaffolds, nanoparticles, solid lipid nano carriers, and liposomes are being employed. Biopolymer textiles have emerged as particularly promising in biomedical applications due to their similarity to the extracellular matrix of human skin tissue. It is important to finding effective methods for tissue regeneration and therapeutic interventions involves facilitating the delivery of cells, drugs, and genes through injectable or implantable approaches [1].

Cellulose is an essential and intriguing biopolymer known for its abundant and renewable nature. The global trend towards utilizing such resources and creating innovative products for science, medicine, and technology has fuelled resurgence in interdisciplinary cellulose research over the last decade. This has led to extensive use of this organic polymer across diverse fields. Cellulose is among the most widely found natural polymers, contributing 700,000 billion tons to total biomass production each year. Most cellulose consists of amphorous and crystalline domain depending upon the nature. The hydroxyl groups in the cellulose framework can be chemically altered to form ester groups that are water-insoluble. The accessibility of cellulose molecules to reagents is pivotal for the efficiency and success of any chemical reaction aimed at modification. The crucial step in obtaining derivatives lies in ensuring effective contact between the reactants. Cellulose presents a unique challenge in this regard due to its biphasic structure, which complicates the process of interaction. In this study, Cellulose Acetate (CA) has been selected as the base polymer due to its unique capability to simultaneously concentrate and separate substances in a single step during ultrafiltration. CA possesses inherent qualities such as strong biocompatibility, widespread availability, renewable

Correspondence to: A Milton Franklin Benial, Department of Physics, N.M.S.S.V.N. College, Nagamalai, Madurai, India; E-mail: miltonfranklin@yahoo.com

Received: 23-Dec-2024, Manuscript No. DDO-26-36105; **Editor assigned:** 26-Dec-2024, PreQC No. DDO-226-36105 (PQ); **Reviewed:** 10-Jan-2025, QC No. DDO-26-36105; **Revised:** 12-Aug-2025, Manuscript No. DDO-26-36105 (R); **Published:** 19-Aug-2025, DOI: 10.35248/2169-0138.25.14.302

Citation: Pushpam S, Hussain S, Joel T, Mathavan T, Benial AMF (2025) Spectroscopic, Quantum Chemical, Molecular Docking Studies on Cellulose Acetate: Polyvinylidene Fluoride Blend Polymer Membrane for Wound Healing. Drug Des. 14:302.

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sourcing, cost-effectiveness, and eco-friendliness. Over the past three decades, cellulose acetate membranes have found extensive use across various fields including bioengineering, pharmaceuticals and food industries. CA has garnered significant interest, especially in the development of electrospun nanofiber membranes and drug development. Due to their low toxicity and excellent compatibility, CA membranes are well-suited for applications such as cell culture, drug delivery, tissue engineering, toxin removal from solutions, bioprocessing, and medical filtration. The moderate hydrophilicity, an adequate mechanical strength, and sufficient chemical stability can be provided when CA blended with other polymers [2].

Poly (vinylidene fluoride), commonly known as PVDF, has a repeating unit of (CH2-CF2). This polymer is often employed as a matrix membrane because of its superior thermal stability, membrane- forming characteristics, and high mechanical strength. However, the hydrophobic properties of PVDF membranes lead to fouling, which impairs their performance and shortens their life span. Enhancing hydrophilicity is essential to minimize fouling in PVDF membranes. Among the various materials used to improve PVDF membrane hydrophilicity, natural polymers are noteworthy for their affordability and availability [3].

To improve these characteristics, various methods have been explored. Chemical modifications, plasma treatments, and surface grafting techniques have been employed to introduce hydrophilic functional groups to PVDF membranes. Typically, PVDF microfiltration membranes are produced using non solvent-induced phase inversion. An alternative and relatively straightforward approach to enhance PVDF membrane performance is to blend PVDF with other membrane materials. PVDF itself is a highly non-reactive thermoplastic fluoropolymer created through the polymerization of vinylidene fluoride. PVDF is a specialized plastic designed for applications demanding the utmost purity and resistance to solvents, acids, and hydrocarbons. With a density of 1.78 g/cm^3, PVDF is lighter than other fluoropolymers such as polytetrafluoroethylene. It is a prominent example of polymeric materials with notable scientific and technological properties [4].

MATERIALS AND METHODS

Materials

CA was purchased from Loba Chemical Pvt. Ltd. Mumbai, Maharashtra, India. The PVDF was purchased from sigma aldrich (average Mw ~534,000 by GPC, powder). The solvent Dimethyl Sulfoxide (DMSO) was also purchased from merck specialities private Ltd., Mumbai, India. All the chemicals have been used without any further purification [5].

Preparation of CA: PVDF flexible film

Solution casting is a simple and easy method to prepare polymer films. In this method the base polymers and complexation material are dissolved in a suitable solvent and stirred well to obtain a homogeneous mixture. The resulting viscous solution is poured onto a petri dish and allowed to evaporate at 60°C for 24 hours. This procedure provides mechanically stable, free standing and flexible films. The films are further vacuum dried for the required time to remove any trace of solvent. The CA and PVDF complex (Table 1) have been prepared by dissolving CA and PVDF in DMSO (50 ml) with proper ratios ((100:0), (95:5), (90:10), (85:15), (80:20) (CA: PVDF)) and stirred continuously until a homogenous solution was obtained. Then the solution has been transferred into petri dish and dried at 60°C to eliminate the solvent. The obtained film was taken for further characterization. Figure 1 shows the schematic representation of solution casting technique. CA and PVDF complex have been synthesized by solution cast-technique with different concentrations [6].

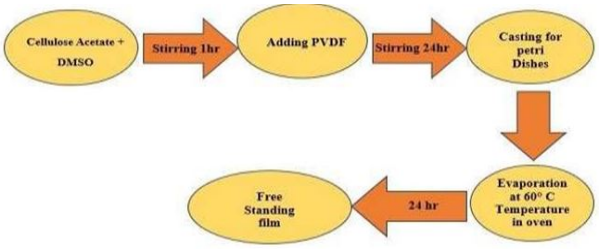


Figure 1: The schematic representation of solution casting technique.

Table 1: The CA and PVDF complex.

Sample code	Cellulose acetate (g)	PVDF (g)
Pure CA	1	-
CA:5% PVDF	1	0.0527 (5% in 1 g)
CA:10% PVDF	1	0.1114 (10% in 1 g)
CA:15% PVDF	1	0.1771 (15% in 1 g)

CA:20% PVDF	1	0.2524 (20% in 1 g)

Thickness measurement of films

The thickness of the film plays a significant role when using the film for packaging applications. The thickness of films was measured using ASTM D6988 standards. A digital vernier calliper (Mitutoyo, Japan) was adopted to determine the thickness of the film. The readings were taken at five different places and the average value is considered.

FTIR instrumentation

The sample was analysed on the JASCO FTIR 4600 device with Fourier transform. The absorption frequencies are expressed in cm^{-1}. FT-IR spectrum (4000-400 cm^{-1}) was recorded as ATR mode in the solid phase at room temperature with the number of scans 4 mm/sec and resolution 4 cm^{-1}.

X-ray diffraction measurements

X-Ray diffractometer using a Bruker D8 Advance ECO XRD machine. The data was collected at room temperature using Cu-Kα through the scanning percentage set at 2O per minute straddling the array of 100-800. The C K-edge spectra for pure and composite films to study the effect of additives on the host polymer matrix [7].

RESULTS AND DISCUSSION

X-ray diffraction analysis

X-ray diffraction analysis is a versatile tool to monitor the changes in structural properties of both crystalline and amorphous region of system. Figure 2 depicts the XRD patterns of pure CA and CA with different concentrations of PVDF. A well-known crystalline peak at 2θ=10°, 13° and 17° have been reported for pure CA film. In order to investigate the influence of different concentration of PVDF to pure CA, relative intensity of peak between 10° and 20° were evaluated. All these information clearly depict that increase the concentration PVDF enhances the amorphous nature of the film. It has been also noted that CA with different concentration of PVDF as shown in the Figure 2. The XRD analysis reveals the qualitative identification and quantitative analysis of the β phase to identify the crystalline phase of PVDF. The XRD spectra (Figure 2a-e) confirm that the peaks at 17.4°, 17.64° and characteristic of the α phase of PVDF, and the peaks at 18.12°, 18.64°, 20.04°(d), 20.4° (e), characteristic of the γ phase. The peak at 2θ=26.96° is related to the diffraction of β phase shown in Figure 2(e). The percentage of the crystallinity of the samples are tabulated in Table 2. It can be observed that the percentage of the crystallinity with increasing the concentration of PVDF [8].

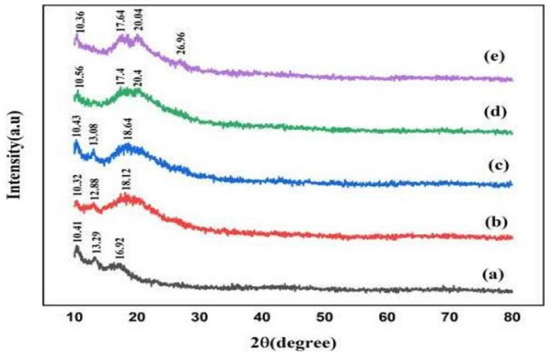


Figure 2: X-RD profile of (a) Pure CA; (b) CA: 5% PVDF; (c) CA: 10% PVDF; (d) CA: 15% PVDF; (e) CA: 20% PVDF.

Table 2: The percentage of crystallinity of the samples.

S. no	Sample code	Area of crystal peak	Total area	Crystallinity (%)
1	Pure CA	367	1213.62	30.2
2	CA:5% PVDF	482.22	1748.69	27.57
3	CA:10% PVDF	422.13	1707.132	24.72
4	CA:15% PVDF	428.1	1938.26	22.08
5	CA:20% PVDF	368.75	1839.39	20.01

FT-IR experimental analysis

The observed FT-IR spectra of the pure CA and CA with different concentration of PVDF (Pure CA, CA+5% PVDF, CA +10% PVDF, CA+15% PVDF, CA+20% PVDF) presented in Figure 3. The change in intensity of the peaks represents the successful introduction of the PVDF in the CA. Moreover, the stretching of carbonyl group at 1441 cm^{-1} is due to strong intermolecular interaction between the oxygen atom of the carbonyl group which result in the CA and PVDF polymer complex. The FTIR results show no extra bands appear with the addition of PVDF which indicates that there is no chemical interaction between PVDF and CA blends.

The spectrum at 605 cm^{-1} is associated in-plane bending or rocking vibration in α-phase of PVDF. In comparison with pure CA, the CA: 5% PVDF, CA: 10% PVDF, CA: 15% PVDF, CA: 20% PVDF, the modes 1065 cm^{-1}, 915 cm^{-1}, 732 cm^{-1}, 605 cm^{-1} was shift to pure CA and spectra at 1441 cm^{-1} are similar to pure CA. On comparing the pure CA and CA: PVDF FTIR spectra bands were shifted but the functional groups were the same, which clearly shows that the composite has good compatibility and better homogeneity/miscibility of composite film. Subsequently the results of FTIR prove that there is no effect of DMSO on CA and CA: PVDF films [9].

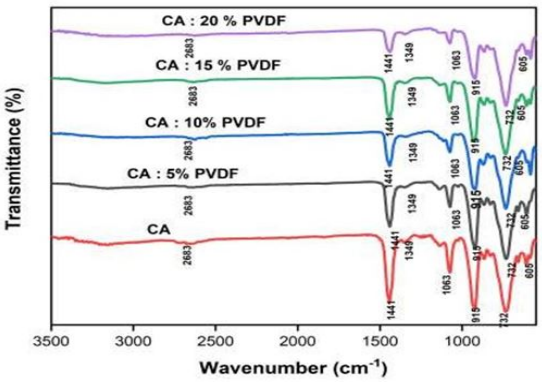


Figure 3: FTIR (experimental) profile of (a) pure CA; (b) CA: 5% PVDF; (c) CA: 10% PVDF; (d) CA: 15% PVDF; (e) CA: 20% PVDF.

Thickness measurement of films

The thicknesses of the pure CA, CA+5% PVDF, CA+10% PVDF, CA+15% PVDF and CA+ 20% PVDF, film values are tabulated in Table 3. From the table, the thickness of the film increases with increasing the concentration of PVDF.

Table 3: The thickness of the flim.

S. no	Sample code	Thickness of the film (mM)
1	Pure CA	0.098
2	CA:5% PVDF	0.148
3	CA:10% PVDF	0.152
4	CA:15% PVDF	0.138
5	CA:20% PVDF	0.141

UV-vis spectral analysis

The electronic properties of the CA: PVDF molecule were investigated based on UV-vis spectral analysis. The UV-vis spectrum was theoretically simulated in the liquid phase using DMSO as a solvent. TD-DFT calculations predict the transitions in the UV-Vis region for CA, PVDF, and CA: PVDF molecules. The transitions was calculated at 186.5 nm with an excitation energy value of 6.6479 eV correspond to the n→π* transition of the CA molecule, similarly for the PVDF and CA: PVDF molecule. The transitions was calculated at 187.1 nm with an excitation energy value of 6.6266 eV correspond to the n→π* transition of the PVDF molecule. The transitions was calculated at 189.5 nm with an excitation energy value of 6.5427 eV correspond to the n→π* transition of the CA: PVDF molecule. This transition is due to the interactions between the lone pair electrons of the electronegative atoms and the π electrons.

Frontier Molecular Orbitals (FMOs) analysis

Frontier molecular orbitals refer to the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO). The HOMO is the outermost higher-energy orbital containing electrons, which acts as an electron donor. The LUMO is the lowest-energy orbital that has to accept electrons, which acts as an electron acceptor. The frontier molecular orbital anlysis predictis reasonable qualitative the excitation properties and the ability of electron transport. The FMOs of the CA, PVDF, and CA: PVDF molecules were computed by the DFT/B3LYP method with a 6-311 ++G (d,p) basis set. The HOMO and LUMO orbitals were visualized.

Mulliken atomic charge distribution analysis

Mulliken charges are directly related to the molecular orbital characteristics of the molecule; they are therefore directly related to the chemical bonds present in the molecule. The Mulliken atomic charge distribution of a molecule has a significant influence on the dipole moment, polarizability, electronic structure, and vibrational modes. The Mulliken atomic charge distribution has been used to describe the process of electronegativity equalization and the model of electrostatic potential outside the molecular surface.

CONCLUSION

The CA: PVDF film was successfully prepared by solution casting technique. The interaction of CA and PVDF was confirmed using FTIR and XRD calculations. FTIR studies reveal that the increase in the concentration of the additive in the CA polymer matrix leads to a change in intensity in the vibrational modes confirming the interaction of CA and PVDF. This change was further investigated using XRD studies and it could be concluded that the interaction between CA and PVDF. Our findings indicate that the sample containing CA: 15% PVDF is significantly more stable and flexible than the others. Through the use of the DFT/B3LYP method with a 6-311G ++ (d,p) basis set, we optimized the molecular structure of the CA: PVDF molecule, allowing us to obtain highly accurate theoretical vibrational frequencies. Additionally, our simulation of the UV-Vis spectrum showed a band gap of approximately 6.6 eV, Furthermore, FMOs analysis revealed that the CA: PVDF molecule has a stable structure, and its energy gap value is comparable to bioactive aromatic compounds. Finally, our Mulliken atomic charge distribution analysis confirmed the presence of Intra-molecular Charge Transfer (ICT) within the molecule, indicating that the carbon atom was highly influenced by the substitution. In these analysis the interaction of the CA: PVDF with the wound healing protein by molecular docking methods. By the binding affinities of receptors showed that the CA: PVDF, which could be a potential ligand by docking methods. Thus it can be used as PVDF molecule, a novel, and natural dug carrier molecule. The CA: PVDF can be used as a promising dressing materials for different types of wound. Overall, our analysis highlights the significant potential of the CA: PVDF molecule for further medical development.

ACKNOWLEDGEMENT

The authors thank the college management for encouragement and permission to carry out this work and PG and Research Department of Physics, N.M.S.S.V.N. College, Nagamalai, Madurai-19 for providing the Gaussian 09program package.

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