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RESEARCH ARTICLE

In Silico Evaluation of Microplastics Interactions for Storage of a Multi-Epitope Vaccine Candidate

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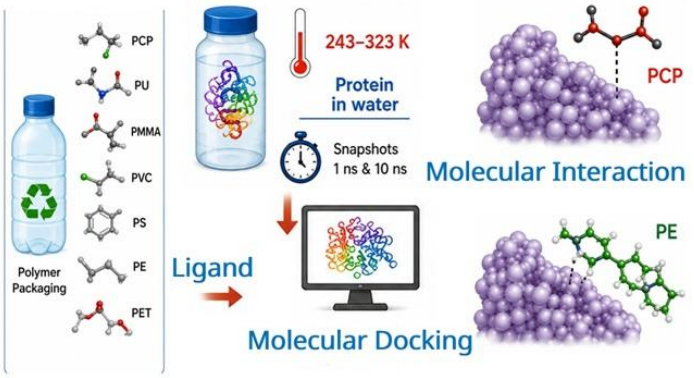
Abstract: The increasing prevalence of multidrug-resistant disease has addressed an urgent requirement for early prophylactic therapies like a vaccine. Their therapeutic efficacy entirely depends on the supply chain & storage parameters. Conventional vaccine formulations have mainly used glass vials, while polymer-based packaging offers reduced package volume, weight and price per dose. But the emergence of microplastics (1-10 µm) as leachable from those polymeric containers may destabilize the vaccine product and toxify the human CYP1A1 protein. Leaching may also occur under different storage temperature conditions. For this, all-atom molecular dynamics simulation on the multi-epitope vaccine was conducted under the OPLS-AA force field, NaCl-neutralized SPC water model, 1atm pressure, and varying storage temperatures. These systems were energy-minimized and equilibrated under constant NVT and NPT conditions for 100 ps, followed by a 10 ns production simulation. Blind & flexible docking of the simulated vaccine snapshots with monomeric polymer structures (i.e., PET, PU, PMMA, PVC, PS, PE, PCP) yielded insights into polymer-vaccine interactions. Initially, both docking methods yielded PCP, a non-biodegradable polymer as weakest binder. Thus, the current investigation may serve as a basis for further studies to validate the suitability of PCP derived vials for vaccine storage.



Keywords: *Vaccine, packaging, storage, microplastics, molecular docking study, molecular dynamics simulation*

Introduction

Modern sustainable way of vaccine development depends on immunological computation to improve its safety and immunogenicity.[1] Such engineered vaccines combine T-cell and B-cell epitopes and have shown advantages over traditional vaccines (cost-effectiveness, specificity, stability).[2] Meanwhile, there is a growing interest in polymer-based vaccine packaging because the polymer vials (e.g., cyclic olefin copolymers) offer the benefits of light weight, flexibility, and low breakage risk.[3] For example, Topas COC polymer has been adopted to alleviate shortages of glass vials for COVID-19 vaccines due to its proven inertness.[4] However, conventional plastic materials i.e. polyethylene (PE), polychloroprene (PCP), polyvinyl chloride (PVC), polystyrene (PS), polyurethane (PU), polymethyl methacrylate (PMMA), and polyethylene terephthalate (PET) can shed micro and nano plastics during storage, raising safety concerns. MPs are well known sourced which contaminate food and water that have been shown to disrupt immune function. They can initiate inflammation, which causes cellular toxicity in experimental models.[5] In the context of vaccines, any interaction between microplastic fragments and protein antigens could affect the structure and immunogenicity of the engineered multi-epitope construct. Despite these concerns, the molecular-level interplay between vaccine antigens and packaging materials has not been extensively studied. Computational methods offer a way to evaluate this scenario and can offer a polymer of choice which can sustain the vaccine molecule in different storage temperature. Molecular dynamics (MD) simulations and Molecular docking have been widely used to predict the stability of vaccine constructs and their binding to receptors.[6] As an example, the multi-epitope vaccine currently studied were previously used 100 ns MD simulation to confirm structural stability.[7] Together with molecular docking study MD simulation claimed its binding to Toll-like receptor 5, signifying its immunotrigerring potential.[8] Building on such approaches, we aim to examine how the monomeric polymers mimicking their micro form interacts with the designed multi-epitope vaccine candidate. In this study, all-atom MD simulations were designed to obtain various conformation of the multi-epitope vaccine construct as snapshots, under various storage temperatures i.e. 243K, 277K, 313K and 323K. Both, rigid body

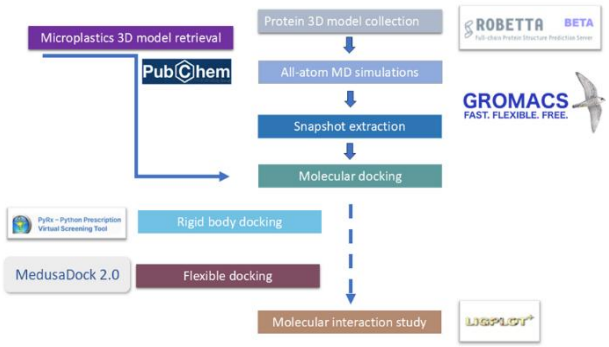


Figure 1. *Workflow of the study showing microplastics and multi-epitope vaccine model retrieval, all-atom MD simulations, snapshot extraction, molecular docking (rigid and flexible) and molecular interaction studies.*

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and flexible molecular docking approaches were aimed to be utilized for the docking of microplastic monomers with the simulation snapshots.[9] Molecular interaction study was conducted on the vaccine-polymer complexes to identify the bonded and non-bonded contacts present between the polymer and the vaccine structure. Together, this study investigates how temperature-induced conformational variations in the multi-epitope vaccine construct impact the interaction profile with microplastics. The overall methodology has been described in Figure 1.

Materials and Methods

1. MD Simulation of the Multi-Epitope Vaccine Construct under Different Storage Temperatures

All-atom molecular dynamics (MD) simulations were performed using the GROMACS 2022 on the designed multi-epitope vaccine construct under different temperature conditions. The 3D structure of the vaccine construct, previously validated in a "protein in water" MD environment at 300K was used as the starting model.[7] Differing the temperature, the system was prepared using the Optimized Potentials for Liquid Simulations (OPLS) force field, while Simple Point Charge (SPC) water model was employed for solvation. The protein structure was centered within a cubic box, maintaining a minimum distance of 1.0 nm between the vaccine model surface and the box. Energy minimization was performed to remove steric clashes. Long-range electrostatic interactions were treated using the Smooth Particle Mesh Ewald (SPME) method, while van der Waals interactions were calculated within 1.0 nm cut-off. The minimization process was conducted for 50,000 steps with an energy tolerance of 1000 kJ/mol/nm, step size 0.01. Following energy minimization, the system was equilibrated under constant number of particles, volume, and temperature (NVT ensemble). Here, the initial velocities were assigned and the leap-frog integrator was used. The simulation was performed with a time step of 0.002 ps for 500 steps. Subsequently, the system was equilibrated under constant pressure and temperature (NPT ensemble) conditions using the checkpoint file obtained from the NVT phase as input. The equilibrated system was then subjected to a 10 ns production MD simulation under NPT conditions.[10] To get the different conformations of the multi-epitope vaccine construct under different storage temperatures, MD simulations were carried out at four different temperatures, i.e. 243K, 277K, 313K and 323K. The radius of gyration (Rg) was analyzed to assess the compactness and structural integrity of the vaccine model in different temperatures. Furthermore, the snapshots were generated for the "Protein" group of trajectories on the 1 ns and 10 ns time frames.

2. Microplastics 3D Structure (Monomers) Retrieval

Three-dimensional (3D) structures of representative polymer monomers associated with common packaging materials were retrieved from PubChem databases. The selected monomers are PET, PU, PMMA, PVC, PS, PE, and PCP. [11] These monomers represent potential microplastic particles that may leach from polymer-based packaging materials during storage.

3. Molecular Docking Study

To evaluate the possible binding affinity between the vaccine construct and microplastic monomers, molecular docking studies were performed. Both rigid and flexible docking approaches were used to explore possible binding orientations and interaction energies.

3.1. Rigid Body Docking

Rigid body molecular docking studies were performed to evaluate the interaction between the multi-epitope vaccine construct and selected polymer molecules using the PyRx platform,[12] which integrates AutoDock Vina for docking calculations.[13] Initially, the protein structures obtained from MD simulation snapshots were imported into the PyRx workspace. They were prepared as macromolecules by converting them into AutoDock compatible formats. Ligand molecules representing different polymers, i.e. PE, PCP, PVC, PS, PU, PMMA, PET were loaded as structure data file (.sdf) format using the Open Babel module integrated within PyRx. Ligand preparation involved geometry optimization by energy minimization. The optimized ligands were then converted into PDBQT format. Docking simulations were carried out using the AutoDock Vina wizard. A grid box (Dimensions in Angstrom, X: 67.2187. Y: 74.5973, Z:68.5257 with a Center X: 67.2187. Y: 74.5973, Z:68.5257) was defined to encompass the entire protein structure, ensuring that all binding regions were included within the search space. To investigate the effect of temperature on vaccine model confirmations following binding affinity evaluation towards different polymers, rigid body docking was performed. The protein snapshots were extracted using the *trjconv* module of GROMACS (command line: gmx trjconv -f md.xtc -s md.tpr -o snapshot_ns.pdb -dump) at 1 ns & 10 ns from all-atom MD simulations conducted at different temperatures i.e. 243K, 277K, 313K and 323K. Each temperature-specific structure was docked independently with all selected polymer ligands. This study was further validated by flexible docking method.

3.2. Flexible Docking

Flexible body molecular docking was performed to further investigate the interaction dynamics between the multi-epitope vaccine construct and selected polymer molecules, allowing conformational flexibility in both receptor and ligand structures. Docking simulations were carried out using the cpiMedusaDock2.0platform(https://dokhlab.med.psu.edu/cpi/#/).[14] 1 ns and 10 ns snapshots from the protein group of trajectories with varying temperatures (243K, 277K, 313K and 323K) subsequently used as receptor inputs. Initially, the protein structure was uploaded and defined as the receptor molecule. Subsequently, ligand molecules representing the selected polymers that include PE, PCP, PVC, PS, PU, PMMA, and PET, were uploaded into the system. Default constraints were applied to guide the docking process. Binding affinity and interaction stability were evaluated using an energy-based scoring function. The resulting docking conformations and corresponding binding energies were analyzed to evaluate the interaction behaviour of the vaccine construct with different polymers.

4. Molecular Interaction Study

Molecular interaction analysis between the vaccine construct and microplastic monomers was performed using LigPlot+ v.2.3.1.[15] From the obtained docking complex

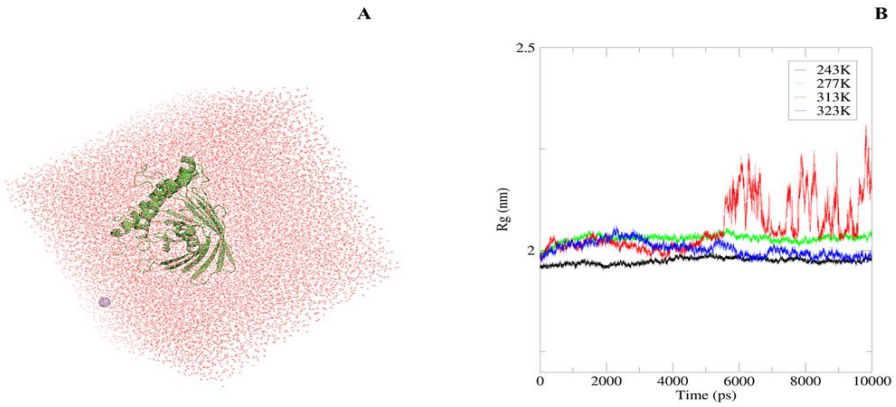


Figure 2. *(A) GROMACS build topology for the multi-epitope vaccine model in a "protein in water" environment. (OPLS-AA ff, NaCl neutralized SPC water model, cubic box 10 Å), varying temperatures, visualized by Open source Pymol software (B) 10 ns Rg plot (backbone) of the multi-epitope vaccine model showing structural changes at different temperatures. This plot was assembled and exported by qtgrace software,*

structures from Medusa Dock web server, complexes exhibiting extreme binding affinity values were selected to capture both favorable and unfavorable interaction profiles.

Results and Discussion

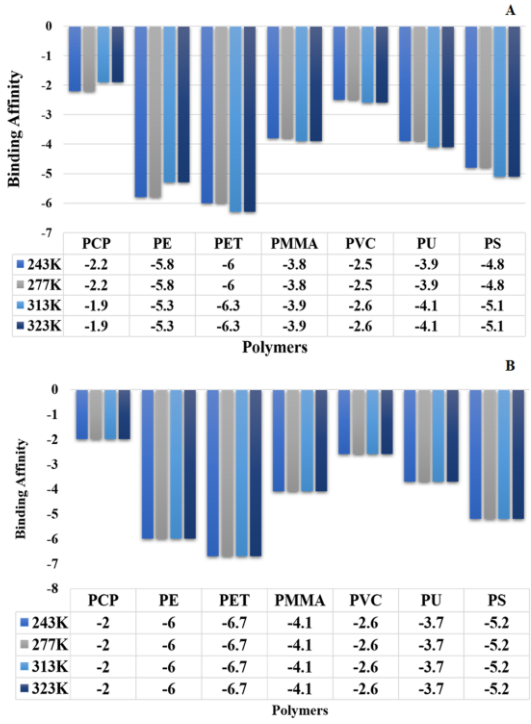
1. MD Simulation Analysis

The molecular dynamics simulations were performed to get the models from different conformational changes of the multi-epitope vaccine construct under different storage temperatures (243K, 277K, 313K and 323K). The radius of gyration (Rg) remained relatively constant throughout the simulations, indicating the compactness of the protein structure was maintained (Figure 2). Representative structural snapshots were obtained at the end (10 ns) of the simulations further demonstrated that the tertiary structure of the vaccine construct remained intact across all temperature conditions.

2. Molecular Docking Study

2.1. Rigid Body Docking

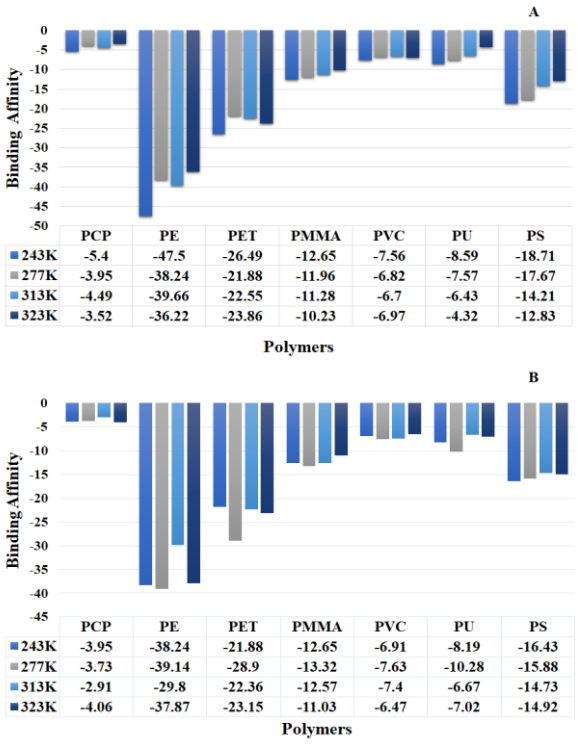
Binding affinities (ΔG in kcal/mol) of seven polymers i.e., PCP, PE, PET, PMMA, PVC, PU, and PS with a vaccine antigen were evaluated using PyRx docking on protein conformations



	PCP	PE	PET	PMMA	PVC	PU	PS
243K	-2.2	-5.8	-6	-3.8	-2.5	-3.9	-4.8
277K	-2.2	-5.8	-6	-3.8	-2.5	-3.9	-4.8
313K	-1.9	-5.3	-6.3	-3.9	-2.6	-4.1	-5.1
323K	-1.9	-5.3	-6.3	-3.9	-2.6	-4.1	-5.1

	PCP	PE	PET	PMMA	PVC	PU	PS
243K	-2	-6	-6.7	-4.1	-2.6	-3.7	-5.2
277K	-2	-6	-6.7	-4.1	-2.6	-3.7	-5.2
313K	-2	-6	-6.7	-4.1	-2.6	-3.7	-5.2
323K	-2	-6	-6.7	-4.1	-2.6	-3.7	-5.2

Figure 3. *Binding affinity (ΔG in kcal/mol) comparison of polymer-vaccine complexes using PyRx software (A) 1 ns and (B) 10 ns snapshots of the vaccine model. Plots were generated through microsoft excel software.*



	PCP	PE	PET	PMMA	PVC	PU	PS
243K	-5.4	-47.5	-26.49	-12.65	-7.56	-8.59	-18.71
277K	-3.95	-38.24	-21.88	-11.96	-6.82	-7.57	-17.67
313K	-4.49	-39.66	-22.55	-11.28	-6.7	-6.43	-14.21
323K	-3.52	-36.22	-23.86	-10.23	-6.97	-4.32	-12.83

	PCP	PE	PET	PMMA	PVC	PU	PS
243K	-3.95	-38.24	-21.88	-12.65	-6.91	-8.19	-16.43
277K	-3.73	-39.14	-28.9	-13.32	-7.63	-10.28	-15.88
313K	-2.91	-29.8	-22.36	-12.57	-7.4	-6.67	-14.73
323K	-4.06	-37.87	-23.15	-11.03	-6.47	-7.02	-14.92

Figure 4. *Binding affinity (ΔG in kcal/mol) comparison of polymer-vaccine complexes by MedusaDock 2.0 webserver using (A) 1 ns and (B) 10 ns snapshots of the vaccine model. Plots were generated through microsoft excel software.*

obtained from molecular dynamics simulations at 1 ns and 10 ns, across four temperatures (243K, 277K, 313K, and 323K) (Figure 3). At 243K and 277K, binding affinities were identical for each polymer: PCP (-2.2), PE (-5.8), PET (-6.0), PMMA (-3.8), PVC (-2.5), PU (-3.9), and PS (-4.8) kcal/mol. At 313K and 323K, affinities shifted to: PCP (-1.9), PE (-5.3), PET (-6.3), PMMA (-3.9), PVC (-2.6), PU (-4.1), and PS (-5.1) kcal/mol. PET consistently showed the strongest binding (up to -6.3 kcal/mol at elevated temperatures), while PCP and PVC displayed the weakest binding (-1.9 to -2.6 kcal/mol). PE showed reduced affinity at higher temperatures (-5.3 vs. -5.8 kcal/mol). The 1ns and 10 ns MD simulation snapshots yielded almost similar binding trends, indicating that longer simulation times did not dramatically alter polymer binding rankings.

2.2 Flexible Docking

MedusaDock 2.0 produced more negative binding affinities (kcal/mol) due to its functions with conformational flexibility (Figure 4). At 1 ns snapshot of the vaccine model, PE consistently showed the binding across all temperatures, ranging from -47.5 kcal/mol at 243K to -36.2 kcal/mol at 323K, followed by PET (-26.5 to -21.9 kcal/mol), PS (-18.7 to -12.8 kcal/mol), PMMA (-12.7 to -10.2 kcal/mol), PU (-8.6 to -4.3 kcal/mol), PVC (-7.6 to - 6.7 kcal/mol), and PCP (-5.4 to -3.5 kcal/mol). At 10 ns, PE remained the strongest binder (-39.1 to -29.8 kcal/mol), while PET achieved its peak affinity of -28.9 kcal/mol at 277K, with other polymers showing similar rankings i.e. PS (-16.4 to -14.7 kcal/mol), PMMA (-13.3 to -11.0 kcal/mol), PU (-10.3 to -6.7 kcal/mol), PVC (-7.6 to -6.5 kcal/mol), and PCP (-4.1 to -2.9 kcal/mol).

3. Molecular Interaction Analysis

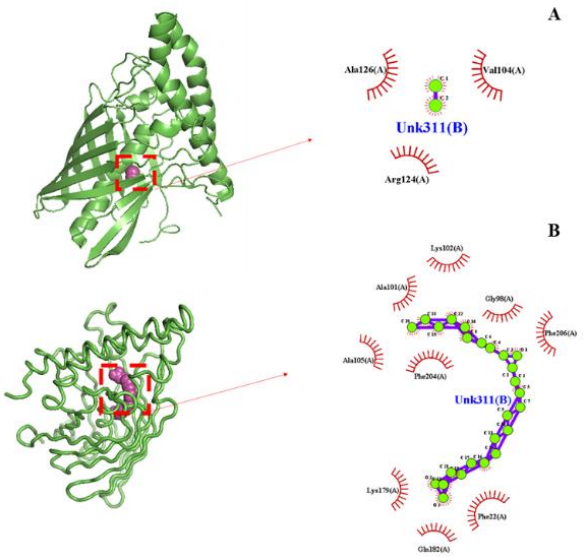


Figure 5. *Molecular Interaction analysis of the polymer [(component Unk311(B)] B chain) and vaccine (A chain) complex obtained from MedusaDock 2.0 resulting highest and lowest binding affinity at 10 ns snapshot simulated under the temperature of 243K (A) PCP shows few weak hydrophobic contacts with residues like Ala126, Arg124, and Val104, indicating minimal binding. (B) PE forms multiple hydrophobic and polar contacts with residues such as Lys102, Gly98, Phe206, Phe204, Lys179, Gln182, and Phe22. Green circles represent ligand atoms, red semicircles show hydrophobic interactions. The interaction maps were generated from LigPlot+ software.*

A detailed molecular interaction analysis was performed using LigPlot+ v.2.3.1 to evaluate the intermolecular contacts between vaccine construct and the polymers. For the PCP monomer (10 ns, 243K), the minimal interaction profile was dominated by hydrophobic contacts. The ligand PCP was found to form 5 non-bonded contacts with the vaccine chain. The observed interactions ranged between 3.69 Å to 3.89 Å. No hydrogen bonds or salt-bridges were detected. In contrast, the PET monomer (10 ns, 243 K) shows 25 non-bonded contacts within distances ranging from 3.39 to 3.89 Å. Related interaction maps were represented as Figure 5.

Discussion

The present study is foundation of a computational perspective on the suitability of polymer-based materials for vaccine storage, examining their interaction with a multi-epitope vaccine construct simulated under different temperature conditions. The different Rg values observed for the simulated vaccine models, indicated that the vaccine protein undergoes minute structural changes as temperature shifts from 243K to 323K.[16] If a polymer binds to an antigen strongly, it can induce misfolding of the antigen structure following masking epitopes and alteration of the immunogenic sites. As a result, the vaccine antigen may be ineffective or potentially harmful. In this study, binding affinities were seen to get decreased with increasing temperature for most of the polymers, although PET shows slightly higher binding at 313K to 323K in rigid docking and achieved its peak at 277K in flexible docking. Whereas, PCP at 313K showing a binding energy of -2.91 kcal/mol, consistent with its weak binding energy across other temperatures. Overall, both docking methods simultaneously ranked PE and PET as the strongest binders, whereas PCP and PVC as the weakest, with flexible docking revealing substantially lower binding energies (up to -47.5 kcal/mol). High binding affinity of the PE and PET monomers towards the vaccine model can harm the storage profiling of this vaccine. This is an important consideration because strong binding could potentially alter antigen conformation or mask immunogenic epitopes. Among the polymers, PCP showed lowest binding affinity in both rigid and flexible docking approaches. A key observation has been addressed from this study, i.e. the consistency of the docking results across different simulation snapshots (1 ns and 10 ns) and temperature conditions. In practical terms, this indicates that the risk associated with microplastic interaction may remain relatively common across storage temperatures.[17] The molecular interaction analysis of the complexes resulting from flexible docking with the highest and lowest binding energies highlighted the nature of these interactions. For PCP and vaccine complex, the absence of hydrogen bonding has highlighted a weak and transient association driven by a few non-bonded contacts. Whereas, the interaction profile of PE revealed the presence of higher counts of non-bonded contacts. These higher counts may affect vaccine stability and functionality. Ghoshal *et al.* (2024) have reported that nanosized polyethylene particles can induce conformational alterations in human α-synuclein, highlighting the potential of micro- and nanoplastics to affect protein structure and behaviour through surface-mediated interactions.[18] Also, Kuttykattil *et al.* (2025) found that PET-derived monomers bind to human inflammatory receptors such as PAFR, β2-AR, CXCR1, and TLR-2. These interactions remained stable during

molecular dynamics simulations, suggesting that microplastics may affect biological function. Together, these findings may contribute to the safety of polymer usage in the field of vaccine packaging. While polymer containers offer practical advantages such as reduced weight and improved durability, concerns about microplastic leaching remain valid.[19,20] The current study suggested that even if such leaching occurs, the resulting interactions with protein-based vaccines may be weak and transient, thereby posing minimal risk to structural integrity. However, it is important to note that this study focuses on monomer-level interactions in a simplified computational environment.[21] In real-world scenarios, additional factors such as polymer degradation products, long-term exposure and biological environments may influence interaction dynamics. Despite its contributions, the study has certain limitations that should be acknowledged. The simulation time (10 ns) represents a relatively short timescale and may not capture long-term structural fluctuations.[22] Additionally, the use of isolated monomers does not fully replicate the complexity of actual microplastic particles or polymer surfaces. Experimental validation, such as spectroscopic or biophysical studies, would be necessary to confirm the computational predictions.

Conclusion

The present study provides a computational insight in the interaction between polymer-derived microplastic monomers and a multi-epitope vaccine candidate under different storage conditions. Molecular dynamics simulations showed that the vaccine structure remains stable across different storage temperatures, indicating good structural integrity. Docking results revealed that polymers such as PE and PET exhibited stronger binding interactions, whereas PCP and PVC showed weaker associations with the vaccine construct. However, binding energies generated by different docking algorithms should be interpreted qualitatively rather than as directly comparable quantitative values. Molecular Interaction analysis further confirmed that stronger binders formed more non-bonded contacts, which may influence the vaccine's instability. These findings may contribute to a safer vaccine packaging technology. While, polymer containers offer practical advantages like reduced weight and improved durability. As this study is based on computational models, further validation of these experiments is needed. Cumulatively, this study suggests that even if polymer leaching occurs, the resulting interactions with protein-based vaccines may be weak and transient especially in case of the PCP, thereby posing minimal risk to structural integrity.

Experimental Section

General Information: The entire study is based on computational techniques. The experimental setup was entirely provided by cellular and molecular immunology laboratory, Department of biotechnology, NIT Durgapur. The molecular dynamics simulation studies were carried out using galaxy Europe web platform.

Preparation of compound: No compound was prepared during this study.

General Procedure: The molecular dynamics plots from the study was obtained from qtgrace software. Whereas, the histograms were designed by microsoft excel software.

Supporting Information

There is no supporting data provided.

Author Contribution Declaration & Information

Contribution

Nibedita conceptualized the study, reviewed the draft manuscript, supervised the progress of the work, and finalized the manuscript. Shveta designed the article, developed the research plan, and wrote the first draft of the manuscript. Pinkan also contributed to the article design, developed the research plan, and reviewed the draft manuscript.

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Data Availability Declaration

The data generated during the current study are included in this published article and its supplementary information. Additional data may be supplied on request.

Declaration of Conflict of Interest

The authors declare that they have no competing interest that could have appeared to influence the work reported in this paper.

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