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Molecular Dynamics Simulation of Cry j 1 Allergen Adsorption on a PET Microplastic Surface

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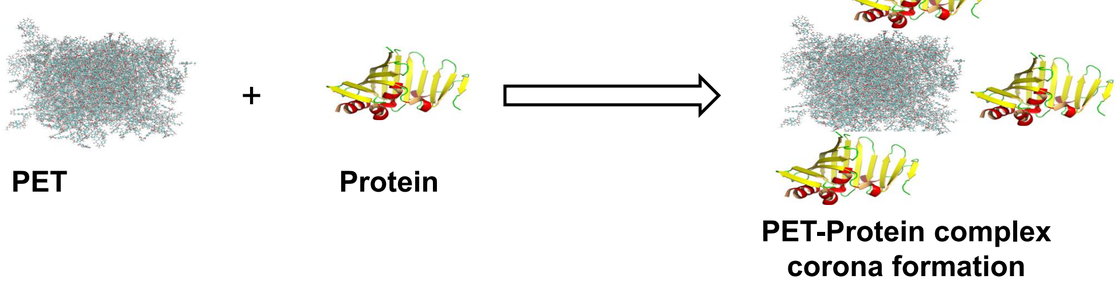
INTRODUCTION & AIM

- Polyethylene terephthalate (PET) microplastics are ubiquitous environmental pollutants increasingly recognized as potential carriers of biomolecules.
- Cry j1, a major Japanese cedar pollen allergen, triggers severe seasonal allergic responses and poses growing health concerns in Japan.
- Emerging studies suggest that plastics can act as vectors for protein adsorption and transport, potentially altering their structure and immunogenicity.
- This study employs molecular dynamics simulation to investigate whether PET surfaces adsorb Cry j1, modify its conformation, and influence its allergenic potential.

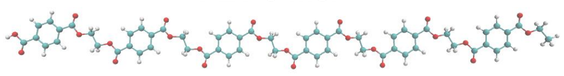
GRAPHICAL ABSTRACT

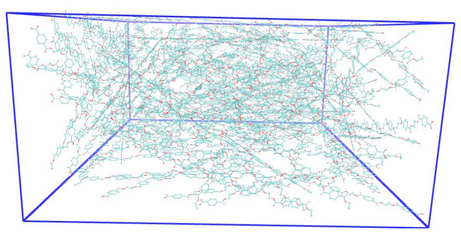


METHOD

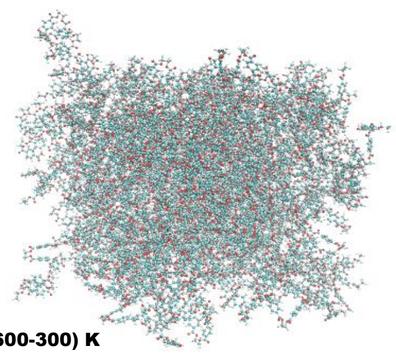
- **PET surface preparation**

PET-6-mer





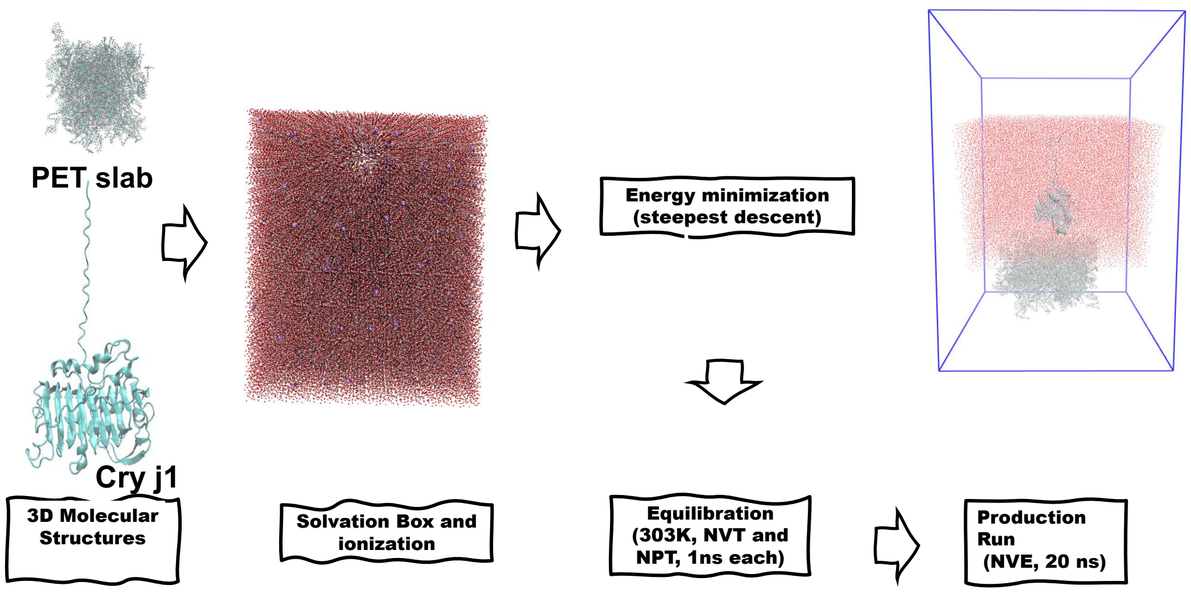
180 X PET-6-mer
Box size: 12 X 12 X 15



1. Simulated annealing (NVT 300-600-300) K
2. NVT (1 ns, 303 K)
3. NPT (9 ns, 303 K

PET slab surface

- **Adsorption behavior of cry j1 in contact with PET surface**



The PET slab was generated by first building a 6-MER PET, 180 of this 6-MER PET molecules was then packed into a box size 12 X 12 X 15. The box was subjected to temperature annealing from 300K to 600K back to 300K using NVT at 1ns each, changing the temperature every 50K. After which the box was further equilibrated using 1ns nvt and a final production run was done in 9ns NPT. The slab was then ready for the simulation.
In the MD simulation, the 3d structure of the cry j1 was solvated, ionized using 0.15 KCl, energy minimized and equilibrated in 1ns NVT and 1 ns NPT before combining with the PET slab. The coupling was done with the Cry j1 set at an orientation in which the epitope active site was facing the PET slab at 3nm distance. After combination, energy minimization was done using steepest decent algorithm and equilibrated using NVT 1ns, followed by NPT 1ns. The production for PET + protein and protein alone was done at 20ns using NVT ensemble, then protein is position 3nm away from the PET surface with the major epitope region facing the PET slab. All analysis was done using charm-36 forcefield jul.21.

RESULTS & DISCUSSION

Fig 1a: Initial Contact between protein and PET

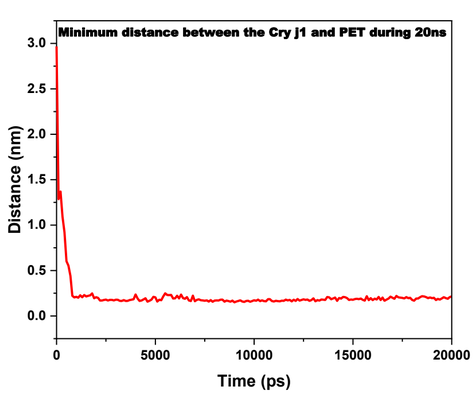
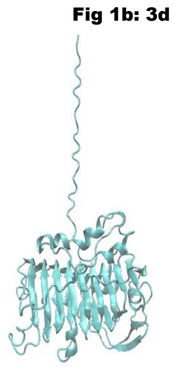


Fig 1b: 3d structure of the cry j1 protein



The protein was placed so that its major T-cell epitopes as reported by Yukiko et al., 2000 (residue (P141-P160). After simulation, after 800 ps, the protein and the PET interaction was observed, and it remained till the end of the simulation

Fig 2a: Hydrogen Bond Analysis of solvated protein, and protein + PET

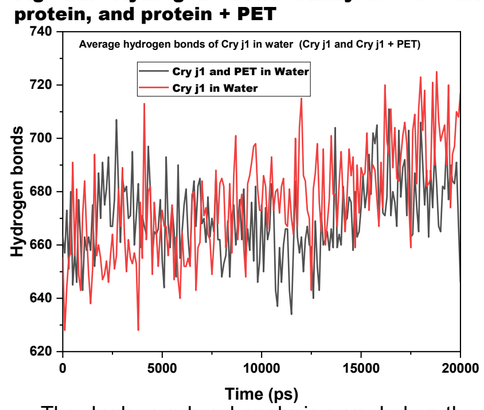
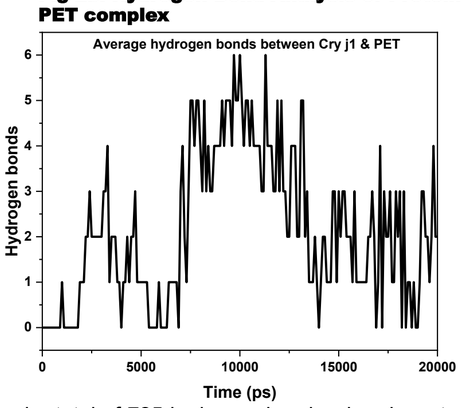


Fig 2b: Hydrogen Bond Analysis of Protein – PET complex



The hydrogen bond analysis revealed on the average, Cry j 1 established a total of 725 hydrogen bonds when in water but when adsorbed on the surface of the PET the number decreases to 711 hydrogen bonds. This 2 % decrease may be due to solvent displacement upon contact with the PET surface. The result hydrophobic residues of Cry j1 also participated in hydrogen bonding with the PET during the adsorption simulation.

Fig 3a: Structural Stability analysis of the Protein (Radius of gyration)

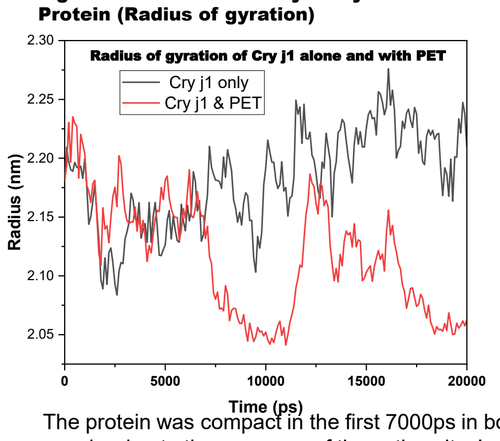
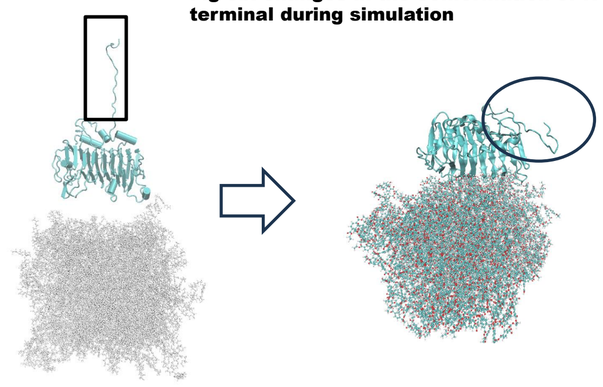


Fig 3b: changes in the conformation of N-terminal during simulation



The protein was compact in the first 7000ps in both simulations after which a change was observed in the Cry j1 – PET. This may be due to the exposure of the active sites' residues to the PET surface. The visuals of the protein before and during simulation showed the N-terminal changed orientation during the simulation.

Fig 4a: RMSF Analysis (Flexibility)

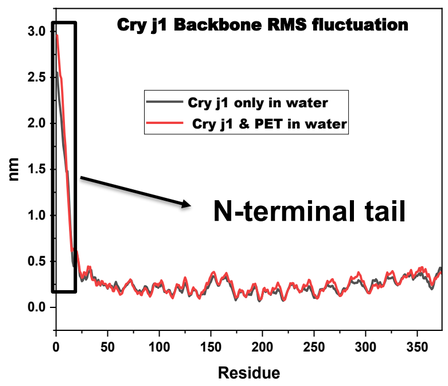
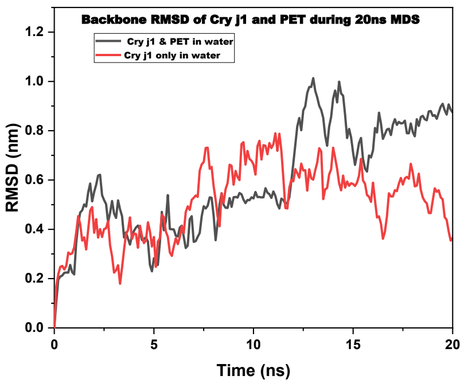


Fig 4b:RMSD Analysis (Overall Stability)



The identical RMSF pattern for both systems shows a highly flexible N-terminal tail and a rigid, and well-folded core. This indicates the flexible tail is an intrinsic property of the protein and is not affected by PET binding. In the RMSD, the protein alone exhibits the classic signature of a stable protein, equilibrating and then settling into a compact, stable conformation, while the PET-bound protein undergoes a large, sustained conformational change, ending in a different, less compact state.

CONCLUSION

- The protein is stable but undergoes a significant substrate-induced conformational change when PET is present.
- RMSD in the PET-bound system suggests the protein must open its structure or rearrange its core to when in contact with the bulky polymer, a behavior consistent with enzymes like PETase that degrade solid substrates.
- This represents a functional transition from a resting state to an active, substrate-bound state.

FUTURE WORK / REFERENCES

- More investigation on the secondary structure stability focusing on the interaction of individual residues and energies
- Increase the simulation time
- Target the individual residues of the binding epitopes to assess the effect of PET on the allergenicity of the cry j1.