Multi-Phase Analysis of Microplastic Contamination on Biological Interactions, Digestive Impact, Adsorption Design, and Concentration in Hawai?i's Foods

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Microplastics have been a growing problem within the biomedical and health fields. However, mechanistic links between dietary exposure, molecular interaction, physiological impact, and mitigation remain unclear. This study provides an integrated pipeline to assess microplastic contamination in foods commonly consumed in Hawai?i, along with biological interactions and prevention strategies. Raman spectroscopy identified microplastic types within food groups. Molecular docking analyzed 100 protein-ligand interactions (10 plastic ligands x 10 important human proteins) with toxicological modeling evaluating biological risk. Molecular dynamics simulations (10 ns) were conducted to assess structural and thermodynamic stability. A standardized in-vitro model examined the effects of microplastics on nutrient digestibility. A computational genetic algorithm was created to engineer a de novo adsorbent molecule capable of removing microplastics from the human digestive system. Microplastics were found in all food groups which confirms dietary exposure. Several complexes had strong binding, like bisphenol A with estrogen receptor alpha (-8.07 kcal/mol) and terephthalic acid with endocrine/metabolic proteins (= -6.5 kcal/mol). Molecular dynamics indicated stable interactions (RMSD: 0.10 - 0.23 nm) indicating molecular inhibition. Digestibility decreased as microplastic concentration increased with changes in ash and organic matter. The novel adsorbent molecule had a binding affinity of -13.28 kcal/mol which is stronger than many adsorbents used today. These findings establish a framework that links dietary exposure to biological interactions and digestive disruption, while proposing a targeted mitigation strategy for this global microplastic problem.

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