In Silico Evaluation of the Interactions of Microplastic-Associated Chemicals with Hormone Receptors in the Context of Biological Variability in Vaccine Responses

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Abstract

Sex steroid hormones and their receptors contribute to the regulation of immune responses and interindividual variability following vaccination. Therefore, determining the potential interactions of microplastic-associated endocrine-disrupting chemicals with hormone receptors is of considerable importance. In this study, the potential binding of bisphenol A (BPA), bisphenol S (BPS), dibutyl phthalate (DBP), and bis(2-ethylhexyl) phthalate (DEHP) within the natural ligand-binding pockets of estrogen receptor alpha (ERα) and the androgen receptor (AR) was investigated using molecular docking. The docking protocol was validated by redocking the native ligands, with low RMSD values supporting its reliability. An integrated evaluation of docking scores, cluster distributions, and protein–ligand interactions indicated that BPA exhibited a consistent binding profile toward both receptors. BPA retained the Glu353 interaction shared with the native ligand in ERα and the Asn705 interaction shared with dihydrotestosterone in AR. BPS displayed a similar interaction pattern, whereas DBP and DEHP binding was predominantly mediated by hydrophobic contacts. Despite its favorable AR docking score, the low cluster convergence observed for DEHP warrants cautious interpretation. Overall, the findings suggest that BPA and BPS may bind within the natural ligand pockets of both receptors, providing a preliminary molecular basis for further experimental investigation of endocrine disruptors in the context of hormonal–immune interactions.