

Nanoplastics penetration across the blood-brain barrier

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ABSTRACT

Microplastics and nanoplastics (MNPs), originating from plastic degradation, have arisen to be a threat to ecology and human health. Alarmingly, the penetration of MNPs across the highly selective blood–brain barrier (BBB) poses an emerging and urgent risk, yet its molecular mechanism remains unexplored.

This study was conducted to investigate the molecular mechanism and energetic favorability of nanoplastic penetration into the blood-brain barrier. Using long-timescale (over 27 μ s) all-atom explicit solvent steered molecular dynamics, the free energy of the passive permeation of four polymer nanoparticles was investigated: polyethylene, polypropylene, polystyrene, and polyethylene terephthalate. It was found that the increase in the polymer hydrophobicity elevated the energetic preference for entering the BBB. Moreover, polymers can enter the BBB as polymerized nanoplastics and exit as dispersed polymer chains as the nanoparticles dissolve within the BBB. This work advances the knowledge about the mechanism of nanoplastic penetration across the BBB, which could aid in the rational design of therapeutics for nanoplastic penetration inhibitors.

