Does Size Matter? Toxicity of Polyethylene Terepthalate Nanoplastics of Different Sizes on Aquatic Organisms based on Molecular Docking and Machine Learning Methodology

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Abstract

Although there is ample evidence that nanoplastics (NPs) are toxic to aquatic life, little is known about how their sizes affect their toxicities. This study examined the toxicity of Polyethylene Terepthalate (PET) Nanoplastics (NPs) of different sizes (1, 4, 9, 16 and 25 nm coded NP1 to NP5) on aquatic organisms such as *Terpedo californica* (electric ray fish) and *Danio rerio* (zebrafish) as model species by molecular docking and machine learning methodology based on Multilayer Perceptrons Artificial Neutral Networks (MLP ANN). The PET NPs were built and characterized *in silico* and then docked on the acetylcholinesterase (TcAChE) and cytochrome P450 (Zf CYP450) of the organisms respectively. The results showed that the binding affinities of the NPs increased steadily from – 7.1 kcal/mol to – 9.9 kcal/mol for NP1 to NP4, and experienced a drop at NP5 (– 8.9 kcal/mol) for TcAChE while also Zf CYP450 had similar pattern which ranged from -5.2 kcal/mol to -8.1 kcal/mol. The binding affinity of NP2, NP3, and NP4 were higher than the control for TcAChE, indicating that they have a higher inhibitory potential at this site and therefore could impact more toxicity on the enzyme than the native inhibitor (-)-galanthamine. However, the abiraterone control for Zf CYP450 showed the highest toxicity with binding affinity of -9.5 kcal/mol compared with the PET NPs. The MLP ANN was able to predict the toxicity of the PET NPs based on the inherent properties with coefficients of 0.986 and 0.965 for Tc AChE and Zf CYP450 respectively. The validation of the ANN was tested by error analysis models which confirmed that the ANN was at high accuracy. The study confirmed that size of PET NPs can influence its toxicity to aquatic organisms and the surface area and reactivity (energy) of the NPs are important for its toxicity.

Keywords: Artificial Neural Networks, Fish, Health risks, Plastic pollution, Simulation, Toxicity

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