Nanoplastics can change the secondary structure of proteins

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Supporting Information

Abbreviations used in this document:
PE: Polyethylene
PP: Polypropylene
PET: Polyethylene terephthalate
N66: Nylon-6,6
Neat: In the absence of plastic nanoparticles

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1. Structural images of the nanoparticles generated and used in the present study

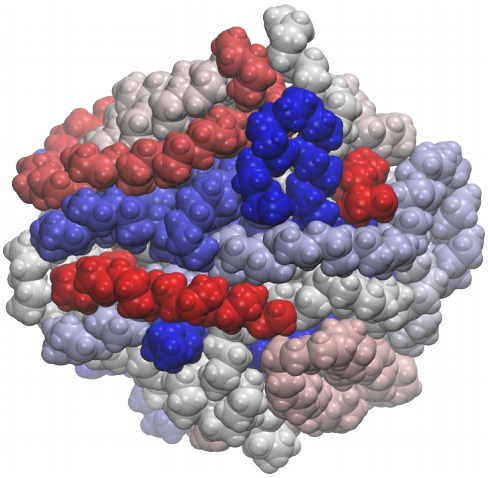


Figure S1: PE Nanoparticle used in the simulations. Each chain is highlighted in a different color.

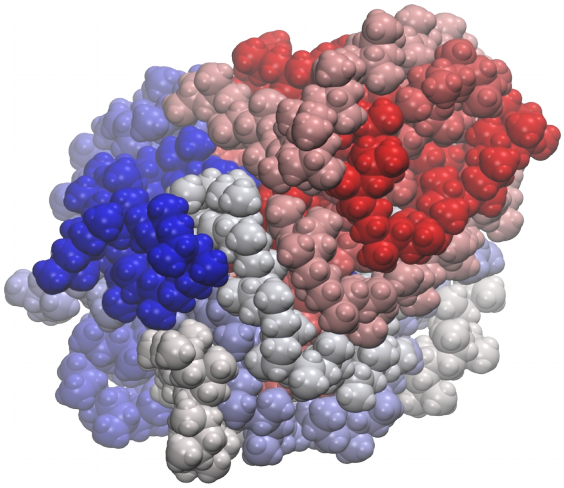


Figure S2: PP Nanoparticle used in the simulations. Each chain is highlighted in a different color.

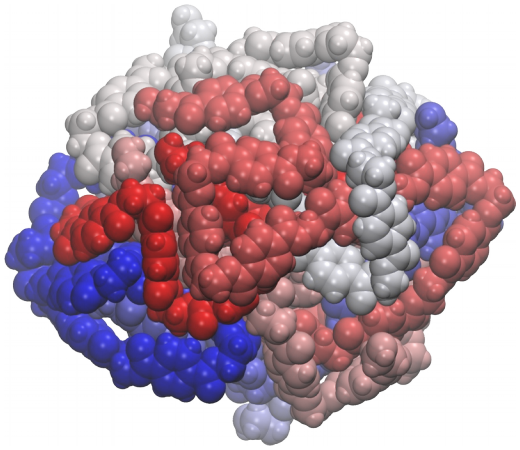


Figure S3: PET Nanoparticle used in the simulations. Each chain is highlighted in a different color.

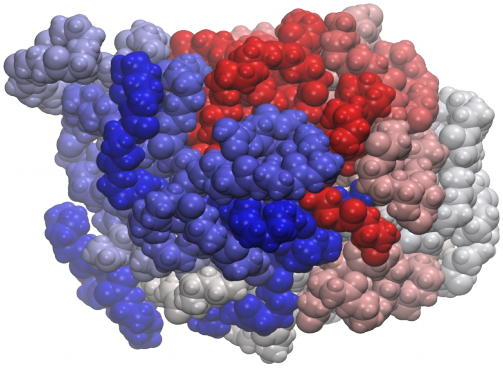


Figure S4: N66 Nanoparticle used in the simulations. Each chain is highlighted in a different color.

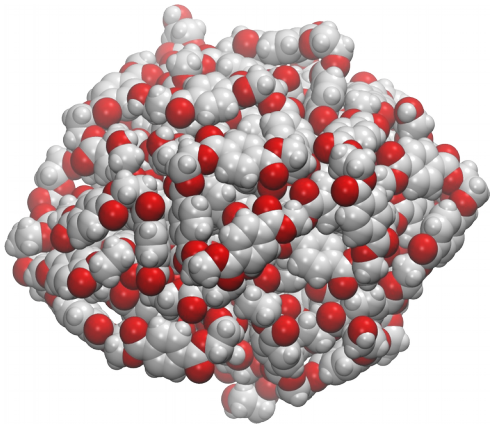


Figure S5: PET Nanoparticle used in the simulations. Oxygen atoms are highlighted in red, showing the scattered interactions sites at the surface of the nanoparticle

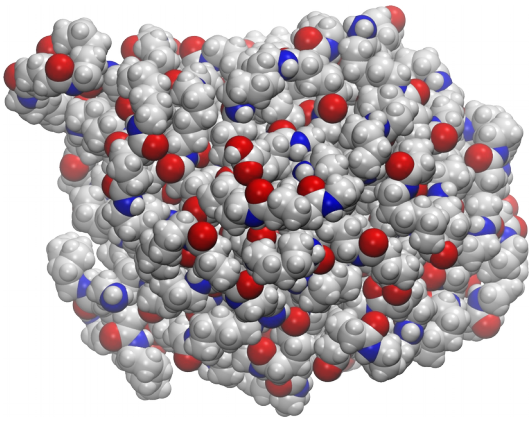


Figure S6: N66 Nanoparticle used in the simulations. The oxygen atoms are highlighted in red, the nitrogen atoms are in blue. The surface shows a distinct scatter of hydrogen bond donor (N-H) and acceptor sites (O).

2. Ramachandran plots of the α-helix and tryptophane zipper structures in aqueous solutions, and adsorbed on the plastic nanoparticles

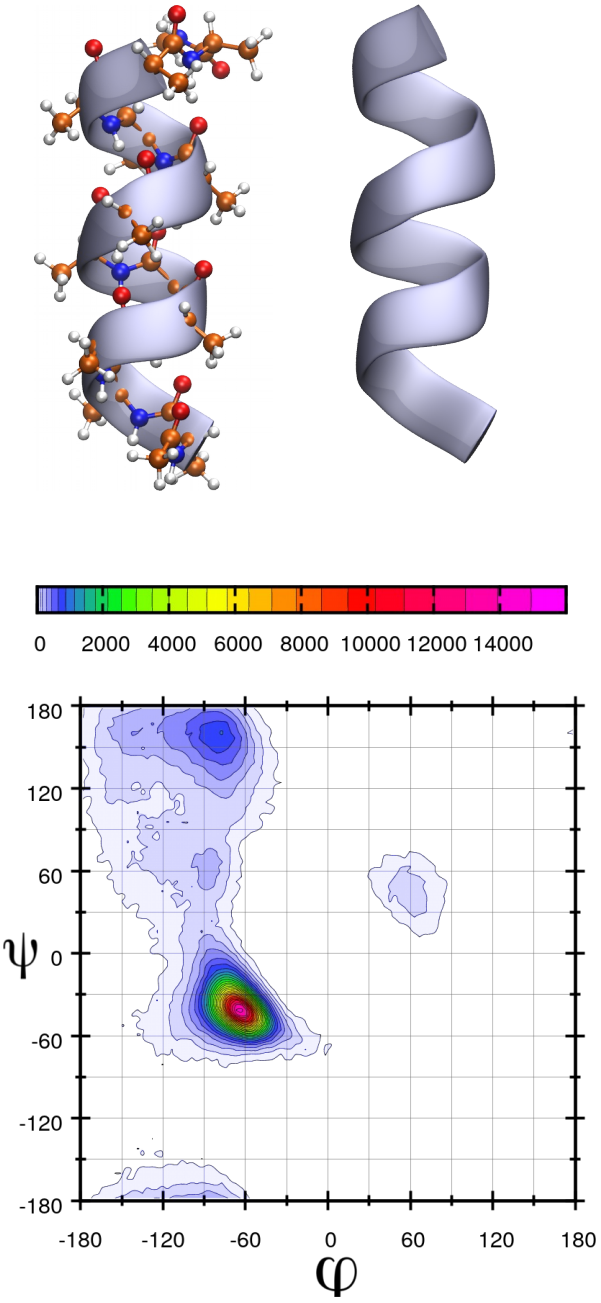


Figure S7: Free α-helix structure in saline solution

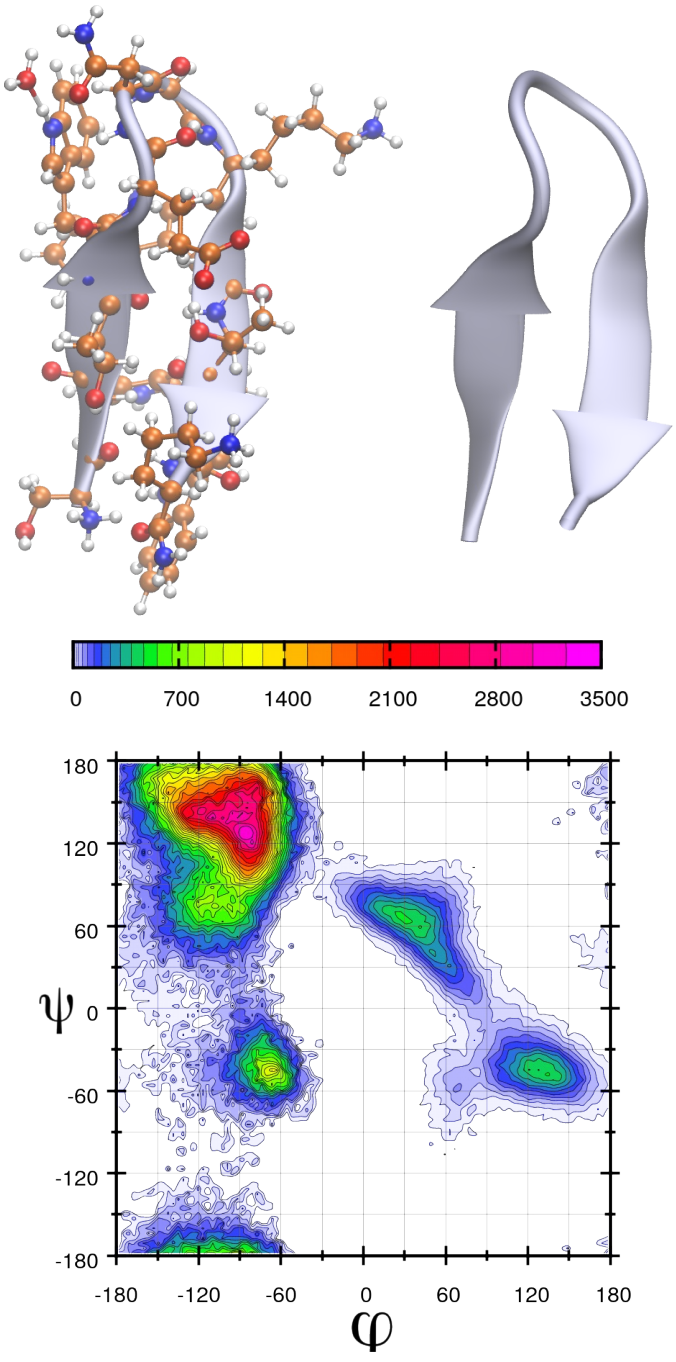


Figure S8: Free tryptophan zipper structure in saline solution

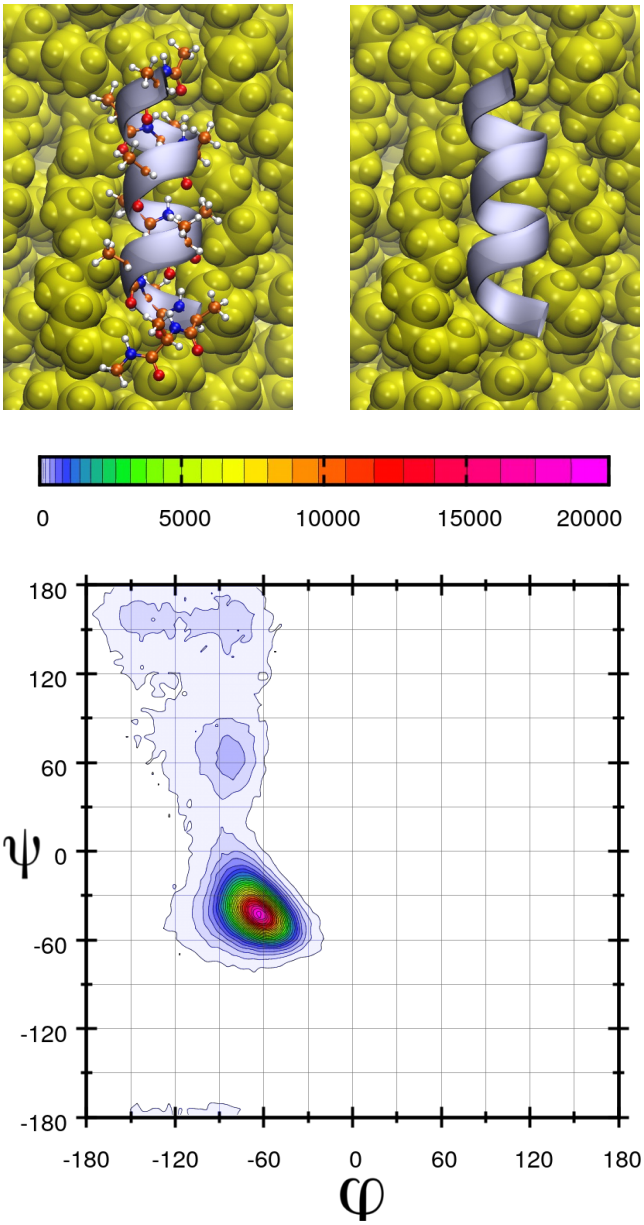


Figure S9: α-Helix structure on PE nanoparticle

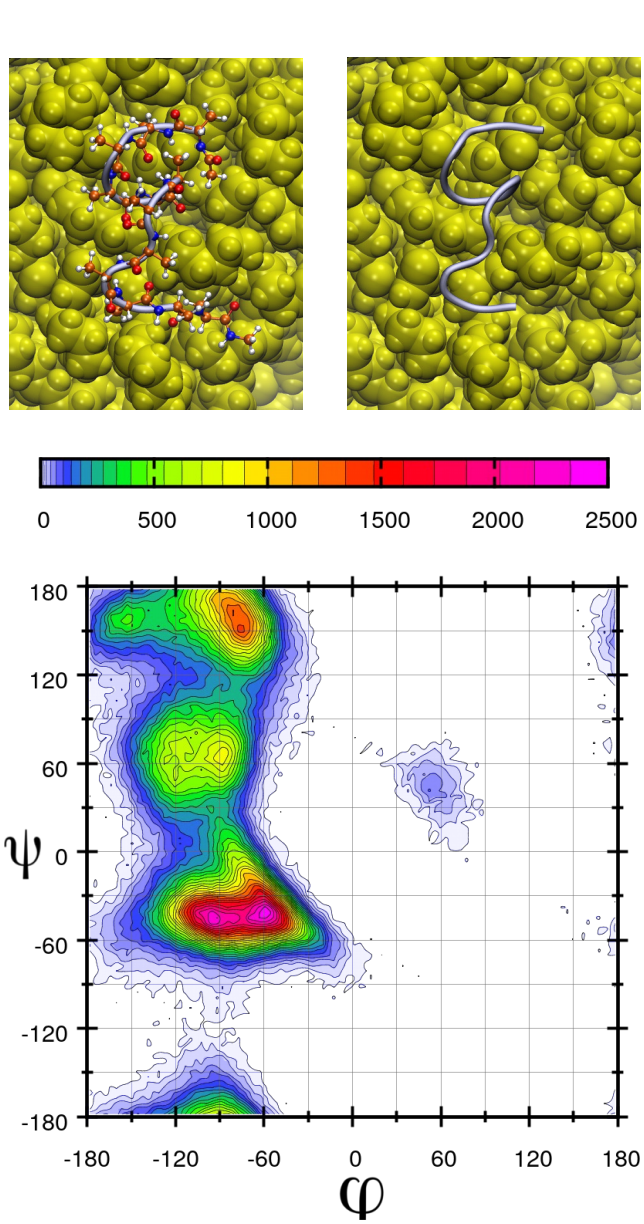


Figure S10: α-Helix structure on N66 nanoparticle

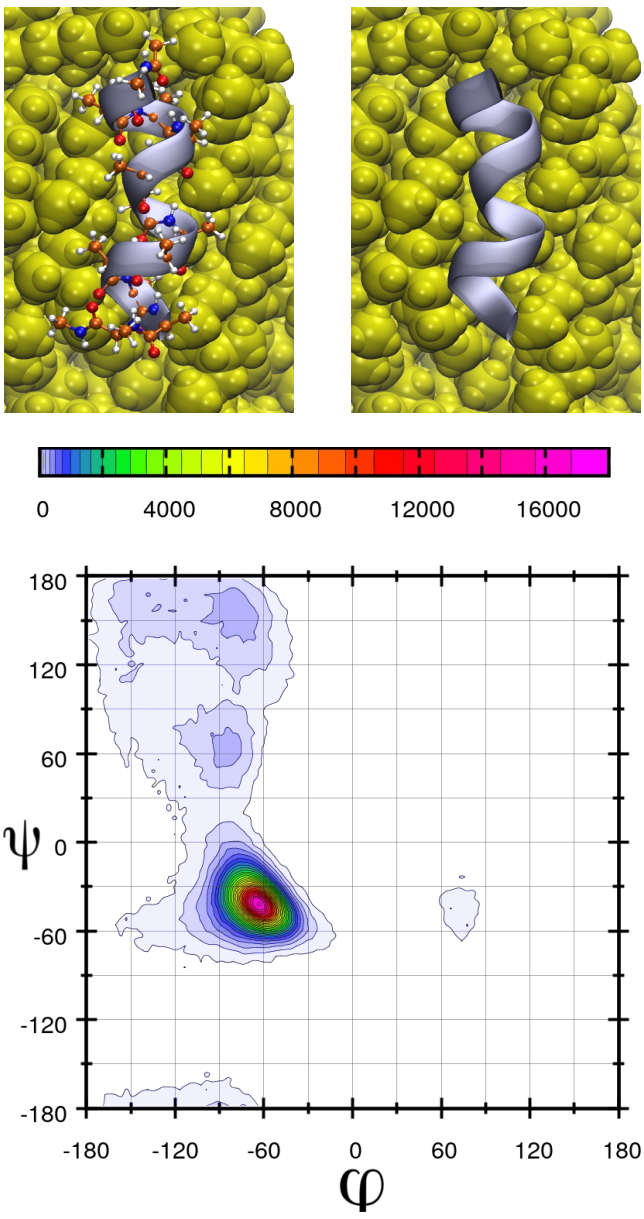


Figure S11: α-Helix structure on PP nanoparticle

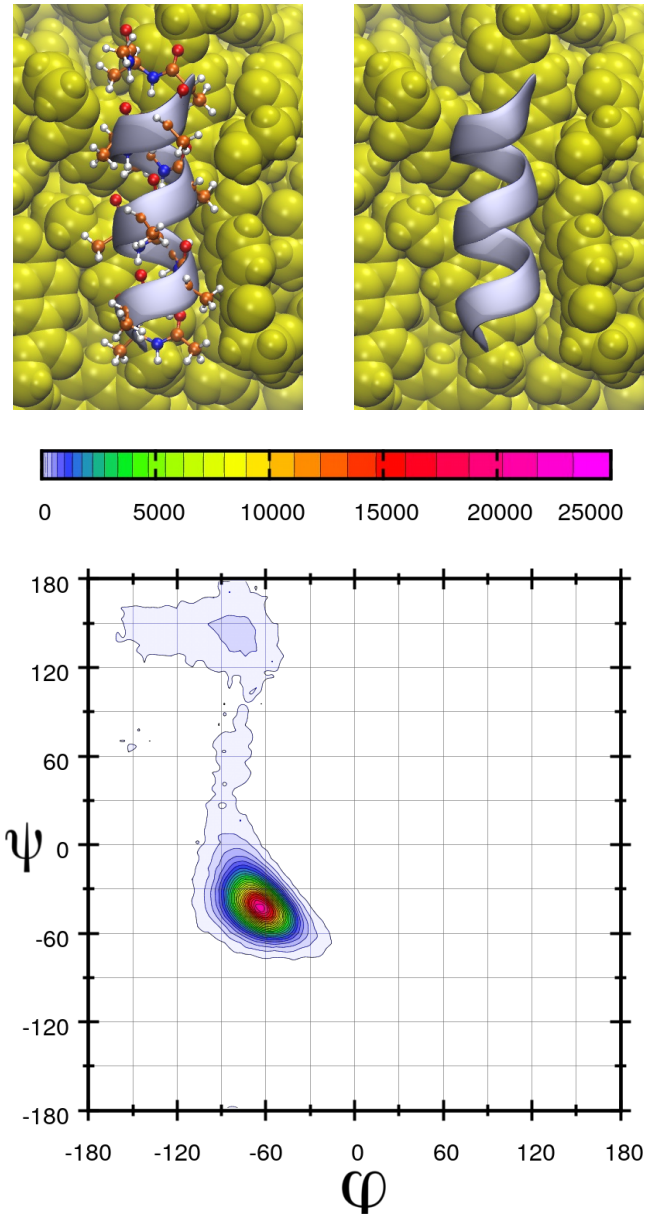
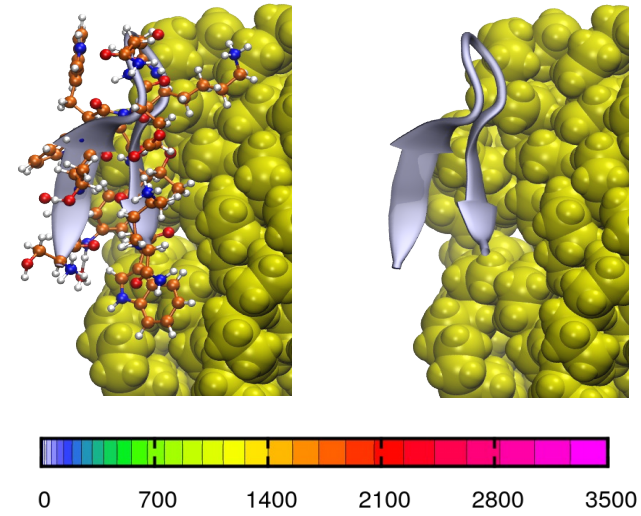


Figure S12: α-Helix structre on PET nanoparticle



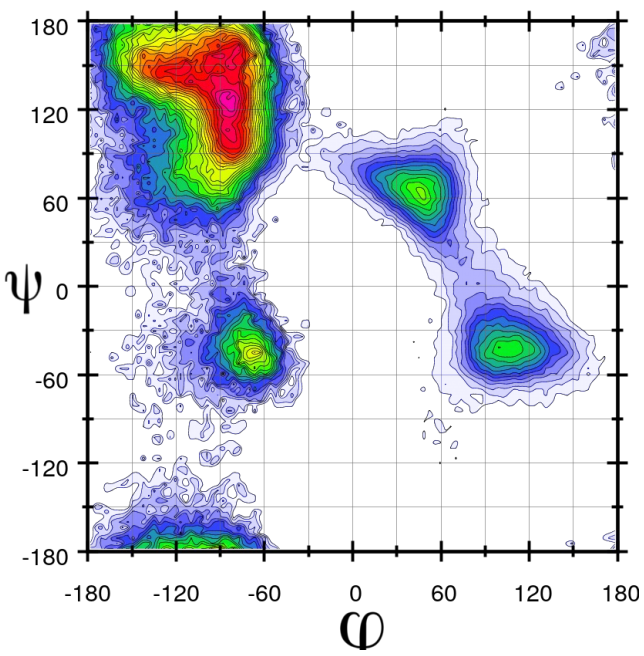
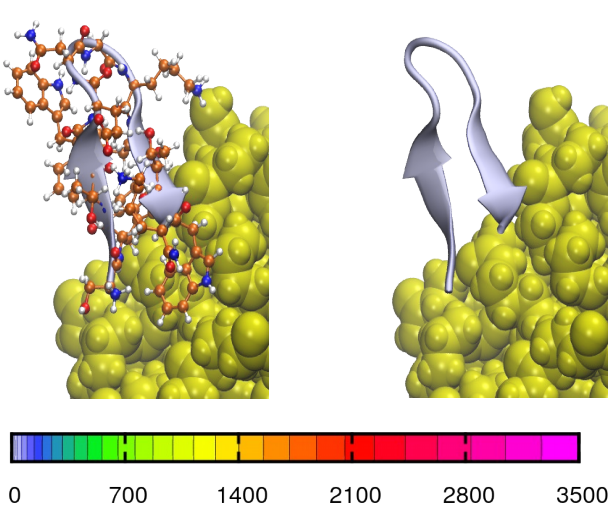


Figure S13: Tryptophan zipper structure on PE nanoparticle



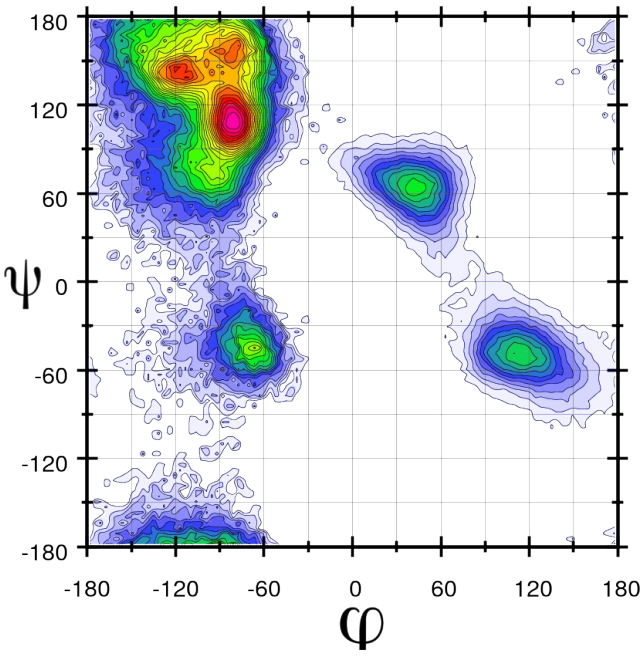


Figure S14: Tryptophan zipper structure on N66 nanoparticle

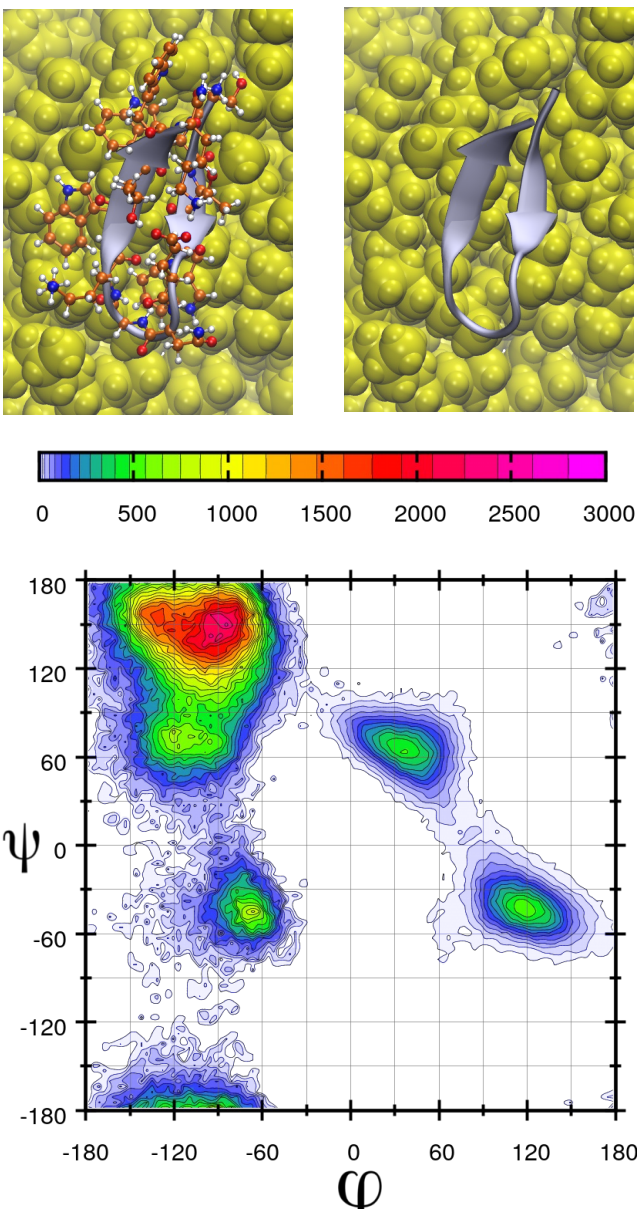


Figure S15: Tryptophan zipper structure on PP nanoparticle

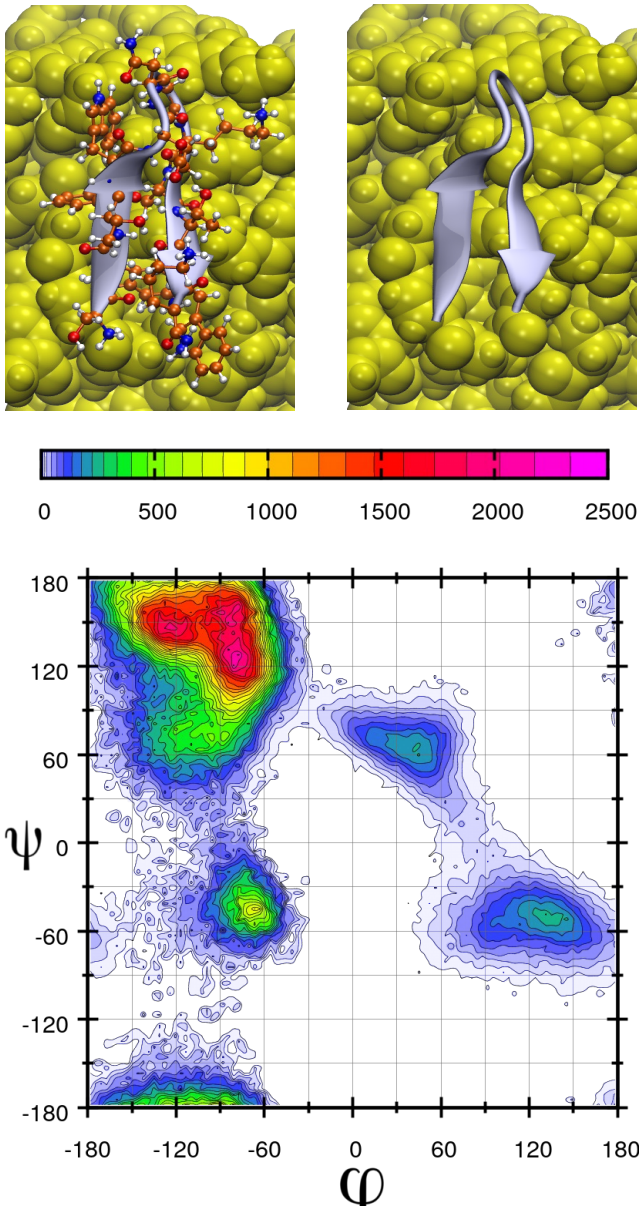


Figure S16: Tryptophan zipper structure on PET nanoparticle

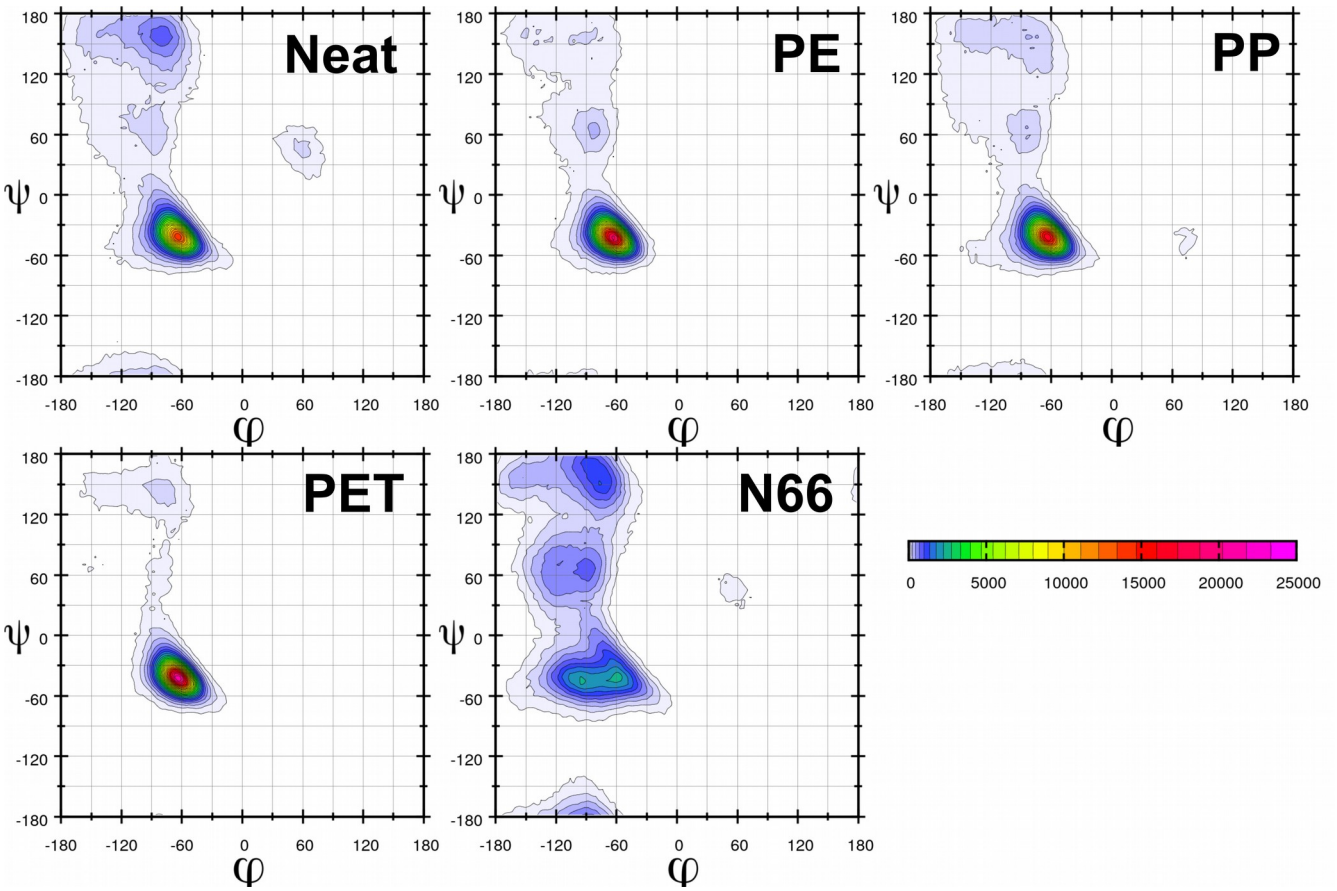


Figure S17. Rescaled Ramachandran plots of the α-helix structures with identical scaling allowing direct quantitative comparison of the plots

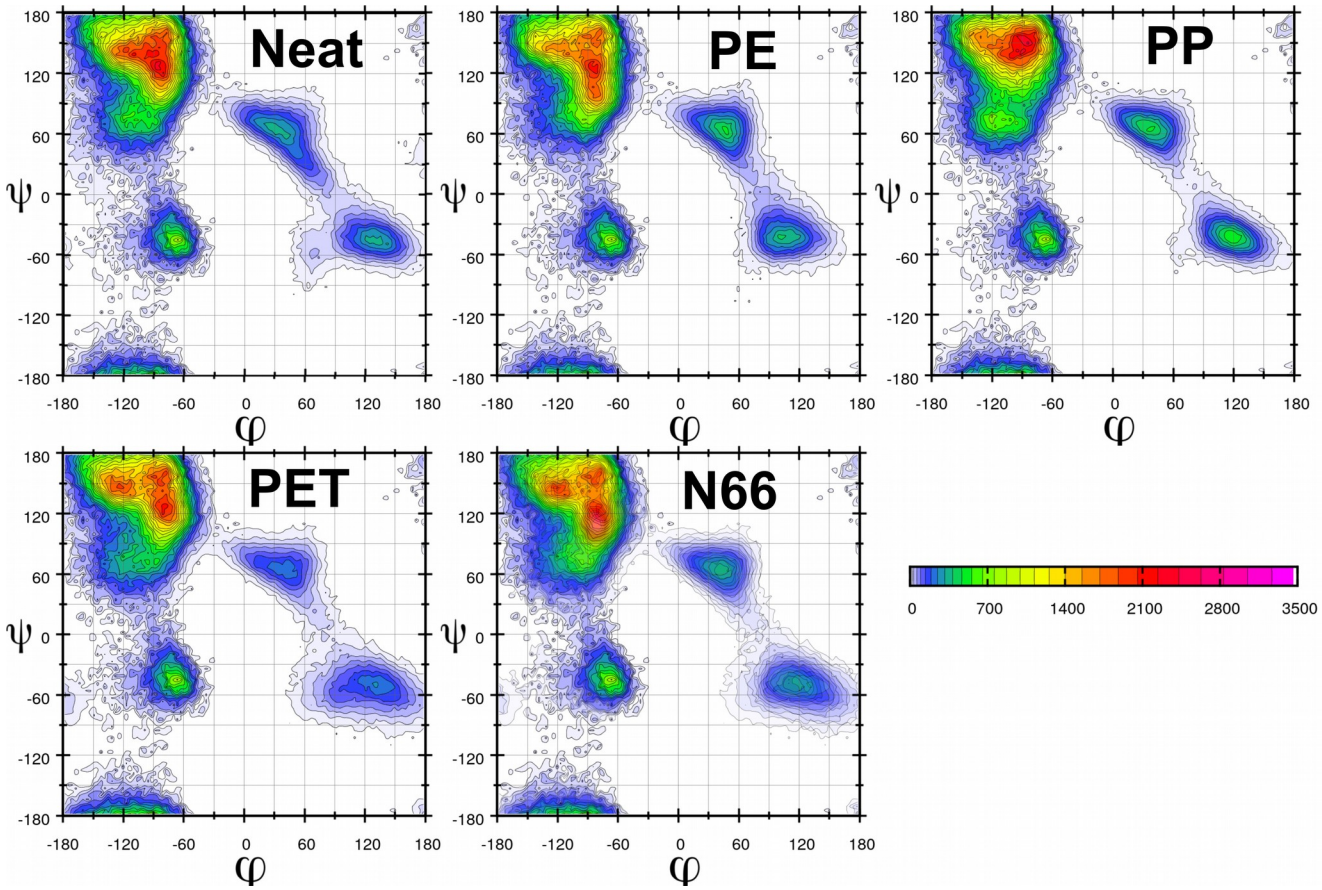


Figure S18. Rescaled Ramachandran plots of the tryptophane zipper structure with identical scaling allowing direct quantitative comparison of the plots

3. Time development of the surface of the nanoplastics covered by the selected amino acids and water in the MD simulations

Simulations of the plastic particles in aqueous saline solutions in the presence of six selected amino acids (glycine, aspartate, arginine, asparagine, phenylalanine, tryptophan) were performed. In one simulation box, one plastic nanoparticle, and one kind of amino acids were present, resulting in altogether 24 simulations. The further details are given in the Methods and Models section of the article.

The graphs shown in this section present the interaction surfaces of the plastic nanoparticle with the surrounding aqueous solution, and with the amino acids for each simulations. These surfaces were calculated through Voronoi tesselation at every picosecond of the simulation, as implemented in the Travis code. High interaction surface of the nanoparticles with the amino acid shows that the amino acid adsorbs on the surface of the plastic, which occurs almost exclusively in case of the amino acids with non-polar (hydrophobic) side chains. It is also possible to observe that the total surface of the plastic particle increases upon the adsorption of these amino acids.

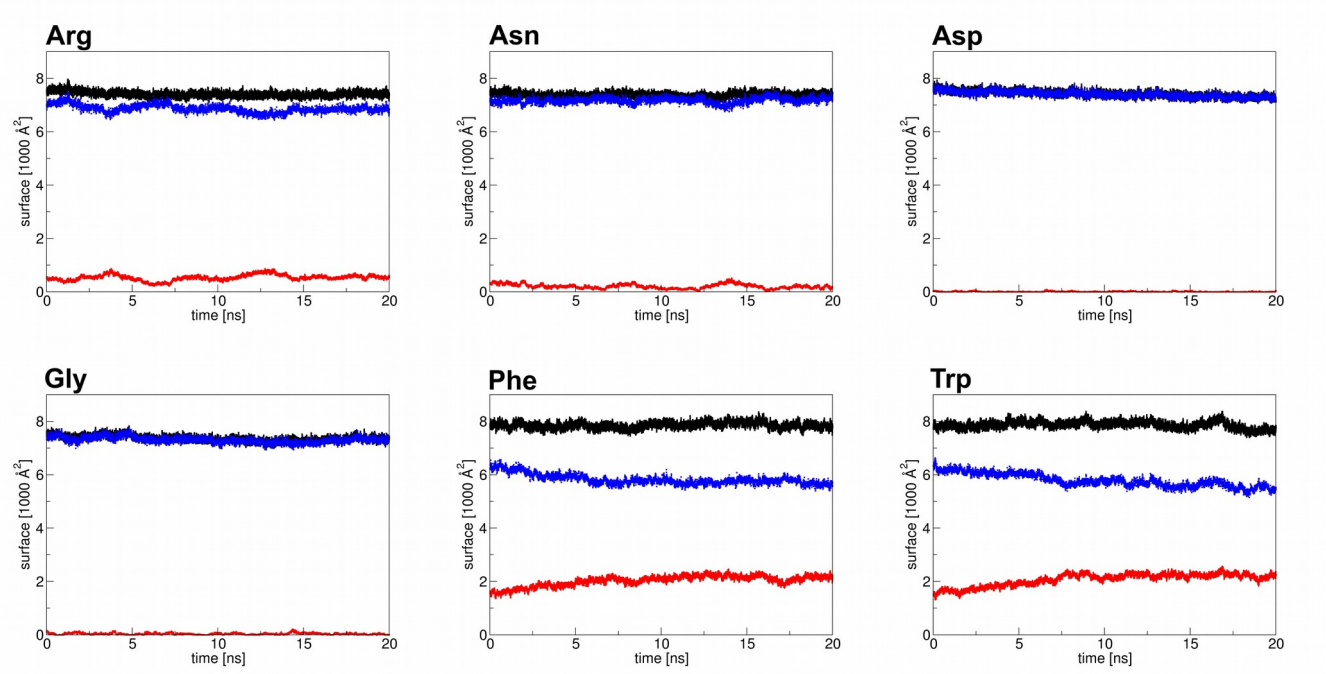


Figure S19. Time development of the total surface area (black), and surface coverages of the ***polyethylene*** *nanoparticle by water (blue) and the amino acids (red) in the molecular dynamics simulation.*

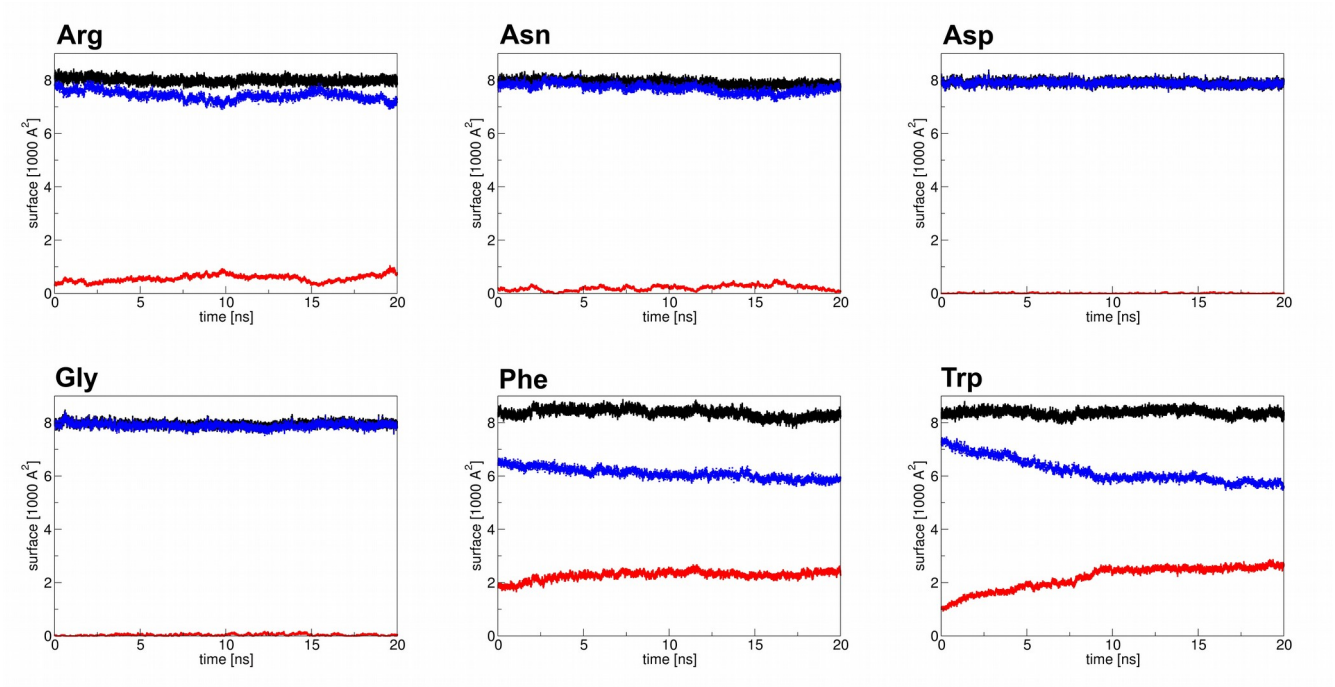


Figure S20. Time development of the total surface area (black), and surface coverages of the ***polypropylene*** *nanoparticle by water (blue) and the amino acids (red) in the molecular dynamics simulation.*

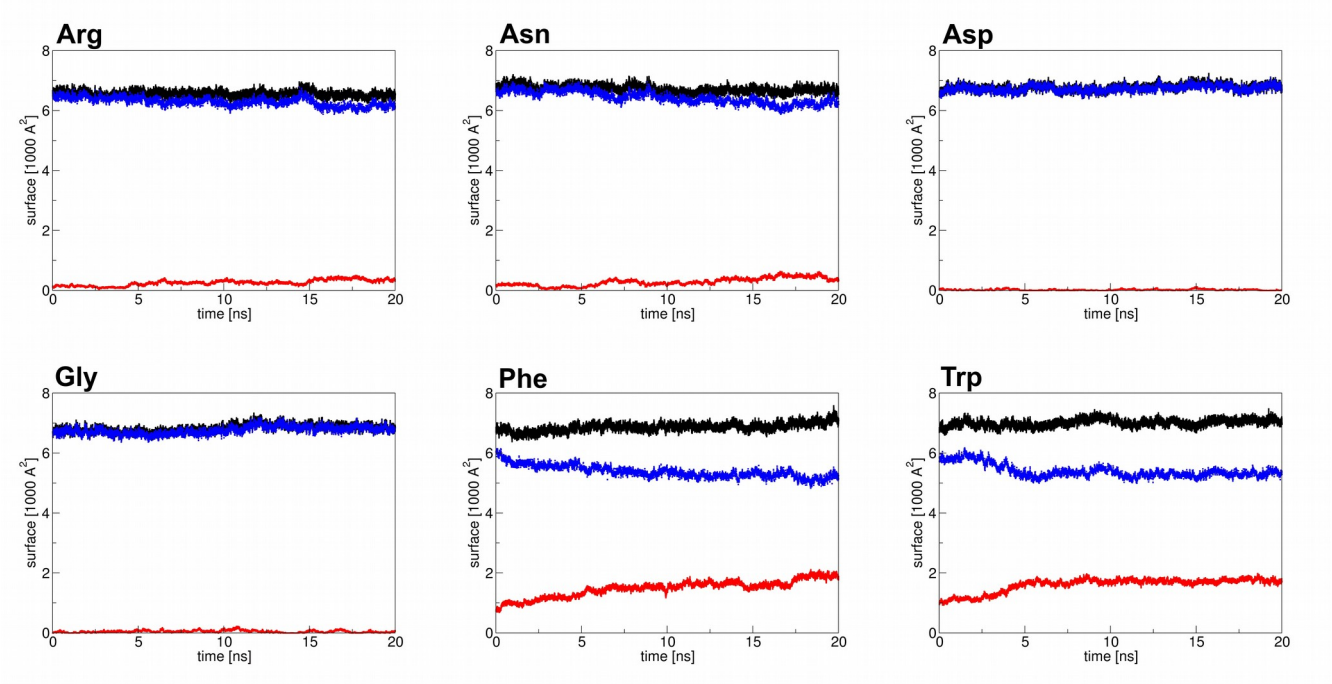


*Figure S21. Time development of the total surface area (black), and surface coverages of the **PET** nanoparticle by water (blue) and the amino acids (red) in the molecular dynamics simulation.*

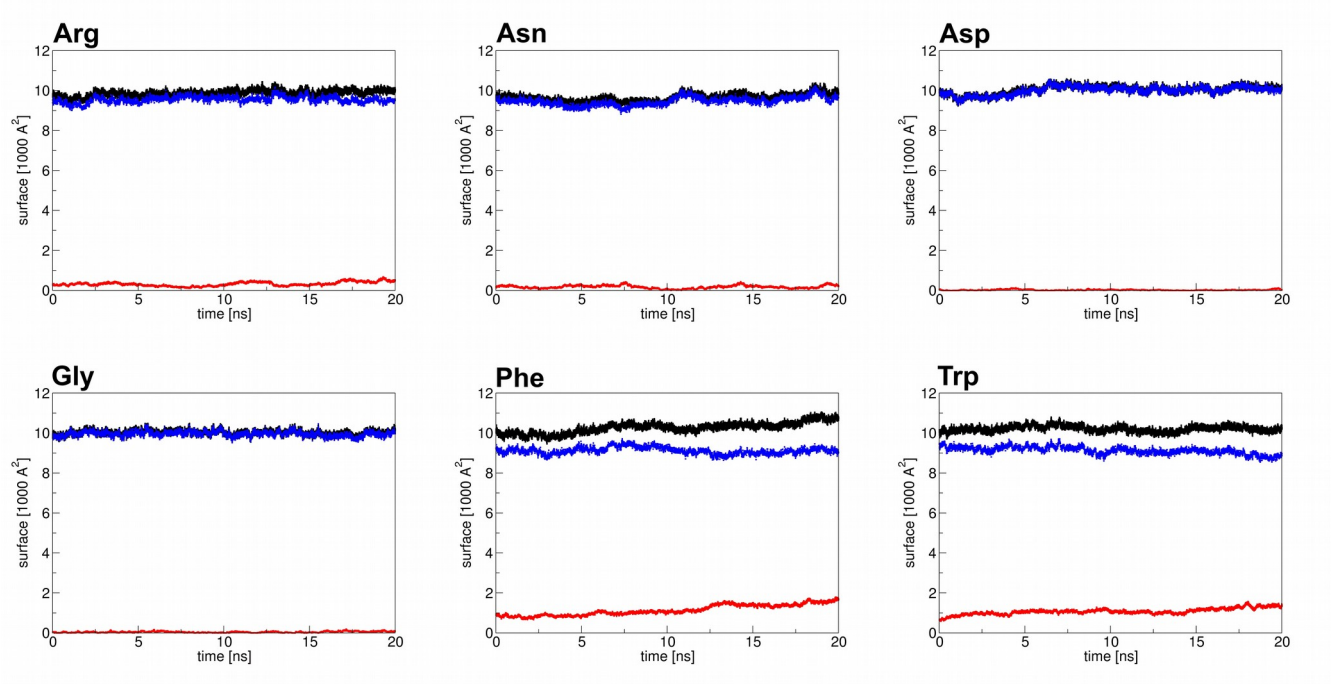


Figure S22. Time development of the total surface area (black), and surface coverages of the ***nylon-6,6*** *nanoparticle by water (blue) and the amino acids (red) in the molecular dynamics simulation.*