Journal of the Serbian Chemical Society
version electronic
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. **00(0)** S1-S3 (2025)
Supplementary material

SUPPLEMENTARY MATERIAL TO

Molecular dynamics-based methodological approach to clarify PFOA binding on Human Serum Albumin

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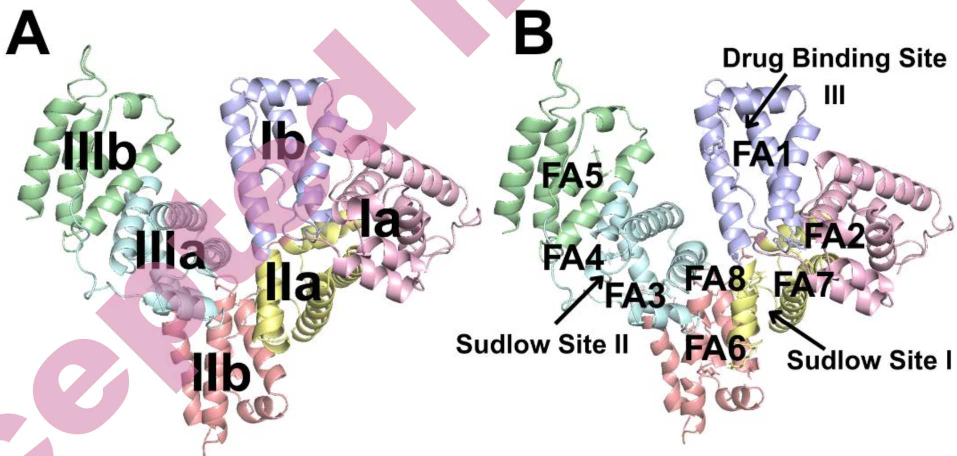

Figure S1. *PyMOL* representation of the crystal structure of HSA (PDB: 1N5U). (A) The overall structure with subdomains highlighted: Domain Ia (light pink), Domain Ib (light blue), Domain IIa (light yellow), Domain IIb (salmon), Domain IIIa (pale cyan), and Domain IIIb (pale green). (B) Binding pockets relevant to ligand interactions are labeled, including eight fatty acid binding sites (FA1–FA8), two Sudlow's drug-binding sites (Sudlow's site I and II), and an additional drug-binding pocket. Binding site annotations are based on literature-reported positions.

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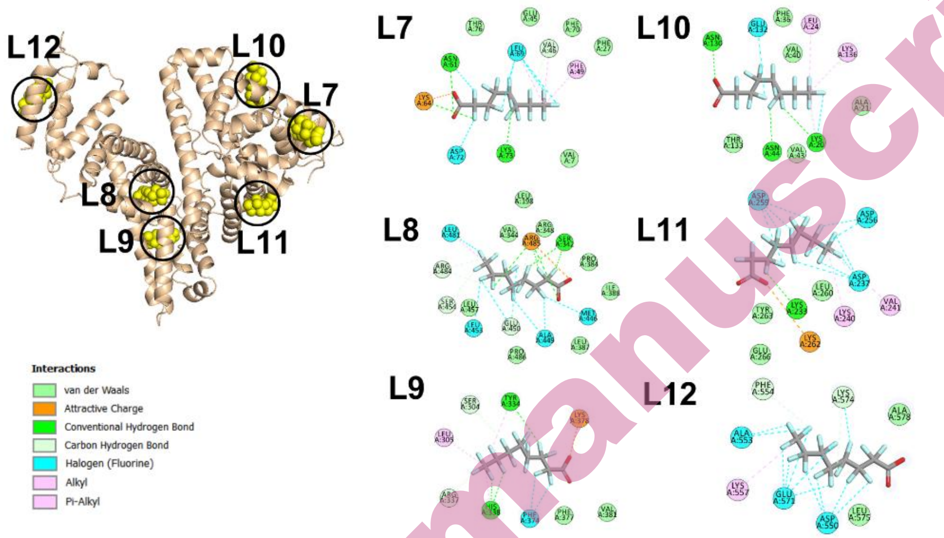

Figure S2. Representation of docking poses with binding energies below –33.4 kJ/mol. Poses L7–L12 are shown on the HSA molecule (left), while the right panels present the interactions for each pose, as generated in the *Discovery Studio* program. The legend for the interaction types is provided below the depiction of the HSA crystal structure (PDB: 1N5U) with bound ligands.

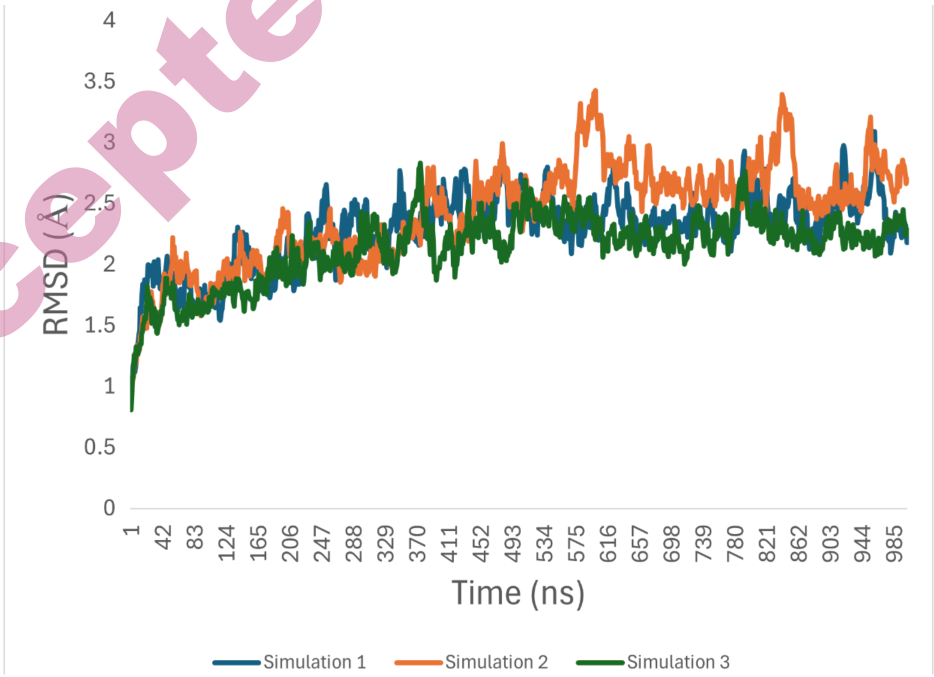

Figure S3. RMSD of HSA during all three 1000-ns MD simulation.

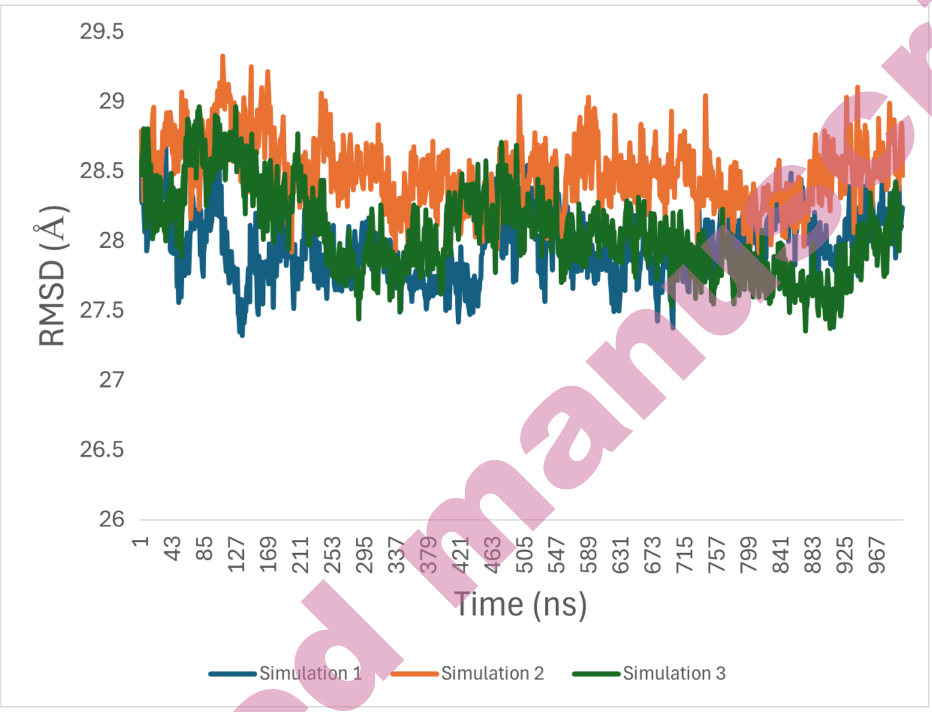

Figure S4. Radius of gyration of HSA during all three 1000-ns MD simulation.

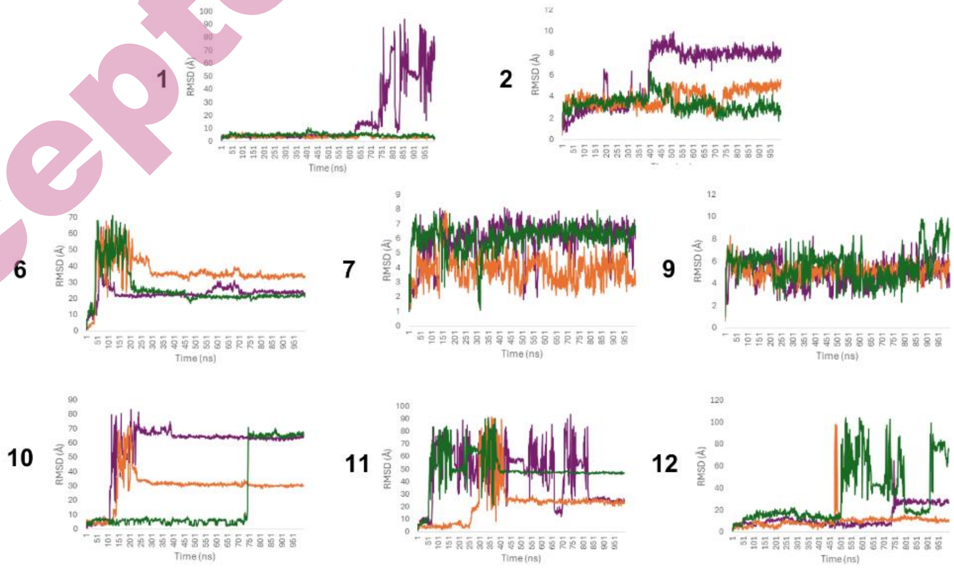

Figure S5. RMSD plots for ligand (L) poses not selected as PFOA binding sites on HSA. The plots were generated from three independent MD simulations.