Supplementary File

A Multimodal Approach Integrating Spectroscopy, Deep Learning guided Molecular Docking, and Molecular Dynamics simulation for predictive assessment of Pioglitazone to albumin binding for Formulation development.

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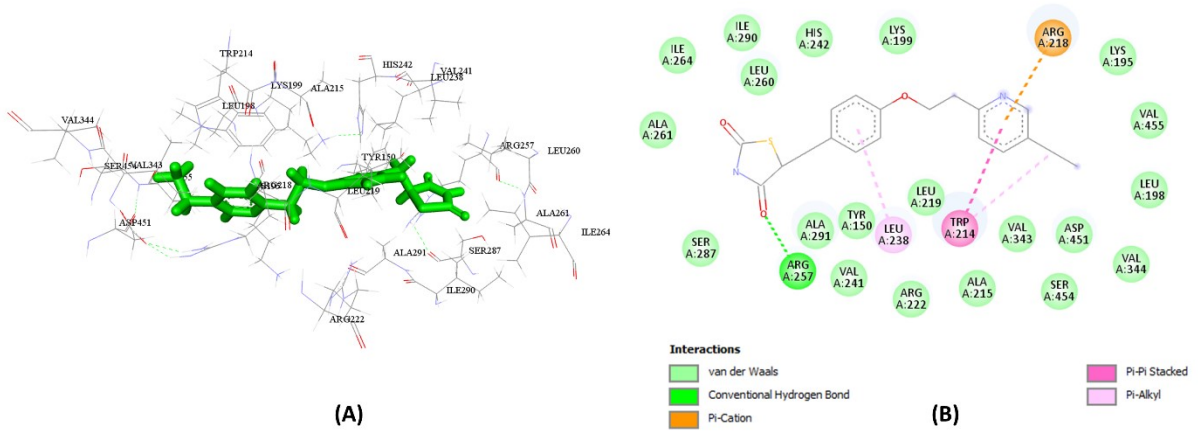

Figure S1. (A) 3D and (B) 2D docking interaction between Human serum albumin and Pioglitazone. The dotted lines of specific color indicating the type of possible interactions observed.

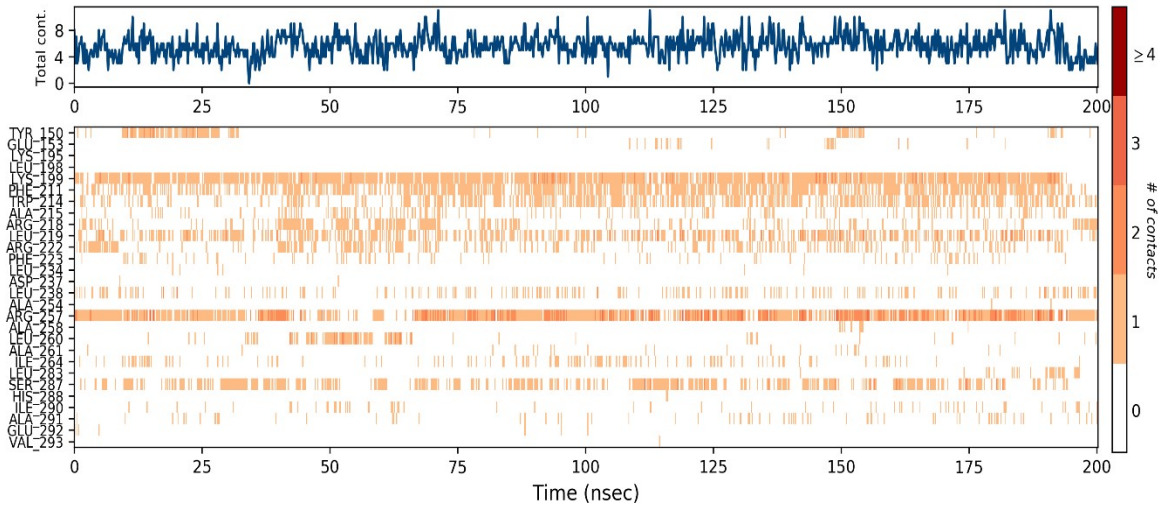

Figure S2. Timeline of pioglitazone and human serum albumin interactions during the 200 ns MD simulation. The top panel displays the total number of contacts (Total cont.) formed over the trajectory, while the bottom panel highlights residue-wise interactions across individual frames. Darker shades indicate residues forming multiple simultaneous interactions with the ligand.