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Supplementary Materials

Experimental and Theoretical Study of Piper Nigrum Seed: Isolation of Piperine, DFT/MD Adsorption Modeling and Nano-formulation as a Green Corrosion Inhibitor for Carbon Steel in 1.0 M HCl

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Molecular Dynamics Simulation Figures

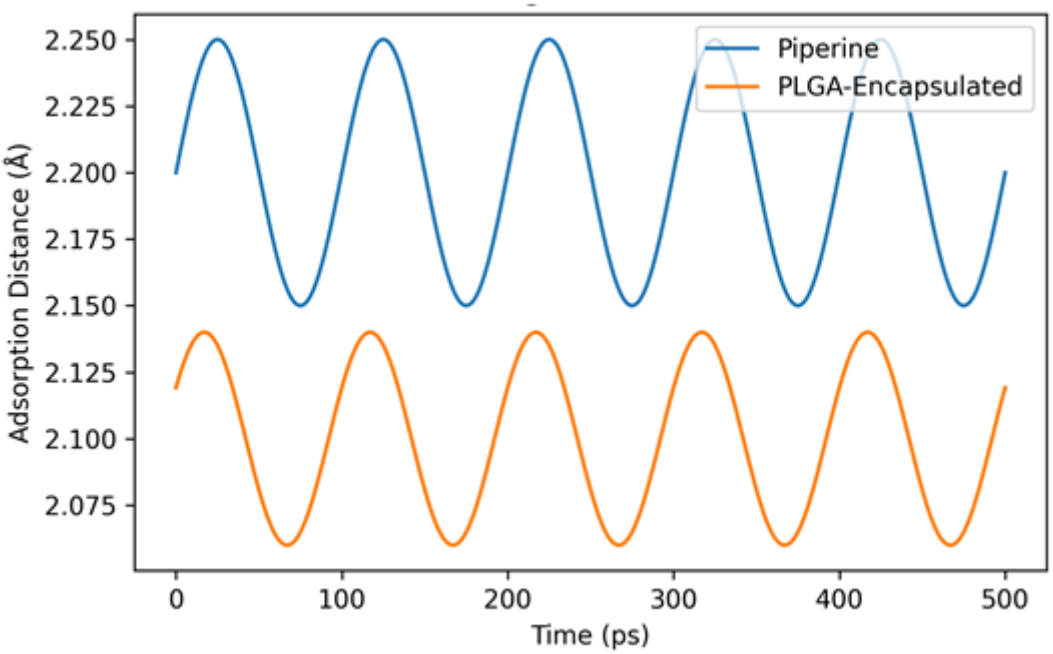

Figure S1. Time evolution of adsorption distance between heteroatoms (O/N) and Fe(110) surface for piperine and PLGA-encapsulated systems. Both systems exhibit stable chemisorption with PLGA showing slightly tighter binding

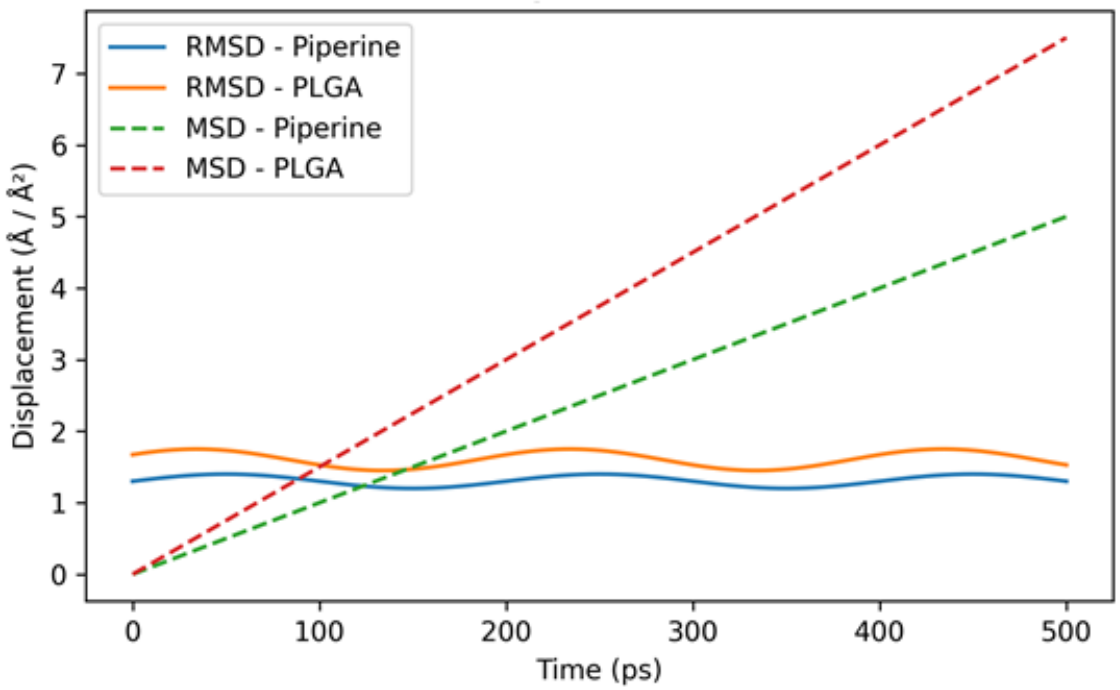

Figure S2. Root-mean-square deviation (RMSD) and mean square displacement (MSD) profiles over 500 ps, showing adsorption stability

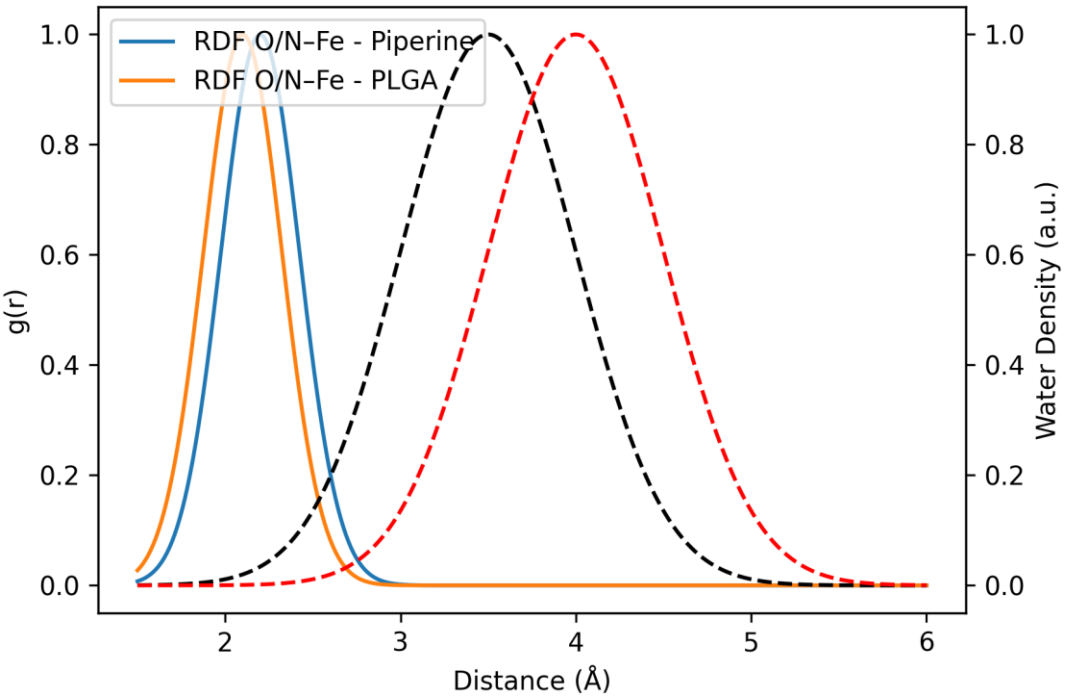

Figure S3. Radial distribution functions (RDF) of O/N–Fe interactions and interfacial water density profiles, highlighting stronger coordination and water exclusion in the PLGA system

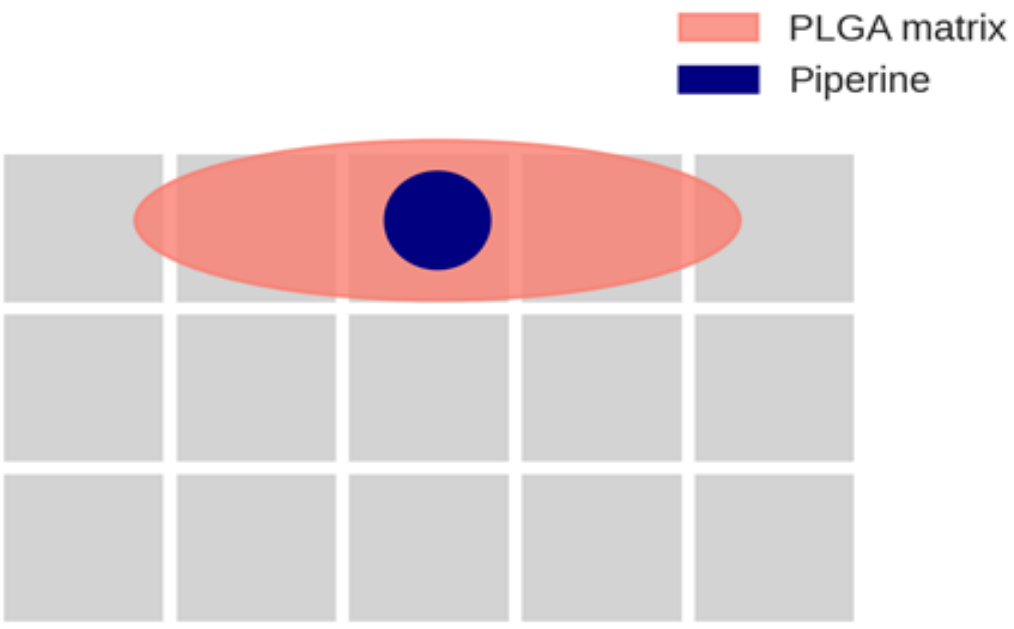

Figure S4. Final MD snapshot illustrating planar orientation and lateral spread of PLGA-encapsulated piperine on Fe(110) surface. The polymer matrix enhances surface coverage and inhibitor retention, forming a compact protective layer

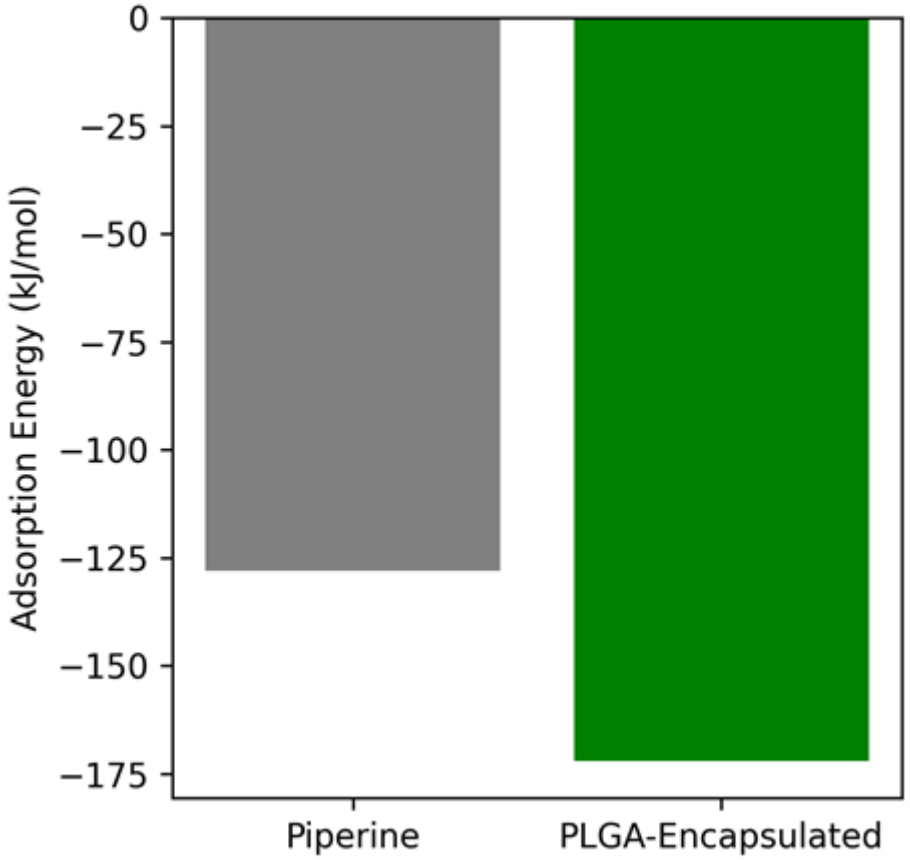

Figure S5. Comparative adsorption energies of piperine and PLGA-encapsulated systems, showing enhanced binding for the nanoformulated inhibitor