Green Synthesis of Platinum and Palladium Nanoparticles Using *Peganum harmala* L. Seed Alkaloids: Biological and Computational Studies

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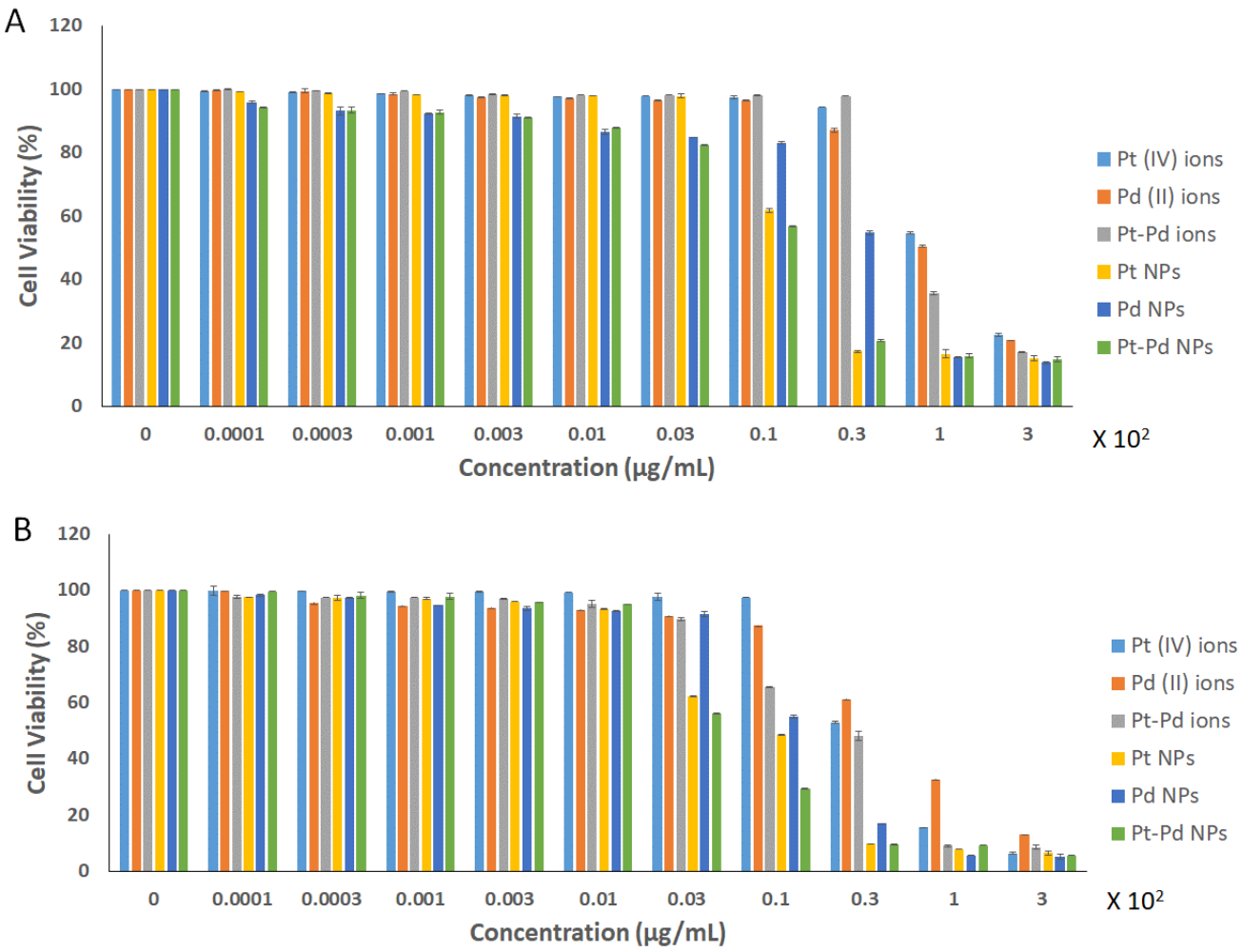

Figure S1. Evaluating the cytotoxicity of Pt NPs, Pd NPs, and Pt-Pd NPs compared to the individual metals ions at various concentrations ranging from 0.01 to 300 µg/mL using SRB assay in (**A**) A549 and (**B**) MCF-7 cells. An overall statistically significant decrease in cell viability was observed with the nanoparticles compared to individual metal ions ($p < 0.05$). Untreated cells were used as negative control and considered as 100%. All experiments were carried out in triplicates, and the mean values were calculated. Error bars represent ± standard deviation.

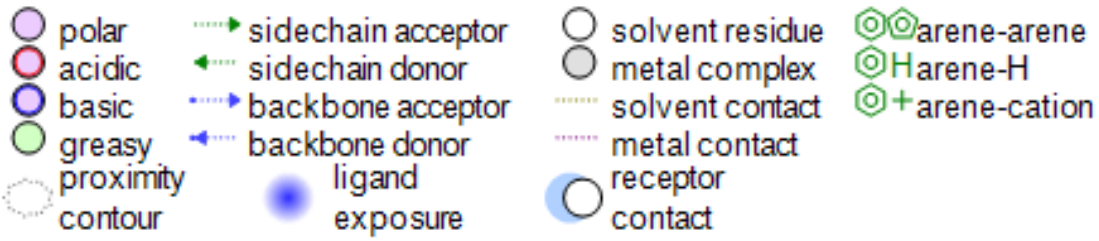

Figure S2. Color map of interaction modes between ligands and enzymes provided by MOE v. 2010.

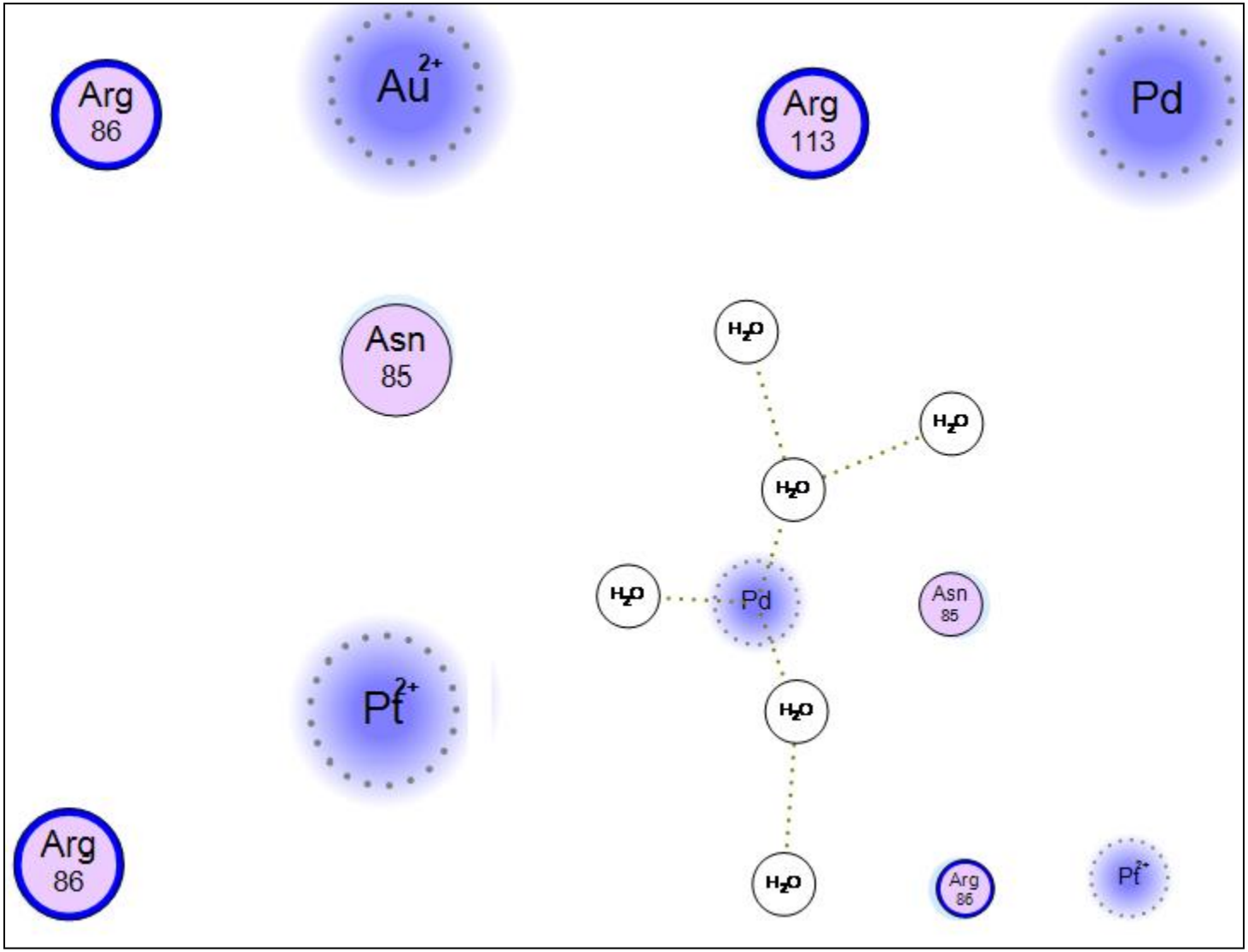

Figure S3:2D interaction-ligand exposure between the four metal dynamic designed nanoparticles (Au^{+2} NPs and tested metals; Pd^{0} NPs, Pt^{+2} NPs and Pd^{0}-Pt^{+2} mixture NPs) and key amino acids of cysteine proteinase displayed by MOE v.2010.

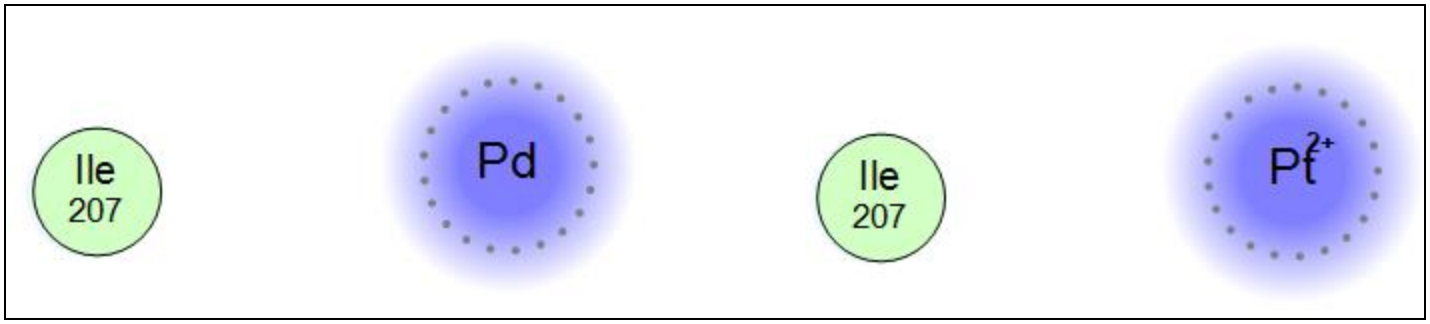

Figure S4:2D interaction-ligand exposure between Pd^{0}NPs and Pt^{+2} NPs designed dynamic models and key amino acids of superoxide dismutase displayed by MOE v.201