Supporting Information

Probing the Role of Imidazopyridine and Imidazophosphorine Scaffolds to Design Novel Proton Pump Inhibitor for H^+,K^+-ATPase: A DFT Study

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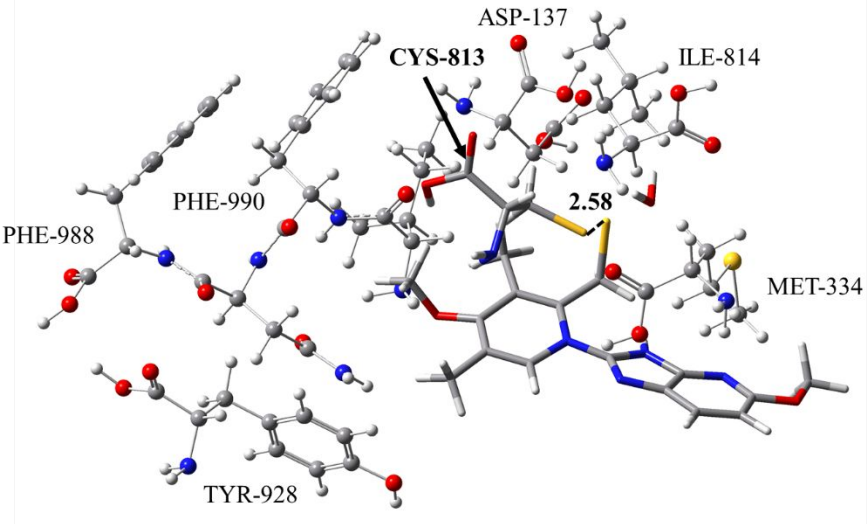

Figure S1: TS4 of Tenatoprazole with binding site residues of H^+,K^+-ATPase

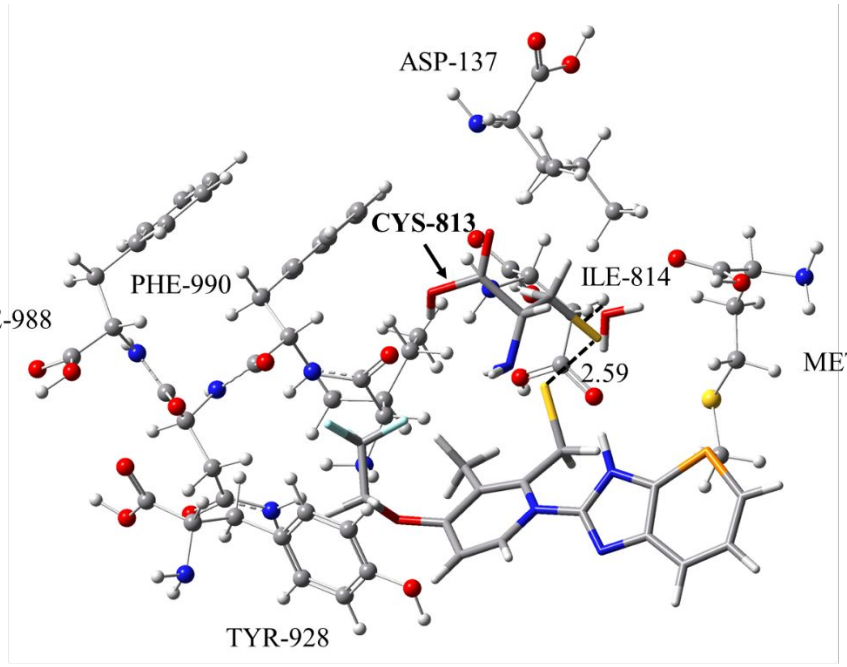

Figure S2: TS4 of Inhibitor-5 with binding site residues of H^+,K^+-ATPase

Tenatoprazole and inhibitor-5 with binding site residues are optimized, The transition state was treated with m062x/6-31g(d) and second layer of residues treated with MM force field uff. The ONIOM optimized geometries were taken for single point calculations at M11L/6-31++G(d,p) in aqueous phase using SMD solvation model to obtain the energies.