

Supplementary Data

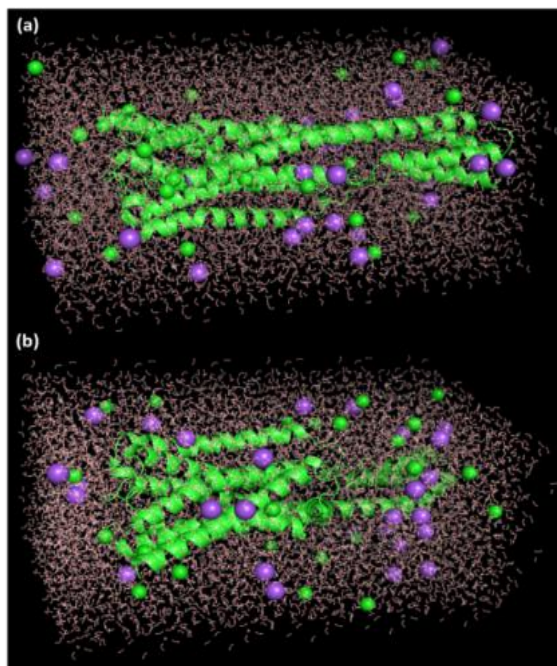


Figure S1. Receptor-ligand complex (a) CuGS and (b) GpnS in triclinic box solvated with water molecules and neutralized with 28 Na⁺ and 27 Cl⁻ ions (0.15 M salt).

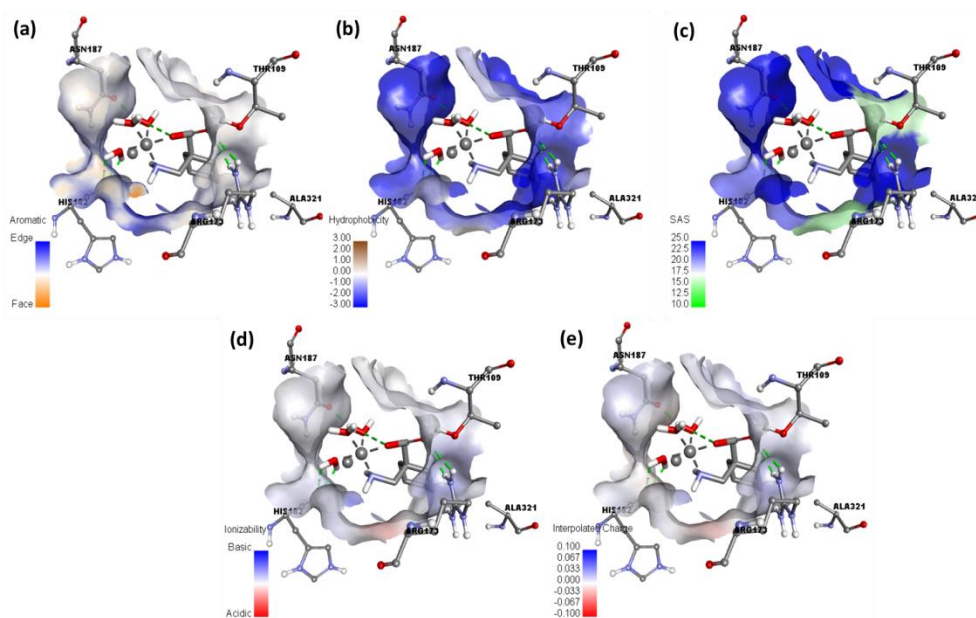


Figure S2. Representation of (a) aromatic surface, (b) hydrophobic surface, (c) solvent accessible surface, (d) ionizability surface, and (e) Interpolated charge; between serotonin and metal complex [Cu(II)-(Gpn)].