Electronic Supplementary Material (ESI) for Molecular BioSystems.

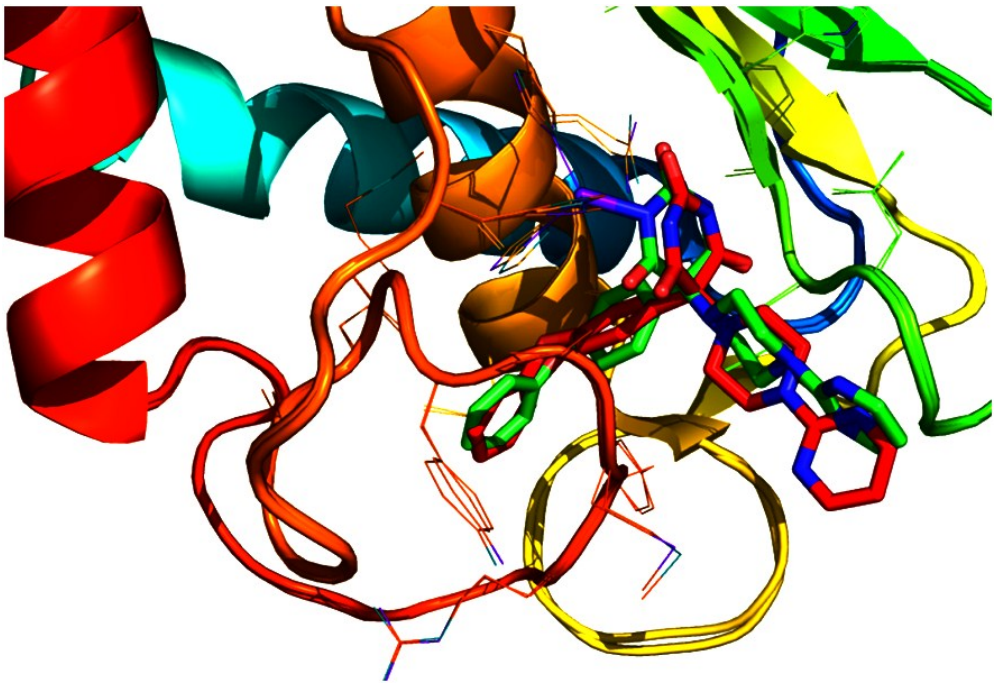

Fig. S1. Docking Program Validation: Alignment of the redocked (red) and co-crystal ligand (green) binding pose using the glide docking module.

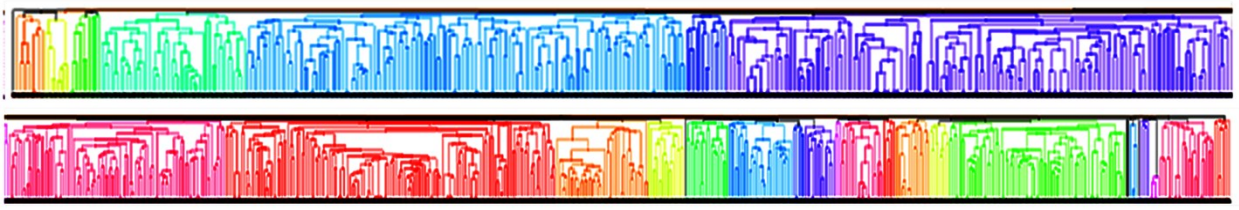

Fig.S2. Hierarchical clustering of the structure based hits obtained during pharmacophore based screening

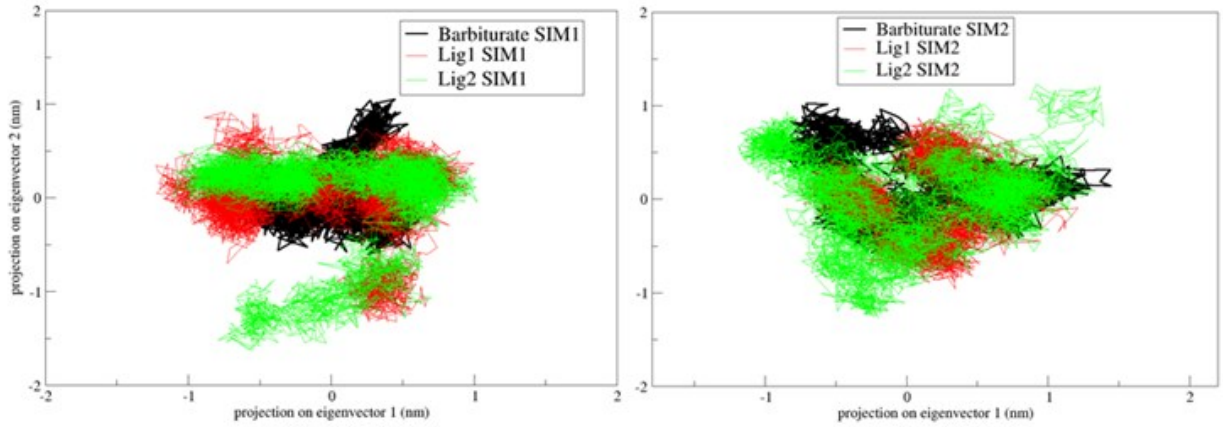

Fig S3: Principal component Analysis (PCA) plot for three individual trajectories for Lig-1,Lig-2 and Barbiturate complex in both SIM1 and SIM2.