

Supplementary Information

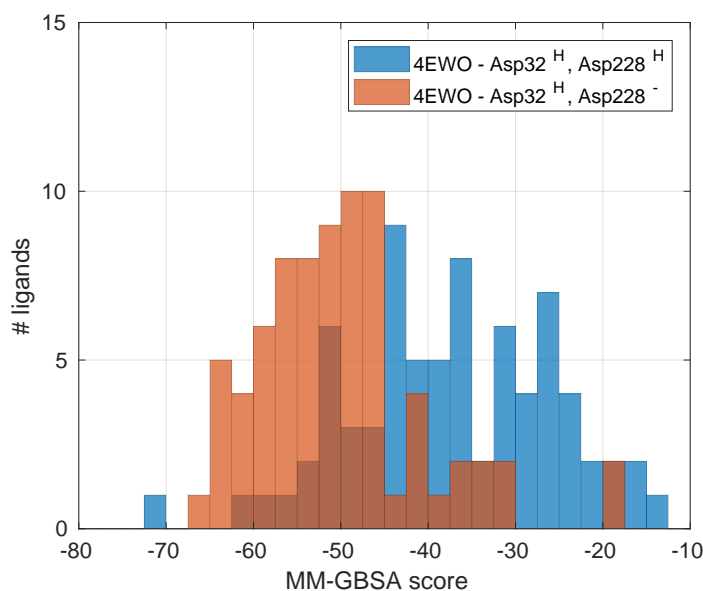


Fig. S1 Distribution of the calculated MM-GBSA scores for different protonation states of the receptor 4EWO. Overall, the single protonation state (Asp32^H, Asp228⁻) resulted in lower MM-GBSA scores than the double protonation state (Asp32^H, Asp228^H).

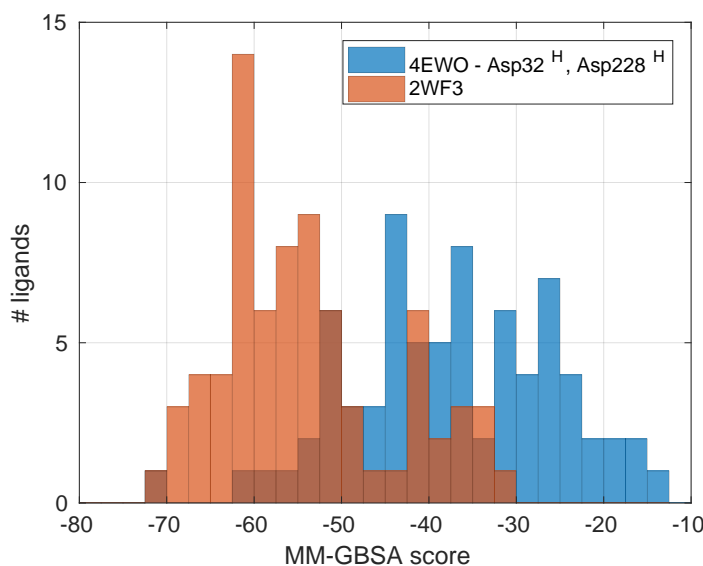


Fig. S2 Distribution of the calculated MM-GBSA scores for the two receptor conformations - 4EWO and 2WF3 for the same set of 75 ligands. In general, the receptor 2WF3 resulted in lower MM-GBSA scores than 4EWO.