

**S2 Fig. Ligand library original GLL/GDD vs racemic GLL/GDD NSQ\_AUC comparisons.**

Comparison of VS performance on groups of binding pockets bound by the same ligand depending on the ligand library used for screening: original GLL/GDD (hatched) or racemic GLL/GDD (plain). Values are NSQ\_AUCs calculated on ROC curves comparing a) known ligands against decoys, and b) agonists against inhibitors (or vice-versa).

