Supplementary Information

Figure S1. The detail results on the distribution of enriched active ligands calculated for each benchmarked software. Horizontal axis indicates top percentage of rank, Vertical axis indicates percentage of selected ones in total known binding ligands.

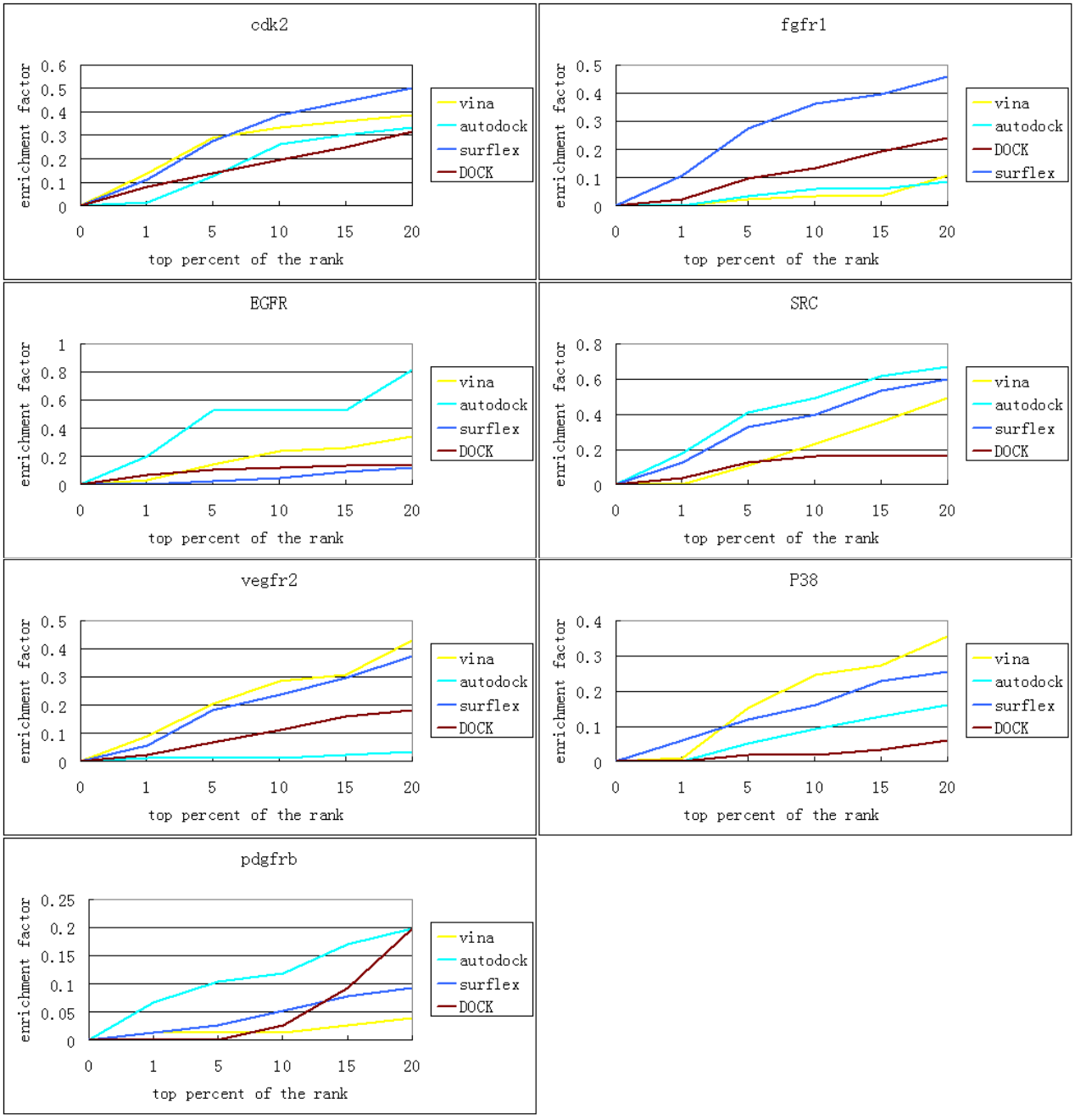

Figure S2. Comparisons of binding pose respectively against IGF1R and IR for each identified IGF1R specific inhibitors. Atoms were colored by the type. Protein residues were represented by lines and ligands were represented by sticks. Green lines and sticks exhibit ligands' binding pose in IGF1R active site, while cyan ones exhibit ligands' binding pose in IR active site. Yellow dash lines indicate H-bonds automatically exhibited by Pymol while the one with a number on it indicate H-bond that was not identified by Pymol [25]. For compound named 640627, no reasonable pose was generated in the active site of IR.

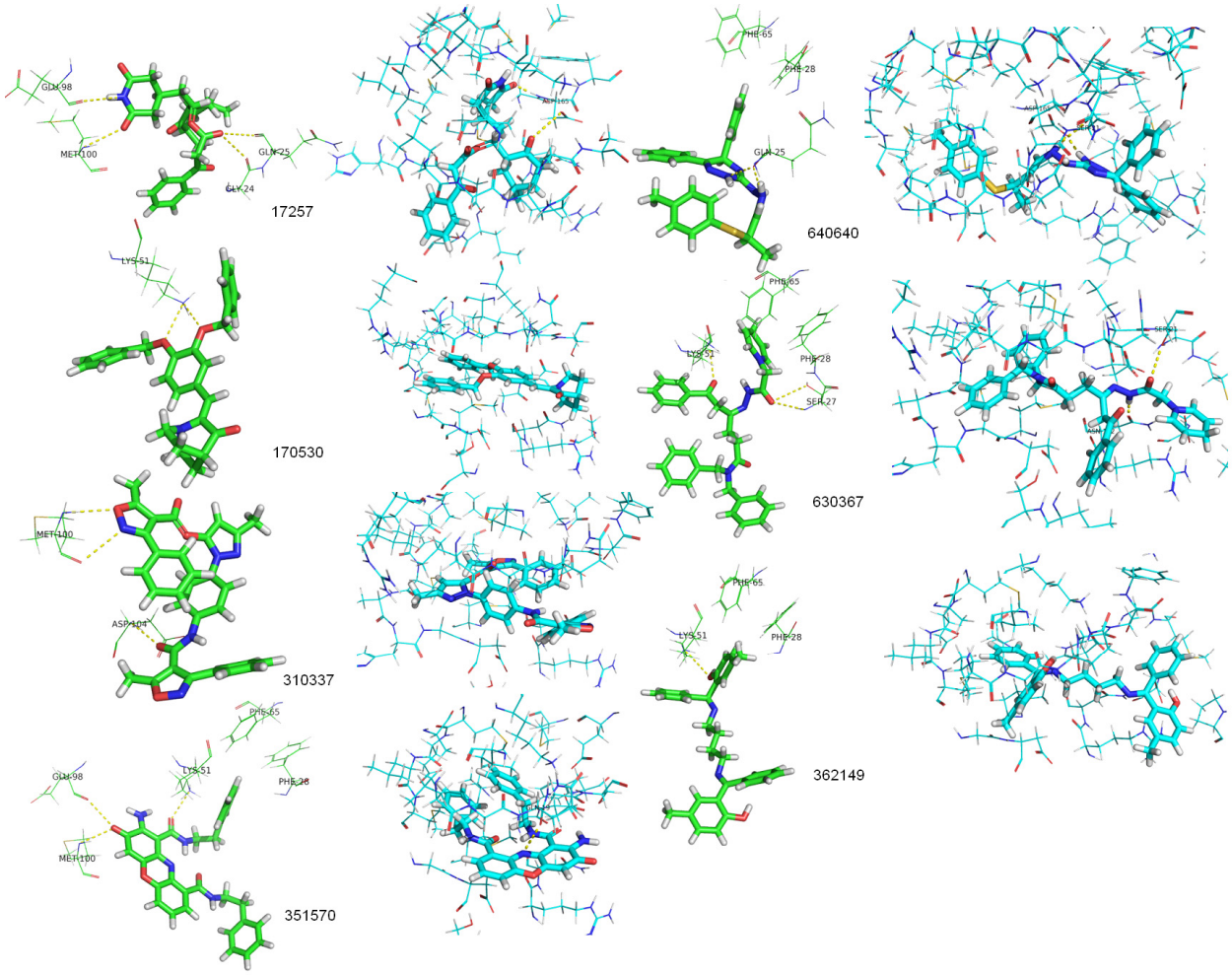

Figure S2. *Cont.*