



Figure S12. The binding free energy terms obtained from the MM-GBSA calculations relative to the binding of ligands as labeled in the plot and the color codes for different energy components as shown in the schema (the values presented are in kcal/mol). The terms consist of van der Waals energy, electrostatic energy, polar solvation energy, solvent-accessible surface area (SASA energy), and total binding free energy. 1P8D (A), 3NMQ (B), 3O96 (C), 4ACG (D), and 5J20 (E).