**RUN1920** -1.4binding -1.6 $\Delta\Delta G$  / kcal mol $^{-1}$ binding (all GENS) -1.8-2.0 -2.2 -2.4-121.0solvent -121.5 -122.0 -122.5 -122.5 -123.0complex -123.5

**GEN**