**RUN1260** binding -0.7 $\Delta\Delta G$  / kcal mol $^{-1}$ binding (all GENS) -0.8-0.9-1.0-1.1<del>-</del>73.25 solvent complex  $\Delta G$  / kcal mol<sup>-1</sup> -73.50**-**73.75 -74.00

