## $\Delta G$ [kcal/mol] FEP+ bace\_p2 jnk1 -3pde2 tyk2 thrombin ros1 -6p38 eg5 ptp1b cdk8 Predicted galectin hif2a cdk2 pfkfb3 pde10 cmet shp2 mcl1 bace syk bace\_hunt tnks2 Experimental