l: 1 | mp: 2 | feat.: 64 params: 3.13e+04 | Test (n=800) Ε D 80 6.79/5.63 [kcal/mol] $1 - r^2$: 4.454E-04 1.13/0.63 [kcal/mol] $1 - r^2$: 1.425E-02 0.08/0.06 [eÅ] 60 -2000 $1 - r^2$: 6.532E-03 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600**-**2 -6050 -2600-2400-2200-2000 -50**-**2 0 0 1 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 0.04 379.14/263.98 [kcal/mol] $1 - r^2$: 6.770E-03 6.81/3.09 [kcal/mol] $1 - r^2$: 9.939E-01 0.01/0.01 [e] 60 0.03 40 pred. [kcal/mol] pred. [kcal/mol] -5000.02 20 -10000.01 0.00 -1500-20-0.01-40-2000-0.02-60 -2500-0.0350 0.02 -2000-1000 0 -500 -0.020.00 0.04 ref. [e] ref. [kcal/mol] ref. [kcal/mol]