l: 1 | mp: 2 | feat.: 32 params: 9.49e+03 | Test (n=800) Ε D 80 19.15/16.01 [kcal/mol] $1 - r^2$: 4.713E-03 1.18/0.66 [kcal/mol] $1 - r^2$: 1.612E-02 0.08/0.05 [eÅ] 60 -2000 $1 - r^2$: 5.695E-03 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -2600 -40-2-60-280050 -2750 -2500 -2250 -2000 -50 0 0 1 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 0.02 380.09/264.88 [kcal/mol] $1 - r^2$: 6.760E-03 0.01/0.00 [e] 6.64/3.01 [kcal/mol] 60 $1 - r^2$: 1.002E+00 40 pred. [kcal/mol] 0.01 pred. [kcal/mol] -50020 pred. [e] -10000.00 -1500-20-0.01-40-2000 -0.02-60 -250050 -2000-1000 0 -500 -0.020.00 0.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]