l: 1 | mp: 4 | feat.: 64 params: 7.04e+04 | Test (n=800) Ε D 80 2 3.92/2.62 [kcal/mol] $1 - r^2$: 1.759E-04 0.56/0.29 [kcal/mol] $1 - r^2$: 3.567E-03 0.05/0.04 [eÅ] 60 $1 - r^2$: 2.511E-03 -2000pred. [kcal/mol] – 2500 1 40 pred. [kcal/mol] pred. [*eÅ*] 20 0 0 -20 -1-40-2600**-**2 -6050 -2600-2400-2200-2000 -50 **-**2 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q $0 = 377.97/263.07 \text{ [kcal/mol]} \\ 1 = r^2: 6.971E-03$ 6.57/2.86 [kcal/mol] 0.01/0.01 [e] 60 0.000 $1 - r^2$: 1.007E+00 kcal/mol 40 pred. [kcal/mol] -0.00520 -0.010-0.015-20-40-2000 -0.020-60 : -2500-0.025-1000 0 50 -0.01-20000 -50-0.020.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]