l: 0 | mp: 4 | feat.: 128 params: 1.44e+0.5 | Test (n=800) Ε D 75 -2 3.68/2.86 [kcal/mol] $1 - r^2$: 1.439E-04 0.86/0.42 [kcal/mol] $1 - r^2$: 8.186E-03 0.05/0.03 [eÅ] $1 - r^2$: 2.399E-03 -200050 1 pred. [kcal/mol] pred. [kcal/mol] pred. [eÅ] 25 -2200 0 0 -2400-25 -2600-50**-**2 **-**75 50 -2600-2400-2200-2000 -50 -10 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 0.02 75 - $0 = 376.92/262.13 \text{ [kcal/mol]} \\ 1 - r^2 : 6.819E-03$ 6.76/2.98 [kcal/mol] 0.01/0.00 [e] $1 - r^2$: 9.930E-01 0.01 50 kcal/mol pred. [kcal/mol] 0.00 25 -0.010 -0.02**-**25 -0.03-2000-50-0.04-2500**-75** -100050 -0.02-20000 -500 -0.040.00 0.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]