l: 1 | mp: 2 | feat.: 128 params: 1.12e+05 | Test (n=800) Ε D 80 3.69/2.75 [kcal/mol] $1 - r^2$: 1.735E-04 0.63/0.33 [kcal/mol] $1 - r^2$: 4.558E-03 0.07/0.04 [eÅ] 60 $1 - r^2$: 4.245E-03 -2000pred. [kcal/mol] -2400 40 1 pred. [kcal/mol] pred. [*eÅ*] 20 0 0 -20 -40-2600-2-6050 -2600-2400-2200-2000 -50**-**2 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 $0 = 378.80/263.86 \text{ [kcal/mol]} \\ 1 - r^2 : 6.766E-03$ 6.63/2.90 [kcal/mol] 0.01/0.00 [e] 0.04 60 $1 - r^2$: 1.004E+00 40 pred. [kcal/mol] pred. [kcal/mol] -5000.02 20 pred. [*e*] -10000.00 -1500-20-40-2000-0.02-60 -25000 50 -2000-1000 0 -50 -0.020.00 0.02 0.04 ref. [e] ref. [kcal/mol] ref. [kcal/mol]