*l*: 2 | mp: 4 | feat.: 32 params: 3.11e+04 | Test (n=800) Ε D 80 2 5.72/4.72 [kcal/mol]  $1 - r^2$ : 3.658E-04 0.59/0.33 [kcal/mol]  $1 - r^2$ : 4.070E-03 0.05/0.03 [eÅ] 60 -2000  $1 - r^2$ : 2.171E-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 0 1 0 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 80  $0 = 377.45/262.68 \text{ [kcal/mol]} \\ 1 = r^2: 7.019E-03$ 6.63/2.91 [kcal/mol]  $1 - r^2$ : 9.973E-01 0.01/0.00 [e] 0.020 60 bred -200 -1000 -1500 40 0.015 pred. [kcal/mol] 20 pred. [*e*] 0.010 0.005 -200.000 -40-2000-60 -0.005-2500-1000 0 50 0.01 -20000 -500.00 0.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]