l: 0 | mp: 2 | feat.: 128 params: 7.30e+04 | Test (n=800) Ε D 80 6.06/3.61 [kcal/mol] $1 - r^2$: 4.203E-04 0.92/0.48 [kcal/mol] $1 - r^2$: 9.767E-03 0.11/0.07 [eÅ] 60 -2000 $1 - r^2$: 1.179E-02 1 40 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400**-**20 -1-40-2600-2-60-280050 -2800-2600-2400-2200-2000 -50 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 386.38/270.49 [kcal/mol] $1 - r^2$: 6.310E-03 6.65/2.96 [kcal/mol] 0.01/0.01 [e] 60 0.04 $1 - r^2$: 1.003E+00 40 pred. [kcal/mol] pred. [kcal/mol] -5000.02 20 pred. [e] -10000.00 -1500-20 -0.02-2000-40-60 -0.04-2500-100050 -0.025 0.000 0.025 0.050 -20000 -500 ref. [kcal/mol] ref. [kcal/mol] ref. [e]