l: 0 | mp: 4 | feat.: 32 params: 1.15e+04 | Test (n=800) Ε D 1.93/0.81 [kcal/mol] $1 - r^2$: 4.233E-02 19.04/14.83 [kcal/mol] 0.08/0.06 [eÅ] 100 -2000 $1 - r^2$: 4.676E-03 $1 - r^2$: 6.211E-03 1 50 pred. [kcal/mol] pred. [*eÅ*] 0 0 -50 -1-100-150**-**2 -2800 100 -2750 -2500 -2250 -2000 -100**-**2 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q $0 = 379.83/264.72 \text{ [kcal/mol]} \\ 1 = r^2: 6.549\text{E-}03$ 7.01/3.08 [kcal/mol] 150 0.02/0.01 [e] 0.2 $1 - r^2$: 1.038E+00 100 bred. [kcal/mol] -1000 -1500 pred. [kcal/mol] 50 0.1 pred. [e] 0 0.0 -50-100-0.1-2000 -150-2500-0.20 100 0.1 0.2 -2000-1000 0 -100-0.2 -0.10.0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]