l: 0 | mp: 2 | feat.: 128 params: 7.30e+0.4 | Test (n=800) Ε D 75 -6.10/3.62 [kcal/mol] $1 - r^2$: 4.309E-04 0.95/0.49 [kcal/mol] 0.11/0.08 [eÅ] $1 - r^2$: 1.033E-02 -2000 $1 - r^2$: 1.297E-02 50 pred. [kcal/mol] pred. [kcal/mol] 25 pred. [*eÅ*] -2200 0 -0 -2400-25 -2600-50**-**75 -280050 -2 -2800-2600-2400-2200-2000 -500 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F 75 - $0 = 385.66/270.03 \text{ [kcal/mol]} \\ 1 - r^2 : 6.221E-03$ 6.64/2.95 [kcal/mol] 0.01/0.01 [e] 0.04 $1 - r^2$: 1.002E+00 50 | Kcal/mol pred. [kcal/mol] 0.02 25 pred. [*e*] 0.00 0 -0.02-25 -2000 -50-0.04-2500-75-100050 -0.050-0.025 0.000 0.025 0.050 -20000 -500 ref. [kcal/mol] ref. [kcal/mol] ref. [e]