*l*: 0 | mp: 4 | feat.: 32 params: 1.15e+04 | Test (n=800) Ε D 75 -13.57/9.68 [kcal/mol]  $1 - r^2$ : 2.297E-03 1.46/0.77 [kcal/mol]  $1 - r^2$ : 2.466E-02 0.07/0.05 [eÅ] -2000  $1 - r^2$ : 5.215E-03 50 1 pred. [kcal/mol] pred. [kcal/mol] 25 -2200pred. [*eÅ*] 0 0 -2400-25 -2600 -50-2-2800-75-5050 -2750 -2500 -2250 -2000 **-**2 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 75 -0.10  $0 = 378.43/263.58 \text{ [kcal/mol]} \\ 1 = r^2: 6.669\text{E-}03$ 6.67/3.02 [kcal/mol] 0.01/0.01 [e]  $1 - r^2$ : 9.976E-01 50 0.05 bred -200 -1000 -1500 ored. [kcal/mol] 25 pred. [e] 0.00 -0.05-25 -0.10-2000-50 -0.15**-75** -2500 -1000 50 -0.10.0 0.1 -20000 -50 0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]