*l*: 1 | mp: 4 | feat.: 128 params: 2.56e+05 | Test (n=800) Ε D 80 2 3.31/2.08 [kcal/mol]  $1 - r^2$ : 1.109E-040.55/0.27 [kcal/mol]  $1 - r^2$ : 3.497E-03 0.03/0.02 [eÅ] 60  $1 - r^2$ : 9.905E-04 -200040 1 ored. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600-2-6050 -2600-2400-2200-2000 -50 **-**2 0 1 0 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 80  $0 = 378.14/263.24 \text{ [kcal/mol]} \\ 1 = r^2: 6.988E-03$ 6.57/2.86 [kcal/mol]  $1 - r^2$ : 9.957E-01 0.00/0.00 [e] 0.020 60 40 0.015 ored. [kcal/mol] pred. [kcal/mol] -50020 pred. [*e*] 0.010 -10000.005 -1500-20 0.000 -2000-40-0.005-60 -2500-0.0100 50 -2000-1000 0 -50-0.010.00 0.01 0.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]