*l*: 2 | mp: 2 | feat.: 64 params: 4.26e+04 | Test (n=800) Ε D 80 2 6.39/4.83 [kcal/mol]  $1 - r^2$ : 2.284E-04 0.65/0.35 [kcal/mol]  $1 - r^2$ : 4.911E-03 0.13/0.10 [eÅ]60  $1 - r^2$ : 1.503E-02 -2000 bred. [kcal/mol] -2500 -2400 40 1 ored. [kcal/mol] pred. [*eÅ*] 20 0 0 -20 -1-40-2600-2-60 50 -2600-2400-2200-2000 -50 **-**2 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 80 0.02  $0 = 378.88/263.74 \text{ [kcal/mol]} \\ 1 = r^2: 6.783E-03$ 6.64/2.91 [kcal/mol]  $1 - r^2$ : 9.911E-01 0.01/0.01 [e] 60 0.01 bred -200 -1000 -1500 40 pred. [kcal/mol] 0.00 20 -0.01-0.02-20-0.03-40-2000 -0.04-60 -2500-0.0550 -0.020.00 -2000-1000 0 -50 0 -0.040.02 ref. [e] ref. [kcal/mol] ref. [kcal/mol]