*l*: 2 | mp: 4 | feat.: 64 params: 1.03e+05 | Test (n=800) Ε D 80 5.03/4.31 [kcal/mol]  $1 - r^2$ : 2.819E-04 0.53/0.27 [kcal/mol]  $1 - r^2$ : 3.184E-03 0.07/0.06 [eÅ] 60  $1 - r^2$ : 5.066E-03 -2000bred. [kcal/mol] -2500 -2400 1 40 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 0.005 377.23/262.51 [kcal/mol]  $1 - r^2$ : 7.003E-03 6.60/2.87 [kcal/mol]  $1 - r^2$ : 9.936E-01 0.01/0.01 [e] 60 0.000 bred -200 -1000 -1500 40 pred. [kcal/mol] -0.00520 -0.010-0.015-20-0.020-40-2000-0.025-60 -2500 -1000 50 -0.01-2000 0 -500 -0.020.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]