*l*: 1 | mp: 2 | feat.: 64 params: 3.13e+04 | Test (n=800) Ε D 80 6.87/4.90 [kcal/mol]  $1 - r^2$ : 5.985E-04 0.78/0.42 [kcal/mol]  $1 - r^2$ : 7.111E-03 0.07/0.05 [eÅ] 60 -2000  $1 - r^2$ : 4.826E-03 40 1 ored. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600-2-60 -280050 -2800-2600-2400-2200-2000 -50 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 80 379.24/264.17 [kcal/mol]  $1 - r^2$ : 6.776E-03 6.60/2.92 [kcal/mol]  $1 - r^2$ : 9.964E-01 0.01/0.00 [e] 0.02 60 40 ored. [kcal/mol] pred. [kcal/mol] -5000.01 20 pred. [e] -10000.00 -1500-0.01-20-40-2000-0.02-60 -2500-0.030 50 -2000-1000 0 -50-0.020.00 0.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]