*l*: 2 | mp: 2 | feat.: 64 params: 4.26e+04 | Test (n=800) Ε D 80 5.88/4.08 [kcal/mol]  $1 - r^2$ : 3.873E-04 1.04/0.58 [kcal/mol]  $1 - r^2$ : 1.251E-02 0.06/0.04 [eÅ] 60 -2000 $1 - r^2$ : 3.983E-03 40 1 ored. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -40-2600-2-60-2800-2800-2600-2400-2200-2000 -5050 **-**2 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 80 379.27/264.12 [kcal/mol]  $1 - r^2$ : 6.752E-03 0.04 6.68/3.03 [kcal/mol] 0.01/0.00 [e] 60  $1 - r^2$ : 1.001E+00 40 ored. [kcal/mol] pred. [kcal/mol] -5000.02 20 pred. [e] -10000.00 -1500-20-0.02-2000-40-60 -2500-0.04Ó 50 0.02 -2000-1000 0 -50-0.04 -0.02 0.000.04 ref. [kcal/mol] ref. [kcal/mol] ref. [e]