*l*: 1 | mp: 5 | feat.: 128 params: 4.91e+05 | Test (n=2000) Ε D 8.0 -5500.92/0.55 [kcal/mol] 0.98/0.22 [kcal/mol] 0.01/0.01 [eÅ]750 0.6  $1 - r^2$ : 2.095E-04  $1 - r^2$ : 8.912E-05  $1 - r^2$ : 1.523E-03 -600 --600 – [kcal/mol] – 650 – 750 500 0.4 pred. [kcal/mol] pred.  $[e ilde{A}]$ 250 0.2 0.0 0 -0.2 -250-0.4-800-500-0.6 -850-750-500 500 0.0 0.5 -800 -700 -600-0.50 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 0.050 750 46.64/40.39 [kcal/mol] 46.79/31.60 [kcal/mol] 0.01/0.01 [e] 200  $1 - r^2$ : 2.032E-01  $1 - r^2$ : 9.596E-01 0.025 500 150 pred. [kcal/mol] pred. [kcal/mol] 0.000 100 250 pred. [e] -0.02550 0 -0.0500 -250-0.075-50 -500-0.100-100-750-100100 200 -5000 500 -0.10-0.050.00 0.05 0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]