*l*: 1 | mp: 5 | feat.: 128 params: 4.91e+05 | Test (n=2000) Ε D 0.8 -550 1.06/0.30 [kcal/mol]  $1 - r^2$ : 2.467E-04 1.07/0.67 [kcal/mol] 0.02/0.01 [eÅ] 750 0.6  $1 - r^2$ : 1.209E-04  $1 - r^2$ : 2.209E-03 -600 -600 Fred -650 -750 -750 500 0.4 ored. [kcal/mol] pred. [*eÅ*] 0.2 250 0.0 0 -0.2-250-0.4-800 -500-0.6-850 -750500 0.0 0.5 -800 -700-600-500-0.50 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs  $E_{\rm ele}$ F Q 0.06 750 36.59/31.85 [kcal/mol] 46.79/31.62 [kcal/mol] 0.01/0.01 [e] 200  $1 - r^2$ : 1.934E-01  $1 - r^2$ : 9.663E-01 0.04 500 ored. [kcal/mol] 150 ored. [kcal/mol] 0.02 250 pred. [e] 100 0.00 0 50 -0.02-250 0 -0.04-500 -50-0.06-750 -100100 -100200 -5000 500 -0.050.00 0.05 0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]