l: 2 | mp: 5 | feat.: 64 params: 1.99e+05 | Test (n=2000) Ε D 0.8 -550 1.69/1.47 [kcal/mol] 0.85/0.24 [kcal/mol] 0.02/0.01 [eÅ] 750 0.6 $1 - r^2$: 1.079E-04 $1 - r^2$: 1.556E-04 $1 - r^2$: 2.275E-03 -600 -600 Fred -650 -750 -750 500 0.4 ored. [kcal/mol] pred. [*eÅ*] 250 0.2 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 0.10 50.59/44.36 [kcal/mol] 46.78/31.56 [kcal/mol] 0.02/0.01 [e] 200 750 $1 - r^2$: 1.800E-01 $1 - r^2$: 9.864E-01 150 500 pred. [kcal/mol] ored. [kcal/mol] 0.05 100 pred. [e] 250 50 0.00 0 0 -250**-**50 -0.05-500-100-0.10-750-0.10 -0.05-1000 100 200 -500 0 500 0.00 0.05 0.10 ref. [kcal/mol] ref. [kcal/mol] ref. [e]