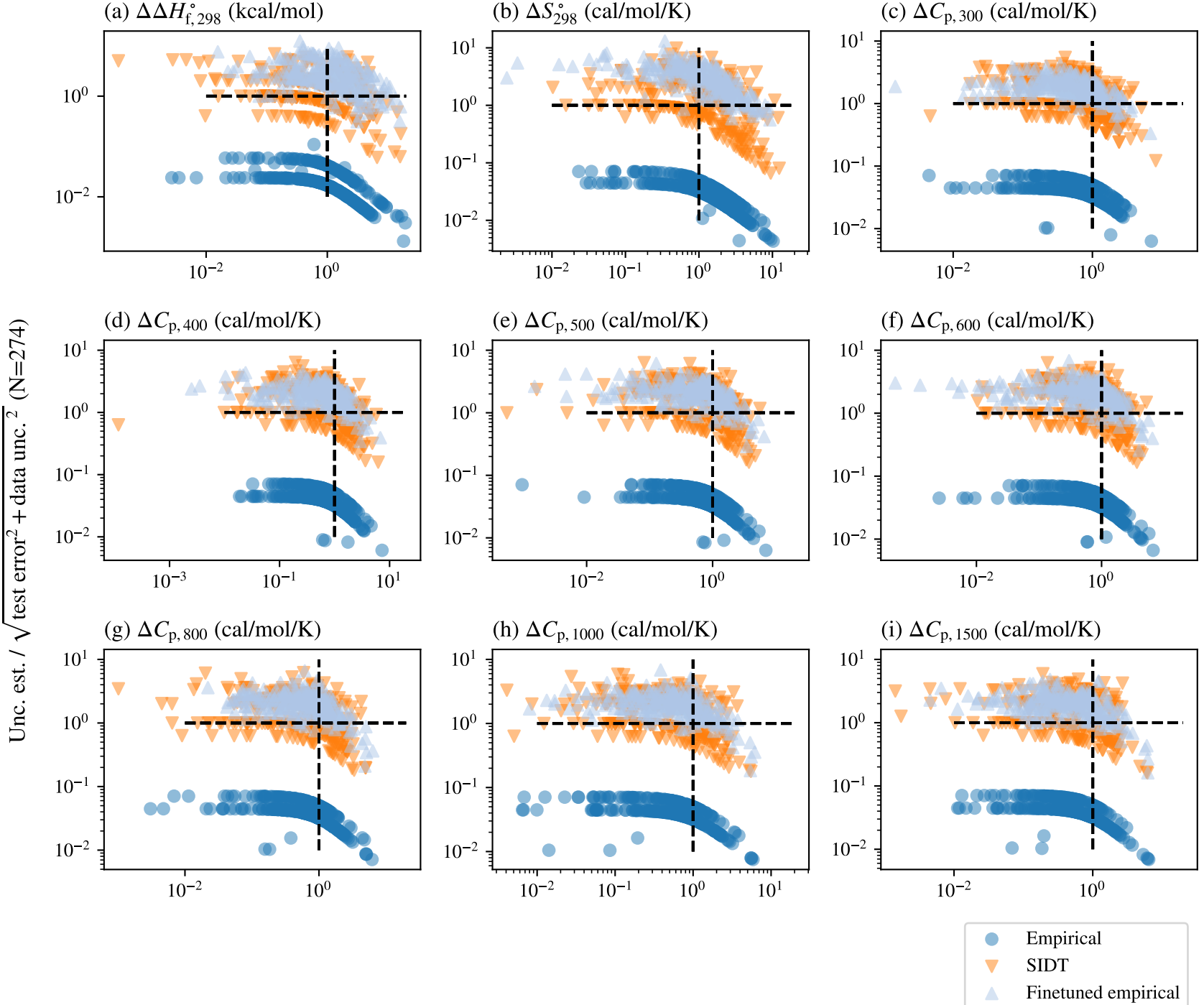
(a) $\Delta\Delta H^\circ_{f,298}$ (kcal/mol)
(b) ΔS°_{298} (cal/mol/K)
(c) $\Delta C_{p,300}$ (cal/mol/K)
(d) $\Delta C_{p,400}$ (cal/mol/K)
(e) $\Delta C_{p,500}$ (cal/mol/K)
(f) $\Delta C_{p,600}$ (cal/mol/K)
(g) $\Delta C_{p,800}$ (cal/mol/K)
(h) $\Delta C_{p,1000}$ (cal/mol/K)
(i) $\Delta C_{p,1500}$ (cal/mol/K)
Unc. est. / $\sqrt{\text{test error}^2 + \text{data unc.}^2}$ (N=274)
| Test error / data unc. |
Empirical
SIDT
Finetuned empirical