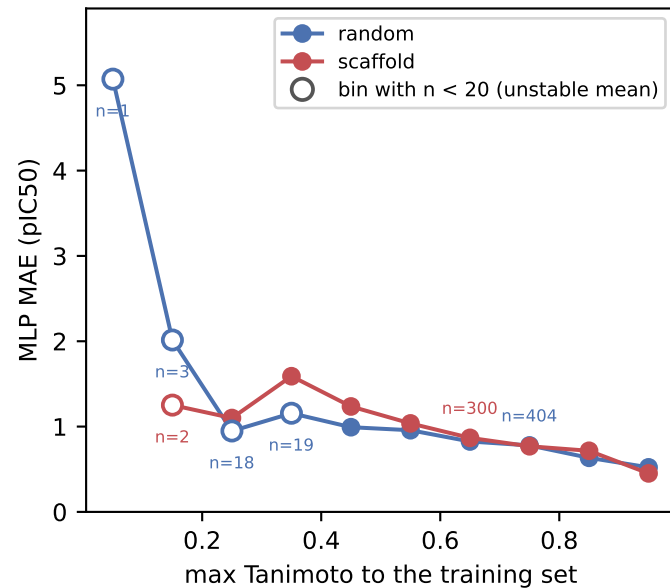
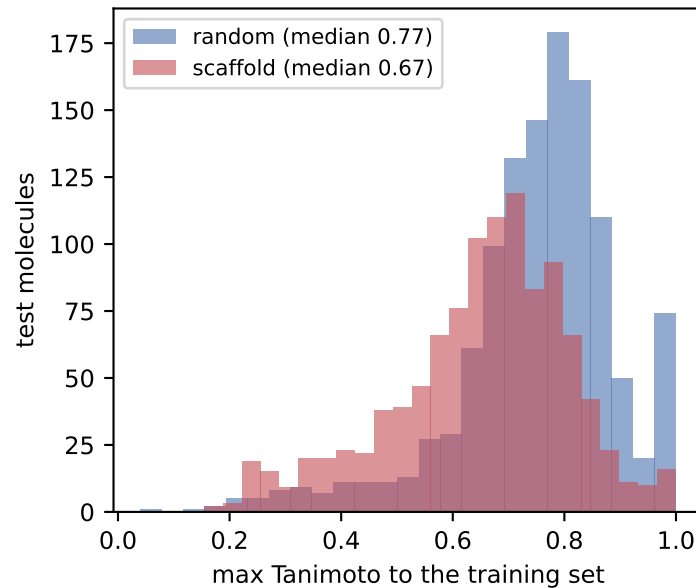


Figure 12 — Applicability domain, and what the regression diagnostics actually say
a slope below 1 can come from weak correlation rather than from predictions being pulled toward the mean

A. MAE is lower at high similarity — a trend, not a monotone curve
(per-bin n shown only where it is unstable or largest; full table in sidecar)



B. Test molecules sit further away under the scaffold split



C. Slope, correlation and spread are three different quantities

