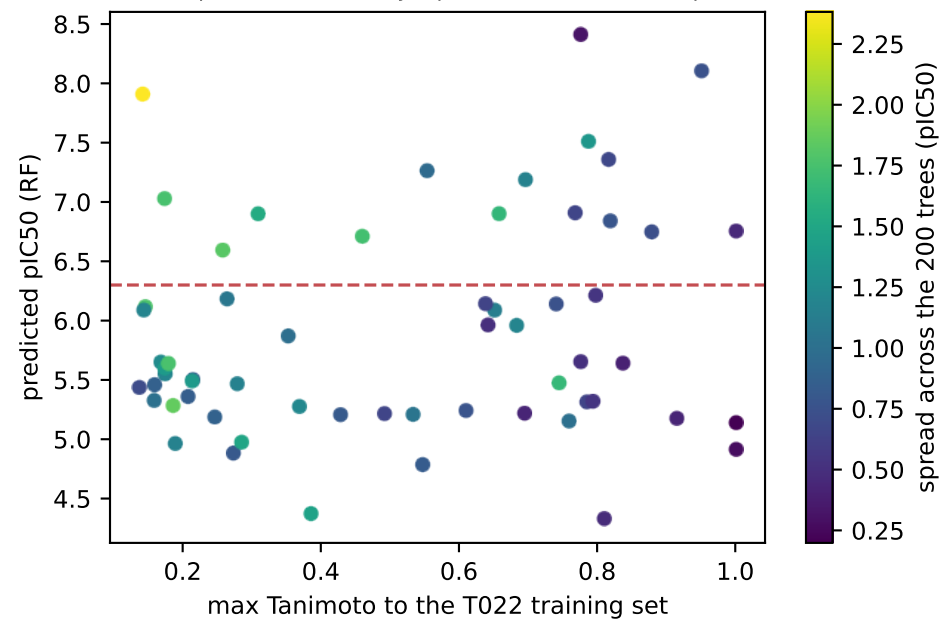


Figure 13 — Applying the regression model to an UNLABELED set: predictions only, no accuracy claim

A. The 60 unlabeled molecules, coloured by tree spread
measured Spearman(similarity, spread) = -0.66 (n=60, p < 0.001)



B. Domain check: median 0.54; 26 below 0.4

