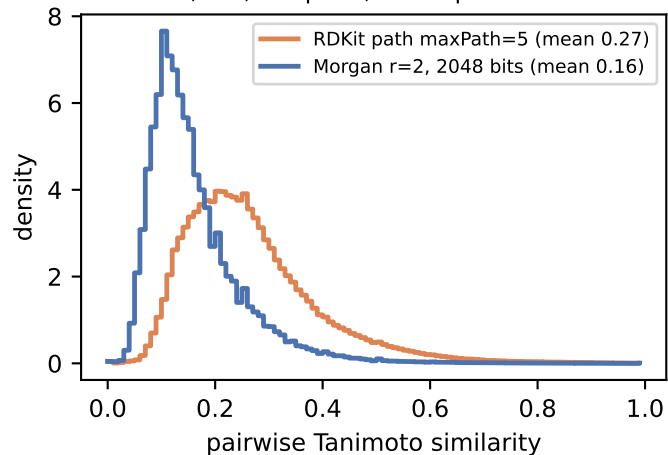
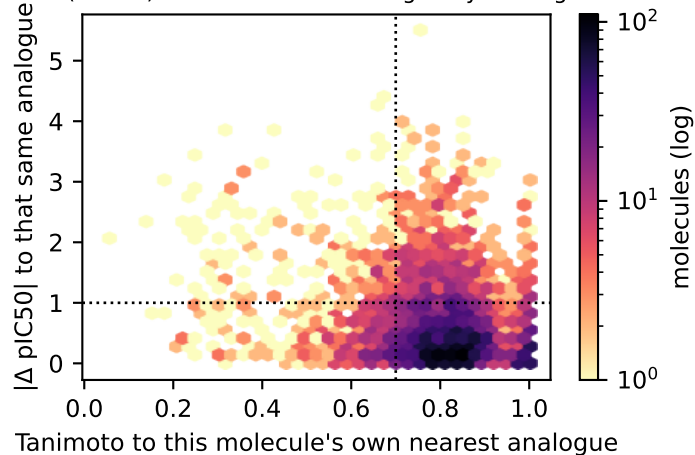


Figure 2 — Similarity structure: representation-dependent, and potency is not a smooth function of similarity
panel B pairs each molecule with its own single nearest analogue (per-molecule relationships, not unique molecule pairs)

A. 10,739,295 pairs, two representations



B. Of the 3887 molecules whose nearest analogue is at sim ≥ 0.7 , 808 (20.8%) differ from that analogue by > 1 log unit



C. Almost every molecule has a close partner

