

Supplementary Material for

"Enabling the hypothesis-driven prioritization of ligand candidates in big databases:
Screenlamp and its application to GPCR inhibitor discovery for invasive species control"
by Sebastian Raschka, Anne M. Scott, Nan Liu, Santosh Gunturu, Mar Huertas, Weiming Li, and
Leslie A. Kuhn,
Journal of Computer-Aided Molecular Design

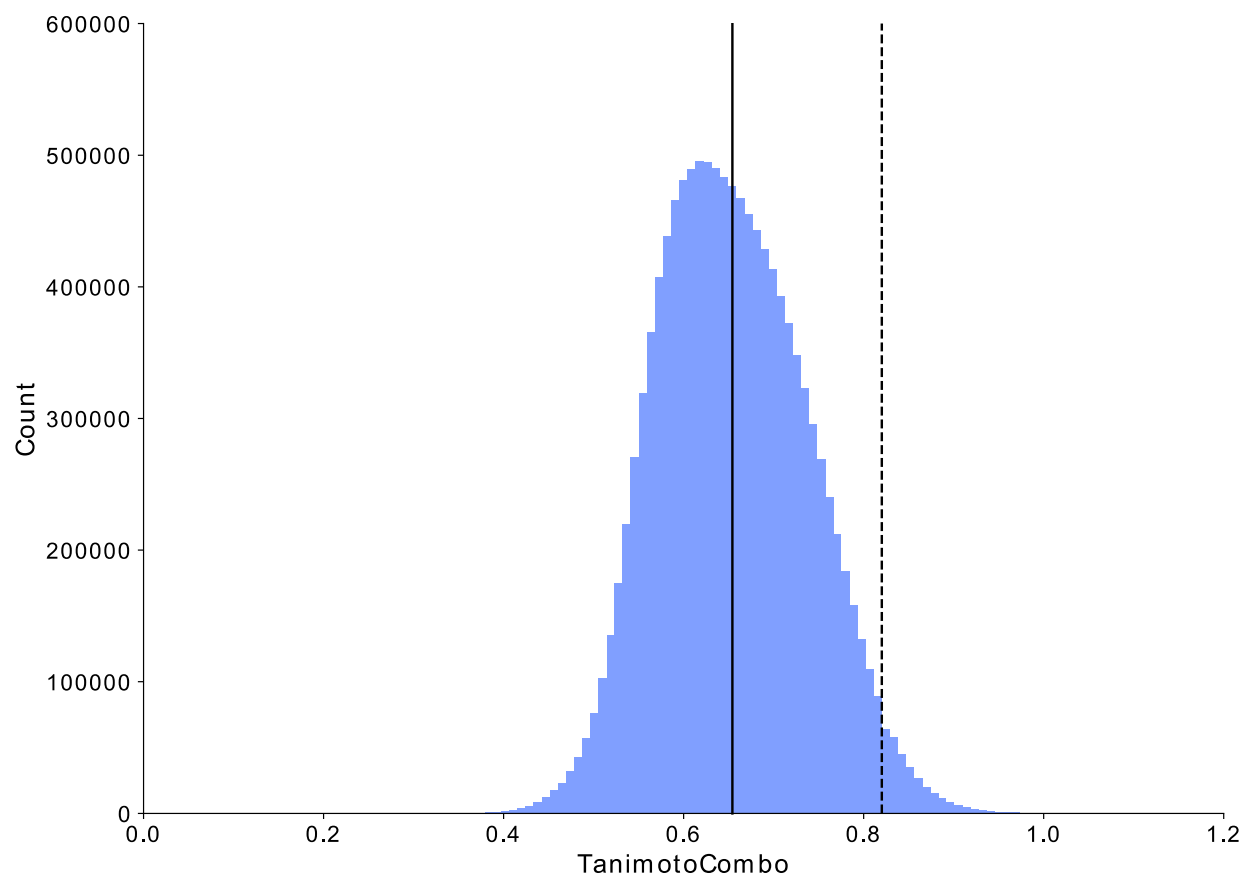


Fig. S1 TanimotoCombo similarity score distribution from overlaying the low-energy conformers of 3kPZS with the single-conformer drug-like database from ZINC. The black vertical line indicates the mean of the distribution, and the dashed line indicates a similarity score threshold two standard deviations above the mean

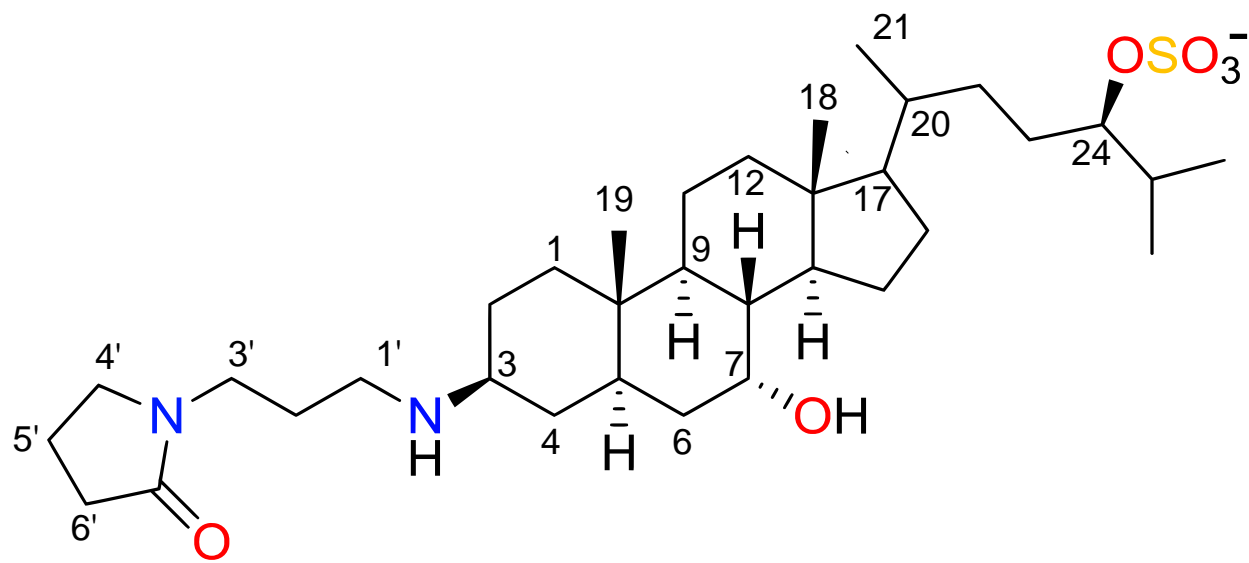


Fig. S2 Structure of PAMS-24