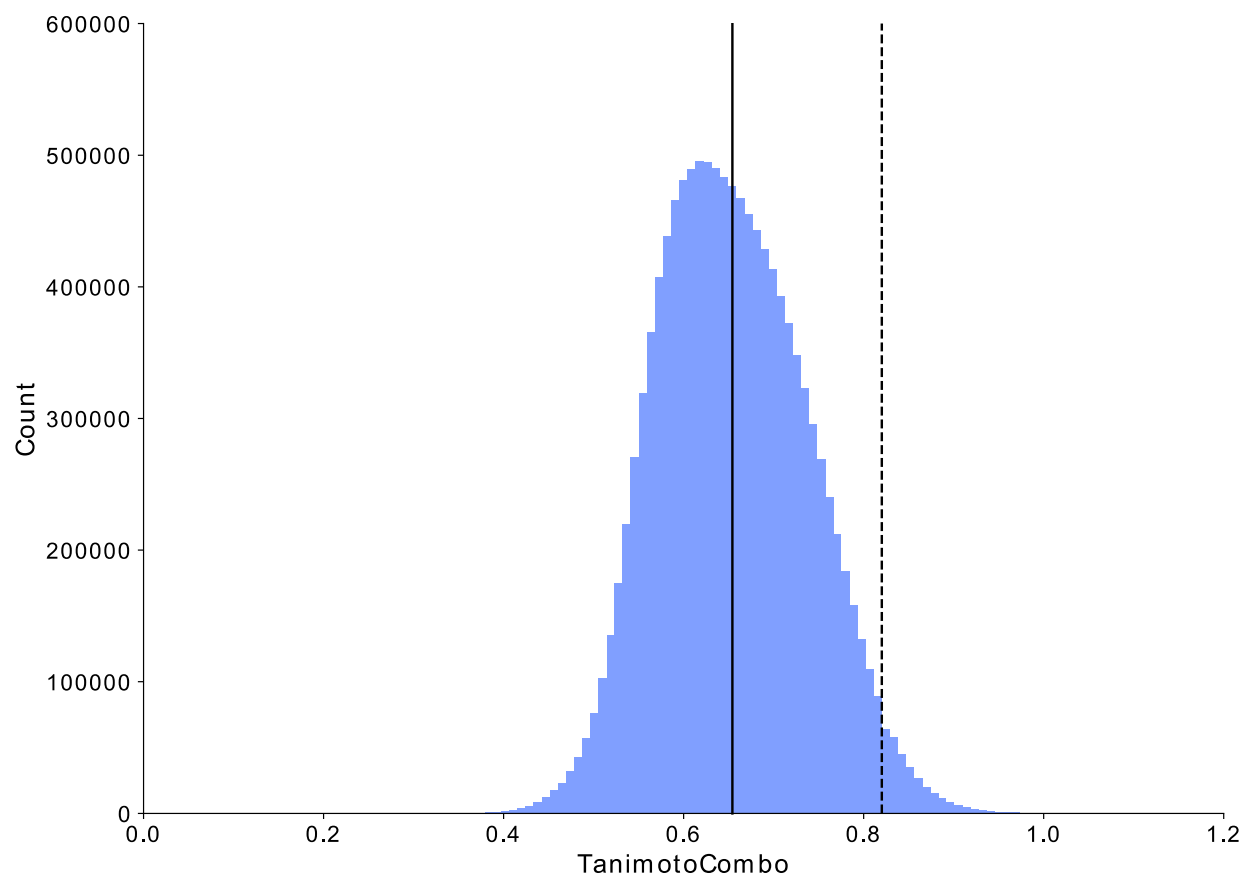**Fig. S1** TanimotoCombo similarity score distribution from overlaying the low-energy conformers of
3kPZS with the single-conformer drug-like database from ZINC. The black vertical line indicates the
mean of the distribution, and the dashed line indicates a similarity score threshold two standard
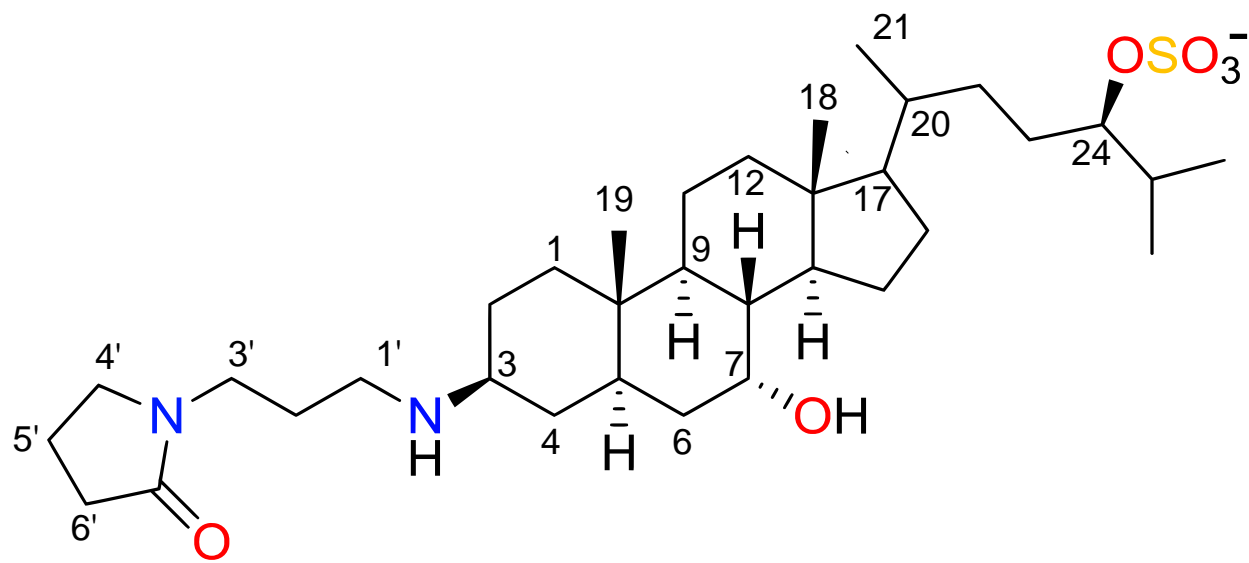deviations above the mean

Fig. S2 Structure of PAMS-24