

Figure S1. Probability density distributions for pairwise similarity scores of actives and decoys for 10 DUD-E targets. For each target, Tanimoto similarity scores were calculated between any two actives (or decoys) using FCFP4 descriptors.

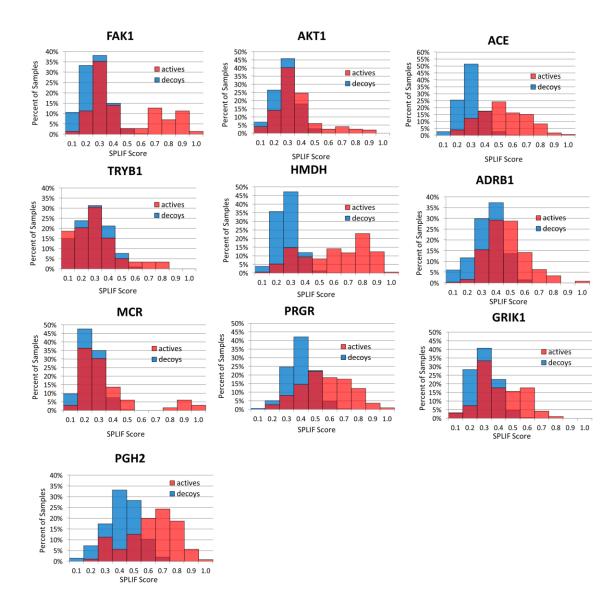


Figure S2. Probability density distributions for SPLIF scores of actives and decoys for 10 DUD-E targets.