

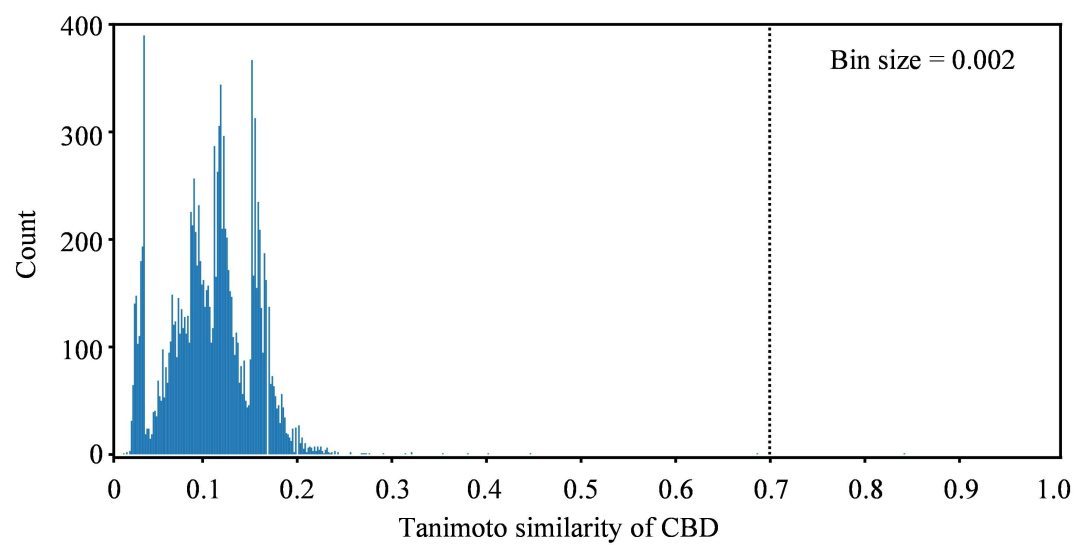


Fig. S1. Histogram of Tanimoto similarities to CBD for compounds across all training sets (ML, LGE-GNN, and DDN).