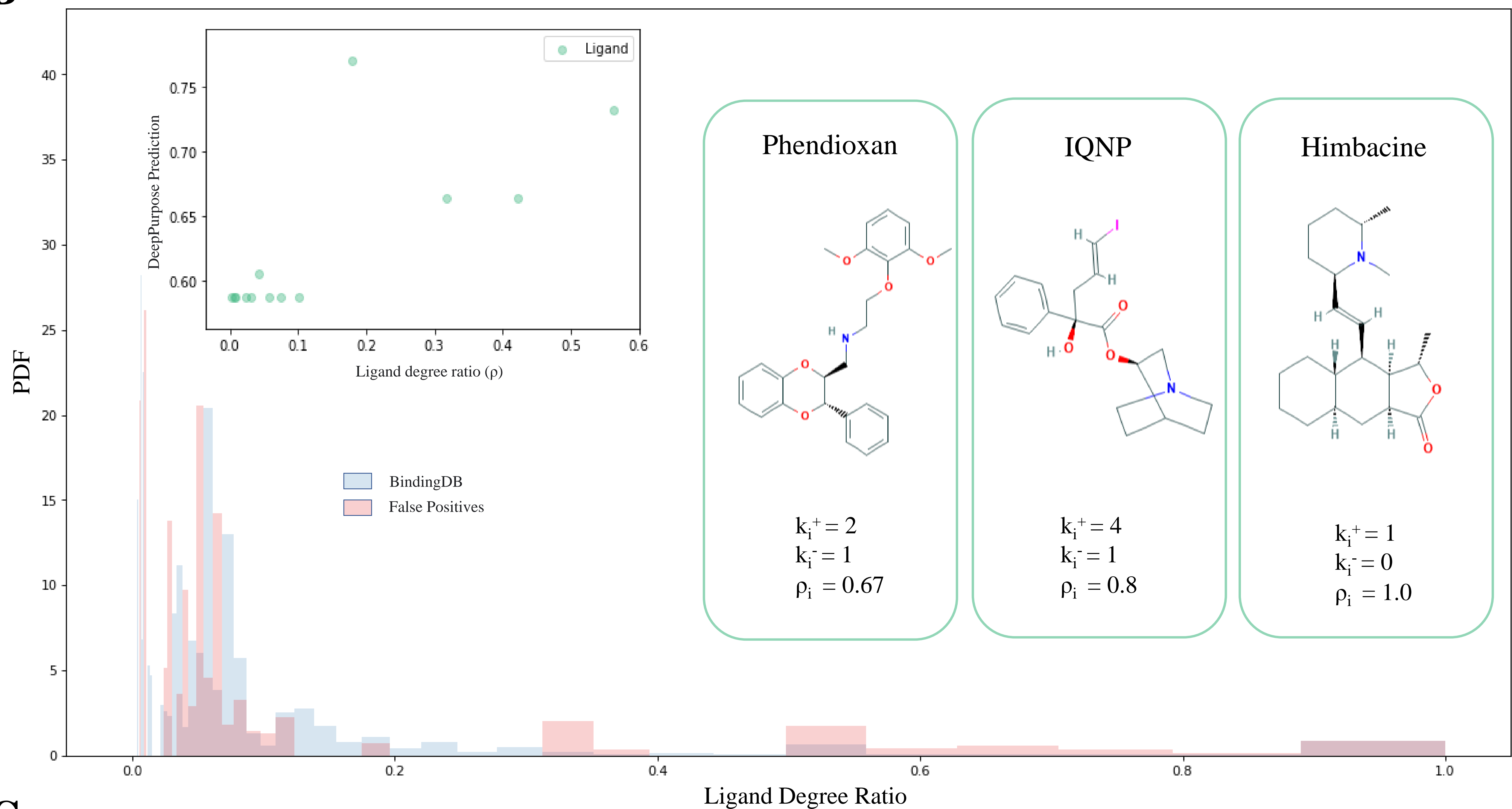


A

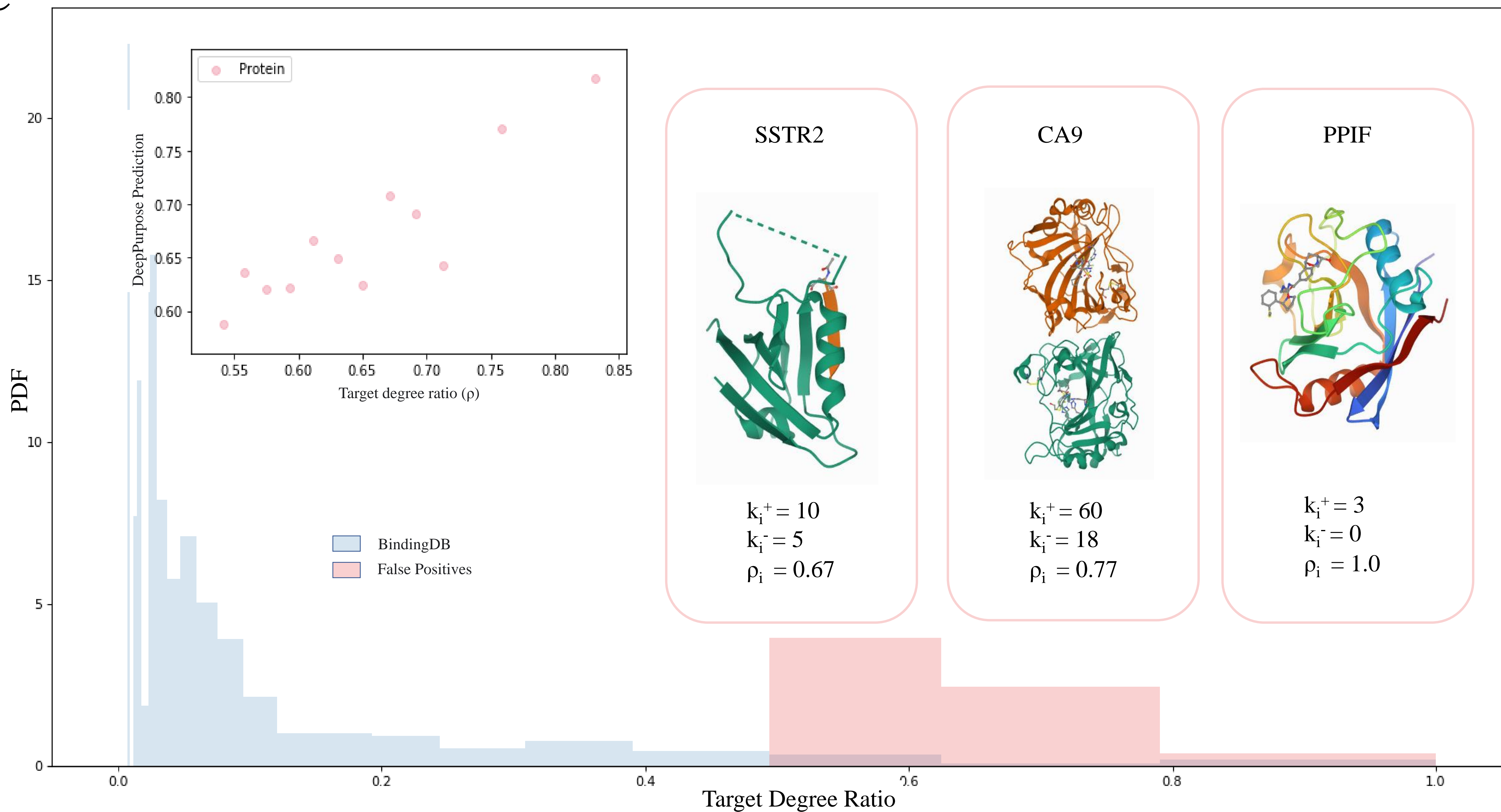
BindingDB Training Data for DeepPurpose

Node Type	Has Only Positive Annotations	Has Only Negative Annotations	Has both annotations	Total Node Count
Ligand	3,084	6,539	793	10,416
Protein	168	556	667	1,391

B



C



D

Assigning SMILES and Amino Acid Sequences Randomly

Version	AUROC	AUPRC
Original	0.85	0.63
Randomized	0.84	0.61