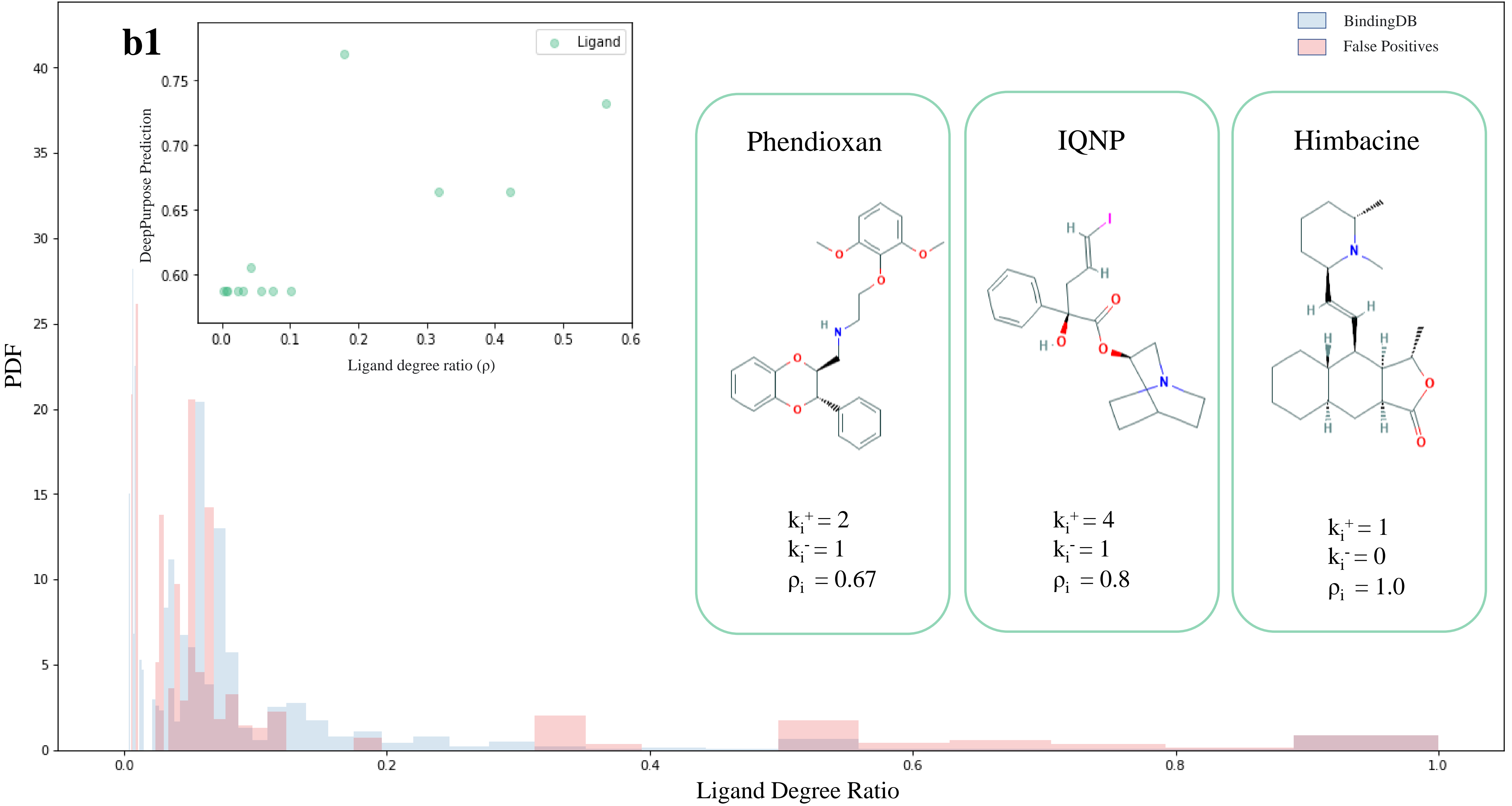
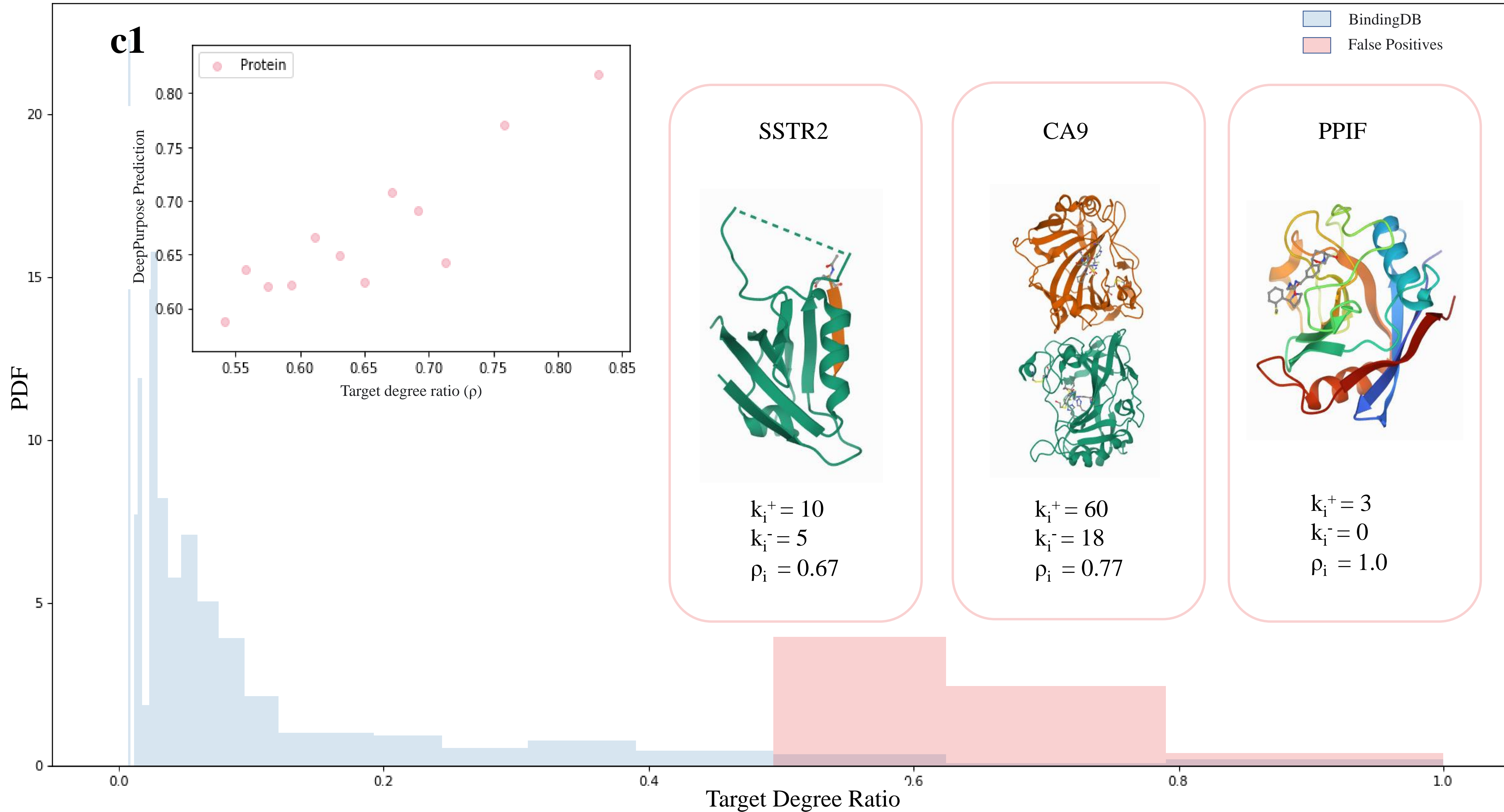


**a****BindingDB Training Data for DeepPurpose**

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