Table S 1. Comparison of ZincExplorer with ZincPred on Zhao_dataset at C, H, E and D separately. The performance was evaluated using the AURPC and the Precision values at a 70% recall control. The comparison was based on 15,628 CHEDs, in which ZincPred can provide the prediction scores.

	CYS			HIS			GLU			ASP		
	Precision	Recall	AURPC									
ZincExplorer	98.3%	70.1%	0.973	78.7%	70.1%	0.821	17.2%	71.4%	0.509	15.4%	71.4%	0.473
ZincPred	96.8%	70.0%	0.963	61.5%	70.6%	0.735	9.2%	71.4%	0.292	13.9%	71.4%	0.423

Table S 2. Comparison of ZincExplorer with ZincFinder on Zhao_dataset at C, H, E and D separately. The performance was evaluated using the AURPC and the Precision values at a 70% recall control. The comparison was based on 5,904 CHEDs, in which ZincFinder can provide the prediction scores.

	CYS			HIS			GLU			ASP		
	Precision	Recall	AURPC									
ZincExplorer	98.4%	70.2%	0.973	77.8%	70.1%	0.815	25.0%	71.0%	0.527	12.6%	74.3%	0.380
ZincFinder	97.6%	70.0%	0.961	63.1%	70.2%	0.742	10.2%	71.0%	0.288	17.3%	71.8%	0.428