

**S5 Table**

Category	Site type	$n_l$	AUC	$sn$	$sp$	MCC	$n_l^*$	AUC*	$sn^*$	$sp^*$	MCC*
Metal binding	Ca	13	0.858	0.077	0.985	0.032	2	0.990	1.00	0.985	0.139
	Fe	42	0.841	0.143	0.985	0.112	23	0.971	0.261	0.985	0.160
	Mg	35	0.877	0.114	0.985	0.081	24	0.958	0.167	0.985	0.103
	Zn	47	0.922	0.489	0.966	0.271	30	0.975	0.767	0.966	0.350
PTMs	Nglyco	11	0.841	0.727	0.791	0.322	2	0.985	0.500	0.992	0.492
	Phos	109	0.779	0.068	0.991	0.144	23	0.981	0.174	0.991	0.260
Catalytic activity	Cat	1226	0.706	0.045	0.985	0.091	204	0.978	0.270	0.985	0.383
Macromolecular binding	DNA	38	0.722	0.105	0.985	0.077	17	0.951	0.235	0.985	0.126
	RNA	52	0.546	0.039	0.988	0.029	1	1.00	1.00	0.988	0.153
	PPI	616	0.631	0.037	0.986	0.067	29	0.990	0.793	0.986	0.540
Ligand binding	ADP	12	0.685	0.083	0.986	0.034	2	0.989	0.500	0.986	0.099
	ATP	121	0.855	0.141	0.988	0.187	50	0.980	0.340	0.988	0.310
	GDP	17	0.543	0.177	0.985	0.092	3	0.995	1.00	0.985	0.236
	GTP	39	0.642	0.051	0.987	0.036	4	0.989	0.500	0.987	0.146
	NAD	16	0.768	0.063	0.985	0.027	7	0.981	0.143	0.985	0.048