

**Table a1.** Comparison with state-of-the-art approaches in terms of AUC

	NetLapRLS	WNN-GIP	RLScore	KBMF2K	CMF	NRLMF	TMF	
S1	EN	0.972±0.002	0.964±0.003	0.962±0.003	0.905±0.003	0.969±0.002	<u>0.987 ±0.001</u>	<b>0.989±0.001</b>
	IC	0.969±0.003	0.959±0.003	0.967±0.003	0.961±0.003	0.981±0.002	<u>0.989 ±0.001</u>	<b>0.989±0.001</b>
	GPCR	0.915±0.006	0.944±0.005	0.925±0.007	0.926±0.006	0.940±0.007	<u>0.969 ±0.004</u>	<b>0.983±0.003</b>
	NR	0.850±0.021	0.901±0.017	0.850±0.030	0.877±0.023	0.864±0.026	<u>0.950 ±0.011</u>	<b>0.978±0.008</b>
S2	EN	0.786±0.023	<b>0.882±0.015</b>	0.791±0.021	0.713±0.029	0.829±0.019	<u>0.871±0.017</u>	0.843±0.012
	IC	0.757±0.025	0.797±0.028	0.778±0.022	0.799±0.019	0.743±0.029	<u>0.813 ±0.027</u>	<b>0.819±0.011</b>
	GPCR	0.817±0.015	0.891±0.010	0.837±0.024	0.839±0.020	0.857±0.014	<b>0.895±0.011</b>	0.882±0.009
	NR	0.789±0.039	<u>0.890±0.023</u>	0.776±0.041	0.844±0.023	0.818±0.036	<b>0.900±0.021</b>	0.886±0.017
S3	EN	0.905±0.014	0.947±0.008	0.931±0.009	0.876±0.012	0.915±0.013	<u>0.966±0.005</u>	<b>0.976±0.001</b>
	IC	0.914±0.012	0.950±0.007	0.937±0.009	0.938±0.008	0.905±0.012	<u>0.964±0.007</u>	<b>0.972±0.002</b>
	GPCR	0.770±0.02	0.926±0.013	0.853±0.017	0.882±0.016	0.837±0.019	<u>0.930±0.012</u>	<b>0.959±0.007</b>
	NR	0.655±0.046	<b>0.935±0.017</b>	0.736±0.034	0.668±0.060	0.680±0.066	0.851±0.027	<u>0.929±0.029</u>
S4	EN	-	-	0.734±0.015	<u>0.755±0.014</u>	-	-	<b>0.802±0.015</b>
	IC	-	-	0.681±0.025	<u>0.739±0.018</u>	-	-	<b>0.751±0.014</b>
	GPCR	-	-	<u>0.716±0.013</u>	0.675±0.011	-	-	<b>0.817±0.012</b>
	NR	-	-	0.594±0.035	<u>0.705±0.029</u>	-	-	<b>0.735±0.026</b>

The best results in each benchmark dataset under four kinds of CVs are highlighted in bold face and the second-best results are underlined.