Supplement for “Comparative assessment of intrinsic disorder predictions with a focus on protein and nucleic acid-binding proteins”

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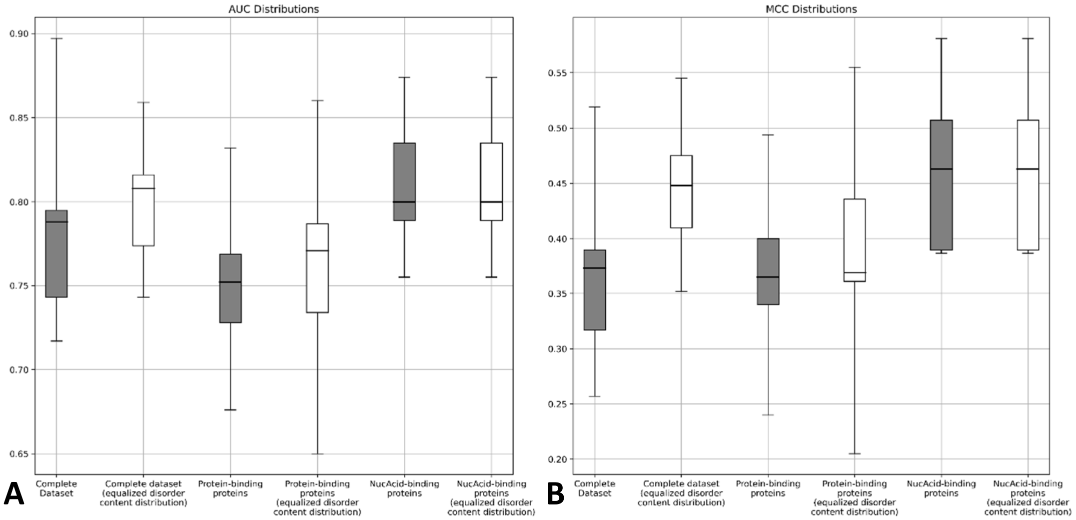
Supplementary Tables

Supplementary Table S1. Predictive performance on the disorder-content equalized subset of the benchmark dataset, the disordered nucleic-acids binding proteins, and the disordered protein-binding proteins. We quantify statistical significance of differences in AUC between the best predictor (identified in bold font) and each the other nine predictors on a given dataset. We bootstrap 50% of the proteins 100 times. For normal measurements (tested with the Anderson-Darling test at 0.05 significance) we use paired t-test; otherwise we use the Wilcoxon rank sum test; = and + mean that the differences are not significant (*p*-value > 0.01) and significant (*p*-value ≤ 0.01), respectively.

Dataset	Predictor	AUC	Precision	Sensitivity	MCC
Disorder-content equalized benchmark dataset	**ESpritz-DisProt**	**0.859**	0.751	0.537	0.545
	SPOT-Disorder	0.819+	0.599	0.751	0.478
	ESpritz-Xray	0.816+	0.634	0.626	0.475
	IUPred-long	0.809+	0.669	0.695	0.472
	VSL2B	0.808+	0.671	0.848	0.410
	IUPred-short	0.801+	0.645	0.606	0.448
	ESpritz-NMR	0.774+	0.599	0.713	0.415
	disEMBL	0.746+	0.570	0.455	0.357
	DISOPRED3	0.743+	0.518	0.635	0.352
	GlobPlot	0.565+	0.364	0.427	0.103
Disorder-content equalized disordered protein-binding proteins	**ESpritz-DisProt**	**0.860**	0.816	0.552	0.555
	ESpritz-Xray	0.796+	0.684	0.648	0.436
	IUPred-long	0.787+	0.701	0.741	0.440
	VSL2B	0.777+	0.710	0.875	0.361
	IUPred-short	0.771+	0.672	0.617	0.394
	ESpritz-NMR	0.745+	0.639	0.738	0.369
	SPOT-Disorder	0.734+	0.587	0.807	0.363
	disEMBL	0.703+	0.610	0.423	0.286
	DISOPRED3	0.65+	0.522	0.668	0.205
	GlobPlot	0.562+	0.479	0.450	0.147
Disorder-content equalized disordered nucleic acids-binding proteins	**SPOT-Disorder**	**0.874**	0.752	0.814	0.581
	ESpritz-DisProt	0.843=	0.687	0.446	0.466
	ESpritz-Xray	0.835=	0.583	0.692	0.536
	IUPred-long	0.804=	0.571	0.685	0.463
	IUPred-short	0.800=	0.575	0.580	0.437
	VSL2B	0.796+	0.522	0.834	0.387
	DISOPRED3	0.789+	0.500	0.720	0.507
	ESpritz-NMR	0.757+	0.493	0.765	0.390
	disEMBL	0.755+	0.548	0.486	0.388
	GlobPlot	0.556+	0.298	0.407	0.061

Supplementary Figures



Supplementary Figure S1. Distribution of the AUCs (panel A) and MCCs (panel B) over nine disorder predictors. We exclude the poorly-performing GlobPlot from this analysis. The box plots show the lowest AUC (bottom error bar), first quartile (bottom of box), median (horizontal line inside box), third quartile (top of box) and highest AUC (top error bar). The grey plots are for the original datasets while the white plots are for the sampled/disorder content-equalized datasets that have similar distribution of the per-protein disorder content. The content distribution similarity was measured using Kolmogorov–Smirnov test at *p*-value of 0.001.

Benchmark Dataset

Each protein is described using five lines:

1. >Uniprot ID
2. AA sequence using 1-letter AA encoding
3. Disorder annotation: 1 for intrinsic disorder; 0 for structure/order; and X for missing annotation (excluded from assessment)
4. Disordered protein binding annotation: 1 for disordered protein-binding region; 0 for other disordered and ordered regions; and X for missing annotation
5. Disordered nucleic acids binding annotation: 1 for disordered nucleic acids-binding region; 0 for other disordered and ordered regions; and X for missing annotation

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FVKQQFIWNKDSEYHGGGDAWFQGGYLKYGNNPLTPTTNSDYRQPGNAFDFLLANDVDNSNPVVQAENLNWLHYLMNFGTITAGQDDANFDSIRIDAVDFIHNDTIQRTYDYLRDAYQVQQSEAKANQHISLVEAGLDAGTSTIHNDALIESNLREAATLSLTN
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