Evaluation of novel computational methods to identify RNA-binding protein footprints from structural data

SUPPLEMENTAL MATERIAL

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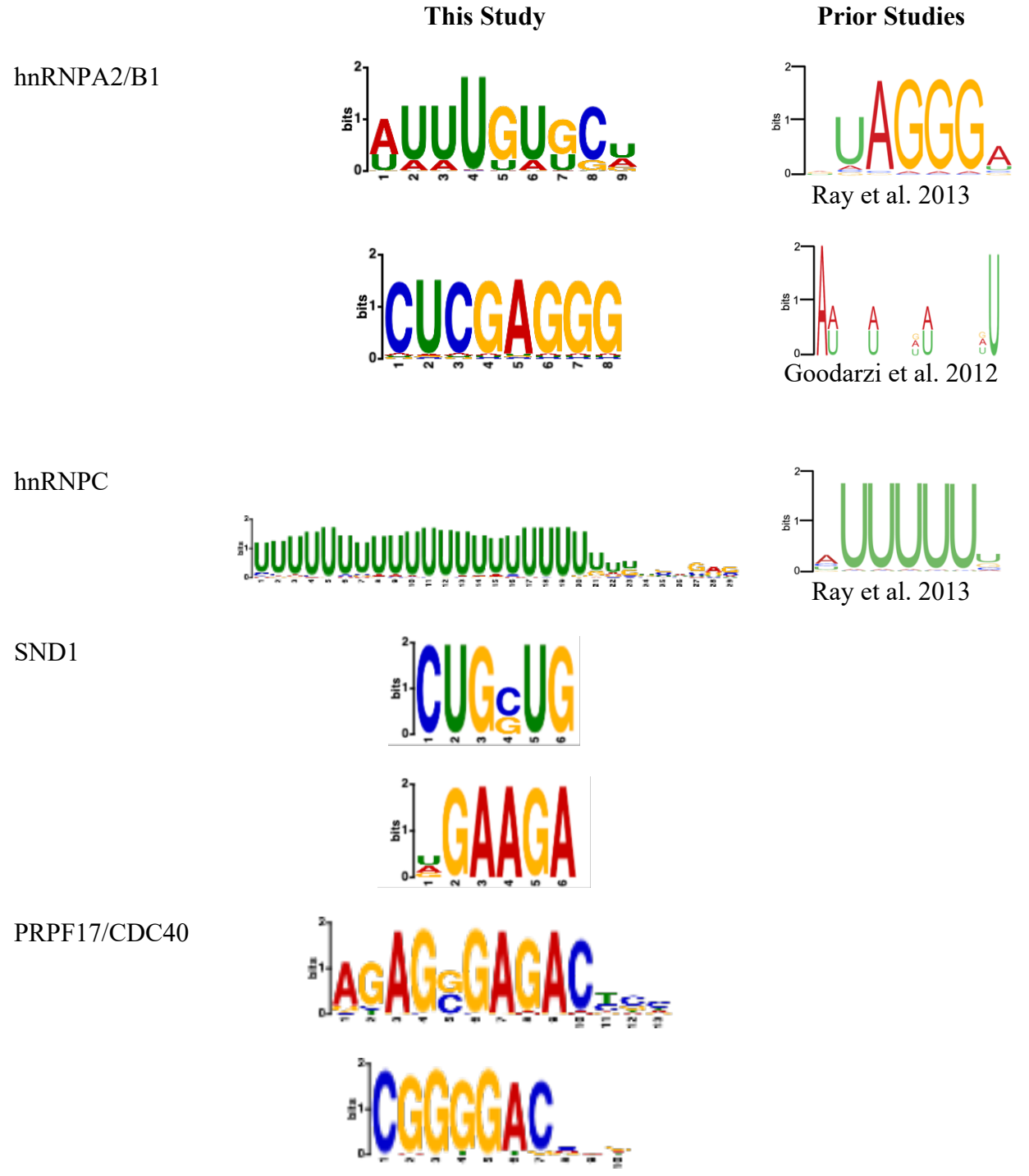
Supplemental Tables

Utility	Input	Prediction	Regions	Notes	Reference
KYG	structure	Yes	98 - 101 108 - 115 178 - 183 196 - 201 224 - 229 248 - 255 264 - 269 285 - 305 353 - 358 370 - 381 432 - 436 453 - 457 488 - 511 533 - 548		Kim et al. 2006
TriPepSVM	sequence	Yes	n/a	overall prediction	Bressin et al. 2019
SPOT-Struct-RNA	structure	No	n/a		Zhao et al. 2011
SPOT-Seq-RNA	sequence	Yes	288, 333, 357, 369		Yang et al. 2014
FastRNABindR	sequence	No	n/a		El-Manzalawy et al. 2016
HybridNAP	sequence	Yes	88 - 113 125 - 141 222 - 235		Zhang et al. 2019
DRNAPred	sequence	No	n/a		Yan and Kurgan 2017

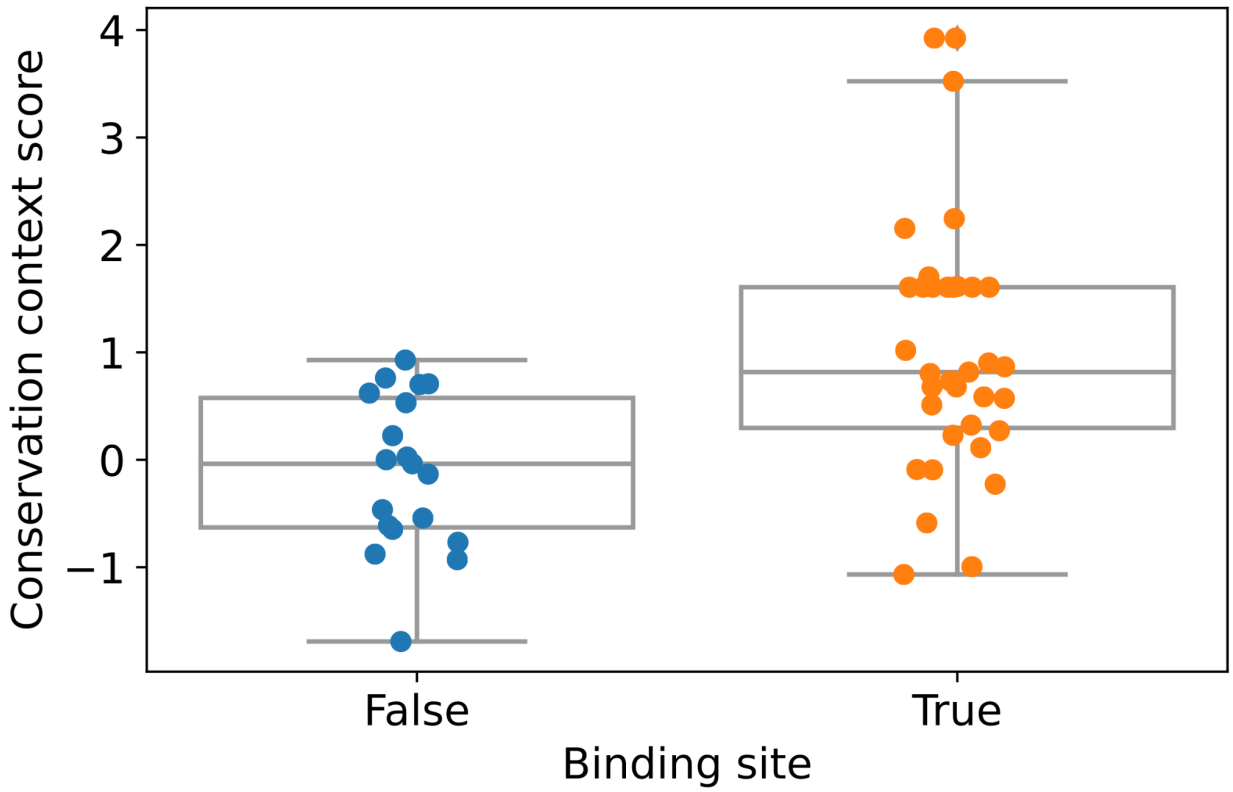
PPrint	sequence	Yes	16 - 21 169 - 184 225 - 231 255 - 265 281 - 289 305 - 311 376 - 383 401 - 412 437 - 450 480 - 493		Kumar et al. 2007
aaRNA	sequence	Yes	40 - 43 126 - 130 153 - 157 216 - 220 298 - 304		Li et al. 2014
Final Prediction	-	Yes	225-229		

Supplemental Table S1. Protein Binding Target Tool Glossary. First column lists utility name, second column states required input (protein sequence or structure), third column denotes if the utility positively predicted that PRPF17 can bind RNA, fourth column indicates predicted binding regions, and fifth column provides the relevant publication. For TriPepSVM, predictions are made at the protein rather than amino acid level, and we indicate this as 'overall prediction' in the Notes column. Overall, six utilities predicted that PRPF17 can bind RNA, but only five of them characterized specific residues as potentially capable of binding. If a region was identified by a majority of these utilities (i.e., three out of five), it was included in our final prediction (see bottom row). Final predictions were validated through protein-RNA specific docking with five RNAs selected for their relative abundance of identified RNA binding motifs in their 3' UTR sequence.

Supplemental Figures



Supplemental Figure S1. Sequence binding motifs found by each team in their top predicted sites and those found by prior studies. For each RBP, motif(s) mined by each team are shown on the left. If available, motif(s) found in prior studies are shown on the right (motifs were created to depict study results). References to these studies are listed below each motif.



Supplemental Figure S2. Conservation context scores in known iron response protein (IRP) binding sites ("True") are higher than in incorrect IRP binding sites ("False"), p-value = 0.0003. Context scores are calculated as the average PhyloP 100way score in the binding site subtracted by the average of the PhyloP 100way scores in flanking sites of the same size. Higher PhyloP 100way scores indicate higher conservation, and higher context scores indicate higher conservation in the binding site relative to its surrounding context. PhyloP 100way scores are available on the UCSC genome browser.

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