

Table S2.

(a) Comparison of different disorder prediction methods for proteins from Table 2. Each protein is referenced below by the PDB code of the monomer. Its family and disordered regions with respect to missing X-ray coordinates in the monomer structure and six prediction methods are listed. Table 2 contains additional information including protein family, interacting partner, and function.

Protein (family)	Missing coordinates	Predicted disordered regions					
		VSL2 [1]	VL3H* [2]	FoldUnfold [3]	IUPred* [4]	RONN [5]	DISOPRED [6]
Ichg smart00020	70-77, 143-153	1-4, 70-82, 151-155 , 189-194, 219-224, 242-245	87-101	71-82	1-6, 242-245	4-9, 70-81 , 113-137, 147-165	1, 5-7, 244, 245
Inuk pfam01404	32-34, 133-136, 177-183	1-9, 24-28, 81-84, 181-183	1-19	-	1-12, 183	82-84	183
In8i cd00728	1,71-76, 302-311, 381-385, 674-677, 728-741	1-6 , 150-160, 182-188, 466-481, 706-741	194-198, 709-741	148-163, 217-227, 722-741	103-105, 153-159, 471-477, 718-741	146-163, 208-220, 468-484, 507-508, 536-557, 705-741	157-158, 721-741
Iuch pfam01088	1-4, 147-166	1-6 , 67-80, 108-139, 148-162 , 192-200, 227-230	1-3 , 112-149, 199-205, 222-230	65-80, 150-164 , 189-202	67-70, 148-159	68-82, 112-130, 145-164 , 190-194	65-78, 150-168
Iym3 cd03378	1-11 (His-tag)** 40-49 215	1-44 , 156-162, 181-182, 210-215	1-35 , 155-170	31-50	1-17 , 27-44	1-49	1-15
Iz9w cd00534	1, 15-25, 121-133	1-6 , 19-20 , 45-47, 128-133	3-6, 103-104, 129-133	-	-	-	-
Itk1 PRK05330	1-2, 37-45, 87-101, 187-201	1-8 , 41-50 , 80-96 , 120-122, 170-175, 216, 244-260	1-14, 249-260	40-53 , 87-100	1-14 , 37-41 , 43-56, 81-94	1 , 35-47 , 81-94 , 249-260	1-4 , 79-92

*For these methods, those residues which are predicted as having >50% probability of being disordered, were considered as disordered.

**His-tag was not considered in evaluations.

(b) Quality of predictions of disordered (and ordered) residues by different methods for proteins from Table 2.

	VSL2	VL3H	FoldUnfold	IUPred	RONN	DISOPRED
<i>TP</i>	83	30	66	53	78	43
<i>FP</i>	262	179	86	97	236	45
<i>TN</i>	1560	1643	1736	1725	1586	1777
<i>FN</i>	94	147	111	124	99	134
<i>Sensitivity</i>	0.47	0.17	0.37	0.30	0.44	0.24
<i>Specificity</i>	0.86	0.90	0.95	0.95	0.87	0.98
<i>1 – Specificity</i>	0.14	0.10	0.05	0.05	0.13	0.02
<i>S _ product</i>	0.40	0.15	0.36	0.28	0.38	0.24

TP (true positives) is number of residues correctly predicted as being disordered;

TN (true negatives) is number of residues correctly predicted as being ordered;

FP (false positives) is number of ordered residues predicted as disordered;

FN (false negatives) is number of disordered residues predicted as ordered;

$$Sensitivity = \frac{TP}{TP + FN};$$

$$Specificity = \frac{FP}{FP + TN};$$

$$S_product = Sensitivity \times Specificity.$$

References:

1. Obradovic Z, Peng K, Vucetic S, Radivojac P, Dunker AK (2005) Exploiting heterogeneous sequence properties improves prediction of protein disorder. *Proteins* 61 Suppl 7: 176-82.
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3. Galzitskaya OV, Garbuzynskiy SO, Lobanov MY (2006) FoldUnfold: web server for the prediction of disordered regions in protein chain. *Bioinformatics* 22: 2948-2949.
4. Dosztanyi Z, Csizmek V, Tompa P, Simon I (2005) IUPred: web server for the prediction of intrinsically unstructured regions of proteins based on estimated energy content. *Bioinformatics* 21: 3433-3434.
5. Yang ZR, Thomson R, McNeil P, Esnouf RM (2005) RONN: the bio-basis function neural network technique applied to the detection of natively disordered regions in proteins. *Bioinformatics* 21: 3369-3376.
6. Ward JJ, Sodhi JS, McGuffin LJ, Buxton BF, Jones DT (2004) Prediction and functional analysis of native disorder in proteins from the three kingdoms of life. *J Mol Biol* 337: 635-645.