

Supplementary material V:

In the present table, we included data resulting from a comparison with MetaDisorder server. In this case, the comparison was quite difficult: the server aims at predicting disordered vs ordered regions. As mentioned in the MetaDisorder related publication, disordered regions are associated with the lack of 3D structure and have unique sequence characteristics. Therefore, our method based on the analysis of high-resolution 3D structures would not be appropriate for predicting such regions. Hence, we diverted the MetaDisorder method and conducted the prediction on our MD set sequences. The results are described in the table below (column labeled MetaDisorder server). More than 70% of the residues were considered as ordered. Consequently, we made a crude approximation and defined these residues as rigid. For obtaining an equivalent population of rigid residues with our approach, the B-factor threshold needs to reach 0.41. In this case, the prediction rates are slightly in favor of our approach. However, it is actually difficult to conclude because ordered regions do not mean necessarily rigid regions as we mentioned previously.

		This study, adapted for comparison			PROEbyal	PredBF	MetaDisorder	Order/Disorder Prediction
		-MD disorder - Jackknife - B-factor _{MD} and RMSF _{MD}	-MD disorder - PROEbyal thresholds - B-factor _{MD} Only	-Large variation disorder - PROEbyal thresholds - B-factor _{MD} Only		MD disorder	MD disorder	MD disorder B-factor only
	threshold value(s) _{MD}	2.3±0.4 ; 1.4±0.5	0.03	0.03	0.03	2.3	0.41	0.41
	% of rigid fragments	78.76	57.80	58.20	57.80 ^a	48.0	71.0	71.0
Strict	% of flexible fragments	21.24	42.20	41.80	42.20 ^a	52.0	29.0	29.0
	ACC	38.73	59.30	55.30	63.1	61.1	60.6	63.7
	COV	55.03	40.43	37.81	46.2	45.8	65.4	71.4
	F-measure	45.46	48.08	44.91	53.3	52.9	62.8	67.3
Non-Strict	threshold value(s) _{MD}	-1.4±0.3 ; -0.7±0.2	-0.3	-0.3	-0.3	-1.4		
	% of rigid fragments	35.09	44.33	45.64	44.33 ^a	37.0		
	% of flexible fragments	64.91	55.67	54.36	55.67 ^a	63.0		
	ACC	74.84	61.23	58.49	70.1	62.4		
	COV	84.54	87.35	86.16	73.9	75.5		
	F-measure	79.39	71.99	69.68	71.9	68.3		
<small>^a: for this study, a threshold line is defined by a B-factor_{MD} and a RMSF_{MD} value respectively ^b: according to our MD dataset</small>								