

Table IV – Comparison of our flexibility prediction results with those using the PROFbval method.

Datasets		This study, adapted for comparison			PROFbval	PredBF
		MD dataset	MD dataset	Large dataset	MD Dataset	MD Dataset
		(a) -B-factor _{Norm} and RMSF _{Norm}	(b) B-factor _{Norm} only	(b) B-factor _{Norm} only	(b) B-factor _{Norm} only	(c) B-factor _{Norm} only
Strict	threshold value(s)	2.3±0.4 ; 1.4±0.5	0.03	0.03	0.03	2.3
	% of rigid fragments	78.76	57.80	58.20	57.80	48.0
	% of flexible fragments	21.24	42.20	41.80	42.20	52.0
	ACC	38.73	59.30	55.30	63.1	61.1
	COV	55.03	40.43	37.81	46.2	45.8
	F-measure	45.46	48.08	44.91	53.3	52.9
Non-Strict	threshold value(s)	-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	37.0
	% of flexible fragments	64.91	55.67	54.36	55.67	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

(a): for this study. two combined criteria, B-factor_{Norm} and a RMSF_{Norm} were used. The values correspond to the intercepts with x and y axes of figure 1 respectively.

(b): for comparison purpose with ProFbval, only B-factor_{Norm} threshold was used and was chosen equal to ProFbVal threshold.

(c): using Bfact_{Norm} thresholds defined in our procedure.