Supplementary Table R3-Q3-2. Calculation of the prediction ratio for the scores of the docking poses

The prediction ratio (p_{δ}^{error}) is defined in *Marillet et al.* (reference) as the percentage of cases such that the difference between the experimental and predicted free energies is equal or smaller than a specified amount δ. We have calculated the prediction ratio for the standard case of δ equal to 2.8 Kcal/mol. We have also added the absolute number of predictions for the prediction ratio in the column *abs*. We have used the scores of the native conformation of the complexes and also the averages with all the poses from a docking search with PatchDock. Several scores are used, some taken from our analysis and others from the CCHarPPI server.

	δ (KCal/mol)	AB2				AB2 Rigid				AB2 Flexible			
		Native		All decoys		Native		All decoys		Native		All decoys	
		%	abs	%	abs	%	abs	%	abs	%	abs	%	abs
FiberDock	δ ≤2.8	68.09	64	71.28	67	56.25	27	64.58	31	80.43	37	78.26	36
	δ >2.8	31.91	30	28.72	27	43.75	21	35.42	17	19.57	9	21.74	10
aVdW	δ ≤2.8	67.02	63	64.89	61	60.42	29	56.25	27	73.91	34	73.91	34
	δ >2.8	32.98	31	35.11	33	39.58	19	43.75	21	26.09	12	26.09	12
rVdW	δ ≤2.8	58.51	55	64.89	61	45.83	22	54.17	26	71.74	33	76.09	35
	δ >2.8	41.49	39	35.11	33	54.17	26	45.83	22	28.26	13	23.91	11
aElec	δ ≤2.8	61.70	58	70.21	66	52.08	25	62.50	30	71.74	33	78.26	36
	δ >2.8	38.30	36	29.79	28	47.92	23	37.50	18	28.26	13	21.74	10
rElec	δ ≤2.8	60.64	57	69.15	65	50.00	24	60.42	29	71.74	33	78.26	36
	δ >2.8	39.36	37	30.85	29	50.00	24	39.58	19	28.26	13	21.74	10
laElec	δ ≤2.8	60.64	57	69.15	65	52.08	25	62.50	30	69.57	32	76.09	35
	δ >2.8	39.36	37	30.85	29	47.92	23	37.50	18	30.43	14	23.91	11
lrElec	δ ≤2.8	56.38	53	70.21	66	45.83	22	62.50	30	67.39	31	78.26	36
	δ >2.8	43.62	41	29.79	28	54.17	26	37.50	18	32.61	15	21.74	10
HB	δ ≤2.8	67.02	63	57.45	54	60.42	29	45.83	22	73.91	34	69.57	32
	δ >2.8	32.98	31	42.55	40	39.58	19	54.17	26	26.09	12	30.43	14
EPAIR	δ ≤2.8	62.77	59	68.09	64	50.00	24	62.50	30	76.09	35	73.91	34
	δ >2.8	37.23	35	31.91	30	50.00	24	37.50	18	23.91	11	26.09	12
ES3DC	δ ≤2.8	65.96	62	73.40	69	56.25	27	70.83	34	76.09	35	76.09	35
	δ >2.8	34.04	32	26.60	25	43.75	21	29.17	14	23.91	11	23.91	11
E3D	δ ≤2.8	67.02	63	58.51	55	58.33	28	47.92	23	76.09	35	69.57	32
	δ >2.8	32.98	31	41.49	39	41.67	20	52.08	25	23.91	11	30.43	14
ZRANK	δ ≤2.8	63.83	60	-	-	52.08	25	-	-	76.09	35	-	-
	δ >2.8	36.17	34	-	-	47.92	23	-	-	23.91	11	-	-
ZRANK2	δ ≤2.8	60.64	57	-	-	52.08	25	-	-	69.57	32	-	-
	δ >2.8	39.36	37	-	-	47.92	23	-	-	30.43	14	-	-
ROSSETADOCK	δ ≤2.8	67.02	63	-	-	60.42	29	-	-	73.91	34	-	-
	δ >2.8	32.98	31	-	-	39.58	19	-	-	26.09	12	-	-
PyDock	δ ≤2.8	60.64	57	-	-	52.08	25	-	-	69.57	32	-	-
	δ >2.8	39.36	37	-	-	47.92	23	-	-	30.43	14	-	-
PISA	δ ≤2.8	65.96	62	-	-	58.33	28	-	-	73.91	34	-	-
	δ >2.8	34.04	32	-	-	41.67	20	-	-	26.09	12	-	-
PIE	δ ≤2.8	64.89	61	-	-	56.25	27	-	-	73.91	34	-	-
	δ >2.8	35.11	33	-	-	43.75	21	-	-	26.09	12	-	-
SIPPER	δ ≤2.8	63.83	60	-	-	56.25	27	-	-	71.74	33	-	-
	δ >2.8	36.17	34	-	-	43.75	21	-	-	28.26	13	-	-