

Supplementary Figure S5

a

	MN	UG1033	UR29	Self-docking	Cross-docking
2B0S	1.41	3.04	5.41	1.41	4.23
2B1A	1.57	3.09	4.79	3.09	3.18
2B1H	1.65	3.72	4.74	4.74	2.69
Average:				3.08	3.37

b

	MN	UG1033	W2RW020 (10aa)	W2RW020 (9aa)	Self-docking	Cross-docking
1Q1Jp	2.08	5.70	1.48	1.66	2.08	2.95
1Q1Jq	1.78	7.07	3.20	1.68	1.78	3.98
3C2Ap	1.69	4.65	3.04	1.19	4.65	1.98
3C2Aq	1.79	2.70	2.22	1.65	2.70	1.89
3GHBp	3.01	6.11	1.76	1.55	1.76	3.56
3GHBq	2.52	6.75	2.93	2.31	2.31	4.06
Average:					2.55	3.07

c

	MN	UG1033	UR29	Self-docking	Cross-docking
2B0S	0.41	0.65	0.72	0.41	0.68
2B1A	0.49	0.55	0.65	0.55	0.57
2B1H	0.60	0.65	0.55	0.55	0.63
Average:				0.50	0.63

d

	MN	UG1033	W2RW020 (10aa)	W2RW020 (9aa)	Self-docking	Cross-docking
1Q1Jp	2.08	3.52	1.48	1.66	2.08	2.22
1Q1Jq	1.78	5.70	3.20	1.68	1.78	3.53
3C2Ap	1.69	1.89	3.04	1.19	1.89	1.98
3C2Aq	1.79	1.35	2.22	1.65	1.35	1.89
3GHBp	3.01	4.20	1.76	1.55	1.76	2.92
3GHBq	2.52	2.92	2.93	2.31	2.31	2.79
Average:					1.86	2.55