

Table S1. Docking affinity and RMSD values of FX-BRD2 complexes

mode	affinity(kcal/mol)	dist from rmsd l.b.	dist from rmsd u.b.
1	-7.6	0.000	0.000
2	-7.6	1.030	1.839
3	-7.5	8.087	20.751
4	-7.4	3.905	17.972
5	-7.3	7.000	12.361
6	-7.3	6.936	12.091
7	-7.2	11.293	18.986
8	-7.2	7.521	20.476
9	-7.2	11.831	23.665

Table S2. Docking affinity and RMSD values of FX-BRD3 complexes

mode	affinity(kcal/mol)	dist from rmsd l.b.	dist from rmsd u.b.
1	-6.4	0.000	0.000
2	-6.4	2.269	17.626
3	-6.3	1.855	2.913
4	-6.2	10.655	15.607
5	-6.2	2.310	17.409
6	-6.1	3.334	18.065
7	-6.1	3.836	17.338
8	-6.1	11.385	16.279
9	-6.0	5.228	8.248

Table S3. Docking affinity and RMSD values of FX-BRD4 complexes

mode	affinity(kcal/mol)	dist from rmsd l.b.	dist from rmsd u.b.
1	-6.8	0.000	0.000
2	-6.7	1.510	2.729
3	-6.6	1.883	2.516
4	-6.6	2.219	3.908
5	-6.5	2.728	16.599
6	-6.4	3.438	17.425
7	-6.4	2.805	17.144
8	-6.4	2.544	3.981
9	-6.4	2.579	3.793