

Supplemental Information S13

FireDock results of BvrR interacting with DNA

Frame 5523

Global Energy (Kcal/mol)	Attractive VdW (Kcal/mol)	Repulsive VdW (Kcal/mol)	ACE (Kcal/mol)
-15.44	-30.65	9.58	7.66

Frame 7507

Global Energy (Kcal/mol)	Attractive VdW (Kcal/mol)	Repulsive VdW (Kcal/mol)	ACE (Kcal/mol)
-17.19	-22.90	5.55	2.71

BvrR with DNA with different motif sequence

Global Energy (Kcal/mol)	Attractive VdW (Kcal/mol)	Repulsive VdW (Kcal/mol)	ACE (Kcal/mol)
-2.91	-15.78	6.16	3.58