MD and FBE Validation

Table S2. MD duplication result

Input	MD Setting			FBE Calculation	
	Force Field	Water model	Frames number	Method	Free energy result (kcal/mol)
Our work DprE1-C6	AMBER99SB	TIP3P	5000	MM/GBSA MM/PBSA	-46.31 -23.61
Kumar et al.[64] DprE1-C6	AMBER14SB	TIP3P	5000	MM/GBSA MM/PBSA	-41.28 -22.36