SUPPORTING INFORMATION

Molecular Mechanism of Dual Intercalation in Sac7d-DNA Complexation

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Definition of rotation angle of protein (Sac7d) around DNA:

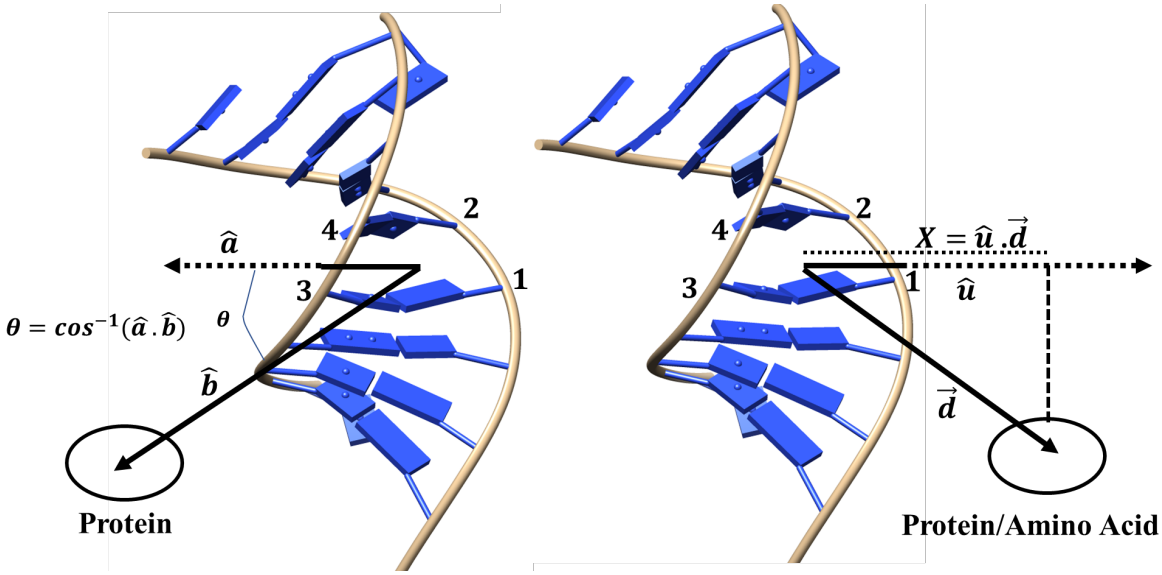

Figure S1: Schematic representation of X and rotation angle used for defining the protein/amino acid intercalation and rotation of protein (Sac7d) around DNA. In left figure, the $\hat{a}$ represents the unit vector from the center of mass of base 1 and 2 to the center of mass of base 3 and 4. The $\hat{b}$ represents the unit vector from the center of mass of 1,2,3 and 4 base to center of mass of protein. The dot product of vector The $\hat{a}$ and $\hat{b}$ define the angle θ . In the right figure, the $\hat{u}$ represents the unit vector from the center of mass of phosphate of base 4 and 1 to the center of mass of base 1,2,3 and 4. The $\vec{d}$ represents the distance vector from the center of mass of 1,2,3 and 4 base to center of mass of protein/amino acid. The dot product of the vector $\hat{u}$ and $\vec{d}$ define the X (reaction coordinate for intercalation of amino acid). the base number 1,2,3 and 4 are the schematic representation of intercalating base pair.

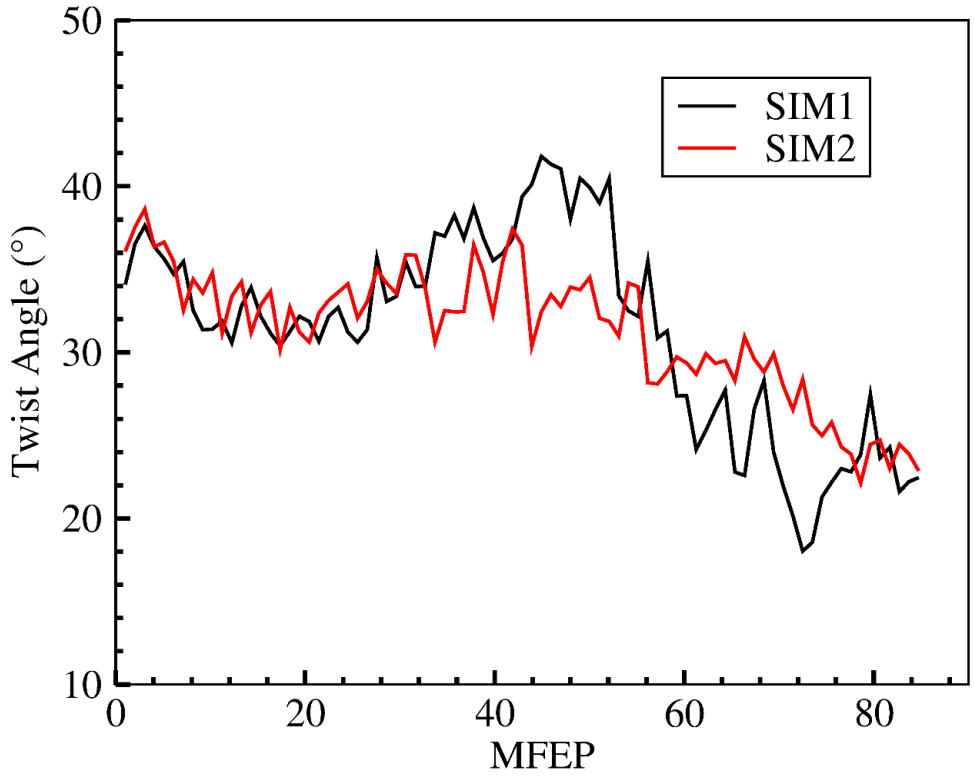

Figure S2: Changes in the twist angle of intercalating DNA base step along the protein intercalation (SIM1 is for MET29 intercalation while SIM2 is for VAL26 intercalation). Note that, the twist angle changes drastically around MFEP 60 where the amino acids intercalate into DNA.

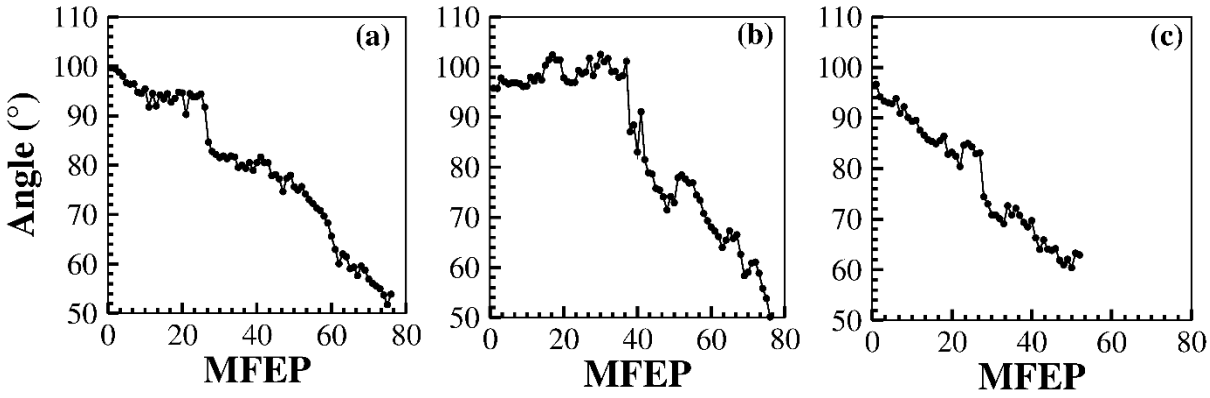

Figure S3: Rotation angle of protein during the dissociation (unbinding) from DNA along the MFEP. (a) SIMD-1 (b)SIMD-2 and (c) SIMD-3.

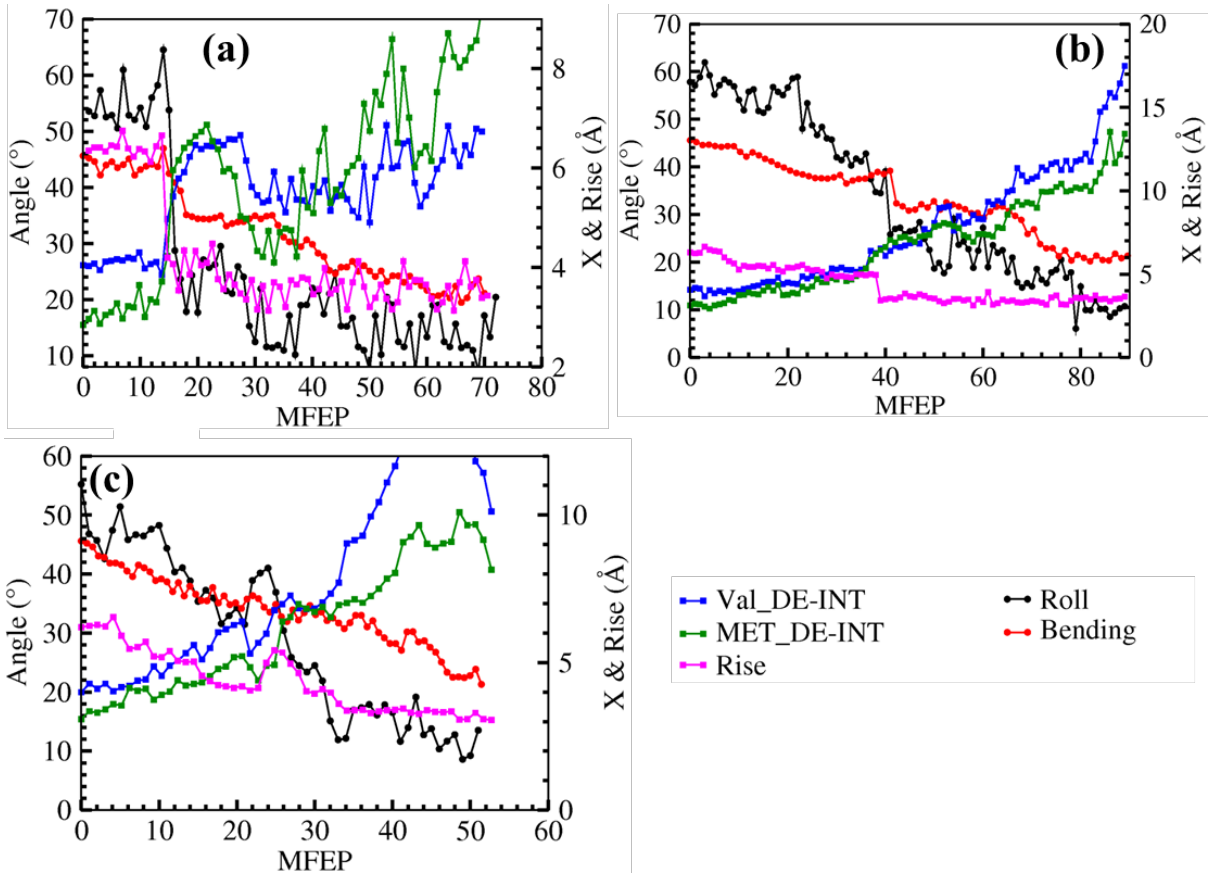

Figure S4: Change in the X_{VAl} (Val_DE-INT), X_{MET} and DNA parameters for I to F simulation. (a) SIMD-1 (b)SIMD-2 and (c) SIMD-3.

Table S1: pKa of all surface amino acid calculated using PropKa module[ref 30,31 of MS].

Residue Name	Residue number	pKa	
HIS	2	6.5	Deprotonated
ARG	5	12.15	Protonated
GLU	17	3.08	Deprotonated
ARG	18	12.5	Protonated
ARG	19	12.5	Protonated
LYS	20	10.5	Protonated
GLU	23	4.5	Deprotonated
ASP	27	3.8	Deprotonated
HIS	29	6.43	Deprotonated
GLU	32	4.41	Deprotonated
LYS	35	10.22	Protonated
ARG	36	12.5	Protonated
LYS	39	10.5	Protonated
ARG	40	12.5	Protonated
LYS	42	10.43	Protonated
LYS	45	10.5	Protonated
ASP	46	3.8	Deprotonated
ASP	48	3.69	Deprotonated
LYS	49	10.5	Protonated
GLU	55	3.7	Deprotonated

GLU	57	4.1	Deprotonated
ARG	58	12.5	Protonated
ARG	60	12.43	Protonated
LYS	62	10.5	Protonated
HIS	63	6.5	Deprotonated
ASP	66	3.8	Deprotonated
TYR	67	10.79	Protonated
ASP	69	3.8	Deprotonated
TYR	70	10	Protonated
LYS	71	10.5	Protonated
TYR	72	9.39	Protonated
ARG	73	12.5	Protonated
ARG	75	12.5	Protonated
LYS	76	10.36	Protonated