Table S1 Number of complexes obtained using different distance filters

Distance (Å) KS-ACP	Distance (Å) AT-ACP	Number of complexes (monomerA+monomer B)
20	**No constraints used**	2+3
30	35	0+0
30	40	0+0
30	55	4+3
30	60	3+3
30	70	12+4
35	35	0+0
40	40	3+4
No constraints used	20	22+14
55	30	1+3
60	30	9+6
70	30	18+13

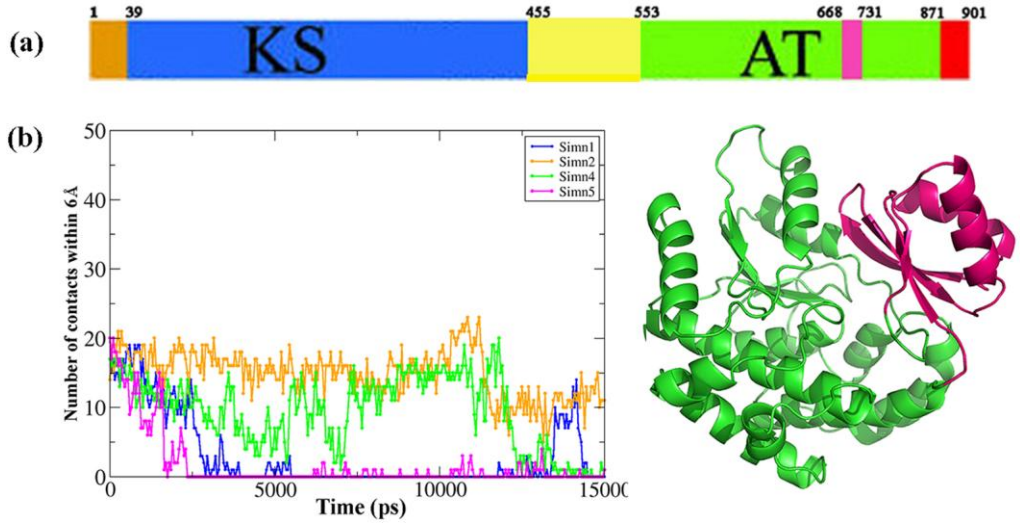

Figure S1

(a) Sequence boundaries of large (green) and small (dark pink) sub-domains of AT domain. The two sub-domains marked have also been shown in different colors on the cartoon representation of AT crystal structure.

(b) Variation of number of contacts between the two subdomains of AT domain over the 15ns MD trajectory with a distance cutoff <6Å.

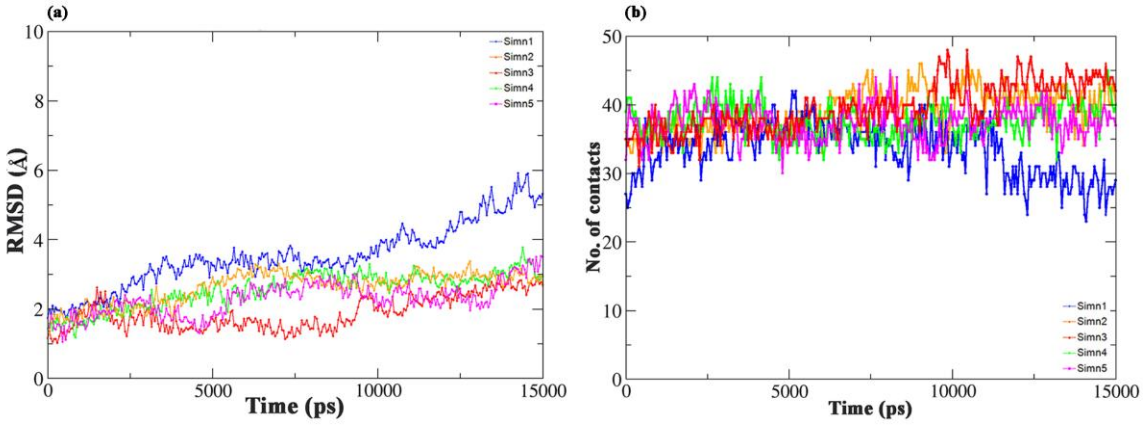

Figure S2

(a) RMSD (Å) vs. Time (ps) plots for docking domain dimer from the five 15ns MD trajectories for the KS-AT di-domain structure.

(b) Variation of the number of contacts between two helices in the docking domain dimer across five 15ns MD trajectories.

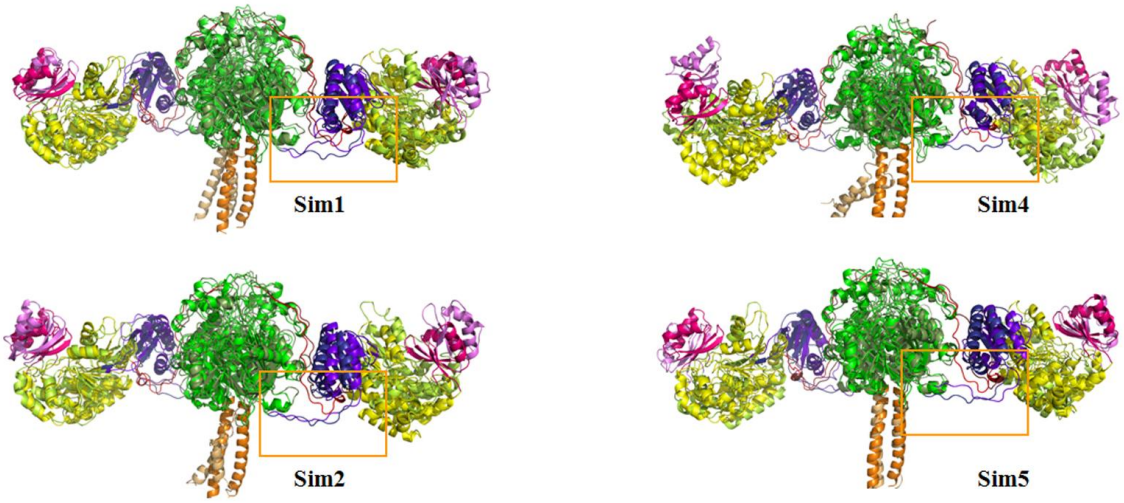

Figure S3
The figure shows typical snapshots of the final structures at the end of 15 ns simulation from the four trajectories, superposed on the starting structures of KS-AT di-domain.

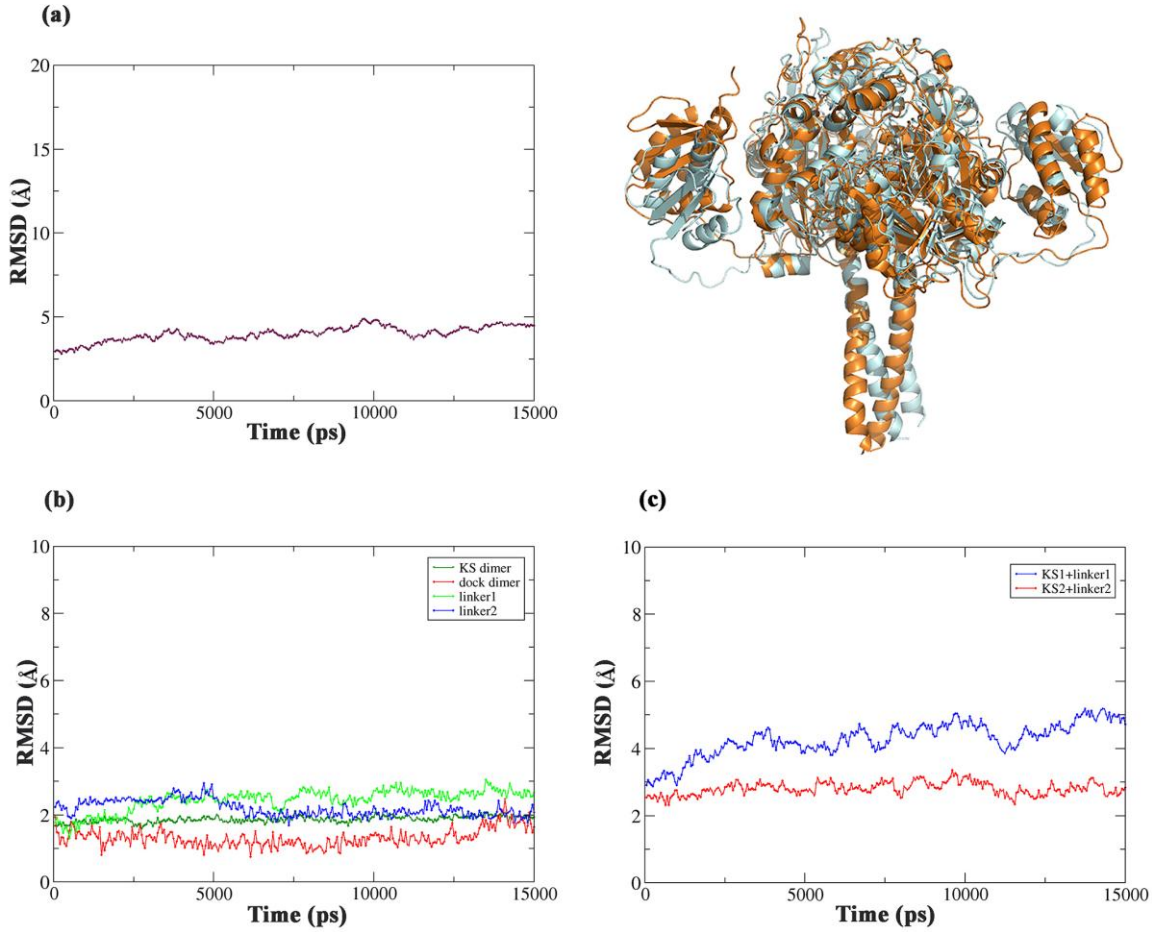

Figure S4

(a) Variation of the RMSD (Å) with Time (ps) for the complete dimeric KS-linker sub-fragment over the 15ns MD trajectory and superposition of the final structure of the KS-linker sub-fragment at the end of 15ns MD simulation on the initial starting structure.

(b) RMSD (Å) vs. Time (ps) plots for the individual KS dimer, docking domain dimer and linker domains across 15ns MD trajectory.

(c) RMSD (Å) vs. Time (ps) plots for both the monomers of KS+linker region over 15ns MD trajectory.

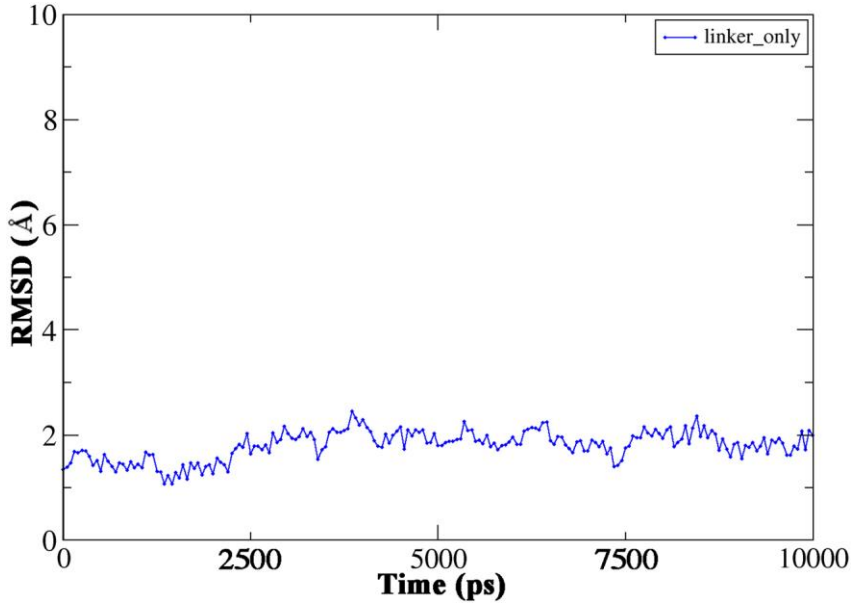

Figure S5
RMSD (Å) vs. Time (ps) plots for MD simulation on linker domain only over the 10ns MD trajectory.

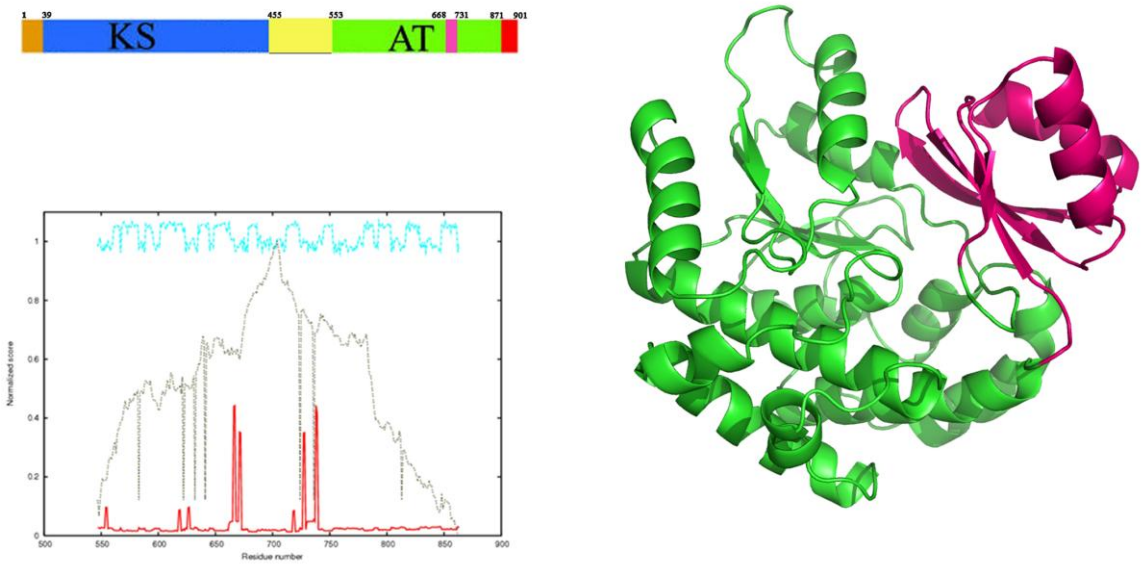

Figure S6
Prediction for hinge regions within the AT domain by using hingemaster software.

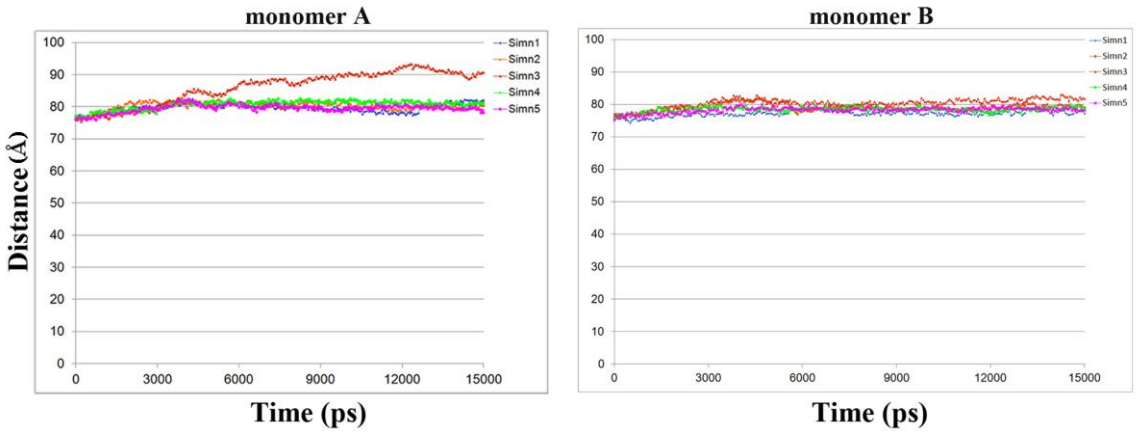

Figure S7
Plot for the distance (Å) between the catalytic centers of KS (Cys-191) and AT (Ser-642) vs. Time (ps) over the five 15ns MD trajectories.

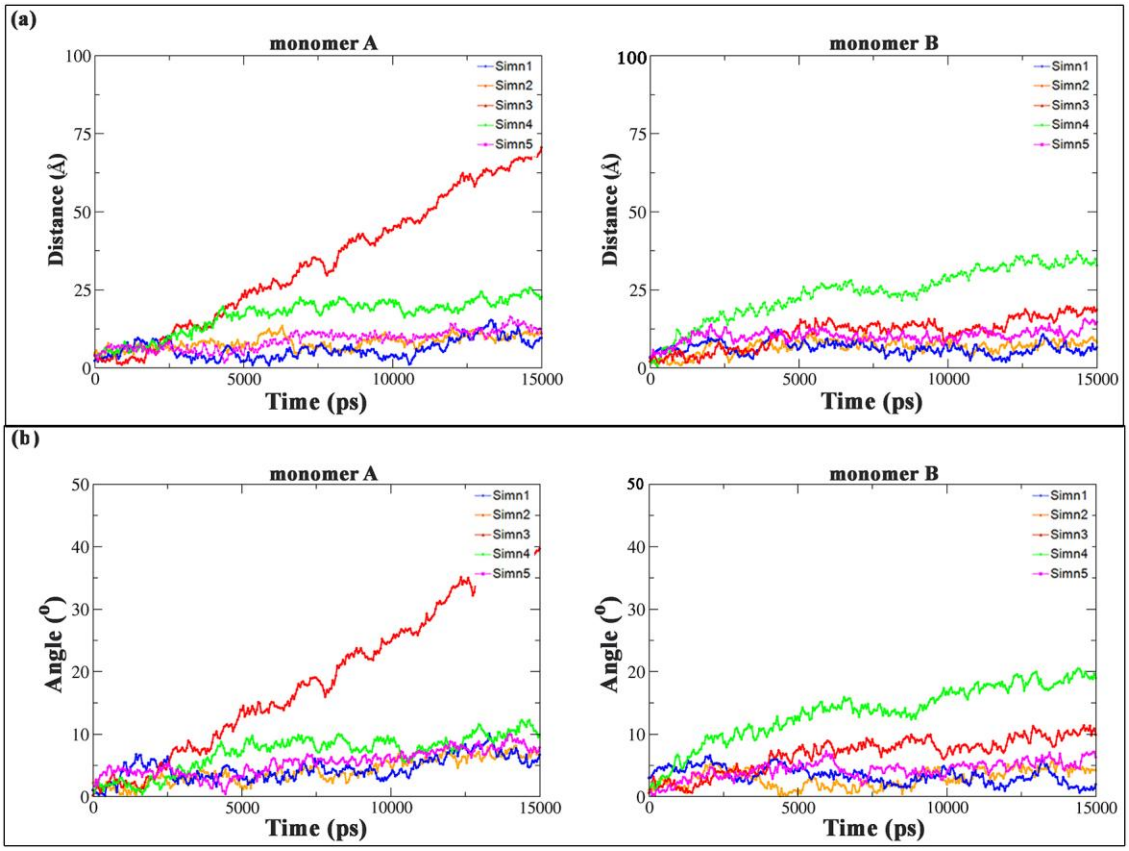

Figure S8

(a) Translation of Gly 676 (outermost residue of AT domain) with respect to its position in the initial structure over five 15ns MD trajecties.

(b) Rotation of the vector joining Cys 199 to Gly 676 with respect to starting orientation over five 15ns MD trajectories.

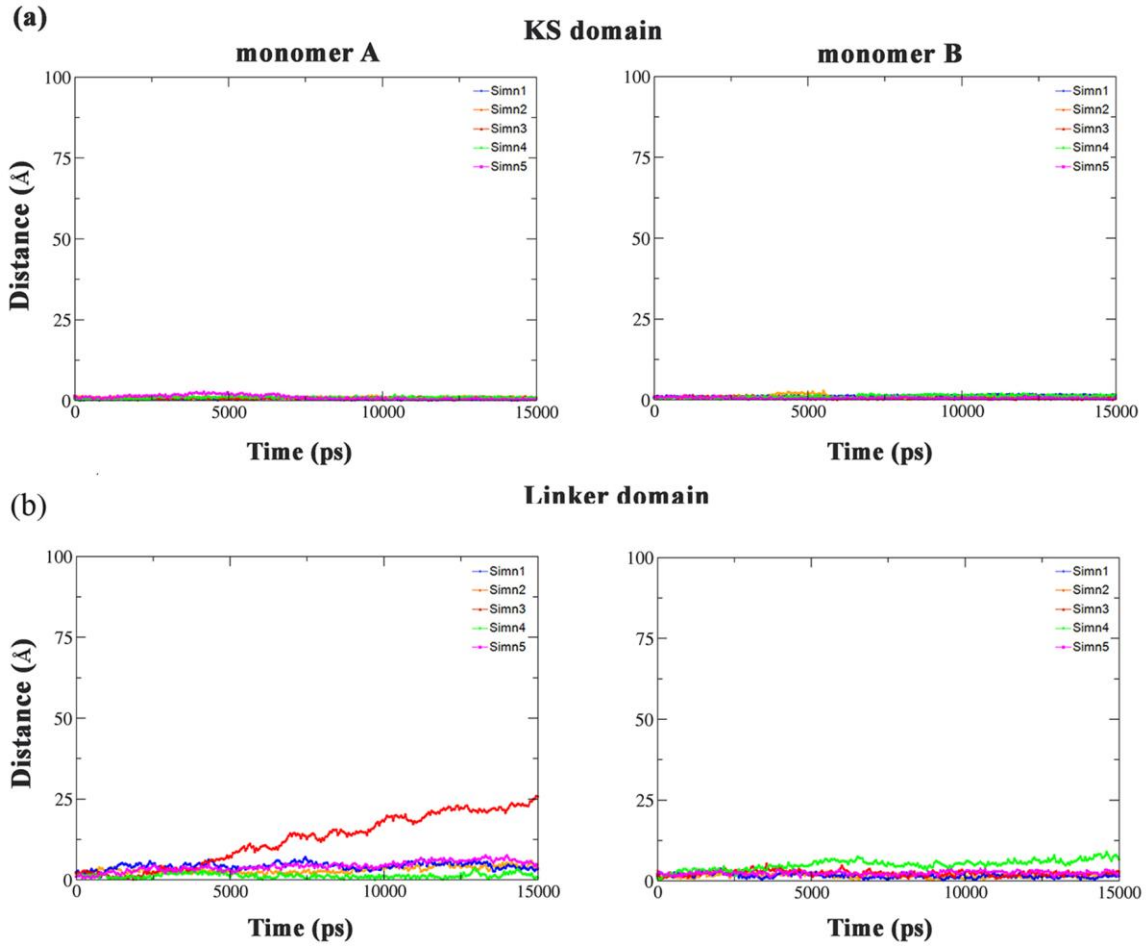

Figure S9

(a) Translation of Val 518 (residue of linker domain) with respect to its position in the initial structure over 15ns MD trajectories.

(b) Rotation of the vector joining Cys 199 to Val 518 with respect to starting orientation over 15ns MD trajectories.

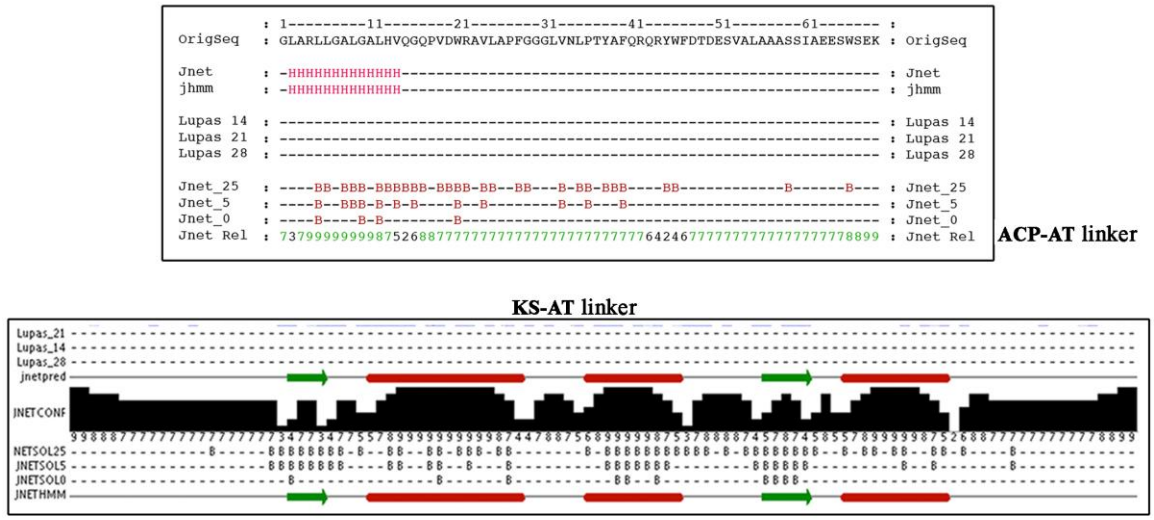

Figure S10
The secondary structure prediction by Jpred server for the 49 AT-ACP linkers