Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Dynamics of the thumb-finger regions in GH11 xylanase *Bacillus circulans*: comparison between the Michaelis and covalent intermediate

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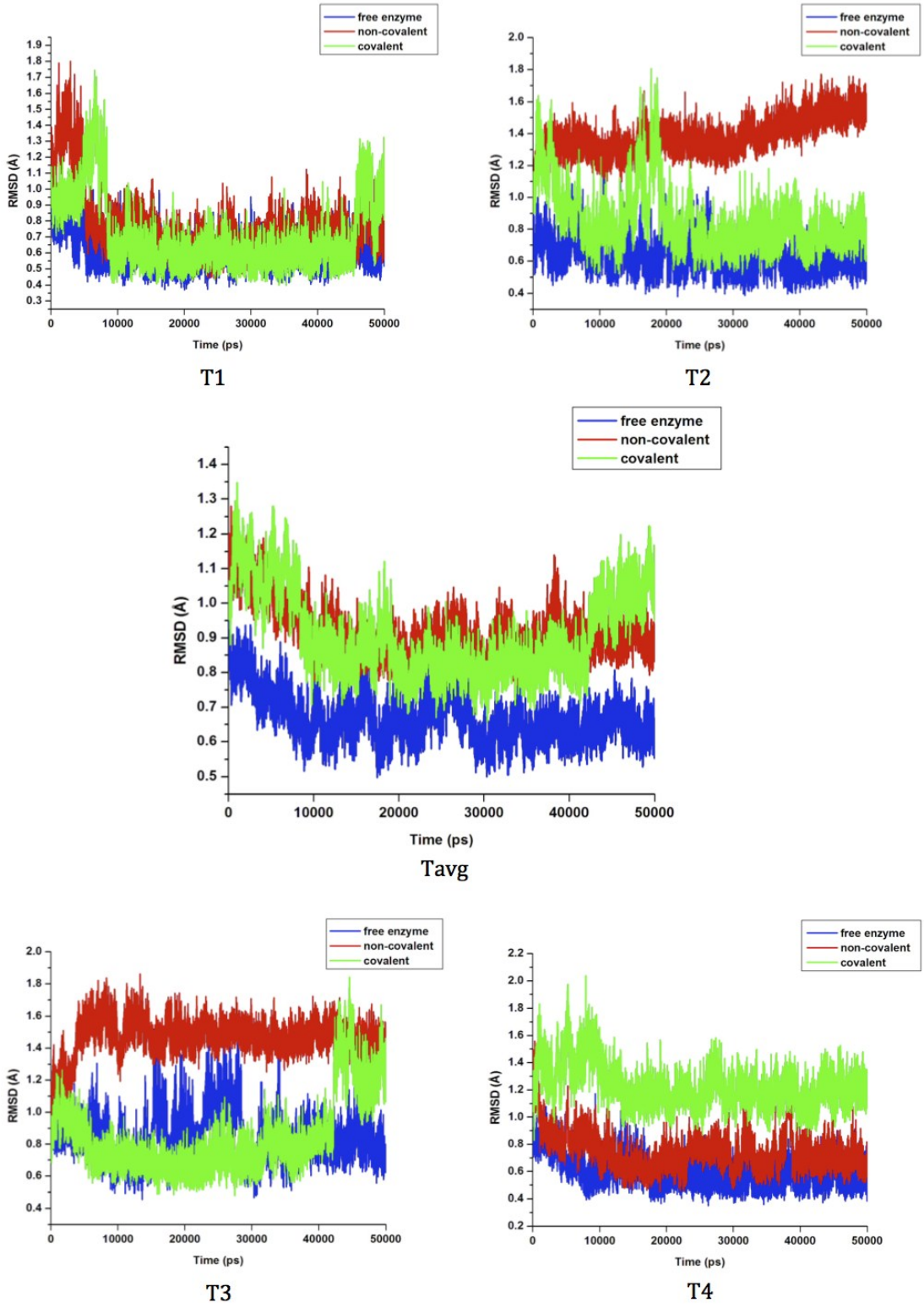
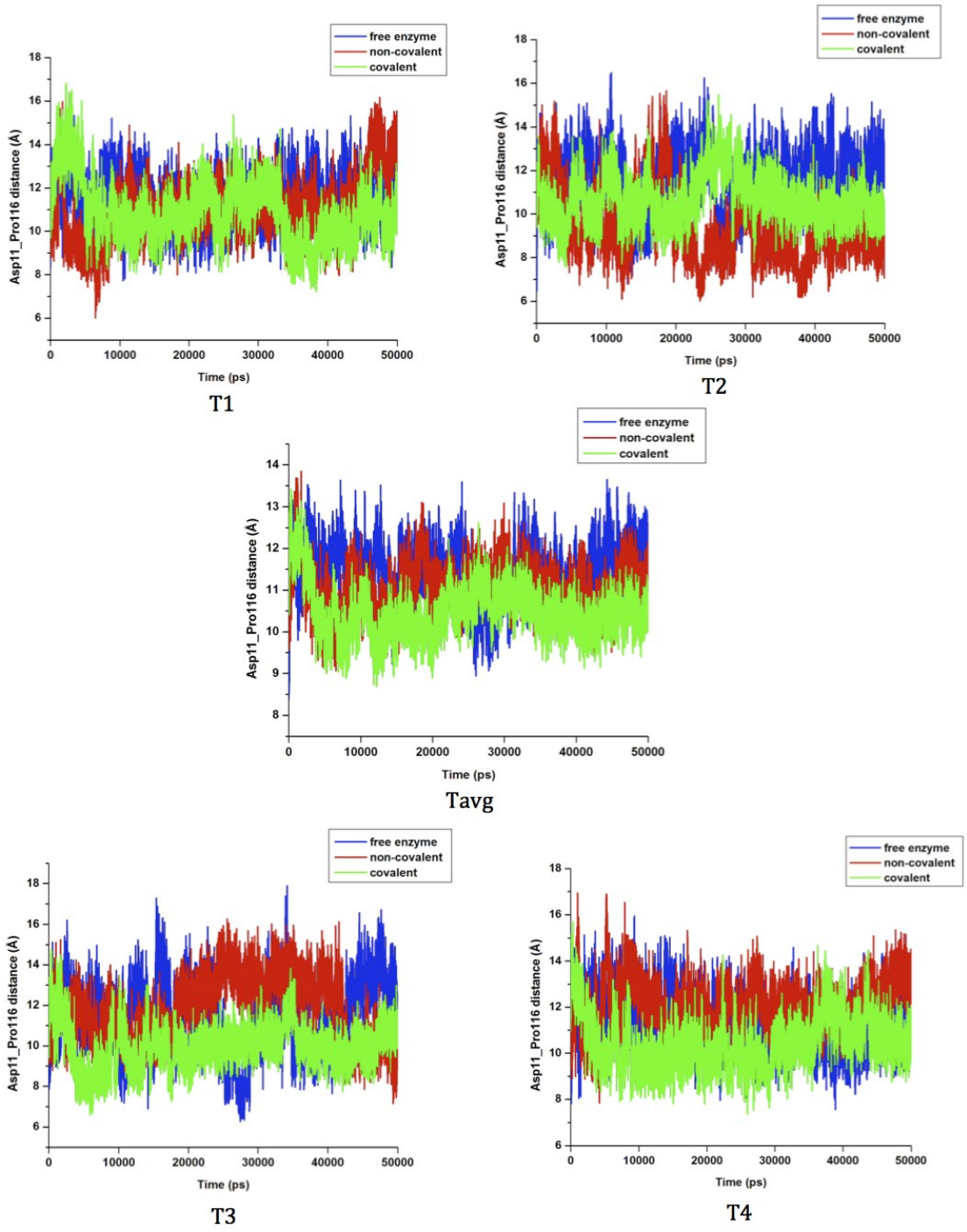
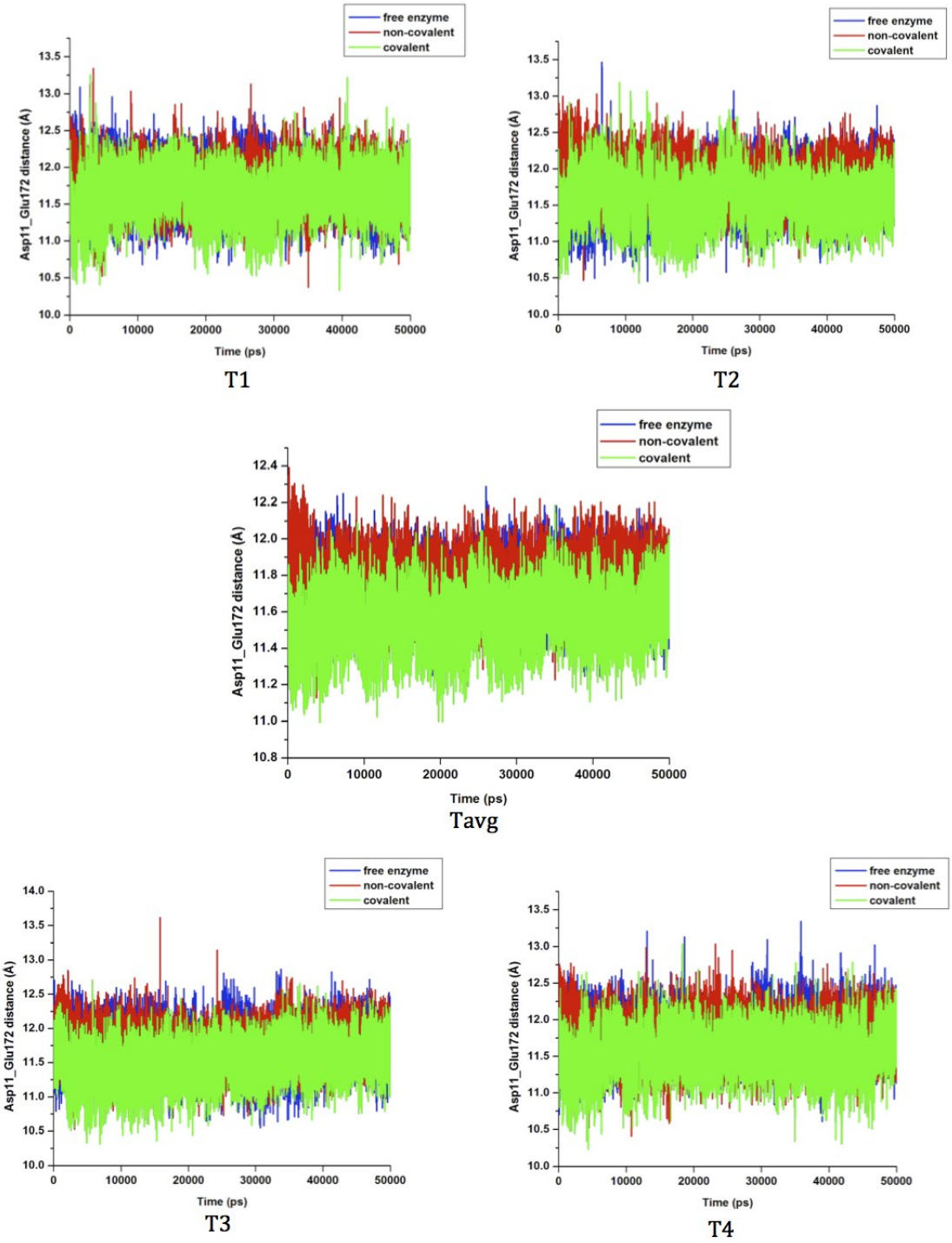


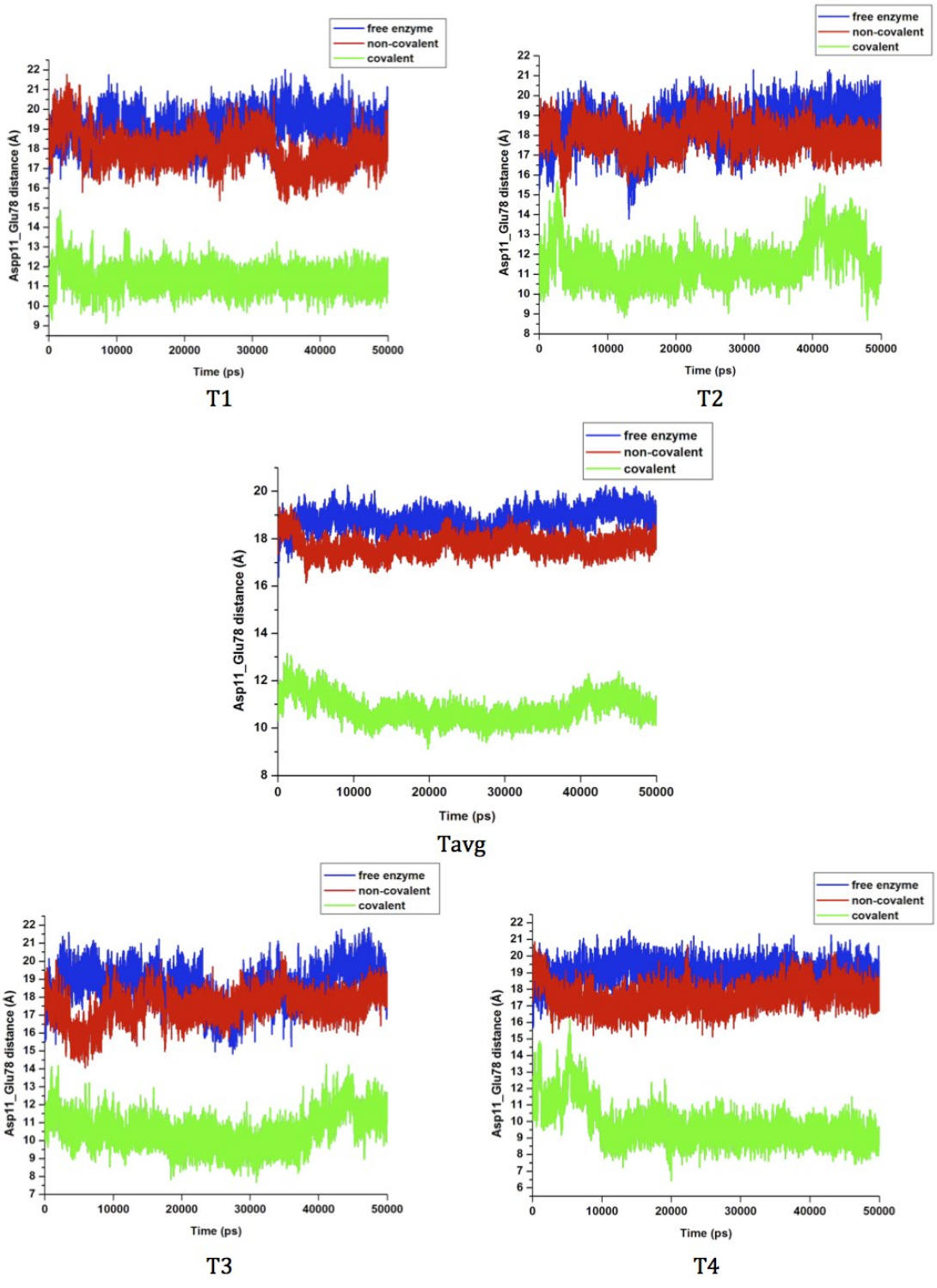
S1: Comparative RMSD for alpha carbon atoms of the respective free enzyme, non-covalently complex and covalent complex: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



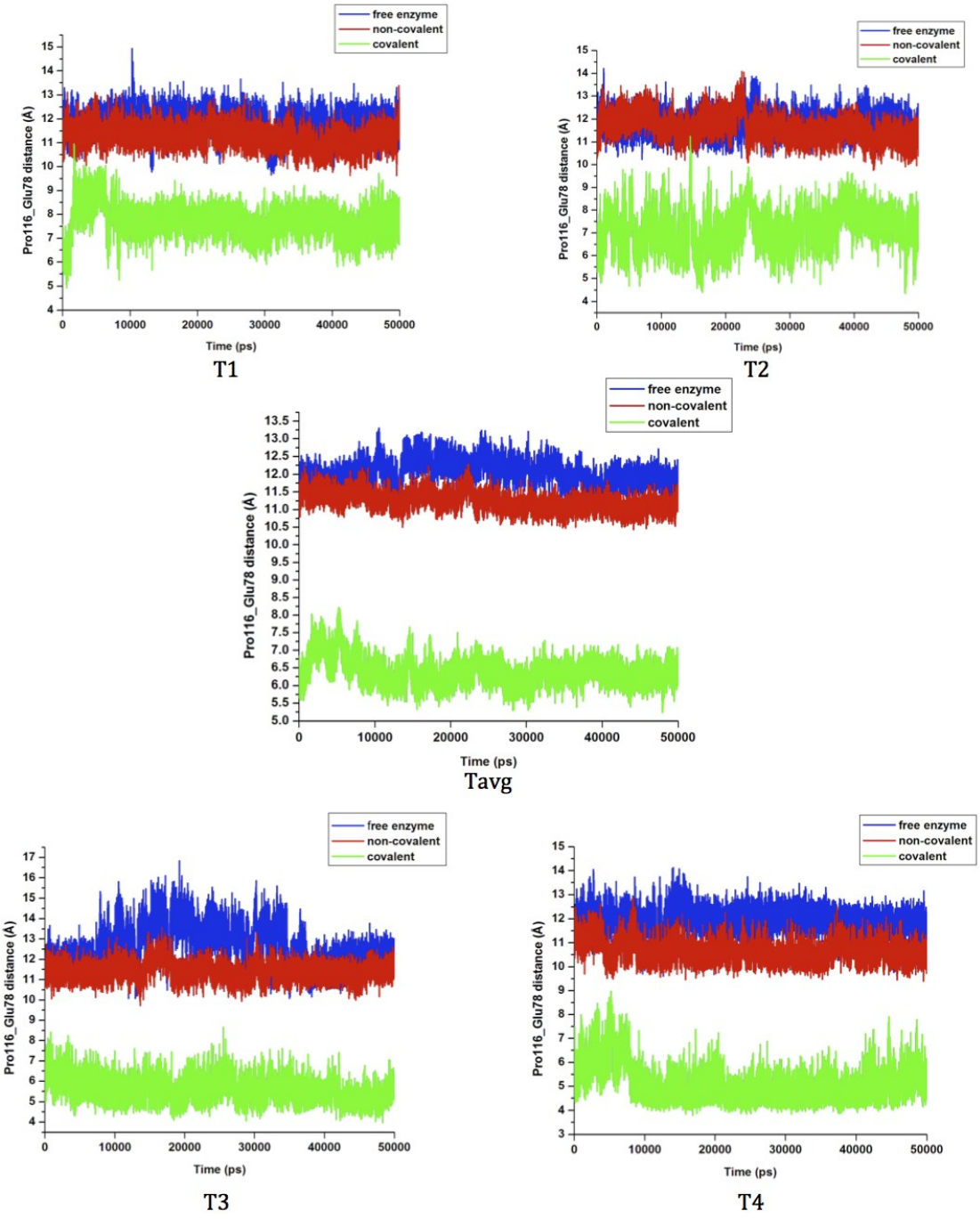
S2: The extent of opening and closing of the enzyme. A thumb-finger distance as a function of time for the free enzyme (blue), non-covalently bound (red) and covalently bound (green) systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



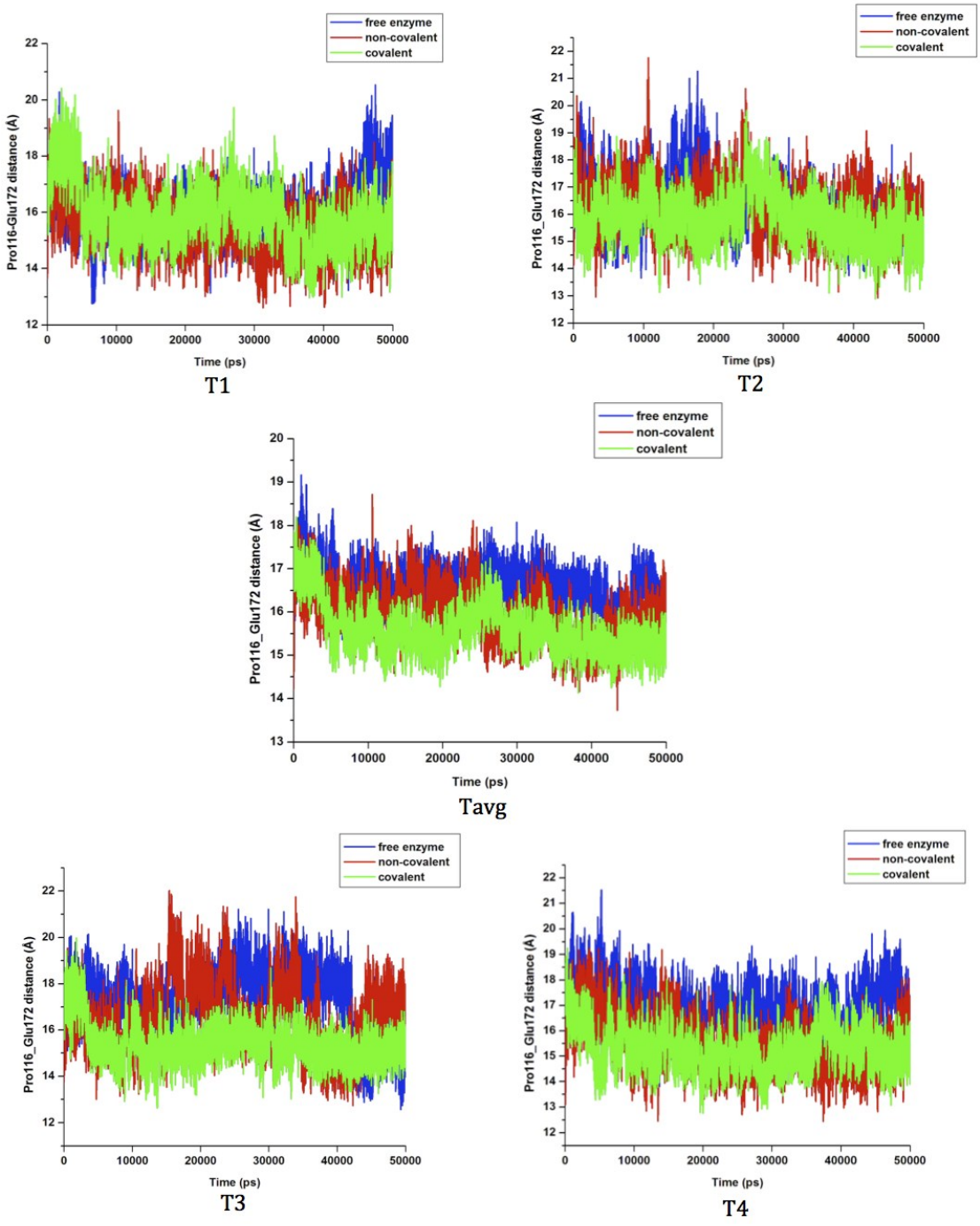
S3: The Asp11-Glu172 distance as a function of time for the free enzyme (blue), non-covalently bound (red) and covalently bound (green) systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



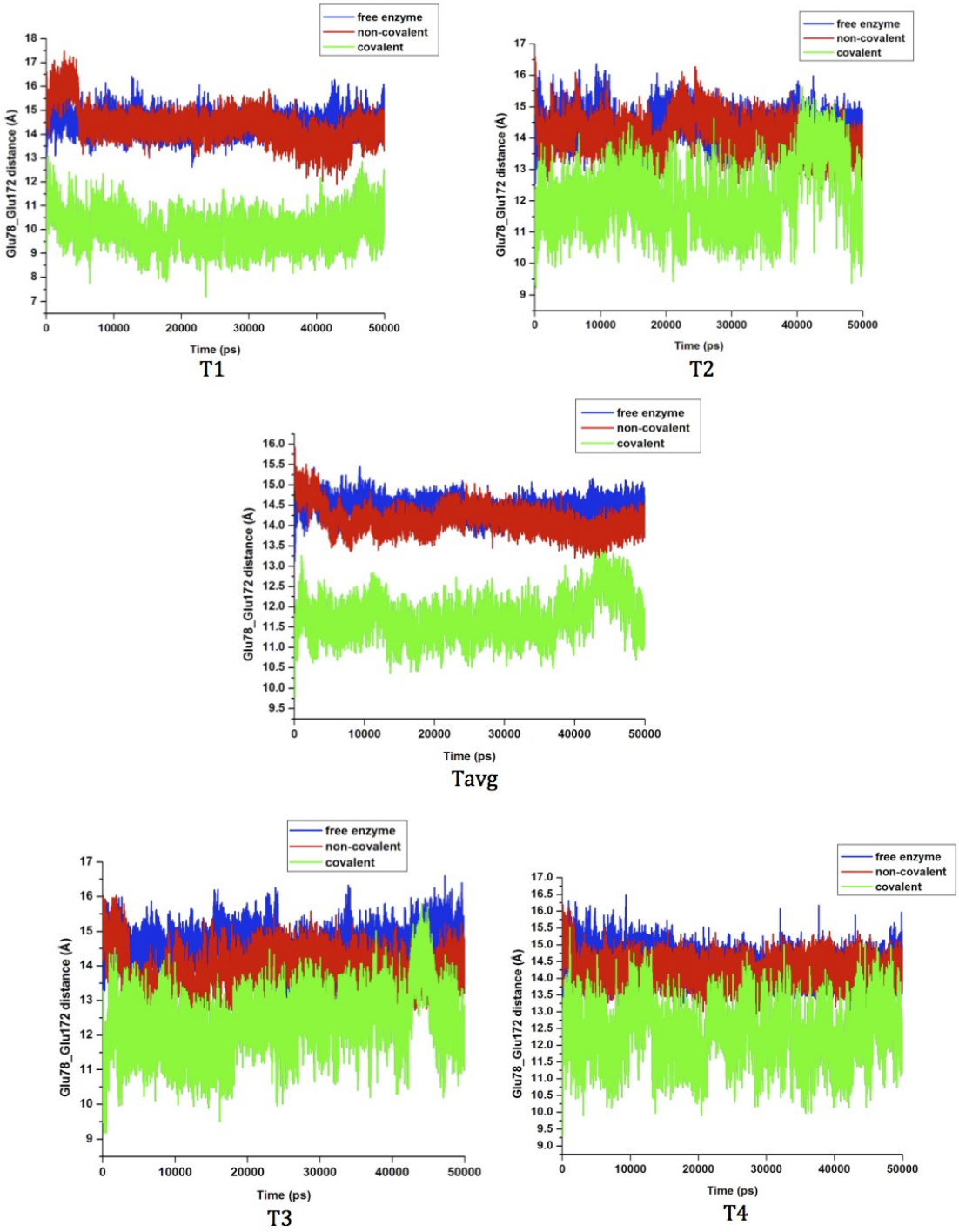
S4: Asp11-Glu78 distance as a function of time for the free enzyme (blue), non-covalently bound (red) and covalently bound (green) systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



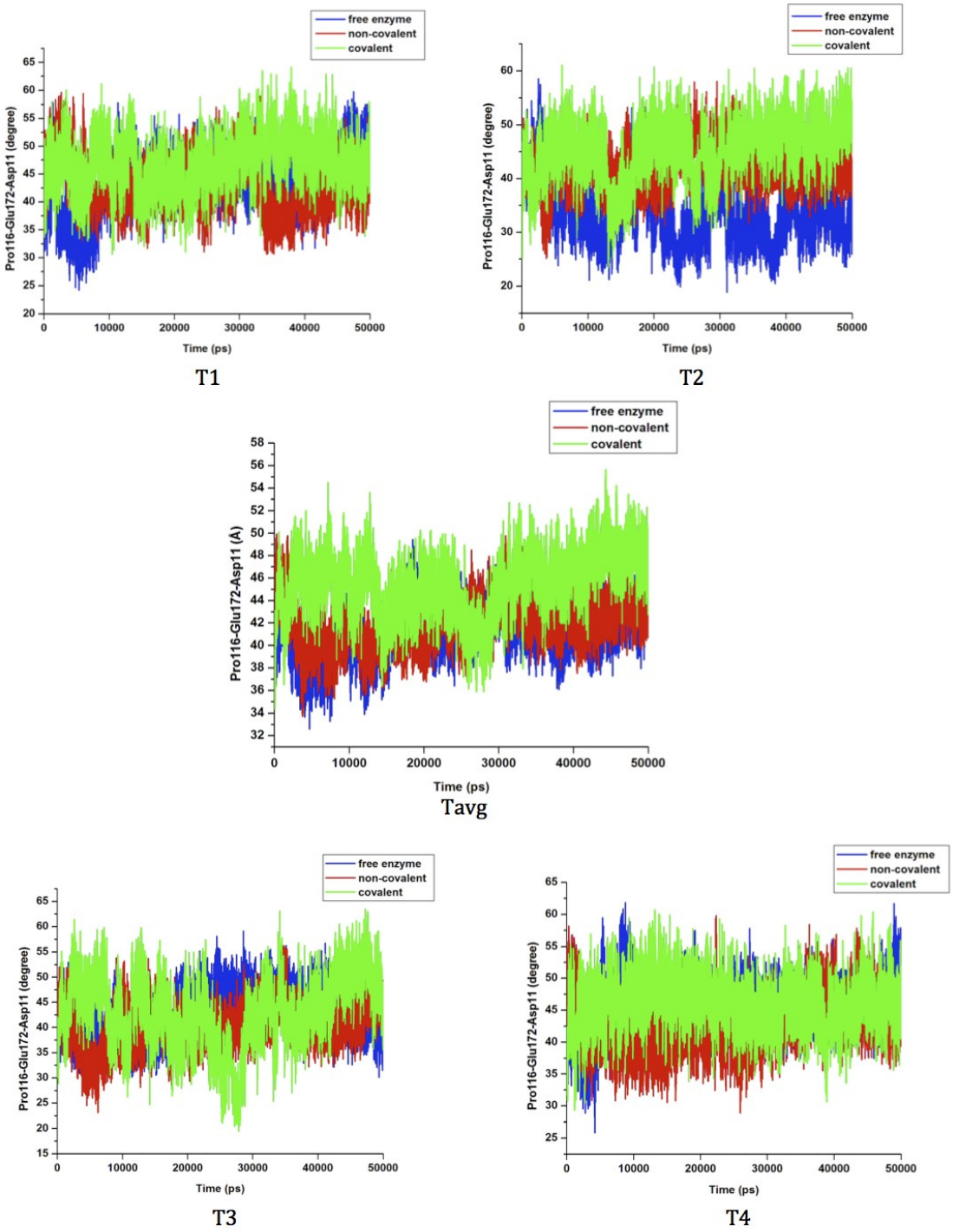
S5: The extent of compression on the thumb region of the enzyme for the free enzyme (blue), non-covalently (red) and covalently bound (green) systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



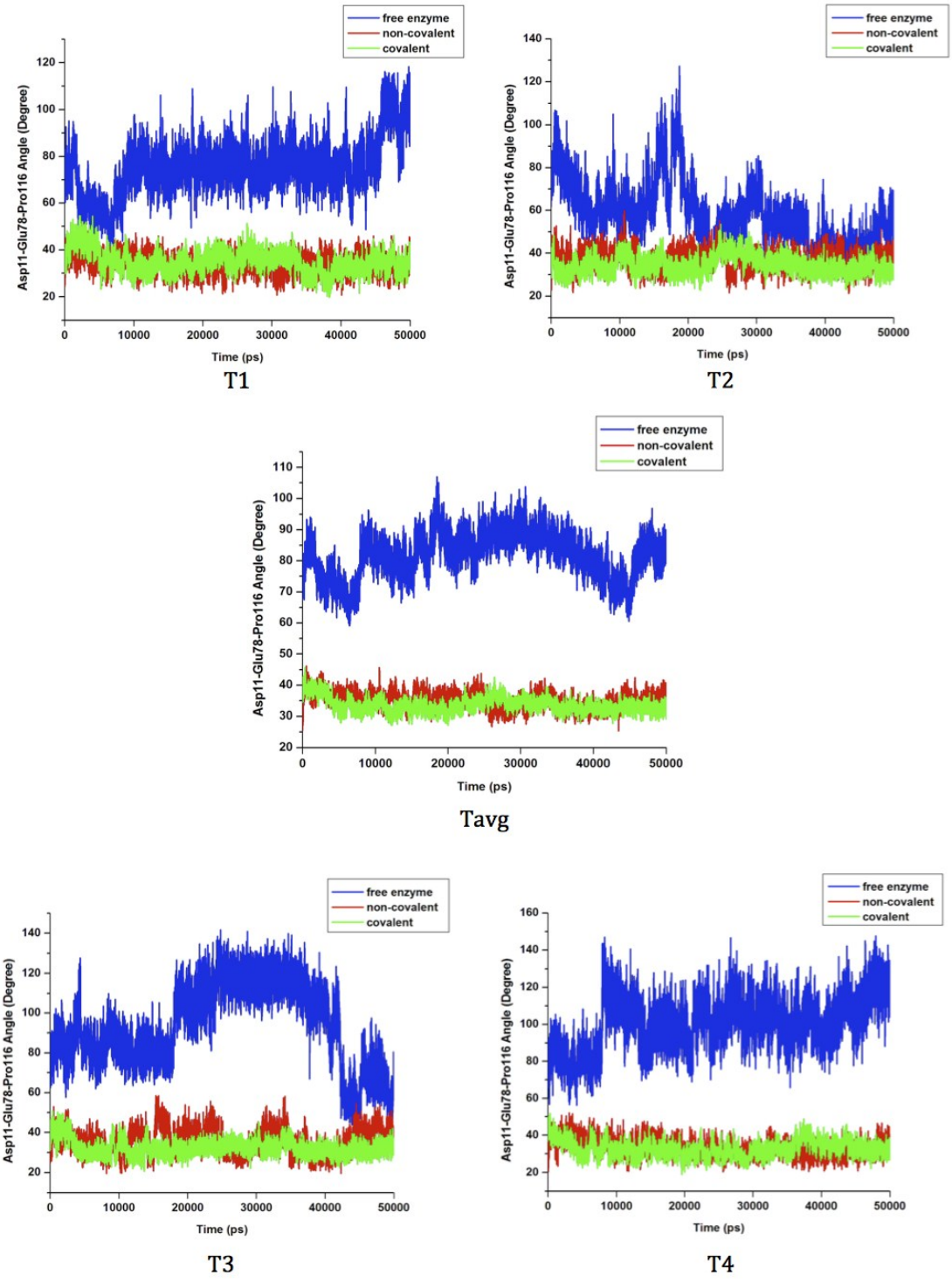
S6: The extent of compression of the thumb region of the enzyme. Pro116-Glu172 cross-distance as a function of time for the free enzyme (blue), non-covalently (red) and covalently bonded (green) systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



S7: The extent of opening of the enzyme active site. Glu78-Glu172 distance as a function of time for the free enzyme (blue), non-covalently (red) and covalently bonded (green) systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



S8: Comparative Pro116-Glu172-Asp11 angle measured for the respective free enzyme, non-covalent and covalent intermediate systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.



S9: Comparative Asp11-Glu78-Pro116 angle measured for the respective free enzyme, non-covalent and covalent intermediate systems: T1, T2, T3, T4 & T_{avg} are represent four distinctive 50 ns MD trajectories and overall average, respectively.

Table S1: Average distance measured for the respective free enzyme, non-covalent intermediate and covalent intermediate complex.

	Free enzyme	**Non-covalent**	**Covalent**
Cα-Cα distance	Dist. (Å)	Dist. (Å)	Dist. (Å)
Asp11-Pro116	11.41±0.68	11.07±0.57	10.48±0.60
Asp11- Glu78	18.80±0.44	17.75±0.37	10.79±0.51
Asp11-Glu172	11.76±0.12	11.71±0.12	11.55±0.13
Pro116-Glu78	12.05±0.33	11.24±0.25	6.38±0.36
Pro116-Glu172	16.64±0.46	15.97±0.59	15.59±0.54
Glu78-Glu172	14.44±0.20	14.14±0.31	11.72±0.44

Table S2: Average angle measured for the respective free enzyme, non-covalent intermediate and covalent intermediate complex.

	Free enzyme	**Non-covalent**	**Covalent**
Cα-Cα angle	Angle (deg.)	Angle (deg.)	Angle (deg.)
Asp11-Glu78-Pro116	81.87±7.17	35.22±2.67	33.60±2.30
Pro116-Glu172-Asp11	45.34±2.76	42.11±2.06	41.33±2.17

Table S3: Average H-bond distances between the substrate and active site residues monitored during MD simulation of the non-covalent intermediate complex.

Non-covalent complex	
Hydrogen Bond	**H-bond avg dist (Å)**
Arg112 (NH_2…O_6) Subs	14.09±1.67
Thr67 (OG_1…O_{11}) Subs	13.63±1.96
Tyr79 (O…O_{10}) Subs	11.90±1.40
Leu68 (O…O_{10}) Subs	13.71±1.46
Glh172 (OE_1…O_{12}) Subs	10.31±1.40

Table S4: Average H-bond distances between the substrate and active site residues monitored during MD simulation of the covalent intermediate complex.

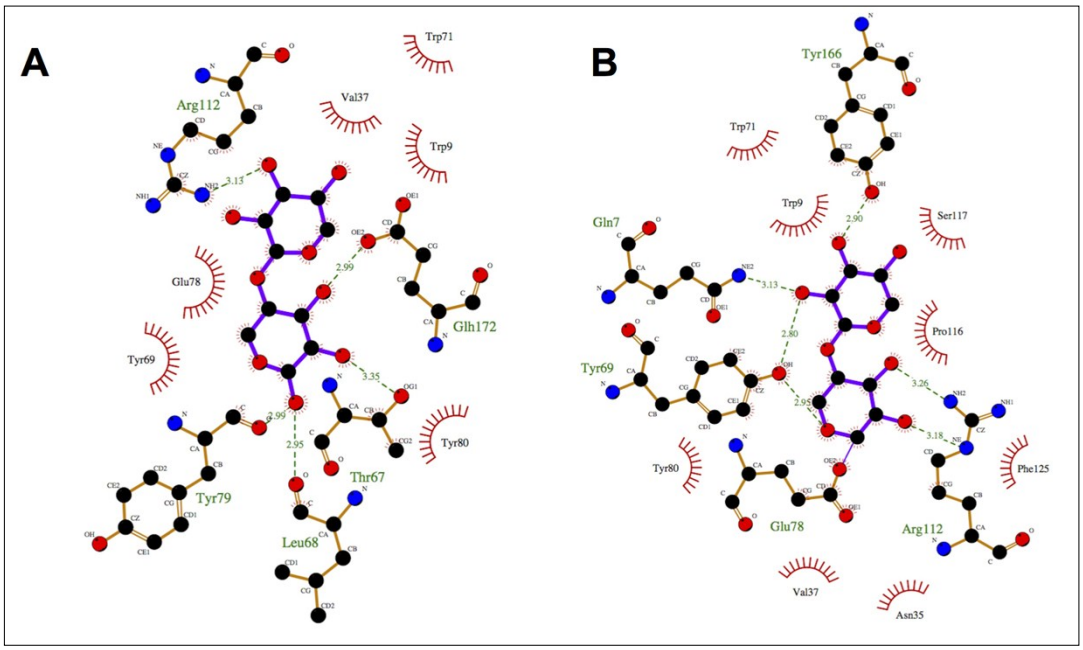
Covalent complex	
Hydrogen Bond	**H-bond avg dist (Å)**
Arg112 (NE…O_1) Subs	6.41±0.82
Arg112 (NH_2…O_3) Subs	6.78±0.97
Gln7 (NE_2…O_{2B}) Subs	7.51±0.55
Tyr69 (OH…O_{2B}) Subs	5.38±0.60
Tyr69 (OH…O_5) Subs	5.21±0.57
Tyr166 (OH…O_{3B}) Subs	5.14±0.60

Table S5: Average radius of gyration (Rg) monitored during MD simulation of the free enzyme, non-covalent complex and covalent complex.

Free enzyme Rg (Å)	Non-covalent Rg (Å)	Covalent Rg (Å)
15.27±0.04	15.26±0.03	15.19±0.04

Table S6: Prominent residues contribution towards motions across distinctive modes of the free enzyme, non-covalent complex and covalent complex systems.

System	Normal Mode	Residue Numbers with High Displacement Frequency
Free enzyme	**1**	**116, 135**
	2	**11, 118**
	3	**11, 118**
Non-covalent	**1**	**11, 47, 99, 137, 139, 140, 171, 184, 120**
	2	**11, 99, 110, 135, 184**
	3	**11, 47, 99**
Covalent	**1**	**11, 111, 116**
	2	**11, 116, 118, 120, 133, 162**
	3	**11, 47, 71, 74, 119, 123, 157**



S10: Interaction of a non-covalently bound (**A**) and a covalently bound (**B**) xylobiose sugar with *B. circulans* endo-β-1,4-xylanase.