Ligand Binding Swaps Between Soft Internal Modes of α,β-Tubulin and Alters Its Accessible Conformational Space

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Supporting Information

Movie no.	File name	Description
M1	M1_Apo_dimer_PC1.avi	Movements of Apo dimer along its PC1
M2	M2_Apo_dimer_PC3.avi	Movements of Apo dimer along its PC3
M3	M3_Apo_dimer_PC4.avi	Movements of Apo dimer along its PC4
M4	M4_E7010_dimer_PC1.avi	Movements of Tubulin-E7010 complex along its PC1
M5	M5_E7010_dimer_PC2.avi	Movements of Tubulin-E7010 complex along its PC2
M6	M6_TN16_dimer_PC1.avi	Movements of Tubulin-TN16 complex along its PC1
M7	M7_TN16_dimer_PC3.mpg	Movements of Tubulin-TN16 complex along its PC3
M8	M8_Apo_Bchain_PC1.avi	Movements of B-chain of the Apo system along the PC1 as viewed from the dimeric interface, as described in the Figure 7 of the main article.
M9	M9_E7010_Bchain_PC1.avi	Movements of B-chain of the Tubulin-E7010 complex system along the PC1 as viewed from the dimeric interface, as described in the Figure 7 of the main article.

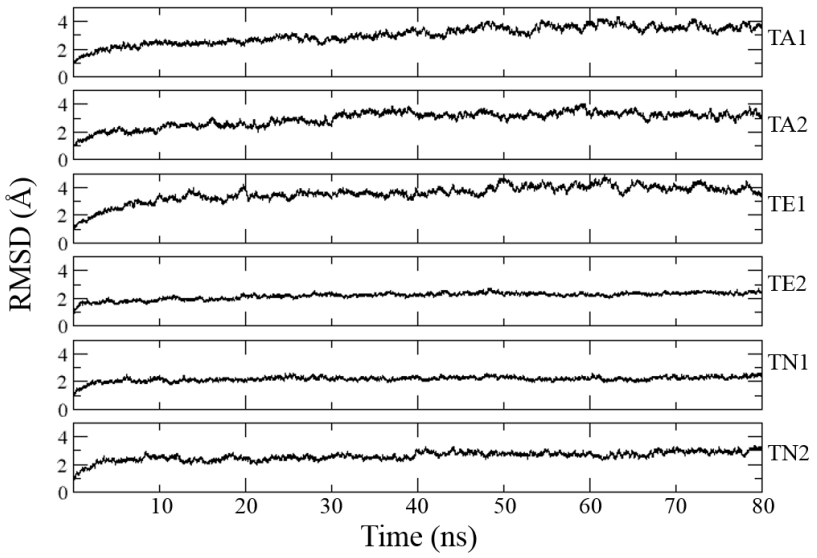

Figure S1: Root mean square deviation (RMSD) values of the tubulin backbone along different trajectories.

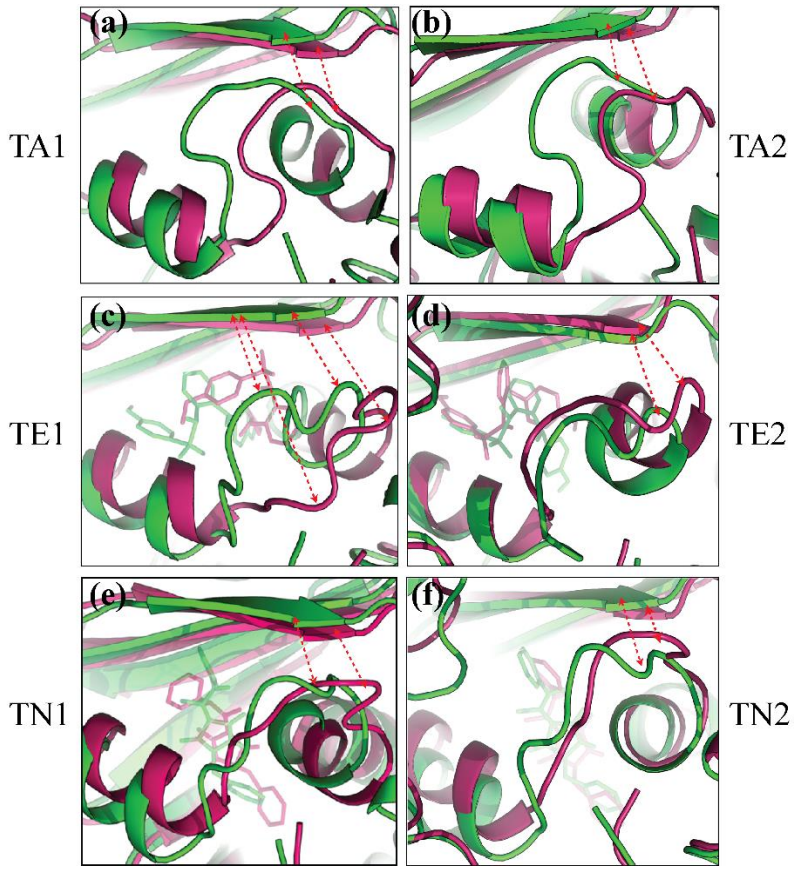

Figure S2: Orientations and positioning of T7 loop observed from different trajectories of tubulin complexed and apo systems. Secondary srtuctures shown in green and magenta are representing the snap shots of starting and end point of simulation respectively. This figure resembles the Figure 2 of the main manuscript; here the spheres have removed to clearly show the positions of the T7 in different snapshots.

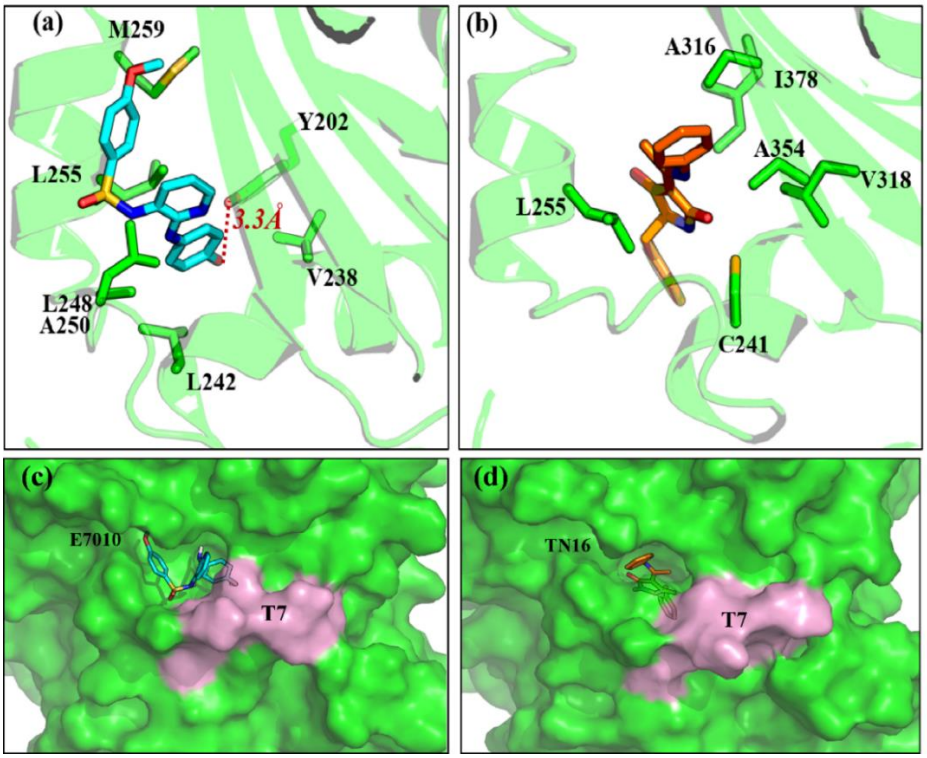

Figure S3: Difference in the topology of interactions of the ligands in the pocket of Tubulin. (a) E7010 complex and (b) TN16 complex, showing their difference in the H-bonds and hydrophobic interactions with the side chains of Tubulin (green) residues shown in sticks; the backbone secondary structure has also been shown in green. (c) and (d) the same complexes have been shown using surface representation, highlighting the T7 loop in pink colour. Only the β subunit has been shown for clarity. The view is from the position of the α-subunit towards the interfacial surface. The transparency of the cartoons, sticks and surface has been duly set to show the deeper penetration of the TN16 inside the cavity.

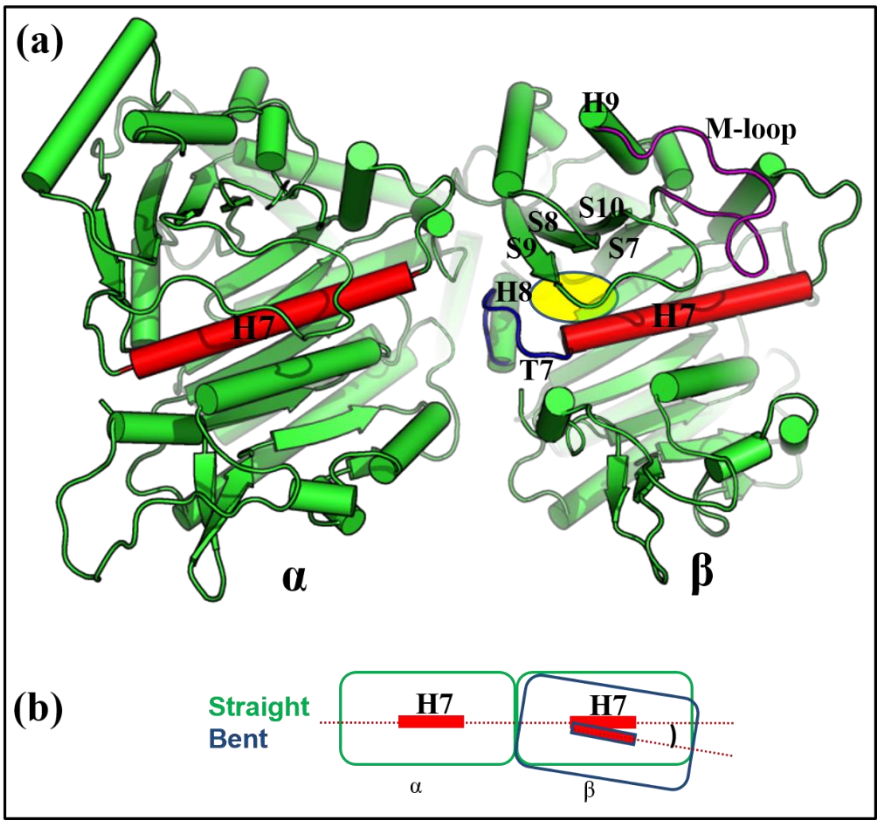

Figure S4: (a) Cartoon representation of the tubulin dimer. The two H7 helices of α and β subunits are particularly shown in red colour.The circle in yellow is representing the colchicine binding domain of tubulin protein. The T7-loop and M-loop are shown in blue and purple color, respectively. (b) Schematic representation to show the angle between the two subunits that makes difference in tubulin's 'Straight' to 'Bent' conformer.

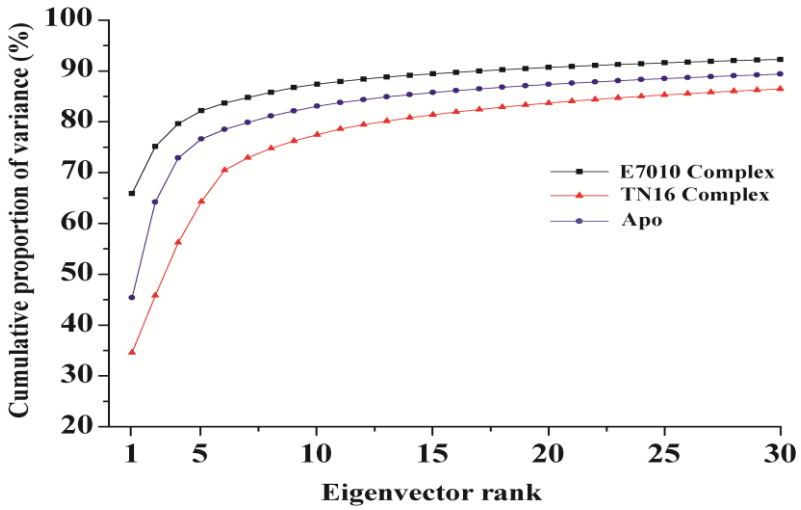

Figure S5: Cumulative sum of the variance (% contribution to the overall dynamics) of the principal modes of motions obtained from principal component analysis (PCA). Only modes no. 1 to 30 have been shown.

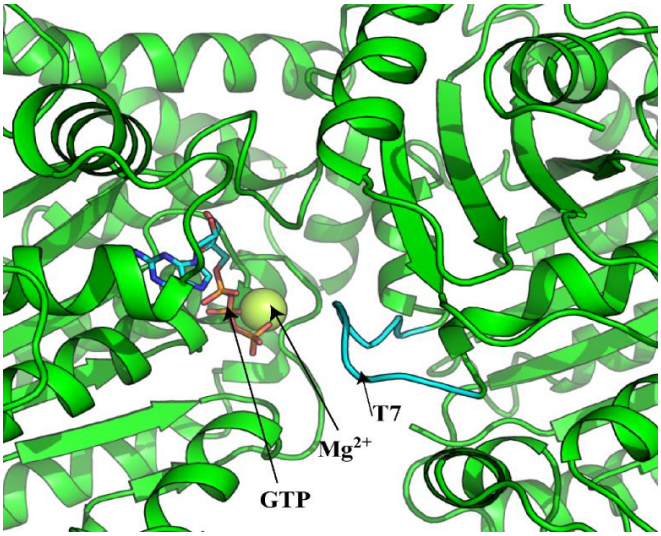

Figure S6: The close proximity of the GTP bound to the α-subunit and the T7 loop of the β-subunit. The structure has been shown using 3HKC after removing the ligand for clarity. Color scheme are same as in main text Figure 1.