SUPPORTING INFORMATION

C-terminal Tail of β -Tubulin and its Role in the Alterations of Dynein Binding Mode

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Table S1: Salt bridge formation across the MT-MTBD interface. Interactions were identified when the distance between oxygen atoms in the carboxyl group (acidic residue side chain) and nitrogen atoms in the amine group (basic residue side chain) fell within 3.2 Å cut-off at least once during 200 ns simulation.

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A				
P34036 Q9JHU4	DYHC_DICDI DYHCI_MOUSE	3317 3231	NEQANQKLKQMVQDQQAAEIKQKDARELQVQLDVRNKEIAVQKVKAYADLEKAEPAIIEA NAAANDKLKKMVKDQQEAEKKKVMSQEIQEQLHKQQEVIADKQMSVKEDLDKVEPAVIEA * **:***:**:*** ** *: ::::: ** :::: ** ::::: ** ::::: ** :::::	3376 3290
P34036	DYHC_DICDI	3377	QEAVSTIKKKHLDEIKSLPKPPTPVKLAMEAVCLMLGGKKLEWADIRKKIMEPNFITSII	3436
Q9JHU4	DYHCI_MOUSE	3291	QNAVKSIKKQHLVEVRSMANPPAAVKLALESICLLLGESTTDWKQIRSIIMRENFIPTIV	3350
Р34036 Q9JHU4 В	DYHC_DICDI DYHC1_MOUSE	3437 3351	NYDTKKMMTPKIREAITKGYLEDPGFDYETVNRASKACGPLVKWAT <mark>AQTYYSEILDRIKP</mark> NFS <mark>AEEI-SDAIREKMKKN</mark> YMSNPSYN <mark>YEIVNRASLACGPMVKWAIAOLNYADMLKRVEP</mark> * ****.******************	3496 3409
P02550 P09733	TBA1A_PIG TBA1_YEAST	1 1	MRECISIHVGQAGVQIGNACWELYCLEHGIQPDGQMPSDK-TIGGGDDSFNTFFSETGAG MREVISINVGQAGCQIGNACWELYSLEHGIKPDGHLEDGLSKPKGGEEGFFTFHETGYG ****	59 60
P02550	TBA1A_PIG	60	KHVPRAVFVDLEPTVIDEVRTGTYRQLFHPEQLITGKEDAANNYARGHYTIGKEIIDLVL	119
P09733	TBA1_YEAST	61	K <mark>FVPRAIYVDLEPNVIDEVRN</mark> GPYKDLFHPEQLISGKEDAANNYARGHYTVGREILGDVL	120
P02550	TBA1A_PIG	120	DRIRKLADQCTGLQGFSVFHSFGGGTGSGFTSLLMERLSVDYGKKSKLEFSIYPAPQVST	179
P09733	TBA1_YEAST	121	DRIRKLADQCDGLQGFLFTHSLGGGTGSGLGSLLEELSAEVGKKSKLEFSIYPAPQVST	180
P02550	TBA1A_PIG	180	AVVEPYNSILTHTTLEHSDCAFMVDNEAIYDICRRNLDIERPTYTNLNRLIGQIVSSIT	239
P09733	TBA1_YEAST	181	SVVEPYNTVLTHTTLEHADCTFMVDNEAIYDMCKRNLDIPRPSFANLNNLIAQVVSSVT	240
P02550	TBA1A_PIG	240	ASLRFDGALNVDLTEFQTNLVPYPRAHFPLATYAPVISAEKAYHEQLSVAEITNACFEPA	299
P09733	TBA1_YEAST	241	ASLRFDGSLNVDLNEFQTNLVPYPRIHFPLVSYSPVLSKSKAFHESNSVSEITNACFEPG	300
P02550	TBA1A_PIG	300	NOMVKCDPRHGKYMACCLLYRGDVVPKDVNAAIATIKTKRTIQFVDWCPTGFKVGINYEP	359
P09733	TBA1_YEAST	301	NOMVKCDPRDGKYMATCLLYRGDVVTRDVQRAVEQVKNKKTVQLVDWCPTGFKIGICYEP	360
P02550	TBA1A_PIG	360	PTVVPGGDLAKVQRAVCMLSNTTAIAEAWARLDHKFDLMYAKRAFVHWYVGEGMEEGEFS	419
P09733	TBA1_YEAST	361	PTAT <mark>PNSQLATVDRAVCMLSNTTSIAEAWKRIDRKFDLMY</mark> AKRAF <mark>VHWYV</mark> GEGMEEGEFT	420
P02550	TBA1A_PIG	420	EAREDMAALEKDYEEVGVDSVEGEGEEEGEEY	451
P09733	TBA1_YEAST	421	EAREDLAALERDYIEVGADSVAEEEEF	447
P02554	TBB_PIG	1	MRE <mark>IVHIQAGQCGNQIGAKFWEVISDEHGIDPTGSY</mark> HGDSDLQLERINYV <mark>YNEA</mark> AGN <mark>KYV</mark>	60
P02557	TBB_YEAST	1	MRE <mark>IIHISTGO GNQIGAAFWETICGE</mark> HGLDFNGTYHGHDDIQKERLNVVFNEASSGKWV	60
P02554	TBB_PIG	61	PRAILVDLEPGTMDSVRSGPFGQIFRPDNFVFGQSGAGNNWAKGHYTEGAELVDSVLDVV	120
P02557	TBB_YEAST	61	PRSINVDLEPGTIDAVRNSAIGNLFRPDNYIFGQSSAGNVWAKGHYTEGAELVDSVDDVI	120
P02554	TBB_PIG	121	RKESESCDCLQ <mark>GFQLTHSLGGGTGSGMGTLLISKIREEYPDRIMNTFSVV</mark> P <mark>SPKVSDTVV</mark>	180
P02557	TBB_YEAST	121	RREAEGCDSLQGFQITHSLGGGTGSGMGTLLISKIREEFPDRMMATFSVLPSPKTSDTVV	180
P02554	TBB_PIG	181	EPYNATLSVHQLVENTDETYCIDNEALYDICFRTLKLTTPTYGDLNHLVSATMSGVTTCL	240
P02557	TBB_YEAST	181	EPYNATLSVHQLVEHSDETFCIDNEALYDICQRTLKLNQPSYGDLNNLVSSVMSGVTTSL	240
P02554	TBB_PIG	241	RFPGQLNADLRKLAVNMVPFPRLHFFMPGFAPLTSRGSQQYRALTVPELTQQMFDAKNMM	300
P02557	TBB_YEAST	241	RYPGQLNSDLRKLAVNLVPFPRLHFFMVGYAPLTAIGSQSFRSLTVPELTQQMFDAKNMM	300
P02554	TBB_PIG	301	AACDPRHGRYLTVAAVFRGRMSMKEVDEQMLNVQNKNSSYFVEWIPNNVKTAVCDIPPRG	360
P02557	TBB_YEAST	301	AAADPRNGRYLTVAAFFRGKVSVKEVEDEMHKVQSKNSDYFVEWIPNNVQTAVCSVAPQG	360
P02554	TBB_PIG	361	L <mark>KMSATFIGNSTAIQELFKRISEQFTAMFRRKAFLHWYT</mark> GEGMDEMEFTEAESNMNDLVS	420
P02557	TBB_YEAST	361	LDMAATFIANSTSIQELFKRVGDQFSAMFKRKAFLHWYTSEGMDELEFSEAESNMNDLVS	420
P02554	TBB_PIG	421	EYQQYQDATADEQGEFEEGEEDEA	445
P02557	TBB_YEAST	421	EYQQYQEATVEDDEEVDENGDFGAPQNQDEPITENFE	457
A				

Turn

Nucleotide binding Coiled coil Sequence conflict Beta strand Modified residue





Figure S4: Number of hydrogen bonds between (A) MTBD and β -tubulin, (B) MTBD and β -H18 and (C) MTBD and β -CTT.



Figure S5: Percent helicity of MTBD-tubulin interface residues, (A) MTBD-H1, (Lys3385- Ser3393, 2-10), (B) MTBD-H3, (Trp3419-Ile3426, 2-9), (C) MTBD-H6, (Tyr3464-Ala3470, 2-8), (D) α-H15 (Val405-Glu411, 2-8), (E) β-H8, (Met149-Glu160, 2-12), (F) β-H9, (Glu183-Asn197, 2-16), and (G) β-H18 (Glu415-Gln436, 2-23).



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N-terminal, (C) MTBD-H1 and α -H14, (D) MTBD-H1 and α -H15, (E) Ser3393 (MTBD-H1) and β-Pro263, (F) α-Glu411 (H15) and Lys3396 (black) and Lys3402 (red) in the MTBD-H1-H2 loop and MTBD-H2 respectively, (G) β-Glu447 (β-tubulin C-terminal) and MTBD Lys3384 (black) in the N-terminal, Lys3386 (red) in H1, His3387 (blue) in H1, Arg3469 (green) in H6, and Lys3472 (orange) in the H6-H7 loop, (H) β -Glu449 (β -tubulin C-terminal) and MTBD Lys3384 (black) in the N-terminal, Lys3386 (red) in H1, His3387 (blue) in H1, Arg3469 (green) in H6, Lys3472 (orange) in the H6-H7 loop and Lys3479 (magenta) in H7, (I) MTBD-H2 and α-H15, (J) Thr3399 (MTBD-H2) and α -Glu414 (H15-H16 loop), (K) MTBD-H3 and β -H8, (L) MTBD-H3 and β -H9, (M) MTBD-H3 and β-H12, (N) MTBD-H3 and β-H18, (O) MTBD-H6 and α-H16, (P) Ser3471 (MTBD-H6-H7 loop) and α-Glu415 (H16), and (Q) α-Gly416 (H16) and Arg3469 (MTBD H6), (R) Oxygen atoms (OE1-9186 and OE2-9187) of the Glu3390 (MTBD-H1) carboxyl group and the nitrogen atoms (NE-4004, NH1-4007 and NH2-4010) of the α -Arg402 (H14-H15 loop) amine group, (S) Oxygen atoms (OE1-4152 and OE2-4153) of the α -Glu415 (H16) carboxyl group and the nitrogen atoms (NE-9977, NH1-9980 and NH2-9983) of the Arg3469 (MTBD-H6) amine group, (T) Oxygen atoms (OE1-4142 and OE2-4143) of the α -Glu414 (H15-H16 loop) carboxyl group and the nitrogen atoms (NE-9977, NH1-9980 and NH2-9983) of the Arg3469 (MTBD-H6) amine group, and (U) oxygen atoms (OE1-4152 and OE2-4153) of the α -Glu415 (H16) carboxyl group and the nitrogen atoms (NE-4004, NH1-4007 and NH2-4010) of the α -Arg402 (H14-H15 loop) amine group.









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R

Т















Figure S7: (A) Radius of gyration (Rg/nm) vs. time (ps), (B) Root mean square deviation (nm)

Figure S8: Sample of conformations presenting the fluctuation of β -CTT.



Table S1: Salt bridge formation across the MT-MTBD interface. Interactions were identified when the distance between oxygen atoms in carboxyl group (acidic residue side chain) and nitrogen atoms in amine group (basic residue side chain) fell within 3.2 Å cut-off at least once during 200 ns simulation.

Interacting Residues					
Residues of α-tubulin/	α-tubulin	MTBD			
MTBD interaction	Glu411	Lys3396			
	-	Lys3402			
	Glu414	Arg3469			
	Arg402	Glu3390			
Residue of β-tubulin/	β-tubulin	MTBD			
MTBD interaction	Glu159	Lys3424			
		Lys3425			
	Asp163	Lys3396			
		Arg3423			
	Glu196	Lys3385			
		Lys3392			
		Lys3424			
	Asp199	Arg3423			
	Arg264	Asp3389			
	Glu420	Lys3385			
		Lys3392			
		Arg3469			
	Asp427	Lys3385			
		Lys3386			
	Glu431	Lys3386			
	Glu447	Lys3384			
		Lys3386			
		His3387			

	Arg3469
	Lys3472
Glu448	Lys3386
	Lys3472
Glu449	His3384
	Lys3386
	Lys3387
	Arg3469
	Lys3472
	Lys3479
Glu451	Lys3384
	Lys3385
	Lys3386
	His3387
Glu452	Lys3384
	Lys3385
	Lys3386
	His3387
	Lys3479
Asp453	Lys3385
	Lys3386
	His3387
Glu454	His3387
	Lys3384