

2, 3-Dihydro-3 β -methoxy Withaferin-A Lacks Anti-Metastasis Potency: Bioinformatics and Experimental Evidences

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Supporting Information:

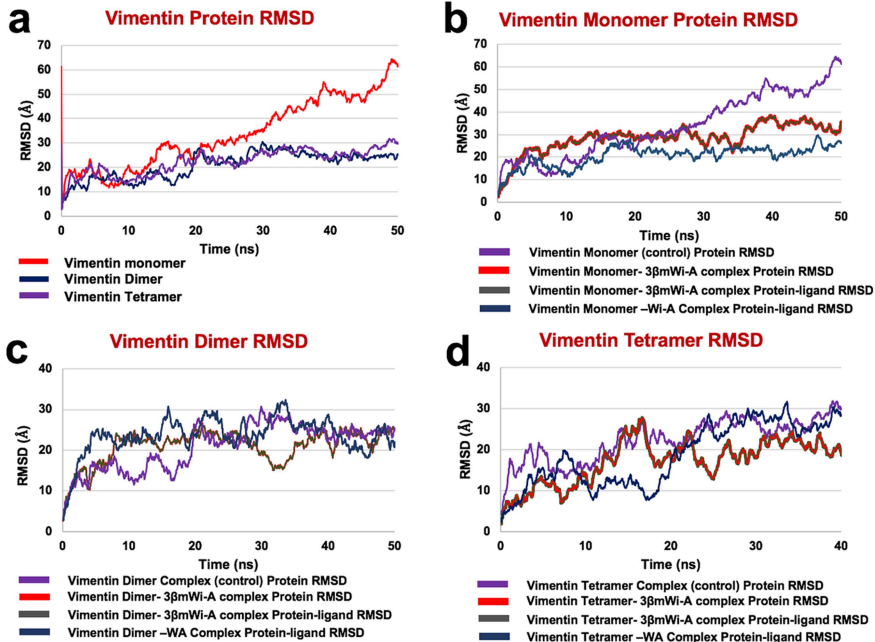
Legends to Supplementary figures-

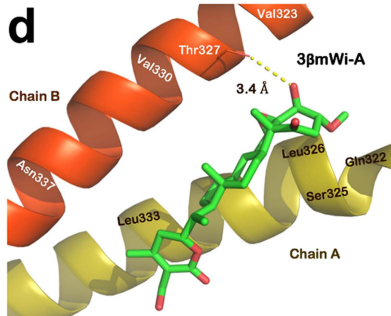
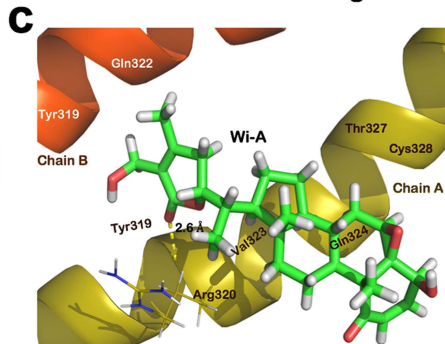
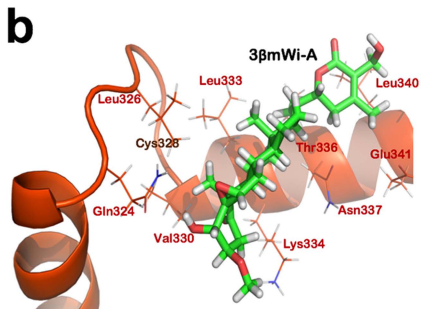
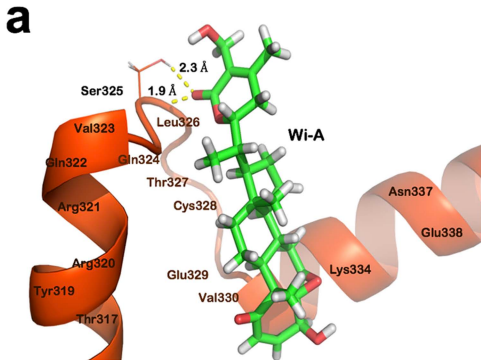
Figure S1. RMSD Fluctuations of vimentin protein with time. (a) RMSD fluctuations of vimentin monomer (red), dimer (blue) and tetramer (purple) structure taken as control. (b) RMSD fluctuations of vimentin monomer protein only for (i) control structure (purple), (ii) in complex with Wi-A (blue) and (iii) in complex with 3 β mWi-A (red). (iv) RMSD of vimentin monomer-3 β mWi-A complex is plotted in green color, which is overlapping with that of protein RMSD. (c) RMSD fluctuations of vimentin dimer protein only for (i) control structure (purple), (ii) in complex with Wi-A (blue) and (iii) in complex with 3 β mWi-A (red). (iv) RMSD of vimentin dimer-3 β mWi-A complex is plotted in green color. (d) RMSD fluctuations of vimentin tetramer protein only for (i) control structure (purple), (ii) in complex with Wi-A (blue) and (iii) in complex with 3 β mWi-A (red). (iv) RMSD of vimentin tetramer-3 β mWi-A complex is plotted in green color.

Figure S2. Molecular docking of Wi-A and 3 β mWi-A with Vimentin. Molecular interactions at vimentin monomer binding site with Wi-A (a) and 3 β mWi-A (b); and molecular binding of Wi-A (c) and 3 β mWi-A (d) with vimentin dimer binding site.

Figure S3. Alignment of vimentin protein sequence with conserved domain sequence of intermediate filament protein family (pfam00038).

Figure S1





[Superfamily] cl25641 (PSSMID 330462) Intermediate filament protein ;Intermediate filament protein.
 CD-length: 313 E-value: 7.31e-139 Bitscore: 405

			10	20	30	40	50	
			*....*....*....*....*....					
Vimentin	102	NEKVELQELNDRFANYIDKVRFL	EQQNKILLAELEQLKGG	---	GKSRLGD	148		
Cdd:pfam00038	1	NEKEQLQELNDRLAS	YIDKVRFL	EQQNKDLET	KISELRQKkg	aEPSRLYS	50	
			60	70	80	90	100	
			*....*....*....*....*....					
Vimentin	149	LYEEEMRELRRQVDQLTNDKARVE	VERDNLAEDIMRLREKLQE	EMLQREE	198			
Cdd:pfam00038	51	LYEREIRDRLRRQLDQLTVERARL	QLEIDNRLAAEDFRQ	YEDELNLRQS	100			
			110	120	130	140	150	
			*....*....*....*....*....					
Vimentin	199	AENTLQSFQDQVDNASLARLDL	ERKVESLQEEIAFLKKLHEEE	IQELQAQ	248			
Cdd:pfam00038	101	AEADLVGLRKDLDEATLARVDL	EMKVESLQEELAF	LKKNH	EEVRELQSQ	150		
			160	170	180	190	200	
			*....*....*....*....*....					
Vimentin	249	IQEQHVQIDVDVS-KPDLTAAL	RDVRQQYESVAAKNLQEA	EAEWYKSFAD	297			
Cdd:pfam00038	151	VQDTQVNVEMDAAR	KLDLTSALAEIRAQYEE	IAAKNREEAEWYQSKLEE	200			
			210	220	230	240	250	
			*....*....*	*....*....				
Vimentin	298	LSEAAARNNDALRQAKQEST	EYRRQVQSLTCEVDALKGT	NESLERQMRE	347			
Cdd:pfam00038	201	LQQAARNGDALRSAKEE	ITELRRQIQSLEIELQSL	KKQKASLERQLAET	250			
			260	270	280	290	300	
			*....*....*....*....*....					
Vimentin	348	EENFAVEAANYQDTIGRLQ	DEIQNMKEEMARHLREYQD	LLNVKMA	LIDIEI	397		
Cdd:pfam00038	251	EERYELQLADYQDLISEL	AEELQQIRQEMARQLREYQ	ELLNVK	LALDIEI	300		
			310					
			*.... ...					
Vimentin	398	ATYRKLLGE	EESR	410				
Cdd:pfam00038	301	ATYRKLLGE	EECR	313				