In-silico investigation of the role of vitamins in cancer therapy through inhibition of MCM7 oncoprotein

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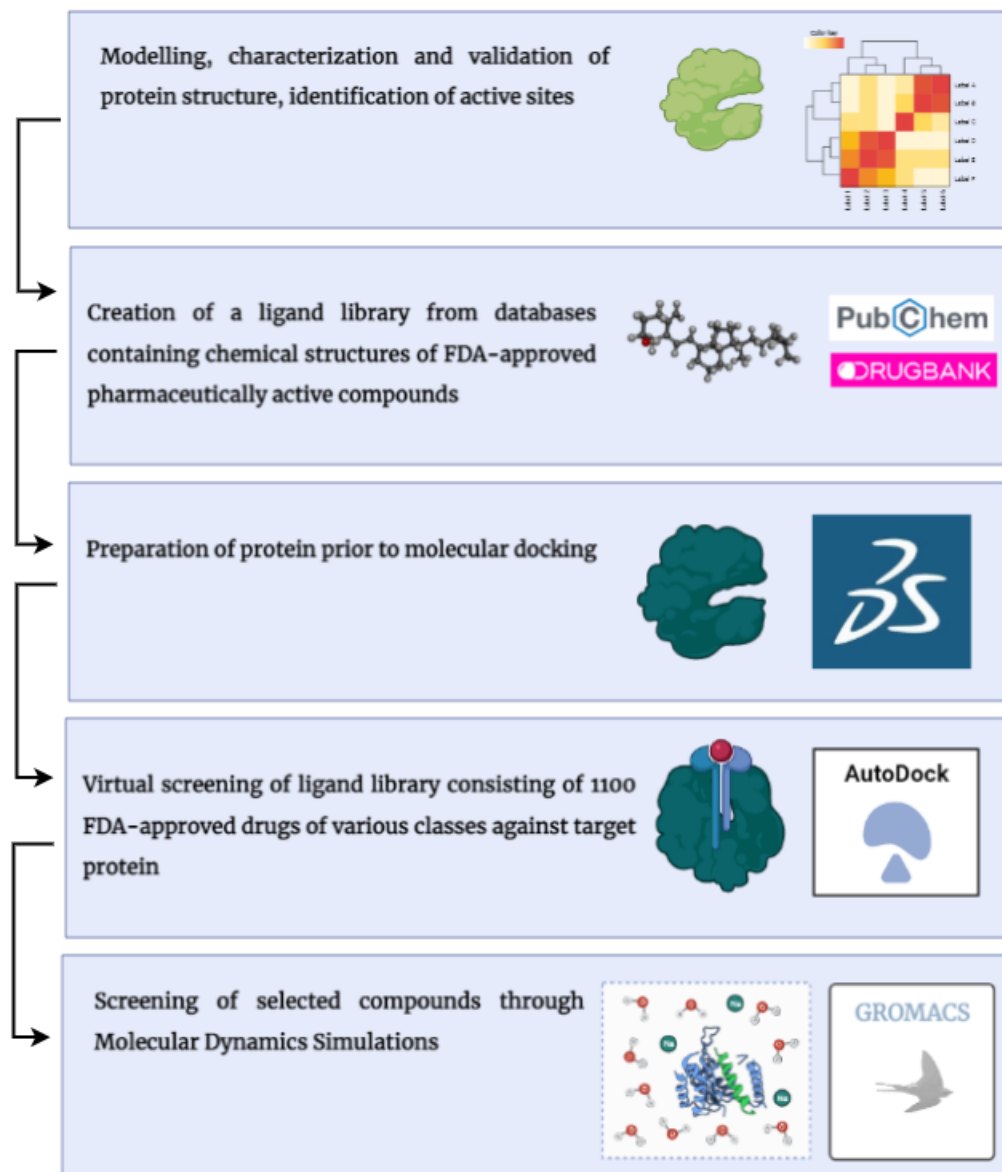
Figure S1: Illustration of the research pipeline for the present study

SOPMA :
Alpha helix   (Hh) :   357 is 49.65%
3₁₀ helix   (Gg) :   0 is   0.00%
Pi helix   (Ii) :   0 is   0.00%
Beta bridge   (Bb) :   0 is   0.00%
Extended strand   (Ee) :   99 is 13.77%
Beta turn   (Tt) :   31 is   4.31%
Bend region   (Ss) :   0 is   0.00%
Random coil   (Cc) :   232 is 32.27%
Ambiguous states (?) :   0 is   0.00%
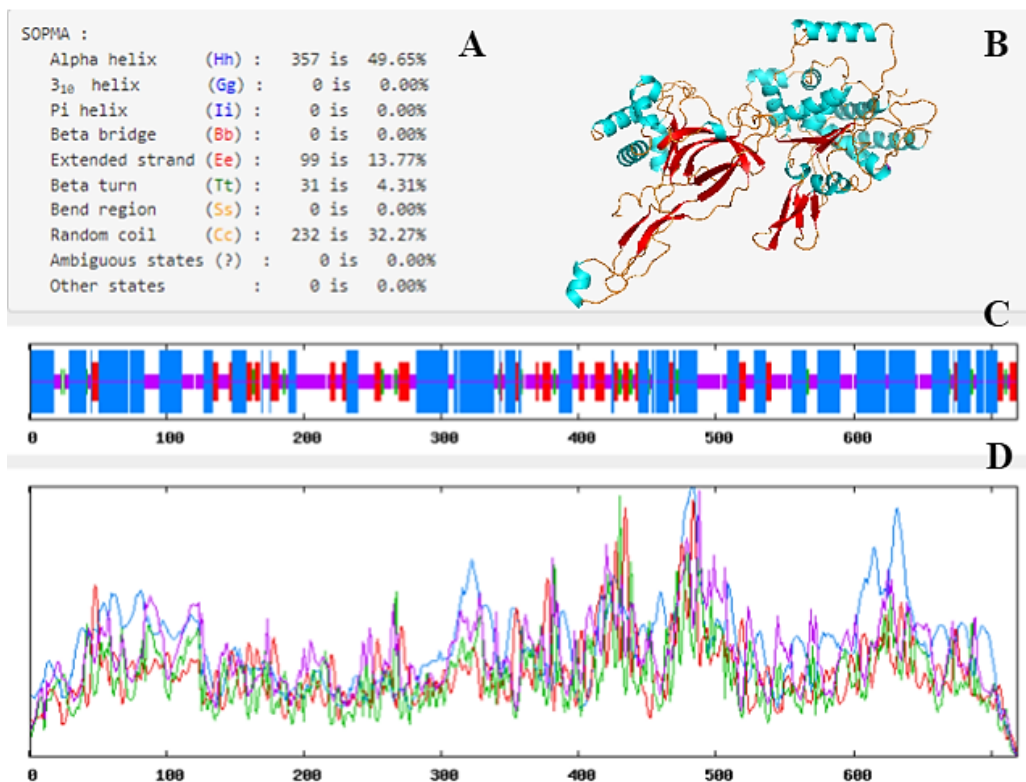Other states   :   0 is   0.00%

Figure S2: SOPMA analysis results reveal the percentage of helices, turns, and loops constituting the secondary structure of MCM7.
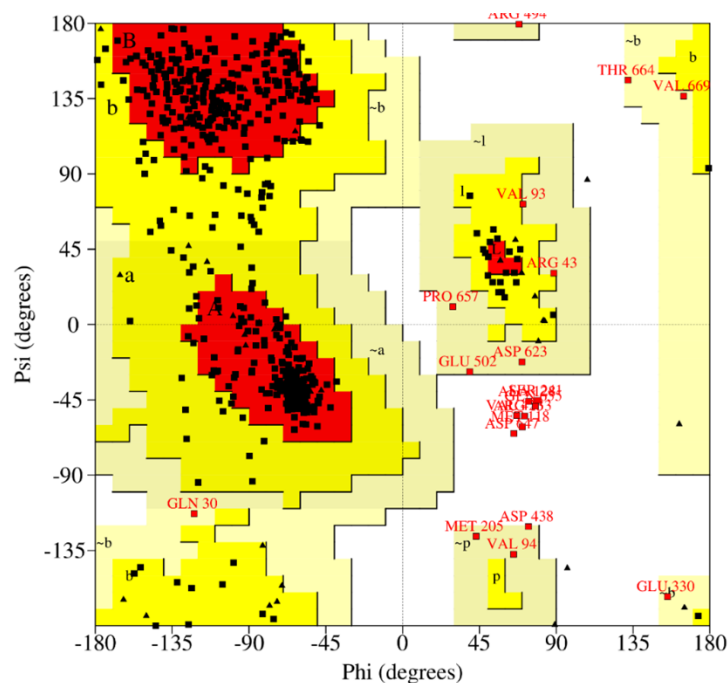

Figure S3: Ramachandran plot illustrating the stereochemical geometry of the predicted model of MCM7 for structure validation

Table S1: List of the average distance between ligand atom and the side chain of the protein residue involved in each of the observed π-alkyl and alkyl-alkyl interactions obtained from the MD simulation

Compound Name	Interaction type	Residues	Distance (Å)
Ergocalciferol	Alkyl	*Tyr 345*	4.32± 1.2
	Pi-Alkyl	*Tyr 539*	3.58±0.8
Cholecalciferol	Alkyl	*Tyr 539*	4.78±1.3
	Pi-Alkyl	*Pro 548*	6.2±2.0
Ergosterol	Alkyl	*Ala 338*	7.6±1.6
	Pi-Alkyl	*Tyr 345*	5.6±0.2
Menaquinone	Alkyl	*Ala 338*	3.6±0.9
	Alkyl	*Pro 547*	5.4±1.06
	Alkyl	*Pro 548*	5.08±0.6
	Pi-sigma	*Phe 551*	8.0±0.93