Supplementary Materials

Discovery of hordenine as a potential inhibitor of pyruvate dehydrogenase kinase 3: Implication in lung cancer therapy

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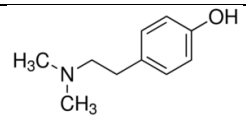
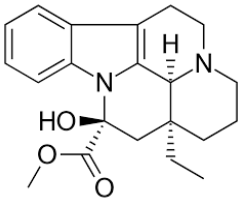
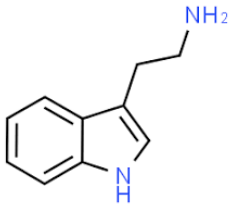
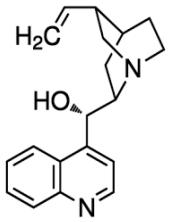
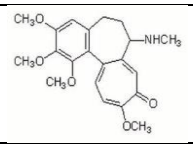
Table S1. Binding parameters of screened natural compounds with PDK3 obtained from molecular docking and fluorescence binding studies.

S.No.	NAME OF THE COMPOUND/LIGAND	CHEMICAL STRUCTURE	PUBCHEM cID	ΔG # (kcal/mol)	Binding constant* (K) M^{-1}
1	Hordenine		68313	–7.1	0.5 X10^6
2	Vincamine		15376	–6.9	NA
3	Tryptamine		1150	–7.1	NA
4	Cinchonine		90454	–8.1	NA
5	Colcemid		2832	–7.0	2.02 X 10^3

#Binding affinity of the selected compounds with PDK3 predicted through Molecular docking. *Binding constant calculated from fluorescence studies. Binding constant values could not be predicted in some cases and mentioned as not applicable (NA).