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Polyphenol MHQP as an allosteric inhibitor of Kinesin-5: Cease the molecular catwalk of "Drunken Sailor"

Manjari Shukla, Sushobhan Maji, Keshav Rajarshi & Sudipta Bhattacharyya*

Department of Bioscience & Bioengineering, Indian Institute of Technology, Jodhpur-342 030, Rajasthan, India

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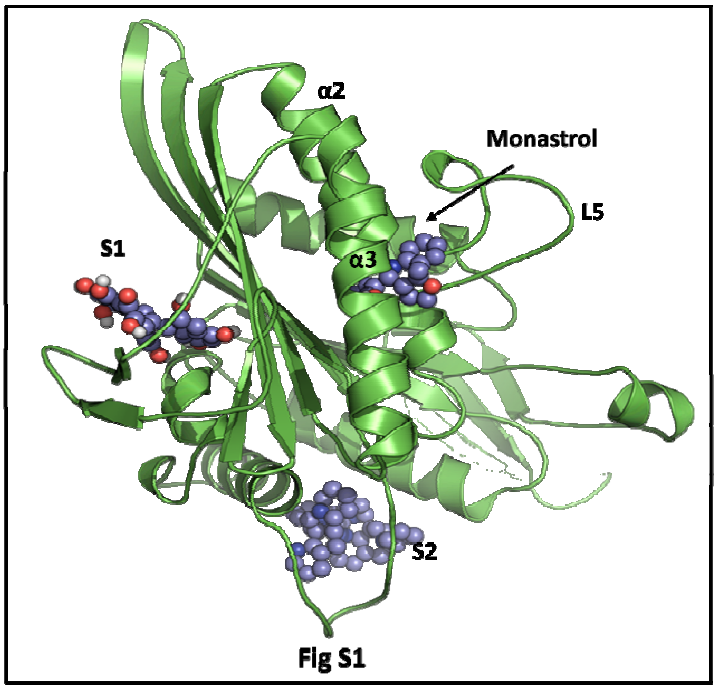
Supplementary Data

Table

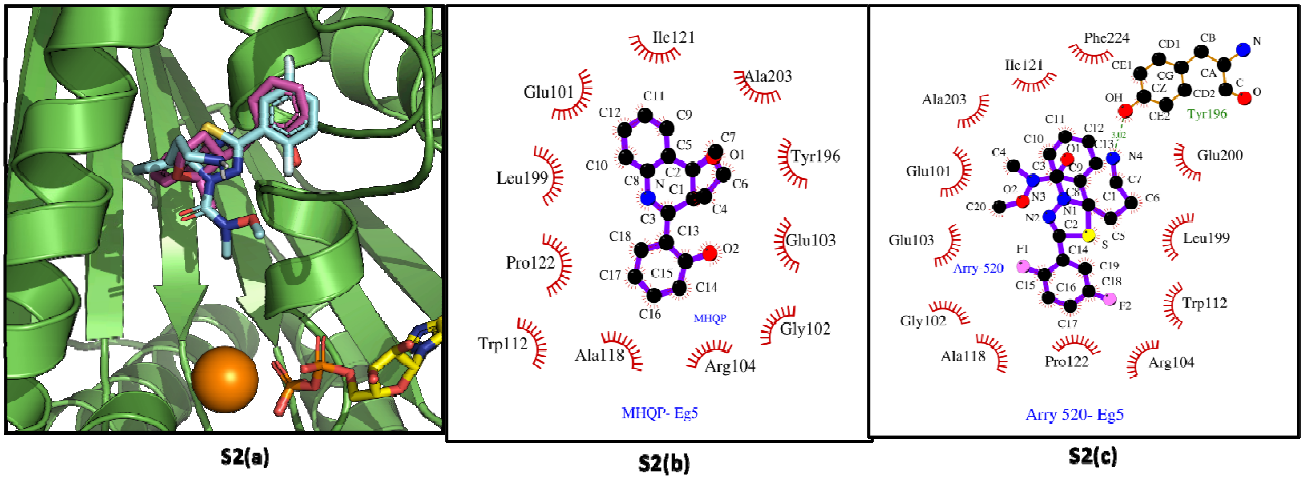
Suppl. Table 1 —*In silico* molecular docking based free energy of binding scores of selected compounds with Kinesin Eg5 motor domain

Sr. No.	Compound Name (PubChem Id)	Chemical Class	Binding site	Binding energy (ΔG) (Kcal/mol)
1	Amentoflavone[5281600]	Biflavonoid	S2	-10.1
2	Theaflavin[135403798]	Polyphenol	S1	-9.3
3	U-74389G[104934]	Aminosteroids	S2	-9.4
4	Ormosinine[90478901]	Alkaloid	Monastrol	-10.1
5	Fumariline[159888]	Alkaloid	Monastrol	-10.3
6	3,3'-Biplumbagin[183757]	Quinones	Monastrol	-10.5
7	Ararobinol[438692]	Anthraquinone	S2	-10.3
8	4,4',4",4'"-(Ethane-1,1,2,2-tetrayl)tetraphenol[82180]	Phenol	Monastrol	-8.2
9	2-Methyltetrahydrofuran-3-one[18552]	Phenol	Monastrol	-10
10	2-[5-(4-fluorophenyl)-1-phenyl-4,5-dihydro-1H-pyrazol-3-yl]phenol[3716559]	Phenol	Monastrol	-9.2
11	2-(9b-methyl-2,3,3a,4,5,9b-hexahydrofuro [3,2-c]quinolin-4-yl)phenol [117066418]	Phenol	Monastrol	-10.6

Figures



Suppl. Fig. S1 — Kinesin Eg5 crystal structure (PDB Id: 2PG2) showing allosteric binding sites, Monastrol binding site (formed by L5/α2/α3), S1 and S2



Suppl. Fig. S2 — Comparison of the binding site of Eg5 docked with Arry-520 and with MHQP in the presence of ADP S2(A) The Eg5 docked with MHQP in the presence of ADP has been super imposed with the co-crystallized structure of Eg5 in the presence of Arry-520; S2(B) The 2D interaction profile of MHQP with Eg5; and S2(C) 2D interaction profile of Arry-520 with Eg5