

## Supplementary material:

**Table 1:** RMSD matrix showing the values generated from super imposition of kinase domains of HKs by MATRAS tool. The values are the determinants of identity among kinase domains of four HKs.

<b>HK1</b>	<b>0.000</b>	<b>0.588</b>	<b>0.674</b>	<b>0.650</b>
<b>HK2</b>	<b>0.588</b>	<b>0.000</b>	<b>0.233</b>	<b>0.520</b>
<b>HK3</b>	<b>0.674</b>	<b>0.233</b>	<b>0.000</b>	<b>0.561</b>
<b>HK4</b>	<b>0.650</b>	<b>0.520</b>	<b>0.561</b>	<b>0.000</b>

**Table 2:** Molecular docking of ATP into the kinase domains of HKs

Hexokinase	Docking score	No. of H-Bonds	Interacting residues	H-bond length (Å)
HK1	-12.417	6	G170	2.6
			K621	3.0
			S682	2.8
			S682	2.8
			S682	2.9
			E742	2.9
HK2	-12.2306	3	H504	2.4
			Q608	2.8
			N609	2.5
HK3	-12.6445	5	T626	2.2
			R520	3.0
			L623	2.7
			N624	2.6
			N624	2.9
HK4	-13.1834	2	H156	1.8
			E157	2.5