

Supplementary Information

Molecular Docking-Guided Screening of Phytoconstituents from *Artemisia princeps* as Allosteric Glucokinase Activators

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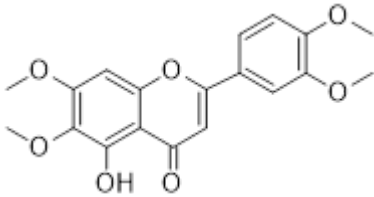
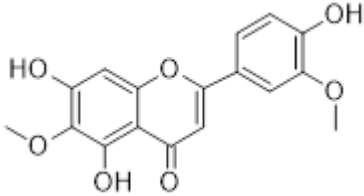
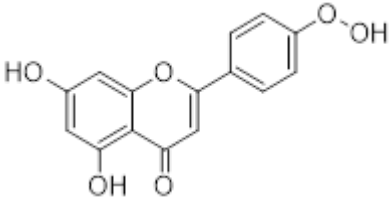
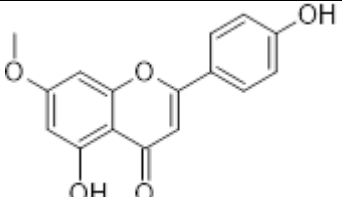
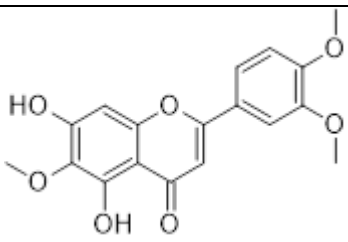
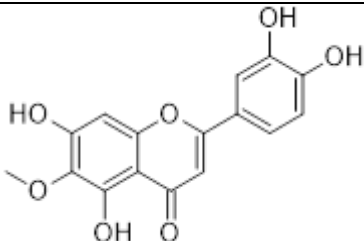
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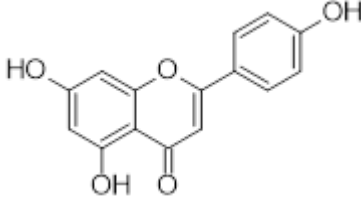
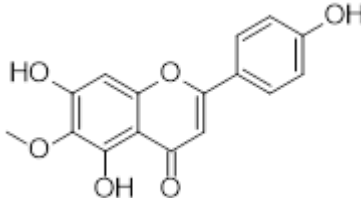
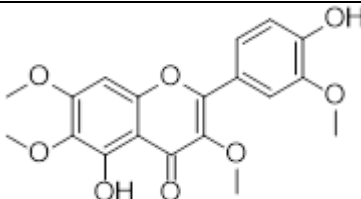
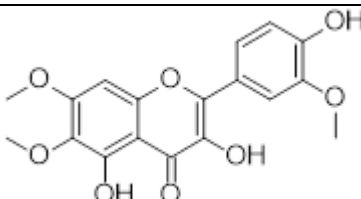
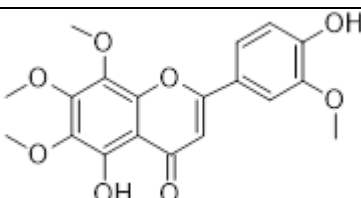
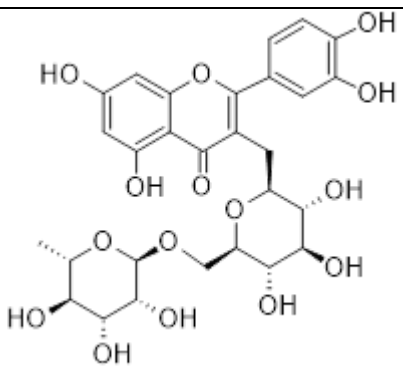
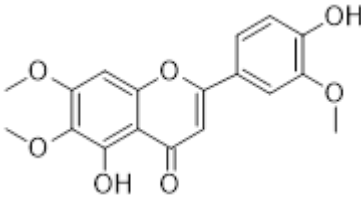
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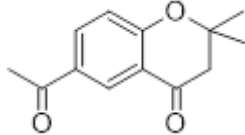
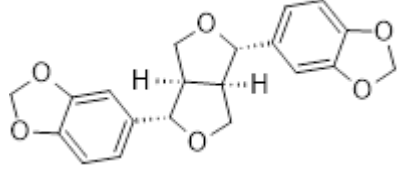
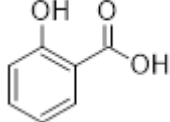
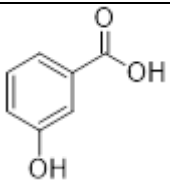
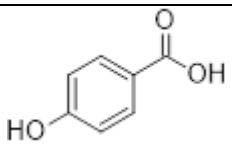
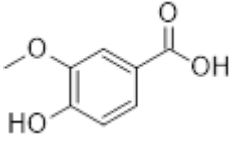
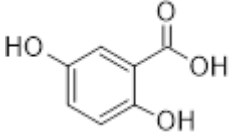
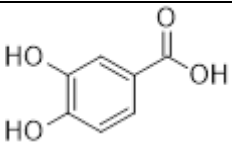
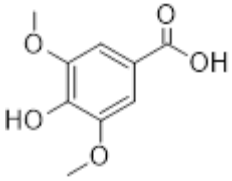
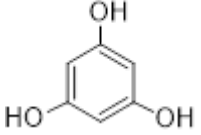
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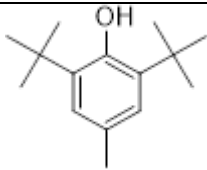
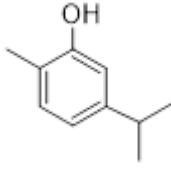
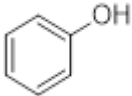
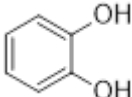
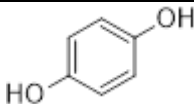
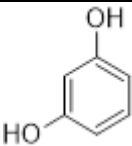
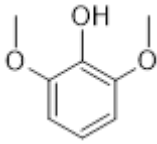
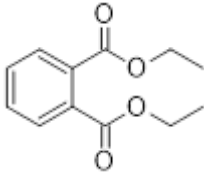
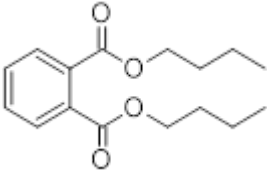
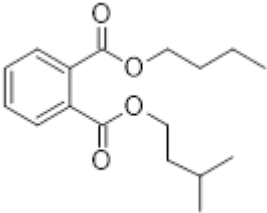
Supplementary Tables

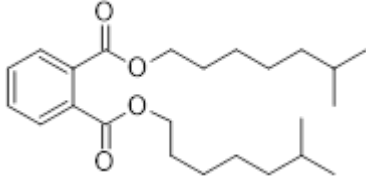
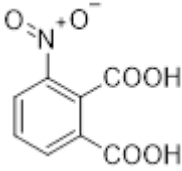
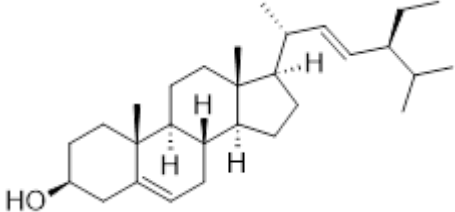
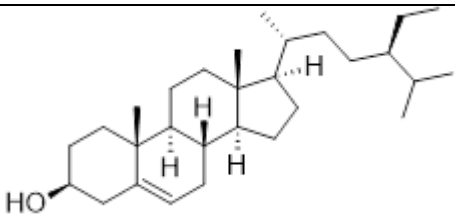
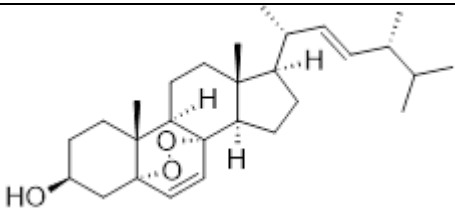
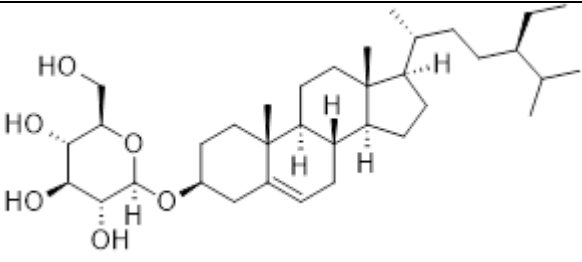
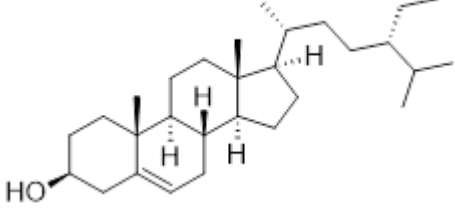
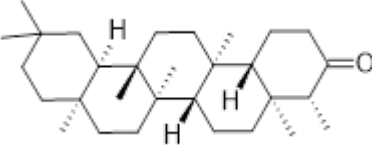
Table S1. List of phytoconstituents selected for the *in silico* docking studies against the GK enzyme.

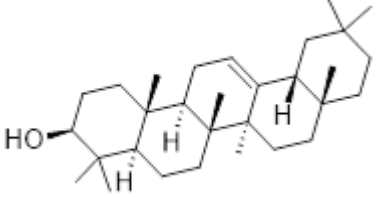
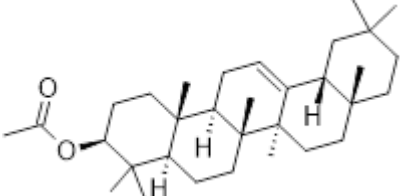
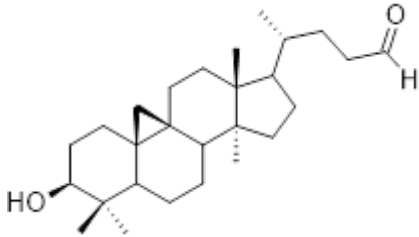
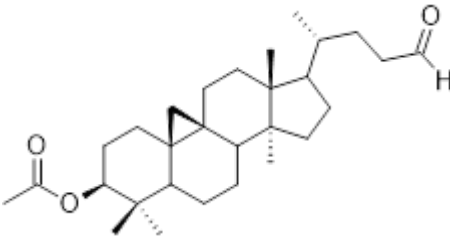
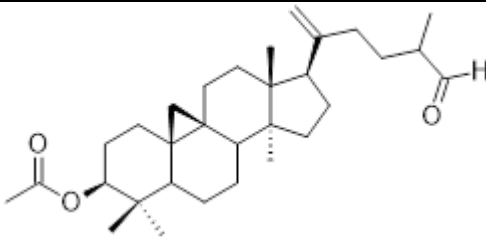
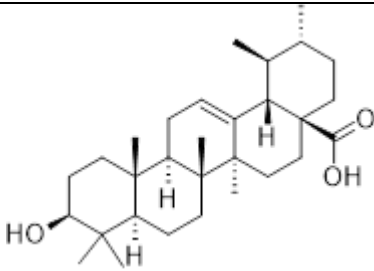
Sr. No.	Compound	Category	Structure
1	5-Desmethyl-sinensetin	Flavanone	
2	Jaceosidin	Flavonoids	
3	Acacetin	Flavonoids	
4	Genkwanin	Flavonoids	
5	Eupatilin	Flavonoids	
6	Eupafolin	Flavonoids	

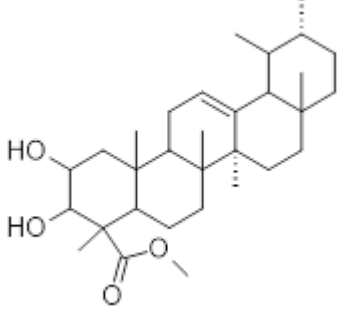
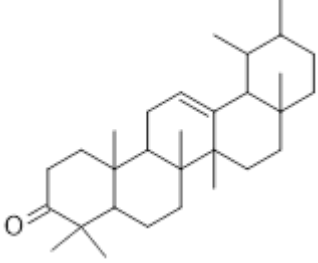
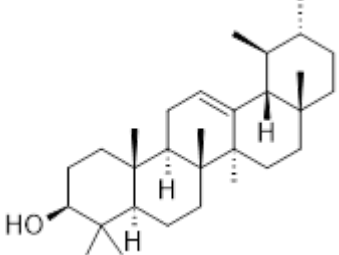
7	Apigenin	Flavonoids	
8	Hispidulin	Flavonoids	
9	Chrysopenetin	Flavonoids	
10	3,5,4'-Trihydroxy-6,7,3'-trimethoxy flavone	Flavonoids	
11	5,4'-Dihydroxy-6,7,3',5'-tetramethoxyflavone	Flavonoids	
12	Rutin	Flavonoids	
13	5,4'-Dihydroxy-6,7,3'-trimethoxyflavone	Flavonoids	

14	6-Acetyl-2,2-dimethylchroman-4-one	Flavonoids	
15	Sesamin	Lignans	
16	Salicylic acid	Phenolic acids	
17	m-Hydroxy benzoic acid	Phenolic acids	
18	p-Hydroxy benzoic acid	Phenolic acids	
19	Vanillic acid	Phenolic acids	
20	Gentisic acid	Phenolic acids	
21	Protocatechuic acid	Phenolic acids	
22	Syringic acid	Phenolic acids	
23	Phloroglucinol	Phenols	

24	6-Methyl-3-isopropylphenol	Phenols	
25	2,6-Di-tert-butyl-4-methylphenol	Phenols	
26	Phenol	Phenols	
27	1,2-Benzenediol (catechol)	Phenols	
28	1,4-Benzenediol (hydroquinone)	Phenols	
29	1,3-Benzenediol (resorcinol)	Phenols	
30	2,6-Dimethoxy phenol	Phenols	
31	Diethyl phthalate	Phthalates	
32	Dibutyl phthalate	Phthalates	
33	Butyl isobutyl phthalate	Phthalates	

34	Diisooctyl phthalate	Phthalates	
35	3-Nitrophthalic acid	Phthalates	
36	Stigmasterol	Steroids	
37	β -Sitosterol	Steroids	
38	Ergosterol peroxide	Steroids	
39	Daucosterol	Steroids	
40	γ -Sitosterol	Steroids	
41	Friedelin	Triterpenes	

42	β -Amyrin	Triterpenes	
43	β -Amyrin acetate	Triterpenes	
44	Wrightial	Triterpenes	
45	Wrightial acetate	Triterpenes	
46	27-Norcycloart-20(21)-ene-25-al-3 β -ol acetate (sajabalal acetate)	Triterpenes	
47	Ursolic acid	Triterpenes	

48	Methyl commateD	Triterpenes	
49	3-Keto-urs-12-ene	Triterpenes	
50	α -Amyrin (viminalol)	Triterpenes	

Supplementary Figures

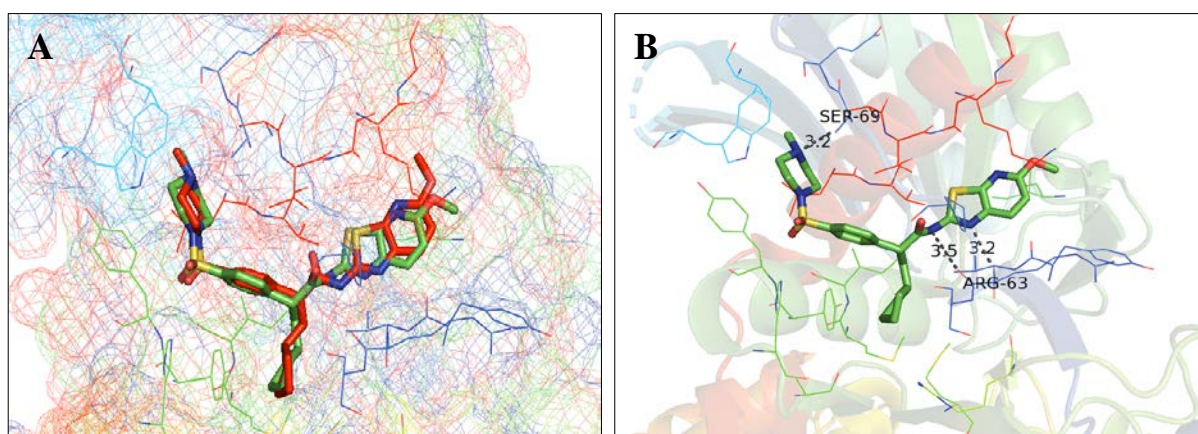


Figure S1. A. Overlay of the docked pose of the 3IMX ligand (green sticks) on that produced by the co-crystallized ligand (red sticks) in the allosteric site of GK. B. Docked pose showing hydrogen bond interactions of the 3IMX ligand (reference GK activator) with allosteric site residues of GK protein.

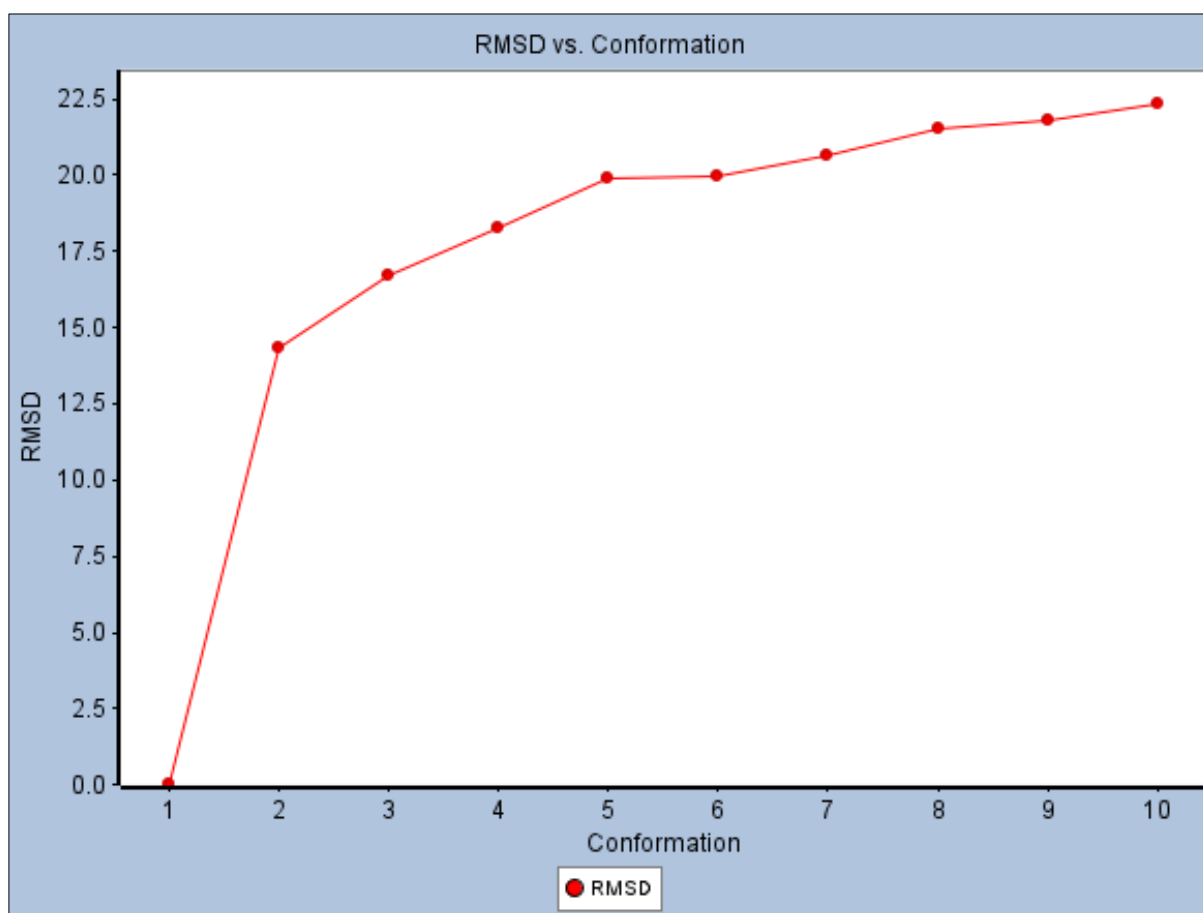


Figure S2. In between each confirmation with respect to the RMSD (molecular dynamics simulation).

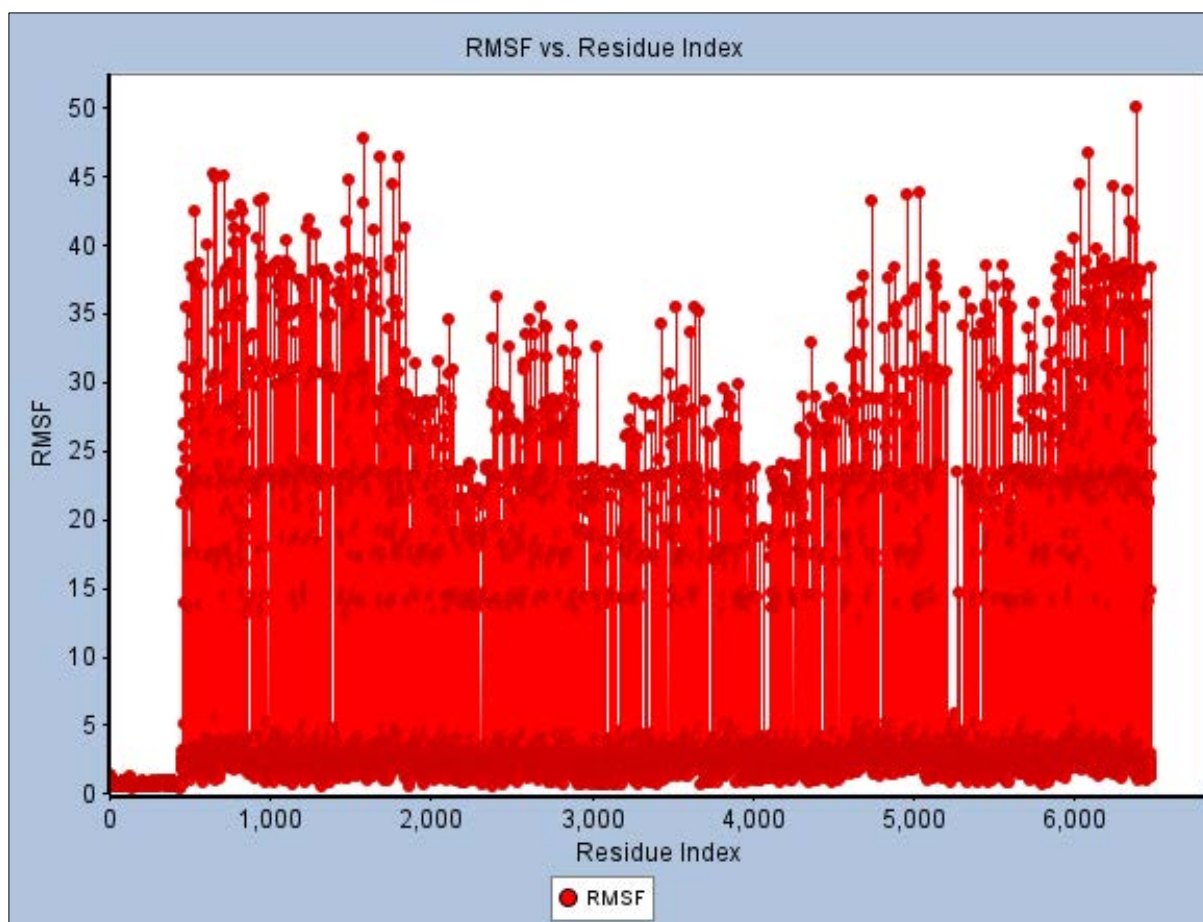


Figure S3. The root mean square fluctuation (RMSF) with respect to each residue (molecular dynamics simulation).