

Supplementary material:

Table 1: Docking results of Natural Compounds with HBx: Natural compounds derived from plants: illustrate minimum free energy required for hydrogen bonding.

S.N.	Natural Compounds	MolDock Score	HBond	Amino acid residues involved in protein-ligand interactions
1	Rutin	-161.65	-10.93	LEU5, ASP48, GLY50, HIS52, LEU93, LYS95, LYS96
2	Bilobatin	-157.37	-6.59	LEU5, HIS52, ALA70, ARG72, THR97
3	Curcumin	-138.55	-2.73	LEU71, SER104
4	Oleanoic acid	-124.15	-2.46	LEU5, SER104
5	Betulinic acid	-127.47	-0.10	SER104
6	Ellagic acid	-99.88	-11.21	LEU71, ARG72, LYS95, THR97, GLY99, SER104
7	Luteoline	-89.42	-7.30	ARG72, SER75, LYS95, THR97
8	Resveratrol	-85.23	-4.48	LEU5, ASP48, GLY50, ALA51, HIS52, LYS96,

Table 2: Docking results of Rutin and its derivative's with HBx protein of HBV: illustrate minimum free energy required for hydrogen bonding

S.N.	Compounds	R ₁	R ₂	R ₃	R ₄	R ₅	R ₆	R ₇	R ₈	R ₉	MolDock Score	HBond	Amino acid residues involved in protein-ligand interactions
1	Rutin	H	OH	H	OH	H	H	OH	OH	H	-161.65	-10.93	LEU5, ASP48, GLY50, HIS52, LEU93, LYS95, LYS96
2	Rutin01	CH ₃	OH	H	OH	H	H	OH	OH	H	-163.16	-13.32	LEU5, PRO42, ALA70, ARG72, LEU93, LYS96, SER104
3	Rutin02	H	CH ₃	H	OH	H	H	OH	OH	H	-159.79	-13.56	LEU5, VAL92, LYS95, LYS96, THR97, LEU98
4	Rutin03	H	OH	CH ₃	OH	H	H	OH	OH	H	-145.14	-11.13	ALA70, VAL92, LYS95, LEU98
5	Rutin04	H	OH	H	CH ₃	H	H	OH	OH	H	-154.96	-12.79	LEU5, PRO46, ASP48, ALA70, VAL92, LYS96, THR97
6	Rutin05	CH ₃	OH	H	CH ₃	H	H	OH	OH	H	-157.06	-09.51	LEU5, PRO46, THR97, SER104
7	Rutin06	H	CH ₃	H	CH ₃	H	H	OH	OH	H	-109.76	-13.97	LEU5, PRO46, ALA70, ARG72, VAL92, LYS96, THR97
8	Rutin07	CH ₃	OH	H	CH ₃	H	H	OH	OH	H	-159.15	-14.71	ALA70, ARG72, VAL92, LYS95, THR97, LEU98
9	Rutin08	CH ₃	H	OH	CH ₃	H	H	OH	OH	H	-165.76	-11.40	LEU5, ARG72, LEU93, LYS96, LEU98
10	Rutin09	OH	OH	H	OH	H	H	OH	OH	H	-149.22	-11.15	ALA70, VAL92, LYS95, LEU98, THR97
11	Rutin10	H	OH	H	OH	H	H	OH	OH	H	-156.96	-06.62	LEU5, LYS96, LEU98, SER104
12	Rutin11	H	H	OH	OH	H	CH ₃	OH	OH	H	-139.00	-17.65	LEU5, ASP48, ALA70, LYS95, LYS96, THR97, LEU98
13	Rutin12	H	OH	H	OH	H	H	OH	OH	CH ₃	-139.44	-11.90	LEU5, ALA51, LYS95, LYS96, THR97
14	Rutin13	H	OH	H	OH	H	H	OH	CH ₃	H	-155.55	-14.45	LEU5, ALA70, LEU98, GLY99, SER104
15	Rutin14	H	OH	H	OH	H	H	CH ₃	OH	H	-156.65	-15.98	LEU5, ALA70, THR97, GLY99, SER104
16	Rutin15	H	OH	H	OH	CH ₃	H	OH	OH	H	-149.60	-11.55	PRO46, SER47, LYS95, THR97, LEU98
17	Rutin16	NH ₂	OH	H	OH	H	H	OH	OH	H	-163.95	-13.01	LEU5, PRO46, GLY67, LEU93, LYS95, LYS96
18	Rutin17	H	OH	NH ₂	OH	H	H	OH	OH	H	-148.62	-17.58	LEU5, ALA51, ALA70, VAL92, LYS95, LEU93, THR97, LEU98
19	Rutin18	H	OH	H	NH ₂	H	H	OH	OH	H	-152.44	-19.05	LEU5, VAL92, LEU93, LYS96, LEU98, THR97
20	Rutin19	H	NH ₂	H	OH	H	H	OH	OH	H	-120.55	-16.26	LEU5, PRO46, LYS96, THR97, LEU98, SER104
21	Rutin20	NH ₂	OH	NH ₂	OH	H	H	OH	OH	H	-144.72	-09.91	LEU5, PRO42, THR97, SER104