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Supplementary Material:

Table 1: The ligands were taken from the plant *Momordica charantia*. The molecular weights are calculated and given in column 4. The ligands that show passing Lipinski's filter based on colors in column 5 and bioavailabilty in column 6.

Sl.no.	Compound Name	IUPAC Name	Molecular Weight	Lipinki's Filter	Bioavailability
1	Charantin	(2S, 3R, 4R, 6R)-5(10.13-dimethyl-17-(6-methylheptan-2-yl)-hexadecahydro-1H-cyclopenta[a]phenathren-3-yloxy)-6-(hydroxymethyl)-tetrahydro-2H-pyran-2,3,4,5-tetracol	574.83	Blue	Red (Six)
2	Momordenol	17-(5-ethyl-6-methylheptan-2-yl)-3-hydroxy-9, 13-dimethyl-1,3,4,7,8,10,11,13,17-decahydro-2H-cyclopenta[a]-16(9H)-one	426.35	Blue	Red (Six)
3	Momordicilin	(E)-4-((2-hydroxyhex-3-en-2-yloxy)methyl)-4,6a,6b,8a,11,12,14b-heptamethyl-octadecahydropicen-3(4H.6bH,14bH)-one	540.86	Yellow	Red (Five)

Table 2: The active site of the receptor (1Q5K), the grid values taken for docking study and the minimum binding energy of the ligands.

Active Site	Residues	Center of Grid Value	Minimum Binding Energy (kcal/mol) of the Selected Compounds		
			Charantin,	Momordenol	Momordicilin
H1	IGNGGVVKQNCD	20.411, 27.175, 11.723	-2.67	-3.92	-4.81
H2	LDPVDPPALHAR	29.722, 30.136, -17.358	-2.95	-3.92	-3.64
H3	QPIFEKVHKVF	38.201, 49.261, 12.182	-3.05	-3.56	-5.48
H4	LHTSSIVRLTPP	15.615, 47.909, -1.702	-2.50	Nil	Nil
H5	VLGQWCSRLEY	29.722, 57.083, 3.762	-2.57	-3.31	-4.22
H6	FKLQKNRELFGS	8.603, 31.714, 13.371	-2.75	-3.50	-4.72
H7	VYRARHSRYGQPE	34.920, 34.918, 12.531	-4.25	-4.06	-4.08
H8	PIFGGVEF	20.499, 54.988, 20.671	-2.42	-4.06	-4.08