



Summarized table Shows the molecular docking analysis results for ligands against proteins, including binding energy, Number of Hydrogen bonds and interacting residues of ligand and receptor.

Protein Name	Ligand Name	Binding Energy (kcal/mol)	No. of H Bonds	Interacting residue
5HRC 3C-Like Protease (3CL-pro)	Baicalin	-5.97	02 H1:Distance= 1.75 Å, H2:Distance= 2.76 Å	LEU220(H1), ARG217(H2)
	Quercetin	-7.02	04 H1:Distance= 2.74 Å,H2: Distance=3.18 Å,H3: Distance= 2.88 Å,H4: Distance=2.59 Å	THR190(H1), GLU166(H2), LEU141(H3), SER144(H4)
	Luteolin	-5.24	05 H1:Distance= 2.11 Å, H2: Distance=3.25 Å,H3: Distance= 2.30 Å,H4: Distance= 2.67 Å,H5: Distance=3.20 Å	ARG188(H1), GLU166(H2), SER144(H3), LEU141(H4), GLY143(H5)
	Rutin	-2.65	03 H1:Distance= 2.26 Å, H2:Distance= 1.75 Å, H3:Distance= 2.05 Å	THR280(H1), GLY215(H2), ASP216(H3)
	Hesperidin	-3.46	03 H1:Distance= 2.19 Å,H2: Distance=2.00 Å,H3: Distance=2.08 Å	VAL125(H1), ARG4(H2), GLN127(H3), SER139, TYR126
	Curcumin	-6.18	02 H1:Distance= 2.80 Å,H2: Distance=2.12 Å	SER144(H1), LEU141(H2), GLN189, PHE140, ASN142
	EGCG	-4.49	03 H1:Distance= 2.60 Å,H2: Distance=2.91 Å,H3: Distance=3.68 Å	THR190(H1), GLU166(H2), CYS145(H3), PRO168
	Piperine	-4.72	01 H1:Distance= 3.69 Å	CYS145(H1), ASN142, PRO168, LEU167
	Glycyrrhizin	-6.55	02 H1:Distance= 2.60 Å,H2: Distance=2.91 Å	GLU14(H1), LYS100(H2), LYS12
6VYB Spike Glycoprotein 6LYEST	Baicalin	-6.82	02 (H1:Distance= 2.61 Å), (H2:Distance= 1.96 Å)	SER50(H1), LEU48(H2), LYS304
	Quercetin	-6.06	01 (H1:Distance= 2.15 Å)	GLY526(H1)
	Luteolin	-6.72	01 (H1:Distance= 1.72 Å)	SER1037(H1)
	Rutin	-3.09	04 (H1:Distance= 3.20 Å) H2:Distance= 2.50 Å H3:Distance= 3.04 Å) H4:Distance= 2.48 Å)	GLN564(H1), ASP578(H2), THR523(H3), ASN360(H4), PRO579



VEDICINALS INDIA PRIVATE LIMITED

	Hesperidin	-4.52	04 (H1:Distance= 2.22 Å,H2: Distance=2.61 Å,H3: Distance=2.42 Å, H4: Distance=2.50 Å)	PHE515(H1), ARG355(H2),GLU516(H3), PRO463(H4)
	Curcumin	-4.90	02 (H1:Distance= 1.83 Å,H2: Distance=2.91 Å)	GLY1093(H1), ARG1107(H2), ALA706, SER711
	EGCG	-5.43	04 (H1:Distance= 2.69 Å,H2: Distance=2.43 Å, H3: Distance=3.23 Å,H4: Distance=2.36 Å)	PHE898(H1), THR883(H2), GLN895(H3), ASP796(H4)
	Piperine	-5.23	01 (H1:Distance= 2.92 Å)	ASN544(H1), LEU546, PHE565
	Glycyrrhizin	-9.42	03 (H1:Distance= 2.80 Å,H2: Distance= 3.28 Å, H3: Distance= 2.53 Å)	LYS378(H1), THR376(H2), VAL503(H3), TYR508
6X6P Envelope Glycoprotein	Baicalin	-6.41	02 (H1:Distance= 3.33 Å,H2:Distance= 2.73 Å)	ASN1108(H1), TYR1047(H2), LYS1038
	Quercetin	-6.51	02 (H1:Distance= 2.25 Å,H2:Distance= 2.52 Å)	VAL362(H1), LEU368(H2), GLY339
	Luteolin	-6.74	01 (H1:Distance= 3.22 Å)	SER371(H1), PHE338,
	Rutin	-3.87	05 (H1:Distance= 2.37 Å,H2:Distance= 3.16 Å, H3:Distance= 2.36 Å, H4:Distance= 3.25 Å, H5:Distance= 2.49 Å)	ASP428(H1), THR430(H2), PHE464(H3), TYR396(H4), PRO463(H5)
	Hesperidin	-4.15	02 (H1:Distance= 2.89 Å,H2: Distance=2.70 Å)	LYS1038(H1), GLN1036(H2), TRP886
	Curcumin	-4.70	01 (H1:Distance= 3.16 Å)	THR1077(H1), PRO1089, PRO1079, ILE1130
	EGCG	-4.91	03 (H1:Distance= 3.15 Å,H2: Distance=2.80 Å, H3: Distance= 2.18 Å)	SER530(H1), LYS529(H2), GLY526(H3), PRO527
	Piperine	-5.44	01 (H1:Distance= 3.11 Å)	ARG567(H1), HIS519, PHE559
	Glycyrrhizin	-9.02	04 (H1:Distance= 3.10 Å,H2: Distance= 2.98 Å, H3: Distance= 3.31 Å, H4: Distance= 2.22 Å)	ASN61(H1), ARG634(H2), ARG237(H3), VAL83(H4), PRO85
	6M3M Nucleocapsid Protein	Baicalin	-5.90	02 (H1:Distance= 2.76 Å,H2:Distance= 2.50 Å)
Quercetin		-5.91	04	ASN155(H1), HIS146(H2), ASN76(H3), ASN78(H4)



VEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 2.25 Å,H2:Distance= 2.52 Å, H3:Distance= 2.25 Å,H4:Distance= 2.52 Å)	
	Luteolin	-5.67	02 (H1:Distance= 2.19 Å) (H2:Distance= 1.84Å)	ALA157(H1), ASN78(H2)
	Rutin	-3.01	03 (H1:Distance= 2.00 Å) H2:Distance= 3.01 Å) H3:Distance= 2.28 Å)	ASN155(H1), ASN78(H2), THR77(H3)
	Hesperidin	-3.64	03 (H1:Distance= 2.18 Å,H2: Distance=2.86 Å, H3: Distance= 3.12 Å)	THR166(H1), TYR173(H2), ALA174(H3), LYS170, THR167
	Curcumin	-5.14	03 (H1:Distance= 2.54 Å,H2:Distance= 3.01 Å, H3:Distance= 2.50 Å)	ASN141(H1), GLY117(H2), THR149(H3), GLY148
	EGCG	-5.11	03 (H1:Distance= 2.77 Å,H2: Distance= 1.97 Å, H3: Distance= 2.86 Å)	ASN78(H1), THR77(H2), ALA156(H3), ASN155
	Piperine	-5.52	01 (H1:Distance= 2.85 Å)	LYS128(H1), TRP133
	Glycyrrhizin	-7.20	02 (H:Distance= 3.08 Å,H2:Distance= 3.18 Å)	ARG89(H1), ARG150(H2), ALA91, PRO118, TYR110, ALA51,
6W9C Papain-Like Protease (PL- pro)	Baicalin	-5.92	01 (H1:Distance= 3.30 Å)	TYR95(H1), PRO96, LYS105
	Quercetin	-5.64	02 (H1:Distance= 2.59 Å, H2:Distance= 2.23 Å)	LYS306(H1), THR259(H2)
	Luteolin	-6.30	03 (H1:Distance= 3.26 Å, H2:Distance= 2.47 Å, H3:Distance= 2.13 Å)	LYS94(H1), TYR95(H2), LYS91(H3), GLY142
	Rutin	2.83	02 (H1:Distance= 2.57 Å, H2:Distance= 1.96 Å)	ASP164(H1), THR301(H2)
	Hesperidin	-4.06	02 (H1:Distance= 1.80 Å, H2:Distance= 1.76 Å)	LYS306(H1), GLY256(H2), HIS255, LYS279,
	Curcumin	-5.80	01 (H1:Distance= 2.39 Å)	GLU252(H1), LEU253, TYR251, PHE258, GLY256
	EGCG	-4.81	03 (H1:Distance= 2.09 Å, H2:Distance= 2.82 Å, H3:Distance= 3.18 Å)	SER278(H1), LYS306(H2), THR259(H3)
	Piperine	-5.32	02 (H1:Distance= 2.96 Å, H2:Distance= 2.60 Å)	THR259(H1), LYS306(H2)
	Glycyrrhizin	-7.05	03	LYS53(H1), ASN88(H2), LYS92(H3)



VEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 2.91 Å, H2:Distance= 2.88 Å, H3:Distance= 2.82 Å)	
7BV2 Rna- DependantRna Polymerase (RdRp)	Baicalin	-6.47	02 (H1:Distance= 3.03 Å, H2:Distance= 2.32 Å)	ASN543(H1), SER501(H2), GLY559, GLY683
	Quercetin	-5.93	03 (H1:Distance= 2.96 Å, H2:Distance= 2.05 Å, H3:Distance= 3.01 Å)	THR319(H1), SER318(H2), ARG349(H3)
	Luteolin	-6.17	02 (H1:Distance= 2.53 Å, H2:Distance= 2.52 Å)	SER318(H1), ILE266(H2)
	Rutin	-3.96	03 (H1:Distance= 2.15 Å, H2:Distance= 2.42 Å, H3:Distance= 3.28 Å)	SER255(H1), ILE266(H2), TRP268(H3), PRO323
	Hesperidin	-4.23	02 (H1:Distance= 2.27 Å, H2:Distance= 2.16 Å, H3:Distance= 2.86 Å, H4:Distance= 2.33 Å)	THR591(H1), SER592(H2), GLY590(H3), ASP865(H4)
	Curcumin	-5.24	01 (H1:Distance= 2.73 Å)	LEU270(H1), ALA383, PRO328
	EGCG	-5.40	03 (H1:Distance= 1.82 Å, H2:Distance= 2.72 Å, H3:Distance= 2.14 Å)	PRO323(H1), VAL398(H2), LEU270(H3), THR324
	Piperine	-6.37	02 (H1:Distance= 3.07 Å, H2:Distance= 3.07 Å)	LYS780(H1), ASP135(H2), CYS139, LEU142, PHE134, ALA130, TYR129
	Glycyrrhizin	-7.37	03 (H1:Distance= 2.26 Å, H2:Distance= 3.00 Å, H3:Distance= 3.38 Å)	LEU544(H1), TYR546(H2), LYS545(H3), LYS500
6WX4 Helicase Inhibitors	Baicalin	-5.92	02 (H1:Distance= 2.55 Å, H2:Distance= 1.82 Å)	GLN122(H1), SER278(H2)
	Quercetin	-5.91	03 (H1:Distance= 2.11 Å, H2:Distance= 3.21 Å, H3:Distance= 3.26 Å)	LYS91(H1), LYS94(H2), TYR95(H3)
	Luteolin	-6.38	03 (H1:Distance= 3.37 Å, H2:Distance= 3.01 Å, H3:Distance= 2.05 Å)	TYR95(H1), LYS94(H2), LYS91(H3)
	Rutin	-4.04	04 (H1:Distance= 2.79 Å) H2:Distance= 2.21 Å H3:Distance= 2.51 Å) H4:Distance= 2.39 Å)	ARG82(H1), ASP76(H2), THR75(H3), HIS73(H4)
	Hesperidin	-4.06	02 (H1:Distance= 2.41 Å, H2: Distance= 2.13 Å)	GLU143(H1), ASN146(H2)



VEDICINALS INDIA PRIVATE LIMITED

	Curcumin	-5.13	01 (H1:Distance= 2.66 Å)	SER309(H1), TYR310, HIS255, LYS279, SER278
	EGCG	-5.10	01 (H1:Distance= 1.98 Å)	ALA141(H1)
	Piperine	-5.40	01 (H1:Distance= 2.73 Å)	LYS306(H1)
	Glycyrrhizin	-7.37	02 (H1:Distance= 3.08 Å,H2: Distance= 2.19 Å)	LYS94(H1), GLN97(H2),ALA145, TYR95
6HZA Furin	Baicalin	-7.29	03 (H1:Distance= 2.49 Å,H2:Distance= 2.73 Å, H3:Distance= 2.05 Å)	LYS449(H1), TYR313(H2), TYR571(H3)
	Quercetin	-5.86	04 (H1:Distance= 2.96 Å, H2:Distance=2.69 Å, H3:Distance= 2.86 Å, H4:Distance= 2.11 Å)	GLY265(H1), ASP264(H2), ASN529(H3), ASP530(H4), SER311
	Luteolin	-6.72	04 (H1:Distance= 2.12 Å, H2:Distance= 1.95 Å, H3:Distance= 2.69 Å, H4:Distance= 3.11 Å)	SER311(H1), ALA532(H2), ASN310(H3), GLY265(H4)
	Rutin	-3.66	03 (H1:Distance= 1.95 Å) H2:Distance= 2.95 Å,H3:Distance= 2.90 Å,	GLY307(H1), ASP530(H2), ASN529(H3), TRP531
	Hesperidin	-4.47	04 (H1:Distance= 2.77 Å,H2: Distance =2.34 Å, H3: Distance=2.97 Å, H4: Distance=2.37 Å)	GLY229(H1), ASP154(H2), ASP191(H3), GLY255(H4), PRO256, TYR308, GLU236
	Curcumin	-5.47	03 (H1:Distance= 3.18 Å, H2: Distance =2.89 Å, H3: Distance=2.48 Å)	ARG490(H1), ASN529(H2), GLY527(H3), SER311, ILE312, TYR313,GLY307,
	EGCG	-5.63	03 (H1:Distance= 3.07 Å, H2:Distance= 2.32 Å, H3: Distance=2.00 Å)	GLY255(H1), ASP264(H2), TYR308(H3)
	Piperine	-6.03	01 (H1:Distance= 2.93 Å)	ARG483(H1), THR442, SER575
	Glycyrrhizin	-6.36	04 (H1:Distance= 3.04Å,H2: Distance= 2.57Å, H3: Distance= 2.56Å, H4: Distance= 2.50Å)	ARG490(H1),GLU271(H2), TYR313(H3), TYR571(H4), VAL263, ALA267, TRP531
1D3G DHODH	Baicalin	-6.7	02 (H1:Distance= 2.76 Å,H2:Distance= 2.78 Å)	LYS184(H1), GLU229(H2),
	Quercetin	-7.2	03 (H1:Distance= 2.45 Å, H2:Distance=2.28 Å, H3:Distance= 2.41 Å)	THR63(H1), LEU67(H2), LEU359(H3)



VEDICINALS INDIA PRIVATE LIMITED

	Luteolin	-7.42	04 (H1:Distance= 2.51 Å, H2:Distance= 3.08 Å, H3:Distance= 2.76 Å, H4:Distance= 2.35 Å)	SER120(H1), TYR356(H2), SER305(H3), THR357(H4)
	Rutin	-3.21	06 (H1:Distance= 2.54 Å, H2:Distance= 2.20 Å, H3:Distance= 2.56 Å, H4:Distance= 2.13 Å, H5:Distance= 2.43 Å, H6:Distance= 2.58 Å)	ASP264(H1), LEU221(H2), VAL213(H3), GLY220(H4), ALA219(H5), THR218(H6)
	Hesperidin	-4.25	03 (H1:Distance= 3.04 Å, H2: Distance =3.14 Å, H3: Distance=2.33 Å)	ARG89(H1), LYS371(H2), PHE73(H3), GLY112, PRO365
	Curcumin	-6.69	01 (H1:Distance= 3.13 Å)	TYR147(H1), LEU359, PRO364, PHE98
	EGCG	-4.73	02 (H1:Distance= 2.14 Å, H2:Distance= 2.25 Å)	ASP259(H1), ALA219(H2)
	Piperine	-8.22	01 (H1:Distance= 2.90 Å)	GLN47(H1)
	Glycyrrhizin	-6.38	02 (H1:Distance= 2.88 Å, H2: Distance= 2.57 Å)	PHE73(H1), ASP174(H2), LYS110
3SCI Angiotensin Converting Enzyme 2 (ACE2)	Baicalin	-5.56	04 (H1:Distance= 3.33 Å, H2:Distance= 2.27 Å, H3:Distance= 3.13 Å, H4:Distance= 2.89 Å)	ASN121(H1), LYS114(H2), THR118(H3), ARG115(H4)
	Quercetin	-6.64	03 (H1:Distance= 1.94 Å, H2:Distance=2.94 Å, H3:Distance= 2.13 Å)	GLN102(H1), ASN210(H2), ALA396(H3), VAL209
	Luteolin	-6.60	04 (H1:Distance= 2.66 Å, H2:Distance= 2.68 Å H3:Distance= 3.23 Å, H4:Distance= 2.75 Å)	LYS562(H1), GLU564(H2), ASN210(H3), GLN102(H4), VAL209, ALA99
	Rutin	-4.48	03 (H1:Distance= 2.35 Å) H2:Distance= 2.02 Å, H3:Distance= 2.52 Å,	PHE390(H1), ARG393(H2), LEU100(H3), ALA99, LEU391,
	Hesperidin	-4.46	01 (H1:Distance= 2.90 Å)	SER511(H1), GLY205, TYR196
	Curcumin	-5.89	01 (H1:Distance= 2.40 Å)	GLU375(H1), ALA396, ASP206
	EGCG	-5.82	02 (H1:Distance= 2.70 Å, H2:Distance= 2.47 Å)	SER128(H1), GLU145(H2)
	Piperine	-5.87	01 (H1:Distance= 2.74 Å)	ASP350(H1), PHE390, LEU391



VEDICINALS INDIA PRIVATE LIMITED

	Glycyrrhizin	-5.36	02 (H1:Distance= 3.29Å,H2: Distance= 3.16 Å)	LYS534(H1), LEU539(H2)
5CE1 Serine protease Hepsin	Baicalin	-6.16	03 (H1:Distance= 2.24 Å,H2:Distance= 3.16 Å,H3:Distance= 2.89 Å)	HIS203(H1), TYR243(H2), TYR301(H3)
	Quercetin	-5.60	03 (H1:Distance= 3.09 Å, H2:Distance=2.32 Å, H3:Distance= 2.64 Å)	GLY282(H1), GLN283(H2), GLU398(H3)
	Luteolin	-5.71	02 (H1:Distance= 2.18 Å, H2:Distance= 2.39 Å)	ASP347(H1), ALA348(H2), CYS381
	Rutin	-3.48	04 (H1:Distance= 2.80 Å) H2:Distance= 3.35 Å,H3:Distance= 2.80 Å, H4:Distance= 2.24 Å)	SER353(H1), ARG208(H2), TYR182(H3),HIS186(H4), ALA185
	Hesperidin	-4.00	05 (H1:Distance= 3.37 Å, H2:Distance= 2.50 Å, H3:Distance= 3.14 Å, H4:Distance= 2.21 Å, H5:Distance= 3.23 Å)	GLU253(H1), ASN254(H2), TYR243(H3), SER353(H4), TYR301(H5), VAL375, HIS203, TRP377
	Curcumin	-5.26	02 (H1:Distance= 2.64 Å, H2:Distance= 2.76 Å)	LYS335(H1), ARG397(H2), ALA281, GLU398, HIS240
	EGCG	-4.94	02 (H1:Distance= 3.39 Å, H2:Distance= 2.54 Å)	TYR301(H1), ASP347(H2), CYS381
	Piperine	-6.50	0	SER353(H1), ALA348(H2)
	Glycyrrhizin	-6.78	02 (H1:Distance= 2.76Å,H2: Distance= 2.09 Å)	GLN283(H1), LYS68(H2), VAL286, ILE363, TYR52,
5T30 AP2-associated protein kinase 1	Baicalin	-6.05	02 (H1:Distance= 2.17 Å,H2:Distance= 2.80 Å)	GLU187(H1), LYS90(H2)
	Quercetin	-5.66	02 (H1:Distance= 2.35 Å, H2:Distance=2.01 Å)	ASN142(H1), GLY117(H2)
	Luteolin	-5.92	03 (H1:Distance= 2.86 Å, H2:Distance= 2.97 Å, H3:Distance= 1.87 Å)	ASN185(H1), TRP186(H2), GLY86(H3),GLY85
	Rutin	-2.97	02 (H1:Distance= 2.98 Å) H2:Distance= 1.98 Å)	GLN119(H1), ALA139(H2), PRO141
	Hesperidin	-3.53	01 (H1:Distance= 2.41 Å)	GLU42(H1), GLN46, LEU49, GLY68
	Curcumin	-4.91	02 (H1:Distance= 2.19 Å, H2:Distance= 3.09 Å)	SER3(H1), ARG192(H2)
	EGCG	-4.15	02	CYS196(H1), GLU191(H2)



MEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 3.66 Å, H2:Distance= 2.71 Å)	
	Piperine	-5.10	01 (H1:Distance= 3.19 Å)	LYS90(H1)
	Glycyrrhizin	-6.30	02 (H1:Distance= 2.13 Å, H2: Distance= 2.33 Å)	ASN142(H1), SER121(H2), VAL118
3GVA Structure of human ABL2	Baicalin	-7.00	02 (H1:Distance= 2.38 Å, H2:Distance= 2.72 Å)	LEU348(H1), LYS340(H2)
	Quercetin	-6.37	03 (H1:Distance= 3.25 Å, H2:Distance=2.03 Å, H3:Distance=2.13 Å)	GLU505(H1), ALA479(H2), GLU508(H3)
	Luteolin	-6.72	01 (H1:Distance= 1.88 Å)	GLU508(H1)
	Rutin	-3.43	02 (H1:Distance= 3.21 Å) H2:Distance= 2.60 Å)	TYR363(H1), GLN346(H2)
	Hesperidin	-5.16	03 (H1:Distance= 2.36 Å, H2:Distance= 2.71 Å, H3:Distance= 3.17 Å)	GLU338(H1), LYS340(H2), TRP281(H3)
	Curcumin	-5.77	02 (H1:Distance= 2.94 Å, H2:Distance= 2.00 Å, H3:Distance= 3.29 Å)	SER395(H1), ASN343(H2), THR391(H3), GLN392, TYR388
	EGCG	-5.01	04 (H1:Distance= 2.31 Å, H2:Distance= 2.33 Å, H3:Distance= 2.24 Å, H4:Distance= 1.99 Å)	GLU338(H1), ASP427(H2), HIS407(H3), ASN404(H4)
	Piperine	-6.74	01 (H1:Distance= 3.38 Å)	LYS317(H1), ALA315, VAL302, VAL345, ALA426, MET336
	Glycyrrhizin	-5.80	02 (H1:Distance= 2.32 Å, H2: Distance= 2.84 Å, H3:Distance= 3.07 Å, H4:Distance= 2.64 Å, H5:Distance= 3.39 Å)	ASN272(H1), LEU348(H2), LEU347(H3), LYS340(H4), GLN346(H5), TRP281
1O86 Angiotensin Converting Enzyme	Baicalin	-7.14	03 (H1:Distance= 2.26 Å, H2:Distance= 2.17 Å, H3:Distance= 3.28 Å)	SER517(H1), GLU123(H2), ARG124(H3)
	Quercetin	-6.38	03 (H1:Distance= 2.83 Å, H2:Distance=2.77 Å, H3:Distance=2.81 Å)	SER219(H1), ARG522(H2), TYR135(H3)
	Luteolin	-6.67	03 (H1:Distance= 3.19 Å, H2:Distance=2.29 Å, H3:Distance=2.13 Å)	GLY404(H1), SER222(H2), GLU123(H3)



VEDICINALS INDIA PRIVATE LIMITED

	Rutin	-3.71	04 (H1:Distance= 3.31 Å, H2:Distance= 2.32 Å, H3:Distance= 3.23 Å H4:Distance= 2.41 Å)	TYR523(H1), SER517(H2), ASN70(H3), ASN66(H4), TRP357, PRO519
	Hesperidin	-5.55	04 (H1:Distance= 2.42 Å, H2:Distance= 2.62 Å, H3:Distance= 2.83 Å, H4:Distance= 2.88 Å)	ASP121(H1), SER219(H2), SER222(H3), GLU403(H4), ARG124, ILE204, ILE88, ALA89, ALA125, THR92
	Curcumin	-7.26	04 (H1:Distance= 2.65 Å, H2:Distance= 2.61 Å, H3:Distance= 2.27 Å, H4:Distance= 2.77 Å)	ASP358(H1), SER355(H2), GLU411(H3), TYR523(H4), ALA63, TYR62, TYR360, HIS353, ALA354,
	EGCG	-6.41	04 (H1:Distance= 3.09 Å, H2:Distance= 2.52 Å, H3:Distance= 2.05 Å, H4:Distance= 2.13 Å)	TYR360(H1), ASP358(H2), ALA356(H3), SER517(H4)
	Piperine	-6.35	01 (H1:Distance= 3.24 Å)	GLY404(H1), HIS410, PRO407, TYR213
	Glycyrrhizin	-5.63	03 (H1:Distance= 3.25 Å,H2: Distance= 2.03 Å, H3:Distance= 2.36 Å)	GLN483(H1), TYR175(H2), HIS263(H3), PRO500, PRO497
6XS6 SARS-CoV-2 Spike D614G mutation	Baicalin	-6.85	04 (H1:Distance= 3.05 Å,H2:Distance= 1.98 Å, H3:Distance= 3.04 Å, H4:Distance= 2.55 Å)	ASN53(H1), ASP31(H2), PHE33(H3), SER102(H4)
	Quercetin	-7.04	02 (H1:Distance= 1.98 Å, H2:Distance=2.48 Å)	SER102(H1), TYR56(H2)
	Luteolin	-6.95	01 (H1:Distance= 2.01 Å)	GLU101(H1)
	Rutin	-3.39	04 (H1:Distance= 2.18 Å, H2:Distance= 3.08 Å, H3:Distance= 2.67 Å, H4:Distance= 2.42 Å)	GLU6(H1), SER7(H2), THR114(H3), GLU155(H4), LYS208, PRO209
	Hesperidin	-4.44	01 (H1:Distance= 3.21 Å)	GLY9(H1), GLY10
	Curcumin	-5.06 (BOTH2)	01 (H1:Distance= 2.13 Å)	GLU155(H1), GLY10, LYS208
	EGCG	-4.88	01 (H1:Distance= 2.01 Å)	ALA121(H1)
	Piperine	-4.92	01 (H1:Distance= 3.38 Å)	PHE33(H1), ASP31, TYR32, TYR104
	Glycyrrhizin	-6.88	02 (H1:Distance= 2.83 Å,H2: Distance= 2.64 Å)	LYS795(H1), LYS814(H2), LEU806, PRO807
4WSI	Baicalin	-6.54	02	LYS410(H1), ASN635(H2)



VEDICINALS INDIA PRIVATE LIMITED

PALS1	Quercetin	-7.17	(H1:Distance= 2.79 Å,H2:Distance= 3.29 Å) 03 (H1:Distance= 2.11 Å, H2:Distance=3.28 Å, H3:Distance=2.84 Å)	THR579 (H1), GLN580(H2), TYR363(H3), ARG578
	Luteolin	-6.96	03 (H1:Distance= 2.99 Å, H2:Distance=3.01 Å, H3:Distance=2.83 Å)	TYR638(H1), GLN633(H2), ASN388(H3)
	Rutin	-3.97	02 (H1:Distance= 2.13 Å, H2:Distance= 2.16 Å)	GLU368(H1), ASP399(H2), LEU371, GLY405
	Hesperidin	-5.50	03 (H1:Distance= 2.11 Å, H2:Distance= 2.85 Å, H3:Distance= 2.44 Å)	PHE639(H1), HIS637(H2), MET469(H3), PRO670, TYR466, GLU467
	Curcumin	-6.30	02 (H1:Distance= 3.14 Å, H2:Distance= 3.39 Å)	ASN388(H1), LYS583(H2), TYR363, PHE354, TYR356, PRO408
	EGCG	-6.56	03 (H1:Distance= 2.81 Å, H2:Distance= 2.63 Å, H3:Distance= 2.33 Å)	ASN388(H1), GLN580(H2), GLY409(H3)
	Piperine	-6.47 (BOTH2)	01 (H1:Distance= 3.38 Å, H2:Distance= 2.90 Å)	GLY409(H1), GLN633(H2),
	Glycyrrhizin	-6.10	02 (H1:Distance= 2.83 Å,H2: Distance= 2.64 Å)	LYS795(H1), LYS814(H2), LEU806, PRO807
ISZT GP41 mutation (HIV)	Baicalin	-6.32	02 (H1:Distance= 2.22 Å,H2:Distance= 2.99 Å)	GLU47(H1), TRP44(H2), TYR51
	Quercetin	-6.17	01 (H1:Distance= 1.98 Å)	GLN18(H1)
	Luteolin	-6.35	02 (H1:Distance= 2.56 Å, H2:Distance=1.92 Å)	GLU47(H1), GLN18(H2)
	Rutin	-3.62	02 (H1:Distance= 2.32 Å, H2:Distance= 2.99 Å)	GLU47(H1), GLN18(H2)
	Hesperidin	-3.66	01 (H1:Distance= 3.08 Å)	TRP44(H1), TRP41, ILE28
	Curcumin	-5.04	02 (H1:Distance= 2.60 Å, H2:Distance= 3.00 Å)	THR52(H1), GLN18(H2), TRP44
	EGCG	-4.21	01 (H1:Distance= 2.10 Å)	THR52(H1)
	Piperine	-5.14	01 (H1:Distance= 3.10 Å)	GLN66(H1), GLN7, LEU11
	Glycyrrhizin	-5.77	01	TRP44(H1), ILE55, ILE48, LEU21



VEDICINALS INDIA PRIVATE LIMITED

4CNI IL-6 (IL-6 - Interleukin 6)	Baicalin	-6.85	(H1:Distance= 2.65 Å) 04 (H1:Distance= 3.05 Å,H2:Distance= 1.98 Å, H3:Distance= 3.04 Å, H4:Distance= 2.55 Å)	ASN53(H1), ASP31(H2), PHE33(H3), SER102(H4)
	Quercetin	-7.04	02 (H1:Distance= 1.98 Å, H2:Distance=2.48 Å)	SER102(H1), TYR56(H2)
	Luteolin	-6.95	01 (H1:Distance= 2.01 Å)	GLU101(H1)
	Rutin	-3.39	04 (H1:Distance= 2.18 Å, H2:Distance= 3.08 Å, H3:Distance= 2.67 Å, H4:Distance= 2.42 Å)	GLU6(H1), SER7(H2), THR114(H3), GLU155(H4), LYS208, PRO209
	Hesperidin	-4.44	01 (H1:Distance= 3.21 Å)	GLY9(H1), GLY10
	Curcumin	-5.06 (BOTH2)	01 (H1:Distance= 2.13 Å)	GLU155(H1), GLY10, LYS208
	EGCG	-4.88	01 (H1:Distance= 2.01 Å)	ALA121(H1)
	Piperine	-4.92	01 (H1:Distance= 3.38 Å)	PHE33(H1), ASP31, TYR32, TYR104
	Glycyrrhizin	-6.88	02 (H1:Distance= 2.83 Å,H2: Distance= 2.64 Å)	LYS795(H1), LYS814(H2), LEU806, PRO807
2IG2 IgG	Baicalin	-5.89	01 (H1:Distance= 2.33 Å)	GLN110(H1), TRP108
	Quercetin	-6.10	02 (H1:Distance= 2.25 Å, H2:Distance=2.36 Å)	ASP106(H1), GLN3(H2)
	Luteolin	-6.07	01 (H1:Distance= 2.01 Å)	GLU101(H1)
	Rutin	-3.62	02 (H1:Distance= 2.28 Å, H2:Distance= 3.56 Å)	ASP106(H1), VAL2(H2), TYR107
	Hesperidin	-4.03	03 (H1:Distance= 2.50 Å, H2:Distance= 2.91 Å, H3:Distance= 2.30 Å)	GLN176(H1), PRO88(H2), TYR181(H3)
	Curcumin	-4.72	01 (H1:Distance= 3.27 Å)	TYR181(H1), VAL116
	EGCG	-5.65	05 (H1:Distance= 1.73 Å, H2:Distance= 3.35 Å, H3:Distance= 2.43 Å, H4:Distance= 2.22 Å, H5:Distance= 3.22 Å)	ASP106(H1), TRP108(H2), VAL2(H3), GLN3(H4), GLN110(H5), GLY109



MEDICINALS INDIA PRIVATE LIMITED

	Piperine	-5.27	01 (H1:Distance= 3.03 Å, H2:Distance= 2.70 Å)	GLN39(H1), TRP108(H1)
	Glycyrrhizin	-6.81	01 (H1:Distance= 2.82 Å)	GLY10(H1), GLY9, VAL11, PRO152
1DN0 IgM/IgA	Baicalin	-5.68	01 (H1:Distance= 1.91 Å)	LYS40(H1)
	Quercetin	-5.80	01 (H1:Distance= 1.91 Å)	GLN167(H1), GLU106
	Luteolin	-6.51	01 (H1:Distance= 2.35 Å)	GLN167(H1), GLU106
	Rutin	-3.68	02 (H1:Distance= 2.72 Å, H2:Distance= 2.24 Å)	PRO41(H1), GLU166(H2)
	Hesperidin	-4.04	02 (H1:Distance= 2.43 Å, H2:Distance= 3.07 Å)	SER169(H1), SER172(H2)
	Curcumin	-5.01	02 (H1:Distance= 1.99 Å, H2:Distance= 2.27 Å)	ASP168(H1), VAL105(H2), LYS104, VAL86
	EGCG	-5.09	03 (H1:Distance= 3.02 Å, H2:Distance= 2.04 Å, H3:Distance= 2.11 Å)	SER169(H1), GLN167(H2), VAL105(H3)
	Piperine	-6.38	01 (H1:Distance= 3.22 Å)	ILE107(H1), LYS104, GLN39
	Glycyrrhizin	-6.12	02 (H1:Distance= 3.40 Å, H2:Distance= 2.76 Å)	GLU162(H1), LYS146(H2)
	1GNH C-reactive protein	Baicalin	-6.25	03 (H1:Distance= 3.23 Å, H2:Distance= 2.51 Å, H3:Distance= 3.07 Å)
Quercetin		-5.44	02 (H1:Distance= 2.07 Å, H2:Distance= 2.25 Å)	ASP112(H1), THR90(H2)
Luteolin		-6.14	02 (H1:Distance= 1.92 Å, H2:Distance= 2.03 Å)	GLU85(H1), THR90(H2)
Rutin		-3.14	06 (H1:Distance= 2.90 Å, H2:Distance= 2.10 Å, H3:Distance= 3.26 Å, H4:Distance= 2.23 Å, H5:Distance= 2.14 Å, H6:Distance= 2.41 Å)	SER74(H1), GLU81(H2), GLN150(H3), ASP140(H4), GLY79(H5), ASN61(H6), SER68
Hesperidin		-4.16	06 (H1:Distance= 2.95 Å, H2:Distance= 2.58 Å, H3:Distance= 2.35 Å, H4:Distance= 2.52 Å, H5:Distance= 2.25 Å, H6:Distance= 2.58 Å)	PRO182(H1), THR27(H2), VAL184(H3), ASN186(H4), ALA189(H5), LYS23(H6), PRO25
Curcumin		-4.92	01	ASN158(H1), PRO179, GLY177



MEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 2.78 Å)	
	EGCG	-4.93	03 (H1:Distance= 2.07 Å, H2:Distance= 2.59 Å, H3:Distance= 1.94 Å)	LEU204(H1), HIS38(H2), ASP112(H3)
	Piperine	-6.25	01 (H1:Distance= 2.59 Å)	SER44(H1), VAL86, VAL111
	Glycyrrhizin	-5.26	02 (H1:Distance= 3.40 Å, H2:Distance= 2.76 Å)	GLU162(H1), LYS146(H2)
4LBJ Galectin-3	Baicalin	-5.84	03 (H1:Distance= 2.46 Å, H2:Distance= 3.02 Å, H3:Distance= 2.75 Å)	SER188(H1), ARG169(H2), PHE190(H3)
	Quercetin	-6.93	02 (H1:Distance= 3.05 Å, H2:Distance= 2.85 Å)	ARG169(H1), ARG168(H2)
	Luteolin	-6.13	01 (H1:Distance= 3.14 Å)	ARG169(H1)
	Rutin	-4.38	01 (H1:Distance= 2.68 Å)	ARG169(H1)
	Hesperidin	-3.97	01 (H1:Distance= 3.18 Å)	ARG169(H1), ARG168, VAL189
	Curcumin	-4.84	01 (H1:Distance= 1.92 Å)	GLN220(H1), HIS217, LEU218
	EGCG	-5.01	04 (H1:Distance= 2.29 Å, H2:Distance= 2.05 Å, H3:Distance= 2.88 Å, H4:Distance= 2.04 Å)	GLU184(H1), GLY182(H2), TRP181(H3), ASN179(H4)
	Piperine	-5.37	02 (H1:Distance= 3.16 Å, H2:Distance= 2.83 Å)	ARG168(H1), ARG169(H2)
	Glycyrrhizin	-6.26	02 (H1:Distance= 2.30 Å, H2:Distance= 3.07 Å)	GLN220(H1), ARG186(H2), HIS217
6JOD Angiotensin II	Baicalin	-7.40	03 (H1:Distance= 1.71 Å, H2:Distance= 3.33 Å, H3:Distance= 2.81 Å)	CYS70(H1), LYS73(H2), LYS76(H3)
	Quercetin	-5.85	02 (H1:Distance= 2.45 Å, H2:Distance= 2.32 Å, H3:Distance= 2.11 Å, H4:Distance= 2.60 Å)	TYR204(H1), ASP279(H2), TYR103(H3), CYS195(H4)
	Luteolin	-6.02	01 (H1:Distance= 2.71 Å, H2:Distance= 2.07 Å, H3:Distance= 2.88 Å)	ARG182(H1), TYR51(H2), THR125(H3), LYS215
	Rutin	-2.59 (Both2)	01 (H1:Distance= 2.25 Å)	ASN85(H1), LYS76
	Hesperidin	-4.72	01	LEU173(H1), TYR180, PHE179



VEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 2.23 Å)	
	Curcumin	-5.34	01 (H1:Distance= 3.10 Å)	THR136(H1), PHE226, CYS137, ILE163
	EGCG	-5.83	04 (H1:Distance= 2.13 Å, H2:Distance= 3.22 Å, H3:Distance= 2.90 Å, H4:Distance= 3.25 Å)	TYR104(H1), MET197(H2), ALA208(H3), LYS215(H4), ILE196
	Piperine	-6.86	01 (H1:Distance= 2.83 Å)	ARG182(H1), LYS215, PHE129, HIS273
	Glycyrrhizin	-9.13	03 (H1:Distance= 2.31 Å, H2:Distance= 2.77 Å, H3:Distance= 2.76 Å)	CYS70(H1), LYS73(H2), LYS76(H3), PRO165, ILE81, VAL164
3RZE Histamine (Histamine H1 receptor)	Baicalin	-6.97	02 (H1:Distance= 3.04 Å, H2:Distance= 2.01 Å)	ARG218(H1), GLN219(H2)
	Quercetin	-5.64	03 (H1:Distance= 2.49 Å, H2:Distance= 2.69 Å, H3:Distance= 2.58 Å)	PHE156(H1), PHE153(H2), LEU149(H3)
	Luteolin	-8.05	04 (H1:Distance= 3.35 Å, H2:Distance= 3.28 Å, H3:Distance= 2.22 Å, H4:Distance= 2.03 Å)	THR194(H1), TYR431(H2), THR112(H3), TYR458(H4), SER111
	Rutin	-3.94	02 (H1:Distance= 2.19 Å, H2:Distance= 2.16 Å)	VAL1103(H1), GLU1011(H2),
	Hesperidin	-4.21	0	PHE153
	Curcumin	-4.72	0	VAL187, HIS167, TRP189
	EGCG	-4.66	04 (H1:Distance= 2.20 Å, H2:Distance= 2.58 Å, H3:Distance= 2.90 Å, H4:Distance= 2.11 Å)	TYR1161(H1), GLU1005(H2), ARG218(H3), LYS215(H4)
	Piperine	-5.26	0	TYR210, MET421
	Glycyrrhizin	-9.03	03 (H1:Distance= 3.37 Å, H2:Distance= 2.31 Å, H3:Distance= 2.75 Å)	ASN474(H1), ARG139(H2), LYS137(H3), LYS57
4IP8 Serum amyloid A is name like C-reactive protein	Baicalin	-6.90	01 (H1:Distance= 2.70 Å)	TYR21(H1)
	Quercetin	-6.35	01 (H1:Distance= 3.11 Å)	HIS37(H1)
	Luteolin	-6.97	04 (H1:Distance= 3.35 Å, H2:Distance= 3.28 Å, H3:Distance= 2.22 Å, H4:Distance= 2.03 Å)	THR194(H1), TYR431(H2), THR112(H3), TYR458(H4), SER111
	Rutin	-3.87	04	ARG25(H1), ASP33(H2), SER32(H3), MET24(H4)



VEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 2.31 Å, H2:Distance= 2.52 Å, H3:Distance= 2.92 Å, H4:Distance= 2.72 Å)	
	Hesperidin	-4.28	0	PHE69
	Curcumin	-6.44	01 (H1:Distance= 3.16 Å)	HIS37(H1), ALA20, PHE36, MET17
	EGCG	-4.57	04 (H1:Distance= 3.04 Å, H2:Distance= 3.20 Å, H3:Distance= 2.05 Å, H4:Distance= 2.00 Å)	HIS71(H1), GLN66(H2), TYR29(H3), SER32(H4)
	Piperine	-6.19	0	TYR210, MET421
	Glycyrrhizin	-5.96	0	TRP18, ILE58, ALA14, ARG62
2QQI Neuropilin 1 (NRP1)	Baicalin	-6.03	01 (H1:Distance= 2.39 Å)	ASP36(H1), ASP146
	Quercetin	-5.53	02 (H1:Distance= 1.90 Å, H2:Distance= 2.11 Å)	VAL44(H1), VAL48(H2)
	Luteolin	-5.62	02 (H1:Distance= 2.10 Å, H2:Distance= 2.71 Å)	LYS170(H1), PRO138(H2)
	Rutin	-3.26	02 (H1:Distance= 3.15 Å, H2:Distance= 2.32 Å)	ASP24(H1), TYR22(H2)
	Hesperidin	-3.43	05 (H1:Distance= 3.11 Å, H2:Distance= 3.40 Å, H3:Distance= 1.89 Å, H4:Distance= 2.29 Å, H5:Distance= 2.18 Å)	GLY77(H1), THR78(H2), THR115(H3), SER26(H4), GLY136(H5), ALA116, LYS137
	Curcumin	-5.06	01 (H1:Distance= 3.07 Å)	TYR46(H1), VAL44
	EGCG	-4.37	03 (H1:Distance= 1.92 Å, H2:Distance= 2.89 Å, H3:Distance= 2.65 Å)	ASP32(H1), ASP24(H2), TYR22(H3)
	Piperine	-5.30	01 (H1:Distance= 3.18 Å)	LYS4(H1)
	Glycyrrhizin	-7.50	02 (H1:Distance= 2.43 Å, H2:Distance= 2.58 Å)	LYS96(H1), LEU158(H2), PHE101, ALA151, LEU98, CYS155
4RN5 Neuropilin-1	Baicalin	-6.28	01 (H1:Distance= 2.49 Å)	LYS373(H1), ILE372
	Quercetin	-6.31	03 (H1:Distance= 2.48 Å, H2:Distance= 2.17 Å, H3:Distance= 2.78 Å)	SER364(H1), ILE400(H2), LYS373(H3)
	Luteolin	-5.97	02 (H1:Distance= 1.84 Å, H2:Distance= 2.11 Å)	ILE400(H1), LYS373(H2), THR401, SER364



VEDICINALS INDIA PRIVATE LIMITED

	Rutin	-4.07	05 (H1:Distance= 2.89 Å, H2:Distance= 2.96 Å, H3:Distance= 2.75 Å, H4:Distance= 2.13 Å, H5:Distance= 2.12 Å)	LYS373(H1), PRO398(H2), LYS397(H3), ILE400(H4), SER364(H5)
	Hesperidin	-3.94	02 (H1:Distance= 2.42 Å, H2:Distance= 2.31 Å)	VAL392(H1), VAL394(H2), CYS275
	Curcumin	-5.61	02 (H1:Distance= 2.10 Å, H2:Distance= 2.90 Å)	ASP368(H1), ILE400(H2), LYS373, LYS397, SER363
	EGCG	-4.81	02 (H1:Distance= 2.18 Å, H2:Distance= 2.67 Å)	GLU304(H1), GLN296(H2), SER295
	Piperine	-5.28	01 (H1:Distance= 3.01 Å)	VAL394(H1), ALA393, VAL379
	Glycyrrhizin	-6.76	02 (H1:Distance= 2.96 Å, H2:Distance= 3.16 Å)	LYS274(H1), GLN382(H2), PHE381, PRO396, VAL379, VAL394
3B5H Emmprin (CD147) Thrombosis factor	Baicalin	-7.73	04 (H1:Distance= 2.66 Å, H2:Distance= 2.68 Å, H3:Distance= 3.15 Å, H4:Distance= 2.35 Å)	GLN100(H1), HIS102(H2), LYS191(H3), ASP32(H4)
	Quercetin	-5.64	04 (H1:Distance= 1.73 Å, H2:Distance= 2.70 Å, H3:Distance= 2.20 Å, H4:Distance= 3.08 Å)	GLN81(H1), HIS102(H2), PRO104(H3), ASP194(H4), GLY103
	Luteolin	-5.53	02 (H1:Distance= 2.64 Å, H2:Distance= 3.09 Å)	HIS102(H1), GLN100(H2)
	Rutin	-2.90	06 (H1:Distance= 3.32 Å, H2:Distance= 2.98 Å, H3:Distance= 2.38 Å, H4:Distance= 2.43 Å, H5:Distance= 3.01 Å, H6:Distance= 2.34 Å)	ILE197(H1), ALA109(H2), SER112(H3), VAL107(H4), GLN195(H5), ASP194(H6), ALA196, LYS108
	Hesperidin	-4.15	02 (H1:Distance= 1.84 Å, H2:Distance= 2.18 Å)	PRO105(H1), SER78(H2), GLY103, ARG106, PRO104, TRP82
	Curcumin	-4.79	01 (H1:Distance= 2.98 Å)	ALA109(H1), VAL107, LYS108, ARG106
	EGCG	-4.76	03 (H1:Distance= 2.48 Å, H2:Distance= 2.47 Å, H2:Distance= 2.33 Å)	HIS102(H1), VAL30(H2), THR29(H3)
	Piperine	-5.25	0	GLN81, PRO104, ARG106
	Glycyrrhizin	-6.04	04 (H1:Distance= 2.94 Å, H2:Distance= 2.80 Å, H3:Distance= 2.89 Å, H4:Distance= 3.18 Å)	VAL60(H1), ASP80(H2), LYS57(H3), LYS127(H4)
5E84	Baicalin	-7.07	02	LYS280(H1), ARG279(H2), LYS113



MEDICINALS INDIA PRIVATE LIMITED

GRP78	Quercetin	-6.09	(H1:Distance= 2.47 Å, H2:Distance= 2.24 Å) 03 (H1:Distance= 2.89 Å, H2:Distance= 2.56 Å, H3:Distance= 2.36 Å)	ASN282(H1), LYS280(H2), PHE117(H3)
	Luteolin	-6.46	02 (H1:Distance= 2.45 Å, H2:Distance= 2.20 Å)	VAL119(H1), ARG279(H2)
	Rutin	-4.08	04 (H1:Distance= 3.13 Å, H2:Distance= 2.79 Å, H3:Distance= 2.83 Å, H4:Distance= 2.02 Å)	LYS435(H1), ARG439(H2), ASP348(H3), ASP350(H4)
	Hesperidin	-4.63	06 (H1:Distance= 2.63 Å, H2:Distance= 3.16 Å, H3:Distance= 2.65 Å, H4:Distance= 2.24 Å, H5:Distance= 2.80 Å, H6:Distance= 2.46 Å)	LYS344(H1), ARG101(H2), ASN248(H3), TYR175(H4), THR251(H5), GLU463(H6), ASP471, GLY464, ASN472, ARG466, LYS340
	Curcumin	-5.45	01 (H1:Distance= 2.56 Å)	ARG279(H1), LYS118, LYS113, GLN109, VAL285
	EGCG	-5.58	03 (H1:Distance= 1.69 Å, H2:Distance= 2.15 Å, H3:Distance= 2.17 Å)	GLU308(H1), GLN304(H2), ARG306(H3), LYS294, GLN302, ALA305
	Piperine	-6.05	02 (H1:Distance= 2.83 Å, H2:Distance= 3.08 Å)	SER365(H1), LYS296(H2), ILE61, CYS41
	Glycyrrhizin	-7.29	02 (H1:Distance= 3.12 Å, H2:Distance= 3.35 Å)	VAL119(H1), LYS280(H2), LYS118, ILE112
4EL1 Antithrombotic	Baicalin	-7.48	02 (H1:Distance= 2.48 Å, H2:Distance= 2.75 Å)	LYS247(H1), ASP181(H2)
	Quercetin	-6.23	02 (H1:Distance= 2.27 Å, H2:Distance= 2.22 Å)	GLU303(H1), VAL437(H2)
	Luteolin	-6.56	03 (H1:Distance= 1.98 Å, H2:Distance= 3.30 Å, H3:Distance= 2.69 Å)	GLU330(H1), LYS328(H2), SER357(H3)
	Rutin	-3.42	03 (H1:Distance= 2.32 Å, H2:Distance= 3.16 Å, H3:Distance= 2.14 Å)	LEU355(H1), LYS352(H2), PRO353(H3), LYS375
	Hesperidin	-4.24	03 (H1:Distance= 2.02 Å, H2:Distance= 2.72 Å, H3:Distance= 2.41 Å)	LYS352(H1), LEU355(H2), LYS328(H3)
	Curcumin	-5.03 (Both2)	01 (H1:Distance= 2.15 Å)	GLU239(H1), PRO235
	EGCG	-5.55	03	LYS352(H1), GLU378(H2), LEU355(H3), LYS328,



VEDICINALS INDIA PRIVATE LIMITED

			(H1:Distance= 2.92 Å, H2:Distance= 2.16 Å, H3:Distance= 2.93 Å)	HIS354
	Piperine	-5.55 (Both2)	01 (H1:Distance= 3.22 Å)	LYS247(H1), PRO235, LEU287
	Glycyrrhizin	-6.82	02 (H1:Distance= 2.58 Å, H2:Distance= 2.13 Å)	THR255(H1), GLU242(H2), ILE318, MET324, ALA245
3SH5 Heparan sulfate proteoglycan (HSPG)	Baicalin	-7.03	02 (H1:Distance= 2.14 Å, H2:Distance= 3.04 Å)	TRP216(H1), SER212(H2), TRP215
	Quercetin	-6.75	03 (H1:Distance= 2.07 Å, H2:Distance= 2.12 Å, H3:Distance= 1.82 Å)	GLU452(H1), PRO510(H2), ARG560(H3)
	Luteolin	-6.90	02 (H1:Distance= 2.20 Å, H2:Distance= 2.24 Å)	THR565(H1), VAL558(H2), SER511
	Rutin	-3.77	04 (H1:Distance= 2.67 Å, H2:Distance= 2.16 Å, H3:Distance= 2.66 Å, H4:Distance= 2.59 Å)	PHE364(H1), TRP305(H2), ALA306(H3), LEU366(H4), ALA409, PRO218
	Hesperidin	-4.75	02 (H1:Distance= 2.65 Å, H2:Distance= 2.07 Å)	PHE364(H1), TRP216(H2), HIS363, TRP305, PRO218, ALA409, GLU408, PHE461
	Curcumin	-6.18	03 (H1:Distance= 3.28 Å, H2:Distance= 2.77 Å, H3:Distance= 2.52 Å)	LYS463(H1), TRP216(H2), TRP305(H3), PRO218
	EGCG	-5.77	04 (H1:Distance= 2.78 Å, H2:Distance= 3.02 Å, H3:Distance= 2.23 Å, H4:Distance= 2.30 Å)	CYS394(H1), MET348(H2), SER349(H3), THR350(H4)
	Piperine	-5.91	02 (H1:Distance= 3.05 Å, H2:Distance= 2.67 Å)	TRP305(H1), THR156(H2), VAL303, TRP215, PRO159, TRP216, PRO109
	Glycyrrhizin	-7.10	03 (H1:Distance= 2.72 Å, H2:Distance= 2.24 Å, H3:Distance= 3.22 Å)	SER59(H1), TYR480(H1), ARG471(H1), PRO109, ARG61
6B1E Dipeptidyl Peptidase-4 (DPP-4) Inhibitor	Baicalin	-7.03	02 (H1:Distance= 2.14 Å, H2:Distance= 3.04 Å)	TRP216(H1), SER212(H2), TRP215
	Quercetin	-6.75	03 (H1:Distance= 2.07 Å, H2:Distance= 2.12 Å, H3:Distance= 1.82 Å)	GLU452(H1), PRO510(H2), ARG560(H3)
	Luteolin	-6.90	02 (H1:Distance= 2.20 Å, H2:Distance= 2.24 Å)	THR565(H1), VAL558(H2), SER511
	Rutin	-3.77	04 (H1:Distance= 2.67 Å, H2:Distance= 2.16 Å H3:Distance= 2.66 Å, H4:Distance= 2.59 Å)	PHE364(H1), TRP305(H2), ALA306(H3), LEU366(H4), ALA409, PRO218



VEDICINALS INDIA PRIVATE LIMITED

	Hesperidin	-4.75	02 (H1:Distance= 2.65 Å, H2:Distance= 2.07 Å)	PHE364(H1), TRP216(H2), HIS363, TRP305, PRO218, ALA409, GLU408, PHE461
	Curcumin	-6.18	03 (H1:Distance= 3.28 Å, H2:Distance= 2.77 Å, H3:Distance= 2.52 Å)	LYS463(H1), TRP216(H2), TRP305(H3), PRO218
	EGCG	-5.77	04 (H1:Distance= 2.78 Å, H2:Distance= 3.02 Å, H3:Distance= 2.23 Å, H4:Distance= 2.30 Å)	CYS394(H1), MET348(H2), SER349(H3), THR350(H4)
	Piperine	-5.91	02 (H1:Distance= 3.05 Å, H2:Distance= 2.67 Å)	TRP305(H1), THR156(H2), VAL303, TRP215, PRO159, TRP216, PRO109
	Glycyrrhizin	-7.10	03 (H1:Distance= 2.72 Å, H2:Distance= 2.24 Å, H3:Distance= 3.22 Å)	SER59(H1), TYR480(H1), ARG471(H1), PRO109, ARG61
7KDJ Spike Glycoprotein (7KDJ-Mutant)	Baicalin	-7.08	02 (H1:Distance= 3.10 Å, H2:Distance= 2.13 Å)	LYS529(H1), SER530(H2)
	Quercetin	-7.06	05 (H1:Distance= 2.19 Å, H2:Distance= 2.08 Å, H3:Distance= 1.82 Å, H4:Distance= 1.94 Å, H5:Distance= 3.03 Å)	GLN218(H1), PRO209(H2), ASP215(H3), LEU212(H4), THR208(H5)
	Luteolin	-6.41	01 (H1:Distance= 2.00 Å)	ALA520(H1)
	Rutin	-2.87	04 (H1:Distance= 2.67 Å, H2:Distance= 2.16 Å, H3:Distance= 2.66 Å, H4:Distance= 2.59 Å)	PHE364(H1), TRP305(H2), ALA306(H3), LEU366(H4), ALA409, PRO218
	Hesperidin	-4.34	02 (H1:Distance= 2.65 Å, H2:Distance= 2.07 Å)	PHE364(H1), TRP216(H2), HIS363, TRP305, PRO218, ALA409, GLU408, PHE461
	Curcumin	-4.83	01 (H1:Distance= 3.18 Å)	ASN544(H1), PHE543, VAL576, PHE565, LEU546, GLY381
	EGCG	-5.40	02 (H1:Distance= 3.37 Å, H2:Distance= 2.23 Å)	ARG567(H1), ALA520(H2)
	Piperine	-5.14	02 (H1:Distance= 3.09 Å, H2:Distance= 3.12 Å)	GLN564(H1), ASN544(H2), VAL576, PHE565
	Glycyrrhizin	-8.57	02 (H1:Distance= 3.02 Å, H2:Distance= 2.58 Å)	THR376(H1), VAL503(H2), TYR508
G476S Spike Glycoprotein	Baicalin	-7.43	02 (H1:Distance= 1.85 Å, H2:Distance= 3.17 Å)	PHE4(H1), VAL3(H2)
	Quercetin	-7.40	04 (H1:Distance= 2.97 Å, H2:Distance= 2.50 Å,	ALA262(H1), ILE312(H2), ASN824(H3), SER813(H4), LYS825



VEDICINALS INDIA PRIVATE LIMITED

			H3:Distance= 2.19 Å, H4:Distance= 2.68 Å)	
	Luteolin	-7.01	01 (H1:Distance= 2.40 Å, H2:Distance= 3.07 Å, H3:Distance= 2.09 Å)	VAL524(H1), ASN17(H2), ALA972(H3),
	Rutin	-4.18	03 (H1:Distance= 2.76 Å, H2:Distance= 2.78 Å, H3:Distance= 3.31 Å)	ARG815(H1), LYS814(H2), GLN314(H3), GLY311
	Hesperidin	-5.06	02 (H1:Distance= 2.04 Å, H2:Distance= 2.06 Å)	LYS310(H1), THR315(H2), LYS814, LEU822
	Curcumin	-6.48	01 (H1:Distance= 2.22 Å)	LEU552(H1), ALA522, GLN14, CYS15, LEU962, PRO9, LEU5, VAL6
	EGCG	-6.80	02 (H1:Distance= 2.21 Å, H2:Distance= 2.16 Å)	ASN536(H1), LEU8(H2), VAL3
	Piperine	-6.60	00	LEU5, LEU962, VAL11, VAL534
	Glycyrrhizin	-7.76	01 (H1:Distance= 2.79 Å)	LYS947(H1), PHE823
V483G	Baicalin	-7.70	02 (H1:Distance= 3.05 Å, H2:Distance= 2.06 Å)	LYS356(H1), SER359(H2)
Spike	Quercetin	-7.29	04 (H1:Distance= 2.89 Å, H2:Distance= 2.36 Å, H3:Distance= 2.58 Å, H4:Distance= 2.85 Å)	GLU1111(H1), ILE1115(H2), ASP1118(H3), THR1117(H4), ILE1114
Glycoprotein	Luteolin	-7.54	01 (H1:Distance= 3.19 Å)	THR1116(H1)
	Rutin	-4.35	04 (H1:Distance= 2.75 Å, H2:Distance= 2.25 Å, H3:Distance= 2.05 Å, H4:Distance= 2.96 Å)	VAL11(H1), VAL534(H2), ASP198(H3), LYS535(H4), TYR200, LEU533
	Hesperidin	-5.59	05 (H1:Distance= 2.37 Å, H2:Distance= 3.18 Å, H3:Distance= 2.53 Å, H4:Distance= 2.06 Å, H5:Distance= 2.93 Å)	PHE592(H1), SER591(H2), ILE231(H3), GLU224(H4), GLN183(H5), LEU223
	Curcumin	-6.97	02 (H1:Distance= 3.07 Å, H2:Distance= 2.81 Å)	PHE79(H1), PRO57(H2), ASP53, ARG78, LEU54, LEU56
	EGCG	-6.36	03 (H1:Distance= 3.20 Å, H2:Distance= 3.38 Å, H3:Distance= 2.06 Å)	ARG905(H1), VAL143(H2), MET902(H3)
	Piperine	-7.72	01 (H1:Distance= 3.09 Å)	LYS310(H1), PHE515, ALA243
	Glycyrrhizin	-8.00	02 (H1:Distance= 2.88 Å, H2:Distance= 2.04 Å)	SER975(H1), ASP950(H2), LEU948, PHE970, VAL976



VEDICINALS INDIA PRIVATE LIMITED

E484K Spike Glycoprotein	Baicalin	-7.18	02 (H1:Distance= 1.94 Å, H2:Distance= 2.51 Å)	GLN599(H1),SER549(H2),ILE351,PHE348,VAL381,CY S544
	Quercetin	-6.56	02 (H1:Distance= 2.71 Å, H2:Distance= 2.10 Å)	SER113 (H1),GLU 115 (H2), ILE120, PHE211,ASN140,TRP123,VAL145,ILE138
	Luteolin	-6.83	02 (H1:Distance= 1.88 Å, H2:Distance= 2.22 Å)	GLY302 (H1),PRO244 (H2),TYR57,LYS60
	Rutin	-3.13	03 (H1:Distance= 2.55 Å, H2:Distance= 2.27 Å, H3:Distance= 3.09 Å)	SER659 (H1),SER656 (H2)ASN625 (H3),VAL629,VAL627,GLN626
	Hesperidin	-4.41	02 (H1:Distance= 2.52 Å, H2:Distance= 2.71 Å)	SER727 (H1),SER730 (H2),PRO1098,ALA1097
	Curcumin	-4.72	02 (H1:Distance= 2.32 Å, H2:Distance= 2.71 Å)	THR143 (H1),ASN141 (H2),SER174,ARG177
	EGCG	-5.62	01 (H1:Distance= 2.14 Å)	LEU884 (H1),LEU847,PRO882,ASP886,HIS1077
	Piperine	-6.92	--	CYS451,LEU532,ALA382,PHE411,TYR388,LEU387,PH E393,PHE396
	Glycyrrhizin	-6.79	04 (H1:Distance= 2.23 Å, H2:Distance= 3.28 Å, H3:Distance= 2.36 Å, H4:Distance= 3.13 Å)	ARG485 (H1),ASN373 (H2),TRP372 (H3),ARG365 (H4),ALA367,ALA371,ILE487
P681H Spike Glycoprotein	Baicalin	-6.80	04 (H1:Distance= 3.19 Å, H2:Distance= 1.86 Å, H3:Distance= 2.93 Å, H4:Distance= 2.49 Å)	ARG273(H1), PRO272(H2), THR274(H3), GLU298(H4), SER50
	Quercetin	-6.17	03 (H1:Distance= 2.59 Å, H2:Distance= 2.39 Å H3:Distance= 2.06 Å)	MET153(H1), SER155(H2), PHE140(H3)
	Luteolin	-6.92	03 (H1:Distance= 2.19 Å, H2:Distance= 2.38 Å H3:Distance= 3.14 Å)	ASP178(H1), GLU224(H2), LYS206(H3)
	Rutin	-4.76	02 (H1:Distance= 2.45 Å, H2:Distance=1.85 Å)	ARG158(H1), GLN134(H2), TYR144
	Hesperidin	-4.43	01 (H1:Distance= 3.06 Å)	HIS66(H1), ASP80
	Curcumin	-6.07	04 (H1:Distance= 2.86 Å, H2:Distance= 2.82 Å, H3:Distance= 2.77 Å, H4:Distance= 3.18 Å)	ARG355(H1), PRO463(H2), THR430(H3), TYR396(H4), GLU516
	EGCG	-6.24	03 (H1:Distance= 2.74 Å, H2:Distance= 2.29 Å,	HIS69(H1), PRO26(H2), TRP64(H3)



VEDICINALS INDIA PRIVATE LIMITED

	Piperine	-6.03	H3:Distance= 2.43 Å) 01 (H1:Distance= 3.10 Å)	THR95(H1), ASN211, LYS97, VAL213
	Glycyrrhizin	-6.94	03 (H1:Distance= 2.90 Å, H2:Distance= 3.16 Å, H3:Distance= 1.77 Å)	SER12(H1), GLN134(H2), VAL6(H3), LEU10, LEU8
K417N Spike Glycoprotein	Baicalin	-7.26	01 (H1:Distance= 2.46 Å)	GLY66(H1), ARG65
	Quercetin	-7.35	06 (H1:Distance= 3.40 Å, H2:Distance= 2.91 Å H3:Distance= 3.34 Å, H4:Distance= 2.54 Å, H5:Distance= 2.14 Å H6:Distance= 1.89 Å)	CYS780(H1), THR755(H2), ILE357(H3), SER356(H4), THR763(H5), ALA684(H6), SER777
	Luteolin	-7.54	04 (H1:Distance= 2.40 Å, H2:Distance= 2.97 Å, H3:Distance= 2.67 Å, H4:Distance= 2.42 Å)	ASP209(H1), SER193(H2), LYS218(H3), ASN216(H4), SER192
	Rutin	-3.81	03 (H1:Distance= 2.13 Å, H2:Distance= 3.16 Å, H3:Distance= 2.29Å)	LEU1043(H1), GLN1042(H2), LYS213(H3)
	Hesperidin	-6.65	01 (H1:Distance= 2.92 Å)	THR1040(H1), ARG221
	Curcumin	-6.89	01 (H1:Distance= 2.26 Å)	SER252(H1), CYS197, LEU1032
	EGCG	-6.89	01 (H1:Distance= 2.01 Å)	ARG189(H1), SER236
	Piperine	-7.38	01 (H1:Distance= 3.10 Å)	LEU257(H1), LEU260, TYR191
	Glycyrrhizin	-7.28	02 (H1:Distance= 2.69 Å, H2:Distance= 1.96 Å)	LYS559(H1), ASN481(H2), TYR480, PRO558
N501Y Spike Glycoprotein	Baicalin	-7.39	03 (H1:Distance= 3.21 Å, H2:Distance= 2.27 Å, H3:Distance= 3.15 Å)	ALA263(H1), LYS310(H2), PHE201(H3), GLY261
	Quercetin	-7.35	02 (H1:Distance= 1.71 Å, H2:Distance= 2.56 Å)	ILE934(H1), PHE562(H2)
	Luteolin	-7.06	02 (H1:Distance= 2.88 Å, H2:Distance= 2.36 Å)	GLY184(H1), GLN787(H2)
	Rutin	-4.75	03 (H1:Distance= 2.30 Å, H2:Distance= 2.16 Å, H3:Distance= 2.70Å)	MET900(H1), GLY1124(H2), ALA930(H3), SER1123



VEDICINALS INDIA PRIVATE LIMITED

	Hesperidin	-5.72	01 (H1:Distance= 3.20 Å, H2:Distance= 3.38 Å, H3:Distance= 2.53 Å, H4:Distance= 3.31 Å)	SER305(H1), ASP364(H2), ILE197(H3), CYS361(H4), THR307, VAL308, ILE358, LEU242, VAL362
	Curcumin	-6.43	01 (H1:Distance= 2.76 Å)	LYS386(H1), SER730, PHE833, LEU727
	EGCG	-7.25	04 (H1:Distance= 2.12 Å, H2:Distance= 2.53 Å, H3:Distance= 2.37 Å, H4:Distance= 2.25 Å)	ILE666(H1), PRO665(H2), PRO681(H3), CYS662(H4)
	Piperine	-6.86	00	VAL1137, LEU455, PRO1140
	Glycyrrhizin	-7.88	01 (H1:Distance= 2.76 Å)	ASN440(H1), PHE140, PRO139, PHE92, LEU441
N440K Spike Glycoprotein	Baicalin	-7.55	04 (H1:Distance= 2.29 Å, H2:Distance= 2.25 Å, H3:Distance= 2.50 Å, H4:Distance= 3.28 Å)	ASP198(H1), SER929(H2), PHE515(H3), TRP886(H4)
	Quercetin	-7.96	06 (H1:Distance= 2.44 Å, H2:Distance= 2.75 Å, H3:Distance= 2.45 Å, H4:Distance= 2.15 Å, H5:Distance= 2.29 Å, H6:Distance= 2.81 Å)	SER685(H1), VAL362(H2), CYS361(H3), ASP364(H4), VAL597(H5), SER366(H6), VAL367
	Luteolin	-7.21	02 (H1:Distance= 2.05 Å, H2:Distance= 2.42 Å)	LYS182(H1), PHE186(H2), ARG246
	Rutin	-4.91	04 (H1:Distance= 2.30 Å, H2:Distance= 3.34 Å, H3:Distance= 2.36 Å, H4:Distance= 2.38 Å)	ILE923(H1), LEU922(H2), GLY910(H3), GLY908(H4), LYS921, ASN919
	Hesperidin	-6.31	03 (H1:Distance= 3.03 Å, H2:Distance= 3.03 Å, H3:Distance= 2.73 Å)	THR376(H1), LYS825(H2), TYR741(H3), TRP152, THR827
	Curcumin	-6.98	01 (H1:Distance= 2.55 Å)	LEU335(H1), CYS336, VAL341
	EGCG	-7.07	05 (H1:Distance= 3.29 Å, H2:Distance= 3.08 Å, H3:Distance= 2.74 Å, H4:Distance= 3.23 Å), H5:Distance= 2.14 Å)	ARG357(H1), SER730(H2), THR791(H3), LYS733(H4), LEU821(H5), PRO793
	Piperine	-7.40	01 (H1:Distance= 3.25 Å)	ILE931(H1), ALA930, TYR200, VAL951, TRP886
Glycyrrhizin	-7.69	06 (H1:Distance= 3.02 Å, H2:Distance= 2.92 Å, H3:Distance= 3.10 Å, H4:Distance= 3.30 Å), H5:Distance= 1.80 Å, H6:Distance= 2.84 Å)	ASN61(H1), LYS129(H2), LYS378(H3), LYS150(H4), PHE140(H5), THR51(H6), PRO412, ILE410	