

Table S 1 Ligands docked to the SARS-CoV-2 proteins; binding energies, dissociation constants and active sites

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
1	4-Caffeoylquinic acid	124136972	Main Protease (MPro)	-7.96	1.45	Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.15	1.07	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Ile ²²² , Pro ²²³
			RNA-dependent RNA polymerase (RdRP)	-7.02	7.1	Tyr ¹⁴⁹ , Ala ¹⁷⁶ , Asn ¹⁷⁷ , Leu ¹⁷⁸ , Gly ¹⁷⁹ , Glu ¹⁸⁰ , Arg ¹⁸¹ , Gln ¹⁸⁴ , Asn ²¹³ , Arg ²⁴⁹ , Thr ²⁵² , Leu ²⁶¹
			Helicase	-8.3	0.826	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Glu ⁴¹⁸ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.43	3.55	Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷
			Spike Open Protein	-7.35	4.1	Gly ⁹⁰⁸ , Ile ⁹⁰⁹ , Gly ⁹¹⁰ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸ , Arg ¹⁰³⁹ , Val ¹⁰⁴⁰ , Asp ¹⁰⁴¹ , Tyr ¹⁰⁴⁷ , His ¹⁰⁴⁸ , Glu ¹⁰⁹² , Gly ¹⁰⁹³ , Arg ¹¹⁰⁷ , Asn ¹¹⁰⁸
			Spike Close Protein	-7.09	6.32	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Leu ³³⁵ , Val ³⁶² , Asp ³⁶⁴ , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰
2	(1S,4R,5R)-3-[3-(3,4-Dihydroxyphenyl)prop-2-enoyloxy]-1,4,5-trihydroxycyclohexane-1-carboxylic acid	60074140	Main Protease (MPro)	-8.01	1.36	Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁸ , Thr ¹⁹⁹ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-9.23	0.17	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸
			RNA-dependent RNA polymerase (RdRP)	-8.29	0.85	Val ⁵⁸⁸ , Ile ⁵⁸⁹ , Gly ⁵⁹⁰ , Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Leu ⁷⁵⁸ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.95	1.495	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.69	2.33	No binding site was found
			Spike Open Protein	-7.21	5.15	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-6.84	9.7	Arg ³⁵⁵ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Lys ⁴⁶² , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Glu ⁴⁶⁵ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷
3	1,2,4-Cyclopentanetrione	534963	Main Protease (MPro)	-6.25	26.05	Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Arg ¹⁸⁸ , Gln ¹⁸⁹
			Papain like protease (PLPro)	-8.2	0.97	Phe ⁶⁹ , His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Tyr ¹⁵⁴ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.02	38.86	Ala ⁴⁶ , Lys ⁴⁷ , Tyr ¹²⁹ , His ¹³³ , Asp ¹³⁵ , Asn ⁷⁰⁵ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Ala ⁷⁷¹ , Ser ⁷⁷² , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-6.68	12.67	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-6.72	11.8	Leu ¹⁹ , Ala ²² , Phe ²³
			Spike Open Protein	-5.87	50.05	Ile ⁷⁸⁸ , Tyr ⁷⁸⁹ , Lys ⁷⁹⁰ , Thr ⁷⁹¹ , Pro ⁷⁹² , Pro ⁷⁹³ , Lys ⁷⁹⁵ , Leu ⁸⁰⁶ , Pro ⁸⁰⁷ , Pro ⁸⁰⁹ , Lys ⁸¹⁴ , Gln ⁸⁷² , Ser ⁸⁷⁵ , Ala ⁸⁷⁹
			Spike Close Protein	-7.31	4.41	Glu ⁹⁶ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
4	11,14,17-Eicosatrienoic acid	5312529	Main Protease (MPro)	-4.53	477.24	Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-6.74	11.45	Arg ¹⁶⁶ , Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-4.79	308.76	Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Tyr ³⁸ , Asn ³⁹ , Val ⁴² , Phe ⁴⁸ , Lys ⁵⁰ , Lys ⁷³ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Tyr ²¹⁷ , Asp ²¹⁸ , Asp ²²¹ , Asn ⁷¹³
			Helicase	-4.99	220.3	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵
			E-channel proteins	-5.74	61.81	Leu ¹⁹ , Ala ²² , Phe ²³

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-3.95	1280.98	Pro ¹⁰⁷⁹ , Phe ¹⁰⁸⁹ , Pro ¹⁰⁹⁰ , Arg ¹¹⁰⁷ , Phe ¹¹²¹ , Ser ¹¹²³ , Gly ¹¹²⁴ , Asn ¹¹²⁵ , Val ¹¹²⁸ , Val ¹¹²⁹ , Ile ¹¹³⁰
			Spike Close Protein	-4.95	236.08	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹
5	11-Eicosenoic acid	5282768	Main Protease (MPro)	-4.11	979.48	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-6.42	19.65	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Ser ²⁴⁵ , Ala ²⁴⁶ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-4.11	969.61	Phe ⁴⁴¹ , Lys ⁵⁴⁵ , Tyr ⁵⁴⁶ , Ala ⁵⁴⁷ , Ile ⁵⁴⁸ , Arg ⁸³⁶ , Ala ⁸⁴⁰ , Phe ⁸⁴³ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Arg ⁸⁵⁸ , Leu ⁸⁶²
			Helicase	-4.76	322.608	Asn ¹⁷⁹ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-6.07	35.41	No binding site was found
			Spike Open Protein	-4.01	1155.66	Ile ¹¹⁹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹ , Pro ²³⁰
			Spike Close Protein	-6.21	28.2	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Leu ²²⁹
6	13-16-Docosadienoic acid	5282807	Main Protease (MPro)	-4.08	1026.88	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Phe ²²³ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-6.26	25.61	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Val ¹⁶⁵ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³
			RNA-dependent RNA polymerase (RdRP)	-5.03	204.88	Ser ²⁵⁵ , Tyr ²⁶⁵ , Ile ²⁶⁶ , Lys ²⁶⁷ , Trp ²⁶⁸ , Leu ²⁷⁰ , Val ³²⁰ , Phe ³²¹ , Pro ³²² , Pro ³²³ , Thr ³²⁴ , Leu ³⁸⁷ , Leu ³⁸⁸ , Leu ³⁸⁹ , Asp ³⁹⁰ , Thr ³⁹⁴ , Cys ³⁹⁵ , Phe ³⁹⁶ , Ser ³⁹⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Helicase	-4.34	655.449	Asp ³²⁸ , Lys ³²⁹ , Cys ³³⁰ , Ser ³³¹ , Arg ³³² , Lys ³⁴⁵ , Phe ³⁴⁶ , Lys ³⁴⁷ , Asn ³⁴⁹ , Ser ³⁵⁰ , Thr ³⁵¹ , Leu ³⁵² , Glu ³⁵³ , Gln ³⁵⁴
			E-channel proteins	-6.28	24.84	No binding site was found
			Spike Open Protein	-3.64	2161.61	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-4.5	500.33	Leu ³³⁵ , Cys ³³⁶ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Val ³⁶² , Ala ³⁶³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴ , Trp ⁴³⁶ , Arg ⁵⁰⁹
7	18, β -Glycyrrhetic acid	404621453	Main Protease (MPro)	-9.19	0.35	Lys ⁵ , Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷² , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-8.71	0.41	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-8.14	1.07	Arg ²⁴⁹ , Thr ²⁵² , Ser ²⁵⁵ , Tyr ²⁶⁵ , Thr ³¹⁹ , Val ³²⁰ , Phe ³²¹ , Pro ³²³ , Arg ³⁴⁹ , Thr ³⁹⁴ , Cys ³⁹⁵ , Phe ³⁹⁶ , Tyr ⁴⁵⁶ , Arg ⁴⁵⁷ , Asn ⁴⁵⁹ , Leu ⁴⁶⁰ , Pro ⁴⁶¹ , Pro ⁶⁷⁷
			Helicase	-9.91	0.054	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-9.72	0.07	No binding site was found
			Spike Open Protein	-7.99	1.38	His ¹¹⁰¹ , Trp ¹¹⁰² , Phe ¹¹⁰³ , Ile ¹¹¹⁴ , Ile ¹¹¹⁵ , Asn ¹¹³⁵ , Thr ¹¹³⁶ , Val ¹¹³⁷ , Tyr ¹¹³⁸ , Asp ¹¹³⁹ , Gln ¹¹⁴² , Pro ¹¹⁴³
			Spike Close Protein	-8.08	1.2	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
			Main Protease (MPro)	-4.55	462.17	Arg ⁴ , Lys ⁵ , Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹
			Papain like protease (PLPro)	-4.86	276.21	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-4.39	607.51	Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Ile ⁸⁶⁴ , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
8	1-Octen-3-ol	18827	Helicase	-4.47	525.43	Gln ²⁸¹ , Asp ⁴⁰¹ , Pro ⁴⁰² , Ala ⁴⁰³ , Pro ⁴¹⁹ , Lys ⁴³⁰ , Pro ⁴³⁴ , Phe ⁴³⁷ , Tyr ⁴⁵⁷ , Asp ⁴⁵⁸ , Asn ⁴⁵⁹ , Asn ⁵⁵⁹
			E-channel proteins	-4.5	503.72	No binding site was found
			Spike Open Protein	-4.16	900.21	Val ⁷²⁹ , Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Gln ⁷⁷⁴ , Thr ⁷⁷⁸ , Phe ⁷⁸² , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Leu ⁸⁶⁵ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-4.15	906.31	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
9	2,5-dihydroxyterephthalic acid	69131	Main Protease (MPro)	-7.22	5.09	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-7.22	5.14	Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.49	17.58	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-6.3	24.305	Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Leu ²³⁵
			E-channel proteins	-5.95	43.44	Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷
			Spike Open Protein	-6.53	16.29	Arg ⁴⁰³ , Tyr ⁴⁵³ , Ser ⁴⁹⁴ , Tyr ⁴⁹⁵ , Gly ⁴⁹⁶ , Phe ⁴⁹⁷ , Asn ⁵⁰¹ , Tyr ⁵⁰⁵
			Spike Close Protein	-6.37	21.42	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
10	2-Hydroxy-5-sulfobenzoic acid	7322	Main Protease (MPro)	-6.44	19.03	Phe ⁸ , Val ¹⁰⁴ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-7.05	6.76	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸
			RNA-dependent RNA polymerase (RdRP)	-5.91	46.71	Ala ³⁸³ , Ser ³⁸⁴ , Gly ³⁸⁵ , Asn ³⁸⁶
			Helicase	-6.74	11.546	Gln ²⁸¹ , Asp ⁴⁰¹ , Pro ⁴⁰² , Ala ⁴⁰³ , Pro ⁴¹⁹ , Met ⁴²⁹ , Lys ⁴³⁰ , Gly ⁴³³ , Pro ⁴³⁴ , Tyr ⁴⁵⁷ , Asp ⁴⁵⁸ , Asn ⁴⁵⁹
			E-channel proteins	-5.77	59.26	Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰

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				(kcal/mol)	(μ M)	
			Spike Open Protein	-5.08	189.89	Ser ⁷⁰⁴ , Val ⁷⁰⁵ , Ala ⁷⁰⁶ , Tyr ⁷⁰⁷ , Ser ⁷⁰⁸ , Ser ⁷¹¹ , Ile ⁷¹² , Ala ⁷¹³ , Asn ¹⁰⁷⁴
			Spike Close Protein	-6.42	19.68	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
11	2-Hydroxycinnamic acid	637540	Main Protease (MPro)	-6.47	18.12	Phe ³ , Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Val ²⁹⁶ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-6.71	12.15	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.15	30.84	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Tyr ⁵⁴⁶ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶ , cser ¹⁵ , cgl ¹⁹ , dmet ⁸⁷
			Helicase	-6.32	23.262	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-6.27	25.52	No binding site was found
			Spike Open Protein	-5.96	42.71	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Gln ⁷⁷⁴ , Val ⁸⁶⁰ , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-6.26	25.78	Val ³⁸² , Leu ³⁹⁰ , Cys ³⁹¹ , Thr ³⁹³ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Ala ⁵²² , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Phe ⁵⁶⁵
12	2R,3S-Catechin	9064	Main Protease (MPro)	-8.49	0.6	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.11	1.14	Arg ¹⁶⁶ , Glu ¹⁶⁷ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.25	4.84	Phe ⁴⁴¹ , Lys ⁵⁴⁵ , Tyr ⁵⁴⁶ , Ala ⁵⁴⁷ , Ile ⁵⁴⁸ , Ser ⁵⁴⁹ , Arg ⁵⁵⁵ , Arg ⁸³⁶ , Ala ⁸⁴⁰ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Arg ⁸⁵⁸ , Leu ⁸⁶²
			Helicase	-7.84	1.794	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹³ , Lys ⁴¹⁴ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , His ⁵⁵⁴
			E-channel proteins	-6.78	10.79	Ala ³² , Ile ³³ , Ala ³⁶

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-6.89	8.87	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-6.95	8.02	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
13	2S,3R-Catechin	73160	Main Protease (MPro)	-8.09	1.18	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-9.26	0.16	Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Tyr ¹⁵⁴ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-7.06	6.72	Lys ⁵⁹³ , Phe ⁵⁹⁴ , Cys ⁸¹³ , Ser ⁸¹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Arg ⁸³⁶ , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.54	2.972	Asn ¹⁷⁹ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.74	2.11	Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰ , Arg ⁶¹
			Spike Open Protein	-6.92	8.45	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-7.24	4.94	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
14	3,4-Dihydroxybenzoic acid	72	Main Protease (MPro)	-5.94	44.4	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-6.85	9.61	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.13	32.22	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Val ⁷⁶³ , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-6.65	13.35	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²²
			E-channel proteins	-5.47	98.32	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.8	55.76	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-6.22	27.54	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
15	3,4-Dimethoxybenzoic acid	7121	Main Protease (MPro)	-6.29	24.43	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Thr ¹¹¹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-6.06	36.02	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸
			RNA-dependent RNA polymerase (RdRP)	-5.35	120.8	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-5.71	64.911	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Leu ²³⁵
			E-channel proteins	-5.57	82.35	Leu ²⁸ , Leu ³¹ , Ala ³² , Thr ³⁵ , Cys ⁴⁰
			Spike Open Protein	-5.25	141.33	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Gly ⁷⁴⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-5.44	103.25	Leu ³³⁵ , Cys ³³⁶ , Pro ³³⁷ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Val ³⁶² , Ala ³⁶³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸
16	3-Acetoxy-4,5-dihydroxy	129855414	Main Protease (MPro)	-6.99	7.58	Arg ⁴⁰ , Pro ⁵² , Asn ⁵³ , Tyr ⁵⁴ , Glu ⁵⁵ , Asp ⁵⁶ , Met ⁸² , Asn ⁸⁴ , Cys ⁸⁵ , Thr ¹⁷⁵ , Gly ¹⁷⁹ , Asn ¹⁸⁰ , Phe ¹⁸¹ , Phe ¹⁸⁵ , Val ¹⁸⁶ , Asp ¹⁸⁷ , Arg ¹⁸⁸
	-3-prenyldihydrostilbene		Papain like protease (PLPro)	-9	0.25	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Glu ¹⁶⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-7.11	6.19	Arg ³³ , Phe ³⁵ , Ile ³⁷ , Asn ³⁹ , Val ⁴² , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Lys ⁷³ , Thr ¹²³ , Asp ²⁰⁸ , Asn ²⁰⁹ , Tyr ²¹⁷ , Asp ²¹⁸ , Asn ⁷¹³
			Helicase	-7.23	5.007	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-8.62	0.48	No binding site was found
			Spike Open Protein	-7.63	2.54	Ile ¹⁰⁵ , Leu ¹¹⁸ , Ile ¹¹⁹ , Val ¹²⁰ , Asn ¹²² , Val ¹²⁷ , Ile ¹²⁸ , Lys ¹²⁹ , Phe ¹³³ , Gln ¹³⁴ , Phe ¹³⁵ , Cys ¹³⁶ , Pro ¹³⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Leu ²⁴¹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-7.48	3.27	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
17	3-Deazaneplanocin A	73087	Main Protease (MPro)	-6.46	18.46	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Gln ¹⁸⁹
			Papain like protease (PLPro)	-7.62	2.61	Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-6.43	19.32	Glu ¹³⁶ , Gly ¹³⁷ , Asn ¹³⁸ , Cys ¹³⁹ , Asp ¹⁴⁰ , Lys ¹⁴³ , Phe ¹⁵⁷ , Asn ¹⁵⁸ , Lys ¹⁵⁹ , Lys ¹⁶⁰ , Asp ¹⁶¹ , Trp ¹⁶² , Tyr ¹⁶³
			Helicase	-6.91	8.608	Pro ⁴⁰⁶ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Glu ⁴¹⁸ , Pro ⁴¹⁹ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-5.78	57.77	Val ²⁹ , Ala ³² , Ile ³³ , Ala ³⁶ , Arg ³⁸
			Spike Open Protein	-5.78	58.46	Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-6.27	25.4	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Val ³⁶² , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰
18	4,7,10,13,16-Docosapentaenoic acid	5282848	Main Protease (MPro)	-4.86	272.04	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-7.77	2.03	Lys ¹⁵⁷ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-5.11	180.21	Lys ⁴²⁶ , Gly ⁴²⁷ , Phe ⁴²⁸ , Phe ⁴²⁹ , Lys ⁴³⁰ , Ser ⁴³³ , Ser ⁴³⁴ , Val ⁴³⁵ , Glu ⁸⁷⁶ , Asp ⁸⁷⁹ , His ⁸⁸² , Leu ⁸⁸³ , Gln ⁸⁸⁶
			Helicase	-5.85	51.772	Asn ¹⁷⁹ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asp ⁵³⁴ , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.04	6.89	No binding site was found
			Spike Open Protein	-5.12	177.5	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-6.18	29.56	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹
19	4-Hydroxybenzoic acid	135	Main Protease (MPro)	-6.04	37.57	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Thr ¹¹¹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³
			Papain like protease (PLPro)	-6.06	36.08	His ⁷³ , Thr ⁷⁴ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Cys ¹⁵⁵ , Asn ¹⁵⁶ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-5.45	101.18	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-5.97	42.28	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²²
			E-channel proteins	-5.42	106.8	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.32	127.07	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-5.92	45.69	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
20	4-Hydroxycinnamic acid	637542	Main Protease (MPro)	-6.68	12.71	Phe ³ , Lys ⁵ , Met ⁶ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-6.83	9.79	His ⁷³ , Thr ⁷⁴ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Cys ¹⁵⁵ , Asn ¹⁵⁶ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.33	23.07	Pro ³²³ , Thr ³²⁴ , Phe ³²⁶ , Gly ³²⁷ , Tyr ³⁴⁶ , His ³⁴⁷ , Phe ³⁴⁸ , Arg ³⁴⁹ , Glu ³⁵⁰ , Phe ³⁹⁶ , Asn ⁶²⁸ , Ser ⁶⁶⁴ , Val ⁶⁷⁵ , Lys ⁶⁷⁶ , Pro ⁶⁷⁷ , basn ¹¹⁸
			Helicase	-6.18	29.612	Val ⁴⁹⁶ , Leu ⁵⁰⁰ , Thr ⁵⁰¹ , Asn ⁵⁰³ , Trp ⁵⁰⁶ , Arg ⁵⁰⁷ , Ala ⁵⁰⁹ , Leu ⁵²⁶ , Gly ⁵²⁷ , Leu ⁵²⁸ , Tyr ⁵⁴³ , Ile ⁵⁴⁵ , Leu ⁵⁷³
			E-channel proteins	-6.29	24.51	No binding site was found
			Spike Open Protein	-6.49	17.55	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-6.65	13.31	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
21	4-o-Methylglycyrrhisoflavone	637542	Main Protease (MPro)	-6.91	8.56	Arg ¹³¹ , Thr ¹⁹⁹ , Ile ²⁰⁰ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-8.61	0.49	Pro ²⁴⁷ , Pro ²⁴⁸ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-7.16	5.65	Arg ¹⁹⁷ , Gly ²³⁰ , Val ²³¹ , Pro ²³² , Phe ²⁸³ , Asp ²⁸⁴ , Lys ²⁸⁸ , Tyr ²⁸⁹ , Trp ²⁹⁰ , Asp ²⁹¹ , Gln ²⁹² , Thr ²⁹³ , Tyr ²⁹⁴
			Helicase	-7.6	2.682	Ala ¹ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³⁰ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-7.95	1.48	No binding site was found
			Spike Open Protein	-6.58	15.15	Ser ⁷³⁰ , Thr ⁷⁷⁸ , Phe ⁸²³ , Val ⁸²⁶ , Thr ⁸²⁷ , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-6.17	30.17	His ¹¹⁰¹ , Trp ¹¹⁰² , Phe ¹¹⁰³ , Ile ¹¹¹⁴ , Ile ¹¹¹⁵ , Thr ¹¹³⁶ , Val ¹¹³⁷ , Tyr ¹¹³⁸
22	4-o-Methylneobavaisoflavone	637542	Main Protease (MPro)	-7.07	6.6	Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁹ , Tyr ²³⁷ , Asn ²³⁸ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Leu ²⁸⁶ , Leu ²⁸⁷ , Asp ²⁸⁹
			Papain like protease (PLPro)	-8.99	0.26	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Met ²⁰⁸
			RNA-dependent RNA polymerase (RdRP)	-6.52	16.51	Ser ²⁵⁵ , Tyr ²⁶⁵ , Ile ²⁶⁶ , Lys ²⁶⁷ , Trp ²⁶⁸ , Leu ²⁷⁰ , Val ³²⁰ , Phe ³²¹ , Pro ³²² , Thr ³²⁴
			Helicase	-7.84	1.782	Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asp ⁵³⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-8.15	1.06	No binding site was found
			Spike Open Protein	-5.89	47.82	Leu ⁵⁴ , Phe ⁸⁶ , Asn ⁸⁷ , Asp ⁸⁸ , Asn ¹⁹⁶ , Ile ¹⁹⁷ , Asn ²³⁴ , Ile ²³⁵ , Thr ²³⁶ , Pro ²⁷²
			Spike Close Protein	-6.52	16.68	Trp ⁸⁸⁶ , Gly ⁸⁸⁹ , Ala ⁸⁹⁰ , Tyr ⁹⁰⁴ , Ser ¹⁰³⁰ , Glu ¹⁰³¹ , Leu ¹⁰³⁴ , Gly ¹⁰³⁵ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸ , Arg ¹⁰³⁹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
23	6,9,12-Octadecatrienoic acid	5353640	Main Protease (MPro)	-4.45	544.39	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷
			Papain like protease (PLPro)	-4.85	276.68	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-4.88	266.59	Phe ⁴⁴¹ , Tyr ⁵⁴⁶ , Ala ⁵⁴⁷ , Ile ⁵⁴⁸ , Arg ⁸³⁶ , Ile ⁸³⁷ , Ala ⁸⁴⁰ , Phe ⁸⁴³ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Arg ⁸⁵⁸ , Ser ⁸⁶¹ , Leu ⁸⁶² , Asp ⁸⁶⁵
			Helicase	-5.63	74.42	Ala ⁴ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Glu ¹²⁸ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶ , Pro ²³⁸
			E-channel proteins	-6.26	25.74	Phe ²⁶ , Val ²⁹ , Thr ³⁰
			Spike Open Protein	-3.78	1698.07	His ⁶⁶ , Ala ⁶⁷ , Ile ⁶⁸ , Pro ⁸² , Asp ¹³⁸ , Pro ¹³⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Gln ²³⁹ , Thr ²⁴⁰ , Leu ²⁴¹ , Leu ²⁴² , Tyr ²⁶⁵
			Spike Close Protein	-5.3	130.33	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹
24	7,10,13,16-Docosatetraenoic acid	2033	Main Protease (MPro)	-4.64	395.7	Arg ¹³¹ , Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹
			Papain like protease (PLPro)	-5.61	76.72	Pro ²⁴⁷ , Pro ²⁴⁸ , Asn ²⁶⁷ , Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-5.36	117.58	Arg ⁵⁸³ , Ser ⁵⁹² , Phe ⁵⁹⁴ , Tyr ⁵⁹⁵ , Ser ⁸⁶¹ , Ile ⁸⁶⁴ , Asp ⁸⁶⁵ , Tyr ⁹¹⁵ , Pro ⁹¹⁸ , Glu ⁹¹⁹
			Helicase	-5.67	69.327	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-6.74	11.57	No binding site was found
			Spike Open Protein	-3.45	2963.8	Leu ⁵⁴ , Phe ⁸⁶ , Asn ⁸⁷ , Asp ⁸⁸ , Asn ¹⁹⁶ , Ile ¹⁹⁷ , Asp ¹⁹⁸ , Gly ¹⁹⁹ , Ile ²³³ , Asn ²³⁴ , Ile ²³⁵ , Pro ²⁷²
			Spike Close Protein	-5.22	148.92	Val ³²⁷ , Val ³⁸² , Ser ³⁸³ , Lys ³⁸⁶ , Asp ³⁸⁹ , Leu ³⁹⁰ , Cys ³⁹¹ , Phe ³⁹² , Thr ³⁹³ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Ala ⁵²² , Lys ⁵²⁸ , Asn ⁵⁴² , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Thr ⁵⁴⁷ , Phe ⁵⁶⁵

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
25	7,10,13,16-Docosatetraenoic acid, methyl ester	5352981	Main Protease (MPro)	-4.43	570.73	Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Gly ²⁷⁸ , Arg ²⁷⁹ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷
			Papain like protease (PLPro)	-6.55	15.78	Asp ¹⁶⁴ , Val ¹⁶⁵ , Arg ¹⁶⁶ , Met ²⁰⁸ , Ser ²⁴⁵ , Ala ²⁴⁶ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹ , Asp ³⁰²
			RNA-dependent RNA polymerase (RdRP)	-5.45	100.67	Val ³³⁵ , Asp ³³⁶ , Val ³³⁸ , Pro ³³⁹ , Phe ³⁴⁰ , Arg ³⁶⁵ , Leu ³⁶⁶ , Leu ³⁷¹
			Helicase	-4.79	309.801	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-6.57	15.38	Leu ¹⁹ , Phe ²⁰ , Ala ²² , Phe ²³ , Val ²⁴ , Phe ²⁶ , Leu ²⁷ , Thr ³⁰
			Spike Open Protein	-4.15	910.91	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-5.68	69.09	Cys ³³⁶ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ala ³⁷² , Ser ³⁷³ , Phe ³⁷⁴ , Ser ³⁷⁵ , Trp ⁴³⁶ , Asn ⁴³⁷ , Ser ⁴³⁸ , Asn ⁴⁴⁰ , Leu ⁴⁴¹ , Arg ⁵⁰⁹
26	8-Prenylmucronulatol	637051	Main Protease (MPro)	-6.99	7.48	Thr ²⁵ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.01	0.25	Pro ²⁴⁷ , Pro ²⁴⁸ , Asn ²⁶⁷ , Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-7.24	4.9	Tyr ³² , Lys ⁴⁷ , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Cys ¹³⁹ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷¹⁴ , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-7.39	3.835	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Gln ⁴⁰⁴ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.8	1.93	No binding site was found
			Spike Open Protein	-6.91	8.61	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Glu ⁴⁶⁵ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-7.07	6.58	Leu ³³⁵ , Cys ³³⁶ , Pro ³³⁷ , Phe ³³⁸ , Gly ³³⁹ , Glu ³⁴⁰ , Phe ³⁴² , Asn ³⁴³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴ , Trp ⁴³⁶
27	Aconitic acid	309	Main Protease (MPro)	-5.75	61.5	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-6.53	16.35	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-5.95	43.73	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-5.7	65.904	Gln ²⁸¹ , Asp ⁴⁰¹ , Pro ⁴⁰² , Ala ⁴⁰³ , Pro ⁴¹⁹ , Met ⁴²⁹ , Lys ⁴³⁰ , Pro ⁴³⁴ , Tyr ⁴⁵⁷ , Asp ⁴⁵⁸ , Asn ⁴⁵⁹ , Asn ⁵⁵⁹
			E-channel proteins	-5.05	198.41	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.33	124.74	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-5.45	100.67	Gly ⁷⁴⁴ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
28	Agaritrine	439517	Main Protease (MPro)	-6.6	14.55	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Ile ¹⁵² , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-7.1	6.24	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Glu ¹⁶⁷ , Tyr ¹⁷¹
			RNA-dependent RNA polymerase (RdRP)	-6.14	31.36	Lys ⁴⁷ , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Cys ¹³⁹ , Asp ¹⁴⁰ , Thr ¹⁴¹ , Leu ¹⁴² , Asn ⁷⁰⁵ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-6.64	13.623	Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵
			E-channel proteins	-6.2	28.63	Leu ²⁸ , Val ²⁹ , Ala ³²
			Spike Open Protein	-5.79	57.1	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-5.76	60.37	Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶
29	Agnuside	442416	Main Protease (MPro)	-7.28	4.61	Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Asp ¹⁵³ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Val ²⁹⁷ , Arg ²⁹⁸ , Ser ³⁰¹ , Val ³⁰³
			Papain like protease (PLPro)	-9.07	0.22	Phe ⁶⁹ , His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Tyr ¹⁵⁴ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.17	29.86	Asp ²⁶⁹ , Leu ²⁷¹ , Lys ²⁷² , Tyr ²⁷³ , Asp ²⁷⁴ , Phe ²⁷⁵ , Glu ²⁷⁷
			Helicase	-7.38	3.874	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵
			E-channel proteins	-7.69	2.33	Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰
			Spike Open Protein	-6	40.12	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Leu ²²⁶ , Val ²²⁷
			Spike Close Protein	-6.14	31.41	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
30	Alizarin	6293	Main Protease (MPro)	-7.42	3.65	Val ¹⁰⁴ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-7.28	4.58	Val ¹⁸⁷ , Gln ¹⁹⁵ , Thr ¹⁹⁷ , Ile ²²² , Pro ²²³ , Cys ²²⁴ , Thr ²²⁵ , Ala ²³⁰ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.19	5.37	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Tyr ⁵⁴⁶ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶ , cser ¹⁵ , cgl ¹⁸ , cgl ¹⁹
			Helicase	-7.75	2.071	Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.24	4.92	No binding site was found
			Spike Open Protein	-6.58	15.15	Glu ⁵⁵⁴ , Ser ⁵⁵⁵ , Asn ⁵⁵⁶ , Lys ⁵⁵⁷ , Lys ⁵⁵⁸ , Phe ⁵⁵⁹ , Leu ⁵⁶⁰ , Arg ⁵⁷⁷ , Leu ⁵⁸² , Glu ⁵⁸³ , Ile ⁵⁸⁴

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-7.05	6.82	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
31	Alpha pinenene	6654	Main Protease (MPro)	-5.37	116.2	Trp ²¹⁸ , Phe ²¹⁹ , Asn ²²¹ , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Asn ²⁷⁷
			Papain like protease (PLPro)	-5.38	113.68	Asp ¹⁶⁴ , Val ¹⁶⁵ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-4.91	250.87	Ser ⁵⁹² , Phe ⁵⁹⁴ , Tyr ⁵⁹⁵ , Ile ⁸⁶⁴ , Tyr ⁹¹⁵
			Helicase	-6.18	29.512	Val ⁴⁹⁶ , Phe ⁴⁹⁹ , Leu ⁵⁰⁰ , Thr ⁵⁰¹ , Asn ⁵⁰³ , Trp ⁵⁰⁶ , Arg ⁵⁰⁷ , Ala ⁵⁰⁹ , Leu ⁵²⁶ , Leu ⁵²⁸ , Tyr ⁵⁴³ , Ile ⁵⁴⁵ , Leu ⁵⁷³
			E-channel proteins	-5.87	49.47	No binding site was found
			Spike Open Protein	-5.68	68.86	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-5.9	47.42	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
32	Anhydrosecoisolariciresinol	9974771	Main Protease (MPro)	-6.55	15.83	Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-7.23	5.02	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Glu ¹⁶⁷ , Tyr ²⁶⁸ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-6.42	19.78	Asp ⁷¹⁷ , Tyr ⁷¹⁹ , Val ⁷²⁰ , Asn ⁷²² , Leu ⁷²³ , Arg ⁷²⁶ , Glu ⁷⁴⁴ , Ala ⁷⁴⁷ , Tyr ⁷⁴⁸ , Lys ⁷⁵¹ , His ⁷⁵² , Tyr ⁷⁷⁰
			Helicase	-7.18	5.504	Gly ³ , Ala ⁴ , Val ⁶ , Arg ²¹ , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-6.48	17.85	Leu ²⁸ , Val ²⁹ , Ala ³²
			Spike Open Protein	-5.78	58.36	Arg ⁴⁰³ , Tyr ⁴⁵³ , Ser ⁴⁹⁴ , Tyr ⁴⁹⁵ , Gly ⁴⁹⁶ , Phe ⁴⁹⁷ , Asn ⁵⁰¹ , Tyr ⁵⁰⁵
			Spike Close Protein	-6.17	30.22	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Glu ¹⁹¹ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Lys ²⁰⁶ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
33	Apigenin	5280443	Main Protease (MPro)	-7.26	4.74	Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , His ¹⁷² , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.21	0.18	Phe ⁶⁹ , His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-7.48	3.28	Gly ⁵⁹⁰ , Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.45	3.489	Asn ¹⁷⁹ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.37	3.99	Ile ⁴⁶ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷
			Spike Open Protein	-6.86	9.4	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-7.38	3.89	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Arg ¹⁹⁰ , Phe ¹⁹² , Ser ²⁰⁵ , Lys ²⁰⁶ , His ²⁰⁷ , Leu ²²⁶
34	Ascorbic acid	54670067	Main Protease (MPro)	-4.96	232.53	Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁸ , Thr ¹⁹⁹ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-5.66	71.1	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶⁷ , Tyr ¹⁷¹
			RNA-dependent RNA polymerase (RdRP)	-5.95	43.29	Tyr ⁴⁵⁶ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Val ⁵⁵⁷ , Asp ⁶²³ , Arg ⁶²⁴ , Lys ⁶⁷⁶ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸²
			Helicase	-6.51	16.994	Trp ¹¹⁴ , Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Lys ¹³¹ , Ala ¹³⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²² , Asn ⁴²³
			E-channel proteins	-4.54	471.63	No binding site was found
			Spike Open Protein	-5.79	56.62	Val ⁷²⁹ , Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Thr ⁷⁷⁸ , Phe ⁷⁸² , Pro ⁸⁶³ , Leu ⁸⁶⁵ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-5.54	86.92	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Val ³⁶² , Cys ⁵²⁵ , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
35	Baicalin	64982	Main Protease (MPro)	-8.85	0.33	Val ¹⁰⁴ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Ile ¹⁵² , Asp ¹⁵³ , Tyr ¹⁵⁴ , Pro ²⁵² , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Val ²⁹⁷ , Arg ²⁹⁸ , Val ³⁰³
			Papain like protease (PLPro)	-10.82	0.01	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Val ¹⁶⁵ , Arg ¹⁶⁶ , Glu ¹⁶⁷ ,
						Tyr ¹⁷¹ , Val ²⁰² , Met ²⁰⁶ , Met ²⁰⁸ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³
			RNA-dependent RNA polymerase (RdRP)	-9.01	0.25	Val ³¹ , Tyr ³² , Lys ⁴⁷ , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Cys ¹³⁹ , Thr ¹⁴¹ , Asn ⁷⁰⁵ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-8.9	0.29	Asn ¹⁷⁷ , Arg ¹⁷⁸ , Thr ¹⁹⁹ , Phe ²⁰⁰ , Glu ²⁰¹ , Lys ²⁰² , Arg ²¹² , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Gln ⁵³¹ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-8.89	0.3	No binding site was found
			Spike Open Protein	-7.47	3.37	Met ⁷⁴⁰ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Gly ⁸⁵⁷ , Val ⁹⁶³ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
36	Balsacone A	71602340	Spike Close Protein	-7.95	1.48	Tyr ⁷⁸⁹ , Lys ⁷⁹⁰ , Thr ⁷⁹¹ , Lys ⁷⁹⁵ , Ser ⁸⁰³ , Gln ⁸⁰⁴ , Leu ⁸⁰⁶ , Pro ⁸⁰⁷ , Asp ⁸⁰⁸ , Pro ⁸⁰⁹ , Ser ⁸¹⁶ , Phe ⁸¹⁷ , Ser ⁸⁷⁵ , Ala ⁸⁷⁶ , Ala ⁸⁷⁹
			Main Protease (MPro)	-7.37	3.93	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.55	0.1	Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Val ¹⁶⁵ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Gly ²⁶⁶ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-7.54	3	Tyr ³² , Ala ⁴⁶ , Lys ⁴⁷ , Tyr ¹²⁹ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷¹⁴ , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-7.69	2.319	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			E-channel proteins	-8.52	0.57	Phe ²³ , Phe ²⁶ , Leu ²⁷ , Thr ³⁰ , Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-6.79	10.63	Arg ⁴⁴ , His ⁴⁹ , Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-6.83	9.85	Gly ⁹⁰⁸ , Ile ⁹⁰⁹ , Gly ⁹¹⁰ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸ , Val ¹⁰⁴⁰ , Asp ¹⁰⁴¹ , Lys ¹⁰⁴⁵ , Gly ¹⁰⁴⁶ , Tyr ¹⁰⁴⁷ , His ¹⁰⁴⁸ , Arg ¹¹⁰⁷ , Asn ¹¹⁰⁸
37	Behenic acid	8215	Main Protease (MPro)	-4.12	959.84	Arg ¹³¹ , Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹
			Papain like protease (PLPro)	-5.6	78.02	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Gly ²⁶⁶ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-4.19	854.32	His ⁶¹³ , Phe ⁷⁶⁶ , Ser ⁷⁶⁸ , Ala ⁷⁷¹ , Ser ⁷⁷² , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Ile ⁷⁷⁹ , Lys ⁷⁸⁰ , Glu ⁷⁹⁶ , Cys ⁷⁹⁹ , Thr ⁸⁰¹ , Thr ⁸⁰³
			Helicase	-4.51	493.62	Gly ³ , Ala ⁴ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.55	86.05	No binding site was found
			Spike Open Protein	-3.21	4414.08	Arg ³⁵⁵ , Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁸
			Spike Close Protein	-5.15	168.16	Leu ³³⁵ , Cys ³³⁶ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Val ³⁶² , Ala ³⁶³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴ , Trp ⁴³⁶ , Asn ⁴³⁷ , Leu ⁴⁴¹
38	Benzoic acid	243	Main Protease (MPro)	-5.93	45.23	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Thr ¹¹¹ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³
			Papain like protease (PLPro)	-6.11	33.44	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.48	17.67	No binding site was found
			Helicase	-6.02	38.531	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Lys ¹³¹ , Ala ¹³⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²²
			E-channel proteins	-5.57	83.05	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-5	215.52	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-5.82	53.91	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
39	Biochanin	5280373	Main Protease (MPro)	-6.85	9.59	Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Met ⁴⁹ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.04	0.24	Thr ⁷⁴ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-7.51	3.12	Arg ³³ , Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Tyr ³⁸ , Lys ⁵⁰ , Val ⁷¹ , Lys ⁷³ , Thr ¹²³ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Tyr ²¹⁷ , Asp ²¹⁸ , Asp ²²¹
			Helicase	-7.31	4.397	Asn ¹⁷⁷ , Asn ¹⁷⁹ , Glu ²⁰¹ , Pro ⁵¹⁴ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³² , Val ⁵³³ , Asp ⁵³⁴ , Arg ⁵⁶⁰
			E-channel proteins	-6.81	10.19	No binding site was found
			Spike Open Protein	-6.29	24.59	Tyr ³⁸ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Gly ²⁸³
			Spike Close Protein	-6.78	10.77	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Thr ³³³ , Leu ³³⁵ , Val ³⁶² , Asp ³⁶⁴ , Cys ⁵²⁵ , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰
40	Butein	5281222	Main Protease (MPro)	-7.74	2.14	Phe ³ , Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Ile ¹⁵² , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-7.76	2.04	Pro ⁵⁹ , Asp ⁶² , Arg ⁶⁵ , Val ⁶⁶ , Ala ⁶⁸ , Phe ⁶⁹ , Tyr ⁷² , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Pro ⁷⁷ , Phe ⁷⁹ , Leu ⁸⁰
			RNA-dependent RNA polymerase (RdRP)	-7.39	3.83	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Tyr ⁵⁴⁶ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶ , Ile ⁸⁴⁷
			Helicase	-7.09	6.342	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Arg ⁵⁶⁰
			E-channel proteins	-7.28	4.64	No binding site was found

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-6.77	10.88	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-7.57	2.81	Tyr ⁷⁸⁹ , Lys ⁷⁹⁰ , Thr ⁷⁹¹ , Pro ⁷⁹² , Asp ⁷⁹⁶ , Phe ⁷⁹⁷ , Ala ⁸⁷⁹ , Ile ⁸⁸² , Thr ⁸⁸³ , Ala ⁸⁹³ , Gln ⁸⁹⁵ , Ile ⁸⁹⁶ , Pro ⁸⁹⁷ , Phe ⁸⁹⁸
41	Caffeic acid	689043	Main Protease (MPro)	-7.09	6.4	Phe ³ , Met ⁶ , Phe ⁸ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-7.28	4.59	His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.76	11.13	Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Ile ⁸⁶⁴ , Asp ⁸⁶⁵ , Ala ⁸⁶⁶ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.15	5.731	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Lys ¹³⁹ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²²
			E-channel proteins	-6.39	20.77	No binding site was found
			Spike Open Protein	-6.65	13.37	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Glu ²²⁴ , Pro ²²⁵ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-6.69	12.58	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
42	Cinnamic acid	444539	Main Protease (MPro)	-6.44	19.09	Phe ³ , Lys ⁵ , Met ⁶ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-6.81	10.26	Lys ¹⁵⁷ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Val ¹⁶⁵ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-6.23	27.17	Pro ³²³ , Thr ³²⁴ , Phe ³²⁶ , Gly ³²⁷ , Tyr ³⁴⁶ , His ³⁴⁷ , Phe ³⁴⁸ , Arg ³⁴⁹ , Glu ³⁵⁰ , Phe ³⁹⁶ , Asn ⁶²⁸ , Ser ⁶⁶⁴ , Val ⁶⁷⁵ , Lys ⁶⁷⁶ , Pro ⁶⁷⁷ basn ¹¹⁸
			Helicase	-6.24	26.535	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-6.41	19.92	No binding site was found

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-6.19	29.21	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-6.15	30.94	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Val ²²⁷
43	Citric acid	311	Main Protease (MPro)	-5.24	145.44	Phe ⁸ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Ile ¹⁵² , Asp ¹⁵³ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-6.18	29.36	His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-5.34	122.03	Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-5.74	61.706	Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-4.83	286.66	No binding site was found
			Spike Open Protein	-5.27	138.26	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-5.71	64.8	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Val ³⁶² , Cys ⁵²⁵ , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰
44	Cryptochlorogenic acid	9798666	Main Protease (MPro)	-7.99	1.4	Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁸ , Thr ¹⁹⁹ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-9.25	0.16	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸
			RNA-dependent RNA polymerase (RdRP)	-7.39	3.82	Tyr ¹⁴⁹ , Cys ¹⁵¹ , Ala ¹⁷⁶ , Asn ¹⁷⁷ , Leu ¹⁷⁸ , Gly ¹⁷⁹ , Glu ¹⁸⁰ , Arg ¹⁸¹ , Gln ¹⁸⁴ , Arg ²⁴⁹ , Thr ²⁵² , Leu ²⁶¹
			Helicase	-7.95	1.501	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.52	3.08	Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰ , Arg ⁶¹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-7.26	4.81	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-7.14	5.8	Gly ⁹⁰⁸ , Ile ⁹⁰⁹ , Gly ⁹¹⁰ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸ , Val ¹⁰⁴⁰ , Gly ¹⁰⁴⁶ , Tyr ¹⁰⁴⁷ , His ¹⁰⁴⁸ , Glu ¹⁰⁹² , Gly ¹⁰⁹³ , Gln ¹¹⁰⁶ , Arg ¹¹⁰⁷ , Asn ¹¹⁰⁸
45	curcumin	969516	Main Protease (MPro)	-7.28	4.62	Lys ⁵ , Arg ¹³¹ , Lys ¹³⁷ , Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-9.09	0.22	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Ala ²⁴⁶ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-7.3	4.46	Tyr ³² , Lys ⁴⁷ , Tyr ¹²² , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asn ¹³⁸ , Cys ¹³⁹ , Asp ¹⁴⁰ , Thr ¹⁴¹ , Leu ¹⁴²
			Helicase	-7.4	3.79	Leu ¹⁷⁶ , Asn ¹⁷⁷ , Arg ¹⁷⁸ , Thr ¹⁹⁹ , Phe ²⁰⁰ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Arg ²¹² , Asn ⁵¹⁶ , Ser ⁵¹⁷ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Gln ⁵³¹ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-8.27	0.87	Ile ⁴⁶ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰
			Spike Open Protein	-6.63	13.93	Ile ¹⁰⁵ , Leu ¹¹⁸ , Val ¹²⁰ , Asn ¹²² , Ala ¹²³ , Asn ¹²⁵ , Val ¹²⁷ , Lys ¹²⁹ , Phe ¹³⁵ , Cys ¹³⁶ , Pro ¹³⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Val ¹⁷¹ , Leu ²⁴¹
			Spike Close Protein	-7.32	4.29	Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷
46	Eicosadienoic acid	6439848	Main Protease (MPro)	-4.84	282.81	Arg ¹³¹ , Thr ¹⁹⁹ , Tyr ²³⁷ , Asn ²³⁸ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹
			Papain like protease (PLPro)	-6.34	22.45	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-4.33	672.25	Arg ³⁰⁵ , Glu ⁴⁷⁴ , Asp ⁴⁷⁷ , Lys ⁴⁷⁸ , Phe ⁴⁸⁰ , Asp ⁴⁸¹ , Val ⁶³⁷ , Arg ⁶⁴⁰ , Lys ⁶⁴¹ , Thr ⁶⁴³ , Val ⁷³⁷ , Thr ⁷³⁹ , Val ⁷⁴² , Asn ⁷⁴³
			Helicase	-5.06	194.762	Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			E-channel proteins	-6.04	37.19	No binding site was found
			Spike Open Protein	-4.37	630.49	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Thr ⁷³⁴ , Val ⁸⁶⁰ , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Val ⁹⁵² , Asn ⁹⁵⁵ , Ala ⁹⁵⁶ , Leu ⁹⁵⁹ , Asn ⁹⁶⁰ , His ¹⁰⁵⁸
			Spike Close Protein	-6.17	29.86	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Leu ²²⁹
47	Ellagic acid	5281855	Main Protease (MPro)	-7.93	1.54	Phe ⁸ , Lys ¹⁰² , Val ¹⁰⁴ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Ile ¹⁵² , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-8.41	0.69	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶²
			RNA-dependent RNA polymerase (RdRP)	-7.59	2.72	Lys ⁴⁷ , Tyr ¹²⁹ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-8.08	1.189	Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-6.77	10.98	Leu ²⁸ , Val ²⁹ , Ala ³² , Ile ³³
			Spike Open Protein	-8.1	1.16	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Gln ⁷⁷⁴ , Thr ⁷⁷⁸ , Phe ⁸²³ , Val ⁸⁶⁰ , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-7.41	3.71	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶
48	Epicatechin	72276	Main Protease (MPro)	-7.18	5.45	Arg ¹³¹ , Lys ¹³⁷ , Asp ¹⁹⁷ , Thr ¹⁹⁹ , Val ²⁰⁴ , Tyr ²³⁷ , Asn ²³⁸ , Tyr ²³⁹ , Leu ²⁷² , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹
			Papain like protease (PLPro)	-9.28	0.16	Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Tyr ¹⁵⁴ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-7.39	3.84	Gly ⁵⁹⁰ , Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.22	5.127	Asn ¹⁷⁹ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Glu ⁴¹⁸ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
49	Eriodictyol	440735	E-channel proteins	-7.06	6.65	Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰
			Spike Open Protein	-7.01	7.26	Tyr ³⁸ , Pro ³⁹ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-7.21	5.18	Asp ⁴²⁰ , Tyr ⁴²¹ , Asn ⁴²² , Tyr ⁴²³ , Lys ⁴²⁴ , Lys ⁴⁶² , Phe ⁴⁶⁴ , Glu ⁴⁶⁵ , Arg ⁴⁶⁶ , Asp ⁴⁶⁷
			Main Protease (MPro)	-7.62	2.58	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.13	1.11	Arg ¹⁸³ , Leu ¹⁸⁵ , Val ¹⁸⁷ , Thr ¹⁹⁷ , Leu ¹⁹⁹ , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.61	2.65	Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.77	2.03	Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
50	Euchrestafavanone A	484588	E-channel proteins	-7.25	4.86	Ile ⁴⁶ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷
			Spike Open Protein	-7.2	5.29	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-7	7.44	Ala ⁹⁵⁸ , Thr ⁹⁶¹ , Leu ⁹⁶² , Gln ⁹⁶⁵ , Phe ⁹⁷⁰ , Gly ⁹⁹⁹ , Gln ¹⁰⁰² , Ser ¹⁰⁰³ , Thr ¹⁰⁰⁶ , Tyr ¹⁰⁰⁷ , Gln ¹⁰¹⁰
			Main Protease (MPro)	-7.94	1.51	Ser ⁴⁶ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Ala ¹⁹¹ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.95	0.05	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Arg ¹⁶⁶ , Glu ¹⁶⁷ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Tyr ²⁶⁸
50	Euchrestafavanone A	484588	RNA-dependent RNA polymerase (RdRP)	-8.25	0.9	Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Tyr ³⁸ , Asn ³⁹ , Val ⁴² , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Asp ²¹⁸ , Asp ²²¹ , Asn ⁷¹³

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Helicase	-8.88	0.308	Pro ¹⁷⁵ , Leu ¹⁷⁶ , Asn ¹⁷⁷ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Asp ²⁰⁴ , Val ⁴⁸⁴ , Asn ⁵¹⁶ , Ser ⁵¹⁷ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³² , Val ⁵³³ , Asp ⁵³⁴
			E-channel proteins	-8.9	0.3	Arg ⁶¹ , Asn ⁶⁴
			Spike Open Protein	-7.58	2.78	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-7.14	5.83	Arg ³⁵⁵ , Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Lys ⁴⁶² , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶
51	Ferulic acid	445858	Main Protease (MPro)	-6.29	24.35	Arg ⁴ , Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-6.62	14.09	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-6.08	34.76	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Phe ⁴⁴¹ , Tyr ⁵⁴⁶ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶
			Helicase	-6.24	26.715	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-6.35	22	No binding site was found
			Spike Open Protein	-5.67	70.03	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-6.94	8.25	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
			Main Protease (MPro)	-8.12	1.12	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Arg ¹⁸⁸ , Gln ¹⁸⁹
			Papain like protease (PLPro)	-10.08	0.04	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Arg ¹⁶⁶ , Glu ¹⁶⁷ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
52	Flemiflavanone D	42607928	RNA-dependent RNA polymerase (RdRP)	-8.05	1.27	Leu ²⁷⁰ , Pro ³²² , Pro ³²³ , Thr ³²⁴ , Arg ³⁴⁹ , Leu ³⁸⁷ , Leu ³⁸⁸ , Leu ³⁸⁹ , Asp ³⁹⁰ , Thr ³⁹³ , Thr ³⁹⁴ , Cys ³⁹⁵ , Phe ³⁹⁶ , Ser ³⁹⁷
			Helicase	-8.21	0.959	Leu ¹⁷⁶ , Asn ¹⁷⁷ , Arg ¹⁷⁸ , Asn ¹⁷⁹ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Asp ²⁰⁴ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Gln ⁵³¹ , Thr ⁵³² , Asp ⁵³⁴ , Ser ⁵³⁵
			E-channel proteins	-8.18	1.01	No binding site was found
			Spike Open Protein	-7.81	1.89	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Thr ⁷⁷⁸ , Phe ⁸²³ , Val ⁸²⁶ , Thr ⁸²⁷ , Val ⁸⁶⁰ , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Val ⁹⁵² , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸
			Spike Close Protein	-8.01	1.34	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Ser ⁴⁵ , Glu ²²⁴ , Pro ²²⁵ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
53	Formononetin	5280378	Main Protease (MPro)	-7.04	6.95	Thr ²⁵ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.17	1.02	Lys ¹⁵⁷ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³
			RNA-dependent RNA polymerase (RdRP)	-6.54	16.13	Phe ³⁵ , Ile ³⁷ , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Asp ²¹⁸ , Asp ²²¹
			Helicase	-7.31	4.375	Pro ¹⁷⁵ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.15	5.75	Leu ²⁸ , Val ²⁹ , Leu ³¹ , Ala ³² , Thr ³⁵ , Cys ⁴⁰
			Spike Open Protein	-6.4	20.29	Tyr ³⁸ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-6.76	11.11	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Leu ³³⁵ , Val ³⁶² , Asp ³⁶⁴ , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰
			Main Protease (MPro)	-4.79	310.85	Met ⁶ , Ala ⁷ , Phe ⁸ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³
			Papain like protease (PLPro)	-5.63	74.8	No binding site was found

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
54	Fumaric acid	444972	RNA-dependent RNA polymerase (RdRP)	-5.6	79.08	Asp ⁴⁵² , Tyr ⁴⁵³ , Tyr ⁴⁵⁵ , Tyr ⁴⁵⁶ , Met ⁵⁴² , Thr ⁵⁵⁶ , Val ⁵⁵⁷ , Ala ⁵⁵⁸ , Asp ⁶²³ , Arg ⁶²⁴ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸²
			Helicase	-6.17	30.065	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Tyr ⁴²¹ , Phe ⁴²² , Asn ⁴²³
			E-channel proteins	-4.39	601.39	No binding site was found
			Spike Open Protein	-4.73	342.82	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Gln ⁷⁷⁴ , Thr ⁷⁷⁸ , Pro ⁸⁶³ , Ile ⁸⁷⁰ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-5.06	195.09	Ser ⁷³⁰ , Thr ⁷⁷⁸ , Pro ⁸⁶³ , Leu ⁸⁶⁵ , Thr ⁸⁶⁶ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸
55	Galangin	5281616	Main Protease (MPro)	-7.88	1.68	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.49	0.6	Arg ¹⁶⁶ , Met ²⁰⁸
			RNA-dependent RNA polymerase (RdRP)	-7.21	5.21	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Tyr ⁵⁴⁶ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶
			Helicase	-7.21	5.214	Ala ¹³⁵ , Leu ¹³⁸ , Lys ¹³⁹ , Glu ¹⁴² , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Met ³⁷⁸ , Ala ³⁷⁹ , Thr ³⁸⁰ , Tyr ³⁸² , Asp ³⁸³ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰
			E-channel proteins	-7.37	3.94	Leu ²⁸ , Val ²⁹ , Ala ³² , Ile ³³ , Ala ³⁶
			Spike Open Protein	-7.24	4.94	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Phe ²⁰¹ , Ile ²⁰³ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
			Spike Close Protein	-7.03	7.03	Leu ³³⁵ , Cys ³³⁶ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Val ³⁶² , Ala ³⁶³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴
			Main Protease (MPro)	-6.59	14.9	Met ⁶ , Ala ⁷ , Phe ⁸ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-7.1	6.25	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.5	17.31	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Val ⁷⁶³ , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
56	Gallic acid	370	Helicase	-5.84	52.21	Val ⁴⁹⁶ , Arg ⁴⁹⁷ , Leu ⁵⁰⁰ , Thr ⁵⁰¹ , Trp ⁵⁰⁶ , Arg ⁵⁰⁷ , Ala ⁵⁰⁹ , Leu ⁵²⁶ , Gly ⁵²⁷ , Leu ⁵²⁸ , Tyr ⁵⁴³ , Ile ⁵⁴⁵ , Leu ⁵⁷³
			E-channel proteins	-5.23	147.92	No binding site was found
			Spike Open Protein	-5.72	63.82	Gly ⁹⁰⁸ , Ile ⁹⁰⁹ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸ , Arg ¹⁰³⁹ , Val ¹⁰⁴⁰ , Asp ¹⁰⁴¹ , Gly ¹⁰⁴⁶ , Tyr ¹⁰⁴⁷ , His ¹⁰⁴⁸
			Spike Close Protein	-6.52	16.63	Cys ³⁹¹ , Phe ³⁹² , Thr ³⁹³ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Pro ⁵²¹ , Ala ⁵²² , Thr ⁵²³ , Phe ⁵⁴³ , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Gln ⁵⁶⁴ , Phe ⁵⁶⁵
57	Gensitic acid	3469	Main Protease (MPro)	-6.59	14.7	Phe ³ , Met ⁶ , Ala ⁷ , Phe ⁸ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Val ²⁹⁶ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-6.56	15.44	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.11	33.16	Phe ³²⁶ , Gly ³²⁷ , Tyr ³⁴⁶ , His ³⁴⁷ , Phe ³⁴⁸ , Arg ³⁴⁹ , Glu ³⁵⁰ , Asn ⁶²⁸ , Ser ⁶⁶⁴ , Val ⁶⁷⁵ , Lys ⁶⁷⁶ , Pro ⁶⁷⁷ , Gly ⁶⁷⁸
			Helicase	-7.09	6.396	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Lys ¹³¹ , Ala ¹³⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²²
			E-channel proteins	-5.56	84.61	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-6.05	36.63	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-6.01	39.65	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Main Protease (MPro)	-6.45	18.71	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Thr ¹¹¹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³
			Papain like protease (PLPro)	-6.51	16.82	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.16	30.42	Arg ³⁰⁵ , Arg ⁴⁶⁷ , Leu ⁴⁷⁰ , Phe ⁴⁷¹ , Glu ⁴⁷⁴ , Cys ⁷³⁰ , Leu ⁷³¹ , Arg ⁷³³ , Asn ⁷³⁴ , Arg ⁷³⁵ , Val ⁷³⁷ , Asp ⁷³⁸

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
58	Gentisic acid	3469	Helicase	-5.99	40.807	Val ⁴⁹⁶ , Arg ⁴⁹⁷ , Phe ⁴⁹⁹ , Leu ⁵⁰⁰ , Thr ⁵⁰¹ , Trp ⁵⁰⁶ , Arg ⁵⁰⁷ , Ala ⁵⁰⁹ , Leu ⁵²⁶ , Tyr ⁵⁴³ , Ile ⁵⁴⁵ , Leu ⁵⁷³
			E-channel proteins	-5.56	84.32	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.89	47.99	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-6.25	26.09	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
59	Glycyrrhisoflavone	5317764	Main Protease (MPro)	-7.65	2.49	Leu ²⁷ , His ⁴¹ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Gly ¹⁷⁰ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.34	0.14	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Glu ¹⁶⁷ , Tyr ¹⁷¹ , Tyr ²⁶⁸ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-8.01	1.34	Arg ³³ , Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Tyr ³⁸ , Asn ³⁹ , Lys ⁵⁰ , Lys ⁷³ , Thr ¹²³ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Tyr ²¹⁷ , Asp ²¹⁸ , Asp ²²¹
			Helicase	-8.58	0.514	Asn ¹⁷⁷ , Asn ¹⁷⁹ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Asp ²⁰⁴ , Val ⁴⁸⁴ , Ser ⁴⁸⁶ , Pro ⁵¹⁴ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Ser ⁵¹⁷ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³² , Val ⁵³³ , Asp ⁵³⁴ , Arg ⁵⁶⁰
			E-channel proteins	-8.06	1.23	Arg ⁶¹ , Asn ⁶⁴ , Leu ⁶⁵
			Spike Open Protein	-7.33	4.22	His ¹¹⁰¹ , Trp ¹¹⁰² , Phe ¹¹⁰³ , Ile ¹¹¹⁴ , Ile ¹¹¹⁵ , Thr ¹¹¹⁶ , Asn ¹¹³⁵ , Thr ¹¹³⁶ , Tyr ¹¹³⁸ , Pro ¹¹⁴⁰
			Spike Close Protein	-7.88	1.67	Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Lys ²⁰⁶ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
			Main Protease (MPro)	-9.57	0.11	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , Gly ²⁹ , His ⁴¹ , Cys ⁴⁴ , Ser ⁴⁶ , Met ⁴⁹ , Tyr ¹¹⁸ , Asn ¹¹⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶
				-9.46	0.76	Arg ¹³¹ , Asn ¹³³ , Thr ¹³⁵ , Val ¹³⁷ , Thr ¹⁶⁹ , Val ¹⁷¹ , Ala ¹⁹⁴ , Gly ¹⁹⁵ , Thr ¹⁹⁶ , Asp ¹⁹⁷ ,

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
60	Glycyrrhizin	14982		-9.46	0.76	Thr ¹⁹⁸ , Thr ¹⁹⁹ , Tyr ²³⁷ , Asn ²³⁸ , Tyr ²³⁹ , Leu ²⁷² , Leu ²⁸⁶ , Leu ²⁸⁷ , Asp ²⁸⁹
			Papain like protease (PLPro)	-9.23	0.17	Gly ²⁰⁹ , Thr ²¹⁰ , Leu ²¹¹ , Ser ²¹² , Tyr ²¹³ , Glu ²¹⁴ , Gln ²¹⁵ , Val ²²⁰ , Gln ²²¹ , Ala ²⁴⁹ , Gln ²⁵⁰ , Tyr ²⁵¹ , Glu ²⁵² , Leu ²⁵³ , Lys ²⁵⁴ , Thr ²⁵⁷ , Phe ²⁵⁸ , Val ³⁰³ , Tyr ³⁰⁵
			RNA Polymerase	-9.96	0.05	Asp ⁴⁵² , Tyr ⁴⁵⁵ , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Lys ⁶²¹ , Cys ⁶²² , Asp ⁶²³ ,
						Arg ⁶²⁴ , Ser ⁷⁵⁹ , Asp ⁷⁶⁰ , Asp ⁷⁶¹ , Lys ⁷⁹⁸ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Cys ⁸¹³ , Ser ⁸¹⁴
				-10.52	0.03	Asp ⁴⁵² , Tyr ⁴⁵⁵ , Lys ⁵⁵¹ , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Tyr ⁶¹⁹ , Pro ⁶²⁰ , Lys ⁶²¹ , Cys ⁶²² , Asp ⁶²³ , Arg ⁶²⁴ , Ser ⁷⁵⁹ , Asp ⁷⁶⁰ , Asp ⁷⁶¹ , Ala ⁷⁶² , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-11.57	0.003	Pro ¹⁷⁵ , Leu ¹⁷⁶ , Asn ¹⁷⁷ , Lys ²⁰² , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Ser ⁴⁸⁵ , Ser ⁴⁸⁶ , Pro ⁵¹⁴ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Thr ⁵³² , Val ⁵³³ , Asp ⁵³⁴ , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-10.07	0.04	Arg ⁶¹ , Asn ⁶⁴
			Spike Open Protein	-9.29	0.16	Val ⁴⁷ , His ⁴⁹ , Lys ³⁰⁴ , Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-9.49	0.11	Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Main Protease (MPro)	-4.09	997.83	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-5.58	80.7	Arg ⁶⁵ , Val ⁶⁶ , Ala ⁶⁸ , Phe ⁶⁹ , Glu ⁷⁰ , Thr ⁷⁴ , Thr ⁷⁵

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
61	Heneicosanoic acid	16898	RNA-dependent RNA polymerase (RdRP)	-3.76	1744.55	Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Lys ⁷³ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Asp ²¹⁸ , Asp ²²¹
			Helicase	-4.81	300.024	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.67	69.68	No binding site was found
			Spike Open Protein	-3.45	2943.86	Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-4.45	547.15	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
62	Hesperetin	72281	Main Protease (MPro)	-7.33	4.22	Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , His ¹⁷² , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.34	0.77	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Glu ¹⁶⁷ , Tyr ¹⁷¹
			RNA-dependent RNA polymerase (RdRP)	-7.59	2.74	Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.8	1.933	Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹¹ , Leu ⁴¹² , Thr ⁴¹³ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.42	3.62	Ile ⁴⁶ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰
			Spike Open Protein	-6.88	9.1	Arg ³⁵⁵ , Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-7.1	6.28	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Main Protease (MPro)	-8.02	1.33	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , His ⁴¹ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , His ¹⁷² , Gln ¹⁸⁹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
63	Hesperidin	10621	Papain like protease (PLPro)	-10.61	0.02	Lys ¹⁵⁷ , Thr ¹⁵⁸ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Val ¹⁶⁵ , Glu ¹⁶⁷ , Leu ¹⁹⁹ , Glu ²⁰³ ,
						Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³² , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Cys ²⁷⁰ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-9.53	0.1	Val ¹⁶⁶ , Tyr ⁴⁵⁶ , Met ⁵⁴² , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Val ⁵⁵⁷ , Ala ⁵⁵⁸ , Asp ⁶¹⁸ , Tyr ⁶¹⁹ , Pro ⁶²⁰ , Lys ⁶²¹ , Cys ⁶²² , Asp ⁶²³ , Arg ⁶²⁴ , Lys ⁶⁷⁶ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸² , Phe ⁷⁹³ , Ser ⁷⁹⁵ , Lys ⁷⁹⁸
			Helicase	-8.93	0.283	Lys ¹³⁹ , Glu ¹⁴² , Glu ¹⁴³ , Lys ¹⁴⁶ , Arg ¹⁷⁸ , Asn ¹⁷⁹ , Val ¹⁸¹ , Glu ¹⁹⁷ , Thr ²²⁸ , His ²³⁰ , Cys ³⁰⁹ , Arg ³³⁷ , Arg ³³⁹ , Met ³⁷⁸ , Ala ³⁷⁹ , Thr ³⁸⁰ , Tyr ³⁸² , Asp ³⁸³ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Thr ⁴¹⁰
			E-channel proteins	-8.82	0.34	Leu ²⁸ , Val ²⁹ , Leu ³¹ , Ala ³² , Leu ³⁴ , Thr ³⁵ , Ala ³⁶ , Cys ⁴⁰
			Spike Open Protein	-8.18	1.01	Asn ⁷¹⁰ , Thr ¹⁰⁷⁶ , Ser ¹⁰⁹⁷ , Gly ¹⁰⁹⁹ , Thr ¹¹⁰⁰ , His ¹¹⁰¹ , Trp ¹¹⁰² , Ile ¹¹¹⁴ , Ile ¹¹¹⁵ , Val ¹¹³³ , Asn ¹¹³⁴ , Asn ¹¹³⁵ , Thr ¹¹³⁶ , Tyr ¹¹³⁸
64	Homogentisic acid	780	Spike Close Protein	-8.53	0.56	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Lys ²⁰⁶ , Phe ²²⁰ , Ser ²²¹ , Ala ²²² , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Main Protease (MPro)	8.99	8.99	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Papain like protease (PLPro)	-6.59	14.87	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-6.65	13.31	Pro ³²³ , Thr ³²⁴ , Phe ³²⁶ , Gly ³²⁷ , Tyr ³⁴⁶ , His ³⁴⁷ , Phe ³⁴⁸ , Arg ³⁴⁹ , Glu ³⁵⁰ , Asn ⁶²⁸ , Ser ⁶⁶⁴ , Val ⁶⁷⁵ , Lys ⁶⁷⁶ , Pro ⁶⁷⁷
			Helicase	-6.2	28.774	Val ⁴⁹⁶ , Phe ⁴⁹⁹ , Leu ⁵⁰⁰ , Thr ⁵⁰¹ , Asn ⁵⁰³ , Trp ⁵⁰⁶ , Arg ⁵⁰⁷ , Ala ⁵⁰⁹ , Leu ⁵²⁶ , Leu ⁵²⁸ , Tyr ⁵⁴³ , Ile ⁵⁴⁵ , Leu ⁵⁷³
			E-channel proteins	-5.52	89.3	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.09	187.35	Gly ⁸⁸⁵ , Trp ⁸⁸⁶ , Thr ⁸⁸⁷ , Ile ⁸⁹⁶ , Met ⁹⁰⁰ , Gln ⁹⁰¹ , Ala ⁹⁰³ , Tyr ⁹⁰⁴ , Arg ⁹⁰⁵
64	Homogentisic acid	780	Spike Close Protein	-6	39.85	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
65	Hydroxytyrosol	82755	Main Protease (MPro)	-6.48	17.73	Met ⁶ , Ala ⁷ , Phe ⁸ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-6.34	22.57	Gln ¹⁷⁴ , His ¹⁷⁵ , Val ²⁰²
			RNA-dependent RNA polymerase (RdRP)	-5.59	80.29	Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-5.38	114.062	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ²¹ , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶
			E-channel proteins	-5.3	129.89	No binding site was found
			Spike Open Protein	-5.5	92.68	Tyr ³⁸ , Pro ³⁹ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-5.06	197.08	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Arg ¹⁰⁰⁰
66	Isoliquiritin	5318591	Main Protease (MPro)	-7.87	1.69	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Val ¹⁸⁶ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Ala ¹⁹¹ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.12	0.21	Met ²⁰⁸ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-7.71	2.23	Tyr ²⁶⁵ , Ile ²⁶⁶ , Lys ²⁶⁷ , Trp ²⁶⁸ , Leu ²⁷⁰ , Pro ³²² , Pro ³²³ , Thr ³²⁴ , Leu ³⁸⁸ , Leu ³⁸⁹ , Asp ³⁹⁰ , Thr ³⁹³ , Thr ³⁹⁴ , Cys ³⁹⁵ , Phe ³⁹⁶ , Ser ³⁹⁷
			Helicase	-7.85	1.75	Asn ¹⁷⁷ , Asn ¹⁷⁹ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Pro ⁵¹⁴ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Thr ⁵³² , Asp ⁵³⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-8.42	0.68	Leu ²⁷ , Ile ⁴⁶ , Val ⁴⁷ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰
			Spike Open Protein	-6.8	10.29	Asn ³⁰ , Thr ³³ , Phe ⁵⁸ , Phe ⁵⁹ , Ser ⁶⁰ , Ala ²⁸⁸ , Val ²⁸⁹ , Asp ²⁹⁰ , Leu ²⁹³ , Asp ²⁹⁴ , Leu ²⁹⁶ , Ser ²⁹⁷ , Lys ³⁰⁰ , Asn ⁶⁰⁶
			Spike Close Protein	-6.98	7.64	Ile ¹⁰⁵ , Leu ¹¹⁸ , Val ¹²⁰ , Asn ¹²² , Asn ¹²⁵ , Val ¹²⁷ , Lys ¹²⁹ , Phe ¹³³ , Gln ¹³⁴ , Phe ¹³⁵ , Cys ¹³⁶ , Pro ¹³⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Val ¹⁷¹ , Leu ²⁴¹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
67	Isorhamnetin	5281654	Main Protease (MPro)	-7.52	3.08	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.46	0.63	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Leu ¹⁹⁹ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.42	3.66	Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.51	3.116	Asn ¹⁷⁷ , Arg ¹⁷⁸ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-6.9	8.73	Leu ²⁸ , Leu ³¹ , Ala ³² , Thr ³⁵ , Ala ³⁶ , Arg ³⁸
			Spike Open Protein	-6.62	14.14	Lys ⁵³⁵ , Glu ⁵⁵⁴ , Ser ⁵⁵⁵ , Asn ⁵⁵⁶ , Lys ⁵⁵⁷ , Lys ⁵⁵⁸ , Phe ⁵⁵⁹ , Arg ⁵⁷⁷ , Leu ⁵⁸² , Glu ⁵⁸³ , Ile ⁵⁸⁴ , Leu ⁵⁸⁵
			Spike Close Protein	-6.84	9.65	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Lys ⁸⁵⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
68	Kaempferol	5280863	Main Protease (MPro)	-7.66	2.44	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.13	1.1	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.14	5.83	Tyr ³² , Lys ⁴⁷ , Tyr ¹²⁹ , His ¹³³ , Asp ¹³⁵ , Asn ¹³⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-7.48	3.317	Ala ¹³⁵ , Leu ¹³⁸ , Lys ¹³⁹ , Glu ¹⁴² , Asn ¹⁷⁹ , Thr ³⁸⁰ , Tyr ³⁸² , Asp ³⁸³ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰
			E-channel proteins	-7.02	7.13	No binding site was found
			Spike Open Protein	-6.82	9.97	Lys ⁵³⁵ , Glu ⁵⁵⁴ , Ser ⁵⁵⁵ , Asn ⁵⁵⁶ , Lys ⁵⁵⁷ , Lys ⁵⁵⁸ , Phe ⁵⁵⁹ , Arg ⁵⁷⁷ , Leu ⁵⁸² , Glu ⁵⁸³ , Ile ⁵⁸⁴ , Leu ⁵⁸⁵
			Spike Close Protein	-7.31	4.37	Leu ³³⁵ , Cys ³³⁶ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Ala ³⁶³ , Asp ³⁶⁴ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴
			Main Protease (MPro)	-5.99	41.01	Phe ⁸ , Lys ¹⁰² , Val ¹⁰⁴ , Arg ¹⁰⁵ , Ile ¹⁰⁶ , Gln ¹⁰⁷ , Gln ¹¹⁰ , Thr ¹¹¹ , Phe ¹¹² , Asn ¹⁵¹ , Ile ¹⁵² , Asp ¹⁵³ , Ser ¹⁵⁸ , Phe ²⁹⁴ , Arg ²⁹⁸

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
69	Kanzonol Y	10001604	Papain like protease (PLPro)	-9.37	0.14	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Glu ¹⁶⁷ , Tyr ¹⁷¹ , Tyr ²⁶⁸ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-7.06	6.68	Ala ⁴⁶ , Lys ⁴⁷ , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Cys ¹³⁹ , Thr ¹⁴¹ , Leu ¹⁴² , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-7.58	2.797	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-7.8	1.91	Leu ¹⁹ , Ala ²² , Phe ²³ , Phe ²⁶
			Spike Open Protein	-5.39	112.15	Trp ⁸⁸⁶ , Gly ⁸⁸⁹ , Ala ⁸⁹⁰ , Tyr ⁹⁰⁴ , Ser ¹⁰³⁰ , Glu ¹⁰³¹ , Leu ¹⁰³⁴ , Gly ¹⁰³⁵ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸
			Spike Close Protein	-6.94	8.14	Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
70	Lauric acid	3893	Main Protease (MPro)	-4.17	877.71	His ⁴¹ , Ser ⁴⁶ , Met ⁴⁹ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-5.28	133.9	Asp ¹⁶⁴ , Val ¹⁶⁵ , Arg ¹⁶⁶ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Gly ²⁶⁶ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-4.74	335.94	Val ³³⁵ , Asp ³³⁶ , Val ³³⁸ , Phe ³⁴⁰ , Arg ³⁶⁵ , Leu ³⁶⁶
			Helicase	-4.91	253.856	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Glu ⁴¹⁸ , Pro ⁴¹⁹ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-5.12	176.6	No binding site was found
			Spike Open Protein	-5.12	177.2	Asn ⁹⁹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
			Spike Close Protein	-5.08	187.98	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
71	Linoleic acid	5280450	Main Protease (MPro)	-4.56	453.67	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷
			Papain like protease (PLPro)	-6.66	13.08	Lys ¹⁵⁷ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-5.24	144.71	Arg ³³ , Ala ³⁴ , Phe ³⁵ , Ile ³⁷ , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Lys ⁷³ , Thr ¹²³ , Asp ²⁰⁸ , Asn ²⁰⁹ , Tyr ²¹⁷ , Asp ²¹⁸ , Asn ⁷¹³
			Helicase	-5.02	208.717	Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-6.24	26.71	No binding site was found
			Spike Open Protein	-4.23	797.2	Arg ³⁵⁵ , Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷
			Spike Close Protein	-5.68	69.09	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Leu ²²⁹
72	Linolenic acid	5280934	Main Protease (MPro)	-4.81	299.52	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-7.03	7.01	Asp ¹⁶⁴ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³
			RNA-dependent RNA polymerase (RdRP)	-5.23	145.69	Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Tyr ³⁸ , Asn ³⁹ , Val ⁴² , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ⁷¹³
			Helicase	-5.25	141.807	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-6.45	18.58	No binding site was found
			Spike Open Protein	-4.68	369.87	Leu ³⁹⁰ , Cys ³⁹¹ , Leu ⁵¹⁷ , His ⁵¹⁹ , Phe ⁵⁴³ , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Thr ⁵⁴⁷ , Gln ⁵⁶⁴ , Phe ⁵⁶⁵ , Thr ⁵⁷³ , Val ⁵⁷⁶ , Arg ⁵⁷⁷ , Pro ⁵⁷⁹
			Spike Close Protein	-5.32	127.07	Val ³⁸² , Leu ³⁹⁰ , Cys ³⁹¹ , Phe ³⁹² , Thr ³⁹³ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Ala ⁵²² , Phe ⁵⁴³ , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Thr ⁵⁴⁷ , Phe ⁵⁶⁵

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
73	Liquiritigenin	114829	Main Protease (MPro)	-7.04	6.89	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-9.11	0.21	Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Tyr ¹⁵⁴ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.95	8.03	Phe ⁴⁰⁷ , Gln ⁴⁰⁸ , Thr ⁴⁰⁹ , Asp ⁴⁴⁵ , Gly ⁴⁴⁶ , Asn ⁴⁴⁷
			Helicase	-7.2	5.25	Asn ¹⁷⁹ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asp ⁵³⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.44	3.54	No binding site was found
			Spike Open Protein	-6.94	8.2	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Lys ²⁰⁶ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-7.13	5.93	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Leu ³³⁵ , Val ³⁶² , Cys ⁵²⁵ , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰
74	Luteolin	5280445	Main Protease (MPro)	-7.62	2.59	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.47	0.62	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Glu ¹⁶⁷ , Tyr ¹⁷¹
			RNA-dependent RNA polymerase (RdRP)	-7.84	1.79	Phe ⁴⁰⁷ , Thr ⁴⁰⁹ , Asp ⁴⁴⁵ , Gly ⁴⁴⁶ , Asn ⁴⁴⁷
			Helicase	-7.83	1.831	Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹¹ , Leu ⁴¹² , Thr ⁴¹³ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-7.36	4.04	Ile ⁴⁶ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷
			Spike Open Protein	-7.05	6.83	Arg ³⁵⁵ , Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-7.28	4.64	Val ³⁸² , Leu ³⁹⁰ , Cys ³⁹¹ , Phe ³⁹² , Thr ³⁹³ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Pro ⁵²¹ , Ala ⁵²² , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Thr ⁵⁴⁷ , Phe ⁵⁶⁵
			Main Protease (MPro)	-4.65	391.05	Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-6.01	39.06	Asp ¹⁶⁴ , Tyr ²⁶⁸

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
75	Malic acid	525	RNA-dependent RNA polymerase (RdRP)	-5.5	92.52	Arg ³⁰⁵ , Arg ⁴⁶⁷ , Leu ⁴⁷⁰ , Phe ⁴⁷¹ , Glu ⁴⁷⁴ , Cys ⁷³⁰ , Leu ⁷³¹ , Arg ⁷³³ , Asn ⁷³⁴ , Arg ⁷³⁵ , Asp ⁷³⁶ , Val ⁷³⁷
			Helicase	-5.63	75.177	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Lys ¹³¹ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Tyr ⁴²¹ , Phe ⁴²² , Asn ⁴²³
			E-channel proteins	-4.05	1078.39	No binding site was found
			Spike Open Protein	-4.82	294.5	Ser ⁷³⁰ , Thr ⁷⁷⁸ , Pro ⁸⁶³ , Leu ⁸⁶⁵ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸
			Spike Close Protein	-4.88	266.59	Leu ³⁹⁰ , Cys ³⁹¹ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Ala ⁵²² , Phe ⁵⁴³ , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Phe ⁵⁶⁵
76	Margaric acid	10465	Main Protease (MPro)	-3.91	1354.36	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Asn ²⁷⁷
			Papain like protease (PLPro)	-5.91	46.79	Asp ¹⁶⁴ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-4.62	408.6	Glu ⁴⁷⁴ , Asp ⁴⁷⁷ , Lys ⁴⁷⁸ , Phe ⁴⁸⁰ , Asp ⁴⁸¹ , Val ⁶³⁷ , Arg ⁶⁴⁰ , Lys ⁶⁴¹ , Thr ⁶⁴³ , Val ⁷³⁷ , Thr ⁷³⁹ , Val ⁷⁴² , Asn ⁷⁴³
			Helicase	-4.72	345.14	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.51	92.21	No binding site was found
			Spike Open Protein	-3.7	1943.56	Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-5.04	203.5	Trp ¹⁰⁴ , Ile ¹¹⁹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹
			Main Protease (MPro)	-7.53	3.03	Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , His ¹⁷² , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.65	0.09	Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Arg ⁸² , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
77	Myricetin	5281672	RNA-dependent RNA polymerase (RdRP)	-7.66	2.44	Asp ⁴⁵² , Tyr ⁴⁵⁶ , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Val ⁵⁵⁷ , Ala ⁵⁵⁸ , Lys ⁶²¹ , Cys ⁶²² , Asp ⁶²³ , Arg ⁶²⁴ , Lys ⁶⁷⁶ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸² , Gly ⁶⁸³
			Helicase	-7.68	2.331	Asn ¹⁷⁷ , Arg ¹⁷⁸ , Glu ²⁰¹ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Gln ⁵³¹ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-6.85	9.49	Leu ²⁸ , Leu ³¹ , Ala ³² , Thr ³⁵ , Ala ³⁶ , Arg ³⁸
			Spike Open Protein	-7.12	6.05	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Thr ⁷⁷⁸ , Val ⁸⁶⁰ , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-7.33	4.22	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
78	Myristic acid	11005	Main Protease (MPro)	-4.03	1107.91	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-5.52	89.3	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-4.45	548.07	Phe ³⁵ , Asp ³⁶ , Ile ³⁷ , Asn ³⁹ , Val ⁴² , Phe ⁴⁸ , Lys ⁵⁰ , Thr ²⁰⁶ , Asp ²⁰⁸ , Asn ²⁰⁹ , Asp ²¹⁸ , Asp ²²¹ , Asn ⁷¹³
			Helicase	-4.66	386.462	Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-4.85	280.44	No binding site was found
			Spike Open Protein	-3.71	1923.97	His ¹¹⁰¹ , Trp ¹¹⁰² , Phe ¹¹⁰³ , Ile ¹¹¹⁴ , Ile ¹¹¹⁵ , Asn ¹¹³⁵ , Thr ¹¹³⁶ , Tyr ¹¹³⁸
			Spike Close Protein	-4.9	256.87	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
			Main Protease (MPro)	-4.51	496.96	Phe ⁸ , Val ¹⁰⁴ , Arg ¹⁰⁵ , Ile ¹⁰⁶ , Gln ¹⁰⁷ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-5.82	54.46	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Ser ²⁴⁵ , Ala ²⁴⁶ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁸ , Thr ³⁰¹ , Asp ³⁰²

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
79	Myristoleic acid	5281119	RNA-dependent RNA polymerase (RdRP)	-5.32	125.16	Val ³³⁵ , Asp ³³⁶ , Val ³³⁸ , Phe ³⁴⁰ , Leu ³⁶⁶
			Helicase	-4.86	273.426	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-5.48	95.7	No binding site was found
			Spike Open Protein	-5.28	135.26	Ser ⁹⁴ , Glu ⁹⁶ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
			Spike Close Protein	-5.43	104.48	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Leu ²²⁶ , Val ²²⁷
80	Naringen	442428	Main Protease (MPro)	-8.05	1.26	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-10.17	0.04	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Arg ¹⁶⁶ , Gln ¹⁶⁷ , Ser ¹⁷⁰ , Leu ¹⁸⁵ ,
						Leu ¹⁹⁹ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Ile ²²² , Pro ²²³ , Lys ²³² , Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-8.54	0.55	Tyr ³² , Lys ⁴⁷ , Tyr ¹²⁹ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷¹⁴ , Ala ⁷⁷¹ , Ser ⁷⁷² , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-8.42	0.673	Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁵¹⁴ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Thr ⁵³² , Val ⁵³³ , Asp ⁵³⁴ , His ⁵⁵⁴ , Ser ⁵⁵⁵ , Arg ⁵⁶⁰
			E-channel proteins	-8.53	0.56	Phe ²³ , Phe ²⁶ , Leu ²⁷ , Val ²⁹ , Thr ³⁰ , Leu ³¹ , Ile ³³ , Leu ³⁴ , Leu ³⁹ , Cys ⁴³ , Ile ⁴⁶ , Val ⁴⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-7.52	3.07	Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Asn ³³⁴ , Asn ³⁶⁰ , Pro ⁵²¹ , Ala ⁵²² , Thr ⁵²³ , Asn ⁵⁴⁴ , Gln ⁵⁶⁴ , Arg ⁵⁷⁷ , Asp ⁵⁷⁸ , Pro ⁵⁷⁹ , Gln ⁵⁸⁰ , Thr ⁵⁸¹ , Leu ⁵⁸²
			Spike Close Protein	-7.64	2.52	His ⁴⁹ , Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
81	Naringenin	932	Main Protease (MPro)	-7.36	4.01	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-9.36	0.14	Phe ⁶⁹ , His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-7.42	3.62	Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.45	3.478	Pro ¹⁷⁵ , Leu ¹⁷⁶ , Asn ¹⁷⁷ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Asp ²⁰⁴ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³²
			E-channel proteins	-7.4	3.75	Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷
			Spike Open Protein	-6.61	14.4	Ser ⁷³⁰ , Thr ⁷³² , Thr ⁷⁷⁸ , Phe ⁸²³ , Val ⁸⁶⁰ , Pro ⁸⁶² , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Ala ¹⁰⁵⁶ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸ , Gly ¹⁰⁵⁹
			Spike Close Protein	-6.95	8.03	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Tyr ²⁷⁹ , Gly ²⁸³
82	Neochlorogenic acid	5280633	Main Protease (MPro)	-8.04	1.28	Thr ²⁵ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.81	0.35	Arg ¹⁸³ , Leu ¹⁸⁵ , Val ¹⁸⁷ , Gln ¹⁹⁵ , Thr ¹⁹⁷ , Leu ¹⁹⁹ , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Ile ²²² , Thr ²²⁵ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.82	1.87	Tyr ³² , Ala ⁴⁶ , Lys ⁴⁷ , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Cys ¹³⁹ , Asp ¹⁴⁰ , Thr ¹⁴¹ , Leu ¹⁴² , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷¹⁴

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
82	Nishindaside	10310589	Helicase	-7.79	1.962	Lys ¹³⁹ , Glu ¹⁴² , Glu ¹⁴³ , Lys ¹⁴⁶ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Val ¹⁸¹ , Glu ¹⁹⁷ , Thr ²¹⁴ , His ²³⁰ , Ala ³³⁶ , Arg ³³⁷ , Arg ³³⁹ , Thr ⁴¹⁰
			E-channel proteins	-7.73	2.15	Ile ⁴⁶ , Ser ⁵⁰ , Leu ⁵¹ , Pro ⁵⁴ , Phe ⁵⁶ , Tyr ⁵⁷ , Ser ⁶⁰ , Arg ⁶¹
			Spike Open Protein	-6.57	15.33	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Lys ²⁰⁶ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-7.38	3.9	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Tyr ²⁷⁹ , Gly ²⁸³
83	Nishindaside	10310589	Main Protease (MPro)	-7.55	2.91	His ⁴¹ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-7.53	3.03	Asp ¹⁰⁸ , Asn ¹⁰⁹ , Gly ¹⁶⁰ , Glu ¹⁶¹ , Leu ¹⁶² , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-6.75	11.28	Tyr ¹²⁹ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Ala ⁷⁷¹ , Ser ⁷⁷² , Gln ⁷⁷³ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-7.19	5.412	Gly ³ , Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³⁰ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-7.04	6.9	Leu ³¹ , Ala ³² , Thr ³⁵ , Ala ³⁶ , Arg ³⁸ , Cys ⁴⁰
			Spike Open Protein	-5.94	43.95	Asp ³⁶⁴ , Tyr ³⁶⁵ , Ser ³⁶⁶ , Tyr ³⁶⁹ , Asn ³⁷⁰ , Pro ³⁸⁴ , Thr ³⁸⁵ , Leu ³⁸⁷ , Asn ³⁸⁸ , Pro ⁵²⁷ , Lys ⁵²⁸
			Spike Close Protein	-7.14	5.83	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Val ¹²⁰ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Val ²²⁷
			Main Protease (MPro)	-7.43	3.57	His ⁴¹ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-7.2	5.24	Tyr ²⁶⁸ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-6.36	21.63	Tyr ⁷¹⁹ , Val ⁷²⁰ , Leu ⁷²³ , Asn ⁷⁴³ , Glu ⁷⁴⁴ , Phe ⁷⁴⁵ , Ala ⁷⁴⁷ , Tyr ⁷⁴⁸ , Lys ⁷⁵¹ , His ⁷⁵²

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
84	Nordihydroguaiaretic	4534	Helicase	-7.01	7.247	Gly ³ , Ala ⁴ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵
			E-channel proteins	-6.57	15.23	Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-6.13	32	Pro ³³⁰ , Ile ³³² , Asn ³⁶⁰ , Pro ⁵²¹ , Ala ⁵²² , Thr ⁵²³ , Asn ⁵⁴⁴ , Gln ⁵⁶⁴ , Arg ⁵⁷⁷ , Asp ⁵⁷⁸ , Pro ⁵⁷⁹ , Gln ⁵⁸⁰ , Leu ⁵⁸²
			Spike Close Protein	-6.25	26.27	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
85	Oleic acid	445639	Main Protease (MPro)	-4.34	663.24	Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Gly ²⁷⁸ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷
			Papain like protease (PLPro)	-6.33	22.8	Asp ¹⁶⁴ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-3.95	1268.08	Tyr ¹²⁹ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ⁷⁰⁵ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Ala ⁷⁷¹ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-4.49	515.764	Ala ⁴ , Val ⁶ , Asn ⁹ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.78	57.87	No binding site was found
			Spike Open Protein	-3.26	4084.33	Thr ³³ , Phe ⁵⁸ , Phe ⁵⁹ , Gln ²¹⁸ , Gly ²¹⁹ , Phe ²²⁰ , Asp ²⁸⁷ , Ala ²⁸⁸ , Val ²⁸⁹ , Asp ²⁹⁰ , Leu ²⁹³ , Asp ²⁹⁴ , Leu ²⁹⁶ , Ser ²⁹⁷ , Lys ³⁰⁰ , Asn ⁶⁰⁶
			Spike Close Protein	-5.06	194.76	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Lys ²⁰⁶ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
			Main Protease (MPro)	-7.8	1.92	Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , His ¹⁷² , Gln ¹⁸⁹
			Papain like protease (PLPro)	-8.5	0.58	Asp ¹⁶⁴ , Arg ¹⁶⁶ , Met ²⁰⁸ , Ala ²⁴⁶ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
86	Oleuropein	5281544	RNA-dependent RNA polymerase (RdRP)	-8.31	0.81	Tyr ³² , Lys ⁴⁷ , Phe ⁴⁸ , Tyr ¹²⁹ , Ala ¹³⁰ , His ¹³³ , Phe ¹³⁴ , Asp ¹³⁵ , Asn ¹³⁸ , Cys ¹³⁹ , Asp ¹⁴⁰ , Thr ¹⁴¹ , Leu ¹⁴² , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷¹⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-7.77	2.003	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-8.3	0.82	Arg ⁶¹ , Asn ⁶⁴ , Leu ⁶⁵
			Spike Open Protein	-6.8	10.42	Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Asn ³³⁴ , Asn ³⁶⁰ , His ⁵¹⁹ , Pro ⁵²¹ , Ala ⁵²² , Thr ⁵²³ , Asn ⁵⁴⁴ , Gln ⁵⁶⁴ , Arg ⁵⁷⁷ , Asp ⁵⁷⁸ , Pro ⁵⁷⁹ , Leu ⁵⁸²
			Spike Close Protein	-7.12	6.05	Arg ³⁵⁵ , Asn ³⁹⁴ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁷ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁸
87	Oxalic acid	971	Main Protease (MPro)	-4.55	461.39	Met ⁶ , Phe ⁸ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹
			Papain like protease (PLPro)	-5.14	171.03	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-4.89	259.93	Phe ⁴⁴⁰ , Phe ⁴⁴¹ , Phe ⁴⁴² , Gln ⁴⁴⁴ , Lys ⁵⁴⁵ , Tyr ⁵⁴⁶ , Ala ⁵⁴⁷ , Ser ⁵⁴⁹ , Lys ⁵⁵¹ , Asn ⁵⁵² , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵
			Helicase	-4.98	222.918	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Leu ¹³⁸ , Asn ³⁸¹ , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²² , Asn ⁴²³
			E-channel proteins	-3.24	4189.06	No binding site was found
			Spike Open Protein	-3.69	1983.32	Gln ⁷⁸⁴ , Val ⁷⁸⁵ , Lys ⁷⁸⁶ , Gln ⁷⁸⁷ , Tyr ⁷⁸⁹ , Phe ⁸⁸⁸ , Gly ⁸⁹¹ , Ala ⁸⁹² , Ala ⁸⁹³
			Spike Close Protein	-4.5	506.28	Asp ⁴²⁰ , Tyr ⁴²¹ , Asn ⁴²² , Tyr ⁴²³ , Lys ⁴²⁴ , Lys ⁴⁶² , Glu ⁴⁶⁵ , Arg ⁴⁶⁶ , Asp ⁴⁶⁷
			Main Protease (MPro)	-4.57	450.62	Phe ⁸ , Val ¹⁰⁴ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Ile ¹⁵² , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-5.58	80.7	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Thr ¹⁵⁸ , Val ¹⁵⁹ , Glu ¹⁶¹ , Glu ¹⁶⁷ , Tyr ¹⁷¹
			RNA-dependent RNA polymerase (RdRP)	-4.35	649.94	Phe ⁴⁴¹ , Ala ⁵⁴⁷ , Ile ⁵⁴⁸ , Arg ⁸³⁶ , Ile ⁸³⁷ , Ala ⁸⁴⁰ , Gly ⁸⁴¹ , Phe ⁸⁴³ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Arg ⁸⁵⁸ , Ser ⁸⁶¹ , Leu ⁸⁶²

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
88	Palmitoleic acid	445638	Helicase	-4.75	330.322	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ²¹ , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³⁰ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.88	48.97	No binding site was found
			Spike Open Protein	-4.21	814.89	Tyr ⁷⁰⁷ , Ser ⁷⁰⁸ , Asn ⁷⁰⁹ , Asn ⁷¹⁰ , Ser ⁷¹¹ , Ile ⁷¹² , Thr ¹⁰⁷⁷ , Ala ¹⁰⁷⁸ , Pro ¹⁰⁷⁹ , Phe ¹⁰⁸⁹ , Pro ¹⁰⁹⁰ , Gly ¹⁰⁹³ , Val ¹⁰⁹⁴ , Phe ¹⁰⁹⁵ , Arg ¹¹⁰⁷ , Phe ¹¹²¹
			Spike Close Protein	-4.55	462.96	Ile ¹⁰⁵ , Leu ¹¹⁸ , Val ¹²⁰ , Asn ¹²² , Val ¹²⁷ , Lys ¹²⁹ , Phe ¹³³ , Phe ¹³⁵ , Cys ¹³⁶ , Pro ¹³⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Leu ²⁴¹
89	p-Cymene	7463	Main Protease (MPro)	-5.62	76.07	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-6.67	12.95	Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-5.5	93.78	Pro ³²³ , Phe ³²⁶ , Gly ³²⁷ , Pro ³²⁸ , Tyr ³⁴⁶ , His ³⁴⁷ , Phe ³⁴⁸ , Arg ³⁴⁹ , Phe ³⁹⁶ , Val ³⁹⁸ , Ser ⁶⁶⁴ , Glu ⁶⁶⁵ , Met ⁶⁶⁶ , Val ⁶⁷⁵ , Lys ⁶⁷⁶ , Pro ⁶⁷⁷ , basn ¹¹⁸
			Helicase	-5.83	53.64	Trp ¹¹⁴ , Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Ala ¹³⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Lys ¹³⁹ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²² , Asn ⁴²³
			E-channel proteins	-6.27	25.44	No binding site was found
			Spike Open Protein	-5.75	61.5	Ser ⁸⁸⁴ , Gly ⁸⁸⁵ , Trp ⁸⁸⁶ , Thr ⁸⁸⁷ , Ile ⁸⁹⁶ , Met ⁹⁰⁰ , Gln ⁹⁰¹ , Tyr ⁹⁰⁴ , Arg ⁹⁰⁵ , Met ¹⁰⁵⁰
			Spike Close Protein	-5.68	68.4	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Main Protease (MPro)	-8.25	0.9	Thr ²⁵ , His ⁴¹ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.86	0.32	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
90	Phloridzin dihydrate	9912668	RNA-dependent RNA polymerase (RdRP)	-7.25	4.87	Glu ⁴⁷⁴ , Asp ⁴⁷⁷ , Lys ⁴⁷⁸ , Phe ⁴⁸⁰ , Asp ⁴⁸¹ , Tyr ⁴⁸³ , Asp ⁴⁸⁴ , Gly ⁴⁸⁵ , Arg ⁶⁴⁰ , Lys ⁶⁴¹ , Thr ⁶⁴³ , Thr ⁶⁴⁴ , Thr ⁷³⁹ , Val ⁷⁴²
			Helicase	-7.68	2.363	Lys ¹³⁹ , Glu ¹⁴² , Glu ¹⁴³ , Lys ¹⁴⁶ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Val ¹⁸¹ , Leu ²²⁷ , Thr ²²⁸ , His ²³⁰ , Cys ³⁰⁹ , Ser ³¹⁰ , Met ³⁷⁸ , Ala ³⁷⁹ , Thr ³⁸⁰ , Tyr ³⁸² , Asp ³⁸³ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹¹
			E-channel proteins	-7.34	4.2	Arg ⁶¹ , Asn ⁶⁴
			Spike Open Protein	-6.16	30.32	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-7.14	5.84	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷
91	Phlorizin	6072	Main Protease (MPro)	-8.75	0.39	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.01	0.25	Arg ⁶⁵ , Val ⁶⁶ , Phe ⁶⁹ , Glu ⁷⁰ , Thr ⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-7.91	1.58	Ser ²⁵⁵ , Tyr ²⁶⁵ , Ser ³¹⁸ , Thr ³¹⁹ , Val ³²⁰ , Phe ³²¹ , Pro ³²² , Pro ³²³ , Arg ³⁴⁹ , Cys ³⁹⁵ , Phe ³⁹⁶ , Tyr ⁴⁵⁶ , Arg ⁴⁵⁷ , Tyr ⁴⁵⁸ , Asn ⁴⁵⁹ , Leu ⁴⁶⁰ , Pro ⁴⁶¹ , Pro ⁶⁷⁷
			Helicase	-8.66	0.447	Asn ¹⁷⁷ , Asn ¹⁷⁹ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Asp ²⁰⁴ , Pro ⁵¹⁴ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Gln ⁵³¹ , Thr ⁵³² , Val ⁵³³ , Asp ⁵³⁴ , His ⁵⁵⁴ , Arg ⁵⁶⁰
			E-channel proteins	-8.66	0.31	No binding site was found
			Spike Open Protein	-7.2	5.27	Ala ⁵²⁰ , Pro ⁵²¹ , Lys ⁵⁵⁷ , Leu ⁵⁶⁰ , Phe ⁵⁶² , Gln ⁵⁶³ , Gln ⁵⁶⁴ , Phe ⁵⁶⁵ , Gly ⁵⁶⁶ , Arg ⁵⁶⁷ , Asp ⁵⁶⁸ , Ile ⁵⁶⁹ , Asp ⁵⁷¹
			Spike Close Protein	-7.56	2.89	Phe ³⁴² , Asn ³⁴³ , Phe ³⁴⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴ , Ser ³⁷⁵ , Trp ⁴³⁶ , Asn ⁴³⁷ , Ser ⁴³⁸ , Asn ⁴⁴⁰ , Leu ⁴⁴¹ , Arg ⁵⁰⁹
			Main Protease (MPro)	-5.91	46.94	Met ⁶ , Ala ⁷ , Phe ⁸ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
92	Pyrogallol	1057	Papain like protease (PLPro)	-5.7	65.9	Thr ⁷⁴ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Cys ¹⁵⁵ , Asn ¹⁵⁶ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-5.69	67.59	Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-6.06	36.016	Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Lys ¹³¹ , Ala ¹³⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Tyr ⁴²¹ , Phe ⁴²² , Asn ⁴²³
			E-channel proteins	-4.61	418.37	Ser ¹⁶ , Leu ¹⁹ , Phe ²⁰ , Phe ²³ , eleu ²¹ , eval ²⁴ , eval ²⁵ , eleu ²⁸
			Spike Open Protein	-4.94	240.51	Ala ⁹⁵⁸ , Thr ⁹⁶¹ , Leu ⁹⁶² , Gln ⁹⁶⁵ , Ser ¹⁰⁰³ , Thr ¹⁰⁰⁶ , Tyr ¹⁰⁰⁷ , Gln ¹⁰¹⁰
			Spike Close Protein	-5.75	61.5	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
93	Quercetin	5280343	Main Protease (MPro)	-7.49	3.25	His ⁴¹ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , His ¹⁷² , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.54	0.55	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.52	3.06	Thr ⁵⁹¹ , Ser ⁵⁹² , Lys ⁵⁹³ , Phe ⁵⁹⁴ , Gln ⁸¹⁵ , Pro ⁸³⁰ , Tyr ⁸³¹ , Pro ⁸³² , Asp ⁸⁶⁵ , Pro ⁸⁶⁸ , Trp ⁹¹⁶
			Helicase	-7.56	2.888	Asn ¹⁷⁷ , Arg ¹⁷⁸ , Glu ²⁰¹ , Asn ⁵¹⁶ , Ser ⁵¹⁷ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-7.03	7.07	Leu ²⁷ , Leu ²⁸ , Val ²⁹ , Leu ³¹ , Ala ³² , Thr ³⁵ , Ala ³⁶ , Arg ³⁸
			Spike Open Protein	-7.14	5.8	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Leu ²²⁶ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-7.43	3.57	Leu ³³⁵ , Cys ³³⁶ , Phe ³³⁸ , Gly ³³⁹ , Phe ³⁴² , Asn ³⁴³ , Ala ³⁶³ , Asp ³⁶⁴ , Tyr ³⁶⁵ , Val ³⁶⁷ , Leu ³⁶⁸ , Ser ³⁷¹ , Ser ³⁷³ , Phe ³⁷⁴
			Main Protease (MPro)	-5.44	102.21	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Phe ²²³ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵
			Papain like protease (PLPro)	-6.75	11.31	No binding site was found

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
94	Quinic acid	6508	RNA-dependent RNA polymerase (RdRP)	-6.15	30.84	Asp ⁴⁵² , Tyr ⁴⁵⁶ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Val ⁵⁵⁷ , Ala ⁵⁵⁸ , Asp ⁶²³ , Arg ⁶²⁴ , Lys ⁶⁷⁶ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸²
			Helicase	-5.93	44.701	Pro ⁴⁰⁶ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Glu ⁴¹⁸ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-5	216.25	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.16	166.47	Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷
			Spike Close Protein	-5.77	58.86	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
95	Reserpine	5770	Main Protease (MPro)	-7.64	2.5	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Gln ¹⁸⁹
			Papain like protease (PLPro)	-8.54	0.55	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Leu ¹⁸⁵ , Val ¹⁸⁷ , Cys ¹⁹² , Gln ¹⁹⁵ , Thr ¹⁹⁷ , Leu ¹⁹⁹ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Ile ²²² , Thr ²²⁵ , Lys ²³² zn ⁵⁰⁰
			RNA-dependent RNA polymerase (RdRP)	-8	1.36	Val ³³⁵ , Asp ³³⁶ , Val ³³⁸ , Phe ³⁴⁰ , Arg ³⁶⁵ , Leu ³⁶⁶ , Ser ³⁶⁷ , Phe ³⁶⁸ , Leu ³⁷¹
			Helicase	-8.63	0.47	Phe ¹⁴⁵ , Tyr ¹⁴⁹ , Arg ¹⁷³ , Pro ¹⁷⁴ , Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Gln ⁴⁰⁴ , Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , Ser ⁴⁸⁵ , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-8.93	0.29	No binding site was found
			Spike Open Protein	-7.4	3.75	Ile ⁷⁸⁸ , Lys ⁷⁹⁰ , Thr ⁷⁹¹ , Pro ⁷⁹³ , Lys ⁷⁹⁵ , Ser ⁸⁰³ , Leu ⁸⁰⁶ , Pro ⁸⁰⁷ , Asp ⁸⁰⁸ , Pro ⁸⁰⁹ , Lys ⁸¹⁴ , Gln ⁸⁷² , Ser ⁸⁷⁵

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Close Protein	-8.13	1.11	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹ , Pro ²³⁰
96	Resveratrol	445154	Main Protease (MPro)	-7.61	2.65	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Thr ¹¹¹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-8.21	0.95	Phe ⁶⁹ , His ⁷³ , Thr ⁷⁴ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.92	8.52	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Tyr ⁵⁴⁶ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶ , Ile ⁸⁴⁷
			Helicase	-6.88	9.04	Lys ⁴⁷³ , Phe ⁴⁷⁵ , Arg ⁵⁷⁹ , Tyr ⁵⁸² , Asp ⁵⁸³ , Leu ⁵⁸⁵ , Gln ⁵⁸⁶ , Phe ⁵⁸⁷ , Thr ⁵⁸⁸ , Ser ⁵⁸⁹
			E-channel proteins	-7.6	2.69	No binding site was found
			Spike Open Protein	-6.24	26.62	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Spike Close Protein	-6.7	12.25	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Ile ²⁰³ , Val ²²⁷
97	Rhamnetin	5281691	Main Protease (MPro)	-7.55	2.91	Met ⁴⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , His ¹⁷² , Val ¹⁸⁶ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-8.82	0.35	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Glu ¹⁶⁷ , Tyr ¹⁷¹ , Gln ²⁶⁹
			RNA-dependent RNA polymerase (RdRP)	-7.49	3.23	Tyr ⁴⁵⁶ , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Ala ⁵⁵⁸ , Tyr ⁶¹⁹ , Pro ⁶²⁰ , Lys ⁶²¹ , Cys ⁶²² , Asp ⁶²³ , Arg ⁶²⁴ , Lys ⁶⁷⁶ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸²
			Helicase	-7.72	2.201	Asn ¹⁷⁷ , Arg ¹⁷⁸ , Thr ¹⁹⁹ , Phe ²⁰⁰ , Glu ²⁰¹ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , Ser ⁵¹⁷ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Gln ⁵³¹ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-6.89	8.96	No binding site was found

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-7.07	6.6	Phe ³²⁹ , Pro ³³⁰ , Asn ³³¹ , Ile ³³² , Thr ³³³ , Asn ³³⁴ , Leu ³³⁵ , Val ³⁶² , Gly ⁵²⁶ , Pro ⁵²⁷ , Lys ⁵²⁸ , Lys ⁵²⁹ , Ser ⁵³⁰ , Gln ⁵⁸⁰
			Spike Close Protein	-7.26	4.81	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Lys ⁸⁵⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
98	Rhodioliin	14778358	Main Protease (MPro)	-9.05	0.23	Thr ²⁵ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Leu ¹⁴¹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , His ¹⁶³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.26	0.16	Val ¹⁸⁷ , Gln ¹⁹⁵ , Thr ¹⁹⁷ , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Ile ²²² , Pro ²²³ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-8.13	1.09	Asp ⁴⁵² , Tyr ⁴⁵⁶ , Arg ⁵⁵³ , Ala ⁵⁵⁴ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Asp ⁶¹⁸ , Tyr ⁶¹⁹ , Pro ⁶²⁰ , Lys ⁶²¹ , Cys ⁶²² , Asp ⁶²³ , Arg ⁶²⁴ , Ser ⁷⁵⁹ , Asp ⁷⁶⁰ , Asp ⁷⁶¹ , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-8.53	0.561	Pro ⁴⁰⁶ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Ser ⁴⁸⁶ , Ala ⁴⁸⁷ , Tyr ⁵¹⁵ , Asn ⁵¹⁶ , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-8.58	0.51	Leu ²⁸ , Val ²⁹ , Ala ³² , Ile ³³ , Ala ³⁶ , Leu ³⁷
			Spike Open Protein	-8.68	0.43	Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Ile ²⁰³ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹
			Spike Close Protein	-7.54	2.97	Ser ⁴⁶ , Val ⁴⁷ , Leu ⁴⁸ , Lys ²⁷⁸ , Thr ³⁰² , Leu ³⁰³ , Lys ³⁰⁴ , Ser ³⁰⁵ , Phe ³⁰⁶ , Thr ³⁰⁷ , Ala ⁹⁵⁶ , Gln ⁹⁵⁷ , Asn ⁹⁶⁰ , Thr ⁹⁶¹ , Lys ⁹⁶⁴
			Main Protease (MPro)	-6.46	18.52	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Thr ¹¹¹ , Ser ¹¹³ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹
			Papain like protease (PLPro)	-6.36	21.93	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-5.81	54.92	Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Val ⁷⁶³ , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
99	Salicylic acid	338	Helicase	-5.98	41.432	Val ⁴⁹⁶ , Phe ⁴⁹⁹ , Leu ⁵⁰⁰ , Thr ⁵⁰¹ , Asn ⁵⁰³ , Trp ⁵⁰⁶ , Arg ⁵⁰⁷ , Leu ⁵²⁶ , Tyr ⁵⁴³ , Ile ⁵⁴⁵ , Leu ⁵⁷³
			E-channel proteins	-5.55	86.19	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-5.09	185.15	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-6.25	26.14	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
100	Secoisolariciresinol	65373	Main Protease (MPro)	-5.51	91.28	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-7.12	6.09	Arg ¹⁸³ , Leu ¹⁸⁵ , Leu ¹⁹⁹ , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Ile ²²² , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-7.04	6.89	Asn ⁴⁰⁴ , Val ⁴⁰⁵ , Ala ⁴⁰⁶ , Phe ⁴⁰⁷ , Thr ⁴⁰⁹ , Asp ⁴⁴⁵ , Gly ⁴⁴⁶ , Asn ⁴⁴⁷
			Helicase	-7.04	6.889	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.93	44.85	Leu ²⁸ , Val ²⁹ , Ala ³² , Ile ³³
			Spike Open Protein	-5.41	108.43	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-6.15	31.2	Asn ³¹⁷ , Arg ³¹⁹ , Gly ⁵⁴⁸ , Thr ⁵⁴⁹ , Gly ⁵⁵⁰ , Asp ⁵⁶⁸ , Thr ⁵⁷² , Thr ⁵⁷³ , Asp ⁵⁷⁴ , Ile ⁵⁸⁷ , Pro ⁵⁸⁹ , Cys ⁵⁹⁰ , Phe ⁵⁹²
101	Shikimic acid	8742	Main Protease (MPro)	-5.19	157.19	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶
			Papain like protease (PLPro)	-5.88	48.64	Cys ¹⁵⁵ , Asn ¹⁵⁶ , Lys ¹⁵⁷ , Glu ¹⁶¹ , Glu ¹⁶⁷ , Tyr ¹⁷¹
			RNA-dependent RNA polymerase (RdRP)	-5.03	206.96	Glu ¹³⁶ , Cys ¹³⁹ , Phe ¹⁵⁷ , Lys ¹⁵⁹ , Lys ¹⁶⁰ , Asp ¹⁶¹ , Trp ¹⁶² , Tyr ¹⁶³
			Helicase	-5.55	85.322	Leu ⁴⁰⁵ , Pro ⁴⁰⁶ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-5.1	184.21	No binding site was found

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
			Spike Open Protein	-5.2	154.82	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Leu ⁹⁷⁷ , Arg ¹⁰⁰⁰
			Spike Close Protein	-5.62	76.07	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Asp ⁹⁷⁹ , Arg ¹⁰⁰⁰
102	Silyhermin	10389806	Main Protease (MPro)	-8.22	0.94	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Val ⁴² , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.44	0.12	Arg ¹⁶⁶ , Val ¹⁸⁷ , Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Ile ²²² , Pro ²²³ , Cys ²²⁴ , Thr ²²⁵ , Ala ²³⁰ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-8.25	0.9	Tyr ¹⁴⁹ , Asn ¹⁵⁰ , Ala ¹⁷⁶ , Asn ¹⁷⁷ , Leu ¹⁷⁸ , Gly ¹⁷⁹ , Glu ¹⁸⁰ , Arg ¹⁸¹ , Gln ¹⁸⁴ , Thr ²⁴⁸ , Arg ²⁴⁹ , Ala ²⁵⁰ , Thr ²⁵² , Ala ²⁵³ , Leu ²⁶¹
			Helicase	-8.81	0.351	Pro ¹⁷⁵ , Asn ¹⁷⁷ , Asn ¹⁷⁹ , Tyr ¹⁸⁰ , Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Thr ⁴¹⁰ , Leu ⁴¹² , Thr ⁴¹³ , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Glu ⁴¹⁸ , Pro ⁴¹⁹ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹
			E-channel proteins	-8.43	0.66	Phe ²⁰ , Phe ²³ , Val ²⁴ , Leu ²⁷ , Ile ⁴⁶ , Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷
			Spike Open Protein	-7.28	4.58	Ser ⁷³⁰ , Met ⁷³¹ , Thr ⁷³² , Lys ⁷³³ , Gln ⁷⁷⁴ , Leu ⁸⁵⁸ , Thr ⁸⁵⁹ , Val ⁸⁶⁰ , Leu ⁸⁶¹ , Pro ⁸⁶² , Pro ⁸⁶³ , Asp ⁸⁶⁷ , Ile ⁸⁷⁰ , Leu ⁹⁵⁹ , Pro ¹⁰⁵⁷ , His ¹⁰⁵⁸
			Spike Close Protein	-8.05	1.25	Arg ³⁵⁵ , Tyr ³⁹⁶ , Pro ⁴²⁶ , Asp ⁴²⁸ , Phe ⁴²⁹ , Thr ⁴³⁰ , Lys ⁴⁶² , Pro ⁴⁶³ , Phe ⁴⁶⁴ , Ser ⁵¹⁴ , Phe ⁵¹⁵ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸
			Main Protease (MPro)	-8.71	0.41	Thr ²⁴ , Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Gly ¹⁴³ , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-9.42	0.13	Pro ⁵⁹ , Arg ⁶⁵ , Val ⁶⁶ , Ala ⁶⁸ , Phe ⁶⁹ , Glu ⁷⁰ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Pro ⁷⁷ , Phe ⁷⁹ , Leu ⁸⁰
			RNA-dependent RNA polymerase (RdRP)	-7.8	1.91	Arg ³⁰⁵ , Glu ⁴⁷⁴ , Asp ⁴⁷⁷ , Asp ⁴⁸¹ , Cys ⁴⁸² , Tyr ⁴⁸³ , Asp ⁴⁸⁴ , Gly ⁴⁸⁵ , Lys ⁵⁷⁴ , Arg ⁶⁴⁰ , Lys ⁶⁴¹ , Thr ⁶⁴³ , Val ⁷³⁷ , Thr ⁷³⁹ , Val ⁷⁴² , Asn ⁷⁴³

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
103	Silymarin	1548994	Helicase	-8.75	0.388	Ala ⁴ , Val ⁶ , Arg ¹⁵ , Ile ²⁰ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³⁰ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Thr ²³¹ , Val ²³² , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-8.89	1.1	No binding site was found
			Spike Open Protein	-7.62	2.6	Ala ²⁷ , Thr ⁶³ , Trp ⁶⁴ , Phe ⁶⁵ , His ⁶⁶ , Ala ⁶⁷ , Pro ⁸² , Asp ¹³⁸ , Pro ¹³⁹ , Phe ¹⁴⁰ , Thr ²⁴⁰ , Leu ²⁴¹ , Leu ²⁴² , Tyr ²⁶⁵
			Spike Close Protein	-7.66	2.44	Tyr ⁷⁸⁹ , Lys ⁷⁹⁰ , Thr ⁷⁹¹ , Lys ⁷⁹⁵ , Ser ⁸⁰³ , Gln ⁸⁰⁴ , Leu ⁸⁰⁶ , Pro ⁸⁰⁷ , Asp ⁸⁰⁸ , Pro ⁸⁰⁹ , Lys ⁸¹⁴ , Ser ⁸⁷⁵ , Ala ⁸⁷⁹
104	Sinapic acid	637775	Main Protease (MPro)	-5.96	43.14	His ⁴¹ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Cys ¹⁴⁵ , His ¹⁶⁴ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Pro ¹⁶⁸ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-7.41	3.7	Phe ⁶⁹ , His ⁷³ , Thr ⁷⁴ , Tyr ¹⁵⁴ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-6.03	38.08	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Phe ⁴⁴¹ , Tyr ⁵⁴⁶ , Val ⁸⁴⁴ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶
			Helicase	-6.01	39.653	Gln ²⁸¹ , Asp ⁴⁰¹ , Pro ⁴⁰² , Ala ⁴⁰³ , Pro ⁴¹⁹ , Lys ⁴³⁰ , Leu ⁴⁵⁵ , Tyr ⁴⁵⁷ , Asp ⁴⁵⁸ , Asn ⁴⁵⁹ , Asn ⁵⁵⁹
			E-channel proteins	-6.47	18.12	No binding site was found
			Spike Open Protein	-5.83	53.64	Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , His ²⁰⁷ , Val ²²⁷
			Spike Close Protein	-5.91	46.94	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , His ²⁰⁷ , Leu ²²⁶
			Main Protease (MPro)	-7.92	1.56	Phe ⁸ , Lys ¹⁰² , Val ¹⁰⁴ , Arg ¹⁰⁵ , Ile ¹⁰⁶ , Gln ¹⁰⁷ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Val ²⁹⁷ , Arg ²⁹⁸ , Val ³⁰³
			Papain like protease (PLPro)	-10.3	0.03	Lys ¹⁵⁷ , Glu ¹⁶¹ , Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Glu ¹⁶⁷ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Asn ²⁶⁷ , Tyr ²⁶⁸ , Gln ²⁶⁹ , Tyr ²⁷³ , Thr ³⁰¹

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
105	Solophenol A	66551634	RNA-dependent RNA polymerase (RdRP)	-6.86	9.38	Tyr ³² , Ala ⁴⁶ , Lys ⁴⁷ , Tyr ¹²⁹ , His ¹³³ , Asp ¹³⁵ , Asn ¹³⁸ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Asp ⁷¹¹ , Lys ⁷¹⁴ , Gly ⁷⁷⁴ , Ser ⁷⁷⁸ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Ser ⁷⁸⁴
			Helicase	-9.4	0.13	Pro ¹⁷⁵ , Leu ¹⁷⁶ , Asn ¹⁷⁷ , Arg ¹⁷⁸ , Thr ¹⁹⁹ , Phe ²⁰⁰ , Glu ²⁰¹ , Lys ²⁰² , Gly ²⁰³ , Asp ²⁰⁴ , Val ²¹⁰ , Tyr ²¹¹ , Arg ²¹² , Val ⁴⁸⁴ , Ser ⁴⁸⁶ , Asn ⁵¹⁶ , Ser ⁵¹⁷ , Asn ⁵¹⁹ , Ala ⁵²⁰ , Thr ⁵³⁰ , Thr ⁵³² , Asp ⁵³⁴
			E-channel proteins	-8.87	0.31	Leu ²⁸ , Val ²⁹ , Leu ³¹ , Ala ³² , Thr ³⁵
			Spike Open Protein	-6.28	24.8	Trp ⁸⁸⁶ , Gly ⁸⁸⁹ , Ala ⁸⁹⁰ , Tyr ⁹⁰⁴ , Ser ¹⁰³⁰ , Glu ¹⁰³¹ , Leu ¹⁰³⁴ , Gly ¹⁰³⁵ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸
			Spike Close Protein	-6.93	8.39	Ile ¹⁰⁵ , Leu ¹¹⁸ , Val ¹²⁰ , Asn ¹²² , Val ¹²⁷ , Lys ¹²⁹ , Phe ¹³³ , Gln ¹³⁴ , Phe ¹³⁵ , Cys ¹³⁶ , Pro ¹³⁹ , Phe ¹⁴⁰ , Leu ¹⁴¹ , Leu ²⁴¹
106	Stearic acid	5281	Main Protease (MPro)	-4.22	805.32	Arg ²¹⁷ , Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Arg ²²² , Phe ²²³ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵
			Papain like protease (PLPro)	-5.69	68.05	Asp ¹⁶⁴ , Met ²⁰⁸ , Pro ²⁴⁷ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³
			RNA-dependent RNA polymerase (RdRP)	-4.81	300.53	His ¹³³ , Asn ⁷⁰⁵ , Ala ⁷⁰⁶ , Ser ⁷⁰⁹ , Thr ⁷¹⁰ , Phe ⁷⁶⁶ , Ser ⁷⁶⁸ , Ala ⁷⁷¹ , Ser ⁷⁷² , Gly ⁷⁷⁴ , Val ⁷⁷⁶ , Ser ⁷⁷⁸ , Ile ⁷⁷⁹ , Lys ⁷⁸⁰ , Asn ⁷⁸¹ , Thr ⁸⁰¹
			Helicase	-4.52	485.359	Gly ³ , Ala ⁴ , Cys ⁵ , Val ⁶ , Gln ¹¹ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.48	95.54	No binding site was found
			Spike Open Protein	-3.38	3335.49	Arg ³⁴ , Leu ¹⁸⁹ , Thr ²⁰⁸ , Pro ²⁰⁹ , Ile ²¹⁰ , Asn ²¹¹ , Leu ²¹² , Pro ²¹⁷ , Gln ²¹⁸ , Gly ²¹⁹ , Ser ²²¹
			Spike Close Protein	-4.94	237.68	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Leu ²²⁶ , Val ²²⁷ , Leu ²²⁹
			Main Protease (MPro)	-4.86	276.21	Met ⁶ , Ala ⁷ , Phe ⁸ , Ser ¹¹³ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹
			Papain like protease (PLPro)	-5.1	181.74	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-5.08	187.66	Arg ³⁰⁵ , Leu ⁴⁷⁰ , Phe ⁴⁷¹ , Glu ⁴⁷⁴ , Cys ⁷³⁰ , Asn ⁷³⁴ , Arg ⁷³⁵ , Asp ⁷³⁶ , Val ⁷³⁷ , Asp ⁷³⁸ , Val ⁷⁴²

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
107	Succinic acid	1110	Helicase	-5.22	148.67	Trp ¹¹⁴ , Tyr ¹²⁰ , Ala ¹²³ , Asn ¹²⁴ , Lys ¹³¹ , Ala ¹³⁴ , Ala ¹³⁵ , Leu ¹³⁸ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Arg ⁴⁰⁹ , Leu ⁴¹⁷ , Tyr ⁴²¹ , Phe ⁴²²
			E-channel proteins	-4.05	1074.76	No binding site was found
			Spike Open Protein	-4.36	633.69	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Leu ⁹⁶⁶ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-4.63	404.48	Cys ³⁹¹ , Phe ³⁹² , Thr ³⁹³ , Glu ⁵¹⁶ , Leu ⁵¹⁷ , Leu ⁵¹⁸ , His ⁵¹⁹ , Ala ⁵²⁰ , Pro ⁵²¹ , Ala ⁵²² , Asn ⁵⁴⁴ , Gly ⁵⁴⁵ , Leu ⁵⁴⁶ , Phe ⁵⁶⁵
108	Syringic acid	10742	Main Protease (MPro)	-5.44	102.9	Phe ⁸ , Val ¹⁰⁴ , Ile ¹⁰⁶ , Gln ¹¹⁰ , Thr ¹¹¹ , Asn ¹⁵¹ , Ile ¹⁵² , Asp ¹⁵³ , Ser ¹⁵⁸ , Thr ²⁹² , Phe ²⁹⁴ , Asp ²⁹⁵ , Arg ²⁹⁸
			Papain like protease (PLPro)	-6.65	13.44	Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , Tyr ¹⁷¹ , Gln ¹⁷⁴ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-5.74	62.44	Met ⁶¹⁵ , Gly ⁶¹⁶ , Trp ⁶¹⁷ , Asp ⁶¹⁸ , Asp ⁷⁶¹ , Ala ⁷⁶² , Lys ⁷⁹⁸ , Cys ⁷⁹⁹ , Trp ⁸⁰⁰ , His ⁸¹⁰ , Glu ⁸¹¹ , Phe ⁸¹² , Cys ⁸¹³ , Ser ⁸¹⁴
			Helicase	-5.86	50.734	Ala ⁴ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶
			E-channel proteins	-5.19	156.66	Leu ²⁸ , Leu ³¹ , Ala ³² , Thr ³⁵ , Cys ⁴⁰
			Spike Open Protein	-5.76	59.66	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³
			Spike Close Protein	-5.43	104.3	Tyr ³⁸ , Pro ³⁹ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Gly ²⁸³ , Thr ²⁸⁴
			Main Protease (MPro)	-6.95	8.1	Thr ²⁵ , Thr ²⁶ , Leu ²⁷ , His ⁴¹ , Cys ⁴⁴ , Thr ⁴⁵ , Ser ⁴⁶ , Met ⁴⁹ , Asn ¹⁴² , Gly ¹⁴³ , Ser ¹⁴⁴ , Cys ¹⁴⁵ , Met ¹⁶⁵ , Glu ¹⁶⁶ , Leu ¹⁶⁷ , Arg ¹⁸⁸ , Gln ¹⁸⁹ , Thr ¹⁹⁰ , Gln ¹⁹²
			Papain like protease (PLPro)	-7.86	1.75	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Ile ²²² , Lys ²³²

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
109	Tangeretin	68077	RNA-dependent RNA polymerase (RdRP)	-6.34	22.68	Phe ³⁵ , Ile ³⁷ , Tyr ³⁸ , Asn ³⁹ , Phe ⁴⁸ , Leu ⁴⁹ , Lys ⁵⁰ , Asp ²⁰⁸ , Asn ²⁰⁹ , Asp ²¹⁸ , Asp ²²¹ , Asn ⁷¹³
			Helicase	-7.12	6.049	Ala ¹³⁵ , Leu ¹³⁸ , Lys ¹³⁹ , Glu ¹⁴² , Arg ¹⁷⁸ , Asn ¹⁷⁹ , Cys ³⁰⁹ , Ser ³¹⁰ , Met ³⁷⁸ , Ala ³⁷⁹ , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Asp ³⁸³ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹
			E-channel proteins	-6.89	8.9	Leu ³¹ , Ala ³² , Leu ³⁴ , Thr ³⁵ , Ala ³⁶ , Cys ⁴⁰
			Spike Open Protein	-5.66	71.35	Met ⁷⁴⁰ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asp ⁷⁴⁵ , Phe ⁸⁵⁵ , Asn ⁸⁵⁶ , Val ⁹⁶³ , Lys ⁹⁶⁴ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
			Spike Close Protein	-6.23	26.94	Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Phe ¹⁹² , Ile ²⁰³ , Ser ²⁰⁵ , Leu ²²⁶ , Val ²²⁷ , Asp ²²⁸ , Leu ²²⁹
110	Tetracosanoic acid	11197	Main Protease (MPro)	-4.51	498.64	Arg ¹³¹ , Lys ¹³⁷ , Thr ¹⁹⁹ , Tyr ²³⁷ , Asn ²³⁸ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-5.49	95.06	Tyr ²⁰⁷ , Met ²⁰⁸ , Gly ²⁰⁹ , Val ²²⁰ , Ile ²²² , Pro ²²³ , Lys ²³² , Tyr ²⁶⁸
			RNA-dependent RNA polymerase (RdRP)	-4.76	326.99	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Phe ⁴¹⁵ , Ser ⁵⁰¹ , Asn ⁵⁴³ , Leu ⁵⁴⁴ , Lys ⁵⁴⁵ , Tyr ⁵⁴⁶ , Val ⁵⁵⁷ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶ , Ile ⁸⁴⁷
			Helicase	-4.54	471.631	Ala ⁴ , Cys ⁵ , Val ⁶ , Arg ¹⁵ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-5.18	159.32	Leu ¹⁹ , Ala ²² , Phe ²³ , Phe ²⁶
			Spike Open Protein	-4.67	378.71	Tyr ⁷⁸⁹ , Lys ⁷⁹⁰ , Thr ⁷⁹¹ , Pro ⁷⁹² , Ile ⁷⁹⁴ , Lys ⁷⁹⁵ , Asp ⁷⁹⁶ , Phe ⁷⁹⁷ , Gly ⁷⁹⁸ , Thr ⁸⁸³ , Ser ⁸⁸⁴ , Ala ⁸⁹³ , Leu ⁸⁹⁴ , Gln ⁸⁹⁵ , Ile ⁸⁹⁶ , Pro ⁸⁹⁷ , Phe ⁸⁹⁸ , Ala ⁸⁹⁹
			Spike Close Protein	-3.71	1911.03	Trp ⁸⁸⁶ , Gly ⁸⁸⁹ , Ala ⁸⁹⁰ , Tyr ⁹⁰⁴ , Ser ¹⁰³⁰ , Glu ¹⁰³¹ , L ^{???} ⁰³⁴ , Gly ¹⁰³⁵ , Gln ¹⁰³⁶ , Lys ¹⁰³⁸
			Main Protease (MPro)	-5.22	149.93	Trp ²¹⁸ , Phe ²¹⁹ , Asn ²²¹ , Ser ²⁶⁷ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶ , Asn ²⁷⁷ , Arg ²⁷⁹
			Papain like protease (PLPro)	-5.7	66.57	Leu ¹⁸⁵ , Val ¹⁸⁷ , Thr ¹⁹⁷ , Leu ¹⁹⁹ , Glu ²⁰³ , Tyr ²⁰⁷ , Met ²⁰⁸ , Lys ²³²

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
111	Thymoquinone	10281	RNA-dependent RNA polymerase (RdRP)	-5.18	160.94	His ⁶¹³ , Met ⁶¹⁵ , Phe ⁷⁶⁶ , Ser ⁷⁶⁸ , Ala ⁷⁷¹ , Ser ⁷⁷² , Ser ⁷⁷⁸ , Ile ⁷⁷⁹ , Lys ⁷⁸⁰ , Thr ⁸⁰¹ , Thr ⁸⁰³
			Helicase	-5.73	63.288	Gln ²⁸¹ , Pro ⁴⁰² , Ala ⁴⁰³ , Lys ⁴³⁰ , Pro ⁴³⁴ , Phe ⁴³⁷ , Tyr ⁴⁵⁷ , Asp ⁴⁵⁸
			E-channel proteins	-5.71	65.57	Leu ³¹ , Ala ³² , Leu ³⁴ , Thr ³⁵ , Cys ⁴⁰
			Spike Open Protein	-4.74	338.22	Glu ⁵⁵⁴ , Ser ⁵⁵⁵ , Lys ⁵⁵⁷ , Lys ⁵⁵⁸ , Phe ⁵⁵⁹ , Arg ⁵⁷⁷ , Leu ⁵⁸² , Glu ⁵⁸³ , Ile ⁵⁸⁴
			Spike Close Protein	-5.59	79.89	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ ??Le ²⁰³ , Ser ²⁰⁵ , Leu ²²⁶ , Val ²²⁷
112	Tyrosine	6057	Main Protease (MPro)	-5.96	42.71	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-7.05	6.85	His ⁷³ , Thr ⁷⁴ , Thr ⁷⁵ , Asp ⁷⁶ , Phe ⁷⁹ , Arg ⁸² , Ala ¹⁵³ , Tyr ¹⁵⁴ , Asn ¹⁵⁶ , His ¹⁷⁵
			RNA-dependent RNA polymerase (RdRP)	-5.52	89.91	Glu ¹³⁶ , Gly ¹³⁷ , Asn ¹³⁸ , Cys ¹³⁹ , Asp ¹⁴⁰ , Lys ¹⁴³ , Phe ¹⁵⁷ , Lys ¹⁵⁹ , Lys ¹⁶⁰ , Asp ¹⁶¹ , Trp ¹⁶² , Tyr ¹⁶³
			Helicase	-5.78	57.58	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Pro ⁴¹⁹ , Phe ⁴²² , Asn ⁵⁵⁷ , Asn ⁵⁵⁹ , Arg ⁵⁶⁰
			E-channel proteins	-5.52	89.91	Leu ³¹ , Thr ³⁵ , Cys ⁴⁰ , Cys ⁴³ , Cys ⁴⁴ , Val ⁴⁷
			Spike Open Protein	-5.97	41.78	Tyr ³⁸ , Asp ⁴⁰ , Lys ⁴¹ , Val ⁴² , Phe ⁴³ , Arg ⁴⁴ , Glu ²²⁴ , Pro ²²⁵ , Tyr ²⁷⁹ , Asn ²⁸² , Gly ²⁸³ , Thr ²⁸⁴
			Spike Close Protein	-5.16	165.35	Asp ⁴²⁰ , Tyr ⁴²¹ , Asn ⁴²² , Tyr ⁴²³ , Lys ⁴²⁴ , Arg ⁴⁵⁴ , Lys ⁴⁶² , Glu ⁴⁶⁵ , Arg ⁴⁶⁶ , Asp ⁴⁶⁷
			Main Protease (MPro)	-6.06	36.02	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Gly ³⁰² , Val ³⁰³
			Papain like protease (PLPro)	-5.92	45.92	Leu ¹⁶² , Gly ¹⁶³ , Asp ¹⁶⁴ , Pro ²⁴⁸ , Tyr ²⁶⁴ , Tyr ²⁶⁸ , Tyr ²⁷³ , Thr ³⁰¹
			RNA-dependent RNA polymerase (RdRP)	-5.18	159.32	Pro ³²³ , Phe ³²⁶ , Gly ³²⁷ , Tyr ³⁴⁶ , Phe ³⁴⁸ , Arg ³⁴⁹ , Asn ⁶²⁸ , Ser ⁶⁶⁴ , Val ⁶⁷⁵ , Lys ⁶⁷⁶ , Pro ⁶⁷⁷

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
113	Tyrosol	10393	Helicase	-5.34	122.441	Ala ¹³⁵ , Leu ¹³⁸ , Lys ¹³⁹ , Glu ¹⁴² , Thr ³⁸⁰ , Asn ³⁸¹ , Tyr ³⁸² , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹
			E-channel proteins	-5.16	163.96	No binding site was found
			Spike Open Protein	-4.48	517.51	Gly ⁹⁰⁸ , Ile ⁹⁰⁹ , Gln ¹⁰³⁶ , Ser ¹⁰³⁷ , Lys ¹⁰³⁸ , Val ¹⁰⁴⁰ , Tyr ¹⁰⁴⁷ , His ¹⁰⁴⁸
			Spike Close Protein	-5.21	150.95	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Asn ⁸⁵⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰
114	Umbelliprenin	1781413	Main Protease (MPro)	-6.84	9.67	Lys ⁵ , Arg ¹³¹ , Lys ¹³⁷ , Thr ¹⁹⁹ , Tyr ²³⁷ , Tyr ²³⁹ , Leu ²⁷¹ , Leu ²⁷² , Gly ²⁷⁵ , Met ²⁷⁶ , Ala ²⁸⁵ , Leu ²⁸⁶ , Leu ²⁸⁷ , Glu ²⁸⁸ , Asp ²⁸⁹ , Glu ²⁹⁰
			Papain like protease (PLPro)	-7.75	2.1	Arg ¹⁶⁶ , Ser ¹⁷⁰ , Leu ¹⁸⁵ , Val ¹⁸⁷ , Gln ¹⁹⁵ , Thr ¹⁹⁷ , Leu ¹⁹⁹ , Val ²⁰² , Glu ²⁰³ , Met ²⁰⁶ , Tyr ²⁰⁷ , Met ²⁰⁸ , Thr ²²⁵ , Lys ²³²
			RNA-dependent RNA polymerase (RdRP)	-6.74	11.49	Thr ⁷⁶ , Phe ⁷⁷ , Tyr ⁸⁰ , Glu ⁸⁴ , Tyr ⁸⁷ , Asn ⁸⁸ , Lys ⁹¹ , His ⁹⁹ , Asp ¹⁰⁰ , Phe ¹⁰¹ , Phe ¹⁰² , Pro ¹¹²
			Helicase	-6.35	22.263	Gly ³ , Ala ⁴ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶ , Pro ²³⁴ , Leu ²³⁵ , Ser ²³⁶
			E-channel proteins	-8.9	0.3	No binding site was found
			Spike Open Protein	-6.5	17.34	Ser ⁸⁸⁴ , Gly ⁸⁸⁵ , Trp ⁸⁸⁶ , Thr ⁸⁸⁷ , Ala ⁸⁹⁰ , Leu ⁸⁹⁴ , Ile ⁸⁹⁶ , Gln ⁹⁰¹ , Tyr ⁹⁰⁴ , Arg ⁹⁰⁵ , Leu ¹⁰³⁴ , Gly ¹⁰³⁵ , Gln ¹⁰³⁶
			Spike Close Protein	-8.12	1.11	Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Phe ¹⁶⁸ , Tyr ¹⁷⁰ , Ser ¹⁷² , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Lys ²⁰⁶ , His ²⁰⁷ , Leu ²²⁶ , Val ²²⁷ , Leu ²²⁹
			Main Protease (MPro)	-5.16	165.07	Met ⁶ , Ala ⁷ , Phe ⁸ , Pro ⁹ , Gln ¹²⁷ , Ile ¹⁵² , Asp ¹⁵³ , Tyr ¹⁵⁴ , Phe ²⁹¹ , Asp ²⁹⁵ , Arg ²⁹⁸ , Gln ²⁹⁹ , Val ³⁰³ , Thr ³⁰⁴
			Papain like protease (PLPro)	-5.4	110.28	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-4.88	265.24	Lys ⁴¹¹ , Pro ⁴¹² , Gly ⁴¹³ , Asn ⁴¹⁴ , Tyr ⁵⁴⁶ , Asp ⁸⁴⁵ , Asp ⁸⁴⁶ , Ile ⁸⁴⁷ , cser ¹⁵

Sr.	Ligands	PubChem ID	Proteins	Binding energy	Dissociation Constant	Active site residues
				(kcal/mol)	(μ M)	
115	Undecanoic acid	8180	Helicase	-4.68	371.12	Pro ⁴⁰⁶ , Ala ⁴⁰⁷ , Pro ⁴⁰⁸ , Arg ⁴⁰⁹ , Leu ⁴¹² , Gly ⁴¹⁵ , Thr ⁴¹⁶ , Leu ⁴¹⁷ , Phe ⁴²² , His ⁵⁵⁴ , Asn ⁵⁵⁷ , Asn ⁵⁵⁹
			E-channel proteins	-5.1	182.97	Leu ⁵¹ , Pro ⁵⁴ , Tyr ⁵⁷ , Ser ⁶⁰ , Arg ⁶¹
			Spike Open Protein	-5.09	187.35	Glu ⁹⁶ , Asn ⁹⁹ , Ile ¹⁰¹ , Arg ¹⁰² , Gly ¹⁰³ , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Ser ²⁰⁵ , Leu ²²⁶ , Val ²²⁷
			Spike Close Protein	-4.79	309.8	Glu ⁹⁶ , Ile ¹⁰¹ , Arg ¹⁰² , Trp ¹⁰⁴ , Ile ¹¹⁹ , Asn ¹²¹ , Val ¹²⁶ , Ile ¹²⁸ , Arg ¹⁹⁰ , Phe ¹⁹² , Phe ¹⁹⁴ , Ile ²⁰³ , Leu ²²⁶ , Val ²²⁷
116	Vanillic acid	8468	Main Protease (MPro)	-5.35	120.39	Trp ²¹⁸ , Phe ²¹⁹ , Leu ²²⁰ , Asn ²²¹ , Phe ²²³ , Glu ²⁷⁰ , Leu ²⁷¹ , Asn ²⁷⁴ , Gly ²⁷⁵ , Met ²⁷⁶
			Papain like protease (PLPro)	-6.6	14.65	No binding site was found
			RNA-dependent RNA polymerase (RdRP)	-5.59	80.56	Tyr ⁴⁵⁶ , Arg ⁵⁵⁵ , Thr ⁵⁵⁶ , Val ⁵⁵⁷ , Ala ⁵⁵⁸ , Asp ⁶²³ , Arg ⁶²⁴ , Lys ⁶⁷⁶ , Thr ⁶⁸⁰ , Ser ⁶⁸¹ , Ser ⁶⁸² , Gly ⁶⁸³
			Helicase	-5.63	74.546	Ala ⁴ , Val ⁶ , Arg ²¹ , Arg ²² , Pro ²³ , Phe ²⁴ , Arg ¹²⁹ , Leu ¹³² , Phe ¹³³ , Glu ¹³⁶
			E-channel proteins	-5.55	85.18	Leu ²⁸ , Leu ³¹ , Ala ³² , Leu ³⁴ , Thr ³⁵ , Cys ⁴⁰
			Spike Open Protein	-5.67	70.15	Met ⁷⁴⁰ , Tyr ⁷⁴¹ , Ile ⁷⁴² , Cys ⁷⁴³ , Gly ⁷⁴⁴ , Ser ⁷⁴⁶ , Leu ⁹⁶⁶ , Ser ⁹⁶⁷ , Ser ⁹⁷⁵ , Val ⁹⁷⁶ , Leu ⁹⁷⁷ , Asn ⁹⁷⁸ , Arg ¹⁰⁰⁰