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ORIGINAL ARTICLE **OPEN ACCESS**

In Silico Screening of Chrysin Derivatives as Drug Leads against Covid- 19

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ABSTRACT
The current investigation was aimed at in silico studies of some selected chrysin derivatives to evaluate their activity in attenuation of COVID 19. In this study 50 chrysin derivatives were selected and Remedesivir was used as standard in assessing the anti viral activity. Primarily drug like properties and bioactivity score was calculated and then the compounds were subjected to ADMET studies. Further the molecular docking studies was performed to ascertain the binding fitness score using PATCHDOCK software towards SARS COV2 protease and Angiotensin Converting Enzyme proteins. The outcome of in silico studies reveals that derivatives of chrysin may ladle out as leads in development of drugs that possess good anti viral properties to combat COVID 19.
KEYWORDS: *Chrysin, Molecular docking, SARS COV-2, Angiotensin converting enzyme, Anti Viral*

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INTRODUCTION

Plants have developed the sophisticated conventional medical systems that have existed since the dawn of mankind [1]. Many indigenous groups have long-standing relationships with medicinal plants, which are used to treat a variety of illnesses [2]. For millennia, phytochemicals have been utilized as medications. Recently, it has been suggested that phytochemicals, which come from plants, are a safer alternative to synthetic medications. Low toxicity, low cost, easy accessibility, and biological properties like antioxidant activities, antineoplastic, detoxification enzyme modulation, immune system stimulation, platelet aggregation reduction, hormone metabolism modulation, and antimicrobial effects are all upsides of phytochemicals [3].

The majority of secondary metabolites present in red wine and tea as well as in vegetables, fruits, seeds, and spices are flavonoids, which are the most prevalent bioactive chemicals. Anthocyanins, flavones, flavanones, and flavanols are some of the classes of flavonoids that can be further subdivided based on their comparable chemical structures. A prominent class of the flavonoid family with a 2-phenyl-1-benzopyran-4-one backbone is called flavones. Flavones have been known to have antiviral properties since the 1990s. Several flavones showed notable antiviral capabilities in in vitro and even in vivo experiments, which indicates that several flavones have been examined for their potential antiviral actions [4].

Among different flavonoids Chrysin is a readily accessible phytoconstituent with significant biological effects. To test their anti-viral effectiveness in battling the SARS-COV-2 Virus, the current work is focused upon the in-silico analysis of semi-synthetic chrysin derivatives.

MATERIAL AND METHODS

Preparation of Chemical Compounds library:

From the Chemical Compounds Database-PubChem, the structure of chrysin was obtained, and 49 compounds that had already been built as semisynthetic derivatives of chrysin were choosen (5-10). Using ChemDraw Ultra 12.0 (2010), selected derivatives' structures were depicted along with their IUPAC names and molecular formulas (Table 1).

Prediction of Molecular properties:

The Lipinski's rule of five compounds was tested using molinspiration, which was also utilized to predict a number of physicochemical properties. For the purpose of predicting a molecule's likelihood of being a medicine, its physicochemical parameters, including molecular weight, volume, polar surface area (PSA),

hydrogen bond acceptor/donor, log P, and the number of rotatable bonds, were computed. The bioactivity score values, which show the overall potential of a chemical to be a therapeutic candidate, are also predicted [11].

ADME properties:

Various parameters like GI absorption, BBB permeability, skin permeability, and toxicity were anticipated using the Swiss ADME and PreADMET web tools to evaluate the ADME features of compounds [12].

Toxicity prediction:

PreADMET was utilized to forecast hERG inhibition and mutagenicity in terms of a compound's potential toxicity [13].

Docking Studies:

The ligand structure is depicted using Chemdraw Ultra12.0, and the energy is reduced using Chemdraw 3d Pro and stored as mol 2 form. The ligand must be saved in pdb form in order to be submitted to the patch dock program. Using MGLtools, the ligand is transformed into pdb format. Protein Data Bank is used to download the necessary protein pdb. The chosen receptor and ligands were docked by submitting them to the online, computerized molecular docking server Patch Dock. In order to receive the results, an email address was provided while keeping the clustering RMSD at 4.0 A°. The provided email address was used to receive and download the result [14].

RESULTS AND DISCUSSION:

Prediction of Molecular properties:

Molinspiration conducted a Lipinski's rule of five analysis for derivatives. Results revealed that all compounds followed Lipinski's rule of five and did not break more than one criterion, demonstrating their high oral bioavailability (Table -2).

Bioactivity scores of compounds:

The bioactivity ratings of substances against receptors were predicted using Molinspiration. All of the compounds were discovered to fall between the range of -5.0 to 5.0, which suggests that they have a moderate to good level of action toward biological targets. These findings come in harmony with previous reports on chrysin derivatives which states that these derivatives exhibit drug like properties and biological actions [15].

ADME properties:

All compounds were found to have caco2 permeability ranging from 02 to 42 nm/sec. apart from L50 compound. This shows that all substances had permeabilities that ranged from moderate to good. All compounds' MDCK values range from 0.02-58 nm/sec. PreADMET measures intestinal absorption in percentage, which is crucial for identifying a potential candidate. Except for (L24-L25, L47-L49, and L51) compounds, all substances were found to have high GI absorption, while all substances had skin permeabilities between -2 and -9 cm/sec.

Because these CYP isoenzymes are essential for drug clearance during phase I of metabolic biotransformation, interactions between compounds and CYP were also anticipated. Results obtained indicated that all chemicals other than (L1, L2, L11, L13, L15, L20, L21, L25, L48-L50) were found to inhibit CYP2C19. These findings come in accordance with the earlier scientific reports which stated that chrysin derivatives exhibit good absorption, distribution and metabolic properties [16,17]

Toxicity predictions:

Studies on toxicity such as mutagenicity and hERG inhibition were anticipated. With the exception of (L20-L22, L24-L25, L36, L37, L38, L48, and L50) compounds, all of the derivatives were determined to be non-mutagens and to exhibit low to medium risk hERG inhibition.

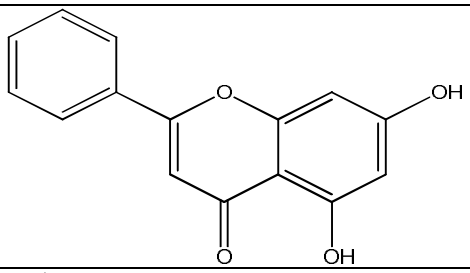
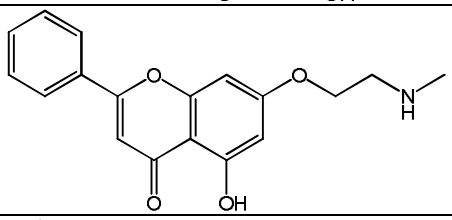
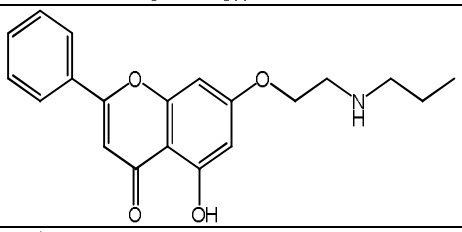
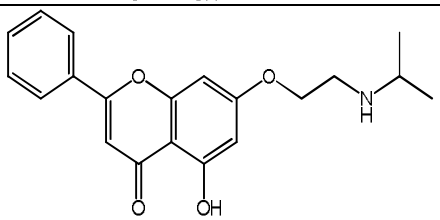
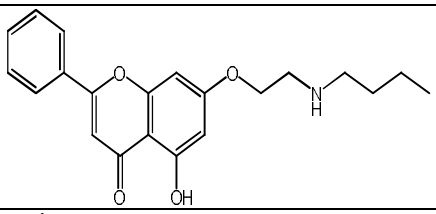
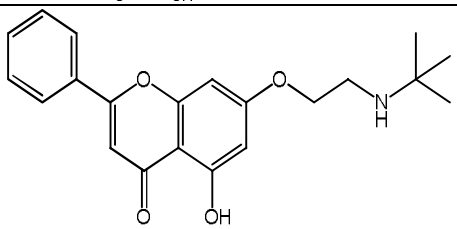
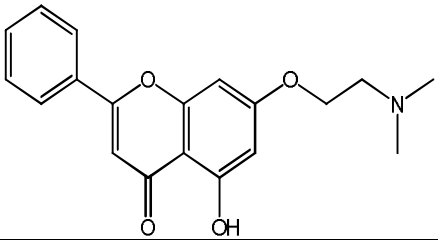
Docking studies:

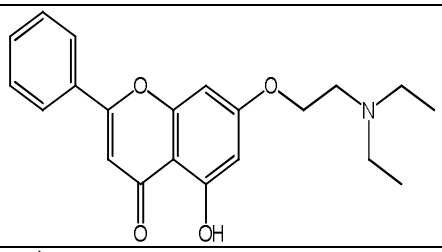
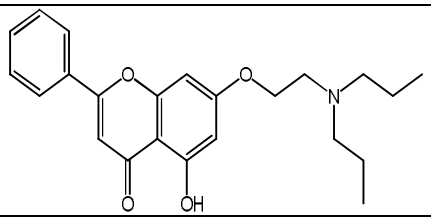
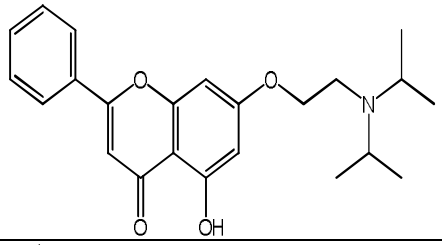
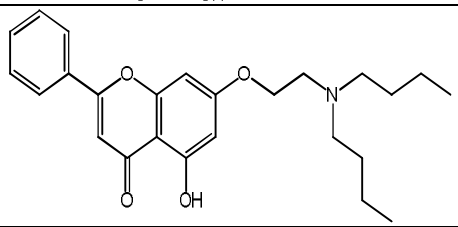
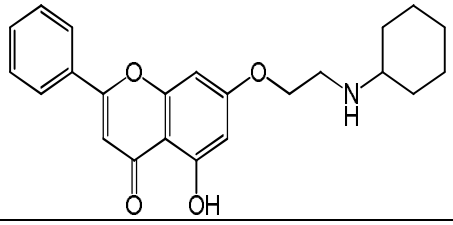
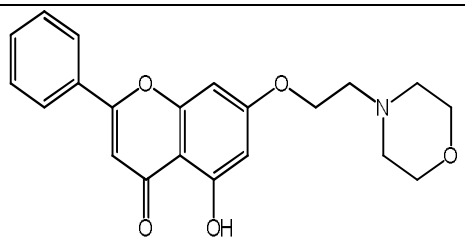
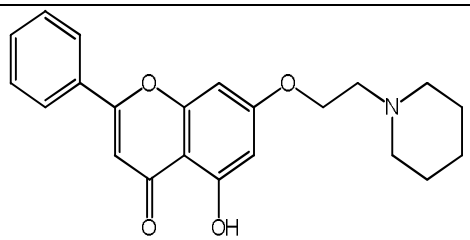
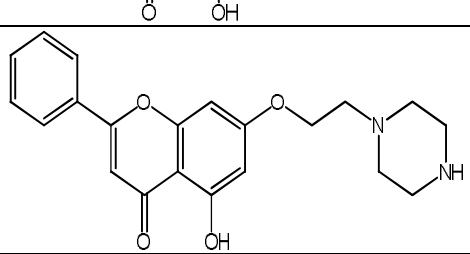
Atomic contact energies between molecules and macromolecular structure were calculated using Patch dock. Strong hydrogen bonding and hydrophobic interactions have been observed between all drugs and the target proteins during binding. One of two cysteine proteases required for viral replication and assembly is the SARS-CoV-2 major protease (Mpro). All of the derivatives, including PL16, PL48, PL37, PL43, PL38, PL12, PL45, and PL19, demonstrated the highest affinity for the target protein, the SARS-CoV-2 protease, with ACE values ranging from -269 to -330 Kcal/mol, respectively. All of the compounds demonstrated higher affinity than the reference drug, remdesivir (Table:3 and Figure 1**)).** These results are further reinforced by earlier studies, which suggested that phytochemicals may be useful in combating viral infections [18].

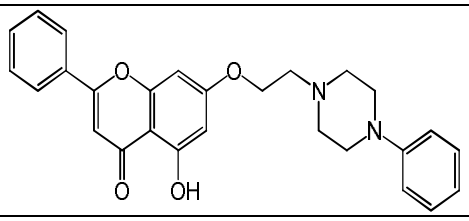
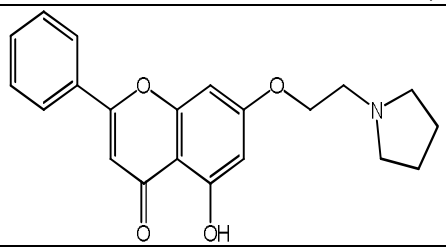
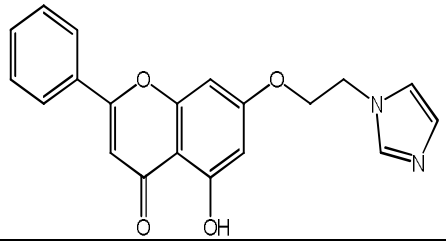
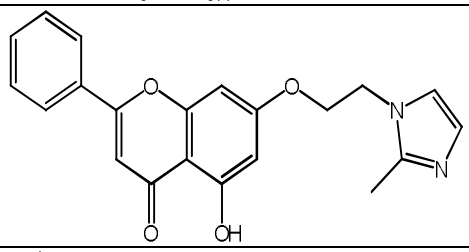
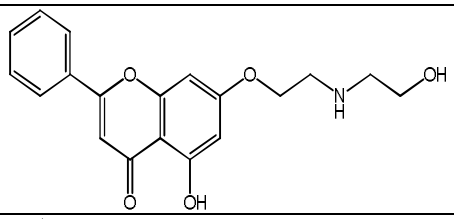
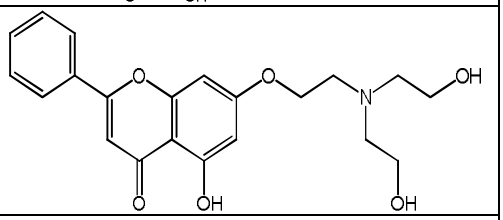
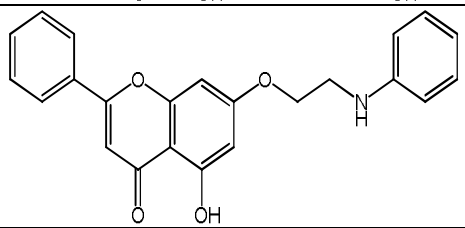
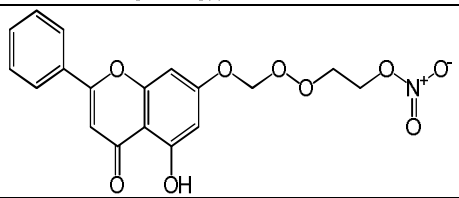
The majority of organs express and function with the type 1 full-length membrane glycoprotein known as ACE2. The kidney, endothelium, lung, and heart all showed the highest expression of ACE2. Regardless of its angiotensinase activity, ACE2 is associated with the function of integrin [19]. Additionally, among all the derivatives, PL23, PL17, PL10, PL11, PL18, PL22, PL44, and PL38 compounds demonstrated the greatest

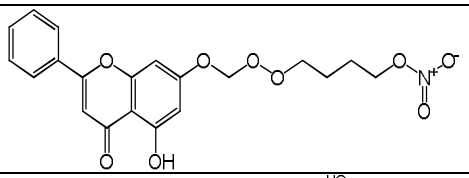
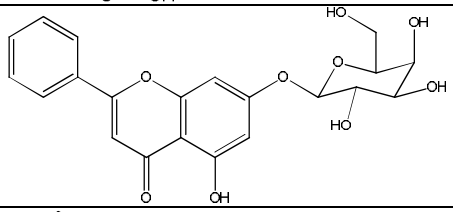
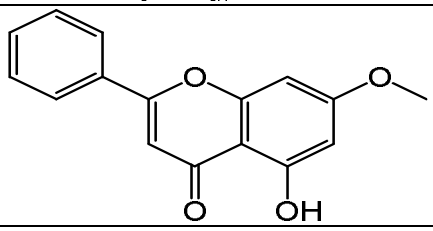
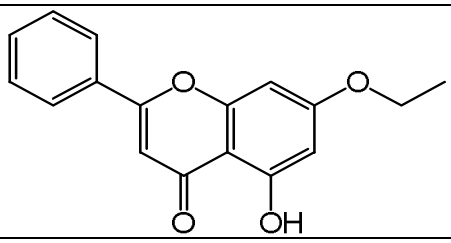
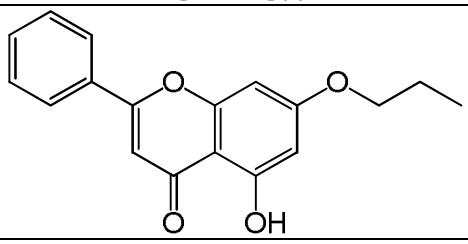
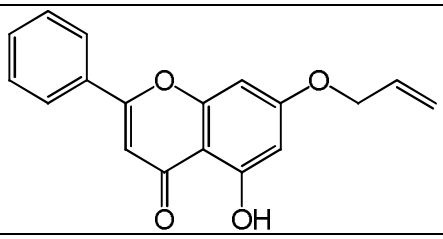
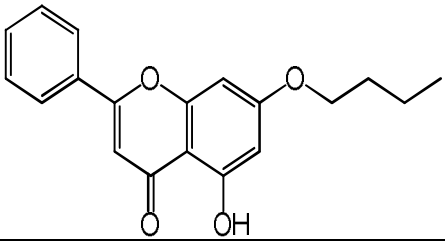
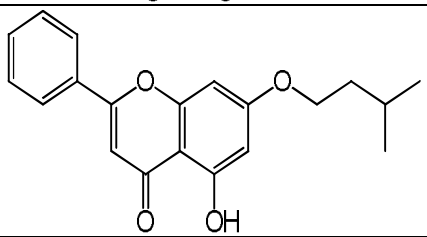
affinity to the Angiotensin Converting Enzyme Inhibitor 2 with ACE values ranging from -331 to -360 Kcal/mol, respectively. All the compounds demonstrated greater affinity than the reference drug Remdesivir (ACE= -330.50) (Table 3 and Figure 2). This is related to prior studies on phytochemical derivatives [20].

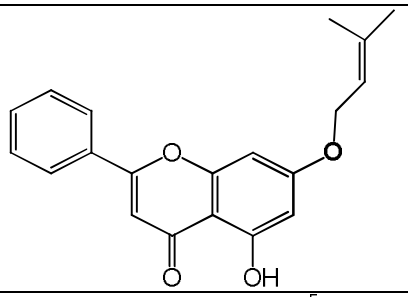
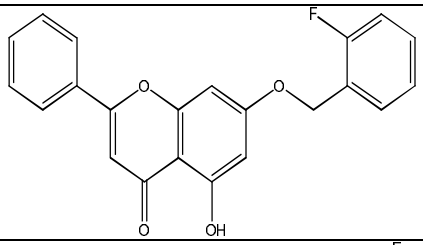
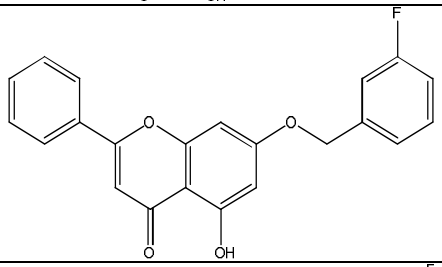
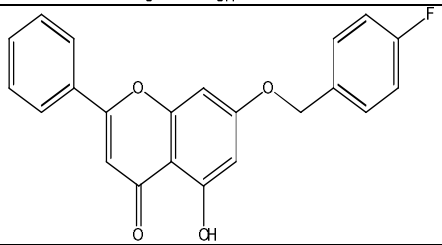
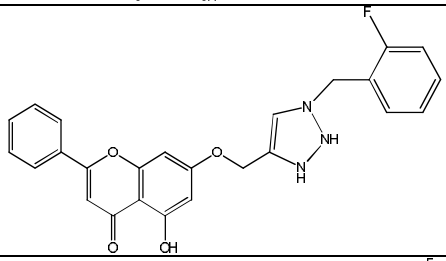
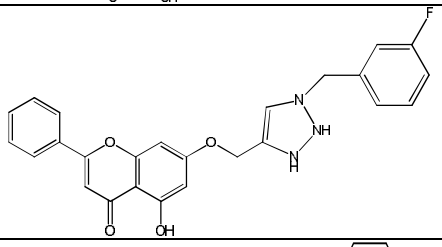
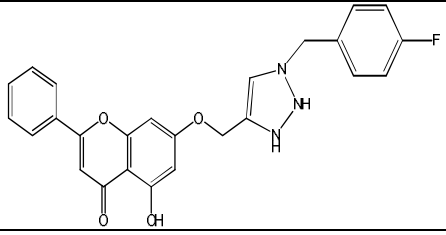
Table 1: SELECTED SEMISYNTHETIC DERIVATIVES OF CHRYSIN

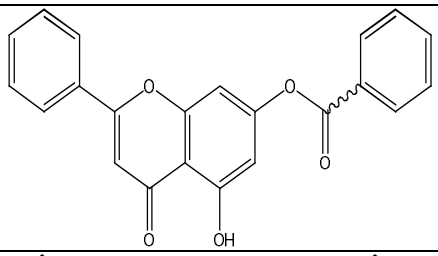
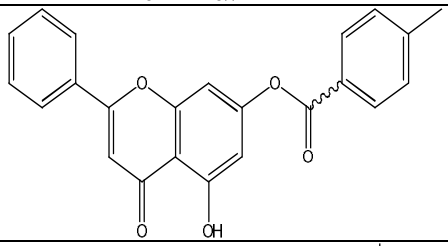
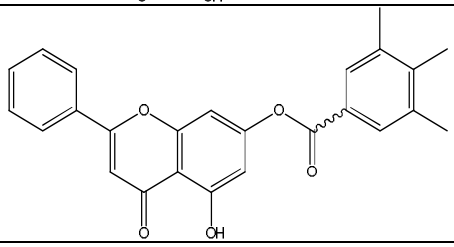
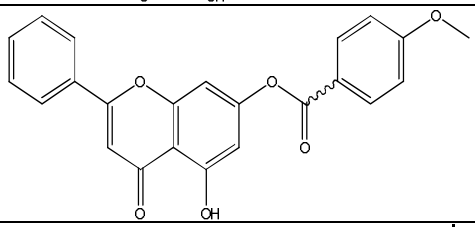
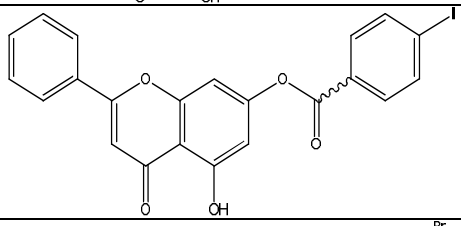
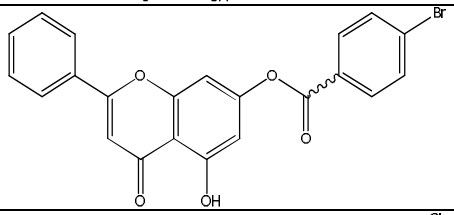
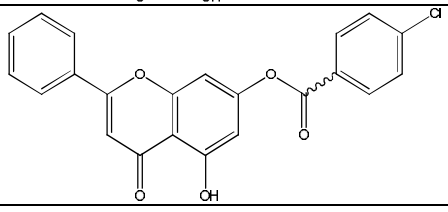
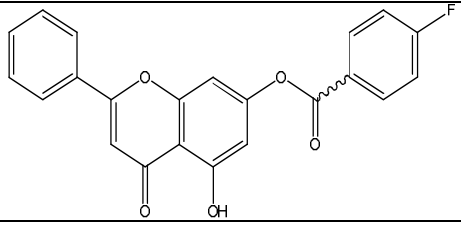
S.no	Name of the compound	Molecular formula	Structure of the compound
01.	5,7-Dihydroxy-2-phenyl-4H-1-benzopyran-4-one (L1)	$C_{15}H_{10}O_4$	
02.	7-(2-(methylamino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L2)	$C_{18}H_{17}NO_4$	
03.	7-(2-(propyl amino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L3)	$C_{20}H_{21}NO_4$	
04.	7-(2-(isopropyl amino) ethoxy)-5-hydroxy-2-phenyl- 4Hchromen-4-one (L4)	$C_{20}H_{21}NO_4$	
05.	7-(2-(butyl amino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L5)	$C_{21}H_{23}NO_4$	
06.	7-(2-(tert-butylamine) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L6)	$C_{21}H_{23}NO_4$	
07.	7-(2-(dimethyl amino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L7)	$C_{19}H_{19}NO_4$	

08.	7-(2-(diethylamino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L8)	$C_{21}H_{23}NO_4$	
09.	7-(2-(dipropyl amino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L9)	$C_{23}H_{27}NO_4$	
10.	7-(2-(diisopropylamino) ethoxy)-5-hydroxy-2-phenyl- 4Hchromen-4-one (L10)	$C_{23}H_{27}NO_4$	
11.	7-(2-(dibutyl amino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L11)	$C_{25}H_{31}NO_4$	
12.	7-(2-(cyclohexyl amino) ethoxy)-5-hydroxy-2-phenyl -4Hchromen-4-one (L12)	$C_{23}H_{25}NO_4$	
13.	7-(2-morpholinoethoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L13)	$C_{21}H_{21}NO_5$	
14.	7-(2-(piperidin-1-yl) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L14)	$C_{22}H_{23}NO_4$	
15.	7-(2-(piperazin-1-yl) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L15)	$C_{21}H_{22}N_2O_4$	

16.	7-(2-(4-phenylpiperazin-1-yl) ethoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L16)	$C_{27}H_{26}N_2O_4$	
17.	7-(2-(pyrrolidin-1-yl) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L17)	$C_{21}H_{21}NO_4$	
18.	7-(2-(1H-imidazol-1-yl) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L18)	$C_{20}H_{16}N_2O_4$	
19.	7-(2-(2-methyl-1H-imidazol-1-yl) ethoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L19)	$C_{21}H_{18}N_2O_4$	
20.	7-(2-(2'-hydroxyethylamino) ethoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L20)	$C_{19}H_{19}NO_5$	
21.	7-(2-bis(2-hydroxyethylamino) ethoxy)-5-hydroxy-2-phenyl-4H-chromen-4-on (L21)	$C_{21}H_{23}NO_6$	
22.	7-(2-(phenylamino) ethoxy)-5-hydroxy-2-phenyl-4Hchromen-4-one (L22)	$C_{23}H_{19}NO_4$	
23.	2-(5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl) oxy) methyl) peroxy) ethyl nitrate (L23)	$C_{18}H_{15}NO_9$	

24.	4-(5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl) oxy) methyl) peroxy) butyl nitrate (L24)	$C_{20}H_{19}NO_9$	
25.	5-hydroxy-2-phenyl-7-(((2R,3S,4R,5S,6S)-3,4,5-trihydroxy-6-(hydroxymethyl) tetrahydro-2H-pyran-2-yl) oxy)-4H-chromen-4-one	$C_{21}H_{20}O_9$	
26.	5-hydroxy-7-methoxy-2-phenyl-4H-chromen-4-one (L26)	$C_{16}H_{12}O_4$	
27.	7-ethoxy-5-hydroxy-2-phenyl-4H-chromen-4-one (L27)	$C_{17}H_{14}O_4$	
28.	5-hydroxy-2-phenyl-7-propoxy-4H-chromen-4-one (L28)	$C_{18}H_{16}O_4$	
29.	7-(allyloxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L29)	$C_{18}H_{14}O_4$	
30.	7-butoxy-5-hydroxy-2-phenyl-4H-chromen-4-one (L30)	$C_{19}H_{18}O_4$	
31.	5-hydroxy-7-(isopentyloxy)-2-phenyl-4H-chromen-4-one (L31)	$C_{20}H_{20}O_4$	

32.	5-hydroxy-7-((3-methylbut-2-en-1-yl) oxy)-2-phenyl-4H-chromen-4-one (L32)	$C_{20}H_{18}O_4$	
33.	7-((2-fluorobenzyl) oxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L33)	C 22 H 15 FO 4	
34.	7-((3-fluorobenzyl) oxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L34)	$C_{22}H_{15}FO_4$	
35.	7-((4-fluorobenzyl) oxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L35)	$C_{22}H_{15}FO_4$	
36.	7-((1-(2-fluorobenzyl)-2,3-dihydro-1H-1,2,3-triazol-4-yl) methoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L36)	$C_{25}H_{20}FN_3O_4$	
37.	7-((1-(3-fluorobenzyl)-2,3-dihydro-1H-1,2,3-triazol-4-yl) methoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L37)	$C_{25}H_{20}FN_3O_4$	
38.	7-((1-(4-fluorobenzyl)-2,3-dihydro-1H-1,2,3-triazol-4-yl) methoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (L38)	$C_{25}H_{20}FN_3O_4$	

39.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-benzoate (L39)	$C_{22}H_{14}O_5$	
40.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-methylbenzoate (L40)	$C_{23}H_{16}O$	
41.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 3,4,5-trimethyl benzoate (L41)	$C_{25}H_{20}O_5$	
42.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-methylbenzoate (L42)	$C_{23}H_{16}O_6$	
43.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-iodobenzoate (L43)	$C_{22}H_{13}IO_5$	
44.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-bromobenzoate (L44)	$C_{22}H_{13}BrO_5$	
45.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-chlorobenzoate (L45)	$C_{22}H_{13}ClO_5$	
46.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-fluorobenzoate (L46)	$C_{22}H_{13}FO_5$	

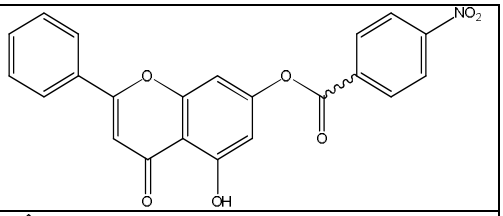
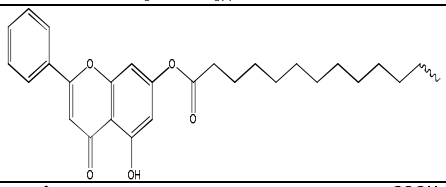
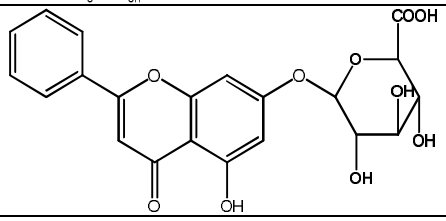
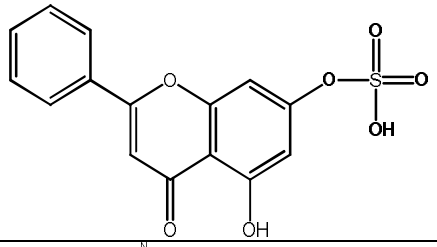
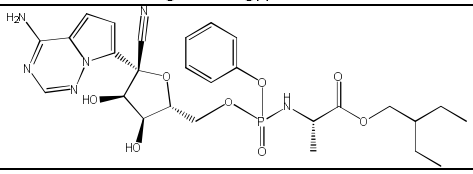
47.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl 4-nitrobenzoate (L47)	$C_{22}H_{13}NO_7$	
48.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl tridecanoate (L48)	$C_{28}H_{34}O_5$	
49.	(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-((5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl) oxy) tetrahydro-2H-pyran-2-carboxylic acid (L49)	$C_{21}H_{18}O_{10}$	
50.	5-hydroxy-4-oxo-2-phenyl-4H-chromen-7-yl hydrogen sulfate (L50)	$C_{15}H_{10}O_7S$	
51.	Remdesivir (L52)	$C_{27}H_{35}N_6O_8P$	

TABLE 2: MOLECULAR PROPERTIES OF CHRYSIN DERIVATIVES

Compound no.	Molecular weight	Rotatable bonds	Hydrogen bond acceptors	Hydrogen bond donors	TPSA	LOG-P	Violations	Volumes
L1	254.24	01	04	02	70.67	2.94	0	216.03
L2	311.34	05	05	02	71.70	3.26	0	279.56
L3	339.39	07	05	02	71.70	3.79	0	313.17
L4	339.39	06	05	02	71.70	3.94	0	312.95
L5	353.42	08	05	02	71.70	4.35	0	329.97
L6	353.42	06	05	02	71.70	4.45	0	329.19
L7	325.36	05	05	01	62.91	3.51	0	296.51
L8	353.42	07	05	01	62.91	4.26	0	330.11
L9	381.47	09	05	01	62.91	5.27	01	363.71
L10	381.47	07	05	01	62.91	4.85	0	363.29
L11	409.53	11	05	01	62.91	6.38	01	397.32
L12	379.46	06	05	02	71.70	5.17	01	353.00
L13	367.40	05	06	01	72.14	3.35	0	328.74
L14	365.43	05	05	01	62.91	4.42	0	336.55
L15	366.42	05	06	02	74.94	2.81	0	332.15
L16	442.51	06	05	01	66.15	5.10	01	403.94
L17	351.40	05	05	01	62.91	3.91	0	319.75
L18	348.36	05	06	02	77.50	3.16	0	303.22
L19	362.38	05	06	02	77.50	3.25	0	319.78
L20	341.36	07	06	03	91.93	2.28	0	304.62
L21	385.42	09	07	03	103.37	2.24	0	346.63
L22	373.41	06	04	02	71.70	4.96	0	334.41
L23	404.35	10	09	01	116.69	-0.83	0	337.96

L24	432.40	12	09	01	116.69	-0.28	0	371.57
L25	416.38	04	09	05	149.82	1.16	0	348.15
L26	268.27	02	04	01	59.67	3.48	0	233.56
L27	282.30	03	04	01	59.67	3.85	0	250.36
L28	296.32	04	04	01	59.67	4.36	0	267.16
L29	294.31	04	04	01	59.67	4.12	0	261.53
L30	310.35	05	04	01	59.67	4.92	0	283.96
L31	324.38	05	04	01	59.67	5.13	01	300.55
L32	322.36	04	04	01	59.67	5.16	01	294.34
L33	362.36	04	05	01	59.67	5.19	01	310.14
L34	362.36	04	05	01	59.67	5.21	01	310.14
L35	362.36	04	05	01	59.67	5.24	01	310.14
L36	445.45	06	08	03	96.19	4.97	0	381.11
L37	445.45	06	08	03	96.19	4.99	0	381.11
L38	445.15	06	08	03	96.19	5.01	01	381.11
L39	358.35	04	05	01	76.74	5.29	01	307.39
L40	372.38	04	05	01	76.74	5.74	01	323.95
L41	400.43	04	05	01	76.74	6.49	01	357.07
L42	388.38	05	06	01	85.98	5.35	01	332.94
L43	484.25	04	05	01	76.74	6.37	01	331.38
L44	437.25	04	05	01	76.74	6.10	01	325.27
L45	392.79	04	05	01	76.74	5.97	01	320.93
L46	376.34	04	06	01	76.74	5.45	01	312.32
L47	403.35	05	07	01	112.57	5.25	01	330.72
L48	450.57	14	05	01	76.74	8.56	01	437.36
L49	430.37	04	10	05	166.89	1.03	0	350.33
L50	334.31	03	07	02	114.04	0.54	0	256.45
L51	598.64	14	10	02	163.12	4.65	02	540.13

TABLE 3: THE MOLECULAR DOCKING STUDIES OF CHRYSIN DERIVATIVES

COMP.NO	SARS-CoV-2		Angiotensin Converting Enzyme 2	
	AREA	ACE	AREA	ACE
PL1	345.00	-183.22	421.90	-236.72
PL2	379.80	-226.64	539.70	-218.21
PL3	443.30	-262.24	591.40	-286.82
PL4	597.30	-244.87	607.30	-260.76
PL5	468.40	-252.53	611.90	-321.80
PL6	582.50	-246.37	602.20	-308.94
PL7	530.40	-250.34	555.00	-307.01
PL8	546.70	-232.25	611.40	-307.75
PL9	608.00	-230.52	594.70	-307.17
PL10	560.40	-256.24	600.70	-341.12
PL11	572.60	-266.94	679.90	-340.27
PL12	614.90	-274.06	644.20	-254.78
PL13	531.30	-241.76	551.10	-241.51
PL14	446.10	-259.54	577.10	-234.34
PL15	545.90	-244.91	601.20	-290.20
PL16	631.20	-326.68	613.90	-278.07
PL17	466.70	-247.51	593.10	-349.50
PL18	543.00	-227.75	574.00	-337.86
PL19	541.40	-269.13	574.20	-315.58
PL20	427.40	-257.44	589.60	-253.58
PL21	525.30	-220.03	558.30	-209.25
PL22	547.20	-266.41	609.90	-336.88
PL23	525.90	-226.54	600.30	-359.38
PL24	507.00	-241.84	613.10	-274.50
PL25	542.20	-223.68	621.60	-287.13
PL26	377.10	-188.88	506.40	-228.64
PL27	387.80	-206.95	544.50	-253.36
PL28	366.00	-219.64	485.80	-215.86
PL29	465.10	-213.20	566.80	-246.03

PL30	502.90	-235.22	579.80	-272.33
PL31	503.30	-212.64	533.40	-261.94
PL32	522.60	-268.57	562.30	-231.60
PL33	519.00	-222.82	605.50	-273.51
PL34	564.40	-214.95	576.60	-250.01
PL35	491.40	-206.87	581.80	-255.96
PL36	593.90	-266.00	645.80	-244.36
PL37	667.20	-312.73	661.80	-232.81
PL38	589.60	-291.12	630.40	-331.28
PL39	507.30	-248.97	582.90	-330.00
PL40	533.00	-246.13	591.90	-240.77
PL41	563.90	-231.14	547.00	-308.10
PL42	510.80	-248.64	635.20	-276.04
PL43	547.70	-291.18	595.60	-330.76
PL44	515.60	-227.60	588.30	-332.43
PL45	555.40	-271.40	562.80	-235.25
PL46	532.60	-244.01	595.00	-312.41
PL47	556.00	-245.50	553.60	-243.50
PL48	644.00	-320.03	733.30	-262.29
PL49	500.30	-207.12	606.50	-325.73
PL50	397.10	-103.79	506.20	-235.31
PL51	581.60	-178.79	849.60	-330.50

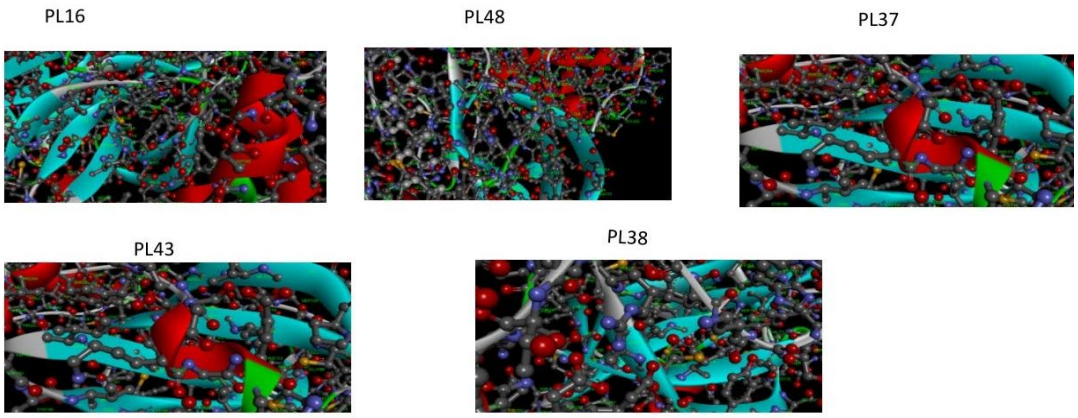
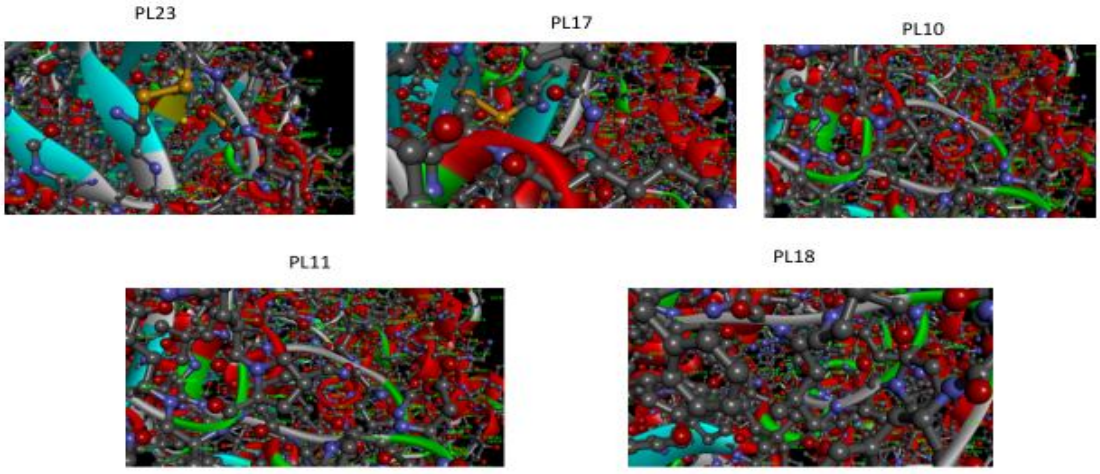


Figure 1: Binding interactions of Chrysin derivatives with SARS Cov2 Protease

Figure 2: Binding interactions of Chrysin derivatives with Angiotensin converting enzyme



CONCLUSION

Based on the findings, it is preferable to concentrate on chrysin derivatives to create effective anti-viral medications. It is abundantly clear from the results of the current computational investigation that chrysin

derivatives have distinct binding interactions with the SARS-CoV-2 Main protease and ACE-2 receptors. Therefore, there is a chance that the examined chrysin compounds will prove to be effective COVID-19 leads.

Author's contribution

Dr. Kaveripakam Sai Sruthi designed, performed the work and prepared the manuscript; Prof. A. Sreedevi aided in giving valuable suggestions throughout the work and others had performed the computational studies.

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