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Sequencing Studies and Evaluation of Efficacy of Selected Medicinal Plant Compounds and Common Indian Spices in Inhibiting the Potential Risk Factors of COVID-19 Viruses- using *In-Silico* Virtual Screening Analysis

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Abstract: **In view of corona virus or COVID-19 global pandemic affecting more than 200 (two hundred) countries, we have taken up extensive studies to evaluate dependable efficacy of selected medicinal plants & common Indian spices (mostly emphasized by Ministry of AYUSH & used as Ayurveda-Rasayana herbs with immuno-modulatory effect) to combat the disease. Molecular docking analysis reveal that several phytocompounds have potent binding affinity against main COVID-19 spike proteins (proteases) and also compounds with a known anti-HIV synthetic drug, Saquinavir (SQV).**

Keywords: **COVID-19, Ayurveda-Rasayana herbs, Homology Modeling, Virtual Screening, Lipinski's rule of five, Saquinavir.**

I. INTRODUCTION:

Despite intense research efforts, how, when and where new diseases appear are still a source of considerable uncertainty. Newly emerging infectious diseases has posed a major threat to public health. The word emerging refers to viruses that have newly appeared in the population or are rapidly expanding their range, corresponding to increase in the number of cases. Several different elements can contribute to the emergence of a new virus disease that may cause epidemic or pandemic around the globe. Most recently, the Middle East respiratory syndrome coronavirus (MERS-CoV) was first identified in Saudi Arabia in 2012 as an emerging global health threat [1].

On December 31, 2019, World Health Organization was informed of a cluster of cases of pneumonia of unknown cause detected in Wuhan City, Hubei Province of China. The corona virus (COVID-2019) was identified as the causative virus by the Chinese authorities on January 7, 2020. Metagenomic RNA sequencing identified the new RNA virus strain to be from the family Corona viridae, which is also referred to as '2019-nCoV'. Of the seven strains of corona virus known to infect humans, SARS- CoV, MERS- CoV and the current strain SARS- CoV-2 are known to cause severe lower respiratory tract dysfunction. Corona viruses are a large family of viruses that can cause illnesses ranging widely in severity. The first known severe illness caused by a corona virus emerged with the 2003 Severe Acute Respiratory Syndrome (SARS) epidemic in China [1, 2, 3].

Indian subcontinent has rich traditional practices, knowledge and experience to mitigate some of the deadly diseases and Indian sages have identified and documented many herbs and Ayurvedic formulations against viral fever, cough and respiratory diseases [4, 5]. Ancient healthcare systems like Ayurveda and Sidda have recommended few antiviral herbs and formations. Some of these medicines may be useful for current COVID19 outbreak in India [4] and abroad since COVID19 is new to India and much there is no previous studies or tests available on herbs and formulations. Hence this proposal was conceived by various experts who are in the field of epidemiology, virology, molecular biology, genomics, data science, Ayurveda and Yoga and we have explored the traditional medicine against COVID19 using herbs and formulations.

Here we put forth a comprehensive research, which identify human and viral proteins and prepare wide spectrum viral inhibitors of influence virus from medicinal plants along with a known anti-HIV synthetic drug, Saquinavir (SQV) [6].

II. METHODOLOGY:

The phytocompounds were downloaded from pubchem and ADME studies was performed using Molinspiration [7] following the Lipinski's rule of five.

The FASTA sequence of the corona virus main protease and spike protein were downloaded from NCBI database (Table 1). Homology modeling studies were performed using their homologous templates given in Table 1. These protein models were docked with the phytocompounds selected (having 0 violations) from ADME studies.

Table 1: Corona virus' main protease and spike protein's NCBI accession number

	NCBI accession number	Homologous template
main protease	QOQ24800	6LU7A
spike protein	QJE37811	7BZ5A

III. RESULTS AND DISCUSSION:

ADME studies: The phytocompounds of the ayurvedic herbs & common Indian spices (mostly emphasized by Ministry of AYUSH & used as Ayurveda-Rasayana herbs) were downloaded from pubchem. ADME studies were performed as per Lipinski's rule of five [8] (Table 2). The phytocompounds showing "0" as 'nviolations' were selected for further docking studies.

Table 2: ADME studies on the ayurvedic herbs & common Indian spices

	Plant with its phyto-compounds	miLogP	TPSA	natoms	MW	nON	nOHNH	nrotb	volume	nviolations
1	***Cinchona cortex***									
	Cinchonidine	3.03	36.36	22	294.40	3	1	3	285.25	0
	quinine	3.06	45.59	24	324.42	4	1	4	310.79	0
	quinidine	3.06	45.59	24	324.42	4	1	4	310.79	0
	cinchonine	3.03	36.36	22	294.40	3	1	3	285.25	0
	Coumarin	2.01	30.21	11	146.15	2	0	0	128.59	0
	Cinnamaldehyde	2.48	17.07	10	132.16	1	0	2	130.44	0
	Cinnamic Acid	1.91	37.30	11	148.16	2	1	2	138.46	0
2	***Berberis aristata***									
	Berberine	0.20	40.82	25	336.37	5	0	2	296.30	0
	oxyberberine	3.13	58.94	26	351.36	6	0	2	301.58	0
	berbamine	6.24	72.87	45	608.74	8	1	3	561.52	2
	aromoline	5.96	83.87	44	594.71	8	2	2	544.00	2
	karachine	3.36	57.24	32	433.50	6	0	2	386.11	0
	palmatine	-0.05	40.82	26	352.41	5	0	4	323.46	0
	oxycanthine	6.24	72.87	45	608.74	8	1	3	561.52	2
	Quercetin	1.68	131.35	22	302.24	7	5	1	240.08	0
	Rutin	-1.06	269.43	43	610.52	16	10	6	496.07	3

	taxilamine	-0.94	78.12	27	370.38	7	1	6	327.70	0
3	***Glycyrrhiza glabra***									
	Glycyrrhizin	2.77	198.76	54	764.99	12	8	7	726.99	3
	Glabridin	4.20	58.92	24	324.38	4	2	1	295.25	0
	Isoliquiritigenin	2.77	77.75	19	256.26	4	3	3	225.91	0
	Liquiritigenin	2.20	66.76	19	256.26	4	2	1	222.24	0
	Liquiritin	0.41	145.91	30	418.40	9	5	4	354.37	0
	Licochalcone A	4.85	66.76	25	338.40	4	2	6	320.79	0
	Glabrene	4.31	58.92	24	322.36	4	2	1	289.04	0
4	***Ocimum sanctum***									
	Oleanolic acid	6.72	57.53	33	456.71	3	2	1	471.14	1
	Ursolic acid	6.79	57.53	33	456.71	3	2	1	471.49	1
	Rosmarinic acid	1.63	144.52	26	360.32	8	5	7	303.54	0
	Eugenol	2.10	29.46	12	164.20	2	1	3	162.14	0
	Carvacrol	3.81	20.23	11	150.22	1	1	1	158.57	0
	Linalool	3.21	20.23	11	154.25	1	1	4	175.59	0
	β-caryophyllene	5.17	0.00	15	204.36	0	0	0	229.95	1
5	***Curcuma longa***									
	Cucumin	1.56	46.67	18	244.29	3	0	0	220.46	0
	curcumin	2.30	93.07	27	368.38	6	2	8	332.18	0
	demethoxycurcumin	2.48	83.83	25	338.36	5	2	7	306.64	0
	bisdemethoxycurcumin	2.67	74.60	23	308.33	4	2	6	281.09	0
	germacrone	4.41	17.07	16	218.34	1	0	0	236.48	0
	α-turmerone	3.78	17.07	16	218.34	1	0	4	236.53	0
	β-turmerones	3.56	17.07	16	218.34	1	0	4	237.09	0
	β-bisabolene	5.46	0.00	15	204.36	0	0	4	234.88	1
	α-curcumene	5.82	0.00	15	202.34	0	0	4	228.14	1
	zingiberene	5.12	0.00	15	204.36	0	0	4	234.35	1
	β-sesquiphellanderene	4.90	0.00	15	204.36	0	0	4	234.90	0
	bisacurone	1.87	57.53	18	252.35	3	2	4	258.48	0
	curcumenone	2.88	34.14	17	234.34	2	0	3	239.94	0
	dehydrocurdione	3.26	34.14	17	234.34	2	0	0	244.87	0
	procurcumadiol	2.29	57.53	18	250.34	3	2	0	247.29	0
	bis-acumol	4.67	20.23	16	218.34	1	1	4	236.18	0
	curcumenol	3.96	29.46	17	234.34	2	1	0	235.26	0
	isoprocurcumenol	3.03	37.30	17	234.34	2	1	0	240.15	0
	epiprocurcumenol	3.24	37.30	17	234.34	2	1	0	239.59	0
	procurcumenol	3.24	37.30	17	234.34	2	1	0	239.59	0
	zedoaronediol	2.25	57.53	18	252.35	3	2	0	253.50	0
	curlone	3.56	17.07	16	218.34	1	0	4	237.09	0
	turmerone	4.10	17.07	16	218.34	1	0	4	236.50	0
	Ar-turmerone	4.48	17.07	16	216.32	1	0	4	230.32	0
	stigmasterole	7.87	20.23	30	412.70	1	1	5	450.33	1
	β-sitosterole	8.62	20.23	30	414.72	1	1	6	456.52	1
	cholesterol	7.62	20.23	28	386.66	1	1	5	423.13	1
	2-hydroxymethyl anthraquinone	2.98	54.37	18	238.24	3	1	1	207.40	0
6	***Picrorhiza kurroa***									
	Kutkin	1.07	151.99	33	460.44	10	4	9	395.50	0
	Picroside I	0.03	167.68	35	492.48	11	5	8	417.89	1
	Picroside III	-0.63	197.14	38	538.50	13	6	9	451.45	3

	Apocynin	1.18	46.53	12	166.18	3	1	2	153.15	0
	Pikuroside	-1.61	214.07	37	530.48	14	7	7	438.27	3
	Picroside IV	-0.45	187.90	36	508.48	12	6	8	425.91	3
	Vanillic acid	1.19	66.76	12	168.15	4	2	2	144.61	0
	Picroside II	-1.05	197.14	36	512.46	13	6	8	424.04	3
7	***Phyllanthus niruri***									
	Phyllanthin,	3.92	55.40	30	418.53	6	0	13	409.59	0
	hypophyllanthin	3.50	64.64	31	430.50	7	0	8	397.16	0
	Methyl brevifolincarboxylate	-0.22	134.27	22	306.23	8	3	2	238.94	0
	niranthin	3.95	64.64	31	432.51	7	0	12	407.97	0
	niruriside	4.54	225.99	55	770.74	17	2	21	667.18	2
	nirtetralin	3.70	64.64	31	430.50	7	0	8	397.16	0
	corilagin	0.31	310.66	45	634.46	18	11	3	487.20	3
	epicatechin	1.37	110.37	21	290.27	6	5	1	244.14	0
8	***Tinospora cordifolia***									
	Berberine	0.20	40.82	25	336.37	5	0	2	296.30	0
	choline	-4.24	20.23	7	104.17	2	1	2	120.16	0
	Tembetarine	-1.60	58.92	25	344.43	5	2	4	328.31	0
	Tinosporin	1.50	118.73	29	406.43	8	2	3	353.42	0
	Palmitine	7.71	72.84	28	400.60	5	1	22	428.97	1
	Jatrorrhizine	-0.35	51.81	25	338.38	5	1	3	305.94	0
	Cordifolioside A	-2.29	197.00	35	504.49	13	7	10	434.44	3
	Palmatine	-0.05	40.82	26	352.41	5	0	4	323.46	0
	Magnoflorine	-1.26	58.92	25	342.42	5	2	2	317.47	0
	Isocolumbin	2.72	85.98	26	358.39	6	1	1	313.96	0
9	***Cubeba officinalis***									
	sabinene	3.10	0.00	10	136.24	0	0	1	152.37	0
	α-thujene	3.31	0.00	10	136.24	0	0	1	151.81	0
	caryophyllene	5.17	0.00	15	204.36	0	0	0	229.95	1
	copaene	5.75	0.00	15	204.36	0	0	1	224.82	1
	α- cubebene	5.82	0.00	15	204.36	0	0	1	224.82	1
	β-cubebene	5.61	0.00	15	204.36	0	0	1	225.37	1
	3-Carene	3.45	0.00	10	136.24	0	0	0	151.81	0
	D-germacrene	5.43	0.00	15	204.36	0	0	1	234.90	1
	δ-cadinene	5.81	0.00	15	204.36	0	0	1	229.72	1
	1,4-cineole	2.72	9.23	11	154.25	1	0	1	166.66	0
	1,8-cineole	2.72	9.23	11	154.25	1	0	0	166.66	0
	cubebol	4.83	20.23	16	222.37	1	1	1	238.72	0
	terpinen-4-ol	2.60	20.23	11	154.25	1	1	1	170.65	0
	γ-elemene	5.42	0.00	15	204.36	0	0	2	234.65	1
10	***Zingiber officinale***									
	gingerol	3.22	66.76	21	294.39	4	2	10	295.61	0
	shogaol	4.35	46.53	20	276.38	3	1	9	281.38	0
	paradol	4.60	46.53	20	278.39	3	1	10	287.57	0
	8-gingerol	4.23	66.76	23	322.44	4	2	12	329.21	0
	10-gingerol	5.24	66.76	25	350.50	4	2	14	362.82	1
	quercetin	1.68	131.35	22	302.24	7	5	1	240.08	0
	zingerone	1.52	46.53	14	194.23	3	1	4	186.75	0
	gingerenone-A	3.32	76.00	26	356.42	5	2	9	336.19	0
	6-dehydrogingerdione	3.81	66.76	21	290.36	4	2	8	283.21	0

	β-bisabolene	5.46	0.00	15	204.36	0	0	4	234.88	1
	α-curcumene	5.82	0.00	15	202.34	0	0	4	228.14	1
	zingiberene	5.12	0.00	15	204.36	0	0	4	234.35	1
	α-farnesene	5.82	0.00	15	204.36	0	0	6	239.27	1
	β-sesquiphellandrene	4.90	0.00	15	204.36	0	0	4	234.90	0
11	***Phyllanthus emblica***									
	ascorbic acid	-1.40	107.22	12	176.12	6	4	2	139.71	0
	ellagitannin	-0.31	447.10	71	992.71	27	13	5	755.62	3
	emblicanin A	2.94	374.26	56	782.53	22	12	6	590.51	3
	emblicanin B	1.57	382.07	56	780.51	22	12	0	579.67	3
	punigluconin	0.69	405.48	57	802.56	23	14	9	614.65	3
	pedunculagin	0.93	377.42	56	784.54	22	13	0	591.77	3
	punicafolin	2.43	444.18	67	938.66	26	15	9	718.03	3
	phyllanemblinin A	0.68	283.34	44	616.44	17	9	4	469.31	3
	kaempferol	2.17	111.12	21	286.24	6	4	1	232.07	0
	ellagic acid	0.94	141.33	22	302.19	8	4	0	221.78	0
	gallic acid	0.59	97.98	12	170.12	5	4	1	135.10	0
12	***Andrographis paniculata***									
	Andrographolide	1.05	86.99	25	350.45	5	3	3	338.33	0
	andrograpanin	2.87	46.53	23	318.46	3	1	4	322.24	0
	7-*O*-methylwogonin	3.27	68.91	22	298.29	5	1	3	259.11	0
	apigenin	2.46	90.89	20	270.24	5	3	1	224.05	0
	onysilin	2.71	65.00	22	300.31	5	1	3	265.32	0
	3,4-dicaffeoylquinic acid	1.21	211.28	37	516.46	12	7	9	431.08	3
13	***Apium graveolens***									
	falcarinol	5.99	20.23	18	244.38	1	1	8	271.09	1
	falcarindiol	5.08	40.46	19	260.38	2	2	8	279.13	1
	panaxidol	5.05	32.76	19	260.38	2	1	8	275.47	1
	d-galacturonic acid	-2.77	127.44	13	194.14	7	5	1	153.99	0
	d-galactose	-2.64	110.37	12	180.16	6	5	1	151.81	0
	1-dodecanol	5.16	20.23	13	186.34	1	1	10	222.03	1
	9-octadecen-12-ynoic acid	6.70	37.30	20	278.44	2	1	12	307.38	1
	Caffeic acid	0.94	77.75	13	180.16	4	3	2	154.50	0
	chlorogenic acid	-0.45	164.74	25	354.31	9	6	5	296.27	1
	apiin	-0.74	228.97	40	564.50	14	8	7	463.10	3
	apigenin	2.46	90.89	20	270.24	5	3	1	224.05	0
	rutaretin	1.89	79.90	19	262.26	5	2	1	226.02	0
	ocimene	3.97	0.00	10	136.24	0	0	3	161.69	0
	bergapten	2.28	52.59	16	216.19	4	0	1	179.69	0
	isopimpinellin	2.26	61.82	18	246.22	5	0	2	205.24	0
	isoimperatorin	3.95	52.59	20	270.28	4	0	3	240.47	0
	osthenol	3.76	50.44	17	230.26	3	1	2	213.94	0
	d-limonene	3.62	0.00	10	136.24	0	0	1	157.30	0
	terpineol	2.60	20.23	11	154.25	1	1	1	170.65	0
14	***Trachyspermum ammi***									
	thymol	3.34	20.23	11	150.22	1	1	1	158.57	0
	para-cymene	3.90	0.00	10	134.22	0	0	1	150.55	0
	γ-terpenine	3.36	0.00	10	136.24	0	0	1	156.74	0

	α-pinene	3.54	0.00	10	136.24	0	0	0	151.81	0
	β-pinene	3.33	0.00	10	136.24	0	0	0	152.37	0
	dipentene	3.62	0.00	10	136.24	0	0	1	157.30	0
	α-terpinene	3.36	0.00	10	136.24	0	0	1	156.74	0
	carvacrol	3.81	20.23	11	150.22	1	1	1	158.57	0
	camphene	3.33	0.00	10	136.24	0	0	0	152.37	0
	myrcene	3.99	0.00	10	136.24	0	0	4	162.24	0
	α-3-carene	3.45	0.00	10	136.24	0	0	0	151.81	0
15	***Cuminum cyminum***									
	carvone	2.51	17.07	11	150.22	1	0	1	159.48	0
	cuminaldehyde	3.24	17.07	11	148.21	1	0	2	152.98	0
	1,8-cineole	2.72	9.23	11	154.25	1	0	0	166.66	0
	o- cymene	3.38	0.00	10	134.22	0	0	1	150.55	0
	safranal	2.95	17.07	11	150.22	1	0	1	158.60	0
	linalool	3.21	20.23	11	154.25	1	1	4	175.59	0
16	***Brassica juncea***									
	Alpha-Tridecene	6.67	0.00	13	182.35	0	0	10	224.94	1
	2,4-Di-tert-butylphenol	5.27	20.23	15	206.33	1	1	2	224.44	1
	7-Hexadecene	8.20	0.00	16	224.43	0	0	12	274.80	1
	Octadecanoic acid	8.07	37.30	20	284.48	2	1	16	325.03	1
	(2-phenyl-1,3-dioxolan-4-yl)-methyl ester	8.56	44.77	30	418.62	4	0	18	438.19	1
	5-Octadecene	8.80	0.00	18	252.49	0	0	14	308.40	1
	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	6.76	20.23	21	296.54	1	1	13	349.38	1
	Cyclododecanol	4.62	20.23	13	184.32	1	1	0	211.46	0
	Gamolenic acid	6.13	37.30	20	278.44	2	1	13	306.47	1
	Oleic acid	7.58	37.30	20	282.47	2	1	15	318.84	1
	Lignocerol	9.44	20.23	25	354.66	1	1	22	423.65	1
	trans-Phytol	6.76	20.23	21	296.54	1	1	13	349.38	1
	Octadecane	9.00	0.00	18	254.50	0	0	15	314.59	1
	Heptadecane	8.79	0.00	17	240.47	0	0	14	297.78	1
	Farnesol	5.05	20.23	16	222.37	1	1	7	253.16	1
	Nonadecanol	8.53	20.23	20	284.53	1	1	17	339.65	1
	n-Octacosane	10.05	0.00	28	394.77	0	0	25	482.60	1
	3-Propionyloxytridecane	6.58	26.30	18	256.43	2	0	13	291.93	1
17	***Camellia sinensis***									
	epigallocatechin gallate	2.25	197.36	33	458.38	11	8	4	367.57	2
	epigallocatechin	1.08	130.60	22	306.27	7	6	1	252.16	1
	epicatechin 3-gallate	2.54	177.13	32	442.38	10	7	4	359.55	1
	epicatechin	1.37	110.37	21	290.27	6	5	1	244.14	0
	catechin gallate	2.54	177.13	32	442.38	10	7	4	359.55	1
	gallocatechin	1.08	130.60	22	306.27	7	6	1	252.16	1
	gallocatechin gallate	2.25	197.36	33	458.38	11	8	4	367.57	2
	catechin	1.37	110.37	21	290.27	6	5	1	244.14	0
18	***Azadirachta indica***									
	nimbolinin	5.75	130.75	47	648.75	10	1	8	587.65	2
	nimbin	3.55	118.36	39	540.61	9	0	8	488.96	1
	salannin	5.40	110.52	43	596.72	9	0	9	551.94	2
	quercetin	1.68	131.35	22	302.24	7	5	1	240.08	0

	nimbandiol	2.17	106.21	33	456.54	7	2	4	415.94	0
	nimbolide	1.94	92.06	34	466.53	7	0	4	417.03	0
	ascorbic acid	-1.40	107.22	12	176.12	6	4	2	139.71	0
	n-hexacosanol	9.65	20.23	27	382.72	1	1	24	457.26	1
	7-desacetyl-7-benzoylazadiradione	5.95	73.59	38	512.65	5	0	4	480.96	2
	17-hydroxyazadiradione	3.65	93.81	34	466.57	6	1	3	433.80	0
	nimbiol	4.92	37.30	20	272.39	2	1	0	272.65	0
	ß-sitosterol	8.62	20.23	30	414.72	1	1	6	456.52	1
19	***Elettaria cardamomum***									
	α tocopherol	9.04	29.46	31	430.72	2	1	12	474.50	1
	γ-tocopherol	8.98	29.46	30	416.69	2	1	12	457.94	1
	Δ-tocopherol	8.60	29.46	29	402.66	2	1	12	441.38	1
20	***Syzygium aromaticum***									
	eugenol	2.10	29.46	12	164.20	2	1	3	162.14	0
	eugenyl acetate	1.90	35.54	15	206.24	3	0	5	198.65	0
	β-caryophyllene	5.17	0.00	15	204.36	0	0	0	229.95	1
	vanillin	1.07	46.53	11	152.15	3	1	2	136.59	0
	crategolic acid	5.81	77.75	34	472.71	4	3	1	479.18	1
	gallotannic acid	7.06	777.98	122	1701.21	46	25	31	1305.93	4
	methyl salicylate	2.13	46.53	11	152.15	3	1	2	136.59	0
	eugenin	1.78	59.67	15	206.20	4	1	1	178.71	0
	kaempferol	2.17	111.12	21	286.24	6	4	1	232.07	0
	rhamnetin	2.22	120.36	23	316.26	7	4	2	257.61	0
	eugenitin	2.16	59.67	16	220.22	4	1	1	195.27	0
	oleanolic acid	6.72	57.53	33	456.71	3	2	1	471.14	1
	methyl amyl ketone	2.31	17.07	8	114.19	1	0	4	131.95	0
	α -humulene	5.30	0.00	15	204.36	0	0	0	234.00	1
	β-humulene	5.09	0.00	15	204.36	0	0	0	234.55	1
	benzaldehyde	1.73	17.07	8	106.12	1	0	1	103.03	0
	β-ylangene	5.54	0.00	15	204.36	0	0	1	225.37	1
	chavicol	2.28	20.23	10	134.18	1	1	2	136.59	0
	α-cubebene	5.82	0.00	15	204.36	0	0	1	224.82	1
	α-copaene	5.75	0.00	15	204.36	0	0	1	224.82	1
	γ-cadinene	5.75	0.00	15	204.36	0	0	1	230.30	1
	δ-cadinene	5.81	0.00	15	204.36	0	0	1	229.72	1
21	***Swertia chirayita***									
	amarogentin	2.04	201.68	42	586.55	13	6	8	494.10	3
	swertiamarin	-1.66	155.15	26	374.34	10	5	4	314.97	0
	mangiferin	-0.16	201.27	30	422.34	11	8	2	335.80	2
	swerchirin	3.05	89.14	21	288.25	6	2	2	239.71	0
	sweroside	-0.71	134.92	25	358.34	9	4	4	307.28	0
	amaroswerin	1.09	221.91	43	602.54	14	7	8	501.79	3
	gentiopicrin	-0.90	134.92	25	356.33	9	4	4	301.06	0
22	***Cinnamomum tamala***									
	Furanogermenone	3.48	30.21	17	232.32	2	0	0	234.89	0
	sabinene	3.10	0.00	10	136.24	0	0	1	152.37	0
	germacrene D	5.43	0.00	15	204.36	0	0	1	234.90	1
	curcumenol	3.96	29.46	17	234.34	2	1	0	235.26	0
	sesquiterpenoid	2.72	83.83	25	350.45	5	2	5	347.78	0
	furanodiene	4.63	13.14	16	216.32	1	0	0	226.49	0

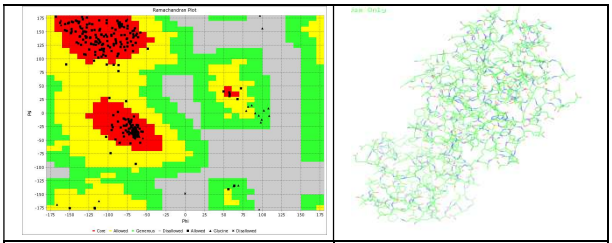
	curzerene	4.54	13.14	16	216.32	1	0	2	226.85	0
	α -pinene	2.74	12.53	11	152.24	1	0	0	155.87	0
	1, 8-cineole	2.50	35.54	15	212.29	3	0	2	211.22	0
	spathulenol	3.91	20.23	16	220.36	1	1	0	233.07	0
	santolina triene	4.20	0.00	10	136.24	0	0	3	162.03	0
	α - bergamotene	5.45	0.00	15	204.36	0	0	3	229.40	1
	α - copaene	5.75	0.00	15	204.36	0	0	1	224.82	1
	α - muurolene	5.97	0.00	15	204.36	0	0	1	229.75	1
	trans -cinnamaldehyde	2.87	62.90	14	211.60	4	0	3	167.31	0
23	***Piper longum***									
	piperine	3.33	38.78	21	285.34	4	0	3	267.74	0
	pipernonaline	5.36	38.78	25	341.45	4	0	7	334.95	1
	piperettine	3.85	38.78	23	311.38	4	0	4	295.16	0
	asarinine	3.69	55.40	26	354.36	6	0	2	300.51	0
	pellitorine	4.26	29.10	16	223.36	2	1	8	249.37	0
	piperundecalidine	5.88	38.78	27	367.49	4	0	8	362.37	1
	piperlongumine	1.62	65.08	23	317.34	6	0	5	289.03	0
	piperlonguminine	3.30	47.57	20	273.33	4	1	5	260.94	0
	retrofractamide A	4.84	47.57	24	327.42	4	1	8	321.96	0
	brachystamide-B	7.87	47.57	30	411.59	4	1	14	422.77	1
	dehydropipernonaline	4.87	38.78	25	339.44	4	0	6	328.76	0
	6-alpha-diol	1.61	65.08	27	369.42	6	0	4	329.70	0
	guineesine	6.86	47.57	28	383.53	4	1	12	389.17	1
24	***Coriandrum sativum***									
	p-cymene	3.90	0.00	10	134.22	0	0	1	150.55	0
	myrcene	3.99	0.00	10	136.24	0	0	4	162.24	0
	cis-ocimene	3.97	0.00	10	136.24	0	0	3	161.69	0
	β-phellandrene	3.79	0.00	10	136.24	0	0	1	156.77	0
	citronellol	3.15	20.23	11	156.27	1	1	5	181.79	0
	nerol	3.20	20.23	11	154.25	1	1	4	175.57	0
	Bornyl acetate	3.05	26.30	14	196.29	2	0	2	202.23	0
	geranyl acetate	3.91	26.30	14	196.29	2	0	6	212.09	0
	Linalyl acetate	3.92	26.30	14	196.29	2	0	6	212.10	0
	α-terpinyl acetate	3.30	26.30	14	196.29	2	0	3	207.16	0
	elemol	4.35	20.23	16	222.37	1	1	3	248.59	0
	nerolidol	5.06	20.23	16	222.37	1	1	7	253.17	1
	tetradecanoic acid	6.05	37.30	16	228.38	2	1	12	257.82	1
	citronellyl acetate	3.86	26.30	14	198.31	2	0	7	218.30	0
	undecanal	5.11	17.07	12	170.30	1	0	9	199.40	1
	cis-beta-ocimene	3.97	0.00	10	136.24	0	0	3	161.69	0
25	***Withania somnifera***									
	withanolide ii	3.73	148.97	42	586.68	10	2	6	530.92	1
	withaferin A	3.86	96.36	34	470.61	6	2	3	442.38	0
	withanolide A	4.15	96.36	34	470.61	6	2	2	441.81	0
	withanone	4.15	96.36	34	470.61	6	2	2	441.81	0
	withanolide B	5.10	76.13	33	454.61	5	1	2	434.12	1
26	***Centella asiatica***									
	Asiatic acid	4.70	97.98	35	488.71	5	4	2	487.79	0
	alpha-Humulene	5.30	0.00	15	204.36	0	0	0	234.00	1
	Arjunolic acid	4.63	97.98	35	488.71	5	4	2	487.44	0

	Asiaticoside	0.37	315.21	67	959.13	19	12	10	875.90	3
	Asiaticoside B	-0.61	335.44	68	975.13	20	13	10	883.59	3
	Asiaticoside C	1.07	321.29	70	1001.17	20	11	12	912.41	3
	Bicyclogermacrene	5.29	0.00	15	204.36	0	0	0	229.40	1
	Castillicetin	2.63	177.88	34	464.38	10	6	5	374.90	1
	Castilliferol	3.60	137.43	32	432.38	8	4	5	358.86	0
	Centellasapogenol A	4.47	97.98	35	488.71	5	4	2	487.42	0
	Centellasaponin A	0.14	315.21	67	959.13	19	12	10	875.52	3
	Centellasaponin B	0.37	276.51	58	828.99	16	11	8	760.08	3
	Centelloside E	-0.14	315.21	67	957.12	19	12	10	869.71	3
	Chavicol	2.28	20.23	10	134.18	1	1	2	136.59	0
	Chebuloside II	2.01	197.36	47	666.85	11	8	5	627.61	3
	Chlorogenic acid	-0.45	164.74	25	354.31	9	6	5	296.27	1
	Corosolic acid	5.87	77.75	34	472.71	4	3	1	479.53	1
	Cryptochlorogenic Acid	-0.67	164.74	25	354.31	9	6	5	296.27	1
	1,3-Dicaffeoylquinic acid	1.42	211.28	37	516.46	12	7	9	431.08	3
	3-Epimaslinic acid	5.81	77.75	34	472.71	4	3	1	479.18	1
	Germacrene B	5.51	0.00	15	204.36	0	0	0	234.30	1
	Madecassic acid	3.78	118.21	36	504.71	6	5	2	495.83	1
	Madecassoside	-0.55	335.44	68	975.13	20	13	10	883.94	3
	Methyleugenol	2.41	18.47	13	178.23	2	0	4	179.67	0
	Myrcene	3.99	0.00	10	136.24	0	0	4	162.24	0
	Naringin	-0.37	225.06	41	580.54	14	8	6	486.25	3
	Neochlorogenic acid	-0.45	164.74	25	354.31	9	6	5	296.27	1
	Patuletin	1.70	140.59	24	332.26	8	5	2	265.63	0
	Pomolic Acid	5.84	77.75	34	472.71	4	3	1	479.18	1
	Quadranoside IV	2.99	177.13	46	650.85	10	7	5	619.91	2
	Scheffuroside B	1.09	312.05	68	971.14	19	11	11	886.86	3
	Stigmasterol	7.87	20.23	30	412.70	1	1	5	450.33	1
	Terminolic acid	3.72	118.21	36	504.71	6	5	2	495.49	1
	Ursolic acid	6.79	57.53	33	456.71	3	2	1	471.49	1
27	***Cinnamomum verum***									
	cinnamyl alcohol	2.03	20.23	10	134.18	1	1	2	136.28	0
	cinnamic aldehyde	4.61	21.60	23	327.25	2	0	5	256.57	0
	5'-hydroxy-5-hydroxymethyl-4''	-1.28	83.83	13	186.16	5	2	3	158.89	0
	Methoxycinnamaldehyde	1.48	26.30	12	162.19	2	0	3	155.99	0
	Cinnamyl acetate	2.74	26.30	13	176.22	2	0	4	172.79	0
	Methyl cinnamate	2.53	26.30	12	162.19	2	0	3	155.99	0
28	***Terminalia chebula***									
	Punicalagin	2.04	518.75	78	1084.72	30	17	0	800.91	3
	terflavin A	2.04	518.75	78	1086.74	30	17	8	811.76	3
	Terchebulin	2.71	507.76	78	1084.72	30	16	0	801.88	3
	Punicalin	0.26	385.23	56	782.53	22	13	0	580.93	3
	1, 6-di-O-galloyl-D-glucose	-0.31	243.90	34	484.37	14	9	7	382.63	2
	Casuarinin	1.49	455.17	67	936.65	26	16	4	706.22	3
	4-O-methylgallic acid	0.86	86.99	13	184.15	5	3	2	152.63	0
	Methyl neochebulagate	0.51	467.33	70	986.71	28	14	11	758.56	3

	Shikimic acid	-1.57	97.98	12	174.15	5	4	1	147.55	0
	Ferulic acid	1.25	66.76	14	194.19	4	2	3	172.03	0
	Vanillic acid	1.19	66.76	12	168.15	4	2	2	144.61	0
	p-Coumaric acid	1.43	57.53	12	164.16	3	2	2	146.48	0
	Melilotic acid	1.82	57.53	12	166.18	3	2	3	152.67	0
	Phloroglucinol	0.43	60.68	9	126.11	3	3	0	108.10	0
	Arjunglucoside I	2.01	197.36	47	666.85	11	8	5	627.61	3
	Maslinic acid	5.81	77.75	34	472.71	4	3	1	479.18	1
	Luteolin	1.97	111.12	21	286.24	6	4	1	232.07	0
29	***Terminalia bellirica***									
	Cardenolide	4.80	26.30	25	342.52	2	0	1	348.90	0
	termilignan	4.58	49.69	22	296.37	3	2	6	286.10	0
	thannilignan	2.79	90.15	24	330.38	5	4	7	307.71	0
	7-hydroxy-3',4'-(methylenedioxy) flavone	3.11	96.61	27	372.33	8	1	4	308.58	0
	anolignan B	4.13	40.46	20	266.34	2	2	5	260.55	0
	bellericoside	1.75	197.36	47	666.85	11	8	6	627.82	3
	Pyridine-3-carboxamide	-0.48	55.99	9	122.13	3	2	1	110.16	0
	1,5-diphenyl-3-pentanone	4.13	17.07	18	238.33	1	0	6	241.64	0
	9-Octadecenoic acid	7.58	37.30	20	282.47	2	1	15	318.84	1
30	***Solanum xanthocarpum***									
	lupeol	8.29	20.23	31	426.73	1	1	1	461.60	1
	carpesterol	9.01	63.60	41	562.84	4	1	9	574.69	2
	campesterol	8.30	20.23	29	400.69	1	1	5	439.71	1
	daucosterol	7.15	99.38	41	576.86	6	4	9	588.64	2
	diosgenin	5.93	38.70	30	414.63	3	1	0	419.38	1
	sitosteryl glucoside	7.15	99.38	41	576.86	6	4	9	588.64	2
	β-solamargine	2.41	238.49	61	868.07	16	9	7	802.65	3
	arachidonic acid	6.42	37.30	22	304.47	2	1	14	333.88	1
31	***Adhatoda vasica***									
	astragalin	0.12	190.28	32	448.38	11	7	4	364.19	2
	vasicine	1.04	35.83	14	188.23	3	1	0	173.66	0
	vasicinone	0.48	55.12	15	202.21	4	1	0	175.84	0
	vasicinol	0.53	56.06	15	204.23	4	2	0	181.67	0
	vasicoline	3.33	18.84	22	291.40	3	0	2	282.95	0
32	***Clerodendrum indicum***									
	Monomelittoside	-3.19	169.30	25	362.33	10	7	4	302.75	1
	Melittoside	-4.64	248.45	36	524.47	15	10	7	434.87	3
	Sammangaoside C	-5.34	327.60	47	686.61	20	13	10	566.99	3
	Inerminoside A	-0.59	251.37	47	676.71	16	8	15	599.13	3
	Euphroside	-2.27	166.14	26	376.36	10	6	4	319.34	1
	Plantarenaloside	-1.33	145.91	25	360.36	9	5	4	311.64	0
	Aucubin	-2.25	149.07	24	346.33	9	6	4	295.06	1
	Harpagide	-2.94	169.30	25	364.35	10	7	3	308.40	1
	Sammangaoside A	0.11	132.14	27	388.46	8	5	5	358.52	0
	Mandarone A	4.17	54.37	23	314.43	3	1	1	308.22	0
	Bungone A	4.33	43.38	23	306.36	3	0	0	280.83	0
	Inerme A	4.41	64.64	30	414.45	7	0	4	369.30	0

	Clerodendrin A	3.52	156.44	43	606.66	12	1	12	543.85	2
	Teuvincenone A	2.50	104.06	26	358.39	6	3	0	316.42	0
	Mandarone E	4.17	54.37	23	314.43	3	1	1	308.22	0
	Formidiol	3.51	96.97	27	368.38	6	2	2	322.09	0
	Teuvincenone E	3.02	83.83	25	340.38	5	2	0	302.52	0
	Coleon U	4.20	97.98	25	346.42	5	4	1	323.88	0
	Friedelin	7.85	17.07	31	426.73	1	0	0	461.05	1
	Clerodone	8.73	17.07	31	426.73	1	0	1	461.40	1
	α-amyrin	8.08	20.23	31	426.73	1	1	0	461.05	1
	Magnificol	8.15	20.23	31	424.71	1	1	1	455.39	1
	Hispidulin	2.48	100.13	22	300.27	6	3	2	249.59	0
	Darendoside B	-1.80	187.77	33	476.48	12	7	8	415.21	2
	Martynoside	0.17	223.31	46	652.65	15	7	13	567.55	3
	Markhamioside F	-2.29	204.84	32	462.40	13	7	8	383.65	2
	Rengyolone	-0.34	46.53	11	154.16	3	1	0	138.09	0
	Cryptojaponol	5.29	46.53	24	330.47	3	1	2	331.58	1
33	***Terminalia arjuna***									
	Arjunin	1.21	451.99	67	934.63	26	15	3	696.34	3
	Arjunic acid	4.89	97.98	35	488.71	5	4	1	487.23	0
	Arjungenin	3.72	118.21	36	504.71	6	5	2	495.49	1
	Terminic acid	6.10	77.75	34	472.71	4	3	2	479.74	1
	Baicalein	2.68	90.89	20	270.24	5	3	1	224.05	0
	Castalagin	1.49	455.17	67	934.63	26	16	0	695.38	3
	Casuariin	0.32	388.41	56	784.54	22	14	1	590.81	3
	Casuarinin	1.49	455.17	67	936.65	26	16	4	706.22	3
34	***Achyranthes aspera***									
	betaine	-5.41	40.13	8	117.15	3	0	2	119.60	0
	tritriacontanol	10.17	20.23	34	480.91	1	1	31	574.87	1
	17-pentatriacontanol	10.27	20.23	36	508.96	1	1	32	608.26	2
	ecdysterone	1.36	138.44	34	480.64	7	6	5	464.48	1
	pentatriacontan	10.25	17.07	36	506.94	1	0	32	602.40	2
	6-pentatriacontanone	10.25	17.07	36	506.94	1	0	32	602.40	2
	hexatriacontane	10.47	0.00	36	506.99	0	0	33	617.02	2
	triacontane	10.17	0.00	30	422.83	0	0	27	516.21	1
	α -Lrhamnopyranosyl	-5.62	882.83	161	2324.38	57	31	35	2010.61	3
	10-octacosanone	9.74	17.07	30	422.78	1	0	25	501.37	1
	4-triacontanone	9.68	37.30	32	452.81	2	1	27	526.43	1

Homology Modelling studies: The FASTA sequence of the corona virus main protease and spike protein were downloaded from NCBI database (Table 1). Homology modeling studies were preformed using modeler [9]. Using Ramachandran plot (generated from VADAR online software [10]) best protein models were selected (Fig. 1, Table 3).



Ramachandran Plot analysis of main protease | 3d structure visualization of main protease in pymol

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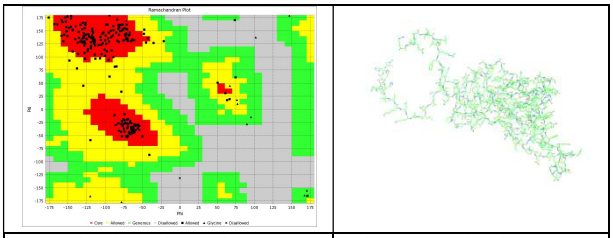


Ramachandran Plot analysis of spike protein	3d structure visualization of spike protein in pymol

Fig. 1: Ramachandran Plot Analysis and 3d structure visualization of corona viral proteins

Table 3a: Ramachandran plot analysis on Spike protein S1

	#res in phipsi core	#res in phipsi allowed	# res in phipsi generous	# res in phipsi outside	
Model 1	196 (85%)	29 (12%)	2 (0%)	2 (0%)	
Model 2	205 (89%)	21 (9%)	3 (1%)	0 (0%)	Selected
Model 3	198 (86%)	30 (13%)	0 (0%)	1 (0%)	
Model 4	201 (87%)	25 (10%)	2 (0%)	1 (0%)	
Model 5	200 (87%)	27 (11%)	1 (0%)	1 (0%)	

Table 3b: Ramachandran plot analysis on main protease

	#res in phipsi core	#res in phipsi allowed	# res in phipsi generous	# res in phipsi outside	
Model 1	286 (93%)	19 (6%)	1 (0%)	0 (0%)	Selected
Model 2	285 (93%)	18 (5%)	2 (0%)	1 (0%)	
Model 3	284 (92%)	20 (6%)	2 (0%)	0 (0%)	
Model 4	284 (92%)	20 (6%)	2 (0%)	0 (0%)	
Model 5	281 (91%)	23 (7%)	2 (0%)	0 (0%)	

Docking studies: Virtual screening/docking studies were performed using the phycompounds selected from the ADME studies having no violations in Lipinski's rule of five, i.e. "0" in 'nviolations' with the selected protein models from Table 3. Results are noted in Table 4 and compared with known anti-HIV synthetic drug, Saquinavir (SQV) (Table 5). Docking was done with patchdock server [11] (except for *Ocimum sanctum, Curcuma longa, Berberis aristata* and *Cinchona cortex* where swiss-dock server [12] was used).

Table 4: Docking analysis

Compound name	Molecular formula	SMILES CODE (Weininger *et.al.*, 1989) [abbreviation for: Simplified molecular-input line-entry system]	Docking score (-kcal/mol)
Achyranthes aspera			
Main Protease			
betaine	$C_5H_{11}NO_2$	C[N+](C)(C)CC(=O)[O-]	2206
Spike protein			
betaine			2068
Terminalia arjuna			
Spike protein			
Arjunic acid	$C_{30}H_{48}O_5$	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)C)O)O)C)C)C2C1O)C)C(=O)O)C	5136
Baicalein	$C_{15}H_{10}O_5$	C1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C=C(C(=C3O)O)O	3614
Main Protease			
Arjunic acid			5044
Baicalein			3774
Clerodendrum indicum			
Spike protein			
Plantarenaloside	$C_{16}H_{24}O_9$	CC1CCC2(C1C(OC=C2C=O)OC3C(C(C(C(O3)CO)O)O)O)O	4016
Sammangaoside A	$C_{19}H_{32}O_8$	CC(C=CC12C(CC(CC1(O2)C)O)(C)C)OC3C(C(C(C(O3)CO)O)O)O	4626
Mandarone A	$C_{20}H_{26}O_3$	CC(C)C1=C(C=C2C(=C1)C(=O)CC3C2(CCC(=O)C3(C)C)C)O	4176
Bungone A	$C_{20}H_{18}O_3$	CC1CC2=C(C(=O)C3=C(C2=O)C=CC4=C3C=CC(=C4C)C)OC1	4066

Inerme A	$C_{45}H_{48}O_{14}$	CC1C(C2C3=CC4=C(C(=C3C5=C(C6=C(C=C5C1O2)OCO6)OC)OC)OCO4)C.CC1C(C2C3=CC(=C(C(=C3C4=C(C5=C(C=C4C1O2)OCO5)OC)OC)OC)OC)C	4698
Teuvincenone A	$C_{20}H_{22}O_6$	CC1CC2=C(C3=C(C(=C2O1)O)C4(CCC(=O)C(C4=C(C3=O)O)(C)C)C)O	4126
Mandarone E	$C_{20}H_{26}O_3$	CC(C)C1=C(C=C2C(=C1)C(=O)CC3C2(CCC(=O)C3(C)C)C)O	4176
Formidiol	$C_{21}H_{20}O_6$	CC1=CC2=C(C3=C(C(=C2O1)O)C4(CCC(=C(C4=CC3=O)C)C(=O)OC)C)O	4424
Teuvincenone E	$C_{20}H_{20}O_5$	CC1CC2=C(C3=C(C(=C2O1)O)C4(CC(=O)C(=C(C4=CC3=O)C)C)C)O	4166
Coleon U	$C_{20}H_{26}O_5$	CC(C)C1=C(C2=C(C(=C1O)O)C3(CCCC(C3=C(C2=O)O)(C)C)C)O	4270
Hispidulin	$C_{16}H_{12}O_6$	COC1=C(C2=C(C=C1O)OC(=CC2=O)C3=CC=C(C=C3)O)O	3736
Rengyolone	$C_8H_{10}O_3$	C1COC2C1(C=CC(=O)C2)O	2500
Main Protease			
Plantarenaloside			4088
Sammangaoside A			4642
Mandarone A			4354
Bungone A			4042
Inerme A			4788
Teuvincenone A			4228
Mandarone E			4354
Formidiol			4662
Teuvincenone E			4192
Coleon U			4052
Hispidulin			4030
Rengyolone			2534
Adhatoda vasica			
Main Protease			
vasicine	$C_{11}H_{12}N_2O$	C1CN2CC3=CC=CC=C3N=C2C1O	3138
vasicinone	$C_{11}H_{10}N_2O_2$	C1CN2C(=NC3=CC=CC=C3C2=O)C1O	3046
vasicinol	$C_{11}H_{12}N_2O_2$	C1CN2CC3=C(C=CC(=C3)O)N=C2C1O	3078
vasicoline	$C_{19}H_{21}N_3$	CN(C)C1=CC=CC=C1C2CCN3C2=NC4=CC=CC=C4C3	4350
Spike protein			
vasicine			2972
vasicinone			2942
vasicinol			2960
vasicoline			4038
Terminalia bellirica			
Spike protein			
Cardenolide	$C_{23}H_{34}O_2$	CC12CCCCC1CCC3C2CCC4(C3CCC4C5=CC(=O)OC5)C	4324
termilignan	$C_{19}H_{20}O_3$	COC1=CC(=C(C=C1)CC(=C)C(=C)CC2=CC=C(C=C2)O)O	4138
thannilignan	$C_{19}H_{22}O_5$	COC1=CC(=C(C=C1)CC(CO)(C(=C)CC2=CC=C(C=C2)O)O)O	4080
7-hydroxy-3',4'-(methylenedioxy) flavone	$C_{19}H_{16}O_8$	COC1=C2C(=C(C(=C1O)O)OC)OC(=C(C2=O)OC)C3=CC4=C(C=C3)OCO4	4434
anolignan B	$C_{18}H_{18}O_2$	C=C(CC1=CC=C(C=C1)O)C(=C)CC2=CC=C(C=C2)O	4126
Pyridine-3-carboxamide	$C_6H_6N_2O$	C1=CC(=CN=C1)C(=O)N	2212
1,5-diphenyl-3-pentanone	$C_{17}H_{18}O$	C1=CC=C(C=C1)CCC(=O)CCC2=CC=CC=C2	3752
Main Protease			
Cardenolide			4294
termilignan			4176
thannilignan			4066
7-hydroxy-3',4'-(methylenedioxy) flavone			4648
anolignan B			3928
Pyridine-3-carboxamide			2262

1,5-diphenyl-3-pentanone			3952
Terminalia chebula			
Main Protease			
4-O-methylgallic acid	$C_8H_8O_5$	COC1=C(C=C(C=C1O)C(=O)O)O	2762
Shikimic acid	$C_7H_{10}O_5$	C1C(C(C(C=C1C(=O)O)O)O)O	2474
Ferulic acid	$C_{10}H_{10}O_4$	COC1=C(C=CC(=C1)C=CC(=O)O)O	3068
Vanillic acid	$C_8H_8O_4$	COC1=C(C=CC(=C1)C(=O)O)O	2674
p-Coumaric acid	$C_9H_8O_3$	C1=CC(=CC=C1C=CC(=O)O)O	2764
Melilotic acid	$C_9H_{10}O_3$	C1=CC=C(C(=C1)CCC(=O)O)O	2774
Phloroglucinol	$C_6H_6O_3$	C1=C(C=C(C=C1O)O)O	2162
Luteolin	$C_{15}H_{10}O_6$	C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O	3582
Spike protein			
4-O-methylgallic acid			2676
Shikimic acid			2438
Ferulic acid			3004
Vanillic acid			2660
p-Coumaric acid			2584
Melilotic acid			2764
Phloroglucinol			2100
Luteolin			3700
Cinnamomum verum			
Spike protein			
cinnamyl alcohol	$C_9H_{10}O$	C1=CC=C(C=C1)C=CCO	2660
cinnamic aldehyde	C_9H_8O	C1=CC=C(C=C1)C=CC=O	4648
5’-hydroxy-5-hydroxymethyl-4’’	$C_8H_{10}O_5$	CC(=O)OC1C=CC(=O)C1(CO)O	2672
Methoxycinnamaldehyde	$C_{10}H_{10}O_2$	COC1=CC=CC=C1C=CC=O	2964
Cinnamyl acetate	$C_{11}H_{12}O_2$	CC(=O)OCC=CC1=CC=CC=C1	2970
Methyl cinnamate	$C_{10}H_{10}O_2$	COC(=O)C=CC1=CC=CC=C1	2852
Main Protease			
cinnamyl alcohol			2560
cinnamic aldehyde			4734
5’-hydroxy-5-hydroxymethyl-4’’			2742
Methoxycinnamaldehyde			2898
Cinnamyl acetate			3198
Methyl cinnamate			3146
Centella asiatica			
Spike protein			
Asiatic acid	$C_{30}H_{48}O_5$	CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1C)C)C(=O)O	5110
Arjunolic acid	$C_{30}H_{48}O_5$	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1)C)C(=O)O)C	5146
Castilliferol	$C_{24}H_{16}O_8$	C1=CC(=CC=C1C=CC(=O)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC=C(C=C4)O)O	5100
Centellasapogenol A	$C_{30}H_{48}O_5$	CC1(CCC2(CCC3(C(=C2C1)CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C)C(=O)O)C	3398
Methyleugenol	$C_{11}H_{14}O_2$	COC1=C(C=C(C=C1)CC=C)OC	3296
Myrcene	$C_{10}H_{16}$	CC(=CCCC(=C)C=C)C	2854
Patuletin	$C_{16}H_{12}O_8$	COC1=C(C2=C(C=C1O)OC(=C(C2=O)O)C3=CC(=C(C=C3)O)O)O	3948
Main Protease			
Asiatic acid			4872
Arjunolic acid			4728
Castilliferol			5124
Centellasapogenol A			3690
Methyleugenol			3324
Myrcene			3114
Patuletin			3848
Withania somnifera			
Spike protein			
withaferin A	$C_{28}H_{38}O_6$	CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3CC5C6(C4(C(=O)C=CC6O)C)O5)C)CO	5000
withanolide A	$C_{28}H_{38}O_6$	CC1=C(C(=O)OC(C1)C(C)(C2CCC3C2(CCC4C3	5248

		C5C(O5)C6(C4(C(=O)C=CC6)C)O)C)O)C	
withanone	$C_{28}H_{38}O_6$	CC1=C(C(=O)OC(C1)C(C)C2(CCC3C2(CCC4C3C5C(O5)C6(C4(C(=O)C=CC6)C)O)C)O)C	4912
Main Protease			
withaferin A			4888
withanolide A			5114
withanone			4746
Coriandrum sativum			
Spike protein			
p-cymene	$C_{10}H_{14}$	CC1=CC=C(C=C1)C(C)C	2780
myrcene	$C_{10}H_{16}$	CC(=CCCC(=C)C=C)C	2854
cis-ocimene	$C_{10}H_{16}$	CC(=CCC=C(C)C=C)C	2890
β-phellandrene	$C_{10}H_{16}$	CC(C)C1CC=C(C)C=C1	2982
citronellol	$C_{10}H_{20}O$	CC(CCC=C(C)C)CCO	3088
nerol	$C_{10}H_{18}O$	CC(=CCCC(=CCO)C)C	3050
Bornyl acetate	$C_{12}H_{20}O_2$	CC(=O)OC1CC2CCC1(C2(C)C)C	3152
geranyl acetate	$C_{12}H_{20}O_2$	CC(=CCCC(=CCOC(=O)C)C)C	3596
Linalyl acetate	$C_{12}H_{20}O_2$	CC(=CCCC(C)(C=C)OC(=O)C)C	3566
α-terpinyl acetate	$C_{12}H_{20}O_2$	CC(=O)OC(C)(C)C1CCC(=CC1)C	3234
elemol	$C_{15}H_{26}O$	CC(=C)C1CC(CCC1(C)C=C)C(C)(C)O	3566
citronellyl acetate	$C_{12}H_{22}O_2$	CC(CCC=C(C)C)CCOC(=O)C	3526
cis-beta-ocimene	$C_{10}H_{16}$	CC(=CCC=C(C)C=C)C	2890
Main Protease			
p-cymene			3030
myrcene			3114
cis-ocimene			3022
β-phellandrene			2874
citronellol			3176
nerol			2950
Bornyl acetate			3028
geranyl acetate			3604
Linalyl acetate			3548
α-terpinyl acetate			3248
elemol			3832
citronellyl acetate			3594
cis-beta-ocimene			3022
Piper longum			
Main Protease			
piperine	$C_{17}H_{19}NO_3$	C1CCN(CC1)C(=O)C=CC=CC2=CC3=C(C=C2)OCO3	4342
piperettine	$C_{19}H_{21}NO_3$	C1CCN(CC1)C(=O)C=CC=CC=CC2=CC3=C(C=C2)OCO3	4404
asarinine	$C_{20}H_{18}O_6$	C1C2C(COC2C3=CC4=C(C=C3)OCO4)C(O1)C5=CC6=C(C=C5)OCO6	4488
pellitorine	$C_{14}H_{25}NO$	CCCCCC=CC=CC(=O)NCC(C)C	4108
piperlongumine	$C_{17}H_{19}NO_5$	COC1=CC(=CC(=C1OC)OC)/C=C/C(=O)N2CCC=CC2=O	4150
piperlonguminine	$C_{16}H_{19}NO_3$	CC(C)CNC(=O)C=CC=CC1=CC2=C(C=C1)OCO2	4110
retrofractamide A	$C_{20}H_{25}NO_3$	CC(C)CNC(=O)C=CC=CCCC=CC1=CC2=C(C=C1)OCO2	4874
dehydropipernonaline	$C_{21}H_{25}NO_3$	C1CCN(CC1)C(=O)C=CC=CCCC=CC2=CC3=C(C=C2)OCO3	4828
6-alpha-diol	$C_{21}H_{23}NO_5$	CC(=O)OC1C=CC2C3CC4=C5C2(C1OC5=C(C=C4)OC(=O)C)CCN3C	4450
Spike protein			
piperine			4252
piperettine			4376
asarinine			4442
pellitorine			3762
piperlongumine			4274
piperlonguminine			4118
retrofractamide A			5022

dehydropipernonaline			5344
6-alpha-diol			4526
Cinnamomum tamala			
Spike protein			
Furanogermenone	$C_{15}H_{20}O_2$	CC1CCC=C(CC2=C(CC1=O)C(=CO2)C)C	3692
sabinene	$C_{10}H_{16}$	CC(C)C12CCC(=C)C1C2	2870
curcumenol	$C_{15}H_{22}O_2$	CC1CCC2C13CC(=C(C)C)C(O3)(C=C2C)O	3608
sesquiterpenoid	$C_{20}H_{28}O_5$	CC1=CC(C(CCC(=C)C(CC1)O)C(=O)C)OC(=O)C=CC(C)(C)O	4748
furanodiene	$C_{15}H_{20}O$	CC1=CCC2=C(CC(=CCC1)C)OC=C2C	3518
curzerene	$C_{15}H_{20}O$	CC1=COC2=C1CC(C(C2)(C)C=C)C(=C)C	
α -pinene	$C_{10}H_{16}$	CC1(C)C2CC3OC3(C)C1C2	2740
1, 8-cineole	$C_{10}H_{18}O_2$	CC(=O)OC1CC2CCC1(OC2(C)C)C	3406
spathulenol	$C_{15}H_{24}O$	CC1(C2C1C3C(CCC3(C)O)C(=C)CC2)C	3500
santolina triene	$C_{10}H_{16}$	CC(=CC(C=C)C(=C)C)C	2984
trans -cinnamaldehyde	C_9H_8O	C1=CC(=C(C=C1Cl)C=CC=O)[N+](=O)[O-]	3110
Main Protease			
Furanogermenone			3698
sabinene			2908
curcumenol			3862
sesquiterpenoid			4374
furanodiene			3606
curzerene			3648
α -pinene			2672
1, 8-cineole			3312
spathulenol			3526
santolina triene			2674
trans -cinnamaldehyde			3242
Swertia chirayita			
Main Protease			
swertiamarin	$C_{16}H_{22}O_{10}$	C=CC1C(OC=C2C1(CCOC2=O)O)OC3C(C(C(C(O3)CO)O)O)O	4308
swerchirin	$C_{15}H_{12}O_6$	COC1=C2C(=C(C=C1)O)C(=O)C3=C(C=C(C=C3O2)OC)O	3756
sweroside	$C_{16}H_{22}O_9$	C=CC1C2CCOC(=O)C2=COC1OC3C(C(C(C(O3)CO)O)O)O	4270
gentiopicrin	$C_{16}H_{20}O_9$	C=CC1C(OC=C2C1=CCOC2=O)OC3C(C(C(C(O3)CO)O)O)O	4454
Spike protein			
swertiamarin			4270
swerchirin			3670
sweroside			4482
gentiopicrin			4580
Syzygium aromaticum			
Spike protein			
eugenol	$C_{10}H_{12}O_2$	COC1=C(C=CC(=C1)CC=C)O	3006
eugenyl acetate	$C_{12}H_{14}O_3$	CC(=O)OC1=C(C=C(C=C1)CC=C)OC	3472
vanillin	$C_8H_8O_3$	COC1=C(C=CC(=C1)C=O)O	2474
methyl salicylate	$C_8H_8O_3$	COC(=O)C1=CC=CC=C1O	2686
eugenin	$C_{11}H_{10}O_4$	CC1=CC(=O)C2=C(C=C(C=C2O1)OC)O	3080
kaempferol	$C_{15}H_{10}O_6$	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	3514
rhamnetin	$C_{16}H_{12}O_7$	COC1=CC(=C2C(=C1)OC(=C(C2=O)O)C3=CC(=C(C=C3)O)O)O	3824
eugenitin	$C_{12}H_{12}O_4$	CC1=CC(=O)C2=C(C(=C(C=C2O1)OC)C)O	3200
methyl amyl ketone	$C_{13}H_{18}N_4O_4$	CCCCCC(=O)C	2436
benzaldehyde	C_7H_6O	C1=CC=C(C=C1)C=O	2166
chavicol	$C_9H_{10}O$	C=CCC1=CC=C(C=C1)O	2672
Main Protease			
eugenol			3148
eugenyl acetate			3538
vanillin			2534
methyl salicylate			2720

eugenin			3054
kaempferol			3774
rhamnetin			3850
eugenitin			3280
methyl amyl ketone			2932
benzaldehyde			2180
chavicol			2718
Camellia sinensis			
Main Protease			
epicatechin	$C_{15}H_{14}O_6$	C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O	3578
catechin	$C_{15}H_{14}O_6$	C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O	3698
Spike protein			
epicatechin			3528
catechin			3596
Azadirachta indica			
Main Protease			
quercetin	$C_{15}H_{10}O_7$	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O	3772
nimbandiol	$C_{26}H_{32}O_7$	CC1=C2C(CC1C3=COC=C3)OC4C2(C(C5(C(C4O)C(C=CC5=O)(C)O)C)CC(=O)OC)C	4750
nimbolide	$C_{27}H_{30}O_7$	CC1=C2C(CC1C3=COC=C3)OC4C2(C(C5(C6C4OC(=O)C6(C=CC5=O)C)C)CC(=O)OC)C	3402
ascorbic acid	$C_6H_8O_6$	C(C(C1C(=C(C(=O)O1)O)O)O)O	2414
17-hydroxyazadiradione	$C_{28}H_{34}O_6$	CC(=O)OC1CC2C(C(=O)C=CC2(C3C1(C4=CC(=O)C(C4(CC3)C)(C5=COC=C5)O)C)C)(C)C	4906
nimbiol	$C_{18}H_{24}O_2$	CC1=CC2=C(C=C1O)C3(CCCC(C3CC2=O)(C)C)C	3792
Spike protein			
quercetin			
nimbandiol			4912
nimbolide			3326
ascorbic acid			2306
17-hydroxyazadiradione			5062
nimbiol			3872
Brassica juncea			
Main Protease			
Cyclododecanol	$C_{12}H_{24}O$	C1CCCCCC(CCCCC1)O	3034
Spike protein			
Cyclododecanol			3100
Cuminum cyminum			
Spike protein			
carvone	$C_{10}H_{14}O$	CC1=CCC(CC1=O)C(=C)C	2940
cuminaldehyde	$C_{10}H_{12}O$	CC(C)C1=CC=C(C=C1)C=O	2910
1,8-cineole	$C_{16}H_{28}O_7$	CC1(C2CCC(O1)(CC2)C)C	2782
o- cymene	$C_{10}H_{14}$	CC1=CC=CC=C1C(C)C	2800
safranal	$C_{10}H_{14}O$	CC1=C(C(CC=C1)(C)C)C=O	2842
linalool	$C_{10}H_{18}O$	CC(=CCCC(C)(C=C)O)C	3108
Main Protease			
carvone			2906
cuminaldehyde			2998
1,8-cineole			2670
o- cymene			2654
safranal			2746
linalool			3110
Apium graveolens			
Spike protein			
d-galacturonic acid			
d-galactose	$C_6H_{12}O_6$	C(C1C(C(C(C(O1)O)O)O)O)O	2364
Caffeic acid	$C_9H_8O_4$	C1=CC(=C(C=C1C=CC(=O)O)O)O	2878
apigenin	$C_{15}H_{10}O_5$	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O	3674

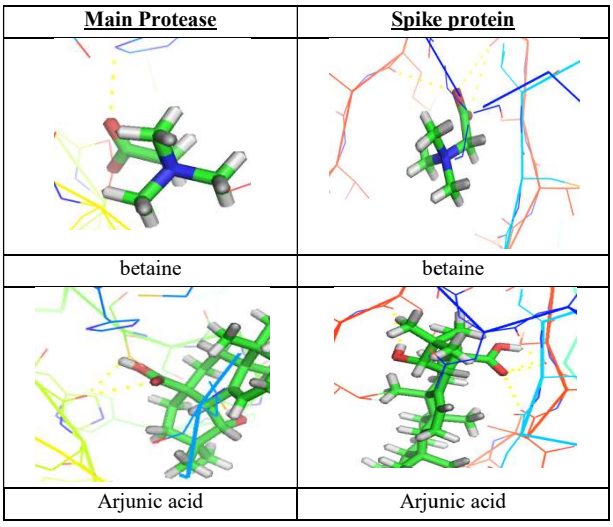
rutaretin	$C_{14}H_{14}O_5$	CC(C)(C1CC2=C(O1)C(=C3C(=C2)C=CC(=O)O3)O)O	3528
ocimene	$C_{10}H_{16}$	CC(=CCC=C(C)C=C)C	3016
bergapten	$C_{12}H_8O_4$	COC1=C2C=CC(=O)OC2=CC3=C1C=CO3	3184
isopimpinellin			
isoimperatorin			
osthenol	$C_{14}H_{14}O_3$	CC(=CCC1=C(C=CC2=C1OC(=O)C=C2)O)C	3534
d-limonene	$C_{10}H_{16}$	CC1=CCC(CC1)C(=C)C	2846
terpineol	$C_{10}H_{18}O$	CC1=CCC(CC1)C(C)(C)O	3000
Main Protease			
d-galacturonic acid			2358
d-galactose			2364
Caffeic acid			2802
apigenin			3652
rutaretin			
ocimene			3118
bergapten			3230
isopimpinellin			
isoimperatorin			3996
osthenol			
d-limonene			2806
terpineol			2824
Trachyspermum ammi			
Spike protein			
thymol	$C_{10}H_{14}O$	CC1=CC(=C(C=C1)C(C)C)O	3024
para-cymene			
γ-terpenine	$C_{10}H_{16}$	CC1=CCC(=CC1)C(C)C	2844
α-pinene	$C_{10}H_{16}$	CC1=CCC2CC1C2(C)C	2754
β-pinene	$C_{10}H_{16}$	CC1(C)C2CCC(=C)C1C2	2702
dipentene	$C_{10}H_{16}$	CC1=CCC(CC1)C(=C)C	2862
α-terpinene	$C_{10}H_{16}$	CC(C)C1=CC=C(C)CC1	2812
carvacrol	$C_{10}H_{14}O$	CC1=C(C=C(C=C1)C(C)C)O	2952
camphene	$C_{10}H_{16}$	CC1(C2CCC(C2)C1=C)C	2680
myrcene	$C_{10}H_{16}$	CC(=CCCC(=C)C=C)C	2854
α-3-carene	$C_{13}H_{20}$	CC1=CCC2C(C1)C2(C)C	2884
Main Protease			
thymol			
para-cymene			3030
γ-terpenine			2830
α-pinene			2504
β-pinene			2602
dipentene			2986
α-terpinene			2918
carvacrol			2950
camphene			2524
myrcene			3114
α-3-carene			2624
Andrographis paniculata			
Main Protease			
Andrographolide	$C_{20}H_{30}O_5$	CC12CCC(C(C1CCC(=C)C2CC=C3C(COC3=O)O)(C)CO)O	4064
andrograpanin	$C_{20}H_{30}O_3$	CC1(CCCC2(C1CCC(=C)C2CCC3=CCOC3=O)C)CO	4106
7-*O*-methylwogonin	$C_{17}H_{14}O_5$	COC1=C(C2=C(C(=C1)O)C(=O)C=C(O2)C3=CC=CC=C3)OC	4012
Apigenin	$C_{15}H_{10}O_5$	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O	3652
onysilin	$C_{17}H_{16}O_5$	COC1=C(C(=C2C(=O)CC(OC2=C1)C3=CC=CC=C3)O)OC	4172
Spike protein			
Andrographolide			4222
andrograpanin			4266
7-*O*-methylwogonin			4052

Apigenin			3674
onysilin			3958
Phyllanthus emblica			
Spike protein			
ascorbic acid	$C_6H_8O_6$	C(C(C1C(=C(C(=O)O1)O)O)O)O	2306
kaempferol	$C_{15}H_{10}O_6$	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	3514
ellagic acid	$C_{14}H_6O_8$	C1=C2C3=C(C(=C1O)O)OC(=O)C4=CC(=C(C(=C43)OC2=O)O)O	3404
gallic acid	$C_7H_6O_5$	C1=C(C=C(C(=C1O)O)O)C(=O)O	2350
Main Protease			
ascorbic acid			2414
kaempferol			3774
ellagic acid			3546
gallic acid			2394
Zingiber officinale			
Main Protease			
gingerol	$C_{17}H_{26}O_4$	CCCCCC(CC(=O)CCC1=CC(=C(C=C1)O)OC)O	4276
shogaol	$C_{17}H_{24}O_3$	CCCCCC=CC(=O)CCC1=CC(=C(C=C1)O)OC	4040
paradol	$C_{17}H_{26}O_3$	CCCCCCCC(=O)CCC1=CC(=C(C=C1)O)OC	4266
8-gingerol	$C_{19}H_{30}O_4$	CCCCCCCC(CC(=O)CCC1=CC(=C(C=C1)O)OC)O	4520
quercetin	$C_{15}H_{10}O_7$	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O	3772
zingerone	$C_{11}H_{14}O_3$	CC(=O)CCC1=CC(=C(C=C1)O)OC	3338
gingerenone-A	$C_{21}H_{24}O_5$	COC1=C(C=CC(=C1)CCC=CC(=O)CCC2=CC(=C(C=C2)O)OC)O	4766
6-dehydrogingerdione	$C_{17}H_{22}O_4$	CCCCCC(=O)C=C(C=CC1=CC(=C(C=C1)O)OC)O	4222
β-sesquiphellandrene	$C_{15}H_{24}$	CC(CCC=C(C)C)C1CCC(=C)C=C1	3782
Spike protein			
gingerol			4144
shogaol			4052
paradol			4314
8-gingerol			4548
quercetin			3634
zingerone			3130
gingerenone-A			4598
6-dehydrogingerdione			4396
β-sesquiphellandrene			3676
Cubeba officinalis			
Spike protein			
sabinene	$C_{10}H_{16}$	CC(C)C12CCC(=C)C1C2	2870
α-thujene	$C_{10}H_{16}$	CC(C)C12CC=C(C)C1C2	2876
3-Carene	$C_{10}H_{16}$	CC1=CCC2C(C1)C2(C)C	2884
1,4-cineole	$C_{10}H_{18}O_2$	CC(C)C12CCC(O1)(CC2)C	2926
1,8-cineole	$C_{16}H_{28}O_7$	CC1(C2CCC(O1)(CC2)C)C	2782
cubebol	$C_{15}H_{26}O$	CC1CCC(C2C13C2C(CC3)(C)O)C(C)C	3646
terpinen-4-ol	$C_{10}H_{18}O$	CC1=CCC(CC1)(C(C)C)O	2904
Main Protease			
sabinene			2908
α-thujene			2802
3-Carene			2624
1,4-cineole			2804
1,8-cineole			2670
cubebol			3762
terpinen-4-ol			2890
Tinospora cordifolia			
Main Protease			
Berberine	$C_{20}H_{19}NO_8S$	COC1=C(C2=C[N+]3=C(C=C2C=C1)C4=CC5=C(C=C4CC3)OCO5)OC	4322
choline	$C_5H_{14}NO^+$	C[N+](C)(C)CCO	2216
Tembetarine	$C_{20}H_{26}NO_4^+$	C[N+]1(CCC2=CC(=C(C=C2C1CC3=CC(=C(C=	4780

		C3)OC)O)O)OC)C	
Tinosporin	$C_{20}H_{22}O_6$	CC12CCC3C(=O)OC(CC3(C1C4C=CC2(C(=O)O4)O)C)C5=COC=C5	4354
Jatrorrhizine	$C_{20}H_{20}NO_4^+$	COC1=C(C2=C[N+]3=C(C=C2C=C1)C4=CC(=C(C=C4CC3)O)OC)OC	4408
Palmatine	$C_{21}H_{22}NO_4^+$	COC1=C(C2=C[N+]3=C(C=C2C=C1)C4=CC(=C(C=C4CC3)OC)OC)OC	4574
Magnoflorine	$C_{20}H_{24}NO_4^+$	C[N+]1(CCC2=CC(=C(C3=C2C1CC4=C3C(=C(C=C4)OC)O)O)OC)C	4590
Isocolumbin	$C_{20}H_{22}O_6$	CC12CCC3C(=O)OC(CC3(C1C4C=CC2(C(=O)O4)O)C)C5=COC=C5	4020
Spike protein			
Berberine			4248
choline			2082
Tembetarine			4448
Tinosporin			4466
Jatrorrhizine			4502
Palmatine			4546
Magnoflorine			4424
Isocolumbin			4208
Phyllanthus niruri			
Spike protein			
Phyllanthin,	$C_{24}H_{34}O_6$	COCC(CC1=CC(=C(C=C1)OC)OC)C(CC2=CC(=C(C=C2)OC)OC)COC	5576
hypophyllanthin	$C_{24}H_{30}O_7$	COCC1CC2=CC(=C3C(=C2C(C1COC)C4=CC(=C(C=C4)OC)OC)OCO3)OC	5544
Methyl brevifolincarboxylate	$C_{14}H_{10}O_8$	COC(=O)C1CC(=O)C2=C1C3=C(C(=C(C=C3C(=O)O2)O)O)O	3632
niranthin	$C_{24}H_{32}O_7$	COCC(CC1=CC(=C(C=C1)OC)OC)C(CC2=CC3=C(C(=C2)OC)OCO3)COC	5214
nirtetralin	$C_{24}H_{30}O_7$	COCC1CC2=CC3=C(C(=C2C(C1COC)C4=CC(=C(C=C4)OC)OC)OC)OCO3	
epicatechin	$C_{15}H_{14}O_6$	C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O	3528
Main Protease			
Phyllanthin,			5192
hypophyllanthin			5732
Methyl brevifolincarboxylate			3644
niranthin			5488
nirtetralin			5240
epicatechin			3578
Picrorhiza kurroa			
Main Protease			
Kutkin	$C_{23}H_{28}O_{12}$	COC1=C(C=CC(=C1)C(=O)OC2C(C(C(C(O2)CO)O)O)O)OC(=O)C=CC3=CC=CC=C3.O.O	5290
Apocynin	$C_9H_{10}O_3$	CC(=O)C1=CC(=C(C=C1)O)OC	2828
Vanillic acid	$C_8H_8O_4$	COC1=C(C=CC(=C1)C(=O)O)O	2674
Spike protein			
Kutkin			5402
Apocynin			2820
Vanillic acid			2660
Ocimum sanctum			
Main Protease			
Eugenol	$C_{10}H_{12}O_2$	COC1=C(C=CC(=C1)CC=C)O	1282.22
Linalool	$C_{10}H_{18}O$	CC(=CCCC(C)(C=C)O)C	1282.03
Carvacrol	$C_{10}H_{14}O$	CC1=C(C=C(C=C1)C(C)C)O	1281.82
Rosmarinic Acid	$C_{18}H_{16}O_8$	C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O	1281.83
Spike protein			
Carvacrol			1165.90
Eugenol			1165.55
Linalool			1165.38
Rosmarinic Acid			1165.50

Curcuma longa			
Spike protein			
Curcumenol	$C_{15}H_{22}O_2$	CC1CCC2C13CC(=C(C)C)C(O3)(C=C2C)O	1154.29
Cucumin	$C_{15}H_{22}O_2$	CC1(CC2=C(C1O)C3(CCCC3(C2=O)C)C)C	1156.10
Cholesterol	$C_{27}H_{46}O$	CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C	1156.33
Bisdemethoxycumin	$C_{19}H_{16}O_4$	OC1=CC=C(C=C1)\C=C\C(=O)CC(=O)/C=C/C2=CC=C(O)C=C2	1156.20
Bisacurone	$C_{15}H_{24}O_3$	CC(CC(=O)C=C(C)C)C1CC(C(C=C1)(C)O)O	1154.33
Bisacumol	$C_{15}H_{22}O$	CC1=CC=C(C=C1)C(C)CC(C=C(C)C)O	1156.22
Arturmerone	$\mathbf{C_{15}H_{20}O}$	CC(CC(=O)C=C(C)C)C1=CC=C(C)C=C1	1156.33
Curcumin	$C_{21}H_{20}O_6$	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	1151.91
Curlone	$C_{15}H_{22}O$	CC(CC(=O)C=C(C)C)C1CCC(=C)C=C1	1156.88
Dehyrocurdione	$C_{15}H_{22}O_2$	CC1CC\C=C(C)/CC(=O)C(CC1=O)=C(C)C	1156.07
Demethoxycucumin	$C_{20}H_{18}O_5$	COC1=C(O)C=CC(=C1)\C=C\C(=O)CC(=O)/C=C/C2=CC=C(O)C=C2	1154.03
Epiprocurcumrnol	$C_{15}H_{22}O_2$	CC(C)=C1CC2C(CCC2(C)O)C(=CC1=O)C	1155.89
Germacrone	$C_{15}H_{22}O$	CC1=CCC(=C(C)C)C(=O)CC(=CCC1)C	1151.03
Isoprocurcumenol	$C_{15}H_{22}O_2$	CC(=C1CC2C(CCC2(C)O)C(=C)CC1=O)C	1156.08
Procurcumadiol	$C_{15}H_{22}O_3$	CC1=CC(=O)C(=C(C)C)CC2(C1CCC2(C)O)O	1156.22
Main Protease			
Ar-Turmeron			1273.17
Bisacumol			1271.99
Bisacurone			1271.21
Bisdemethoxycurcum			1274.20
Cholesterol			1273.16
Cucumin			1274.17
Curcumenol			1274.23
Curcumin			1273.09
Curlone			1273.18
Dehydrocurdione			1269.18
Demethoxycurcumin			1273.09
Epiprocurcumenol			1268.85
Procurcumadioal			1270.65
Isoprocurcumenol			1268.85
Germacrone			1270.56
Glycyrrhiza glabra			
Main Protease			
Glabridin	$C_{20}H_{20}O_4$	CC1(C=CC2=C(O1)C=CC3=C2OCC(C3)C4=C(C=C(C=C4)O)O)C	4088
Isoliquiritigenin	$C_{15}H_{12}O_4$	C1=CC(=CC=C1C=CC(=O)C2=C(C=C(C=C2)O)O)O	3570
Liquiritigenin	$C_{15}H_{12}O_4$	C1C(OC2=C(C1=O)C=CC(=C2)O)C3=CC=C(C=C3)O	3506
Liquiritin	$C_{21}H_{22}O_9$	C1C(OC2=C(C1=O)C=CC(=C2)O)C3=CC=C(C=C3)OC4C(C(C(C(O4)CO)O)O)O	4674
Licochalcone A	$C_{21}H_{22}O_4$	CC(C)(C=C)C1=C(C=C(C(=C1)C=CC(=O)C2=CC=C(C=C2)O)OC)O	4594
Glabrene	$C_{20}H_{18}O_4$	CC1(C=CC2=C(C=CC(=C2O1)C3=CC4=C(C=C(C=C4)O)OC3)O)C	4200
Spike protein			
Glabridin			4102
Isoliquiritigenin			3616
Liquiritigenin			3550
Liquiritin			4586
Licochalcone A			4748
Glabrene			4132
Berberis aristata			
Main Protease			
Karachine	$C_{26}H_{27}NO_5$	CC12CC3C4=C(C1C5(N3CCC6=CC7=C(C=C65)OCO7)CC(=O)C2)C=CC(=C4OC)OC	1140.91

Taxilamine	$C_{20}H_{20}NO_6^+$	COC1=C(OC)C=C2C=[N+](C=CC2=C1)C3=CC(=C(OC)C=C3C(O)=O)OC	1138.29
Berberine	$C_{20}H_{18}NO_4^+$	COC1=C(C2=C[N+]3=C(C=C2C=C1)C4=CC5=C(C=C4CC3)OCO5)OC	1248.72
Oxyberberine	$C_{20}H_{17}NO_5$	COC1=C(C2=C(C=C1)C=C3C4=CC5=C(C=C4CCN3C2=O)OCO5)OC	1140.92
Palmatine	$C_{21}H_{22}NO_4^+$	COC1=C(C2=C[N+]3=C(C=C2C=C1)C4=CC(=C(C=C4CC3)OC)OC)OC	1248.68
Quercetin	$C_{15}H_{10}O_7$	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O	1145.64
Spike protein			
Karachine			1027.00
Oxyberberine			1022.68
Quercetin			1022.94
Taxilamine			1021.46
Berberine			1128.96
Palmatine			1129.03
Cinchona cortex			
Spike protein			
Cinchonidine	$C_{19}H_{22}N_2O$	C=CC1CN2CCC1CC2C(C3=CC=NC4=CC=CC=C34)O	1108.35
Cinchonine	$C_{19}H_{22}N_2O$	C=CC1CN2CCC1CC2C(C3=CC=NC4=CC=CC=C34)O	1107.67
Cinnamic Acid	$C_9H_8O_2$	C1=CC=C(C=C1)C=CC(=O)O	1174.17
Cinnamaldehyde	C_9H_8O	C1=CC=C(C=C1)C=CC=O	1108.31
Quinidine	$C_{20}H_{24}N_2O_2$	COC1=CC2=C(C=CN=C2C=C1)C(C3CC4CCN3CC4C=C)O	1134.49
Quinine	$C_{20}H_{24}N_2O_2$	COC1=CC2=C(C=CN=C2C=C1)C(C3CC4CCN3CC4C=C)O	1108.16
Coumarin	$C_9H_6O_2$	C1=CC=C2C(=C1)C=CC(=O)O2	1134.48
Main Protease			
Cinnamaldehyde			1269.85
Cinnamic Acid			1289.88
Quinidine			1249.72
Quinine			1218.40
Coumarin			1249.70
Cinchonidine			1218.93
Cinchonine			1219.69



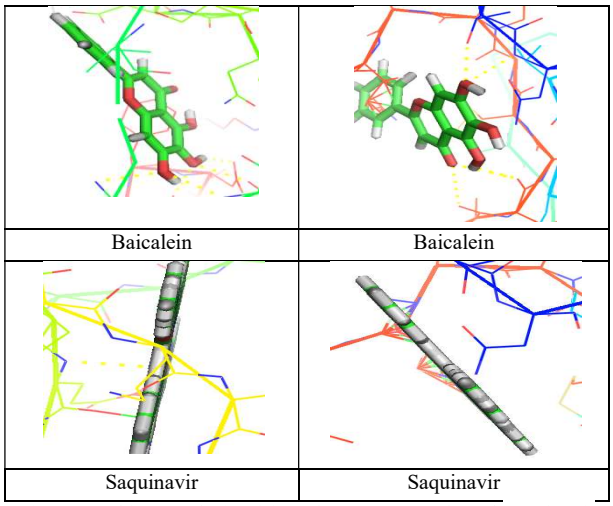


Fig. 2: Docking Analysis of few phyto-compounds and Saquinavir with corona viral proteins

Table 5: Docking with Saquinavir

Main Protease with Saquinavir	Spike protein with Saquinavir
-5322 kcal/mol	-5076 kcal/mol

CONCLUSION:

The global COVID 19 pandemic is caused by a new strain of pre-existing corona virus. In the present paper we have presented elaborate studies (*in-silico*) on some of the important compounds from selected medicinal plants and commonly used Indian spices to evaluate their effectiveness to combat the disease. Also, our studies emphasizes on the utility of some ayurvedic immuno-modulatory herbs such as *Tinospora cordifolia, Withania somnifera, Phyllanthus niruri, Andrographis paniculata, Glycyrrhiza glabra, Ocimum sanctum* etc. Besides looking after anti-viral effects, restoring immune homeostasis is more important factor towards overall management of the disease.

As per docking studies it is seen that arjunic acid from *Terminalia arjuna*, all compounds selected from ADME studies of *Clerodendrum indicum* except Rengyolone, vasicoline from *Adhatoda vasica*, all compounds selected from ADME studies compounds of *Terminalia bellirica* except Pyridine-3-carboxamide, cinnamic aldehyde from *Cinnamomum verum*, all compounds selected from ADME studies of *Centella asiatica, Withania somnifera, Piper longum, Swertia chirayita, Camellia sinensis, Andrographis paniculata, Zingiber officinale, Phyllanthus niruri, Ocimum sanctum, Curcuma longa, Glycyrrhiza glabra, Berberis aristata* and *Cinchona cortex*, Sesquiterpenoid from *Cinnamomum tamala*, all compounds selected from ADME studies compounds of *Azadirachta indica* except ascorbic acid, all compounds selected from ADME studies compounds of *Tinospora cordifolia* except choline and Kutkin from *Picrorhiza kurroa* docks with a good score with selected proteins of corona virus.

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