Supplementary file

Antiviral activity of traditional medicinal plants against SARS-CoV-2 and its cellular receptor

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Table S1: Canonical SMILES used for the calculation of toxicity, pharmacokinetics and target prediction of active constituents.

S.No	Name	Canonical SMILES
1.	Amarogentin	C=CC1C2CCOC(=O)C2=COC1OC3C(C(C(C(O3)CO)O)O)OC(=O)C4=C(C=C(C=C4O)O)C5=CC(=CC=C5)O
2.	Sawertiamarine	C=CC1C(OC=C2C1(CCOC2=O)O)OC3C(C(C(C(O3)CO)O)O)O
3.	α-amyrin	CC(=O)OC1CCC2(C(C1(C)C)CCC3(C2CC=C4C3(CCC5(C4CC(CC5)(C)C)C)C)C)C
4.	β-sitosterol	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
5.	Caesalpinins	CC(=O)OC1CC(C2(C3CC4=C(C=CO4)C(=C)C3CCC2(C1(C)C)O)C)OC(=O)C
6.	Kutkin	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
7.	Vanillic acid	COC1=C(C=CC(=C1)C(=O)O)O
8.	6-gingerol	CCCCCC(CC(=O)CCC1=CC(=C(C=C1)O)OC)O
9.	glycyrrhetic acid	CC1(C2CCC3(C(C2(CCC1O)C)C(=O)C=C4C3(CCC5(C4CC(CC5)(C)C(=O)O)C)C)C)C
10.	Piperine	C1CCN(CC1)C(=O)C=CC=CC2=CC3=C(C=C2)OCO3
11.	Magnoflorine	C[N+]1(CCC2=CC(=C(C3=C2C1CC4=C3C(=C(C=C4)OC)O)O)OC)C
12.	alliin	C=CCS(=O)CC(C(=O)O)N
13.	Allicin	C=CCSS(=O)CC=C
14.	N-acetylcysteine	CC(=O)NC(CS)C(=O)O
15.	Thymoquinone	CC1=CC(=O)C(=CC1=O)C(C)C
16.	Atropine	CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC=CC=C3
17.	Hyoscyamine	CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC=CC=C3
18.	Scopolamine	CN1C2CC(CC1C3C2O3)OC(=O)C(CO)C4=CC=CC=C4
19.	Belladonnine	CN1C2CCC1CC(C2)OC(=O)C3CCC(C4=CC=CC=C34)(C5=CC=CC=C5)C(=O)OC6CC7CCC(C6)N7C
20.	Eufoliatorin	CC=C(C)C(=O)OC1CC2=C3C(CC(C3C4C1C(C(=O)O4)C)(C)O)OC2=O
21.	Eupafolin	COC1=C(C2=C(C=C1O)OC(=CC2=O)C3=CC(=C(C=C3)O)O)O
22.	Caffeic acid	C1=CC(=C(C=C1C=CC(=O)O)O)O
23.	Amarogentin	C1=CC(=CC=C1C(=O)OC2=CC3=C(C=C2)C=C(C=C3)C(=N)N)N=C(N)N
24.	Sawertiamarine	CC(CS)C(=O)N1CCCC1C(=O)O

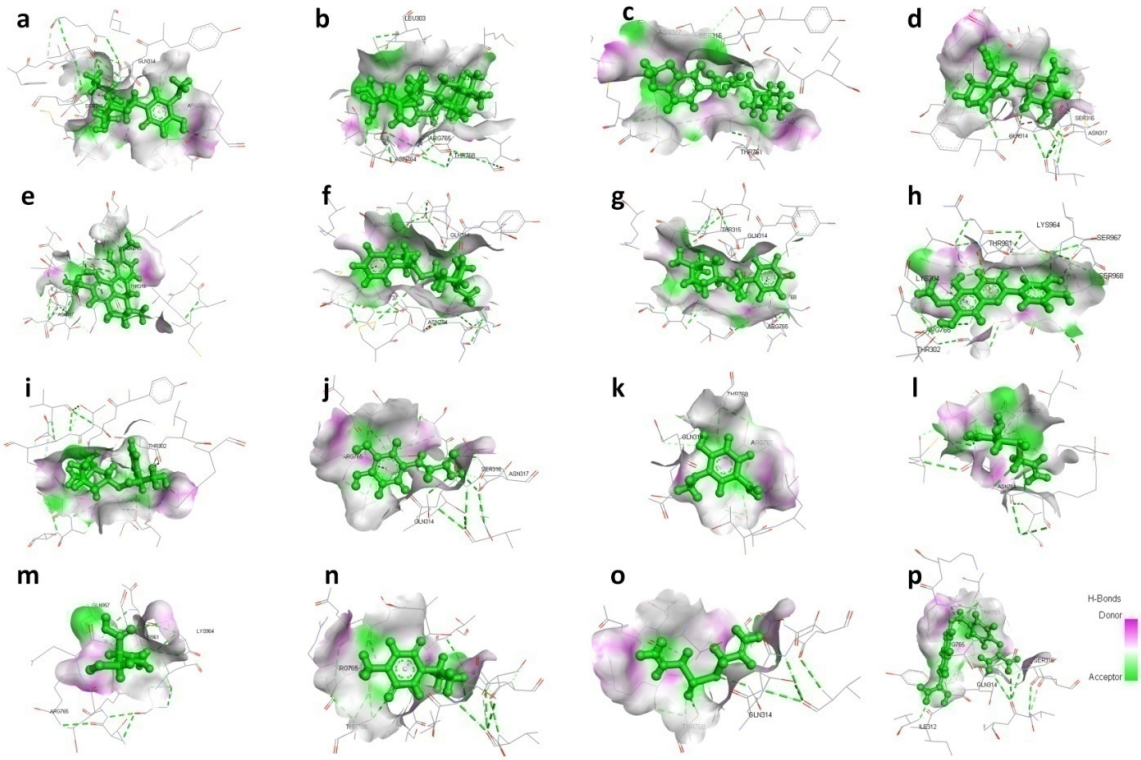

Figure S1: 3 D structure view of protein ligand interaction site. (a) 6-gingerol,(b) glycyrrhetic acid, (c) piperine, (d) sawertiamarine, (e) magnoflorine, (f) scopolamine, (g) atropine, (h) eupafolin, (i) hyoscyamine, (j) caffeic acid, (k) vanillic acid, (l) alliin, (m) n-acetylcysteine, (n) thymoquinone, (o) allicin, (p) nafamostat with spike glycoprotein of SARS-CoV-2.

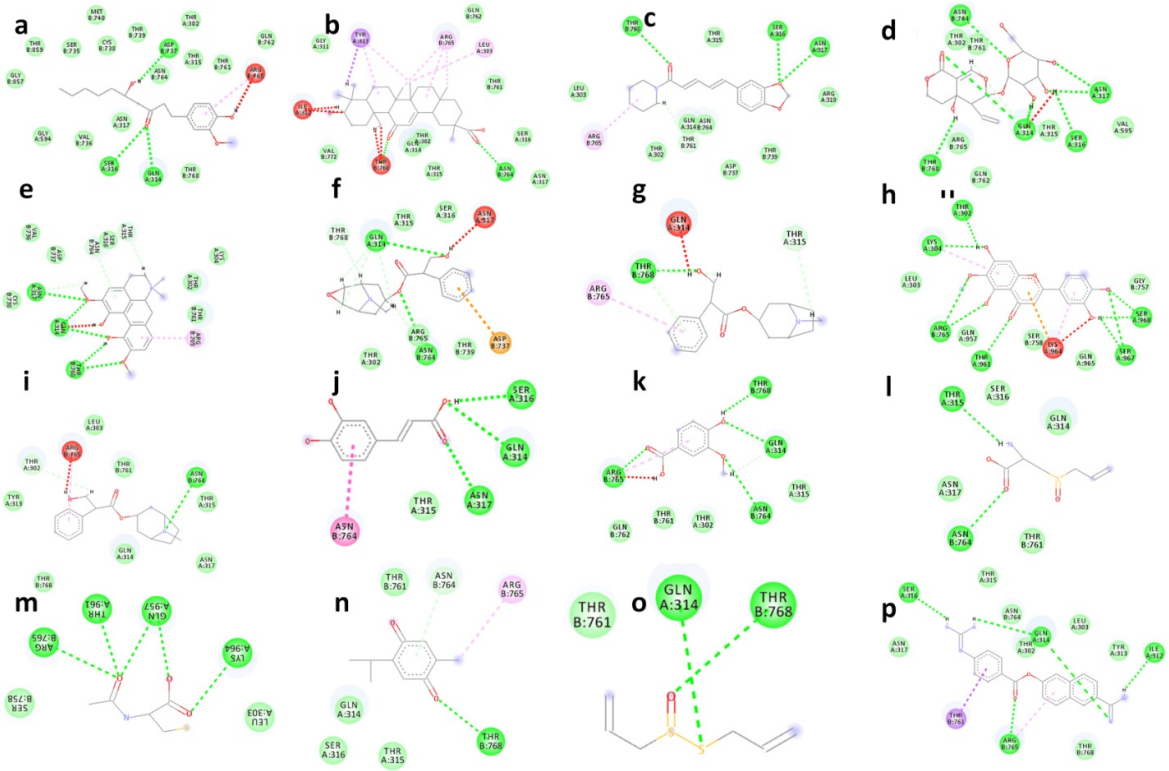

Figure S2: 2 D structure view of protein ligand interaction site (a) 6-gingerol,(b) glycyrrhetic acid, (c) piperine, (d) sawertiamarine, (e) magnoflorine, (f) scopolamine, (g) atropine, (h) eupafolin, and(i) hyoscyamine, (j) caffeic acid, (k) vanillic acid, (l) alliin, (m) n-acetylcysteine, (n) thymoquinone, (o) allicin, (p) nafamostat

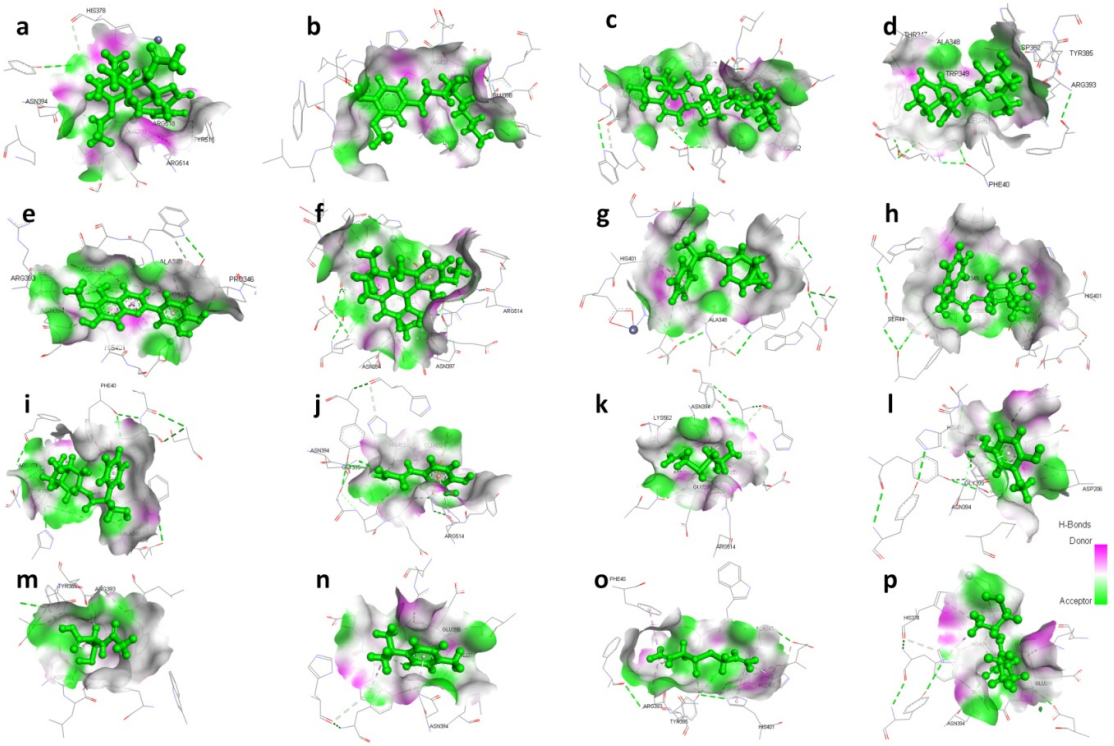

Figure S3: 3 D structure view of protein ligand interaction site. (a) caesalpinins, (b) 6-gingerol, (c) β-sitosterol, (d) sawertiamarine, (e) eupafolin, (f) magnoflorine, (g) scopolamine, (h) atropine, (i) hyoscyamine, (j) caffeic acid, (k) alliin, (l) vanillic acid, (m) n-acetylcysteine, (n) thymoquinone, (o) allicin, (p) captopril with ACE2.

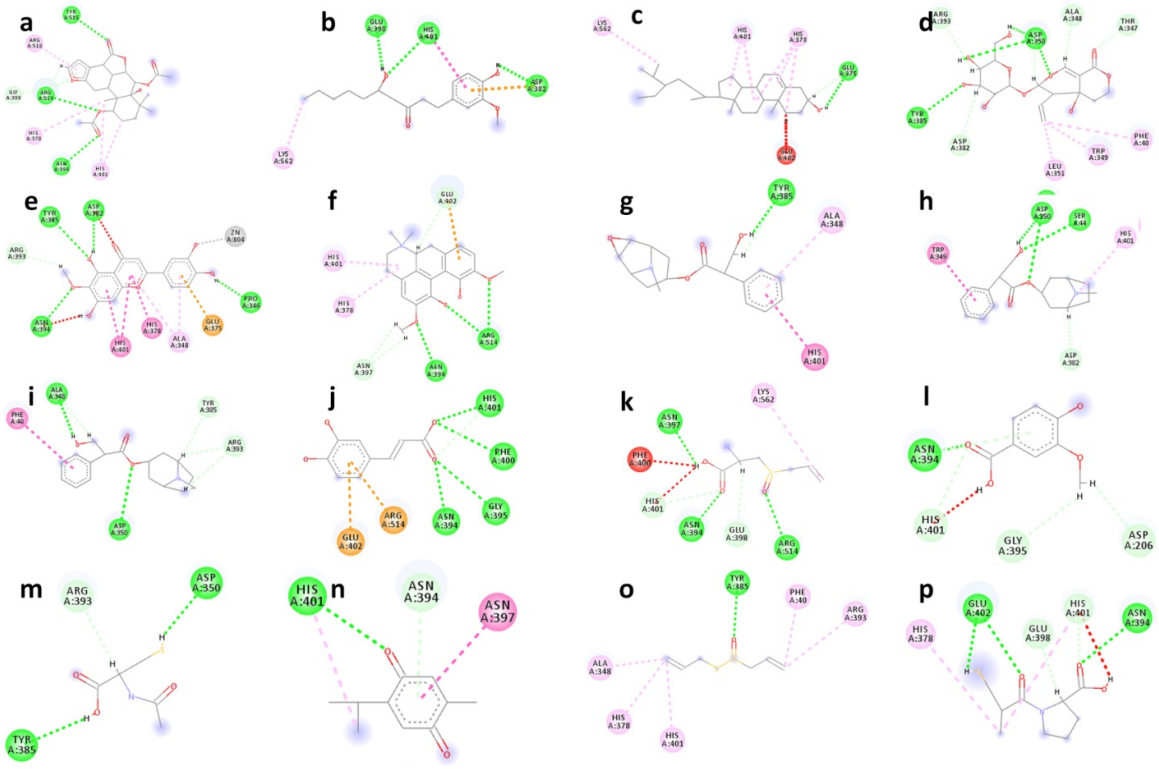

Figure S4: 2 D structure view of protein-ligand interaction site. (a) caesalpinins, (b) 6-gingerol, (c) β-sitosterol, (d) sawertiamarine, (e) eupafolin, (f) magnoflorine, (g) scopolamine, (h) atropine, (i) hyoscyamine, (j) caffeic acid, (k) alliin, (l) vanillic acid, (m) n-acetylcysteine, (n) thymoquinone, (o) allicin, (p) captopril with ACE2.

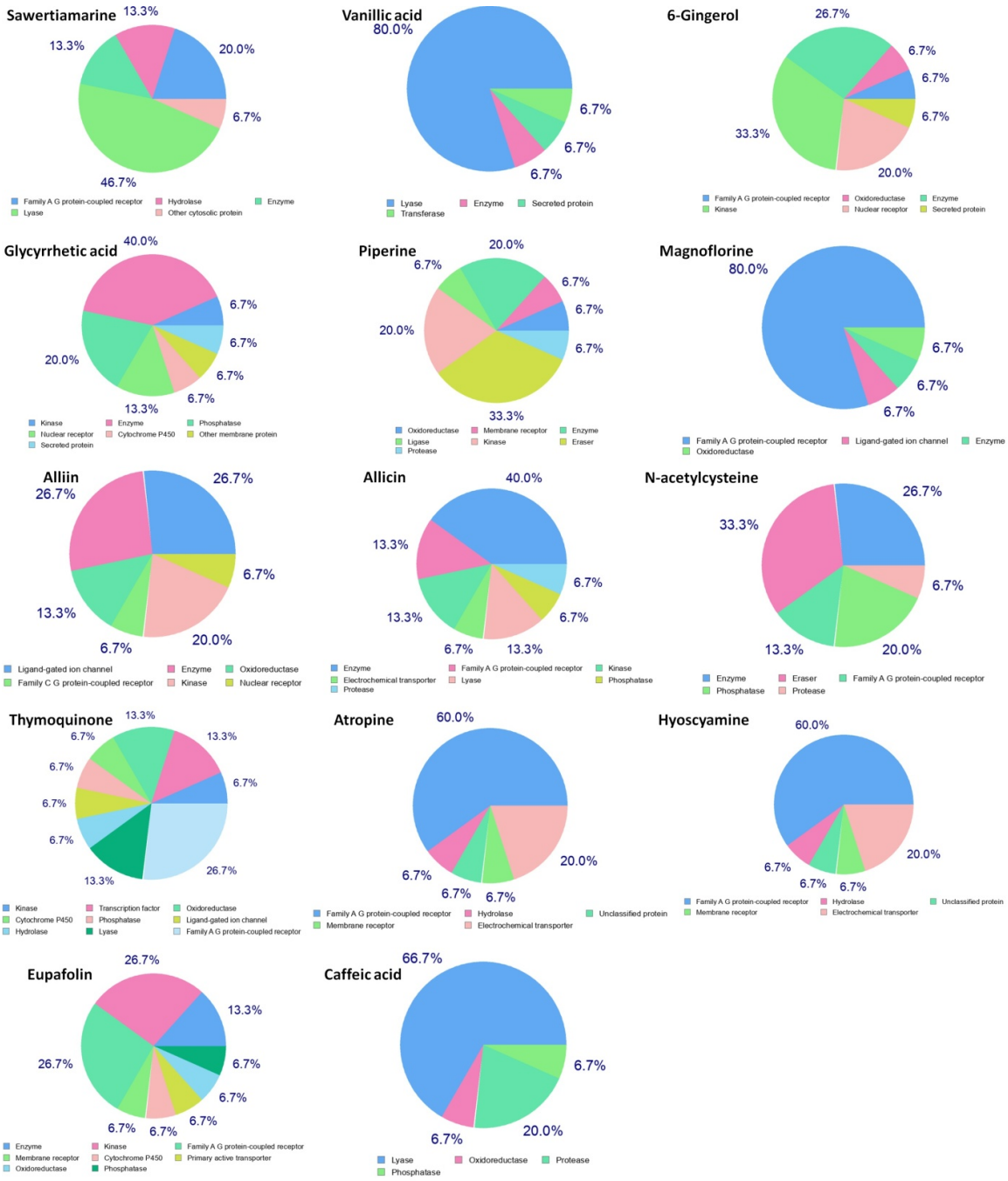

Figure S5: Target prediction analysis of sawertiamarine, vanillic acid, 6-gingerol, glycyrrhetic acid, piperine, magnoflorine, alliin, allicin, n-acetylcysteine, and thymoquinone, atropine, hyoscyamine, eupafolin, caffeic acid.