Supporting Information

Exploring Broccoli's Secondary Metabolites as Promising Inhibitors Against Monkeypox: In silico Approach

Upanshu Gangwar*,†, Pooja‡, Shashank Deep†

† Department of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India. 110016
‡ J. C. Bose University of Science and Technology, Faridabad, 121006
* Email: gangwarupanshu@gmail.com

Library

Table S1: Library used for docking

Serial Number	Metabolite name	Canonical smile	MW	PubChem id
1	Butyronitrile	CCCC#N	69.11	8008
2	Allyl Isothiocyanate	C=CCN=C=S	99.16	5971
3	2-Methyl-2-nitropropane	CC(C)(C)[N+](=O)[O-]	103.12	11672
4	4-(Methylthio)-butanenitrile	CSCCCC#N	115.2	100962
5	Butyl isothiocyanate	CCCCN=C=S	115.2	11613
6	Isobutyl isothiocyanate	CC(C)CN=C=S	115.2	68960
7	Iberin	CS(=O)CCCN=C=S	163.3	10455
8	4-Isothiocyanato-1-butene	C=CCCN=C=S	113.18	76922
9	3-Methylbutyl isothiocyanate	CC(C)CCN=C=S	129.23	79086
10	Isoamyl methyl sulfoxide	CC(C)CCS(=O)C	134.24	143316
11	Erucin	CSCCCCN=C=S	161.3	78160
12	Sulforaphene	CS(=O)C=CCCN=C=S	175.3	6433206
13	Sulforaphane	CS(=O)CCCCN=C=S	177.3	5350
14	Indole-3-carbinol	C1=CC=C2C(=C1)C(=CN2)CO	147.17	3712
15	Indole-3-carboxylic acid	C1=CC=C2C(=C1)C(=CN2)C(=O)O	161.16	69867
16	Indole-3-acetic acid	C1=CC=C2C(=C1)C(=CN2)CC(=O)O	175.18	802
17	1-Methoxyindole-3-carbaldehyde	CON1C=C(C2=CC=CC=C21)C=O	175.18	398554
18	Sinigrin	C=CCC(=NOS(=O)(=O)[O-])SC1C(C(C(C(O1)CO)O)O)O.[K+]	397.5	23682211
19	Gluconapin	C=CCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	373.4	9548620
20	Progoitrin	C=CC(CC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O)O	389.4	5281139
21	Glucocochlearin	CCC(C)C(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	375.4	5281135
22	Glucoiberverin	CSCCCC(=NOS(=O)(=O)[O-])SC1C(C(C(C(O1)CO)O)O)O	406.5	9548637
23	Glucosativin	C(CCS)CC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	407.5	102154672
24	Glucoiberin	CS(=O)CCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	423.5	9548622
25	Glucoraphenin	CS(=O)C=CCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	435.5	15559531
26	3-Methylbutyl-GLS	CC(C)CC/C(=N\OS(=O)(=O)O)/SC1C(C(C(C(O1)CO)O)O)O	389.4	131752360
27	3-Methylpentyl-GLS	CCC(C)CCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	403.5	131751970
28	4-Methylpentyl-GLS	CC(C)CCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	403.5	131752366
29	Glucoerucin	CSCCCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	421.5	656539
30	Glucoraphanin	CS(=O)CCCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	437.5	9548634
31	Glucoalyssin	CS(=O)CCCCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	451.5	9589398
32	Glucohirsutin	CS(=O)CCCCCCCCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO)O)O)O	493.6	101613195
33	Glucosinalbin	C1=CC(=CC=C1CC(=NOS(=O)(=O)O)SC2C(C(C(C(O2)CO)O)O)O)O	425.4	9601115
34	Gluconasturtiin	C1=CC=C(C=C1)CCC(=NOS(=O)(=O)O)SC2C(C(C(C(O2)CO)O)O)O	423.5	656555
35	Glucobrassicin	C1=CC=C2C(=C1)C(=CN2)CC(=NOS(=O)(=O)O)SC3C(C(C(C(O3)CO)O)O)O	448.5	6602378
36	Neoglucobrassicin	CON1C=C(C2=CC=CC=C21)CC(=NOS(=O)(=O)O)SC3C(C(C(C(O3)CO)O)O)O	478.5	9576416
37	Benzoic acid	C1=CC=C(C=C1)C(=O)O	122.12	243
38	Salicylic acid	C1=CC=C(C(=C1)C(=O)O)O	138.12	338
39	p-Hydroxybenzoic acid	C1=CC(=CC=C1C(=O)O)O	138.12	135
40	Protocatechuic acid	C1=CC(=C(C=C1C(=O)O)O)O	154.2	72
41	Gentisic acid	C1=CC(=C(C=C1O)C(=O)O)O	154.12	3469
42	Gallic acid	C1=C(C=C(C(=C1O)O)O)C(=O)O	170.12	370
43	Vanillic acid	COC1=C(C=CC(=C1)C(=O)O)O	168.15	8468
44	p-Coumaric acid	C1=CC(=CC=C1C=CC(=O)O)O	164.16	637542
45	Esculetin	C1=CC(=O)OC2=CC(=C(C=C21)O)O	178.14	5281416
46	Caffeic acid	C1=CC(=C(C=C1C=CC(=O)O)O)O	180.16	689043
47	Ferulic acid	COC1=C(C=CC(=C1)C=CC(=O)O)O	194.18	445858
48	Sinapic acid	COC1=CC(=CC(=C1O)OC)C=CC(=O)O	224.21	637775
49	Gallic acid hexoside	C1=C(C=C(C(=C1O)O)O)C(=O)OC2C(C(C(C(O2)CO)O)O)O	332.26	4628122
50	Gallic acid 4-O-glucoside	C1=C(C=C(C(=C1O)OC2C(C(C(O2)CO)O)O)O)O)C(=O)O	332.26	10088114
51	Sinapoyl malate	COC1=CC(=CC(=C1O)OC)C=CC(=O)OC(CC(=O)O)C(=O)O	340.28	14605050
52	Isochlorogenic acid	C1C(C(C(CC1(C(=O)O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O	354.31	6436237
53	Chlorogenic acid	C1C(C(C(CC1(C(=O)O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O	354.31	1794427
54	Caffeoyl-quinic acid	C1C(C(C(CC1(C(=O)O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O	354.31	1794427
55	5-O-Sinapoylquinic acid	COC1=CC(=CC(=C1O)OC)C=CC(=O)OC2CC(CC(C2O)O)(C(=O)O)O	398.4	72193641
56	Apigenin	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O	270.24	5280443
57	Kaempferol	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	286.24	5280863
58	Luteolin	C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O	286.24	5280445
59	Quercetin	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O	302.23	5280343
60	Myricetin	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	318.23	5281672
61	Astragalin	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O	448.4	5282102
62	Rutin	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O	610.5	5280805
63	Choline	C[N+](C)(C)CCO	104.17	305
64	trigonelline	C[N+]1=CC=CC(=C1)C(=O)[O-]	137.14	5570
65	Linolenic acid	CCC=CCC=CCC=CCCCCCCCC(=O)O	278.4	5280934
66	Linoleic acid	CCCCCC=CCC=CCCCCCCCC(=O)O	280.4	5280450
67	Oleic acid	CCCCCCCCC=CCCCCCCCC(=O)O	282.5	445639
68	Stearic acid	CCCCCCCCCCCCCCCCCC(=O)O	284.5	5281
69	Campesterol	CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C	400.7	173183

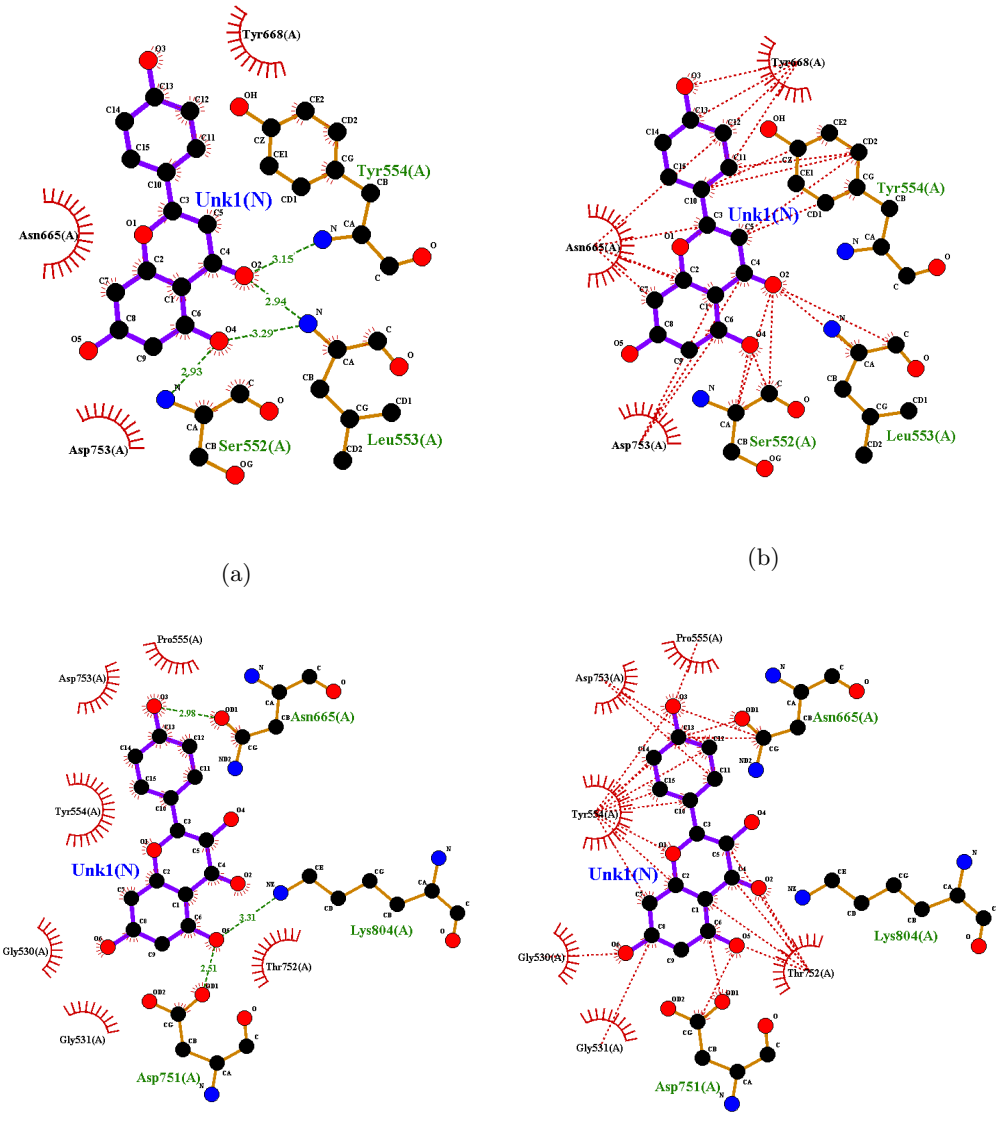

Fig. S1: Interactions obtained after using Ligplot for the MPVX-ligand complexes. Only hydrogen bonds are being shown.

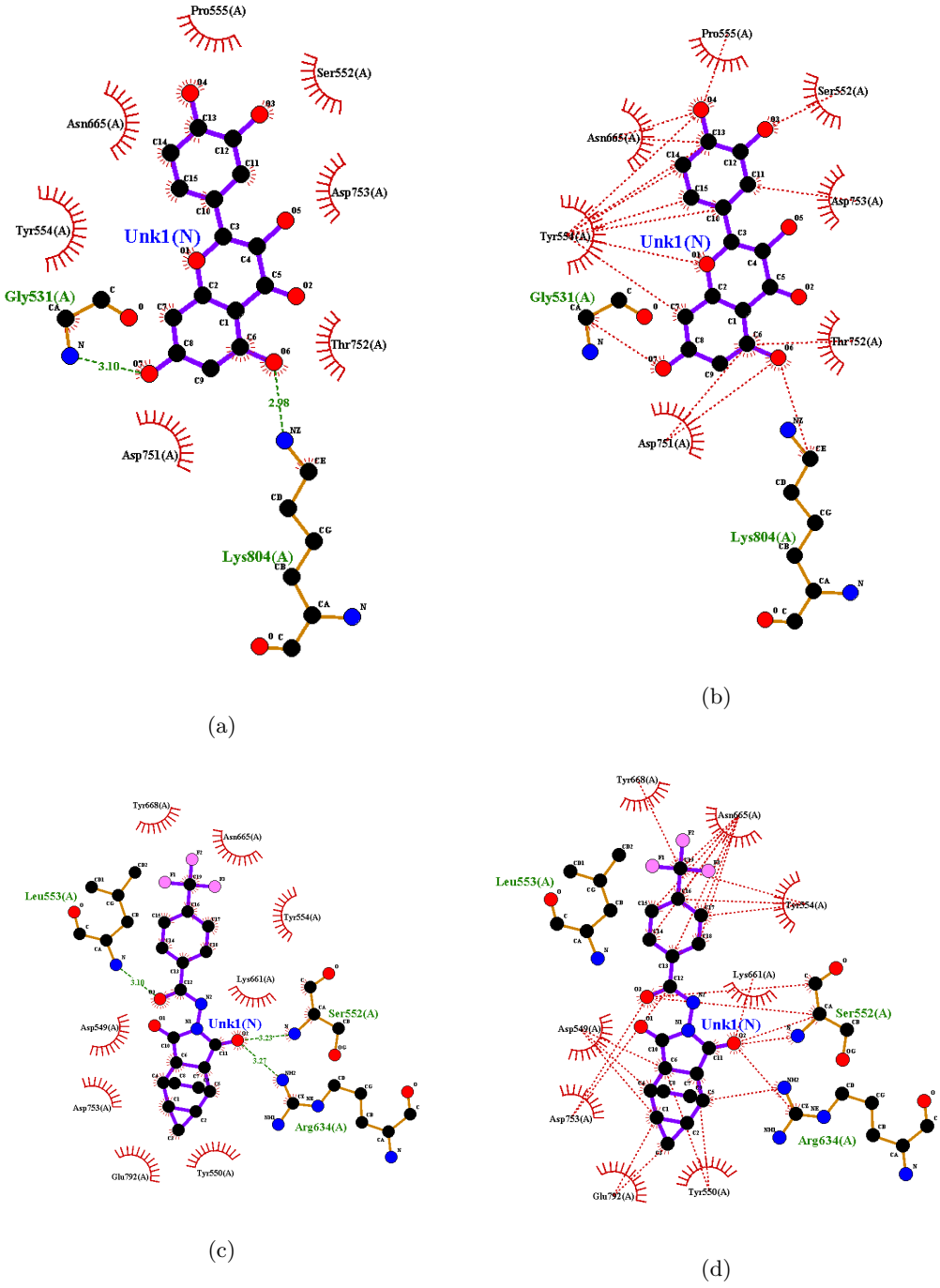

Fig. S2: Interactions obtained after using Ligplot for the MPVX-ligand complexes. Only hydrophobic interactions are being shown.

Structure of the compounds selected for MD simulations

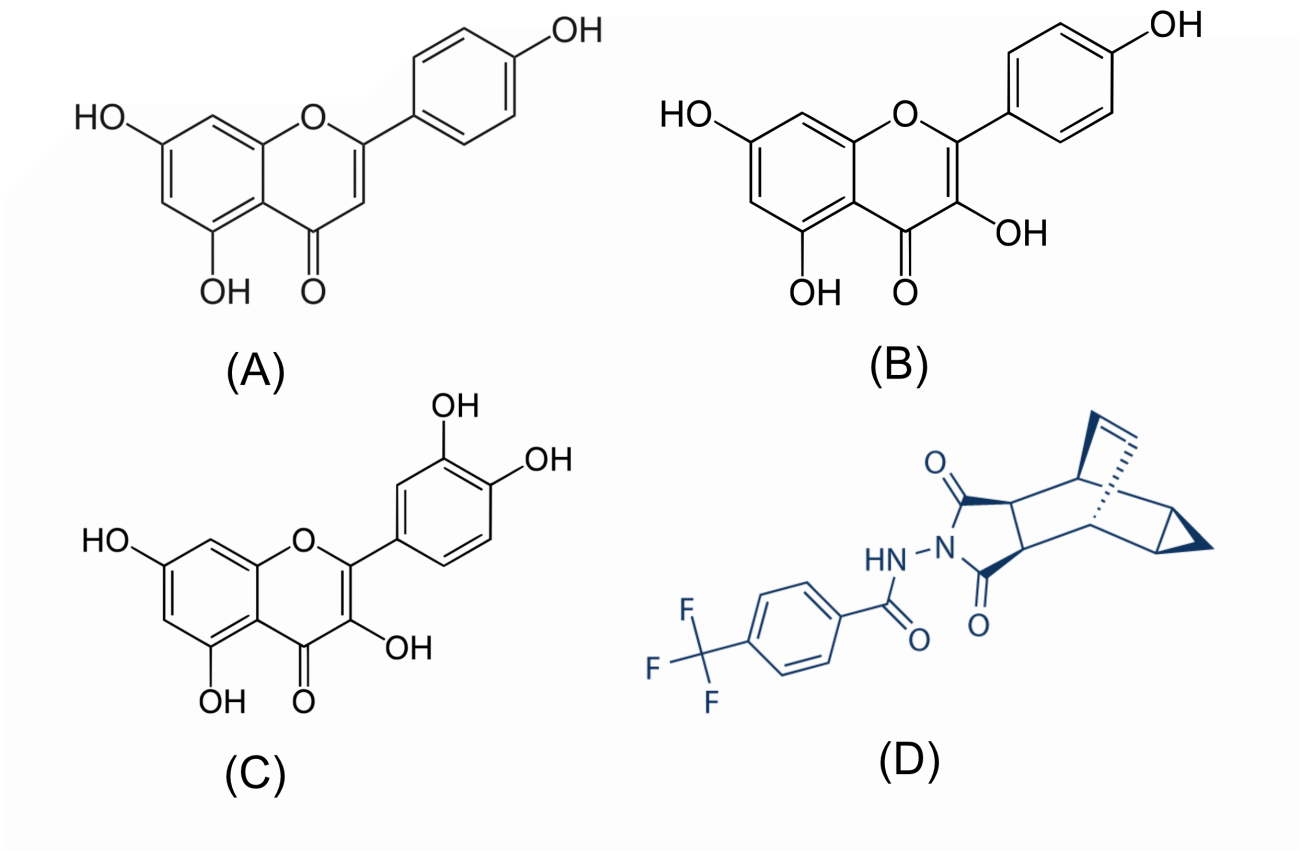

Fig. S3: Structure of the screened compounds for Docking and MD simulations (A) Apigenin, (B) Kaempferol, (C) Quercetin, and (D) Tecovirimat

Binding energy obtained for the drug-like molecules

Table S2: Binding energy for screened Broccoli's metabolites

S. No.	Molecule Number in library	Metabolites	Binding Energy (kcal/mol)
1	70	Tecovirimat	-7.8
2	59	Quercetin	-7.9
3	57	Kaempferol	-7.8
4	56	Apigenin	-7.8
5	55	5-O-Sinapoylquinic acid	-6.8
6	58	Luteolin	-6.9
7	19	Gluconapin	-6.1
8	51	Sinapoyl malate	-5.7
9	18	Sinigrin	-5.8
10	22	Glucoiberverin	-5.6
11	28	4-Methylpentyl-GLS	-6.0
12	29	Glucoerucin	-5.7
13	21	Glucocochlearin	-6.2
14	23	Glucosativin	-5.5
15	45	Esculetin	-5.9
16	16	Indole-3-acetic acid	-5.6
17	48	Sinapic acid	-5.1
18	46	Caffeic acid	-5.3
19	15	Indole-3-carboxylic acid	-5.5
20	39	p-Hydroxybenzoic acid	-5.5
21	47	Ferulic acid	-5.2
22	41	Gentisic acid	-5.3
23	42	Gallic acid	-4.9
24	44	p-Coumaric acid	-5.2
25	38	Salicylic acid	-5.3
26	17	1-Methoxyindole-3-carbaldehyde	-5.0
27	14	Indole-3-carbinol	-5.1
28	40	Protocatechuic acid	-5.1
29	43	Vanillic acid	-5.1
30	37	Benzoic acid	-5.2
31	64	trigonelline	-4.8
32	13	Sulforaphane	-3.6
33	9	3-Methylbutyl isothiocyanate	-3.8
34	12	Sulforaphene	-3.8
35	6	Isobutyl isothiocyanate	-3.3
36	10	Isoamyl methyl sulfoxide	-3.7
37	3	2-Methyl-2-nitropropane	-3.5
38	4	4-(Methylthio)-butanenitrile	-2.9
39	7	Iberin	-3.6
40	11	Erucin	-3.3
41	5	Butyl isothiocyanate	-3.4
42	1	Butyronitrile	-3.2
43	2	Allyl isothiocynate	-3.0
44	8	4-Isothiocyanato-1-butene	-3.3
45	63	Choline	-3.1