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Supplementary Material

In Silico Study of Pubchem Compounds for *Solanum torvum* as Antiviral Agent against SARS-CoV-2

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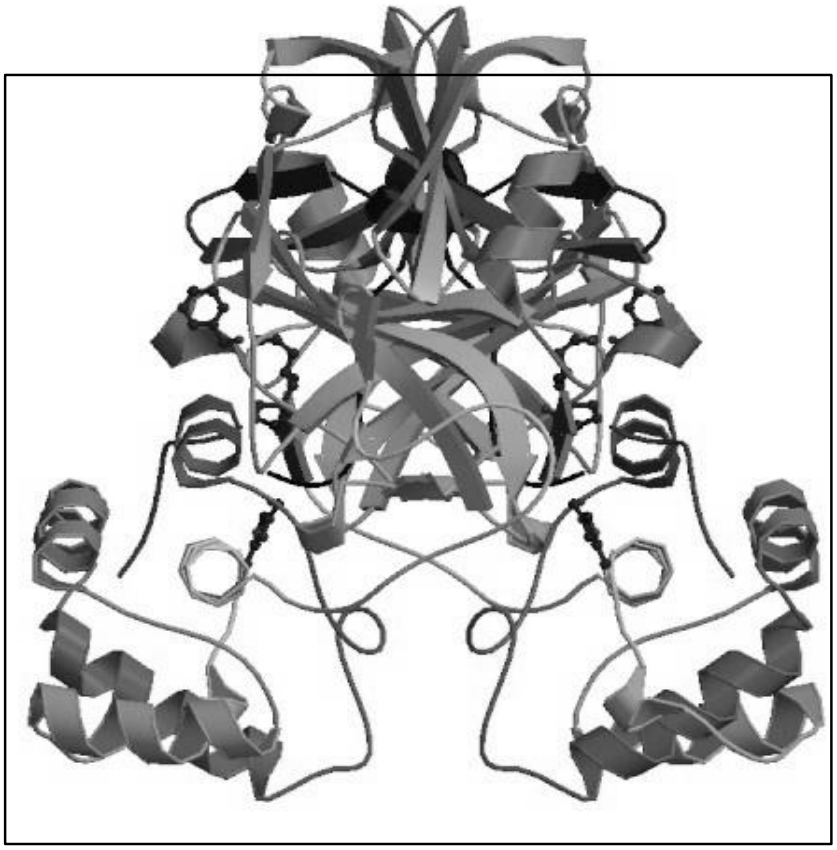

Fig. (S1). Crystal structure of COVID-19 main protease (PDB ID: 6lu7).

Below is the standard PDB format of the top 6 pocket sites from the top 6 ranked clusters:

```
ATOM      1  C3  CON     1     -10.167  16.624  65.875   2  -0.03
ATOM      2  C3  FPK     1      -9.724  14.806  63.577   1   1.96
ATOM      3  C3  GHE     1      -8.778  16.990  66.987   1   2.75
ATOM      4  C3  LCS     1     -10.207  16.096  66.048   1   4.79
ATOM      5  C3  PAS     1      -8.574  18.748  67.234   2   1.18
ATOM      6  C3  SFN     1     -10.049  25.828  65.482   1   5.28
ATOM      7  C3  CON     2     -36.386  12.114  56.464   1   1.64
ATOM      8  C3  FPK     2     -35.460  16.434  55.676   2   1.48
ATOM      9  C3  GHE     2     -37.886   6.662  59.428   2   1.15
ATOM     10  C3  LCS     2     -37.724   6.929  57.237   3   1.05
ATOM     11  C3  SFN     2     -37.297  13.132  54.912   3   3.01
ATOM     12  C3  LCS     3     -25.674   2.646  45.165   2   1.23
ATOM     13  C3  PAS     3     -25.506   2.857  45.207   3   0.29
ATOM     14  C3  SFN     3     -25.399   3.321  47.873   2   3.07
ATOM     15  C3  FPK     4     -18.151  33.468  53.189   3   1.42
ATOM     16  C3  GHE     4     -15.861  33.282  55.351   3   1.15
ATOM     17  C3  PAS     5     -35.003 -14.607  43.817   1   2.15
ATOM     18  C3  CON     6     -26.277  -3.481  54.674   3  -0.80
TER
ATOM      1  C3  MPT     1      -9.583  18.182  65.867   6  15.93
ATOM      2  C3  MPT     2     -36.951  11.054  56.743   5   8.33
ATOM      3  C3  MPT     3     -25.526   2.941  46.082   3   4.59
ATOM      4  C3  MPT     4     -17.006  33.375  54.270   2   2.57
ATOM      5  C3  MPT     5     -35.003 -14.607  43.817   1   2.15
ATOM      6  C3  MPT     6     -26.277  -3.481  54.674   1  -0.80
```

The potential 6 ligand binding sites in your protein:

```
HEADER binding site ID: 1
RESI    PHE_A^140^   HIS_A^163^   MET_A^165^   GLU_A^166^   HIS_A^172^
RESI    VAL_C^3^     LEU_A^141^   SER_A^144^   CYS_A^145^   LEU_C^4^
RESI    ASN_A^142^   GLY_A^143^   HIS_A^41^    LEU_A^27^    MET_A^49^
RESI    THR_A^26^    THR_A^25^    GLN_A^189^   CYS_A^44^    THR_A^45^
RESI    THR_A^24^    SER_A^46^    THR_A^21^    LEU_A^167^   TYR_A^118^
HEADER binding site ID: 2
RESI    ILE_A^106^   GLN_A^110^   THR_A^111^   ASN_A^151^   GLN_A^107^
RESI    ARG_A^105^   ILE_A^152^   ASP_A^153^   PHE_A^294^   SER_A^158^
RESI    PHE_A^8^     GLN_A^127^   THR_A^292^   ASP_A^295^   ARG_A^298^
RESI    VAL_A^104^   GLY_A^109^   VAL_A^202^   ASN_A^203^   PRO_A^293^
RESI    ILE_A^200^   PRO_A^108^   HIS_A^246^   ILE_A^249^   THR_A^243^
RESI    ASP_A^245^   GLU_A^240^   PRO_A^241^   THR_A^201^   LYS_A^102^
HEADER binding site ID: 3
RESI    PHE_A^3^     TRP_A^207^   LEU_A^282^   PHE_A^291^   GLU_A^288^
RESI    ARG_A^4^     LYS_A^5^     GLY_A^283^   SER_A^284^
HEADER binding site ID: 4
RESI    GLY_A^11^    GLU_A^14^    LYS_A^97^    GLY_A^15^    LYS_A^12^
RESI    THR_A^98^    PRO_A^99^    TRP_A^31^    ALA_A^70^    VAL_A^73^
RESI    LEU_A^75^    PRO_A^96^    THR_A^93^    MET_A^17^    GLY_A^71^
RESI    PRO_A^122^   GLY_A^120^   CYS_A^16^    VAL_A^18^    ASN_A^95^
RESI    ALA_A^94^    GLN_A^69^    SER_A^121^   GLN_A^19^    ASN_A^72^
RESI    ASN_A^119^
HEADER binding site ID: 5
RESI    GLU_A^270^
HEADER binding site ID: 6
RESI    LYS_A^5^     LEU_A^286^   LEU_A^287^   GLU_A^288^   ASP_A^289^
RESI    GLU_A^290^   ARG_A^131^   THR_A^199^   TYR_A^239^   LYS_A^137^
RESI    LEU_A^272^   TYR_A^237^
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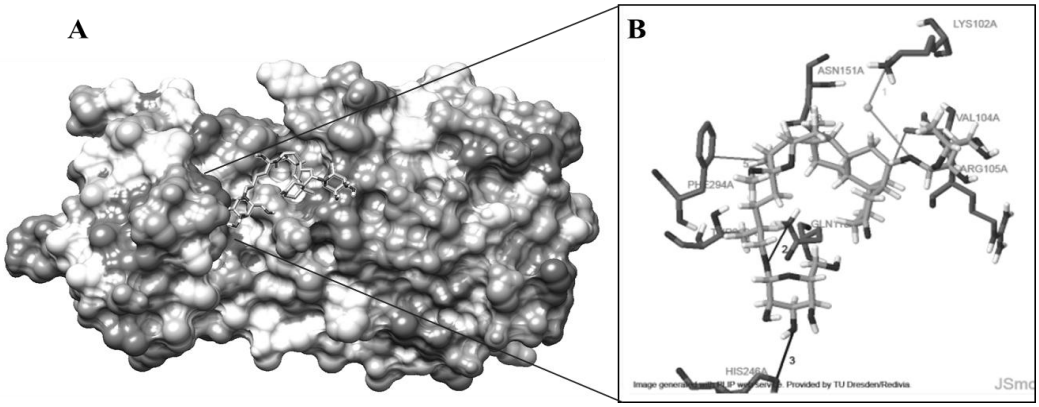

Fig. (S3). (A) Docking result of with Torvoside A ($C_{45}H_{76}O_{18}$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of the SARS-CoV2 Main Protease (6lu7) with Torvoside A ($C_{45}H_{76}O_{18}$) Ligand.

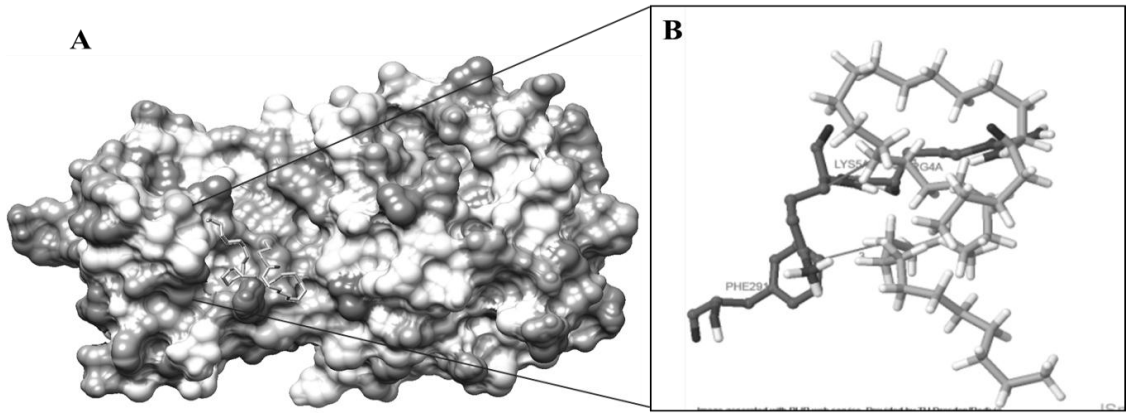

Fig. (S4). (A) Docking result of with 2,3,4-trimethyltriacontane ($C_{33}H_{68}$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of the SARS-CoV2 Main Protease (6lu7) with 2,3,4-trimethyltriacontane ($C_{33}H_{68}$) Ligand.

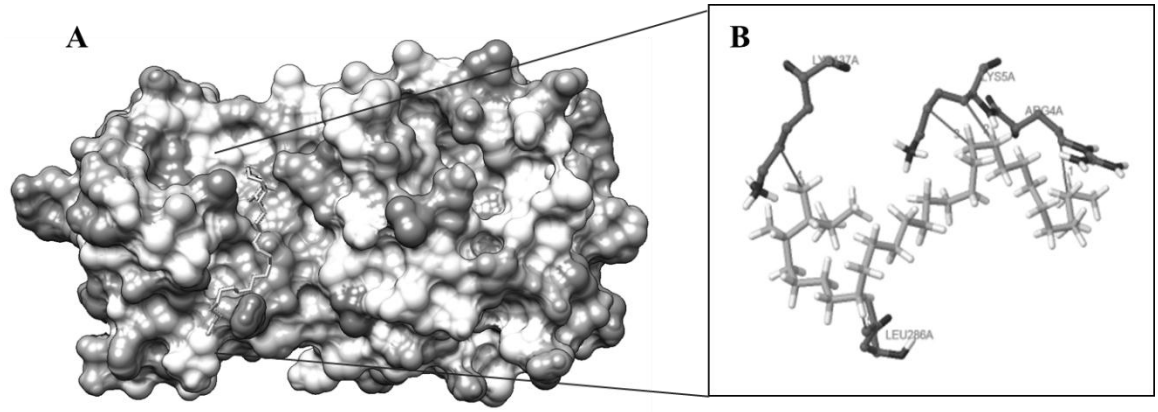

Fig. (S5). (A) Docking result of with Torvanol A Q27134802 rel-potassium (3R,4S)-3-{5-[(E)-2-carboxyethenyl]-2-hydroxy-3-methoxyphenyl}-6-methoxy-3,4-dihydro-2H-chromen-4-yl sulfate ($C_{20}H_{19}KO_{10}S$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of the SARS-CoV2 Main Protease (6lu7) Torvanol A Q27134802 rel-potassium (3R,4S)-3-{5-[(E)-2-carboxyethenyl]-2-hydroxy-3-methoxyphenyl}-6-methoxy-3,4-dihydro-2H-chromen-4-yl sulfate ($C_{20}H_{19}KO_{10}S$) Ligand.

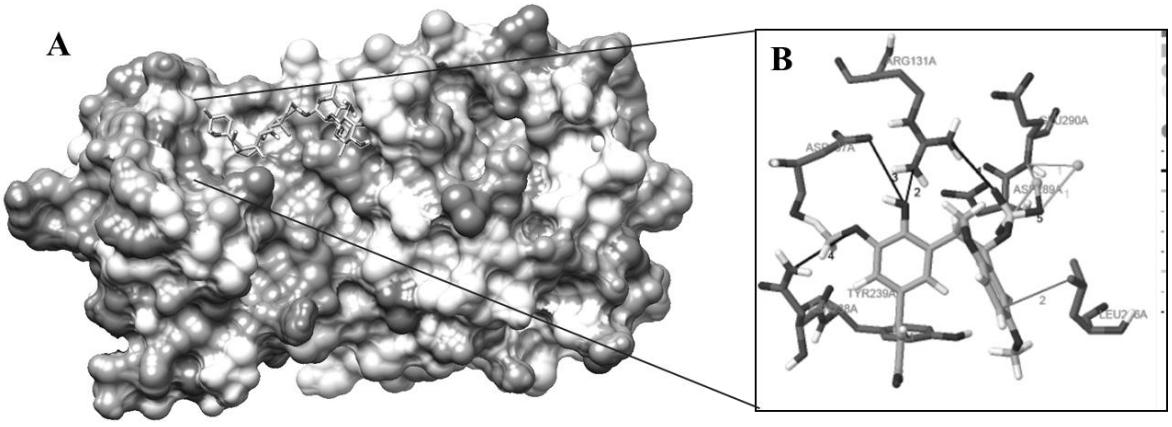

Fig. (S6). (A) Docking result of 5-hexatriacontanone ($C_{36}H_{72}O$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of SARS-CoV2 Main Protease (6lu7) with 5-hexatriacontanone ($C_{36}H_{72}O$) Ligand.

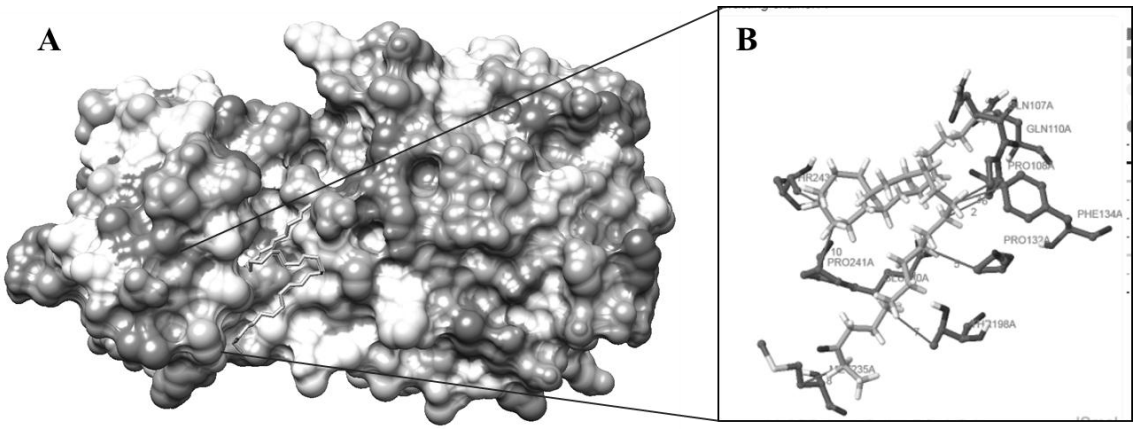

Fig. (S7). (A) Docking result of Torvanol A ($C_{20}H_{20}O_{10}S$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of SARS-CoV2 Main Protease (6lu7) with Torvanol A ($C_{20}H_{20}O_{10}S$) Ligand.

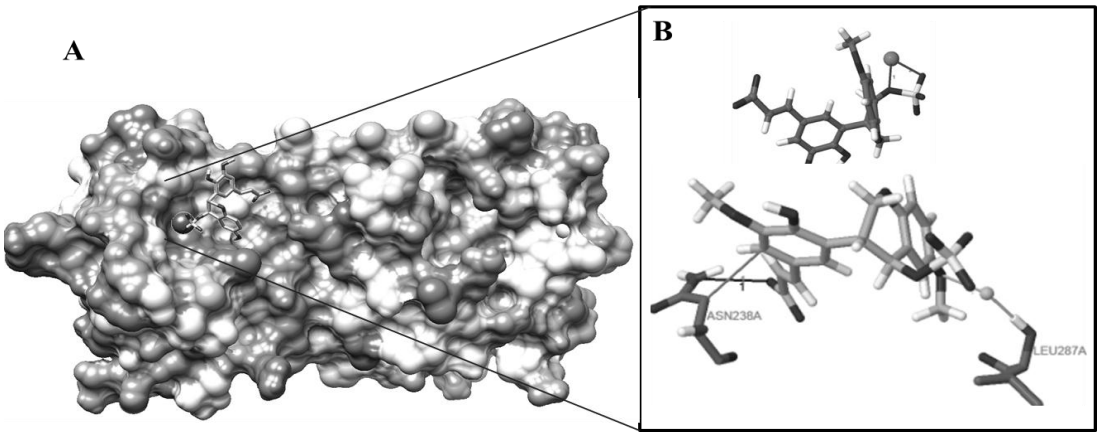

Fig. (S8). (A) Docking result of Jurubine ($C_{33}H_{57}NO_8$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of SARS-CoV2 Main Protease (6lu7) with Jurubine ($C_{33}H_{57}NO_8$) Ligand.

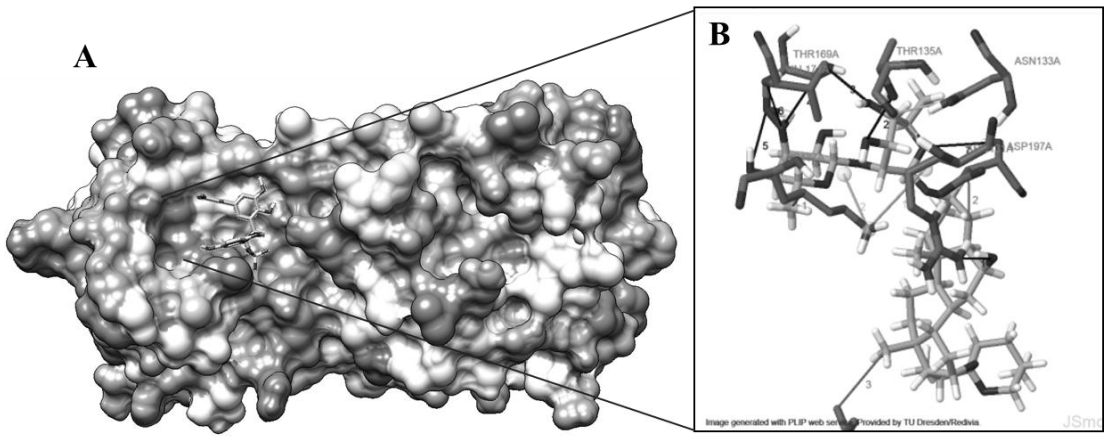

Fig. (S9). (A) Docking result of Tritriacontan-3-one ($C_{33}H_{66}O$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of SARS-CoV2 Main Protease (6lu7) with Tritriacontan-3-one ($C_{33}H_{66}O$) Ligand.

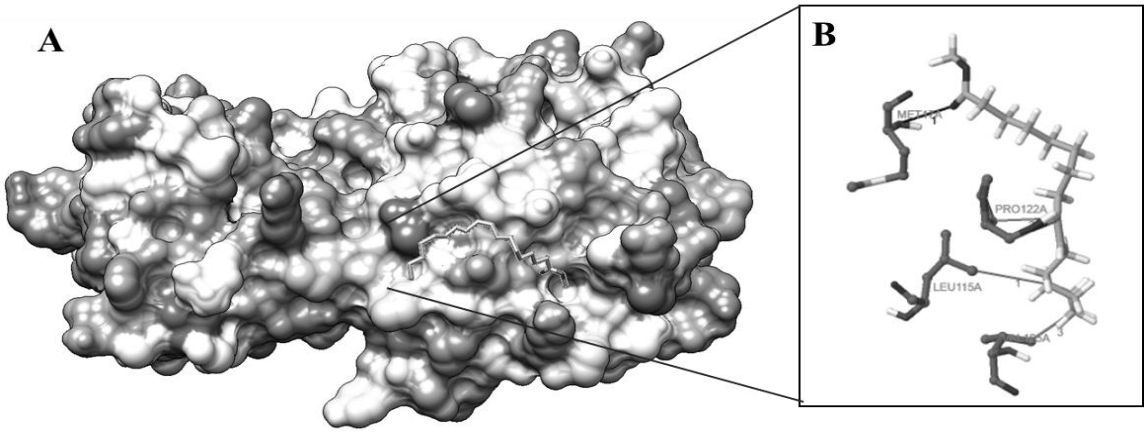

Fig. (S10). (A) Docking result of Torvoside F ($C_{45}H_{74}O_{18}$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of SARS-CoV2 Main Protease (6lu7) with Torvoside F ($C_{45}H_{74}O_{18}$) Ligand.

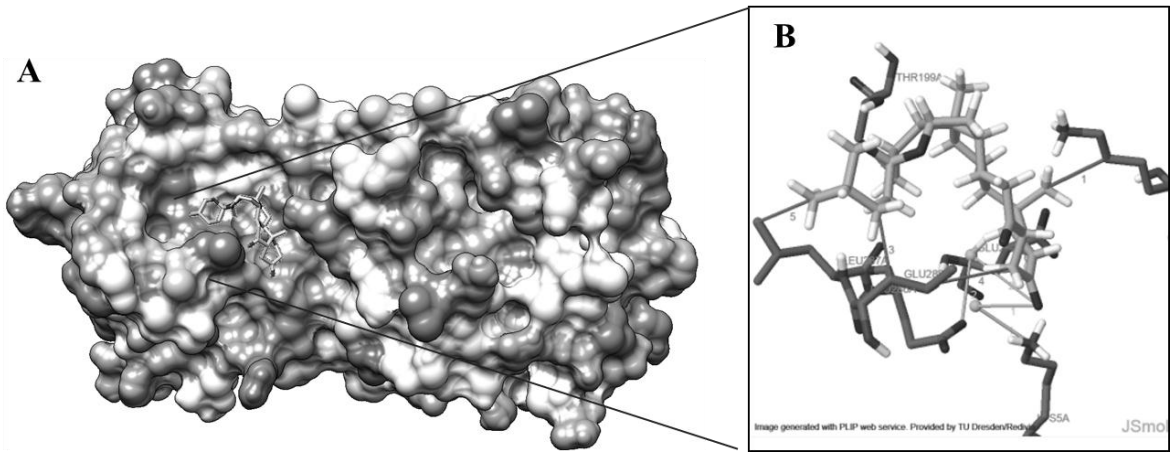

Fig. (S11). (A) Docking result of Chlorogenone, Spirostane-3,6-dione ($C_{27}H_{40}O_4$) Ligand with SARS-CoV2 Main Protease (6lu7). **(B)** Residues interaction of SARS-CoV2 Main Protease (6lu7) with Chlorogenone, Spirostane-3,6-dione ($C_{27}H_{40}O_4$) Ligand.

Fig. (S12). *Solanum torvum* Sw. (Family: Solanaceae), commonly known as Turkey Berry.

Table S1. List of *Solanum torvum* phytochemical compounds downloaded from NCBI Pubchem database.

S.No.	Compound Name	Pub Chem ID:	Molecular Formula	Molecular Weigh
1.	Torvoside H (25S)-26-O-(beta-D-glucopyranosyl)-6alpha,26-dihydroxy-5alpha-spirostan-3-one 6-O-[alpha-L-rhamnopyranosyl-(1->3)-beta-D-quinovopyranoside	70697829	$C_{45}H_{74}O_{18}$	903.1 g/mol
2.	Torvonin A	131751074	$C_{39}H_{64}O_{12}$	724.9 g/mol
3.	Torvoside E	131753159	$C_{40}H_{66}O_{14}$	770.9 g/mol
4.	Torvoside A	131753157	$C_{45}H_{76}O_{18}$	905.1 g/mol
5.	2,3,4-trimethyltriacontane	129837279	$C_{33}H_{68}$	464.9 g/mol
6.	Torvanol A Q27134802 rel-potassium (3R,4S)-3-{5-[(E)-2-carboxyethenyl]-2-hydroxy-3-methoxyphenyl}-6-methoxy-3,4-dihydro-2H-chromen-4-yl sulfate	70697823	$C_{20}H_{19}KO_{10}S$	490.5 g/mol
7.	5-hexatriacontanone	129847814	$C_{36}H_{72}O$	521 g/mol
8.	Torvanol A	5321987	$C_{20}H_{20}O_{10}S$	452.4 g/mol
9.	Jurubine	12304761	$C_{33}H_{57}NO_8$	595.8 g/mol
10.	Tritriacontan-3-one	545660	$C_{33}H_{66}O$	478.9 g/mol
11.	Torvoside F	131753160	$C_{45}H_{74}O_{18}$	903.1 g/mol
12.	Chlorogenone, Spirostane-3,6-dione	13889197	$C_{27}H_{40}O_4$	428.6 g/mol

Table S2. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvoside H (25S)-26-O-(beta-D-glucopyranosyl)-6alpha,26-dihydroxy-5alpha-spirostan-3-one 6-O-[alpha-L-rhamnopyranosyl -(1->3)-beta-D-quinovopyranoside ($C_{45}H_{74}O_{18}$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	5A	LYS	3.77	3072	50
2	126A	TYR	3.34	3072	1194
3	126A	TYR	3.33	3058	1197
4	127A	GLN	3.34	3072	1208
5	137A	LYS	3.82	3047	1307
6	286A	LEU	3.69	3070	2686

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Sidechain**	**Donor Atom**	**Acceptor Atom**
1	127A	GLN	3.29	4.03	132.62			1204 [Nam]	3026 [O3]
2	131A	ARG	2.63	3.47	141.35			1248 [Ng+]	3036 [O3]
3	137A	LYS	2.60	3.54	151.08			1311 [N3+]	3022 [O3]
4	199A	THR	3.00	3.92	157.10			3036 [O3]	1865 [O3]
5	199A	THR	2.67	3.02	102.15			1865 [O3]	3039 [O3]
6	199A	THR	2.41	3.02	119.65			3039 [O3]	1865 [O3]

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	5A	LYS	3.67	3.04	133.38	95.57		53 [N3+]	3024 [O3]	2941

(Table S2) contd.....

Salt Bridges						
Index	**Residue**	**AA**	**Distance**	**Protein positive?**	**Ligand Group**	**Ligand Atoms**
1	5A	LYS	3.29		Carboxylate	3028, 3031
2	5A	LYS	4.55		Carboxylate	3023, 3026
3	131A	ARG	4.63		Carboxylate	3029, 3032
4	137A	LYS	4.94		Carboxylate	3029, 3032

Table S3. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvonin A ($C_{39}H_{64}O_{12}$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	137A	LYS	2.71	3083	1307
2	197A	ASP	3.06	3054	1846
3	199A	THR	3.98	3056	1866

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Side chain**	**Donor Atom**	**Acceptor Atom**
1	5A	LYS	3.28	4.04	131.69			53 [N3+]	3033 [O3]
2	236A	LYS	3.07	3.77	125.46			2235 [N3+]	3034 [O3]
3	287A	LEU	2.57	3.17	118.61			2689 [Nam]	3025 [O3]
4	288A	GLU	3.49	3.84	103.27			3027 [O3]	2706 [O2]

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	288A	GLU	2.59	3.14	103.81	108.33		2705 [O3]	3027 [O3]	2991
2	289A	ASP	3.58	3.84	123.07	96.83		2708 [Nam]	3027 [O3]	2941

Salt Bridges						
Index	**Residue**	**AA**	**Distance**	**Protein positive?**	**Ligand Group**	**Ligand Atoms**
1	5A	LYS	4.74		Carboxylate	3028, 3031
2	137A	LYS	5.17		Carboxylate	3023, 3026

Table S4. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvoside E ($C_{40}H_{66}O_{14}$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	5A	LYS	2.23	3063	51
2	5A	LYS	3.25	3071	49
3	126A	TYR	2.95	3043	1194
4	126A	TYR	3.20	3047	1197
5	126A	TYR	3.75	3040	1195
6	141A	LEU	3.54	3072	1346
7	141A	LEU	2.91	3073	1348
8	288A	GLU	3.92	3083	2703
9	291A	PHE	3.93	3083	2736

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Sidechain**	**Donor Atom**	**Acceptor Atom**
1	5A	LYS	3.10	3.78	125.83			45 [Nam]	3032 [O3]
2	5A	LYS	3.31	3.77	107.83			53 [N3+]	3024 [O3]
3	123A	SER	3.51	3.97	111.28			3033 [O3]	1172 [O2]

(Table S4) contd.....

4	123A	SER	3.11	3.56	111.06			1174 [O3]	3035 [O3]
5	139A	SER	3.19	3.86	128.62			1326 [O3]	3027 [O3]
6	207A	TRP	2.66	3.57	154.39			1937 [Nar]	3038 [O3]
7	282A	LEU	2.16	2.77	119.02			3038 [O3]	2655 [O2]

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	282A	LEU	3.52	2.71	115.89	99.89		3036 [O3]	2655 [O2]	2986

Salt Bridges						
Index	**Residue**	**AA**	**Distance**	**Protein positive?**	**Ligand Group**	**Ligand Atoms**
1	5A	LYS	4.19		Carboxylate	3029, 3032

Table S5. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvoside A ($C_{45}H_{76}O_{18}$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	104A	VAL	3.72	3069	1000
2	104A	VAL	3.75	3053	1001
3	151A	ASN	2.89	3051	1423
4	292A	THR	3.31	3067	2745
5	294A	PHE	3.37	3055	2762

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Sidechain**	**Donor Atom**	**Acceptor Atom**
1	105A	ARG	2.67	3.65	165.97			1003 [Nam]	3027 [O3]
2	110A	GLN	3.18	3.63	109.02			1061 [N3]	3028 [O3]
3	246A	HIS	3.05	3.49	108.69			3033 [O3]	2344 [Nar]

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	102A	LYS	4.09	3.10	115.74	85.47		978 [N3+]	3023 [O3]	2954

Table S6. Interaction of the SARS-CoV2 Main Protease (6lu7) with 2,3,4-trimethyltriacontane ($C_{33}H_{68}$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	4A	ARG	3.63	3027	32
2	5A	LYS	2.71	3029	49
3	291A	PHE	3.33	3036	2737

Table S7. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvanol A Q27134802 rel-potassium (3R,4S)-3-{5-[(E)-2-carboxyethenyl]-2-hydroxy-3-methoxyphenyl}-6-methoxy-3,4-dihydro-2H-chromen-4-yl sulfate ($C_{20}H_{19}KO_{10}S$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	4A	ARG	3.66	3052	33
2	5A	LYS	3.43	3044	49
3	5A	LYS	3.48	3043	51
4	137A	LYS	3.61	3028	1309
5	286A	LEU	3.78	3033	2687

Table S8. Interaction of the SARS-CoV2 Main Protease (6lu7) with 5-hexatriacontanone ($C_{36}H_{72}O$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	137A	LYS	3.07	3072	1308
2	197A	ASP	2.86	3051	1846
3	286A	LEU	3.76	3049	2687

Hydrogen Bonds									
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Sidechain	Donor Atom	Acceptor Atom
1	131A	ARG	3.30	3.98	127.37			1248 [Ng+]	3024 [O3]
2	135A	THR	3.22	4.00	140.40			1290 [O3]	3028 [O3]
3	169A	THR	2.11	2.95	146.03			1600 [O3]	3029 [O3]
4	169A	THR	2.95	3.69	133.60			3032 [O3]	1600 [O3]
5	169A	THR	2.80	3.51	129.07			3033 [O3]	1598 [O2]
6	171A	VAL	3.09	3.44	102.23			1609 [Nam]	3032 [O3]
7	197A	ASP	3.01	3.88	146.61			1842 [Nam]	3026 [O3]

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	133A	ASN	3.94	2.77	157.46	101.40		1269 [Nam]	3026 [O3]	2976

Salt Bridges						
Index	**Residue**	**AA**	**Distance**	**Protein positive?**	**Ligand Group**	**Ligand Atoms**
1	137A	LYS	5.37		Carboxylate	3025, 3026
2	137A	LYS	4.35		Carboxylate	3027, 3030

Table S9. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvanol A ($C_{20}H_{20}O_{10}S$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	107A	GLN	2.37	3053	1033
2	108A	PRO	3.40	3034	1045
3	108A	PRO	3.00	3032	1046
4	110A	GLN	2.22	3053	1058
5	132A	PRO	3.78	3038	1259
6	134A	PHE	4.00	3032	1283
7	198A	THR	3.79	3046	1857
8	235A	MET	3.54	3054	2222
9	240A	GLU	3.52	3040	2284
10	241A	PRO	3.15	3033	2294
11	243A	THR	3.29	3031	2311

Table S10. Interaction of the SARS-CoV2 Main Protease (6lu7) with Jurubine ($C_{33}H_{57}NO_8$) Ligand.

Metal Complexes						
Index	**Residue**	**AA**	**Metal**	**Target**	**Distance**	**Location**
Complex 1: K, linear (2)						
1	2Z	LIG	3022	3025	2.68	Protein.mainchain
2	2Z	LIG	3022	3030	2.48	Protein.mainchain

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**

(Table S10) contd.....

1	238A	ASN	3.18	3048	2258

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Side Chain**	**Donor Atom**	**Acceptor Atom**
1	238A	ASN	3.36	3.93	117.89			2261 [Nam]	3033 [O.co2]

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	287A	LEU	3.66	2.79	173.41	91.33		2689 [Nam]	3027 [O3]	2980

Table S11. Interaction of the SARS-CoV2 Main Protease (6lu7) with Tritriacontan-3-one ($C_{33}H_{66}O$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	239A	TYR	3.89	3048	2273
2	286A	LEU	3.60	3046	2687

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Side chain**	**Donor Atom**	**Acceptor Atom**
1	131A	ARG	3.19	3.81	121.44			1247 [Ng+]	3030 [O2]
2	131A	ARG	3.00	3.34	100.90			1248 [Ng+]	3025 [O3]
3	197A	ASP	3.10	3.71	121.93			3025 [O3]	1849 [O2]
4	238A	ASN	3.12	3.74	121.08			2261 [Nam]	3027 [O3]
5	289A	ASP	2.45	3.28	140.88			2708 [Nam]	3029 [O3]

Water Bridges										
Index	Residue	AA	Dist. A-W	Dist. D-W	Donor Angle	Water Angle	Protein donor?	Donor Atom	Acceptor Atom	Water Atom
1	290A	GLU	3.50	3.49	134.66	93.63		2717 [Nam]	3029 [O3]	2941
2	290A	GLU	3.10	3.85	112.02	87.50		2717 [Nam]	3028 [O2]	2991

Table S12. Interaction of the SARS-CoV2 Main Protease (6lu7) with Torvoside F ($C_{45}H_{74}O_{18}$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	115A	LEU	3.93	3025	1108
2	122A	PRO	3.47	3038	1166
3	125A	VAL	2.88	3028	1187

Hydrogen Bonds									
Index	**Residue**	**AA**	**Distance H-A**	**Distance D-A**	**Donor Angle**	**Protein donor?**	**Sidechain**	**Donor Atom**	**Acceptor Atom**
1	17A	MET	2.39	3.05	122.86			148 [Nam]	3023 [O2]

Table S13. Interaction of the SARS-CoV2 Main Protease (6lu7) with Chlorogenone, Spirostane-3,6-dione ($C_{27}H_{40}O_4$) Ligand.

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
1	137A	LYS	3.46	3045	1309
2	199A	THR	3.68	3043	1866
3	286A	LEU	2.83	3048	2684
4	286A	LEU	3.82	3046	2686

(Table S13) contd.....

Hydrophobic Interactions					
Index	**Residue**	**AA**	**Distance**	**Ligand Atom**	**Protein Atom**
5	287A	LEU	3.81	3052	2695
6	290A	GLU	3.61	3047	2722

Water Bridges										
Index	**Residue**	**AA**	**Dist. A-W**	**Dist. D-W**	**Donor Angle**	**Water Angle**	**Protein donor?**	**Donor Atom**	**Acceptor Atom**	**Water Atom**
1	5A	LYS	3.83	3.04	133.38	126.57		53 [N3+]	3025 [O2]	2941
2	288A	GLU	3.90	3.14	103.81	113.88		2705 [O3]	3025 [O2]	2991