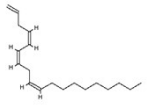
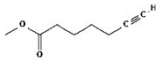
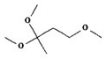
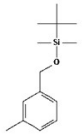
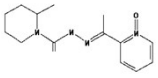
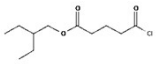
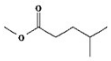
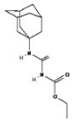
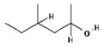
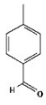
Research Article

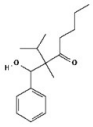
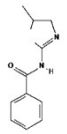
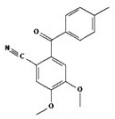
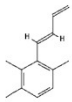
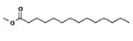
GC–MS analysis of phytoconstituents from Ruellia prostrata and Senna tora and identification of potential anti-viral activity against SARS-CoV-2

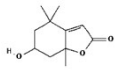
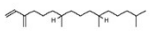
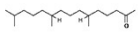
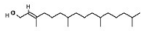
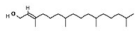
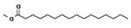
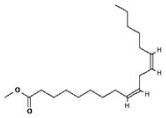
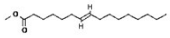
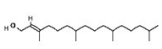
Supplementary Table

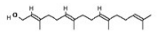
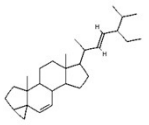
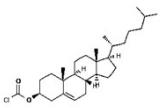
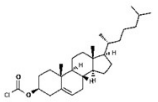
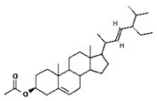
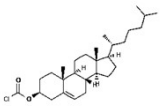
Table S1. Phytochemical compounds structure from GC-MS analysis of *R. prostrata* aerial parts.

Compound name	CID	Compound Structure
Z,Z,Z-1,4,6,9-Nonadecatetraene	5362676	
6-Heptynoic acid, methyl ester	557075	
Cyclopentanol, 1-(1-methylene-2-propenyl)-	549059	
1,5,9,9-Tetramethyl-2-oxatricyclo[6.4.0.0(4,8)]dodecane	586811	
1-Oxaspiro[2.2]pentane, 5-isopropylidene-2,2,4,4-tetramethyl-	549662	
1,3,3-Trimethoxybutane	81084	
3-Methylbenzyl alcohol, TBDMS derivative	22967275	

Cycloheptanone, 4-methoxy-	551377	
o-Xylene	7237	
2-Methylpiperidine-1-thiocarboxylic acid 2-[1-[2-pyridyl 1-oxide]	249948356	
Glutaric acid, monochloride, 2-ethylbutyl ester	91714556	
Styrene	7501	
Pentanoic acid, 4-methyl-, methyl ester	17008	
Ethyl (1-adamantylamino)carbothioylcarbamate	2728763	
Decane	15600	
4-Methyl-2-hexanol	123156	
Benzaldehyde, 4-methyl-	7725	

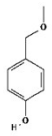
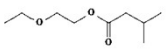
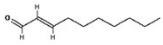
Cyclopentanone, 2-methyl-3-(1-methylethyl)-	41124	
3-(Hydroxy-phenyl-methyl)-2,3-dimethyl-octan-4-one	559104	
5-Methyl-2-benzoylimino-1,3-thiazolidine	569357	
4,5-Dimethoxy-2-[(4-methylphenyl)carbonyl]benzonitrile	25247358	
Dodecane	8182	
(E)-1-(2,3,6-trimethylphenyl)buta-1,3-diene (TPB, 1)	20585933	
Tetradecane	12389	
Phenol, 3,5-bis(1,1-dimethylethyl)-	70825	
2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	6432173	
Methyl tetradecanoate	31284	

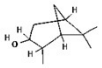
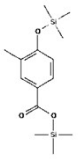
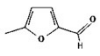
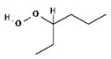
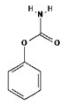
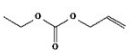
6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one	14334	
Neophytadiene	10446	
2-Pentadecanone, 6,10,14-trimethyl-	10408	
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	5366244	
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	5366244	
Hexadecanoic acid, methyl ester	8181	
9,12-Octadecadienoic acid, methyl ester	5284421	
7-Hexadecenoic acid, methyl ester, (Z)-	5364431	
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	5366244	
Methyl stearate	8201	

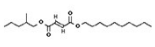
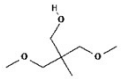
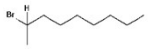
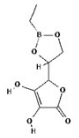
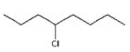
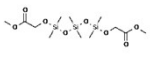
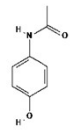
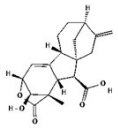
trans-Geranylgeraniol	5281365	
Stigmastan-6,22-dien, 3,5-dedihydro-	5364573	
Cholest-5-en-3-ol (3.beta.)-, carbonochloridate	111262	
Cholest-5-en-3-ol (3.beta.)-, carbonochloridate	111262	
Stigmasta-5, 22-dien-3-ol, acetate, (3.beta.)-	6432445	
Cholest-5-en-3-ol (3.beta.)-, carbonochloridate	111262	

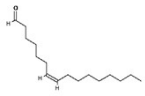
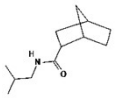
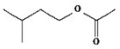
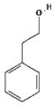
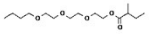
Supplementary Table 2. Phytochemical compounds structure from GC-MS analysis of *Senna tora (L.)* Roxb. leaves.

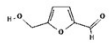
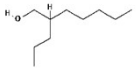
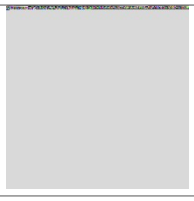
Compound name	**CID**	**Compound Structure**
2-Piperidinecarboxylic acid	849	

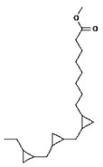
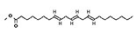
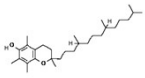
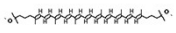
1,1-Cyclohexanedimethanol	250594	
Phenol, 4-(methoxymethyl)-	79310	
3-Furaldehyde	10351	
4-Cyclopentene-1,3-dione	70258	
2-Ethoxyethyl 3-methylbutanoate	91698641	
3-Methylbenzyl alcohol, TBDMS derivative	22967275	
2-Decenal, (E)-	5283345	
o-Xylene	7237	
Cyclopent-4-ene-1,3-dione	70258	

1,3,5,7-Cyclooctatetraene	637866	
2(5H)-Furanone	10341	
Bicyclo[3.1.1]heptan-3-ol, 2,6,6-trimethyl-, (1.alpha.,2.beta.,3.alpha.,5.alpha.)-	99038	
Trimethylsilyl 3-methyl-4-[(trimethylsilyl)oxy]benzoate	91740684	
4,2,7-Ethanylylidenecyclopenta[b]pyran, octahydro-7a-methyl-	565150	
2-Furancarboxaldehyde, 5-methyl-	12097	
Hydroperoxide, 1-ethylbutyl	141085	
Carbamic acid, phenyl ester	69322	
Carbonic acid, ethyl 2-propenyl ester	137020	

Fumaric acid, decyl 2-methylpentyl ester	91737497	
1-Propanol, 3-methoxy-2-(methoxymethyl)-2-methyl-	542357	
2-Bromononane	98219	
l-Ascorbic acid, 5,6-O-ethylboranediyl-	54685836	
Octane, 4-chloro-	33574	
Methyl 6,6,8,8,10,10-hexamethyl-3-oxo-2,5,7,9,11-pentaoxa-6,8,10-trisilatridecan-13-oate	91738767	
Acetaminophen	1983	
2-Methyl-3-(methylthio) furan	526618	
Ent-3a-acetoxy-2b-hydroxy-13-iodomethyl-16-oxo-8,13-epi-17,20-dinorgibberell-1(10)-en-7,19-dioic acid,19,2-lactone,7-methyl est	51136328	

7-Hexadecenal, (Z)-	5364438	
1,5-Diazabicyclo[4.3.0]non-5-ene	76349	
Bicyclo[2.2.1]heptane-2-carboxylic acid isobutyl-amide	565668	
1-Butanol, 3-methyl-, acetate	31276	
3-(Hydroxy-phenyl-methyl)-2,3-dimethyl-octan-4-one	559104	
Levoglucosenone	699486	
Phenylethyl Alcohol	6054	
2-(2-(2-Butoxyethoxy)ethoxy)ethyl 2-methylbutanoate	91693497	
Benzofuran, 2,3-dihydro-	10329	

5-Hydroxymethylfurfural	237332	
Resorcinol	5054	
2-Propyl-1-heptanol	24847	
Tetradecane	12389	
Phenol, 3,5-bis(1,1-dimethylethyl)-	70825	
Pentadecane	12391	
Neophytadiene	10446	
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	5366244	
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	5366244	

Hexadecanoic acid, methyl ester	8181	
Cyclopropaneoctanoic acid, 2-[[2-[(2-ethylcyclopropyl)methyl]cyclopropyl]methyl]-, methyl ester	534619	
8,11,14-Docosatrienoic acid, methyl ester	5364473	
Methyl stearate	8201	
Stigmasta-5,22-dien-3-ol, acetate, (3.beta.)-	6432445	
dl-.alpha.-Tocopherol	2116	
3,4,3',4'-Tetrahydrospirilloxanthin	5366411	

Supplementary Table 3. Docking Score of *R. prostrata* 43 compounds with SARS-CoV-2 M^{pro}

CID	Docking score
CID: 25247358	-6.53
CID: 70825	-6.427
CID: 41124	-5.719
CID: 5364573	-5.68
CID: 551377	-5.673
CID: 569357	-5.409
CID: 7725	-5.285
CID: 249948356	-5.168

CID: 6432173	-5.114
CID: 7501	-5.1
CID: 7237	-5.057
CID: 549662	-5.054
CID: 20585933	-4.945
CID: 22967275	-4.943
CID: 559104	-4.713
CID: 14334	-4.711
CID: 549059	-4.643
CID: 81084	-4.442
CID: 2728763	-4.344
CID: 586811	-3.906
CID: 111262	-3.896
CID: 17008	-3.822
CID: 123156	-3.783
CID: 6432445	-3.418
CID: 91714556	-3.06
CID: 5281365	-2.36
CID: 15600	-2.348
CID: 557075	-2.151
CID: 10408	-1.136
CID: 5284421	-1.116
CID: 5362676	-0.66
CID: 5364431	-0.486
CID: 8181	-0.406
CID: 31284	-0.224
CID: 10446	-0.033
CID: 8201	0.501
CID: 8182	1.291
CID: 12389	1.469

Supplementary Table 4. Docking Score of *S. tora* 53 compounds with SARS-CoV-2 M^{pro}

CID	**Docking score**
CID: 70825	-6.427
CID: 54685836	-6.222
CID: 1983	-6.067
CID: 5054	-5.954
CID: 6054	-5.717
CID: 69322	-5.655
CID: 6432445	-5.584
CID: 51136328	-5.521
CID: 565668	-5.453

CID: 699486	-5.357
CID: 10351	-5.334
CID: 849	-5.321
CID: 99038	-5.307
CID: 565150	-5.296
CID: 637866	-5.196
CID: 526618	-5.171
CID: 534619	-5.089
CID: 7237	-5.057
CID: 22967275	-4.943
CID: 237332	-4.923
CID: 10329	-4.912
CID: 12097	-4.807
CID: 70258	-4.774
CID: 70258	-4.774
CID: 91740684	-4.774
CID: 559104	-4.713
CID: 79310	-4.67
CID: 250594	-4.607
CID: 76349	-4.593
CID: 10341	-4.451
CID: 98219	-4.136
CID: 5364473	-3.867
CID: 2116	-3.742
CID: 31276	-3.617
CID: 91698641	-3.603
CID: 33574	-3.592
CID: 542357	-3.495
CID: 141085	-3.157
CID: 24847	-3.104
CID: 137020	-2.138
CID: 8181	-0.406
CID: 10446	-0.033
CID: 5364438	0.172
CID: 8201	0.501
CID: 12391	1.428
CID: 12389	1.469
CID: 5283345	1.517

Supplementary figure 1.

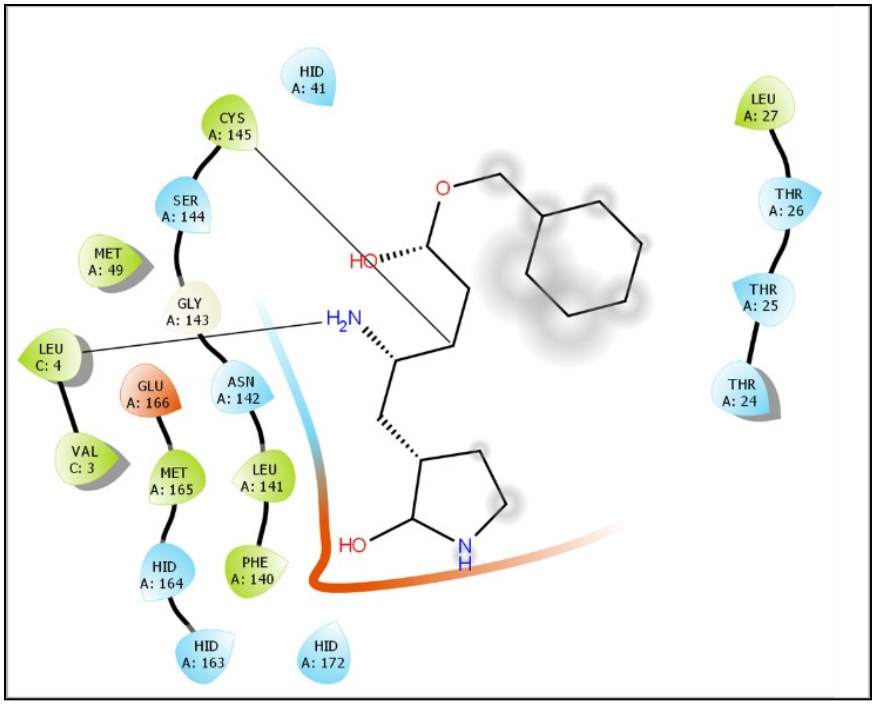


Figure S1. Binding residue with 6LU7 and N3 inhibitor.