

Supplementary data

Table 1S: Binding affinities and interactions of the top three bioactive compounds from *S. surattense* and the positive control Boceprevir against the HCV-NS3 protein (PDB ID: 4A92), focusing on both the helicase/ATPase and protease domains.

S No.	Compound Name	Docking Score (Kcal/mol)	Interacted Residues	Interacted Domain
1	Boceprevir	-7.2	Arg462, Arg467, Gln460, Gly463, Pro205, Ser459, Thr206 (fig. 5a).	Helicase/ATPase
		-6.1	Ala156, Ala157, Arg155, His57, Leu135, Lys136, Phe154, Ser139, val132 (fig. 6a).	Protease
2	Quercetin 3-glycoside [3- <i>O</i> -[β -D-Glucopyranosyl-(1 \rightarrow 4)- β -D-mannopyranoside]	-9.9	Ala234, Arg464, Arg467, Asp290, Gln460, Gly207, Gly209, Lys210, Met415, Phe238, Pro205, Pro230, Ser211, Thr206, Thr212 (fig. 5b).	Helicase/ATPase
		-6.4	Arg481, Gly137, His57, Lys136 (fig. 6b).	
		-9.1	Arg464, Asp290, Gln460, Glu291, Gly207, Gly237, Gly463, Lys210, Met415, Phe238, Pro230, Ser211, Thr419, Tyr418 (fig. 5c).	Protease
3	Delphinidin 3,5-diglycoside [3- <i>O</i> -[α -L-Rhamnopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside], 5- <i>O</i> - β -D-glucopyranoside]	-8.5	Asp81, Asp487, Gln41, Gln526, Gly58, Gly137, His57, Lys136, Phe486, Pro452, Ser139, Thr38, Thr40 (fig. 6c).	Helicase/ATPase
4	Catechin	-8.2	Ala234, Asp290, Gln460, Glu291, Phe238, Pro230, Ser211 (fig. 5d).	Helicase/ATPase
		-6.8	Ala156, Ala157, Asp437, Cys159, Gln526, His57, His528, Lys136, Ser139, val132 (fig. 6d).	Protease

Table 2S: Top eight bioactive compounds from *S. surattense* and positive control boceprevirs' interactions with helicase/ATPase domain residues of the HCV NS3/4A protein (PDB ID: 4A92)

S No.	Compound name	Docking Score (Kcal/mol)	Interacted residues
1	Isorhamnetin 3,7-diglycoside [3,7-Di- <i>O</i> - β -D-glucopyranoside]	-8.7	Ala234, Arg464, Arg467, Asp290, Asp412, Gln460, Glu291, His293, Met415, Pro230, Ser211, Ser231, Ser294.
2	3,3',4',5,5',7-Hexahydroxyflavone [3,7-Di- <i>O</i> - β -D-glucopyranoside]	-8.4	Arg464, Asp290, Gly463, His293, Met415, Ser211, Ser294
3	α -Solanine	-6.7	Ala413, Arg393, Asp296, Cys431, Gly554, Met415, Pro230, Ser297, Thr295, Trp501, Val232, Val432, Val456.
4	Spirostane-3,6,23-triol [6- <i>O</i> -[β -D-Xylopyranosyl-(1 \rightarrow 3)-6-deoxy- β -D-glucopyranoside]	-8.5	Arg464, Asp454, Asp487, Gln460, Met485, Pro230, Ser457, Thr295, Thr433, Val456
5	3,3',4',5,5',7-Hexahydroxy-8-methylflavone [3,4',7-Tri-Me ether]	-5.6	Ala275, Asp555, Gly271, Gly554, Lys272, Pro230, Ser297, Thr269, Thr298, Trp501, Tyr502,
6	Chlorogenic acid	-7.5	Ala234, Arg464, Arg467, Gln460, Glu291, Gly207, Ser231, Thr419, Tyr241
7	1- <i>O</i> - <i>p</i> -Coumaroylglucose [β -D-	-6.6	Arg464, Asn229, Gln460, Glu291, Met415, Phe238, Thr419, Tyr 241
8	Sinapic acid	-6.3	Ala 234, Lys210, Pro230, Ser208, Thr419

Table 3S: Cytotoxic effects of the flowers extract against HepG2 cells

Concentration	Cell viability %	STDs	SEM	95% CI (Min-Max)	P value
Control	100	2.5064948	1.44713		1.000
DMSO (0.7 %)	99.61	6.8109473	3.93230	-16.0109 - 16.7973	1.000
50 µg/ml	104.14723	7.3841089	4.26322	-20.5513 - 12.2569	0.952
100 µg/ml	88.776568	1.8025234	1.04069	-1.6283 - 24.0751	0.101
150 µg/ml	67.21099	7.3364602	4.23571	19.6511 - 45.9269	0.000
200 µg/ml	49.611198	5.2099533	3.00797	37.2530 - 63.5246	0.000
250 µg/ml	30.222913	5.5588332	3.20939	56.4969 - 83.0572	0.000
300 µg/ml	22.783826	2.1675521	1.25144	59.3735 - 95.0589	0.000
350 µg/ml	20.736133	5.2787485	3.04769	68.4371 - 90.0907	0.000
400 µg/ml	16.018663	2.0262542	1.16986	73.7025 - 94.2602	0.000

Table 4S: Cytotoxic effects of the leaves extract against HepG2 cells

Concentration	Cell viability %	STDs	SEM	95% CI (Min-Max)	P value
Control	100	2.5064948	1.44713		1.000
DMSO (0.7 %)	99.61	6.8109473	3.93230	-16.0109 - 16.7973	1.000
50 µg/ml	100.80353	4.9999053	2.88670	-17.2076 - 15.6006	1.000
100 µg/ml	92.068429	5.8320373	3.36713	-4.9201 - 20.7833	0.361
150 µg/ml	71.314152	4.1874082	2.41760	15.5480 - 41.8237	0.000
200 µg/ml	58.475894	5.1321928	2.96307	28.3883 - 54.6599	0.000
250 µg/ml	49.818559	5.0933621	2.94065	36.9013 - 63.4616	0.000
300 µg/ml	41.031623	12.655944	7.30691	41.1257 - 76.8111	0.000
350 µg/ml	28.589943	1.2832446	0.74088	60.5833 - 82.2369	0.000
400 µg/ml	22.757906	4.5900655	2.65008	66.9632 - 87.5210	0.000

Table 5S: Effects of the leaves extract on full-length HCV genome replication in Huh7 cells ($IC_{50} = 19.69 \pm 2.73 \mu\text{g/ml}$)

Concentration (µg/ml)	HCV Survival %	STDs	SEM	95% CI (Min-Max)	P value
Control (HCV genome)	100.00	2.899552	1.67406		1.000
12.5 µg/ml	61.89383	23.59387	11.7969	-4.081 - 76.6205	0.053
25 µg/ml	34.33262	9.620563	5.55444	34.0371 - 97.2977	0.000
50 µg/ml	38.38468	20.17047	10.0852	26.0138 - 97.2168	0.001
100 µg/ml	16.23128	13.73810	6.86905	52.8952 - 114.6423	0.000
Daclatasvir (100 nM)	30.00079	18.60541	8.32059	35.9577 - 104.0407	0.000

Table 6S: Effects of the flowers extract on HCV NS3 gene expression ($IC_{50} = 7.24 \pm 0.56 \mu\text{g/ml}$)

Concentration	HCV NS3 Gene Expression %	STDs	SEM	95% CI (Min-Max)	P value
Control(NS3+)	100	3.403818	1.96519		1.000
3.125 µg/ml	226.6463855	9.681228	6.84566	-141.9125 - -111.3802	0.000
6.25 µg/ml	80.91012118	10.19612	7.20975	3.0118 - 35.1679	0.021
12.5 µg/ml	132.603553	0.175905	0.12438	-32.8861 - -32.3210	0.000
25 µg/ml	469.9504371	60.40875	42.7154	-465.2072 - -274.6936	0.000
50 µg/ml	65.35768672	5.170879	3.65636	26.4883 - 42.7963	0.000
100 µg/ml	75.40063395	9.244154	6.53660	10.0224 - 39.1763	0.001

Table 7S: Effects of the leaves extract on HCV NS3 gene expression ($IC_{50} = 5.42 \pm 2.38 \mu\text{g/ml}$)

Concentration	HCV NS3 Gene Expression %	STDs	SEM	95% CI (Min-Max)	P value
Control(NS3+)	100	3.403818	1.96519		1.000
3.125 µg/ml	46.2538592505	16.59282	9.57987	20.6501 - 86.8422	0.003
6.25 µg/ml	41.9085330863	8.007982	4.62341	42.1187 - 74.0643	0.000
12.5 µg/ml	75.9592139075	16.45561	9.50065	-8.7816 - 56.8632	0.176
25 µg/ml	24.4115468623	10.27629	5.93302	55.0913 - 96.0856	0.000
50 µg/ml	30.6563780833	2.340078	1.35104	64.6759 - 74.0114	0.000