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Fenugreek as a Potential Antiviral Agent against Crimean-Congo Hemorrhagic Fever Virus: an In-depth Theoretical Analysis

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Supplementary Information

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_4aqg.pdb          1 AMENKIEVNNKDEMNRWFEEFKKGNGLVDTFTNSYSFCESIPNLDRFVFQ     50
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_model_01.pd       1 --ENKIEVNNKDEMNRWFEEFKKGNGLVDTFTNSYSFCESIPNLDRFVFQ     48

_4aqg.pdb         51 MASATDDAQKDSIYASALVEATKFCAPIYECAWVSSTGIVKKGLEWFEKN    100
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_model_01.pd      49 MASATDDAQKDSIYASALVEATKFCAPIYECAWVSSTGIVKKGLEWFEKN     98

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_model_01.pd      99 AGTIKSWDESYTELKVDVPKIEQLTGYQQAALKWRKDIGFRVNANTAALS    148

_4aqg.pdb        151 NKVLAEYKVPGEIVMSVKEMLSDMIRRRNLILN----------SHEHVD    189
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_model_01.pd     349 STPMKWGKKLYELFADDSFQQNRIYMHPAVLTAGRISEMGVCFGTIPVAN    398

_4aqg.pdb        390 PDDAAQGSGHTKSILNLRTNTETNNPCAKTIVKLFEVQKTGFNIQDMDIV    439
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_model_01.pd     449 ASEHLLHQSLVGKQSPFQNAYNVKGN    474
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Fig. S1. The sequence alignment results from EMBOSS Needle providing an optimal global alignment between the two input sequences.

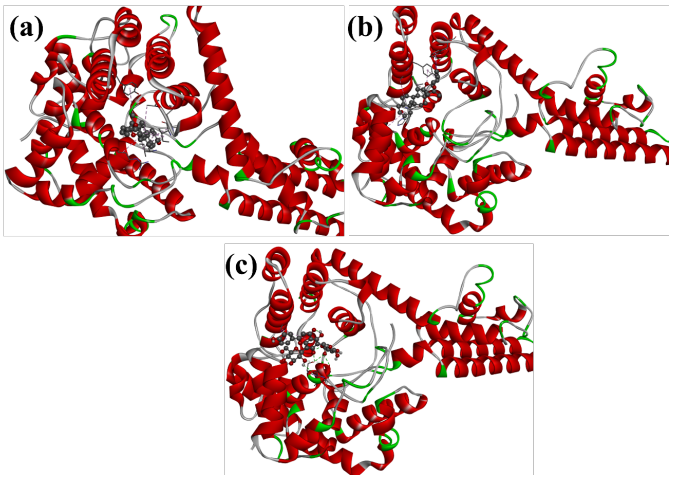

Fig. S2. Ligand-Protein Complex for **(a)** Diosgenin, **(b)** Tigogenone and **(c)** Vicenin2 with CCHFV protein.

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Table S1. Amino acids involved during the important interactions of key constituents of fenugreek with the CCHFV protein.

Ligand	Hydrogen Bonding	Hydrophobic Bonding
4-Hydroxyisoleucine	Gly409	Leu335
Calycosin	Ala300, Ser387, Thr411	Ile305, Ile374, Ile449, Ala451
Diosgenin	Ile305, Arg373	Tyr64, Ile449, Ala451
Formononetin	Arg373, Thr382, Arg385	Ile305, Arg373, Arg385, Ile449
Schaftoside	Gly341, Ser387, Gly409, His410, Thr411	Asp61, Tyr64, And Phe442
HiyodorilactoneA	Thr342	Ala65, Leu335, Pro339, Thr342, Ile386
Irolone	Ser387, Thr411	Ile305, Ile449, Ala451
Isoorientin	Ile305, Gly384, Ser387, Thr411	Ile374, Ile449
Isovitexin	Ala2.33, Gly384, Ser387, Thr411	Ile374, Ile449, Ala451
Kaempferol	Ala300, Arg385, Ser387	Ile374, Thr411, Ile449, His454
Luteolin	Ala303, Ile305, Arg373, Thr382, His454	Gln304, Arg373, Ile374
Mairin	Gly341, Gln438, Ala451	Tyr66, Val69, Ala451
Quercetin	Tyr64, Arg385, Ser387, Glu388, Thr411	Ile449
Sitosterol	Ala303, Ile305	Tyr64, Ile449, Ala451
Tigogenone	Ala65, Phe442	
Vicenin2	Leu335, Ala383, Gly384, Ser387, Thr411	Asp61, Tyr64, Ala65
Vitexin	Tyr64, Arg373, Gly384, Arg385, Gln438, Ala451, His454	Arg373, Ile449, His454