Supplementary Materials

Article

Molecular docking of SP40 peptide towards cellular receptors for Enterovirus 71 (EV-A71)

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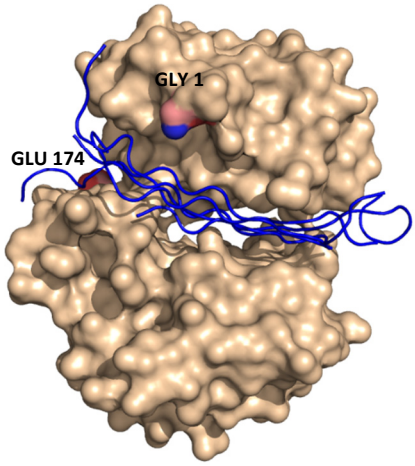
Table S1: General molecular docking of SP40 peptide with different target cellular receptors using HPEPDOCK software.

Receptors	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6	Model 7	Model 8	Model 9	Model 10
Nucleolin	-249.4	-244.6	-238.7	-235.1	-233.1	-228.7	-227.9	-224.4	-223.4	-222.9
Human cyclophilin	-231.8	-223.8	-217.3	-212.7	-212.4	-210.1	-209.7	-209.3	-209.1	-207.7
Human galectin	-229.2	-198.7	-197.3	-193.7	-188.7	-186.9	-186.3	-186.1	-185.6	-185.0
Fibronectin	-227.3	-203.5	-186.4	-186.3	-183.5	-182.0	-181.3	-180.6	-179.9	-179.2
SCARB2	-224.2	-215.1	-211.1	-210.2	-202.7	-200.4	-199.6	-199.5	-197.5	-196.6
DC-SIGN	-194.9	-189.9	-187.0	-186.0	-183.1	-181.8	-181.7	-181.1	-180.7	-178.6
Annexin	-193.4	-179.5	-178.6	-177.6	-177.4	-174.1	-173.6	-170.9	-170.0	-169.4
Human tryptophanyl-tRNA synthetase	-191.4	-189.7	-185.2	-185.1	-185.1	-184.4	-180.5	-177.2	-176.6	-176.0
Vimentin	-182.5	-180.2	-167.7	-167.5	-159.8	-157.8	-156.7	-156.6	-153.4	-151.4
Human prohibitin	-156.1	-152.3	-149.9	-149.5	-146.2	-145.2	-141.9	-140.6	-140.3	-140.1

(A)



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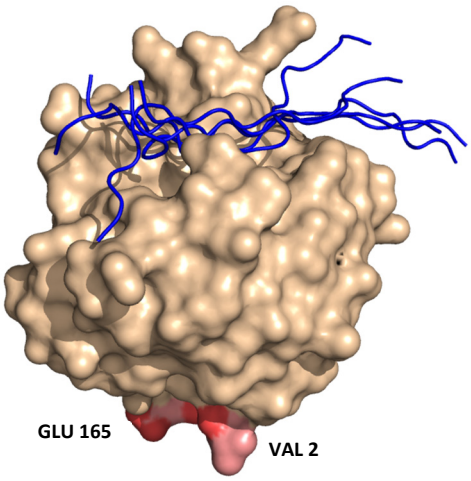
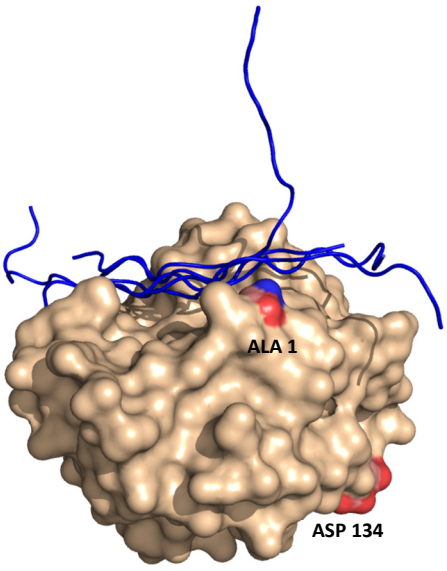
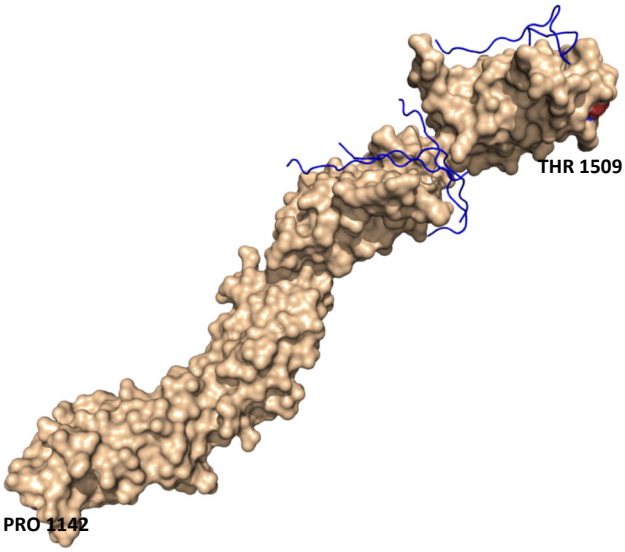


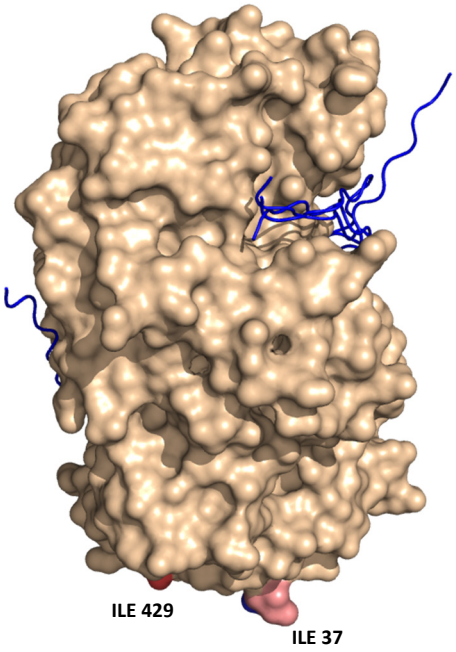
(C)



(D)



(E)



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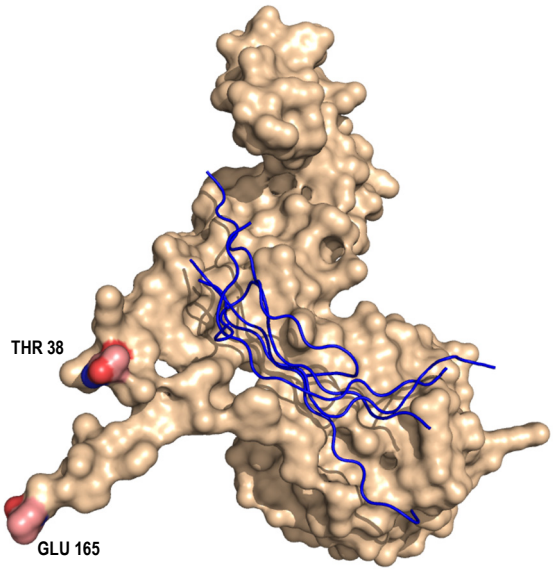
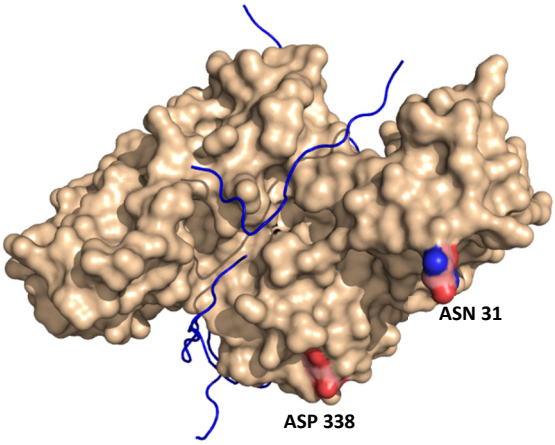
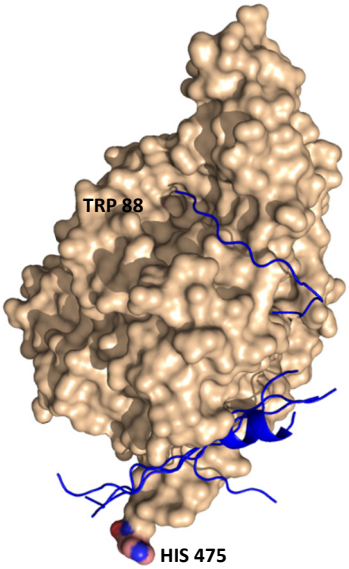


(G)



(H)



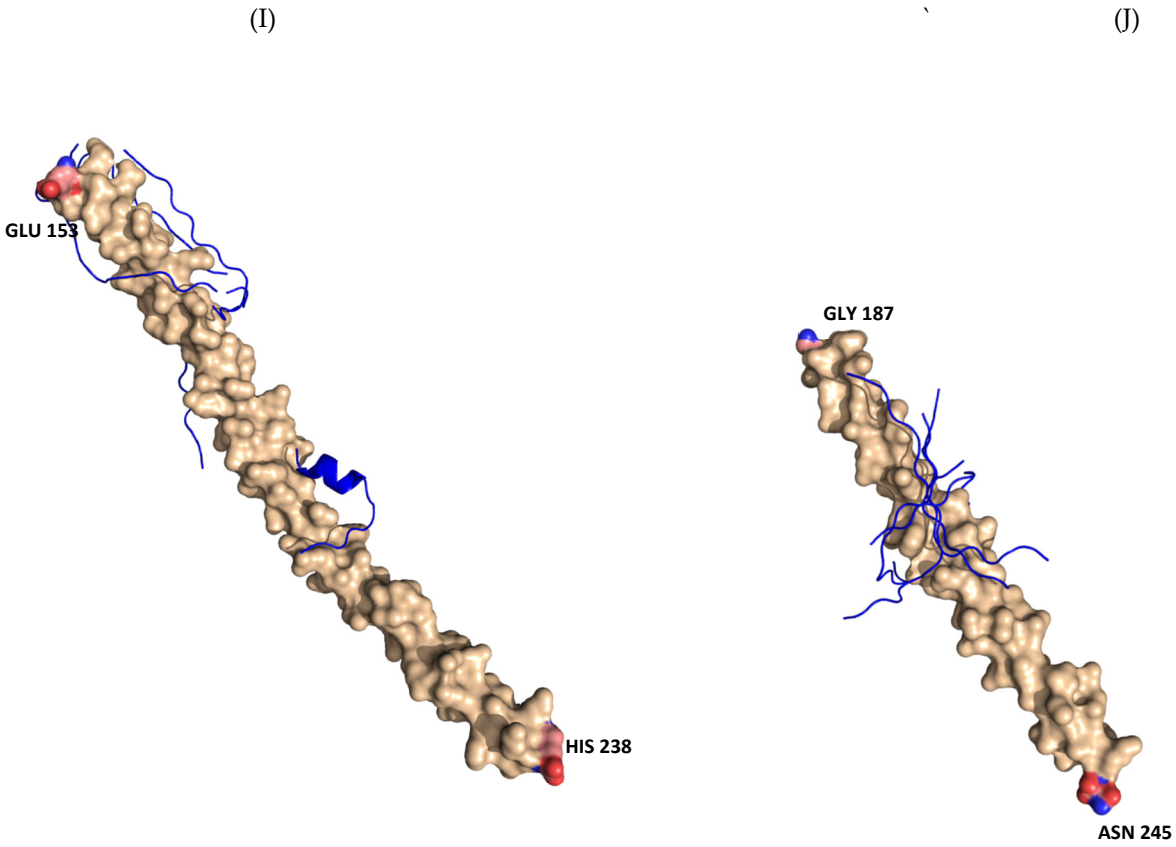


Figure S1: The top- five binding poses of SP40 peptide interacting with the receptors in global molecular docking via HPEPDOCK. The surface of the receptors and SP40 peptides are shown in wheat and blue colors, respectively. A: Nucleolin, B: Human cyclophilin, C: Human galectin, D: Fibronectin, E: SCARB2, F: DC-SIGN, G: Annexin A2, H: Human tryptophanyl-tRNA synthetase l, I: Vimentin and J: Human prohibitin.

Table S2: Fitness Gold score of local molecular docking of SP40 peptide with different target cellular receptors using GOLD software

Receptors	Model 1	Model 2	Model 3	Model 4	Model 5
Nucleolin	**125.25**	116.64	101.35	90.92	114.91
Annexin A2	97.22	107.62	91.01	**113.48**	104.27
SCARB2	94.39	**110.9**	96.55	107.16	87.86
Vimentin	79.24	67.92	54.97	**109.19**	65.73
Human tryptophanyl-tRNA synthetase	96.75	92.98	100.05	**108.5**	97.49
Human cyclophilin	**107.75**	105.87	86.73	84.53	93.33
Fibronectin	88.94	82.72	105.53	**107.02**	106.83
DC-SIGN	79.87	94.49	89.58	60.3	**105.74**
Human galectin	81.06	86.3	98.83	95.46	**99.2**
Human prohibitin	54.05	**55.43**	11	0	40.91