KSN 2021
FULLY VIRTUAL MEETING
September 02 (Thu) - 05 (Sun)

Oral Communication Abstract
Presentation No. OC9-02 (Abstract Submission No. 2400)

Oral Communications 9 Sep. 4 (Sat), 17:00-19:00

In-silico Interaction Studies Of Marine Organisms Metabolites With Drug Target SIRT1 Of Diabetic Kidney Disease

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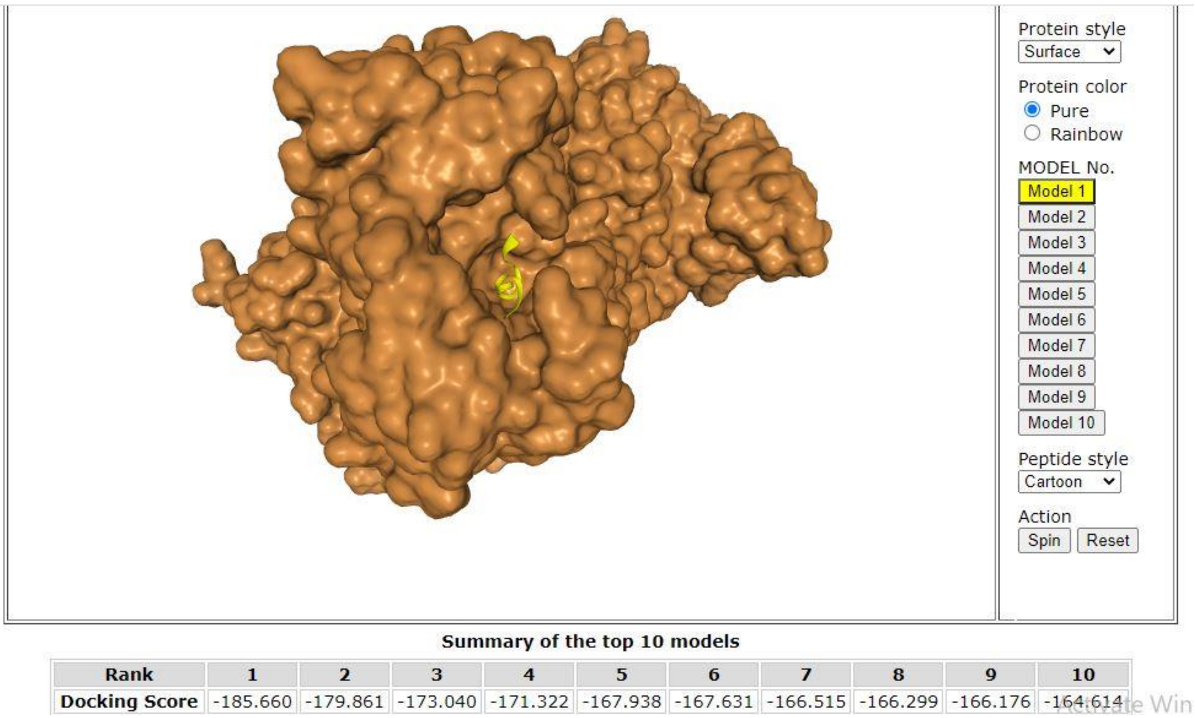
Objectives: Diabetic Kidney Disease or Diabetic nephropathy (DN) is very common, poorly prognosed and found approx. 20–40% in diabetic persons and one of the cause behind kidney failure leading the mortality
Natural products like peptides often have lower side effect, less immunogenic and more stable as compare to chemical drug molecules used in the treatment.
we are investigating the potential use of natural anti cancer peptide (GFFALIPGIE) of Pardaxin 1 obtained from red sea fish *P. marmoratas* and *P. pavoninus* and its dual role as antidiabtic peptide in diabetic kidney diseases against sirtuin-1 (SIRT1) (PDB ID: 5BTR.pdb), a potential drug target for diabetic kidney disease
objective is to explore the potential use of anticancer and antimicrobial natural peptides derieved from marine organisms towards diabetic kidney diseases through in-silico interection study

Methods: downlaoded the strcutrue of drug target Sirtuin-1 (SIRT1) (PDB ID: 5BTR.pdb) from www.rcsb.org
peptide sequence GFFALIPGIE of Pardaxin 1 released by red sea fish *Pardachirus marmoratus* and *Pardachirus pavoninus* to repel the sharks , has been downloaded from uniprot (https://www.uniprot.org/uniprot/P81863)
The known antidiabetic peptide (LLPLPVLK) from soya protein has been taken as positive control
The computational interaction (blind docking has been performed through online tool HPEPDOCK server (http://huanglab.phys.hust.edu.cn/hpepdock/.)

Results: The docking score : -185.66 of drug target -marine paptide Pardaxin 1 where as control (soya peptide) docking score was -155.096 obtained from HPEPDOCK server which reflect that marine organisms anticancer peptide has better inerection /docking as compare to control (soya protien)

Conclusions: The peptide pardaxin 1 (anticancer peptide) produced in red sea sole which is a alpha-helical cationic peptide with , helix-hinge-helix structure
has shown considerably better docking score (-185.66) then soya protein on computational platform and shown its dual role. Hence can be a potential lead for wet lab experimentation for further validations

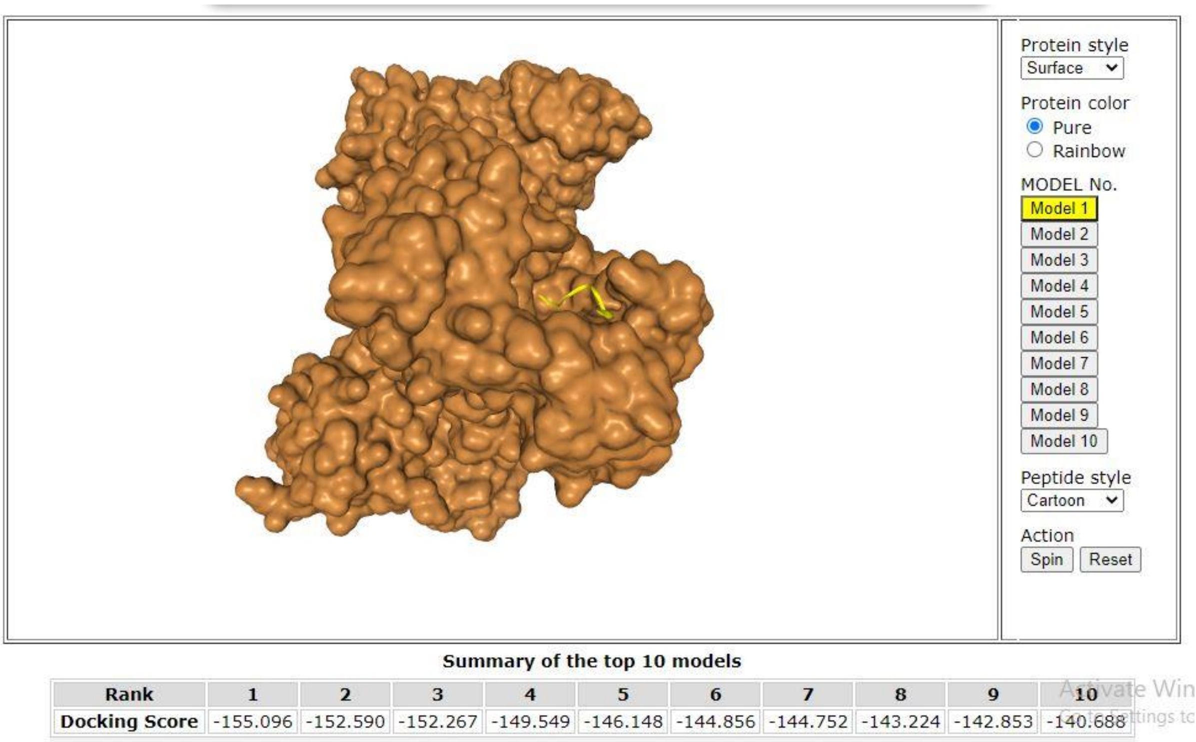
docking of Sea peptide Pardaxin 1 with 5BTR.jpg



Summary of the top 10 models

Rank	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Docking Score	-185.660	-179.861	-173.040	-171.322	-167.938	-167.631	-166.515	-166.299	-166.176	-164.614

Docking soya protein with 5BTR



Summary of the top 10 models

Rank	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Docking Score	-155.096	-152.590	-152.267	-149.549	-146.148	-144.856	-144.752	-143.224	-142.853	-140.688