KSN 2020
FULLY VIRTUAL MEETING

Abstract Type : Oral
Abstract Submission No. : OR-1361

To investigate the computational interactions and comparative binding of angiotensin converting enzyme (ACE) drug target of Diabetic Nephropathy and different plant peptides

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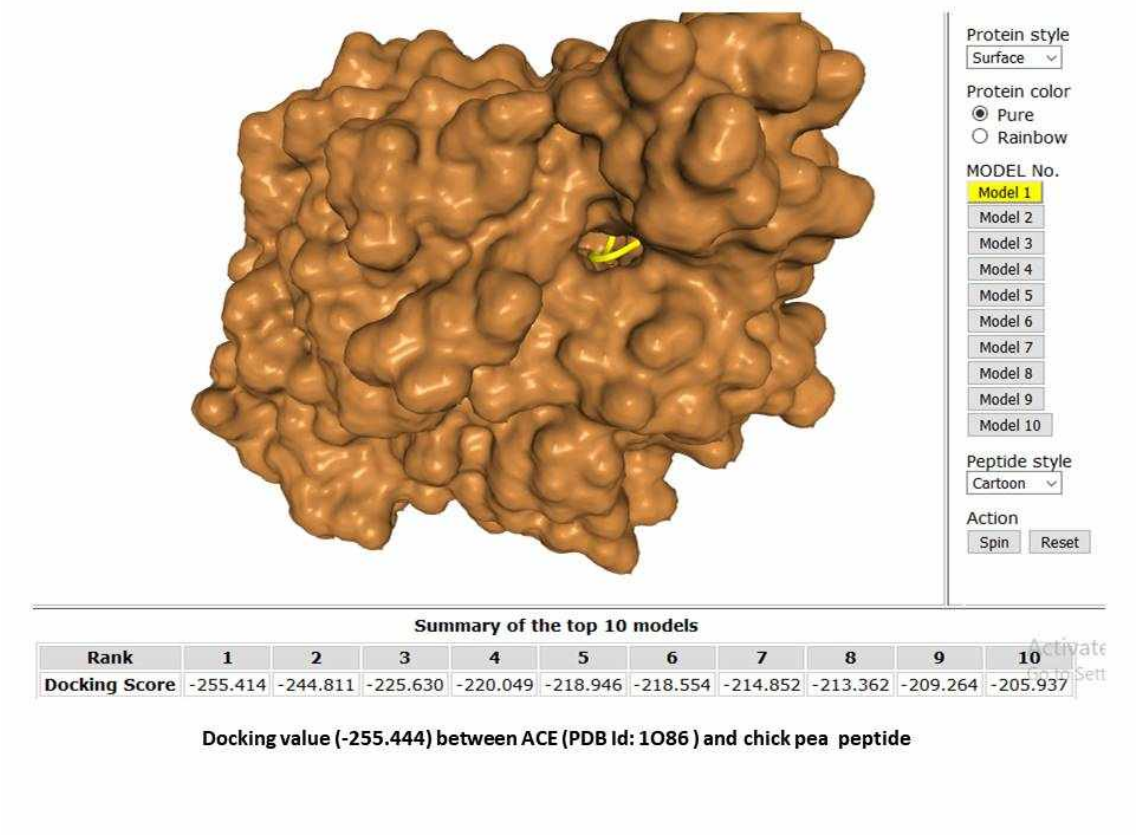
Objectives: To investigate the computational interactions and comparative binding of angiotensin converting enzyme (ACE) drug target of Diabetic Nephropathy and different plant peptides

Methods: Diabetic nephropathy (DN) is directly linked with diabetes and one of the leading cause to disrupt the function of kidney and finally its failure. it has been characterised by proteinuria (mostly albuminuria), elevated serum creatinine levels, and decreased eGFR. The management strategies of DN is totally associated with renin-angiotensin-aldosterone system (RAAS) control. Currently many angiotensin-converting enzyme (ACE) inhibitors i.e benazepril, captopril, fosinopril etc which exerts side effect like drowsiness,, weakness, headache, low bp, dizziness etc Plant peptide are cysteine-rich (defensins), natural and known to be used as a potential alternative therapeutic agents. These peptides exhibits antimicrobial, antibacterial antioxidant and anti-proliferative effects
1. The structure of ACE has been downloaded from protein databank (www.pdb.org) with (pdb ID: 1O86) .
2. A total seven plant peptides having antimicrobial to anti carcinogenic properties and belonging to different classes such as defensins, thionins, cyclotides etc. have been selected from (*l*eguminous *: Vigna sesquipedalis(*KTCENLADTY)*, Phaseolus lunatus(*KTCENLADTFRGPCFATSNC)*, Glycine max(*SKWQHQQDSCRKQLQGVNLTPCEKHIMEKIQGRGDDDDDDDDD), Phaseolus vulgaris(ANDISFNFVRFNETNLILGG), *Cicer* arietinum (ARQSHFANAQP) non-leguminous : *Viola arvensis*(GLPVCGETCVGGTCNTPGCSCSWPVCTRN), *Viola odorata(*GIPCGESCVWIPCISSAIGCSCKSKVCYRN).
3. To study the computational interaction/docking the hpepdock server has been used which is based on blind protein-peptide docking and implemented on hierarchical algorithm

Results: The results reveal that antimicrobial peptides from leguminous plants have shown higher binding affinity/docking as compare to peptides from non-leguminous plants agaisnt drug target 1O86
Peptide from Chickpea (*Cicer arietinum*) of length (ARQSHFANAQP) 11 amino acid has shown the highest affinity /docking with -255.414

Conclusions: chick pea (leguminous plant) has been found to demonstrate the better use with multiple properties such as antimicrobial and anti-cancerous as well as anti-diabetic and proved to be therapeutically important towards diabetic nephropathy, the experiment could be extended with MD simulation studies

Fig 1 Docking of Chick pea with ACE molecule



Summary of the top 10 models

Rank	1	2	3	4	5	6	7	8	9	10
Docking Score	-255.414	-244.811	-225.630	-220.049	-218.946	-218.554	-214.852	-213.362	-209.264	-205.937

Docking value (-255.444) between ACE (PDB Id: 1O86) and chick pea peptide