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BIOMEDICAL INFORMATICS

www.bioinformation.net
Volume 17(1)

Research Article

Molecular modeling of cornulin (CRNN) for docking with phytocompounds from *Justicia adhatoda L.*

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Received December 29, 2020; Revised December 31, 2020; Accepted January 26, 2021, Published January 31, 2021

DOI: 10.6026/97320630017200

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Abstract:
Cornulin (CRNN) is linked with tumour progression. Therefore, it is of interest to document data on the molecular modeling of cornulin (CRNN) for docking with phytocompounds (Pyrazinamide, Anisotine, Vasicinone, Vasicoline) from Justicia adhatoda L. Thus, we document the optimal binding features of these compounds with the cornulin model for further consideration.

Key words: Oral Squamous Cell Carcinoma, cornulin, molecular modeling, and molecular docking.

Background:
Cornulin (CRNN) is linked with tumour progression **[1-7]**. Therefore, it is of interest to document data on the molecular modeling of cornulin (CRNN) for docking with phytocompounds (Pyrazinamide, Anisotine, Vasicinone, Vasicoline) from Justicia adhatoda L.

Materials and Methods:
Sequence retrieval and 3D model building:
The full amino acid (495aa) sequence of CRNN is downloaded from the Uniprot Knowledgebase database in FASTA format with accession number Q9UBG3. The NCBI Simple Local Alignment Search Tool (Psi-BLAST) **[8]** was used to search the Protein Databank (PDB) for templates. The template with PDB ID: 4PCW was chosen having a 41.76 percent identity score. The Swiss model server was used for creating the protein model.

Model evaluation:
ProCheck **[9]** was used for model validataion.

Prominent binding site prediction:
The Cavity Plus server **[10]** was used to identify the binding pockets.

Ligand retrieval:
The structure data for 12 compounds from *Justicia adhatoda L* was downloaded from PubChem database. All the compounds were downloaded in SDF format and converted to the PDB format using Pymol.

Molecular docking and interaction analysis:
Molecular docking and visualization were done using a standard procedure using PyRx, AutoDock 4 and Pymol **[11-13].**

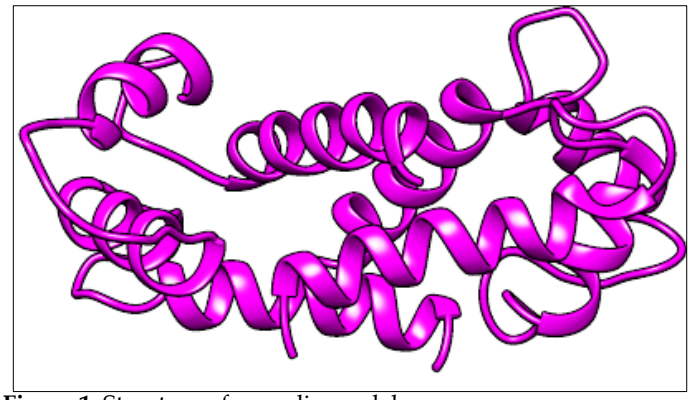

Figure 1: Structure of cornulin model.

Table 1: List of Selected compounds from Justicia adhatoda L

S.No	Compound Name
1	Amrinone
2	Anisotine
3	Sulforaphane
4	methyl_ether
5	Pyrazinamide
6	Squalene
7	Stigmasterol
8	Vasicinone
9	Vasicoline
10	Hexadecanoic acid
11	Adhatodine
12	Ethambutol

Table 2: Molecular Docking Results of phytocompounds with Cornulin

S.No	Compound Name	Binding Energy Kcal/mol	Hydrogen Bond Interaction	Distance Å
1	Pyrazinamide	-6.8	PRO-2	1.9
			GLY-10	2.5
2	Anisotine	6.6	GLN-83	2
3	Vasicinone	-6.2	LYS-80	2.8
4	Vasicoline	-6	LYS-80	2.7

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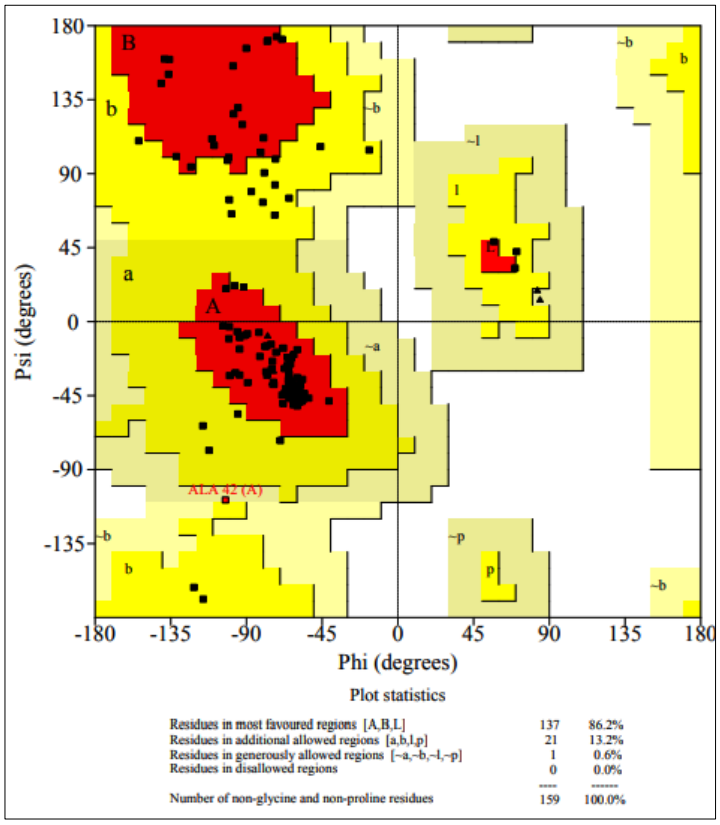

Figure 2: Ramachandran plot analysis of cornulin model.

Results and discussion:

The SWISS-MODEL homology \cornulin was created **(Figure 1)** using a known structure (PDB ID 4PCW) with 41.7% sequence identity as a template evaluated using Ramachandran plot analysis **(Figure 2)**. Cavity Plus was used to predict binding pockets **(Figure 3)**. The binding pockets are made of PRO: 2, GLN: 3 LEU:4, LEU:5: GLN:6: ILE:8: ASN:9: GLY:10: ILE:11, ILE:12, GLU:13, ALA:14, ARG:16, LEU:37, GLU:38, GLN:39, GLU:40, PHE:41, ALA:42, ASP:43, VAL:44, ILE:45, LEU:77, LYS:80, VAL:81, ALA:82, ALA:84, CYS:85, PHE:86, LYS:87, THR:88 and LEU:89.. Molecular docking of the protein model with the compounds shows that PRO-2, GLY-10, GLN-83, LYS-80, LYS-80 residues show strong binding interactions with the phytochemicals **(Figure 4)** for further consideration in the development of optimal drugs against oral cancer.

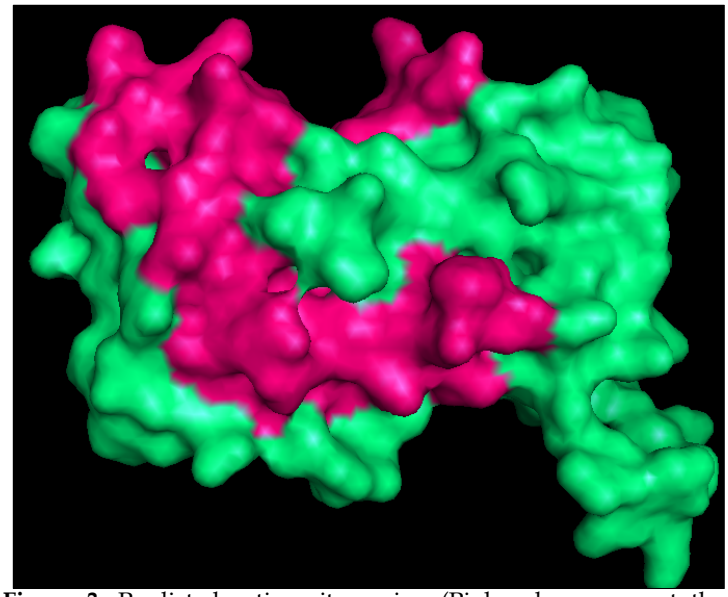

Figure 3: Predicted active site region (Pink color represent the predicted binding site region).

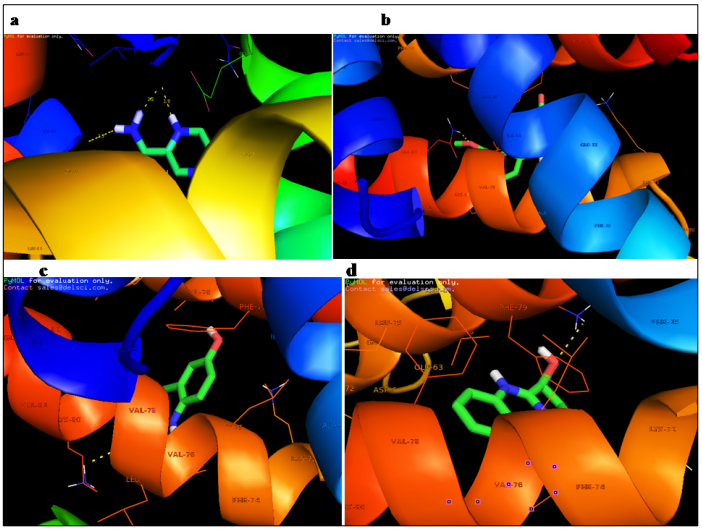

Figure 4: Molecular interaction of cornulin with (a) Pyrazinamide; (b) Anisotine; (c) Vasicinone and (d) Vasicoline.

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Conclusion:
We document the optimal binding features of phytocompounds (Pyrazinamide, Anisotine, Vasicinone, Vasicoline) from *Justicia adhatoda* L with Cornulin in the context of cancer for further consideration.

Conflict of interest: Nil

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Edited by P Kangueane
Citation: Selvaraj ***et al.*** Bioinformation 17(1): 200-205 (2021)

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ISSN 0973-2063 (online) 0973-8894 (print)
Bioinformation 17(1): 200-205 (2021)

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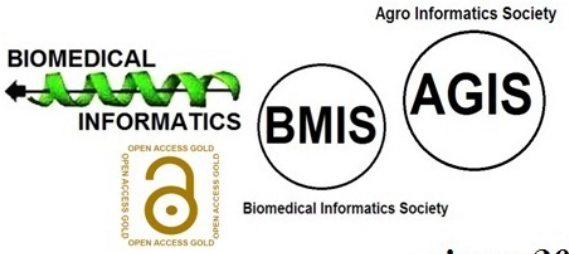

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