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DOCKING STUDIES OF RP2 (X-LINKED RETINITIS PIGMENTOSA) PROTEIN USING VALPROIC ACID AS POTENTIAL INHIBITOR

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Abstract

Mutation in X-Linked retinitis pigmentosa (RP2) can cause regional damage and eventually cause damage. Due to disease complications, there is no curable treatment until now. In the present study, the RP2 crystal structure was improved with the help of Glide software's protein preparation. Insert Anticrobin compounds, such as Velopro Acid Artenine and Cindianine, into RP2 function. Molecular docking was performed by using Auto Dock vina.

Keywords: *X-Linked retinitis pigmentosa (RP2), Anthocyanin, Valproic acid, AutoDock vina*

Introduction

Visual impairment spreads as age related disease worldwide. Retinitis pigmentosa (RP) affect crowd 20-60 years old patients with disease [1]. The retinal copier (bar) has deteriorated, resulting in a lack of darkness. Retinal black parts appear, peripheral vision loss are some major disease symptoms [2,3]. Two million people around the world are affected. Because of reproductive degradation, there are several genes which makes it more complex. These symptoms are different in the patient. Over the past few years, interest in these mixtures has begun again. Different parts of different plants have made a lot of research on their processing requirements. Natural populations of compounds, including plants, microorganisms and animals, are the basis for the discovery of drugs. In biological compounds, this phenomenon is important because of its high antioxidant activity. Silicone methods are widely used to identify many errors in lead moles. In this respect, we present the utility of autologous genes isolated from Seoggium rods as the best disease prevention [4].

Methods

During the molecular docking of the above compound following materials were used in docking: 1) Valproic acid pubchem CID. 2) RP2 (X-Linked retinitis pigmentosa), Structure retrieval: Human degradation at 2.1 ° C was derived from the crystal structure PDB containing 350 amino acids human retinitis pigmentosa protein 2 (PDB ID: 2BX6). 3) m.g.l tools software. 4) Autodock vina. 5) Discovery studio. 6) Pymol. 7) Python. First of all the ligand Valproic acid was downloaded from pubchem.ncbi.org as sdf file. Then it is opened in discovery studio which was already installed. Hydrogen is added to the ligand to fulfill its valency, then further modification was done to the original ligand molecule and it was saved as PDB file. After that this PDB ligand file is opened in autodock to convert it to PDBQT file to use it in autodock vina. Then target molecule RP2 (X-Linked retinitis pigmentosa) was downloaded from the RCSB as a text file. This file was opened in discovery studio and ligand which was already present in the protein was selected and deleted to proceed our docking as the already present ligand disturbs the docking with a new ligand. The file was saved as PDB in discovery studio. Then the protein PDB file was opened in autodock and water was deleted and hydrogen was added to the protein molecule. Then the ligand attachment site was selected by making grid box which covered the protein molecule and the values of dimensions and centers were noted [5].

Then ligand and protein files was copied to the vina folder and the values of grid was put and target and inhibitor names was changed as the names of the files copied. Then the conf file was saved and auto docking was started through opening the command prompt. The docking started after command and the program completed docking itself [6].

Results

In our study, glutamate and CGDM tolerance were identified by a crude bar, with other octagonal compounds firmly limiting RP2 protein. In particular, it is found that there are very many anthocyanins, and their benefits are widely used in human heal. The docking results using AutoDock vina is given in the table as binding affinity in kcal/mol. The docking result of Valproic acid showed -5.3 kcal/mol. Then it was modified using Discovery studio and changes were made in the original Valproic acid compound and modified it to enhance its binding affinity. After modification, the modified compounds of valproic acid among all the three compounds used, gave more binding energy as compared to original one.

Discussion

In our study, the docking results using AutoDock vina are given in the table as binding affinity in kcal/mol. The docking result of Valproic acid showed -5.3 kcal/mol. Then it was modified using Discovery studio and changes were made in the original Valproic acid compound and modified it to enhance its binding affinity. After modification, it was noted that most of the derivatives gave less binding energy as compared to the original compound [7]. Therefore, our results suggest that there should be new compounds, one of our modified to be a good drug.

Binding Affinities of compounds (Kcal/mol):

Its binding energy after modification were at different valuse (kcal/mol), which were less than the original valproic acid.

Interaction between valproic acid01 and target protein:

In the above figure the interaction between valproic acid and the target protein RP2 is shown by using pymol software. The binding pocket is shown at the active site of protein.

It was concluded from this study that Cyanidin gave binding energy as -8.5 kcal/mol

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Table 1: Binding affinities of compounds

Structure name	1	2	3	4	5	6	7	8	9
Valproic acid	-5.1	-4.9	-4.4	-4.4	-4.3	-4.1	-4.0	-3.7	-3.7
Valproic acid01	-5.3	-5.2	-4.8	-4.7	-4.7	-4.7	-4.5	-4.5	-4.5
Aurintinidin	-8.3	-8.1	-7.9	-7.9	-7.8	-7.7	-7.5	-7.4	-7.4
Aurintinidin01	-8.3	-8.1	-8.0	-7.9	-7.7	-7.6	-7.2	-7.1	-6.9
Aurintinidin02	-8.2	-8.0	-8.0	-7.6	-6.7	-6.7	-6.7	-6.7	-6.7
Cyanidin	-8.5	-8.1	-8.0	-7.7	-7.7	-7.6	-7.4	-7.3	-7.3
Cyanidin1	-7.5	-7.4	-7.3	-7.3	-7.2	-7.2	-7.1	-7.0	-6.9

Table 2: ADMT properties of compounds

Structure Name	MlogP	S+logP	S+logD	Role of 5	Rule of 5 -code	MWt	M_NO	T_PSA	HBDH
Valproic acid	1.654	2.610	0.180	0.000		144.215	2.000	37.300	1.000
Valproic acid01	-1.232	-0.660	-2.894	0.000		254.304	6.000	118.220	5.000
Aurintinidin	0.850	0.241	-0.977	0.000		301.278	6.000	114.290	5.000
Aurintinidin01	-1.581	-0.650	-234	0.000		325.785	4.000	112.345	4.000
Aurintinidin02	-0.177	-0.189	-1.117	1.000	Hb	397.426	8.000	134.520	8.000

Table 3: Drug Scoring

Structure name	Rmsd	Rank score	Score
Valproic acid	None	1	-90
Valproic acid01	None	1	-88
Aurintinidin	None	1	-89
Aurintinidin01	None	1	-90
Aurintinidin02	none	1	-104

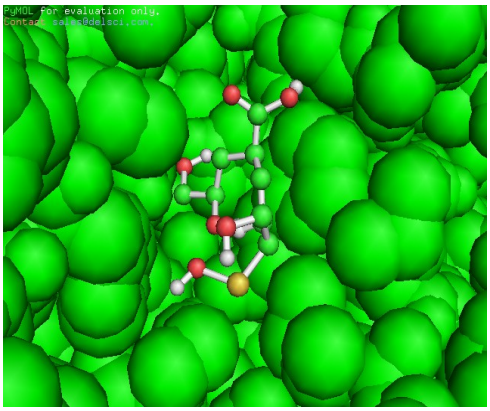

Figure 1. Binding of Cyanidin with the target