QUERCETIN IS MORE POTENT THAN MELPHALAN AS A CDK4, CDK6, PRB INHIBITOR IN RETINOBLASTOMA

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Introduction

Retinoblastoma occurs due to gene mutations that have the potential to cause death. Retinoblastoma occurs due to mutations in the allele of the Retinoblastoma gene (RB1) which acts as a tumor suppressor gene, causing retinal cells to undergo uncontrolled proliferation. Mutations in the RB1 gene due to changes in the coding of this gene indirectly cause overexpression of the CDK4 and CDK6 proteins.

Purpose

Analyzed the potential of Quercetin in the treatment of retinoblastoma by examining its binding to CDK4, CDK6 and pRB proteins in In Silico with molecular docking techniques and comparing them with Melphalan.

Methods

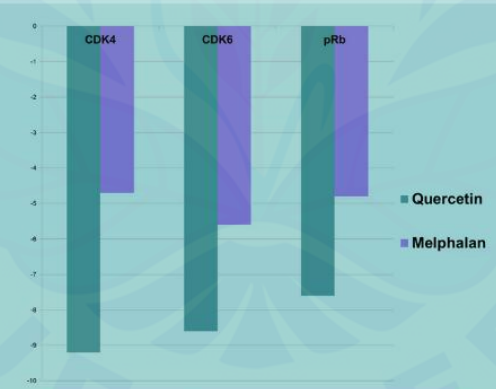
Protein Rb with code 3N5U, CDK4 with code 2W96 and CDK6 with code 3NUP. Quercetin was obtained from the site https://www.rcsb.org/. Quercetin enzyme with code 1JUH. The docking method is done by tethering the ligand to the CDK4, CDK6, pRb receptors. AutoDock Vina was used in the simulation of the docking of the test ligand against the CDK4, CDK6, pRb receptors. The docking results were scored and the best value (most negative G) was observed in the ligand binding area to the CDK4, CDK6, pRb receptors.

Results

Quercetin has a binding affinity for CDK4, CDK6, pRb proteins of -9.2, -8.6, -7.8. Melphalan has a binding affinity value for CDK4, CDK6, pRb proteins of -4.7, -5.6, -4.8.

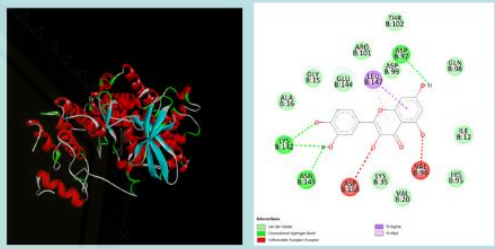
Conclusion

Quercetin has potential as a drug candidate in retinoblastoma.

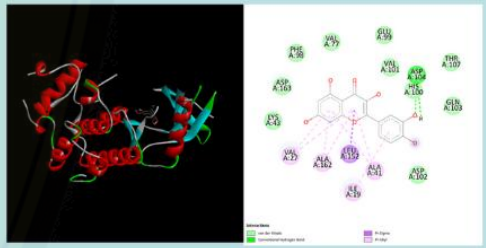


	Quercetin	Melphalan
CDK4	-9,2	-4,7
CDK6	-8,6	-5,6
pRb	-7,8	-4,8

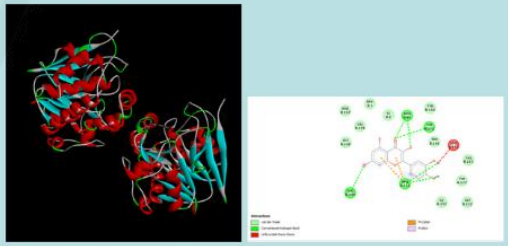
Table 1. Result Comparison



Picture 1. Quercetin CDK4



Picture 2. Quercetin CDK6



Picture 3. Quercetin pRb