International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.9, No.09 pp 210-215, 2016

Natural Flavonoids as CDK5 inhibitors: A Homology modeling and Molecular Docking Study

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Abstract : In this study, homology modeling and molecular docking studies were performed to explore structural features and binding mechanism of natural flavonoid derivatives as Cyclin-dependent kinase 5 (CDK5) inhibitors. A homology modeling procedure was employed to construct a 3D model of CDK5 of Mus musculus protein by using MODELLER9.15. For this procedure, the X-ray crystal structure of FCHO2 F-BAR DOMAIN (PDB ID: 2V0O) at 2.30 Å resolution was used as template. The predicted model was analyzed by PROCHECK. The 3D structure of predicted model shows 93.0% of amino acids in most favored region. The predicted model was used for molecular docking studies by using Autodock4.2. All the selected natural flavonoid derivatives show good binding energy and interactions with the model. Compound Gardenin-B shows two interactions with Lys89 and Glu81.
Key words: Natural Flavonoids, Homology modeling, Modeller9.15, Molecular docking.

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