

Poster Presentation

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Crystal and Molecular docking studies of biscyclohexane diol with FAK

M. K. Kokila¹, KS Kiran², GURUPRASAD RAMAKRISHNA³

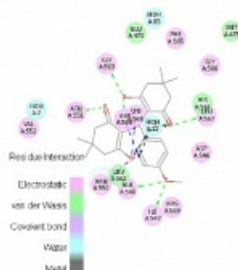
¹Bangalore University, Bangalore, India, ²Department Of Physics, Jain University, Bangalore, India, ³Durga Femto Technologies and Reserach, Bangalore, India
E-mail: drmkkokila@gmail.com

In the present study crystal structure of 3-hydroxy-2-((2-hydroxy-4, 4-dimethyl-6-oxocyclohex-1-enyl) (4-methoxyphenyl) methyl)-5, 5-dimethylcyclohex-2-enone was determined using single crystal X-ray diffraction. Cyclohexane is a non planar molecule the shape of which vaguely resembles a chair. The conformation of cyclohexane molecule is constantly changing, with the atom on the left which is currently pointing down flipping up, and the one on the right flipping down. Further the structural feature was extrapolated to molecular docking studies with focal adhesion kinase (FAK) domain using Autodock to study its anticancerous property. The compound exhibited considerable bacterial inhibition of lower to moderate concentrations. We conclude that these derivatives can be used in medicine and have enormous potential as pharmaceutical agents due to their biological activities. The above titled receptor gain functional and structural insights into their mechanism of inhibition and explore its potential as an anticancer agent.

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