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## Identification of the small molecules targeting *Mdm2* and inhibiting *P53* binding to be a promising approach to treat cancer by structure based virtual screening, docking and molecular dynamic simulation studies

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*P53* is an important tumor suppressor gene with a known role in the later stages of cancer. Since its discovery in 1979, *p53* has become the focus of intensive cancer based research in laboratories around the world. Tumor suppressor gene *p53* is an attractive cancer therapeutic target because it can be functionally activated to eradicate tumors. *Mdm2* has been identified as a *p53* interacting protein towards represses *p53* transcriptional activity. *Mdm2* achieves this repression by binding to and blocking the N- terminal trans-activation domain of *p53*. *Mdm2* is a *p53* responsive gene that is; its transcription can be activated by *p53*. When *p53* is stabilized, the transcription of *Mdm2* is also induced, resulting in higher *Mdm2* protein levels causing recognition and repair, transcription regulation problems leading to cancer. Thus inhibiting the *Mdm2- p53* interactions has been proven to be most promising approach for cancer therapy. In this present paper an investigation was carried out on the mode of interaction between *p53* and *Mdm2* at molecular level. Then a structure based virtual screening approach was used to identify the target specific *Mdm2* inhibitors by docking studies. The best compound will be subjected to molecular dynamic simulations for further validating the docking studies and to reveal interactions during the conformational changes. The identified compounds are compared to that of the FDA drug Nutlin compound that which has already proven. Finally the paper was concluded by proposing a potent lead compound suitable for the inhibition of *p53- Mdm2* complex and recommended for the further studies based on the above mentioned results.

### Biography

Vijay Raj Bollapalli has completed his M Phil in Biochemistry, submitted thesis for the award of the PhD in Dept. of Biotechnology at Acharya Nagarjuna University. He is the Associate Director of DAWN, a premier service organization. He has published more than 5 papers in reputed journals and serving as a Member of (ABAP) Association of Biotechnology and Pharmacy, a reputed journal.

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