

## An *in vitro* and molecular informatics study to evaluate the antioxidative and $\beta$ -hydroxy- $\beta$ -methylglutaryl-CoA reductase inhibitory property of *Ficus virens Ait*

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It is accepted that currently used hypocholesterolemic drugs have severe side effects and are also not competent to attenuate the hypercholesterolemia-induced oxidative stress. Therefore, the present study was initially intended to evaluate antioxidant and  $\beta$ -hydroxy- $\beta$ -methylglutaryl-CoA reductase (HMGR) inhibitory property of *Ficus virens Ait.*, first by *in vitro* analyses followed by a corroboratory molecular informatics study. Our results illustrated that of the entire sequentially extracted fractions of *F. virens* stem bark and leaves extract, *F. virens* bark methanol (FVBM) extract exhibited strong radical scavenging, antioxidant and oxidative DNA damage protective activity, which was well correlated with its total phenolic content. In addition, the preliminary screening of all the extracts of *F. virens* leaves and bark fractions against HMGR inhibitory activity revealed that FVBM extract ( $IC_{50}$ ,  $8.2 \pm 0.45 \mu\text{g/ml}$ ) strongly and significantly inhibited the enzyme activity as compared to other extracts. Moreover, this extract also found to be non-cytotoxic at various concentrations. Further, the mechanism of action of the bioactive compounds, revealed via GC-MS analysis, of this extract was authenticated by molecular docking studies with HMGR. The HMGR inhibition, predicted in term of binding energy, for the first time implied that quinic acid ( $\Delta G$ :  $-8.14 \text{ Kcal/mol}$ ) and paravastatin ( $\Delta G$ :  $-8.22 \text{ Kcal/mol}$ ) exhibited almost same binding energy while other compounds also showed good binding energy, which in turn suggest that quinic acid alone or in combination with other major bioactive compounds were might be responsible for the HMGR inhibitory property of this extract. Our results exemplify that this extract or bioactive compounds with antioxidant and anti-HMGR property may be used in the *in vivo* system for the management, prevention and alleviation of hypercholesterolemia as well as hypercholesterolemia-induced oxidative stress.

**Keywords:** Ficus virens, HMG-CoA reductase, Antioxidant, Molecular docking.

### Biography

Danish Iqbal has completed his Master (biotechnology) degree at the age of 23 years from C.C.S. University and dissertation from PLIM, Department of AYUSH, India. He is a research scholar (J.R.F.) under SERB project, department of science and technology, Govt. of India, and pursuing Ph.D. (biotechnology) from Integral University. He is working on partial purification of bioactive secondary metabolites, enzyme inhibitors from plants, and their docking analysis for the treatment of hyperlipidemia. He is a Secretary in Aqsa Educational Welfare Society for education and development. He has presented oral and poster presentation in more than 3 national and international conferences.

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