

## IN- Silico studies of novel TTF protein related to *Mycobacterium tuberculosis*

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**M**ycobacterium tuberculosis (Mtb) is a successful pathogen causing tuberculosis (TB). One third of the world population is affected by Mtb. Tuberculosis Transcription Factor F (TTF) protein belongs to ECF – sub family, helps in the specific transcription initiation. TTF controls the expression of 14 induced genes and plays a significant role in the expression of SigB and SigC Proteins which are important for virulence.

In the present study TTF homology model was generated with the help of comparative homology modeling techniques using pair wise sequence alignment. The predicted 3D model was subjected to refinement and validated. Virtual screening studies were performed with an In-house library to identify a lead molecule that can inhibit the TTF protein. The TTF protein is considered as novel target for the development of new molecular entities (NMEs) useful for tuberculosis treatment.

### Biography

M. Kiran Kumar is Assistant Professor (C) at The Department of Chemistry, Nizam College, Osmania University since 2010. He is a doctoral research fellow working on identifying novel leads for Tuberculosis therapy. His field of research interest includes identification of new molecular entities (NME's) using Computational Chemistry, Chemical - Biology and Cheminformatics and Bioinformatics related Software tools. He received an award for Best Oral Presentation at the 30<sup>th</sup> Annual Conference Indian Council of Chemists - 2011. He has been mentoring M. Sc. and M. Pharmacy students in their dissertation work and actively involved in organizing Seminars and workshops for students. Mr. M. Kiran Kumar published 04 research articles in reputed international journals and has presented about 20 papers at various International and National Conferences.

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## Investigation of a pantropical weed, *Phyllanthus amarus* schum and thonn for a medicinally important molecule- quercetin

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**P**hyllanthus amarus is a widely distributed pan-tropical herb under an angiosperm family Euphorbiaceae precious for quercetin. Quercetin is a naturally occurring glycosylated flavonoid, synthesized in plant tissues; it is classified under P-vitamins and resembles the non-sugar part of other complex flavonoids viz., rutin, quercetrin, isoquercetrin and hyperoside. Quercetin is found to induce antioxidant, anti-allergenic, antibacterial, anti-fungal, anti-carcinogenic and pharmacological responses, and it is used for the treatment of ailments that range from allergies and pathogenic manifestations to high risk coronary diseases, like cancer and HIV. It is highly valued in the 'Ayurveda' for its therapeutic properties and cosmetology. It is also used as a potential natural dye to color fabrics; in analytical chemistry as a chelating agent to determine magnetic properties of metals, to determine oxidation state of lanthanides, and recently, to synthesize nano-particles of metals that find a great importance in drug targeting in cancerous tissues. It is a secondary metabolite found in quite small quantities in plant tissues out of the total polyphenols (polyphenols 25-30% w/w dry weight). The various applications of quercetin foresee potential industrial demand, and envisage development of biotechnological process to enhance its synthesis, extraction and production from the natural sources using a "green process".

In our laboratory, we optimized the medium composition for callus induction, Biomass enhancement and selection of high yielding cell lines for Quercetin. A thorough investigation for cell culture, extraction of the active principle and validation, are being worked out to enhance production of quercetin, and establish commercial potential of Biotech Quercetin.

**Keywords:** Phyllanthus amarus, Quercetin, Callus, Cell selection, Green Process.

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