Notification No: 520/202
Date: 06/09/2022

Name of the Scholar: Md. Amjad Beg

Name of the Supervisor: Dr. Fareeda Athar

Name of the Department/Centre: Centre for Interdisciplinary Research in Basic Sciences

Topic of Research: Impact of natural compounds against target protein/pathway and antituberculosis approaches

PhD Findings

Tuberculosis is still an important threat to world in respect of its mortality cases. Due to the dramatic change in *M. tuberculosis* (the causative agent of disease) nature, we are in the urgent need for novel therapeutic. Natural products are good source of antibacterial activities and therefore *Achyranthes aspera*, *Calotropis gigantea* and *Calotropis procera* were examined to their anti-tuberculosis activity. The ethyl acetate plant extracts of *A. aspera* aerial part and *C. gigantea* flower ash was found as good source of phytochemicals, secondary metabolites and showed anti-mycobacterial activity with MIC 64µg/ml. GC-MS analysis was conducted to determine the compound content of plants. In the search of mycobacterial protein target, ten proteins were shortlisted which showed the efficient binding with beta-Amyrin compound resulted from GC-MS analysis. *In silico* protein network analysis finalized *Rv1636* protein which is mycobacterial universal stress protein. Molecular docking showed that β-amyrin interacted with most of the proteins and its highest binding affinity was with *Rv1636*. Further biochemical, biophysical, and computational characterization of *Rv1636* was done. The protein contains very minute ATPase activity which gets affected by the addition of β-amyrin. The reason was the structural deformation of *Rv1636* in presence of beta-Amyrin. The binding of β-amyrin to *Rv1636* was further confirmed by molecular docking and MD simulation and thus the study suggests that β-amyrin might affect the functioning of *Rv1636* which makes the bacterium vulnerable to different stress conditions.