Notification No: F.N.O.COE/PhD/(Notification)/520,2022

Date of Award: 06.09.2022

Name of Scholar: Amaduddin

Name of Supervisor: Dr. Mohammad Abid

Name of Department/Centre: Biosciences

Topic of Research **:** Rational drug design and computational approachs for anti-malarial drug discovery

Summary:

The study focused on the identification of molecules using target based virtual high-throughput screening to find potential hits from the ZINC database of natural compounds and a synthetic In-house library against cysteine proteases falcipain (FP2 and FP3). Further, biochemical studies and were performed which resulted in a compound ST72 from natural library and JMI-105 from synthetic library showed potent inhibitory effect on purified proteins. The work focused on the synthesis of a novel series of piperazine tethered 7-chloroquinoline-triazole conjugates. All these derivatives were evaluated for their antimalarial efficacy against (3D7) and (RKL-9) of *P. falciparum* strains. The parasite growth-inhibitory potency of QP11 was correlated with its falcipain targeting activity by the in-silico studies. In total, we have synthesized more than hundred compounds and some of these exhibited the potent antimalarial activity aginst sensitive as well as resistant strain of *P. falciparum*. The results illustrated that the computational approaches and conjugates formation i.e. combination of qunoline-triazole with flanking substituent with promosing biological application into a single molecule is a prominent approach for the development of chemotherapeutic agents against these malarial infection.