Name of the Scholar: Shoaib Manzoor
Name of the Supervisor: Prof. Nasimul Hoda
Name of the Department/Centre: Department of Chemistry,
Topic of Research: In Silico Design, Synthesis and Biological Screening of Anti-Neurodegenerative Agents

ABSTRACT

The present research work deals with the design of new multitarget-direct ligands (MTDLs), synthesis and biological screening against Alzheimer's disease and other neurodegenerative diseases. The thesis described the design and synthesis of different series of new MTDLs for Alzheimer's disease treatment (AD). The thesis also described the design and synthesis of new neuroprotective agents, anti-neuroinflammatory agents and carbonic anhydrase (CA) inhibitors. All the synthesized compounds were validated by ^{1}HNMR, ^{13}CNMR, HRMS, and some the compounds were structurally validated by X-Ray single diffraction analysis. Most of the synthesized compounds displayed moderate to excellent *in vitro* enzyme inhibitory activity against AChE at nanomolar to micromolar concentration. In this thesis, we have reported some dual inhibitors of AChE and *Aβ* inhibitors, and AChE and Tau inhibitors. Our study also indicated that most of the novel triazole-pyrimidine-based compounds displayed promising neuroprotective and anti-inflammatory properties. The study also suggested the benzene and benzothiazole-sulfonamide derivatives displayed remarkable inhibitory activity CA. In summary, the present thesis addresses the synthesis of designed compounds that hit two or more targets in AD and other neurodegenerative diseases. Altogether, the thesis provides preclinical evidence that the lead molecules are therapeutic agents of high potency with multiple functions against AD and other neurodegenerative diseases.