Name: Shaban Ahmad **Notification No: 574/2025**

Name of the Supervisor: Dr Khalid Raza **Date of Award: 07-02-2025**

Topic: AI-based Predictive Modelling and Molecular Enumeration against Lung Cancer

Department / Faculty: Computer Science, Faculty of Sciences.

Findings from PhD Thesis: Lung cancer remains one of the deadliest forms of cancer, claiming over 1.8 million lives annually, with projections exceeding 3.2 million by 2050. My research leveraged artificial intelligence (AI) to accelerate drug discovery, focusing on multitargeted drug identification. We identified Imidurea, Tiaprofenic Acid, and Theodrenaline through computational methods and attempted experimental validation. Using ChEMBL and PubChem Lung Cancer BioAssay data with a stringent 5.0 μM threshold, we generated a dataset of 26,396 compounds and applied advanced deep learning models—Residual Neural Network, Feed Forward Neural Network, and Recurrent Neural Network—achieved near-perfect accuracy (0.99–1) in predicting highly active compounds. Docking studies against ALK, HSP5, KRas, MMP-8, and tRNA DHDS2 identified three potent candidates (PubChem CIDs 144074375, 440810382, and 48426893) with strong docking and MM/GBSA scores. Additionally, molecular enumeration strategies led to the discovery of Ammetazebenpro, Pheammethpuzetidine, and Amthofluoquinoxaline, which exhibited superior efficacy compared to Erlotinib (FDA-approved). DFT, pharmacokinetics, WaterMap, and MD simulations confirmed their stability and enhanced potency. Notably, Pheammethpuzetidine showed the highest binding stability and lowest free energy values. These findings suggest these novel compounds possess up to five times greater therapeutic potential than Erlotinib, supporting their advancement for preclinical and clinical evaluations.