Synthesis, Characterization and Biological Evaluation of Some Fused Heterocyclic Derivatives

A Thesis

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by

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Summary

Chapter 1: I have synthesized 27 novel drivatives of piperidine-indole with amide and urea linkage in the 1st chapter of this thesis. All compounds are characterized at NIH US in total 60 cell lines. In which Compound **9c**, **11d**, **13b**, and **13e** had noteworthy anticancer effects against kidney cancer (UO-31). Compound **11f** demonstrated noteworthy anticancer action against breast cancer (MDA-MB-468) and leukemia (RPMI-8286), with inhibition levels indicating their potential for therapeutic use. While compound **9j** (SNB-75) had efficacy against CNS cancer. All 27 compounds are characterised by TLC, LC-MS, ^{1}H NMR, ^{13}C NMR, IR, Elimental analysis and Melting point.

Chapter 2: I have synthesized 14 novel drivatives of piprazine-benzoxazole with amide linkage in the 2nd chapter of this thesis. All novel compounds are characterized by antimicrobial activity. In which Compounds **9b** and **9f** shows highest active in both gram positive and gram negetive pathogens in antimicrobial activity. All compounds are characterised by TLC, LC-MS, ^{1}H NMR, ^{13}C NMR, IR, Elemental analysis and melting point. Compounds **9b** and **9f**, which shows the highest docking scores of -7.7 kcal/mol and -7.8 kcal/mol respectively. With the exception of compounds **9k** and **9l**, which had molecular weights more than 500, all produced compounds adhered to Lipinski's rule of five. Interestingly, the lipophilicity ratings of all benzoxazole derivatives ranged from 1.94 to 4.31. Using SwissADME, the computational analysis was carried out.

Chapter 3: A series of hybrid naphthalene-imidazole derivatives was synthesized in the 3rd chapter of this thesis. All novel compounds are characterized by antimicrobial activity. In which compounds **9k** and **9p** shows highest active in both gram positive and gram negetive pathogens in antimicrobial activity. All Compounds are characterised by TLC, LC-MS, ^{1}H NMR, ^{13}C NMR, IR, Elemental analysis and melting point. Also compounds **9k** and **9p** both had significant antibacterial action, achieving the highest docking scores of -8.7 kJ/mol and -8.5 kJ/mol, respectively.

Chapter 4: A series of hybrid furan-indoline and pyrrole-indoline derivatives were synthesized in the 4th chapter of this thesis. All compounds are characterized by TLC, LC-MS, ^{1}H NMR, ^{13}C NMR, IR and Elemental analysis. Compound **6k** possesses the greatest binding affinity (-8.4 kcal/mol) in the **6a-k** series. While compound **13e**

possesses the greatest binding affinity (-9.8 kcal/mol) in the **13a-k** series. Also these both compounds are more active in gram-positive and gram-nagetive pathogens.