Abstract of Ph.D. Thesis (Chemistry) of Siji T. B. entitled

SYNTHESIS, CHARACTERISATION AND APPLICATIONS OF SOME NITROGEN AND SULPHUR BASED HETEROCYCLES

Cyclic organic compounds with at least one hetero atom in the ring structure are known as heterocycles. Major parts of the living cells are composed of heterocycles that play vital roles in various biochemical processes. Heterocyclic compounds are the major constituent of various drugs including antimalarial, antimicrobial, antidiabetic, antidepressant, antibiotic and anti-HIV agents. Heterocyclic compounds exhibiting bio and chemiluminescent properties are used as fluorescent sensors.

The work presented in this dissertation consists of developing efficient synthetic strategies for some heterocyclic compounds and studying their applications. We describe the whole work in 7 chapters. Since majority of the synthetic transformations presented in this dissertation utilises β-oxodithioesters, a review of its synthetic utility has been described in **chapter 2**.

The synthesis, characterisation and applications of chromene-2-thiones have been explained in **chapter 3**. Chromene-2-thiones have been synthesised from β-oxodithioesters. The protocol involves the synthesis of β-oxodithioesters followed by their conversion to chromene-2-thiones. For the conversion of β-oxodithioesters to chromene-2-thiones, we have developed two methods: conventional heating and microwave irradiation. Characterisation of the chromene-2-thiones has been carried out using elemental analysis, FT-IR, ^{1}H NMR, ^{13}C NMR, mass spectroscopy and single crystal XRD. *In vitro* cytotoxic activity of the compounds has been studied in cancer cell lines as well as in normal cell lines. The *in silico* molecular docking studies provided theoretical support for the anticancer activity.

Chapter 4 depicts the synthesis, characterisation and applications of 1,2-dithiole-3-thiones. Here, β-oxodithioesters were converted to 1,2-dithiole-3-thiones *via* microwave heating method. Microwave irradiation provided the product with high yields within a few minutes. The techniques such as FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy were used for the characterisation of the synthesised compounds. The *in vitro* cytotoxic activity of the compounds has been studied in cancer cell lines as well as in normal cell lines. *In silico* molecular docking studies provided theoretical support for the anticancer activity.

Chapter 5 describes the synthesis, characterisation and applications of dihydropyridine-2-thione and 3,4-diphenyl thiophene. The reaction between thioamide derived from β-oxodithioester was treated with chalcone to furnish dihydropyridine-2-thione. On the other hand, the reaction between β-oxodithioester and phenacyl bromide afforded 3,4-diphenyl thiophene. The characterisation and biological applications of the synthesised compounds are discussed in this chapter. Characterisation of the synthesised compounds has been carried out using FT-IR, ^{1}H NMR, ^{13}C NMR and single crystal XRD. The anticancer and antibacterial properties of the compounds were theoretically studied using *in silico* molecular docking method.

Chapter 6 gives a description of the synthesis, characterisation and applications of triazoles, triazole functionalized coumarin and fluorene derivatives. The reaction between alkyne, sodium azide and excess of dihaloethane in the presence of copper supported polymer catalyst CuPVPNNMBA yielded 1,2,3-triazole. CuPVPNNMBA catalysed reaction between phenylacetylene, sodium azide and chloromethyl coumarin afforded highly fluorescent triazole functionalized coumarin. Triazole functionalized fluorene, a thorium ion detector, has been synthesised by the reaction between 2-acetylfluorene, phenylacetylene and sodium azide in the presence of catalyst CuPVPNNMBA. 2-Acetylfluorene on reaction with phenylisothiocyanate afforded fluorescent thioamide functionalized fluorene. The techniques such as FT-IR, ^{1}H NMR and ^{13}C NMR and mass spectroscopy were used for the characterisation of the synthesised compounds. The applications of the compounds as antibacterial agents and fluorescence detectors of metal ions have been studied. **Chapter 7** includes a summary and conclusion of the present work.