Organic chemists synthesize hundreds of new heterocyclic compounds every day. In most cases the chemist has specific reasons for synthesizing a particular compound, usually based on theoretical considerations, medicinal chemistry, biological mechanisms or a combination of all three. Heterocyclic compounds have known held center stage in the development of molecules to enhance quality of human life. For example, around seventy percent of drugs used today are heterocyclic compounds. The heterocyclic compounds are very widely distributed in nature and are very essential to living organisms. They play a vital role in the metabolism of all the living cells. Among large number of heterocycles found in nature, nitrogen heterocycles are the most abundant specially those containing oxygen or sulphur due to their wide distribution in nucleic acid illustration and their involvement in almost every physiological process of plants and animals. Heterocyclic compounds possess great applicability in industry as well as in our life in various ways.

Taking in view of the applicability of heterocyclic compounds, the present work was undertaken to synthesize some new heterocycles bearing Pyrrole, oxadiazole and oxadiazepine nucleus.

CHAPTER-I: Introduction to Biological Importance of Pyrroles, 1,2,4-Oxadiazoles and Oxadiazepines.

Chapter I deals with general introduction to of pyrroles, 1,2,4-oxadiazoles and oxadiazepines and their biological importance. A detailed review in this regard is presented.
CHAPTER-II: Synthesis, Characterization and Biological Evaluation of Tetra Substituted Pyrrole Analogue.

Chapter 2 deals with the useful protocol for the synthesis of tetra substituted pyrroles by employing graphite as a catalyst through one–pot four component condensation reaction of aromatic aldehyde, aromatic amine, ethyl acetoacetate and nitromethane as shown in (Scheme 42).

\[
\begin{align*}
\text{Scheme 42. Graphite mediated synthesis of functionalized pyrroles.}
\end{align*}
\]

Synthesized tetra substituted pyrrole derivatives were screened for anti-proliferative activity against different cell lines. Interestingly few of the synthesized compounds showed significant improvement in the cytotoxicity in K562 and HeLa cell lines in concentration dependent manner, in particular compound [134o] showed prominent cytotoxicity against K562 cell line. Herein, we report a mild and simple protocol for synthesis of tetra substituted synthesis of pyrrole derivatives [134 (a-o)] and their anti-proliferative activities against K562 and HeLa cell lines.

Compound [134o] which showed significant inhibition on cell cycle and mitochondrial membrane potential assay.
The main advantage of this method includes simplicity of the procedure, easy reaction work up, excellent yields, short reaction times, easy handling and use of ecofriendly, non-volatile, less expensive reagents are the advantages claimed by this method. The synthesized tetra substituted pyrrole derivatives were characterised by elemental analysis and spectroscopic techniques such as $^1$H NMR, $^{13}$C NMR, IR and mass spectra.

**CHAPTER-III: Synthesis, Characterization and Biological Evaluation of 3, 5 Substituted 1, 2, 4-Oxadiazole Analogues.**

Chapter 3 deals with the synthesis of 3,5 diaryl substituted 1,2,4-oxadiazole analogous. The 3,5 diaryl substituted 1,2,4-oxadiazole ring skeletons are described as bioisosteres for amides or esters as result of the increased hydrolytic and metabolic study of the ring, and is found in several drugs.

We are developed an efficient method for the synthesis of 3,5 diaryl substituted 1,2,4-oxadiazole derivatives using dithioester under heating condition in (Scheme51). All synthesized a new series of the 1,2,4-oxadiazole compounds were evaluated using a antimicrobial screen. The antimicrobial activity of the synthesized compounds may be due to the presence of mono and difluoro group linker and aryl group. The data revealed that compound $[172g]$ and $[172h]$ having mono and di fluoro linker between aromatic nucleuses showed antibacterial activity, which mean fluoro group linker is tolerated for activity. Compound $[172f]$ with 2-hydroxy-6-methylpyridine linker between aromatic nucleus and amide is also responsible for radical scavenger activity.
The synthesized 3,5 diaryl substituted 1,2,4-oxadiazole analogous were characterised by elemental analysis and spectroscopic techniques such as $^1$H NMR, $^{13}$C NMR and IR.

Scheme 51. Synthesis of 3, 5-diaryl 1,2,4-oxadiazole derivatives.
Compounds 172g and 172h showed good antibacterial activity against E. coli and B. subtilis.

Compound 172f showed highest radical scavenging property.

CHAPTER-IV: Synthesis and Characterization of 3-(aryl/alkyl Substituted),5,5-Difluoro-1,2,4-Oxadiazepin-4(5H)-yl(1H-Imidazol-1-yl)Methanone Derivatives.

Chapter 4 deals with the synthesis of heterocyclic molecules via, mild, and simple procedures is currently receiving considerable attention. Here we are developed the synthesis of 1,2,4-oxadiazepine from amidoximes with a 3,3,3-trifluoropropinoic acid, and CDI under mild conditions (Scheme 60).
Scheme 61. Synthesis of 3-(aryl/alkyl substituted), 5,5-difluoro-1,2,4-oxadiazepin-4(5H)-yl)(1H-imidazol-1-yl) methanone derivatives.
CHAPTER-V: Crystal and Molecular Structure Studies of Pyrrole Derivatives.

Chapter 5 deals with the synthesis, crystal and molecular structure studies of pyrrole derivatives

The chemical structure of the title compound [197] and [198]