ABSTRACT OF THESIS

One of the most fascinating families of synthetic compounds in organic chemistry are molecules with the quinoid structure that have a hydroxy group on the quinone ring. These molecules are also abundantly found in nature. Because of their pharmacological properties, naphthoquinone compounds in particular are receiving a lot of interest. One of the simplest naturally occurring naphthoquinones with a variety of uses is 2-hydroxy-1,4-naphthoquinone (Lawsone). Reactions of lawsone, which have been thoroughly described in several studies, have made it feasible to synthesize a wide range of physiologically active chemicals that may be used to treat a variety of illnesses in addition to the normal application of lawsone as a hair and skin colour. Because of this, further research into this molecule's chemistry is necessary.

The creation of novel derivatives of the naturally occurring substance 2-hydroxy-1,4-naphthoquinone (Lawsone) and their metal complexes was the aim of the research that went into this thesis in order to learn more about their biological properties and potential applications in catalysis. Five sections make up the bulk of the thesis. The synthesis of novel Mannich bases and their Structure Activity Relationship (SAR) are covered in **Chapter 2**. The chemistry of complexes generated from Mannich bases of lawsone is discussed in Chapters 3 and 4, along with their use in anticancer and antibacterial activity, as well as interactions with biomolecules including DNA and BSA. Chapter 5 discusses the production and application of lawsone vanadium complex for catalytic oxidation. A study of the synthesis, anticancer effectiveness, and molecular docking of novel isoindolinones is presented in Chapter 6's conclusion.

Chapter 2 comprises the synthesis, characterization, and investigation of anticancer activity of a series of 3-aminomethyl-1,4-naphthoquinone (Mannich bases) derived from lawsone via a one-pot multicomponent Mannich reaction. The structure of compounds was confirmed by ^{1}H NMR, ^{13}C NMR, FT-IR, Mass spectrometry, and elemental analysis along with single crystal XRD. The IC_{50} values were determined by MTT assay on HepG2 cell line and structure activity relationship (SAR) was established. The compounds exhibited good to moderate activity and were found to be hemocompatible. The DAPI and AO/EB staining of the most effective drugs revealed that cytotoxicity was caused by the induction of apoptosis.

In **Chapter 3**, a number of low- or no-activity Mannich bases from chapter 2 are converted into a range of anticancer-active Cu(II) and V(IV) complexes. These synthetic compounds' structures were established using a variety of spectroscopic methods. The redox properties of the complexes were studied by cyclic voltammetry (CV). The complex comprising copper atoms was found to have slightly distorted square planar geometry using single crystal X-ray diffraction analysis, which was further verified by EPR analysis. A few significant parameters, including bond length, bond angle, HUMO and LUMO energy gap (ΔE), and MEP diagram were also determined using theoretical DFT analysis. With the use of UV-vis and florescence methods, the interactions of complexes with biomolecules (CT-DNA and BSA) were

thoroughly studied to show their biological potential. Additionally, the in vitro anticancer activity of particular complexes based on DFT research was successfully assessed against HepG2 utilising the MTT assay in conjunction with the assessment of apoptosis (AO/EB staining). This information demonstrated that incorporation of metal ion to an organic Mannich base increases the potency of a possible medication candidate and comparable to standard drug.

On the basis of the findings from chapter 3, chapter 4 discusses novel V(IV), Ru(II), and Ni(II) metal complexes that were successfully synthesised with the oxygen and two nitrogen atoms (ONN) donor Mannich base ligand. Various spectroscopic and analytical techniques and essential geometry optimization parameter mentioned in chapter 3 confirms the formation of complexes. The intercalative and groove binding interactions of complexes with biomolecules such as CT-DNA and BSA were verified using UV-visible and fluorescence spectroscopy. V(IV) and Ru(II) complexes clearly exhibit the strongest interaction with both DNA and BSA, according to all known spectroscopic techniques, whereas Ni(II) complex showed very weak contact. DFT analysis supported the experimental findings. The cytotoxic potential evaluated against HepG2 cell line revealed Ru(II) complex has higher activity. Ruthenium complex also showed antibacterial activity against B. Subtilis and S. Aureus bacteria.

In **Chapter 5**, a vanadium (IV) complex was created from naturally occurring lawsone and characterised using a variety of spectroscopic methods, including powder XRD, FTIR, UV, and mass spectrometry. Additionally, DFT computations verified the complex's creation and established the optimised geometry. Furthermore, it was used for the high conversion and 92% isolated yield of diphenylmethane with TBHP at 50°C in acetonitrile. Additionally, it preferentially transforms substituted arylalkanes into the appropriate ketones. This study can be studied for various substituted arylalkanes and in organic synthesis, and it may offer some guidelines for future use.

In **Chapter 6**, we have developed an effective method for the synthesis of physiologically active substituted isoindolinone via a three-component Mannich cascade cyclization reaction. This method has the advantage of using an environmentally friendly solvent, acetic acid as a catalyst, and a workup procedure without the use of column chromatography. The molecular structure, dipole moment, MEP maps, and global reactivity parameters of synthesised compounds were all calculated using DFT. The ADME parameters revealed that compounds have good bioavailability. Additionally, the MTT test was used to assess the in vitro anticancer potential of chosen drugs against HepG2 cell line. The substances with high activity were even more substantiated by molecular docking on Alpha fetoprotein (AFP).This is a serum tumour biomarker of disease and is a liver cancer-associated protein showed interaction via hydrogen bonding. It was also examined for *in vivo* research and found to be effective as an anticancer drug.