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***Thesis Title*: Design and Synthesis of Multifunctional Biomimetic Metal Complexes: Some Having Application as Chemotherapeutic Agents, Some as Radio-protective Agents**

This thesis focuses on the design and synthesis of multifunctional biomimetic complexes with immense potential as chemotherapeutic and radio-protective agents. Among these complexes, some exhibit remarkable anticancer properties, while others possess the unique ability to safeguard DNA against radiation-induced damage. To establish their multifunctionality, rigorous testing was conducted to evaluate their capability to mimic Haloperoxidase enzymes, further enhancing their versatility in application.

The synthesis and characterization of a novel [Mn^{II}(sal-oxime)$_2$(H_2O)$_2$] complex were carried out using various spectroscopic techniques, including IR, UV-vis, ESI-MS, and EPR studies. Molecular geometry was determined through DFT calculations, which showed excellent agreement with experimental results. Physicochemical investigations, such as UV-vis spectroscopy and viscosity measurements, provided compelling evidence of the complex's interaction with DNA. These findings were further supported by molecular docking studies. Notably, the compound exhibited significant nuclease activity, as demonstrated by the Gel electrophoresis technique.

Additionally, detailed synthesis and characterization were conducted on Dioxomolybdenum complexes [*cis*-MoO_2(BHAN)$_2$ and *cis*-MoO_2(OV)$_2$] employing *β*-hydroxy-*α*-naphthaldehyde (BHAN) and ortho-vanillin (OV) as ligands in different chapters. Thorough characterization involved IR, UV-vis, ESI-MS, NMR, and single-crystal X-ray crystallographic analysis for *cis*-MoO_2(OV)$_2$. DFT studies were employed to establish the molecular geometry, with TD-DFT calculations validating experimental observations.

The ligands BHAN and OV, along with the complexes *cis*-MoO_2(BHAN)$_2$ and *cis*-MoO_2(OV)$_2$, demonstrated their ability to protect calf thymus DNA and pUC19 plasmid DNA against radiation-induced damage. Emission spectral studies, as well as viscosity measurements, were employed to determine the binding affinities and mode of binding of the ligands and complexes with DNA. The results indicated that

both complexes interacted with calf thymus DNA through the groove. Furthermore, since radicals produced during radiolysis contribute significantly to DNA damage, the complexes' capacity to scavenge these radicals was assessed using EPR spectroscopy. Encouragingly, both complexes displayed considerable potential as reliable radioprotective agents for normal tissues during radiotherapy.

Moreover, an investigation into the Haloperoxidase (HPO) mimicking properties of the synthesized Mo-complexes, *cis*-$MoO_2(BHAN)_2$ and *cis*-$MoO_2(OV)_2$, was conducted. Specifically, their ability to catalyze the single-pot bromination of phenol red to bromophenol blue was evaluated. The results unequivocally confirmed the complexes' mimicry of HPO, exhibiting positive responses and demonstrating catalytic activity. This study represents a significant advancement in the development of HPO mimics, with promising implications for future applications in catalysis.

Overall, this comprehensive research contributes valuable insights into the design and synthesis of multifunctional biomimetic complexes capable of serving as potent chemotherapeutic agents, radio-protective agents, and HPO mimics. The findings have significant implications for the advancement of multifaceted therapeutic approaches and hold great promise for the future of cancer treatment and radiation-induced damage protection for DNA during radiotherapy.

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04-Aug-2023.

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04/08/2023