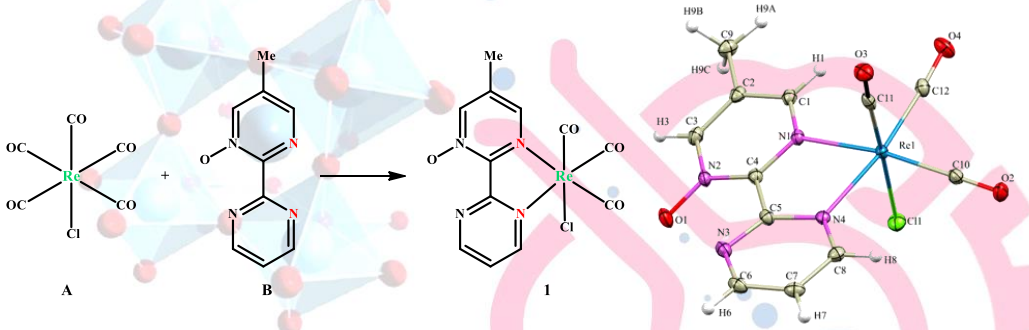
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A Bioactive Rhenium(I) Tricarbonyl Complex Bearing a Bidentate Nitrogen Ligand: Experimental and Theoretical Calculations

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Scheme 1: Synthetic route for the preparation of **1** (left) and its crystal structure (right).

Cancer continues to be one of the world's leading causes of mortality, despite the rising corpus of research. The majority of cancer treatments include photodynamic therapy and chemotherapy, with chemotherapy continuing to be the most successful method for increasing patient survival. But on the other hand, chemotherapy uses non-selective cytotoxic substances that cause cell death in both malignant and healthy tissue[1]. Platinum-based chemotherapy is used to treat more than 50% of cancers. Nevertheless, these medications suffer from serious flaws that hinder their effectiveness and show physiological side effects, such as toxicity toward healthy, non-tumorigenic cells and innate or acquired chemoresistance[2]. In this regard, organorhenium complexes possess several intrinsic properties advantageous for the development of novel anti-cancer drug candidates.

As shown in Scheme **1**, the reaction of $[Re(CO)_5Cl]$, **A**, *via* 5-methyl-[2,2'-bipyrimidine]-1-*N*-oxide (bpyNO) ligand afforded a new Re^I complex $[Re(CO)_3(bpyNO)Cl]$, **1**. The crystal structure of **1** was obtained, and this complex was characterized by means of several spectroscopic and analytical techniques, such as NMR and HR ESI-Mass. Also, theoretical calculations were carried out on this complex, and the *in vitro* cytotoxicity effect of **1** was investigated against a panel of cancer cell lines.

Keywords: Re(I) tricarbonyl complex, Nitrogen donor ligand, Theoretical elucidation, Biological investigation.

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