The role of single crystal diffraction in rhenium complexes having biomedical relevance

Chiranthy Kaushalya and **Theshini Perera**

Email; theshi@sjp.ac.lk

Department of Chemistry, University of Sri Jayewardenepura, Colombo, Sri Lanka.

The focus would be on rhenium complexes which have potential biomedical applications such as biological imaging and anti-cancer properties. The synthesis and characterization of novel sulfonamide complexes would be discussed with a special focus on S-N bond distances involving tertiary sulfonamide linkages. Previous work has paved the way by establishing that near normal Re-N bond distances were observed in crystal structures containing rhenium complexes bearing dipicolylamine based sulfonamide ligands. A significant part of drug discovery in the last forty years has been focused on agents to prevent or treat cancer. Neutral and cationic rhenium complexes providing both hydrophilic as well as hydrophobic properties bearing the robust tridentate ligand system of biphenyl sulfonyl dipicolylamine ($N(SO_2bip)dpa$) and biphenyl sulfonyl dien ($bipSO_2$-dienH) have been synthesized and when coordinated to the $[Re(CO)_3]^+$ core, hold a high potential for the development of metal base anti-cancer drugs. The obtained S–N bond length is comparable with the S–N bond lengths of 1.6194(11) Å for $N(SO_2pip)dpa$ and 1.602(9) Å for N-methyltoluene-p-sulfonamide. However that has not depicted by the shortening of S–N bond length in $N(SO_2bip)dpa$ as that of the most common cases.

Specific examples where single crystal diffraction and NMR spectroscopy have worked hand in hand to identify different isomers of rhenium tricarbonyl complexes bearing iminoether ligands and how structural characterization of a series of rhenium complexes bearing linear NNN donors paved the way to propose a mechanistic approach towards forming a novel insitu ligand will also be discussed.

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