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Synthesis and characterization of dipicolylamine sulfonamide ligands with iodobenzene and trifluoromethyl pyridine pendant groups and their rhenium tricarbonyl complexes

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The dipicolylamine (dpa) moiety has been used in synthetic inorganic chemistry as a tridentate coordinating ligand. Synthesis and study of rhenium complexes have also garnered interest due to non-radioactive rhenium being an analogue to technetium which is widely used as imaging agent used in medicinal chemistry. In this study synthesis of two novel sulfonamide ligands as well as their respective rhenium analogues was carried out. Formation of $N(SO_2(Iodobenz))dpa$ (L1) and $N(SO_2(tfm)py)dpa$ (L2) were confirmed by using spectroscopic techniques such as ^1H NMR spectroscopy, single crystal X-ray diffraction, UV-visible spectroscopy and FTIR spectroscopy. In ^1H NMR spectra of ligands in DMSO-d_6, a singlet peak given by methylene protons; 4.54 ppm for L1 and 4.66 ppm for L2, appeared as two doublets (C1; 5.56 and 4.59, C2; 5.66 and 4.72) in the rhenium complexes. Furthermore, structural data obtained from single crystal X-ray diffraction of ligands revealed that S-N bond distances of L1, 1.6205(14) and L2, 1.6366(15) are within the normal range of S-N bond distances. When considering UV-visible spectra in methanol, $\pi \rightarrow \pi^*$ transitions were observed for both ligands in the 200-265 nm range. In FTIR spectra, the S-N stretching observed at 916 cm^{-1} for L1 and 919 cm^{-1} for L2 are in an agreement with that of similar compounds. Ligands displayed good fluoresence in methanol. Utilizing $[Re(H_2O)_3(CO)_3]^+$ precursor, $[Re(CO)_3L1]PF_6$ (C1) and $[Re(CO)_3L2]PF_6$ (C2) were synthesized. Formation of C2 has been confirmed by single crystal X-ray diffraction data. Prediction of biological activity using Swiss TargetPrediction suggested that these ligands may be useful as prostaglandin G/H synthase enzyme inhibitors. Docking studies were done for ligands with human prostaglandin G/H synthase 2 enzyme (COX-2) using PyRx software and visualized with Discovery Studio. Results suggested that there is a high probability for binding with COX-2 enzyme hence can be pursued as anti-inflammatory drug leads.