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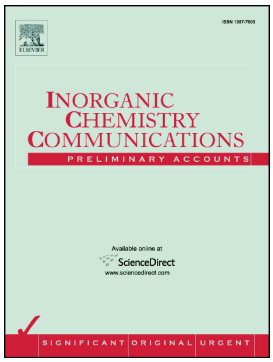

(Pyrazolyl)pyridine ruthenium(III) complexes: Synthesis, kinetics of substitution reactions with thiourea and biological studies

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(Pyrazolyl)pyridine ruthenium(III) complexes: Synthesis, kinetics of substitution reactions with thiourea and biological studies

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Abstract

Reactions of 2-bromo-6-(3,5-dimethyl-1H-pyrazol-1-yl)pyridine (**L1**), 2,6-di (1H-pyrazol-1-yl) pyridine (**L2**) and 2,6-bis(3,5-dimethyl-1H-pyrazol-1-yl)pyridine (**L3**) with $RuCl_3 \cdot 3H_2O$ led to the formation of their respective metal complexes [$RuCl_3$(**L1**)] (**1**), [$RuCl_3$(**L2**)] (**2**) and [$RuCl_3$(**L3**)] (**3**). Solid state structure of complex **3** established the formation of a six-coordinate mononuclear compound in which **L3** is tridentately bound. The order of reactivity of the studied complexes with thiourea (**TU**) nucleophile is in the form **1** > **2** > **3**, in line with density functional theory (DFT) studies. The complexes displayed minimal cytotoxic activity against the HeLa cell line, consistent with molecular docking experiments which showed weaker DNA binding affinities.

Keywords: ruthenium complexes; ligand substitution; cytotoxicity, anti-cancer activities; DFT; molecular docking

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