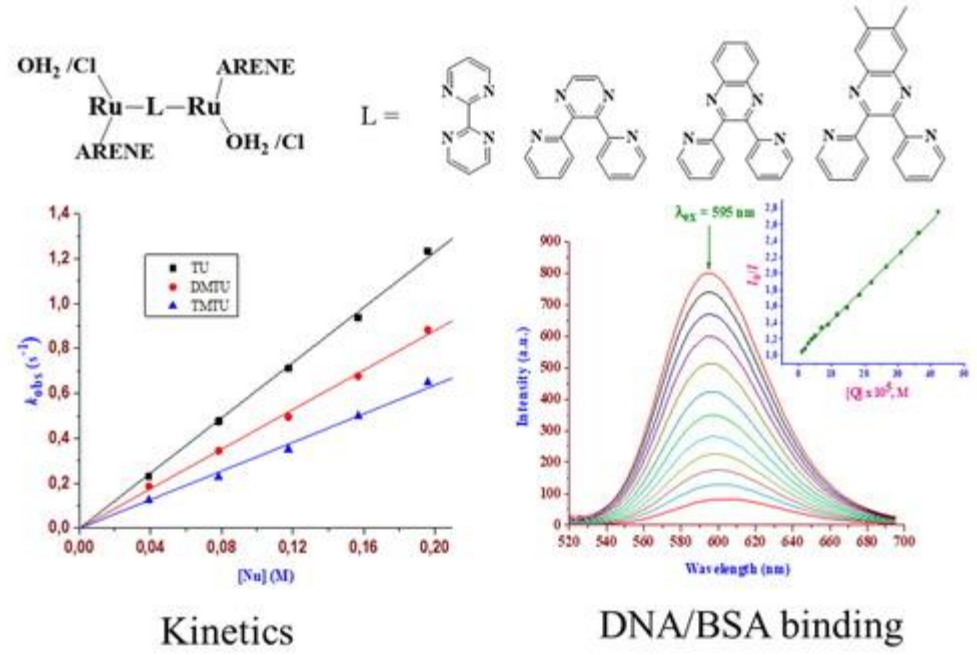
The role of N,N-chelate ligand on the reactivity of (?(6)-p-cymene)Ru(II) complexes: kinetics, DNA and protein interaction studies.

Abstract.

This study reports the kinetic studies of aqua complexes (**Ru1–Ru6**) as well as the calf-thymus DNA (CT-DNA) and bovine serum albumin binding studies of their chloro derivatives (**Ru7–Ru11**). The rate of substitution of the aqua ligand(s) in **Ru1**–**Ru6** by thiourea nucleophiles (thiourea, *N,N*-dimethylthiourea and *N,N,N′,N′*-tetramethylthiourea) in 0.1 M $HClO_4$/$NaClO_4$ aqueous medium was investigated as a function of nucleophile concentration and temperature under *pseudo*-first order conditions. The reactivity of the binuclear and mononuclear complexes decreased in the order **Ru3** > **Ru4** > **Ru5** > **Ru6** and **Ru1** > **Ru2**, respectively. The trend in reactivity of the binuclear complexes showed a dependence on the electronic and static factors of the rigid N,N-chelate bridging ligand in the complexes. The reactivity trends are well supported by the DFT-calculated data. The activation parameters ($\Delta H^{\neq} > 0$, $\Delta S^{\neq} < 0$) for the substitution process in all complexes support an associative mechanism of activation. The complexes effectively bind to CT-DNA *via* intercalation and this was corroborated by the molecular docking results. Likewise, the complexes bind favorably with bovine serum albumin. The order of CT-DNA and bovine serum albumin interactions with these complexes are in line with the trends in aqua ligand substitution.



Kinetics DNA/BSA binding

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