The continual development of drug design has lead to an interest in the methods utilised to coordinate biomolecules to technetium and rhenium for potential use as therapeutic or diagnostic radiopharmaceutical agents. The trend in the design of new radiopharmaceuticals is often conducted with a “hit-and-miss” approach. A logical approach to the synthesis of new pharmaceuticals can be accomplished by a good understanding of the transition metal chemistry of the specific reagents involved. [1]

One of the appealing features of Alberto’s fac-[M(CO)₃(H₂O)]⁺ complex (M = Tc, Re), is the ease whereby the aqua ligand can be substituted by a variety of ligands to produce potential radiopharmaceuticals [2]. As the fac-[M(CO)]³⁺ core accepts many types of ligands, [3-5] it is possible to design bifunctional chelator ligand systems which may affect the hydro/lipophilic properties of the organometallic complex if the coordination and reactivity of the final complex is fully understood. Our study focuses on the fac-[M(CO)₃]⁺ complex using the {2+1} mixed ligand concept, [6] which allows the labeling of bioactive molecules containing monodentate or bidentate donor sites on to the tricarbonyl moiety. Several model complexes were synthesised and investigated for improving the linker possibilities between a biomolecule and the radionuclide. This study focuses on the kinetic and crystallographic properties of the fac[Re(L, L')(CO)]³⁺(S) complex. [7-9] The significant labilisation caused by the coordinated bidentate ligand and the isostructural behaviour of the crystallised complexes will be highlighted.