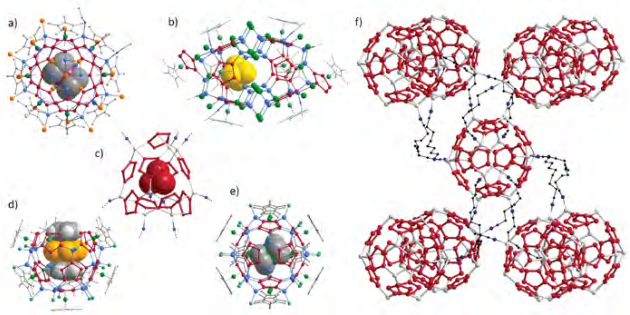

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Keywords: self-assembly, host-guest compounds, pentaphosphaferrocene

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Modifying the RheManTec Triad – a small molecule meanders into the macromolecular world

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Drug development can be approached from numerous angles especially when including the use of transition metal complexes. The utilisation of structural analysis in small molecules can provide a valuable platform whereby additional functionalization of the model pharmaceutical can be evaluated. Particularly when considering the possible bio-activity and receptor binding of the small molecule. Kinetic and mechanistic studies can further describe the coordination tendencies of the small molecule and is critical for understanding reactivity and stability which may be associated to the structural effects. Furthermore to expand the library of information into a system which realistically mimics a biological environment, structural analysis can be conducted by the combination of the small molecules with proteins in a methodology similar to fragment based drug development.

Our research interest is in the modification of bifunctional chelators coordinated to the tricarbonyl complexes of the group 7 Manganese Triad. Particular interest is focused on the radionuclides of ^{99m}technetium(I) and $^{186/188}$rhenium(I) for their application in diagnostic or therapeutic nuclear medicine. To this end we have meandered our way from a small molecule study, involving the kinetic and crystallographic properties of the *fac*-$[M(CO)_3]^+$ core (M = Re, Tc) and crossed over into the world of macromolecular crystallography. The coordination possibilities of multiple amino acid residues to the *fac*-$[Re(CO)_3]^+$ complex in a protein is described. Furthermore, the formation of mono-nuclear versus multi-nuclear complexes can be observed in both small molecule and macromolecular studies.

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