COORDINATION CHEMISTRY OF FUNCTIONALISED TRIAZACYCLONONANE LIGANDS AND APPLICATIONS IN ^{18}F PET IMAGING

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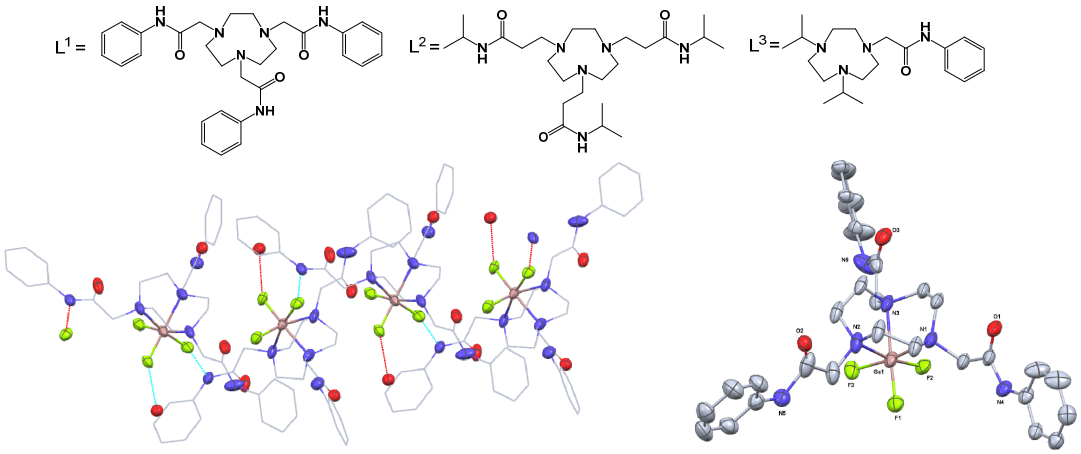
Limitations to ^{18}F-radiolabelling of traditional C-^{18}F based radiotracers for PET imaging have led to several advancements in the use of inorganic metal complexes as alternatives. [1] These allow for rapid and late-stage radiolabelling *via* halide or isotopic exchange. Due to their inherent fluorophilicity and the strength of the M–F bond, Group 13 metals are of particular interest. [2] These are often bound to aza-macrocycles, which offer increased thermodynamic and kinetic stability *via* the macrocyclic effect. Additionally, several d- and f- block metals have been considered as candidates. [3] Typically, these are metals which are stable in the +3 oxidation state (e.g. Fe^{3+}), but also includes metals which can access higher coordination numbers (e.g. Sc, Y and Lu).

This work focuses on complexes of functionalised triazacyclononane ligands. The nature of the pendant arm can influence the geometry, coordination number and behaviour of the ligand. We present the first metal fluoride complexes (M = Al, Ga, Fe) bound to amide-substituted tacn ligands (L^1, L^2, L^3). SCXRD data obtained for [$GaF_3(L^1)$] shows hydrogen bonding between amide NH groups and adjacent, neighbouring fluorine ligands. It is postulated that these hydrogen bonding interactions will enhance stability and assist with directing incoming ^{18}F to the metal centre – presenting an easy entry for ^{18}F into the metal coordination sphere. [4] Other pendant arms, including phosphinate, will also be investigated. It is thought that these may bind more favourably to metals with less Lewis acidity than the early Group 13 metals. Due to previously reported success with $BnMe_2$-tacn complexes of Ga and Fe, we will look towards radiolabelling the GaF_3 and FeF_3 amide-substituted tacn complexes. [5]



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