Electronic Supporting information

\[ \text{AlCl}_3(\text{BnMe}_2\text{-tacn}) \] – a new metal chelate scaffold for radiofluorination by Cl/F exchange

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Infrared spectra were recorded as Nujol mulls between CsI plates using a Perkin-Elmer Spectrum100 spectrometer over the range 4000–200 cm\(^{-1}\). \(^1\)H NMR spectra were recorded using a Bruker AV300 spectrometer. \(^{19}\)F\{\(^1\)H\} and \(^{27}\)Al NMR spectra used a Bruker AV400 spectrometer and are referenced (externally) to CFCl\(_3\) and aqueous [Al(H\(_2\)O)\(_6\)]\(^{3+}\) (pH 1), respectively. Microanalyses were undertaken by London Metropolitan University. AlCl\(_3\) was used as received (Sigma). BzMe\(_2\)-tacn\(^i\) was prepared via the literature method.

\[ \text{AlCl}_3(\text{BzMe}_2\text{-tacn})\]: AlCl\(_3\) (0.067 g, 0.50 mmol) was added to a solution of BnMe\(_2\)-tacn (0.13 g, 0.50 mmol) in CH\(_3\)CN (5 mL) at room temperature with stirring which leads to the rapid formation of a precipitate. After 30 mins. the solvent was removed by filtration. The white precipitate was washed with a small amount of CH\(_2\)Cl\(_2\) solvent and dried \textit{in vacuo}. Yield: 0.13 g, 66%. Required for C\(_{15}\)H\(_{25}\)AlCl\(_3\)N\(_3\): C, 47.3; H, 6.6; N, 11.0. Found: C, 47.0; H, 6.6; N, 11.2. \(^1\)H NMR (CD\(_2\)Cl\(_2\), 298 K): \(\delta\) 7.31 (m, [5H], ArH), 4.58 (s, [2H], Ar-CH\(_2\)), 3.54 (m, [2H], tacn-CH\(_2\)), 3.29 (m, [4H], tacn-CH\(_2\)), 2.92 (s, [6H], CH\(_3\)), 2.65 (m, [4H], tacn-CH\(_2\)), 2.28 (m, [2H], tacn-CH\(_2\)). IR (Nujol, v/cm\(^{-1}\)): 398, 385 (Al–Cl).
Figure S1. $^1$H NMR spectrum of [AlCl$_3$(BnMe$_2$tacn)] in CD$_2$Cl$_2$.

Figure S2. $^{27}$Al NMR spectrum of [AlCl$_3$(BnMe$_2$tacn)] in CD$_2$Cl$_2$. 
Figure S3. $^1$H NMR spectrum of [AlF$_3$(BnMe$_2$tacn)] in CD$_3$CN.

Figure S4. $^{19}$F-$^1$H NMR spectrum of [AlF$_3$(BnMe$_2$tacn)] in CD$_3$CN (the broad background is due to Teflon in the probe).
Figure S5. $^{27}$Al NMR spectrum of [AlF$_3$(BnMe$_2$tacn)] in CD$_3$CN.

Figure S6. Analytical radio-HPLC chromatogram of the crude product from reaction of [AlCl$_3$(BnMe$_2$tacn)] (1 mg, 2.63 μmol) in MeCN (0.6 mL) with 2.99 eq of KF doped with 0.4 mL of aqueous [$^{18}$F]F$^-$ at 80 °C for 30 mins. Peak 1: Rt = 2.54 min 91% ($^{18}$F$^-$). Peak 2: Rt = 6.68 min 9% ([Al$^{18}$F$_2$F$_2$(BnMe$_2$tacn)]).