Electronic Supporting information

$[AlCl_3(BnMe_2\text{-tacn})]$ – 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}. ^1H NMR spectra were recorded using a Bruker AV300 spectrometer. $^{19}F\{^1H\}$ and ^{27}Al NMR spectra used a Bruker AV400 spectrometer and are referenced (externally) to $CFCl_3$ and aqueous $[Al(H_2O)_6]^{3+}$ (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.

$[AlCl_3(BzMe_2\text{-tacn})]$: $AlCl_3$ (0.067 g, 0.50 mmol) was added to a solution of $BnMe_2$-tacn (0.13 g, 0.50 mmol) in CH_3CN (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_2Cl_2 solvent and dried *in vacuo.* Yield: 0.13 g, 66%. Required for $C_{15}H_{25}AlCl_3N_3$: C, 47.3; H, 6.6; N, 11.0. Found: C, 47.0; H, 6.6; N, 11.2. ^1H NMR (CD_2Cl_2, 298 K): δ 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, ν/cm^{-1}): 398, 385 (Al–Cl).

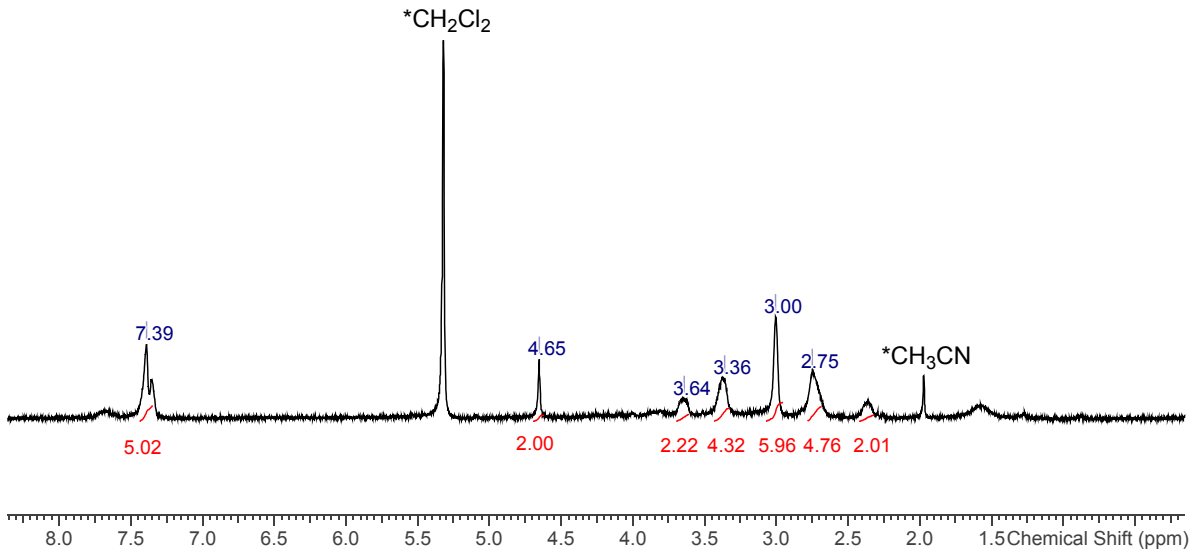

Figure S1. ^{1}H NMR spectrum of [$AlCl_3$($BnMe_2$tacn)] in CD_2Cl_2.

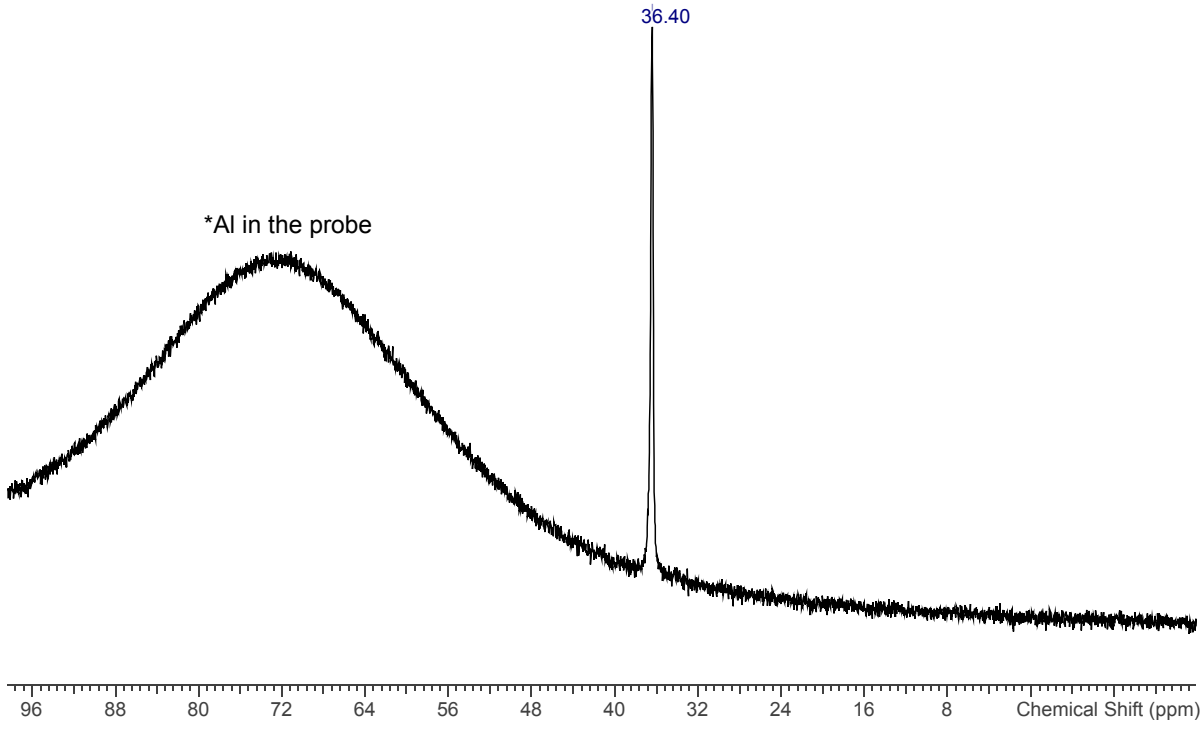

Figure S2. ^{27}Al NMR spectrum of [$AlCl_3$($BnMe_2$tacn)] in CD_2Cl_2.

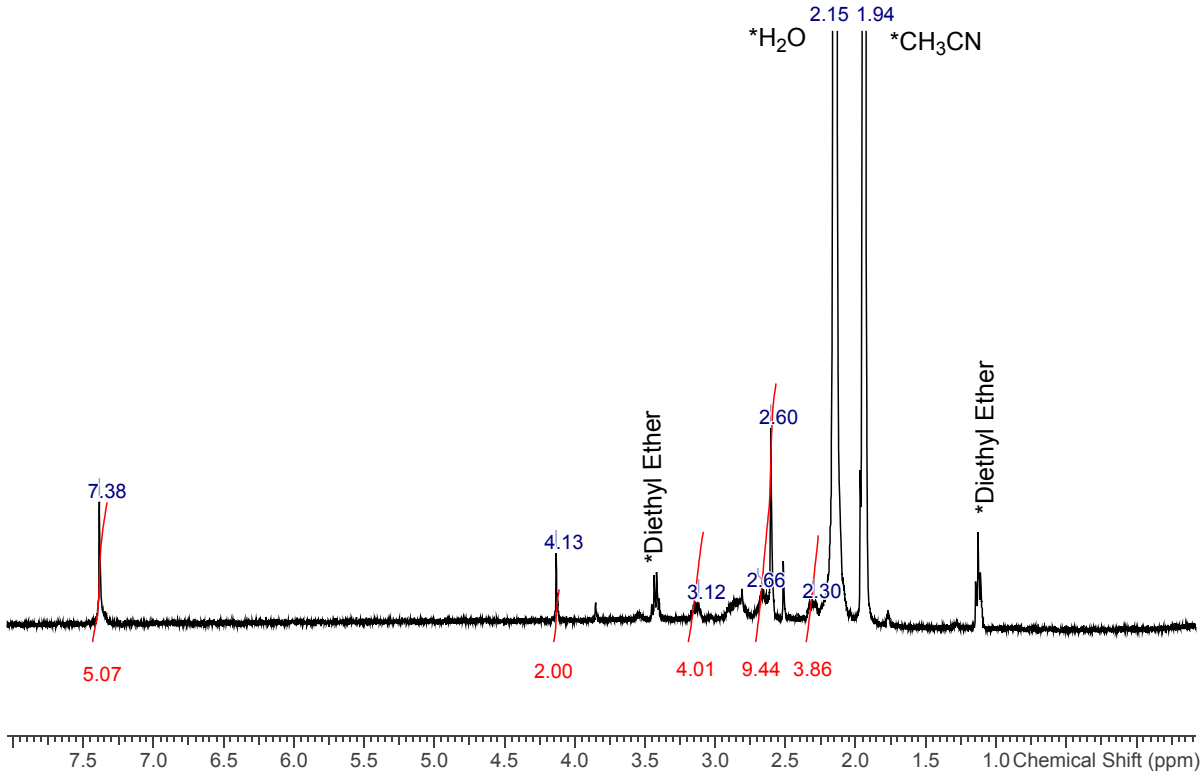

Figure S3. ^{1}H NMR spectrum of [AlF_3($BnMe_2$tacn)] in CD_3CN.

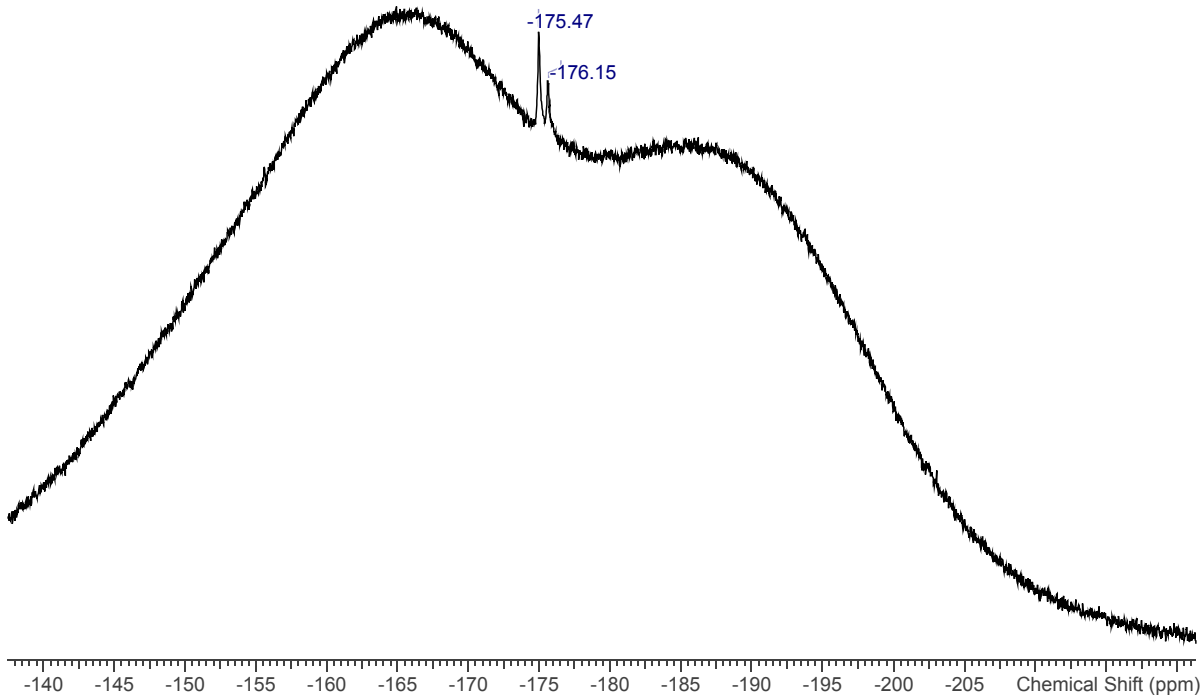

Figure S4. $^{19}F\{^{1}H\}$ NMR spectrum of [AlF_3($BnMe_2$tacn)] in CD_3CN (the broad background is due to Teflon in the probe).

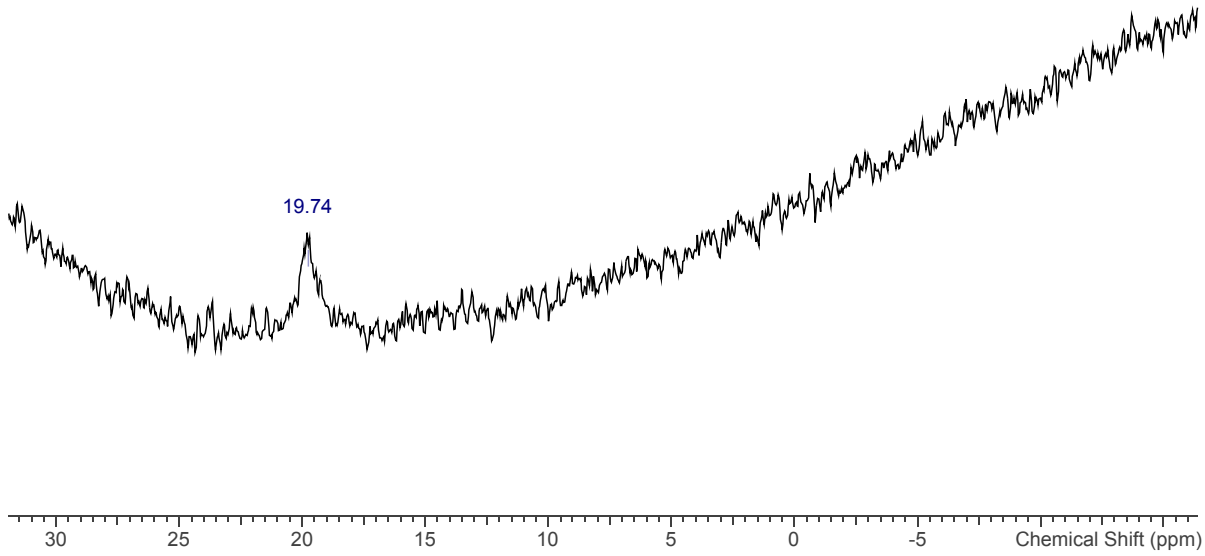

Figure S5. ^{27}Al NMR spectrum of [AlF_3($BnMe_2$tacn)] in CD_3CN.

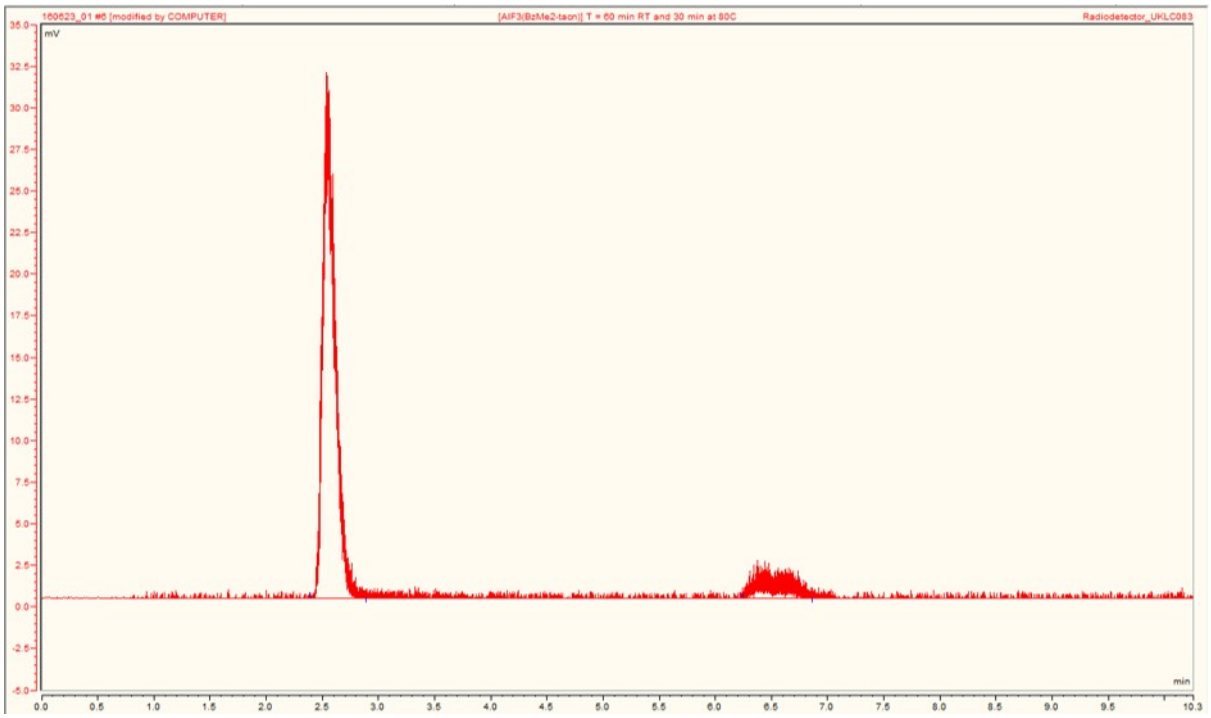

Figure S6. Analytical radio-HPLC chromatogram of the crude product from reaction of [$AlCl_3$($BnMe_2$-tacn)] (1 mg, 2.63 µmol) in MeCN (0.6 mL) with 2.99 eq of KF doped with 0.4 mL of aqueous [^{18}F]F^- at 80 °C for 30 mins. Peak 1: Rt = 2.54 min 91% ($^{18}F^-$). Peak 2: Rt = 6.68 min 9% ([$Al^{18}F^{19}F_2$($BnMe_2$tacn)]).

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i. M. J. Belousoff, M. B. Duriska, B. Graham, S. R. Batten, B. Moubaraki, K. S. Murray, L. Spiccia, *Inorg. Chem.,* 2006, **45**, 3746.