Supplementary Material (ESI) for Dalton Transactions

Supporting Information for:

Induction of B- to Z-DNA transition by copper and zinc complexes with C(15) substituted macrocyclic pentaaza ligands.

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The ligand **1** crystallised by vapour diffusion of CH_2Cl_2 and heptane into a solution of ethanol (Figure S1).

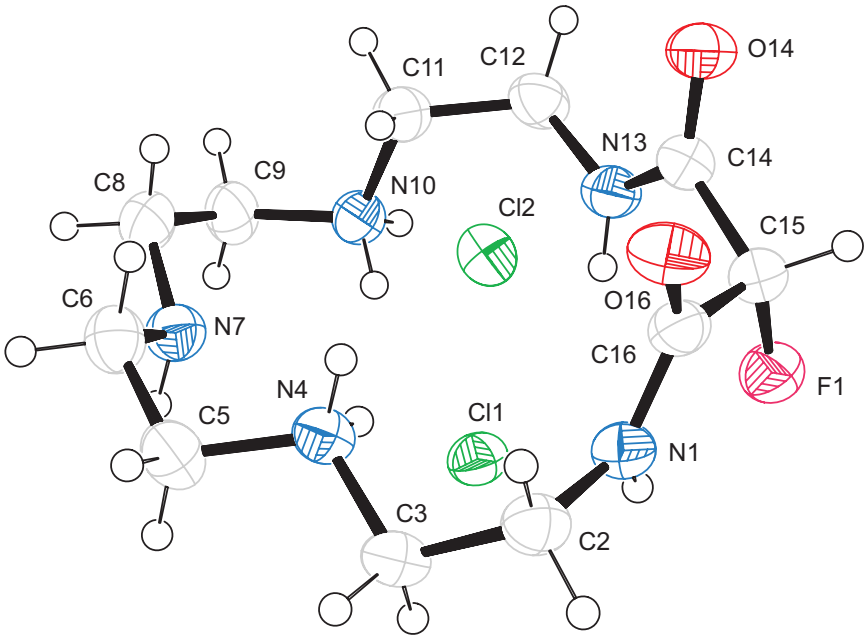

Figure S1. ORTEP plot of ligand 1. (ellipsoids drawn at 50% probability).

The complex crystallised as a di-hydrochloride due to chloride abstraction from the solvent. The fluorine atom is in an axial position relative to the macrocyclic ring. Most likely this arrangements minimises the overall dipole moment of the carbonyl groups and the carbon - fluorine bond.

Crystals of **2** were grown as a di-hydrochloride salt by slow evaporation of ethanol (Figure S2). The chlorine atoms come from the tetraethylenepentamine used for the cyclisation that was not completely hydrochloride-free. To remove the hydrochlorides, **2** was purified by ion-exchange chromatography over AMBERLYST A-26 OH. In the crystal, ligand **2** is sitting on a mirror plane. The fluorine atom is occupying the axial position while the methyl group is in the equatorial position.

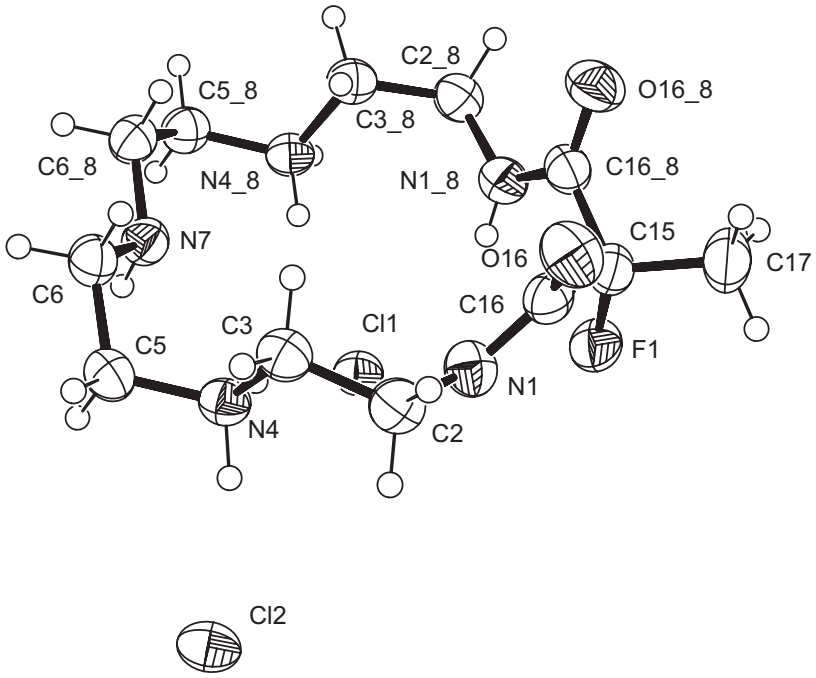

Figure S2. ORTEP plot of ligand 2. (ellipsoids drawn at 50% probability)

Ligand **3** crystallised by slow evaporation from an ethanolic solution. In the crystal structure the two carbonyl groups are pointing in opposite directions (Figure S3).

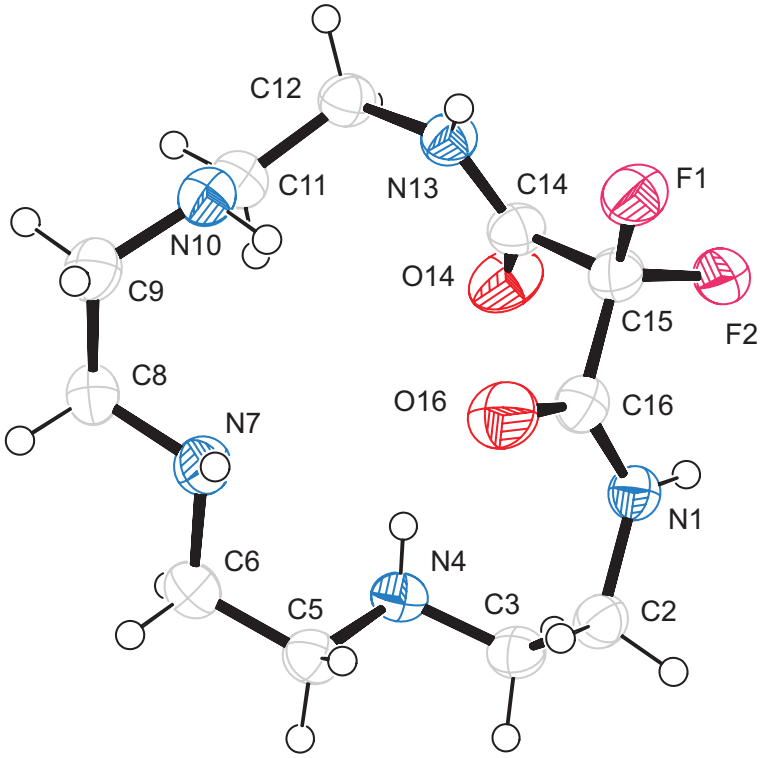

Figure S3. ORTEP plot of ligand 3. (ellipsoids drawn at 50% probability).

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Table S1: Crystallographic table for 1*2 HCl, 2*2 HCl, 3

	1*2 HCl	**2***2 HCl	**3**
Empirical formula	$C_{11}H_{24}Cl_2FN_5O_2$	$C_{12}H_{26}Cl_2FN_5O_2$	$C_{11}H_{21}F_2N_5O_2$
Colour	Colourless	Colourless	Colourless
Formula weight [g mol^{-1}]	348.25	362.28	293.33
Crystal system	Triclinic	Orthorhombic	Monoclinic
Crystal dimensions (mm)	0.19 x 0.14 x 0.11	0.67 x 0.50 x 0.38	0.63 x 0.60 x 0.12
Space group	P-1	Pnma	$P2_1/c$
a [Å]	9.2491(9)	10.8155(5)	9.8251(7)
b [Å]	9.902(1)	10.2095(5)	8.6399(5)
c [Å]	10.053(1)	16.5041(11)	16.781(1)
α [º]	82.753(12)	90	90
β [º]	82.007(12)	90	96.343(8)
γ [º]	65.594(11)	90	90
Volume [$Å^3$]	827.88(14)	1822.40(17)	1415.78(15)
Z	2	4	4
Absorption coefficient (μ, mm^{-1})	0.414	0.379	0.115
Theta range for data collection [º]	2.94 to 30.53	3.01 to 30.51	3.29 to 30.44
Reflections collected	17872	19450	18180
Independent reflections	4567 [R(int) = 0.0472]	2905 [R(int) = 0.0895]	4178 [R(int) = 0.0521]
Data/restraints/parameters	4567/1/218	2905/0/125	4178/0/201
Goodness-of-fit on F^2	1.110	1.057	1.123
Final R indices [I>2sigma(I)]	R1 = 0.0581	R1 = 0.0526	R1 = 0.0631
	wR2 = 0.1541	wR2 = 0.1508	wR2 = 0.1792
Largest diff. peak and hole (e $Å^{-3}$)	0.580 and –0.576	0.526 and –0.719	0.393 and –0.261

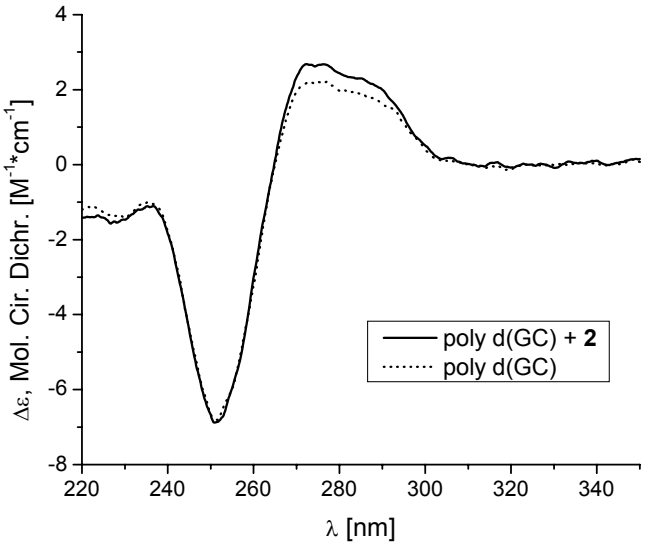

Figure S4. CD spectra of poly d(GC) before (dashed line) and after (straight line) the addition of ligand 2.