Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

DNA binding by pixantrone

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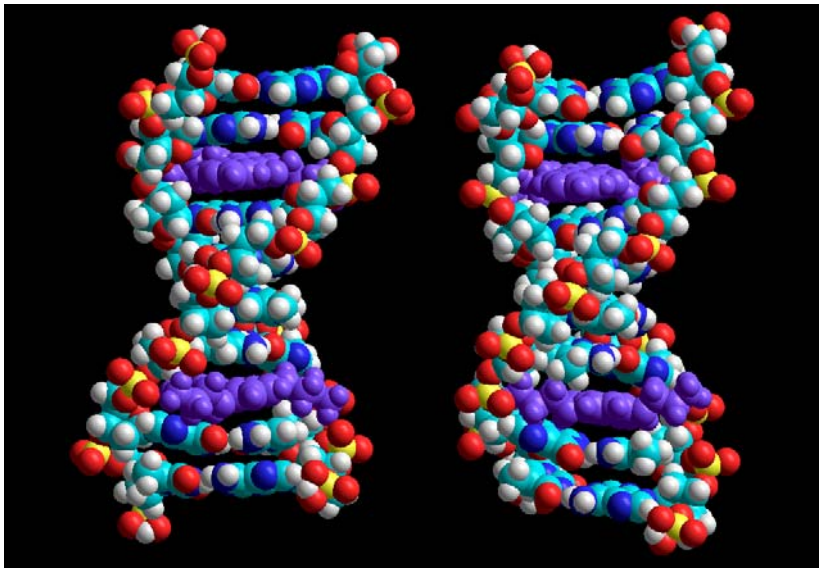
Supplementary Information Table 1	^{1}H NMR assignments of the resonances of free d(ACGATCGT)$_2$ and with added pixantrone at R = 0.6
Supplementary Information Table 2	^{1}H NMR assignments of the resonances of free d(A^{5Me}CGAT^{5Me}CGT)$_2$ and with added pixantrone at R = 2.0
Supplementary Information Figure 1	Models of two pixantrone molecules intercalated into the symmetric 5'-CG or 5'-^{5Me}CG sites in d(ACGATCGT)$_2$ and d(A^{5Me}CGAT^{5Me}CGT)$_2$.

Supplementary Information Table 1 ^{1}H NMR assignment of the DNA resonances of d(ACGATCGT)$_2$ with added pixantrone, at R = 0.6 molar ratio in pH 7 phosphate buffer at 25 ºC. Changes in chemical shift upon pixantrone binding are given in brackets, with a negative sign indicating an upfield shift.

Residue	**H8/H6**	**H2/H5**	**H1'**	**H2'**	**H2"**	Methyl
A_1	8.17 (-0.05)	7.87 (-0.16)	6.13 (-0.10)	2.58 (-0.05)	2.76 (-0.01)	
C_2	7.38 (-0.02)	5.35 (-0.10)	5.35 (-0.02)	2.11 (0.01)	2.32 (-0.03)	
G_3	7.88 (-0.02)		5.62 (-0.07)	2.68 (-0.03)	2.79 (-0.03)	
A_4	8.18 (-0.04)	7.77 (-0.05)	6.23 (-0.06)	2.60 (-0.05)	2.92 (-0.06)	
T_5	7.12 (-0.04)		5.89 (-0.04)	1.99 (-0.04)	2.42 (-0.01)	1.30 (-0.06)
C_6	7.40 (-0.02)	5.54 (-0.06)	5.72 (-0.01)	1.94 (-0.01)	2.36 (0.00)	
G_7	7.94 (-0.03)		5.98 (-0.09)	2.62 (-0.06)	2.72 (0.03)	
T_8	7.34 (-0.07)		6.18 (-0.05)	2.26 (-0.01)	2.26 (-0.01)	1.54 (-0.10)

Supplementary Information Table 2 ^{1}H NMR assignment of the DNA resonances of d(A^{5Me}CGAT^{5Me}CGT)$_2$ with added pixantrone at R = 2 in pH 7 phosphate buffer at 25 ºC. Changes in chemical shift upon pixantrone binding are given in brackets, with a negative sign indicating an upfield shift.

	H8/H6	**H2**	**H1'**	**H2'**	**H2"**	**Methyl**
A_1	8.18 (-0.02)	7.99 (-0.04)	6.11 (-0.10)	2.48 (-0.08)	2.76 (-0.05)	
C_2Me	7.21 (-0.02)		5.80 (0.43)	2.21 (-0.10)	2.30 (-0.04)	1.43 (-0.15)
G_3	7.92 (0.03)		5.45 (-0.18)	2.67 (-0.06)	2.72 (-0.00)	
A_4	8.21 (-0.03)	7.78 (-0.07)	6.20 (-0.10)	2.64 (-0.03)	2.84 (-0.11)	
T_5	7.07 (-0.11)		5.88 (-0.07)	1.67 (-0.26)	2.39 (-0.13)	1.23 (-0.14)
C_6Me	7.29 (0.02)		5.83 (0.20)	2.08 (-0.01)	2.36 (0.04)	1.59 (-0.14)
G_7	7.96 (-0.02)		5.96 (-0.11)	2.67 (-0.04)	2.76 (0.02)	
T_8	7.30 (-0.10)		6.18 (-0.07)	2.23 (-0.02)	2.23 (-0.02)	1.43 (-0.18)



Supplementary Information Figure 1 Energy minimised HyperChem models of two pixantrone molecules intercalated into the symmetric 5'-CG or 5'-^{5Me}CG sites in d(ACGATCGT)$_2$ (left-hand side) and d(A^{5Me}CGAT^{5Me}CGT)$_2$ (right-hand side). The pixantrone intercalative-binding is shown from the minor groove (top) and the major groove (bottom).