Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Structural analysis of the binding of the diquaternary pyridophenazine derivative dqdppn to B-DNA oligonucleotides

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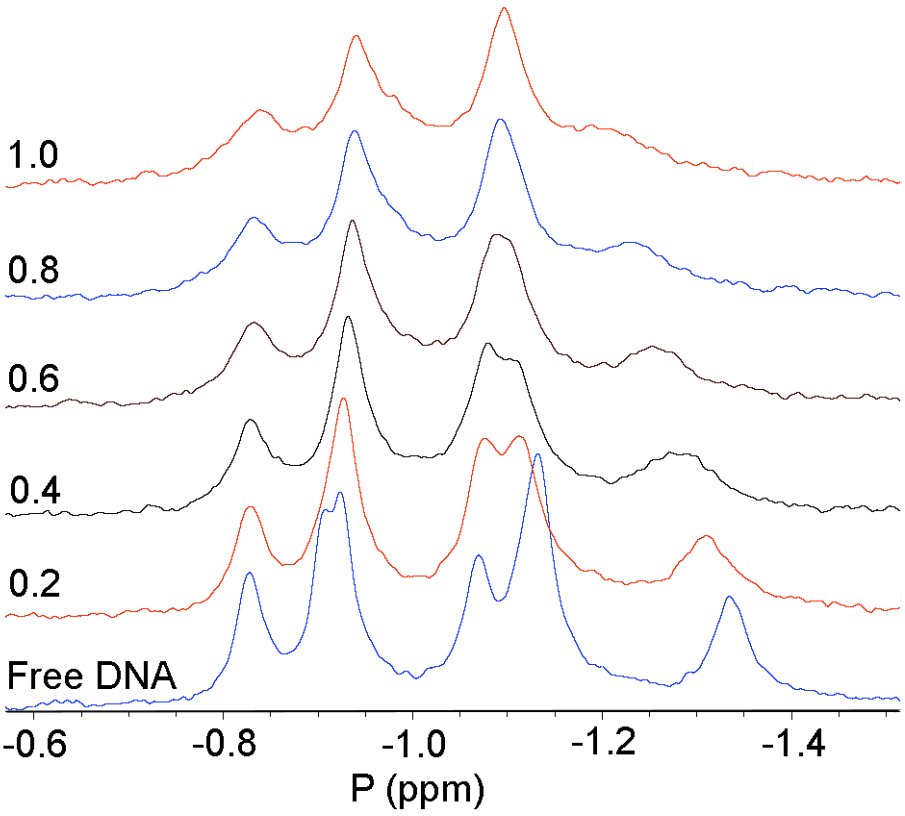
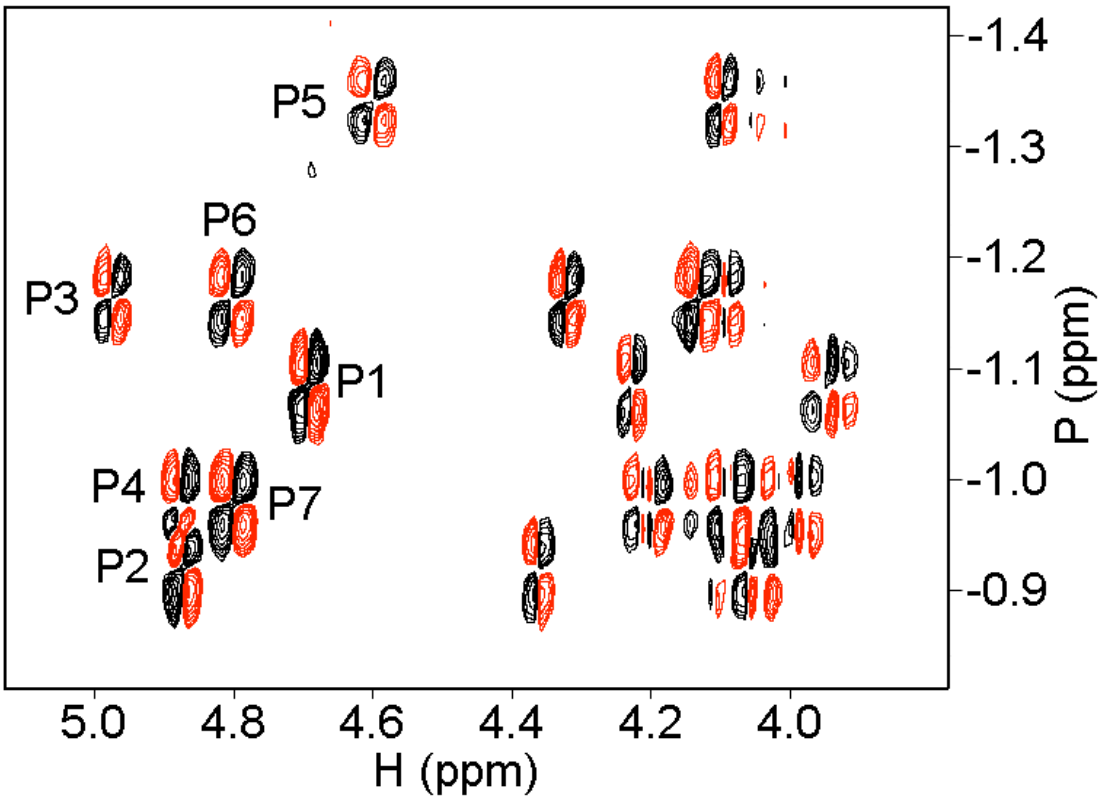
Supporting Information

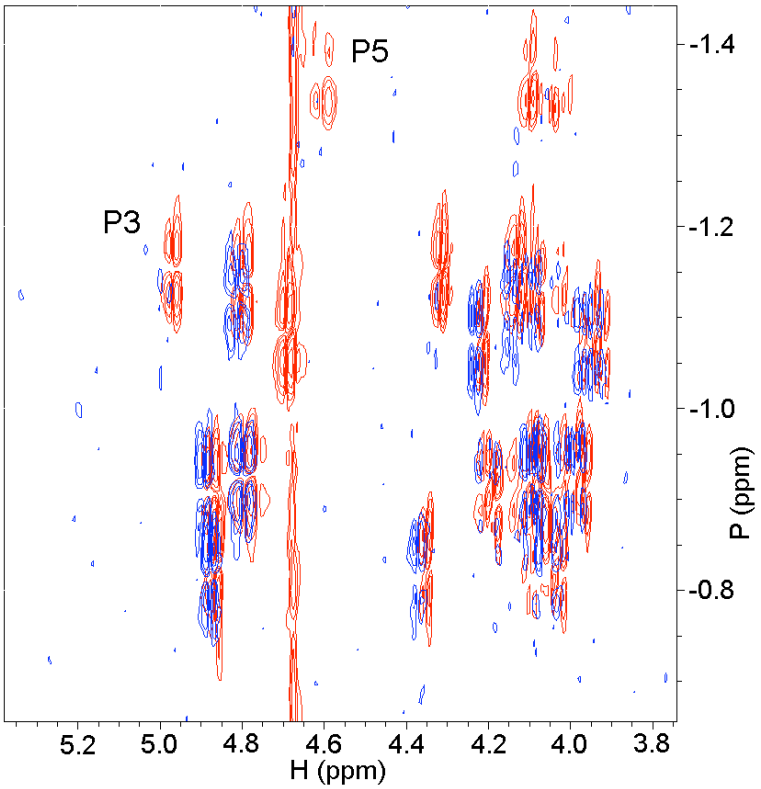
S1. The ^{31}P-^{1}H COSY spectrum of free d(AGAGCTCT)$_2$. The intra-nucleotide correlations between the ^{31}P nuclei of the phosphate groups and the H3' protons are labeled according to the position of the phosphate group.



S2. ^{31}P NMR experiments showing the step-wise addition of dqdppn to d(AGAGCTCT)$_2$. The amount of added ligand is indicated to the left of each spectrum (in molar equivalents).



S3. An overlay of the 2D $^{1}H/^{31}P$ correlation spectra of free $d(AGAGCTCT)_2$, shown in red, and the complex of this sequence with 0.2 molar equivalents of dqdppn, shown in blue.



S4. Intermolecular NOE contacts in the 2:1 complex formed by dqdppn and $d(GAGCTC)_2$

dqdppn	**$d(GAGCTC)_2$**					
	G1	A2	G3	C4	T5	C6
CH_2			1'	H6		
H1	2' / 2"					
H2	1'	2' / 2", 1', H8	2' / 2"	2', 2", 1'	2' / 2", 1'	2' / 2"
H3	1'	2' / 2", 1'	2' / 2"	2' / 2", 1'	Me, 2' / 2", 1'	2' / 2"
H4					Me	
H5	1'	2' / 2"		2' / 2", 1'	Me, 2' / 2", 1'	2' / 2", 1'
H6	1'			2', 2", 1'	Me, 2' / 2", 1'	2' / 2", 1'