Supporting Information

for

Molecular recognition of AT-DNA sequences by the induced CD pattern of dibenzotetraaza[14]annulene (DBTAA)–adenine derivatives

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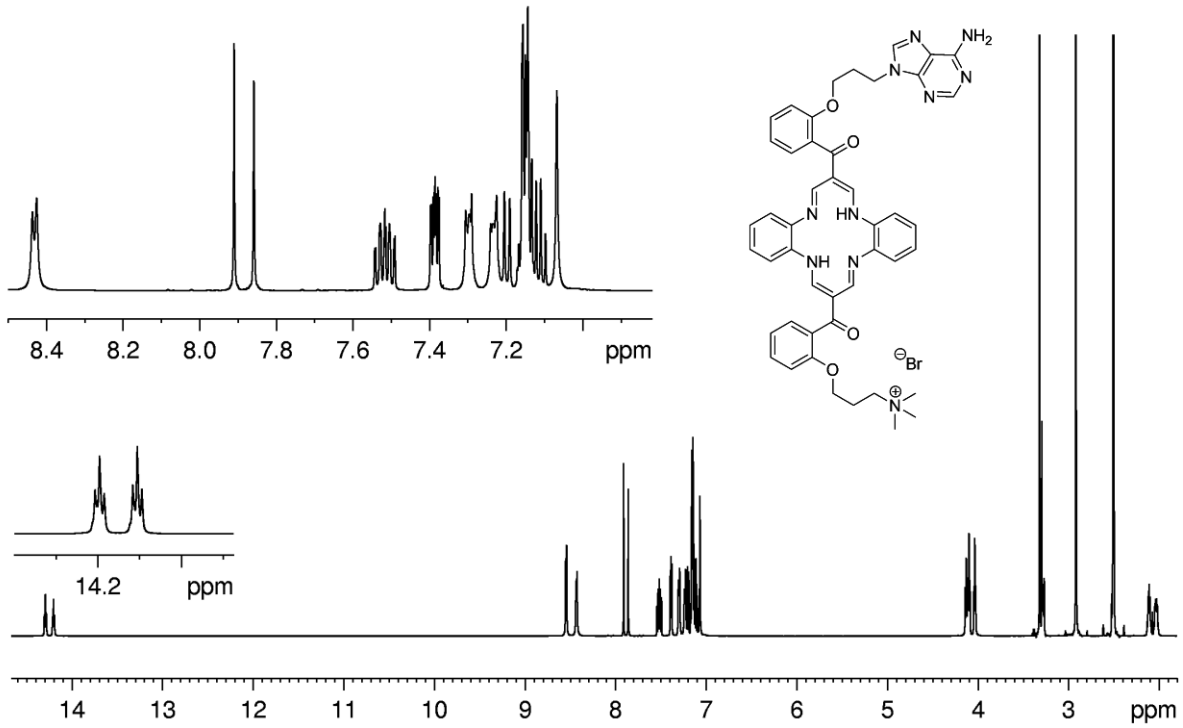
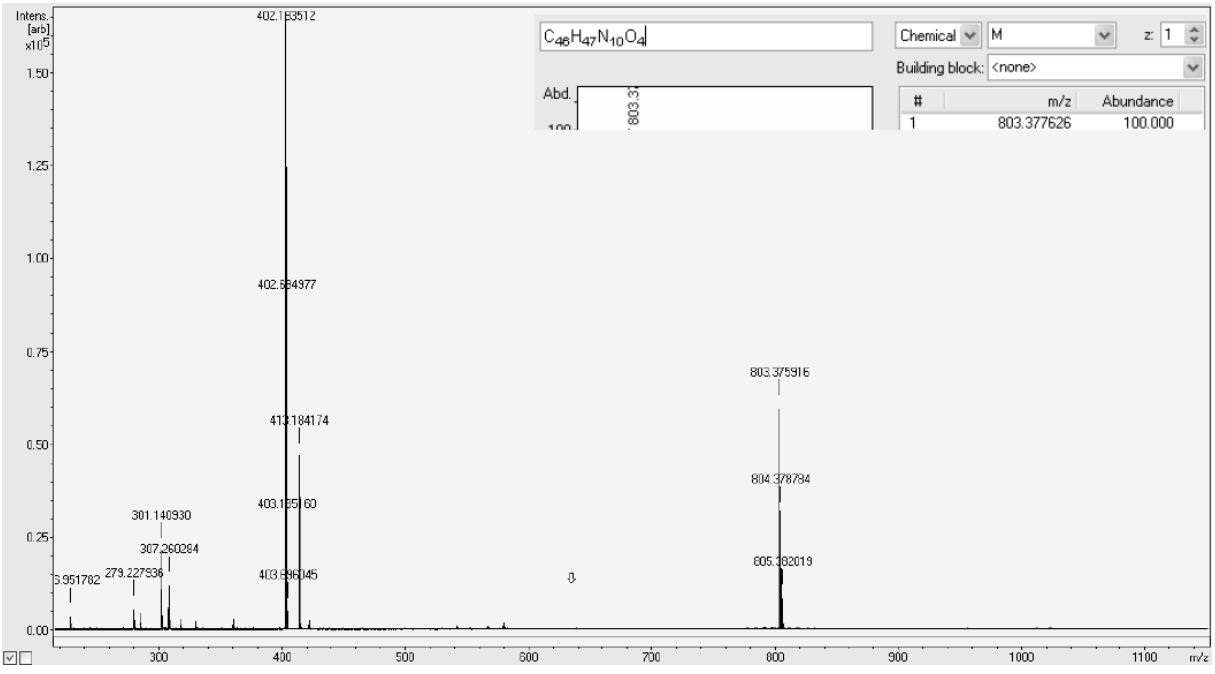
Additional NMR spectra for new compounds characterisation, additional UV–vis and CD spectra

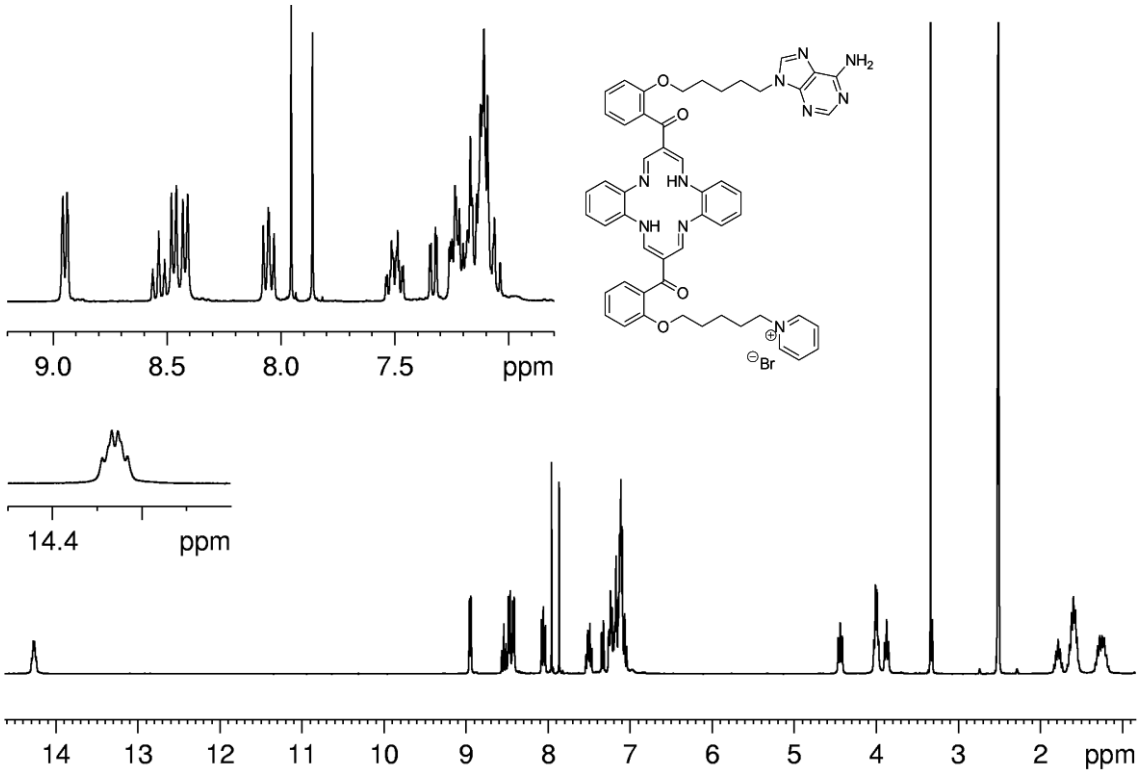
^{1}H NMR and HRMS–ESI spectra of **AP3am** and **AP5**



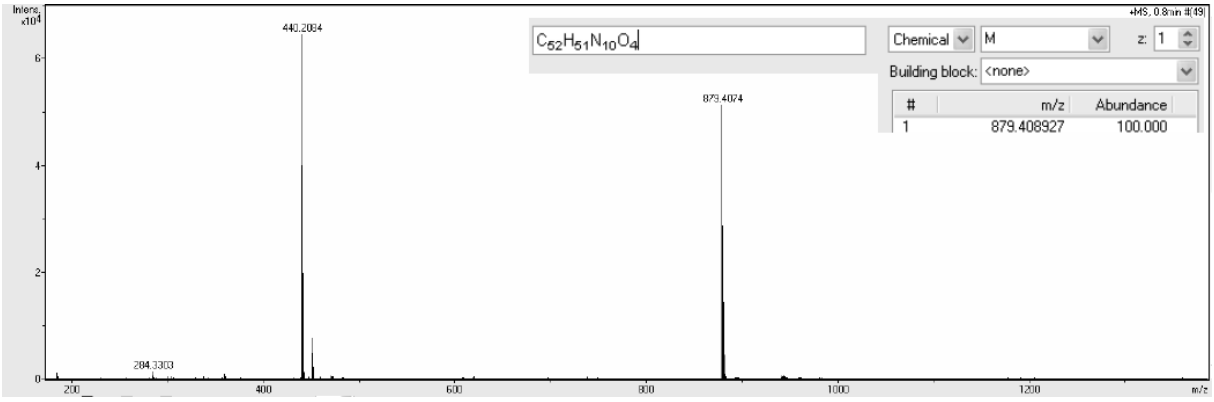
^{1}H NMR spectrum of **AP3am**



ESI-HRMS spectrum of **AP3am**



^{1}H NMR spectrum of **AP5**



ESI-HRMS spectrum of **AP5**

UV–vis experiments:

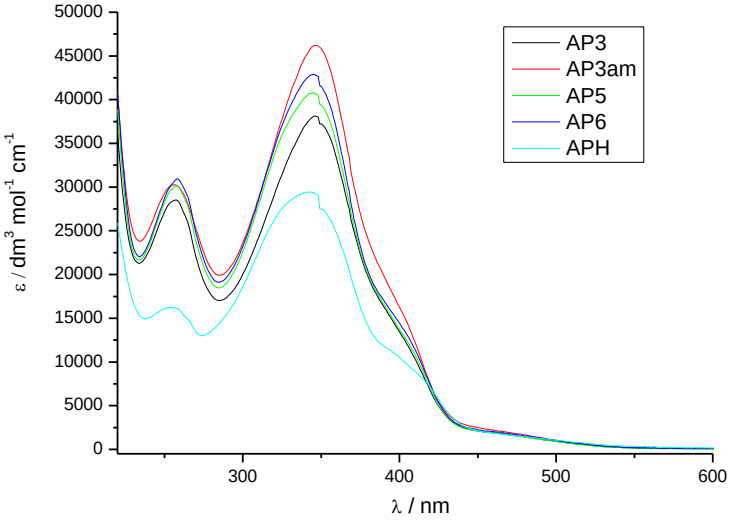
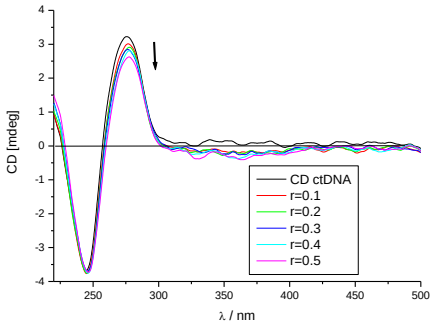
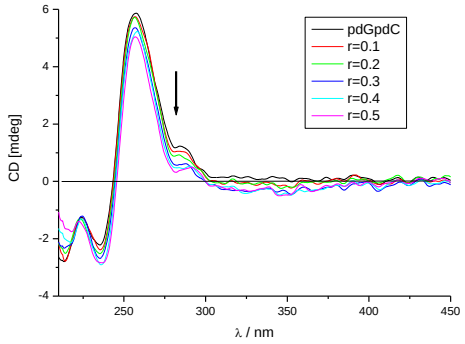
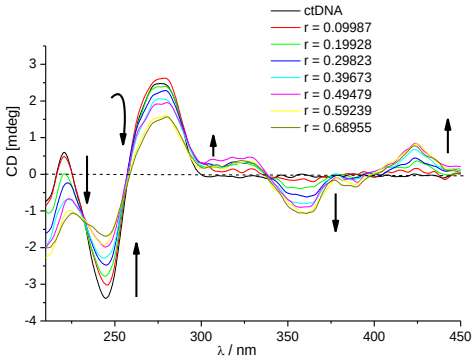
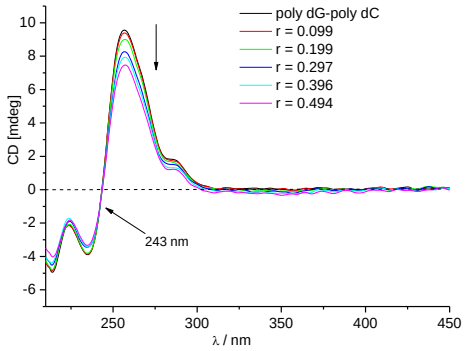
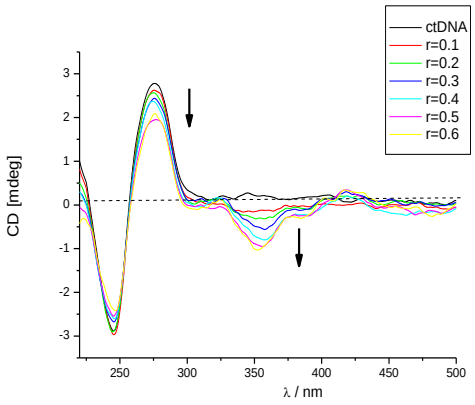
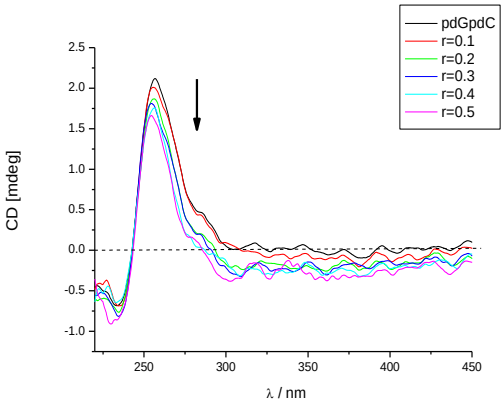


Figure S1. UV–vis spectra of **AP compounds** at c = 1.6 × 10^{-5} mol dm^{-3}; pH 7.0, sodium cacodylate/HCl buffer, *I* = 0.05 mol dm^{-3}.

CD experiments:

	ctDNA	poly dG–poly dC
APH		
AP3		
AP3am		

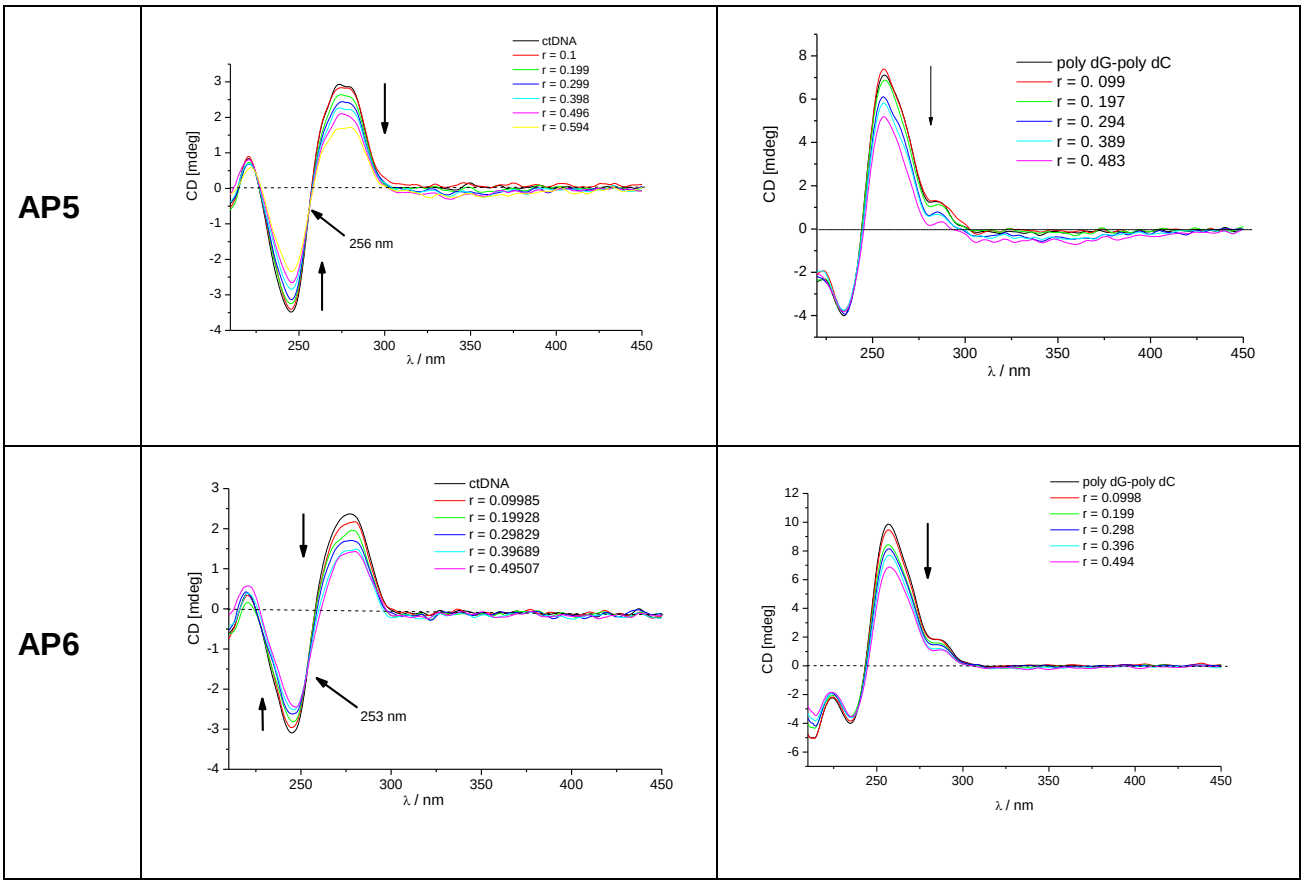
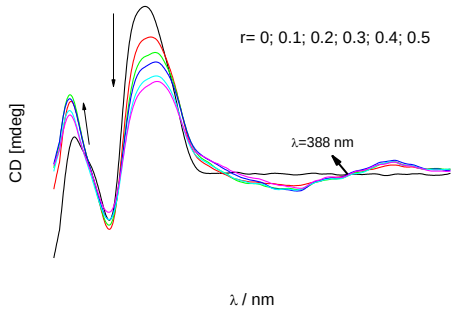
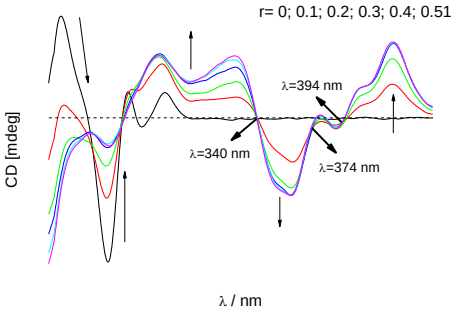
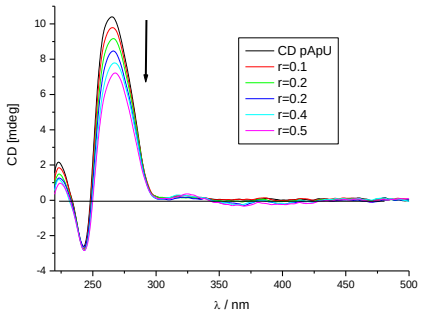
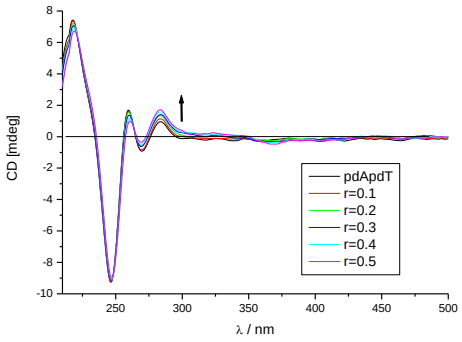
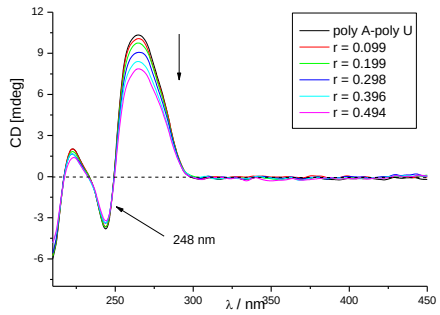
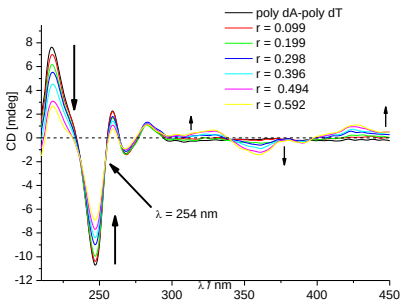
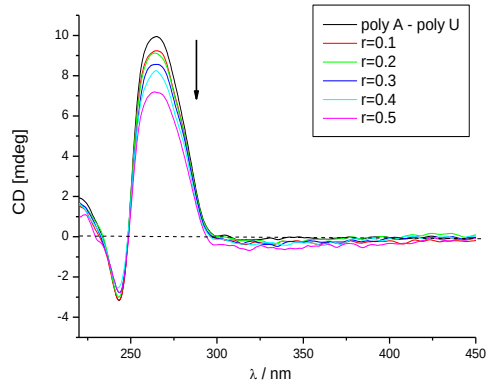
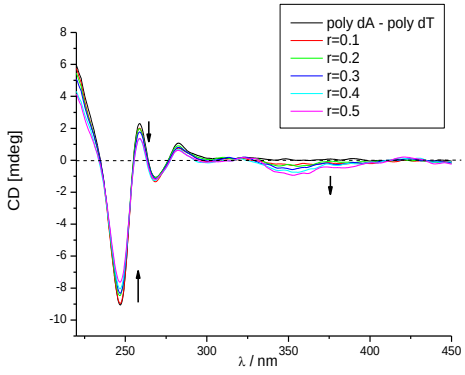


Figure S2. CD titration of **ctDNA** (c = 3.0 × 10^{-5} mol dm^{-3}) and **poly dG–poly dC** (c = 3.0 × 10^{-5} mol dm^{-3}) with **APH**, **AP3**, **AP3am, AP5** and **AP6** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I = 0.05 mol dm^{-3}).

	poly A–poly U	poly dA–poly dT
DP77		
APH		
AP3		
AP3am		

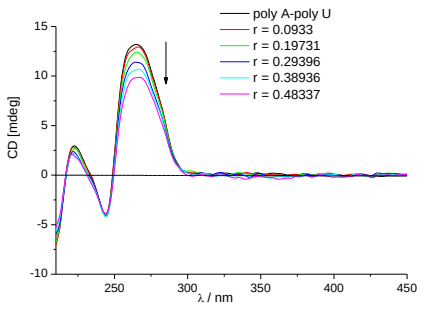
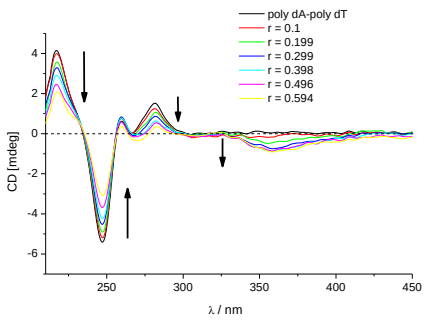
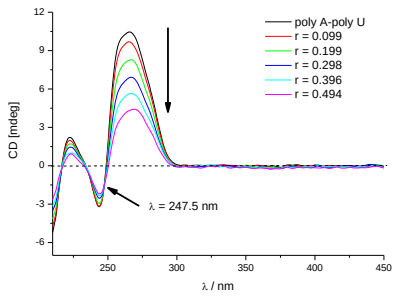
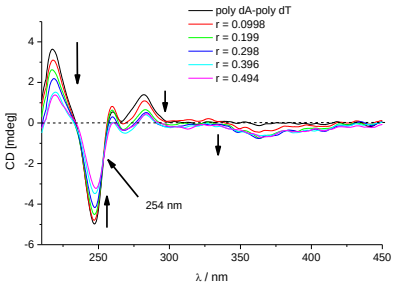
AP5		
AP6		

Figure S3. CD titration of poly A–poly U (c = 3.0 × 10^{-5} mol dm^{-3}) and poly dA–poly dT (c = 3.0 × 10^{-5} mol dm^{-3}) with **DP77, APH**, **AP3**, **AP3am, AP5** and **AP6** at molar ratios r = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I = 0.05 mol dm^{-3}).

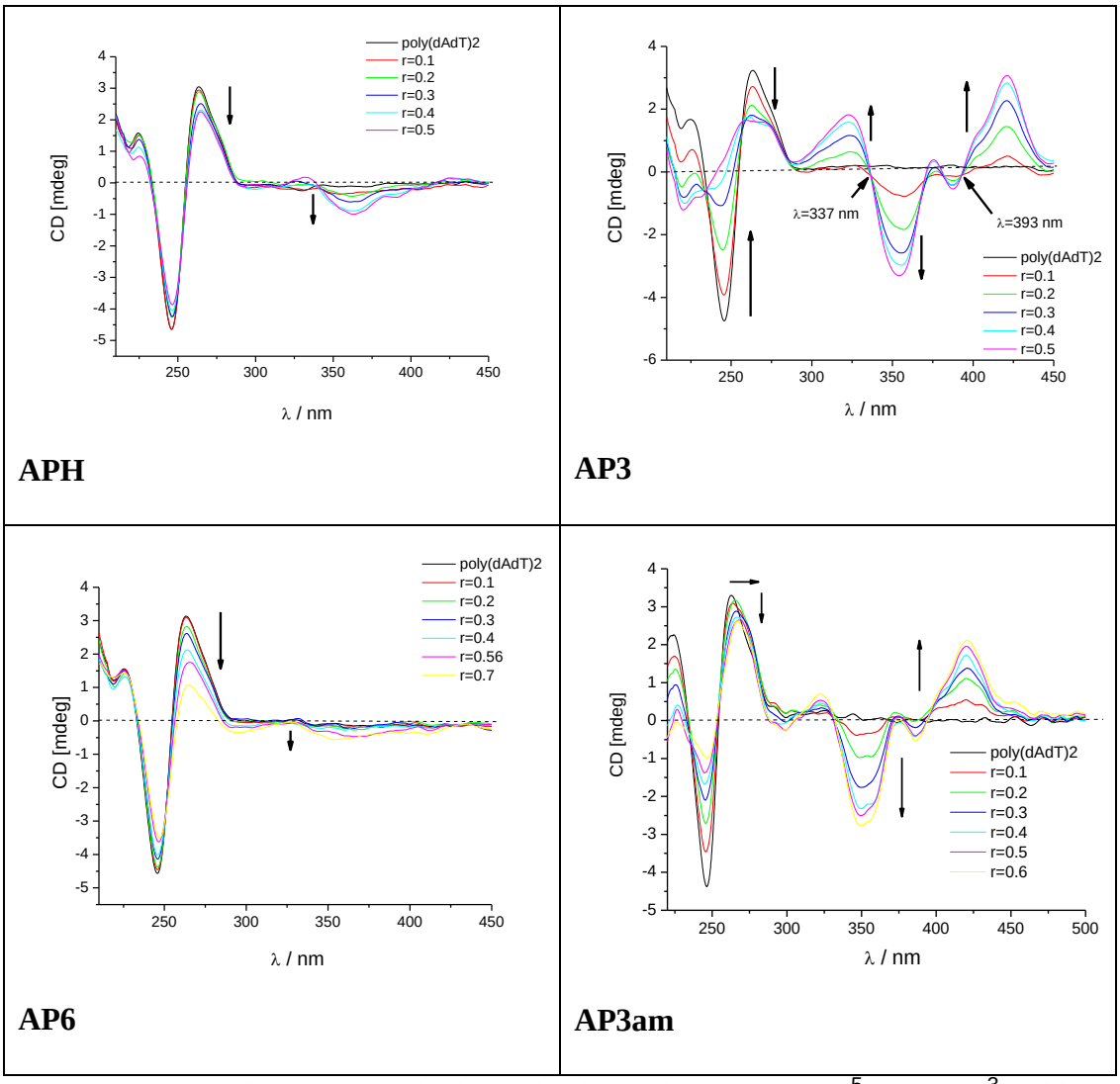


Figure S4. CD titration of poly dAdT–poly dAdT (c = 3.0 × 10^{-5} mol dm^{-3}) with **AP3**, **AP3am** and **AP6** at molar ratios r = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I = 0.05 mol dm^{-3}).

Table S1. Groove widths and depths for selected nucleic acid conformations [1].				
	Groove width [Å]		Groove depth [Å]	
	major	minor	major	minor
[b] poly dAdT–poly dAdT	11.2	6.3	8.5	7.5
[c] poly dA–poly dT	11.4	3.3	7.5	7.9
[a] poly rA–poly rU	3.8	10.9	13.5	2.8
[b] poly dGdC–poly dGdC	13.5	9.5	10.0	7.2
[a] A-helical structure (e.g. A-DNA). [b] B-helical structure (e.g. B-DNA); [c] C-helical structure (e.g. C-DNA).				

1 a) Saenger, W. *Principles of Nucleic Acid Structure*, Springer-Verlag: New York, 1983; b) Cantor, C. R.; Schimmel, P. R. *Biophysical Chemistry*, WH Freeman & Co: San Francisco, 1980.