Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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The effect of the 4-amino functionality on the photophysical and DNA binding properties of alkyl-pyridinium derived 1,8-naphthalimides

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Electronic Supplementary Information (ESI)

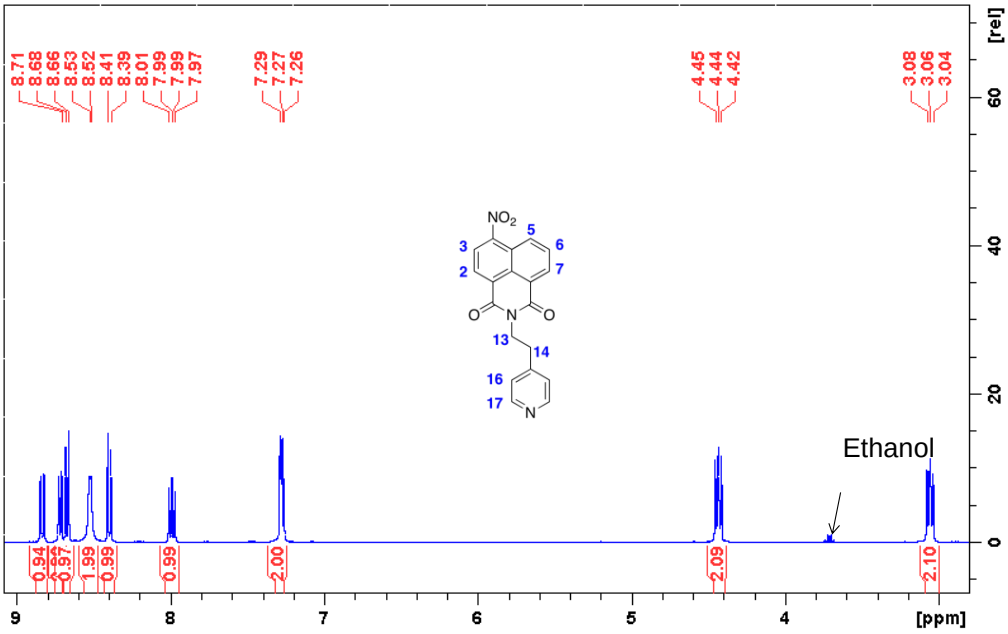

Figure ESI 1A: ^{1}H-NMR of **5** in $CDCl_3$ (400 MHz).

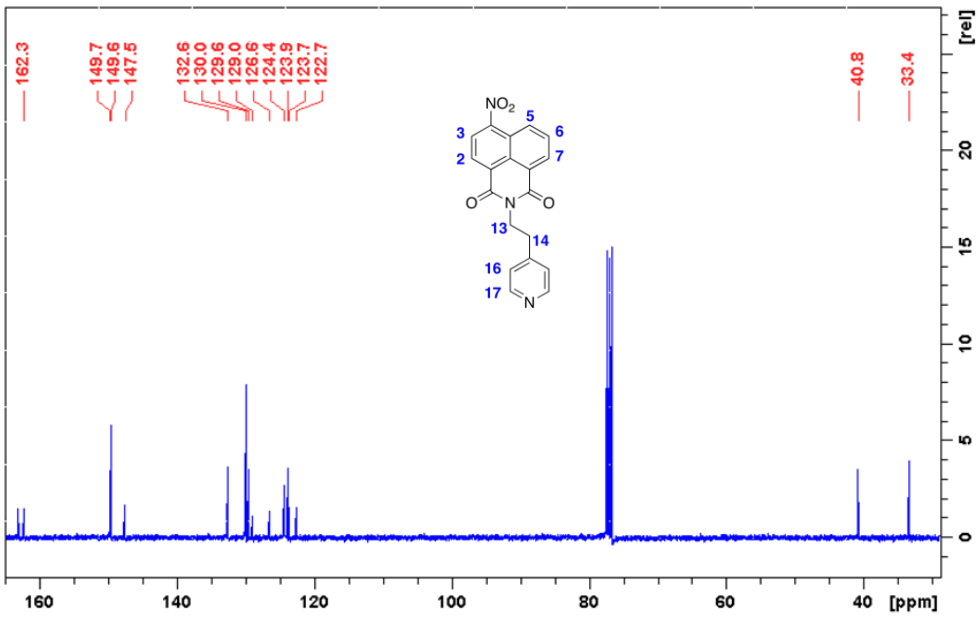

Figure ESI 1B: ^{13}C-NMR of **5** in $CDCl_3$ (100 MHz).

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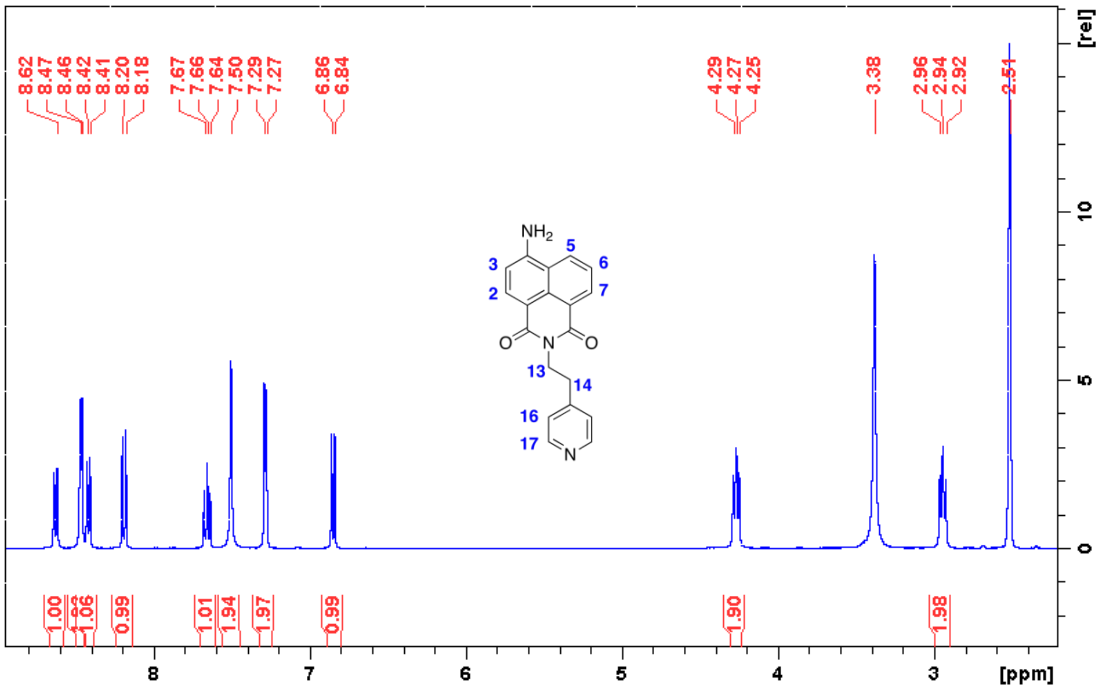

Figure ESI 1c: ^{1}H-NMR of **4** in DMSO-d$_6$ (400 MHz).

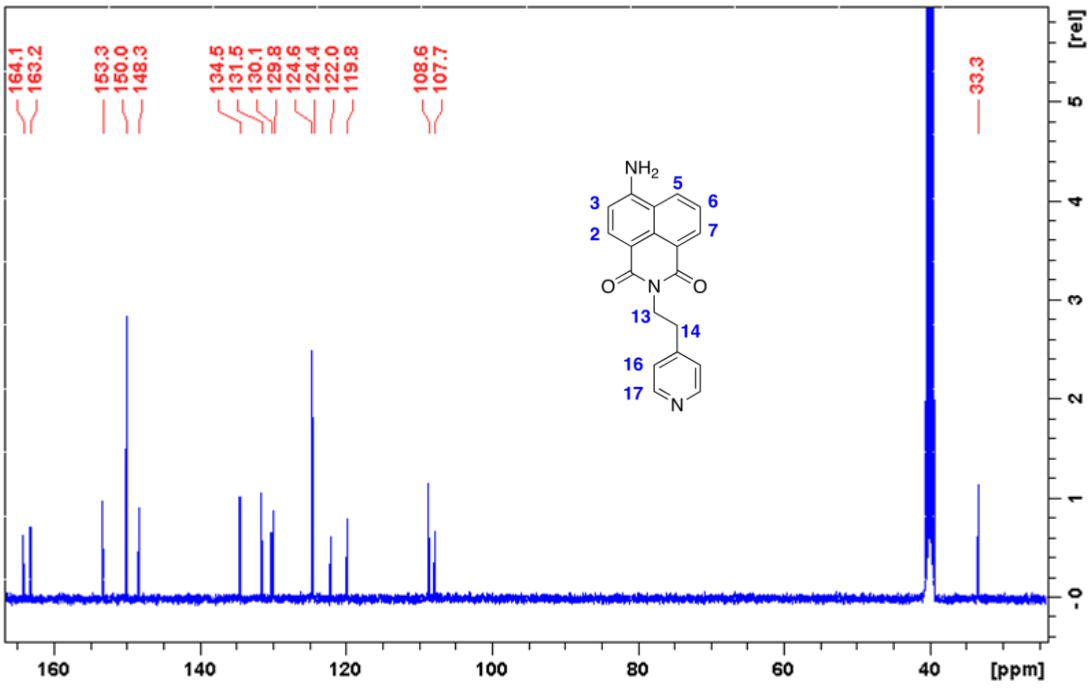

Figure ESI 1d: ^{13}C-NMR of **4** in DMSO-d$_6$ (100 MHz).

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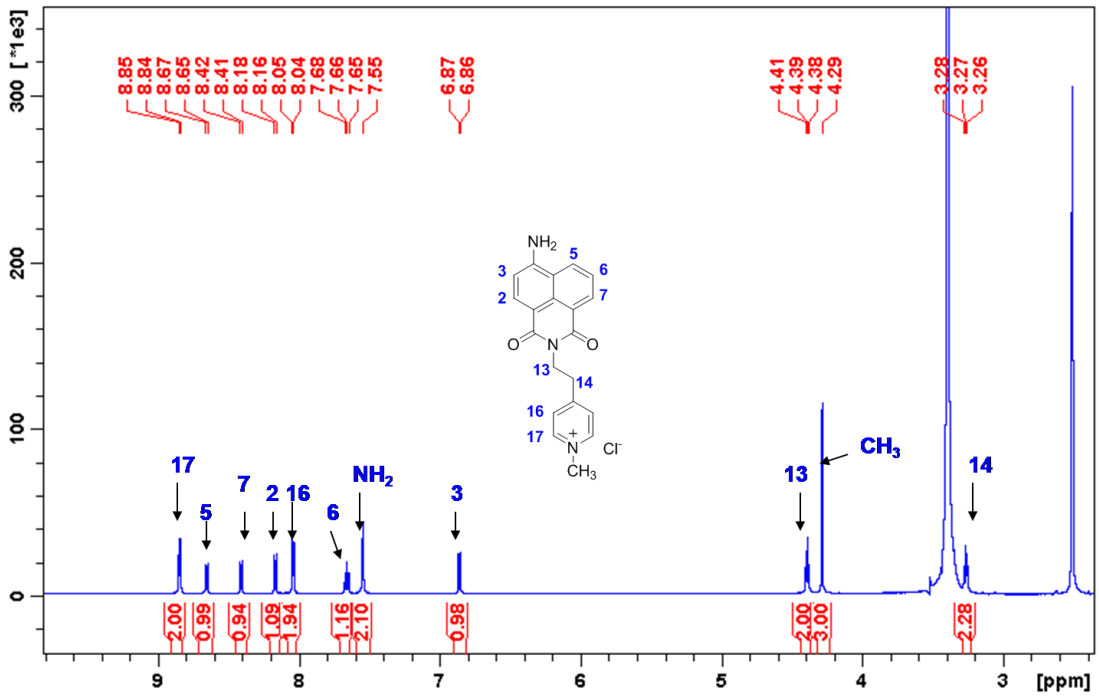

Figure ESI 1e: ^{1}H-NMR of **2** in DMSO-d_6 (600 MHz).

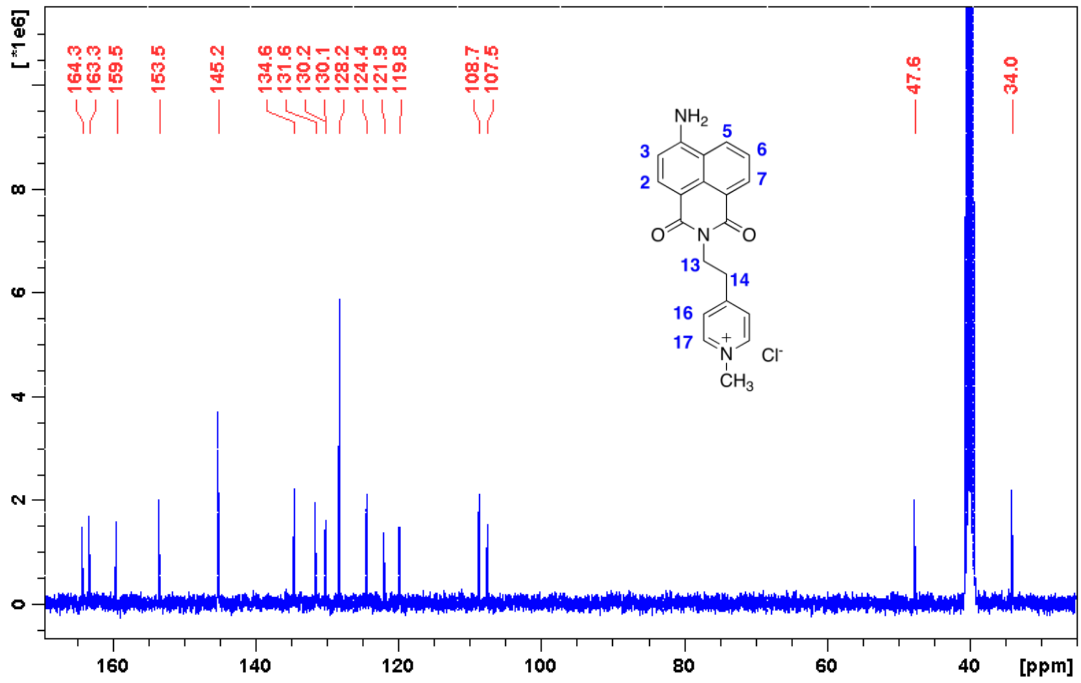

Figure ESI 1f: ^{13}C-NMR of **2** in DMSO-d_6 (150 MHz).

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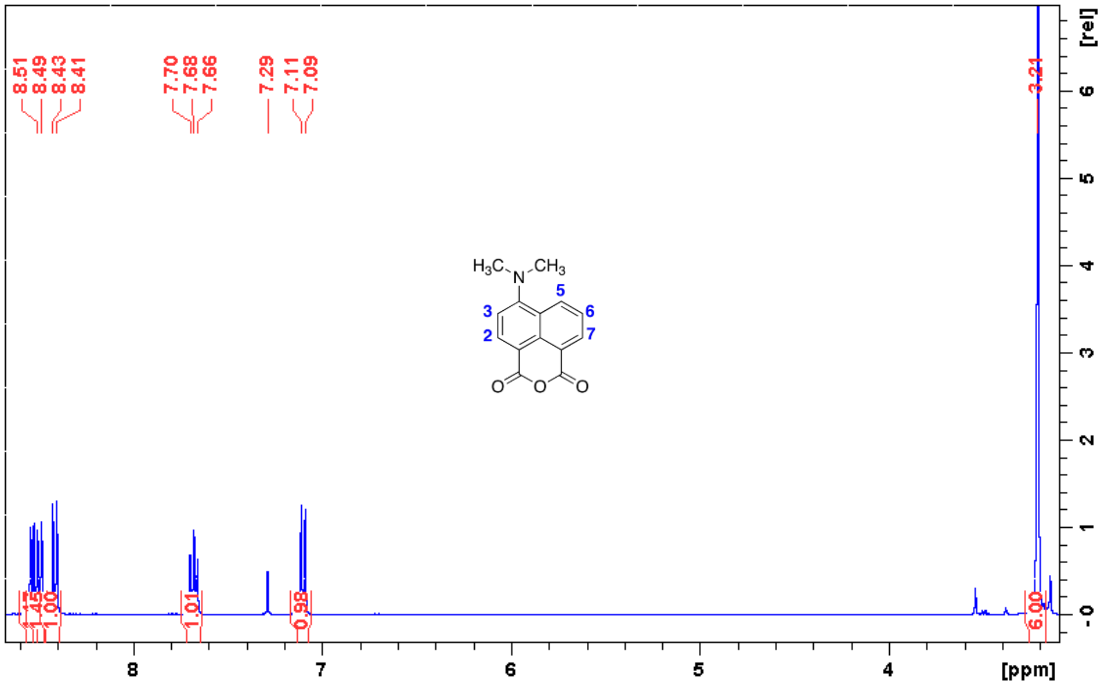

Figure ESI 2a: ^{1}H-NMR of **7** in $CDCl_3$ (400 MHz).

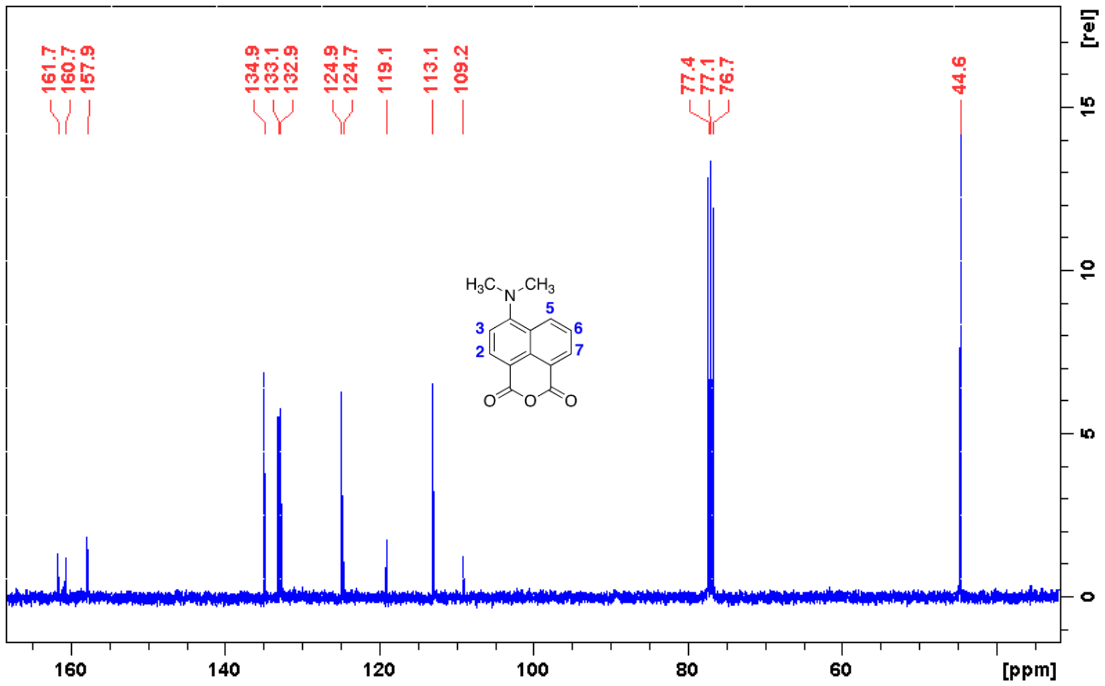

Figure ESI 2b: ^{13}C-NMR of **7** in $CDCl_3$ (100 MHz).

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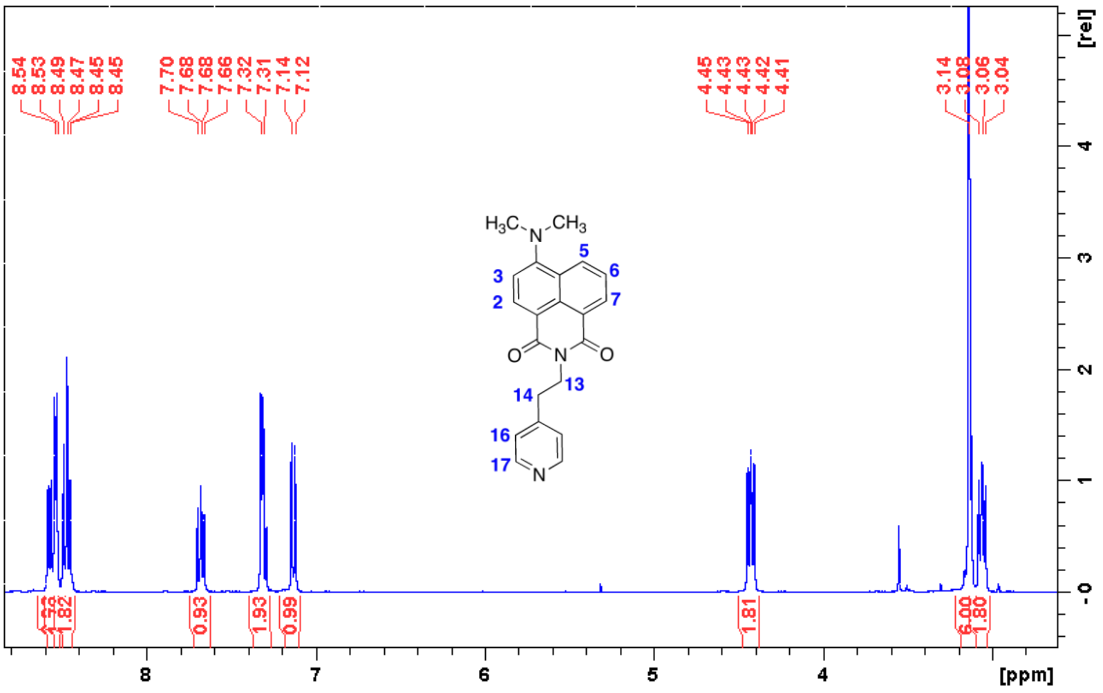

Figure ESI 2c: ^{1}H-NMR of **6** in $CDCl_3$ (400 MHz).

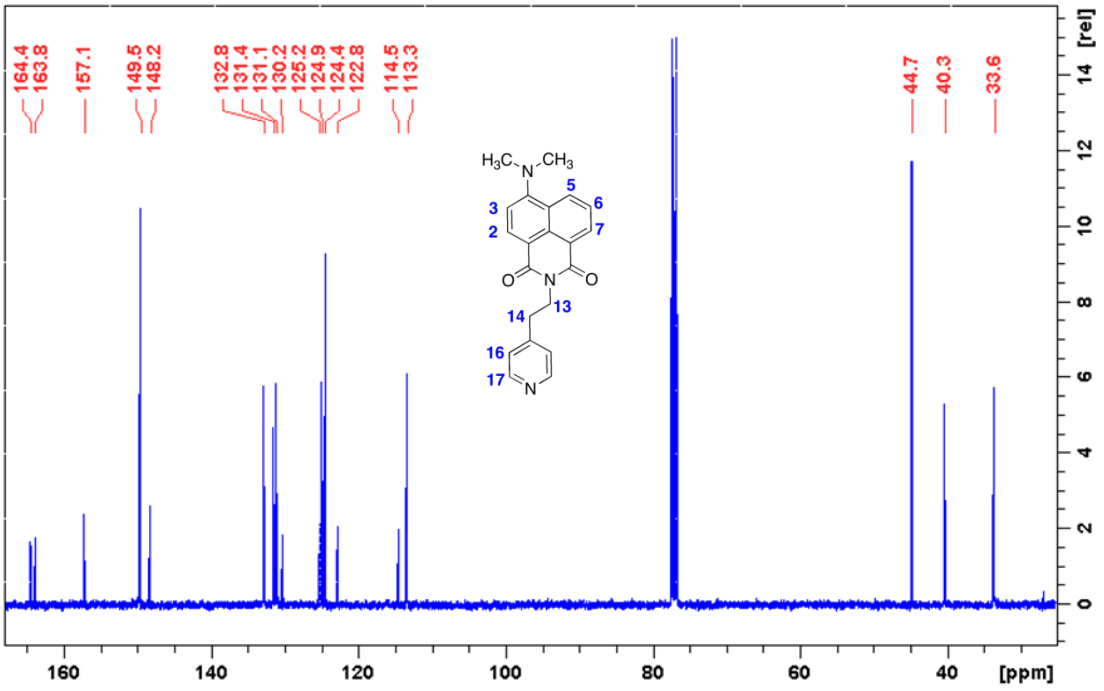

Figure ESI 2d: ^{13}C-NMR of **6** in $CDCl_3$ (100 MHz).

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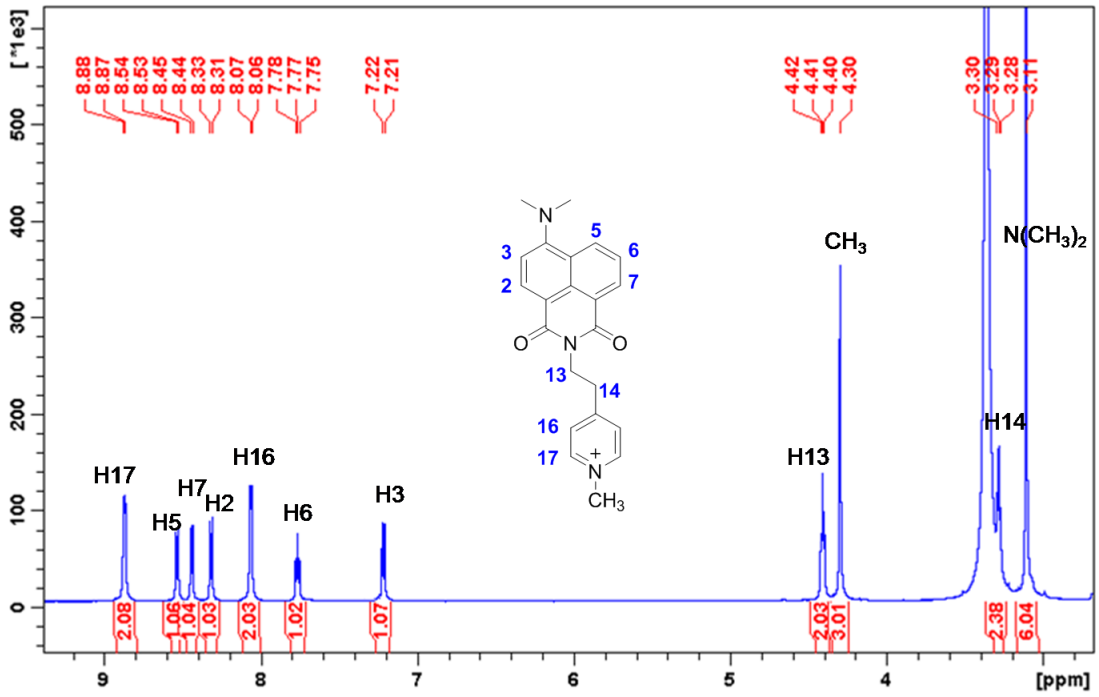

Figure ESI 2e: ^{1}H-NMR of **3** in DMSO-d_6 (600 MHz).

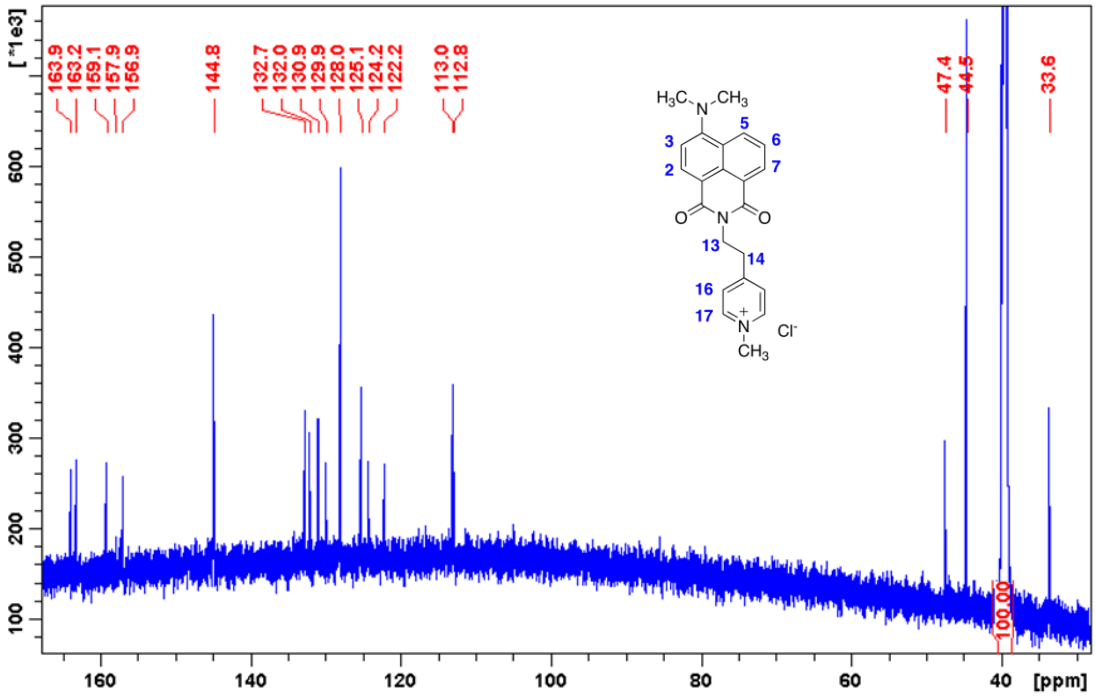

Figure ESI 2f: ^{13}C-NMR of **3** in DMSO-d_6 (150 MHz).

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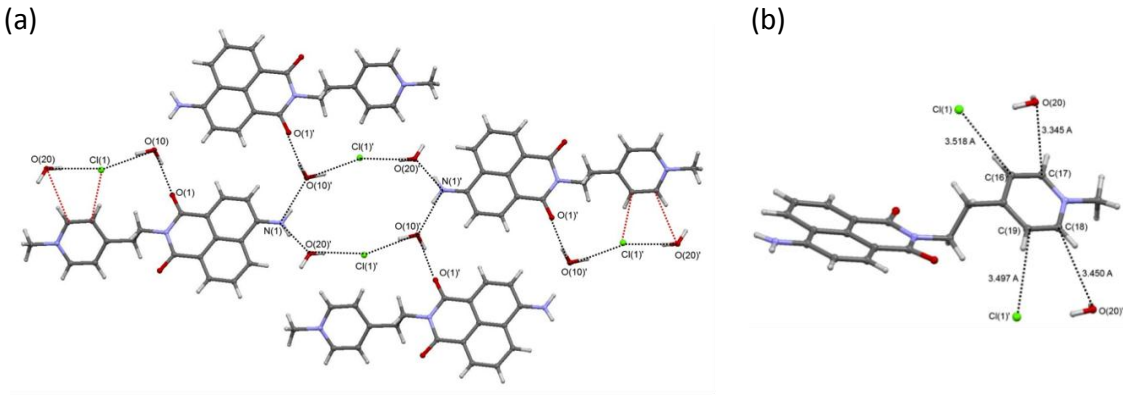

Figure ESI 3: (a) The packing of **2** showing the π–π interactions (c) H-bonding network, where (.....) shows classical NH or OH hydrogen bonding interactions and (.....)denotes non-classical CH based hydrogen bonding, (b) Demonstration of out of plane orientation of pyridyl ring in the solid- state structure of **2** due to non-classical H-bonding interactions

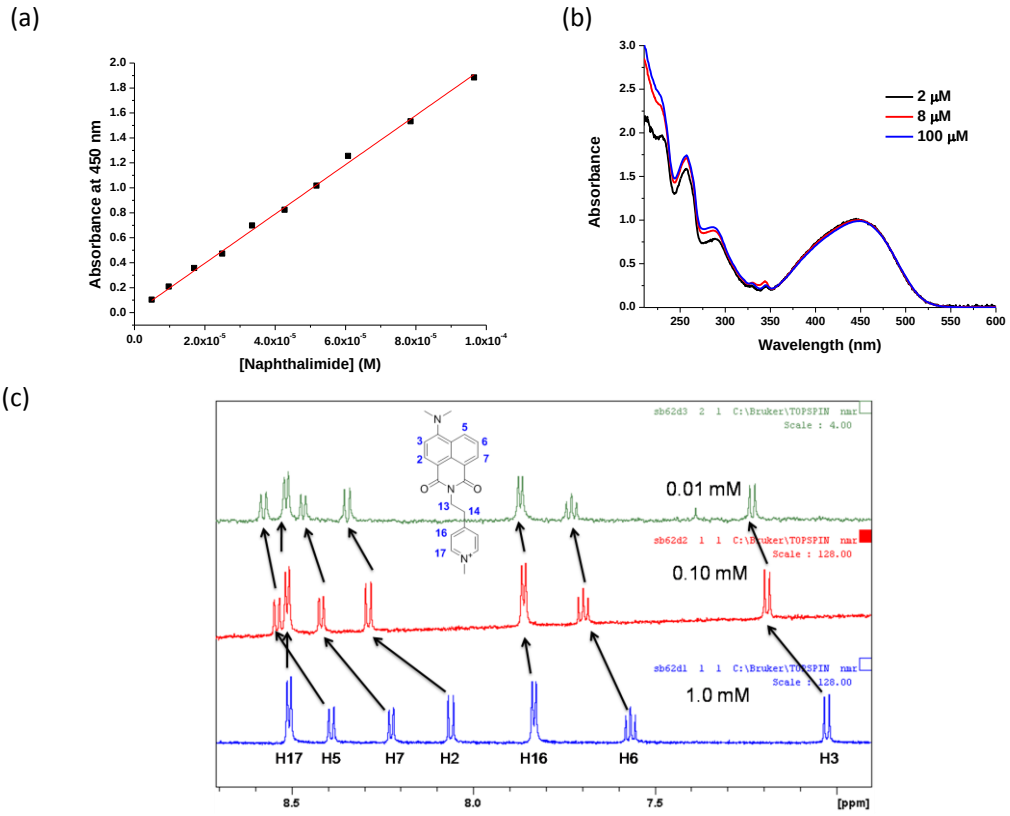

Figure ESI 4: (a) The plot of concentration of **3** vs. absorbance at 450 nm, (b) Normalised UV/vis absorption spectrum of **3** at various concentrations in water, (c) ^{1}H NMR spectrum (600 MHz) of **3** in D2O at various concentrations.

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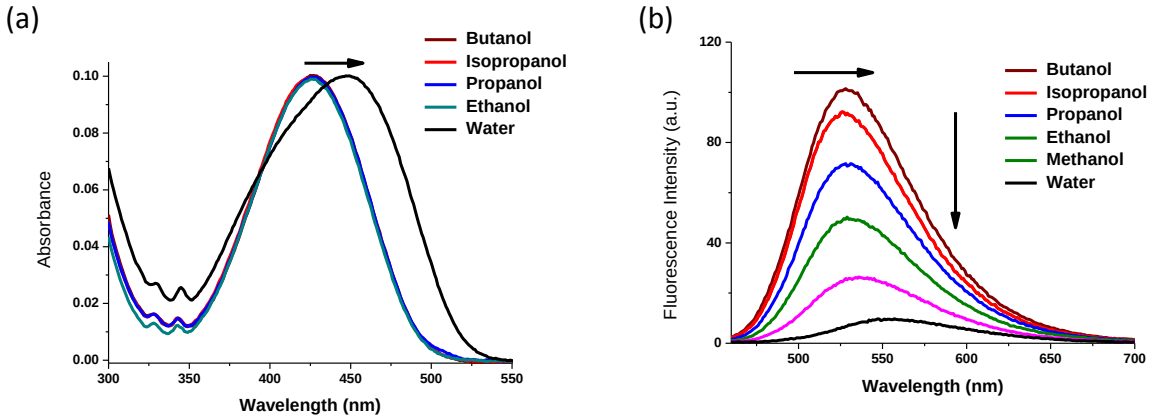

Figure ESI 4: Effect of solvent polarity on the (a) UV/vis and (b) fluorescence spectra of **3.**

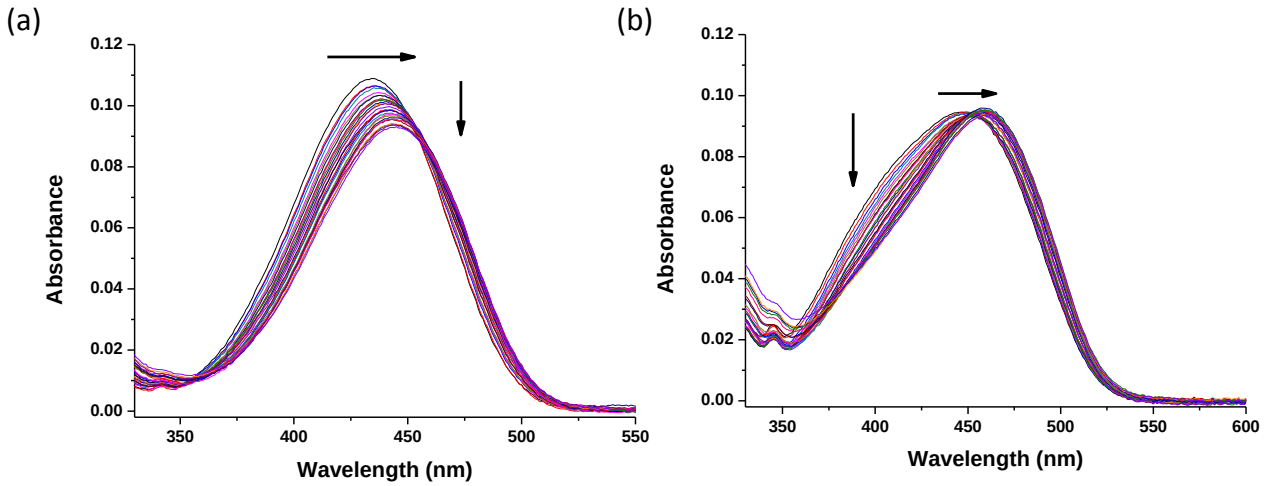

Figure ESI 5: The changes in the UV/vis absorption spectra of (a) **2** (6.9 μM) and **3** (7.9 μM) in the presence increasing concentration of AMP (0-100 mM) in 10 mM phosphate buffer (pH 7.0).

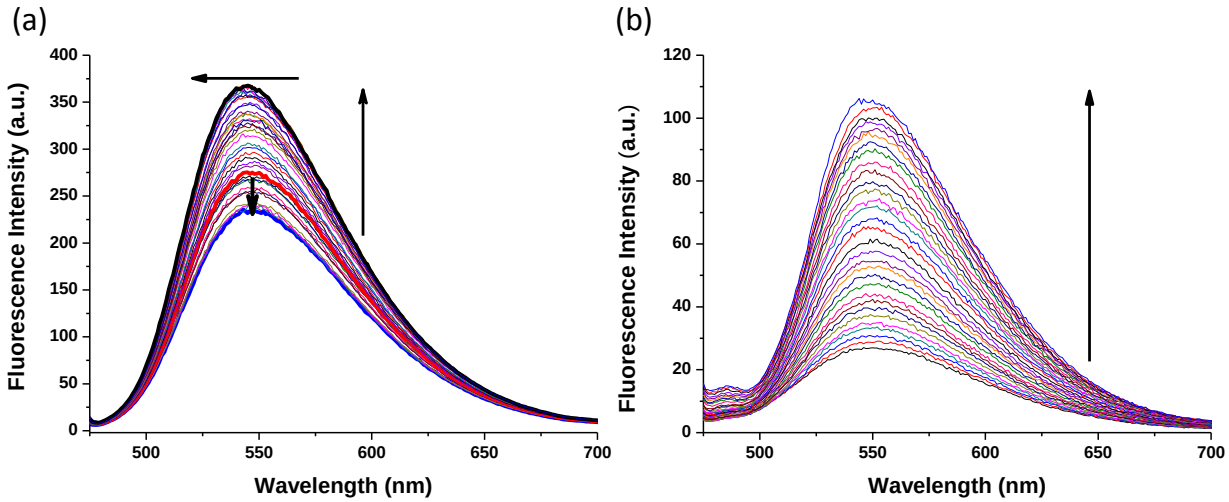

Figure ESI 6: The changes in the fluorescence spectra of (a) **2** (6.9 μM) (λ_{ex} = 460 nm) and **3** (7.9 μM) (λ_{ex} = 450 nm) in the presence of increasing concentration of AMP (0-100 mM) in 10 mM phosphate buffer (pH 7.0).

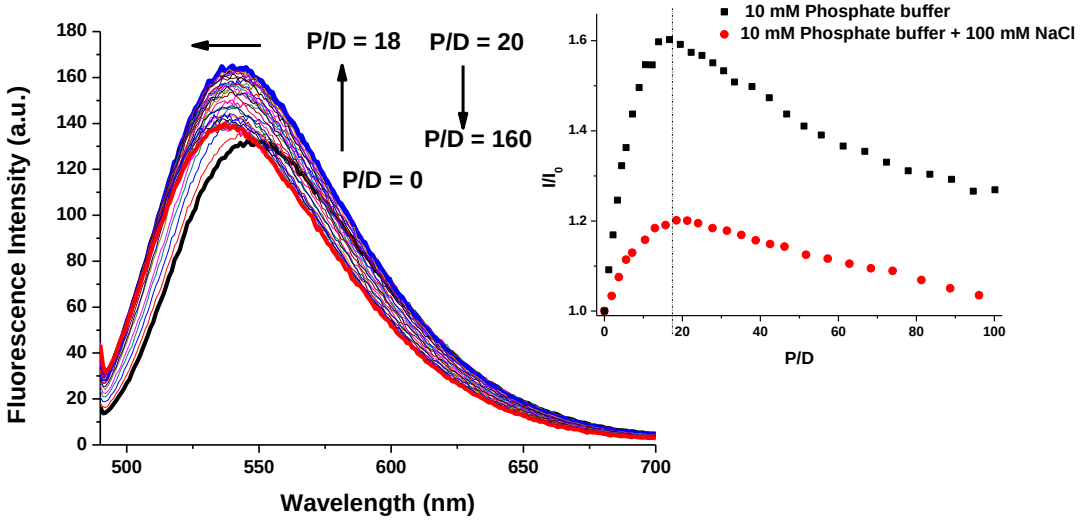

Figure ESI 7: Overall changes in the steady state emission spectra of **2** (7.0 μM) in the presence of increasing concentration of st-DNA (0–1120 μM) in 10 mM phosphate buffer containing 100 mM NaCl (pH 7.0) (λ_{ex} = 480 nm). Inset: Plot of I/I_0 vs. P/D for **2** in 10 mM phosphate (■) and 10 mM phosphate buffer containing 100 mM NaCl (●).

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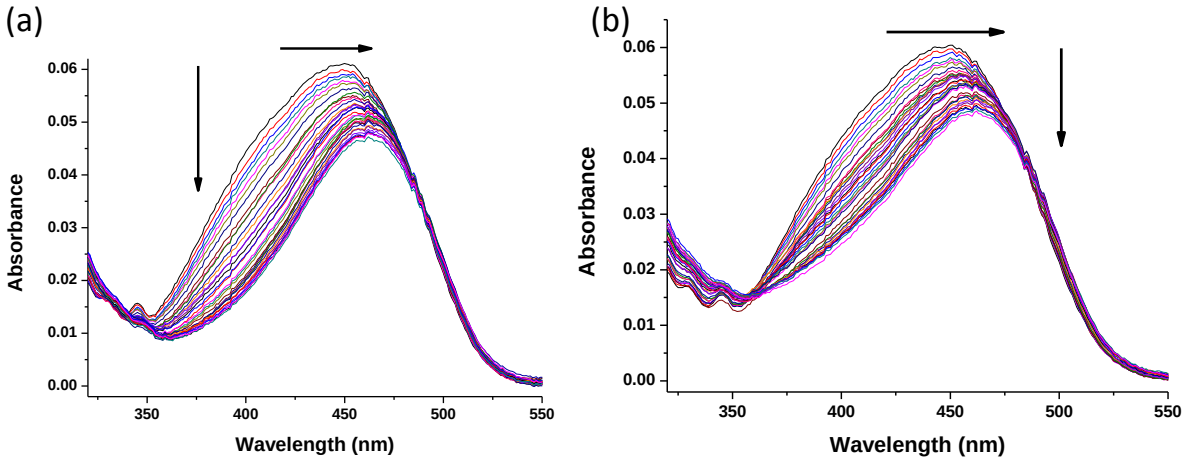

Figure ESI 8: The changes in the UV/vis absorption spectra of **3** (5.2 μM) in the presence of (a) poly $(dA\text{-}dT)_2$ (0-172 μM) and (b) poly $(dG\text{-}dC)_2$ (0-190 μM)CD in 10 mM phosphate buffer (pH 7.0).

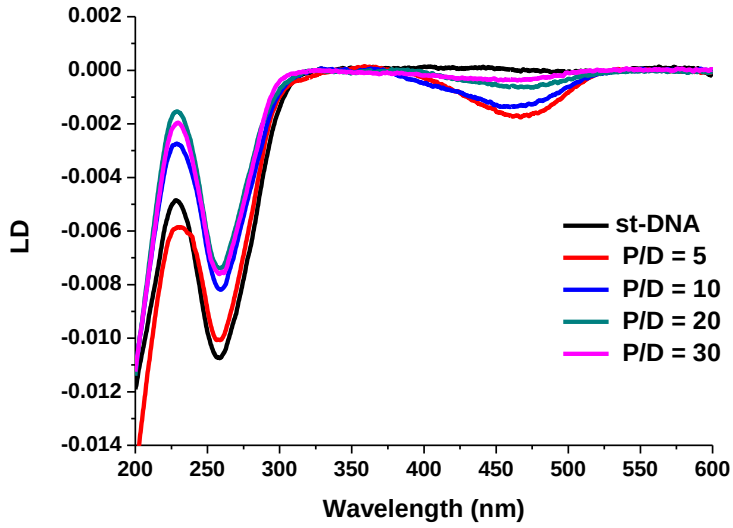

Figure ESI 9: The LD spectra of st-DNA (400 μM) in the presence of varying concentration of **3** (P/D 0→30) in 10 mM phosphate buffer (pH 7.0).

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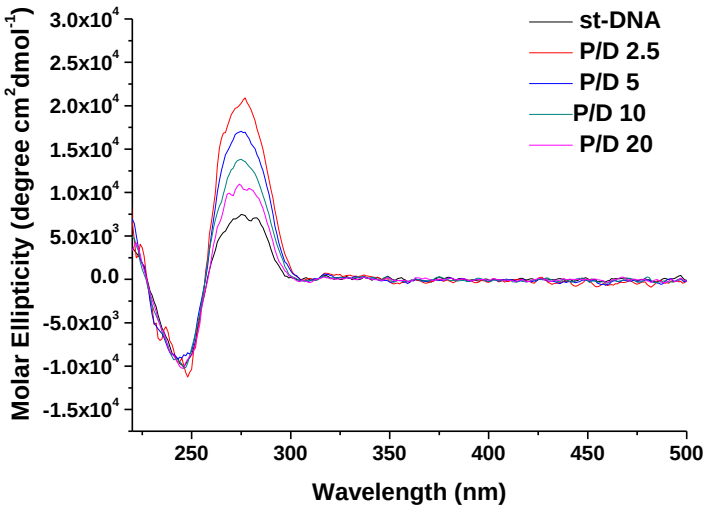

Figure ESI 10: The CD spectra of st-DNA (150 μM) in the presence of varying concentration of **3** (P/D 0→20) in 10 mM phosphate buffer (pH 7.0).

Table ESI 1: Crystal data and structure refinement for **2**.

Identification code	sb29	
Empirical formula	$C_{20}H_{22}ClN_3O_4$	
Formula weight	403.86	
Temperature	108(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.1105(16) Å	α = 98.63(3)°.
	b = 8.8677(18) Å	β = 96.32(3)°.
	c = 14.245(3) Å	γ = 110.67(3)°.
Volume	932.9(3) $Å^3$	
Z	2	
Density (calculated)	1.438 Mg/m^3	
Absorption coefficient	0.238 mm^{-1}	
F(000)	424	
Crystal size	0.21 x 0.13 x 0.08 mm^3	
Theta range for data collection	2.51 to 24.99°.	
Index ranges	-9<=h<=9, -10<=k<=10, -16<=l<=16	
Reflections collected	10726	
Independent reflections	3166 [R(int) = 0.0537]	
Completeness to theta = 24.99°	95.7 %	

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Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9812 and 0.9517
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3166 / 0 / 254
Goodness-of-fit on F^2	1.220
Final R indices [I>2sigma(I)]	R1 = 0.0691, wR2 = 0.1633
R indices (all data)	R1 = 0.0730, wR2 = 0.1656
Largest diff. peak and hole	1.018 and -0.338 e.Å^{-3}

Table ESI 2: Crystal data and structure refinement for **3**.

Identification code	sbpf6	
Empirical formula	C_{22} H_{22} F_6 N_3 O_2 P	
Formula weight	505.40	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.8081(4) Å	α= 85.580(2) °
	b = 9.2489(4) Å	β= 89.039(2) °
	c = 14.9085(6) Å	γ = 62.137(2) °
Volume	1070.27(8) Å^3	
Z	2	
Density (calculated)	1.568 Mg/m^3	
Absorption coefficient	1.866 mm^{-1}	
F(000)	520	
Crystal size	0.24 x 0.11 x 0.04 mm^3	
Theta range for data collection	8.34 to 63.95°.	
Index ranges	-10<=h<=9, -10<=k<=10, -17<=l<=17	
Reflections collected	7357	
Independent reflections	3360 [R(int) = 0.0301]	
Completeness to theta = 63.95∞	95.1 %	

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Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7526 and 0.5895
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3360 / 0 / 310
Goodness-of-fit on F^2	1.074
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1445
R indices (all data)	R1 = 0.0521, wR2 = 0.1468
Largest diff. peak and hole	0.595 and -0.358 e.Å^{-3}

Table ESI 3 Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1X)...O(10)[a]	0.85	2.05	2.882(4)	166.2
N(1)-H(1Y)...O(20)[b]	0.85	2.17	2.978(4)	158.2
O(10)-H(10X)...O(1)[c]	0.85	2.00	2.838(3)	170.0
O(10)-H(10Y)...Cl(1)	0.99	2.19	3.168(3)	166.9
O(20)-H(20X)...Cl(1)	0.83	2.33	3.150(3)	170.6
O(20)-H(20Y)...Cl(1)[d]	0.97	2.21	3.167(3)	168.2

Symmetry transformations used to generate equivalent atoms:

[a] *-x,-y,-z* [b] *x-1,y-1,z-1* [c] *x,y+1,z* [d] *-x+2,-y+2,-z+1*