

Supplementary Materials: Low-Dimensional Compounds Containing Bioactive Ligands. Part XX: Crystal Structures, Cytotoxic, Antimicrobial Activities and DNA/BSA Binding of Oligonuclear Zinc Complexes with Halogen Derivatives of 8-Hydroxyquinoline

Michaela Harmošová, Martin Kello, Michal Goga, Ludmila Tkáčiková, Mária Vilková, Danica Sabolová, Simona Sovová, Erika Samolová, Miroslava Litecká, Veronika Kuchárová, Juraj Kuchár and Ivan Potočný

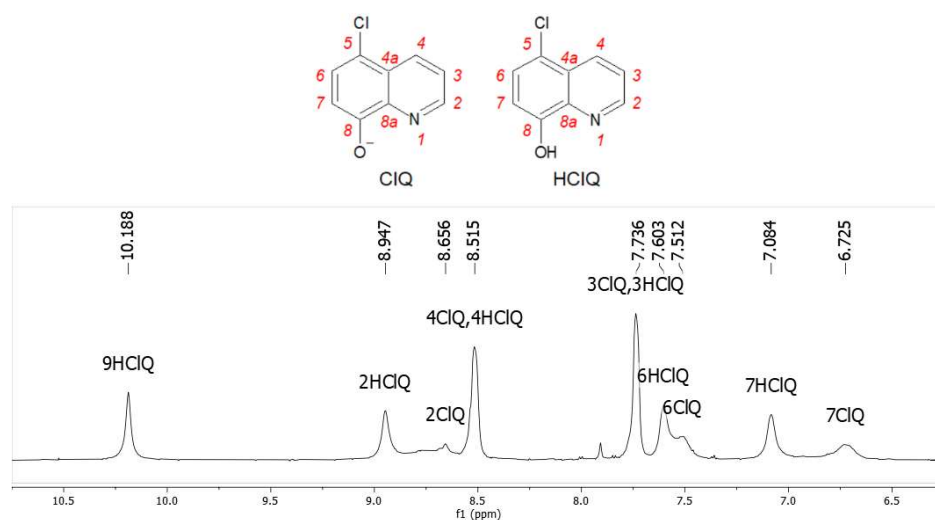


Figure S1. ^1H NMR (600 MHz, DMSO-d_6) spectrum of complex 3.

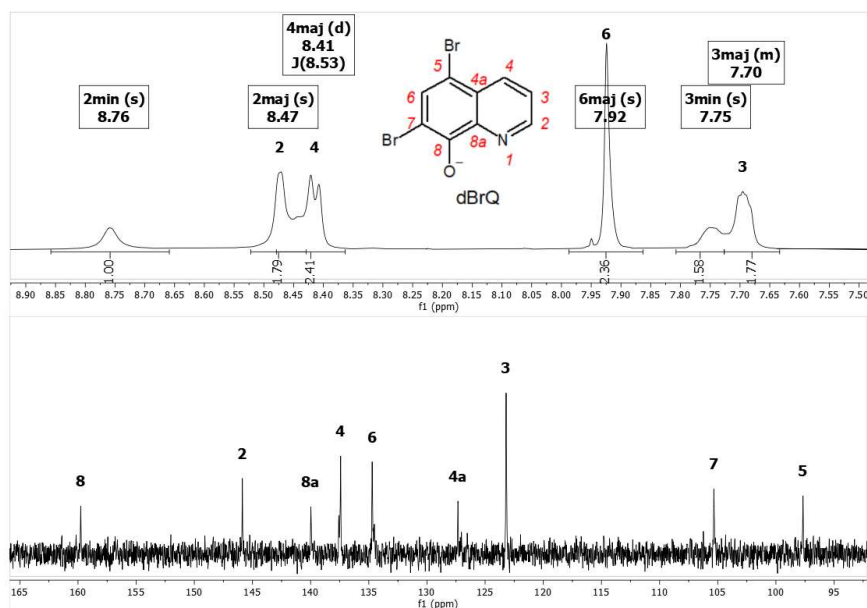


Figure S2. ^1H (600 MHz, DMSO-d_6) and ^{13}C (150 MHz, DMSO-d_6) NMR spectrum of complex 5.

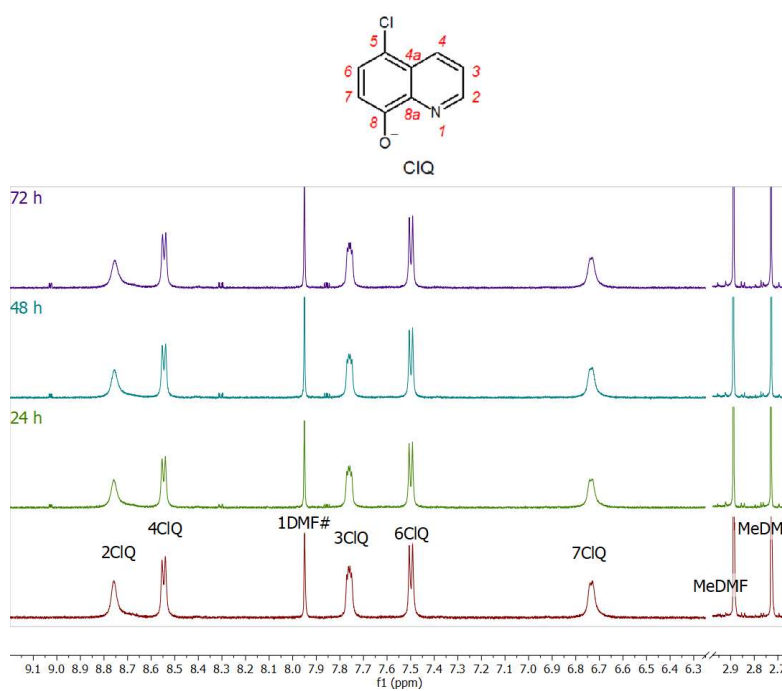


Figure S3. Time-dependent ^1H NMR (600 MHz, DMSO-d_6) spectra of complex 2.

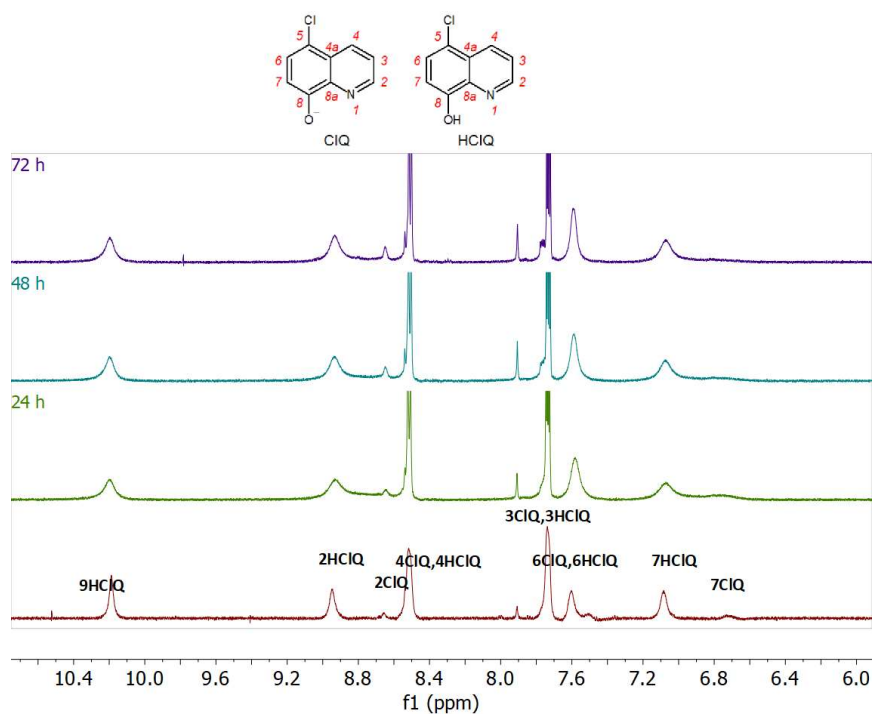


Figure S4. Time-dependent ^1H NMR (600 MHz, DMSO-d_6) spectra of complex 3.

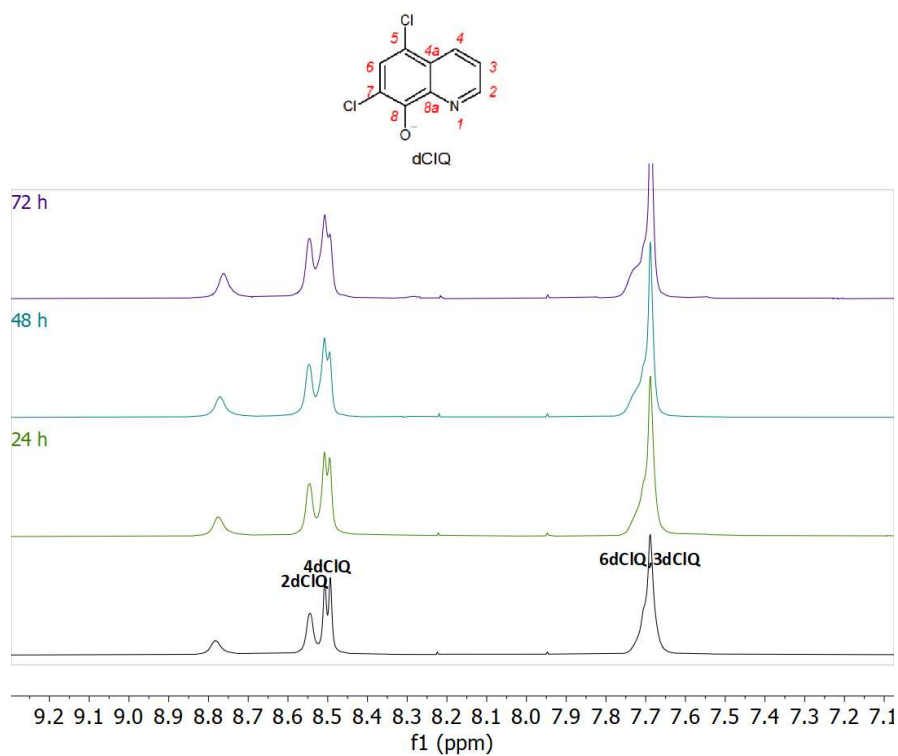


Figure S5. Time-dependent ^1H NMR (600 MHz, DMSO-d_6) spectra of complex 4.

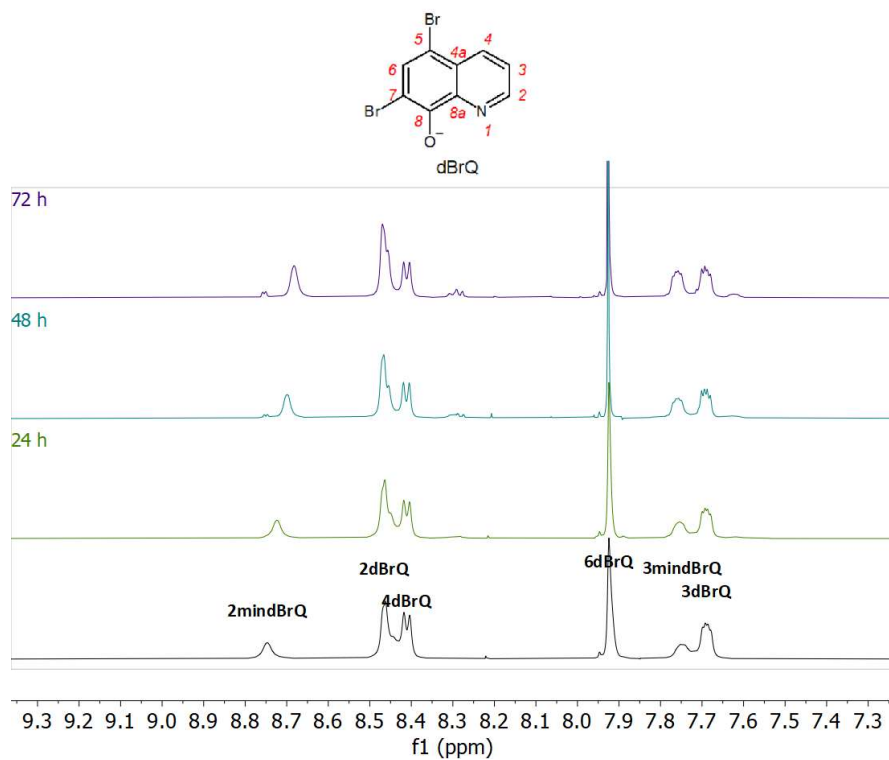


Figure S6. Time-dependent ^1H NMR (600 MHz, DMSO-d_6) spectra of complex 5.

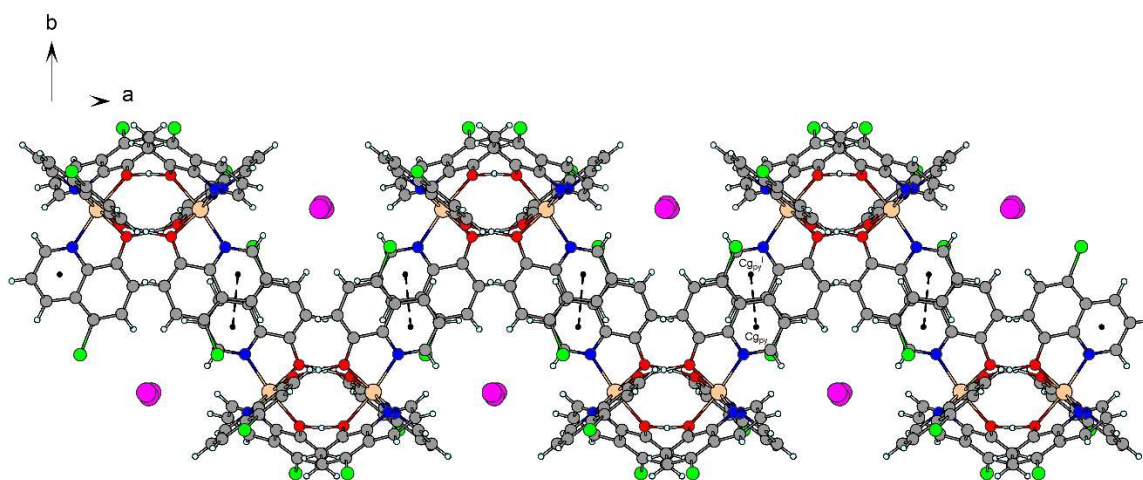


Figure S7. Part of the one-dimensional structure of 3 viewed along the c axis with π - π interactions (black dashed lines).

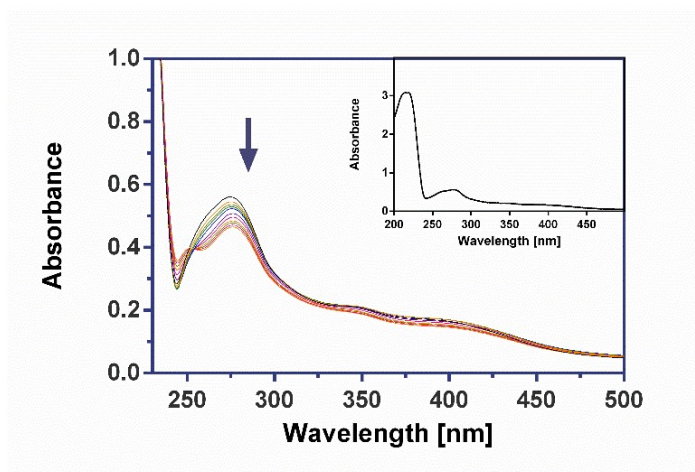


Figure S8. UV-vis spectrum of complex **1** (6.14×10^{-6} M) with ctDNA. The arrow indicates changes in absorbance upon increasing DNA concentration. Inset: UV-vis absorption spectrum of **1**.

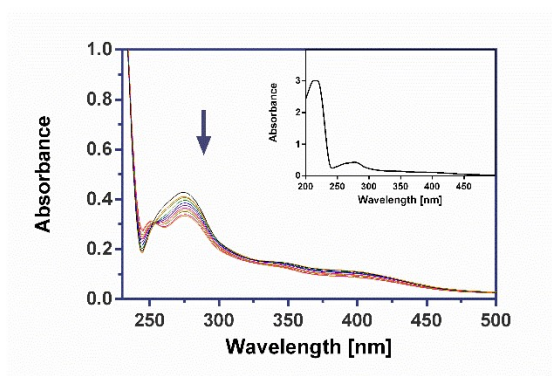


Figure S9. UV-vis spectrum of complex **2** (6.14×10^{-6} M) with ctDNA. The arrow indicates changes in absorbance upon increasing DNA concentration. Inset: UV-vis absorption spectrum of **2**.

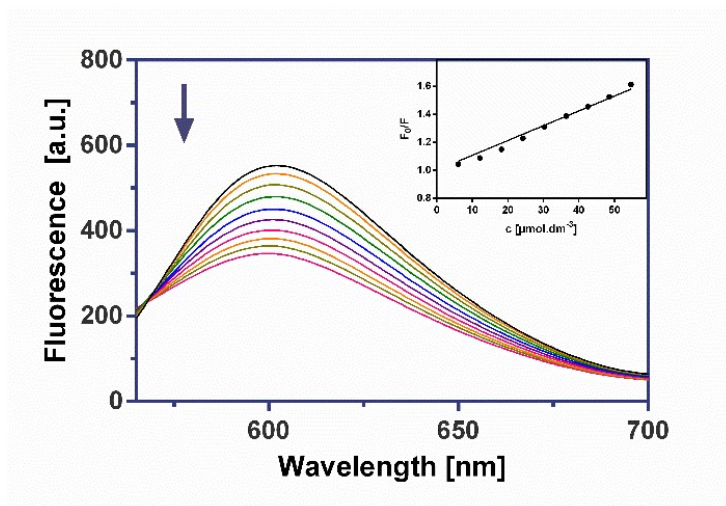


Figure S10. Fluorescence spectrum of DNA-EB complex in the absence (black line) and presence of complex **1**. Inset: The corresponding Stern-Volmer plot for quenching process of EB by **1**.

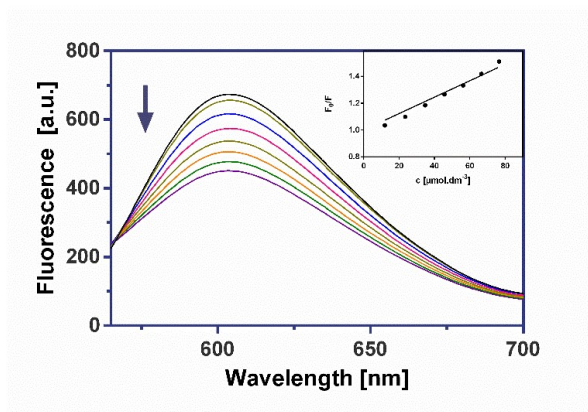


Figure S11. Fluorescence spectrum of DNA-EB complex in the absence (black line) and presence of complex **2**. Inset: The corresponding Stern-Volmer plot for quenching process of EB by **2**.

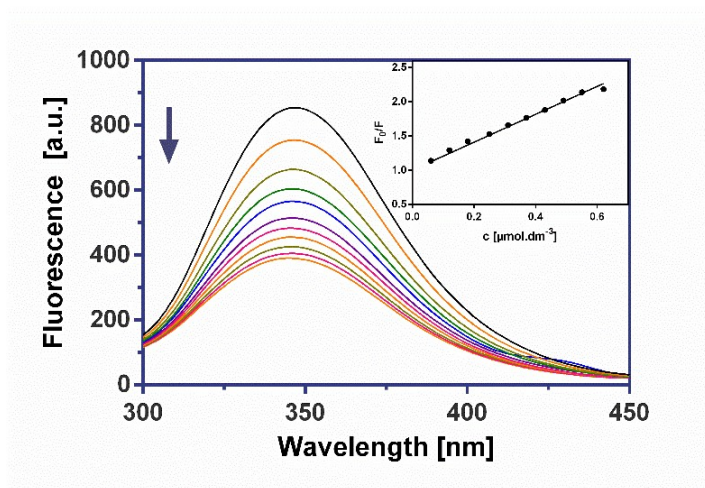


Figure S12. Fluorescence quenching spectra of BSA in presence of complex **1**. Inset: The corresponding Stern-Volmer plot for **1** at 25 °C.

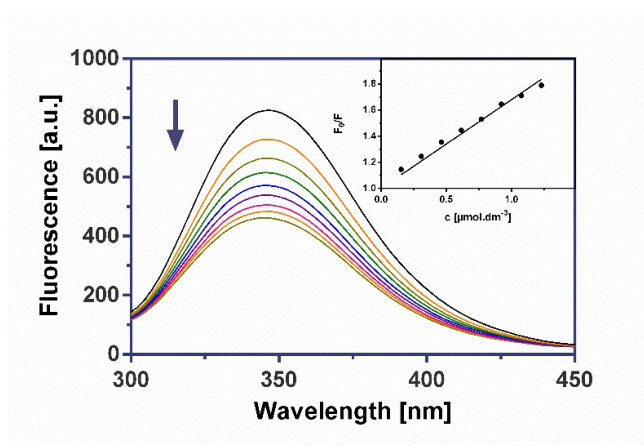


Figure S13. Fluorescence quenching spectra of BSA in presence of complex **2**. Inset: The corresponding Stern-Volmer plot for **2** at 25 °C.

Table S1. ^{13}C NMR (150 MHz, DMSO- d_6) chemical shifts δC [ppm] for complexes **1** – **5**.

		δC								
		C-2	C-3	C-4	C-4a	C-5	C-6	C-7	C-8	C-8a
1*	ClQ	145.6	122.8	135.0	126.6	108.9	130.0	111.6	162.3	139.7
2*	ClQ	145.7	122.8	135.0	126.6	109.0	130.0	111.7	162.3	140.2
3										
4**	dClQ	146.1	122.7	135.1	125.7	108.5	129.5	114.8	158.2	140.0
		147.0			125.4				157.2	139.6
5**	dBrQ	145.9	123.2	137.4	127.3	97.7	134.7	105.3	159.8	140.0
				137.6			134.6			

*162.3 (C=ODMF), 35.8 (MeDMF), 30.8 (MeDMF)

**chemical shifts for major form are in the first line and for the minor form in the second line

Table S2. Data describing different polyhedral distortions for **1** – **5**.

Complex	Σ ^a	CShM ^b	τ	CShM ^c	CShM ^d
1	121.32	2.968	0.6953	3.083	4.070
2	101.34	2.407	0.0843	4.314	1.030
3	88.48	1.594			
4	53.6	0.708			
5	(Zn1) 54	0.761			
	(Zn2) 57.3	0.977			

^a octahedral distortion parameter $\Sigma = (|90 - \varphi_i|)$ [$\Sigma = 0^\circ$ for an ideal octahedron; φ_i represents the twelve smallest L–M–L angles]^b CShM represents result from continuous shape measures of donor atoms positions relative to the vertices of an ideal octahedron^c CShM represents result from continuous shape measures of donor atoms positions relative to the vertices of an ideal trigonal bipyramid^d CShM represents result from continuous shape measures of donor atoms positions relative to the vertices of an ideal spherical square pyramid

Table S3. Cg...Cg distances and angles (Å, °) characterizing π - π interactions in **1** and **2**.

Complex	Cg(I)···Cg(J) ^a	Cg···Cg	α^b	β	γ
1	Cg _{py1} ···Cg _{ph1} ⁱ	3.4821(15)	18.69(13)	14.2	5.2
2	Cg _{py1} ···Cg _{py2} ⁱ	3.5821(1)	7.16(9)	17.2	15.6
	Cg _{ph1} ···Cg _{ph2} ⁱ	3.6236(1)	8.81(9)	14.1	16.5

[Symmetry codes: (i) = -x+1, -y+1, -z+1 (**1**), (**2**)]^aCg_{py1} represents centroid of the pyridine ring containing N1 atomCg_{py2} represents centroid of the pyridine ring containing N2 atomCg_{ph1} represents centroid of the phenyl ring containing C18 atomCg_{ph2} represents centroid of the phenyl ring containing C28 atom^b α is the dihedral angle between planes I and J. β is the angle between Cg(I)···Cg(J) vector and normal to plane I. γ is the angle between Cg(I)···Cg(J) vector and normal to plane JTable S4. Cg...Cg distances and angles (Å, °) characterizing π - π interactions in **3**.

Cg(I)···Cg(J) ^a	Cg···Cg	α^b	β	γ
Cg _{py} ···Cg _{py} ⁱ	3.7466	0	29.4	29.4

[Symmetry code: (i) = -x+1.5, -y+2.5, -z+1.5]

^aCg_{py} represents centroid of the pyridine ring containing N2 atom^b α is the dihedral angle between planes I and J. β is the angle between Cg(I)···Cg(J) vector and normal to plane I. γ

is the angle between Cg(I)···Cg(J) vector and normal to plane

Table S5. Cg...Cg distances and angles (Å, °) characterizing π - π interactions in **5**.

Cg(I)···Cg(J) ^a	Cg···Cg	α^b	β	γ
Cg _{ph1} ···Cg _{ph6} ⁱ	3.773(5)	1.4	20.7	20.2
Cg _{ph1} ···Cg _{ph6} ⁱⁱ	3.792(5)	1.4	17.8	18.4

[Symmetry codes: (i) = 1-x, 1-y, 1-z; (ii) = 2-x, 1-y, 1-z]

^aCg_{ph1} represents centroid of the carbocyclic ring containing C18 atomCg_{ph6} represents centroid of the carbocyclic ring containing C68 atom^b α is the dihedral angle between planes I and J. β is the angle between Cg(I)···Cg(J) vector and normal to plane I. γ

is the angle between Cg(I)···Cg(J) vector and normal to plane J