Electronic Supplementary Material (ESI) for New Journal of Chemistry.

NMR-spectroscopic investigation of the complex between tetraazonia-pentapheno[6,7-*h*]pentaphene and quadruplex DNA Tel26

Heiko Ihmels,* Katharina Löhl, Thomas Paululat, Sandra Uebach

Department of Chemistry and Biology, University of Siegen, Adolf-Reichwein-Str. 2,

57068 Siegen, Germany

E-mail: ihmels@chemie.uni-siegen.de

Table of content

Figure S1. 2D NOESY spectra of **Tel26** with cold probe S2

Figure S2. 2D NOESY spectra of **Tel26** of the imino protons range with cold probe S3

Figure S3. 2D NOESY spectra of **Tel26** of the aromatic protons range with cold probe; S4

Figure S4. 2D NOESY spectra of **Tel26** of the deoxyribose protons with cold probe S5

Table 1. ^{1}H chemical shifts of **Tel26** with cold probe S6

Figure S5. 2D NOESY of **Tel26** with HCN inverse probe S7

Table 2. ^{1}H chemical shifts of **Tel26** with HCN inverse probe S8

Figure S6. Superposed 2D NOESY spectra of **Tel26** in the absence and in the presence of ligand **2** S9

Figure S7. ^{1}H-NMR spectra of the imino protons of **Tel26** with increasing amount of ligand **2** S10

Figure S8. Shifts of the imino protons of the guanine residues of **Tel26** upon addition of 0.5 molar equivalents of ligand **2**. S11

Figure S9. Fluorimetric titration of quadruplex **Tel22** to the ligand **2**. S12

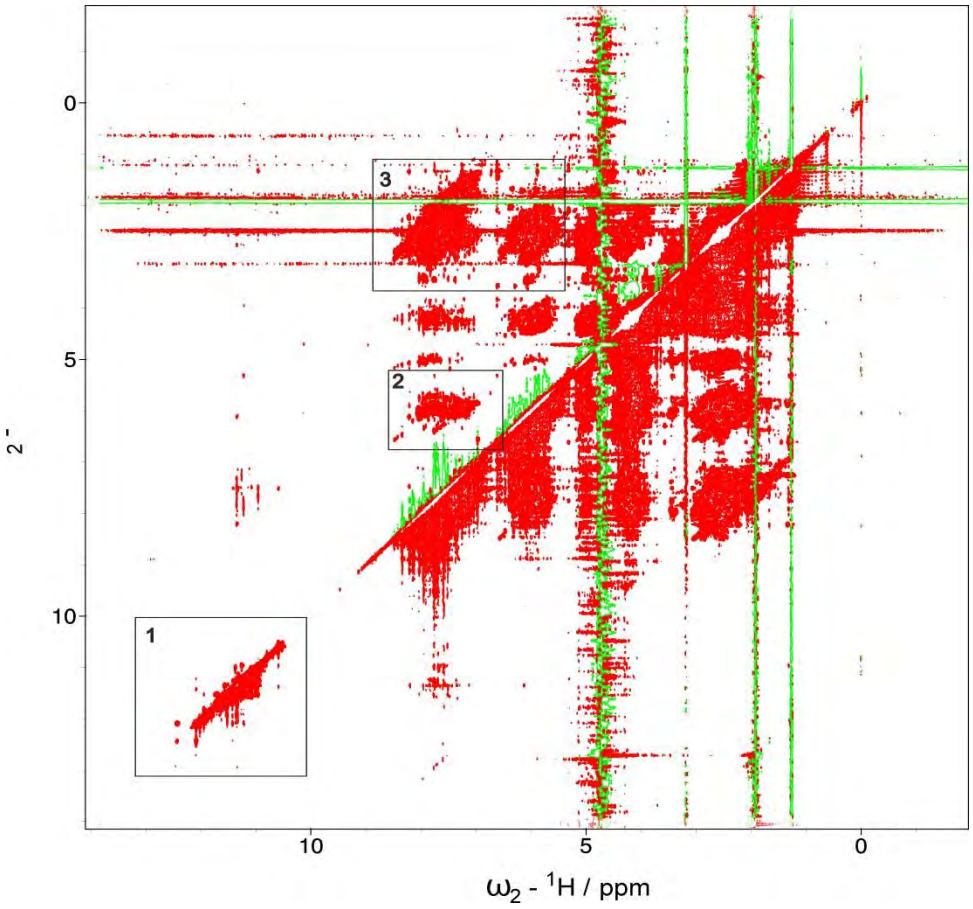

Figure S1. 2D NMR spectra (NOESY) of **Tel26** (2.5 mM, in bases) with cold probe; H_2O-D_2O (9:1); K-phosphate buffer (95 mM, pH 7.0); *T* = 33 °C.

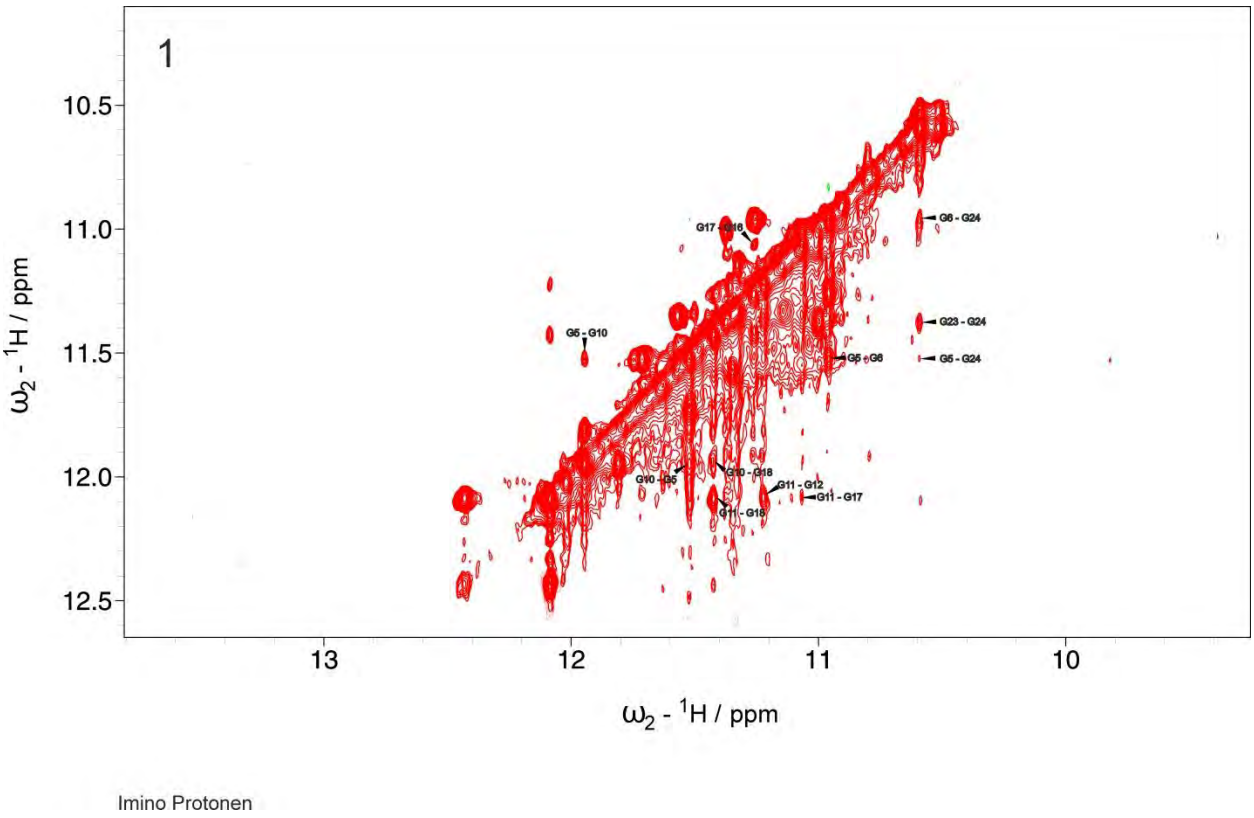

Figure S2. 2D NMR spectra (NOESY) of **Tel26** (2.5 mM, in bases) of the imino protons with cold probe; H_2O-D_2O (9:1); K-phosphate buffer (95 mM, pH 7.0); *T* = 33 °C.

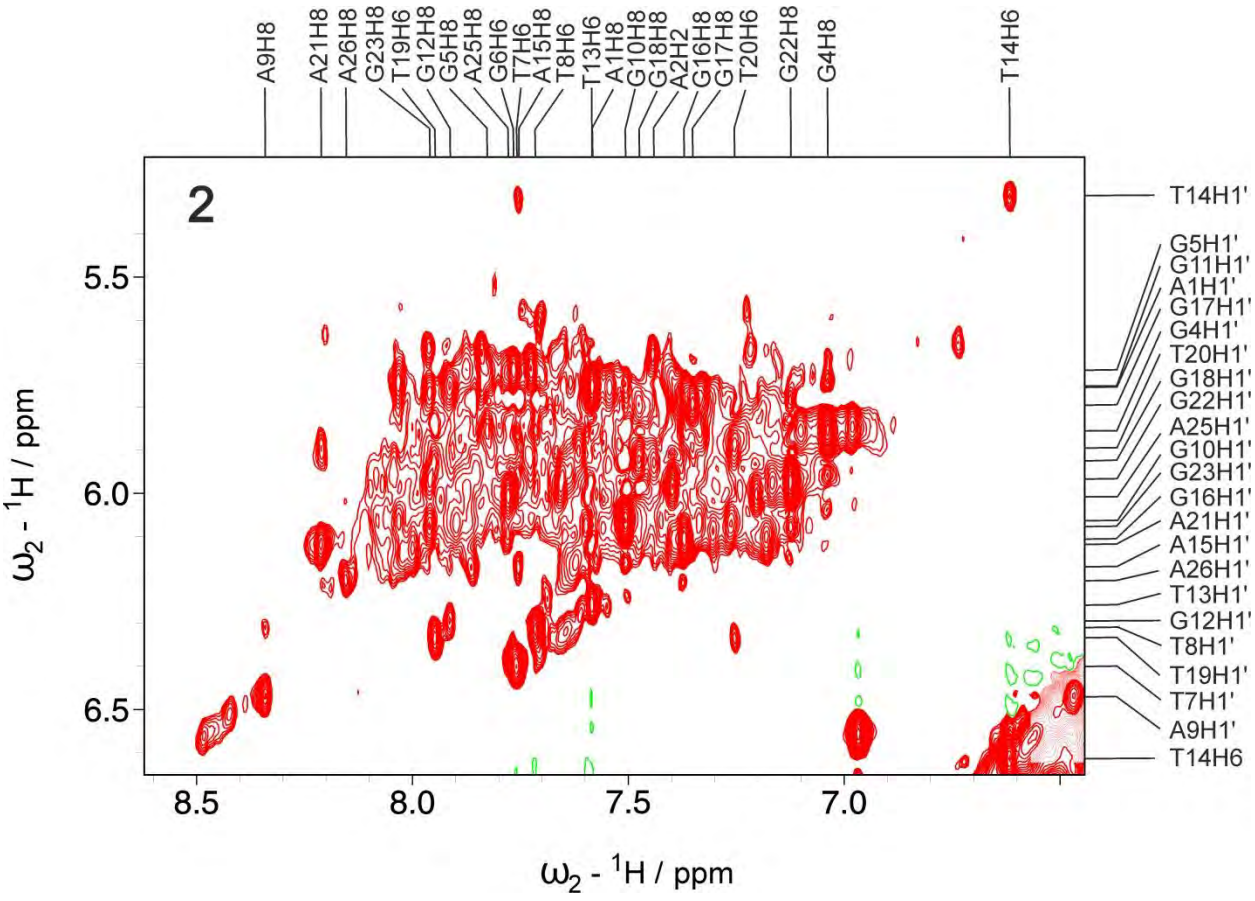

Figure S3. 2D NMR spectra (NOSEY) of **Tel26** (2.5 mM, in bases) of the aromatic protons with cold probe; H_2O-D_2O (9:1); K-phosphate buffer (95 mM, pH 7.0); *T* = 33 °C.

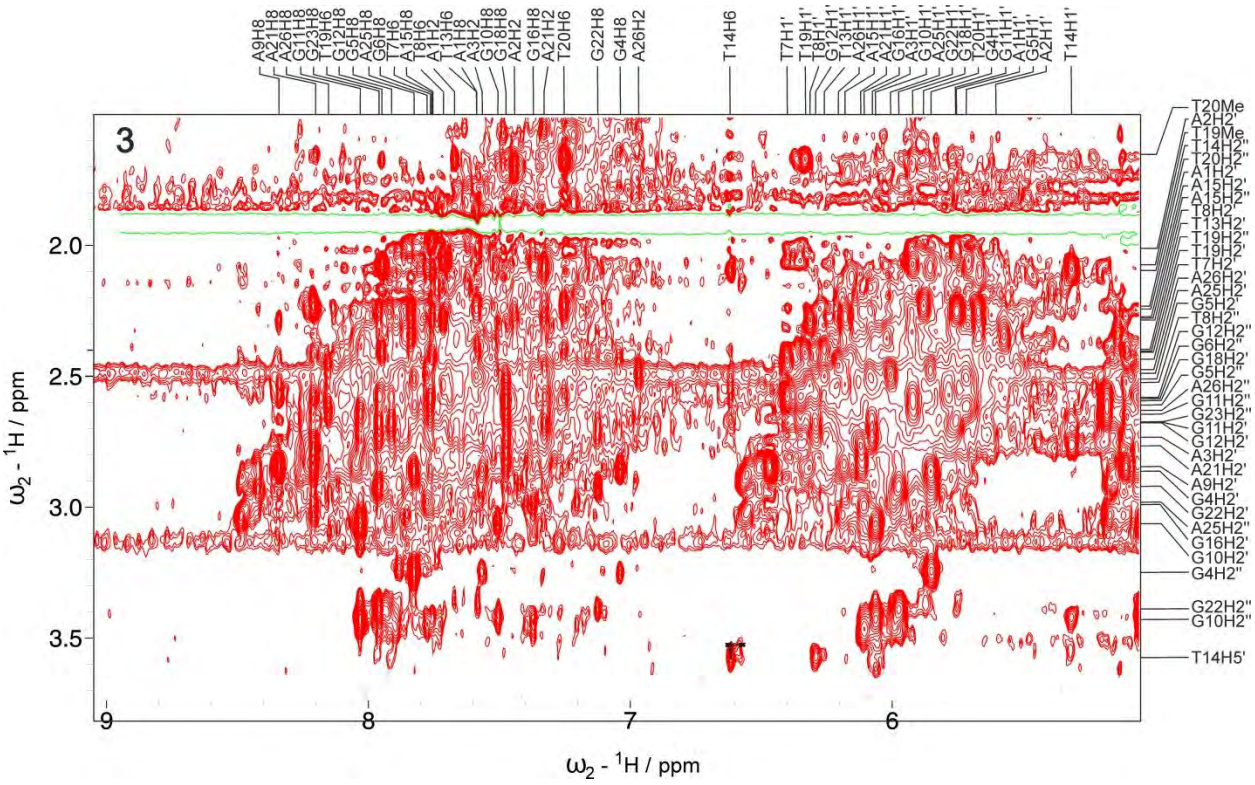

Figure S4. 2D NMR spectra (NOESY) of **Tel26** (2.5 mM, in bases) of the deoxyribose protons with cold probe; H_2O-D_2O (9:1); K-phosphate buffer (95 mM, pH 7.0); *T* = 33 °C.

Table 1. ^{1}H Chemical Shifts of **Tel26** at 33 °C with Cold Probe

	NH1	H2	H6	H8	Me	H1‘	H2‘	H2“	H3‘	H4‘	H5‘	H5“
A 1		7.69		7.58		5.75	2.25					
A 2		7.44		7.81		5.61	2.01					
A 3		7.56		7.87		6.08	2.73					
G 4	11.34			7.02		5.85	2.86	3.25				
G 5	11.52			7.83		5.72	2.51	2.61				
G 6	10.96			7.76		6.35	2.58		5.03			
T 7			7.76			6.40	2.44					
T 8			7.72		1.99	6.31	2.29	2.53	4.93		4.15	
A 9		8.12		8.34		6.47	2.85		5.11		4.24	
G 10	11.95			7.51		6.06	3.06	3.43				
G 11	12.09			8.03		5.76	2.67	2.64				
G 12	11.22			7.91		6.29	2.68	2.58	5.08			
T 13			7.59		1.88	6.26	2.40					
T 14			6.62		1.32	5.31	1.29	2.09	4.51	3.95	3.57	3.83
A 15		7.67		7.76		6.18	2.27	2.28				
G 16	11.26			7.37		6.11	3.00					
G 17	11.07			7.35		5.79			5.01			
G 18	11.42			7.48		5.92	2.59		5.18			
T 19			7.95		2.08	6.33	2.41					
T 20			7.25		1.67	5.88	1.33	2.23	4.98			
A 21		7.33		8.21		6.12	2.77		5.07			
G 22	11.35			7.13		5.97	2.92	3.39				
G 23	11.38			7.96		6.08	2.67					
G 24	10.59			7.35		5.85						
A 25		7.52		7.78		6.01	2.49	2.98	4.93			
A 26		6.97		8.15		6.21	2.47	2.63				

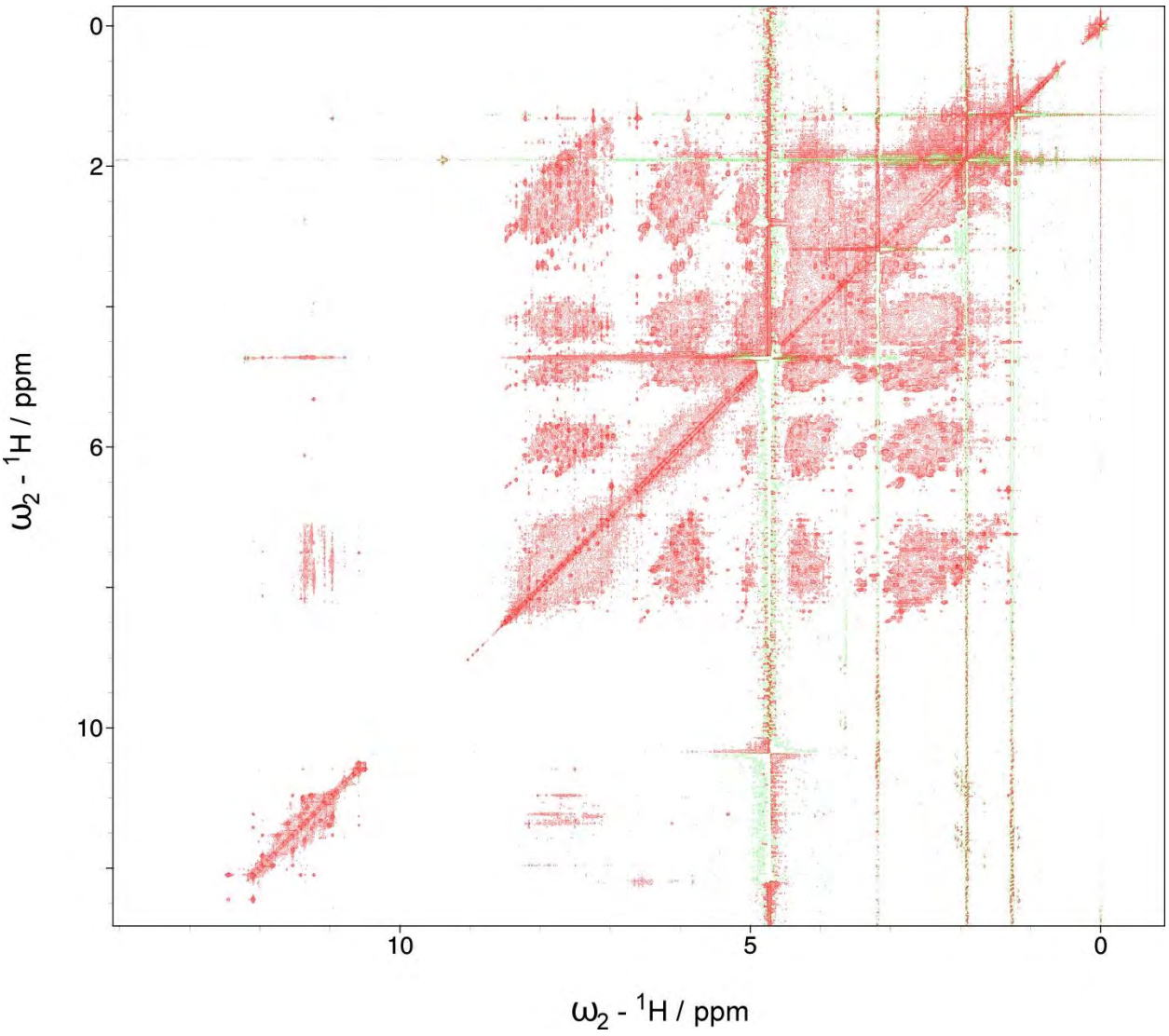

Figure S5. 2D NMR spectra (NOESY) of **Tel26** (2.5 mM, in bases) with HCN inverse probe; H_2O-D_2O (9:1); K-phosphate buffer (95 mM, pH 7.0); *T* = 31 °C.

Table 2. ^{1}H Chemical Shifts of **Tel26** at 31 °C with HCN Inverse Probe

	NH1	H2	H6	H8	Me	H1‘	H2‘	H2“	H3‘	H4‘	H5‘	H5“
A 1		7.68		7.59		5.76	2.25					
A 2												
A 3				7.92		6.06	2.72					
G 4	11.34			7.04		5.86	2.86	3.25				
G 5	11.53			7.83		5.71						
G 6	10.96			7.76		6.36	2.57					
T 7			7.76			6.40	2.44					
T 8			7.71		1.99	6.31	2.28	2.52				
A 9				8.34		6.47	2.85		5.11			
G 10	11.96			7.51		6.06	3.06	3.43				
G 11	12.09			8.03		5.75						
G 12	11.23			7.92		6.29						
T 13			7.58		1.88	6.26	2.40					
T 14			6.62		1.31	5.32		2.10		3.95	3.57	3.83
A 15				7.75		6.18	2.27					
G 16	11.26			7.37		6.11	2.99					
G 17	11.07			7.35		5.79						
G 18	11.41			7.46		5.92	2.60		5.18			
T 19			7.95		2.08	6.34						
T 20			7.24		1.66	5.88	1.63	2.23	4.99			
A 21		7.33		8.21		6.12	2.77		5.07			
G 22	11.36			7.12		5.98	2.92	3.39				
G 23	11.38			7.97								
G 24	10.59			7.85								
A 25		7.51		7.78		6.00	2.49	2.99				
A 26				8.15		6.21						

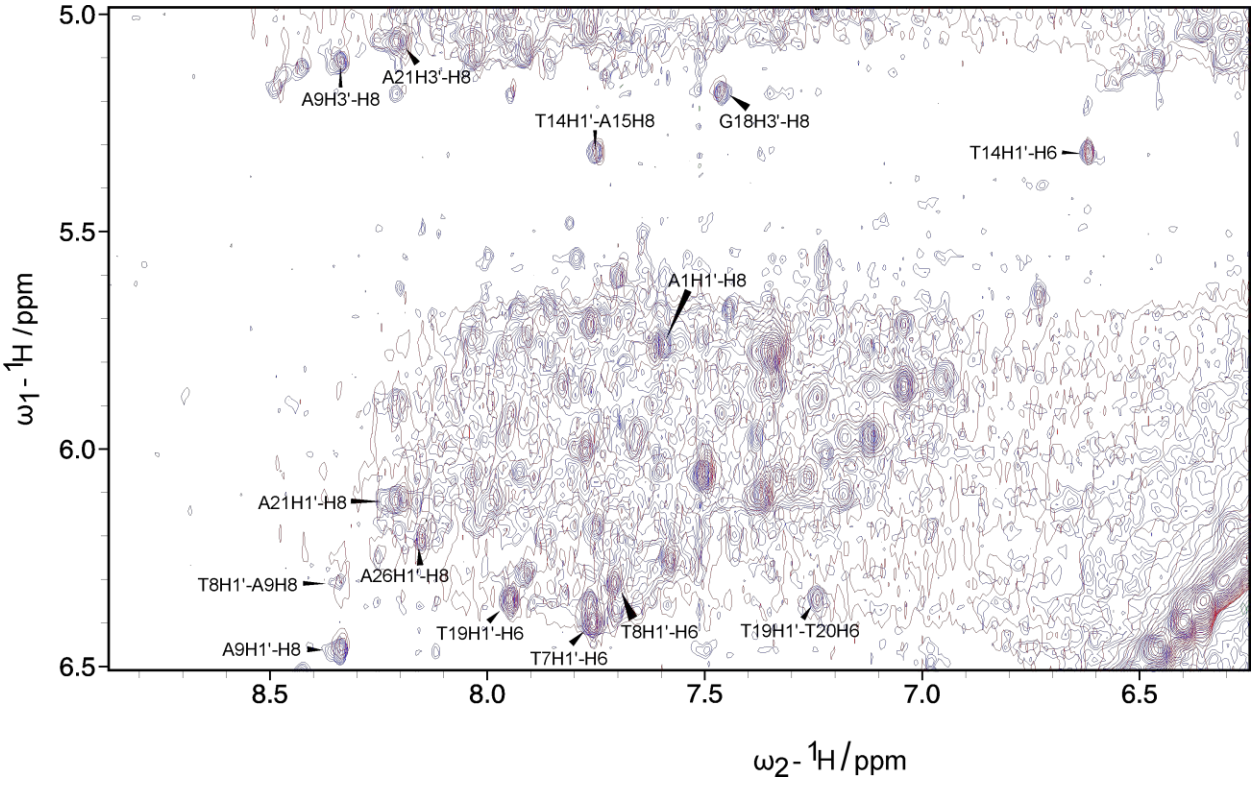

Figure S6. Superposed 2D NMR spectra (NOESY) of **Tel26** (2.5 mM, in bases) in the absence (blue) and in the presence (red) of ligand **2** (0.5 molar equivalent); in K-phosphate buffer in H_2O/D_2O (9:1) (95 mM, pH 7.0); *T* = 31 °C. In the labels "Gx-Gy" within the spectrum, Gx refers to the guanine proton signal at the ω_1 axis and Gy refers to the one at the ω_2 axis.

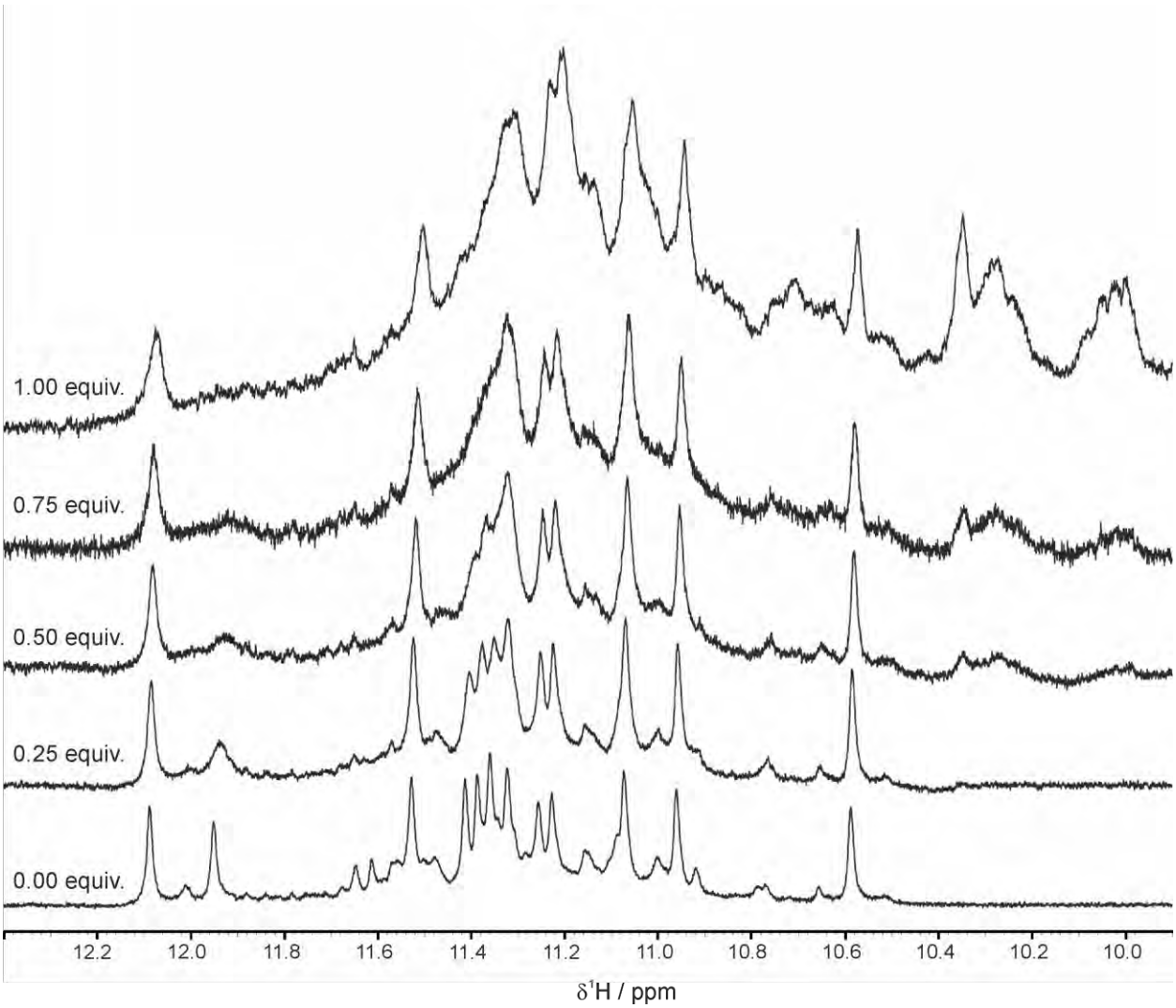

Figure S7. ^{1}H-NMR spectra of the imino protons (10.3-12.5 ppm) of **Tel26** (2.5 mM in bases) with increasing amount of ligand **2**; in K-phosphate buffer H_2O/D_2O (9:1) (95 mM, pH 7.0); *T* = 31 °C.

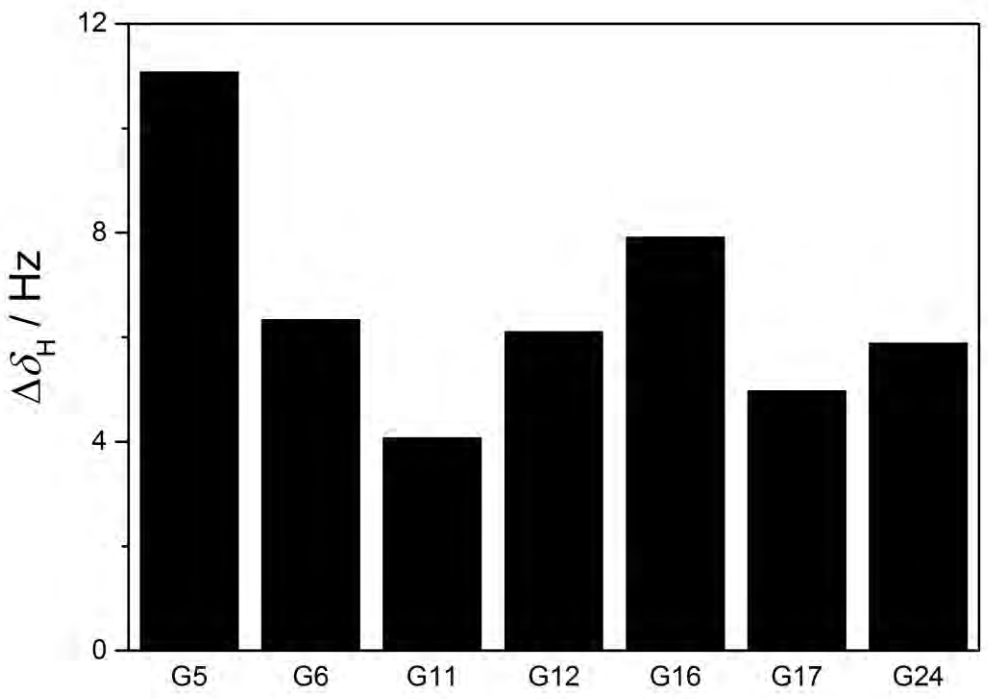

Figure S8. Shifts of the imino protons, $\Delta\delta$ (in Hz), of the guanine residues of **Tel26** upon addition of 0.5 molar equivalents of ligand **2**.

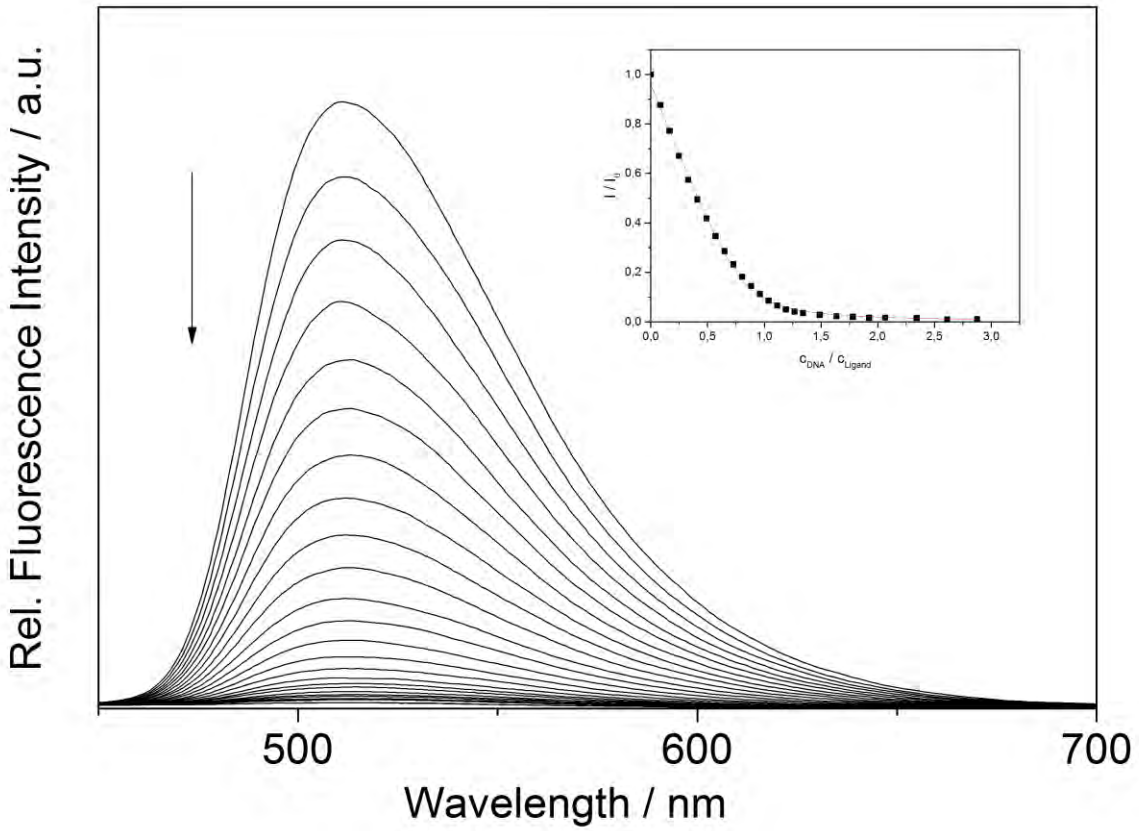

Figure S9. Fluorimetric titration of quadruplex **Tel26** to the ligand **2**. Inset: Plot of (I / I_0) *versus* DNA-to-ligand ratio; continuous line represents the best fit of the experimental data to the independent-site model; λ_{ex} = 386 nm.