Structure of a two-G-tetrad intramolecular G-quadruplex formed by a variant human telomeric sequence in K^+ solution: insights into the interconversion of human telomeric G-quadruplex structures

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Supplementary Information

Figure S1. Imino regions of 1D ^{1}H NMR spectra of multiple telomeric sequences (Figure 1A) at 20°C, with the assignment of I14-Tel23 and the partial assignment of Tel21-T (based on the numbering system shown in Figure 1A). The assignment of G16 in the A-Tel21-TT sequence (Figure 1A), which has been shown to form the hybrid-2 structure[1], is also shown. The G10H1 protons of Tel21-T and A-Tel21-T are labeled with asterisks.

Figure S2. The imino proton regions of the 1D ^{1}H NMR spectra of I14-Tel23 in K^{+} solution in the variable temperature study. The G10H1 proton is labeled with an asterisk.

Figure S3. CD melting curves of multiple telomeric sequences (see Figure 1A for sequences) in K^{+} solution monitored at 287 nm.

Reference:

1. Dai, J. X.; Carver, M.; Punchihewa, C.; Jones, R. A.; Yang, D. Z., *Nucleic Acids Research* **2007,** 35, (15), 4927-4940.

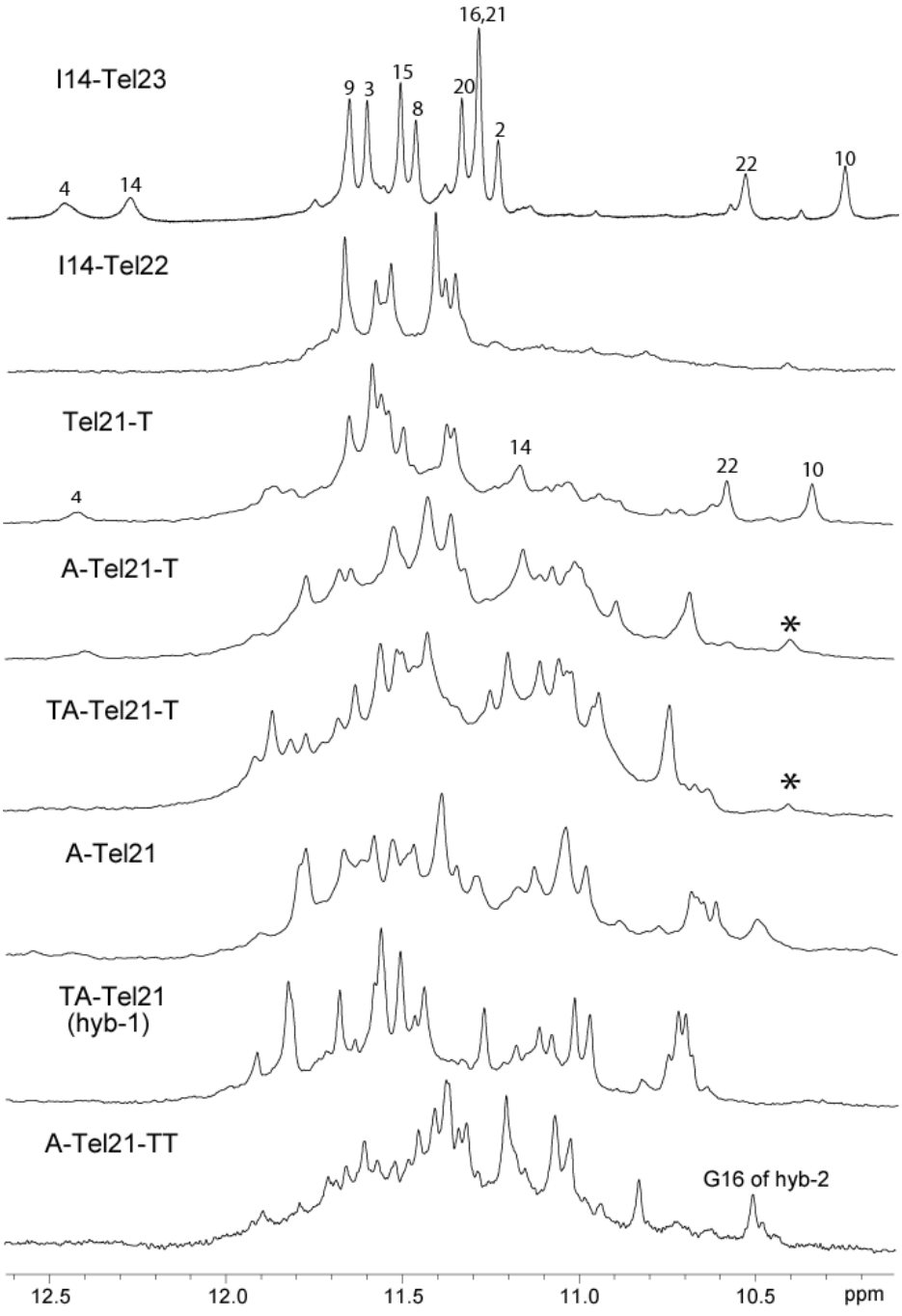
I14-Tel23
16,21
9
3
15
8
20
2
22
10
4
14
I14-Tel22
Tel21-T
14
22
10
4
A-Tel21-T
*
TA-Tel21-T
*
A-Tel21
TA-Tel21
(hyb-1)
A-Tel21-TT
G16 of hyb-2
12.5
12.0
11.5
11.0
10.5
ppm

Figure S1.

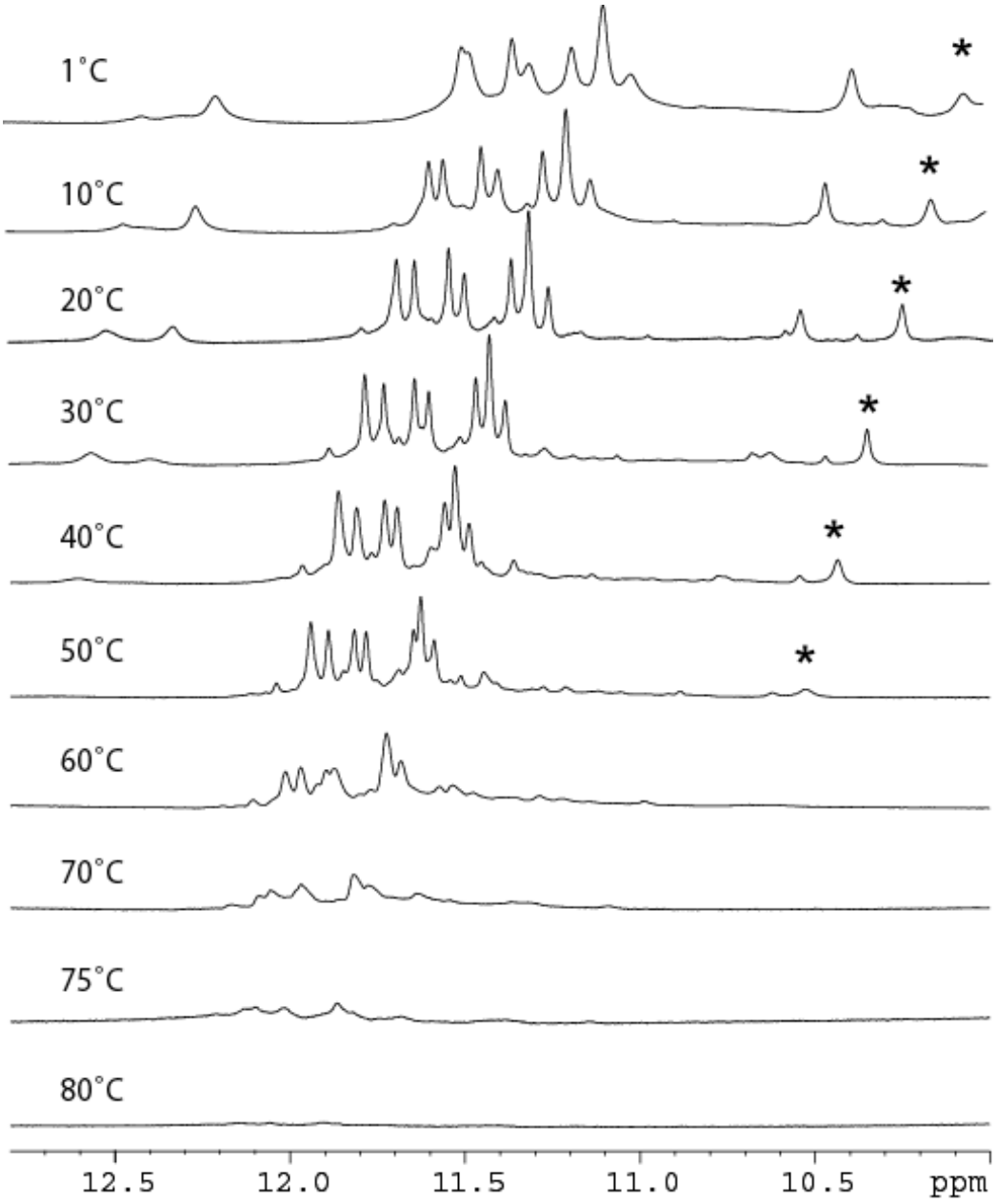

Figure S2.

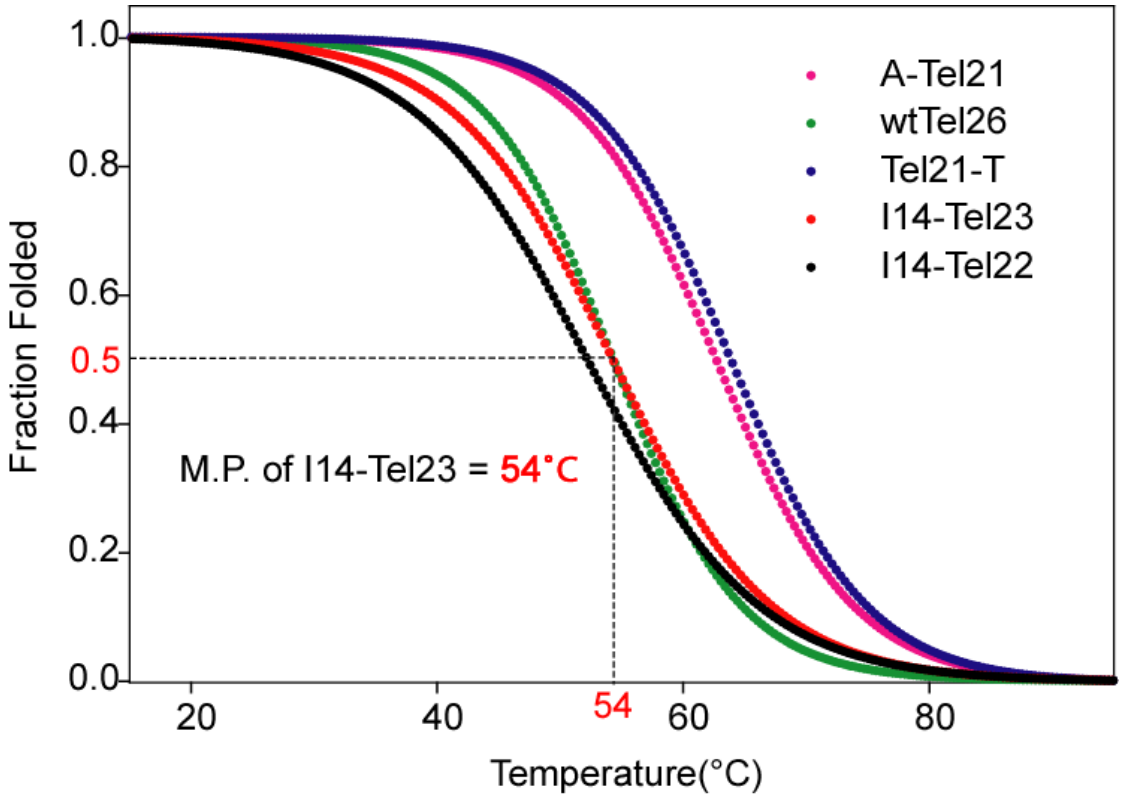
1.0
0.8
0.6
0.5
0.4
0.2
0.0
Fraction Folded
A-Tel21
wtTel26
Tel21-T
I14-Tel23
I14-Tel22
M.P. of I14-Tel23 = 54°C
20
40
54
60
80
Temperature(°C)

Figure S3.

Table S1. Summarized NOE interactions of the loop residues.

A1		A1	
		H8	H1'
I14	H8		6.00
	H1'		5.70
G15	H8		5.18
	H1'		5.40
A13	H4'	4.48	5.50

G4		G4							
		H1	NH21	H8	H1'	H2'	H2"	H3'	H4'
G3	H1		5.03						
	H8			4.97					
	H1'			4.36					4.35
	H2'			3.73					
	H2"			3.21					
	H3'			4.43					
	H4'			4.49					
T5	H6			5.3	4.53	4.2	5.1	5.3	5.93
	Me			6	6	5.5	5.1	5.5	5.5
	H3'			5.5				6	
T6	Me			5.5	4.8	4.6	5.6	6	6.2
G16	H1	5.18							
A19	H2	3.88	3.57						

T5		T5							
		H6	Me	1'	2'	2"	H3'	4'	5'
G4	H8	5.3	5.3				5.5		
	H1'	4.53	6						
	H2'	4.2	5.5						
	H2"	5.1	5.1						
	H3'	5.3	5.5				6		
	H4'	5.93	5.5						
T6	Me	weak	6.2	5	weak	weak	6		
	H6	7.5		6	weak	weak			
	H4'			5.5					
	H5'			4.8					
A7	H2	4.61	4.5		weak			4.6	5

T6		T6							
		Me	H6	H1'	H2'	H2''	H3'	H4'	H5'
G4	H8	5.5							
	H1'	4.8							
	H2'	4.6							
	H2''	5.6							
	H3'	6							
	H4'	6.2							
T5	H6	weak	7.5						
	Me	6.2							
	H1'	5	6					5.5	4.8
	H2'	weak	weak						
	H2''	weak	weak						
A7	H2			weak					
	H8		6	weak	weak	weak	4.3	3.66	4.25
	H1'							5.95	

A7		A7				
		H2	H8	H1'	H2''	H3'
G3	H1	5.2				
	H6	4.61				
	Me	weak				
	4'	4.6				
	H2'	weak				
	5'	5				
T5	Me	4.5				
T6	H6		6			
	H1'	weak	weak			
	H2'		weak			
	H2''		weak			
	H3'		4.3			
	H4'		3.66	5.95		
	H5'		4.25			
G8	H1		4.44	5	4.5	5.3
	H8	5.05				
	H1'	5.5				
	H3'			4.6		
A19	H2	5.5				
G20	H1		5.44			

G10		G10							
		H1	H8	H1'	H2',2"	H3'	H4'	H5'	H5"
T11	Me		5.80	4.78		5.57	4.20		
	H6			3.60	4.50	5.40	4.89		
	H1'								
	H2'	6.00		3.39					
	H2"	6.00		4.20					
	H3'			4.16					
	H4'								
	H5'			4.70					
T12	Me		4.60	4.80	3.96	5.00			
	H6	4.50	5.80	5.80	6.00				
	H1'	3.80							
	H2'	5.29							
	H2"	5.24							
	H3'	5.25							
	H4'	4.00							
	H5'*	4.62							
G9	H1'		4.00						
	H1	4.11							
	H21	5.37							
	H22	5.25							
	H8		4.87						
I14	H1	4.84							
	H2	6.00							
	H8	5.50							
A13	H1'	5.50							
G22	H1	5.00	4.39						

T11		T11							
		Me	H6	H1'	H2'	H2"	H3'	H4'	H5"
G10	H1				6.00	6.00			
	H8	5.80							
	H1'	4.78	3.60		3.39	4.20	4.16		4.70
	H2',2"		4.50						
	H3'	5.57	5.40						
	H4'	4.20	4.89						
T12	Me		5.99	5.00	4.50		4.00	5.00	
	H6			5.46	4.50	4.00	4.04	5.67	
	H5'			5.00					
	H5"		5.80	4.80					
I14	H8		6.50	4.80	6.00	5.50			
	H1'			6.50					

T12		T12								
		Me	H6	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G10	H1		4.50	3.80	5.29	5.24	5.25	4.00	4.62	
	H8	4.60	5.80							
	H1'	4.80	5.80							
	H2',2"	3.96	6.00							
	H3'	5.00								
T11	H6	5.99								5.80
	Me									
	H1'	5.00	5.46						5.00	4.80
	H2'	4.50	4.50							
	H2"		4.00							
	H3'	4.00	4.04							
	H4'	5.00	5.67							
A13	H8		5.48	4.80	4.17	3.50	4.40	5.81		
	H4'			4.96						
I14	H1		5.68	5.42				4.66		
	H8							5.00	4.80	

A13		A13			
		H8	H1'	H4'	H5',5"
A1	H8			4.48	
	H1'			5.50	
G10	H1		5.50		
T12	H6	5.48			
	H1'	4.80		4.96	
	H2'	4.17			
	H2"	3.50			
	H3'	4.40			
	H4'	5.81			

I14		I14				
		H1	H8	H1'	H2	H2'*
A1	H1'		6.00	5.70		
G2	H1'	5.00			5.50	
	H21				5.90	
	H22	5.23			5.60	5.01
G10	H1	4.84	5.50		6.00	
T11	H6		6.50			
	H1'		4.80	6.50		
	H2'		6.00			
	H2"		5.50			
T12	H6	5.68				
	H1'	5.42				
	H4'	4.66	5.00			
	H5"		4.80			
G15	H1'				4.00	
	H8		5.50	4.99	6.00	

T17		T17							
		Me	H6	H1'	H2'	H2"	H3'	H4'	H5"
G16	H1	5.98							
	H8		6		5.8	5.61			
	H1'	4.32	4.46						
	H2',2"	5.1	4.31						
	H3'	6	4.83						
	H4'	4.25	4.3						
	H5'	5.3							
T18	Me		6.57	4.3	4.5	4.3	5	5.2	5.86
	H2"						5		
	H3'			6					
	H6			5.04	5.14	5	4.51	5.48	
A19	H8				5.7				

T18		T18					
		Me	H6	1'	2'	2"	3'
T17	H6	6.57					
	H1'	4.3	5.04				6
	H2'	4.5	5.14				
	H2"	4.3	5				
	H3'	5	4.51			5	
	H4'	5.2	5.48				
	H5"	5.86					
A19	H8		5.03	4.99	3.96	3.61	4.36

A19		A19					
		H2	H8	H1'	H2'	H2"	H3'
G3	H1	4.36					
G4	H1	3.88					
	NH21	3.57					
A7	H2	5.5					
G8	H1	4.9					
G16	H1	4.04					
	H8		4	5.93	4.39		4.38
	H1'		5.53				
	H3'		4.7				
T17	H2'		5.7				
T18	H6		5.03				
	H1'		4.99				
	H2'		3.96				
	H2"		3.61				
	H3'		4.36				
G20	H1	4	5.5	3.8	4.5	4	6
	H21			4.22			
	H22	3.99	4.52	4.42	4.51	4.1	5.28

G22		G22						
		H1	H8	H1'	H2'	H2"	H3'	H4'
G9	H1	4.94						
	H2'	5.00						
	H2"	6.00						
	H8	4.50						
G10	H1	5.00						
	H8	4.39						
G21	H1	4.13		5.35				
	H22	5.36						
	H1'		3.36					
	H2'*		3.20					
	H3'		4.65					
T23	Me	5.76	4.86	5.07	4.70	4.90	4.80	5.76
	H6		5.50	4.30	3.20	3.00	4.20	6.54
	H4'			5.03				
	H5'			5.00				
	H5"			5.00				

T23		T23				
		Me	H6	H4'	H5'	H5"
G22	H1	5.76				
	H8	4.86	5.50			
	H1'	5.07	4.30	5.03	5.00	5.00
	H2'	4.70	3.20			
	H2"	4.90	3.00			
	H3'	4.80	4.20			
	H4'	5.76	6.54			