Structure of an unprecedented G-quadruplex scaffold in the human *c-kit* promoter

Anh Tuân Phan[1,3,*], Vitaly Kuryavyi[1,#], Sarah Burge[2,4,#],
Stephen Neidle[2,*] & Dinshaw J. Patel[1,*]

Supplementary Materials

Table S1. List of 2% ^{15}N-labeled samples of *c-kit87up*[a].

Name	Sequence									
		1		2		3		4		
ck2	A	GGG	A	GGG	C	G	CT	GGG	AGGAG	**G**G
ck3	A	GGG	A	GGG	C	G	CT	GGG	AGGA**G**	GG
ck4	A	GGG	A	GGG	C	G	CT	GGG	AG**G**AG	GG
ck5	A	GGG	A	GGG	C	G	CT	GGG	A**G**GAG	GG
ck6	A	GGG	A	GGG	C	G	CT	GG**G**	AGGAG	GG
ck7	A	GGG	A	GGG	C	G	CT	G**G**G	AGGAG	GG
ck8	A	GGG	A	GGG	C	G	CT	**G**GG	AGGAG	GG
ck9	A	GGG	A	GGG	C	**G**	CT	GGG	AGGAG	GG
ck10	A	GGG	A	GG**G**	C	G	CT	GGG	AGGAG	GG
ck11	A	GGG	A	G**G**G	C	G	CT	GGG	AGGAG	GG
ck12	A	GGG	A	**G**GG	C	G	CT	GGG	AGGAG	GG
ck13	A	GG**G**	A	GGG	C	G	CT	GGG	AGGAG	GG
ck14	A	G**G**G	A	GGG	C	G	CT	GGG	AGGAG	GG
ck15	A	**G**GG	A	GGG	C	G	CT	GGG	AGGAG	GG

[a] 2% ^{15}N-labeled residues are in boldface and labeled in red. Loop numbers are labeled in blue.

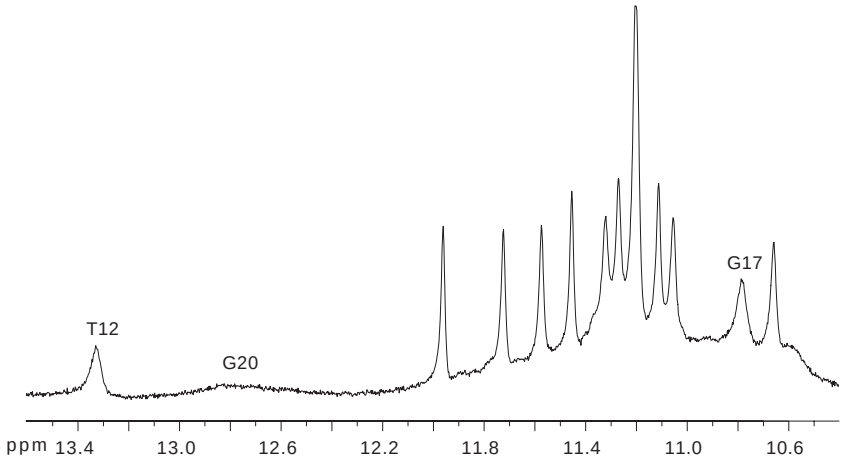

Figure S1. The 600 MHz imino proton spectrum of the *c-kit87up* sequence at 5 ºC. Imino proton of T12, G20, and G17 are indicated. Imino proton of T12 was assigned in a natural abundance $^{15}N,^{1}H$-HMQC spectrum. Imino proton of G17 was assigned in a ^{15}N-filtered experiment on a sample that was 2% ^{15}N-labeled at this position. The broad peak at 12.8 ppm was assigned to the G20 imino proton, because this peak was down-field shifted when G20 was substituted by either T or I.

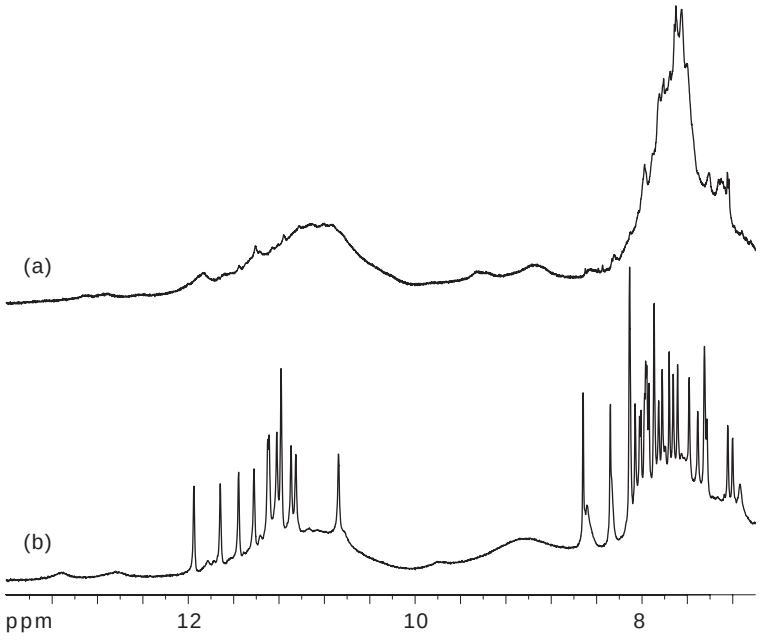

Figure S2. The 600 MHz proton spectra (7.0-13.6 ppm) of *c-kit87up* in (a) Na^+ and (b) K^+ solution at 25 ºC.

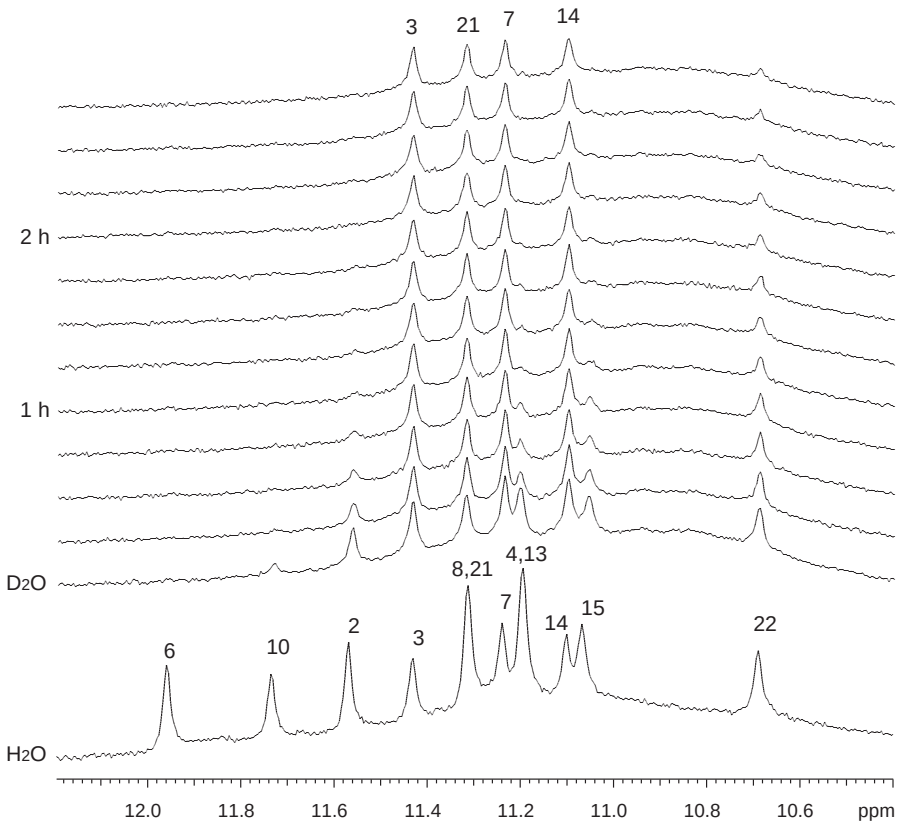

Figure S3. Real-time hydrogen exchange experiments for *c-kit87up*. Imino proton spectra in H_2O and after different periods of time in D_2O at 25 ºC.