HIV-1 integrase inhibitor *T30177* forms a stacked dimeric G-quadruplex structure containing bulges

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Supporting Information

Table S1. Inosine substituted sequences tested in this work

Name	Sequences
T30177-I1	**I** T GG T GGG T GGG T GGG T
T30177-I3	G T **I**G T GGG T GGG T GGG T
T30177-I4	G T G**I** T GGG T GGG T GGG T
T30177-I6	G T GG T **I**GG T GGG T GGG T
T30177-I7	G T GG T G**I**G T GGG T GGG T
T30177-I8	G T GG T GG**I** T GGG T GGG T
T30177-I10	G T GG T GGG T **I**GG T GGG T
T30177-I11	G T GG T GGG T G**I**G T GGG T
T30177-I12	G T GG T GGG T GG**I** T GGG T
T30177-I14	G T GG T GGG T GGG T **I**GG T
T30177-I15	G T GG T GGG T GGG T G**I**G T
T30177-I16	G T GG T GGG T GGG T GG**I** T

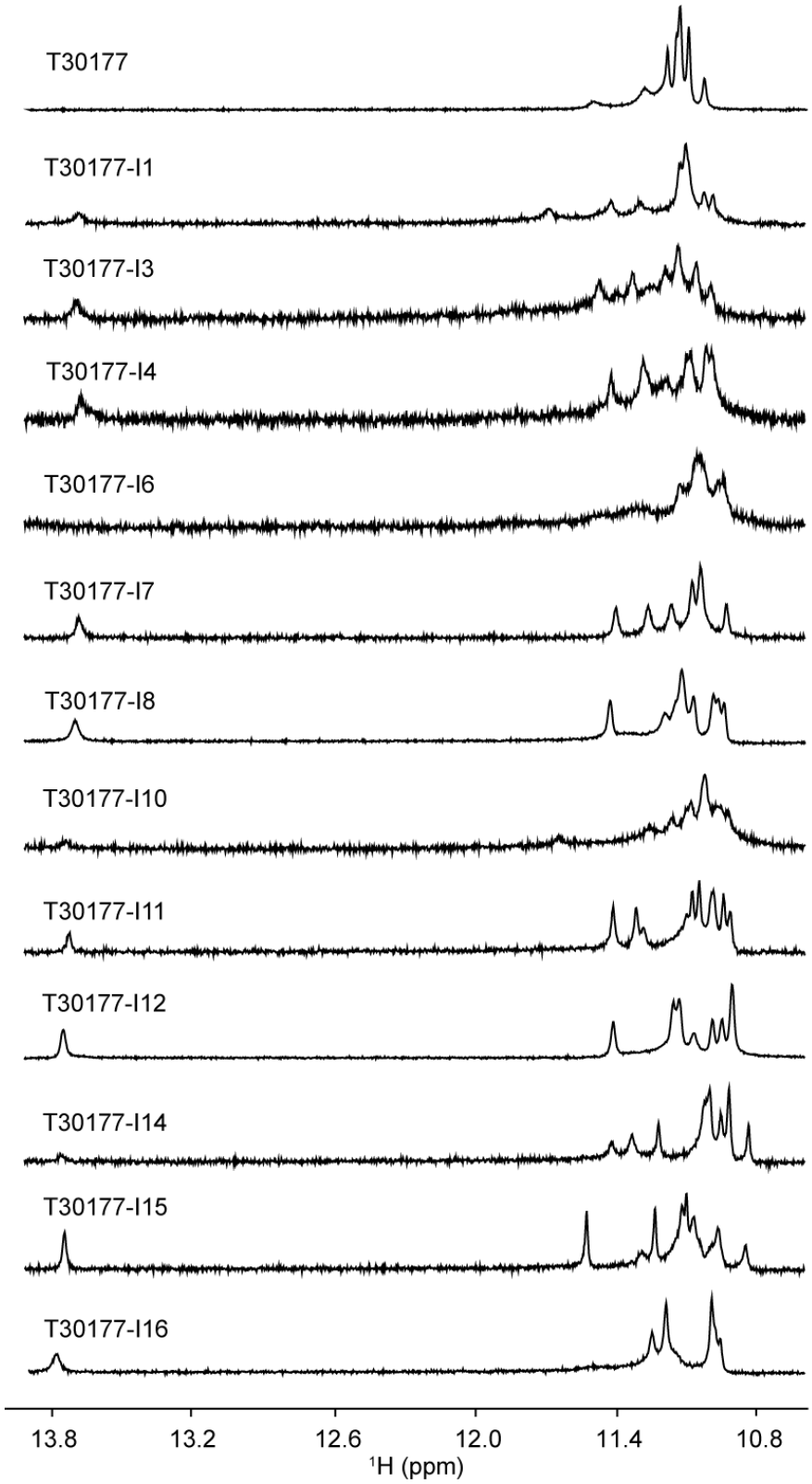
Table S2. Site-specific labeled DNA sequences used in this study[a-c]

Type	Sequences
^{15}N-labeled	G*TGGTGGGTGIGTGGGT
	GTG*GTGGGTGIGTGGGT
	GTGG*TGGGTGIGTGGGT
	GTGGTG*GTGIGTGGGT
	GTGGTGG*TGIGTGGGT
	GTGGTGGG*TGIGTGGGT
	GTGGTGGGTG*IGTGGGT
	GTGGTGGGTGIG*TGGGT
	GTGGTGGGTGIGTG*GGT
	GTGGTGGGTGIGTGG*GT
	GTGGTGGGTGIGTGGG*T
^{2}H-labeled	G#TGGTGGGTGIGTGGGT
	GTG#GTGGGTGIGTGGGT
	GTGG#TGGGTGIGTGGGT
	GTGGTG#GTGIGTGGGT
	GTGGTGG#TGIGTGGGT
	GTGGTGGG#TGIGTGGGT
	GTGGTGGGTG#IGTGGGT
	GTGGTGGGTGIG#TGGGT
	GTGGTGGGTGIGTG#GGT
	GTGGTGGGTGIGTGG#GT
	GTGGTGGGTGIGTGGG#T

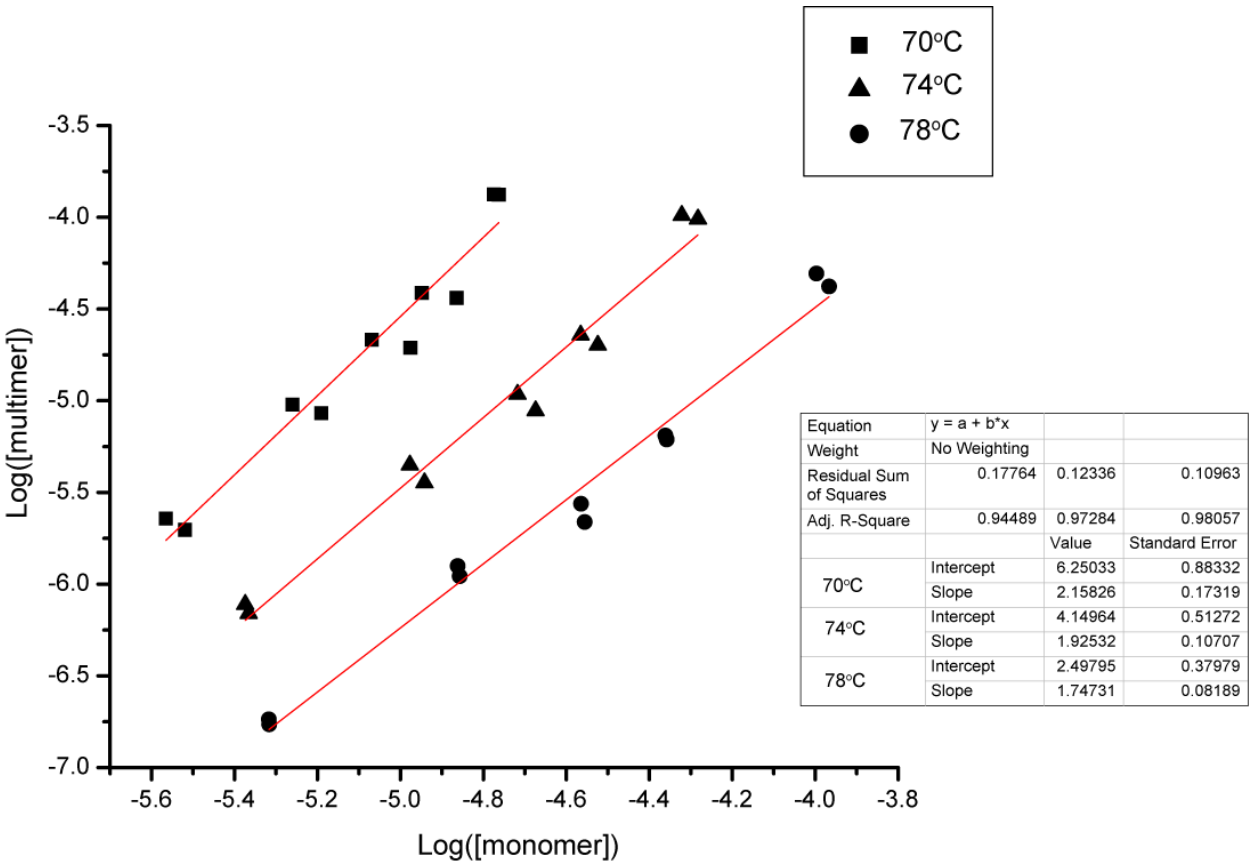
[a] Individual guanines 2%-^{15}N-labeled are marked by asterisks.

[b] Individual guanines ^{2}H-labeled at the H8 position are marked by hash signs.

[c] I is Inosine.

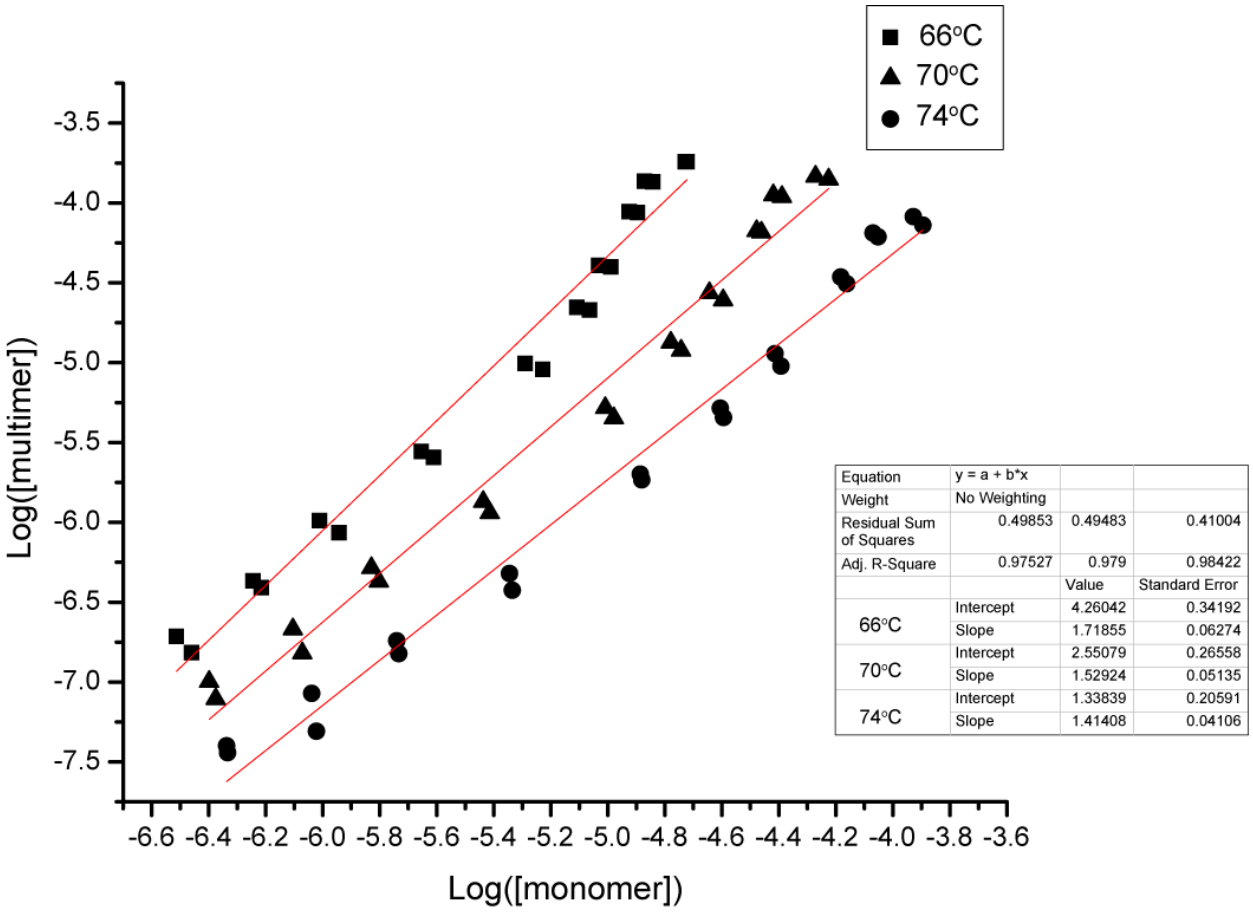


Figures S1. Imino proton spectra of *T30177* and guanine-to-inosine substituted sequences.



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.17764	0.12336	0.10963
Adj. R-Square	0.94489	0.97284	0.98057
		Value	Standard Error
70°C	Intercept	6.25033	0.88332
	Slope	2.15826	0.17319
74°C	Intercept	4.14964	0.51272
	Slope	1.92532	0.10707
78°C	Intercept	2.49795	0.37979
	Slope	1.74731	0.08189

Figures S2. Plots of multimer concentrations against monomer concentrations at three different temperatures of *T30177-I11* for experiments performed in ~100 mM K^+ solution. Data were obtained from the melting curves in Figure 3a. Concentrations were expressed in Moles before taking logarithms. Lines represent best fits of through the data points. The fitting results are shown on the right.



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.49853	0.49483	0.41004
Adj. R-Square	0.97527	0.979	0.98422
		Value	Standard Error
66°C	Intercept	4.26042	0.34192
	Slope	1.71855	0.06274
70°C	Intercept	2.55079	0.26558
	Slope	1.52924	0.05135
74°C	Intercept	1.33839	0.20591
	Slope	1.41408	0.04106

Figures S3. Plots of multimer concentrations against monomer concentrations at three different temperatures of *T30177-I11* for experiments performed in ~60 mM K^+ solution. Data were obtained from the melting curves in Figure 4a. Concentrations were expressed in Moles before taking logarithms. Lines represent best fits of through the data points. The fitting results are shown on the right.