Electronic Supplementary Information

The interaction of cyclic naphthalene diimide with G-quadruplex under molecular crowding condition

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Table of contents

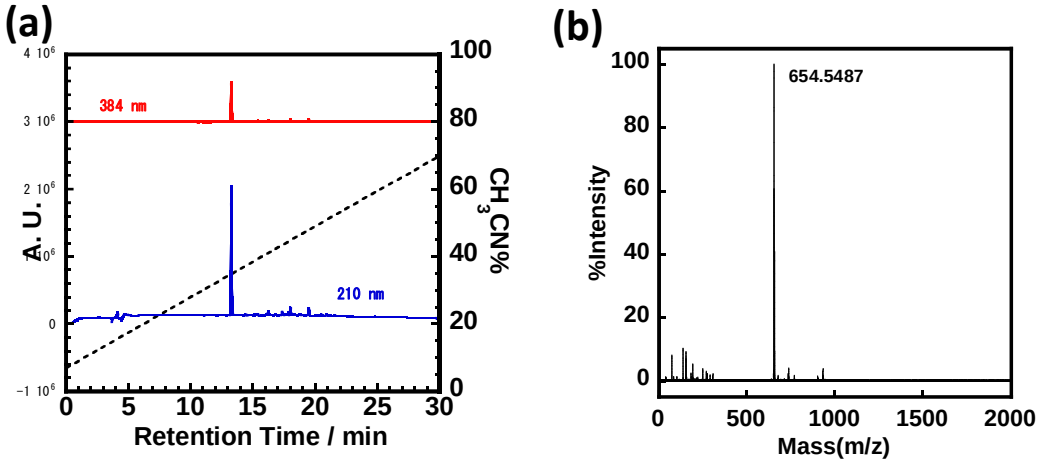


Figure S1. (a) HPLC and (b) MALDI-TOF-MS confirmation of **2.** HPLC conditions; The concentration of acetonitrile (CH_3CN) was changed (from 7% to 70%, 30 min) in water containing 0.1% trifluoroacetic acid at 40 °C.

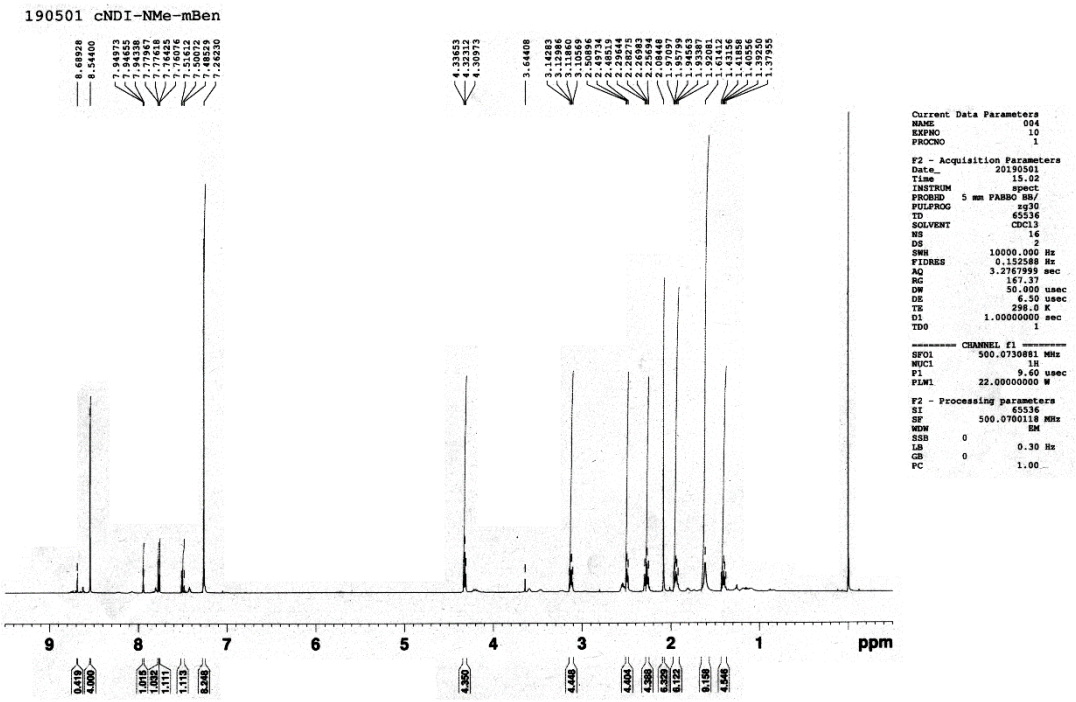


Figure S2. ^{1}H-NMR confirmation of **2**.

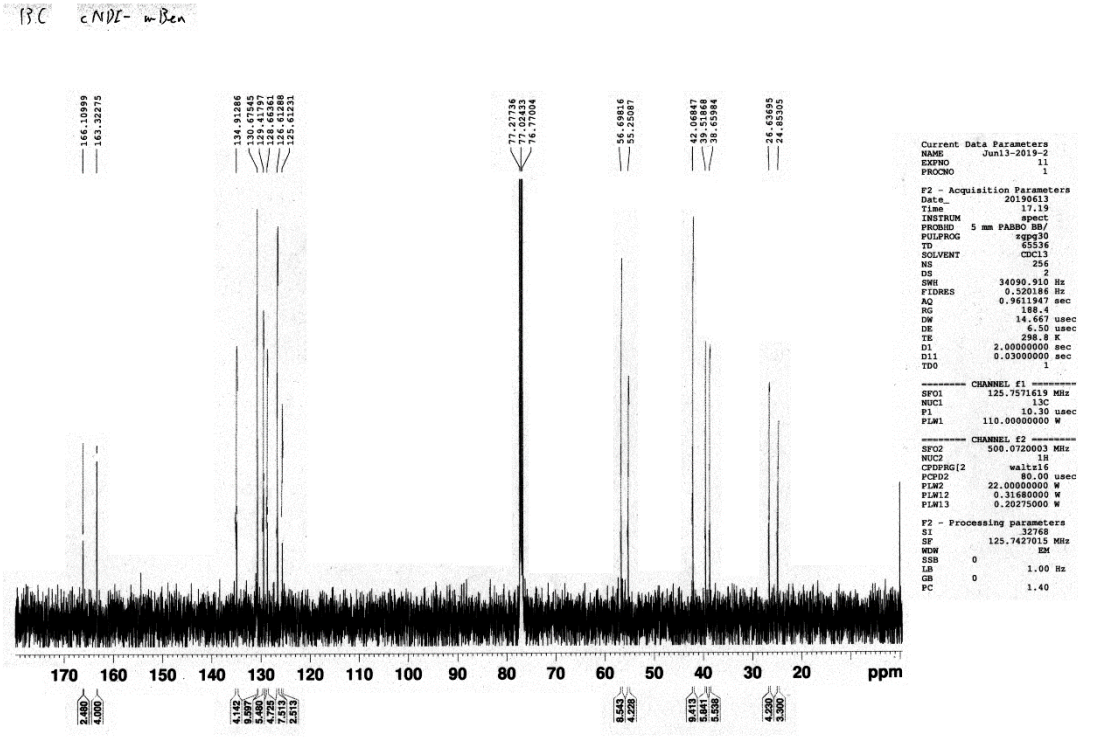


Figure S3. ^{13}C-NMR confirmation of **2**.

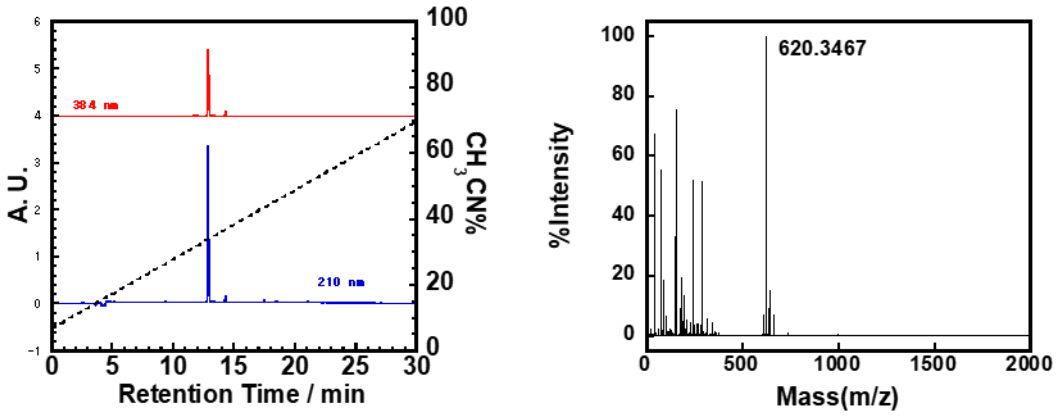


Figure S4. (a) HPLC and (b) MALDI-TOF-MS confirmation of **3**. HPLC conditions; The concentration of acetonitrile (CH_3CN) was changed (from 7% to 70%, 30 min) in water containing 0.1% trifluoroacetic acid at 40 °C.

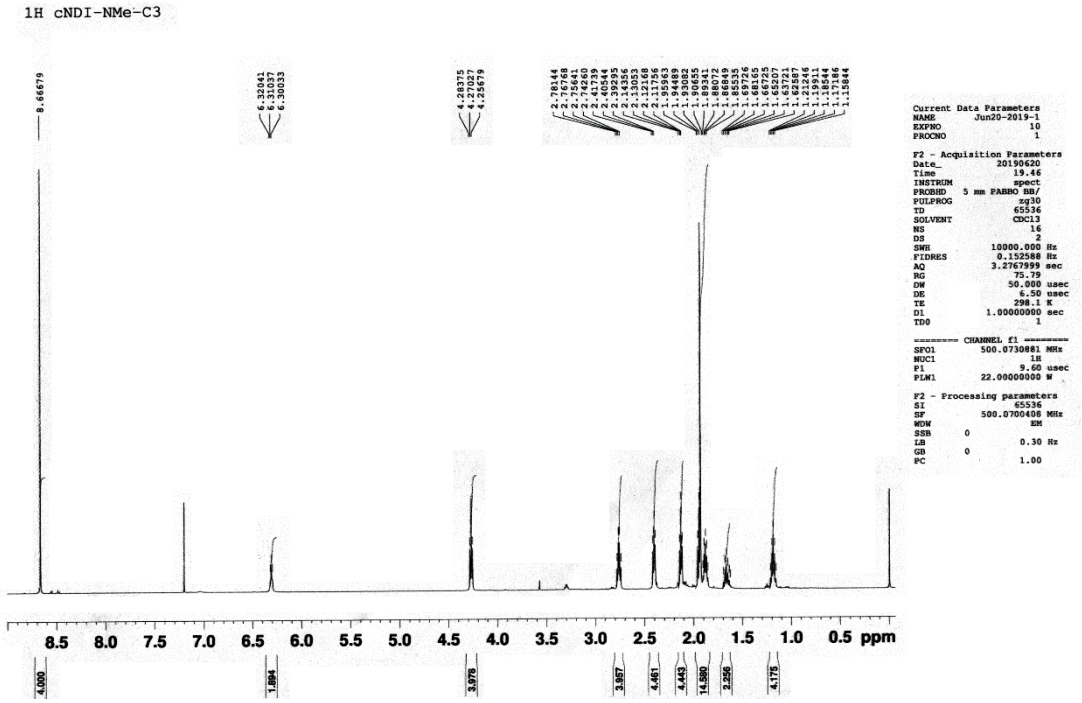


Figure S5. [1]H-NMR confirmation of **3**.

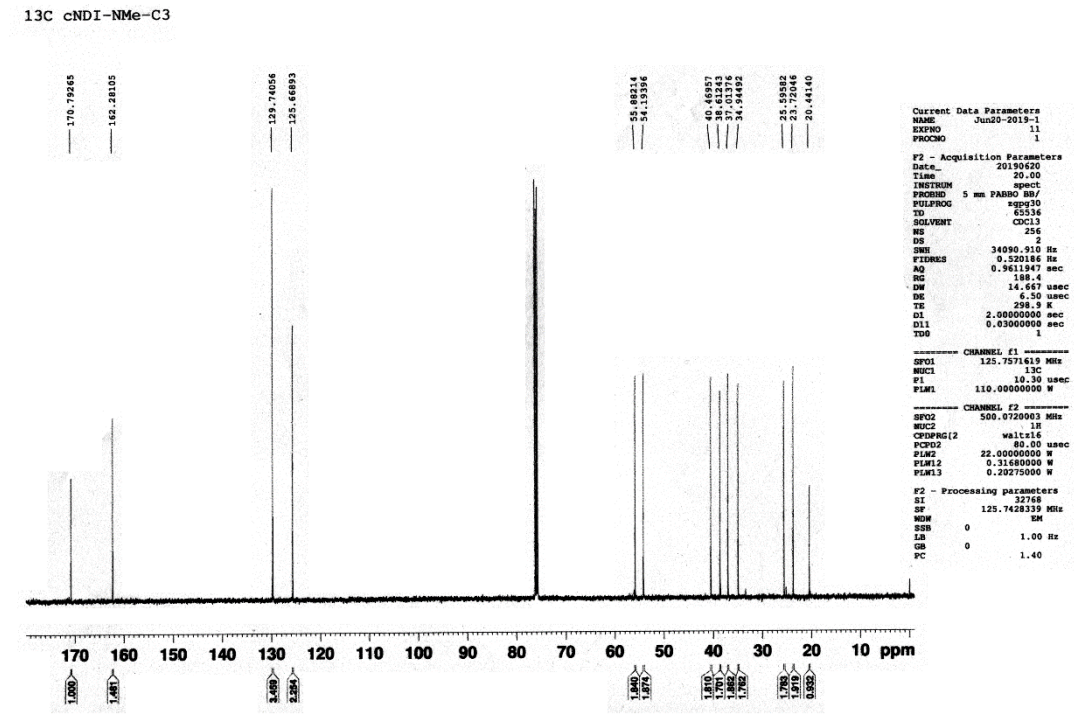


Figure S6. [13]C-NMR confirmation of **3**.

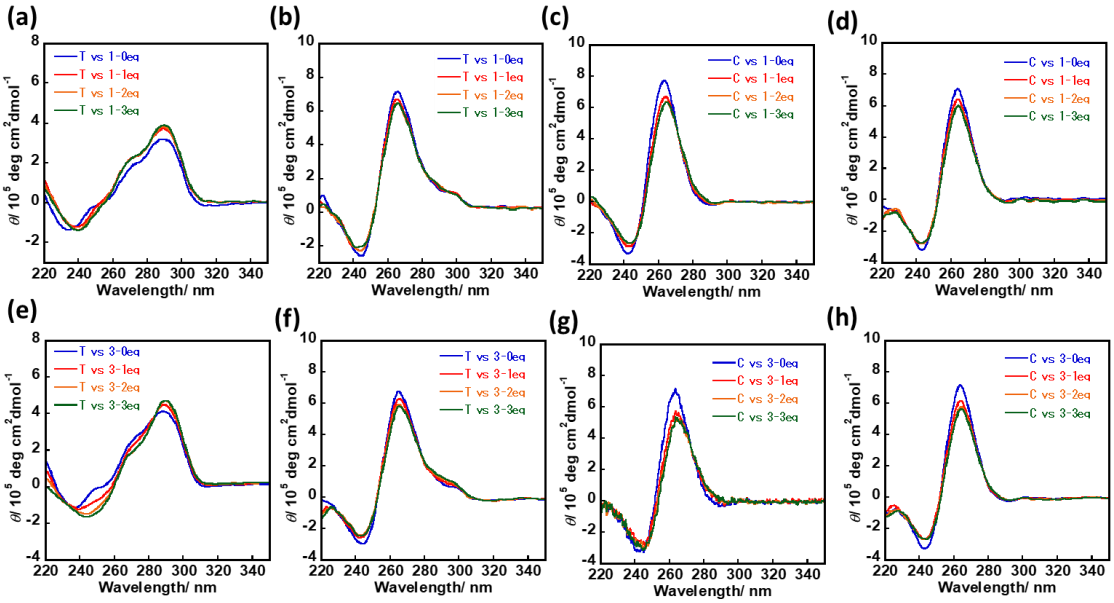


Figure S7. CD spectra of **1** recognizing telomere G1 (a) and c-*myc* (c) under dilute condition, and for telomere G1 (b) and c-*myc* (d) under molecular crowding condition; CD spectra of **3** recognizing telomere G1 (e) and c-*myc* (g) under dilute condition, and for telomere G1 (f) and c-*myc* (h) under molecular crowding condition. Dilute condition: 50 mM Tris-HCl buffer (pH 7.4) and 100 mM KCl; Molecular crowding condition: 50 mM Tris-HCl buffer (pH 7.4), 100 mM KCl, and 40%(v/v) PEG 200. T: telomere G1; C: c-*myc*; eq: equivalent.

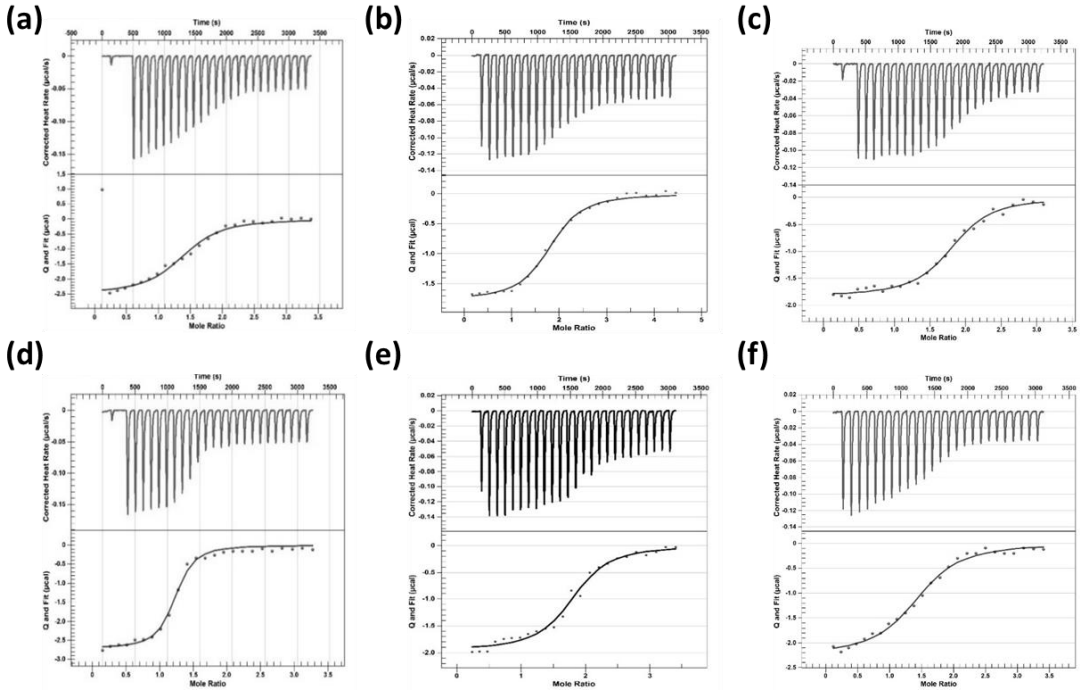


Figure S8. ITC fitting curve of Telomere G1 with **1** (a), **2** (b) and **3** (c), c-*myc* with **1** (d), **2** (e) and **3** (f) under dilute condition. 50 mM KH_2PO_4-K_2HPO_4 buffer (pH 7.0) at 25 °C

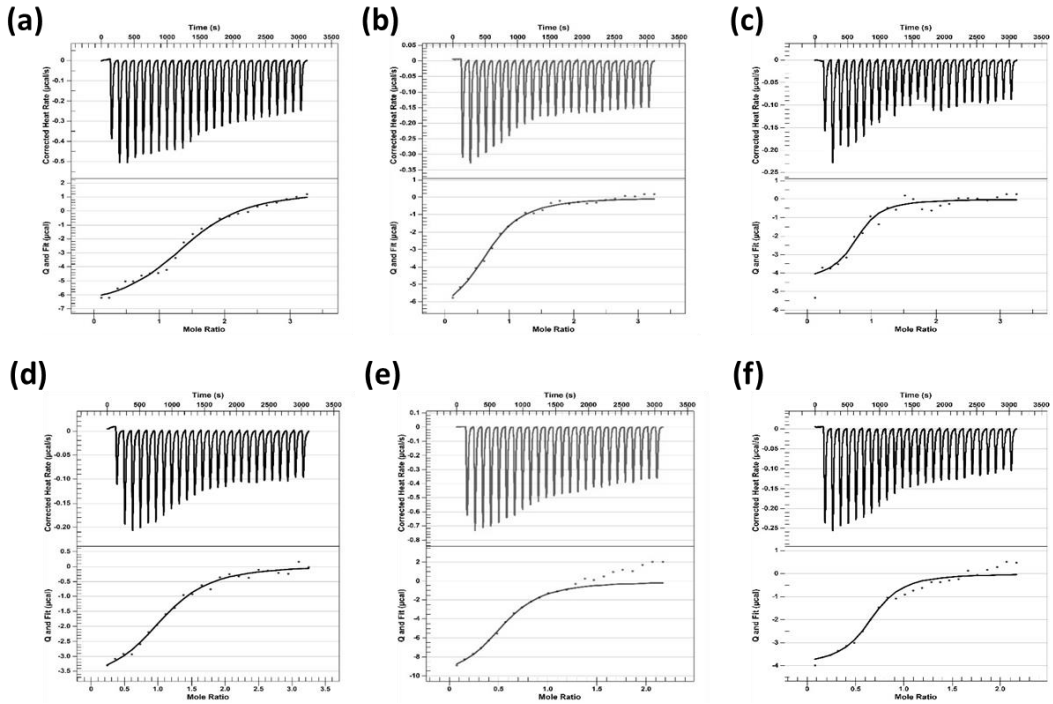


Figure S9. ITC fitting curve of Telomere G1 with **1** (a), **2** (b) and **3** (c), c-*myc* with **1** (d), **2** (e) and **3** (f) under dilute condition. 50 mM KH_2PO_4-K_2HPO_4 buffer (pH 7.0) with 40%(v/v) PEG 200 at 25 °C**.**

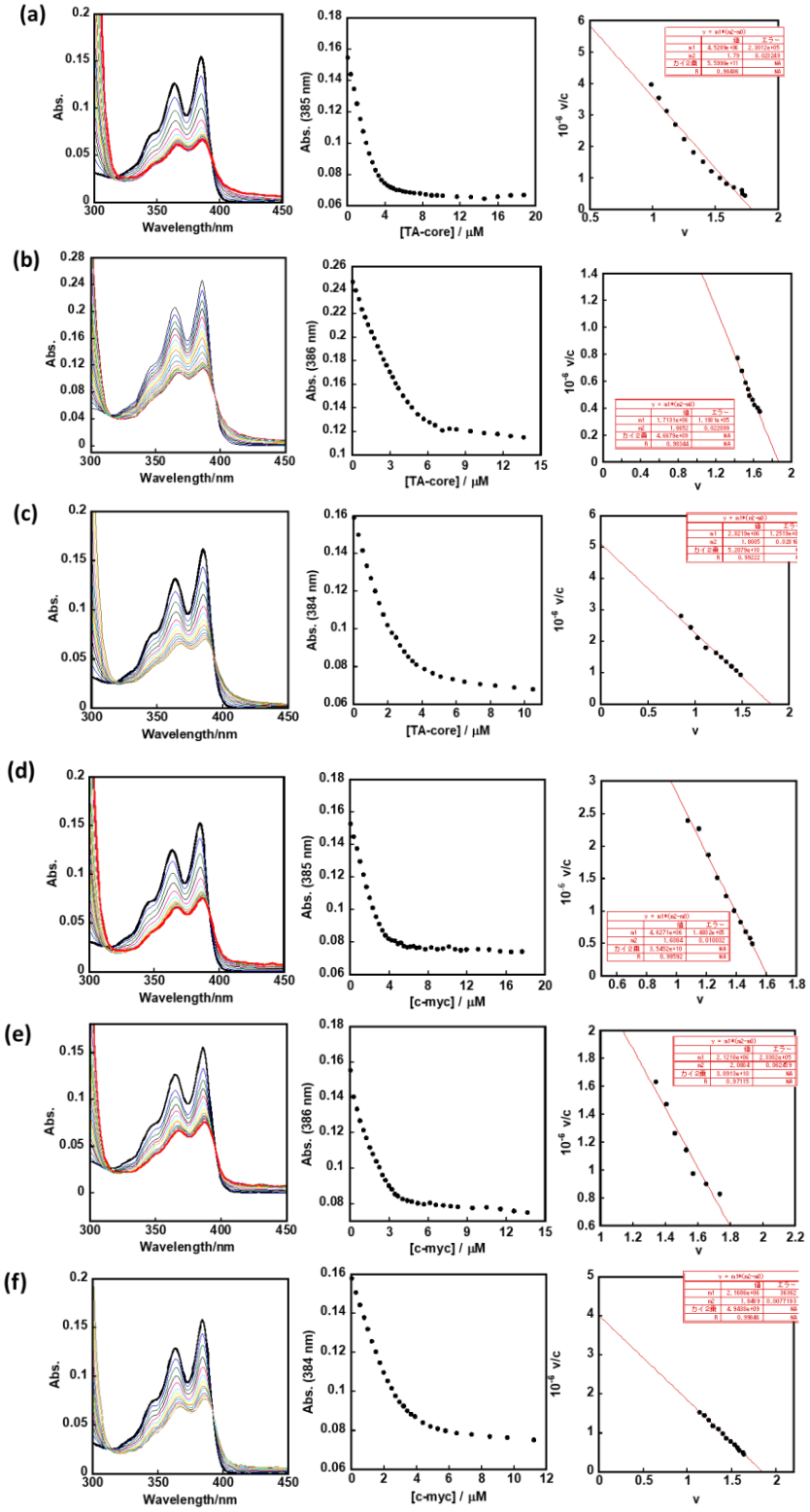


Figure S10. UV-Vis absorbance spectra, titration curve and scatchard plot of Telomere G1 with **1** (a), **2** (b) and **3** (c), c-*myc* with **1** (d), **2** (e) and **3** (f) under dilute condition. 50 mM Tris-HCl buffer (pH 7.4) and 100 mM KCl for telomere G1, 50 mM Tris-HCl buffer (pH 7.4) and 5 mM KCl for c-*myc* at 25 °C.

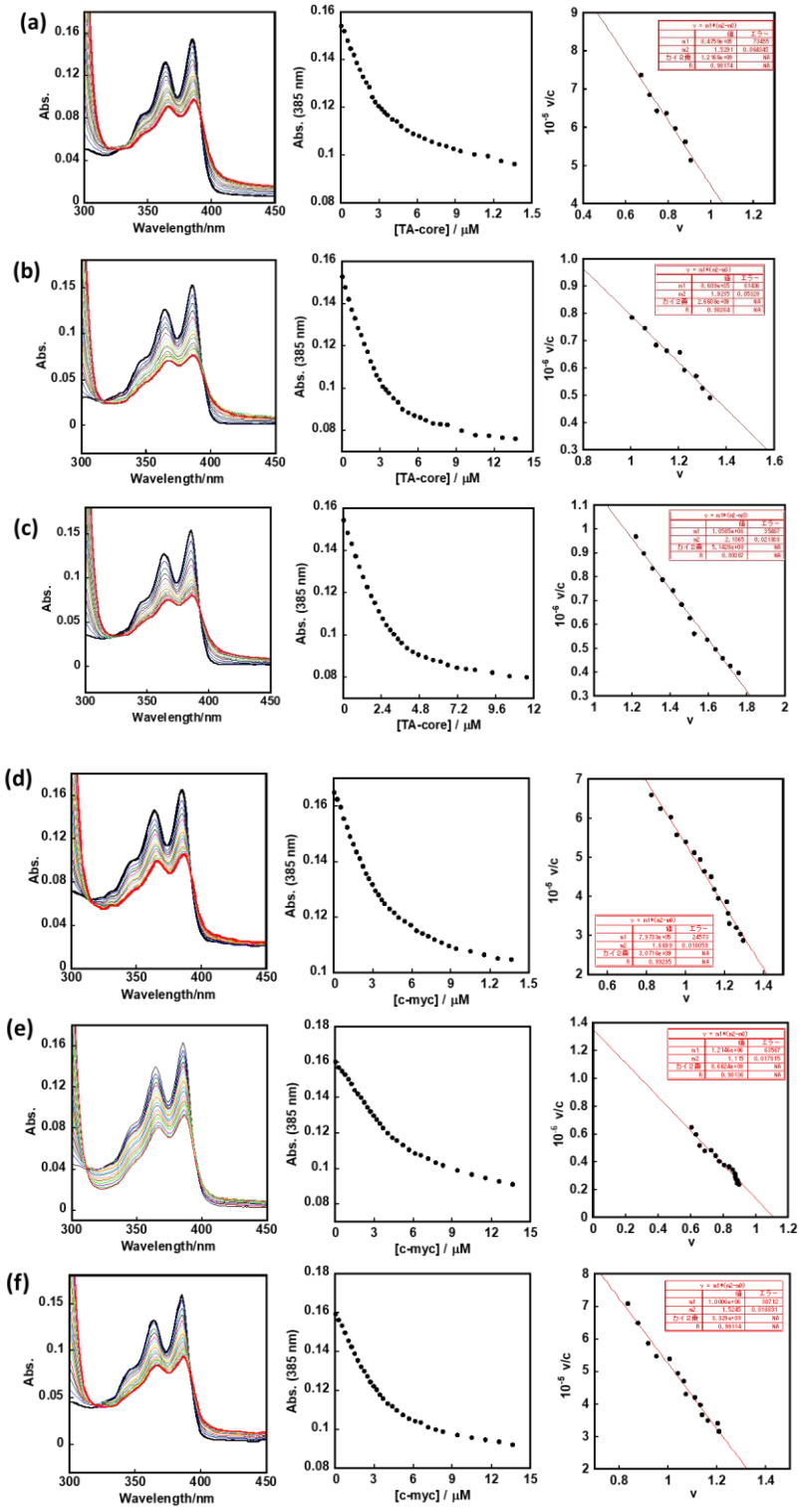


Figure S11. UV-Vis absorbance spectra, titration curve and scatchard plot of Telomere G1 with **1** (a), **2** (b) and **3** (c), c-*myc* with **1** (d), **2** (e) and **3** (f) under molecular crowding condition. 50 mM Tris-HCl buffer (pH 7.4), 100 mM KCl and 40%(v/v) PEG 200 for telomere G1, 50 mM Tris-HCl buffer (pH 7.4), 5 mM KCl and 40%(v/v) PEG 200 for c-*myc* at 25 °C.

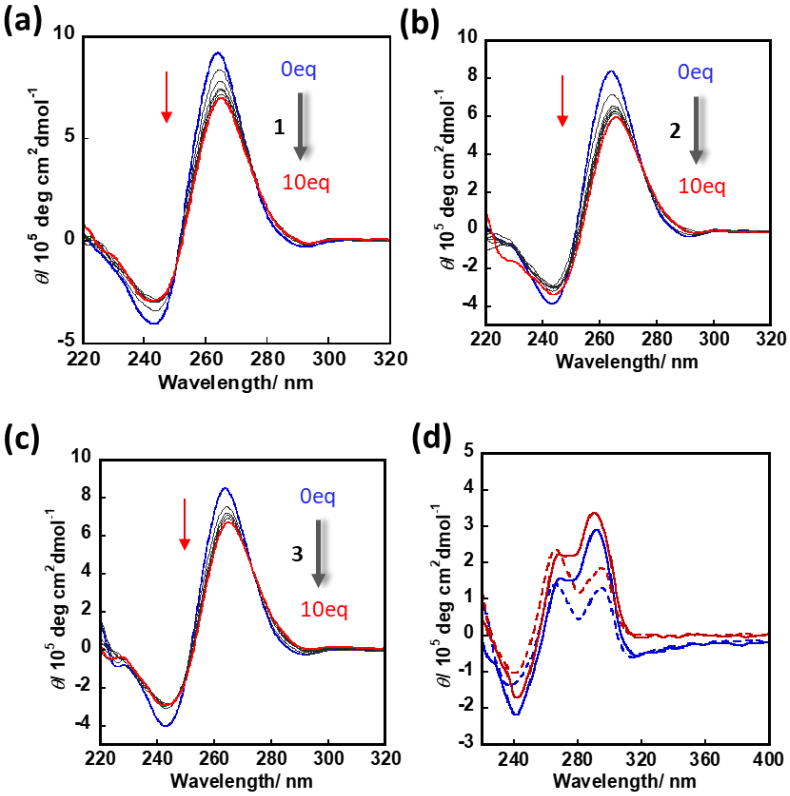
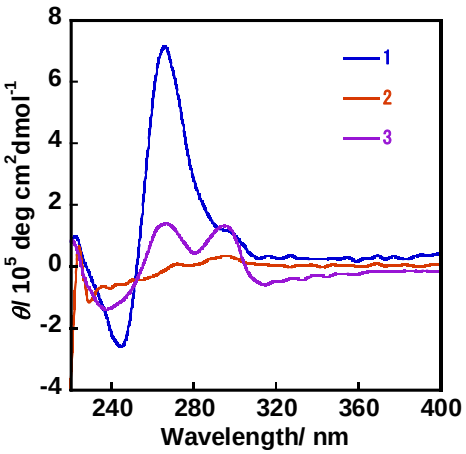
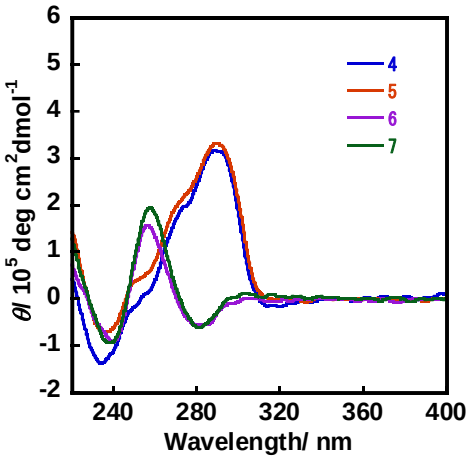


Figure S12. cNDI derivatives enhance the formation of parallel c-*myc* G-quadruplex under cation-deficient molecular crowding condition. Adding **1** (a), **2** (b), **3** (c) to c-*myc* from 0 to 10 equivalents under molecular crowding condition without K^+ (50 mM Tris-HCl buffer (pH 7.4) and 40%(v/v) PEG 200); (d) CD spectra of un-annealed Telomere G1 under molecular crowding condition without K^+, blue dash and red dash line, Telomere G1 only; blue solid and red solid line, Telomere G1 with **1** in 10 eq.

Table S1. CD spectra of Telomere G1 under different condition.

	40%*v*/*v* PEG200	K^+	Annealing	G-quadruplex Structure	CD spectra
1	+	+	+	parallel	
2	+	-	+	No signal	
3	+	-	-	Parallel/hybrid mixture	
4	-	+	+	hybrid	
5	-	+	-	hybrid	
6	-	-	+	ssDNA	
7	-	-	-	ssDNA	