Supplementary Information

# Naphthalene diimides carrying two β-cyclodextrins prefer Telomere RNA G-quadruplex recognition

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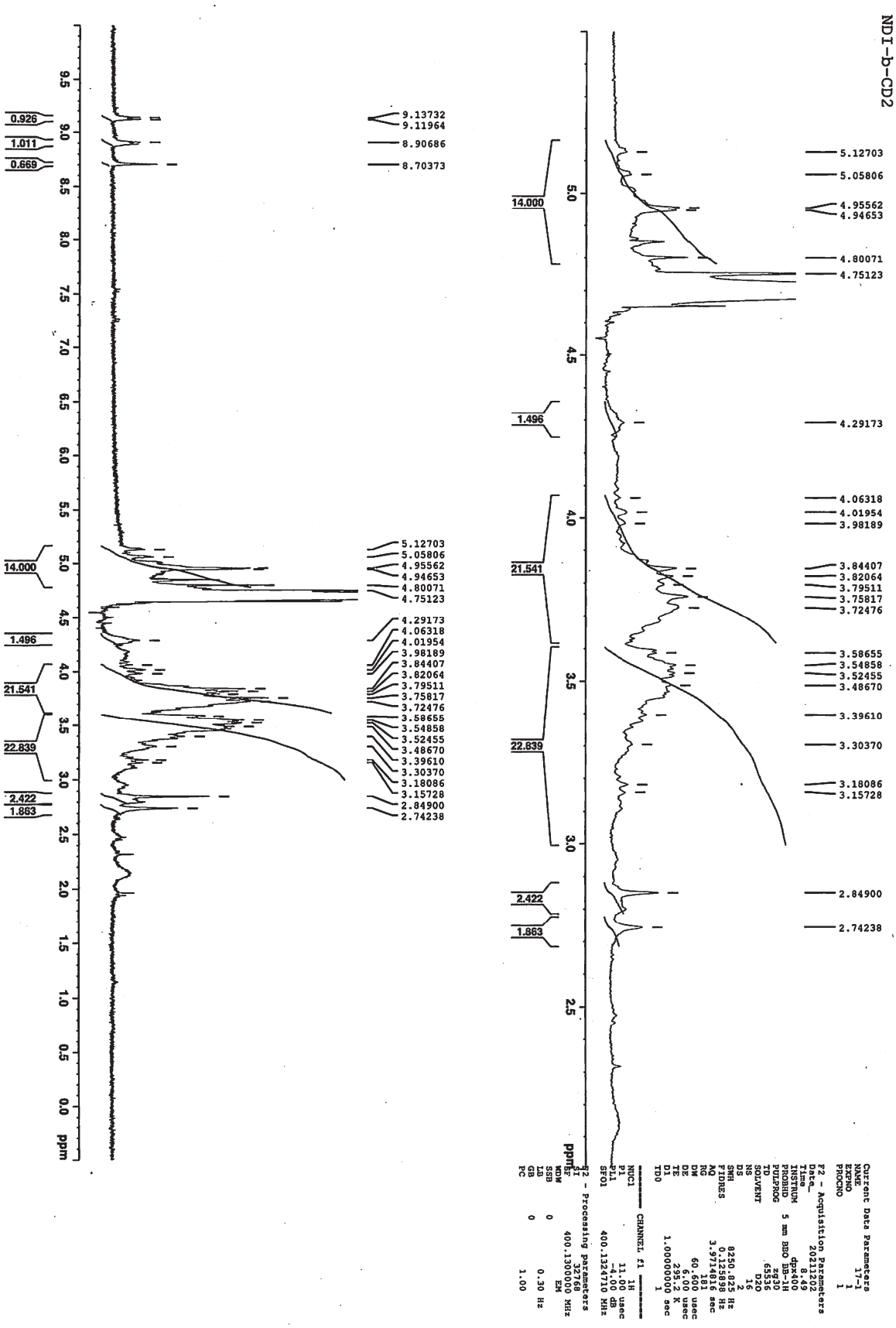


**Figure S1.** $^{1}$H-NMR spectra of **1** in $D_2O$.

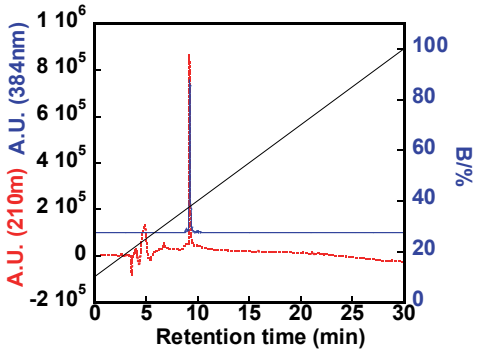


**Figure S2.** RT-HPLC of **1**. HPLC conditions; the concentration of solution B was changed (from 10% to 100%, 30 min) at 40 °C. Solution A： 0.1% trifluoroacetic acid, Solution B：70% acetonitrile, 0.1% trifluoroacetic acid. Flow rate: 1 mL/min. Column: Inertsil ODS-4 (GL Sciences Inc., Tokyo, Japan).

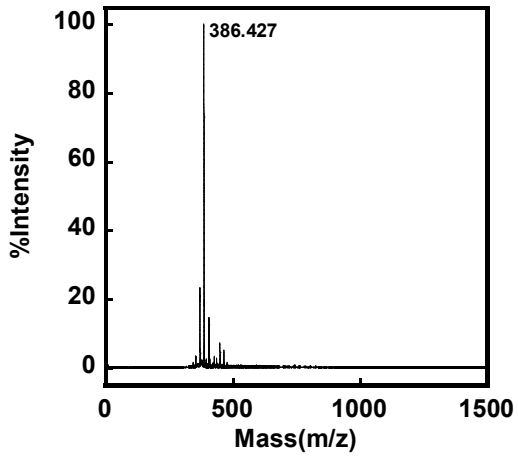


**Figure S3.** MALDI-TOF-MS spectra of **4** under positive mode (Matrix: DHBA). m/z = 386.427 (calculated value of $C_{18}H_{10}N_2O_8$+$H^+$ = 383.289).

**Figure S4.** [1]H-NMR spectra of **4** in DMSO.

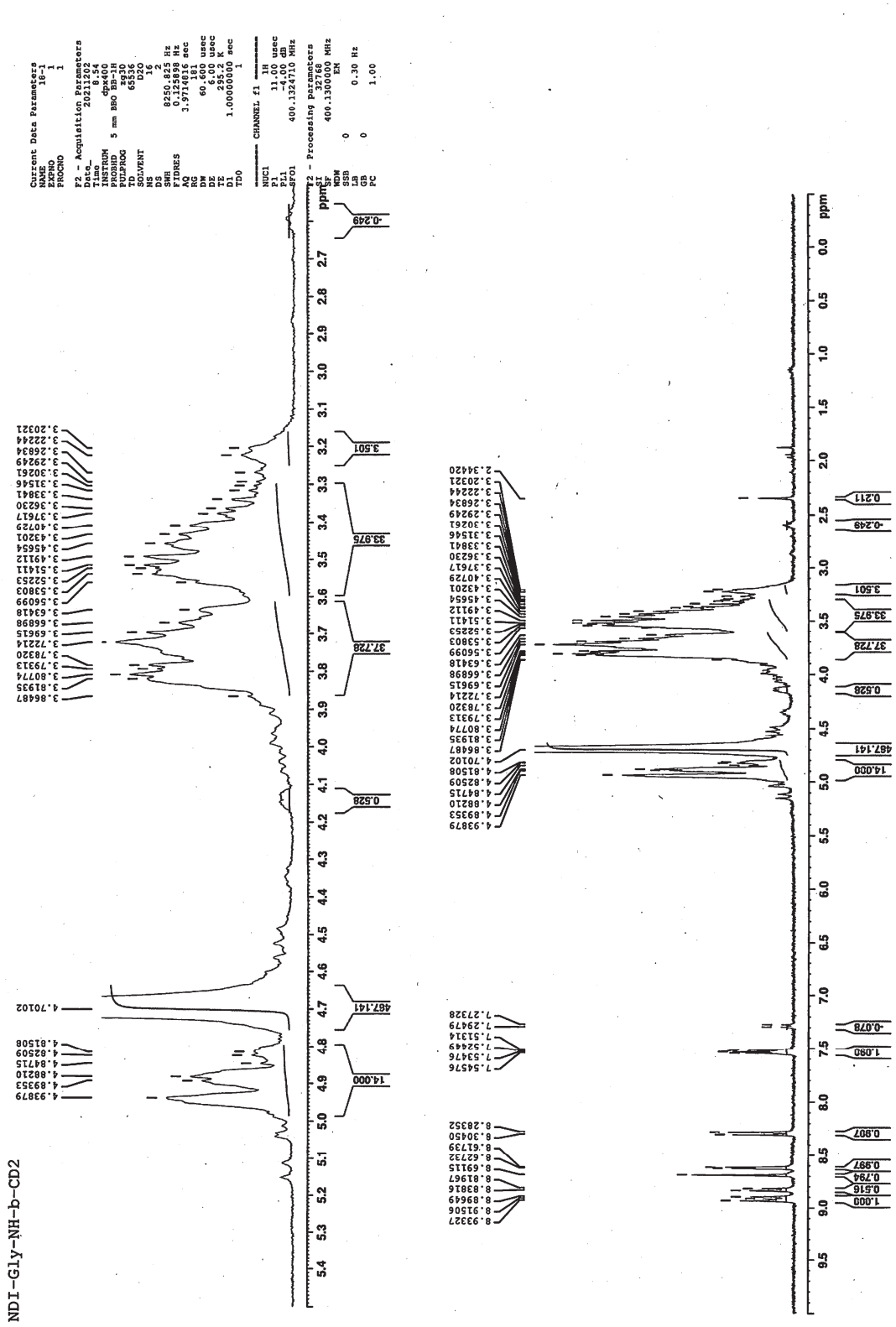


**Figure S5.** $^{1}$H-NMR spectra of **2** in $D_2O$.

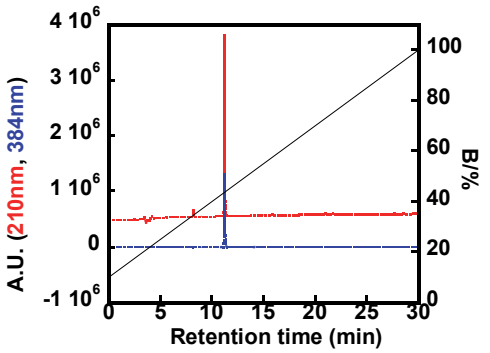


**Figure S6.** RT-HPLC of 2. HPLC conditions; the concentration of solution B was changed (from 10% to 100%, 30 min) at 40 °C. Solution A： 0.1% trifluoroacetic acid, Solution B：70% acetonitrile, 0.1% trifluoroacetic acid. Flow rate: 1 mL/min. Column: Inertsil ODS-4 (GL Sciences Inc., Tokyo, Japan).

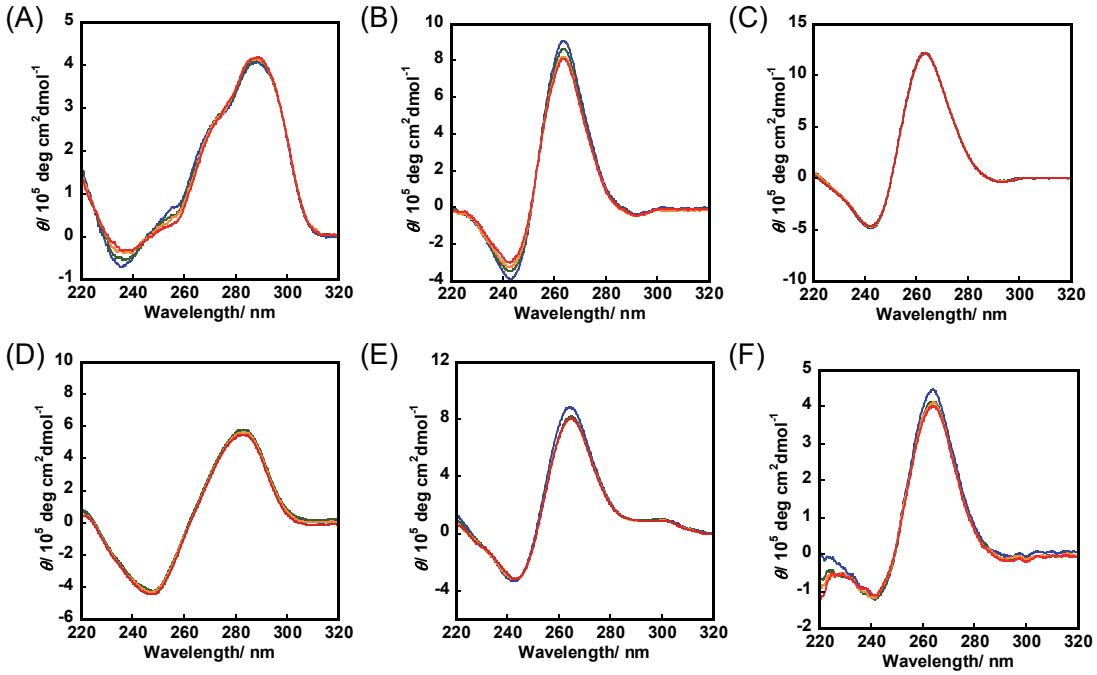


**Figure S7.** CD spectra of (A) Telomere G1, (B) c-myc, (C) c-kit, (D) ds-oligo, (E) G1-r23t, and (F) G1-r12t after adding **2**. 1.5 μM DNA, 0-4.5 μM **2**, 50 mM Tris-HCl buffer (pH 7.4) with 100 mM KCl at 25 °C. [DNA] : [**2**]=1:0 (blue), 1:1 (green), 1:2 (orange), 1:3 (red).

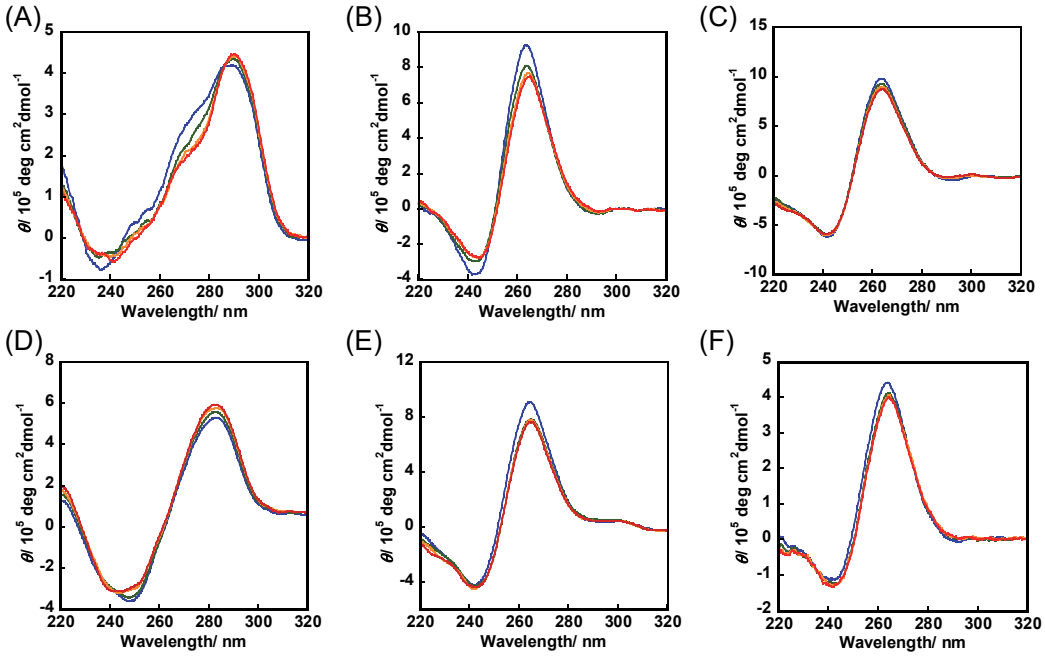


**Figure S8.** CD spectra of (A) Telomere G1, (B) c-myc, (C) c-kit, (D) ds-oligo, (E) G1-r23t, and (F) G1-r12t after adding **3**. 1.5 μM DNA, 0-4.5 μM **3**, 50 mM Tris-HCl buffer (pH 7.4) with 100 mM KCl at 25 °C. [DNA] : [**3**]=1:0 (blue), 1:1 (green), 1:2 (orange), 1:3 (red).

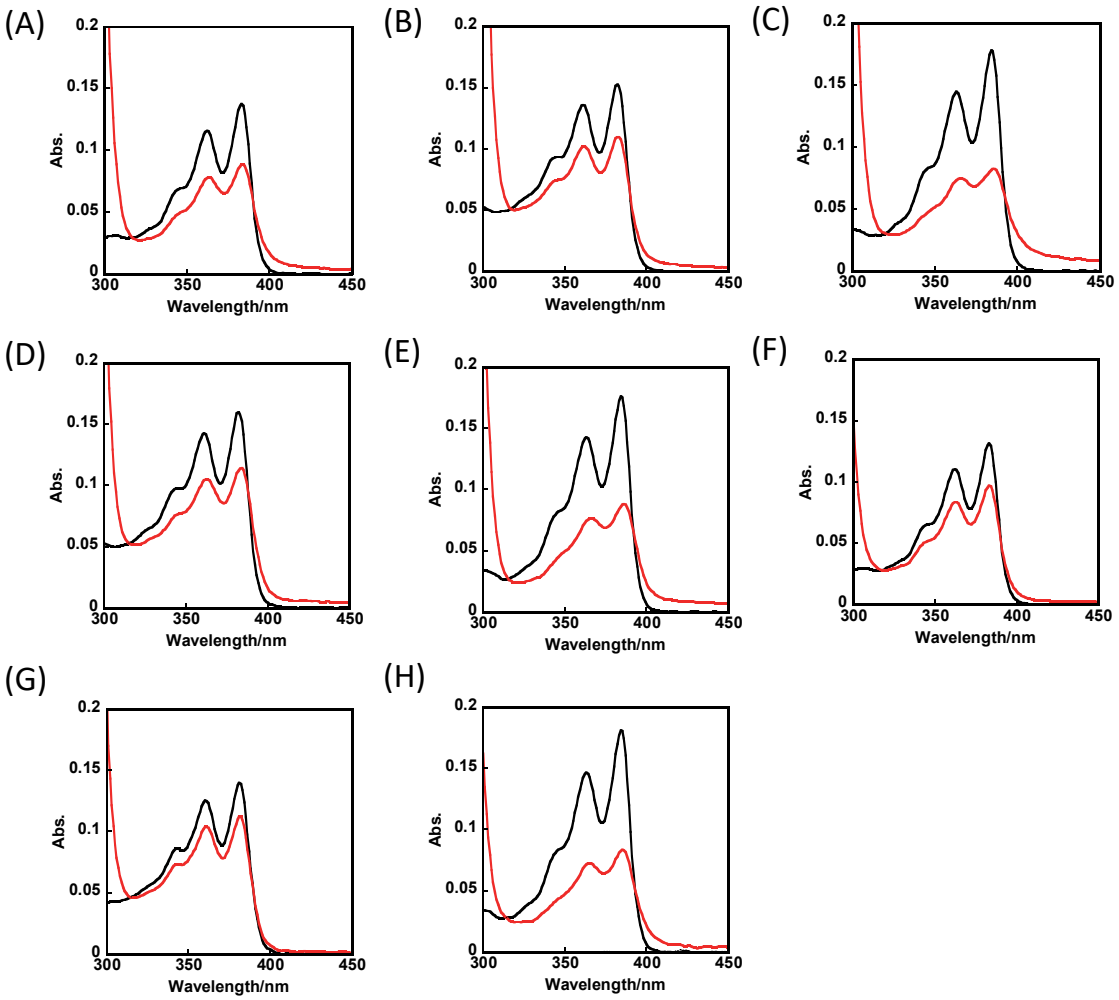


**Figure S9.** UV-Vis spectra of (A) **1** with Telomere G1, (B) **2** with Telomere G1, (C) **3** with Telomere G1, (D) **2** with c-myc, (E) **3** with c-myc, (F) **1** with ds-oligo, (G) **2** with ds-oligo, and (H) **3** with ds-oligo in 50 mM Tris-HCl buffer (pH 7.4) with 100 mM KCl at 25 °C (Before adding DNA: black line, after adding DNA: red line).

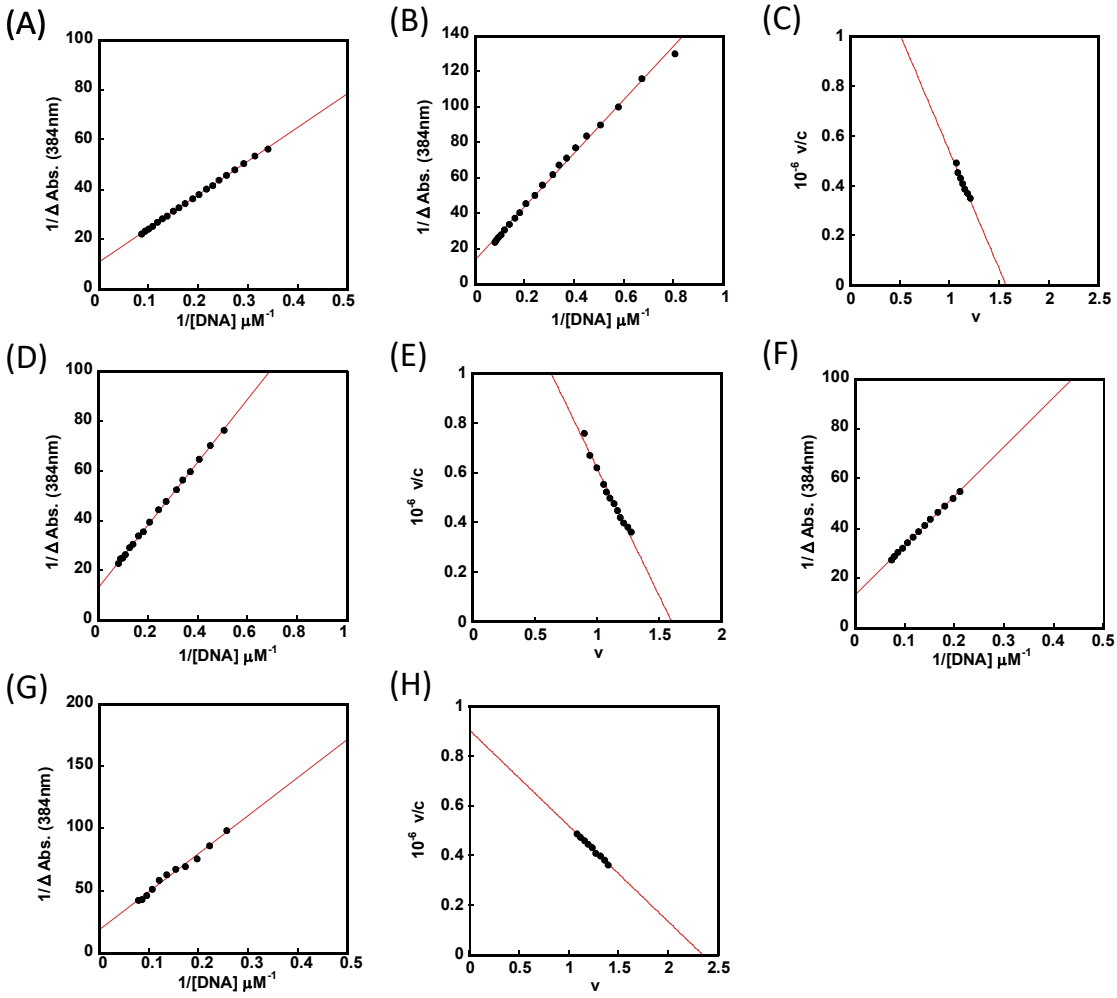


**Figure S10.** Binding analysis of (A) **1** with Telomere G1 (Benesi-Hildebrand analysis), (B) **2** with Telomere G1 (Benesi-Hildebrand analysis), (C) **3** with Telomere G1 (Scatchard analysis), (D) **2** with c-myc (Benesi-Hildebrand analysis), (E) **3** with c-myc (Scatchard analysis), (F) **1** with ds-oligo (Benesi-Hildebrand analysis), (G) **2** with ds-oligo (Benesi-Hildebrand analysis), and (H) **3** with ds-oligo (Scatchard analysis) in 50 mM Tris-HCl buffer (pH 7.4) with 100 mM KCl at 25 °C.

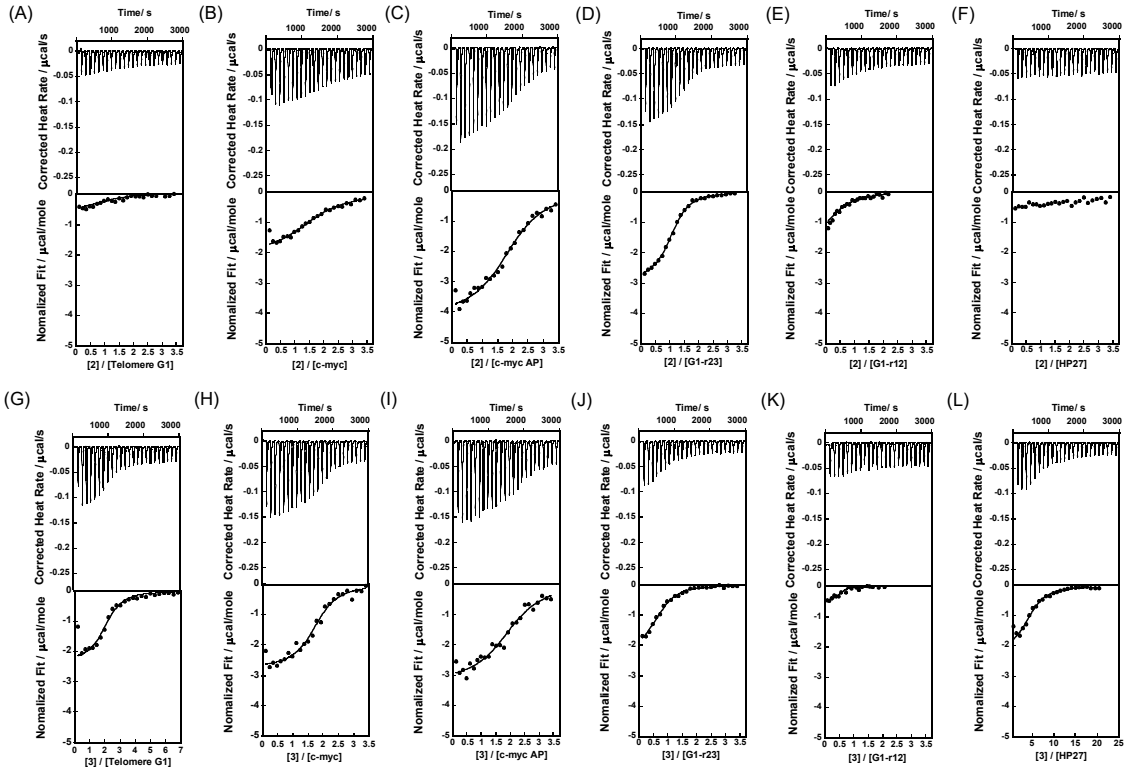


**Figure S11.** ITC measurement of (A, G) Telomere G1, (B, H) c-myc, (C, I) c-myc AP site, (D, J) HP27, (E, K) G1-r23nt and (F, L) HP27 with adding **2** (A-F) or **3** (G-L) in 50 mM $KH_2PO_4$-$K_2HPO_4$ buffer (pH 7.0), 25 °C.

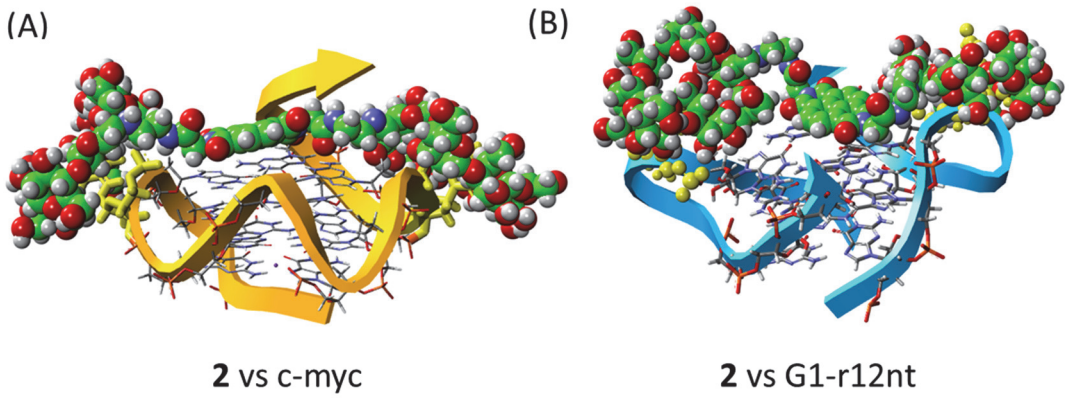


**Figure S12.** Binding model simulation of NDI-β-CyDs conjugator **2** with (A) c-*myc* G-quadruplex (PDB:1xav); (B) 12nt of telomere RNA G-quadruplex (PDB: 2kbp).