

Supplementary Information

Selective *c-MYC* G4 DNA recognition based on a fluorescent light-up probe with disaggregation-induced emission characteristics

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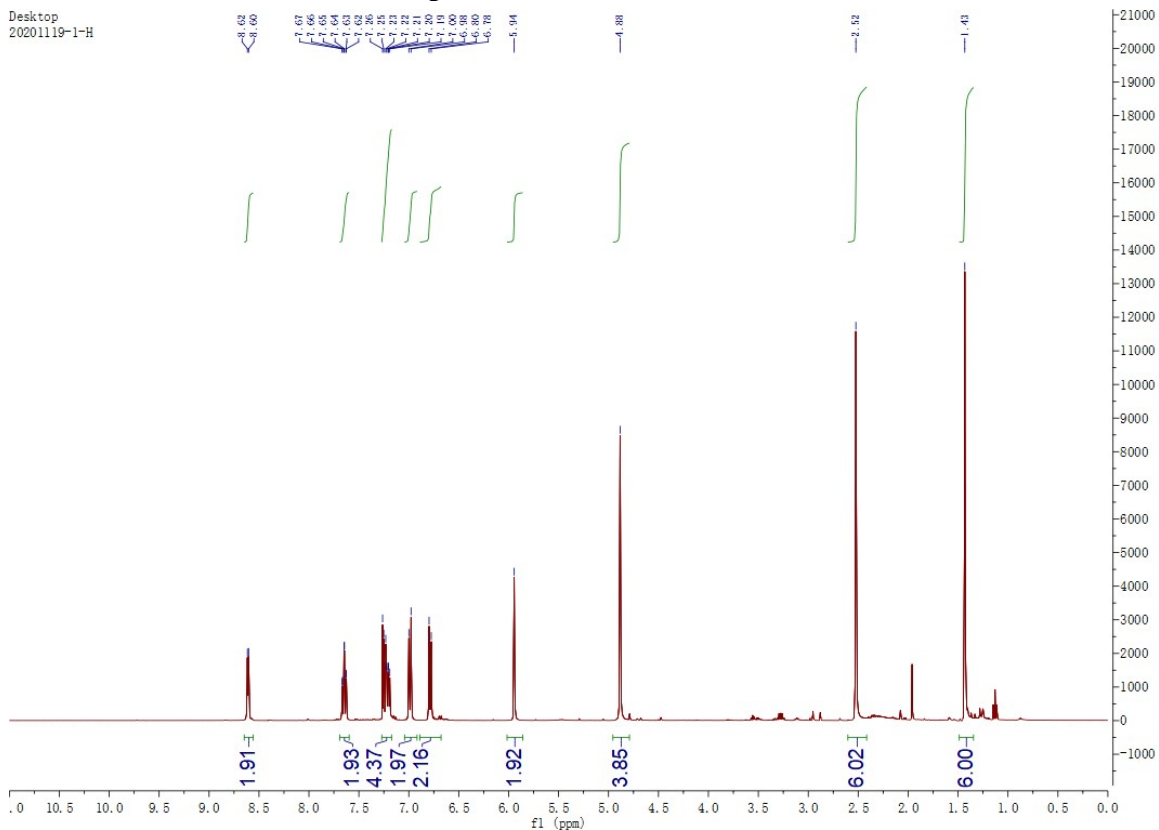
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1. Sequence alignments of oligonucleotides

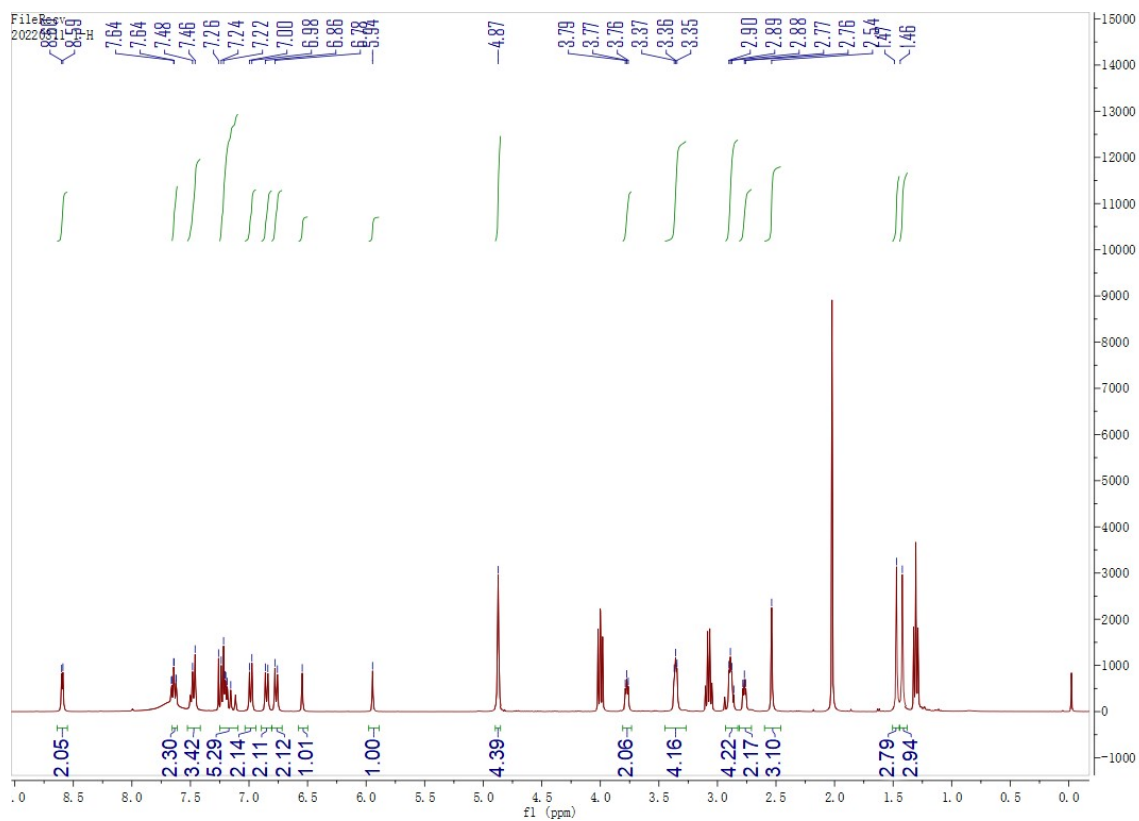
Name	Sequence (from 5' to 3')	Structure in K ⁺ solution
EAD	CTGGGTGGGTGGGTGGGA	G-quadruplex
TBA	GGTTGGTGTGGTTGG	G-quadruplex
c-MYC	TTGAGGGTGGGTAGGGTGGGTA	G-quadruplex
21CTA	GGGCTAGGGCTAGGGCTAGGG	G-quadruplex
TRF2	CGGG AGGG CGGG GAGG GC	G-quadruplex
VAV1	GGGC AGGG AGGG AACT GGG	G-quadruplex
Ckit1	AGGG AGGG CGCT GGA GGA GGG	G-quadruplex
Hum24	TTAGGGTTAGGGTTAGGGTTAGGG	G-quadruplex
ODN	GGGATGGGACACAGGGGACGGG	G-quadruplex
ACS20	GGCTTAGGCTTAGGCTTAGG	G-quadruplex
Ckit3	GG CGA GG AGGGG CGT GG CC GGC	G-quadruplex
HRAS	TC GGGTTGCGGG CGCAGGGCACGGG CG	G-quadruplex
bm	TAGGTTAGGTTAGGTTAGG	G-quadruplex
22AG	AGGG TTAG GGTT AGGG TTAG GG	G-quadruplex
G3T3	GGGTTTGGGTTTGGGTTTGGG	G-quadruplex
BC12	GGGCGGGCGCGGGAGGAAGGGGGCGGG	G-quadruplex
VEGF	GGGGCGGGCCGGGGGGCGGGG	G-quadruplex
Polyd(A-T) ₉	ATATATATATATATATAT	Duplex
Polyd(A-T) ₂	GCA TGC GCG CGC GCA TGC	Duplex
Polyd(A-T) ₅	GCGCAT ATA TAT ATGCGC	Duplex
ds26	CAATCGGATCGAATTCGATCGATTG	Duplex
ss26	ATACGATGCTTCACGGTGCTATCTG	Single-stranded

Table S1. Sequence alignments of oligonucleotides used in the present study.

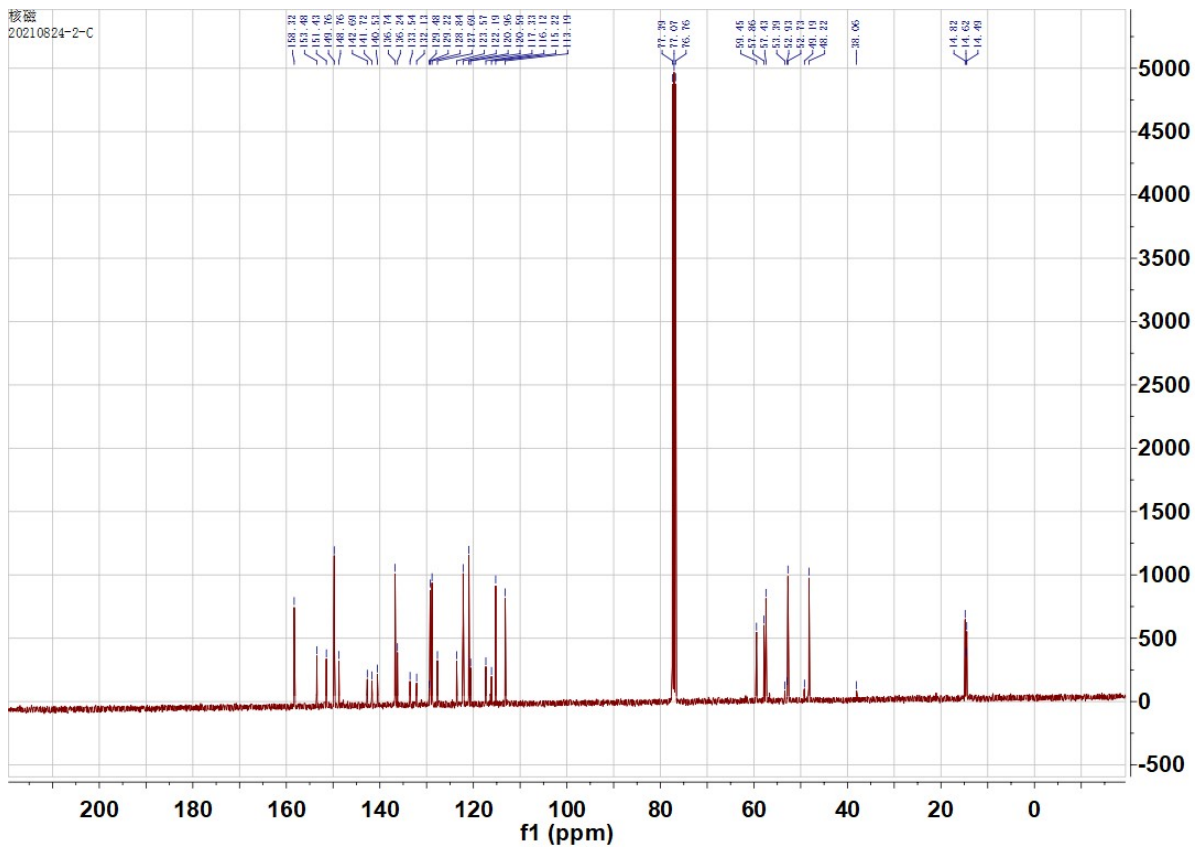
2. ¹H NMR, ¹³C NMR and HRMS spectra



¹H NMR spectrum of compound 1

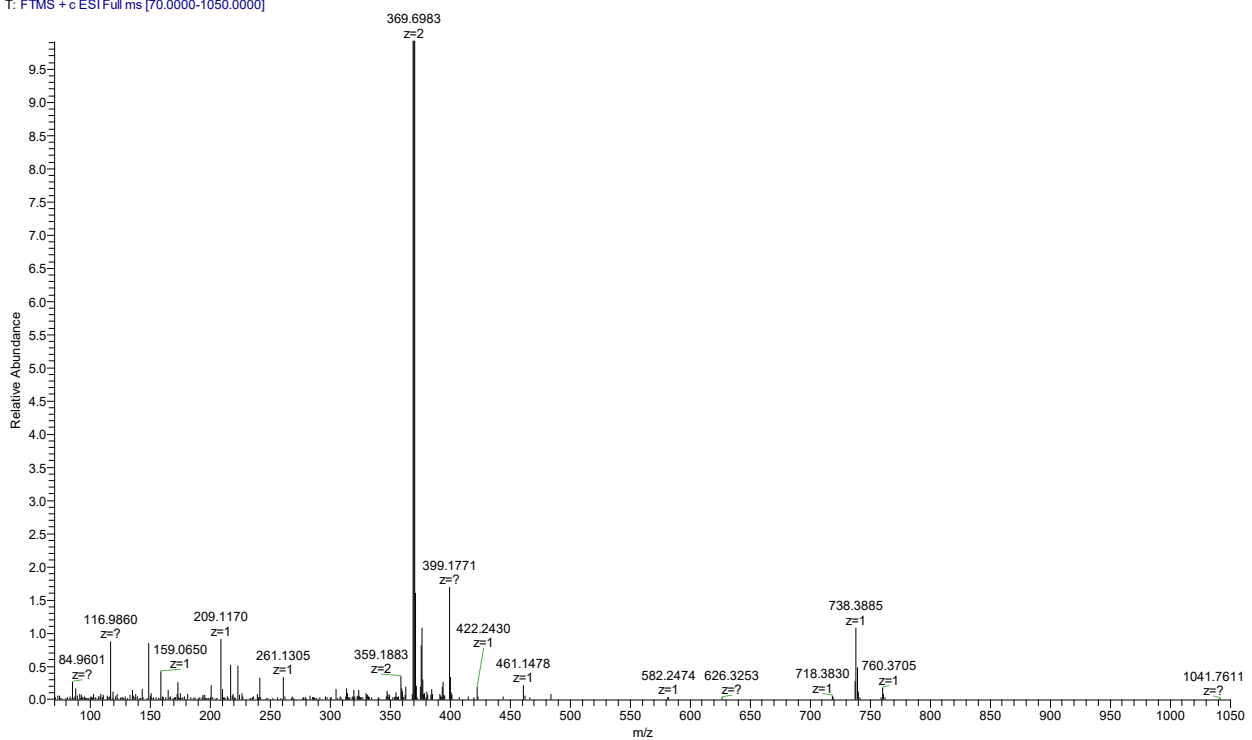


¹H NMR spectrum of compound MRY-3



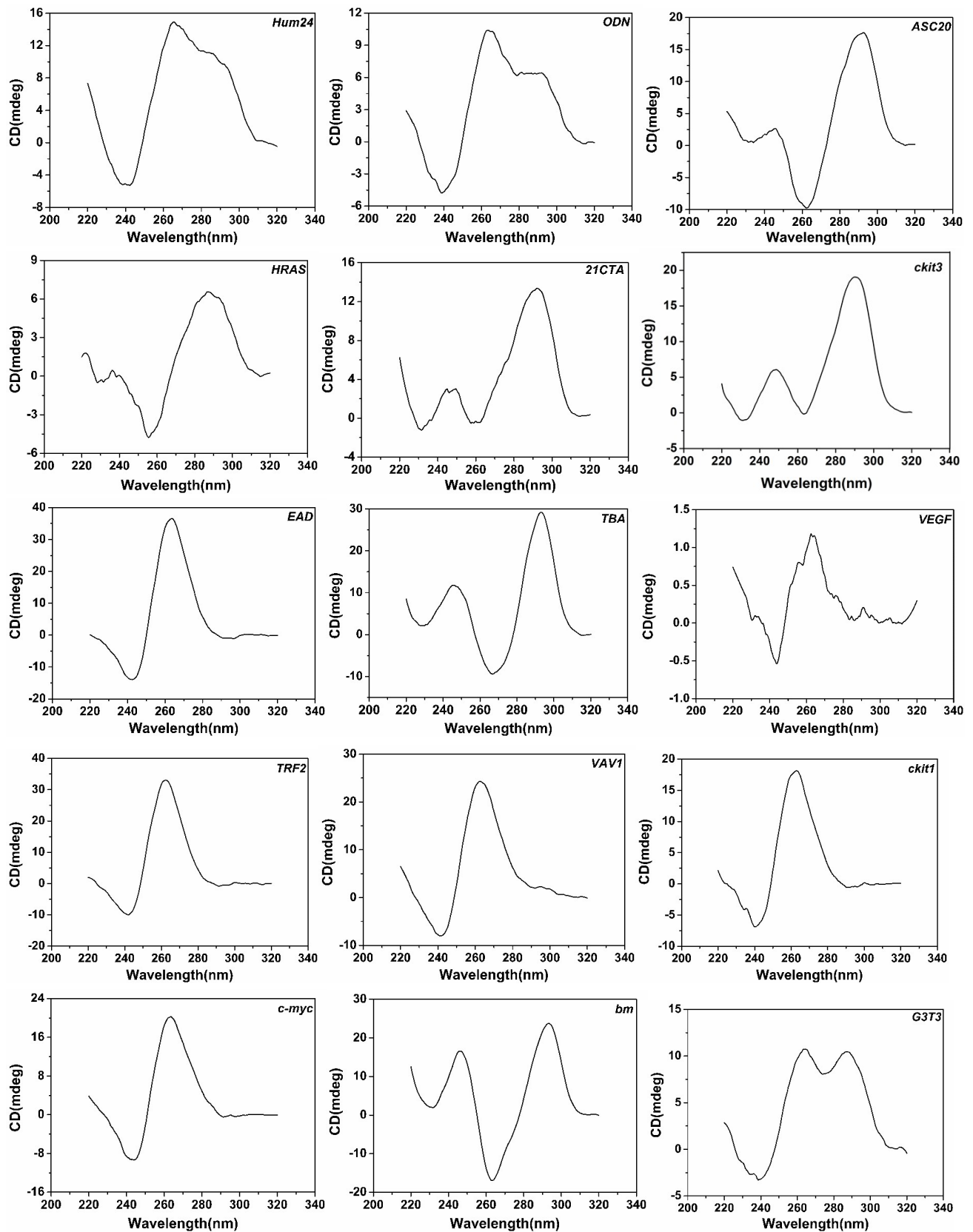
^{13}C NMR spectrum of MRY-3

MRY #829 RT: 4.26 AV: 1 NL: 5.51E9
T: FTMS + c ESI Full ms [70.0000-1050.0000]



HRMS spectrum of MRY-3

3. CD spectra for various G4 structures.



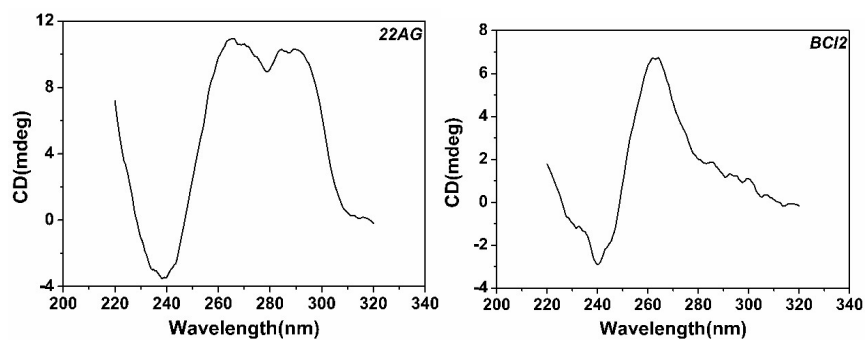


Fig. S1. CD spectra for various G4 structures (4 μ M) in 10 mM Tris-HCl, pH = 7.4, 60 mM KCl.

4. Fluorescence titration curve of MRY-3 with c-MYC G4 DNAs.

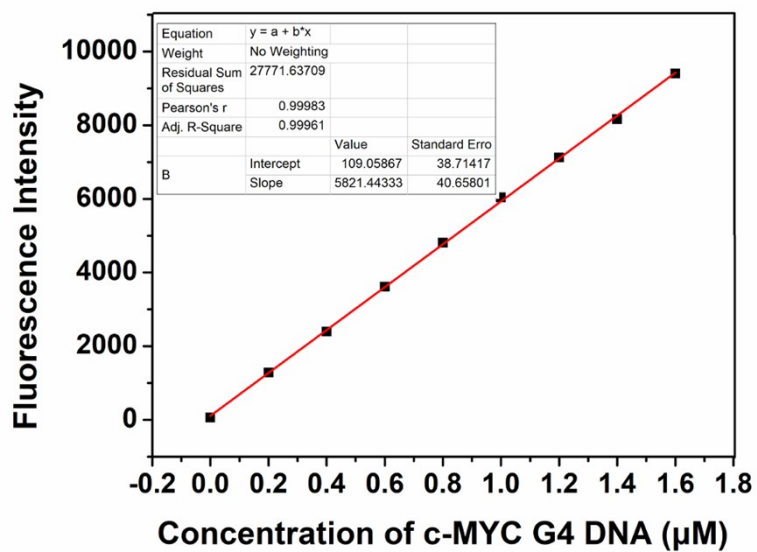
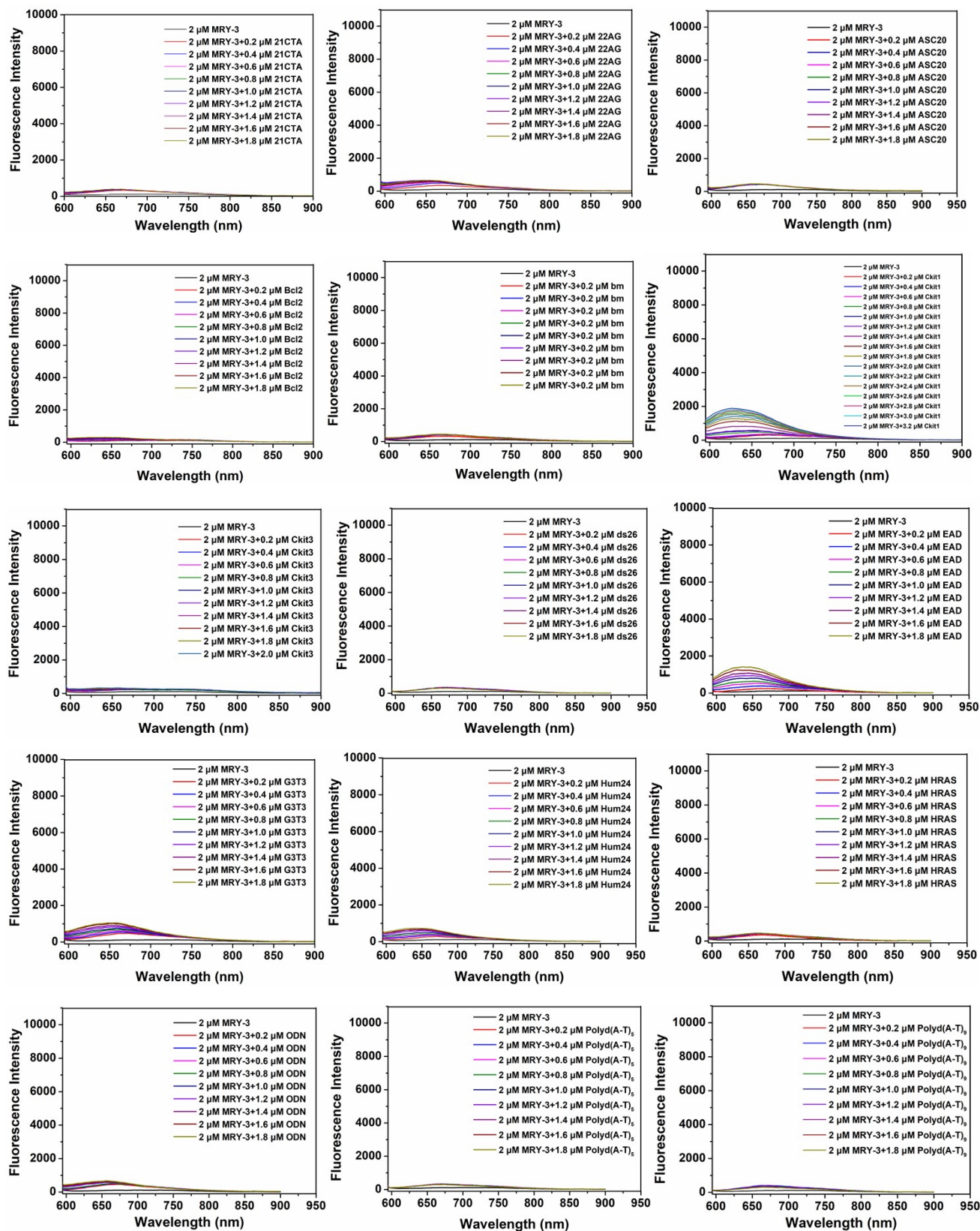


Fig. S2. The linear fit equation for calculating LOD value between MRY-3 and c-MYC G4 DNA at 600 nm.

5. Fluorescence titrations of MRY-3 with G4 and non-G4 DNAs.



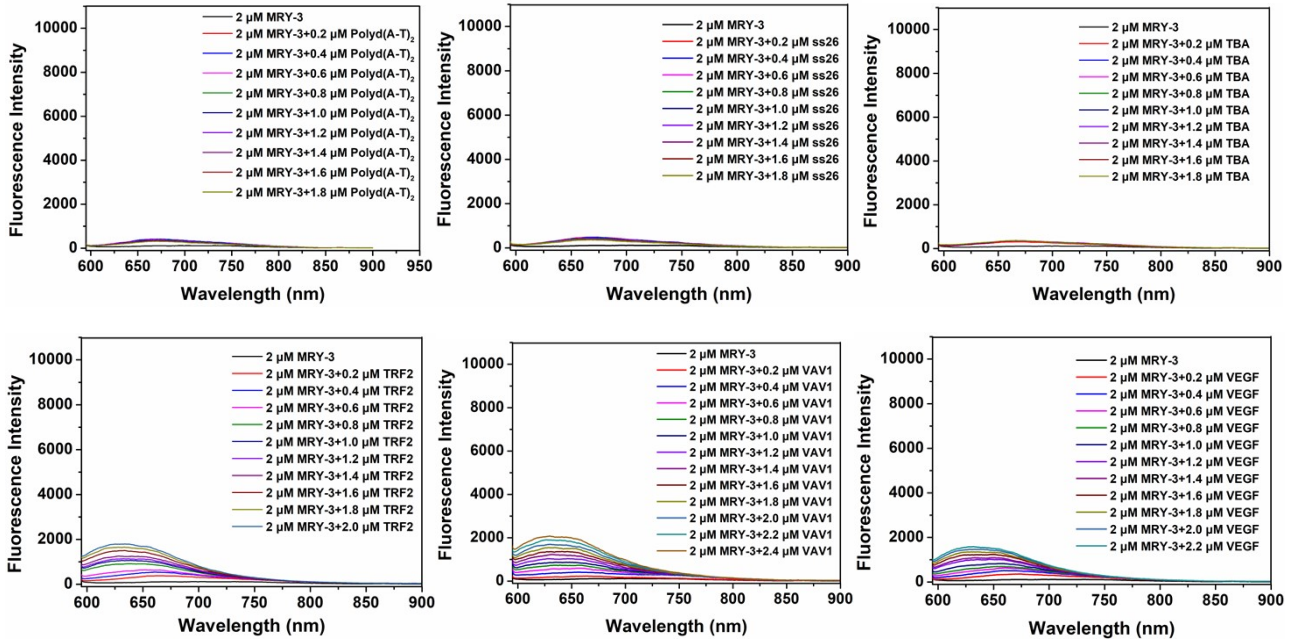


Fig. S3. Fluorescence titrations of **MRY-3** (2 μM) upon addition of increasing amount of anti-parallel G4 DNAs-21CTA, ASC20, bm, Ckit3, HRAS, TBA; hybrid DNAs-22AG, hum24, ODN, G3T3; parallel G4 DNAs- Bcl2, Ckit1, EAD, TRF2, VAV1, VEGF; double-stranded DNAs-Polyd(A-T)₅, Polyd(A-T)₉, Polyd(A-T)₂, ds26 and single-stranded DNA-ss26.

6. Competition experiments.

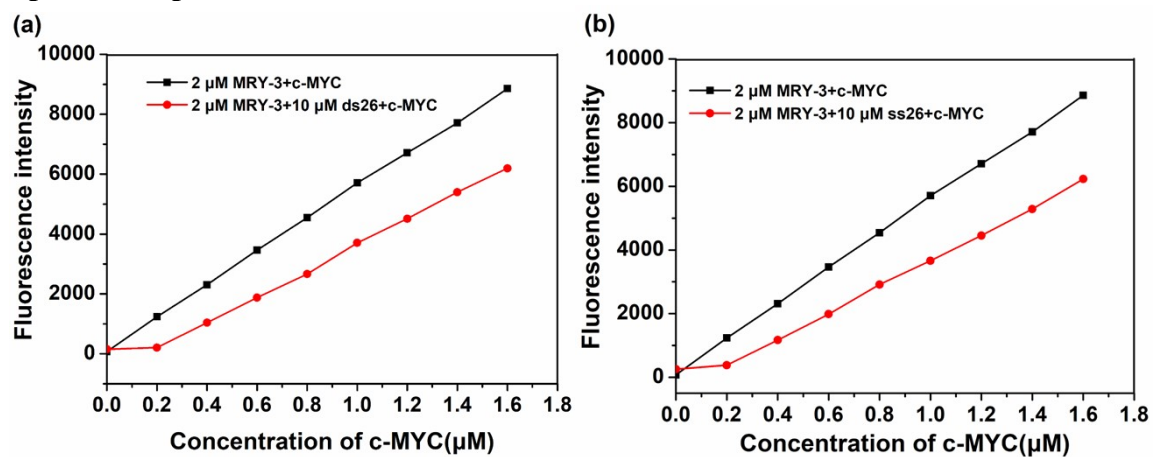
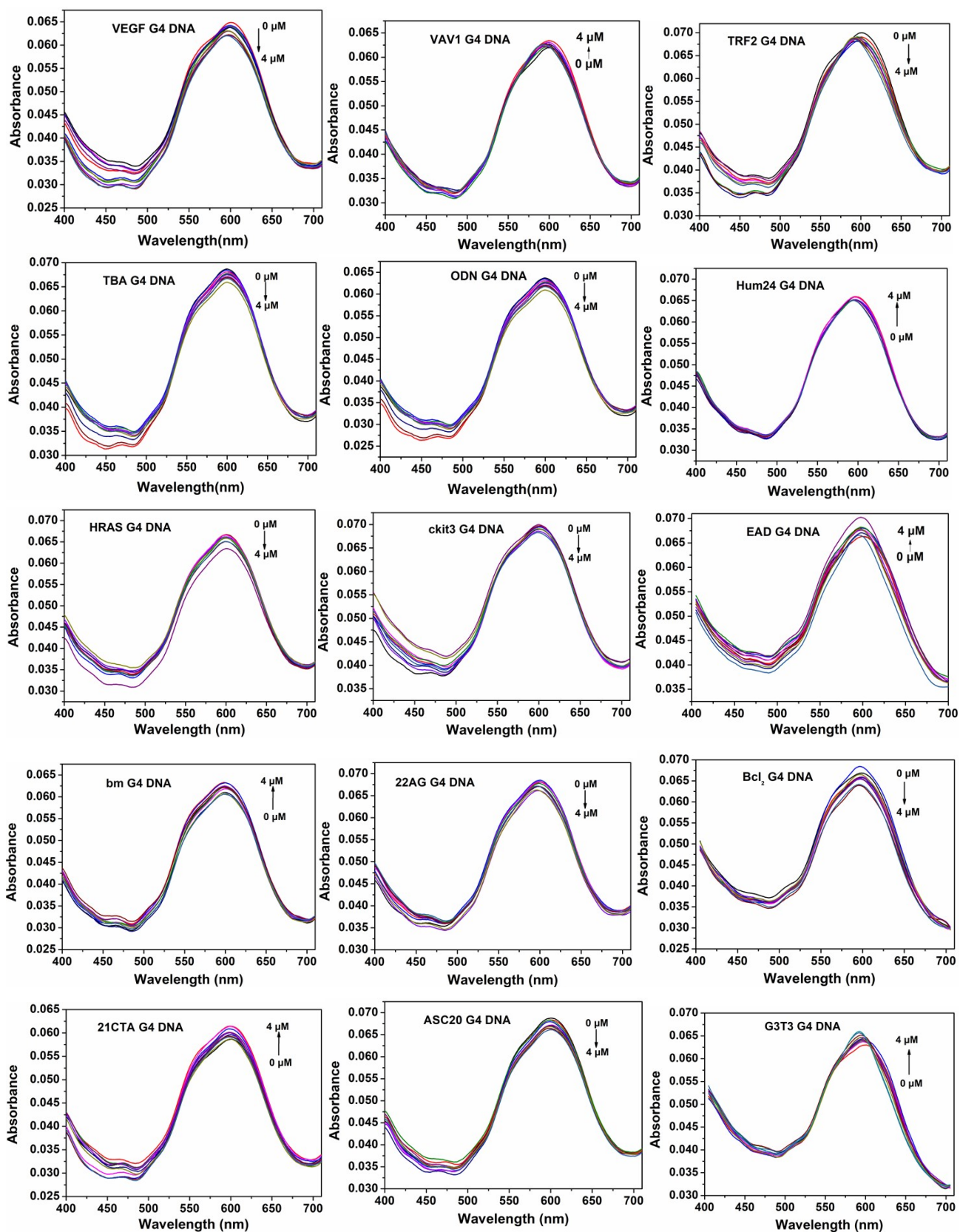


Fig. S4. The fluorescence titration of 2 μM MR-3 with the stepwise addition of the c-MYC without and with 10 μM ds26 (a) or ss26 (b) in 10 mM Tris-HCl/DMSO (95:5, v/v), 60 mM KCl, pH 7.4

7. Absorbance titrations of MRY-3 with G4 and non-G4 DNAs.



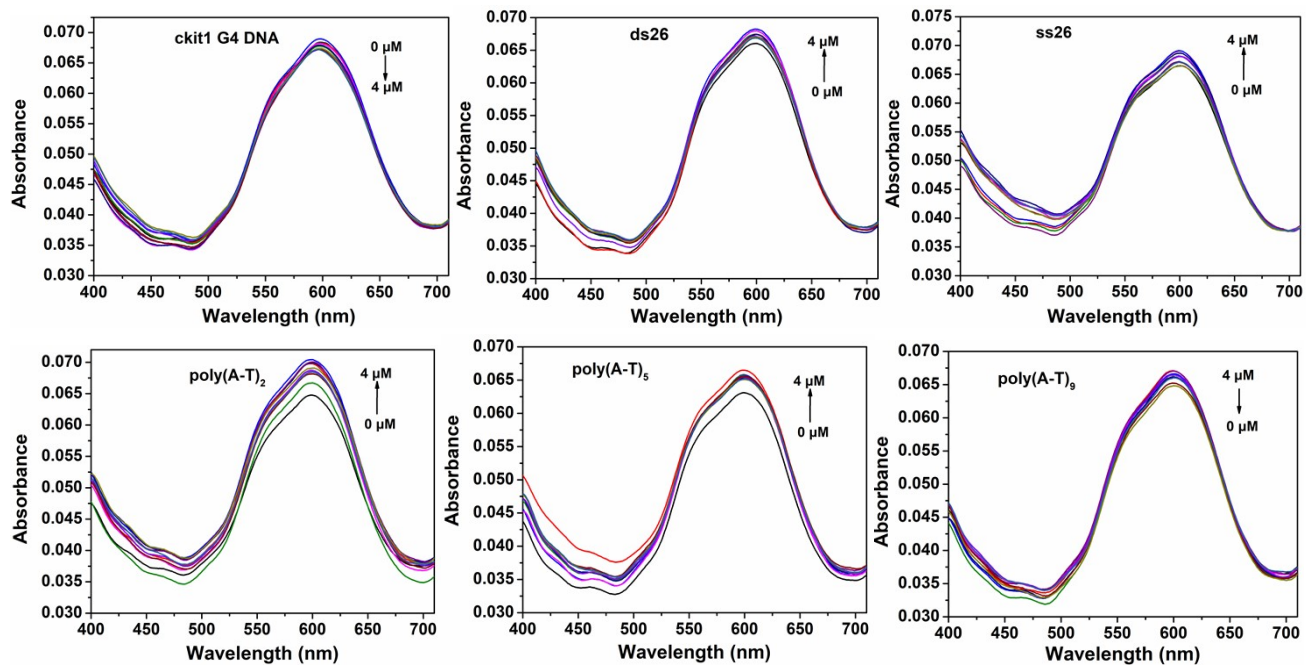


Fig. S5. Absorption titrations of **MRY-3** upon addition of increasing amount of anti-parallel G4 DNAs-21CTA, ASC20, bm, Ckit3, HRAS, TBA; hybrid DNAs-22AG, hum24, ODN, G3T3; parallel G4 DNAs- Bcl2, Ckit1, EAD, TRF2, VAV1, VEGF; double-stranded DNAs-Polyd(A-T)₅, Polyd(A-T)₉, Polyd(A-T)₂, ds26 and single-stranded DNA-ss26 in 10 mM Tris-HCl buffer (pH 7.4, containing 60 mM KCl); Condition: [**MRY-3**] = 1 μ M, [DNA] = 0-4 μ M.

8. Absorption properties of MRY-3 with DNAs.

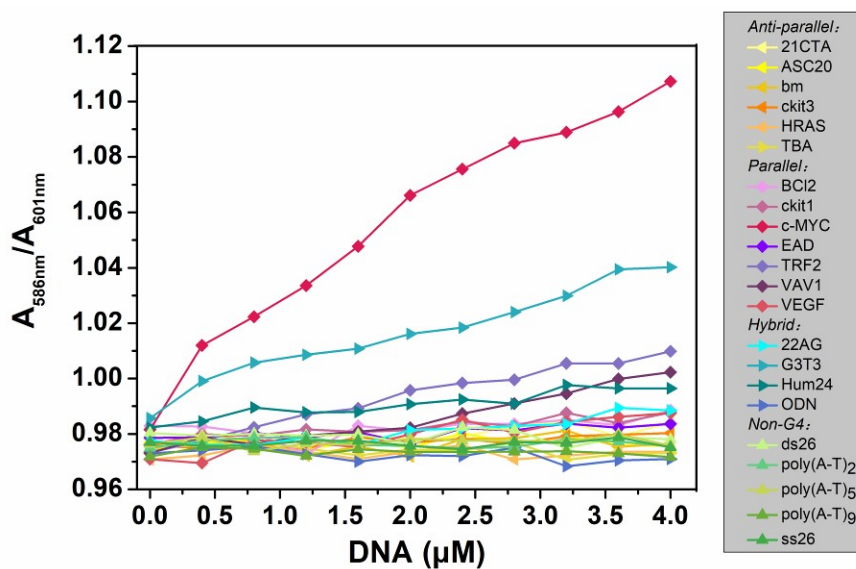


Fig. S6. Plots of $A_{586\text{ nm}}/A_{601\text{ nm}}$ of 1 μM MRY-3 against various DNA concentrations in 10 mM Tris-HCl buffer (pH 7.4, containing 60 mM KCl);

9. CD spectra for mutated C-MYC structures.

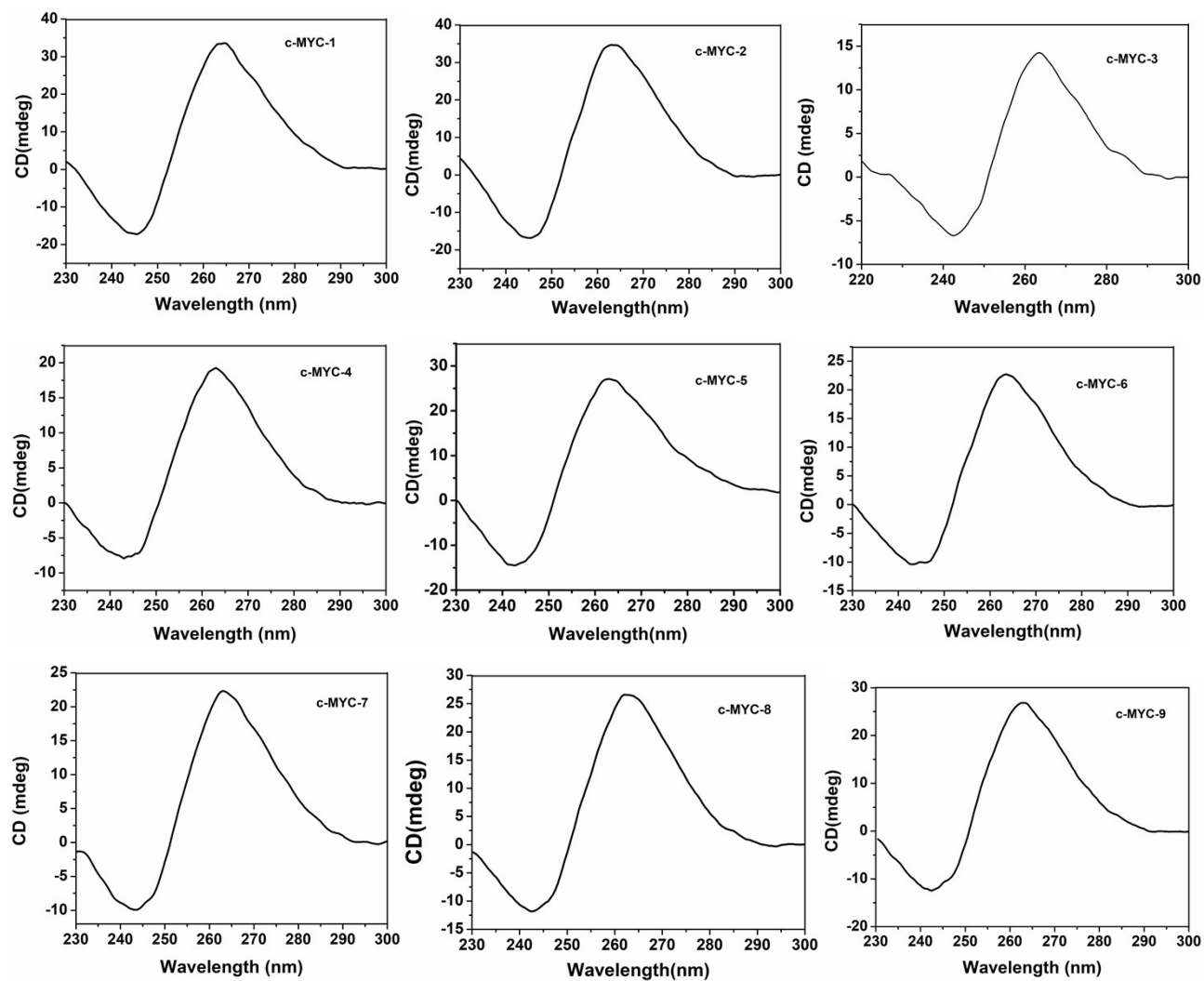


Fig. S7. CD spectra for various mutated C-MYC sequences in 10 mM Tris-HCl/DMSO (95:5, v/v), 60 mM KCl, pH 7.4

10. Fluorescence titrations of MRY-3 with mutated C-MYC structures.

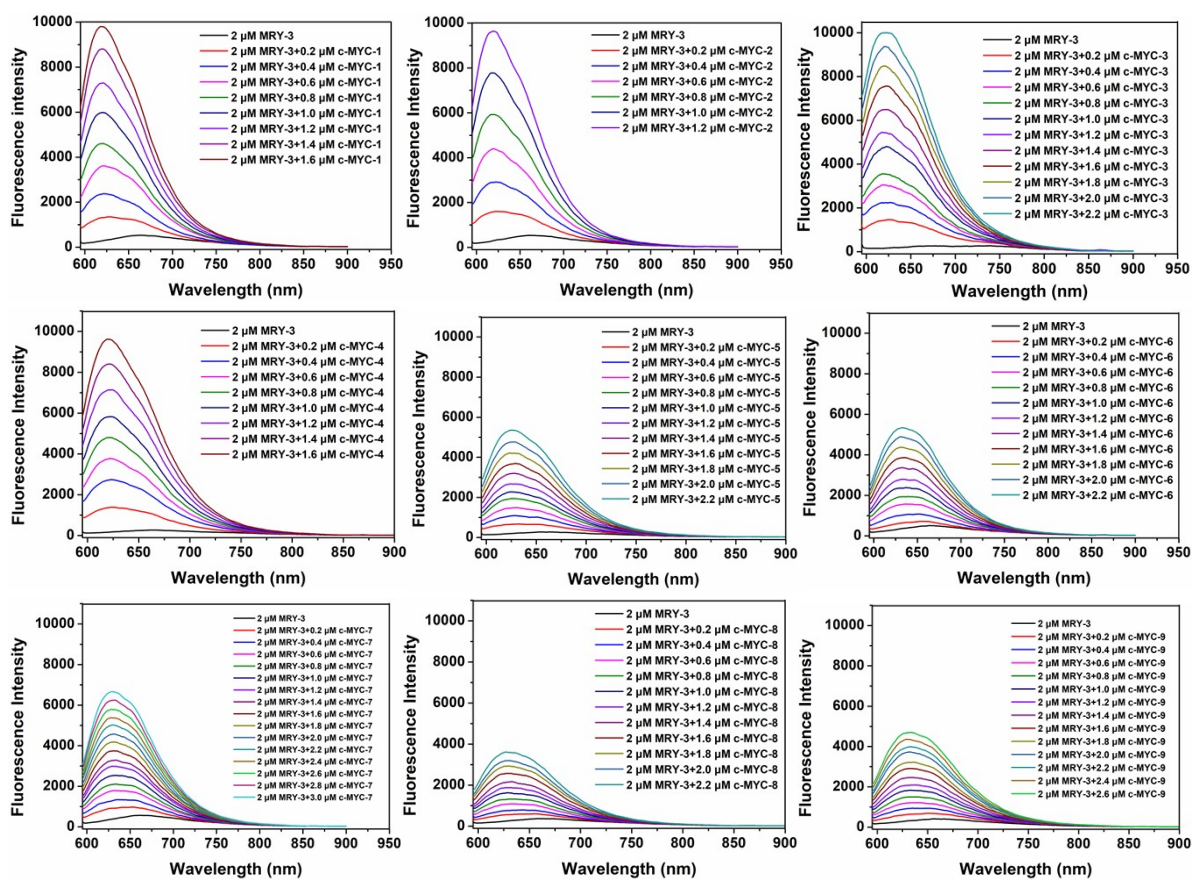


Fig. S8. Fluorescence titrations of MRY-3 (2 μM) upon addition of increasing amount of mutated c-MYC sequences in 10 mM Tris-HCl/DMSO (95:5, v/v), 60 mM KCl, pH 7.4.

11. Fluorescence titrations of MRY-3 with AMCA labeled C-MYC DNA structures.

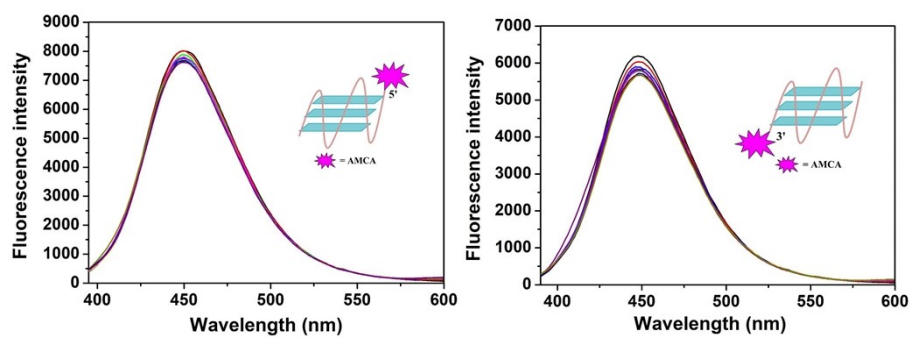


Fig. S9. The fluorescence intensity of 5'/3' AMCA-labeled *c-MYC* G4 (0.2 μ M) with the addition of **MRY-3** (0-1 μ M) in 10 mM Tris-HCl/DMSO (95:5, v/v), 60 mM KCl, pH 7.4. λ_{ex} = 353 nm.