Supplementary Information (SI) for Analyst.

Supporting Information

Selectively aggregating natural ligands into efficient AIEgens by human telomeric duplex-G-quadruplex junction

Ying Xu, Yulu Ru, Xueni Li, Yilin Wang, Dandan Wang, Xiao-Shun Zhou, and Yong Shao*

Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, College of Chemistry and Materials Science, Zhejiang Normal University, Jinhua 321004

*E-mail: yshao@zjnu.cn (S. Y.). Fax: 86 579 82282595

Table S1. Sequences used in this work

Entry	Sequence (from 5′to 3′)
Q	GGGTTAGGGTTAGGGTTAGGG
AQ	AGGGTTAGGGTTAGGGTTAGGG
AQTT	AGGGTTAGGGTTAGGGTTAGGGTT
TAQ	TAGGGTTAGGGTTAGGGTTAGGG
TAQT	TAGGGTTAGGGTTAGGGTTAGGGT
TAQTT	TAGGGTTAGGGTTAGGGTTAGGGTT
TTQA	TTGGGTTAGGGTTAGGGTTAGGGA
TTAQ	TTAGGGTTAGGGTTAGGGTTAGGG
TTAQTT	TTAGGGTTAGGGTTAGGGTTAGGGTT
TTAQTTA	TTAGGGTTAGGGTTAGGGTTAGGGTTA
TAQ-3iG	5′ -TAGGGTTAGGGTTAGGGTTAGG-3′-3′-G-5′
TAQ-5iG	5′-TA-3′-3′-G-5′-GGTTAGGGTTAGGGTTAGGG-3′
TAQ-5iTAG	3′-TAG-5′-5′-GGTTAGGGTTAGGGTTAGGG-3′
mPu22	TGAGGGTGGGGAGGGTGGGGAA
ckit2	CGGGCGGGCGCGAGGGAGGGT
PS2.M	GTGGGTAGGGCGGGTTGG
1XAV	TGAGGGTGGGTAGGGTGGGTAA
PW17	GGGTAGGGCGGGTTGGG
T3TT	GGGTTTGGGTGGGTGGG
T2T2T2	GGGGTTGGGGTTGGGGTTGGGG
NHEIII	TGGGGAGGGTGGGGAGGGTGGGGAAGG
TBA	GGTTGGTGTGGTTGG
D	CCCTAACCCTTAGGGTTAGGG
D-TTAQTT	CCCTAACCCTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTT
D-TTAQTT	ACCCTAACCCTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTT
D-TTAQTT	AACCCTAACCCTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTT
D-TTAQTT	TAACCCTAACCCTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTT
$(TTAQ)_2TT$	TTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTTAGGGTT

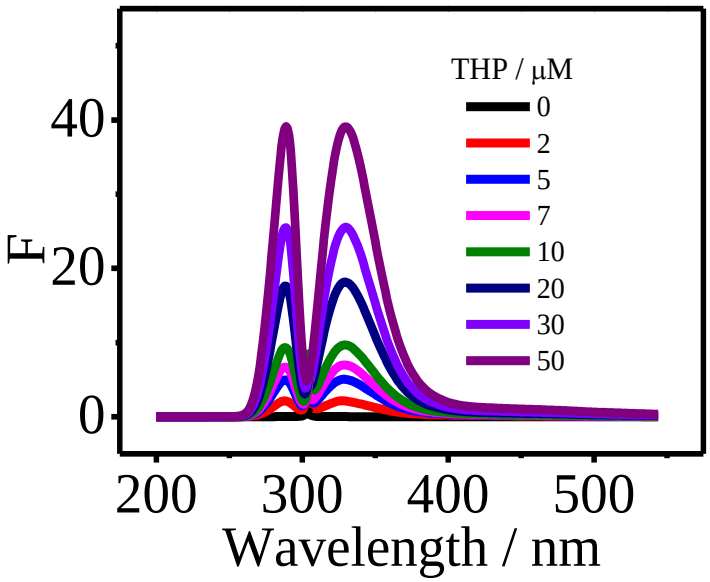

Fig. S1. Fluorescence excitation and emission spectra of THP in formamide.

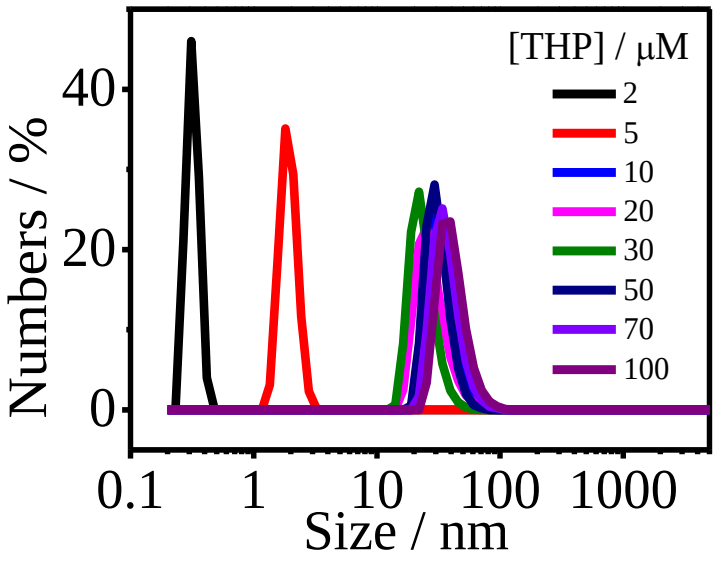

Fig. S2. DLS measurements of THP aggregating at variant concentrations in water.

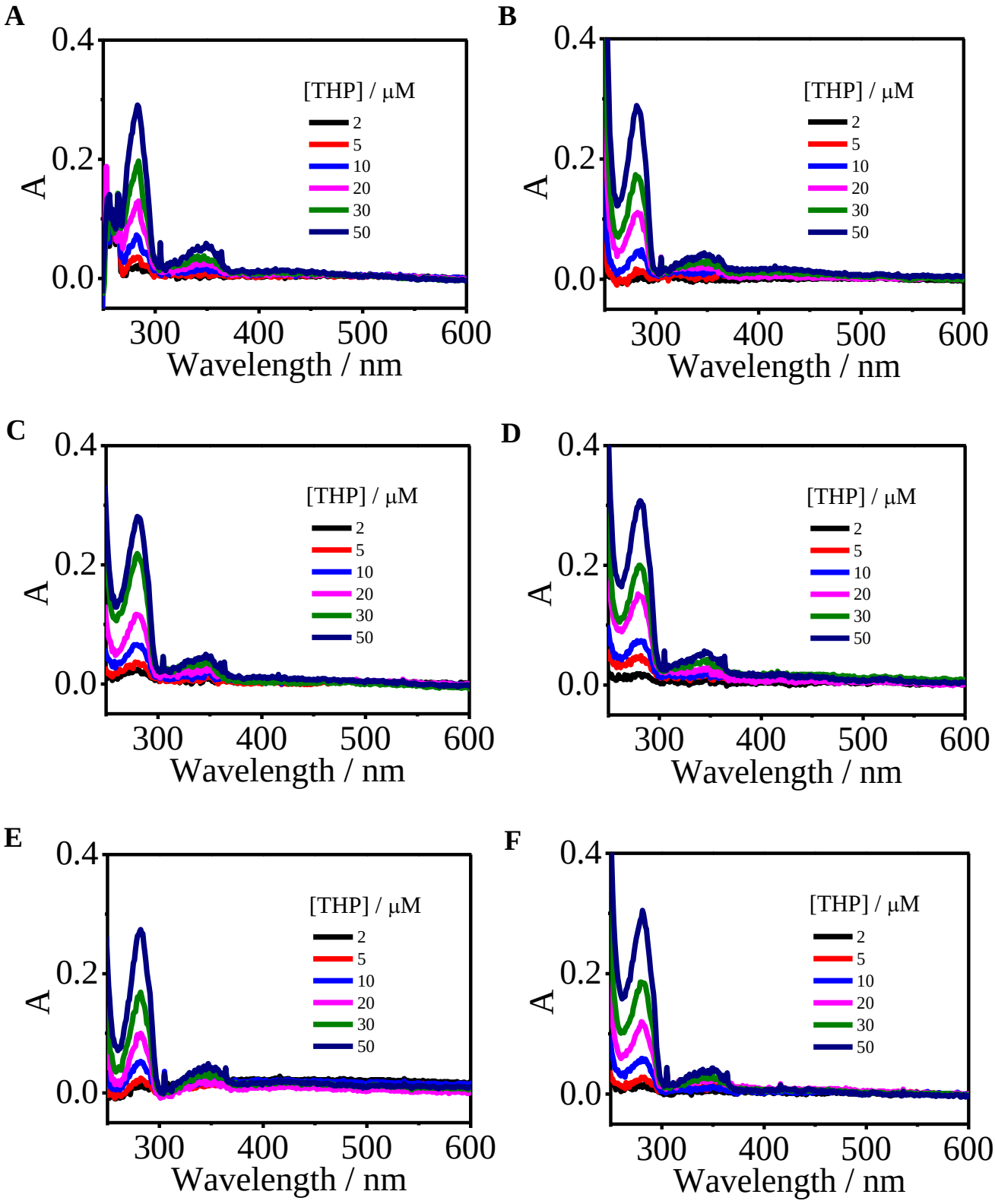

Fig. S3. Absorption spectra of THP in (A) DMF, (B) acetonitrile, (C) methanol, (D) ethanol, (E) glycol, and (F) isopropanol, respectively.

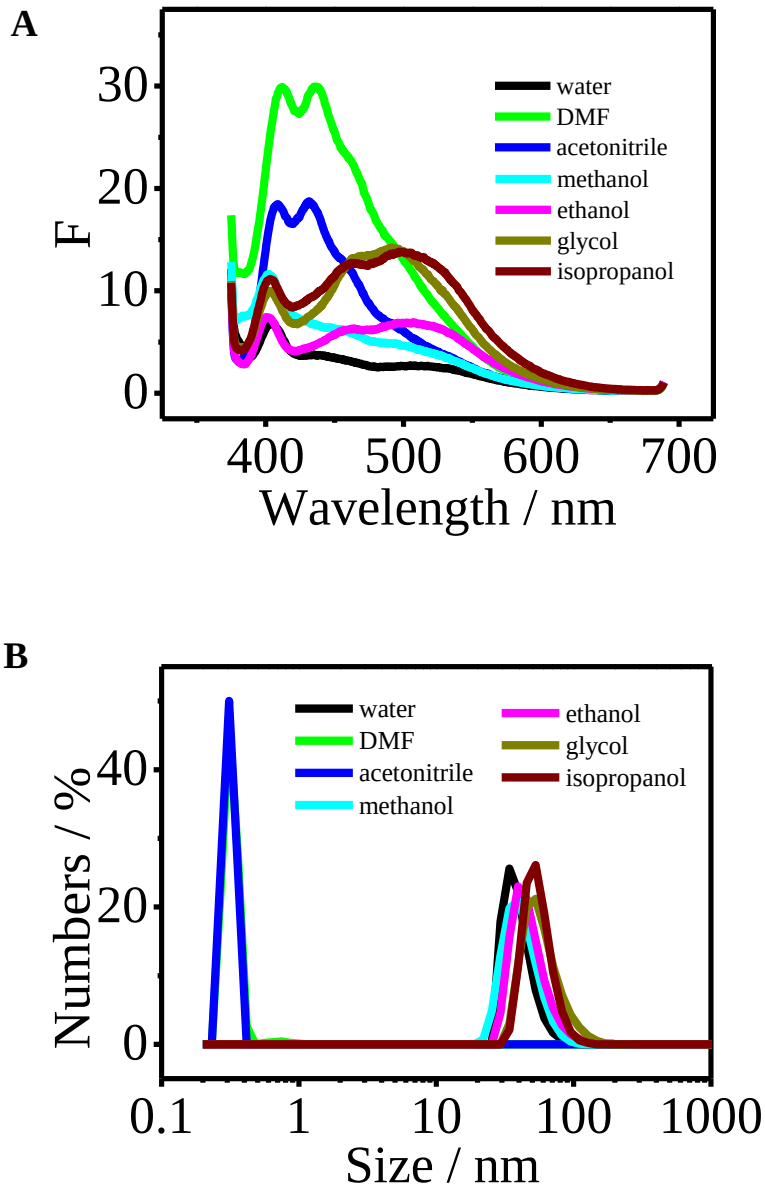

Fig. S4. Emission spectra (A, excitation at 355 nm) and (B) particle size measurements of THP (50 μM) in variant solvents.

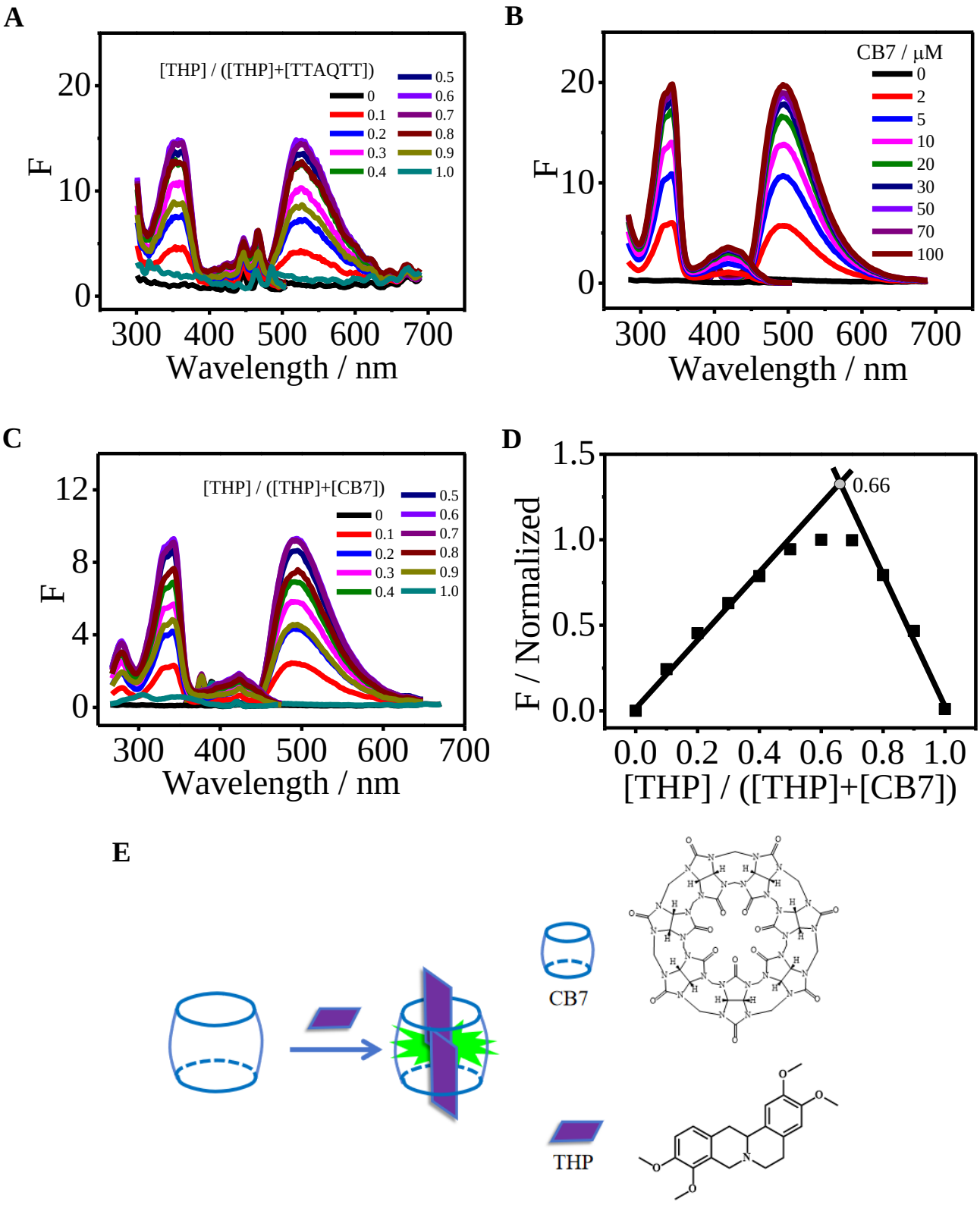

Fig. S5. (A) Fluorescence excitation and emission spectra of THP in bindng with TTAQTT in PBS by systematically changing the [THP]/([THP]+[TTAQTT]) ratio, but keeping their total concentration at 2 μM. (B) Fluorescence excitation and emission spectra of THP (10 μM) in water by increasing the CB7 concentration. (C) Fluorescence excitation and emission spectra of THP in bindng with CB7 in water by systematically changing the [THP]/([THP]+[CB7]) ratio, but keeping their total concentration at 5 μM. (D) The corresponding fluorescence responses at 495 nm in (C) as a function of [THP]/([THP]+[CB7]. (E) The CB7 structure and the predicted binding mode of CB7 with THP.

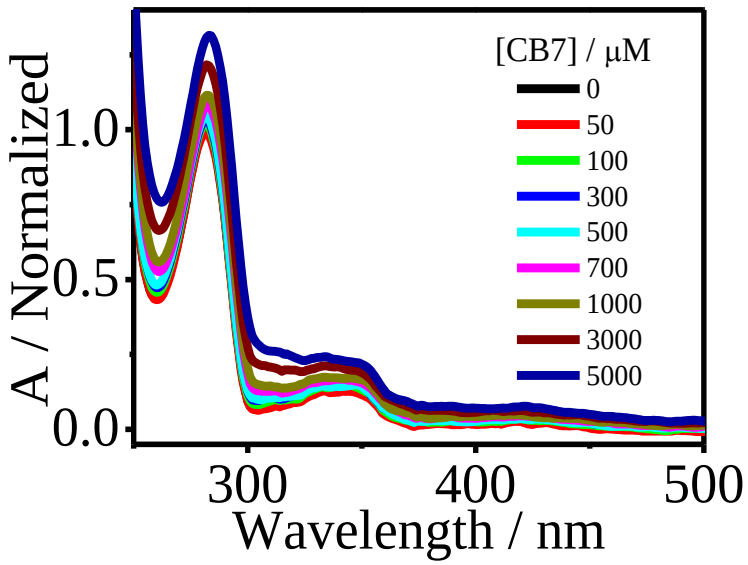

Fig. S6. Normalized absorption spectra with gradual addition of CB7 to THP (35 μM) in water.

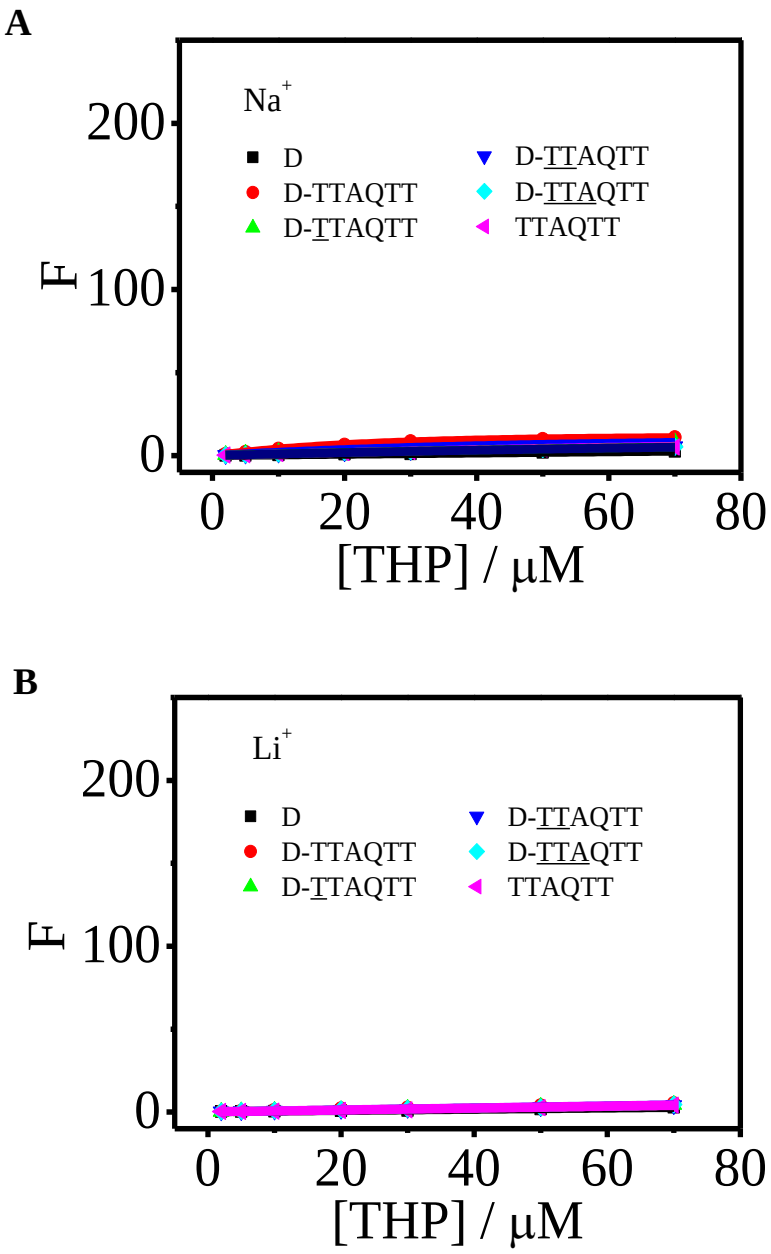

Fig. S7. Fluorescence responses of THP at variant concentration in the presence of DNA (1 μM) in 20 mM PBS (pH 7.0) containing 100 mM (A) Na^+ and (B) Li^+, respectively.

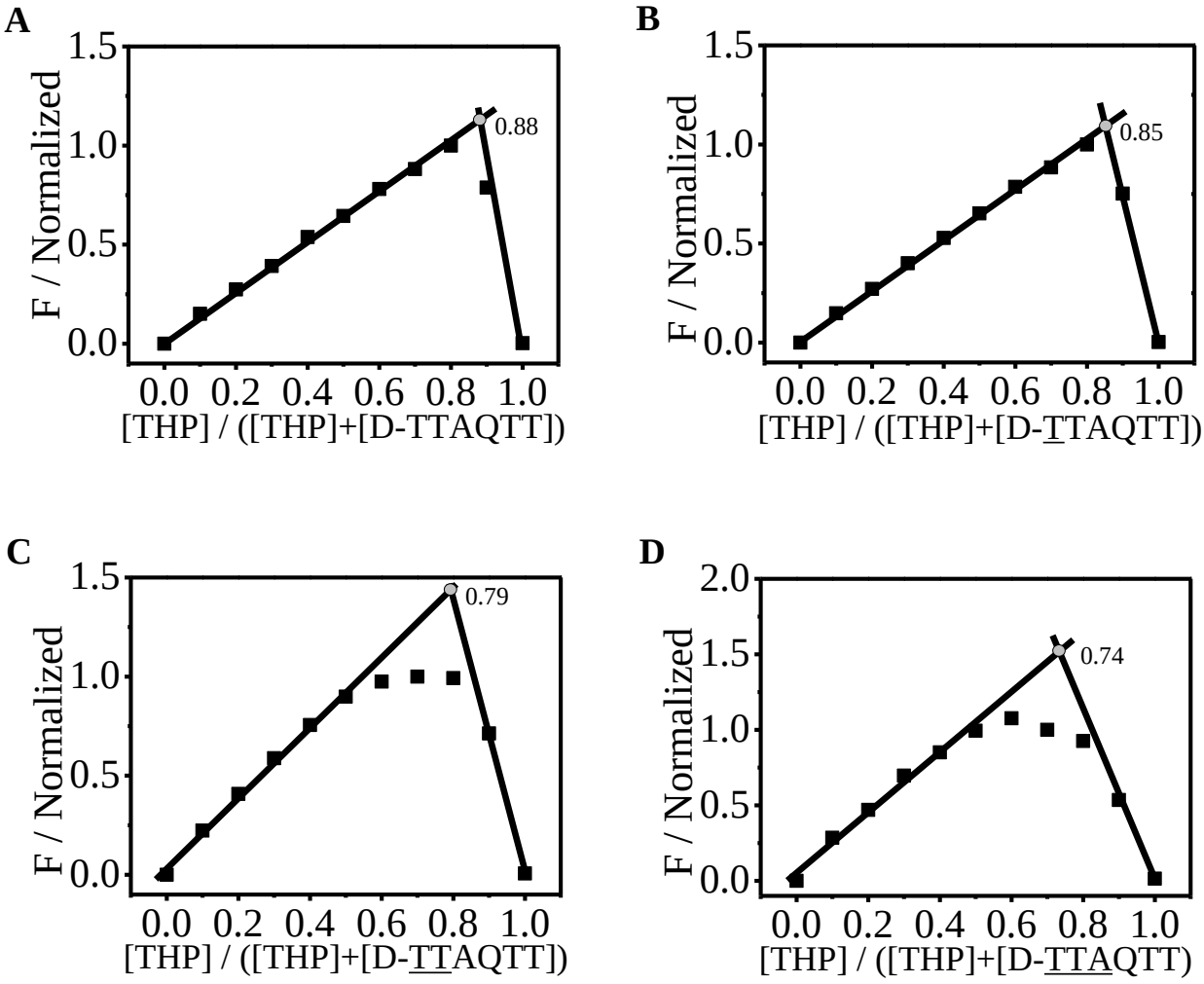

Fig. S8. Job's plot analysis of binding stoichiometry of THP with (A) D-TTAQTT, (B) D-TTAQTT, (C) D-TTAQTT, and (D) D-TTAQTT in 20 mM PBS (pH 7.0) containing 100 mM K^+, respectively.

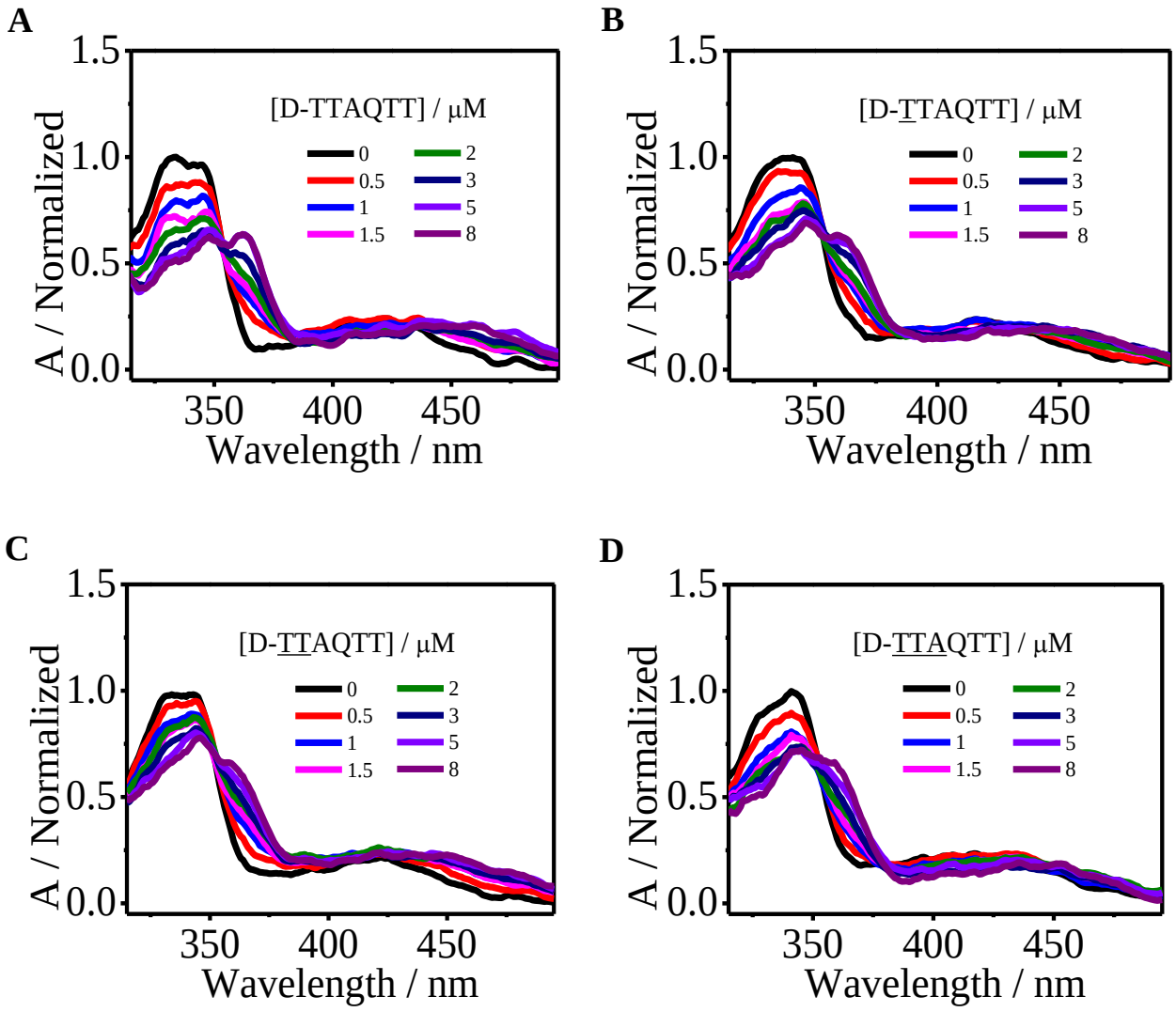

Fig. S9. Normalized absorption spectra of THP (30 μM) with increasing concentration of (A) D-TTAQTT, (B) D-TTAQTT, (C) D-TTAQTT, and (D) D-TTAQTT, respectively.

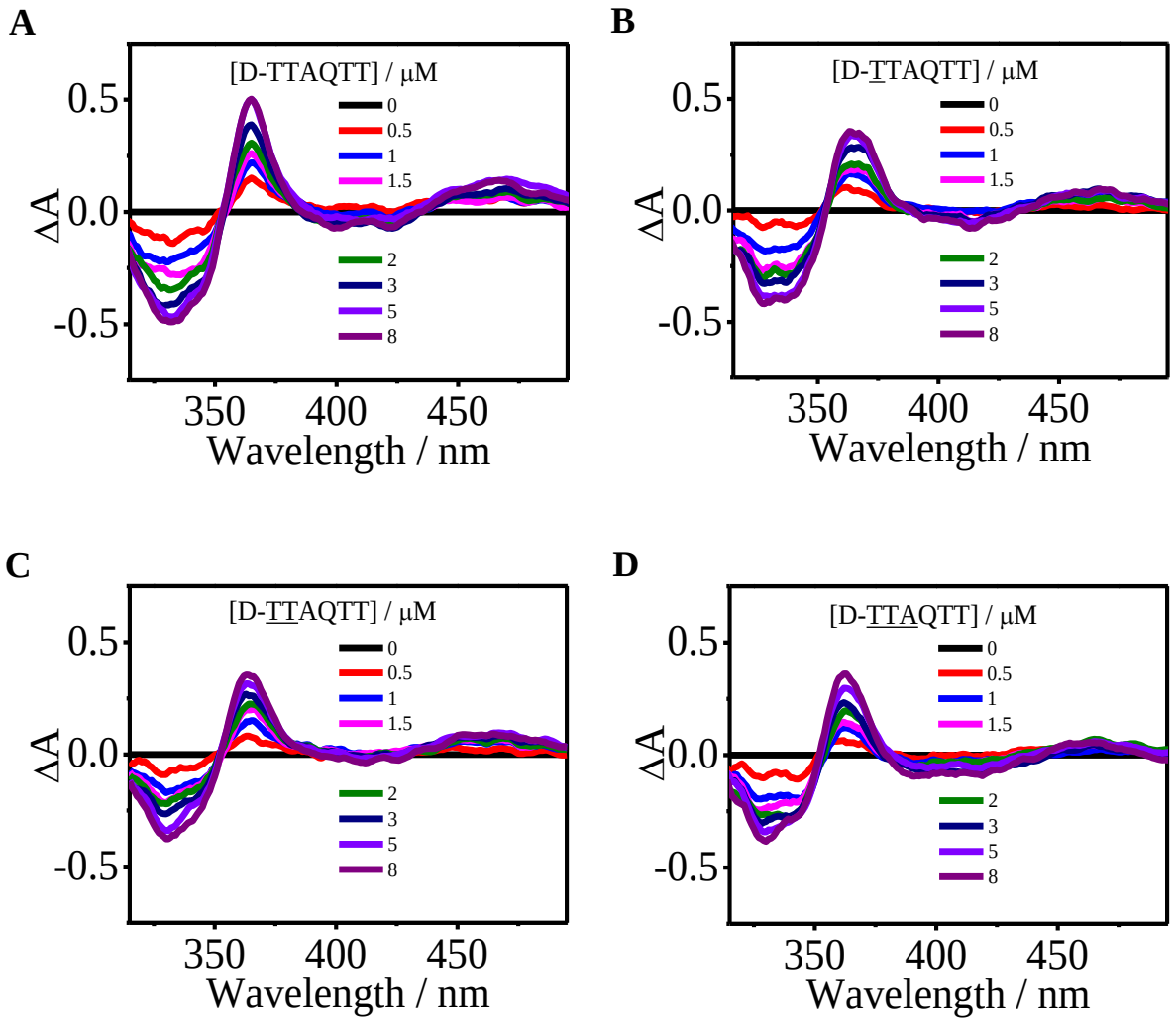

Fig. S10. Difference absorption spectra according to Fig. S9.

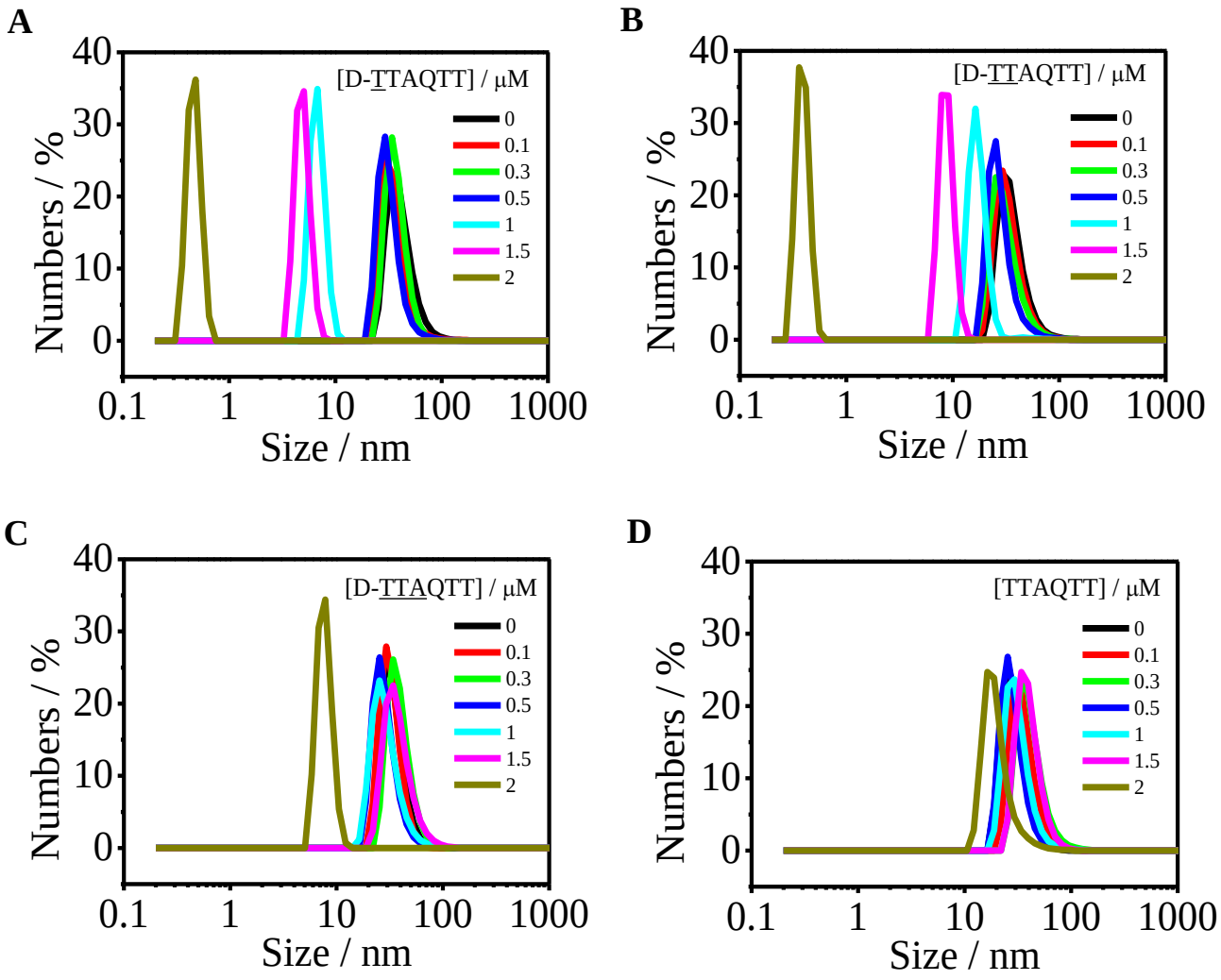

Fig. S11. DLS analysis of THP (10 μM) in interacting with (A) D-TTAQTT, (B) D-TTAQTT, (C) D-TTAQTT, and (D) D-TTAQTT, respectively.

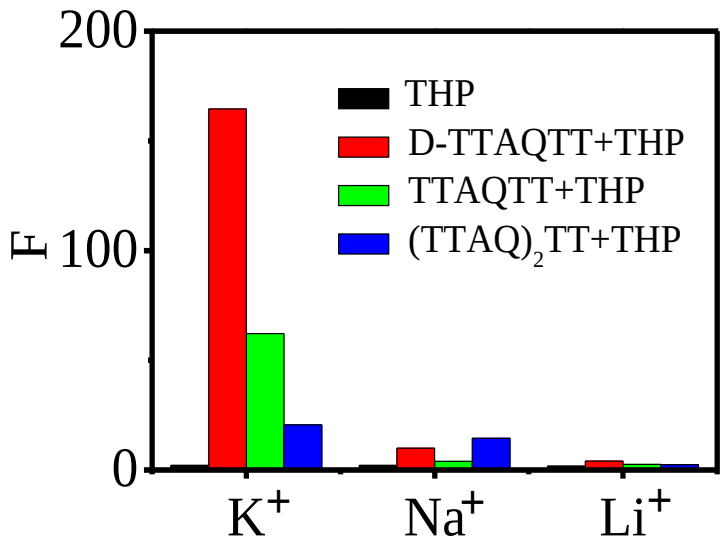

Fig. S12. Effect of monovalent cation ions (K^+, Na^+ and Li^+) on the fluorescence response of THP (50 μM) in the absence and presence of D-TTAQTT, TTAQTT, and $(TTAQ)_2TT$ (1 μM in G4 unit).