Supporting Information

Highly selective, sensitive and fluorescent sensing of dimeric G-quadruplexes by a dimeric berberine

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Figure Legend

Table S1. Optical data of compound **1** with different DNA sequences [a]

DNA	A_F	Abs	φ_F	DNA	A_F	Abs	φ_F
Blank	314.9	0.030	0.002	G_1 (K^+) [c]	2127.3	0.010	0.069
ss-AT DNA	995.6	0.028	0.012	G_1	9276.0	0.023	0.133
ds-AT DNA	1077.1	0.028	0.013	G_2T_1(K^+) [c]	5764.4	0.014	0.133
ss-CG DNA	824.5	0.027	0.010	G_2T_1	26504.3	0.020	0.447
ds-CG DNA	967.8	0.027	0.012	G_2T_2	20551.6	0.021	0.325
CT DNA	356.3	0.027	0.005	G_2T_4	10079.6	0.020	0.164
c-kit2 [b]	1677.2	0.019	0.029	G_2T_6	6447.5	0.019	0.111

[a] Measured in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). The molar ratio of compound **1** to the DNA sequences was 1 : 1.

[b] Measured at 355 nm.

[c] Prepared in 10 mM Tris-HCl buffer (100 mM KCl, pH 7.2).

Table S2. Optical data of compound **1** in different solvents

Solvent	N	A_F	Abs [a]	φ_F	Solvent	N	A_F	Abs [a]	φ_F
H_2O	1.00	18.8	0.021	0.000	EtOH	1.00	266.2	0.043	0.002
$CHCl_3$	1.45	53.6	0.038	0.001	Toluene	1.50	163.4	0.042	0.003
CH_2Cl_2	1.42	102.5	0.034	0.002	90% glycerol	1.43	1606.4	0.045	0.025
CH_3COCH_3	1.36	314.5	0.035	0.006	DMSO	1.48	101.6	0.043	0.002
MeOH	1.33	133.7	0.042	0.002					

[a] Measured at 355 nm.

Table S3. CD melting temperature (T_m, ºC) of G_1 and G_2T_1 without and with compound **1** [a]

DNA	T_m without **1**	T_m with **1**	ΔT_m [b]
G_1	63.3±0.3	62.5±0.2	-0.7±0.1
G_2T_1	53.1±0.2	52.6±0.3	-0.5±0.1

[a] Measured in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). The concentrations of G-quadruplex samples and compound **1** were 3 μM and 10 μM, respectively.

[b] $\Delta T_m = T_m$ (DNA+compound **1**) - T_m (DNA).

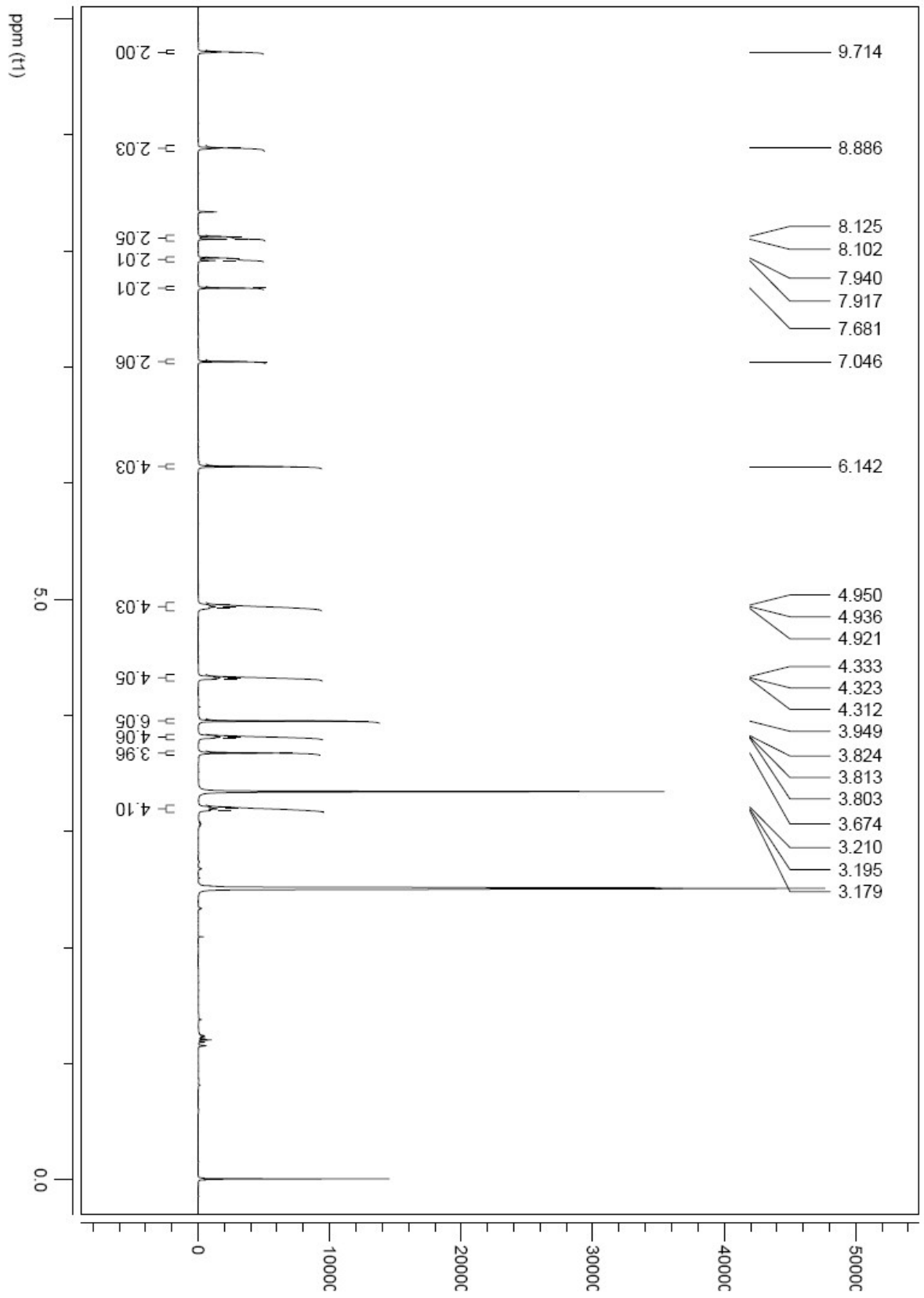


Fig. S1 ^{1}H NMR (400 MHz) of compound **1** in d_6-DMSO.

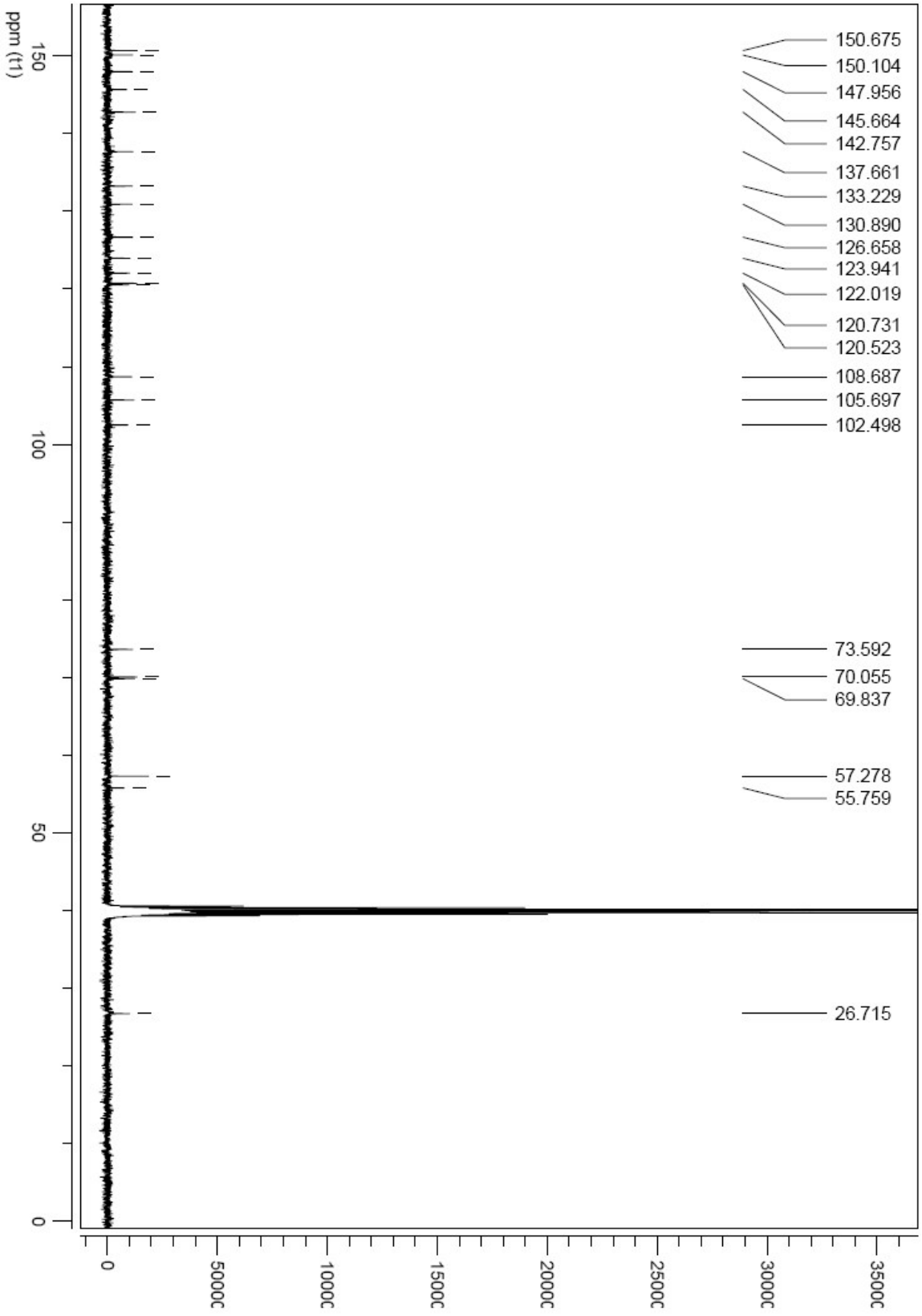


Fig. S2 ^{13}C NMR (100 MHz) of compound **1** in d_6-DMSO.

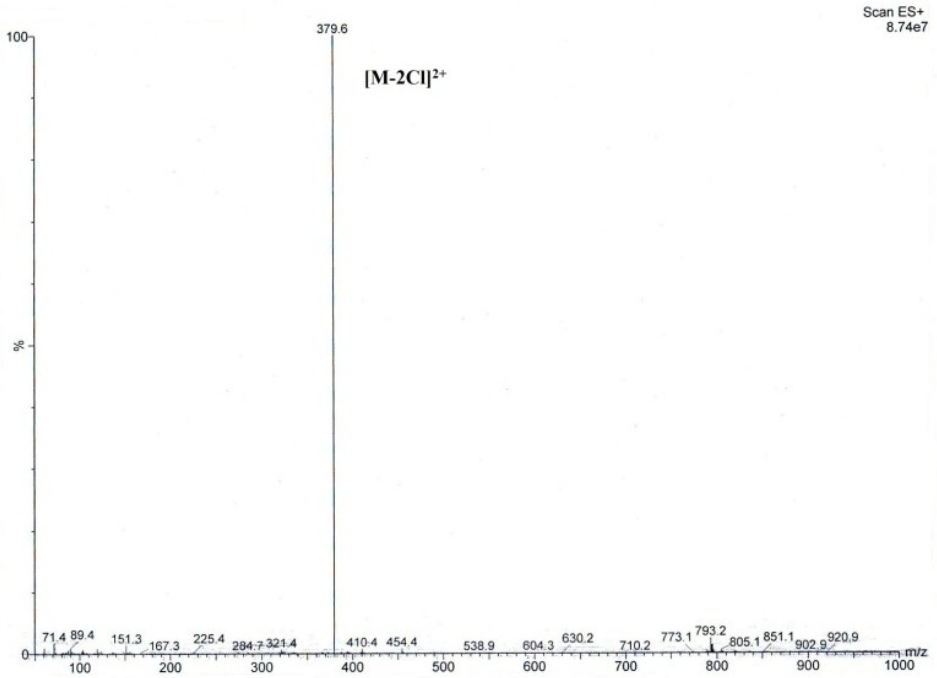
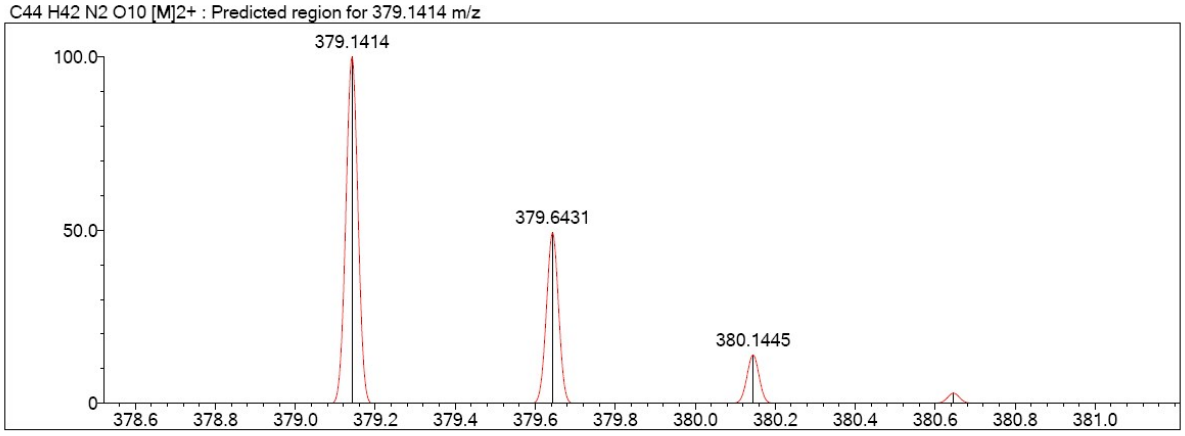


Fig. S3 LR-ESI-MS of compound **1**.



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	41.99	C44 H42 N2 O10	[M]2+	379.1403	379.1414	-1.1	-2.90	44.08	25.0

Fig. S4 HR-ESI-MS of compound **1**.

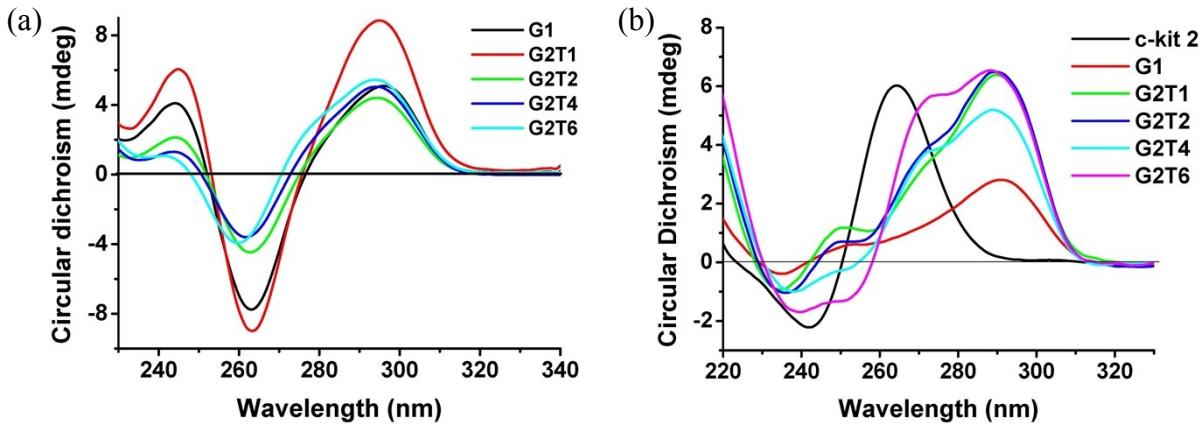


Fig. S5 (a) CD spectra of G_1, G_2T_1, G_2T_2, G_2T_4 and G_2T_6 (5 μM) in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2); (b) CD spectra of c-kit2, G_1, G_2T_1, G_2T_2, G_2T_4 and G_2T_6 (5 μM) in 10 mM Tris-HCl buffer (100 mM KCl, pH 7.2)

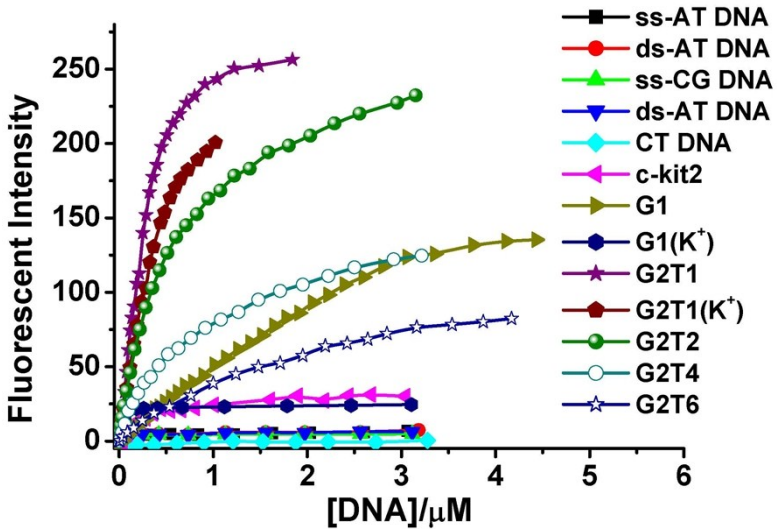


Fig. S6 Plots of the fluorescence intensity at 530 nm of compound **1** (0.5 μM) against the concentrations of various DNA sequences.

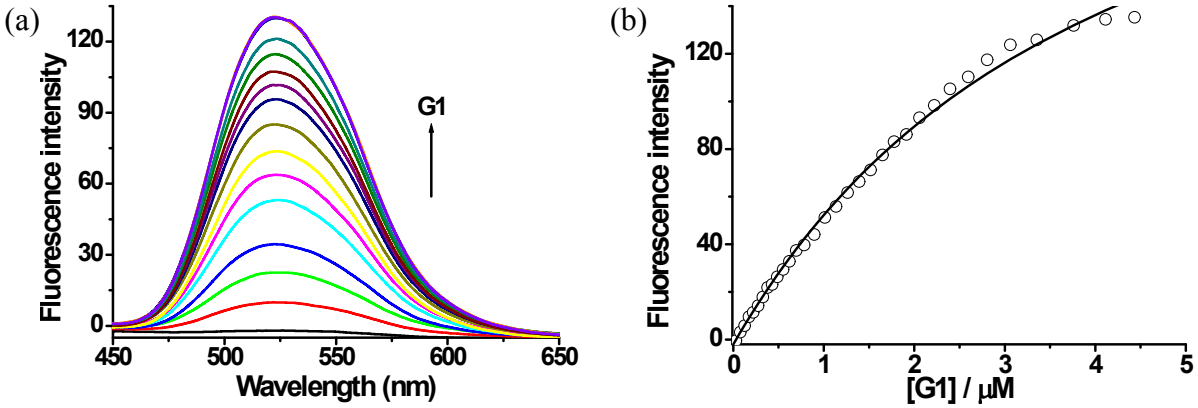


Fig. S7 (a) Fluorescence emission spectra of compound **1** (0.5 μM) in the presence of G_1 of varying concentrations. (b) Plot of the fluorescence intensity of compound **1** (0.5 μM) against the concentrations of G_1 in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). $\lambda_{ex}/\lambda_{em}$ = 355/530 nm.

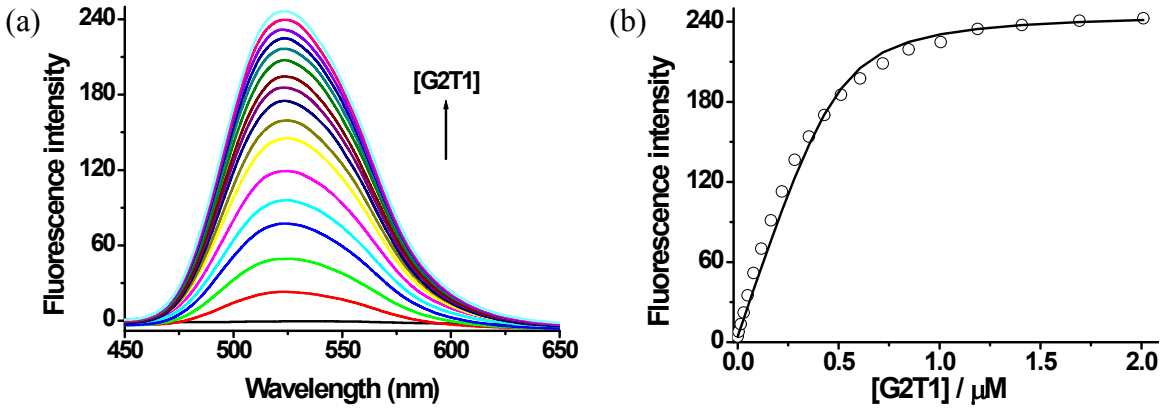


Fig. S8 (a) Fluorescence emission spectra of compound **1** (0.5 μM) in the presence of G_2T_1 of varying concentrations. (b) Plot of the fluorescence intensity of compound **1** (0.5 μM) against the concentrations of G_2T_1 in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). $\lambda_{ex}/\lambda_{em}$ = 355/530 nm.

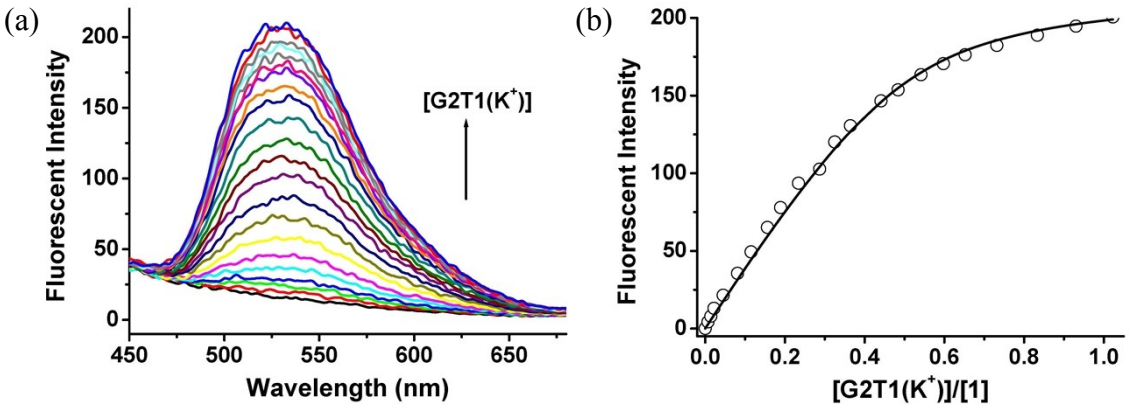


Fig. S9 (a) Fluorescence emission spectra of compound **1** (0.5 μM) in the presence of G_2T_1 (K^+) of varying concentrations. (b) Plot of the fluorescence intensity of compound **1** (0.5 μM) against the concentrations of G_2T_1 (K^+) in 10 mM Tris-HCl buffer (100 mM KCl, pH 7.2). $\lambda_{ex}/\lambda_{em}$ = 355/530 nm.

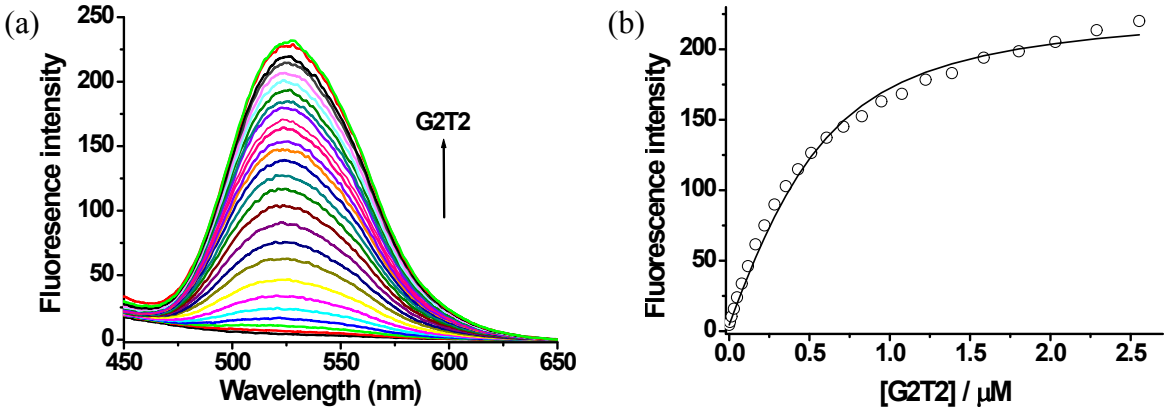


Fig. S10 (a) Fluorescence emission spectra of compound **1** (0.5 μM) in the presence of G_2T_2 of varying concentrations. (b) Plot of the fluorescence intensity of compound **1** (0.5 μM) against the concentrations of G_2T_2 in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). $\lambda_{ex}/\lambda_{em}$ = 355/530 nm.

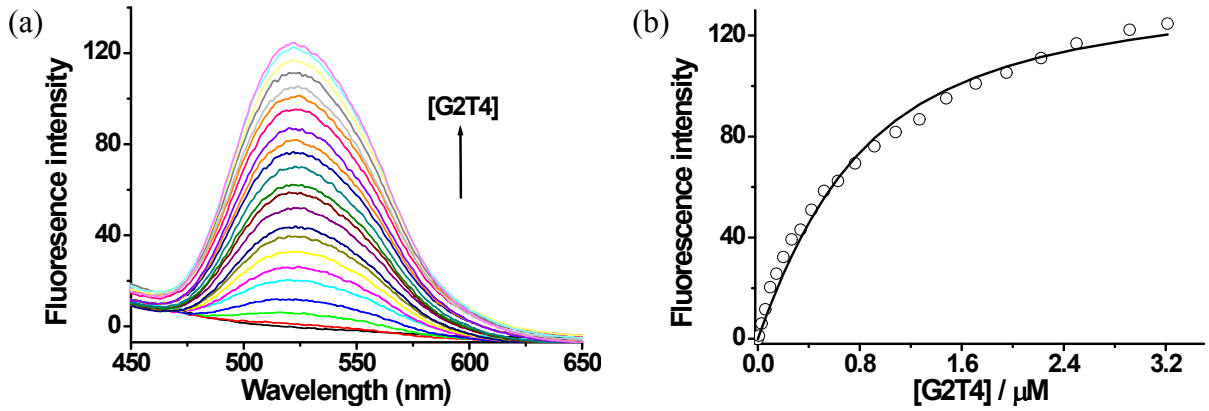


Fig. S11 (a) Fluorescence emission spectra of compound **1** (0.5 μM) in the presence of G_2T_4 of varying concentrations. (b) Plot of the fluorescence intensity of compound **1** (0.5 μM) against the concentrations of G_2T_4 in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). $\lambda_{ex}/\lambda_{em}$ = 355/530 nm.

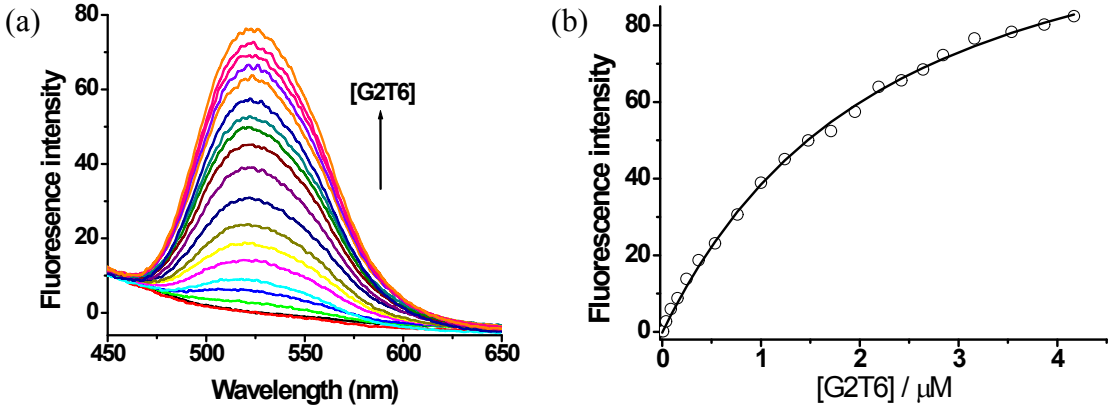


Fig. S12 (a) Fluorescence emission spectra of compound **1** (0.5 μM) in the presence of G_2T_6 of varying concentrations. (b) Plot of the fluorescence intensity of compound **1** (0.5 μM) against the concentrations of G_2T_6 in 10 mM Tris-HCl buffer (100 mM NaCl, pH 7.2). $\lambda_{ex}/\lambda_{em}$ = 355/530 nm.

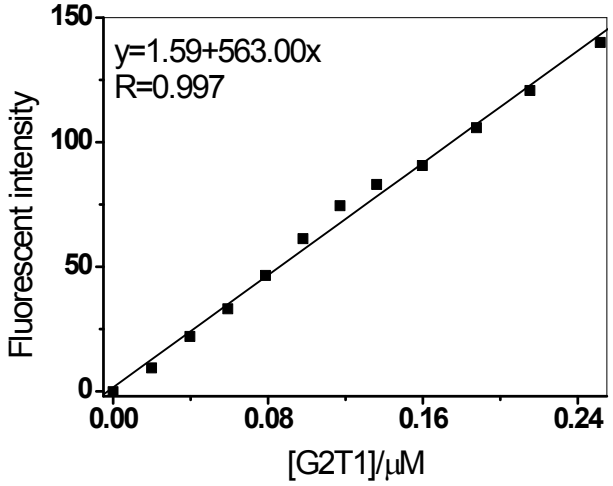


Fig. S13 Plot of the fluorescence intensity at 535 nm of compound **1** (0.5 μM) against the concentrations of G_2T_1 (0~0.5 μM).

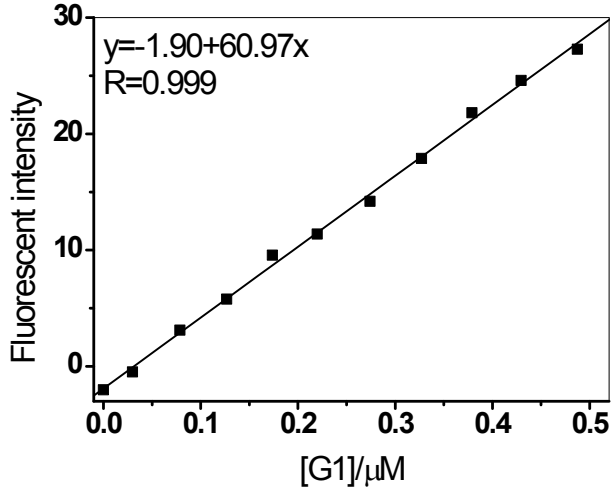


Fig. S14 Plot of the fluorescence intensity at 535 nm of compound **1** (0.5 μM) against the concentrations of G_1 (0~0.5 μM).