A Molecular Container Providing Supramolecular Protection Against Acetylcholine Hydrolysis

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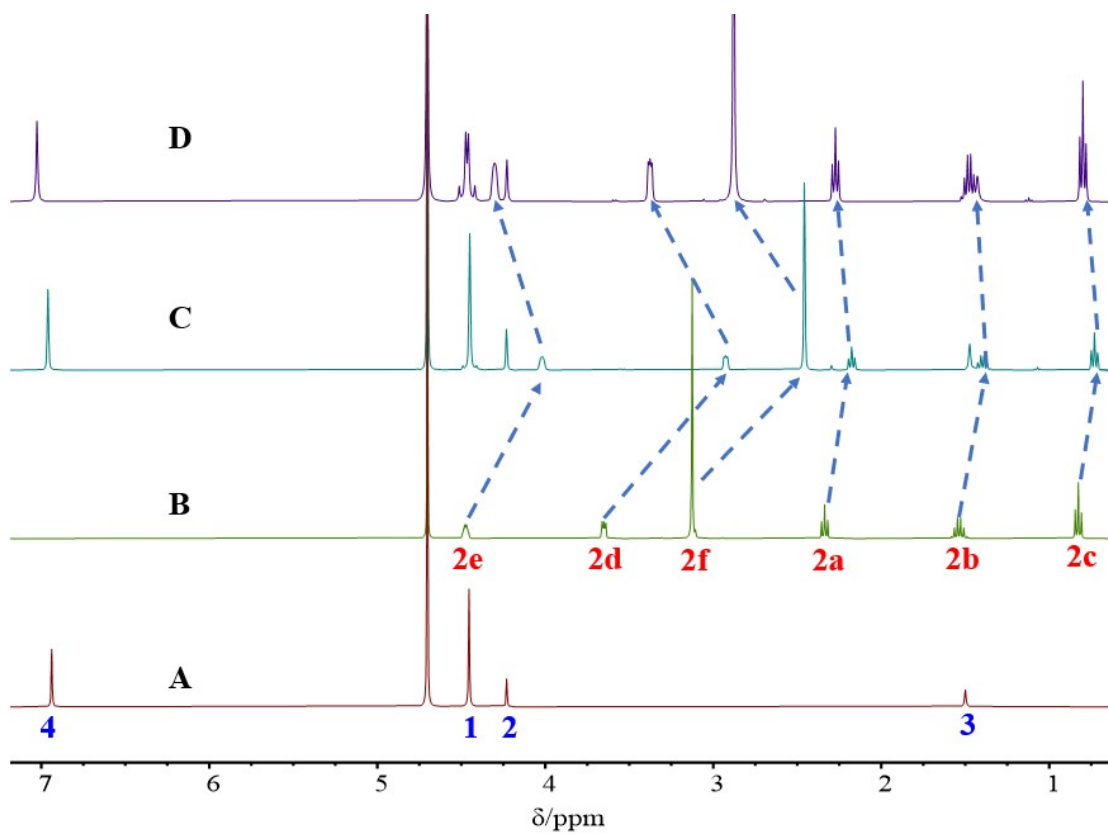*J.-W. Li (E-mail: jianwei.li@utu.fi)*

Fig. S1 ^{1}H NMR spectra (400 MHz, D$_2$O, 295 K): A. **TBTQ-C6** (2 mM); B. **G2** (2 mM); C. **TBTQ-C6** (2 mM) and **G2** (2 mM); D. **TBTQ-C6** (2 mM) and **G2** (6 mM).
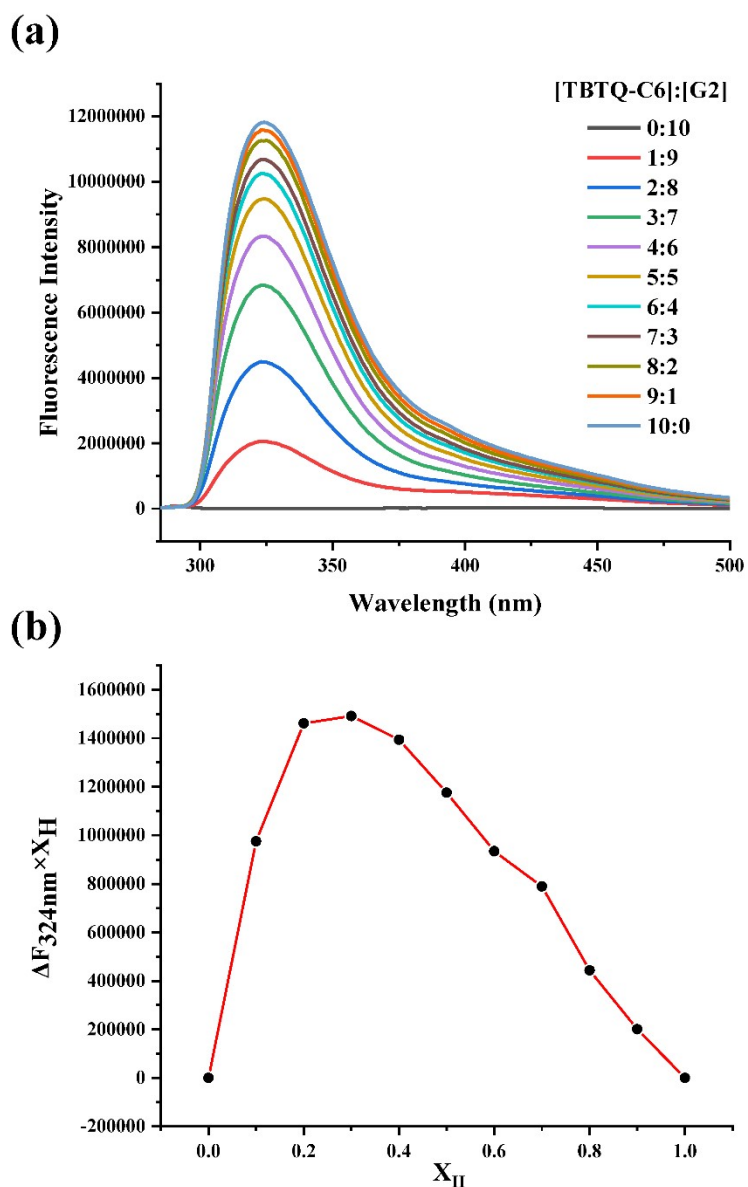
Fig. S2 (a) Fluorescence spectra of the mixture of **TBTQ-C6** and **G2** in different molar ratios at a constant total concentration of 10 μM; (b) Job's plot curve of **TBTQ-C6** and **G2** obtained by plotting fluorescence changes at 324 nm against the molar fraction of **TBTQ-C6** (X_H).
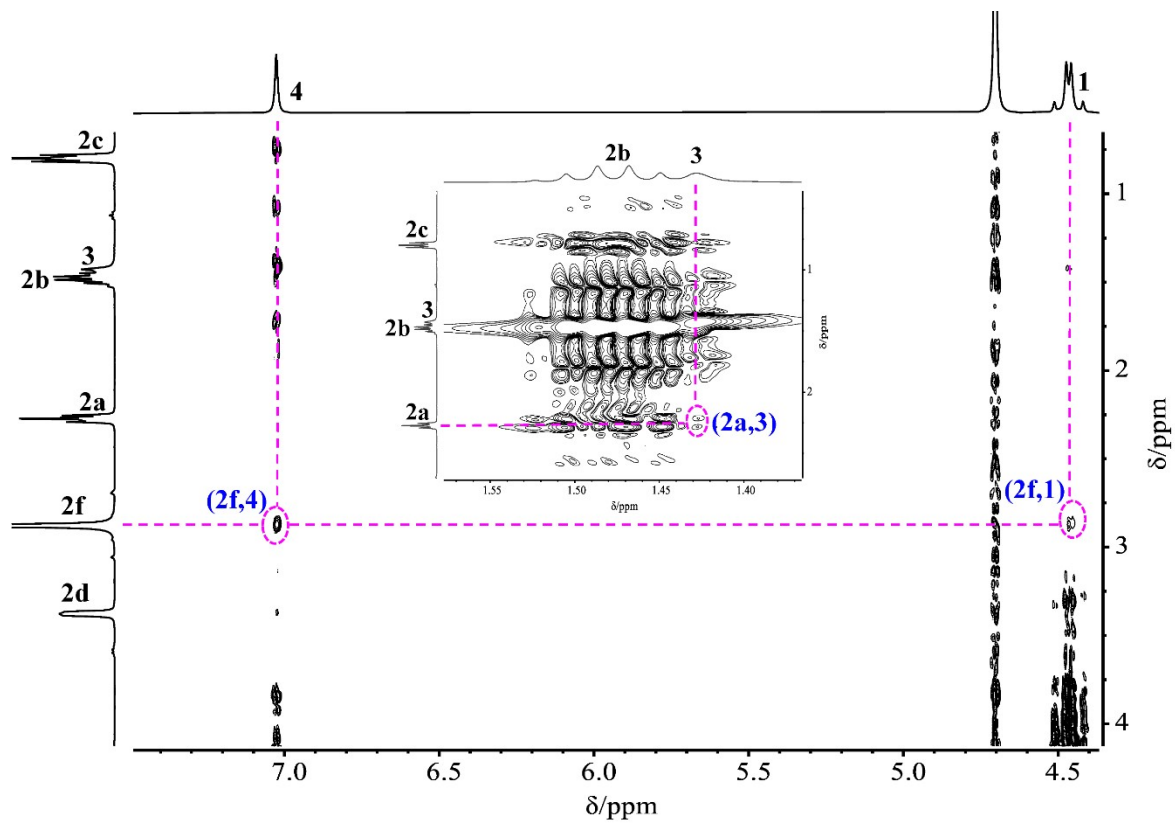
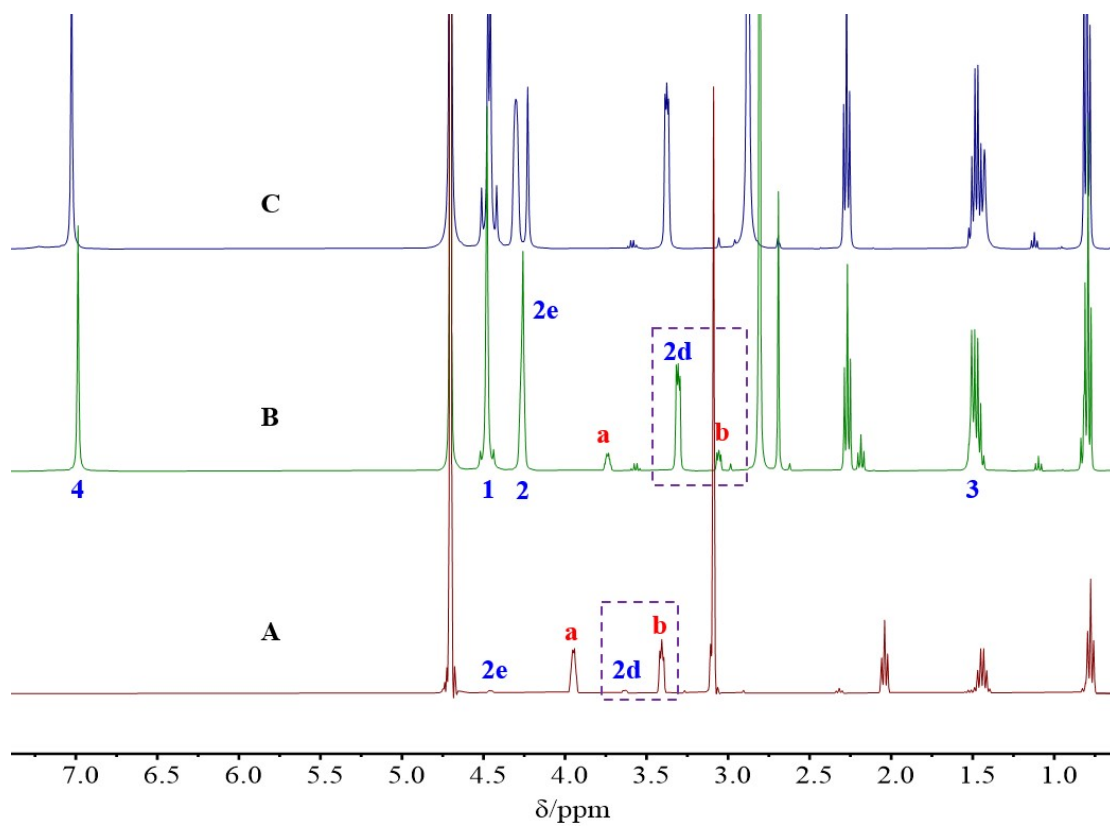Fig. S3 Partial 2D NOESY NMR spectra (400 MHz, D$_2$O, 295 K) of **TBTQ-C6** (30 mM) and **G2** (90 mM).

Fig. S4 ^{1}H NMR spectra (400 MHz, D$_2$O, 295 K): A. **G2** (90 mM) + BChE (1 U/mL); B. **TBTQ-C6** (30 mM) + **G2** (90 mM) + BChE (1 U/mL); C. **TBTQ-C6** (30 mM) + **G2** (90 mM).

Table S1. Association constants (K), thermodynamic data and interaction factor (a), for the host-guest complexation of **TBTQ-C6** with **G1** and **G2** determined from ITC experiments in water at 298.15 K.

Guest		K (M^{-1})		ΔH (kJ/mol)		ΔS (J/mol·K)		ΔG (kJ/mol)	a_1[a]	a_2[a]
	K_1	(9.03±1.73)E4	ΔH_1	−2392±101	ΔS_1	(−7.93±0.34)E3	ΔG_1	−28.19±0.53		
G1	K_2	(2.94±0.33)E4	ΔH_2	2762±106	ΔS_2	(9.35±0.35)E3	ΔG_2	−25.47±0.28	0.98	5.53
	K_3	(5.42±0.23)E4	ΔH_3	−1802±85	ΔS_3	(−5.95±0.28)E3	ΔG_3	−27.01±0.11		
	K_1	(1.70±0.12)E2	ΔH_1	−61.70±4.6	ΔS_1	(−1.64±0.16)E2	ΔG_1	−12.75±0.18		
G2	K_2	(2.19±0.07)E3	ΔH_2	76.75±5.6	ΔS_2	(3.02±0.19)E2	ΔG_2	−13.35±0.08	38.65	0.09
	K_3	(6.78±0.41)E1	ΔH_3	−99.24±11.9	ΔS_3	(−2.78±0.40)E2	ΔG_3	−16.15±0.15		

[a] Interaction factor $a_1 = 3\ K_2/K_1$, $a_2 = 3\ K_3/K_2$ (a_1 or $a_2 > 1$: positive cooperativity; a_1 or $a_2 < 1$: negative cooperativity; a_1 or $a_2 = 1$: no cooperativity).