Supporting Information for:

A Surfactant-Assisted Unimolecular Platform for Multicolor Emissions

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Synthesis of TTC4L

2, 2':5', 2''-Terthiophene (3T, Puyang Huicheng Chemical Co., Ltd., 96%) was used directly without further purification. THF and DMF were A.R. grade and purified to remove water before use. Sodium hydride was dealt with ultrasound dispersed in petroleum ether. Other reagents were A.R. grade and used without further purification.

2, 2':5', 2''-Terthiophene-5-carbaldehyde (1)

1 was synthesized according to literature procedures. ^{1}HNMR ($CDCl_3$) δ 7.28 (d, *J*=3.82Hz, 2H), 7.30(s, 2H), 7.67(d, *J*=3.97Hz, 2H), 9.87(s, 1H). Anal. Calcd for $C_{13}H_8OS_3$ (%): C, 56.49; H, 2.92. Found: C, 56.76; H, 3.13.

2, 2':5', 2''-Terthiophen-5-yl-methanol (2)

Sodium borohydride (600 mg, 15.8 m mol) was added to a solution of 1(1.38 g, 5 m mol) in ethanol (40ml). The mixture was stirred at room temperature under nitrogen until the raw materials disappeared detected by the thin layer chromatography (TLC). The yellow solution was concentrated by evaporation. Ether (80ml) was added and the organic layer was washed with water (3×20ml). The combined organic layers were dried with $MgSO_4$ and the solvent removed under reduced pressure. Chromatography of the residue (silica, ethyl acetate and petroleum ether) yielded product 2 as yellowish powder: ^{1}HNMR ($CDCl_3$) δ 4.82 (s, 2H), 6.92(d, *J*=3.54Hz, 1H), 7.03(t, *J*=2.72Hz, 2H), 7.07(q, *J*=3.86Hz, 2H), 7.18(d, *J*=3.12Hz, 1H), 7.22(d, *J*=5.02Hz, 1H).

5-(4-Bromo-butoxymethyl)-2, 2':5', 2''-terthiophene (3)

Sodium hydride (0.24 g, 10 m mol) was added into the solution of 2 (1.39 g, 5 m mol) in THF (60 ml) under nitrogen. After the initial gas evolution ceased, 1, 4-dibromo-butane (3.24 g, 15 m mol) was added. The reaction mixture was refluxed for several hours till the raw materials disappeared. After cooled to room temperature and concentrated by evaporation, the reaction was quenched with water (3×30 ml) and extracted with ethyl ether (100 ml) for three times. After dried with $MgSO_4$ and concentrated, the residue was further purified by chromatography (silica, dichloromethane and petroleum ether) and gave the product 3 as light yellowish brown crystals: ^{1}HNMR ($CDCl_3$) δ 1.75(m, *J*=6.07Hz, 2H), 1.95(m, *J*=4.75Hz, 2H), 3.43(t, *J*=6.45Hz, 2H), 3.51(t, *J*=6.15Hz, 2H), 4.60(s, 2H), 6.85(d, *J*=6.00Hz, 1H), 7.01(m, *J*=3.80Hz, 2H), 7.06(q, *J*=3.80Hz, 2H), 7.14(d, *J*=4.00Hz, 1H), 7.09(d, *J*=4.95Hz, 1H).

4-Hydroxy-pyridine-2, 6-dicarboxylic acid diethyl ester (4)

Thionyl chloride (30 ml) was added dropwise to ethanol (100ml) cooled in an ice bath. 4-Hydroxy-pyridine-2, 6-dicarboxylic acid (8g) was added into the solution when its temperature reverted to room temperature. The mixture was allowed to stir overnight and then reflux for 2h while the white suspension turned gradually transparent. An oily yellow liquid occurred after the solvent removed under reduced pressure. 80ml water was added into the liquid and white precipitate appeared. The mixture was cooled to zero and then 10% Na_2CO_3 aqueous solution was added dropwise slowly until the mixture remained unchanged of yellow transparent solution and white precipitate. After the vacuum filtration, the precipitate was washed with water and recrystallization was carried out with ethanol / water (1/2) once to give the white crystals: ^{1}HNMR ($CDCl_3$) δ 1.43(t, *J*=7.05Hz, 6H), 4.47(q, *J*=7.2Hz, 4H), 7.28(s, 2H). Anal. Calcd for $C_{11}H_{13}NO_5$ (%): C, 55.23; H, 5.48; N, 5.86. Found: C, 55.31; H, 5.47; N, 5.96.

TTC4L

A solution of 3 (2.07 g, 5 m mol)、4 (1.25 g, 5.2 m mol) and K_2CO_3 (2.07 g, 15 m mol) in butanone (150 ml) was refluxed for 3 days under nitrogen. The suspension gradually turned red which was then concentrated by evaporation and washed with water to remove the excess K_2CO_3. Chromatography of the residue (silica, ethyl acetate and petroleum ether) yielded product 3TC4L-ester as a red oily liquid: ^{1}HNMR (d_6-DMSO) δ 1.37(t, *J*=4.70Hz, 6H), 1.74(m, *J*=7.20Hz, 2H), 1.85(m, *J*=7.50Hz, 2H), 3.56(t, *J*=6.00Hz, 2H), 4.24(t, *J*=6.45Hz, 2H), 4.39(q, *J*=7.10Hz, 4H), 4.66(s, 2H), 7.03(d, *J*=3.90Hz, 1H), 7.14(d, *J*=2.80Hz, 1H) , 7.22(m, *J*=3.40Hz, 3H) , 7.35(d,

J=0.90Hz, 1H), 7.55(d, *J*=1.20Hz, 1H), 7.73(s, 2H). The liquid (0.57 g, 1 m mol) was refluxed overnight with equivalent K_2CO_3 (0.15 g, 1.08 m mol) in ethanol / water (1/1) (50 ml). The solvent removed under reduced pressure and the product 3TC4L occurred as yellowish brown solid: Anal. Calcd for $C_{24}H_{19}NO_6S_3K_2$ (%): C, 48.71; H, 3.24; N, 2.37. Found: C, 47.61; H, 3.86; N, 2.32.

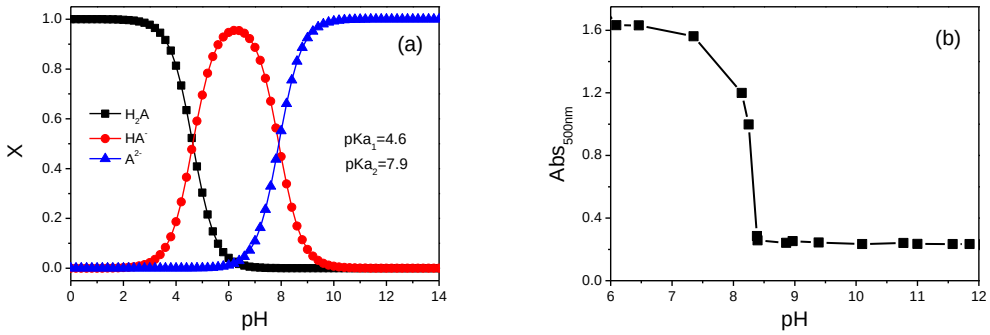


Figure S1. (a) Species distribution of TTC4L solution within pH range of 0-14. (b) Turbidity curve of 1mM TTC4L aqueous solution.

Table S1. Fluorescence lifetime data for TTC4L aqueous solutions

C_{TTC4L}/ mM (λ_{em}/nm) [a]	Component lifetime (ns) [b]			
	τ1 (%)	τ2 (%)	χ2	τ_{avg} [c]
0.02(455)	0.33(16.3)	2.61(83.7)	1.036	2.24
0.10(455)	0.27(14.6)	2.75(85.4)	1.295	2.39
0.50(465)	0.30(16.0)	2.72(84.0)	1.192	2.33

[a] Values in parenthesis shows the monitoring emission wavelength.

[b] Values in parenthesis shows the decay contribution corresponding to each lifetime.

[c] Average lifetimes (τ_{avg}) were calculated using the following equation: $\tau_{avg} = a_1\tau1 + a_2\tau2$, where a1 and a2 represent the percentage of components with life time being τ1 and τ2.

Table S2. Fluorescence lifetime data for TTC4L-DEAB aqueous solutions.

$C_{TTC4L-DEAB}$ / mM (λ_{em}/nm) [a]	Component lifetime (ns) [b]				
	τ1 (%)	τ2 (%)	τ3 (%)	χ2	τ_{avg} [c]
0.1-0(455)	0.27(14.6)	2.75(85.4)	----	1.295	2.39
0.1-12(505)	0.26(32.0)	1.37(49.3)	5.16(18.7)	1.039	1.73
0.1-20(440)	0.22(85.8)	2.07(10.1)	8.98(4.11)	1.066	0.77
0.1-30(440)	0.23(94.7)	1.22(4.04)	6.14(1.28)	0.968	0.35

[a] Values in parenthesis shows the monitoring emission wavelength.

[b] Values in parenthesis shows the decay contribution corresponding to each lifetime.

[c] Average lifetimes (τ_{avg}) were calculated using the following equation: $\tau_{avg} = a_1\tau1 + a_2\tau2 + a_3\tau3$.

The meaning of a1, a2 and a3 is the same as that in Table S1.

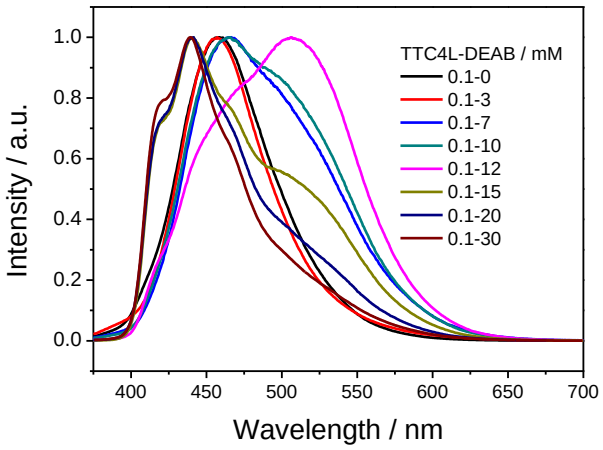


Figure S2. Normalized emission spectra of TTC4L-DEAB aqueous solutions of various ratios.

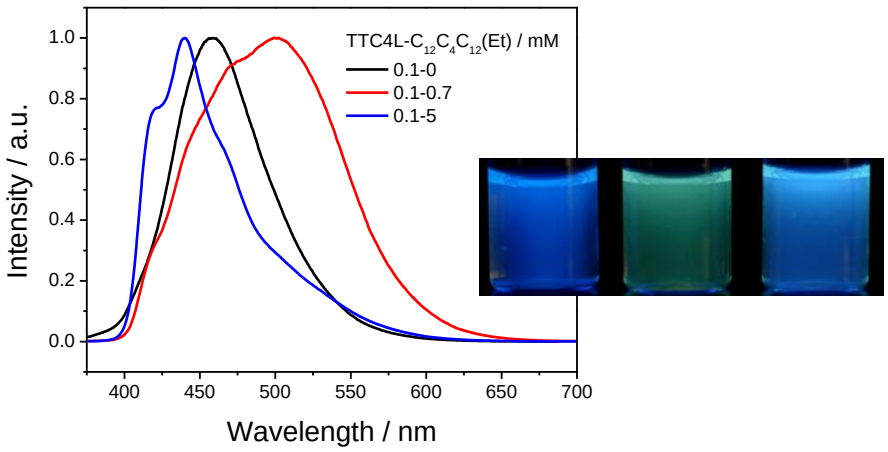


Figure S3. Normalized emission spectra of TTC4L-$C_{12}C_4C_{12}$(Et) aqueous solutions of 0.1-0mM, 0.1-0.7mM and 0.1-5mM system, respectively (excited at 360nm). The right picture shows three colors corresponding to each other (from left to right) under 365nm UV light.

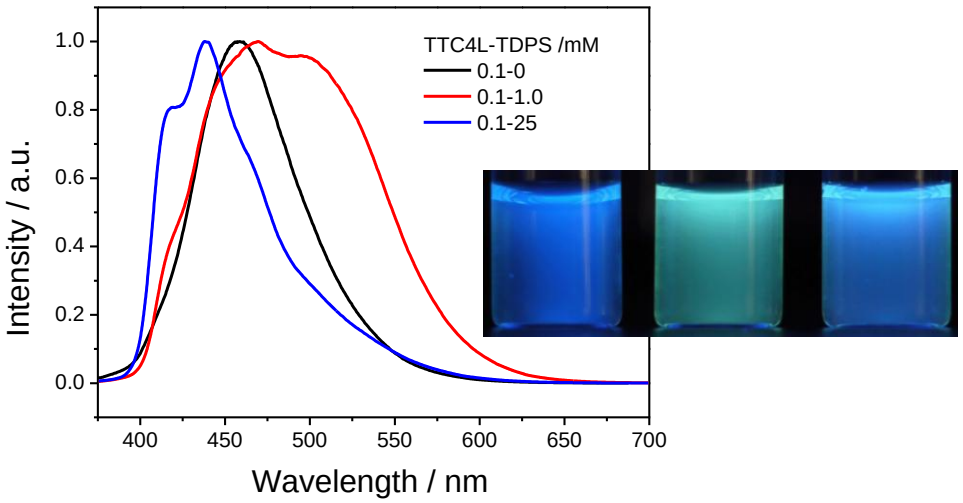


Figure S4. Normalized emission spectra of TTC4L-TDPS aqueous solutions of 0.1-0mM, 0.1-1mM and 0.1-25mM system, respectively (excited at 360nm). The right picture shows three colors corresponding to each other (from left to right) under 365nm UV light.

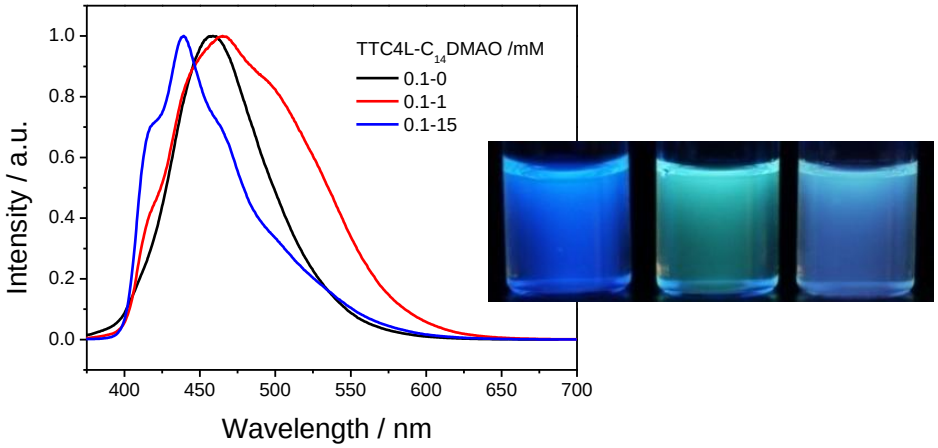


Figure S5. Normalized emission spectra of TTC4L-C_{14}DMAO aqueous solutions of 0.1-0mM, 0.1-1mM and 0.1-15mM system, respectively (excited at 360nm). The right picture shows three colors corresponding to each other (from left to right) under 365nm UV light.

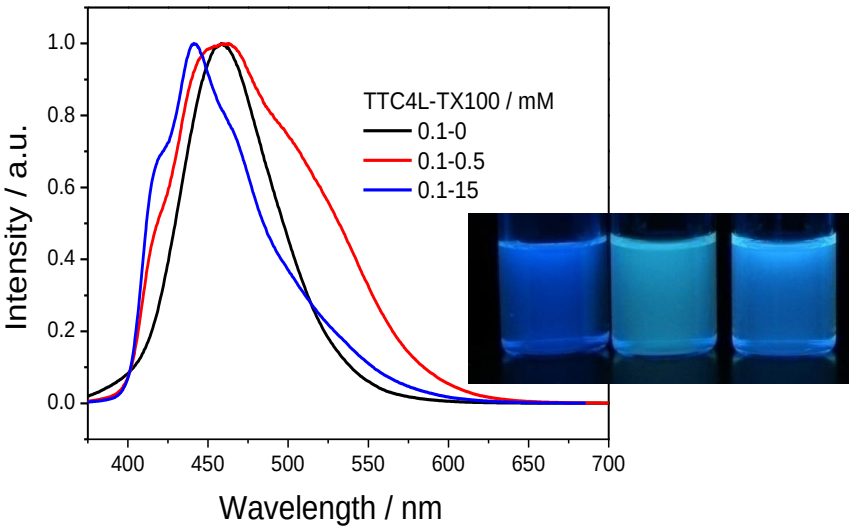


Figure S6. Normalized emission spectra of TTC4L-TX100 aqueous solutions at various ratios (excited at 360nm). The right picture shows sample colors corresponding to 0.1-0, 0.1-0.5, 0.1-15mM (from left to right) under 365nm UV light.

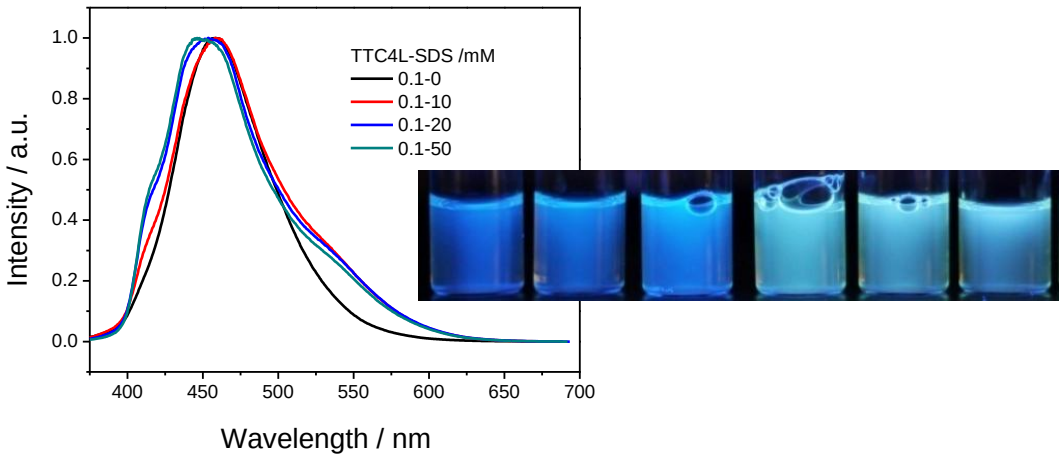
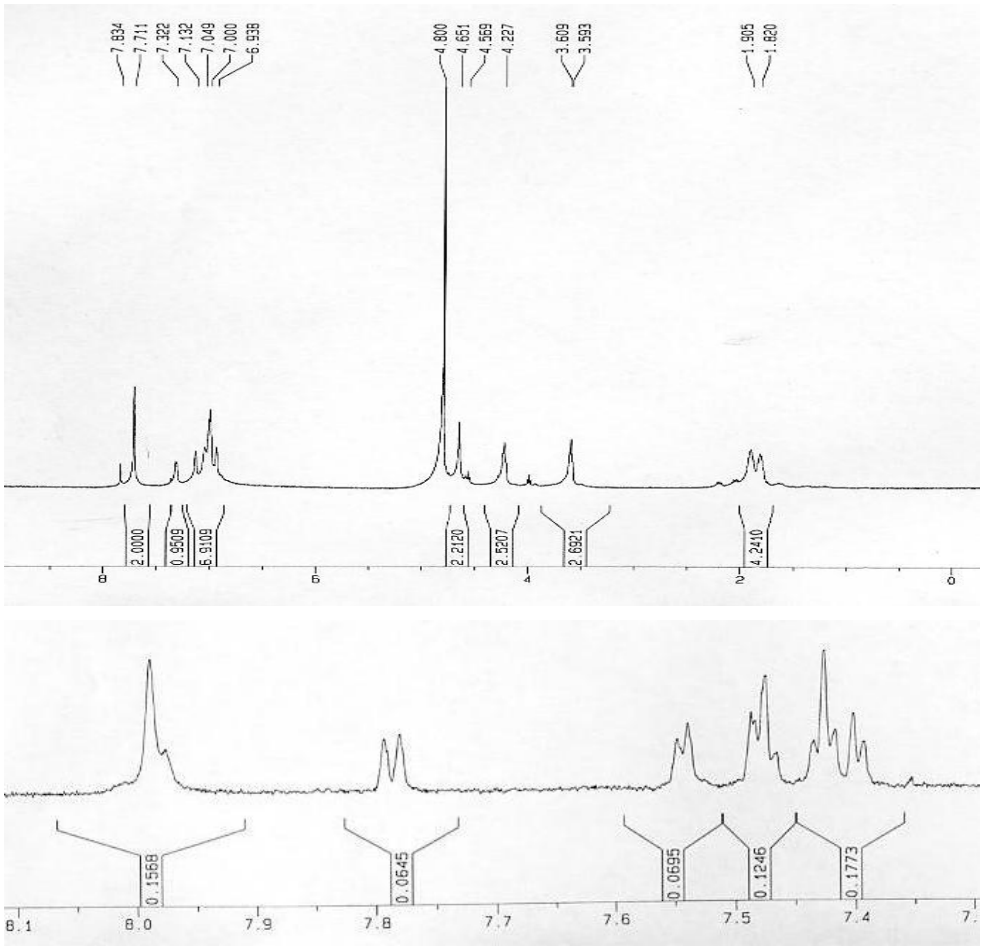


Figure S7. Normalized emission spectra of TTC4L-SDS aqueous solutions at various ratios (excited at 360nm). The right picture shows sample colors corresponding to 0.1-0, 0.1-5, 0.1-10, 0.1-20, 0.1-50, 0.1-90mM (from left to right) under 365nm UV light.



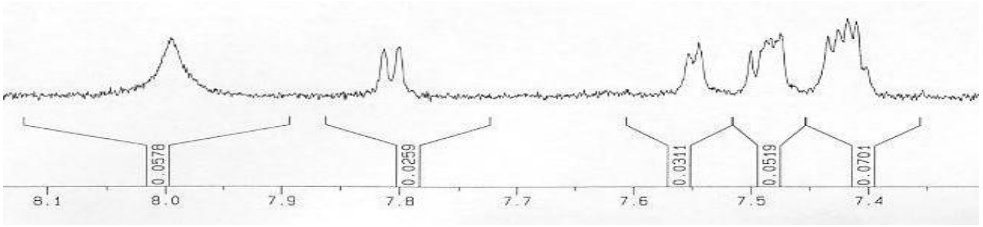


Figure S8. ^{1}HNMR spectra of the TTC4L (upper), 1:3 (middle), and 1:10 (lower) inclusion system with β-CD.

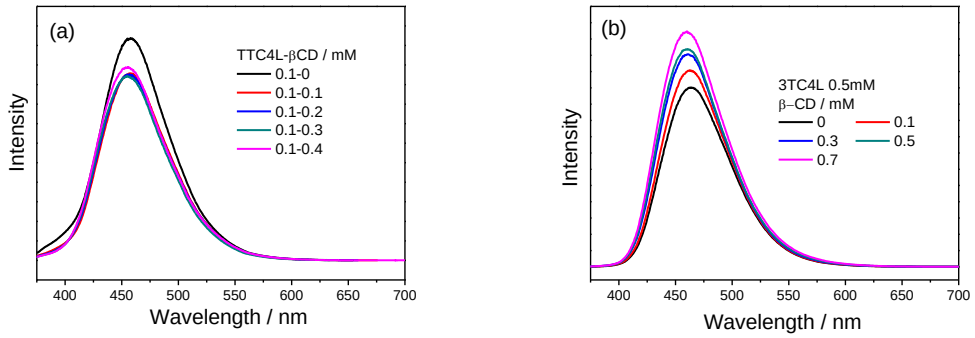


Figure S9. Normalized emission spectra of TTC4L-β-CD aqueous solutions at various β-CD concentrations (excited at 360nm).