Supplementary Information

Highly selective and sensitive macrocycle-based dinuclear foldamer for fluorometric and colorimetric sensing of citrate in water

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Table of contents

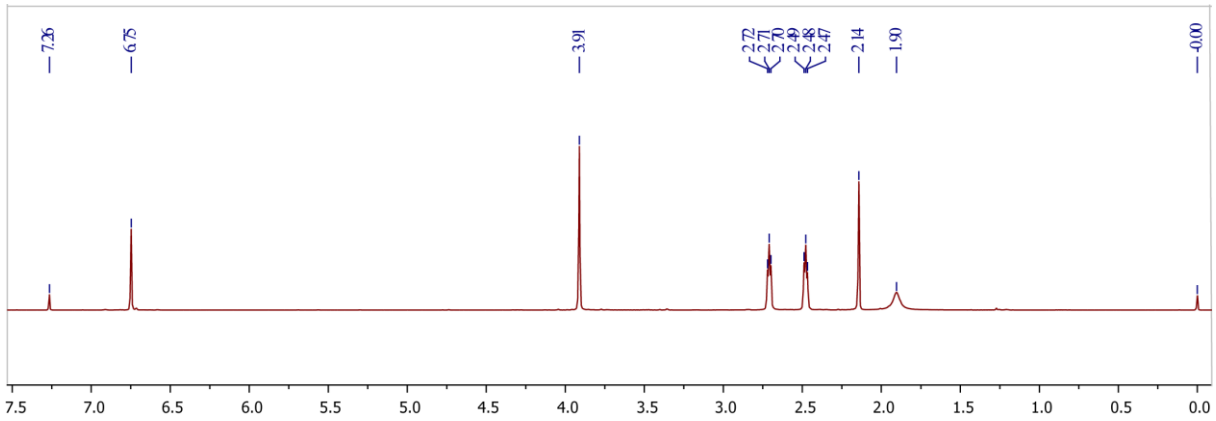

Figure S1. ^{1}H NMR of **L** in $CDCl_3$.

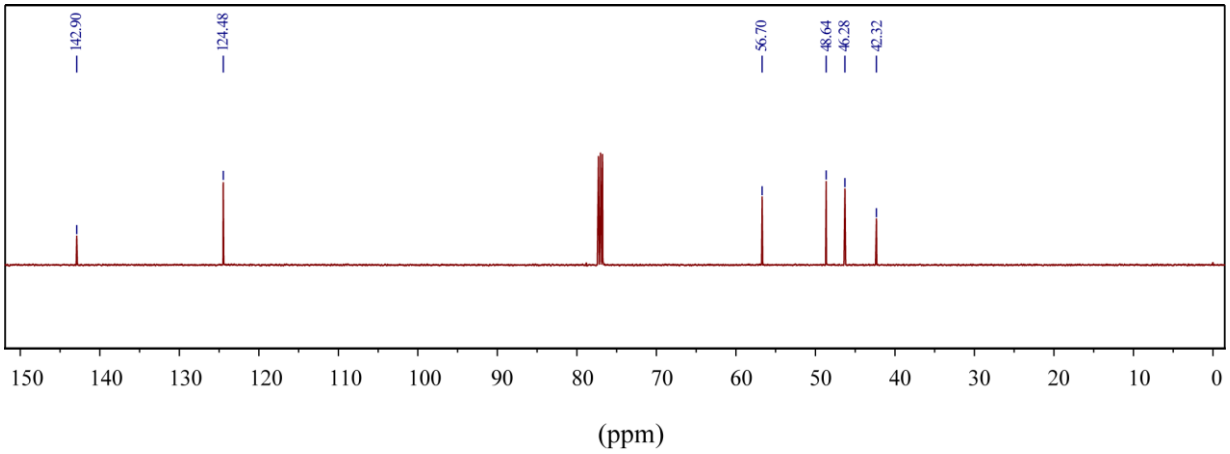

Figure S2. ^{13}C NMR of **L** in $CDCl_3$.

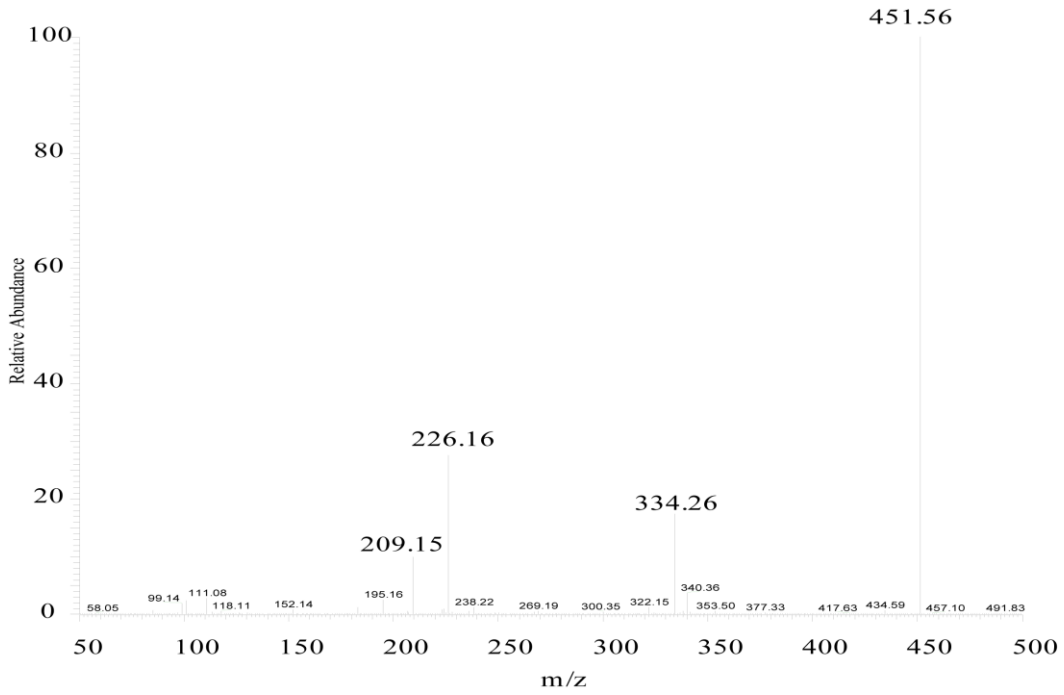

Figure S3. ESI-MS (+) spectra of **L**.

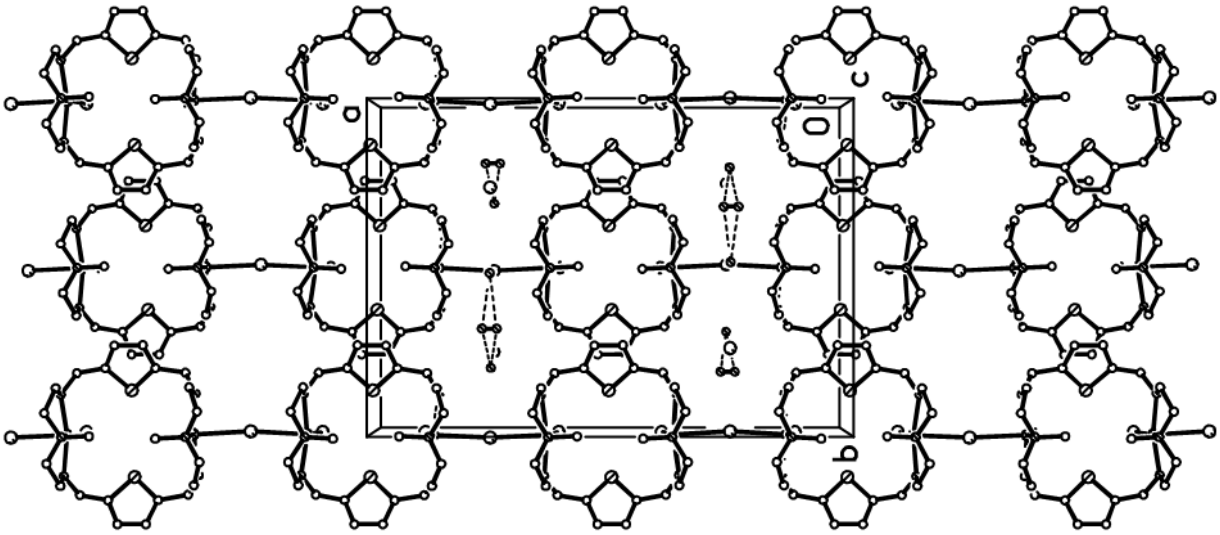

Figure S4. Packing diagram of **1'** showing an infinite polymer along the *a*-axis.

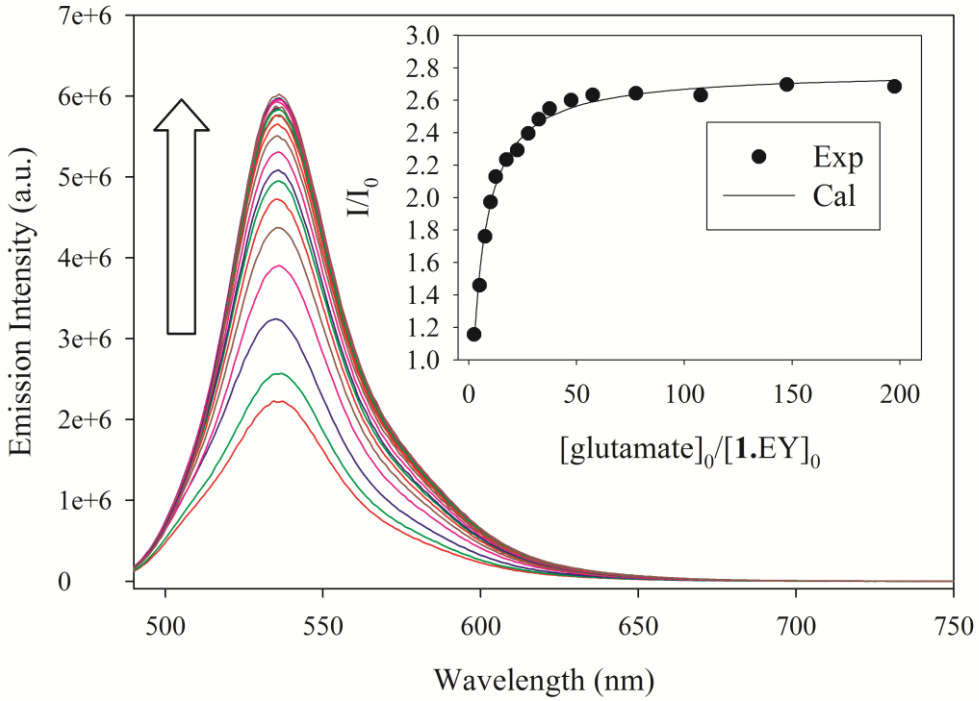

Figure S5. The enhancement of fluorescence intensity of [**1**·EY] (**1**/EY = 5:1) upon the addition of glutamate ([**1**·EY]$_0$ = 2 x 10^{-6} M, [glutamate]$_0$ = 2 x 10^{-3} M) in water buffered with 20 mM HEPES at pH 7.0. λ_{ex} = 470 nm, λ_{em} = 536 nm. The inset shows the titration plot of I/I_o against [glutamate]$_0$/[**1**·EY]$_0$ at λ_{em} = 536 nm.

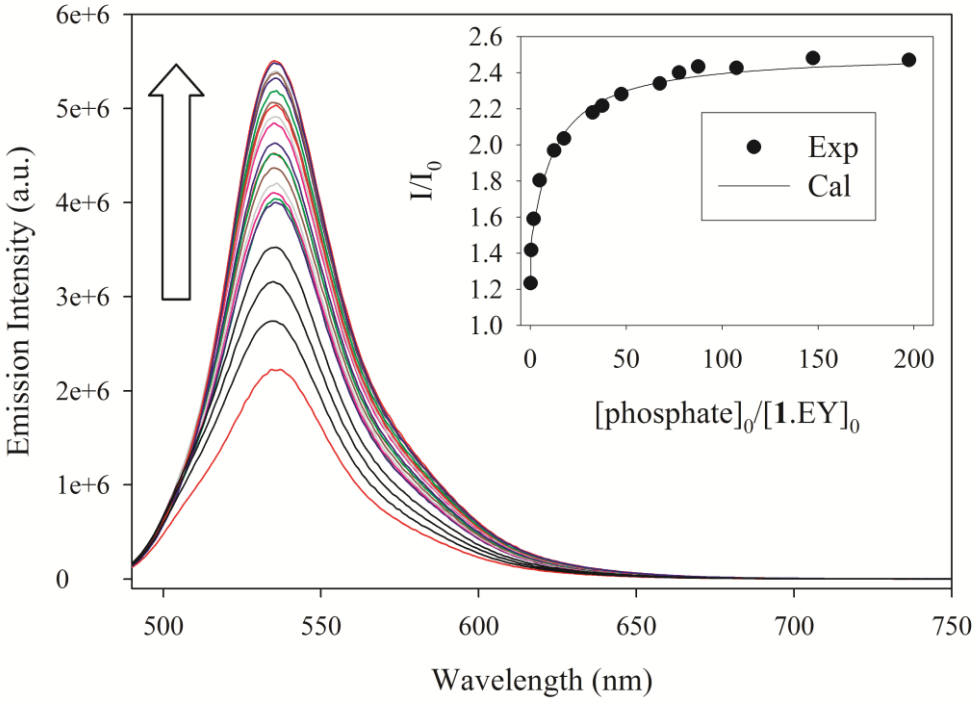

Figure S6. The enhancement of fluorescence intensity of [**1**·EY] (**1**/EY = 5:1) upon the addition of K_2HPO_4 ($[\mathbf{1}\cdot EY]_0$ = 2 x 10^{-6} M, $[K_2HPO_4]_0$ = 2 x 10^{-3} M) in water buffered with 20 mM HEPES at pH 7.0. λ_{ex} = 470 nm, λ_{em} = 536 nm. The inset shows the titration plot of I/I_o against $[K_2HPO_4]_0/[\mathbf{1}\cdot EY]_0$ at λ_{em} = 536 nm.

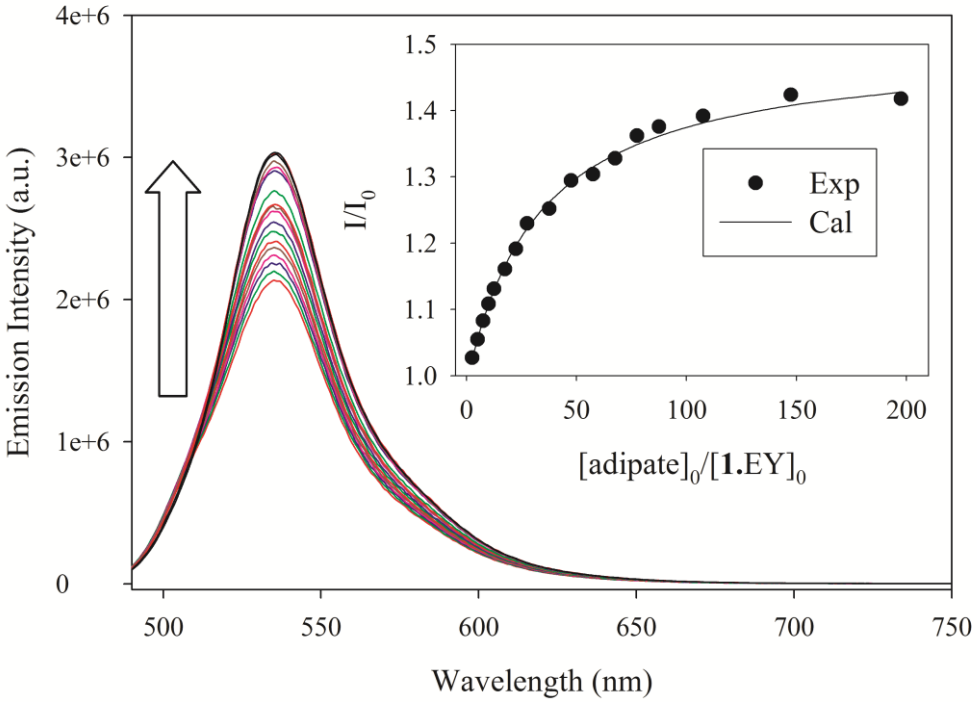

Figure S7. The enhancement of fluorescence intensity of [**1**·EY] (**1**/EY = 5:1) upon the addition of adipate ($[\mathbf{1}\cdot EY]_0$ = 2 x 10^{-6} M, $[adipate]_0$ = 2 x 10^{-3} M) in water buffered with 20 mM HEPES at pH 7.0. λ_{ex} = 470 nm, λ_{em} = 536 nm. The inset shows the titration plot of I/I_0 against $[adipate]_0/[\mathbf{1}\cdot EY]_0$ at λ_{em} = 536 nm.

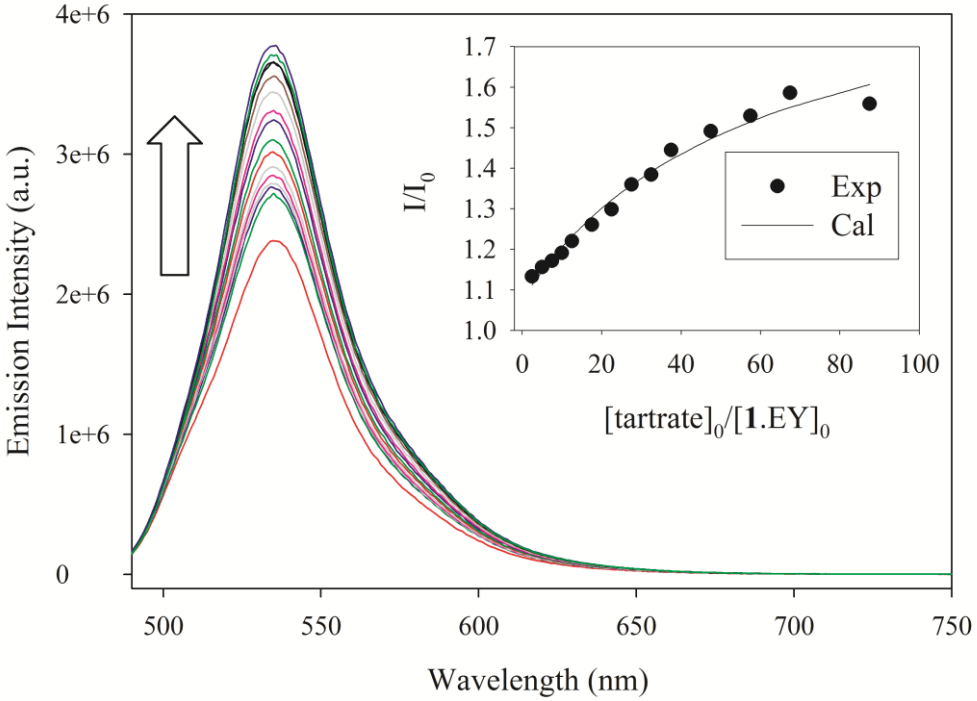

Figure S8. The enhancement of fluorescence intensity of [**1**·EY] (**1**/EY = 5:1) upon the addition of tartrate ($[\mathbf{1}\cdot EY]_0$ = 2 x 10^{-6} M, $[tartrate]_0$ = 2 x 10^{-3} M) in water buffered with 20 mM HEPES at pH 7.0. λ_{ex} = 470 nm, λ_{em} = 536 nm. The inset shows the titration plot of I/I_0 against $[tartrate]_0/[\mathbf{1}\cdot EY]_0$ at λ_{em} = 536 nm.

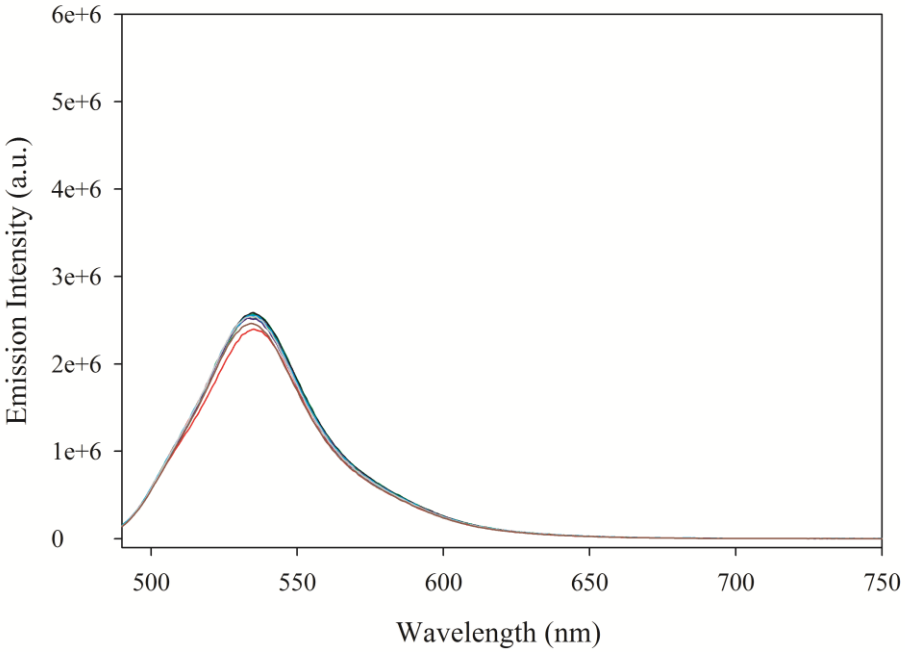

Figure S9. The fluorescence intensity of [**1**·EY] (**1**/EY = 5:1) upon the addition of benzoate ($[\mathbf{1}\cdot EY]_0$ = 2 x 10^{-6} M, $[benzoate]_0$ = 2 x 10^{-3} M) in water buffered with 20 mM HEPES at pH 7.0. λ_{ex} = 470 nm, λ_{em} = 536 nm, showing insignificant change in fluorescence intensity.

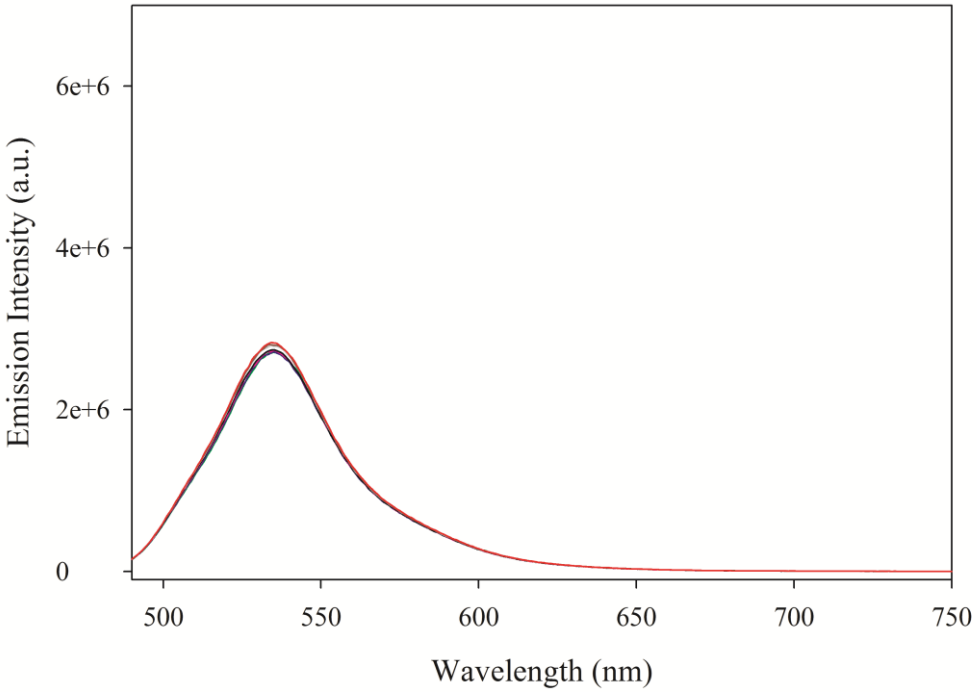

Figure S10. The fluorescence intensity of [**1**·EY] (**1**/EY = 5:1) upon the addition of acetate ([**1**·EY]$_0$ = 2 x 10^{-6} M, [acetate]$_0$ = 2 x 10^{-3} M) in water buffered with 20 mM HEPES at pH 7.0. λ_{ex} = 470 nm, λ_{em} = 536 nm, showing insignificant change in fluorescence intensity.

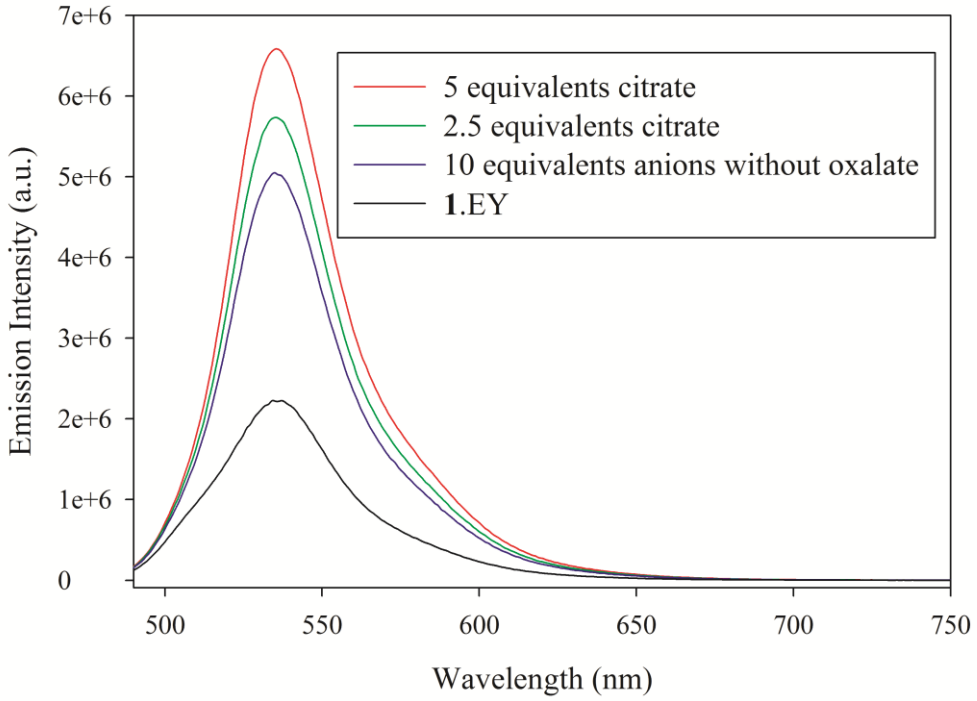

Figure S11. The selectivity of citrate in presence of 10 equivalents of other anions without oxalate, λ_{ex} = 470 nm, λ_{em} = 536 nm, d_{ex} = 2, d_{em} = 3.

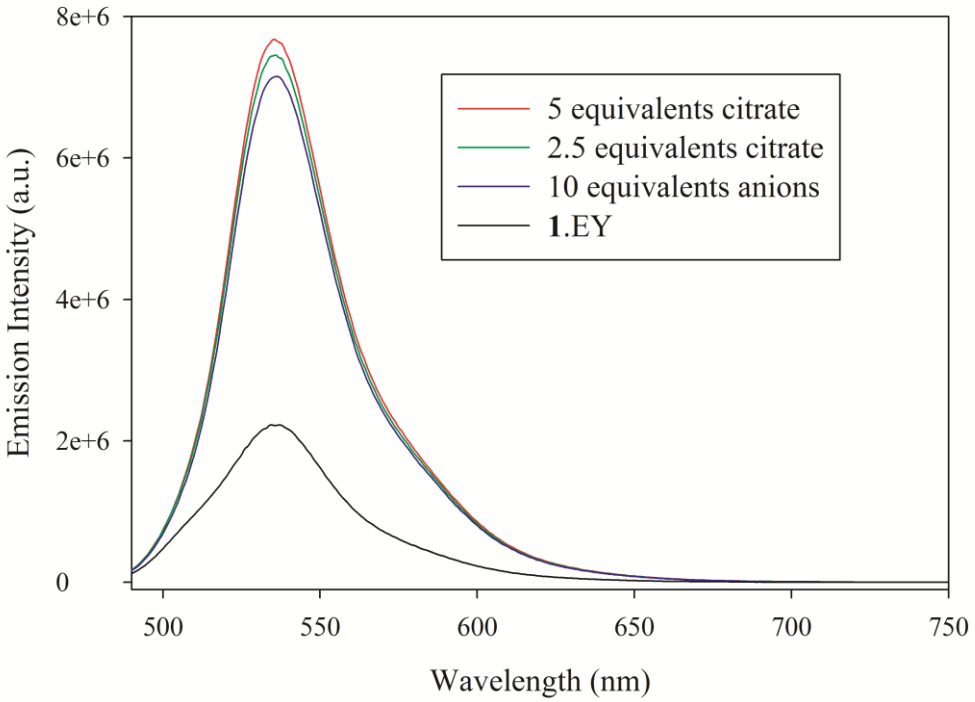

Figure S12. The selectivity of citrate in presence of 10 equivalents of other anions, λ_{ex} = 470 nm, λ_{em} = 536 nm, d_{ex} = 2, d_{em} = 3.

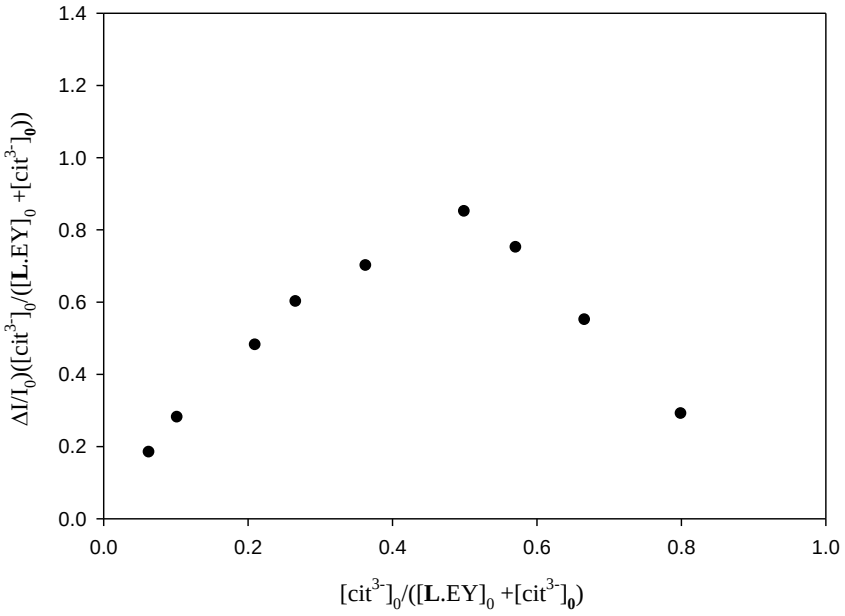

Figure S13. Job's plot for the formation of the citrate complex with **1**.EY. The data was obtained from the titration of **1**.EY with citrate as shown in Figure 4 in the main manuscript.