

Electronic Supplementary Information (ESI)

Dimethoxy triarylamine-derived terpyridine-zinc complex: a fluorescence light-up sensor for citrate detection based on the aggregation-induced emission

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S1. Fig. S1

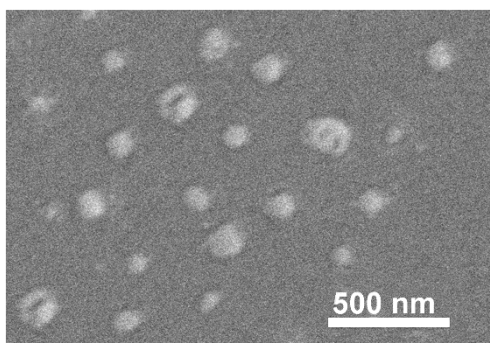


Fig. S1 Scanning electronic microscope (SEM) image of **DTPA-TPY** in the THF/H₂O mixture (f_w = 90 vol%, containing 1 vol% DMSO).

S2. Fig. S2

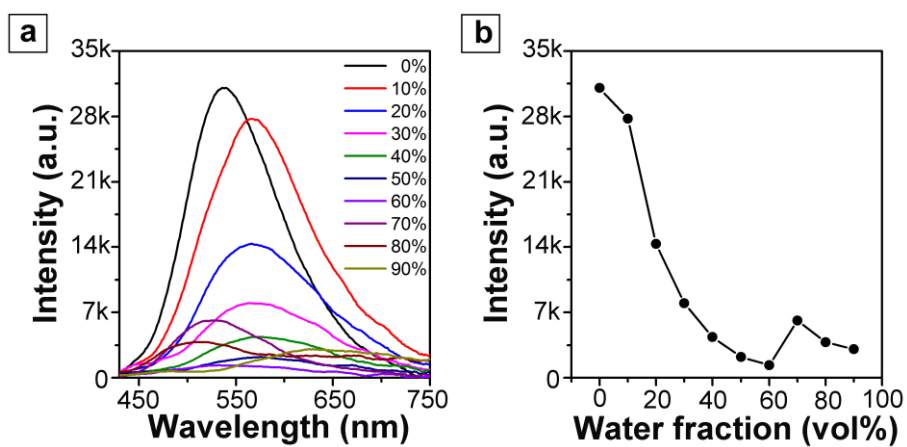


Fig. S2 (a) Emission spectra of **DTPA-TPY-Zn** in the THF/H₂O mixtures with different water fractions (containing 1 vol% DMSO). (b) Plot of maximum emission intensity of **DTPA-TPY-Zn** versus water fraction in the aqueous mixture. Dye concentration: 100 μ M. Excitation wavelength: 410 nm.

S3. Fig. S3

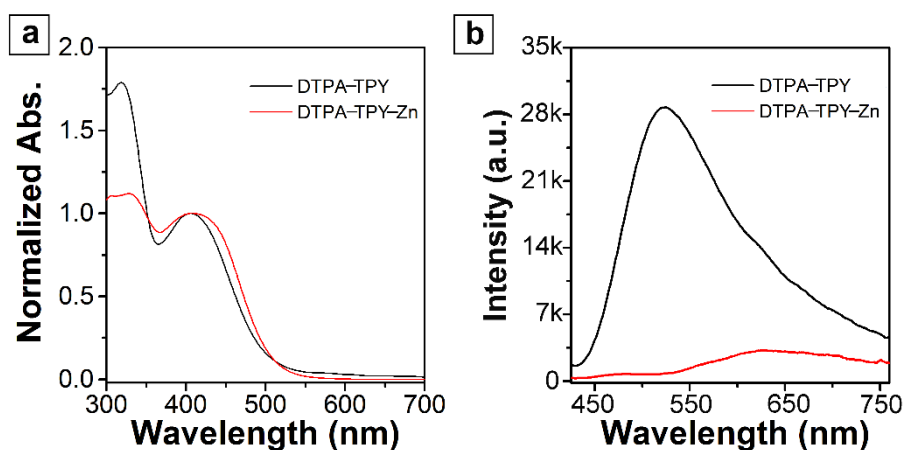


Fig. S3 (a) Normalized absorption spectra of **DTPA-TPY** and **DTPA-TPY-Zn** in the THF/H₂O mixtures ($f_w = 65$ vol%, containing 1 vol% DMSO). (b) Fluorescence spectra of **DTPA-TPY** and **DTPA-TPY-Zn** in the THF/H₂O mixtures ($f_w = 90$ vol%, containing 1 vol% DMSO). Dye concentration: 100 μ M. Excitation wavelength: 410 nm.

S4. Fig. S4

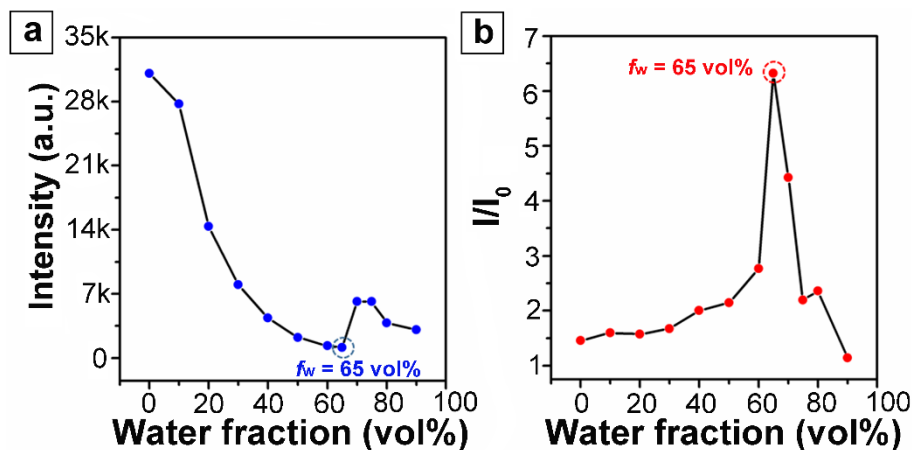


Fig. S4 (a) Fluorescence spectra of **DTPA-TPY-Zn** (100 μ M) at the different THF/H₂O mixtures (containing 1 vol% DMSO) in the absence of citrate. (b) Fluorescence spectra of **DTPA-TPY-Zn** (100 μ M) at the different THF/H₂O mixtures (containing 1 vol% DMSO) in the presence of citrate (100 μ M). I/I_0 represents the ratio between the fluorescence intensity of detection system with (I) and without (I_0) citrate.

S5. Fig. S5

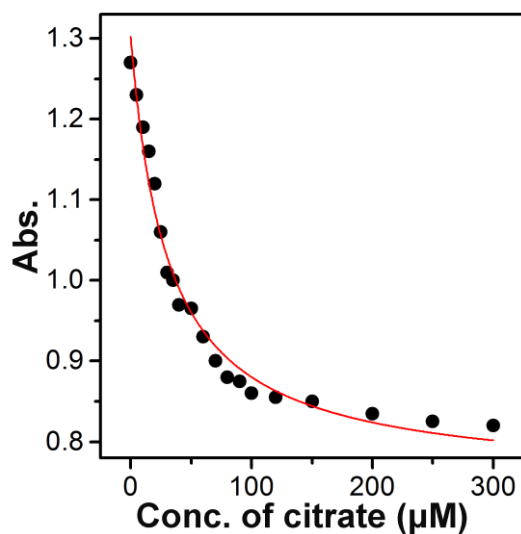


Fig. S5 Binding constant curve for **DTPA-TPY-Zn** (100 µM) with citrate in the THF/H₂O mixtures ($f_w = 65$ vol%, containing 1 vol% DMSO). [Working formula: $y = (A_0 + A \cdot K \cdot x) / (1 + K \cdot x)$. $x =$ [analyte], $y =$ absorbance. $\lambda_{\text{abs}} = 418$ nm.

S6. Fig. S6

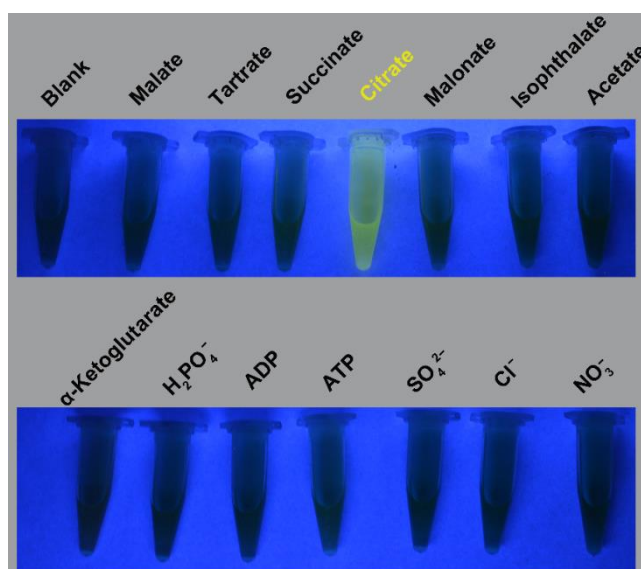


Fig. S6 Photographs of **DTPA-TPY-Zn** in the absence and presence of citrate (100 µM) in the THF/H₂O mixtures solution ($f_w = 65$ vol%, containing 1 vol% DMSO, pH = 7) under 365 nm UV irradiation.

S7. Fig. S7

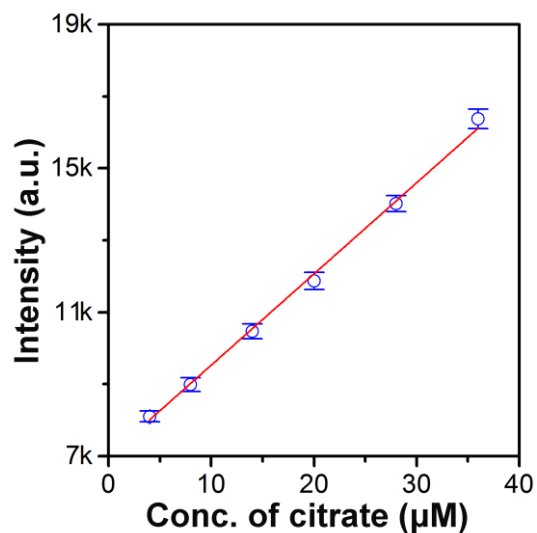
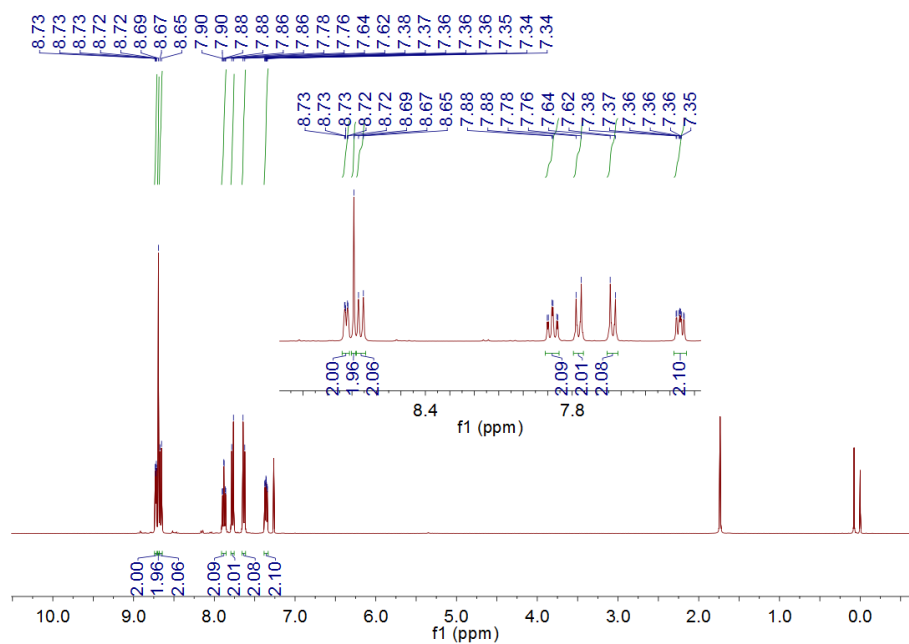


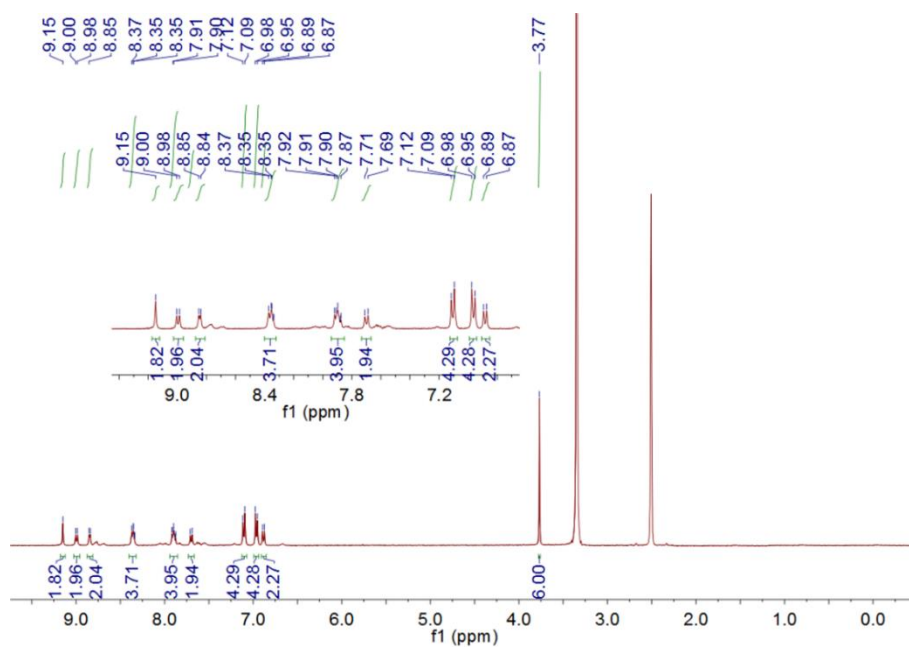
Fig. S7 Plotting the fluorescence intensity (value of the emission maxima at 525 nm) as a function of low citrate concentration (4–36 μM) for **DTPA-TPY-Zn** (100 μM) in the THF/H₂O mixtures (f_w = 65 vol%, containing 1 vol% DMSO).

S8. Characterization Data

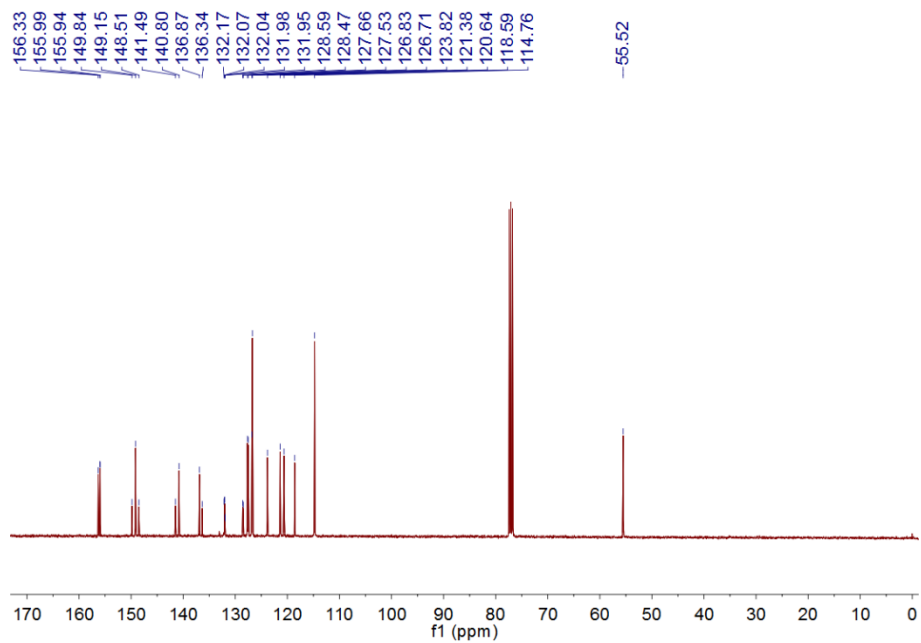
¹H NMR of compound 3



¹H NMR of compound DTPA-TPY



¹³C NMR of compound DTPA-TPY



High-Res ESI-TOF mass spectrum of DTPA-TPY

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-41 H: 0-33 N: 0-4 O: 0-2

JL-HUA

ECUST institute of Fine Chem

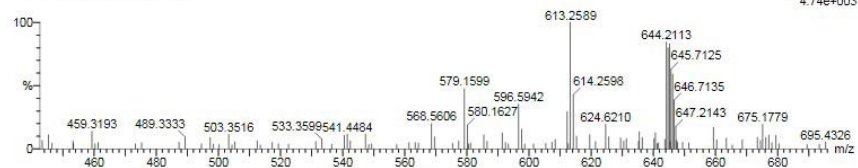
30-Dec-2015

20:51:46

1: TOF MS ES+

4.74e+003

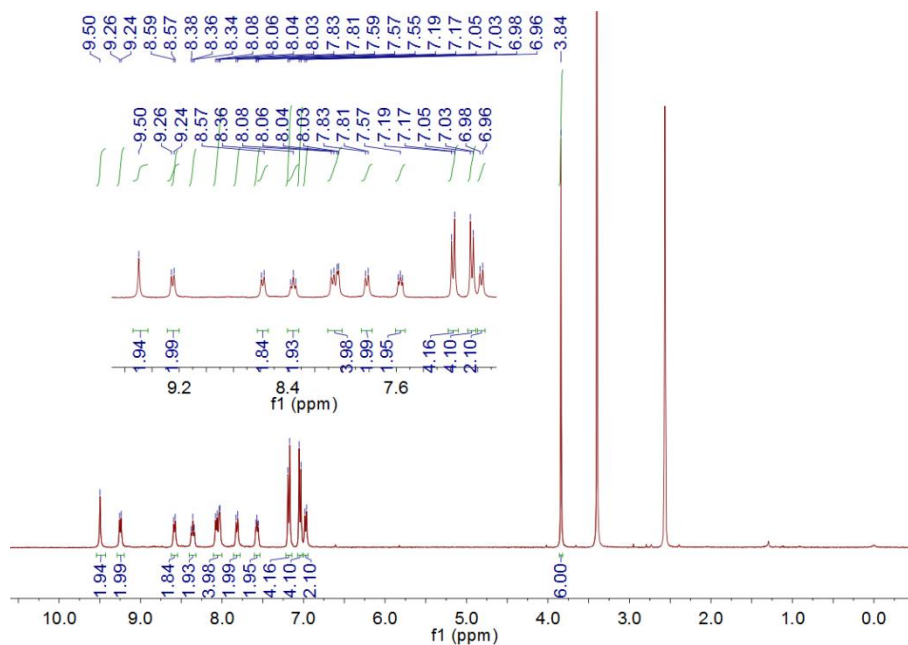
HL-JT-12.65 (0.497) Cm (63:67)



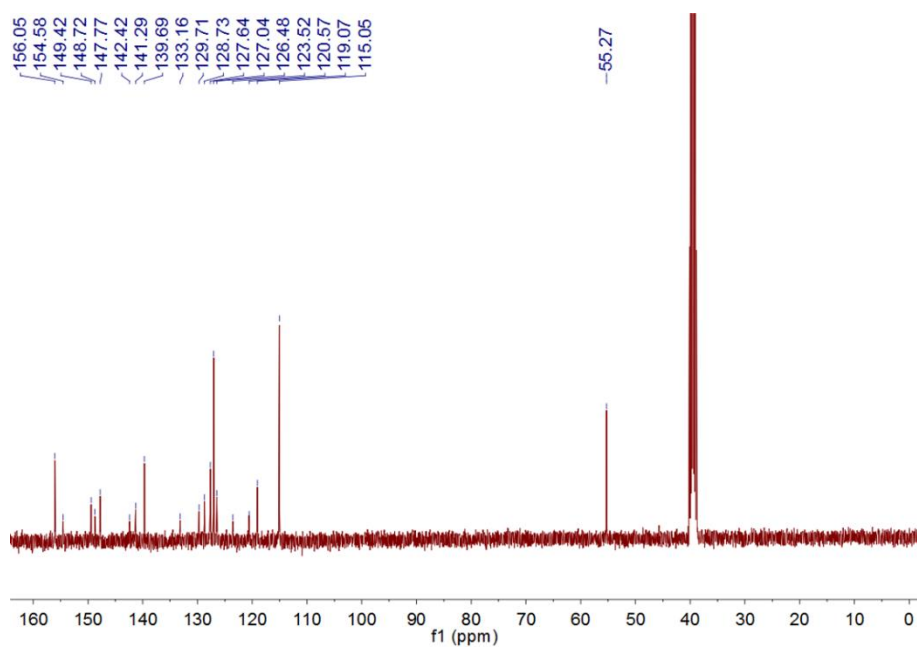
Minimum: 300.0 50.0 -1.5
Maximum: 613.2589 100.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
613.2589	613.2598	-2.5	-4.1	27.5	11.2	0.0	C41 H33 N4 O2

¹H NMR of compound DTPA-TPY-Zn



^{13}C NMR of compound DTPA-TPY-Zn



MALDI-TOF mass spectrum of DTPA-TPY-Zn

