Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Data

Near-Infrared cyanine-based sensor for Fe^{3+} with high sensitivity: its intracellular imaging application in colorectal cancer cells

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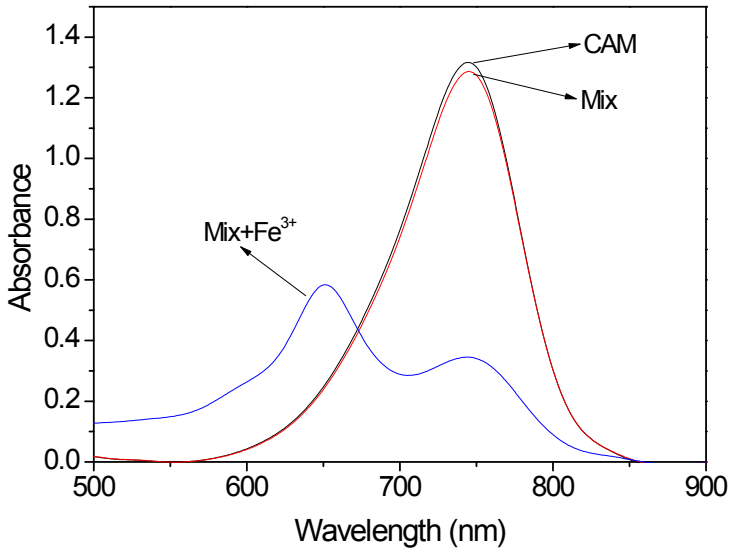
Contents

1. **Selectivity of CAM**

(A)



(B)

Figure S1. (Top) **(A)** Color change of CAM in the presence of different metal cations in a mixed solution. From left to right: Na^{+}, Fe^{2+}, Hg^{2+}, K^{+}, Ca^{2+}, Cr^{3+}, Zn^{2+}, blank, Fe^{3+}, Cu^{2+}, Ni^{2+}, Mg^{2+}, Co^{2+}, Pb^{2+}, Mn^{2+}, Cd^{2+}, Sn^{2+}, Ag^{+} (each 10 equiv except 5 equiv for Fe^{3+}); (Bottom) **(B)** Absorbance spectra change of CAM (10 μM) upon addition of mixed cations (each 1 equiv) and subsequent addition of 5 equiv of Fe^{3+}. Note: Mix= Na^{+} + Fe^{2+} + Hg^{2+}+ K^{+} + Ca^{2+} + Cr^{3+} + Zn^{2+} + Cu^{2+} + Ni^{2+} + Mg^{2+} + Co^{2+} + Pb^{2+} + Mn^{2+} + Cd^{2+} + Sn^{2+} + Ag^{+} .

2. **Benesi-hildebrand plot**

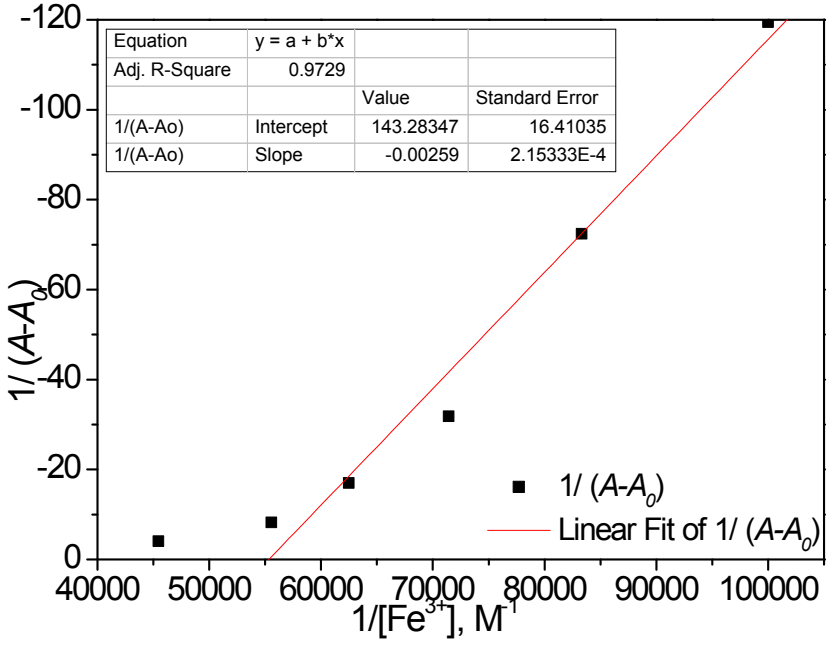


Figure S2. Benesi-Hildebrand plot of CAM (10 μM) with Fe^{3+}.

3. ESI-Mass spectrum of CAM with Fe3+

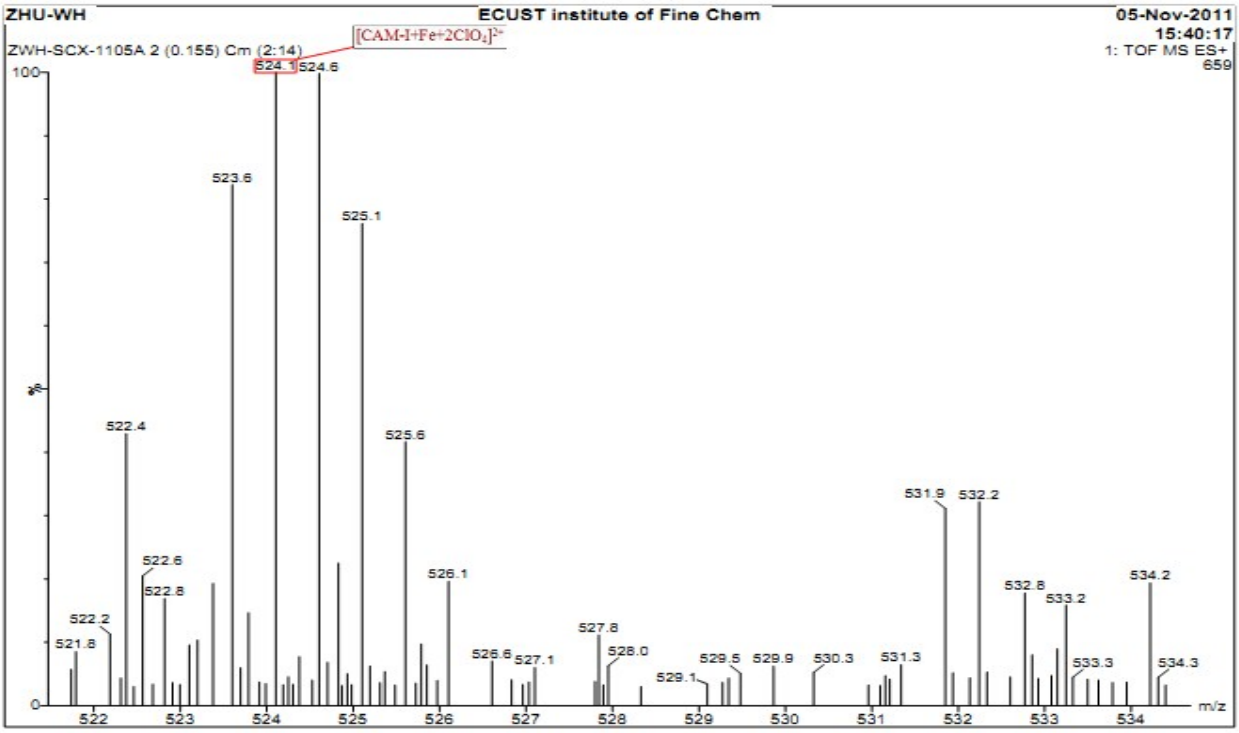


Figure S3. ESI-Mass spectrum of CAM with Fe^{3+}.

4. Detection limit of CAM

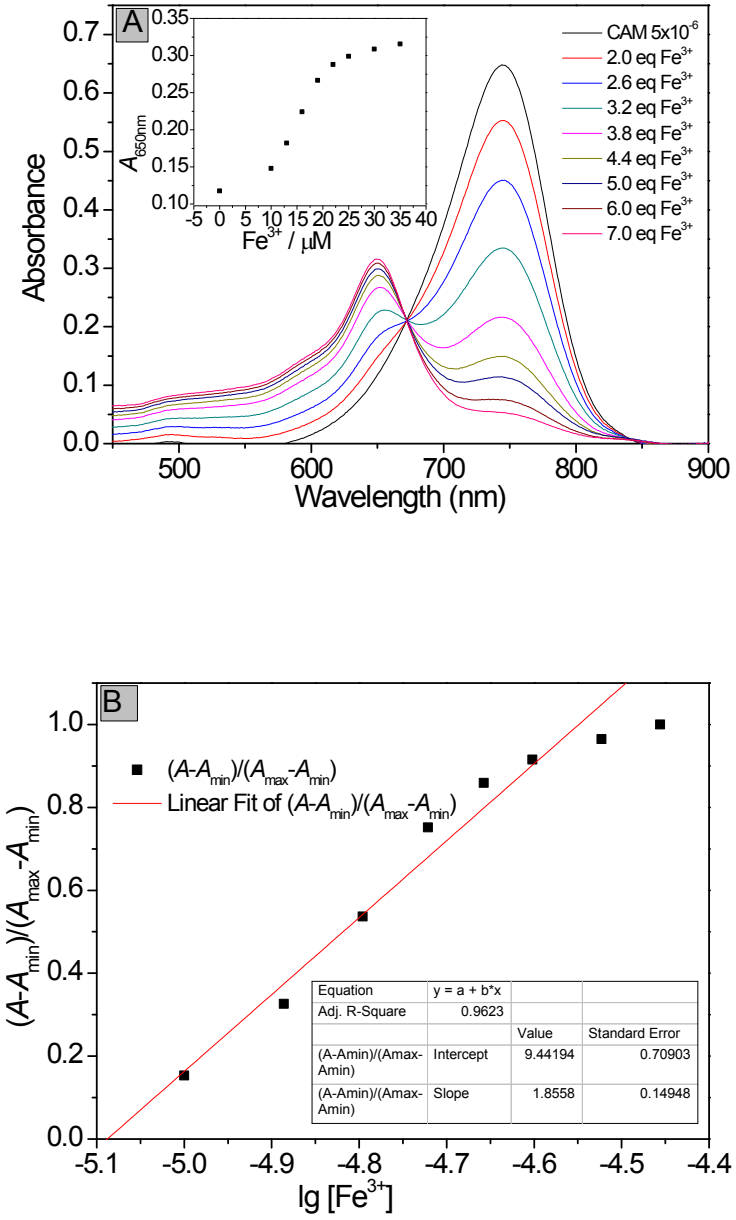


Figure S4. (A) Absorbance changes during the titration of CAM (5 μM) with Fe^{3+} (0-35 μM) in methanol. Inset: The absorbance intensity of CAM at 650 nm versus Fe^{3+} concentration. (B) A plot of $(A-A_{min})/(A_{max}-A_{min})$ at 650 nm versus lg $[Fe^{3+}]$, the calculated detection limit of sensor CAM is 8.2 μM [3].

5. Selectivity of CAT

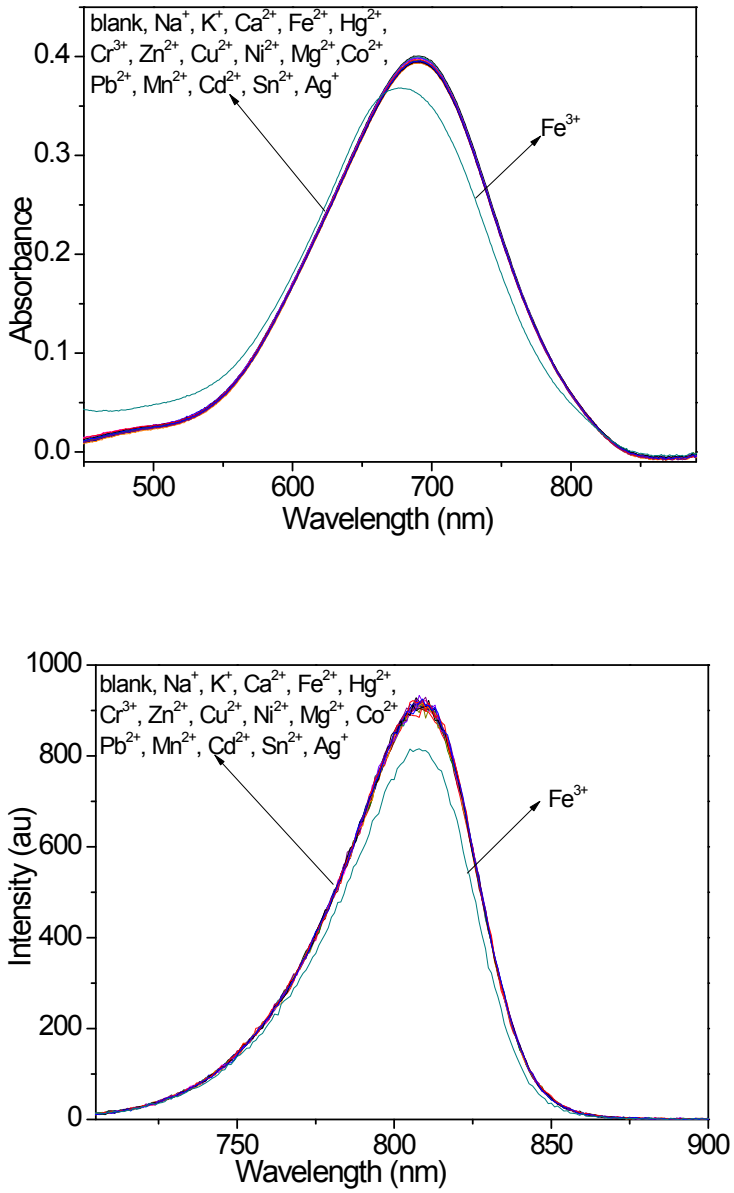


Figure S5. Absorbance and emission spectra change of CAT (10 μM) upon addition of different metal cations (each 10 equiv).

6. Absorbance and emission spectra of CAM with addition of EDTA

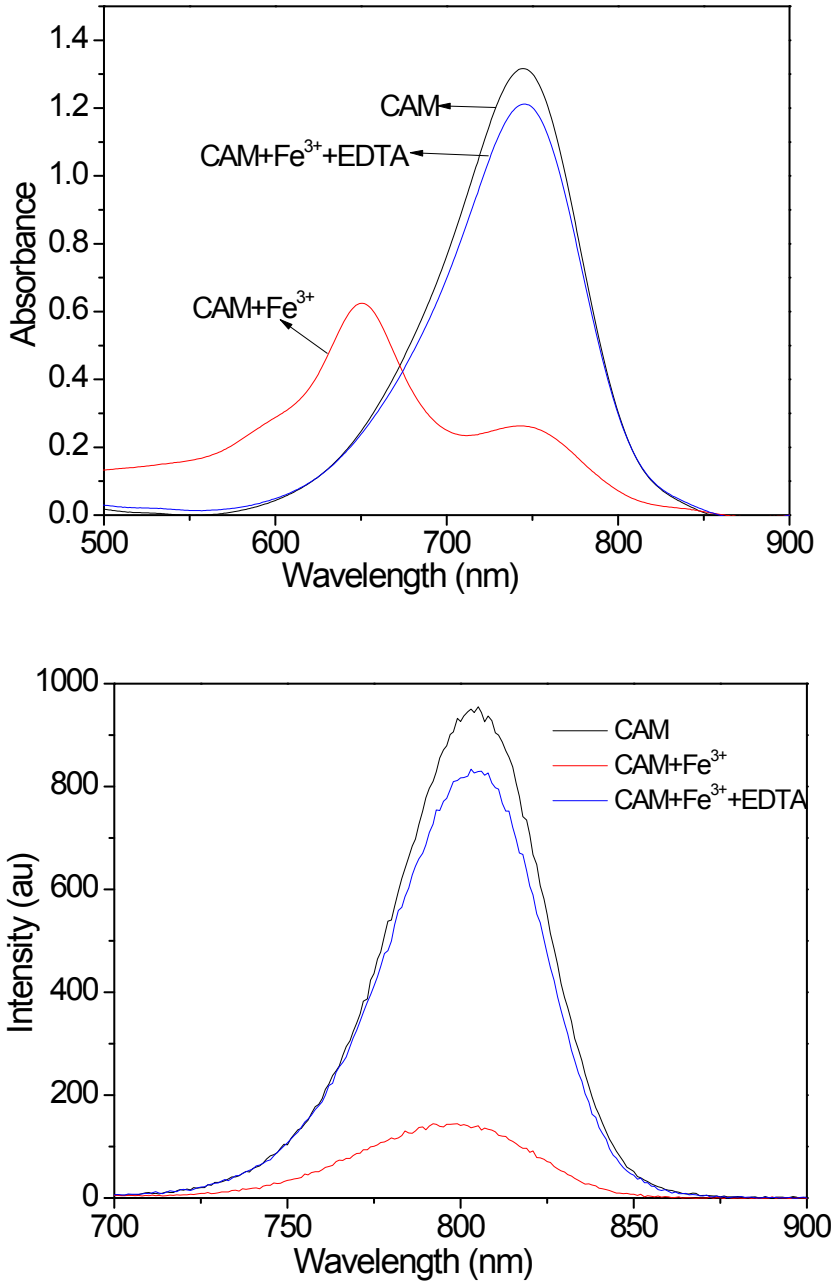


Figure S6. Absorbance and emission spectra of CAM (10 μM) upon addition of Fe^{3+} ions (5 equiv) and subsequent addition of EDTA (5 equiv).

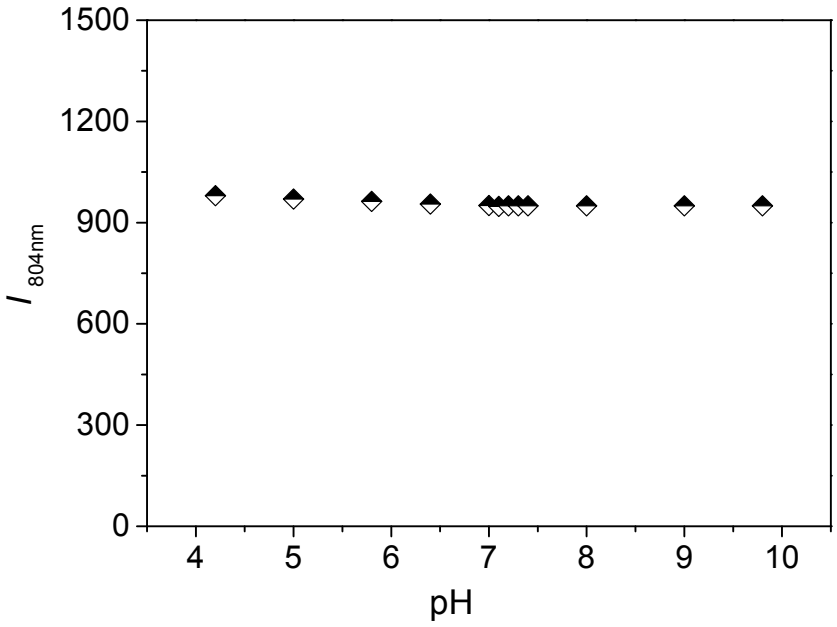
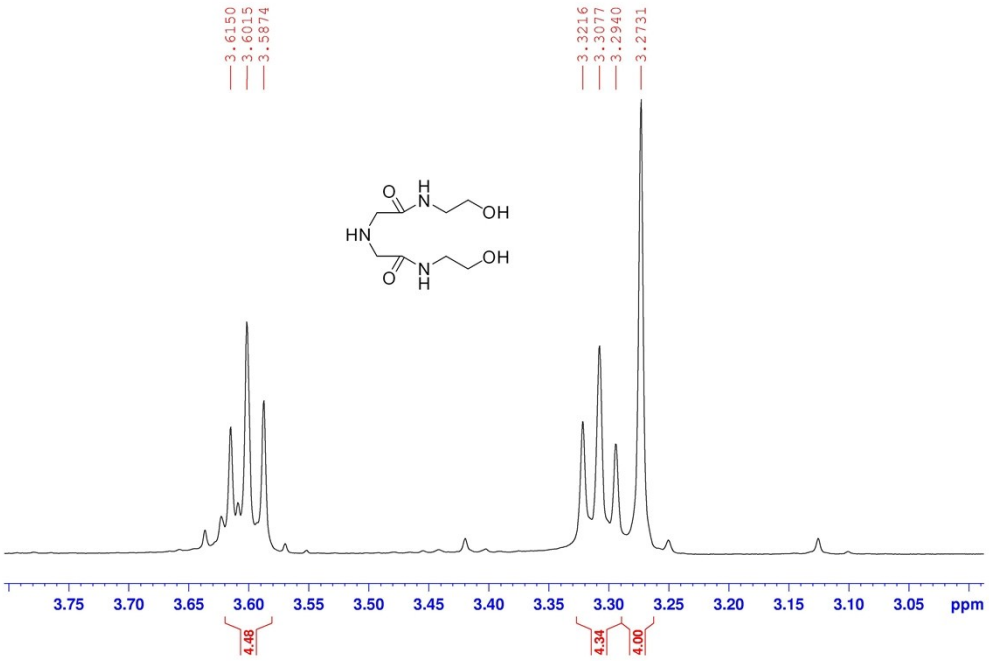
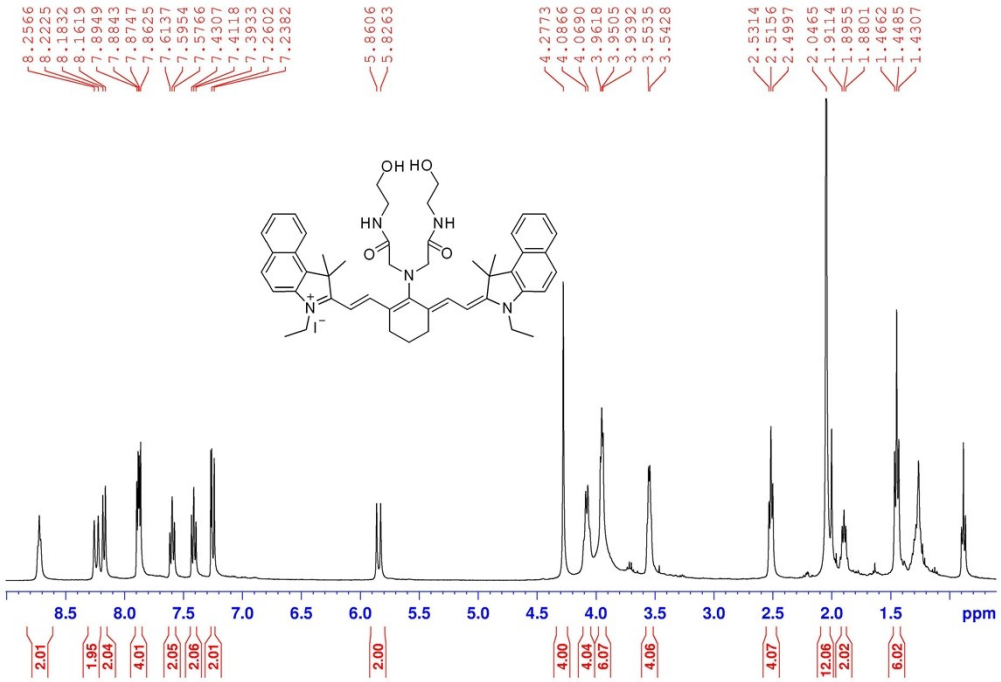


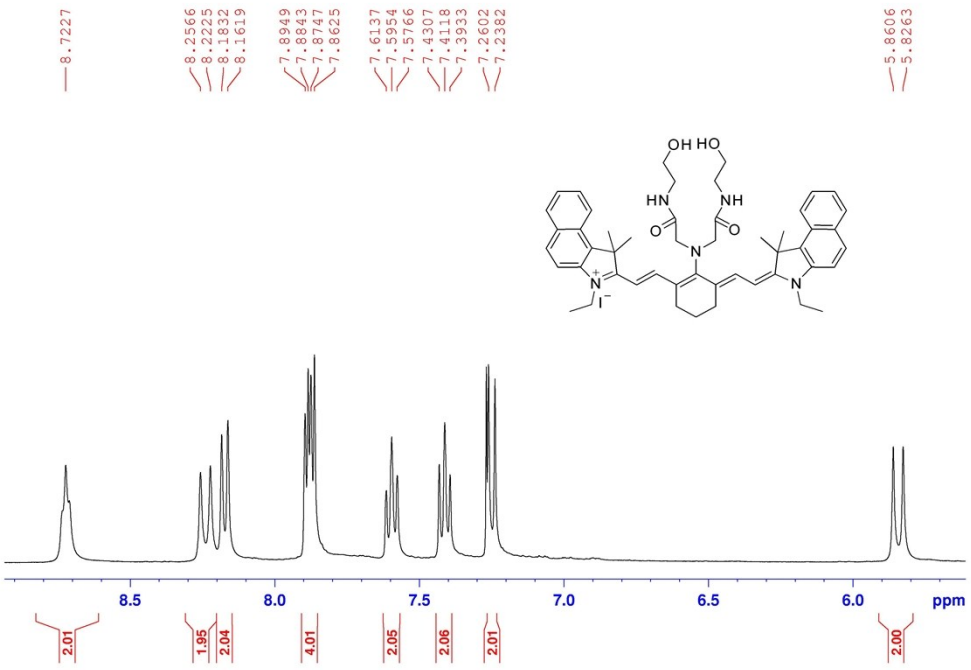
Figure S7. pH-dependent fluorescence intensity at 804 nm of CAM (10 μM, and excited at 671 nm).

7. Characterization data of all compounds

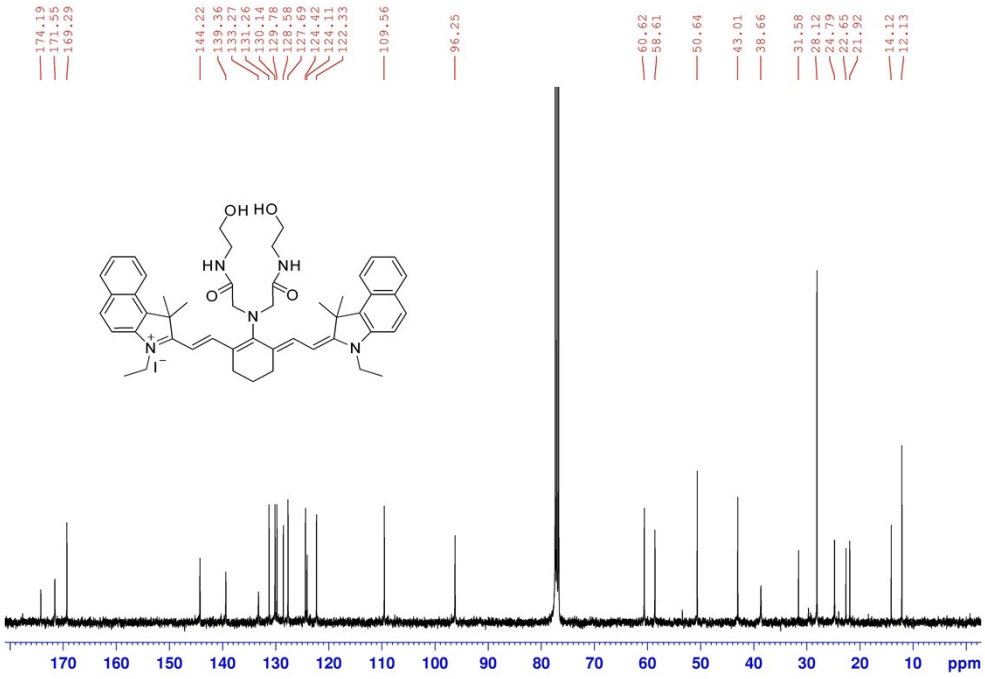


^{1}H NMR spectra of compound 2 in D_2O





Overall and part of ^{1}H NMR spectra of compound CAM in $CDCl_3$



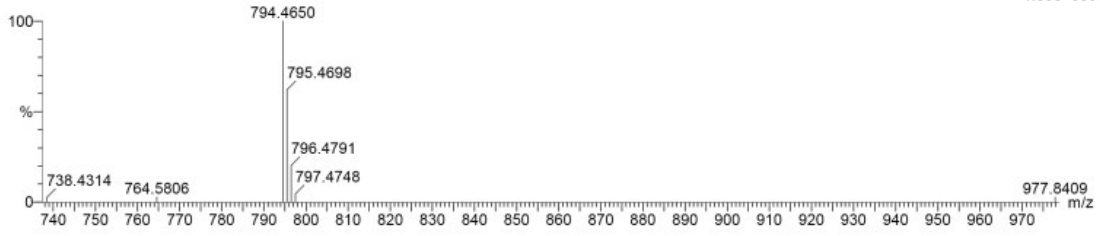
^{13}C NMR spectra of compound CAM in $CDCl_3$

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

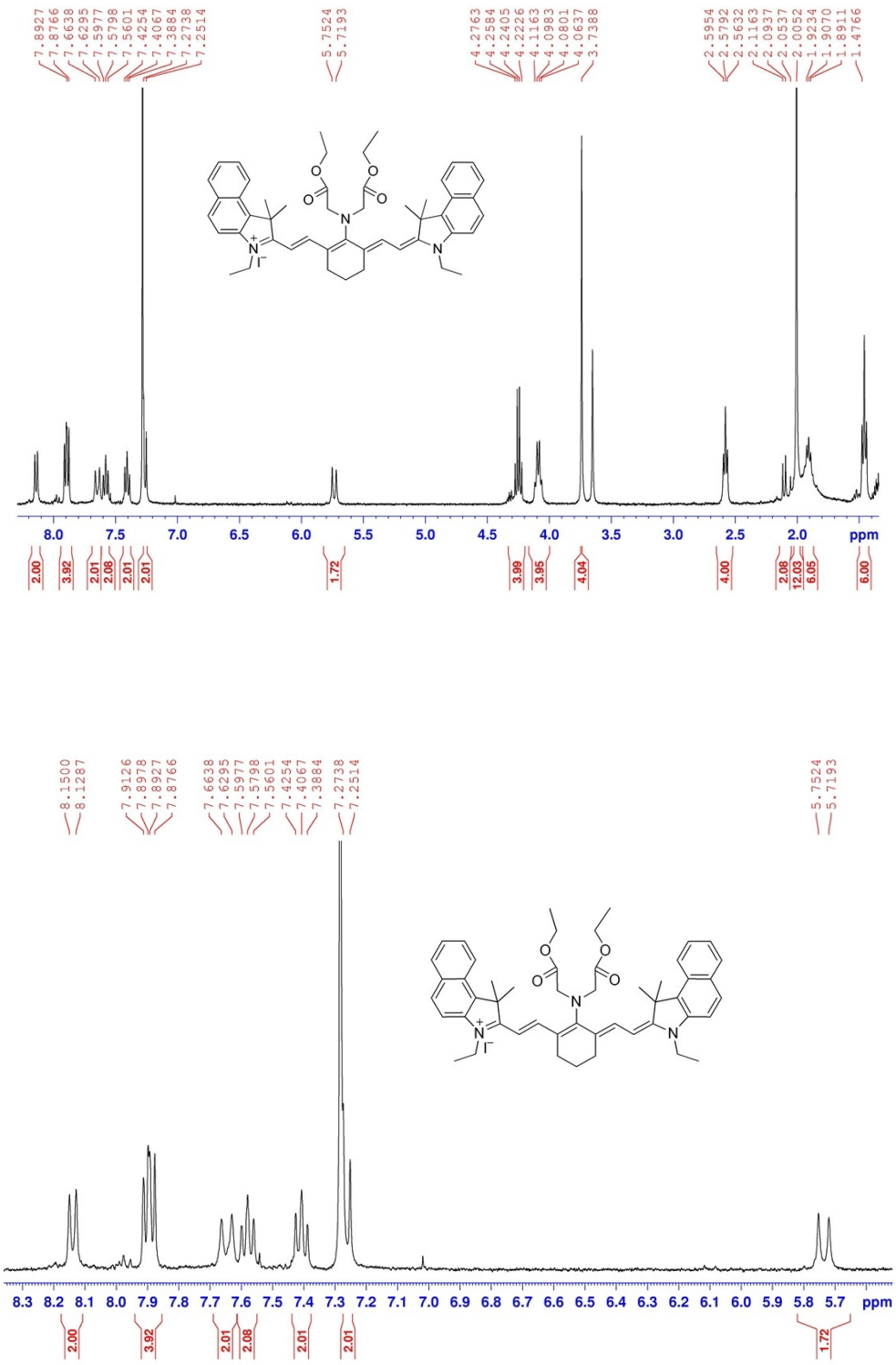
Monoisotopic Mass, Even Electron Ions
63 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-55 H: 0-65 N: 0-5 O: 0-5
ZHU-WH
ZWH-SCX-005-3 3 (0.176) Cm (3)

1: TOF MS ES+
1.53e+003

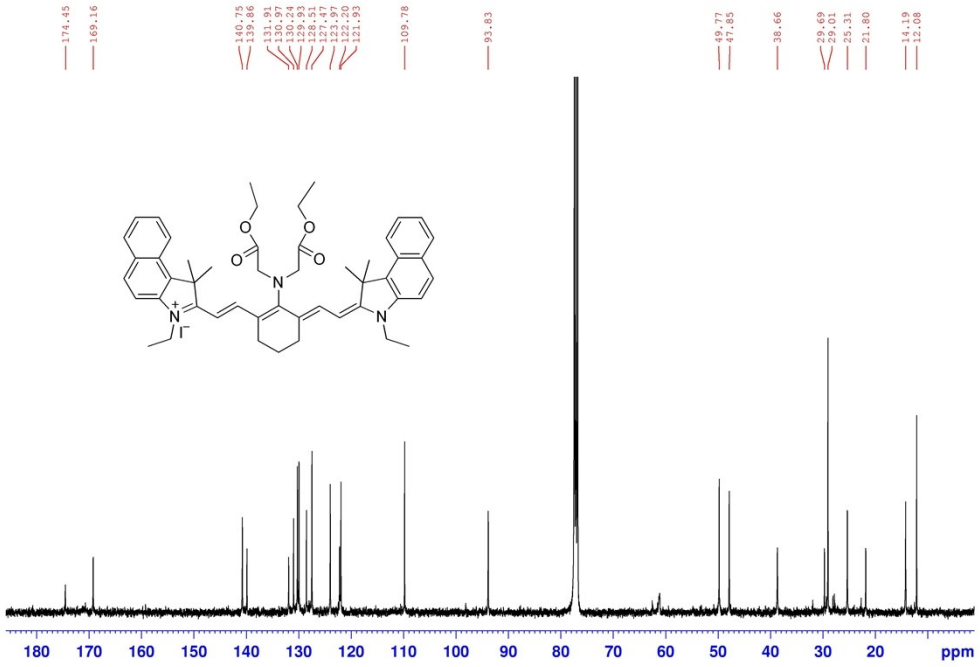


Minimum:				-1.5			
Maximum:		3.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
794.4650	794.4645	0.5	0.6	23.5	9.2	0.0	C50 H60 N5 O4

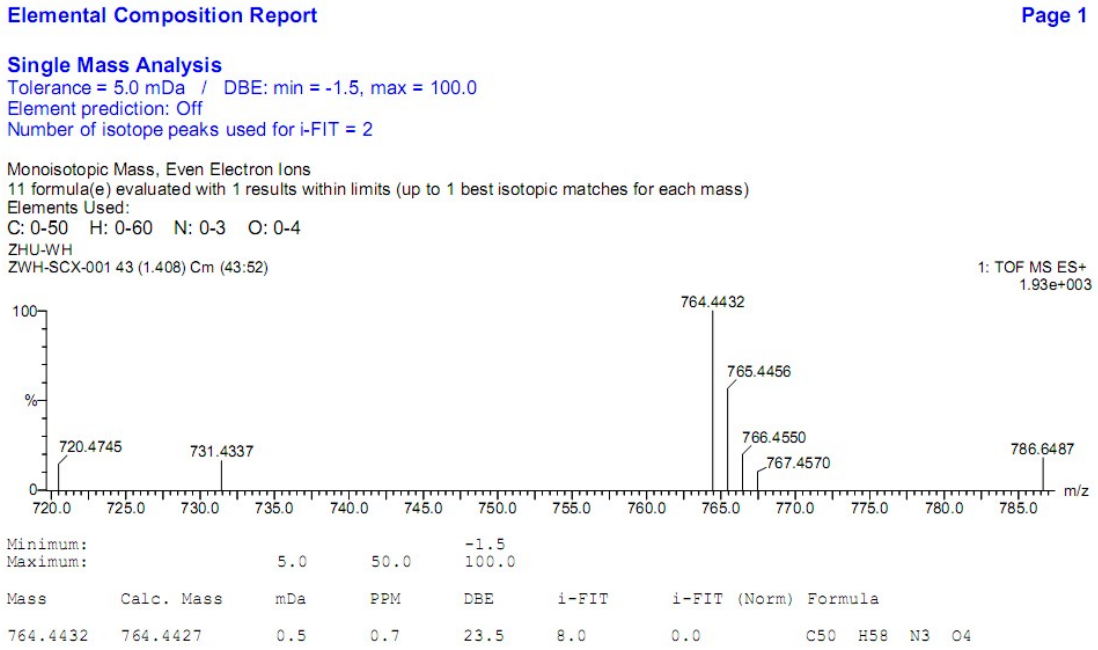
HR EI mass spectra of CAM



Overall and part of ^{1}H NMR spectra of compound CAT in $CDCl_3$



^{13}C NMR spectra of compound CAT in $CDCl_3$



HR EI mass spectra of CAT

References

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2. EI-Ashgar, N. M.; Abdel-latif, M. S. *Anal. Lett.* **2008**, *41*, 3074-3087.
3. Shortreed, M.; Kopelman, R.; Kuhn, M.; Hoyland, B. *Anal. Chem.* **1996**, 68, 1414-1418.