

**Methionine-based turn-on chemical sensor for monitoring Hg(II) ions in 100%
aqueous solution**

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Supplementary Information

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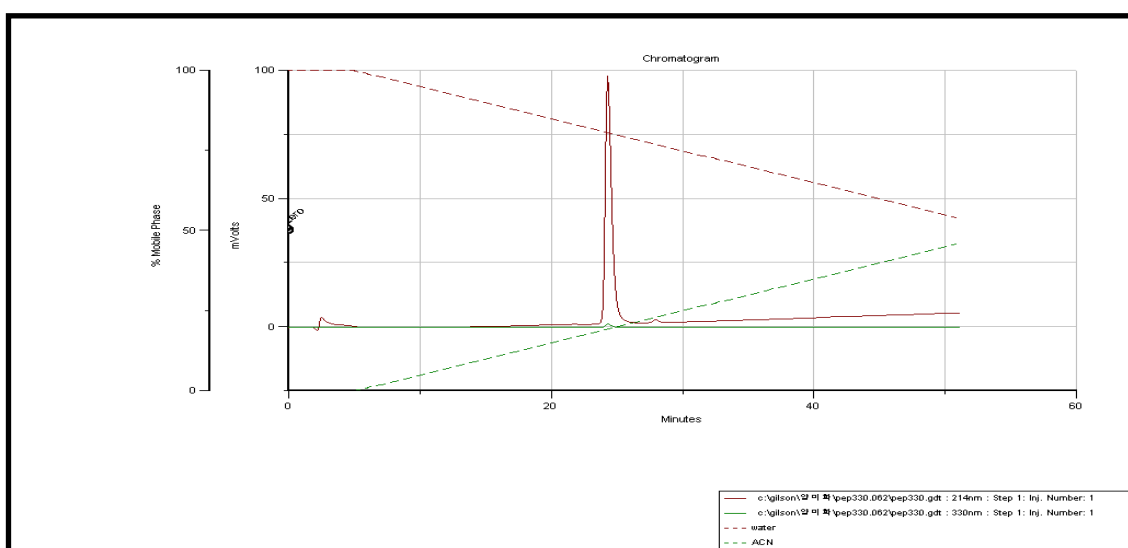


Figure S1. HPLC Chromatogram of **Dansyl-Met**

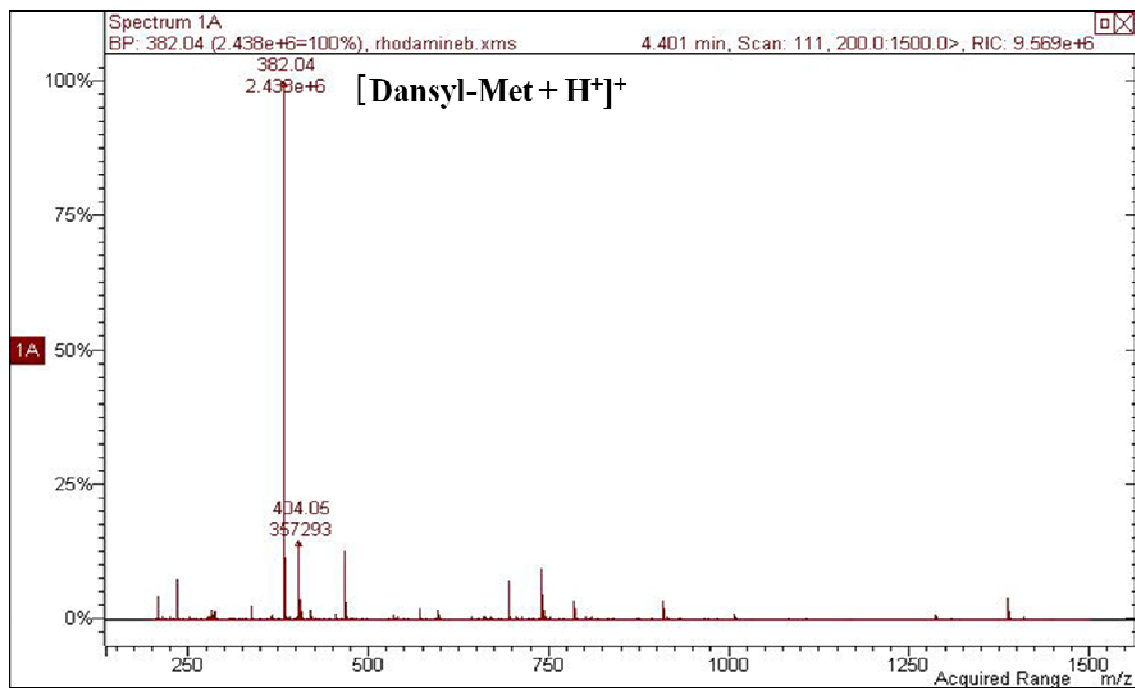


Figure S2. ESI-mass of **Dansyl-Met**

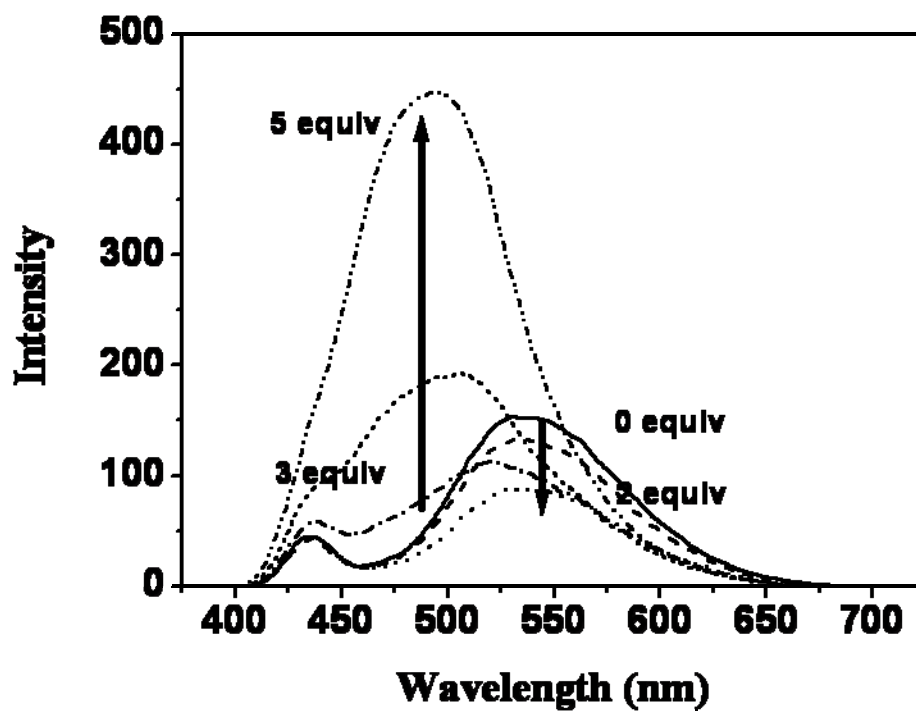


Figure S3. Emission spectra of **Dansyl-Met** (5 μM) in the presence of increasing concentration of Hg (II) (0, 1, 2, 3, 4, and 5 equiv) in 10 mM HEPES buffer solution at pH 7.4

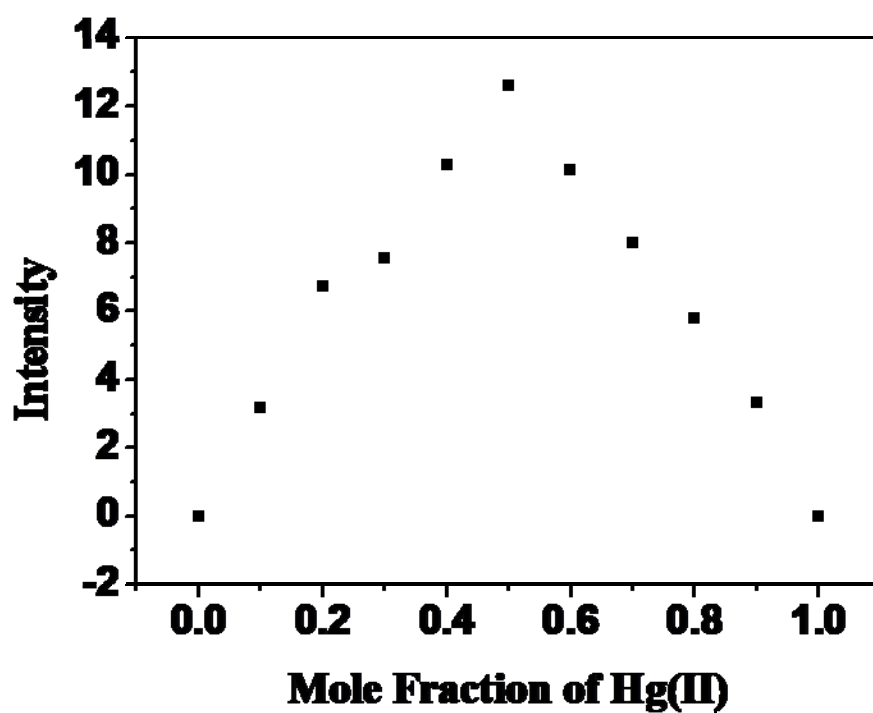


Figure S4. A Job plot for **Dansyl-Met**.

The concentration of **Dansyl-Met** and Hg(II) was 10 μ M in 10mM HEPES buffer (pH 7.4)

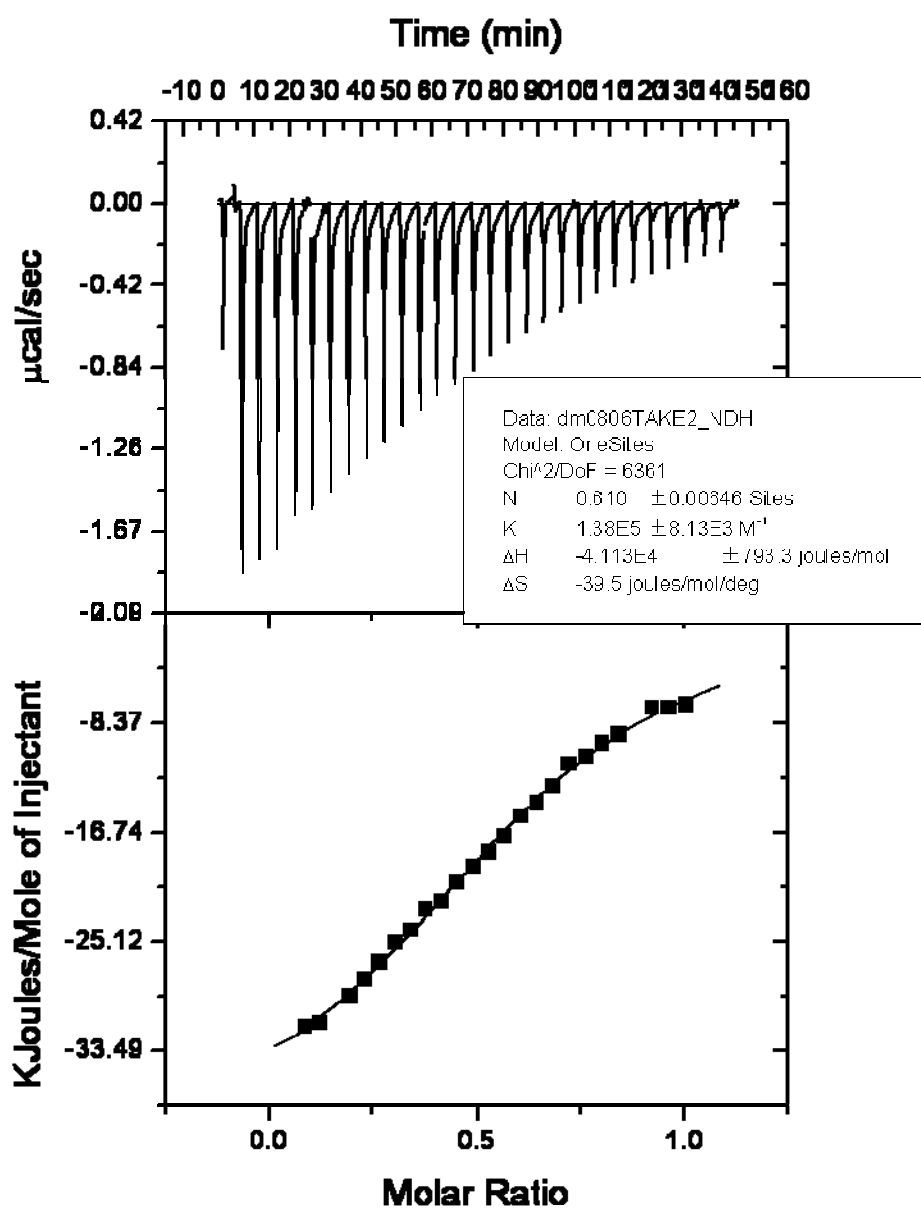


Figure S5. Isothermal calorimetry titration of **Dansyl-Met** (200 μM) in 10 mM HEPES buffer pH 7.4

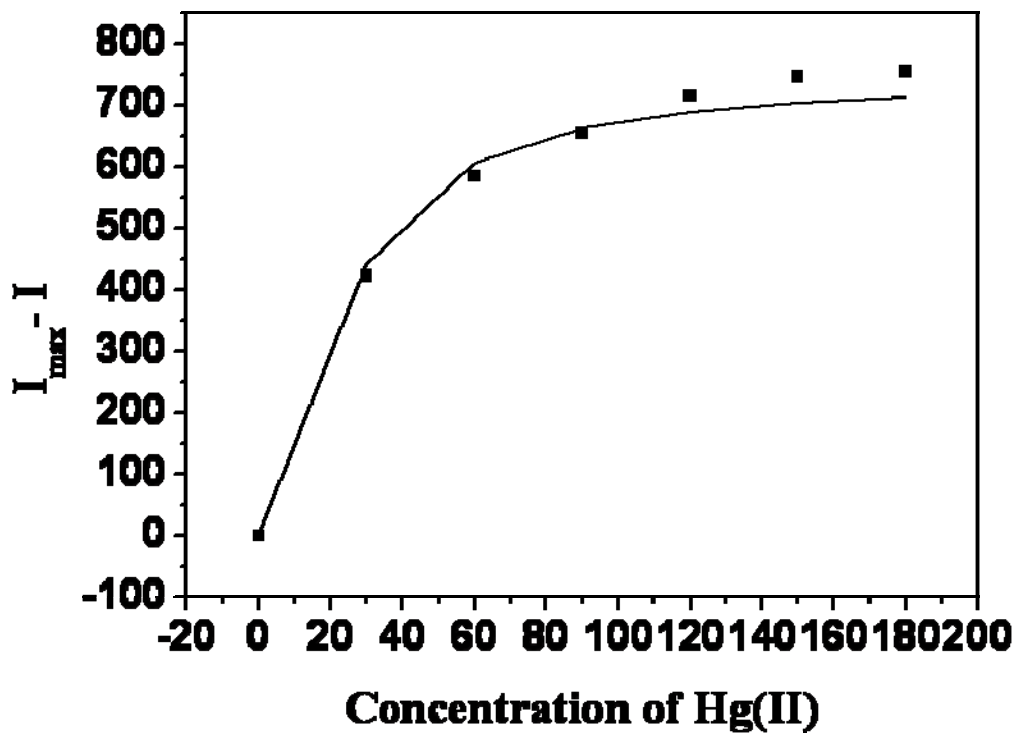


Figure S6. Titration curve with Hg(II) in 50% CH₃CN/HEPES buffer solution and non-linear least square fitting by 1:1 complex model

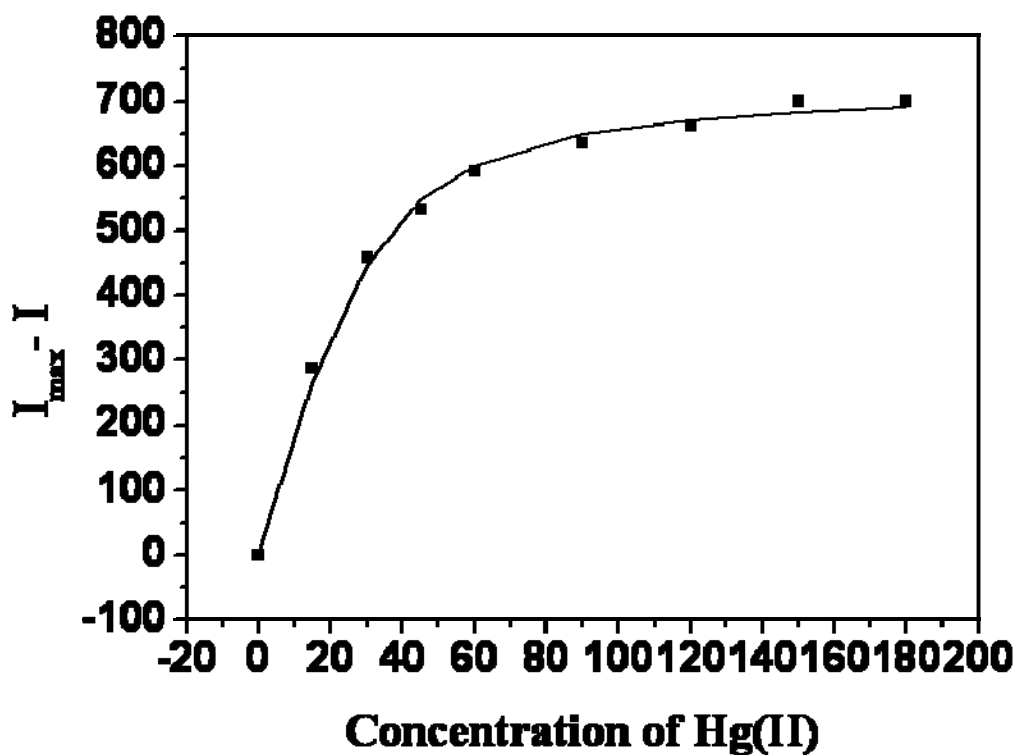


Figure S7. Titration curve with Hg(II) in 100% CH₃CN and non-linear least square fitting by 1:1 complex model

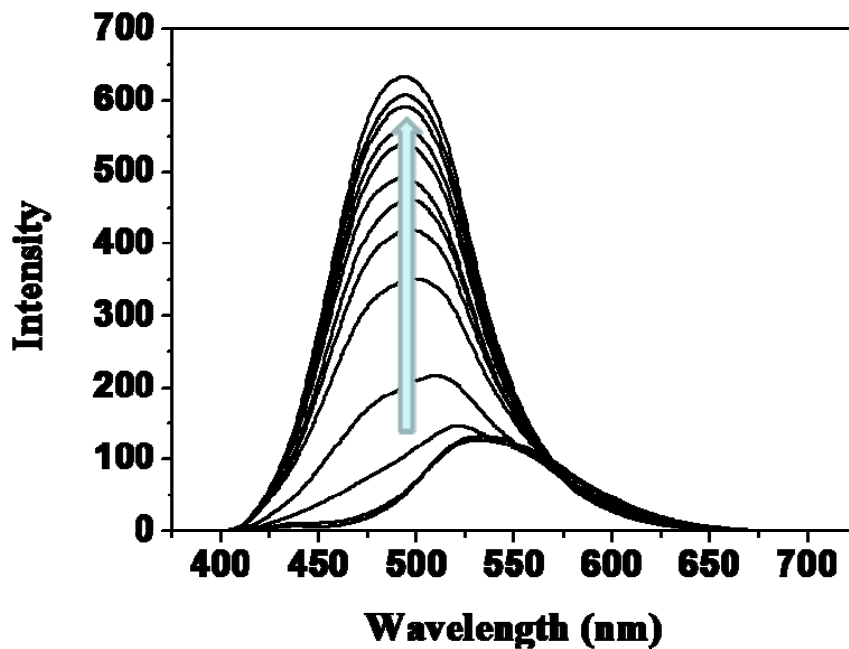
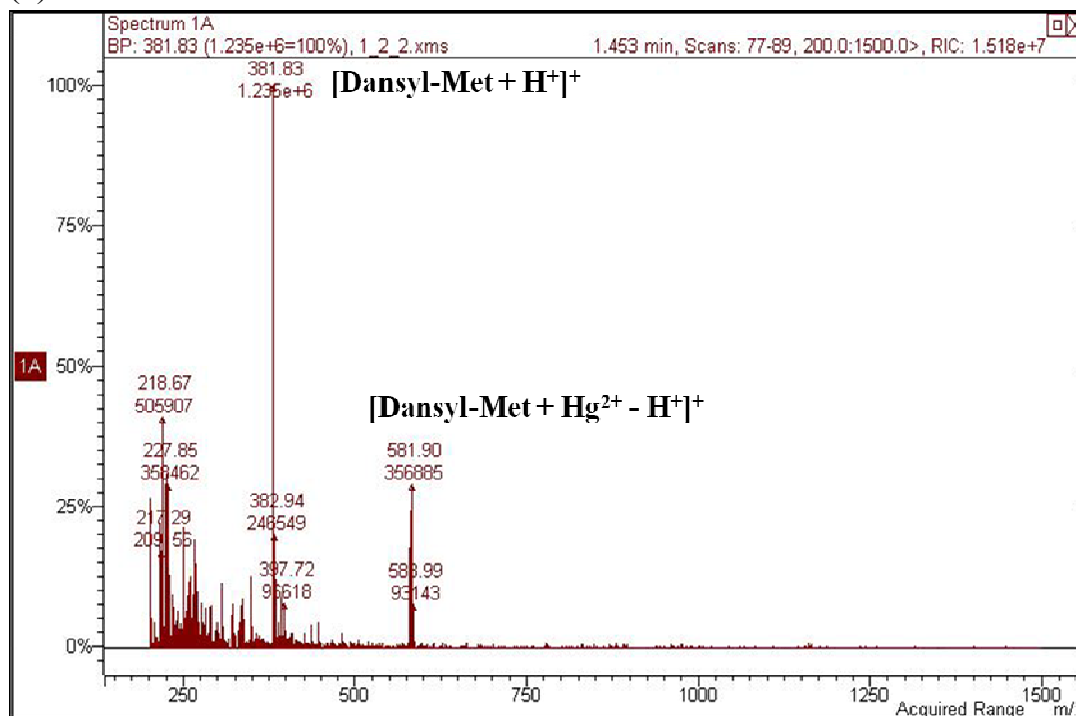
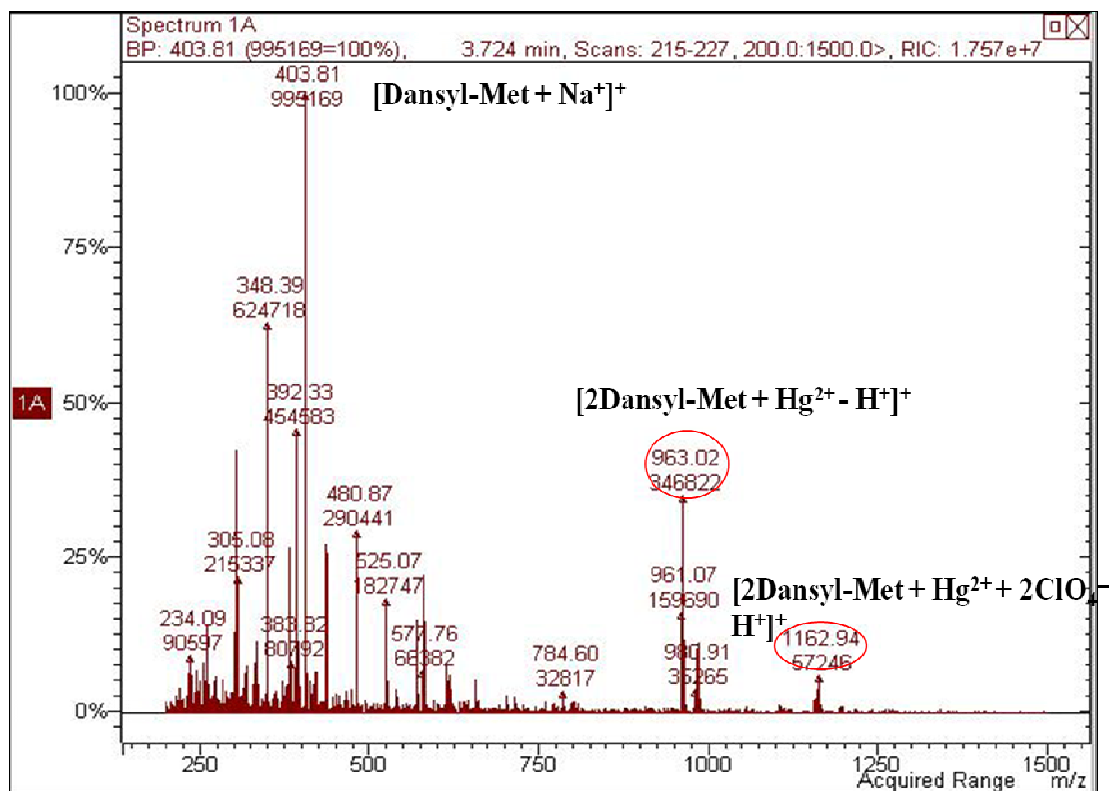


Figure S8. Emission spectra of **Dansyl-Met** (30 μM) in the presence of increasing concentration of Hg (II) in 10% CH₃CN/HEPES buffer solution

(a)



(b)



(c)

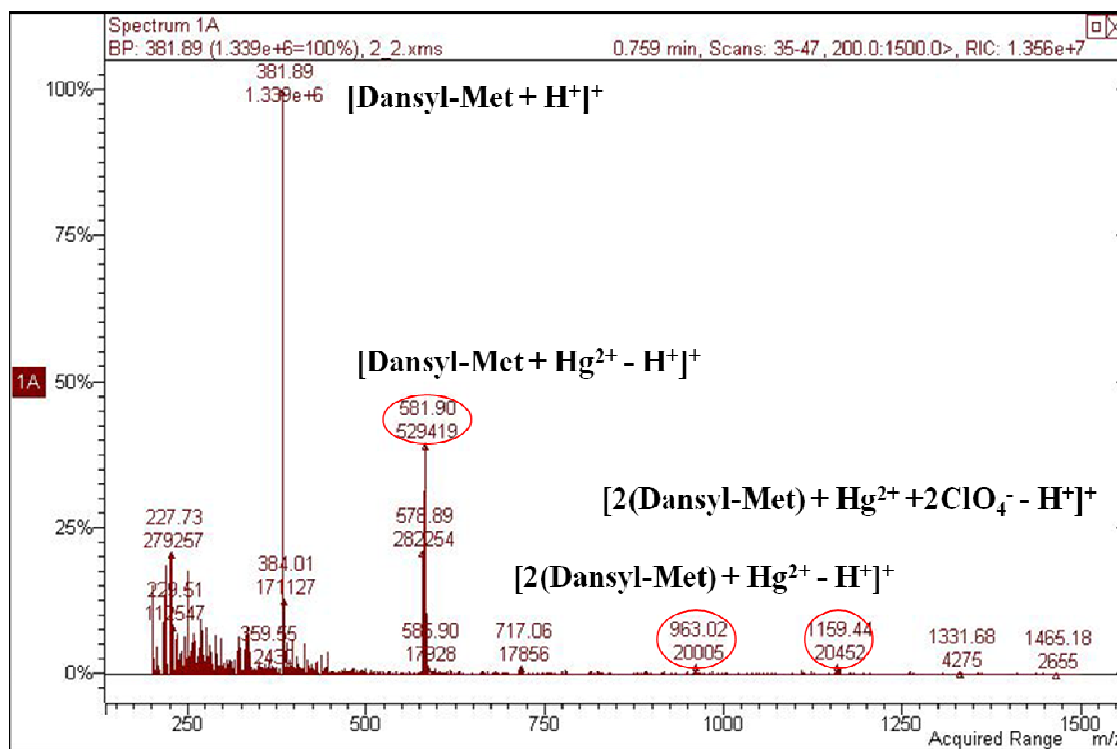
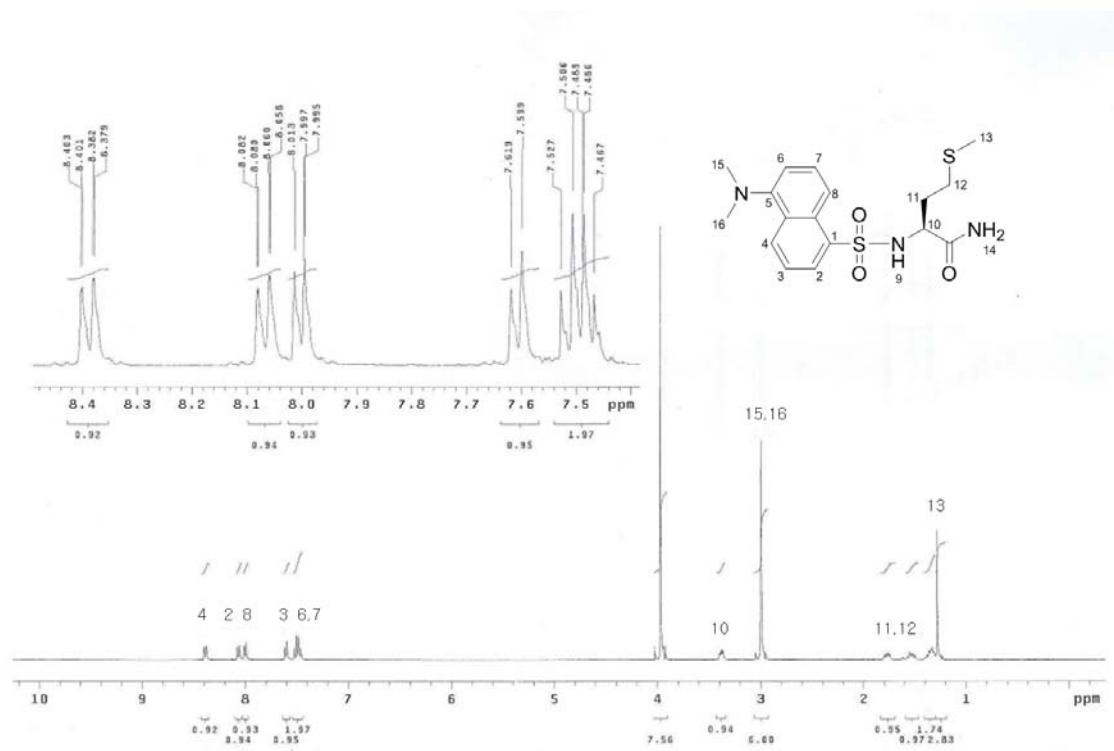


Figure S9. ESI mass spectra of **Dansyl-Met** (600 μM) in (a) 50% CH_3CN /HEPES buffer solution including 5 equiv. of $\text{Hg}(\text{ClO}_4)_2$, (b) 10% CH_3CN /HEPES buffer solution including 3 equiv. of $\text{Hg}(\text{ClO}_4)_2$, and (c) 10% CH_3CN /HEPES buffer solution including 0.1 equiv. of $\text{Hg}(\text{ClO}_4)_2$.



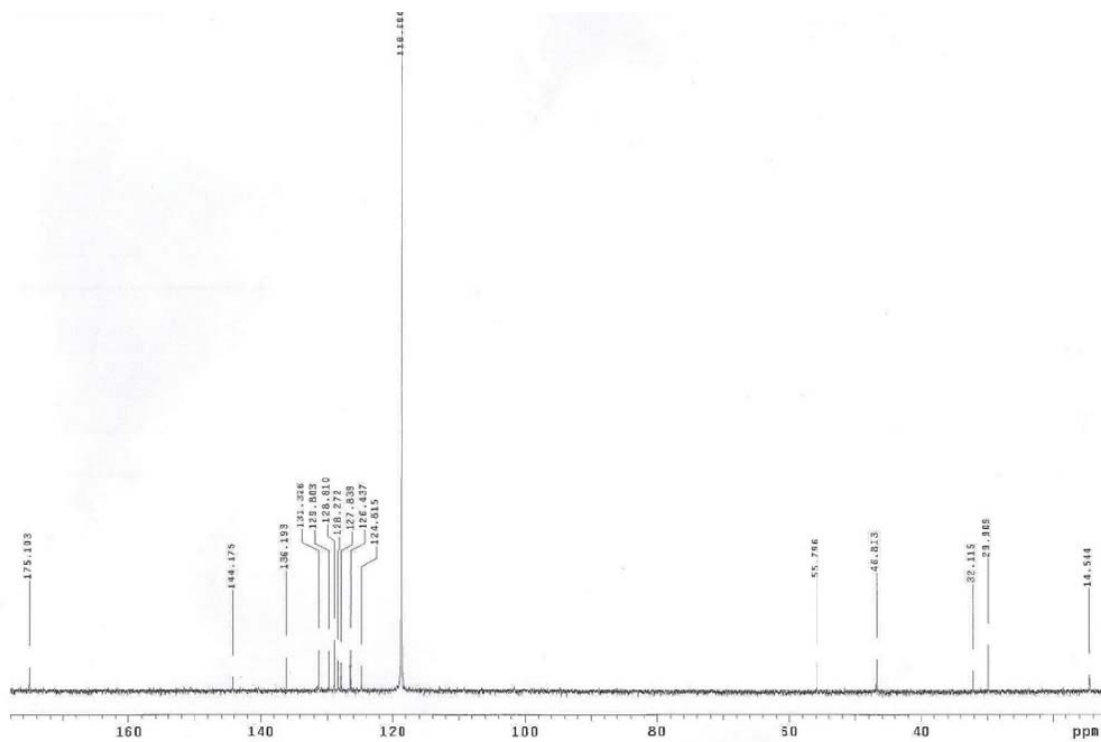
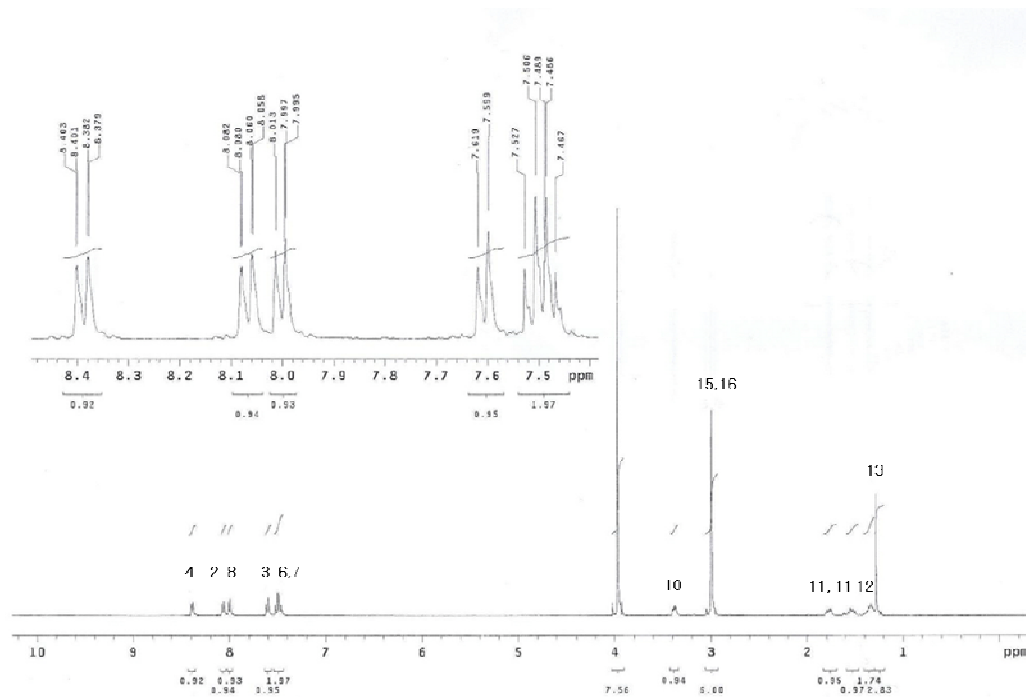


Figure S11. ^{13}C NMR spectra for **Dansyl-Met** in $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (1:1, v/v)

(a)



(b)

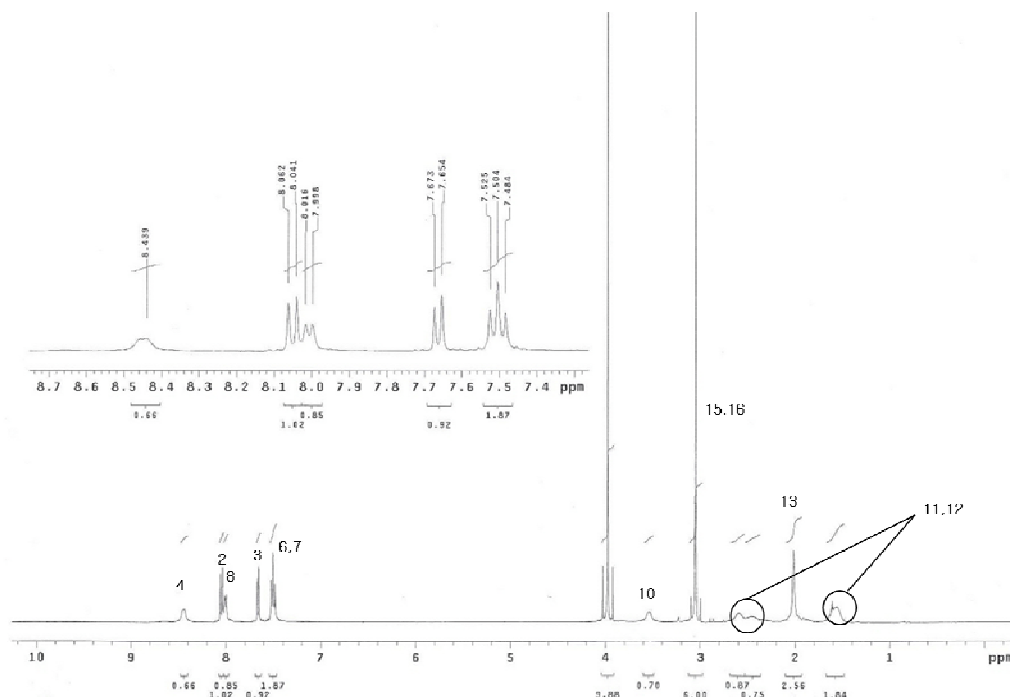


Figure S12. ¹H NMR (400 MHz) of **Dansyl-Met** (5.7 mM) in 50% CD₃CN/D₂O at 25 °C in the absence (a) and presence (b) of 3 equiv of Hg(ClO₄)₂.

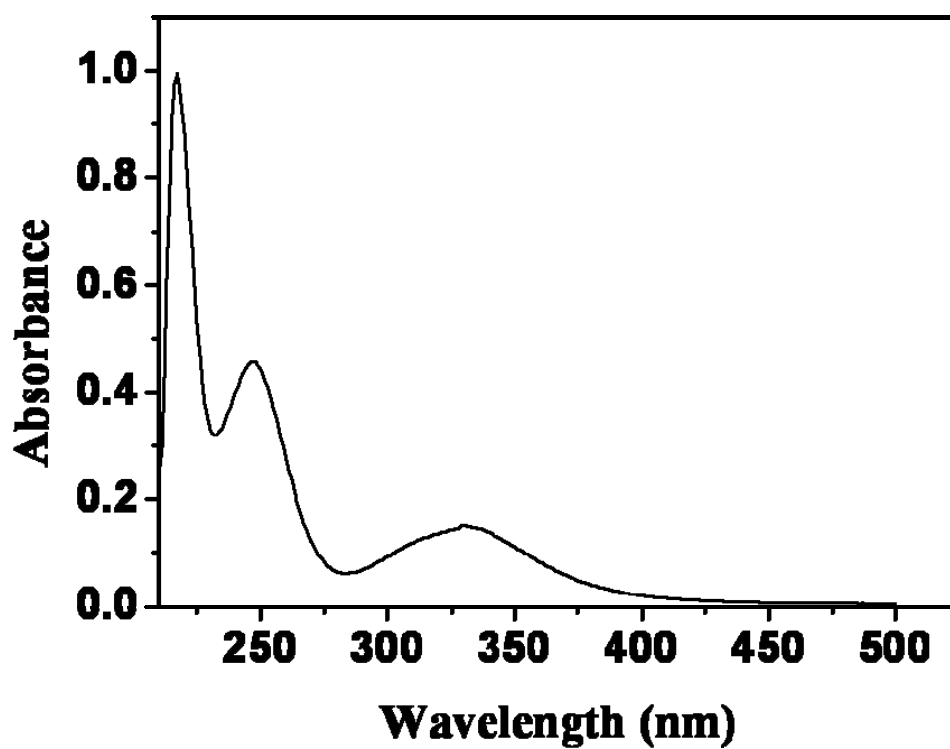


Figure S13. UV absorbance for **Dansyl-Met** (30 μM) in 10 mM HEPES buffer pH 7.4