SUPPORTING INFORMATION

A water-soluble bithiophene with increased photoluminescence efficiency and metal recognition ability

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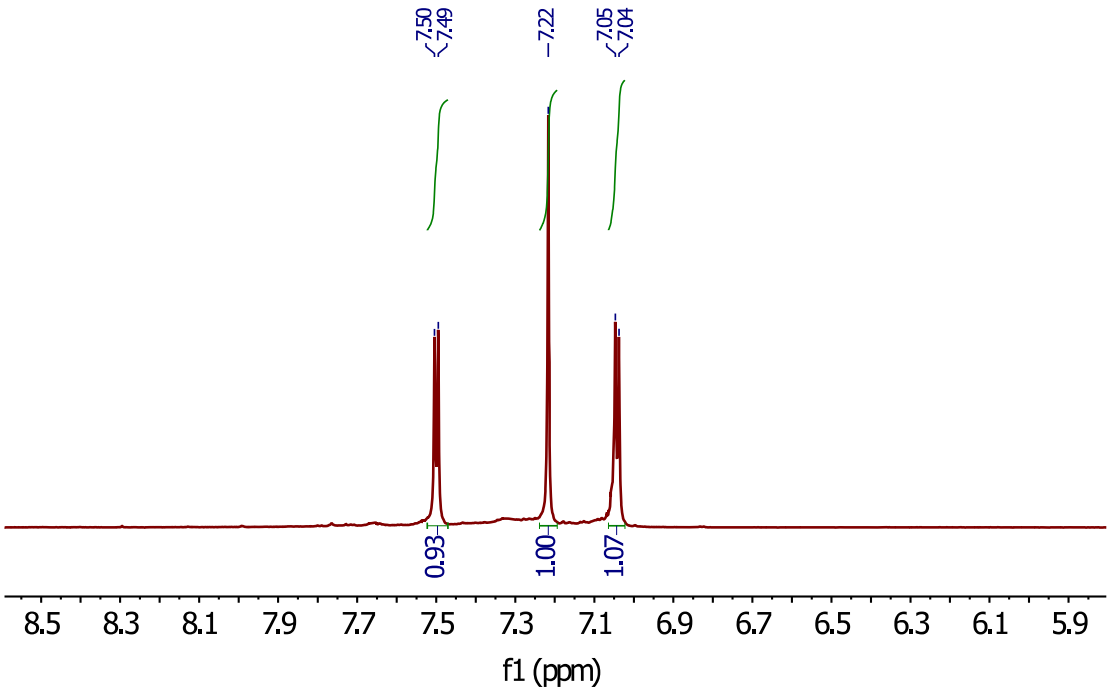

Figure S1. ^{1}H NMR spectrum of **α2-Cl**

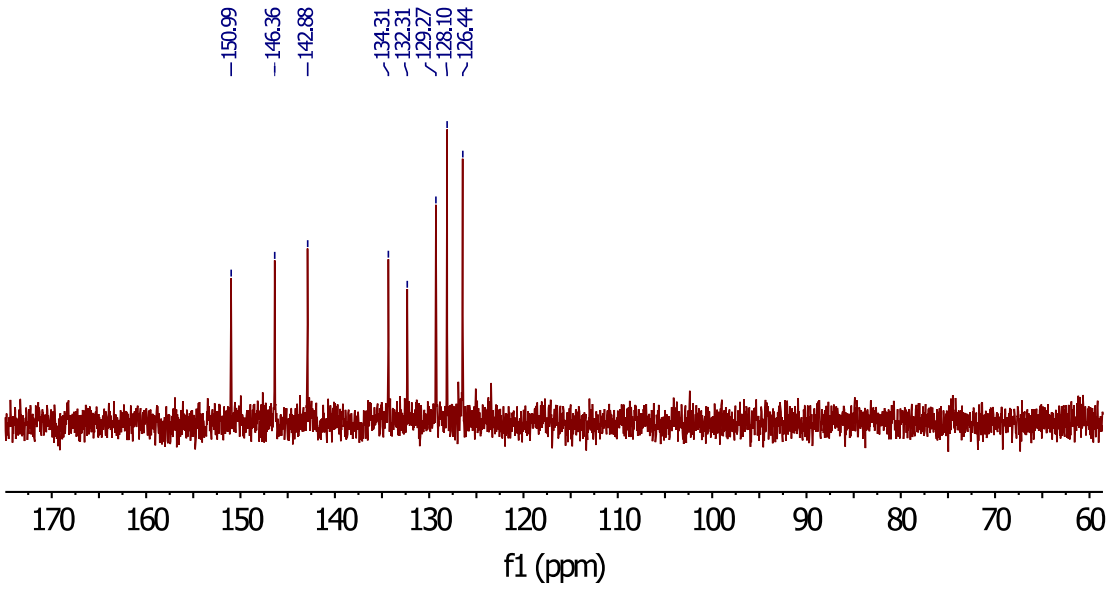

Figure S2. ^{13}C NMR spectrum of **α2-Cl**

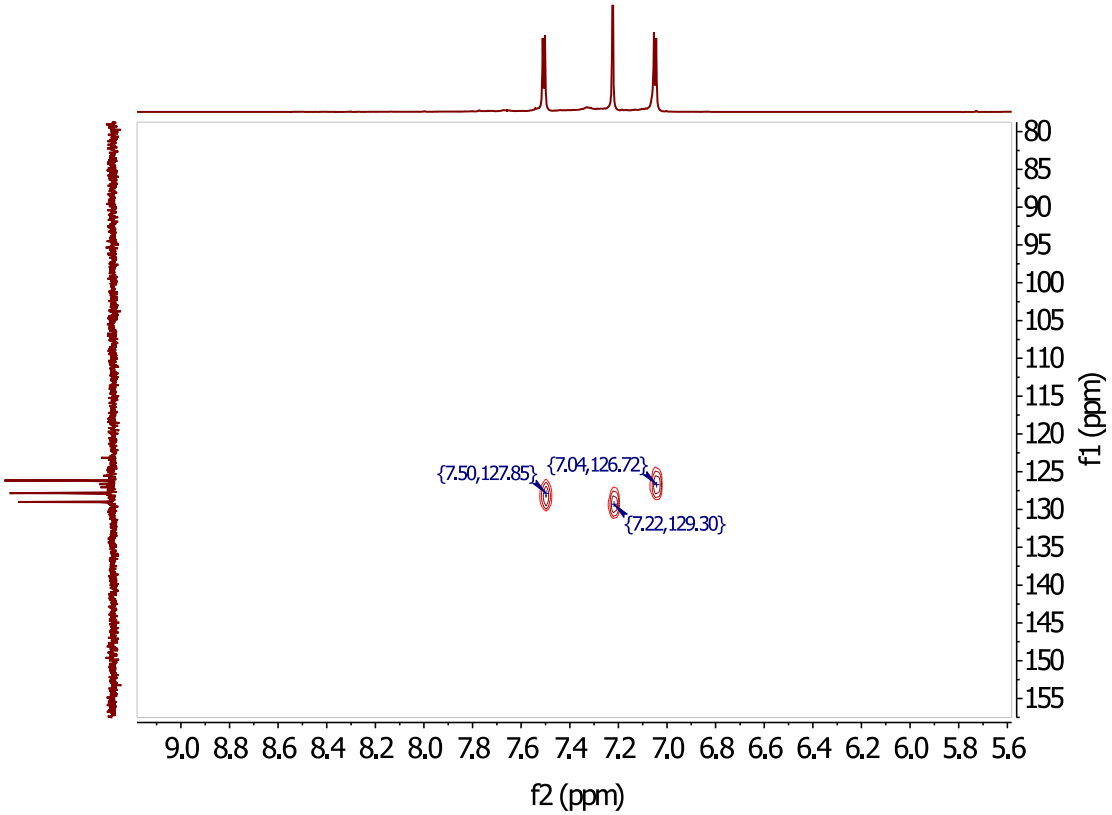

Figure S3. HSQC NMR spectrum of **α2-Cl**

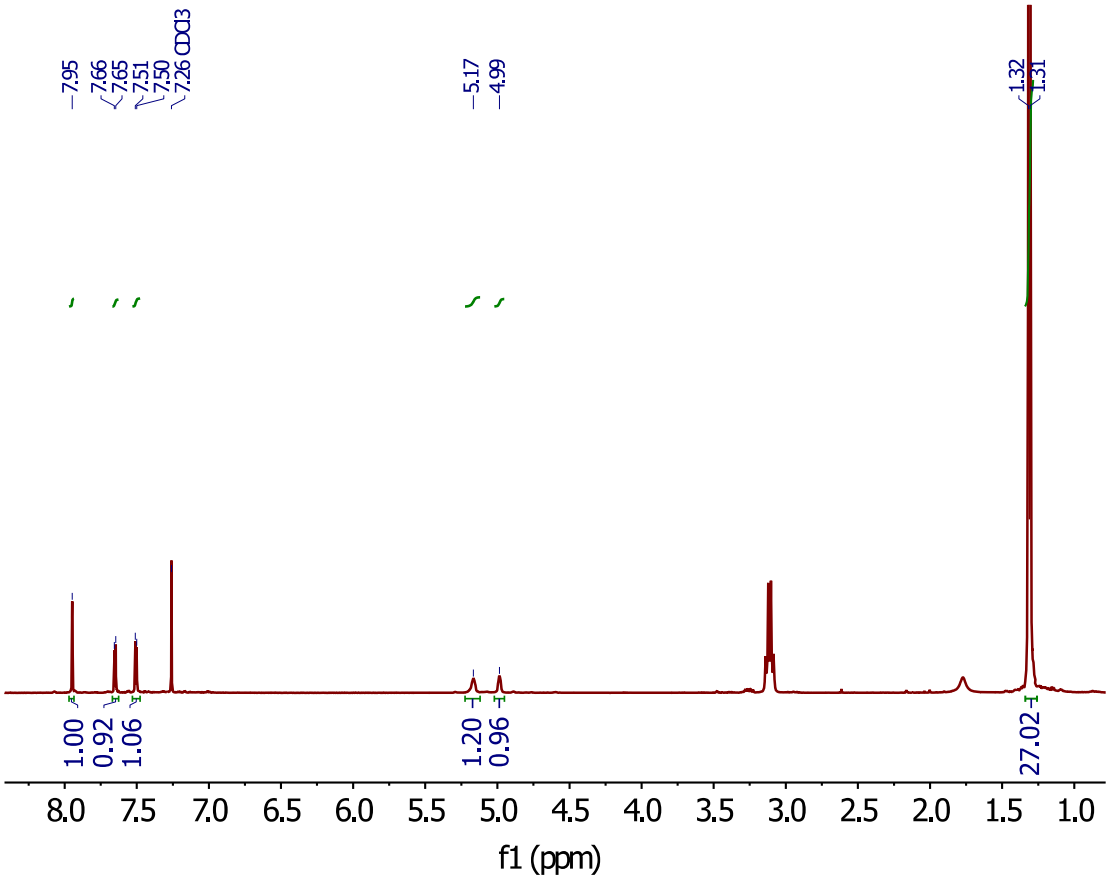

Figure S4. ^{1}H NMR spectrum of **α2-tbS**

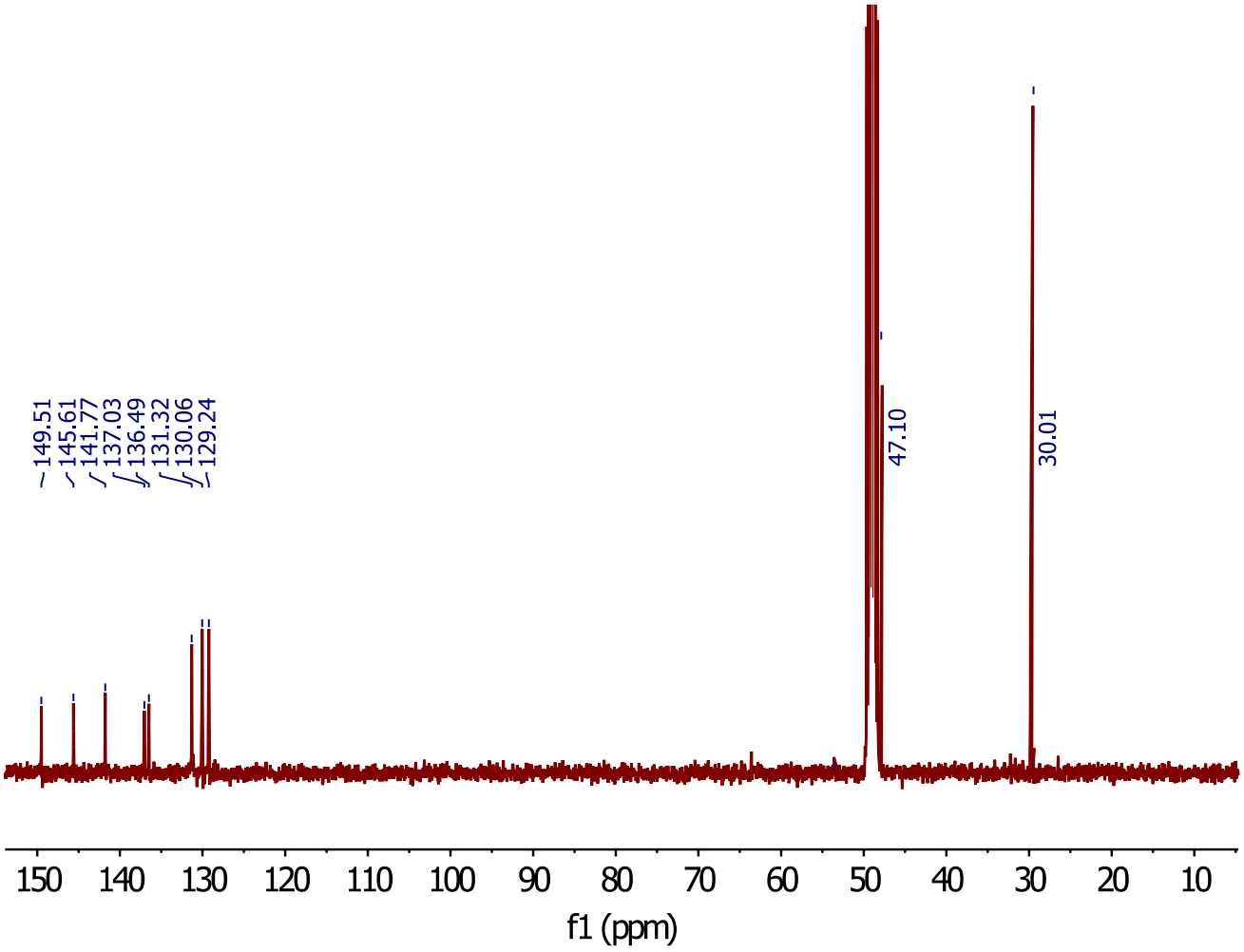

Figure S5. ^{13}C NMR spectrum of **α2-tbS**

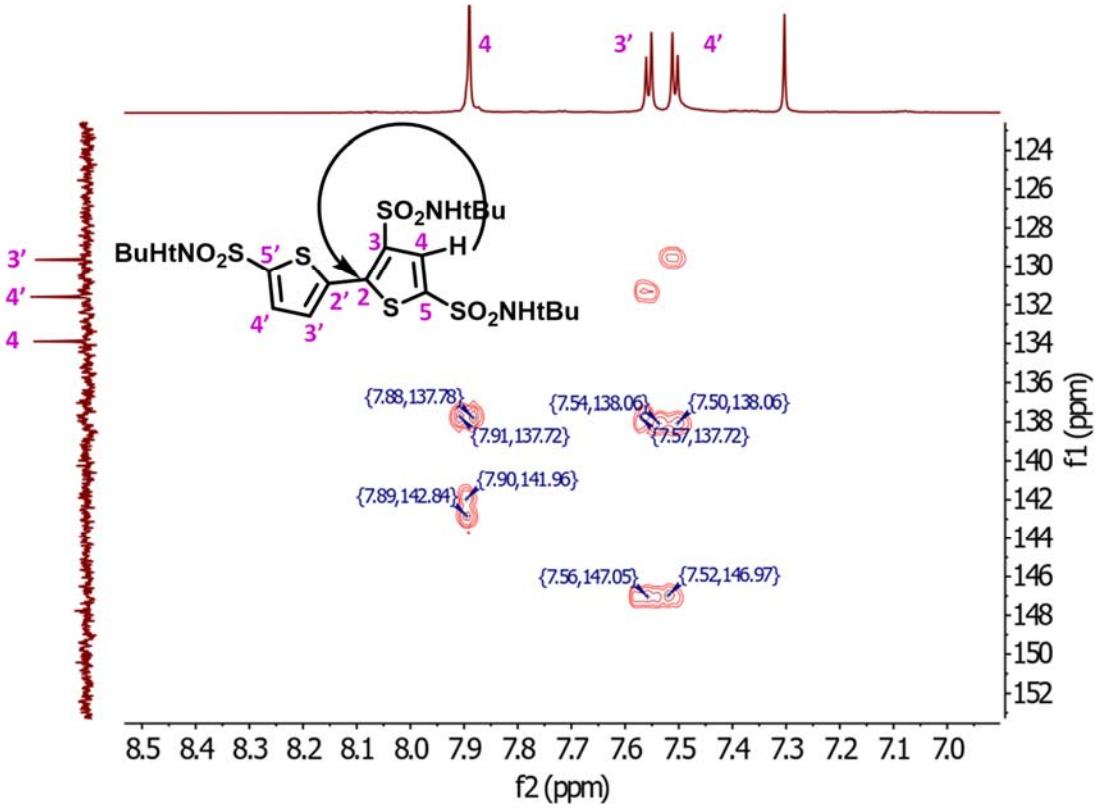

Figure S6. HMBC spectrum of **α2-tbS**

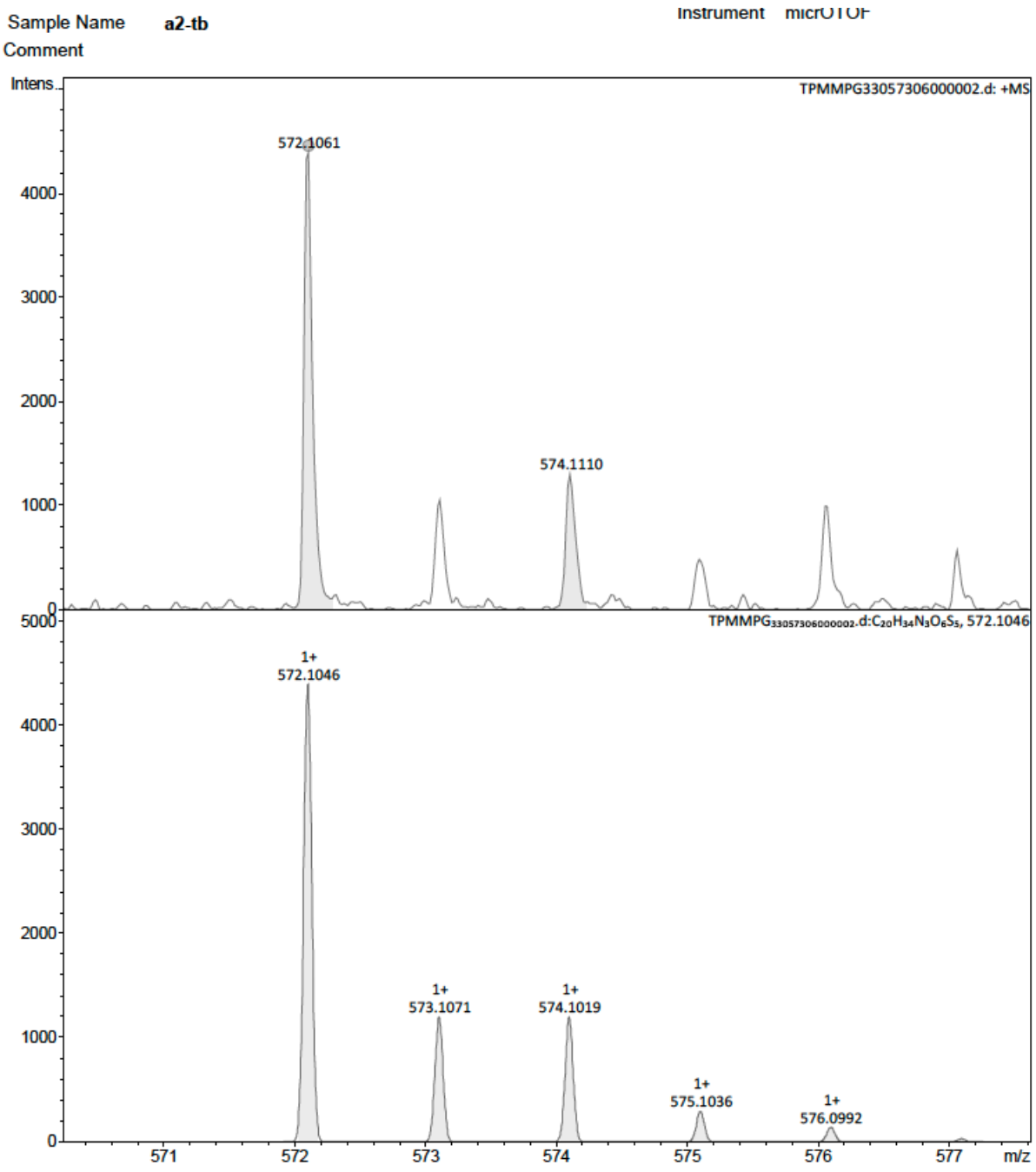

Figure S7. Mass spectrum of **α2-tbS**

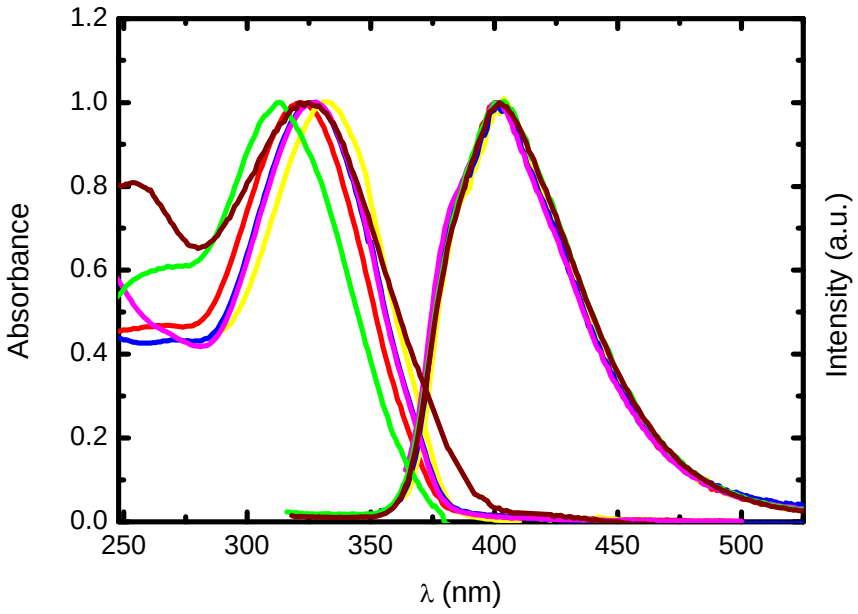

Figure S8. Normalized absorption and fluorescence emission spectra in dioxane (blue), methanol (red), 2-methyltetrahidrofurane (pink), dimethylformamide (yellow) and water at two pH's (acidic pH = 0.35 (green), and basic pH ≈ 13 (brown)) solutions for **α2-tbS** at T = 293K

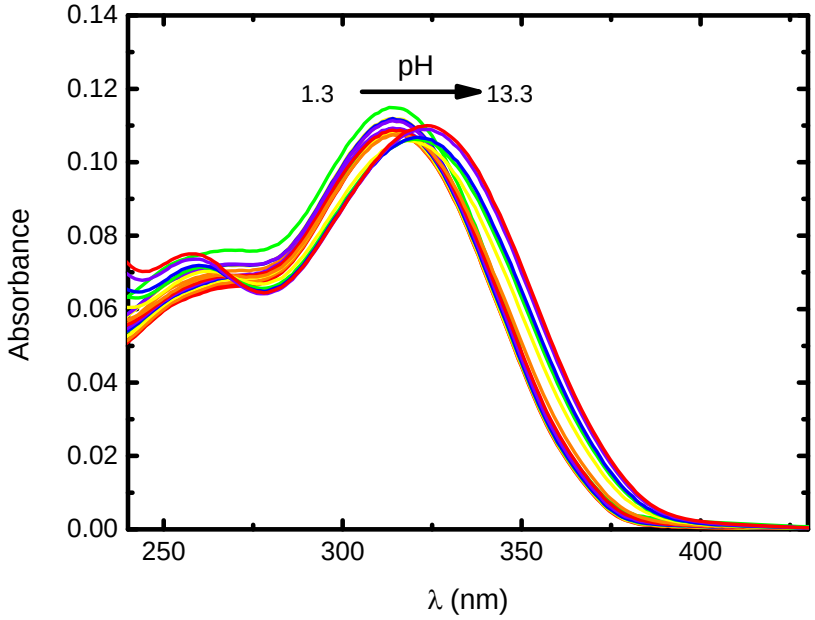

Figure S9. Absorbance of **α2-tbS** recorded at 298.1 ± 0.1 K as function of pH

Scheme S1. Equations for cumulative and stepwise constants. A cumulative or overall constant, given the symbol β, is the equilibrium constant for the formation of a complex from reagents, and can always be expressed as the product of stepwise constants. A stepwise constant refers to the formation of the species one step at a time. In the case of $p\beta_{13}$ for **α2-tbS**:

*Stepwise constants for the triprotonated **α2-tbS***

$$\boldsymbol{\alpha 2\text{-}tbS^{3-}} + H^+ \leftrightarrows \boldsymbol{\alpha 2\text{-}tbS^{2-}} \quad \boldsymbol{K_1} = {[\boldsymbol{\alpha 2 - tbS^{2-}}]}/{[\boldsymbol{\alpha 2 - tbS^{3-}}][\boldsymbol{H^+}]}$$

$$\boldsymbol{\alpha 2\text{-}tbS^{2-}} + H^+ \leftrightarrows \boldsymbol{\alpha 2\text{-}tbS^{-}} \quad \boldsymbol{K_2} = {[\boldsymbol{\alpha 2 - tbS^{-}}]}/{[\boldsymbol{\alpha 2 - tbS^{2-}}][\boldsymbol{H^+}]}$$

$$\boldsymbol{\alpha 2\text{-}tbS^{-}} + H^+ \leftrightarrows \boldsymbol{\alpha 2\text{-}tbS} \quad \boldsymbol{K_3} = {[\boldsymbol{\alpha 2 - tbS}]}/{[\boldsymbol{\alpha 2 - tbS^{-}}][\boldsymbol{H^+}]}$$

*Cumulative constant for the triprotonated **α2-tbS***

$$\boldsymbol{\alpha 2\text{-}tbS^{3-}} + 3H^+ \leftrightarrows \boldsymbol{\alpha 2\text{-}tbS} \quad \boldsymbol{\beta_{13}} = {[\boldsymbol{\alpha 2 - tbS}]}/{[\boldsymbol{\alpha 2 - tbS^{3-}}][\boldsymbol{H^+}]^3}$$

Being $p\beta_{13} = \log K_1 + \log K_2 + \log K_3$

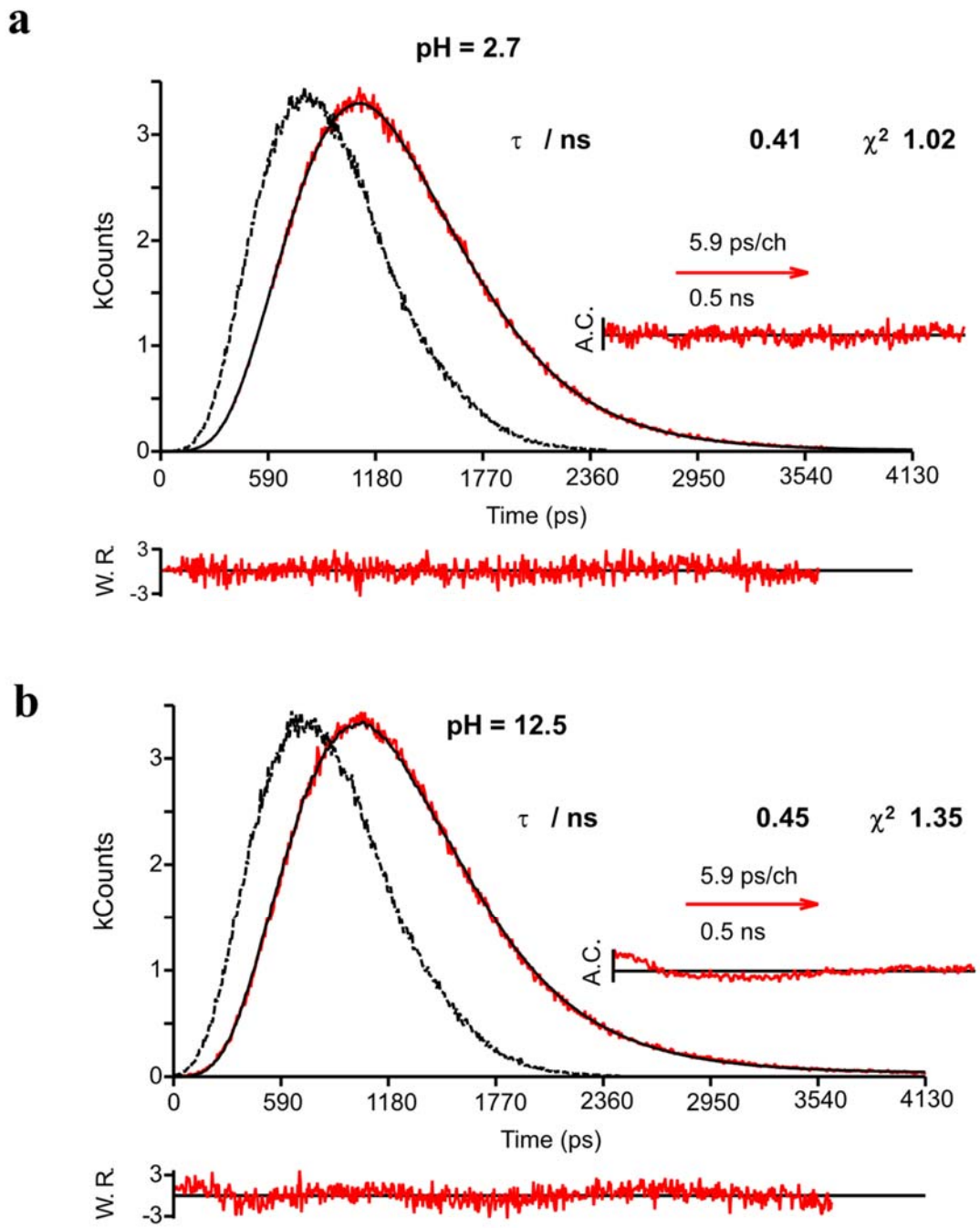

Figure S10. Fluorescence decays of **α2-tbS** in water a) pH = 2.7 and b) pH = 12.5 at T=293 K. The fluorescence decay times (τ_i) are presented as insets. The dashed line in the decays is the pulse IRF. For a better judgment of the quality of the fits, the weighted residuals (WRs), autocorrelation functions (ACs), and chi-squared (χ^2) values are also shown

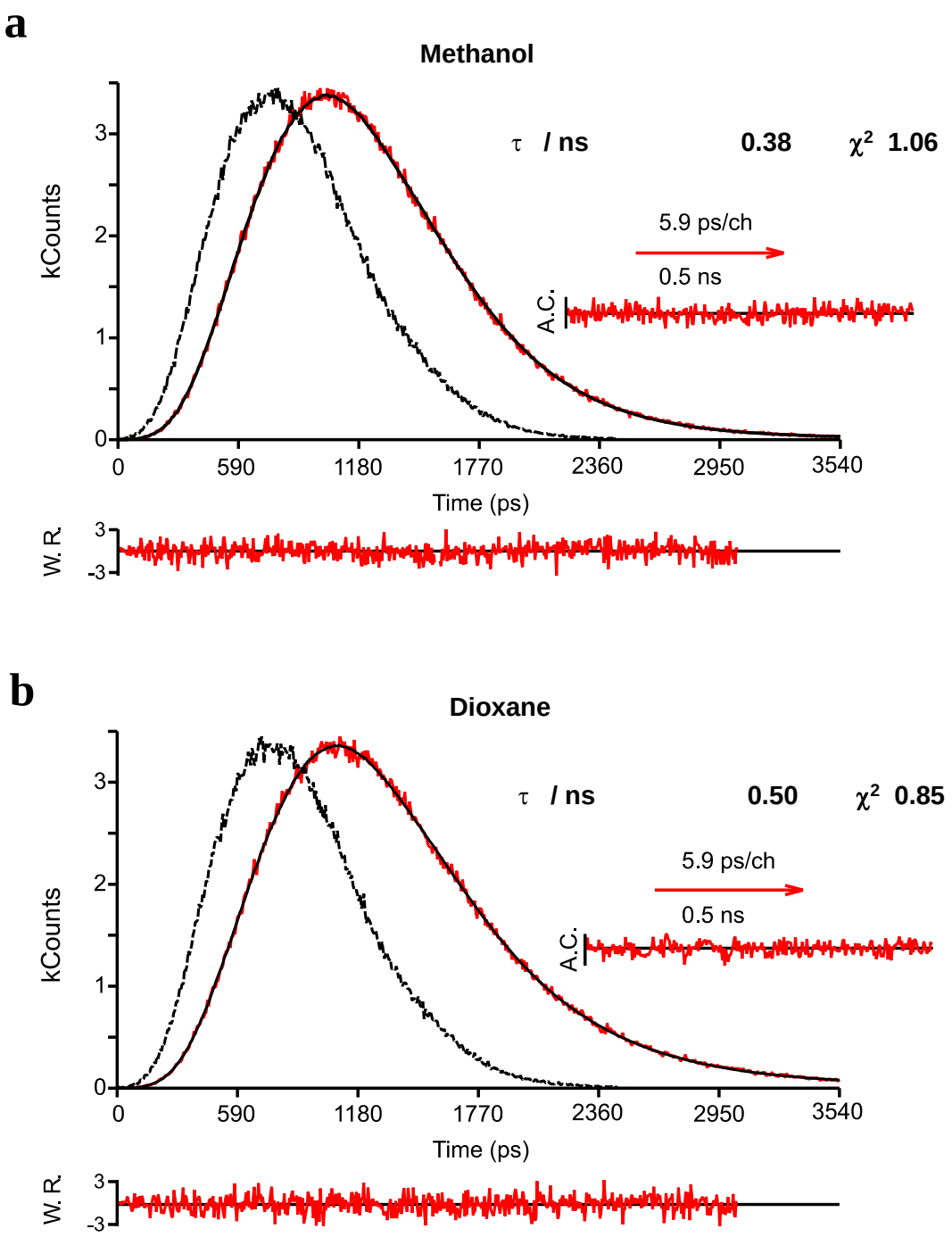

Figure S11. Fluorescence decays of **α2-tbS** in a) methanol and b) dioxane at T=293 K. The fluorescence decay times (τ_i) are presented as insets. The dashed line in the decays is the pulse IRF. For a better judgment of the quality of the fits, the weighted residuals (WRs), autocorrelation functions (ACs), and chi-squared (χ^2) values are also shown

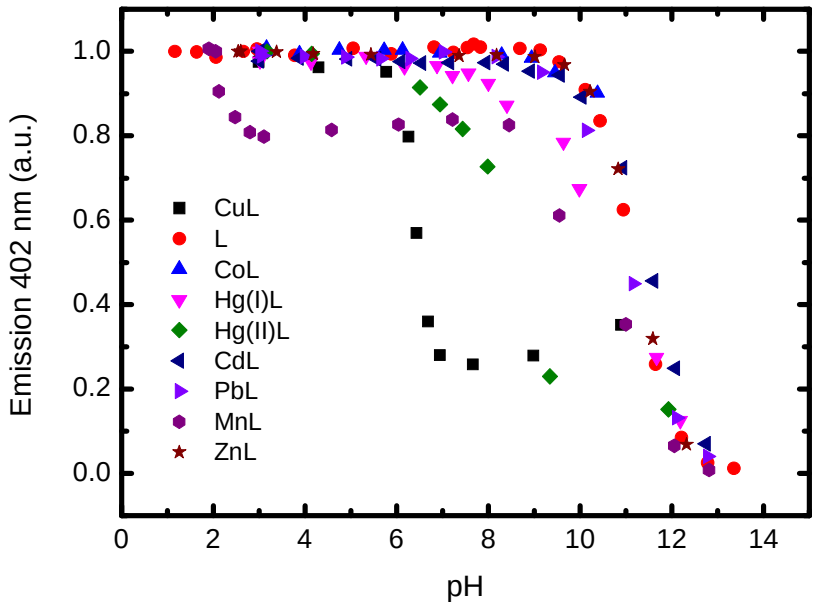

Figure S12. Fluorescence emission intensity *vs* pH curves recorded in water for **α2-tbS (L)** after the addition of an excess of the corresponding metal. [**α2-tbS**] = 1.3x10-5 M; λ_{exc} = 317 nm

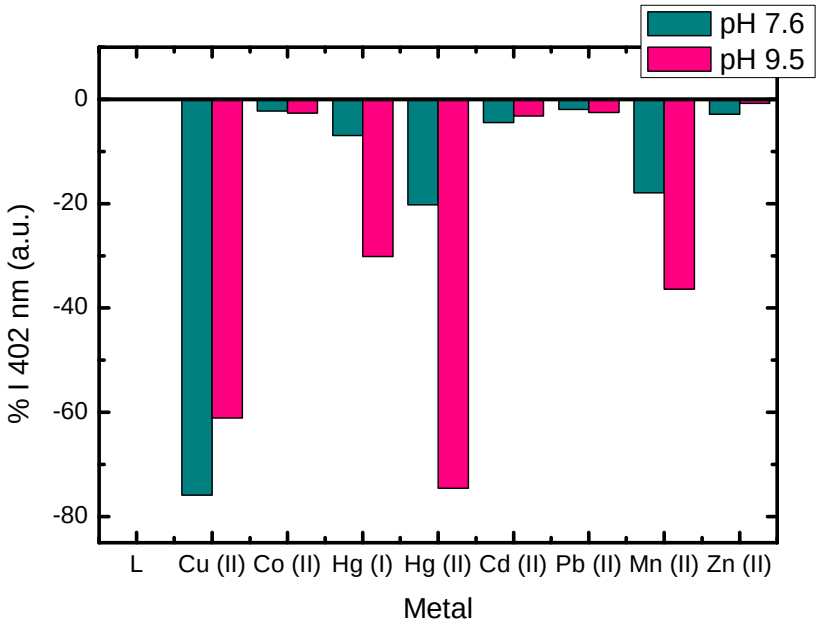

Figure S13. Bar diagram representation of the percentage of response relative to the fluorescence intensity of **α2-tbS** at 402 nm (% I 402 nm) upon addition of divalent metal ions at pH 7.6 and 9.5. In the yy´-axes the fluorescence of the free ligand is leveled to 0. Titrations performed in water at T = 298 K, [**α2-tbS**] = 1.3x10-5 M with λ_{exc} = 317 nm