

Supporting Information for

Specific colorimetric detection of Fe³⁺ ions in aqueous solution by squaraine-based chemosensor

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1. General Information

Reagents and apparatus

Unless stated, all the reagents used were of analytical grade from commercial sources without further purification. ^1H NMR (400 MHz) and ^{13}C NMR (400 MHz) spectra were recorded on a Bruker AV-400 spectrometer (TMS as internal standard). Mass spectrometry analysis was performed on a Q exactive mass spectrometer (Thermo Fisher Scientific, USA). Absorption spectra were measured on M5 spectrometer.

Nuclear Magnetic Resonance Spectroscopy

Proton nuclear magnetic resonance (^1H NMR) and carbon nuclear magnetic resonance (^{13}C NMR) spectroscopy were performed on 400 MHz NMR spectrometers. Chemical shifts are reported as δ in units of parts per million (ppm) downfield from tetramethylsilane ($\delta 0.00$), using the residual solvent signal as an internal standard: chloroform-d, CDCl_3 , (^1H NMR, δ 7.26, singlet; ^{13}C NMR, δ 77.04, triplet). Multiplicities are given as: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplets). The number of protons (n) for a given resonance is indicated by numbers of H.

UV-vis titration measurements

10 mM stock solution of **TSQ** was prepared by dissolving the required amount in DMSO. Further dilutions were made to prepare 100 μM of **TSQ** by adding mixed solution. The different concentrations of metal ions were consequently were added in to make total volume of 200 μL . Absorption measurements were made in 96 well plates.

2. NMR Spectra for TSQ

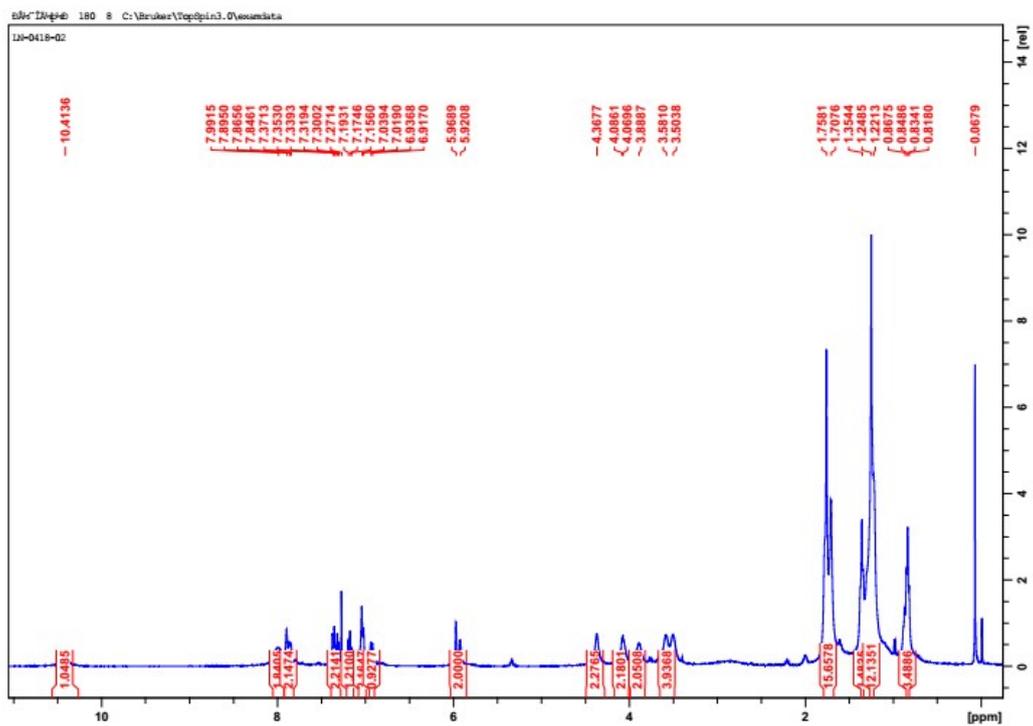


Figure S1. ¹H NMR spectrum for compound TSQ

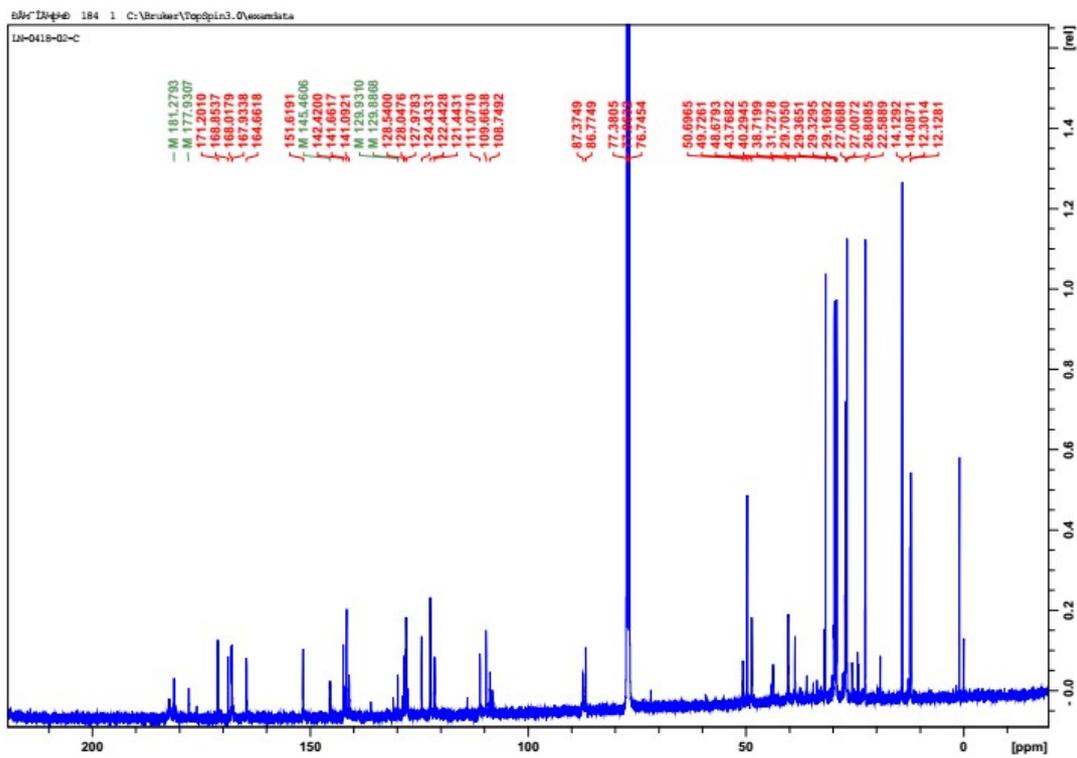


Figure S2. ¹³C NMR spectrum for compound TSQ

3. Comparison of TSQ with recently reported chemosensors

Table S1 Comparison of TSQ with recently reported chemosensors

Sensor	Target	Response type	LOD (μM)	Reaction media	Reversibility	Reference
Sugar-functioned coumarin	Fe^{3+}	Color	4.6	H_2O	No	58
Julolidine derivative	Fe^{3+}	Color	6.8	DMF	No	59
Hetarylazo	Fe^{3+}	Color	2.0	CH_3CN	No	41
Our work	Fe^{3+}	Color	1.0	20% AcOH- H_2O	Yes	/

4. Mass spectrum of TSQ and TSQ- Fe^{3+} complex

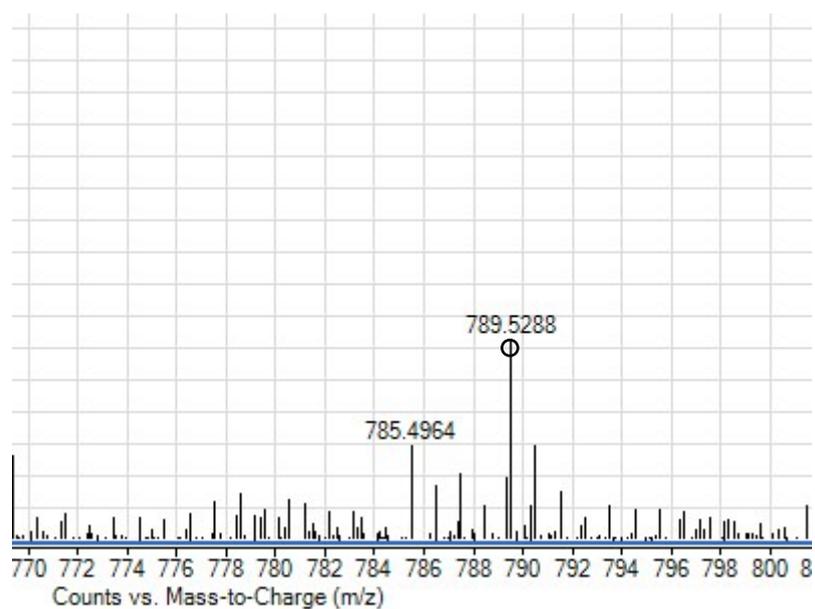


Figure S3a. High resolution mass spectrum for TSQ

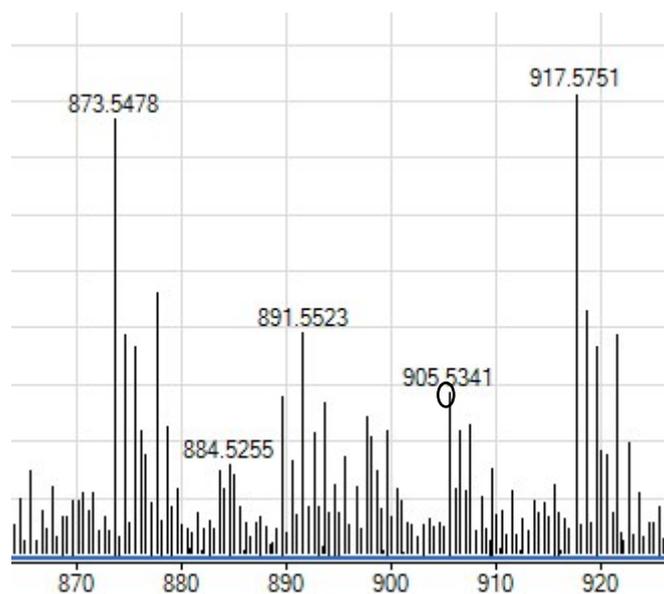


Figure S3b. High resolution mass spectrum for $[\text{TSQ}+\text{Fe}^{3+}+\text{CH}_3\text{COOH}+\text{H}^+]$

5. Reversibility study of TSQ- Fe^{3+} with EDTA

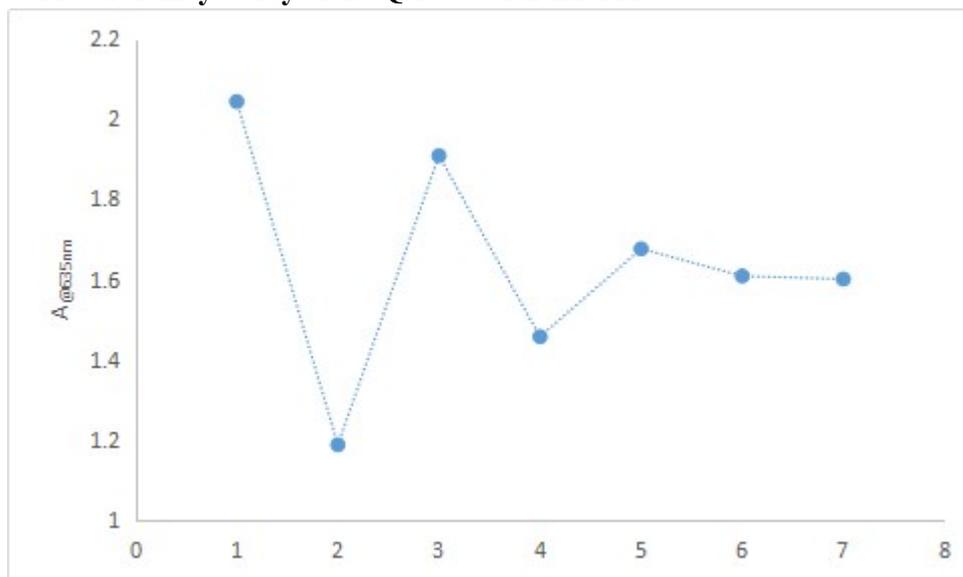


Figure S4. Stepwise complexation/decomplexation cycles were carried out in 20% AcOH- H_2O solution with TSQ and Fe^{3+}