Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

Fluorescent probe for Fe^{3+} and CN^- in aqueous media mimicking a memorized molecular crossword puzzle

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1. ^{1}H NMR spectrum of **2** in $CDCl_3$.

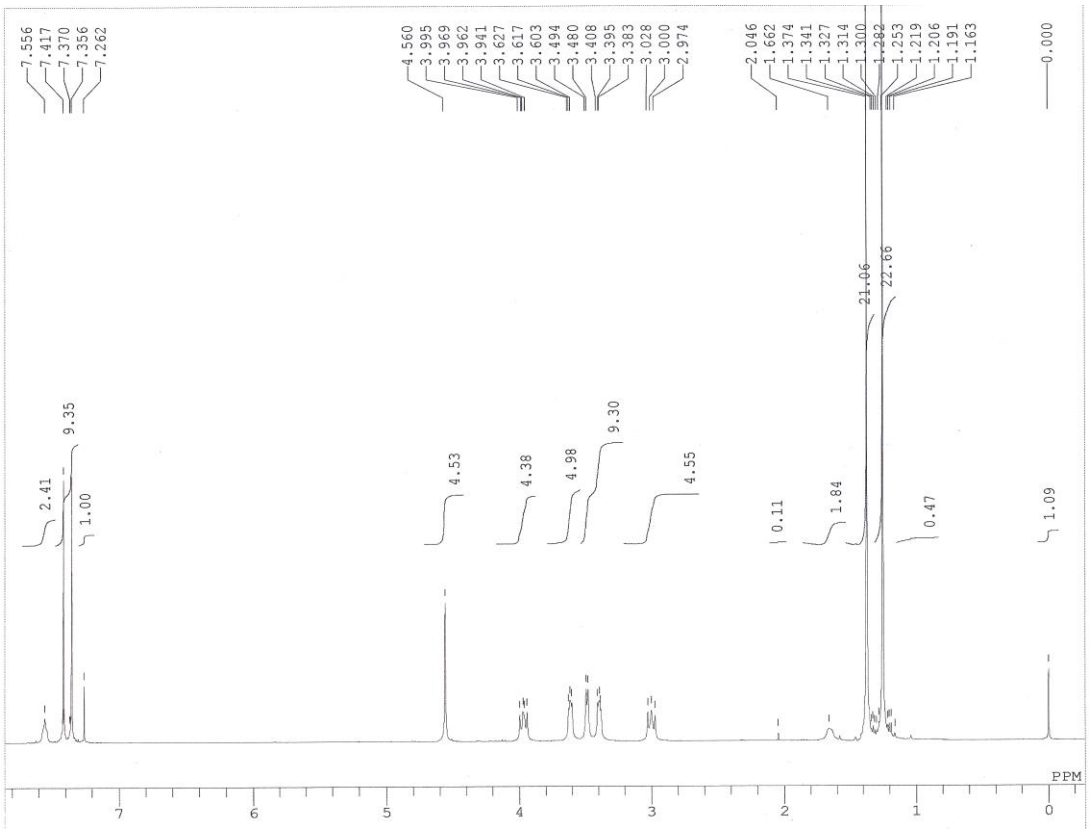


Figure S1. ^{1}H NMR spectrum of **2** in $CDCl_3$.

2. ^{13}C NMR Spectrum of **2** in $CDCl_3$.

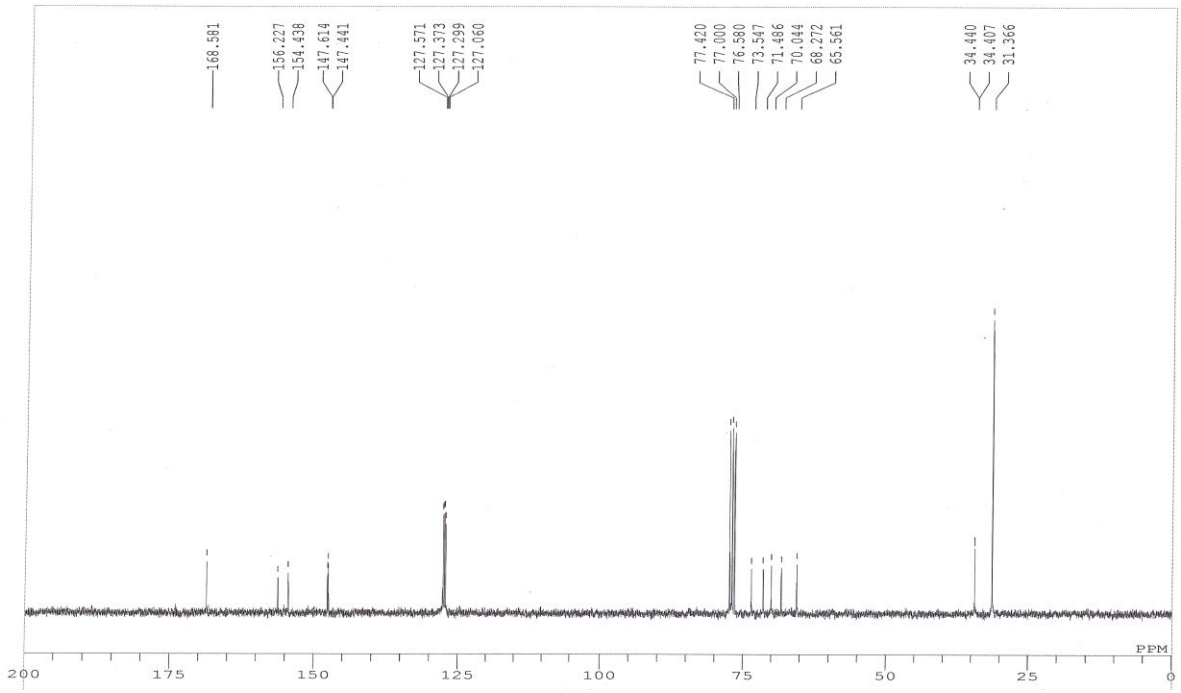


Figure S2. ^{13}C NMR spectrum of **2** in $CDCl_3$.

3. FAB mass spectrum of **2**.

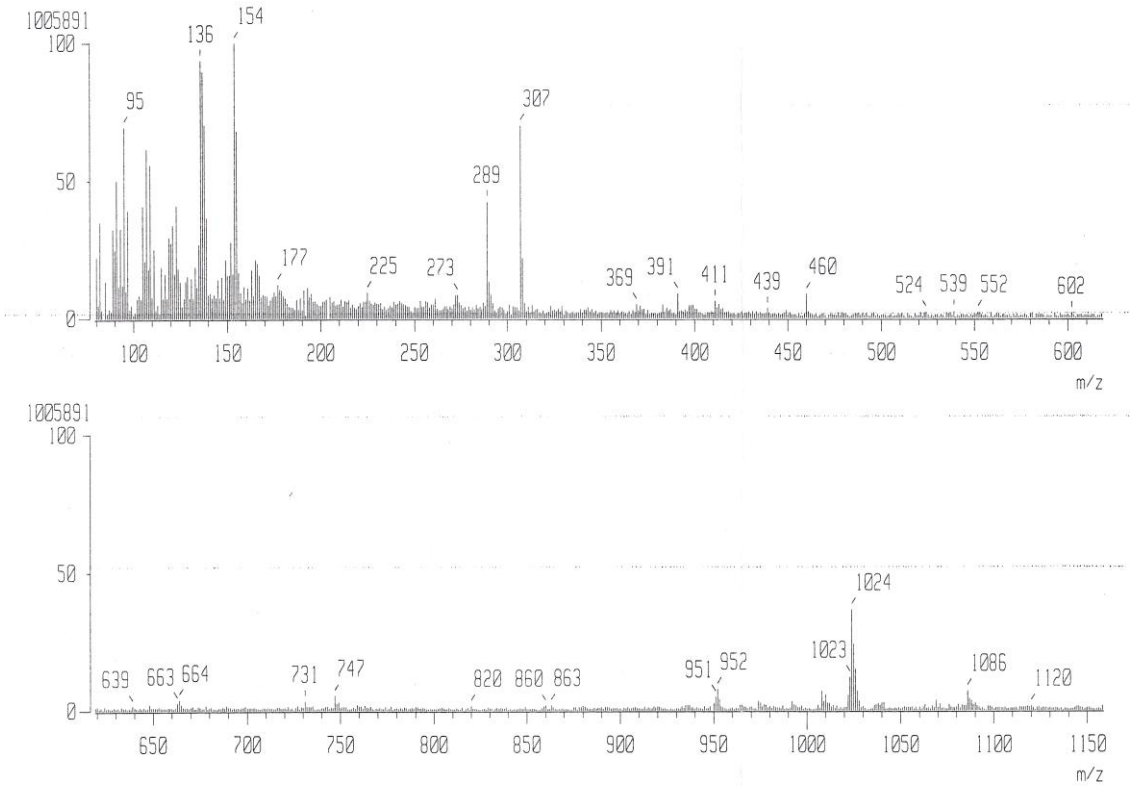


Figure S3. FAB mass spectrum of **2**.

4. ^{1}H NMR spectrum of **4** in $CDCl_3$.

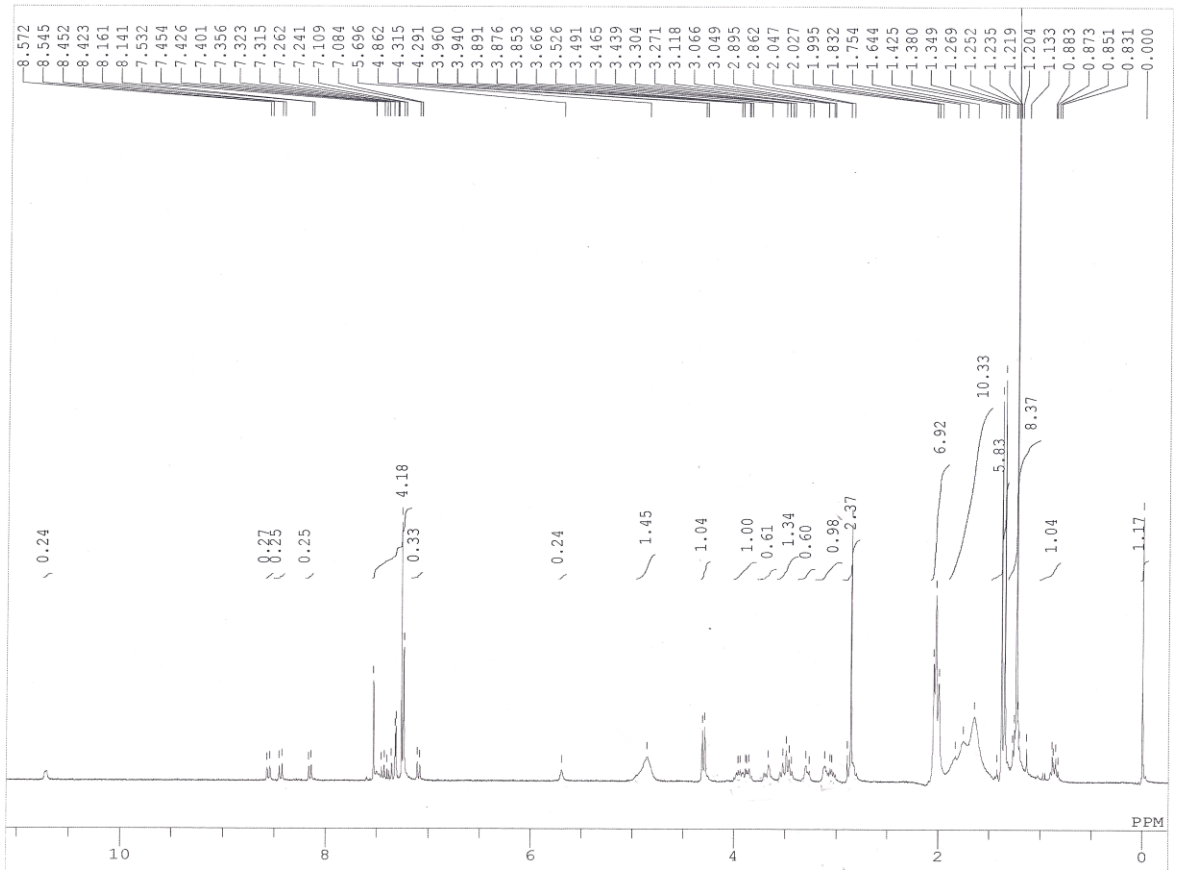


Figure S4. ^{1}H NMR spectrum of **4** in $CDCl_3$.

5. ^{13}C NMR spectrum of **4** in $CDCl_3$.

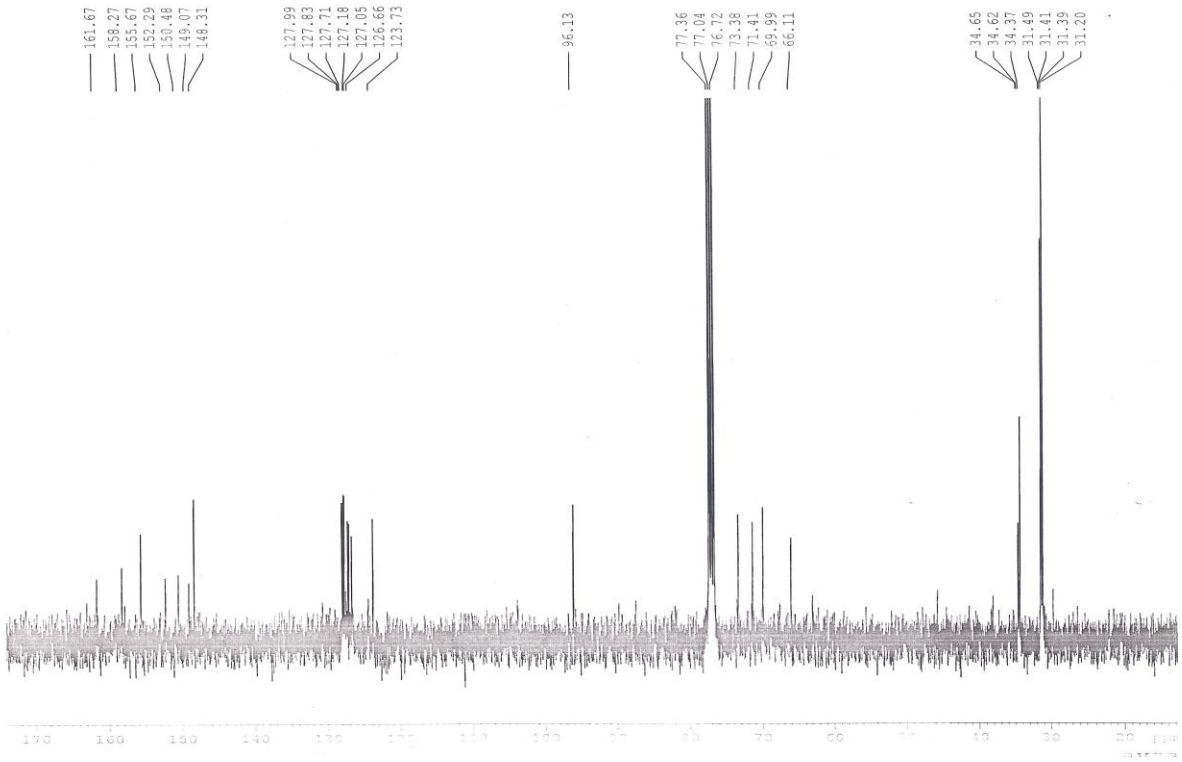


Figure S5. ^{13}C NMR spectrum of **4** in $CDCl_3$.

6. FAB mass spectrum of **4**.

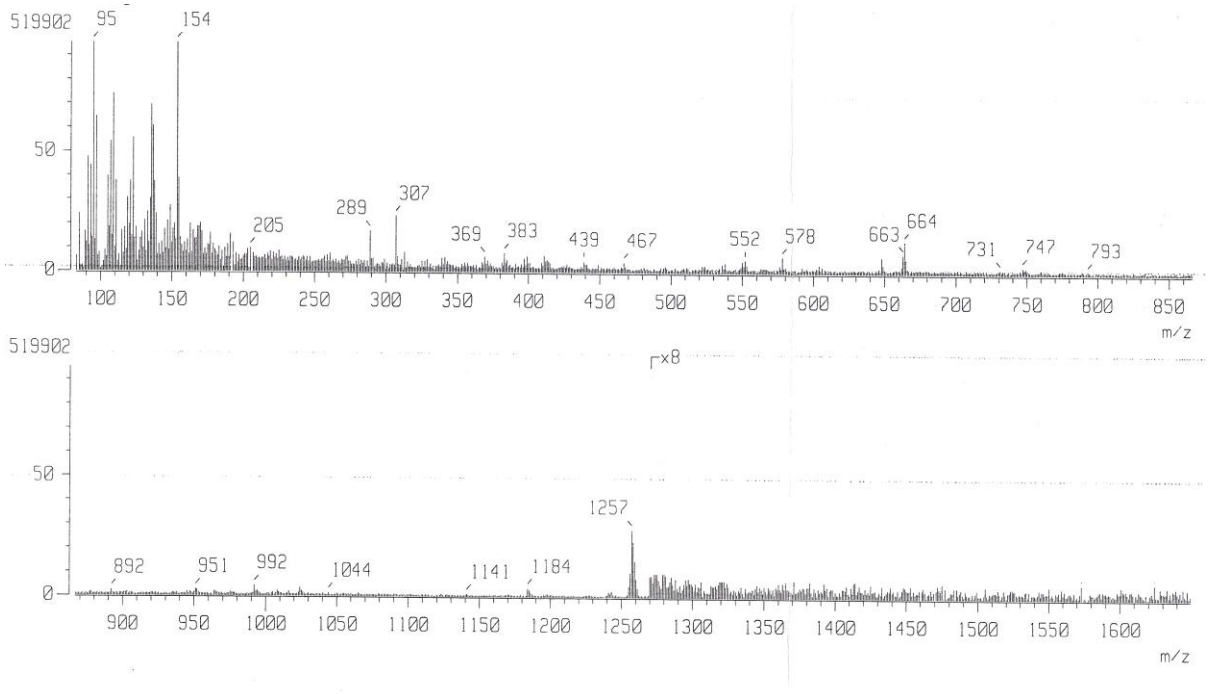


Figure S6. FAB mass spectrum of **4**.

7. Pictorial representation of binding modes of compound **4** with Fe^{3+} ions.

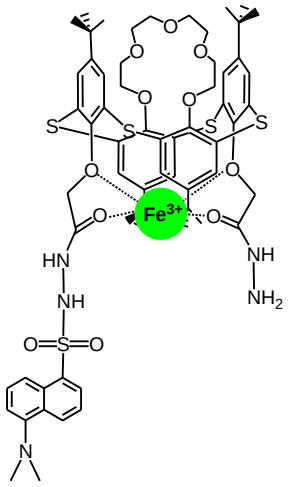


Figure S7. Pictorial representation of binding modes of compound **4** with Fe^{3+} ions

8. Selectivity of receptor **4** for Fe^{3+} ion over other metal ions.

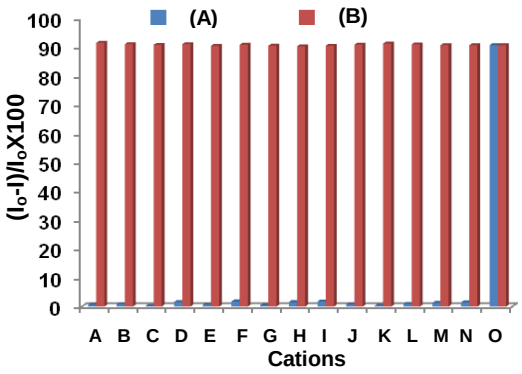


Figure S8. (A) Selectivity of **4** (5.0 µM) towards Fe^{3+} upon addition of different cations and (B) Competitive selectivity of **4** (5.0 µM) towards Fe^{3+} in the presence of different cations in 10% aqueous ethanol. A = Li^{+}, B = Na^{+}, C = K^{+}, D = Ba^{2+}, E = Mg^{2+}, F = Ni^{2+}, G = Cu^{2+}, H = Zn^{2+}, I = Ag^{+}, J = Cd^{2+}, K = Hg^{2+}, L = Pb^{2+}, M = Co^{2+}, N = Fe^{2+}, O = Fe^{3+}.

9. Job plot for **3** and Fe^{3+}/ CN^- in 10% aqueous ethanol.

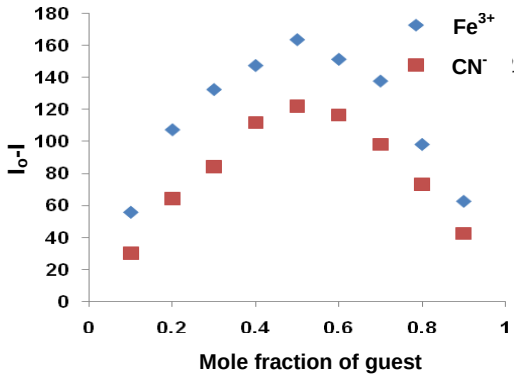


Figure S9. Job plot for **4** and guest (Fe^{3+} or CN^-) in 10% aqueous ethanol.

10. Ratiometric selectivity of compound **4** towards CN^- ions over other anions.

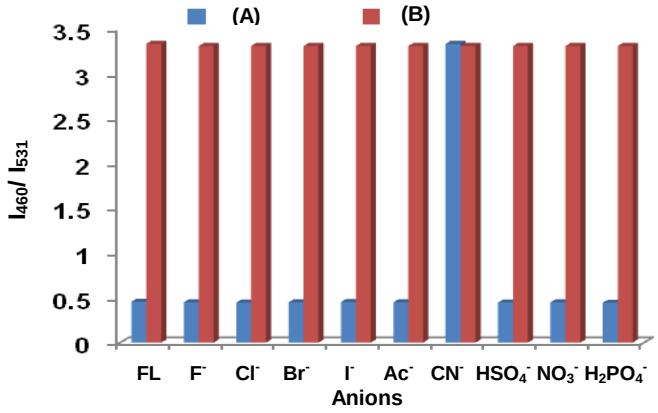
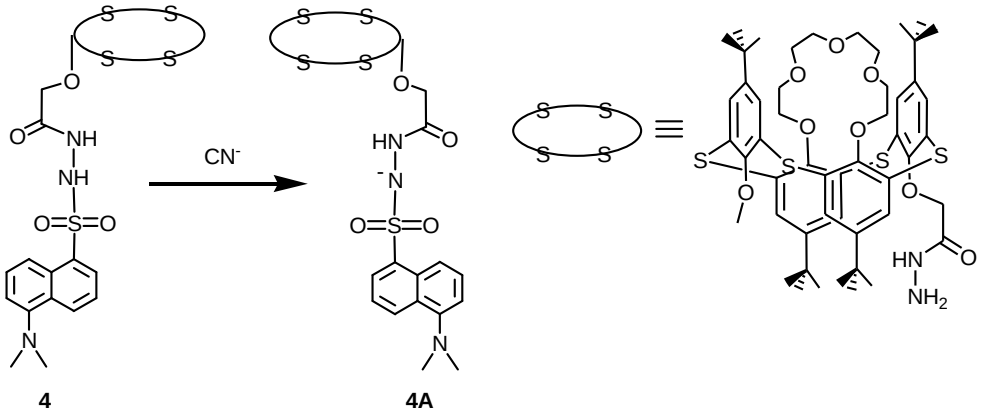


Figure S10. (A) Ratiometric selectivity of **4** (5.0 µM) towards CN^- upon addition of different anions and (B) Competitive selectivity of **4** (5.0 µM) towards CN^- in the presence of different anions in 10% aqueous ethanol

11. The intermolecular proton transfer between cyanide and N-H group of sulphonamide group of thiacalix[4]podand **4**.



Scheme S1. The intermolecular proton transfer between cyanide and N-H group of sulphonamide group of thiacalix[4]podand **4**.

12. ^{1}H NMR spectra of compound **4** with CN^- ions in $CDCl_3$.

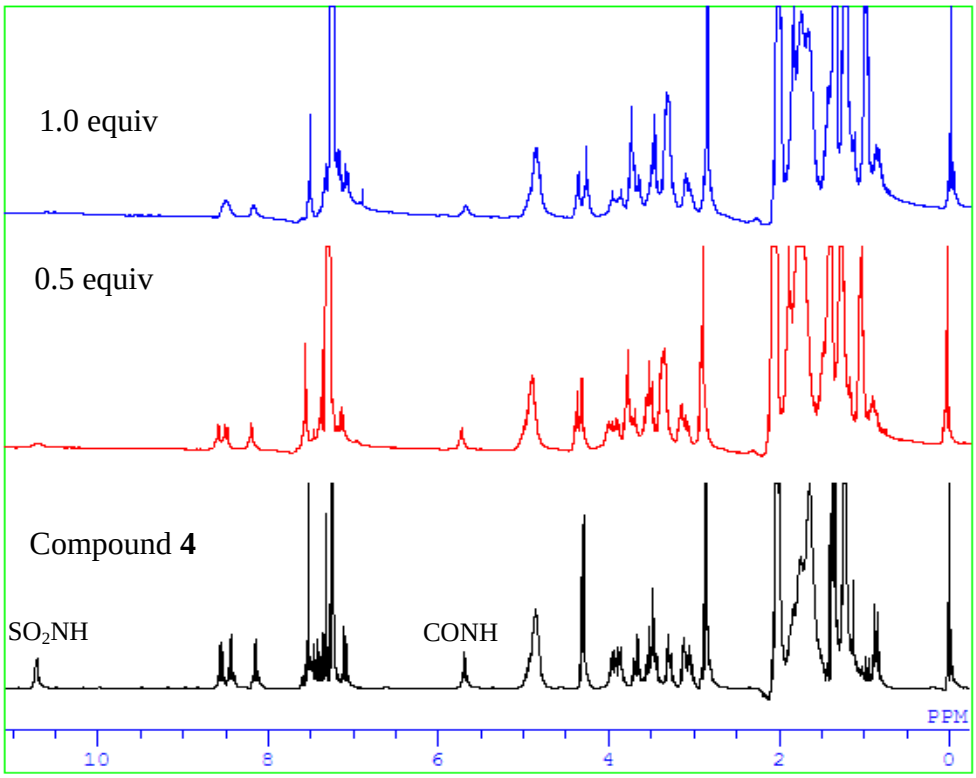


Figure S11. ^{1}H NMR spectra of compound **4** with CN^- ions in $CDCl_3$.

13. Sequential logic circuit for the second sequence with two input strings *In*C and *In*F at λ 460 nm and 531 nm.

(A)

Entry	*In* C (CN^-)	*In* F (Fe^{3+})	Output 1 (λ 460 nm)	Output 2 (λ 531 nm)
1	0	0	0	1
2	1	0	1	0
3	0	1	0	0
4	1	1	0	0

(B)

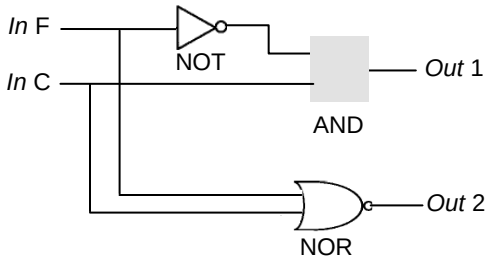


Figure S12. (A) Truth table for the second sequence (addition of first input *InC* followed by second input *InF*) of molecular crossword puzzle; (B) Sequential logic circuit for the second sequence with two input strings *In*C and *In*F at λ 460 nm and 531 nm.