Electronic Supplementary Material (ESI) for Dalton Transactions
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Supplementary Information

Ratiometric/'turn-On' fluorescent chemosensor for CN^-: mimicking XNOR logic function with Fe^{3+} ions

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Contents **Page No.**

1. ^{1}H NMR spectrum of **5** in $CDCl_3$.

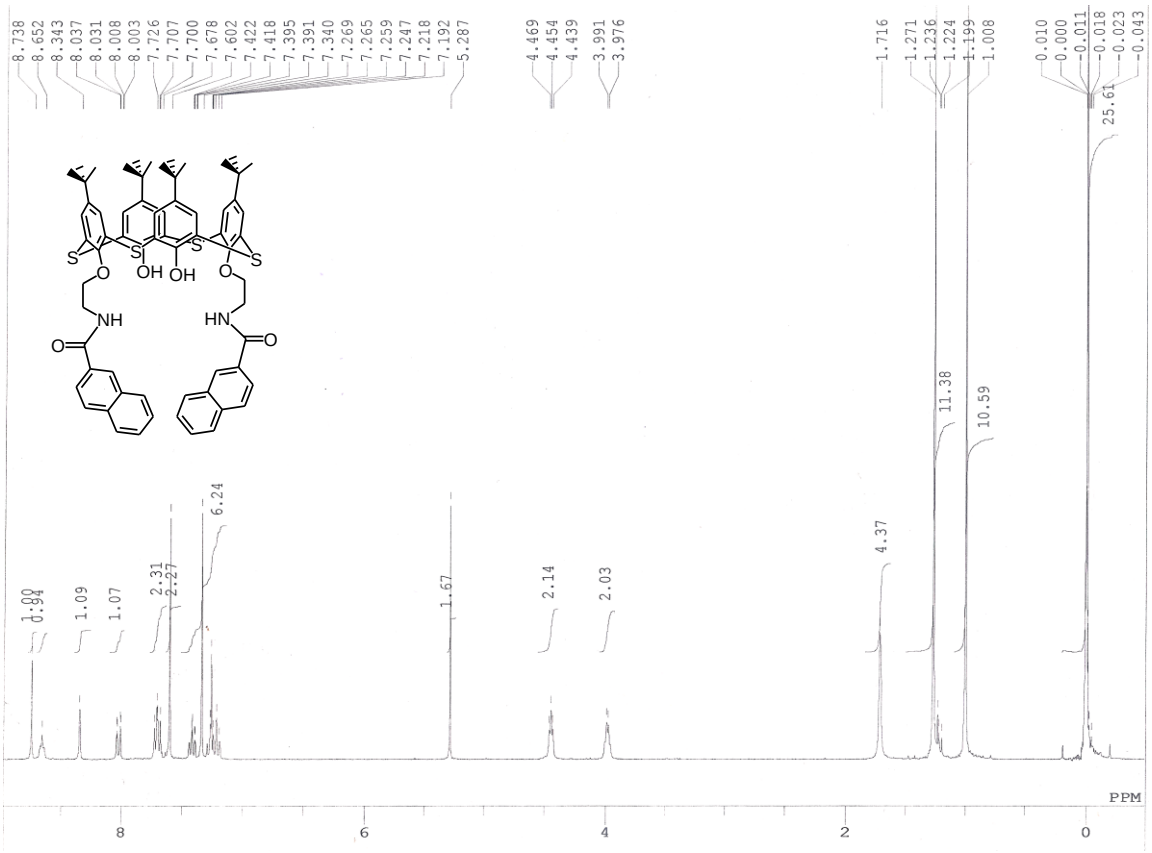

Figure S1. ^{1}H NMR spectrum of **5** in $CDCl_3$.

2. FAB mass spectrum of **5**.

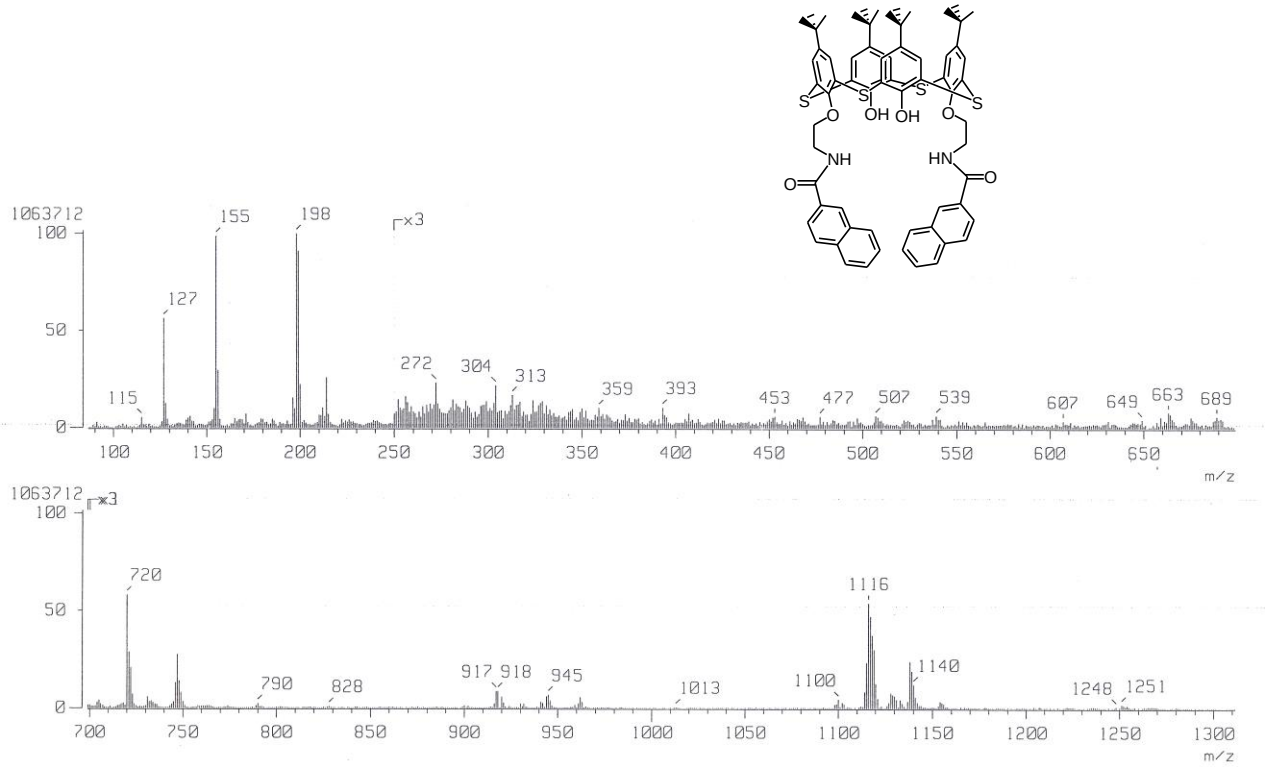

Figure S2. FAB mass spectrum of **5**.

3. ^{1}H NMR spectrum of **6** in $CDCl_3$.

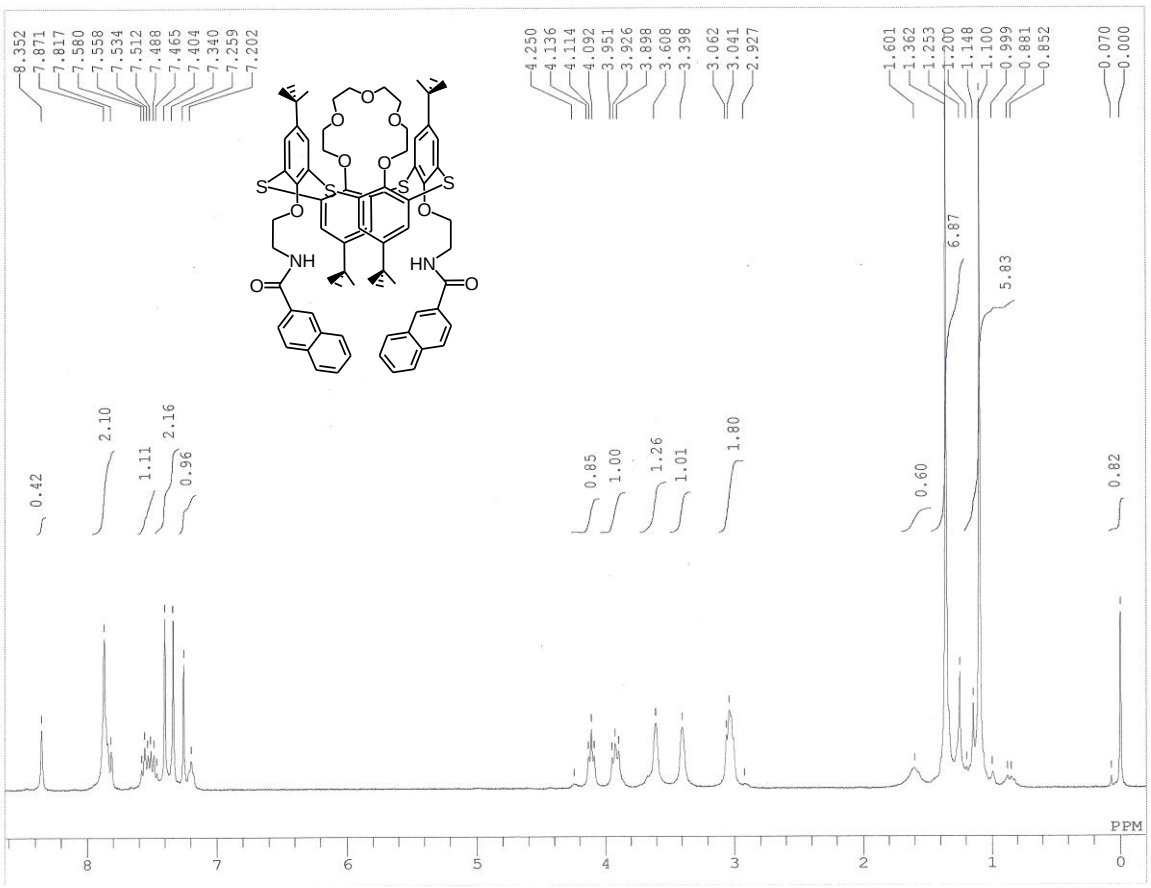

Figure S3. ^{1}H NMR spectrum of **6** in $CDCl_3$.

4. ^{13}C NMR Spectrum of **6** in $CDCl_3$.

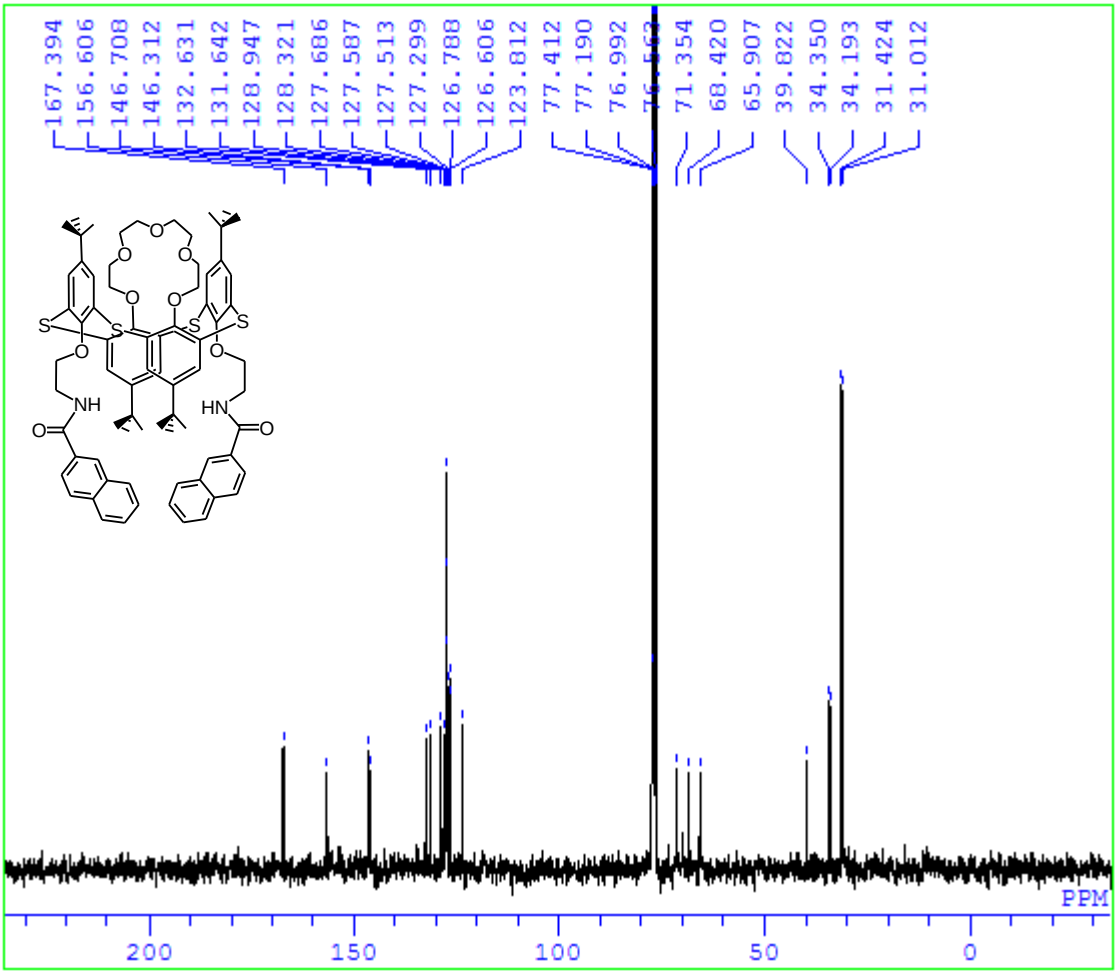

Figure S4. ^{13}C NMR spectrum of **6** in $CDCl_3$.

5. ESI mass spectrum of **6**.

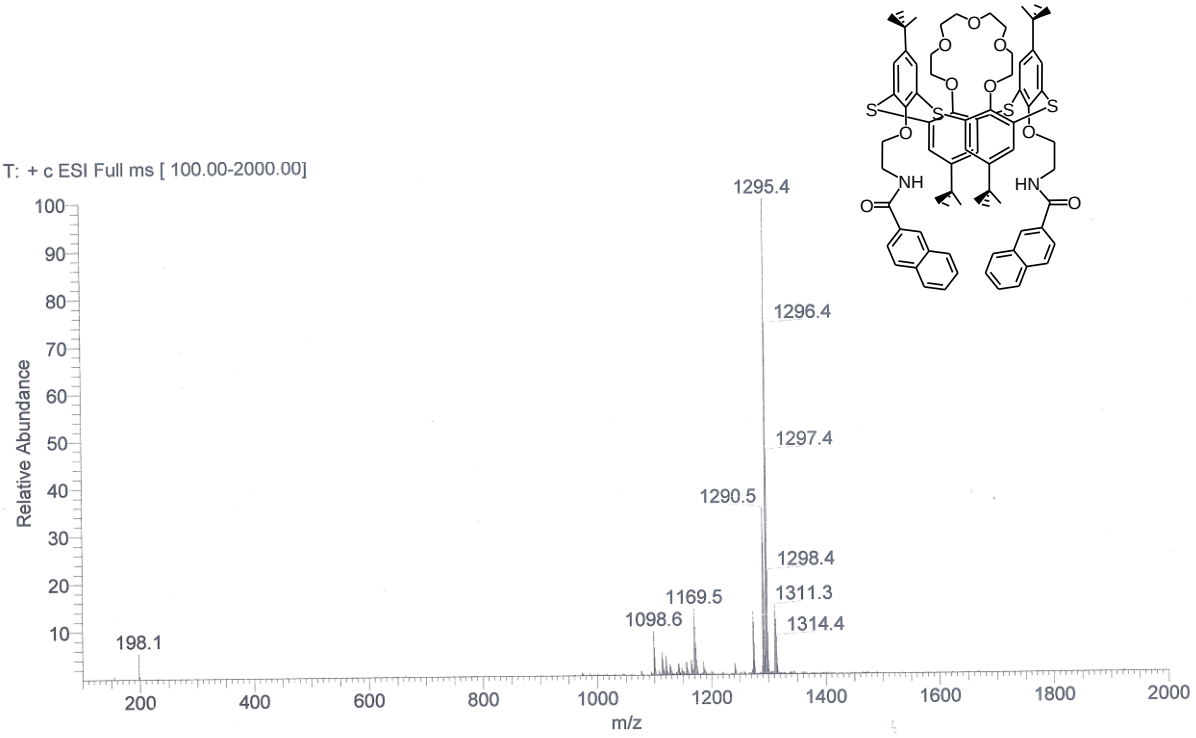

Figure S5. ESI-MS mass spectrum of **6**.

6. ^{1}H NMR spectrum of **7** in $CDCl_3$.

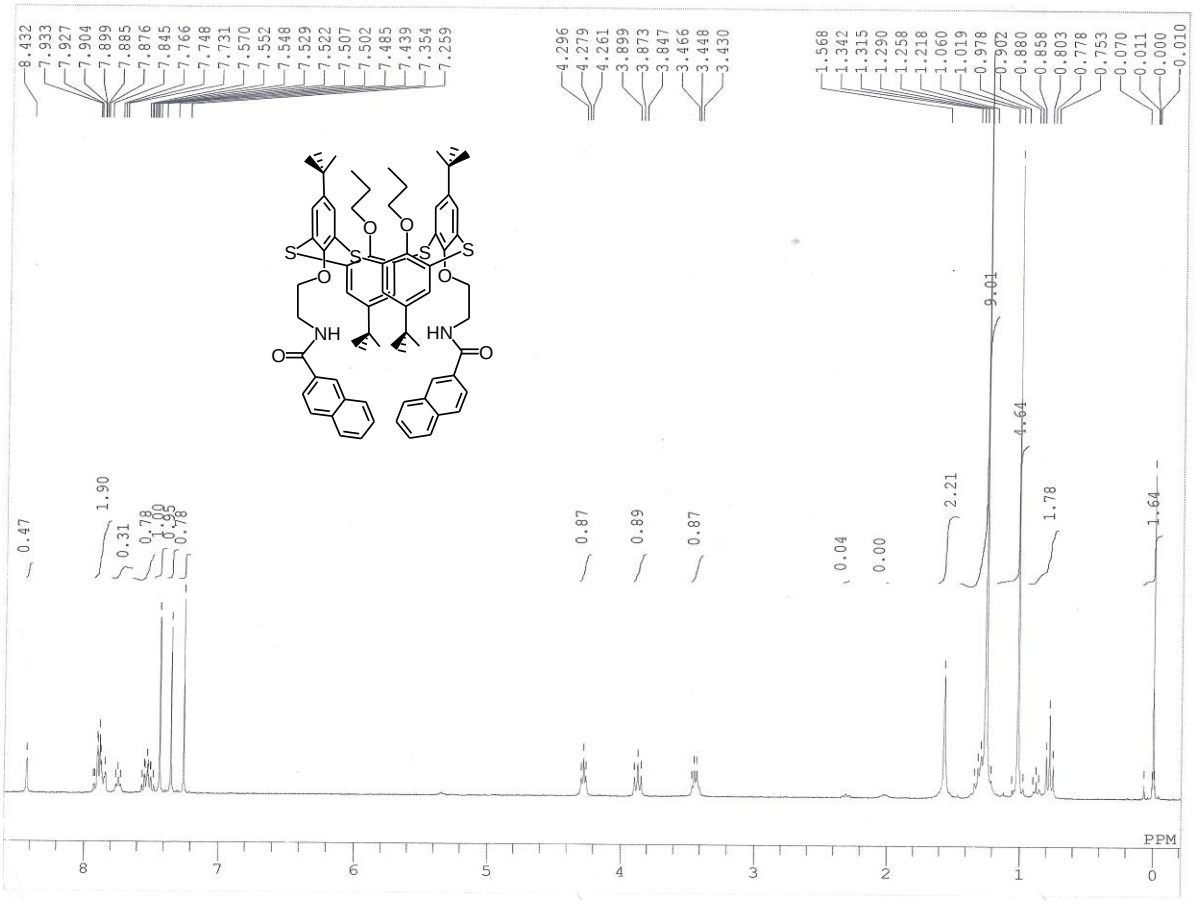

Figure S6. ^{1}H NMR spectrum of **7** in $CDCl_3$.

7. ^{13}C NMR Spectrum of **7** in $CDCl_3$.

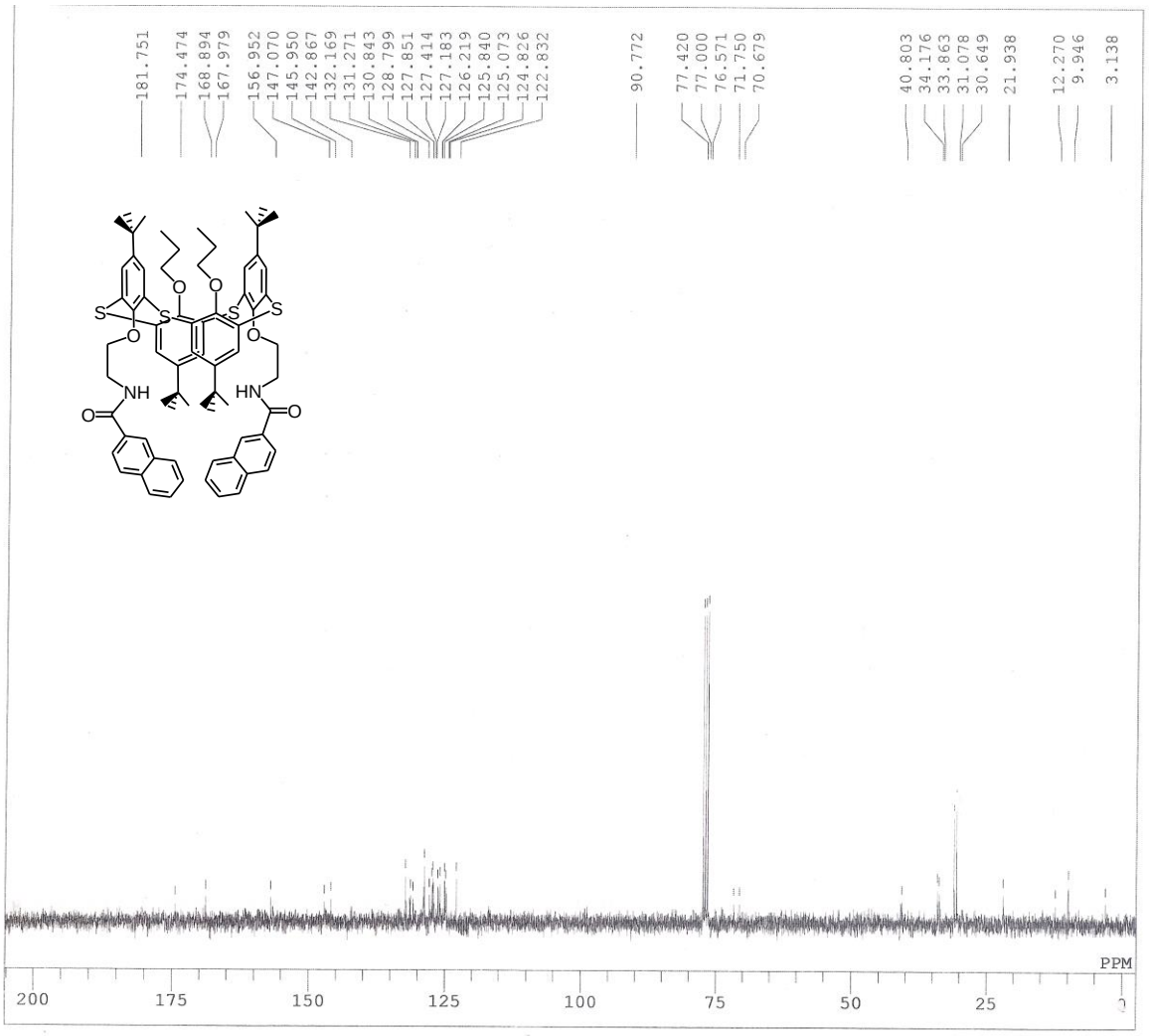

Figure S7. ^{13}C NMR spectrum of **7** in $CDCl_3$.

8. FAB-MS mass spectrum of **7**.

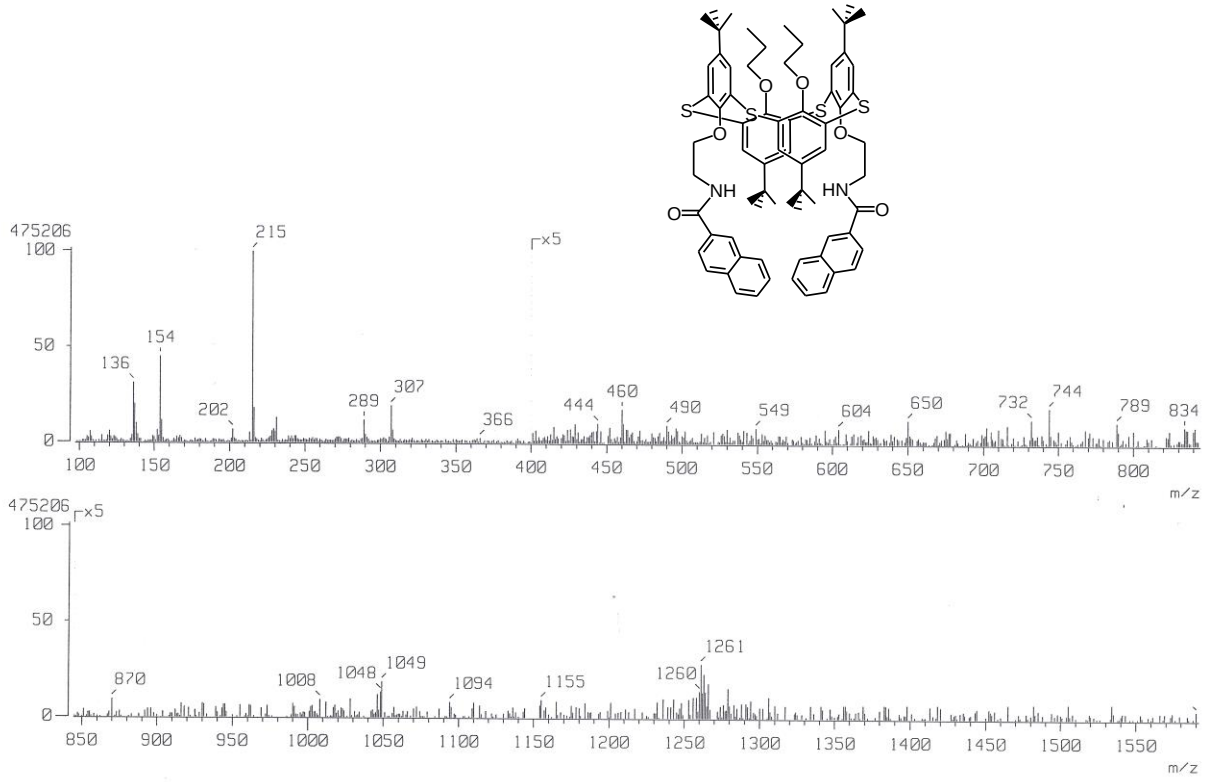

Figure S8. ESI-MS mass spectrum of **7**.

9. Fluorescence spectra of compound **7** with CN^- in THF.

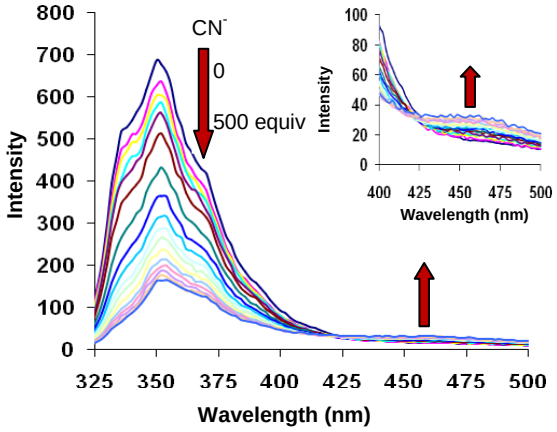

Figure S9 Fluorescence emission spectra of receptor **7** (10 μM) upon various addition of CN^- (0-500 equiv) in THF.

10. Selectivity of compound **7** towards CN^- in the presence of different anions in THF.

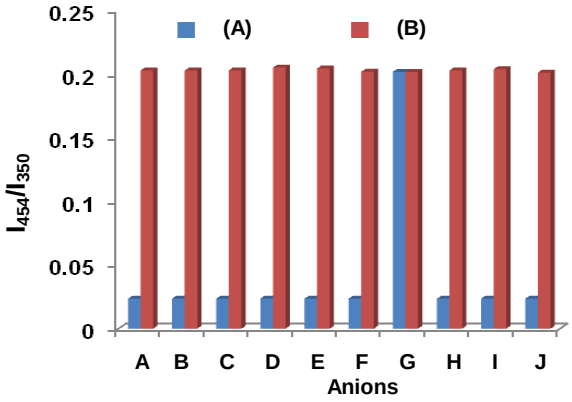

Figure S10. (A) Ratiometric selectivity of **7** (10 μM) towards CN^- upon addition of different anions and (B) Ratiometric competitive selectivity of **7** (10 μM) towards CN^- in the presence of different anions in THF. A=FL, B=F^-, C=Cl^-, D=Br^-, E=I^-, F=OAc^-, G=CN^-, H=HSO_4, I= NO_3^-, J=$H_2PO_4^-$.

11. ^{1}H NMR of compound **5** + CN^- ions in $CDCl_3$.

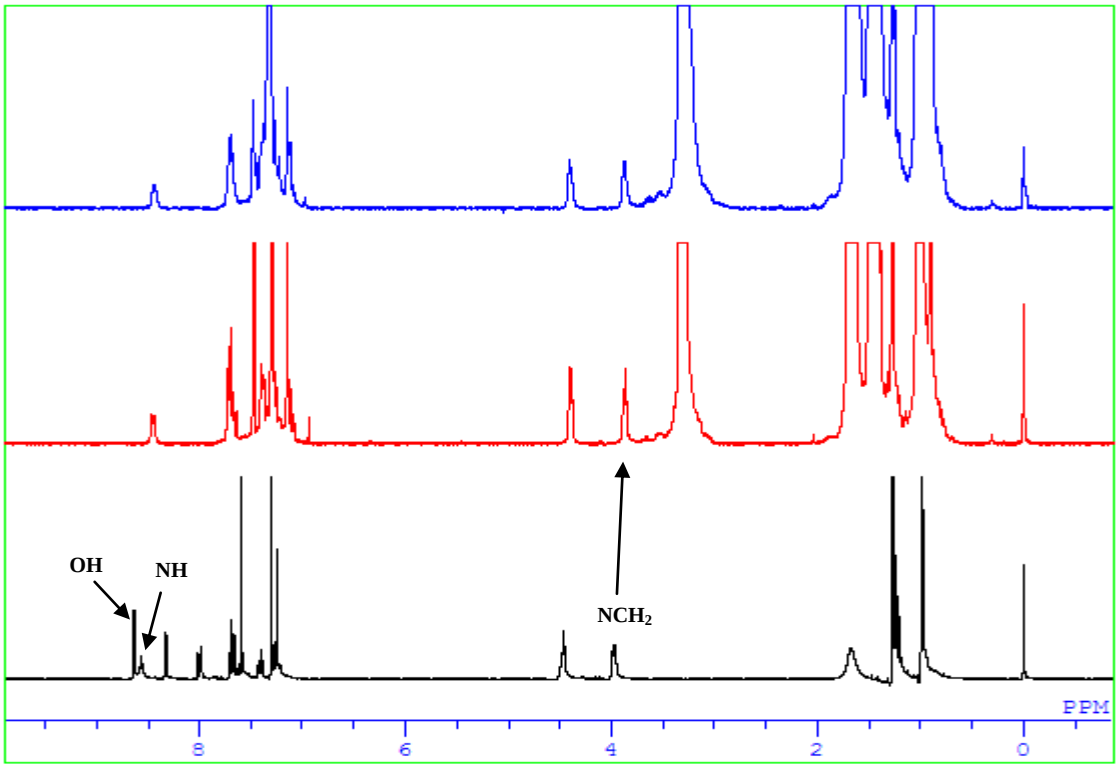

Figure S11. ^{1}H NMR of compound **5** + CN^- ions in $CDCl_3$.

12. ^{1}H NMR of compound **6** + CN^- ions in $CDCl_3$.

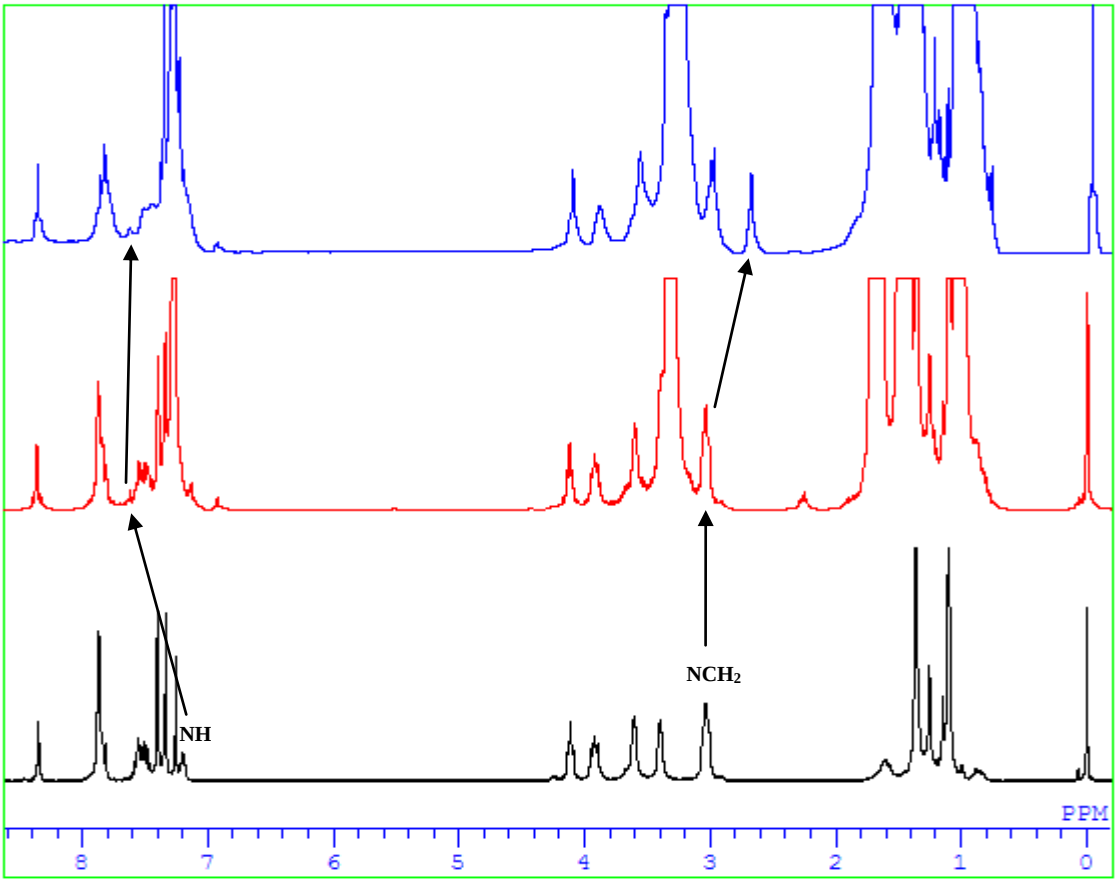

Figure S12. ^{1}H NMR of compound **6** + CN^- ions in $CDCl_3$.

13. Selectivity of compound **5** towards CN^- in the presence of different anions in THF.

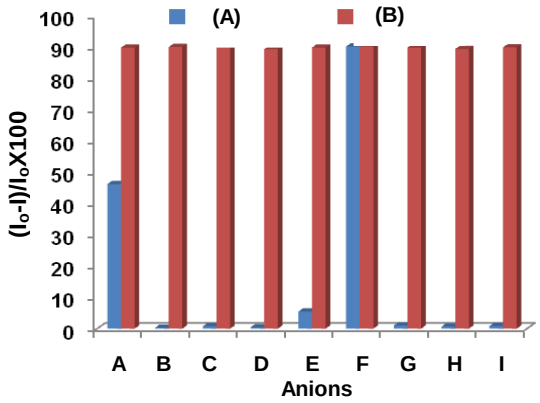

Figure S13. (A) Selectivity of **5** (10 µM) towards CN^- upon addition of different anions and (B) Competitive selectivity of **5** (10 µM) towards CN^- in the presence of different anions in THF. A=F^-, B=Cl^-, C=Br^-, D=I^-, E=OAc^-, F=CN^-, G=HSO_4^-, H= NO_3^-, I=$H_2PO_4^-$.

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14. Job plot of compounds **5-7** with CN^- in THF.

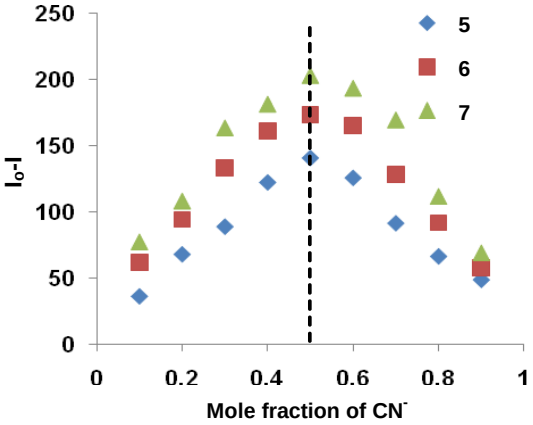

Figure S14. Job's plot of **5-7** with CN^- in THF.

15. Fluorescence spectra of compound **6** with Fe^{3+} in THF.

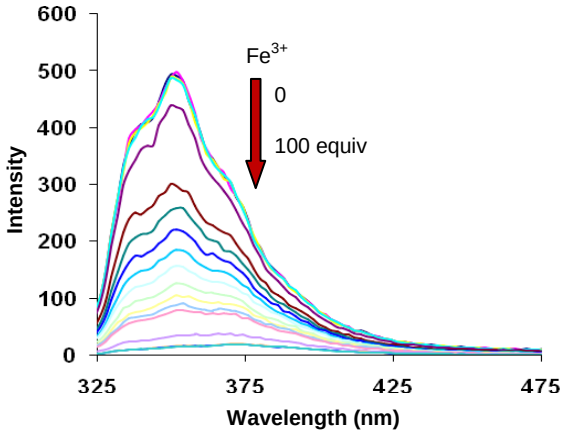

Figure S15 Fluorescence emission spectra of receptor **6** (10 μM) upon various addition of Fe^{3+} (0-100 equiv) in THF.

16. Fluorescence emission spectra of receptor **7** upon various addition of Fe^{3+} in THF.

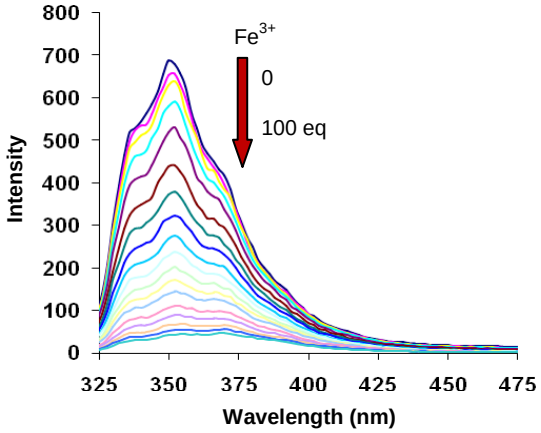

Figure S16. Fluorescence emission spectra of receptor **7** (10 µM) upon various addition of Fe^{3+} (0-100 equiv) in THF.

17. Pictorial representation of binding modes of compound **5**-**7** upon addition of Fe^{3+} ion.

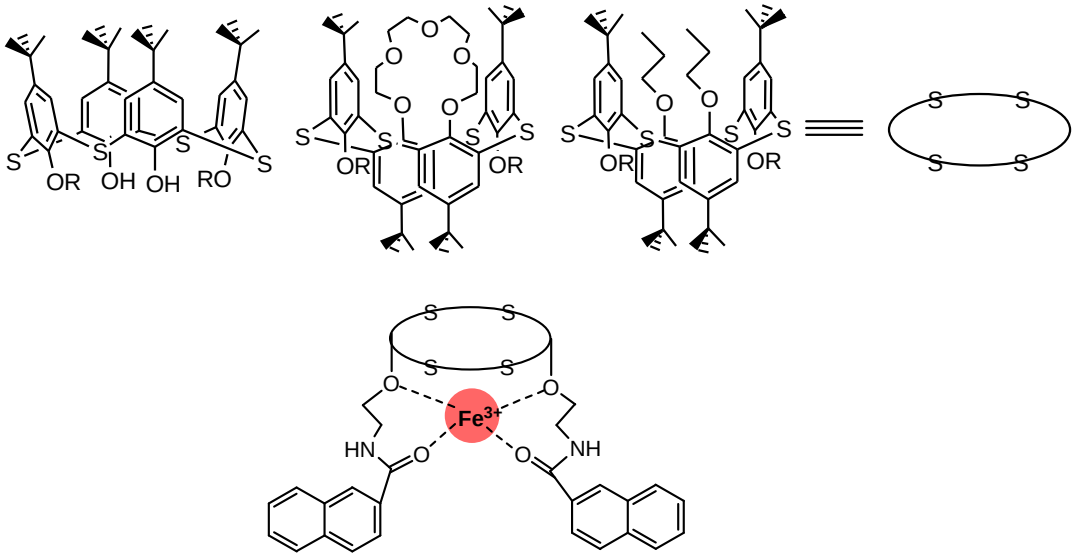

Figure S17. Pictorial representation of binding modes of compound **5**-**7** upon addition of Fe^{3+} ion.

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18. Selectivity of compounds **5** and **6** towards Fe^{3+} in THF.

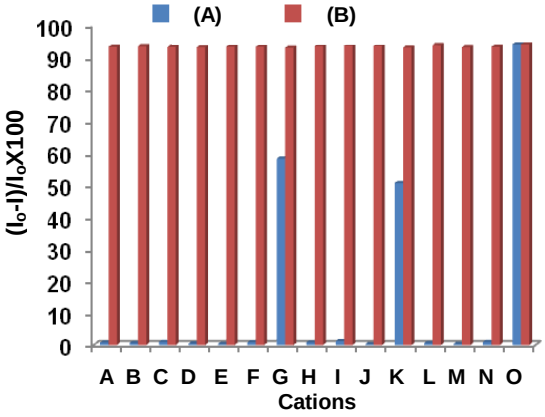

Figure S18. (A) Selectivity of **5** (10 μM) towards Fe^{3+} upon addition of different cations and (B) Competitive selectivity of **5** (10 μM) towards Fe^{3+} in the presence of different cations in 10% aqueous ethanol. A=Li^{+}, B=Na^{+}, C=K^{+}, D=Ba^{2+}, E=Mg^{2+}, F=Ni^{2+}, G=Cu^{2+}, H= Zn^{2+}, I=Ag^{+}, J= Cd^{2+}, K=Hg^{2+}, L=Pb^{2+}, M=Co^{2+}, N=Fe^{2+}, O=Fe^{3+}.

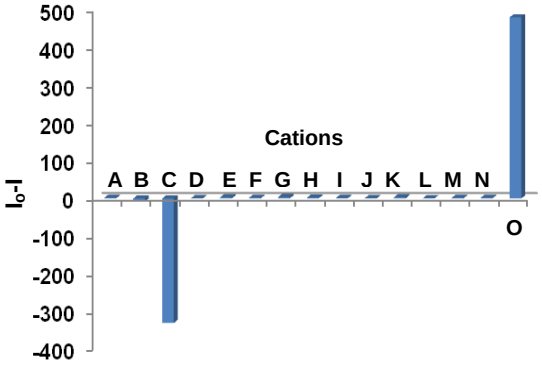

Figure S19. Selectivity of **6** (10 μM) towards Fe^{3+} and K^{+} upon addition of different cations in THF. A=Li^{+}, B=Na^{+}, C=K^{+}, D=Ba^{2+}, E=Mg^{2+}, F=Ni^{2+}, G=Cu^{2+}, H= Zn^{2+}, I=Ag^{+}, J= Cd^{2+}, K=Hg^{2+}, L=Pb^{2+}, M=Co^{2+}, N=Fe^{2+}, O=Fe^{3+}.

19. Selectivity and competitive selectivity of **7** towards Fe^{3+} in THF.

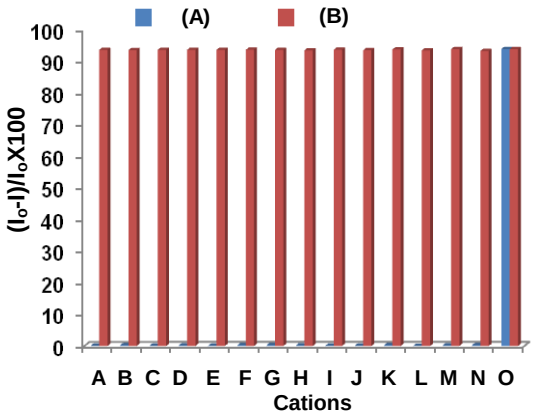

Figure S20. (A) Selectivity of **7** (10 µM) towards Fe^{3+} upon addition of different cations and (B) Competitive selectivity of **7** (10 µM) towards Fe^{3+} in the presence of different cations in 10% aqueous ethanol. A=Li^{+}, B=Na^{+}, C=K^{+}, D=Ba^{2+}, E=Mg^{2+}, F=Ni^{2+}, G=Cu^{2+}, H= Zn^{2+}, I=Ag^{+}, J= Cd^{2+}, K=Hg^{2+}, L=Pb^{2+}, M=Co^{2+}, N=Fe^{2+}, O=Fe^{3+}.

20. Job plot of compounds **5-7** with Fe^{3+} in THF.

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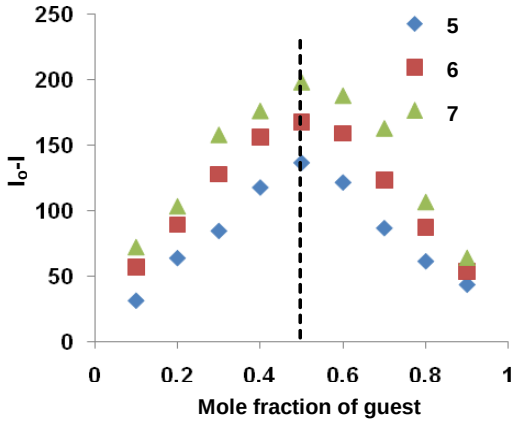

Figure S21. Job's plot of **5-7** with Fe^{3+} in THF.

21. Fluorescence emission spectra of **6.Fe^{3+}** and **7.Fe^{3+}** complexes upon addition of CN^- in THF.

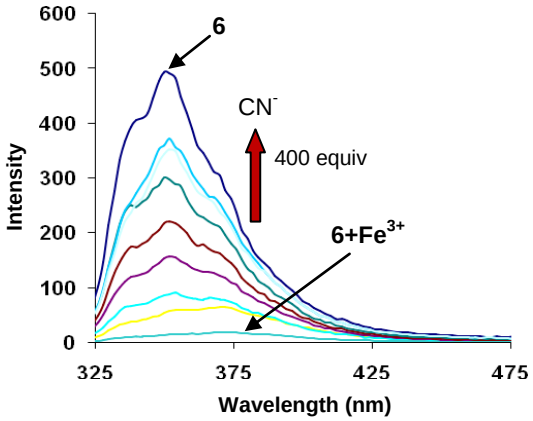

Figure S22 Fluorescence emission spectra of receptor **6.Fe**$^{3+}$ complex upon various addition of CN^- (0-400 equiv) in THF.

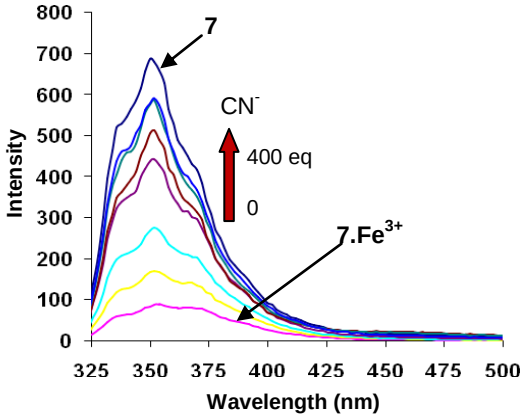

Figure S23. Fluorescence emission spectra of receptor **7.Fe**$^{3+}$ complex upon various addition of CN^- (0-400 equiv) in THF.

22. Reversibility of **5.Fe**$^{3+}$ complex with addition of CN^- ion.

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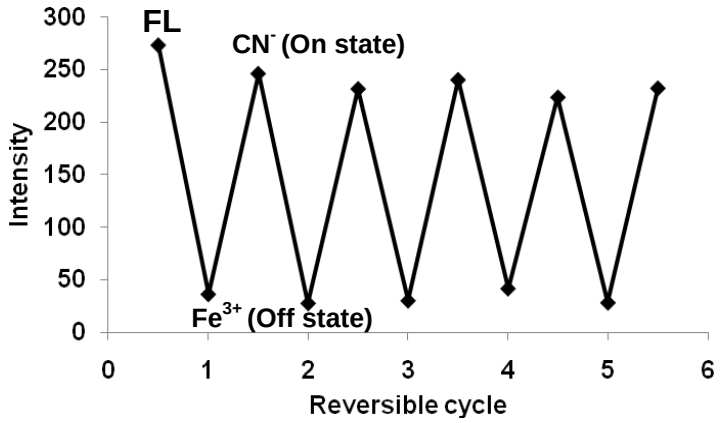

Figure S24. Reversibility of **5.Fe**$^{3+}$ complex with addition of CN^- ion.

23. Selectivity of **5.Fe**$^{3+}$ complex towards CN^- in the presence of other anions in THF.

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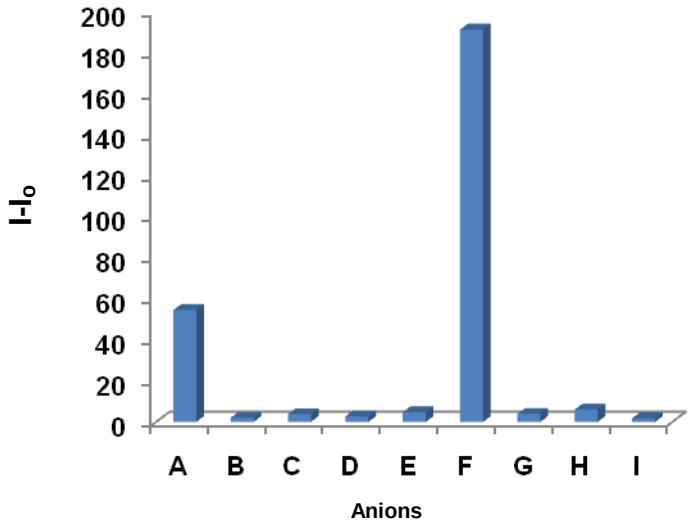

Figure S25. Selectivity of **5.Fe^{3+}** complex towards CN^- upon addition of different anions in THF. A=F^-, B=Cl^-, C=Br^-, D=I^-, E=OAc^-, F=CN^-, G=HSO_4^-, H= NO_3^-, I=$H_2PO_4^-$. I_o indicates fluorescence intensity of **5.Fe^{3+}** complex and I indicate fluorescence intensity of **5.Fe^{3+}-anion** complex.