Electronic Supplementary Information

Concurrent detection and treatment of cyanide contaminated water using mechanosynthesized receptors

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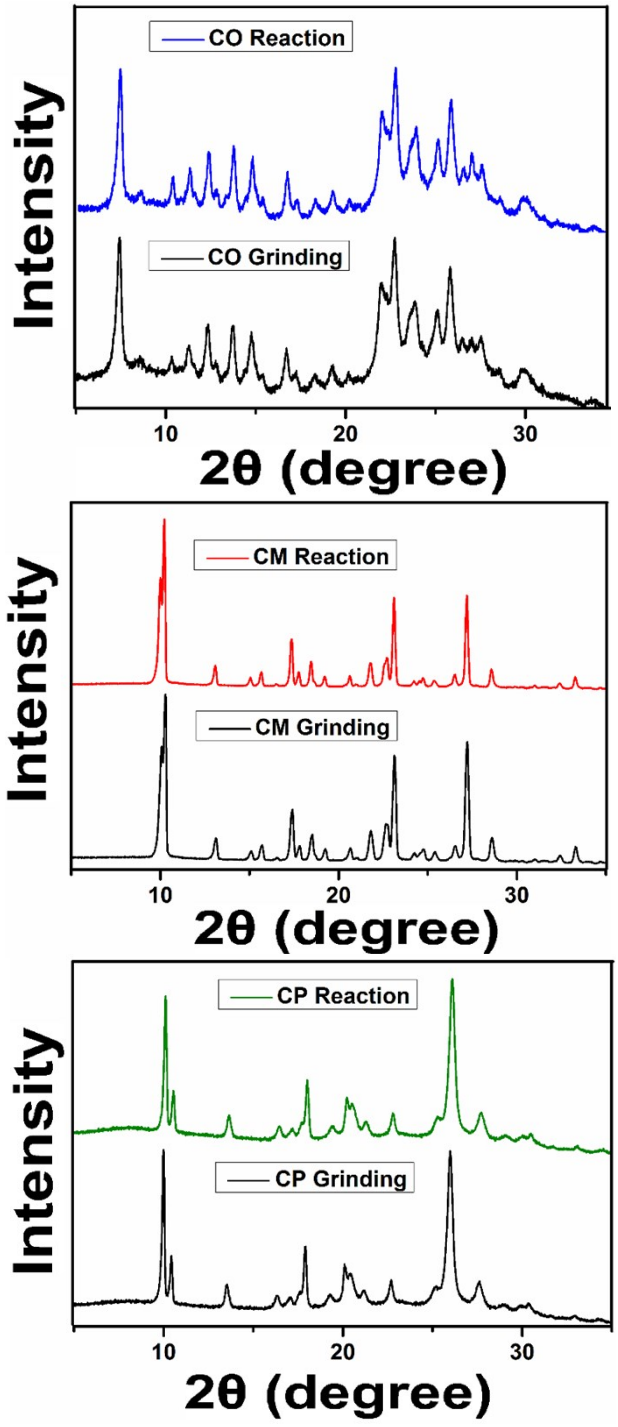

Fig. S1. Comparison of the PXRD patterns of CO, CM, and CP synthesised via MC and solution-based refluxing routes.

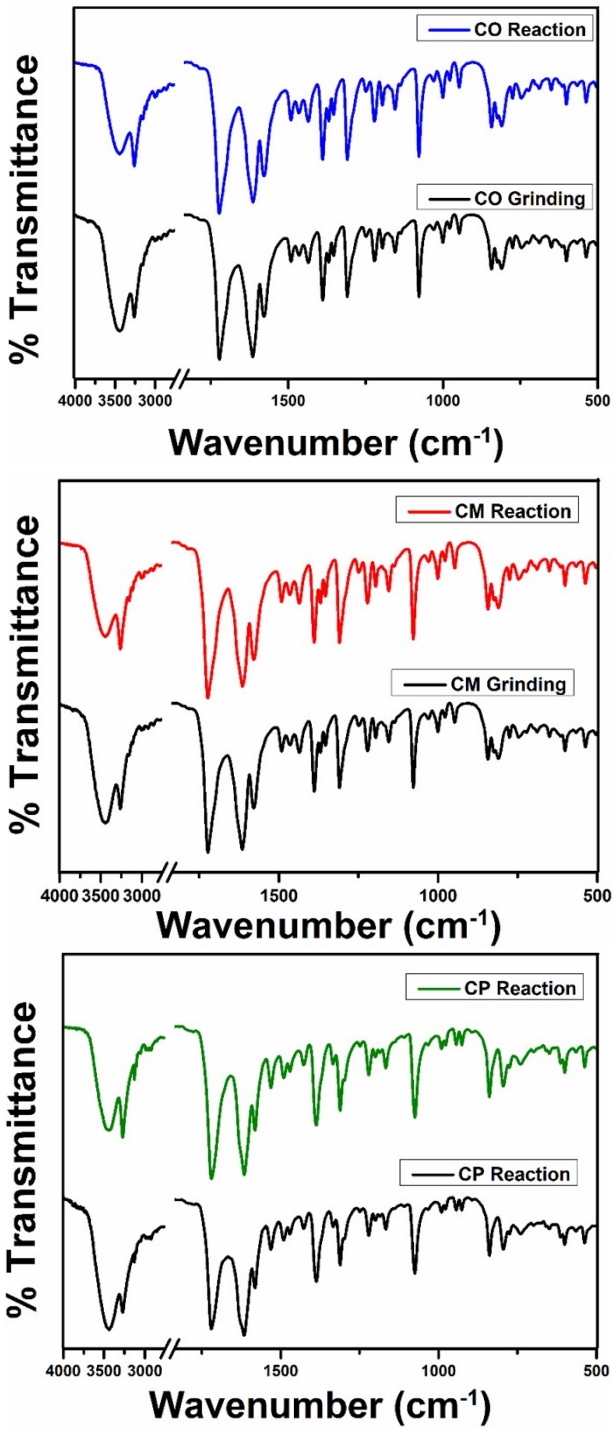

Fig. S2. FTIR profiles of CO, CM, and CP synthesised by two different pathways such as MC and solution-based refluxing.

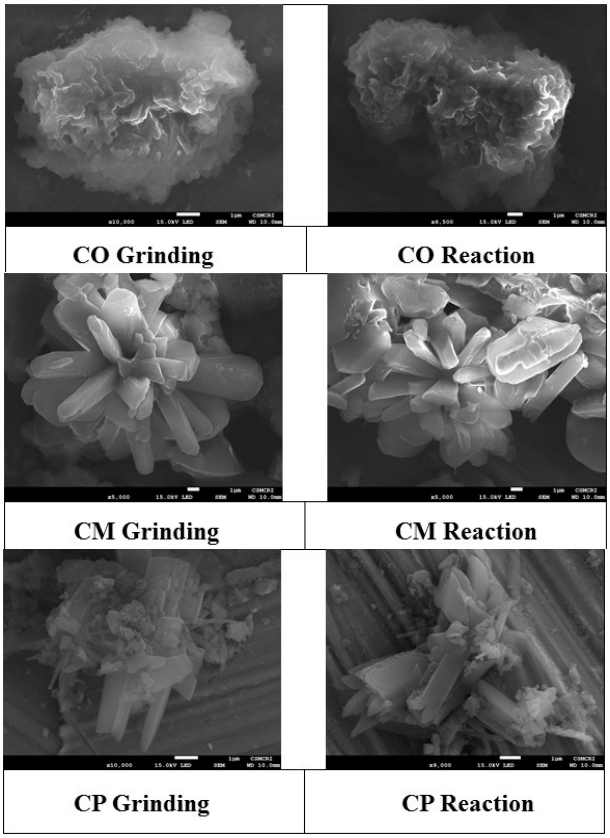

Fig. S3. FE-SEM images of the molecular probes CO, CM, and CP prepared via MC and solution-based refluxing methods.

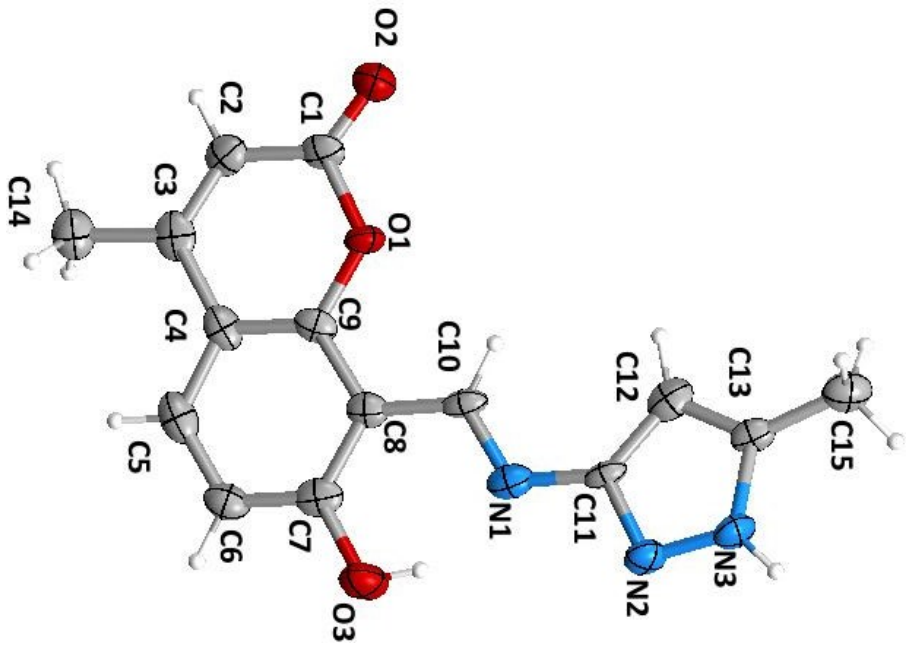

Fig. S4. ORTEP view and atom-numbering scheme of the molecular probe CM. The lattice methanol is omitted for clarity. The ellipsoids represent 50 % probability factor.

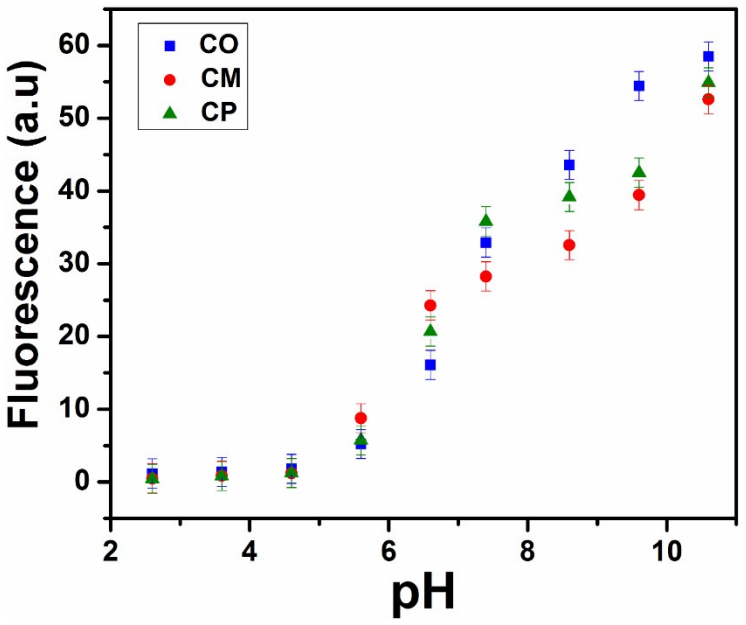

Fig. S5. Fluorescence based pH studies for CO, CM, and CP (20 μM, 2.5 % DMSO in water) in aqueous solution.

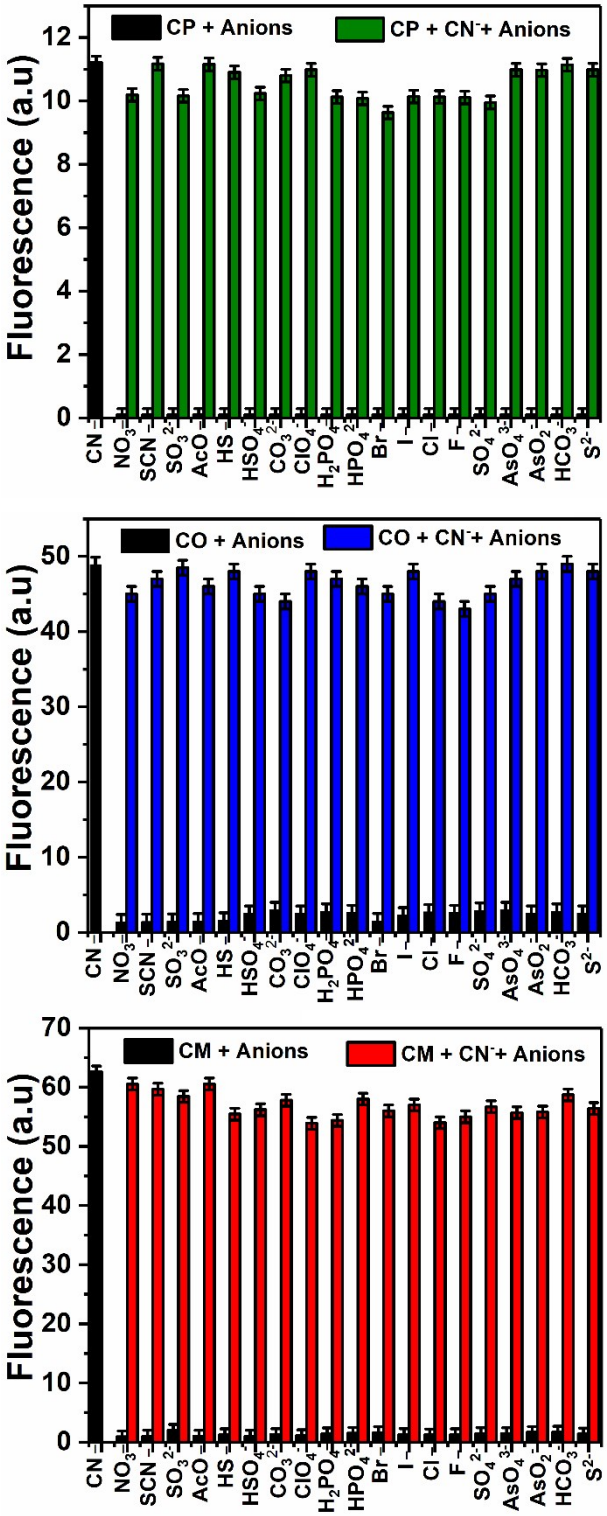

Fig. S6. Competitive fluorescence study of CP, CO, and CM (20 µM in 2.5 % DMSO in water) for cyanide sensing in presence of double excess other anions in HEPES buffer (50 mM) at pH 7.4.

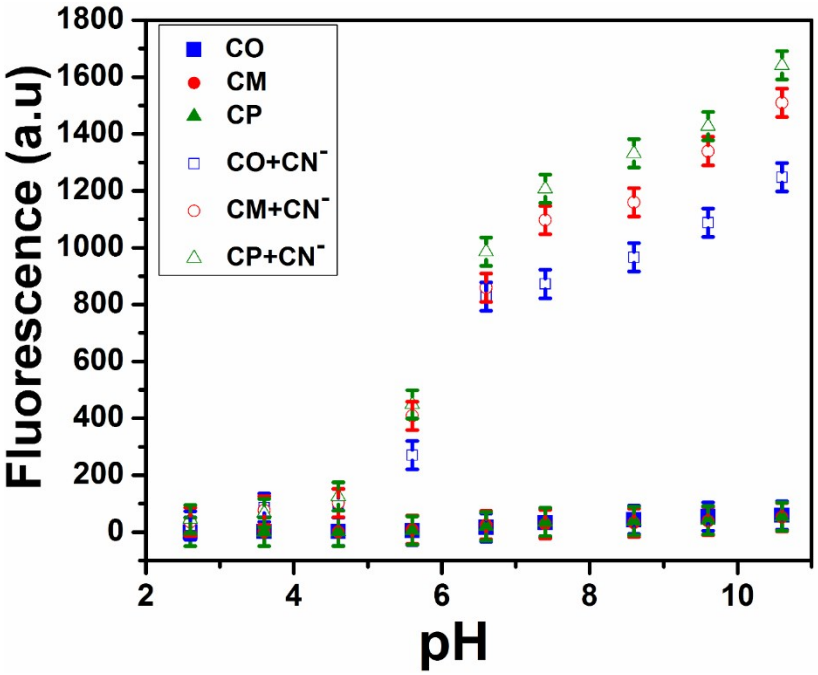

Fig. S7. Fluorescence based pH studies for CO, CM, and CP (20 μM, 2.5 % DMSO in water) in presence of cyanide (2.5 mM) in aqueous solution.

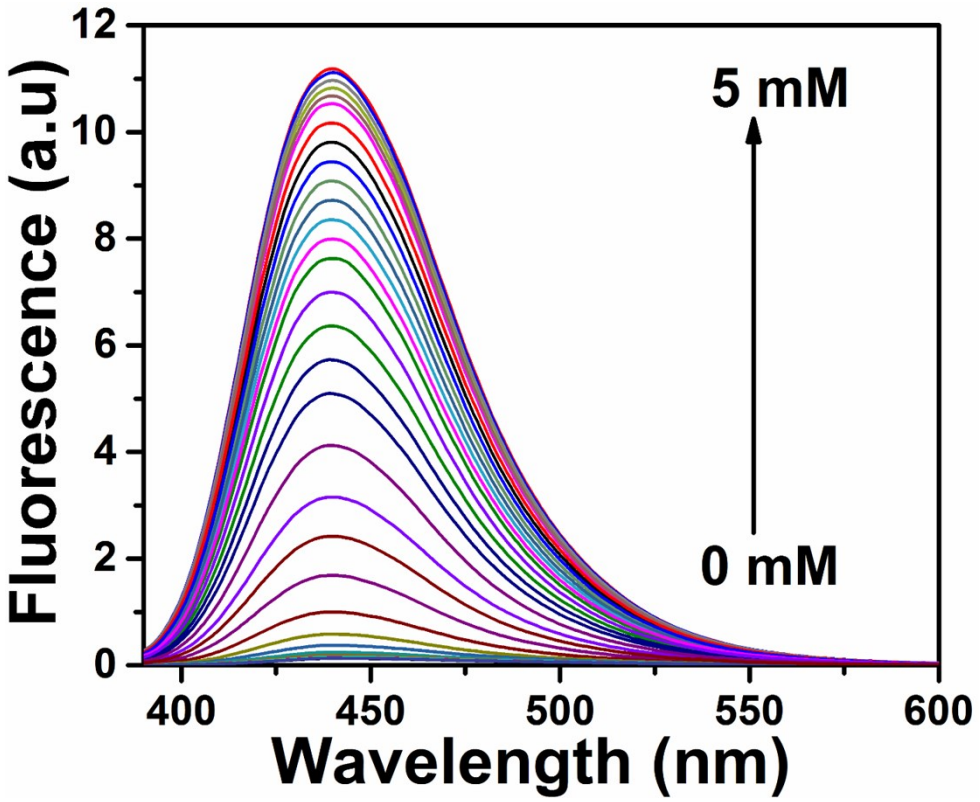

Fig. S8. Fluorescence titration profiles of CP (20 μM, 2.5 % DMSO in water) upon addition of increasing concentrations of cyanide (0-5 mM) in HEPES (50 mM) buffer at physiological pH 7.4.

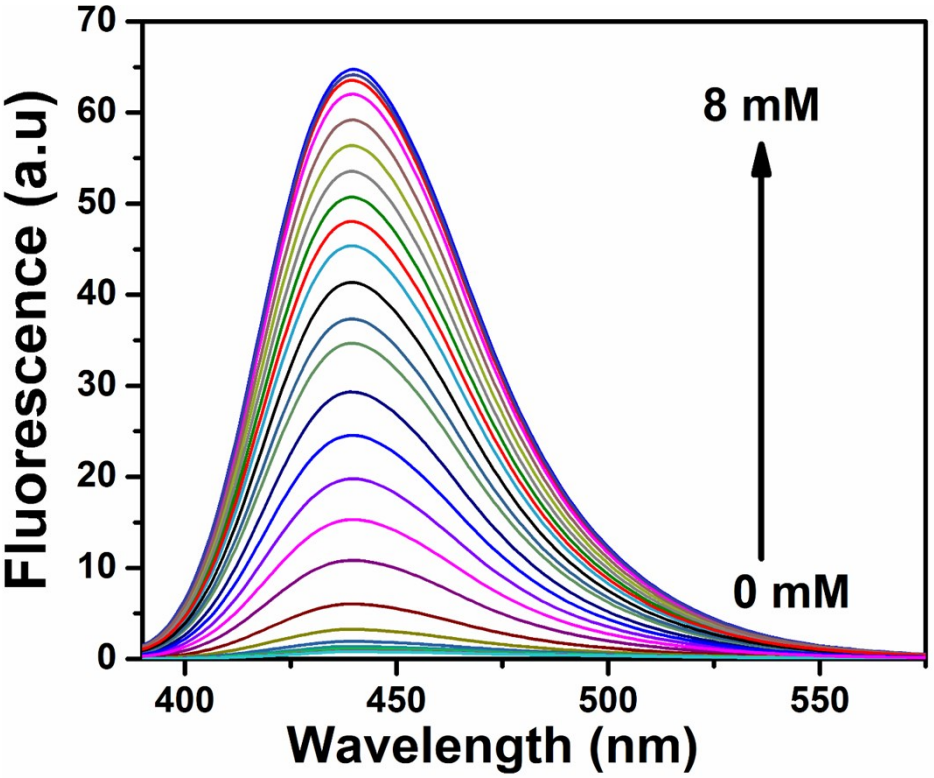

Fig. S9. Fluorescence titration profiles of CO (20 μM, 2.5 % DMSO in water) upon addition of increasing concentrations of cyanide (0-8 mM) in HEPES (50 mM) buffer at physiological pH 7.4.

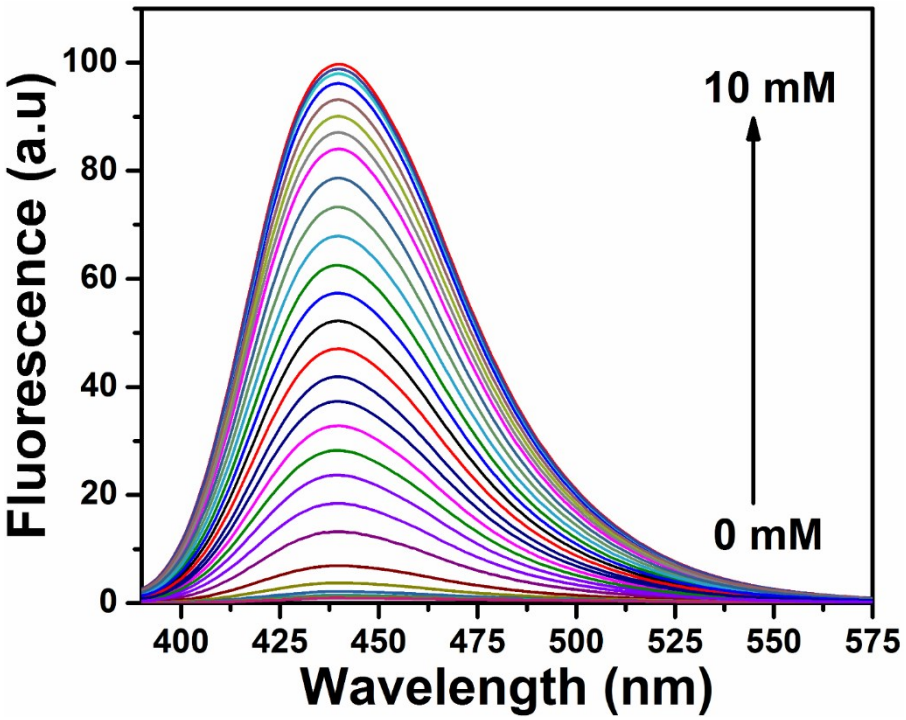

Fig. S10. Fluorescence titration profiles of CM (20 μM, 2.5 % DMSO in water) upon addition of increasing concentrations of cyanide (0-10 mM) in HEPES (50 mM) buffer at physiological pH 7.4.

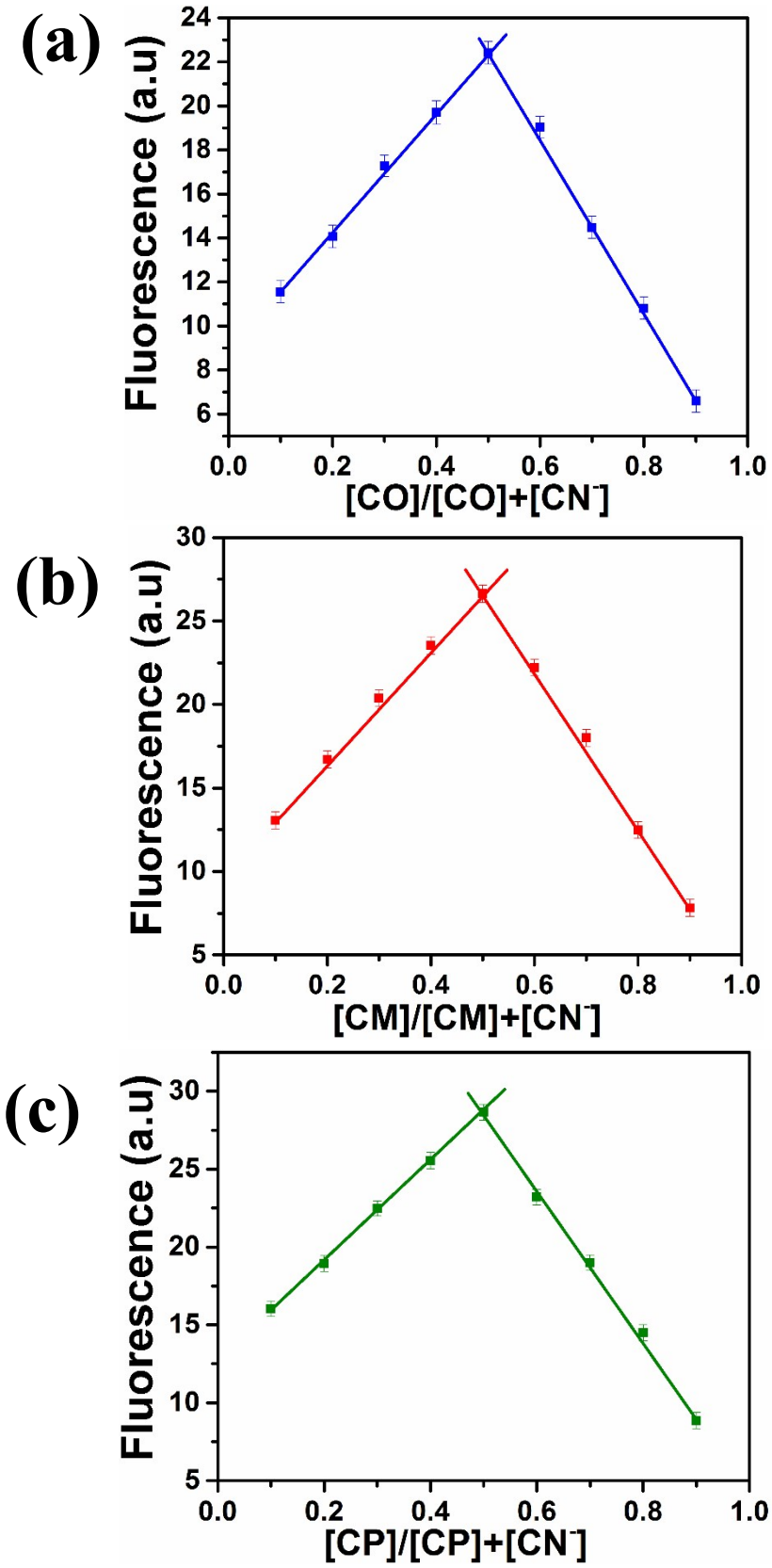

Fig. S11. Job's plots for (a) CO, (b) CM, and (c) CP in presence of different concentrations of cyanide in 50 mM HEPES aqueous buffer solutions.

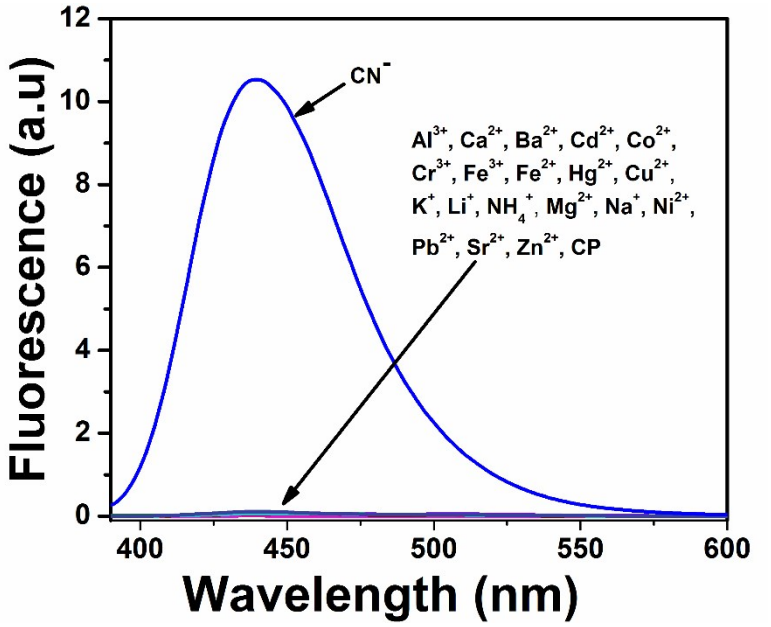

Fig. S12. Fluorescence spectra of mechanosynthesized CP (20 μM, 2.5 % DMSO in water) in HEPES (50 mM aqueous buffer) upon addition of different metal ions. λ_{exi} = 370 nm and λ_{emi}= 444 nm.

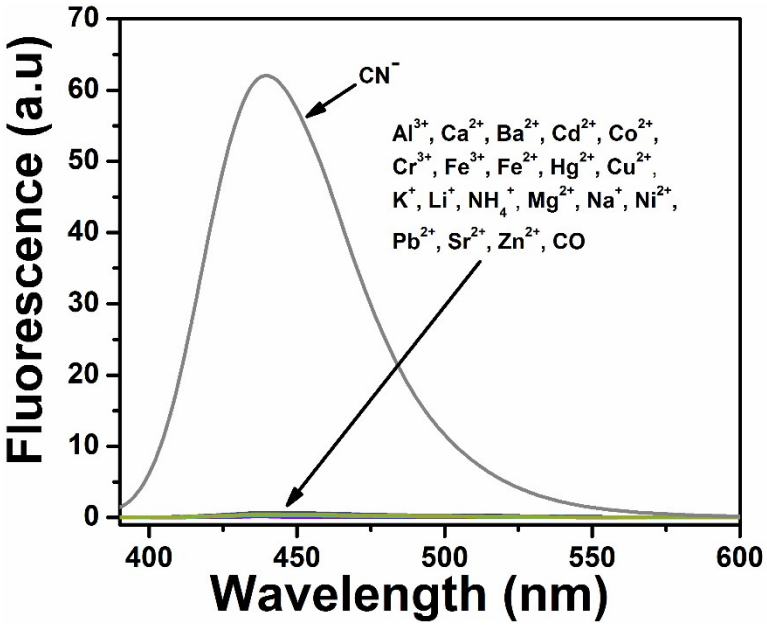

Fig. S13. Fluorescence spectra of mechanosynthesized CO (20 μM, 2.5 % DMSO in water) in HEPES (50 mM aqueous buffer) upon addition of different metal ions. λ_{exi} = 370 nm and λ_{emi}= 444 nm.

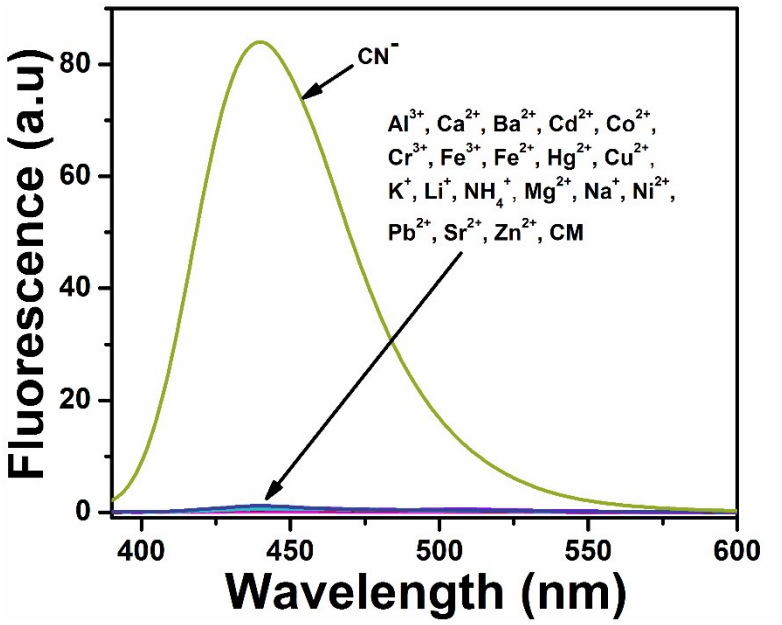

Fig. S14. Fluorescence spectra of mechanosynthesized CM (20 μM, 2.5 % DMSO in water) in HEPES (50 mM aqueous buffer) upon addition of different metal ions. λ_{exi} = 370 nm and λ_{emi}= 444 nm.

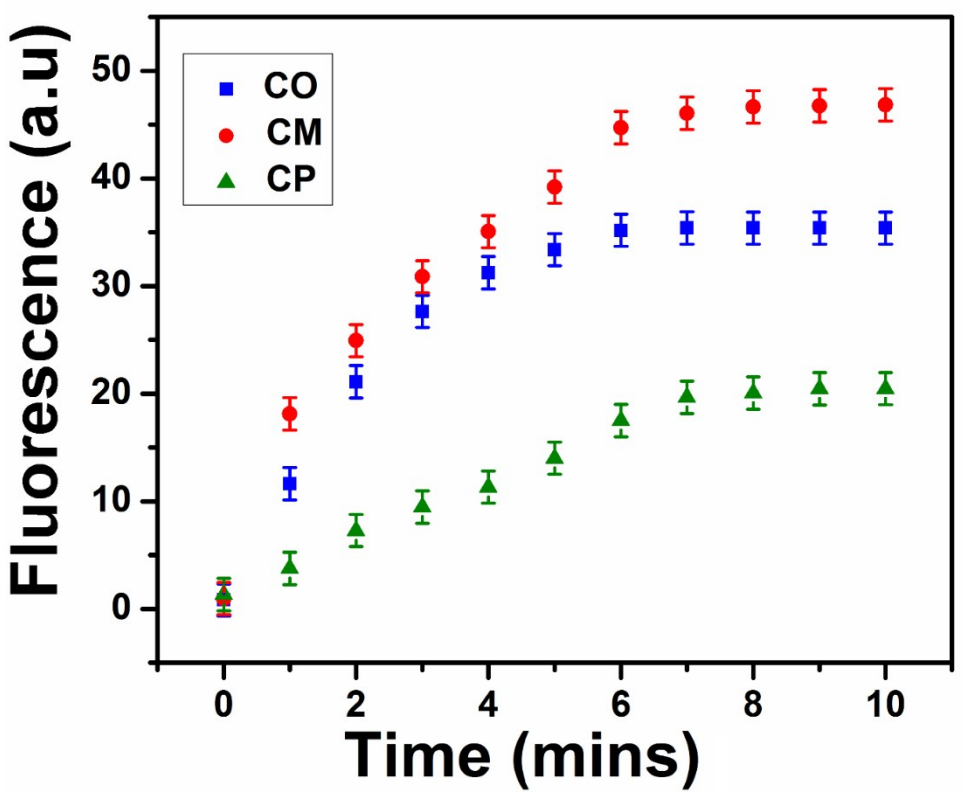

Fig. S15. Time dependent emission changes in the fluorescence profiles of CO, CM, and CP (20 μM, 2.5 % DMSO in water) in HEPES (50 mM aqueous buffer) on addition of cyanide.

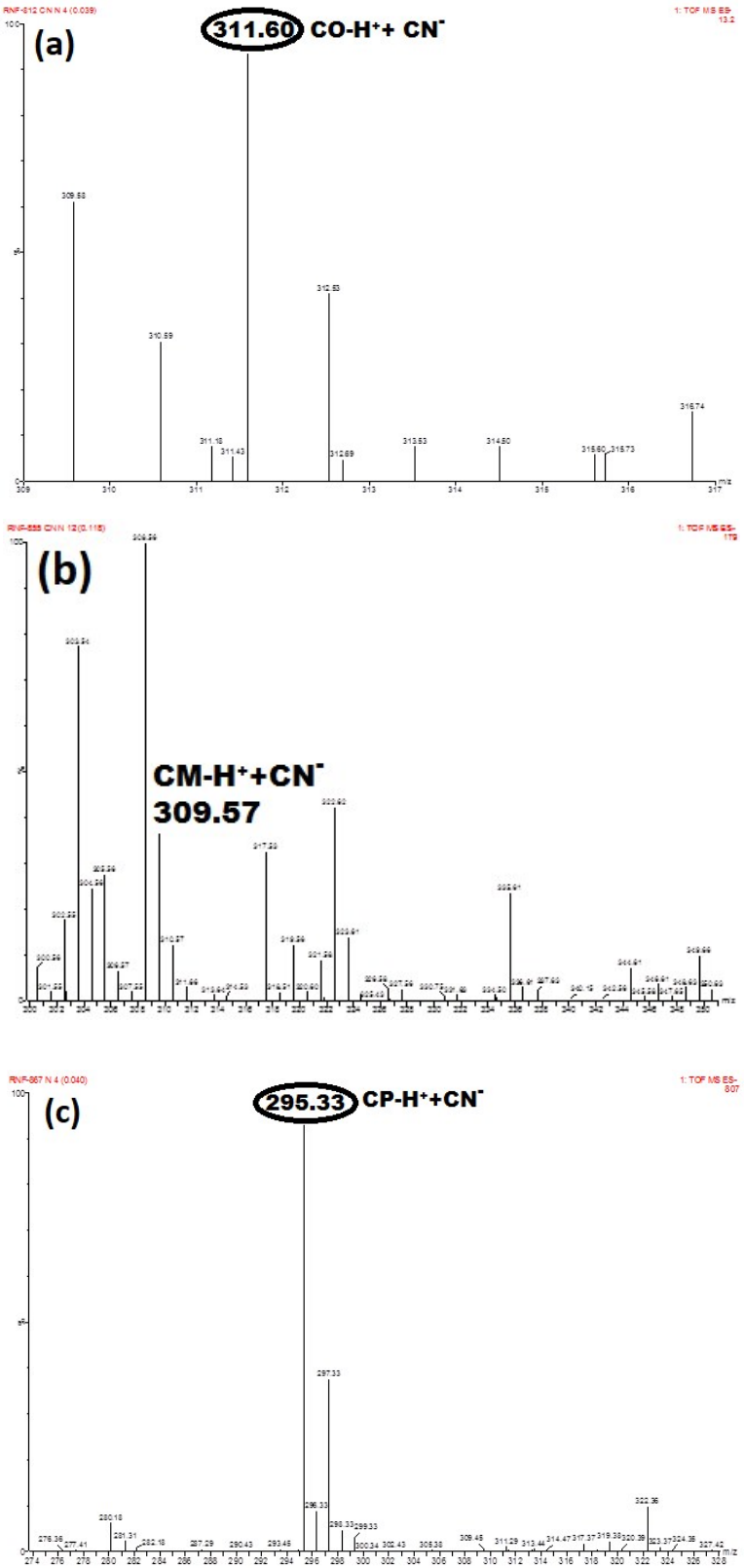

Fig. S16. Mass spectra of (a) CO, (b) CM, and (c) CP in presence of cyanide.

Parameters	CP	CM
Composition	$C_{14}H_{11}N_3O_3$	$C_{32}H_{34}N_6O_8$
Formula wt.	269.26	630.65
Crystal System	Monoclinic	Triclinic
Space Group	$P2_1/n$	P-1
Crystal Color	Intense Yellow	Yellow
a (Å)	7.5911(11)	7.513(3)
b(Å)	9.7485(15)	15.043(6)
c(Å)	16.594(3)	16.048(6)
α(º)	90	66.018(6)
β(º)	98.556(6)	76.843(6)
γ (º)	90	85.708(7)
V(Å^3)	1214.3(3)	1613.3(11)
Density (Mg/m^3) / Z	1.473/4	1.298/2
2 θ_{max} [deg]	56.88	56.58
Temp (K)	150(2)	150(2)
μ mm^{-1}	0.107	0.095
Reflections collected/unique	3041/2626	5000/3223
R(int)	0.0388	0.0584
Data/restraints/parameters	3041/0/225	5000/0/425
R1(F_0), *wR*2(F_0) (I≥ 2 σ(*I*))	0.0419,0.1287	0.1178,0.3305
R1(F_0 2), *wR*2(F_0 2) (all data)	0.0492/0.1219	0.1472,0.3468
F(000)/GOF on F ^{2}	560/1.050	664/1.243
CCDC No.	1911311	1855812

Table S1. X-ray crystallographic data of CP and CM.