

Supporting Information

Coumarin-hemicyanine conjugates as novel reaction-based sensors for cyanide detection: convenient synthesis and ICT mechanism

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ESI 1. NMR spectra of the sensors

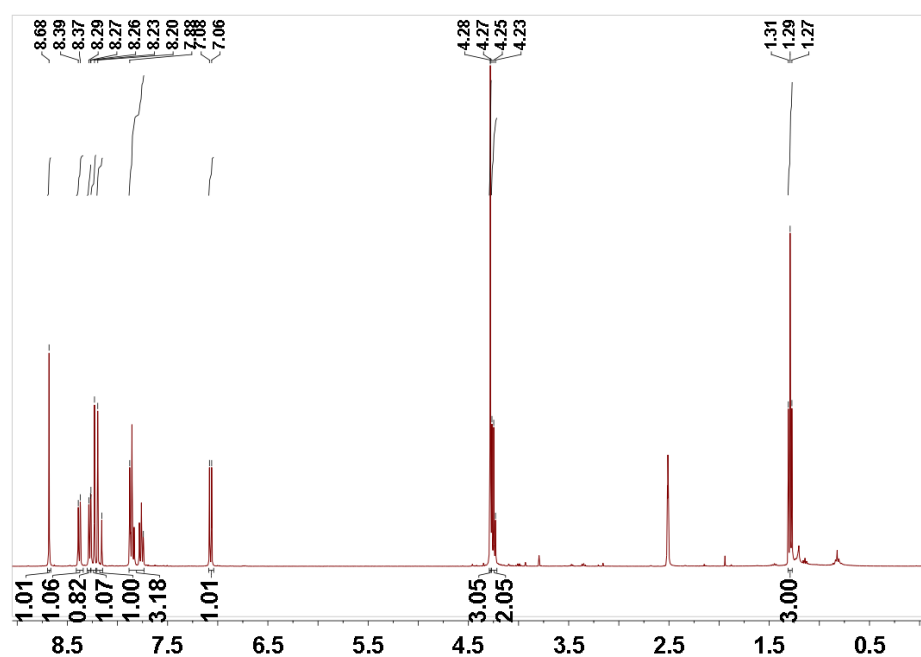


Fig.S1 ¹H NMR charts of COC-1 in DMSO-d₆-CF₃COOD

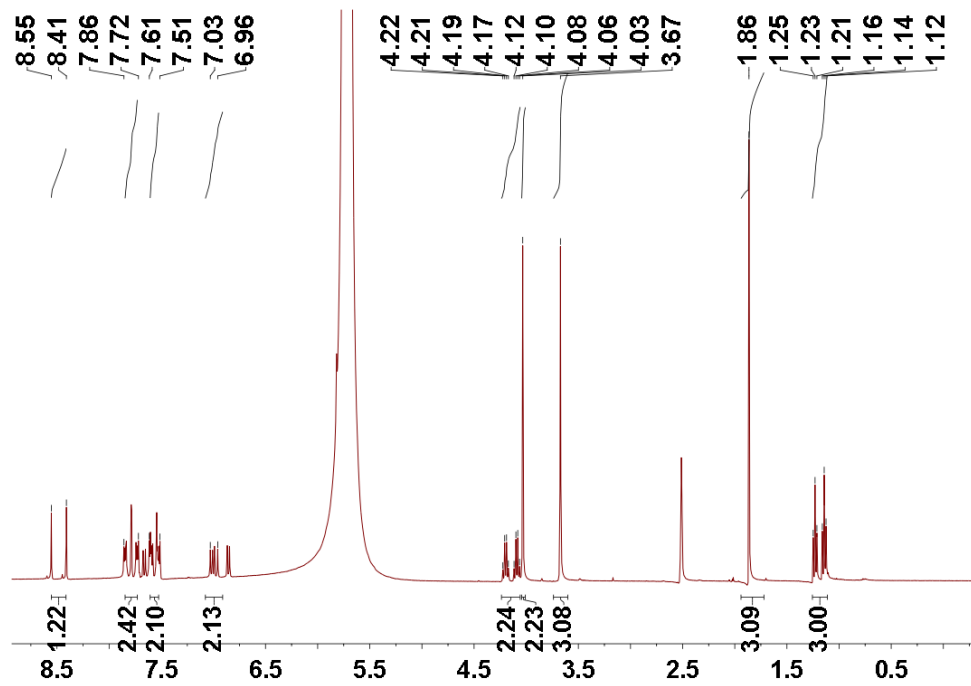


Fig.S2 ¹H NMR charts of COC-2 in DMSO-d₆-CF₃COOD

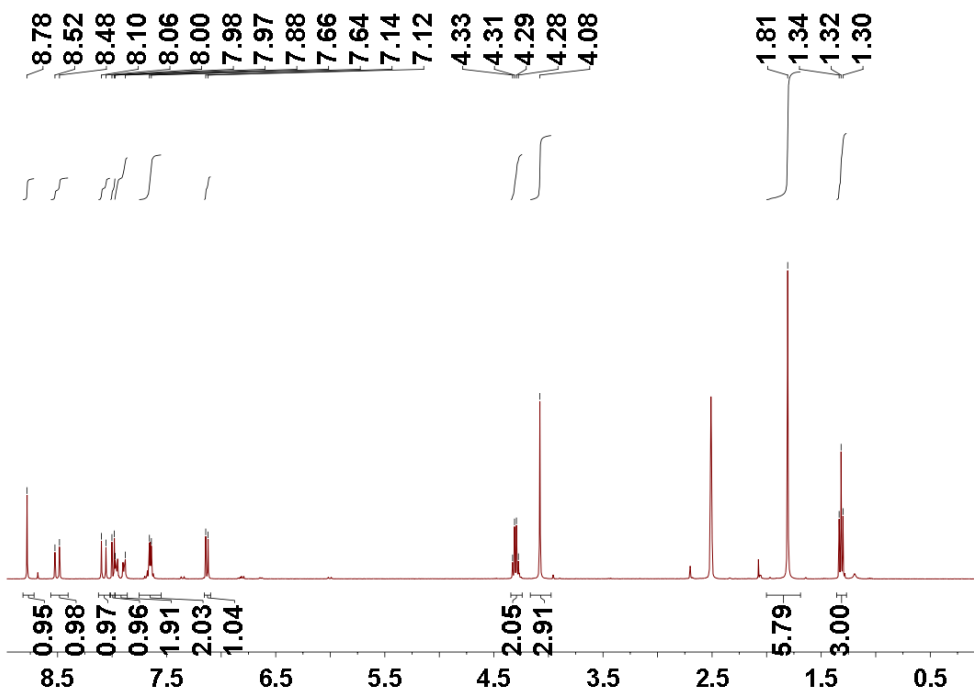


Fig.S3 ¹H NMR charts of COC-3 in DMSO-d₆-CF₃COOD

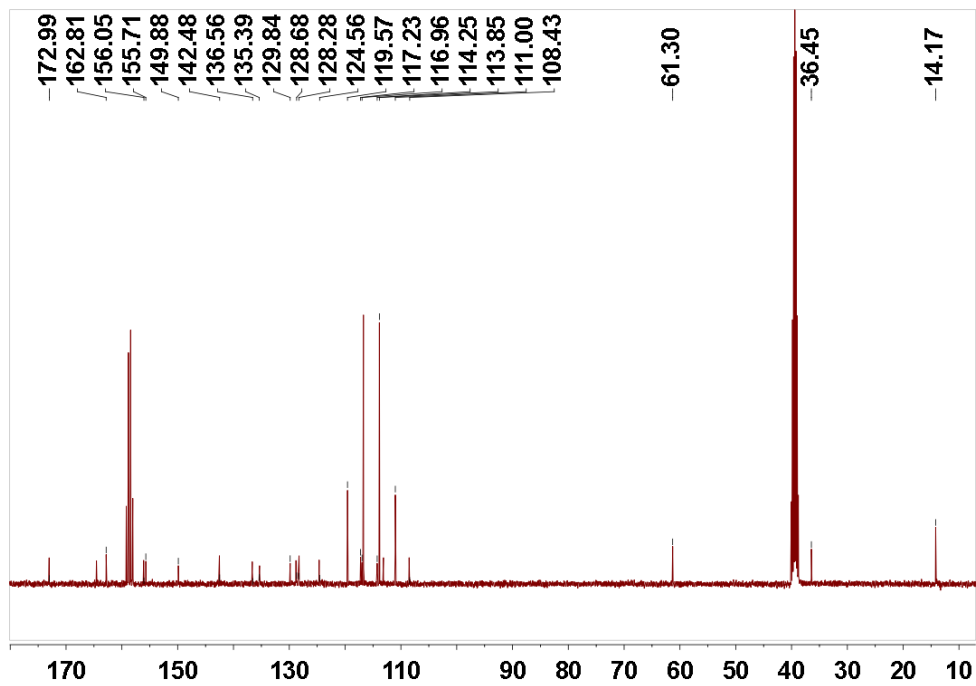


Fig.S4 ^{13}C NMR charts of COC-1 in $\text{DMSO-d}_6\text{-CF}_3\text{COOD}$

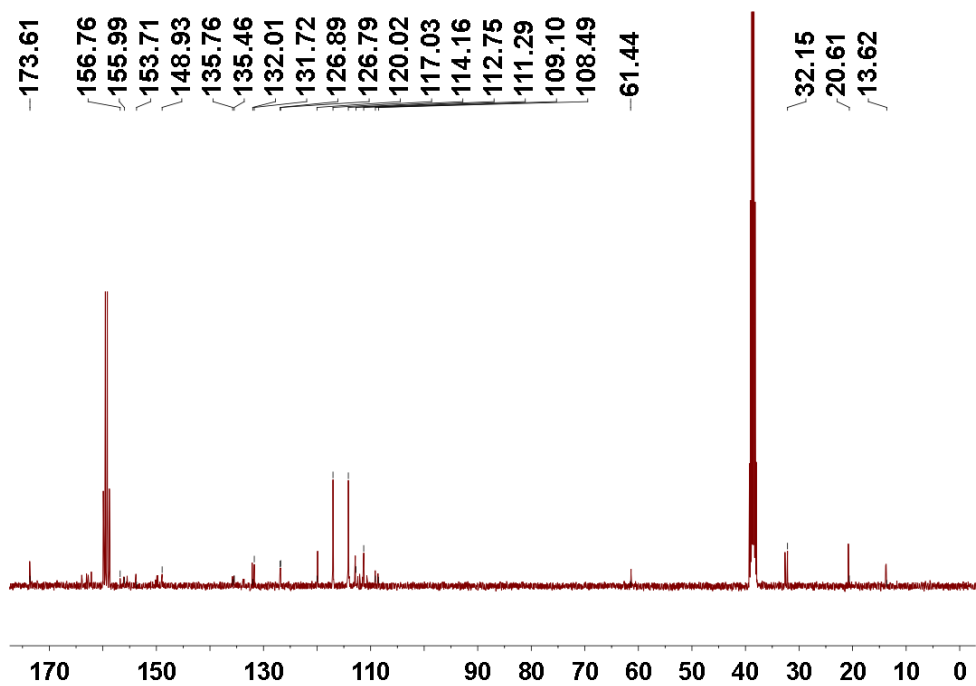


Fig.S5 ^{13}C NMR charts of COC-2 in $\text{DMSO-d}_6\text{-CF}_3\text{COOD}$

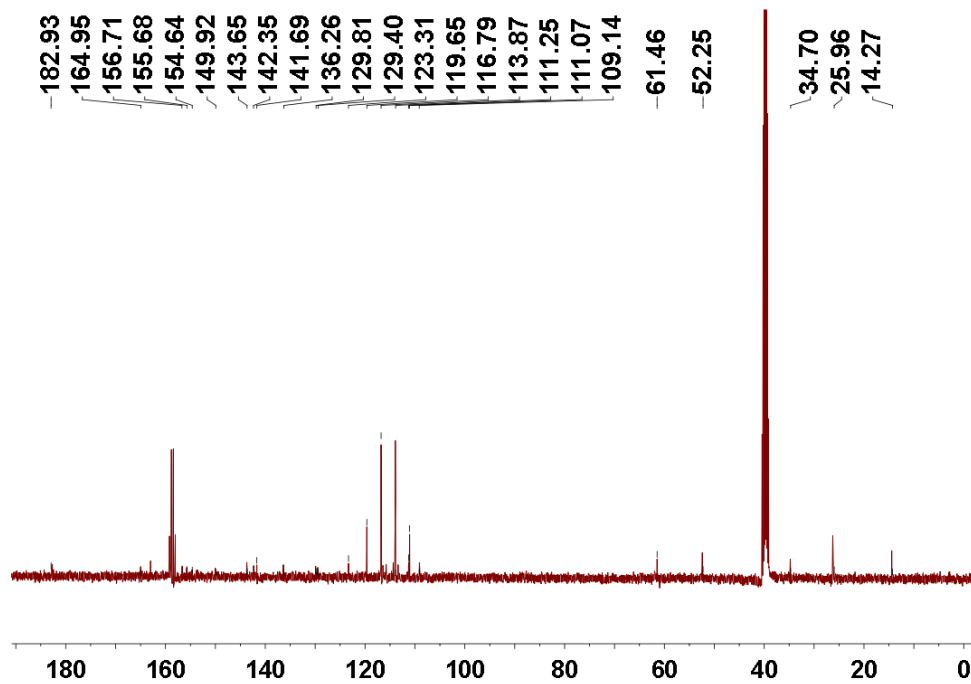


Fig.S6 ^{13}C NMR charts of COC-3 in $\text{DMSO-d}_6\text{-CF}_3\text{COOD}$

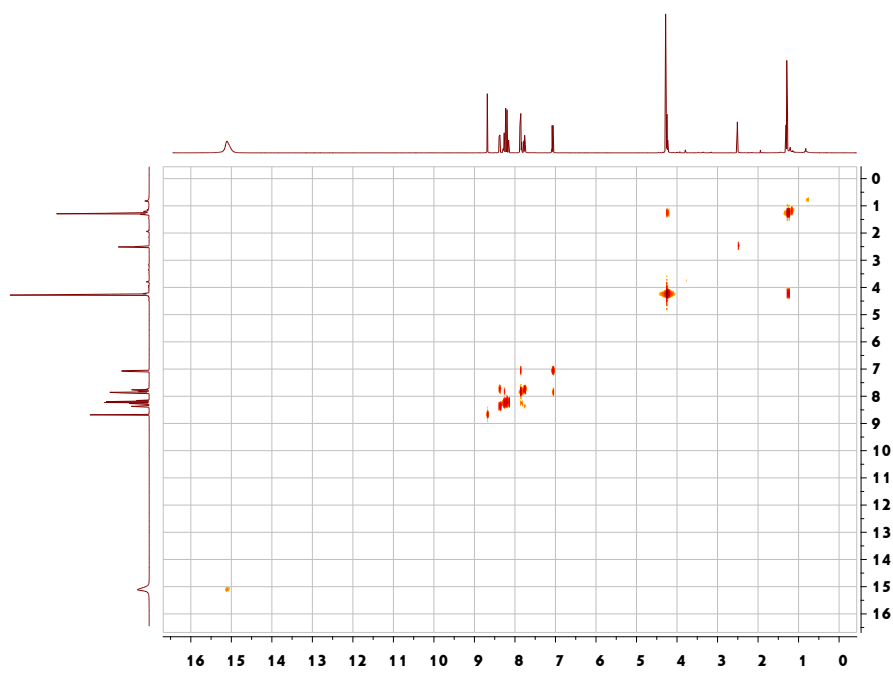


Fig.S7 ^1H - ^1H COSY of COC-1

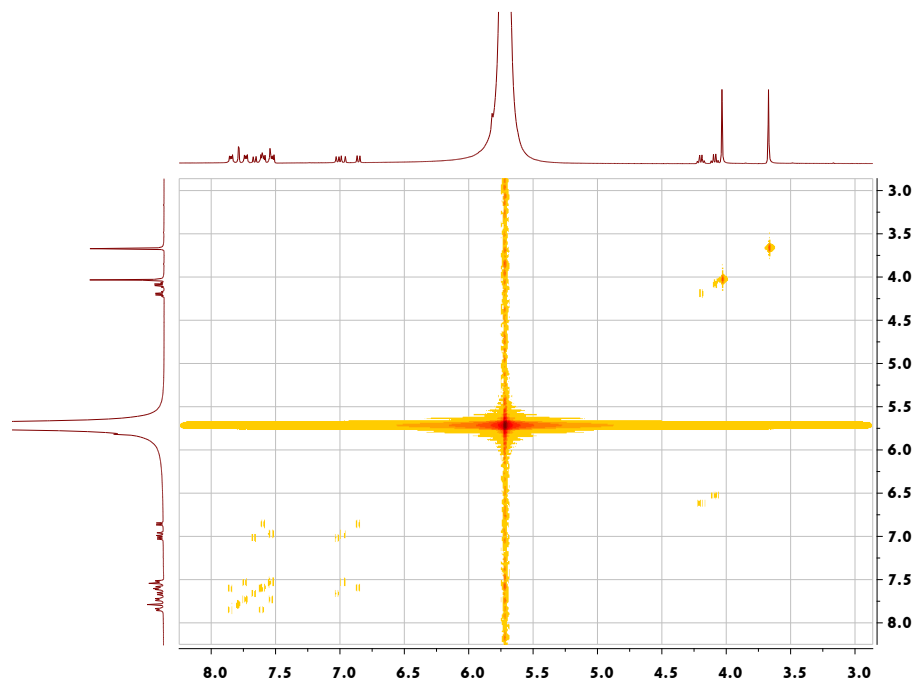


Fig.S8 ^1H - ^1H COSY of COC-2

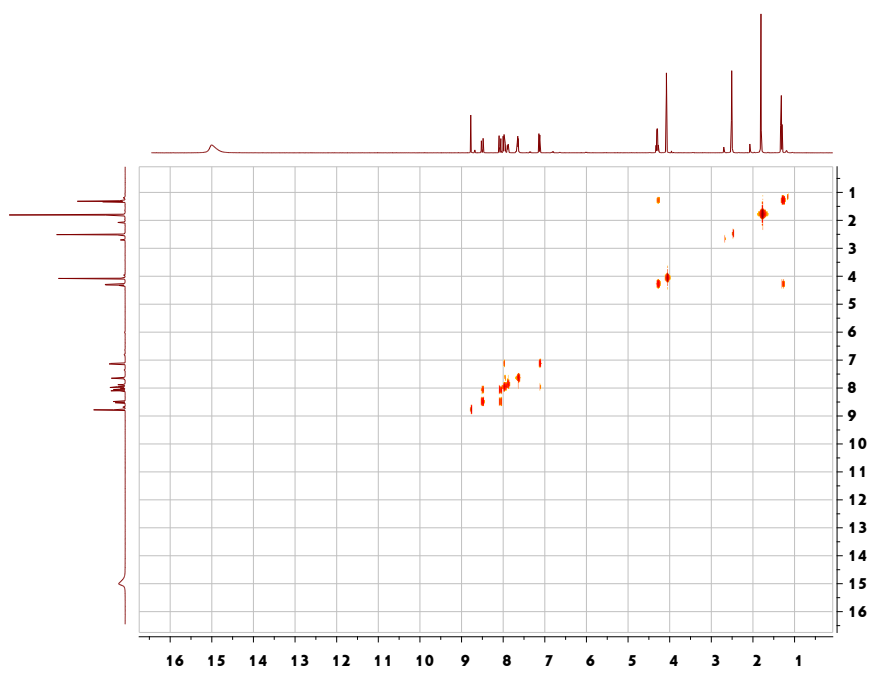


Fig.S9 ^1H - ^1H COSY of COC-3

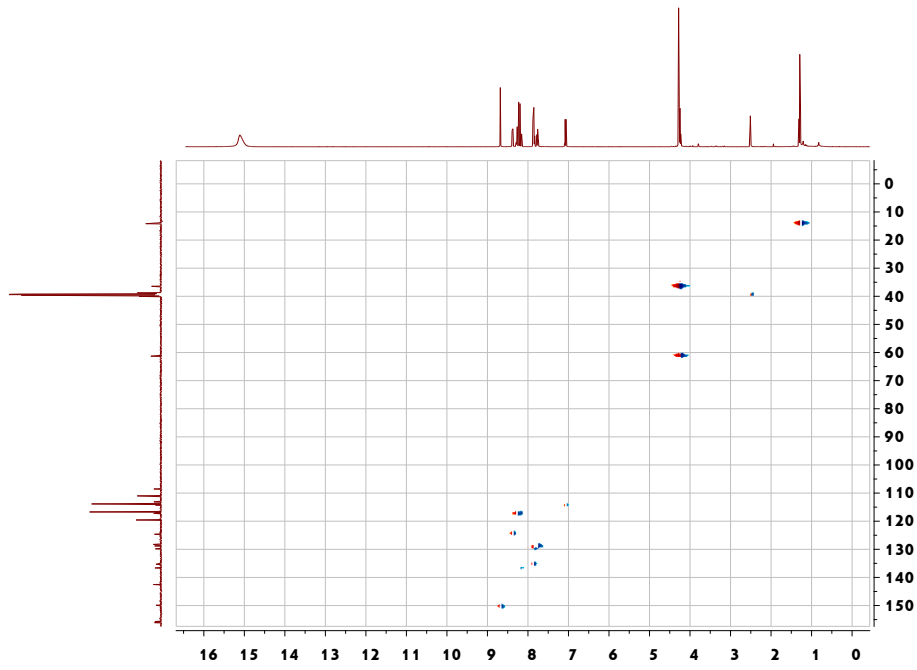


Fig.S10 HSQC of COC-1

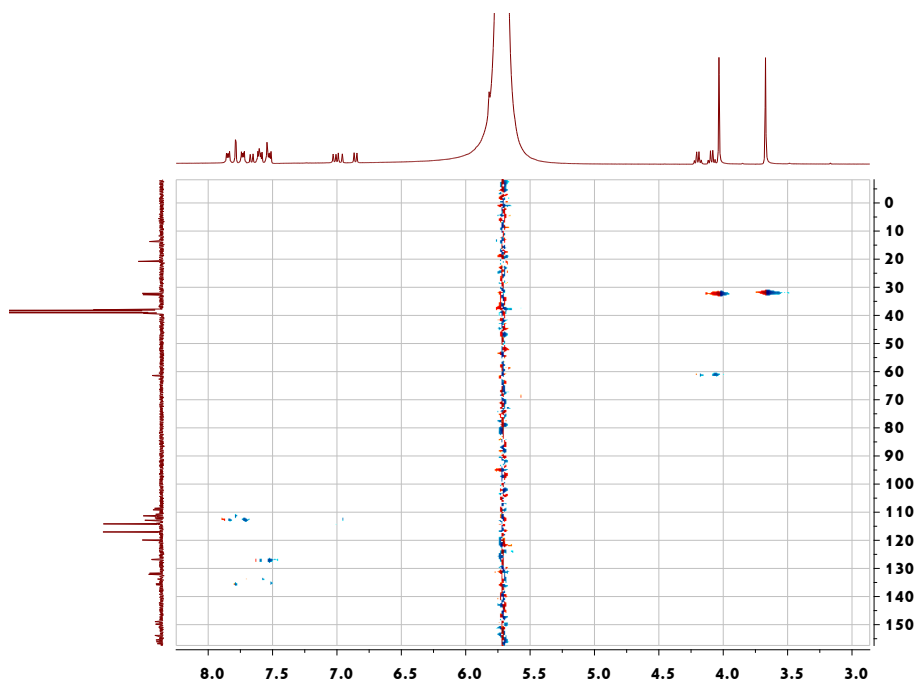


Fig.S11 HSQC of COC-2

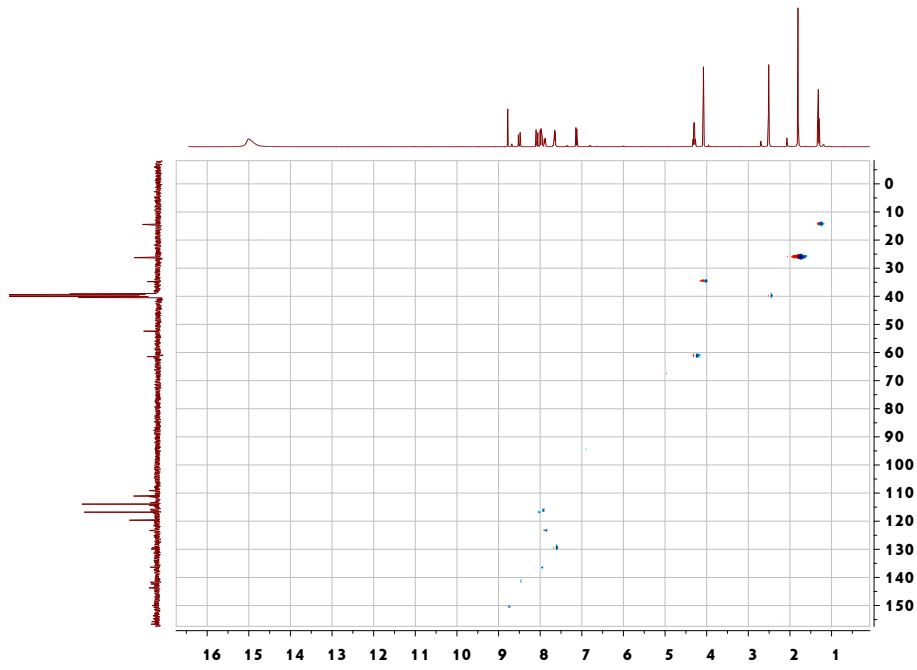


Fig.S12 HSQC of COC-3

ESI 2. Mass spectra of the sensors

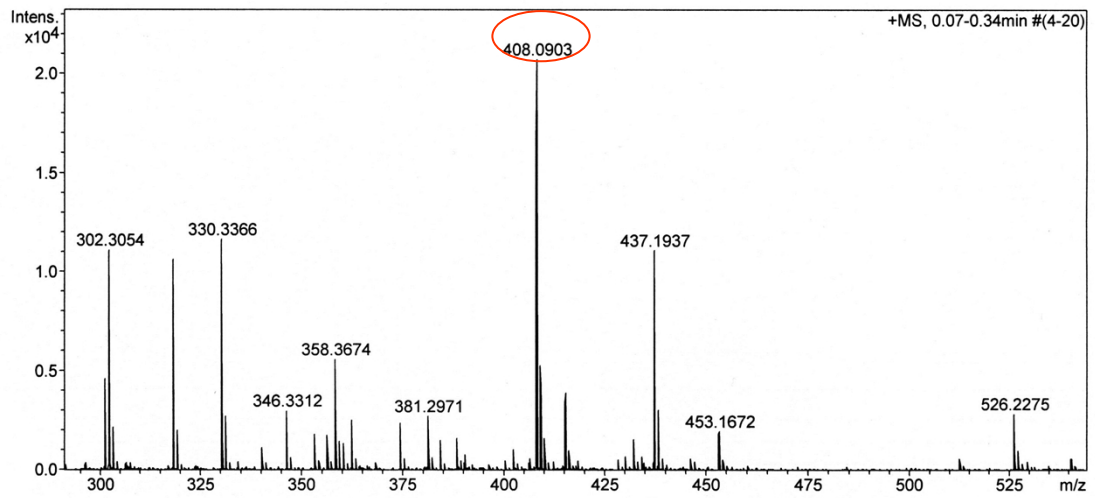


Fig. S13 The HRMS for COC-1

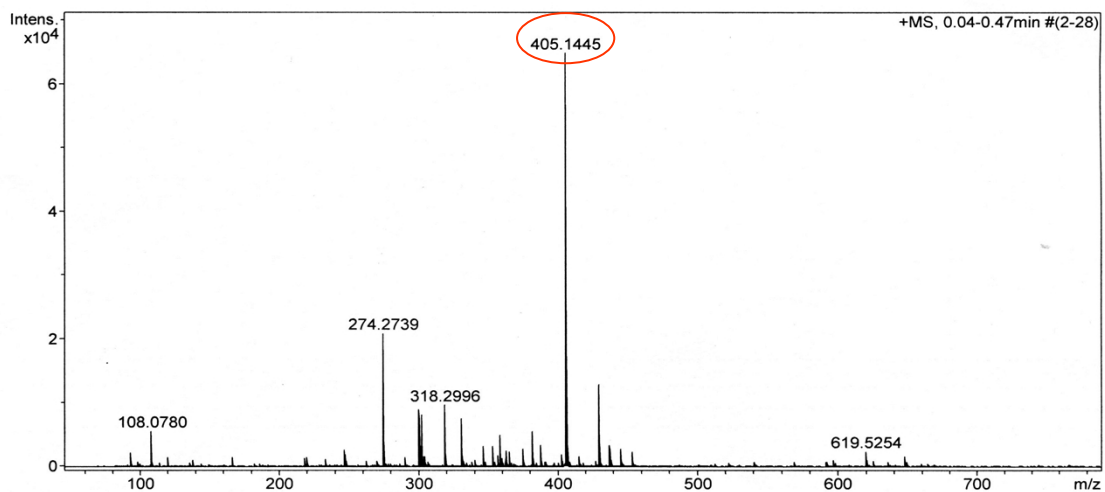


Fig. S14 The HRMS for COC-2

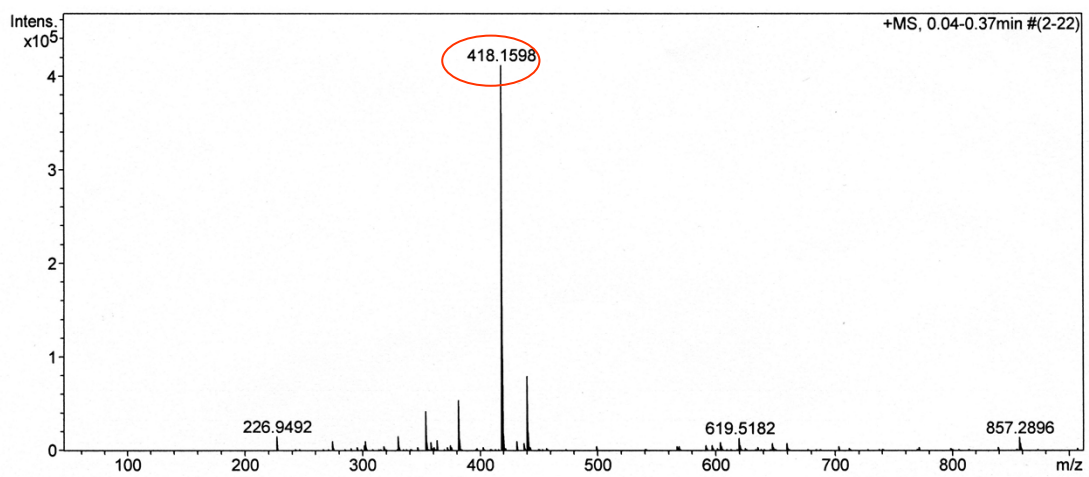


Fig. S15 The HRMS for COC-3

ESI 3. IR of the sensors

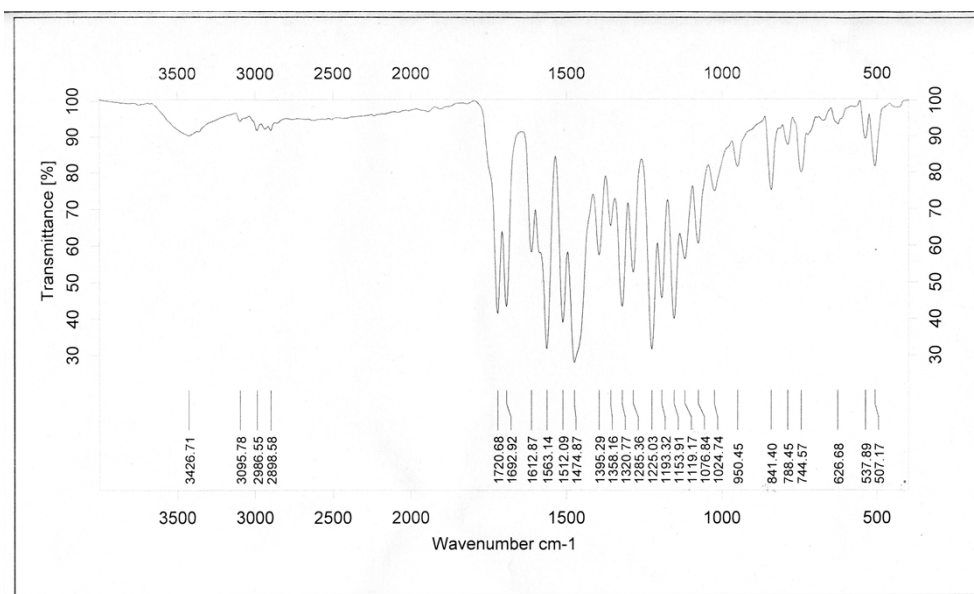


Fig. S16 The IR spectrum of COC-1

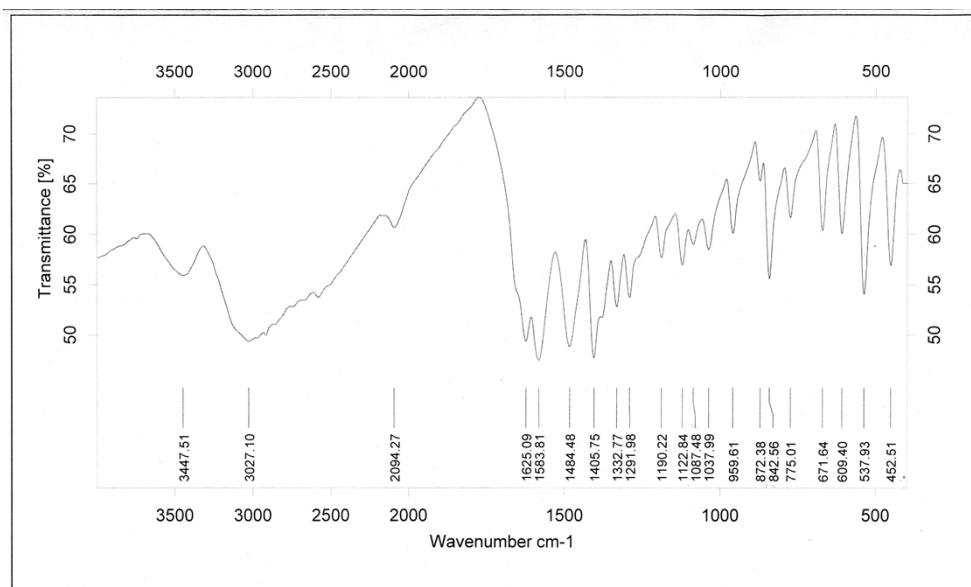


Fig. S17 The IR spectrum of COC-2

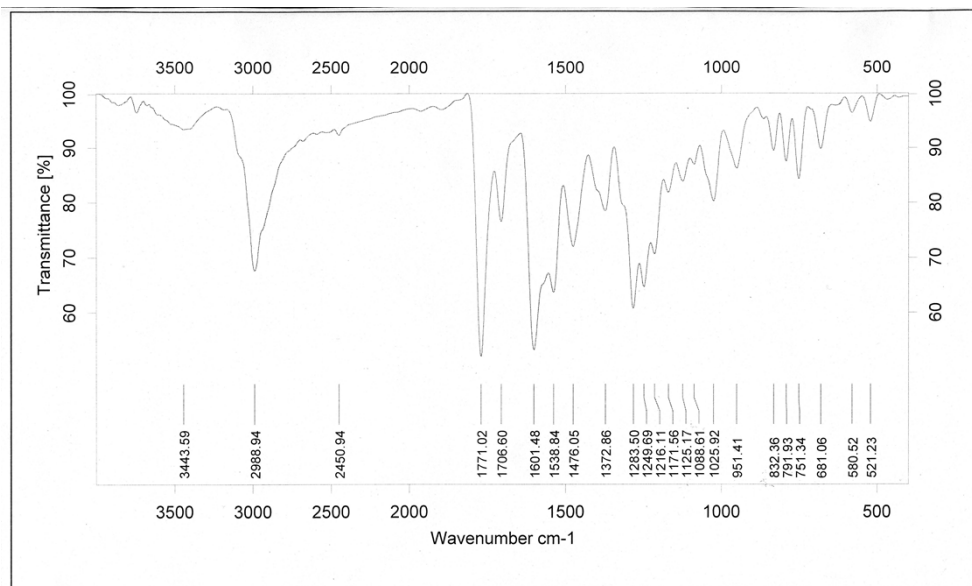
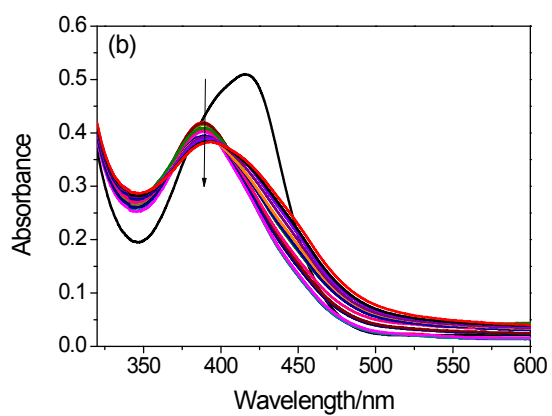
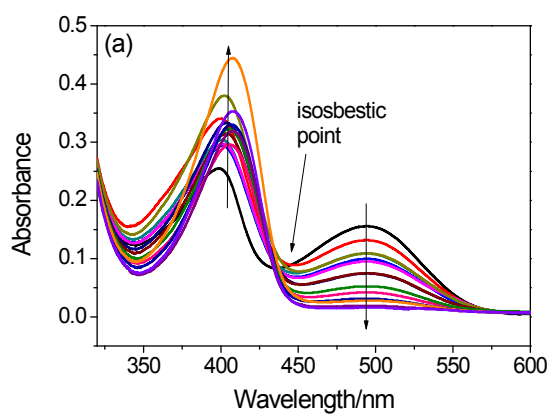


Fig. S18 The IR spectrum of COC-3

ESI 4. Absorption responses of the sensors toward cyanide



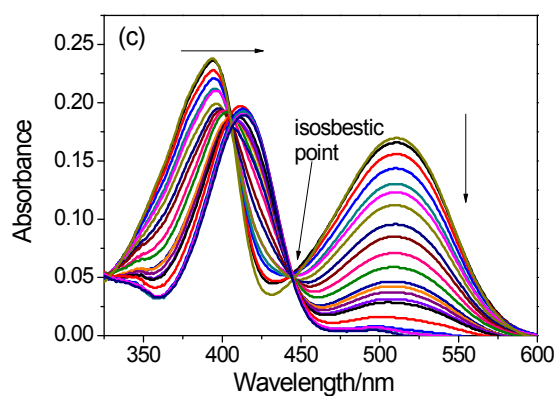


Fig. 4. Changes in absorption spectra of the sensors measured upon addition of CN^- . (a) **COC-1** ($10 \mu\text{M}$); Cyanide concentration (μM): 0, 5, 50, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, respectively; MeCN-buffer (Na_2CO_3 - NaHCO_3 , 10.0 mM, pH = 9.4, 1 : 1, v/v); (b) **COC-2** ($10 \mu\text{M}$); Cyanide concentration (μM): 0, 100, 1000, 3000, 5000, 7000, 9000, 10000, 15000, 20000, 25000, 30000, 35000, 40000, 45000, 50000, respectively; MeCN-buffer (Na_2CO_3 - NaHCO_3 , 10.0 mM, pH = 9.4, 1 : 1, v/v); (c) **COC-3** ($5 \mu\text{M}$); Cyanide concentration (μM): 0, 10, 20, 40, 60, 80, 95, 150, 200, 300, 400, 500, 600, 700, 900, 1000, 2000, 4000, 6000, 10000, respectively; MeOH-buffer (Na_2CO_3 - NaHCO_3 , 10.0 mM, pH = 9.4, 1 : 1, v/v).