Selective naked-eye cyanide detection in aqueous media using a carbazole-derived fluorescent dye

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Electronic Supplementary Information

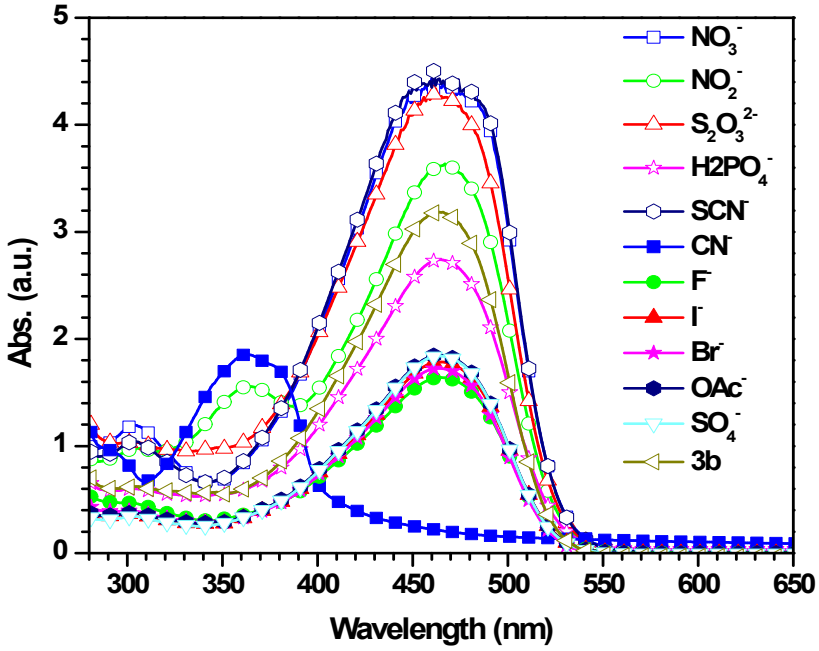


Fig. S1 Absorption spectra of **3b** in the presence of different anions.

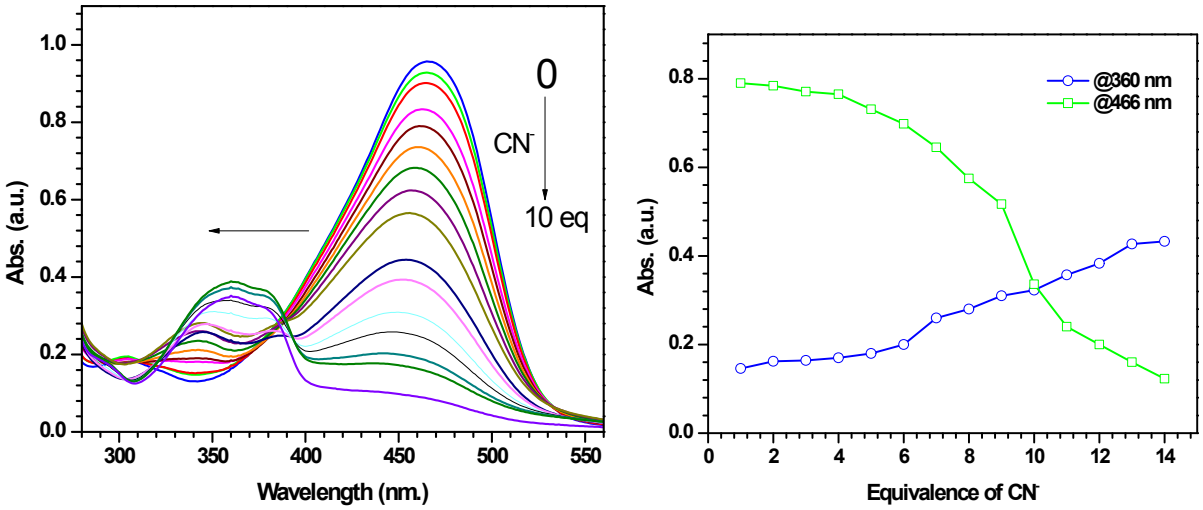


Fig. S2 Absorption changes for **3b** on addition of cyanide in aqueous acetonitrile.

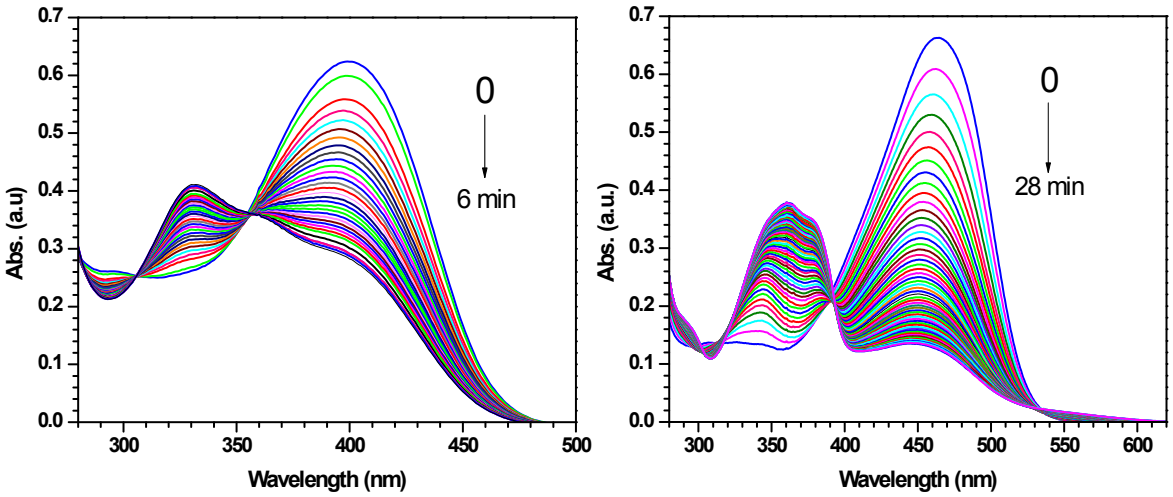


Fig. S3 Time dependent absorption changes of **3a** (left) and **3b** (right) upon addition of 2 equiv. and 10 equiv. of .CN$^-$ respectively.

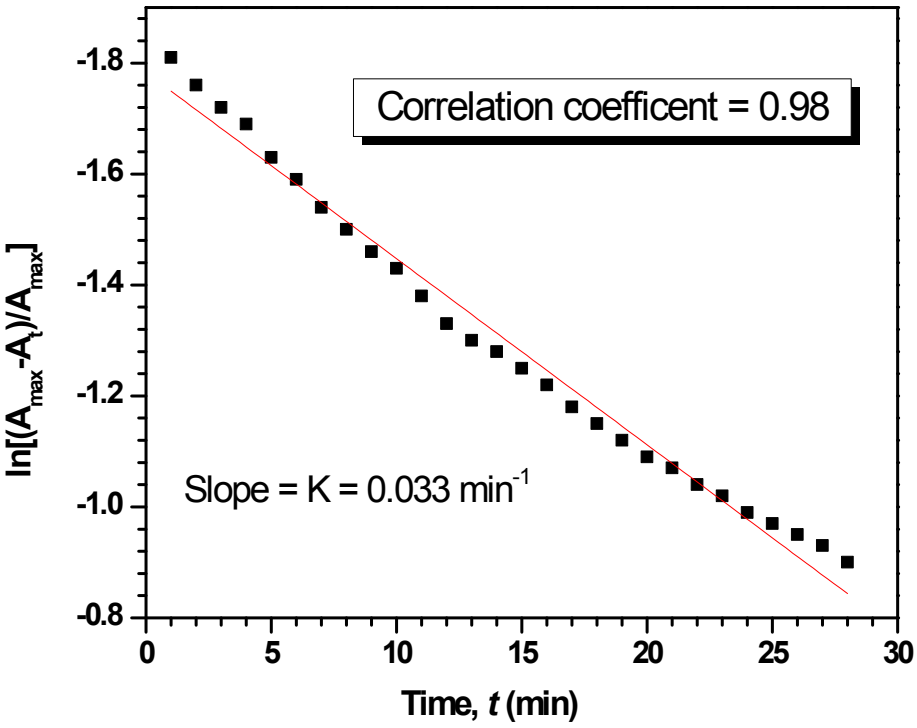


Fig. S4 Kinetics of sensor **3b** action.

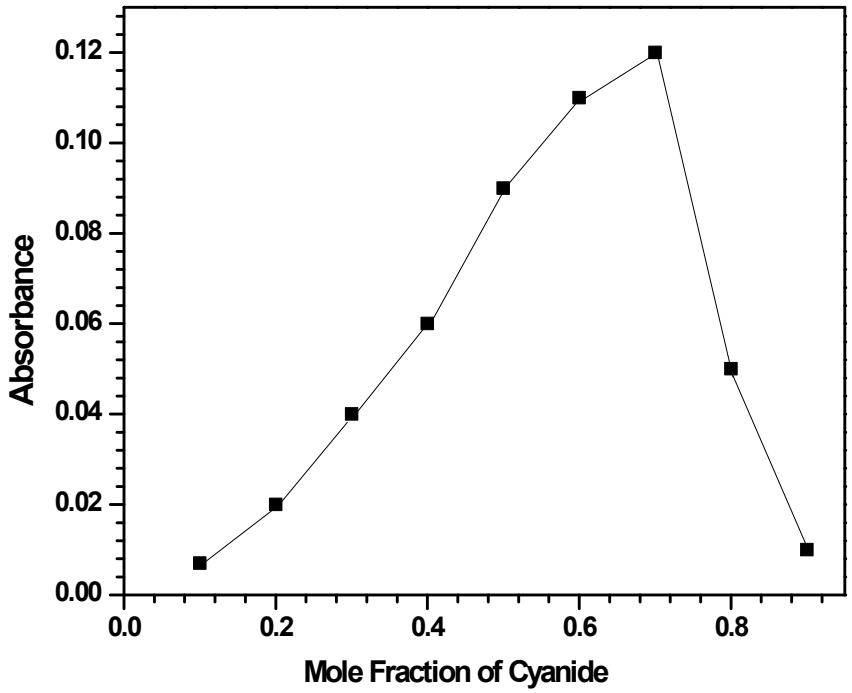


Fig. S5 Jobs plot for **3b.**

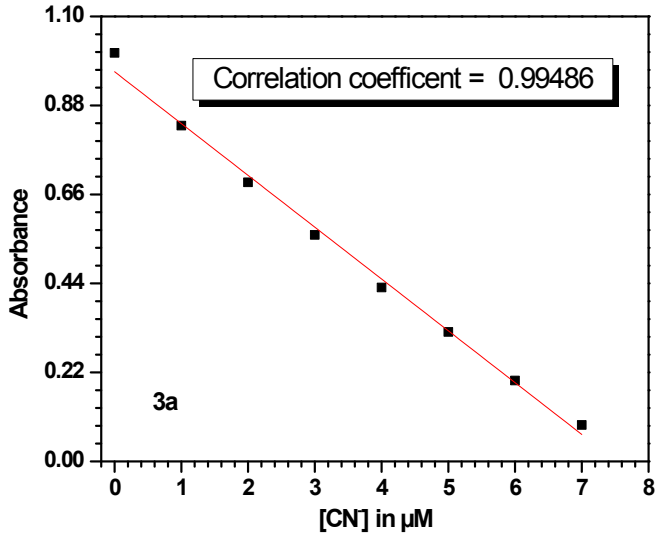
Detection limit determination

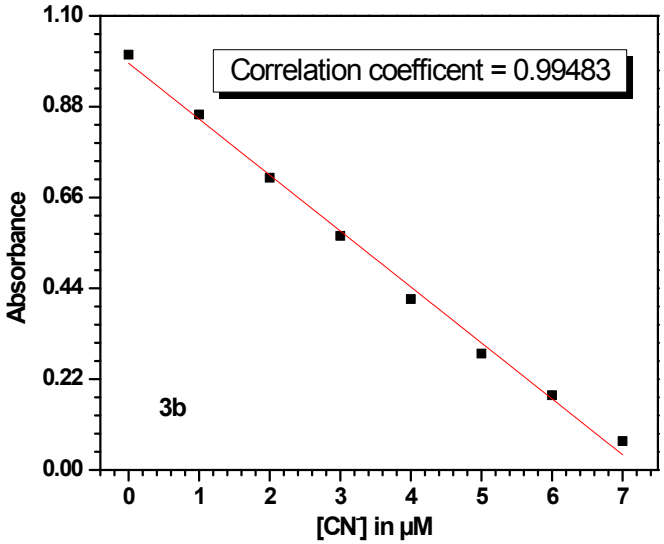
The detection limit of the probes 3a and 3b for cyanide was estimated by using the formula,

$$Detection\ limit = \frac{k \times \sigma}{S}$$

Where $k = 3$, σ is the standard deviation of the blank solution and S is the slope of the calibration curve.

The calibration graphs observed for the dyes **3a** and **3b** are shown below:





Dye	σ	*S*, μM^{-1}	Detection limit, µM
3a	0.0054	0.128	0.136
3b	0.0063	0.135	0.140

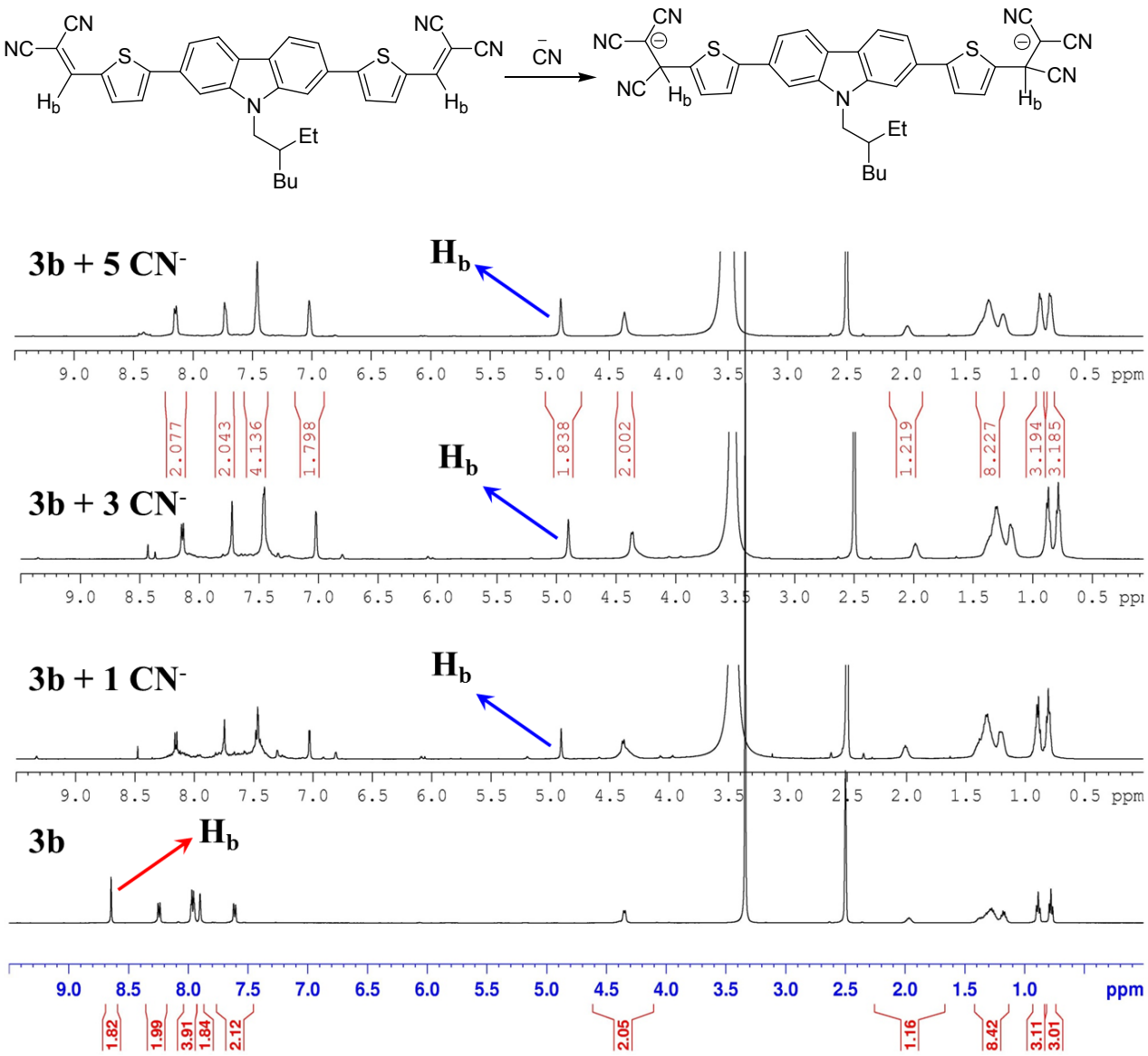


Fig. S6 ^{1}H NMR spectral changes observed for the dye **3b** on addition of various amounts of cyanide in DMSO-d_6.

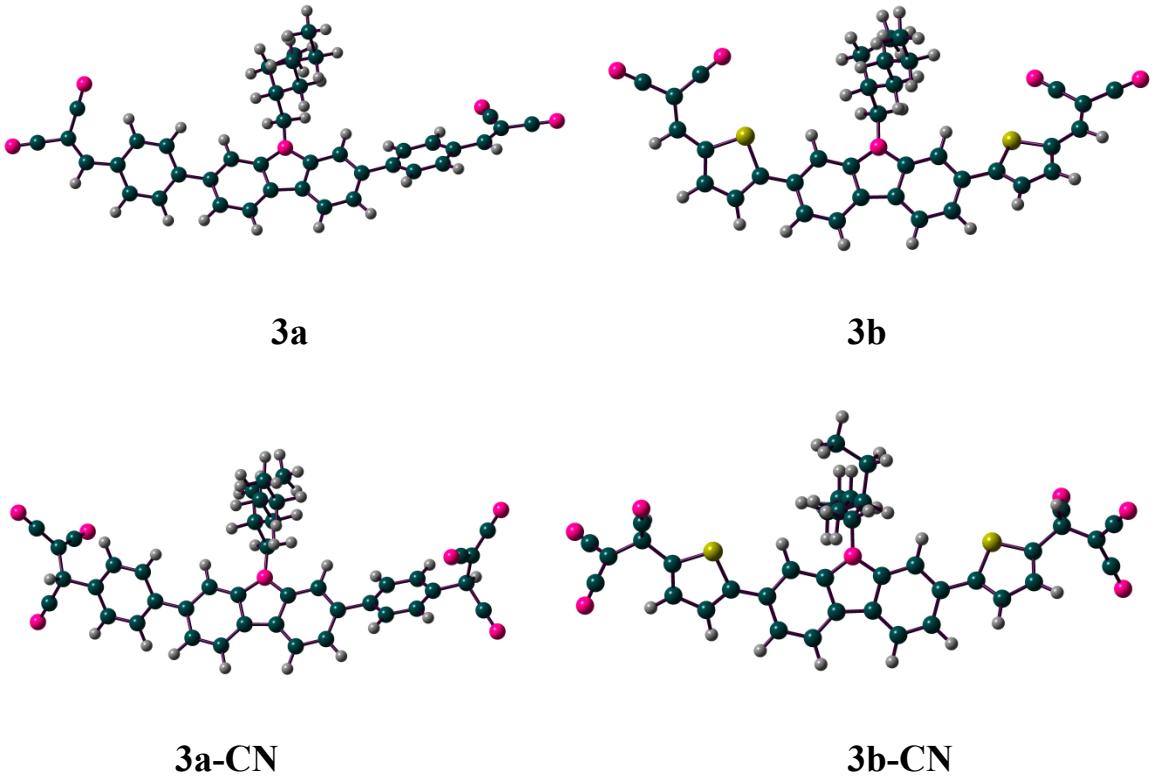


Fig. S7 Optimized geometries for **3a, 3b, 3a-CN$^-$,** and **3b-CN$^-$.**

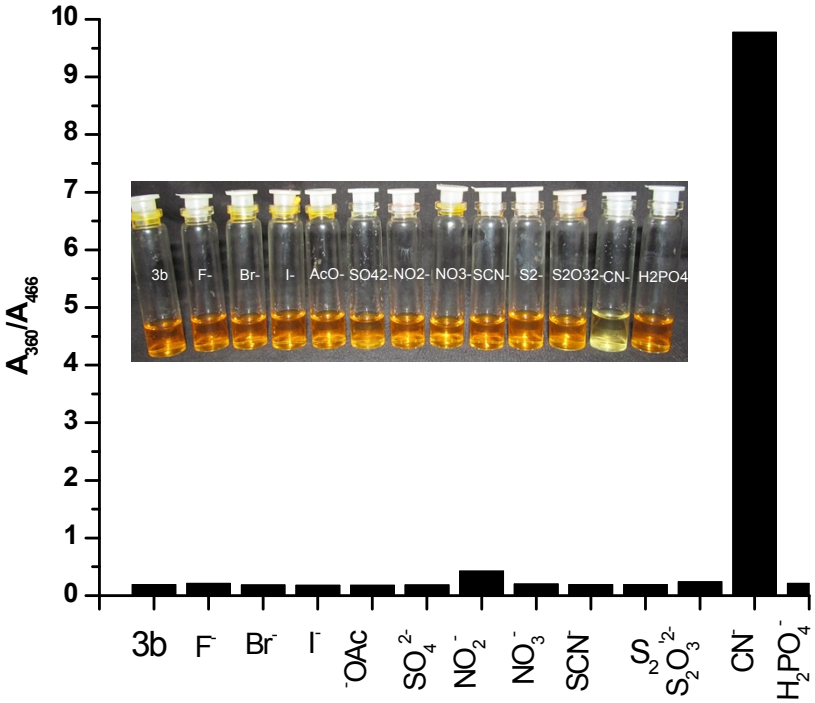


Fig. S8 Absorbance response of **3b** upon addition of 10 equiv of other anions and 2 eq of CN$^-$

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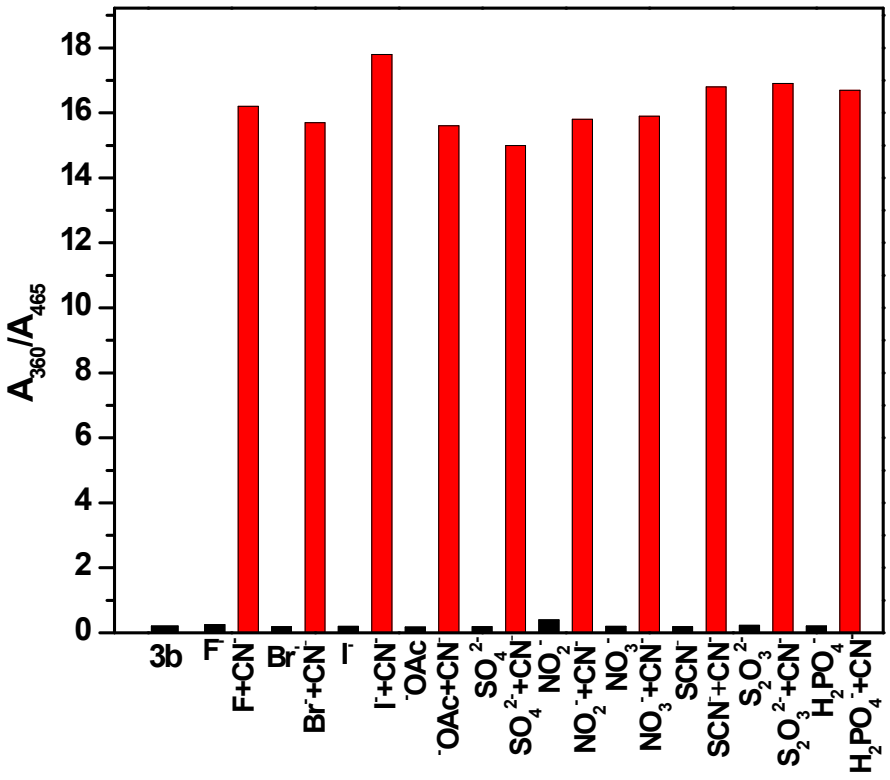

Fig. S9 Ratiometric absorbance changes (A_{330}/A_{405}) of **3b** on addition of 2 equiv of CN^- and 10 equiv of other anions. Black bars indicate the blank and various anions, and red bars indicate the addition of CN^- to the interfering anions.

Table S1 Computed vertical transition energies and their oscillator strengths and configurations for the dyes.

Dye	λ_{max}, nm	f	configuration
3a	457.7	1.3582	HOMO-1 → LUMO (96%)
	338.5	0.1077	HOMO-2 → LUMO (98%)
	331.5	0.6820	HOMO-2 → LUMO+1 (93%)
	310.3	0.4822	HOMO-3 → LUMO (63%), HOMO-1 → LUMO+2 (28%)
3b	492.1	1.3592	HOMO → LUMO (99%)
	377.5	0.3741	HOMO-2 → LUMO (89%), HOMO → LUMO+1 (11%)
	361.7	0.3144	HOMO-2 → LUMO+1 (92%)
	329.6	0.1159	HOMO-3 → LUMO (66%), HOMO → LUMO+2 (32%)
3a-CN	330.7	1.2431	HOMO-1 → LUMO
3b-CN	373.6	1.4307	HOMO-2 → LUMO

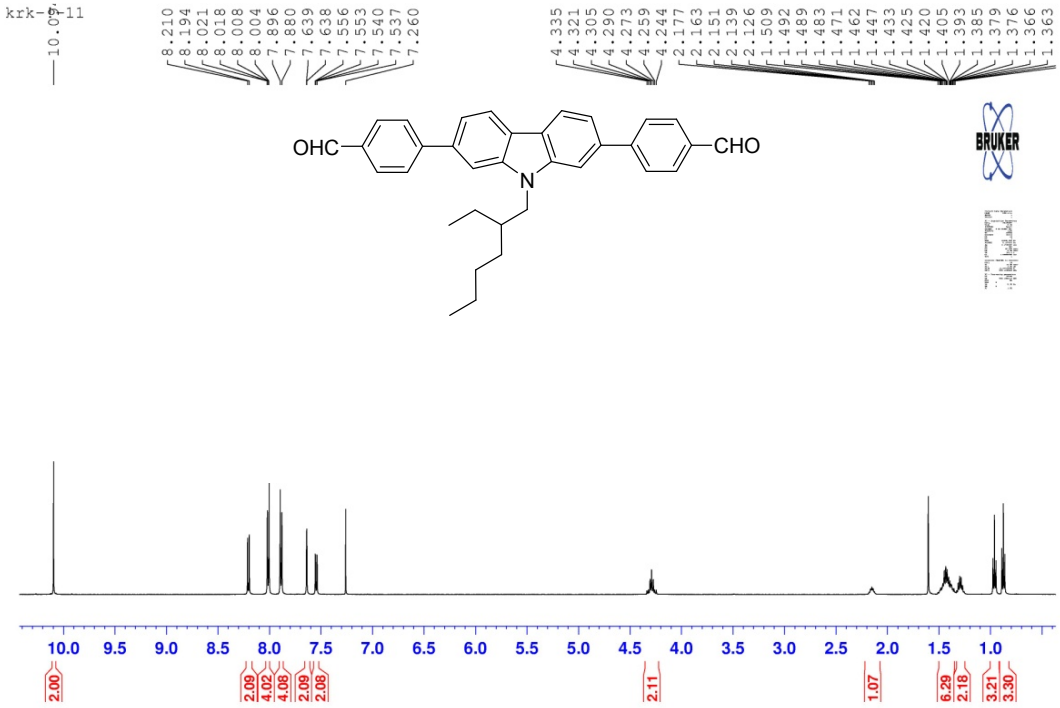

Fig. S10 ^{1}H NMR spectra for **2a** in $CDCl_3$.

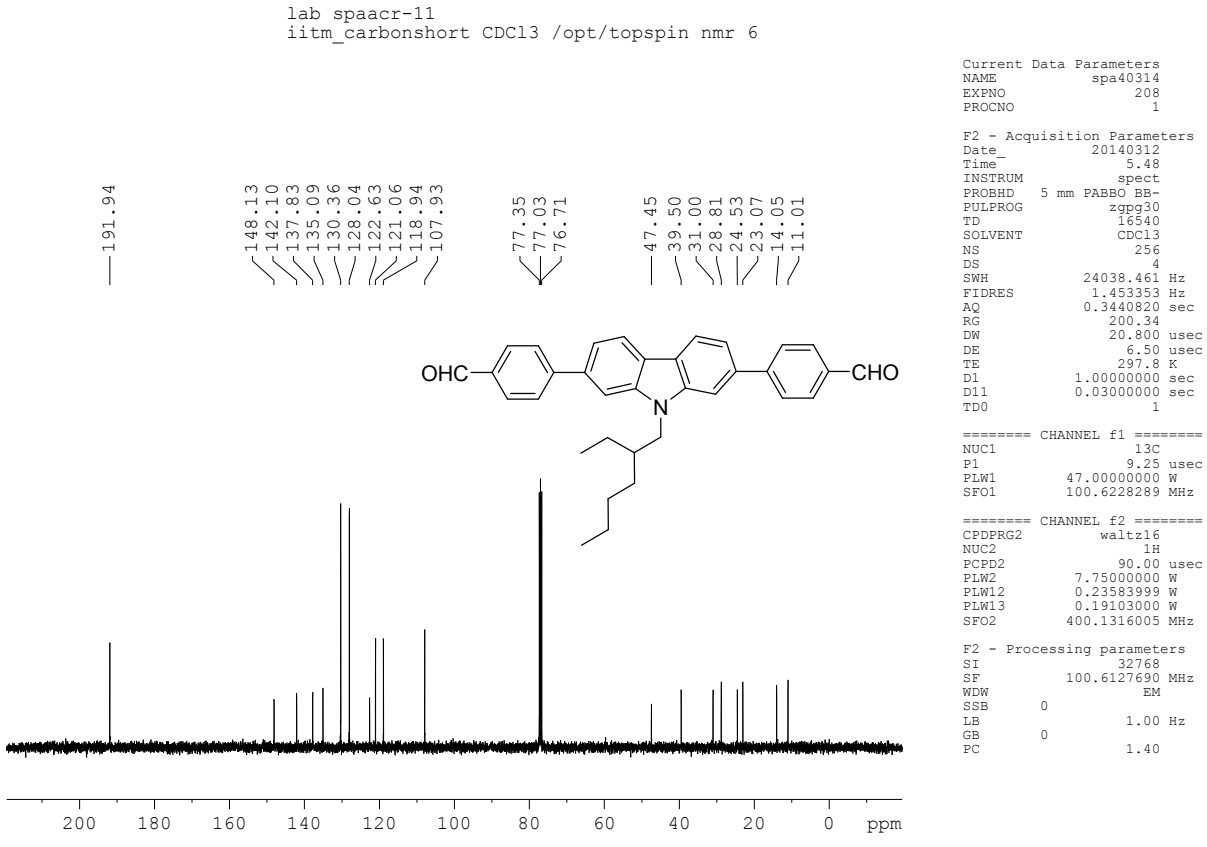

Fig. S11 ^{13}C-NMR spectra of compound **2a.**

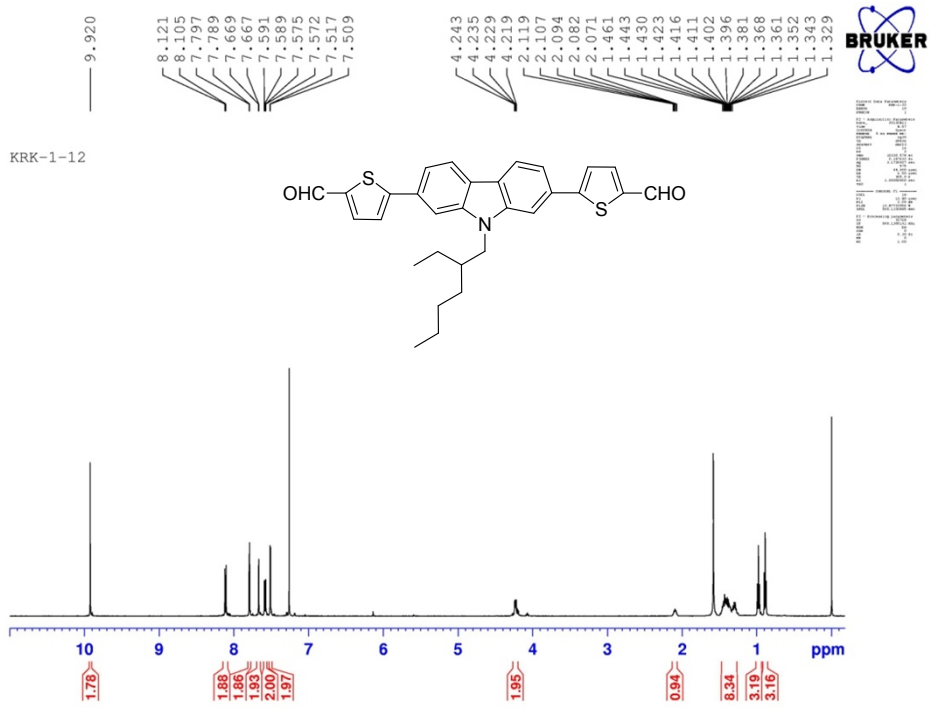

Fig. S12 ^{1}H NMR spectra for **2b** in $CDCl_3$.

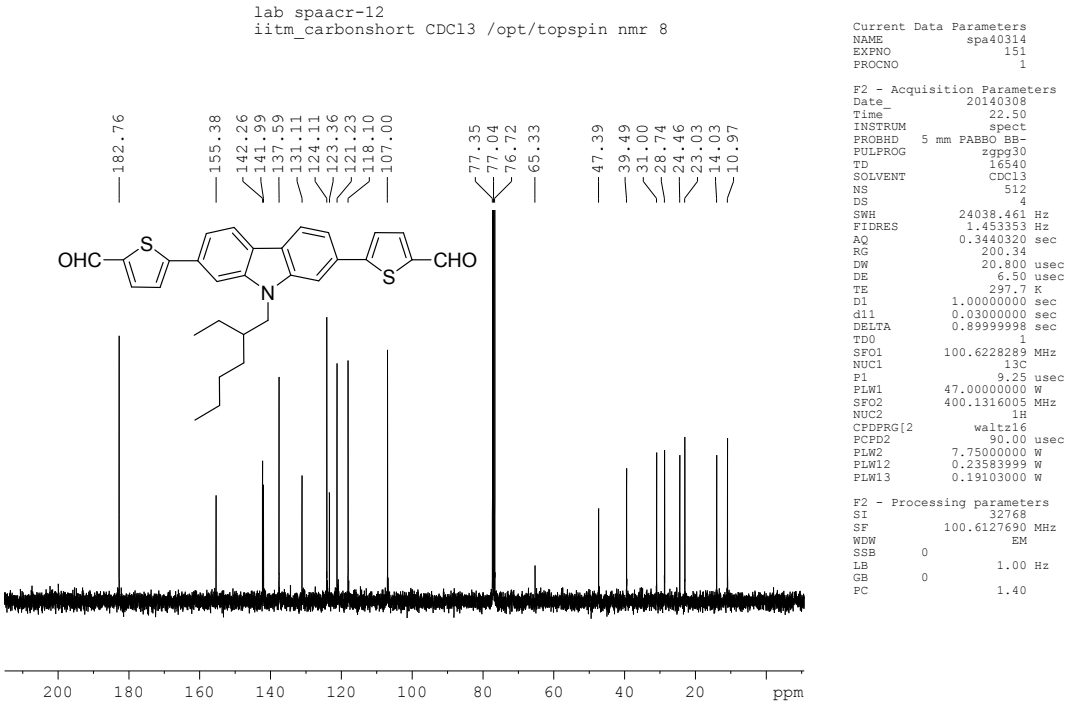


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Fig. S13 ^{13}C NMR spectra for **2b** in $CDCl_3$.

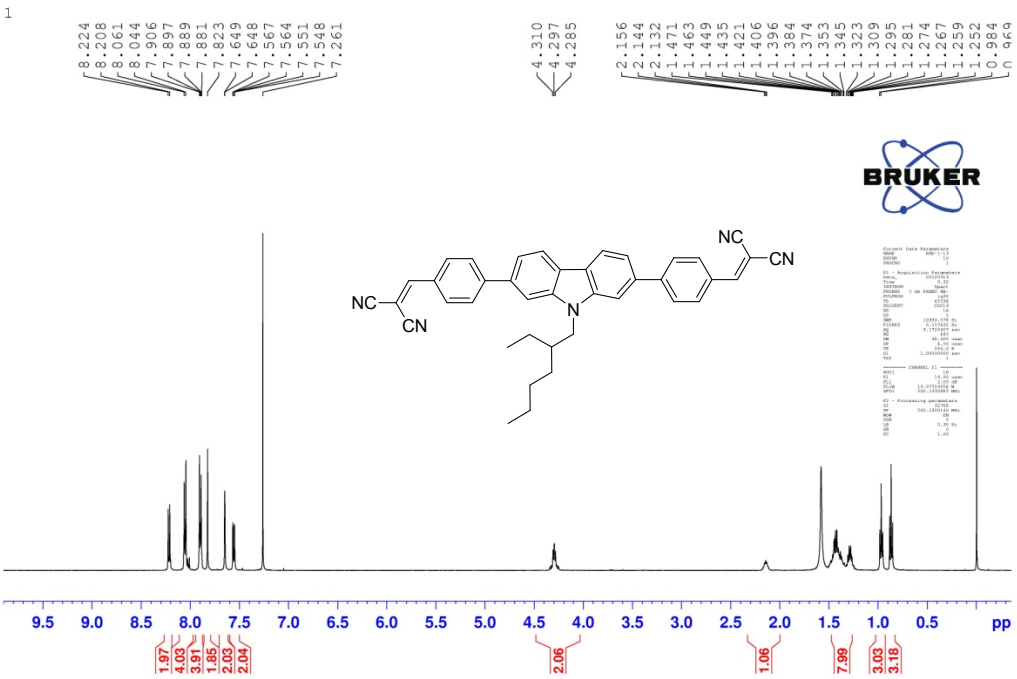

Fig. S14 ^{1}H NMR spectra for **3a** in $CDCl_3$.

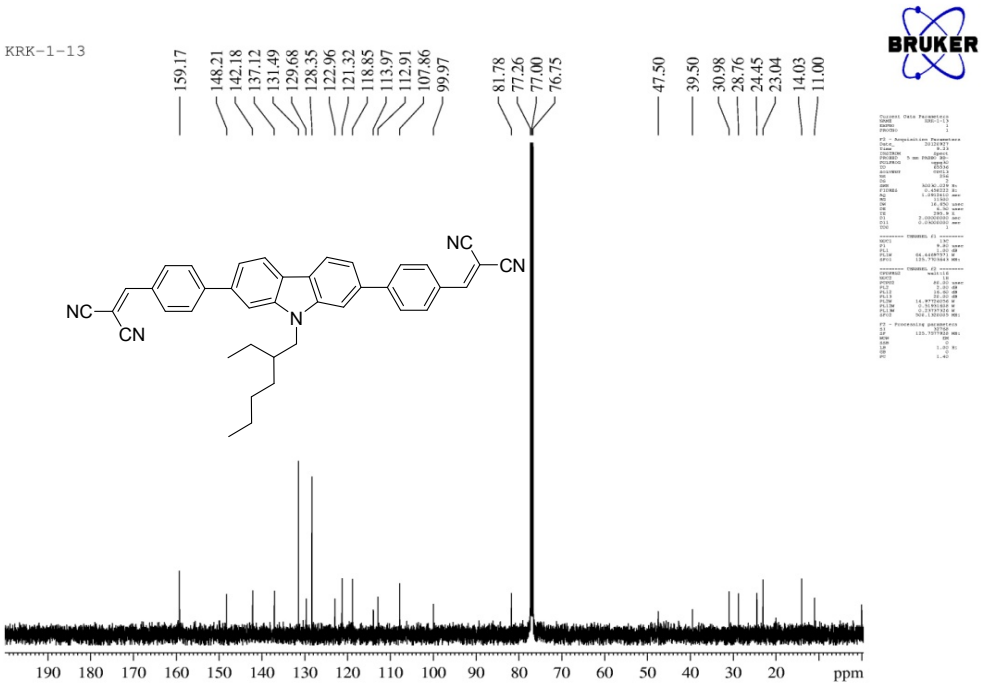

Fig. S15 ^{13}C NMR spectra for **3a** $CDCl_3$.

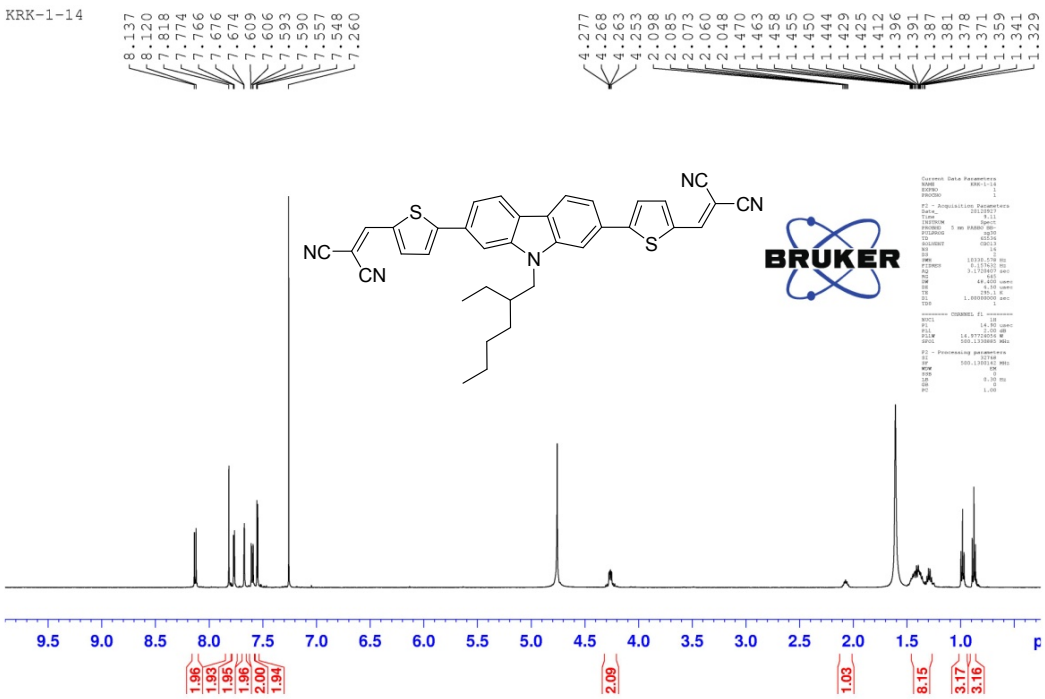

Fig. S16 ^{1}H NMR spectra for **3b** in $CDCl_3$.

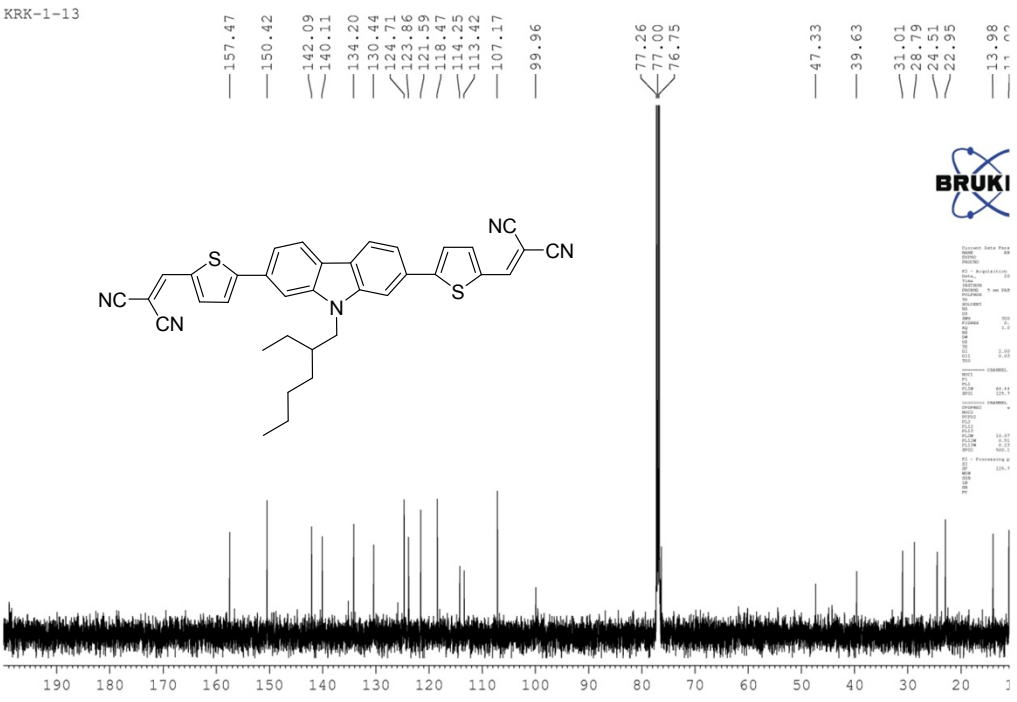

Fig. S17 ^{13}C NMR spectra for **3b** in $CDCl_3$.