

Supplementary Information

Expression of fluorescence property by self-PET (photo-induced electron transfer) suppression both in solution and in the solid state

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Experimental Section:

General:

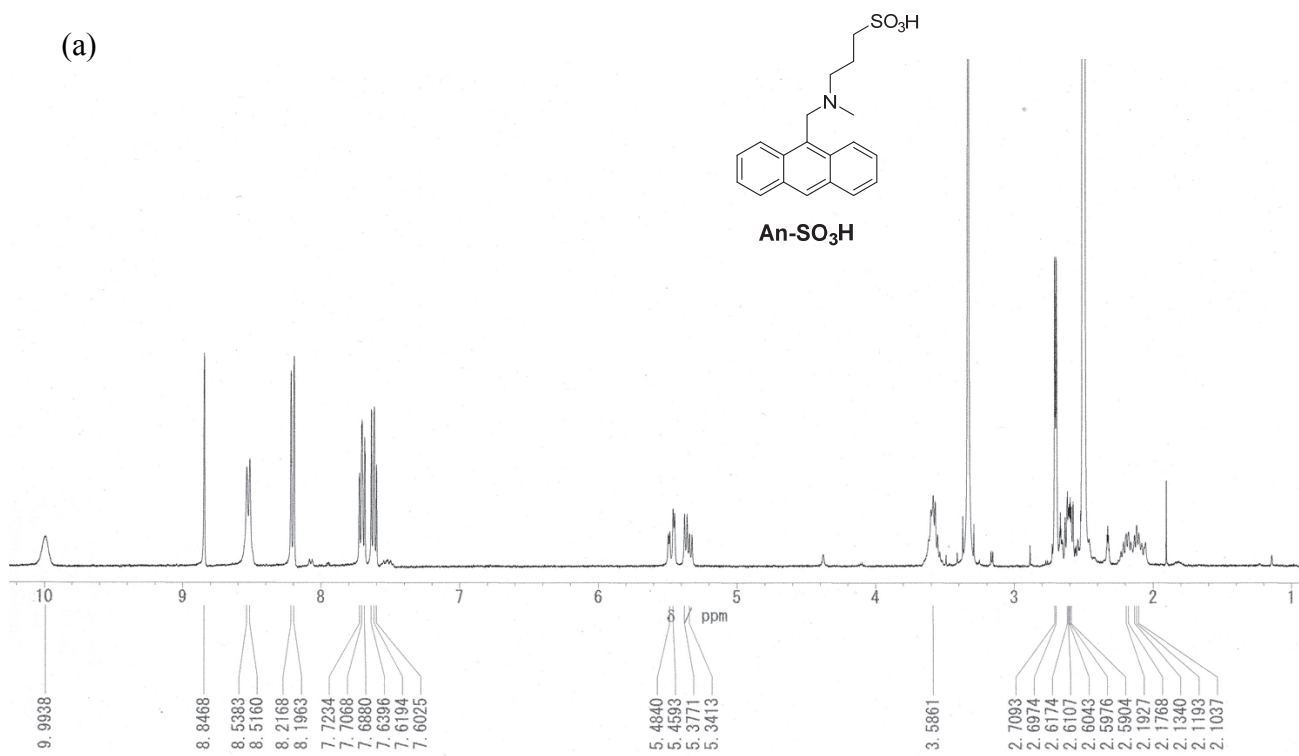
IR spectra were recorded on a SHIMADZU IRAffinity-1 spectrometer by ATR method. ^1H and ^{13}C NMR spectra were recorded on a Varian-400 or Varian-500 FT NMR spectrometer. High-resolution mass spectral data by ESI were acquired on a Thermo Fisher Scientific LTQ Orbitrap XL. Absorption spectra of solution were observed with a HITACH U-2910 spectrophotometer and absorption spectrum of the solid was recorded by a Shimadzu UV-3600 plus spectrophotometer with a calibrated integrating sphere system. fluorescence spectra were measured with a HORIBA FluoroMax-4 spectrofluorometer. The fluorescence quantum yields in solution were determined by a HORIBA FluoroMax-4 spectrofluorometer by using a calibrated integrating sphere system. Fluorescence decay measurements were performed on a HORIBA DeltaFlex modular fluorescence lifetime system, using a Nano LED pulsed diode excitation source (318 nm).

Preparation of 3-((anthracen-9-ylmethyl)(methyl)amino)propane-1-sulfonic acid (**An-SO₃H**)

A solution of 9-(methylaminomethyl)anthracene (0.75 g, 3.4 mmol) and 1,3-propane sultone (0.46 g, 3.7 mmol) in DMF (35 ml) was stirred for 1 day at 100°C. The resulting precipitate was filtered and was washed by DMF to give **An-SO₃H** (0.71 g, yield 62 %) as a colorless solid; FT-IR (ATR): $\tilde{\nu}$ = 2727, 1215, 1175, 1153, 1030 cm^{-1} ; ^1H NMR (400 MHz, DMSO- d_6) δ = 2.05-2.20 (m, 2H), 2.59-2.62 (m, 2H), 2.70 (d, 3H), 3.55-3.60 (m, 2H), 5.34-5.48 (m, 2H), 7.62 (t, 2H), 7.71 (t, 2H), 8.21 (d, J = 8.2 Hz, 2H), 8.53 (d, J = 8.9 Hz, 2H), 8.85 (s, 1H), 9.99 (br, 1H); ^{13}C NMR (125 MHz, DMSO- d_6) δ = 20.15, 49.26, 51.29, 56.58, 121.34, 124.33, 125.57, 127.52, 129.31, 130.89 ppm (one aliphatic carbon signal and two aromatic carbon signals were not observed owing to overlapping with carbon in DMSO- d_6 and overlapping resonance, respectively); HRMS (ESI): m/z (%):[M-H^-] calcd for $\text{C}_{19}\text{H}_{20}\text{O}_3\text{NS}$, 342.11694; found 342.11658.

Preparation of sodium 3-((anthracen-9-ylmethyl)(methyl)amino)propane-1-sulfonate (**An-SO₃Na**)

A solution of **An-SO₃H** (0.18 g, 0.51 mmol) in aqueous NaOH (25 ml, 0.02 M) and ethanol (25 ml) was stirred for 1 day at reflux. After concentrating under reduced pressure, the resulting residue was chromatographed on reverse-phase silica gel (methanol as eluent) to give **An-SO₃Na** (0.19 g, yield 87 %) as an orange-yellow solid; FT-IR (ATR): $\tilde{\nu}$ = 1182 (br), 1045 cm^{-1} ; ^1H NMR (400 MHz, DMSO- d_6) δ = 1.78-1.85 (m, 2H), 2.06 (s, 3H), 2.32-2.36 (m, 2H), 2.59 (t, J = 7.2 Hz, 2H), 4.38 (s, 2H), 7.48-7.57 (m, 4H), 8.07 (d, J = 9.0 Hz, 2H), 8.50 (d, J = 9.0 Hz, 2H), 8.56 (s, 1H); ^{13}C NMR (125 MHz, DMSO- d_6) δ = 23.13, 40.88, 49.47, 53.09, 56.71, 125.00, 125.11, 125.69, 127.06, 128.79, 130.75, 130.95 ppm (one aromatic carbon signal was not observed owing to overlapping resonance); HRMS (ESI): m/z (%):[M-H^-] calcd for $\text{C}_{19}\text{H}_{20}\text{O}_3\text{NS}$, 342.11694; found 342.11670.



(b)

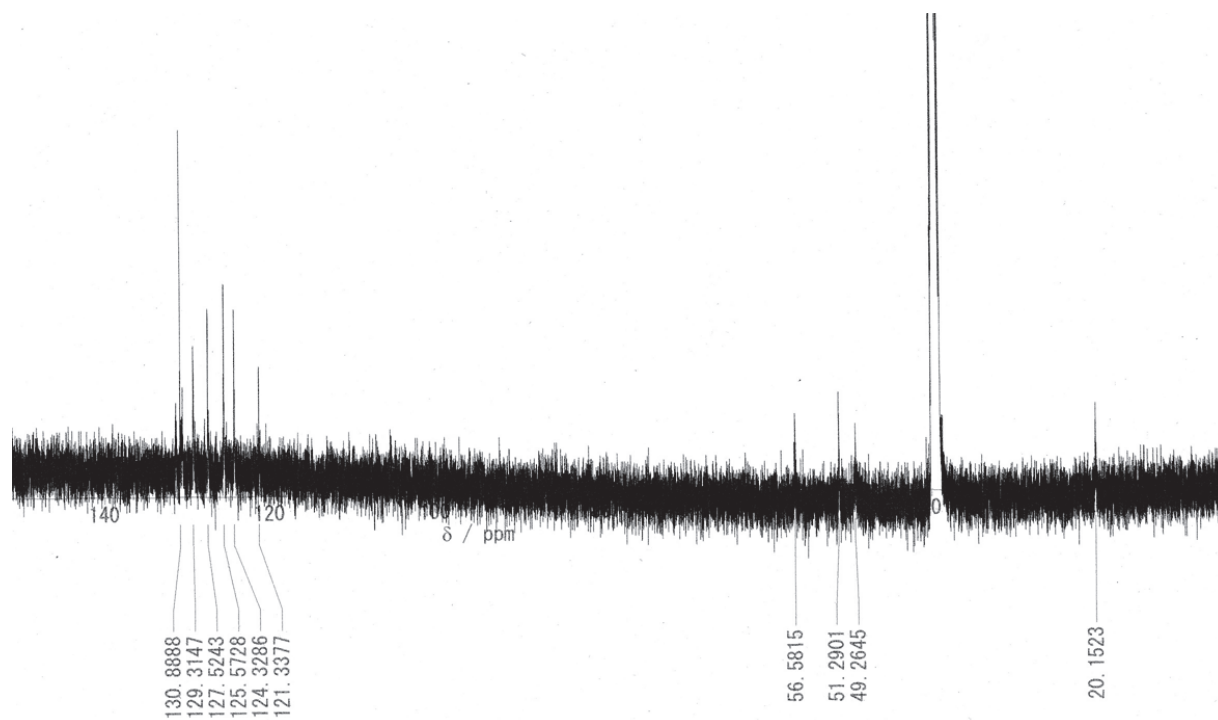


Fig. S1 (a) ¹H HMR (400 MHz) and (b) ¹³C HMR (125 MHz) of An-SO₃H in DMSO-d₆.

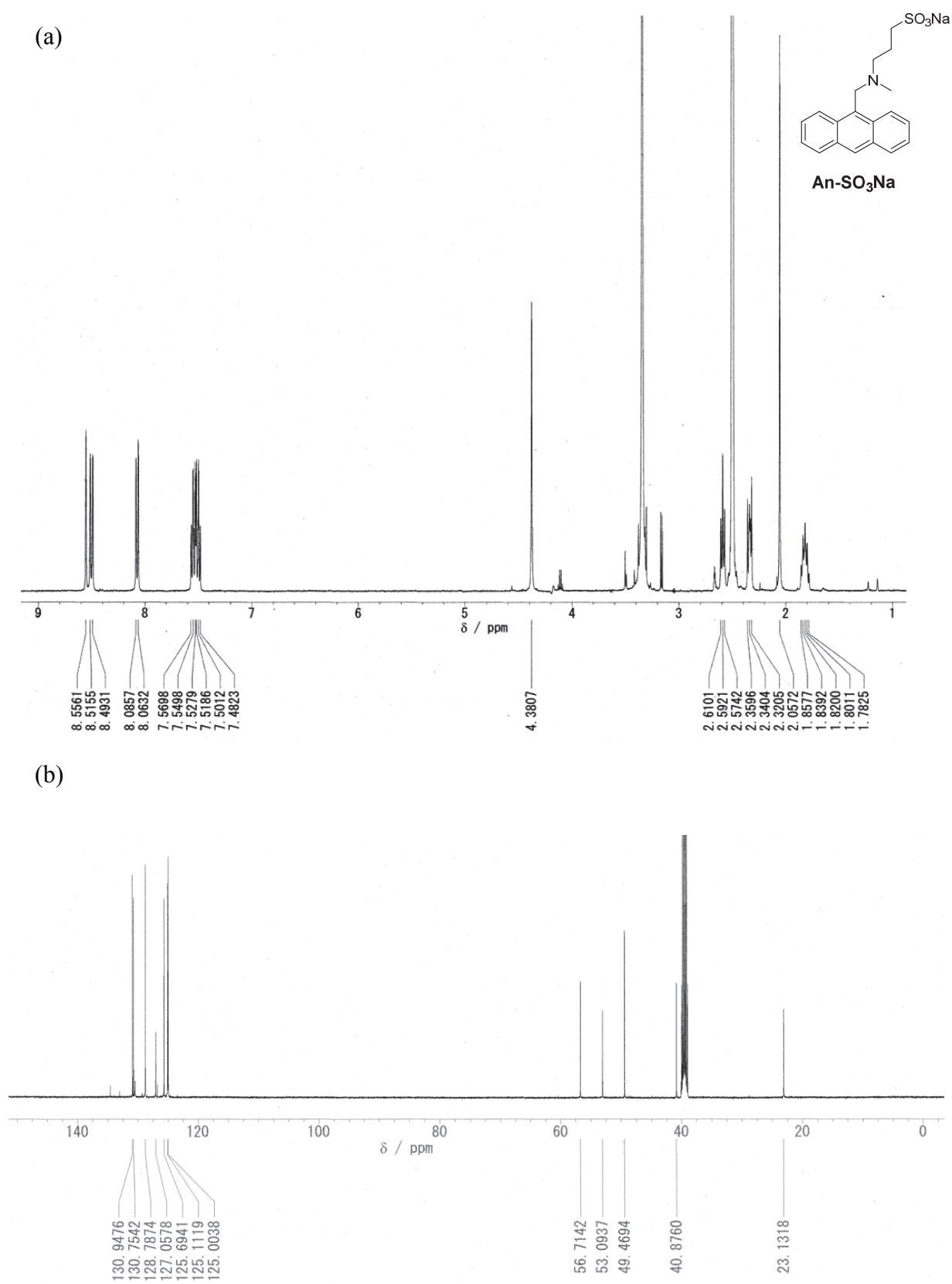
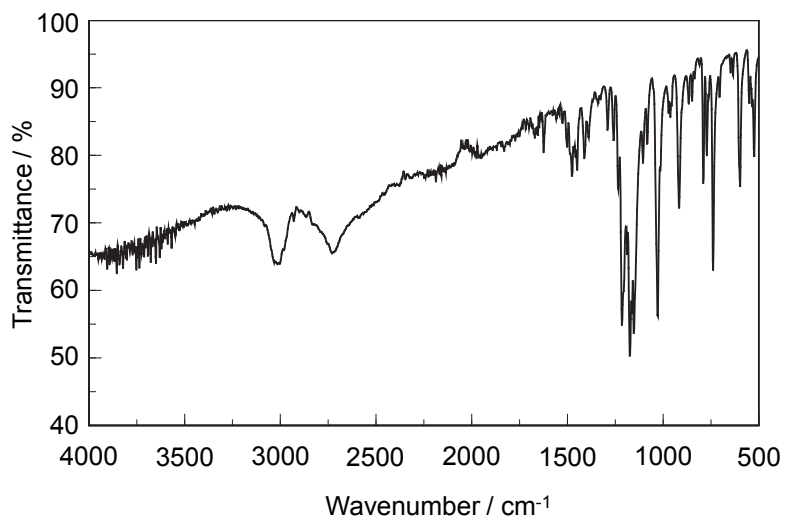


Fig. S2 (a) ^1H HMR (400 MHz) and (b) ^{13}C HMR (125 MHz) of **An-SO₃Na** in DMSO-*d*₆.

(a)



(b)

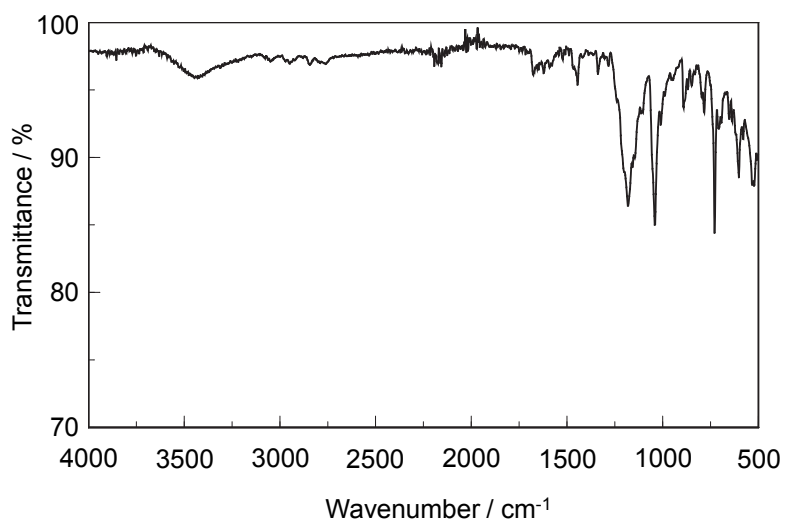


Fig. S3 FTIR spectra of (a) **An-SO₃H** and (b) of **An-SO₃Na**.