Supplementary Information

Dual-mode of assembly of anthracene-based imidazolium salts both in non-polar organic solvents and in aqueous solution

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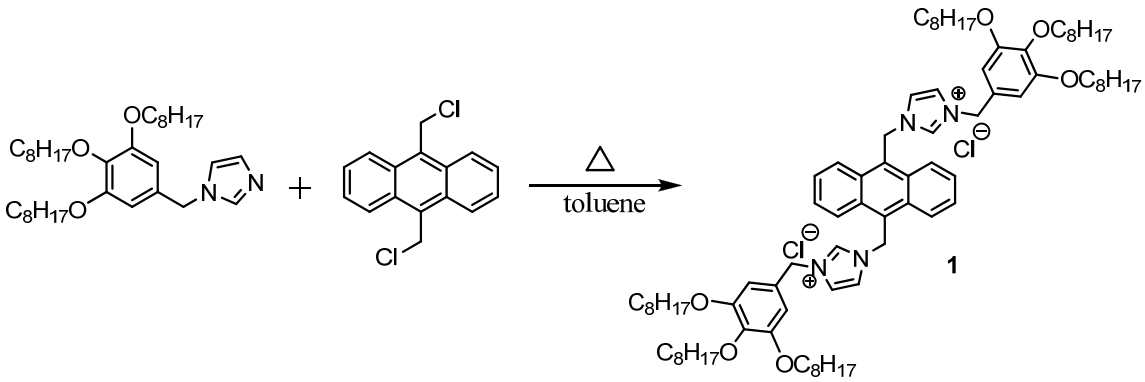
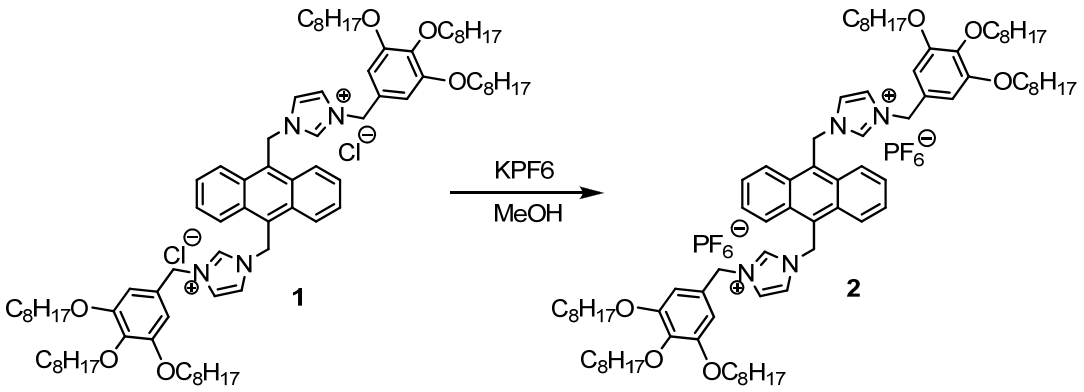
Synthesis of 1,1'-(anthracene-9,10-diylbis(methylene))bis(3-(3,4,5-tris(octyloxy)-benzyl)-1*H*-imidazolium) dichloride (1).



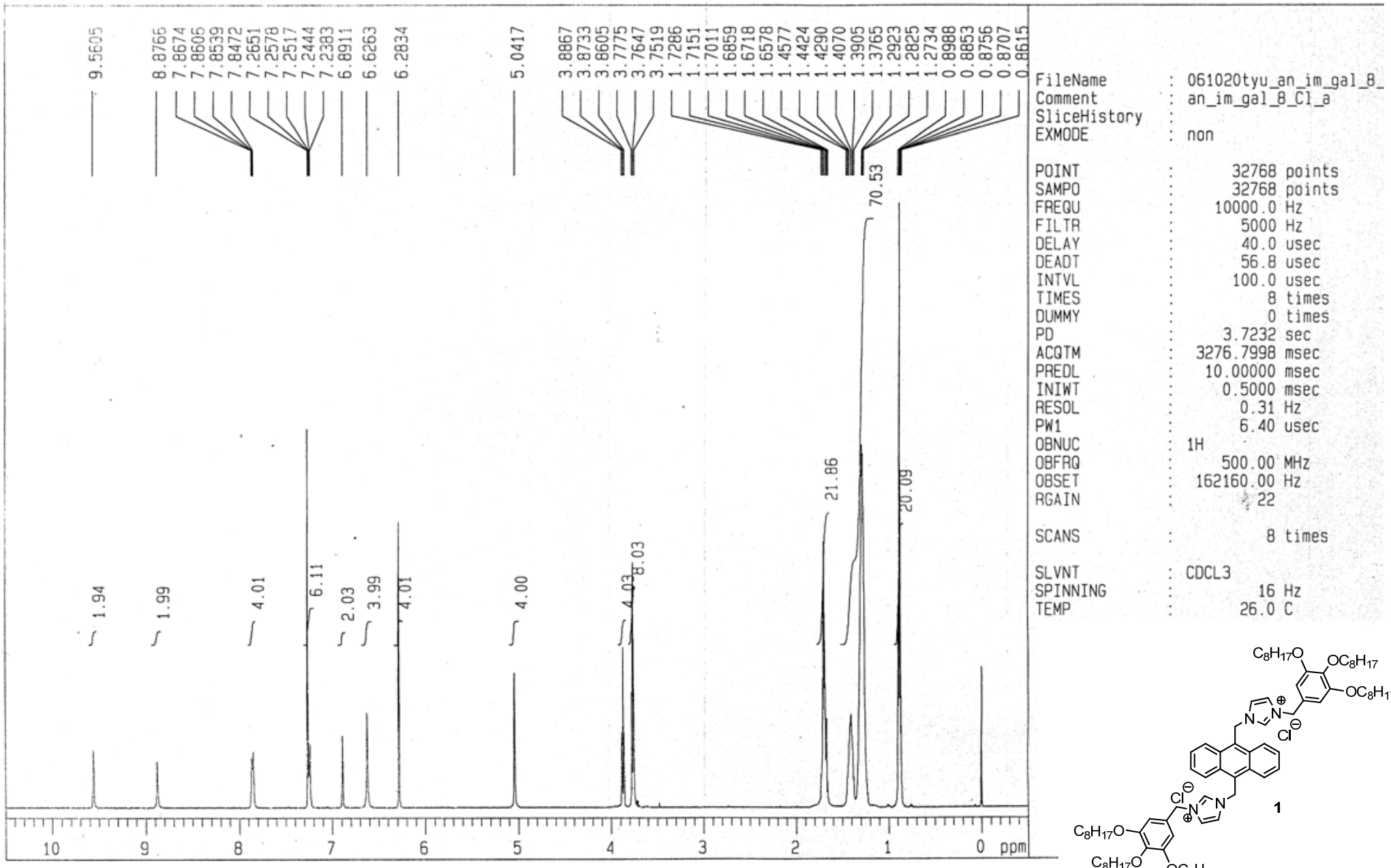
A solution of 1-(3,4,5-tris(octyloxy)benzyl)imidazole (0.470 g, 0.919 mmol) and 9,10-bis(chloromethyl)anthracene (0.126 g, 0.460 mmol) in toluene (20 ml) was refluxed for 3 days under stirring. The solvent was removed in vacuo and the crude product was purified by silica gel chromatography (eluent: $CHCl_3$/MeOH = 95/5 to 4/1) to obtain 0.362 g (61 %) of **1** as a yellow solid. Mp. 204.3–208.1 ºC; ^{1}H NMR (395.75 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8 Hz, 18H), 1.28-1.47 (m, 60H), 1.65-1.79 (m, 12H), 3.76 (t, J = 6.3 Hz, 8H), 3.87 (t, J = 6.5 Hz, 4H), 5.04 (s, 4H), 6.28 (s, 4H), 6.62 (s, 4H), 6.89 (s, 2H), 7.25 (m, 4H), 7.85 (m, 4H), 8.87 (s, 2H), 9.54 (s, 2H); ^{13}C NMR (99.45 MHz, $CDCl_3$): δ 14.12, 22.70, 26.11, 29.40, 30.30, 31.91, 46.25, 53.32, 69.29, 73.43, 107.40, 120.53, 123.38, 124.44, 127.43, 127.60, 130.11, 136.59, 138.83, 153.60; HRMS(ESI) m/z, calcd for $C_{84}H_{128}ClN_4O_6$ $[M - Cl]^+$ 1323.9517, found 1323.9498, calcd for $C_{84}H_{128}N_4O_6$ $[M - 2Cl]^{2+}$ 644.4911, found 644.4903.

Synthesis of 1,1'-(anthracene-9,10-diylbis(methylene))bis(3-(3,4,5-tris(octyloxy)-benzyl)-1*H*-imidazolium) dihexafluorophosphate (2).



A solution of **1** (0.200 g, 1.09 mmol) and KPF_6 (0.412 g, 2.29 mmol) in MeOH (10 mL) was stirred at ambient temperature for 1 day. The solvent was removed in vacuo and dissolved in n-hexane. After filtration, the solvent was evaporated solvent to obtain a yellow solid. The crude product was purificated by silica gel chromatography (eluent: $CHCl_3$/MeOH = 95/5 to 4/1) to obtain 0.362 g (61 %) of **2**. Mp. 119.0–123.6 ºC; ^{1}H NMR (395.75 MHz, $CDCl_3$): δ 0.88 (t, J = 6.8, 18H), 1.28-1.47 (m, 60H), 1.69-1.77 (m, 12H), 3.90 (m, 12H), 4.96 (s, 4H), 6.00 (s, 4H), 6.43 (s, 4H), 6.99 (s, 2H), 7.33 (s, 2H), 7.39 (m, 4H), 7.86 (m, 4H), 8.28 (s, 2H); ^{13}C NMR (99.45 MHz, $CDCl_3$): δ 14.08, 22.66, 26.07, 29.36, 30.31, 31.89, 45.59, 53.95, 69.17, 73.42, 107.30, 121.77, 122.81, 123.12, 124.29, 126.81, 128.05, 130.24, 134.65, 138.89, 153.78; HRMS(ESI) m/z, calcd for $C_{84}H_{128}F_6N_4O_6P$ $[M - PF_6]^+$ 1433.9470, found 1433.9440, calcd for $C_{84}H_{128}N_4O_6$ $[M - 2PF_6]^{2+}$ 644.4911, found 644.4897.

^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **1**



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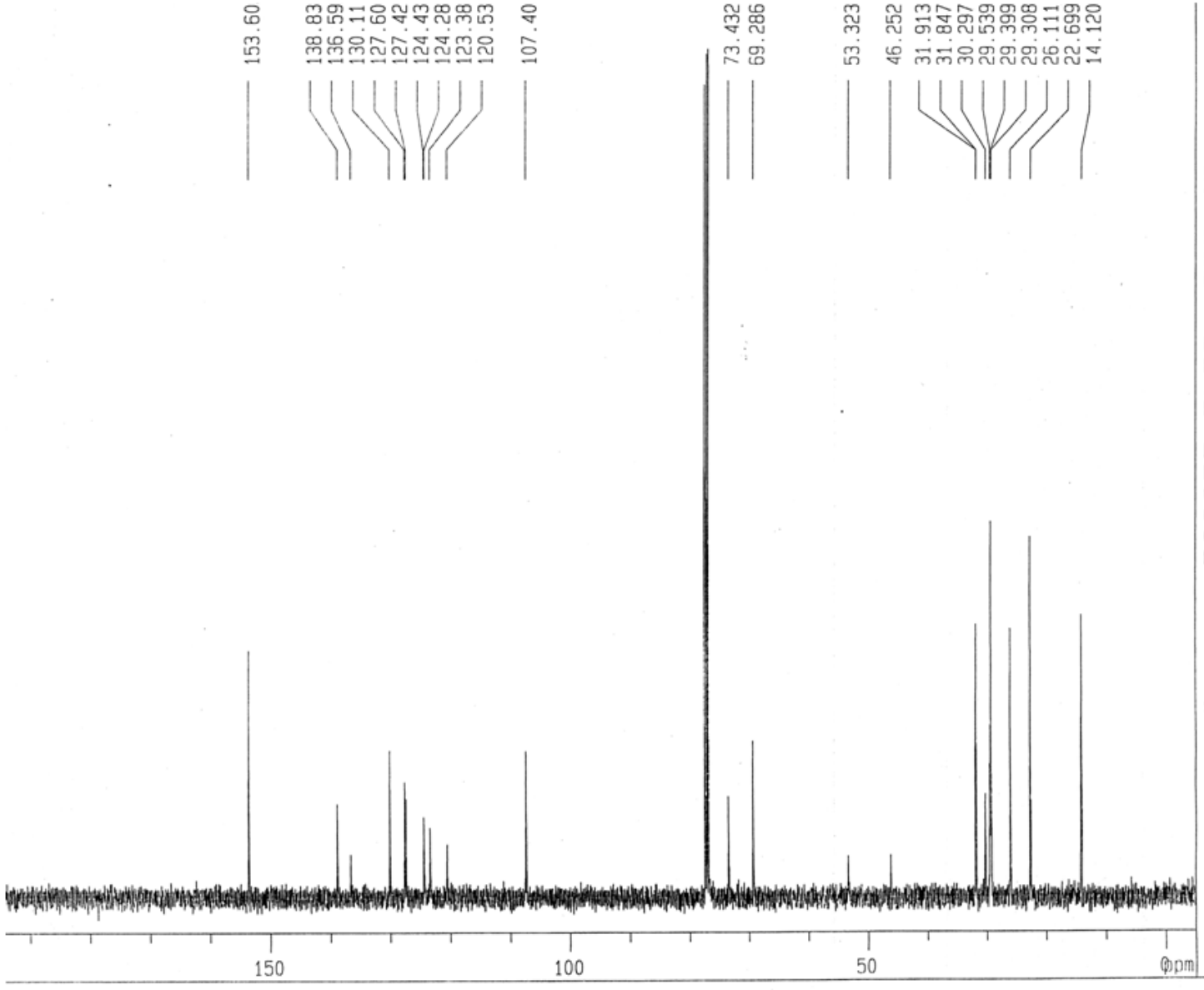
^{13}C NMR (99.45 MHz, $CDCl_3$) spectrum of **1**



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DEADT	:	19.8 usec
INTVL	:	37.2 usec
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DUMMY	:	1 times
PD	:	1.7810 sec
ACQTM	:	1218.9696 msec
PREDL	:	10.00000 msec
INIWT	:	10.0000 msec
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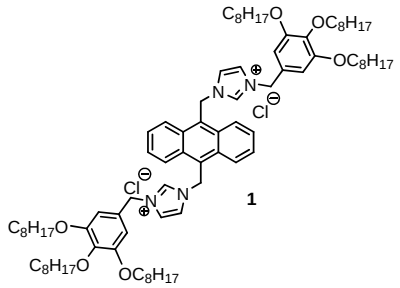
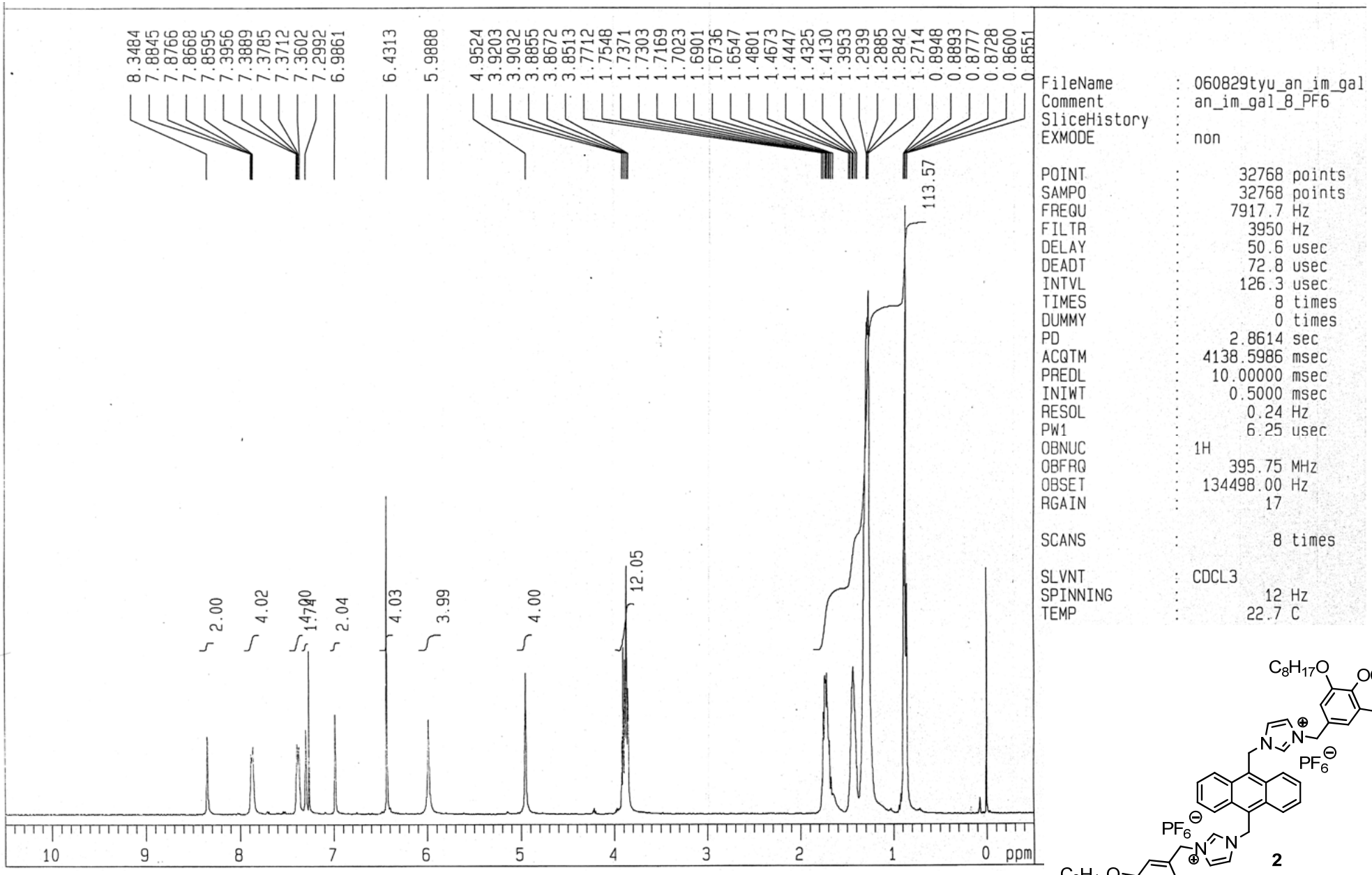


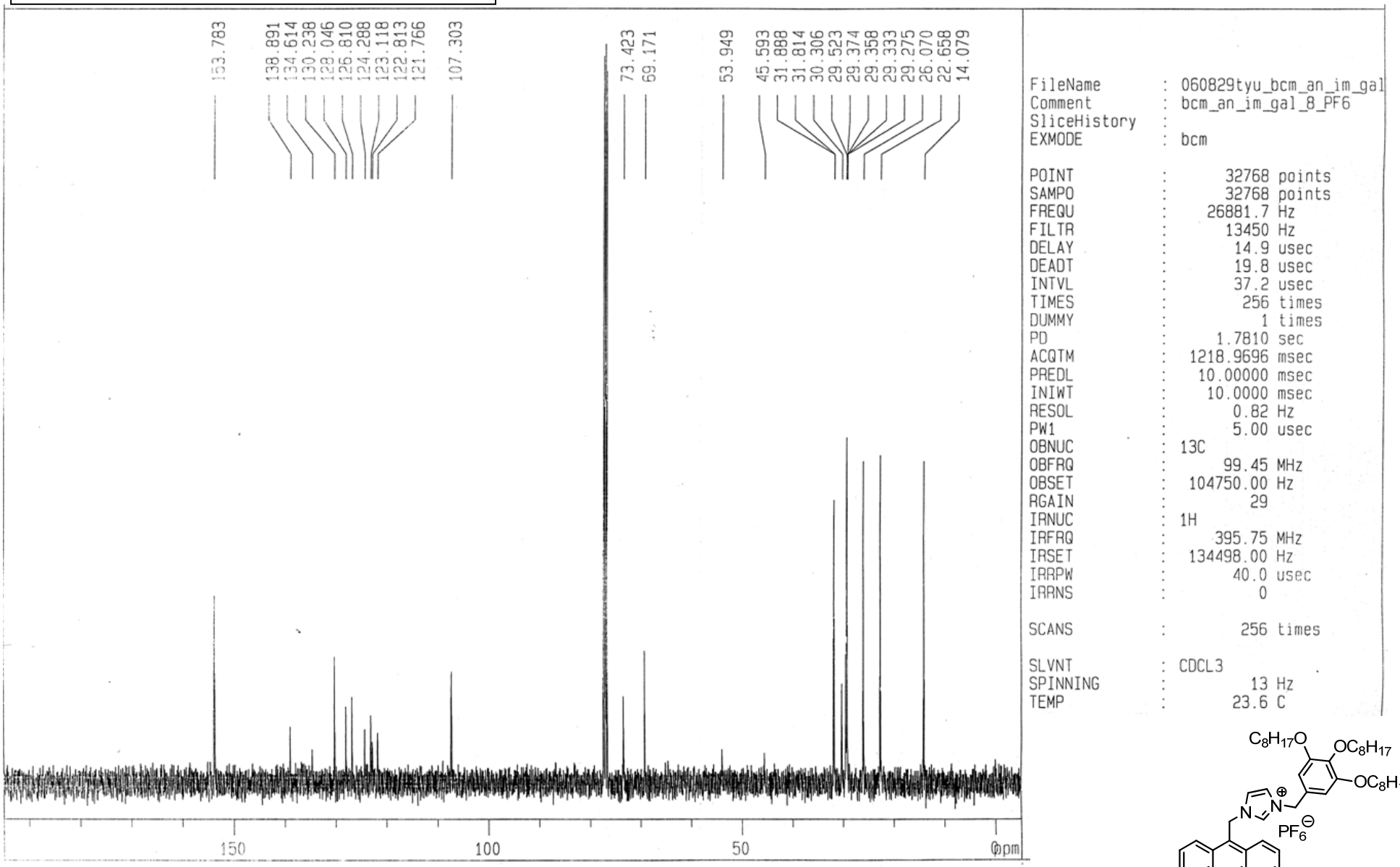
1

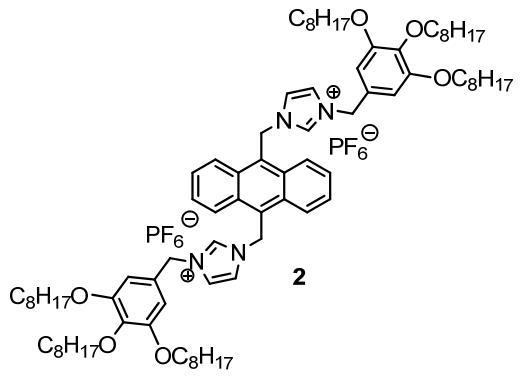
^{1}H NMR (395.75 MHz, $CDCl_3$) spectrum of **2**



2

^{13}C NMR (99.45 MHz, $CDCl_3$) spectrum of **1**





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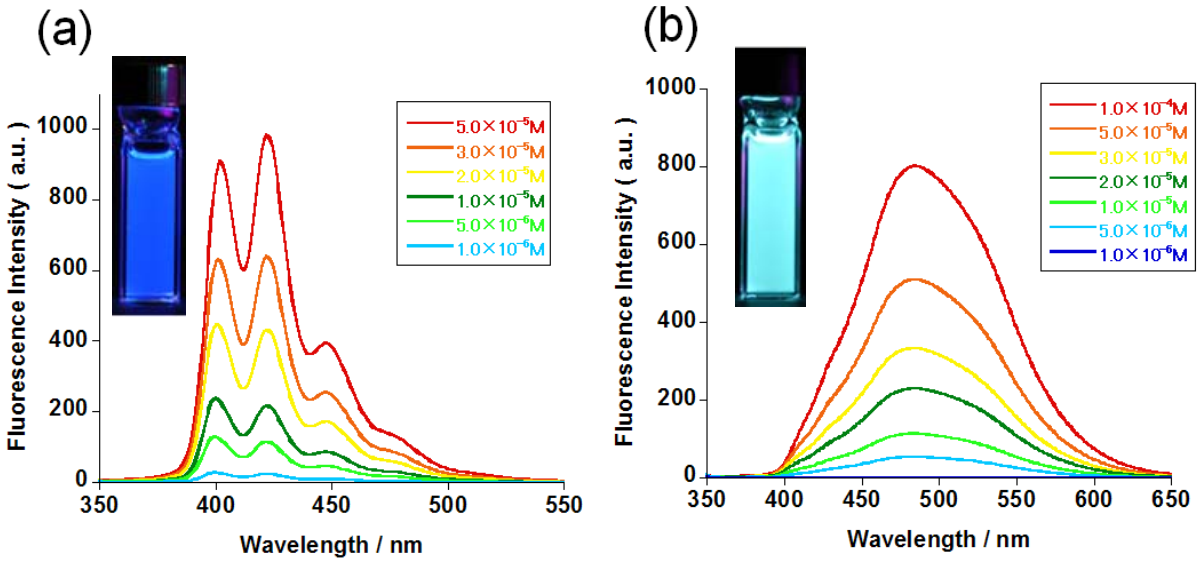

Figure S1. Fluorescence spectra of **2** in EtOH (a) and in hexane (b). λ_{ex} 342 nm. The inset photographs show the color of fluorescence at concentration 5.0 x 10^{-5} M with λ_{ex} 365 nm.

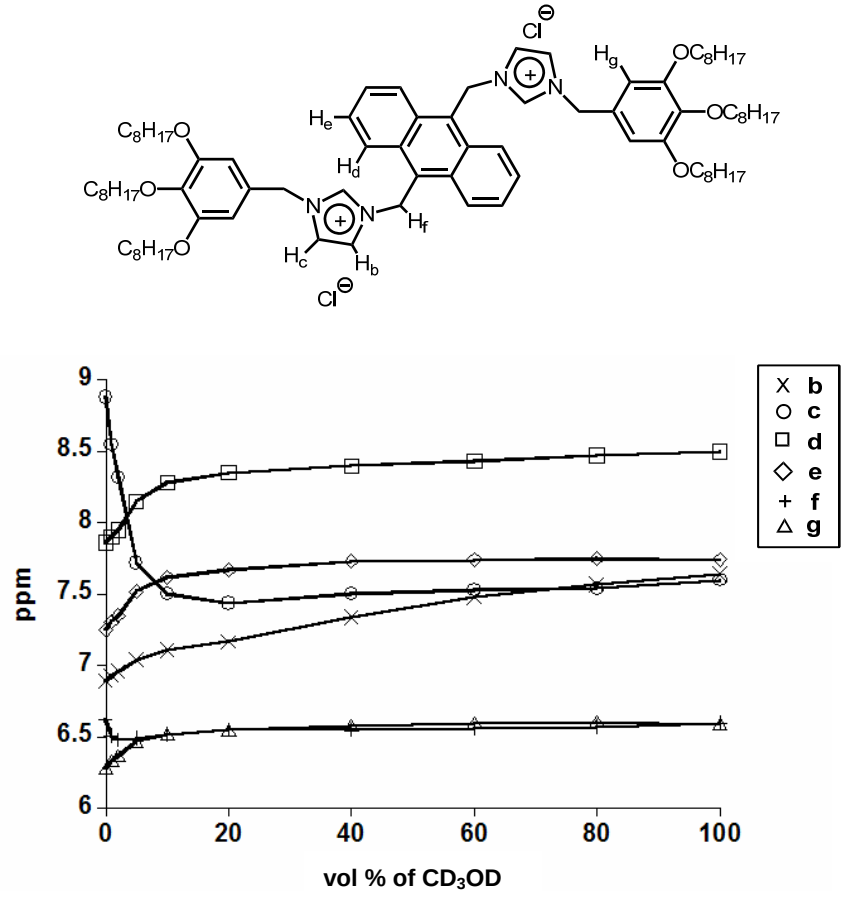

Fig. S2. Solvent-polarity-dependent chemical shift of compound **1** in $CDCl_3/CD_3OD$ at ca. 25ºC (concentration ca. 7.0 x 10^{-3} M).

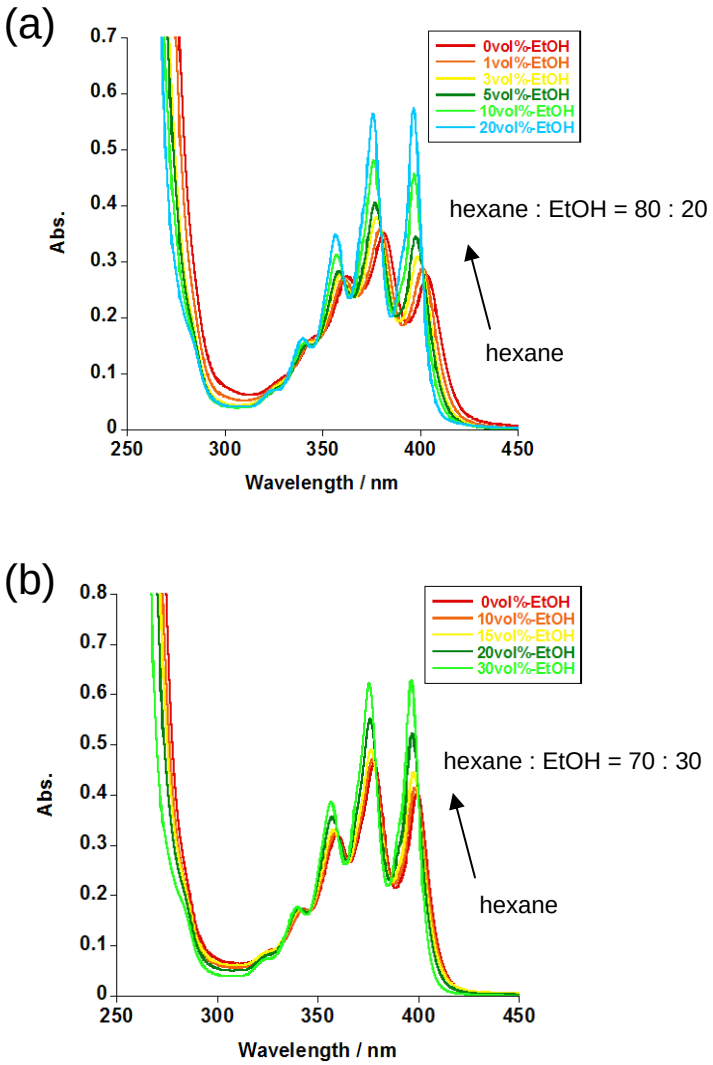

Fig. S3. Solvent-polarity-dependent uv-vis spectra of **1** (a) and **2** (b) in hexane with varying amount of ethanol.