

Supplementary Information for:

Cyanurate-Guided Self-Assembly of a Melamine-Capped Oligo(*p*-phenylenevinylene)

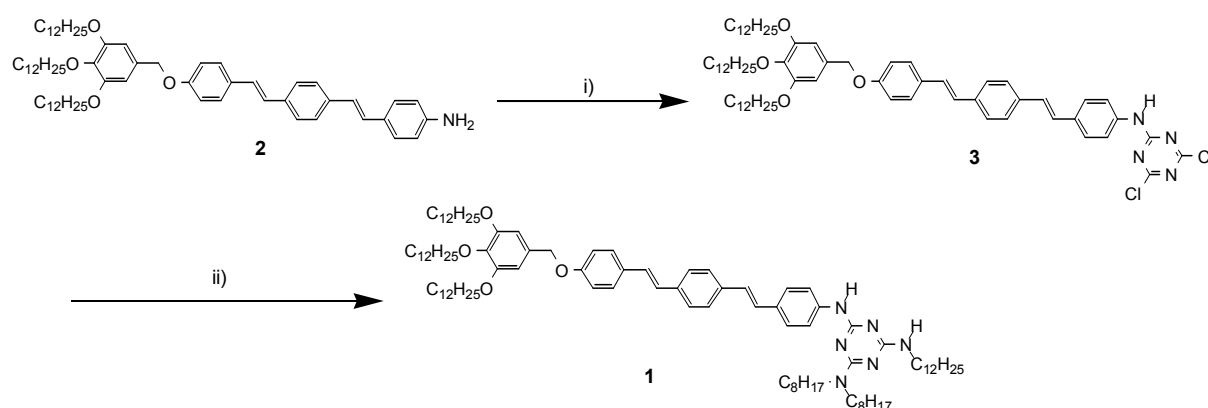
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Materials and methods

Column chromatography was performed using 63–210 μm silica gel. All other commercially available reagents and solvents were of reagent grade and used without further purification. ^1H NMR spectra were recorded on JEOL LA400 or LA500 spectrometer and chemical shifts are reported in ppm with the signal of TMS as internal standard. FAB-MS spectra were measured on a JEOL JMS-AX500 mass spectrometer. Elemental analyses were performed in Analytical Center of Chiba University. The solvents for the spectroscopic measurements were all spectral grade and used without further purification. UV/Vis and fluorescence spectra were recorded on a JASCO V570 spectrophotometer and JASCO FP6600 spectrofluorometer, respectively. SEM observation was carried out using a JEOL JSM-6330F field emission scanning electron microscopy. Dried samples were coated with Os using a Meiwafoysis Neoc Pure Osmium Coater.

Synthesis

OPV **1** was synthesized from amino-OPV derivative **2**¹ according to Scheme S1.



Scheme S1. i) 2,4,6-trichloro-1,3,5-triazine, THF, 20 °C; ii) dodecylamine, THF, 30 °C, and then dioctylamine, 70 °C.

Compound 3: To a THF solution (15 mL) of 2,4,6-trichloro-1,3,5-triazine (19.9 mg, 0.108 mmol) and diisopropylethylamine (30 μ L), compound **2** (103 mg, 0.108 mmol) dissolved in 5 mL of THF was added at 20 °C under N₂. After stirring for 3 h, the solvent was removed by evaporation and the residue was purified by column chromatography over silica gel (hexane: AcOEt = 4:1) to give 105 mg of compound **3** (yield 88%).

¹H NMR (400 MHz, CDCl₃): δ = 7.58 (s, 1H), 7.55 (s, 4H), 7.49 (s, 4H), 7.47 (d, J = 8.9 Hz, 2H), 7.09 (s, 2H), 7.09 (d, J = 16.4 Hz, 1H), 6.98 (d, J = 16.4 Hz, 1H), 6.98 (d, J = 8.7 Hz, 2H), 6.63 (s, 2H), 4.97 (s, 2H), 4.00-3.92 (m, 6H), 1.83-1.70 (m, 6H), 1.52-1.42 (m, 6H), 1.37-1.20 (m, 48H), 0.88 (t, J = 6.9 Hz, 9H).

Compound 1: Compound **3** (105 mg, 0.095 mmol) and diisopropylethylamine (30 mL) were dissolved in 15 mL of dry THF. To this solution, dodecylamine (17.6 mg, 0.095 mmol) in dry THF (5 mL) was added and stirred for 30 min at 30 °C. When TLC showed complete disappearance of **3**, dioctylamine (242 mg, 0.95 mmol) was added and stirred overnight at 70 °C. After cooling to r.t., water and chloroform was added and separated organic layer was washed with water and 2% HCl aq, and dried over Na₂SO₄. After evaporation, the residue was purified by column chromatography over silica gel (hexane: AcOEt = 4:1) to give compound **1** as yellow solid (94.6 mg, 72% yield).

¹H-NMR (500 MHz, CDCl₃) δ = 7.62 (d, J = 7.3 Hz, 2H), 7.47-7.42 (m, 8H), 7.10-6.95 (m, 6H), 6.73 (bs, 1H), 6.63 (s, 2H), 4.97 (s, 2H), 4.80 (t, J = 6.3 Hz, 1H), 4.00-3.93 (m, 6H), 3.51-3.49 (m, 4H), 3.37 (q, J = 6.7 Hz, 2H), 1.83-1.71 (m, 6H), 1.70-1.55 (m, 6H), 1.52-1.42 (m, 6H), 1.37-1.20 (m, 48H), 0.92-0.86 (m, 18H); MS (FAB): 1458 (MH⁺); Anal. Calcd for C₉₆H₁₅₆N₆O₄: C 79.07, H 10.78; N 5.76; found C 78.94, H 11.21, N, 5.63.

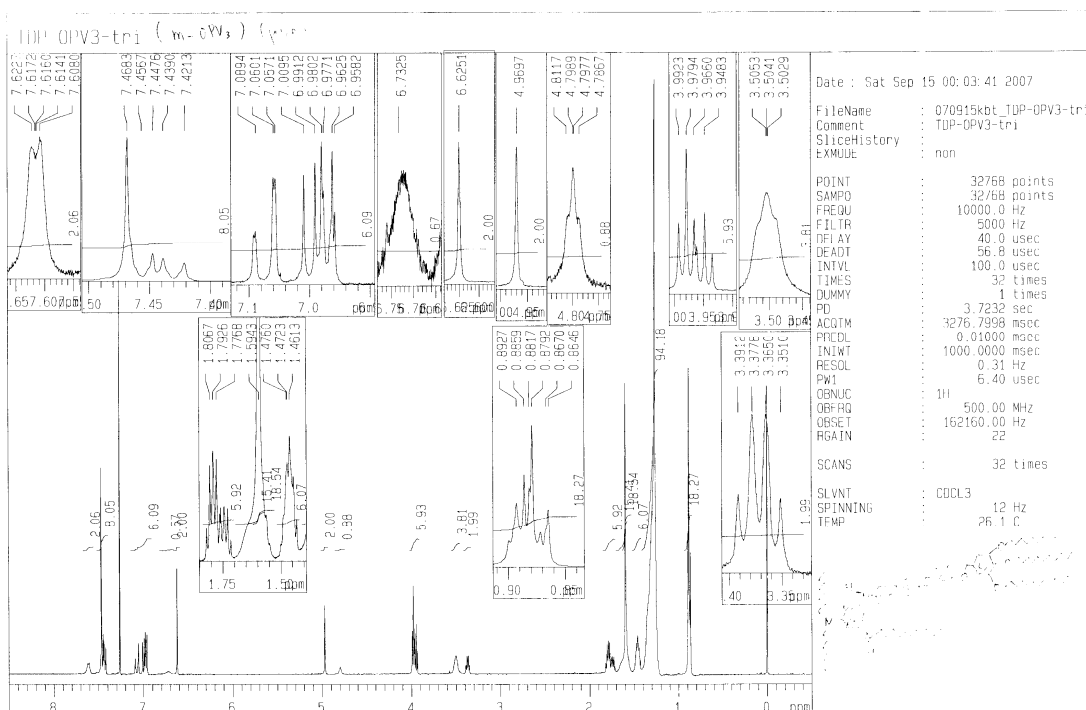


Fig. S1 ¹H NMR spectrum of 1.

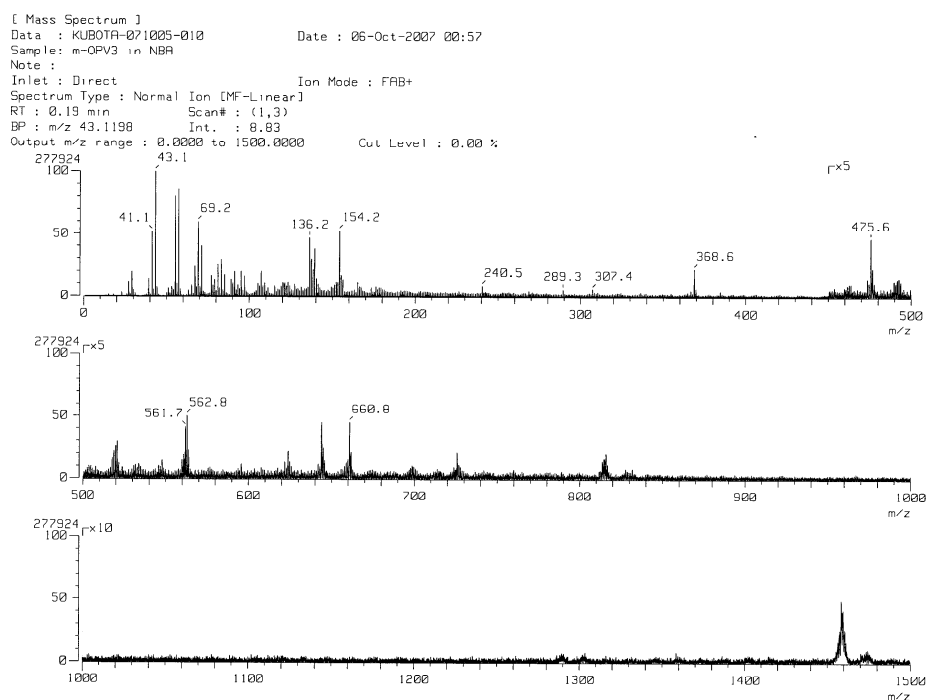


Fig. S2 FAB-MS spectrum of 1.

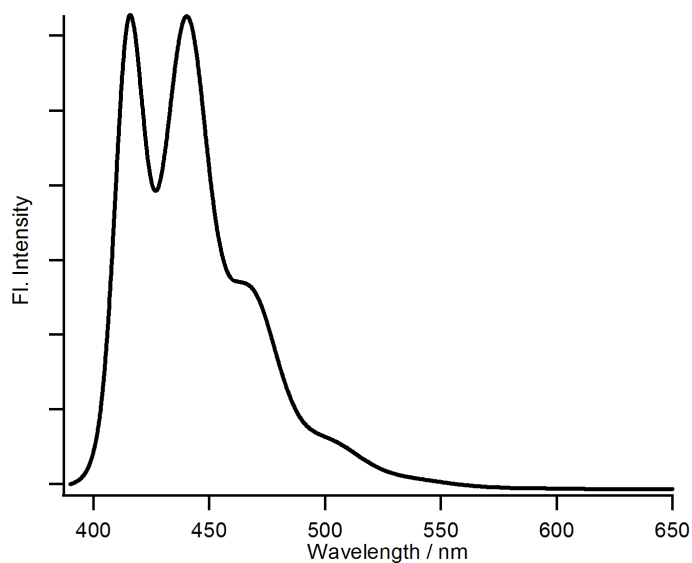


Fig. S3 Fluorescence spectrum of monomeric **1** (1×10^{-5}) in MCH at 10 °C. $\lambda_{\text{ex}} = 365$ nm.

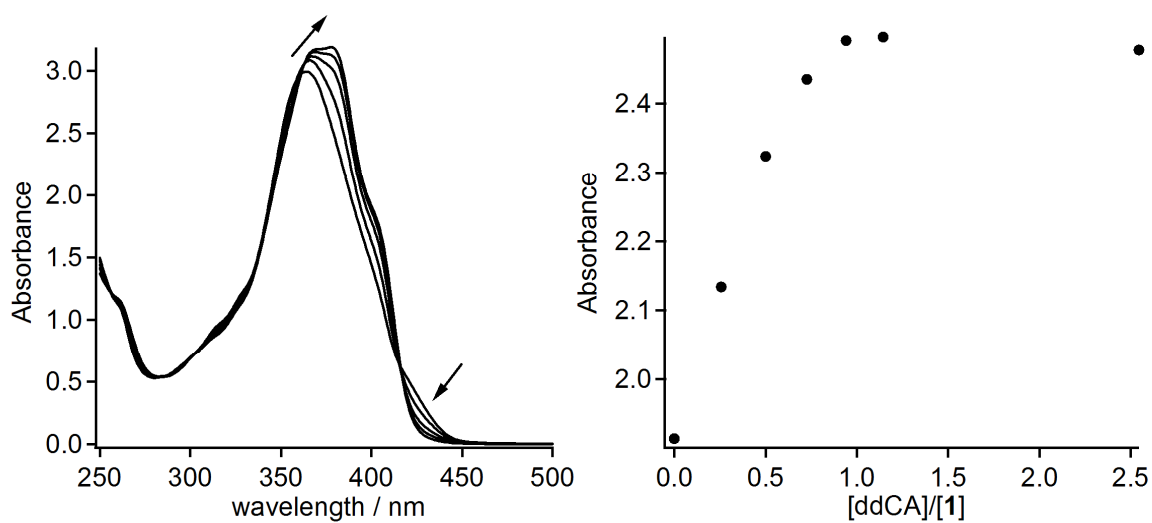


Fig. S4 (a) UV-vis titration of **1** (5×10^{-4}) with ddCA in MCH at 10 °C. (b) Plot of the absorbance at 390 nm versus $[\text{ddCA}]/[\mathbf{1}]$.

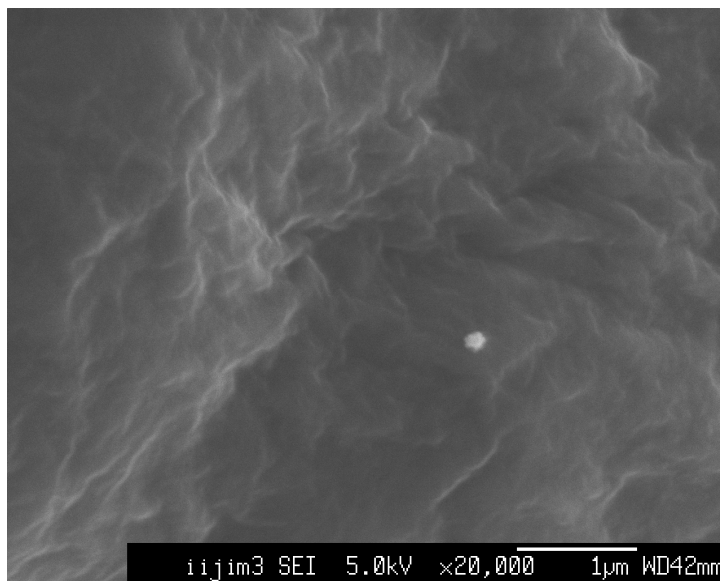


Fig. S5 SEM image of 1_2 -dCA.

References

1. S. Yagai, S. Kubota, T. Iwashima, K. Kishikawa, T. Nakanishi, T. Karatsu and A. Kitamura, *Chem. Eur. J.*, 2008, **14**, 5246-5257.