Supplementary Information (SI) for Soft Matter.
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Unravelling the Self-assembly of a Novel Cationic Pseudo-gemini Surfactant and Its Monomeric Counterpart: Interactions with DNA and BSA in Aqueous Medium at Neutral pH

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Experimental section

Synthesis of NHS-ester

NHS-ester was synthesized according to the reported procedure [1]. 4-dodecyloxybenzoic acid (1 equivalent, 3.2 mmol) and N-Hydroxy succinimide (1 equivalent, 3.2 mmol) was dissolved in dry THF. 1,3-dicyclohexylcarbodiimide (1 equivalent, 3.2 mmol) in dry THF was added to it, and the reaction mixture was stirred for 24 hours at room temperature. After 24 hours of reaction solvent was removed using rotary evaporator and was allowed to dry overnight in desiccator. The product was then recrystallized several times with Ethanol/water to get the pure product.

Synthesis of precursor molecules (PCS)

NHS ester (1 equivalent, 1.2 mmol) was dissolved in dry DCM in a round-bottom flask, after which N, N′-dimethylethylenediamine (2 equivalents, 2.4 mmol) was added. The reaction was allowed to proceed for 24 hours. After 24 hours of reaction, the solvent was removed using a rotary evaporator, yielding a semi-solid product. A small amount of water was added, and the mixture was basified to a pH of 8-10. The precipitate was then filtered and allowed to dry overnight in a desiccator. The foamy appearance of the synthesized product in acidic water indicates that the desired product was successfully formed, with a melting point of 50°C.

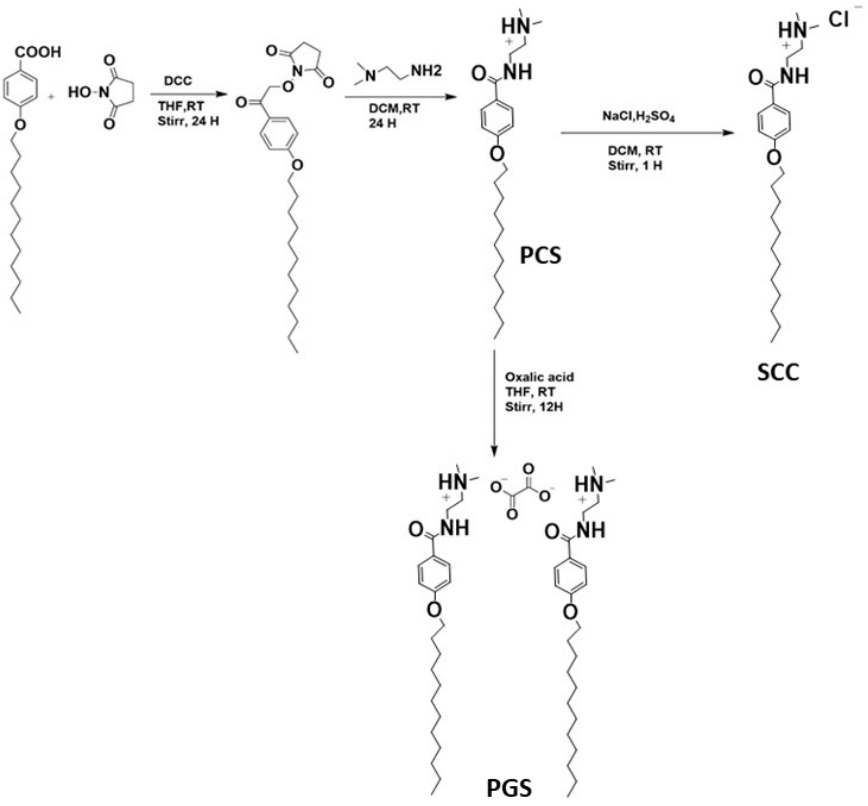
Synthesis of pseudo-gemini surfactant (PGS)

To synthesize the pseudo-gemini surfactant, PGS, the product from the previous step (PCS) (2.3 equivalents, 0.43 mmol) was dissolved in THF in a 50 mL round-bottom flask with a small bar magnet. Oxalic acid (1 equivalent, 0.18 mmol) was then added to the mixture, and the reaction was allowed to proceed for 12 hours. The reaction mixture was filtered to obtain the precipitate, which was washed several times with dry THF before being dried overnight in a desiccator.

Synthesis of single chain counterpart (SCC)

The corresponding monomeric counterpart was synthesized from the product obtained in step 2, i.e. PCS, which was dissolved in dry DCM in a round-bottom flask. HCl gas was then passed through the mixture, using sodium chloride and sulfuric acid as the source of HCl gas, for 1-2 hours. Afterward, the solvent was evaporated using a rotary evaporator, and the product was allowed to dry overnight in a desiccator. The melting point of the final product is 90°C.

The reaction scheme of the detailed synthetic procedure is furnished in **Scheme 1**. The chemical identification data, including representative ^{1}H and ^{13}C-NMR, spectra (**Fig. S1-S4**) are provided below.



Scheme S1: Synthesis scheme for cationic surfactants PGS and SCC

Chemical Identifications

PCS: White solid; Yield: 80 %; **^{1}H-NMR** (500 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.35 (s, 1H), 6.81 (d, *J* = 8.3 Hz, 2H), 3.90 (t, *J* = 6.5 Hz, 2H), 3.58 (q, *J* = 5.5 Hz, 2H), 2.72 (t, *J* = 5.6 Hz, 2H), 2.42 (s, 6H), 1.76 – 1.69 (m, 2H), 1.37 (p, *J* = 7.2 Hz, 2H), 1.30 – 1.17 (m, 16H), 0.81 (t, *J* = 6.8 Hz, 3H). **^{13}C-NMR** (500 MHz, Chloroform-*d*) δ 167.36, 162.03, 129.29, 125.58, 114.23, 68.18, 58.90, 44.32, 35.66, 32.41, 31.91, 29.65, 29.62, 29.58, 29.55, 29.37, 29.33, 29.14, 25.99, 22.67, 14.08.

PGS: White solid; Yield: 95 %; **^{1}H-NMR** (400 MHz, Chloroform-*d*) δ 8.52 (s, 2H), 7.91 (d, *J* = 8.3 Hz, 4H), 6.87 (d, *J* = 8.2 Hz, 4H), 3.93 (t, *J* = 6.6 Hz, 4H), 3.85 (s, 4H), 3.29 (s, 4H), 2.84 (s, 12H), 1.76 (p, *J* = 6.9 Hz, 4H), 1.46 – 1.22 (m, 36H), 0.90 (t, *J* = 6.5 Hz, 6H). **^{13}C-NMR** (400 MHz, Chloroform-*d*) δ 172.65 167.64, 162.07, 129.23, 125.33, 114.25, 77.22, 68.19, 58.09, 44.18, 35.43, 31.93, 29.71, 29.67, 29.64, 29.61, 29.58, 29.40, 29.36, 29.15, 26.00, 22.70, 14.13.

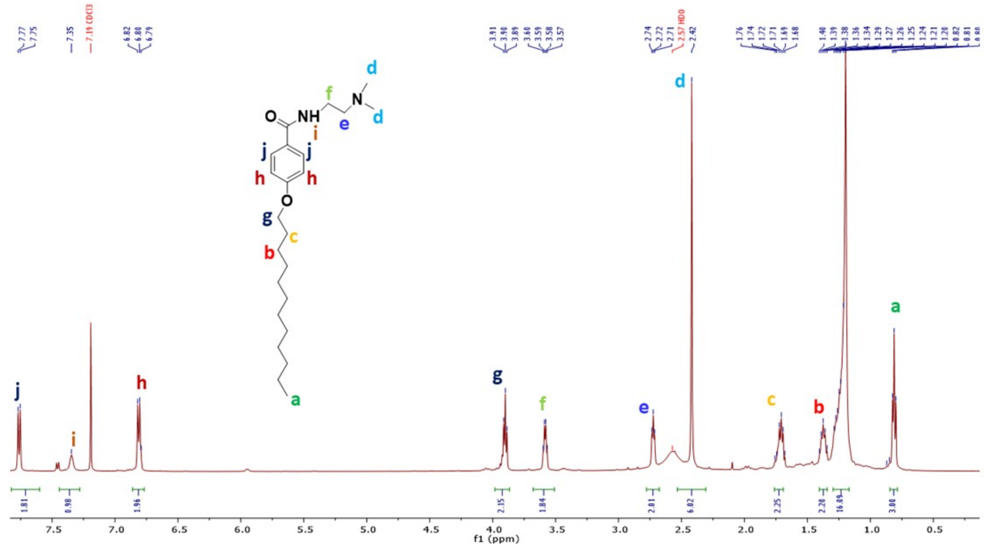


Fig. S1 ^{1}H-NMR spectrum of precursor molecule (PCS) in $CDCl_3$

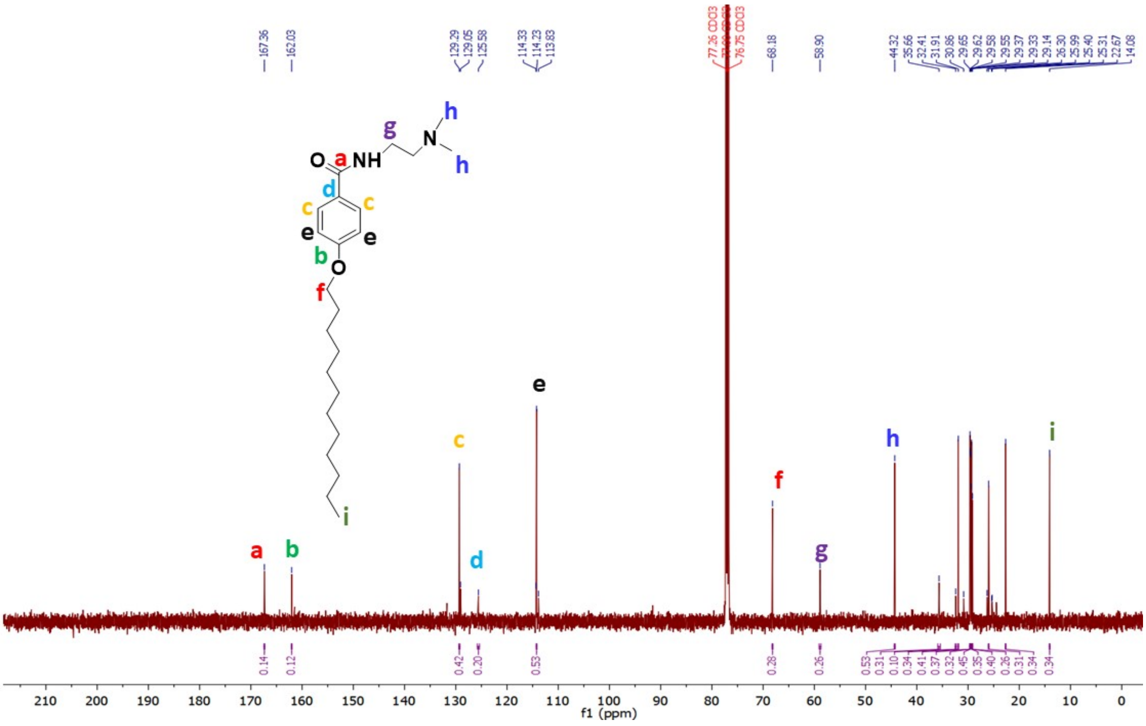


Fig. S2 ^{13}C-NMR spectrum of precursor molecule (PCS) in $CDCl_3$

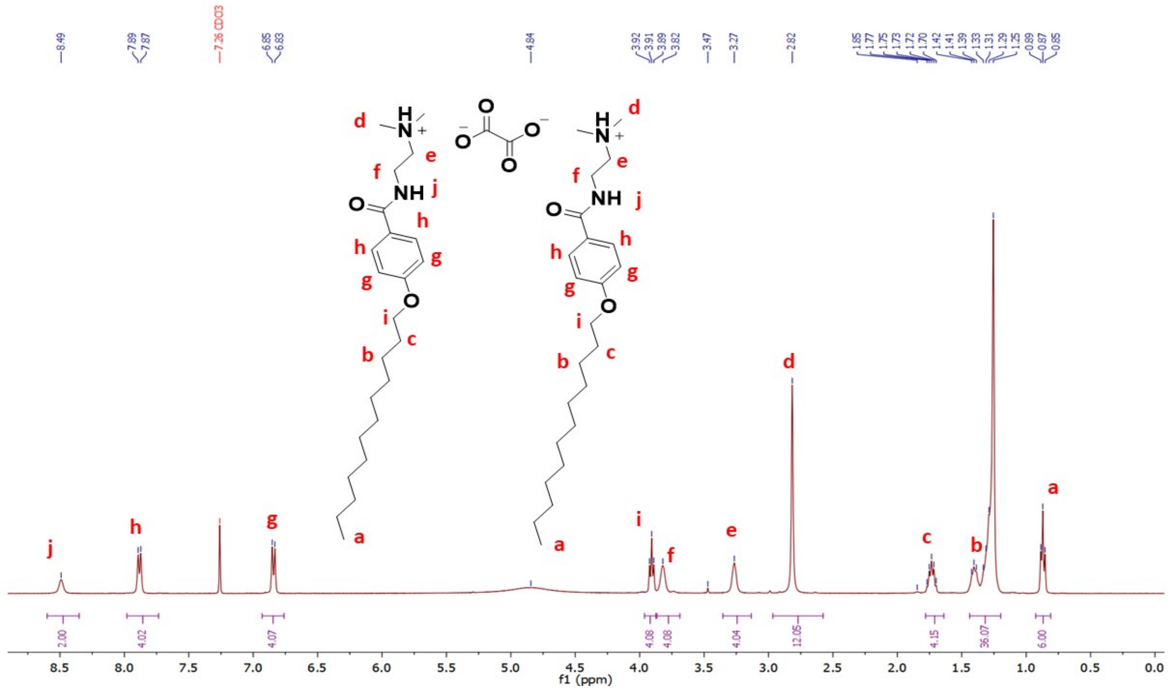


Fig. S3 ^{1}H-NMR Spectrum of PGS in $CDCl_3$

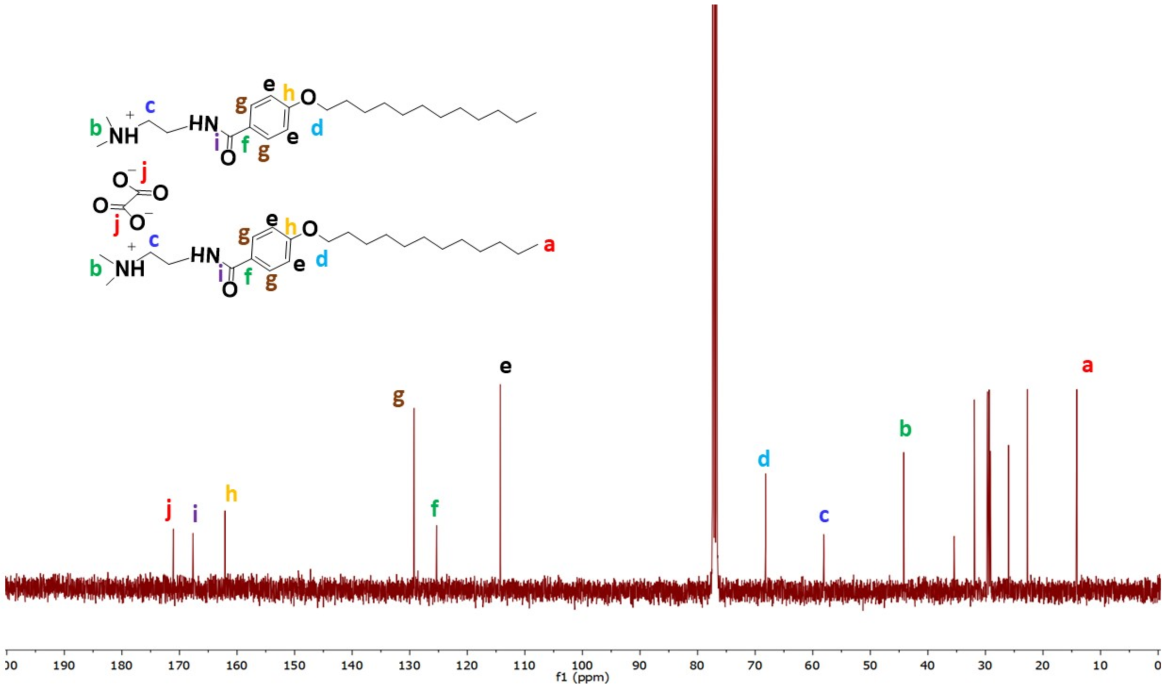


Fig. S4 ^{13}C-NMR Spectrum of PGS in $CDCl_3$

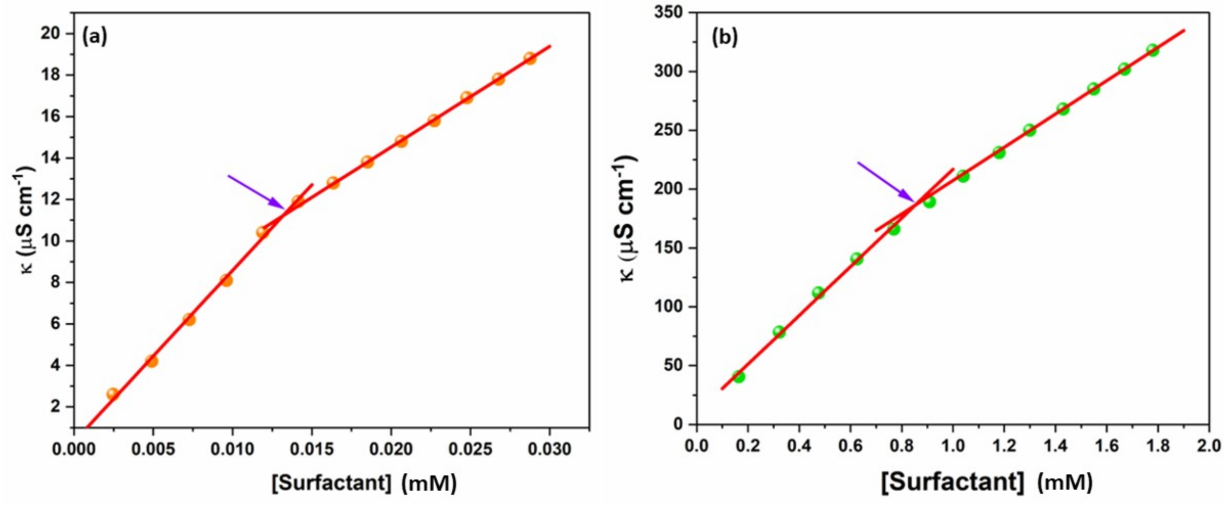


Fig. S5 Conductivity **(**κ) Vs surfactant concentration plot for (a) PGS, and (b) SCC at 25 ^{o}C.

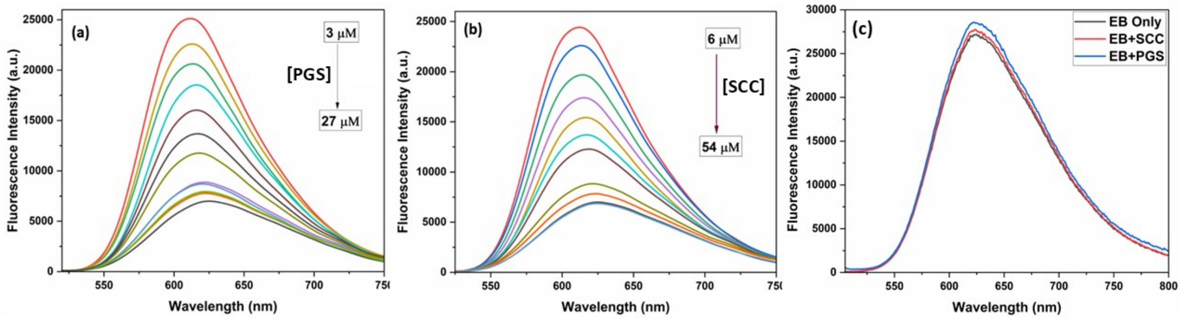


Fig. S6 Fluorescence emission spectra of EB-DNA complex with increasing concentration of (a) PGS, (b) SCC at 25 ^{o}C; (c) Fluorescence emission spectra for EB in absence and presence of PGS and SCC.

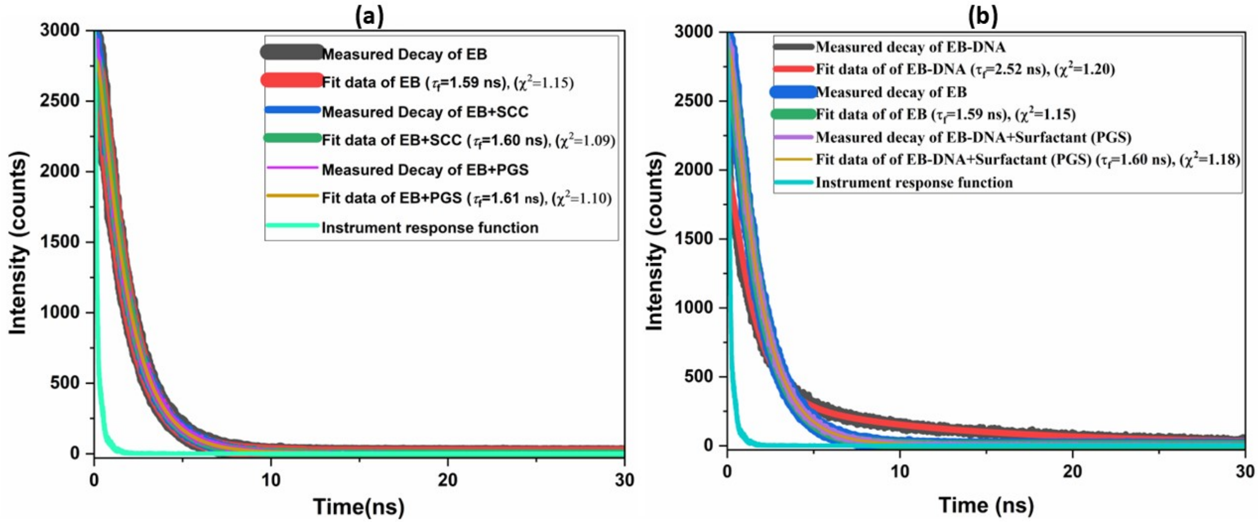


Fig. S7 (a) Fluorescence lifetime decay curves for EB in absence and presence of surfactants; (b) Fluorescence lifetime decay curves for EB and EB-DNA in absence and presence of surfactants.

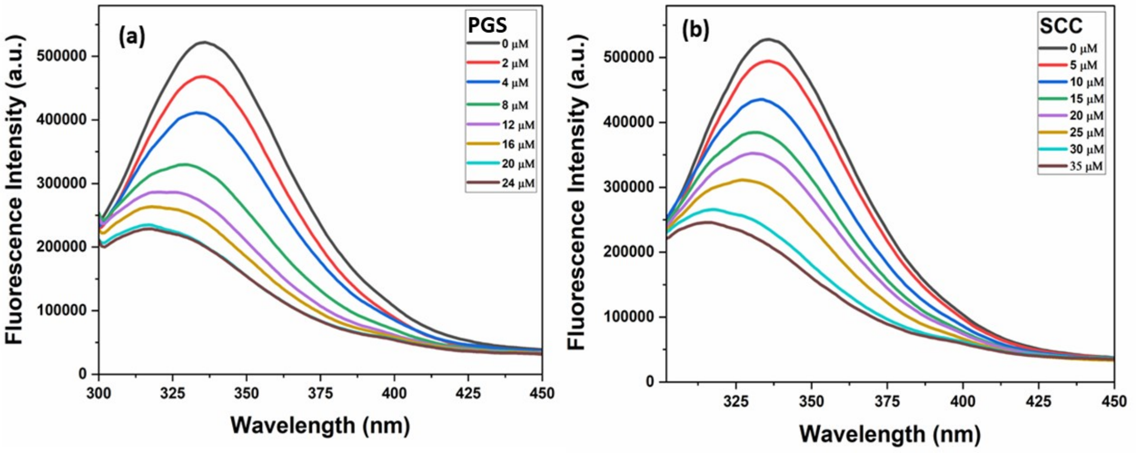


Fig. S8 Fluorescence spectra of BSA (2 μM) with increasing concentration of (a) PGS, (b) SCC, and 25 °C.

Reference

1. Mohanty, A.; Dey, J. A Giant Vesicle Forming Single Tailed Chiral Surfactant for Enantioseparation by Micellar Electrokinetic Chromatography. *Chem. Commun.* **2003**, *12*, 1384-1385.