

Supplementary Information for

Photoswitching and Sensor Applications of a Spiropyran-Polythiophene Conjugate

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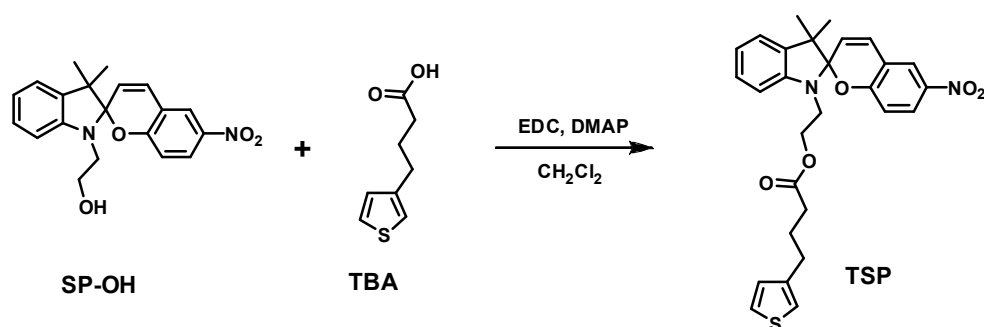
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Materials: 1'-(2-Hydroxyethyl)-3',3'-dimethyl-6-nitrospiro[1(2H)-benzopyran-2,2'-indoline] (SP-OH) was purchased from TCI. 4-(3-thienyl)butanoic acid (TBA) and 3-hexylthiophene (3-HT) were purchased from Rieke fine chemicals.

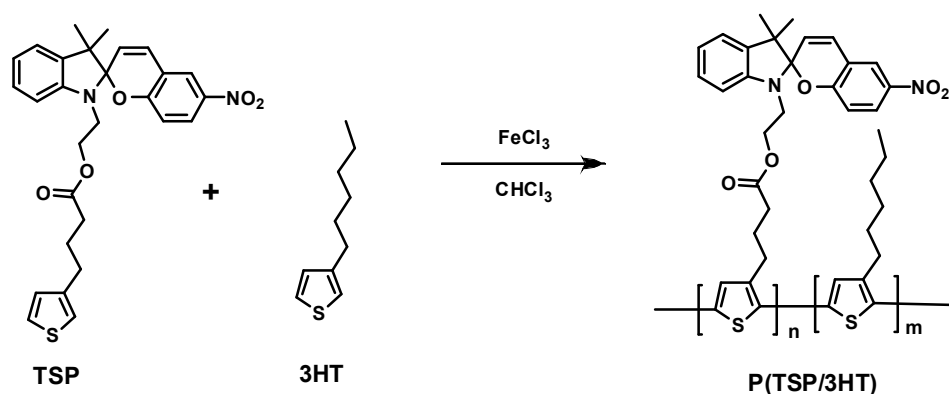
Preparation of monomer TSP



To a solution of 4,3'-thienylbutyric acid (TBA) (100mg, 0.59 mmol) in 5 ml of CH₂Cl₂ was added EDC (225 mg, 1.18 mmol), N,N-dimethylaminopyridine (DMAP) (7.33 mg, 0.06 mmol) and 1'-(2-hydroxyethyl)-3',3'-dimethyl-6-nitrospiro[1(2H)-benzopyran-2,2'-indoline] (SP-OH). The mixture was stirred for 6 h at room temperature, concentrated in vacuo, and the residue was dissolved in ethyl acetate. The solution was washed with water and the organic layer was dried over MgSO₄, filtered and the filtrate was concentrated in vacuo. The residue was subjected to a silica gel column chromatography to afford the desired product TSP (226mg, 76%). mp 63 °C; IR (NaCl) ν_{\max} (cm⁻¹): 746, 810, 954, 1026,

1089, 1170, 1273, 1338, 1458, 1481, 1518, 1578, 1612, 1648, 1736, 2866, 2926, 2960, 3054; ^1H NMR (300 MHz, CDCl_3): δ = 8.02 (1H, d, J = 3Hz), 7.99 (1H, t, J = 3Hz), 7.23 (1H, m), 7.18 (1H, dd, J = 8Hz, J = 1Hz), 7.10 (1H, d, J = 3Hz), 6.90 (4H, m), 6.74 (1H, d, J = 8Hz), 6.68 (1H, d, J = 8Hz), 5.87 (1H, d, J = 10Hz), 4.21 (2H, m), 3.43 (2H, m), 2.62 (2H, t, J = 8Hz), 2.27 (2H, t, J = 8Hz), 1.89 (2H, q, J = 8Hz), 1.27 (3H, s), 1.15 (3H, s); ^{13}C NMR (75 MHz, CDCl_3): δ = 19.8, 25.4, 25.8, 29.3, 33.4, 42.4, 52.8, 62.4, 106.4, 106.7, 115.5, 118.4, 119.9, 120.4, 121.7, 121.8, 122.7, 125.5, 125.9, 127.8, 128.0, 128.3, 135.6, 141.0, 141.5, 146.7, 159.4, 173.2.

Preparation of copolymer P(TSP/3HT)



A suspension of FeCl_3 (648 mg, 2.0 mmol) in 10 mL CHCl_3 was stirred for 30 min at room temperature and the flask was filled with N_2 gas. The monomer TSP (100 mg, 0.20 mmol) and 3HT (168.36mg, 1.00mmol) which were dissolved in 10 mL of CHCl_3 were added to the flask. The mixture was stirred for 24 h and poured into excess methanol. The precipitate was collected by filtration. The powder obtained was washed for 12 h with methanol using a Soxhlet extractor. The remaining powder was extracted with CHCl_3 using the same extractor. The solvent was evaporated to yield the copolymer as a dark brown powder (147 mg, 55%). ^1H NMR (300 MHz, CDCl_3): δ = 7.95 (2H, m), 7.16 (1H, m), 7.02 (7H, m), 6.86 (2H, m), 6.67 (2H, m), 5.85 (1H, d, J = 10Hz), 4.22 (2H, m), 3.43 (2H, m), 2.81 (9H, t, J = 7Hz), 2.56 (3H, s), 2.31 (2H, m), 1.98 (2H, m), 1.71 (10H, m), 1.36 (36H, m), 0.92 (15H, t, J = 7Hz).

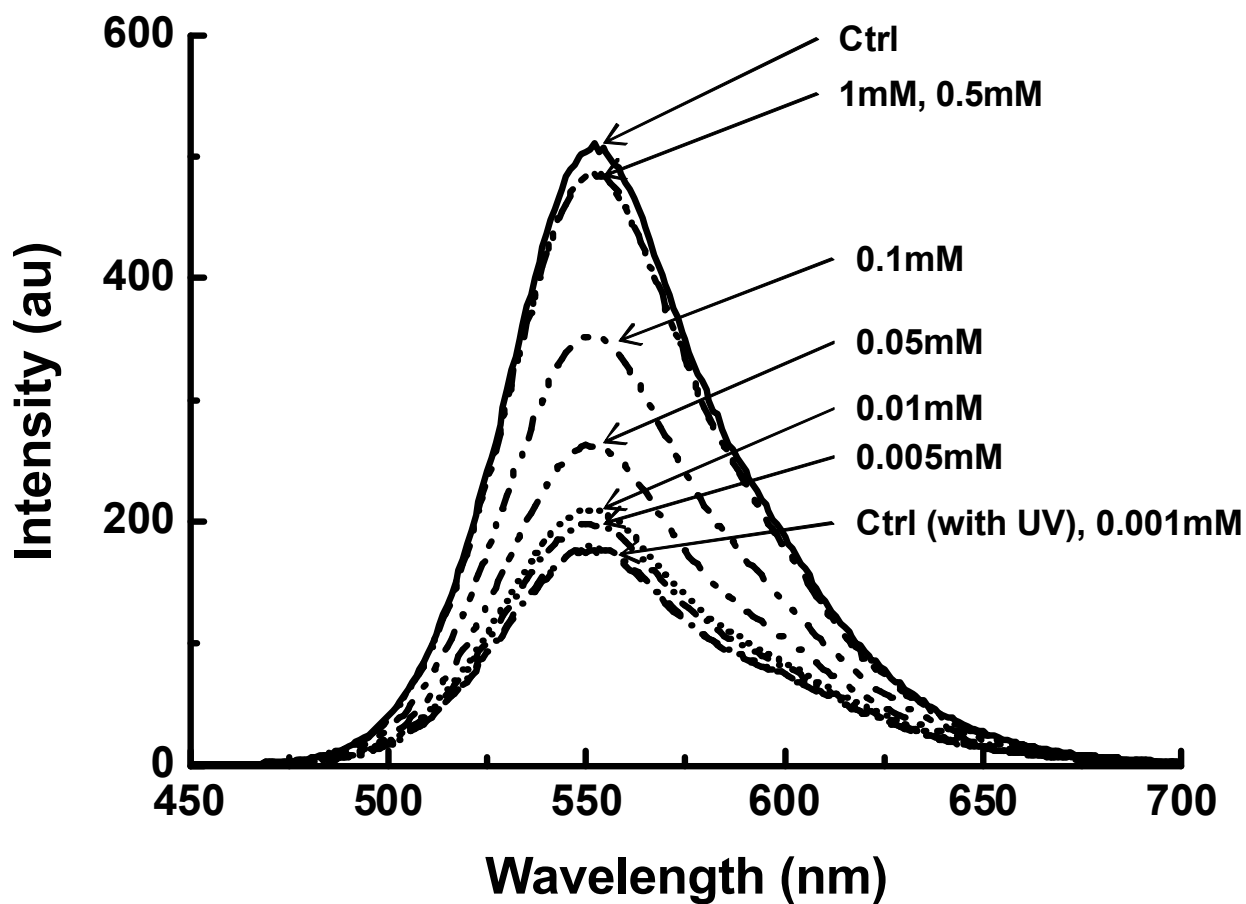


Figure S1. Fluorescence spectra of P(TSP/3HT) (0.1 mM) in the presence of different concentrations of cyanide anion.

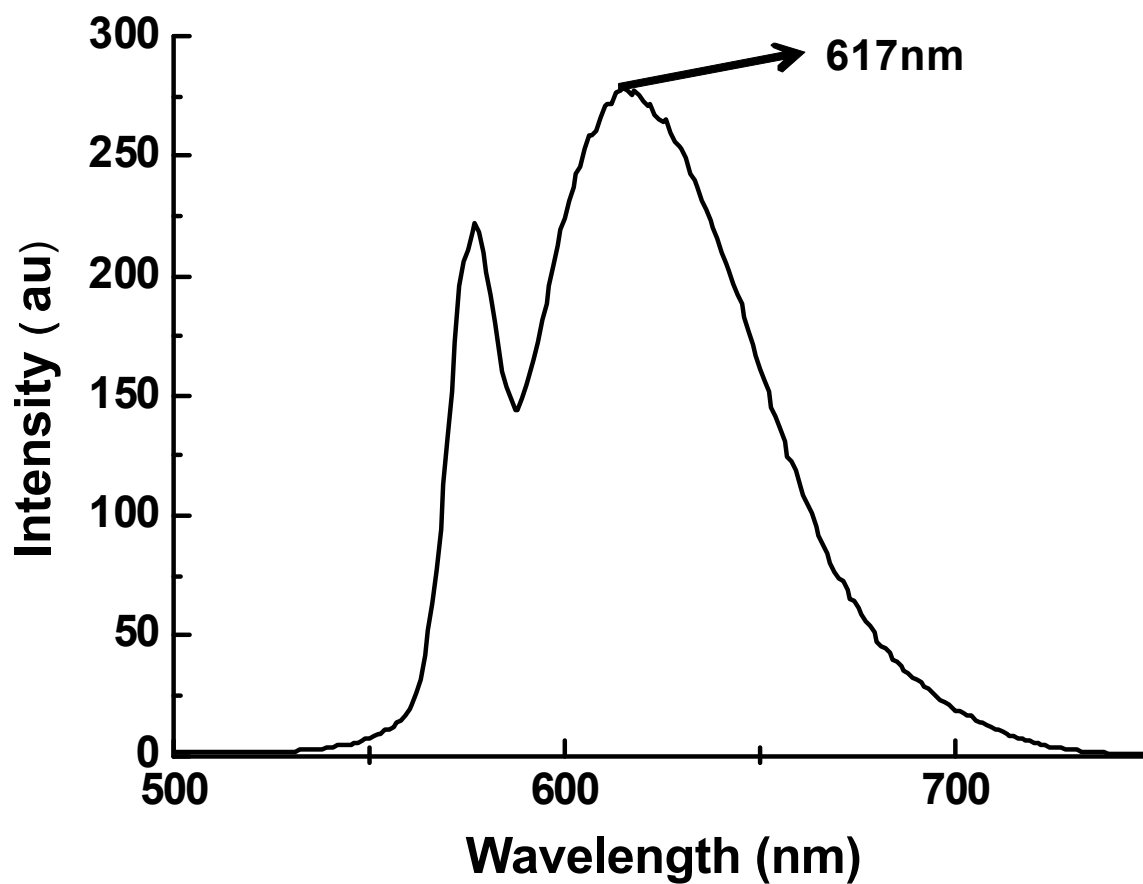


Figure S2. Fluorescence spectra of spiropyran (MC form) (0.1 mM) in THF (excitation at 577 nm).

