Supporting Information for

Water-Soluble Anionic Poly(p-phenylene vinlylenes) with High Luminescence

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Section S4: Fluorescence studies of PDMonoG and PDDiG in DMSO and water.

Section S5: Fluorescence studies and Quantum yield measurements of PDMonoG and PDTriG in DMSO and DMSO: water mixtures.

Section S6: Electrochemical properties of PMDH, PDDMe, PDMonoG and PDTriG.
**Section S1: Synthesis of Side Chains**

Methyl 6-bromohexanoate (1)

To a stirred solution of 6-bromohexanoic acid (1.00 g, 5.12 mmol) in methanol (14 mL) at 0 °C, thionyl chloride (0.67 g, 5.63 mmol) was added dropwise. The mixture was allowed to warm to room temperature and stirred for 24 h. Methanol was removed *in vacuo* and the residue dissolved in ethyl acetate (7 mL) and then washed in order with water (3 mL), sodium bicarbonate (3 mL), water (3 mL), brine (3 mL) and dried (MgSO₄). The solvent was then removed *in vacuo* to yield the title compound 1 (1.05 g, 96%) as a yellow oil.

δ<sub>H</sub> (300 MHz; CDCl₃; Me₄Si): 3.67 (3H, s, CH₃), 3.41 (2H, t, J = 6.0 Hz, CH₂), 2.33 (2H, t, J = 3.0 Hz, CH₂), 1.90-1.85 (2H, m, CH₂), 1.66-1.56 (2H, m, CH₂), 1.52-1.42 (2H, m, CH₂).

IR: ν<sub>max</sub>(neat)/cm<sup>-1</sup>; 3463 (CH, aromatic), 1720 (C=O), 1253, 1170 and 1196 (C-O, ether) and 560 (C-Br). HRMS (ESI): found (MNa<sup>+</sup>): 230.9990 C₁₇H₁₃NaO₂Br requires 230.9991. The <sup>1</sup>H NMR data was in agreement with literature values.<sup>1</sup>

1-Chloro-2-(2-(2-methoxyethoxy)ethoxy)ethane (3)

To a solution of 2-(2-(2-methoxyethoxy)ethoxy)ethanol (5.00 g, 30.4 mmol) and pyridine (2.40 g, 30.4 mmol) in chloroform (20 mL) at 0 °C was added dropwise a solution of thionyl chloride (4.70 g, 39.5 mmol) in chloroform (5 mL). The mixture was then stirred at reflux for 3 h, under an atmosphere of nitrogen. The mixture was then cooled and washed with water (3 x 50 mL), brine (50 mL) and dried (MgSO₄). The solvent was removed *in vacuo* to yield the title compound 3 (5.50 g, 92 %) as a pale yellow oil.

δ<sub>H</sub> (300 MHz; CDCl₃; Me₄Si): 4.18-4.09 (2H, m, CH₂Cl), 3.77-3.70 (2H, m, CH₂), 3.69-3.65 (4H, m, OCH₂), 3.55-3.48 (4H, m, OCH₂), 3.39 (3H, s, OCH₃). IR: ν<sub>max</sub>(neat)/cm<sup>-1</sup>; 2875 (CH, aromatic), 1299, 1245, 1199 and 1102 (C-O, ether) and 749 (C-Cl). HRMS (ESI): found (MNa<sup>+</sup>): 205.0610 C₁₇H₁₅NaO₃Cl requires 205.0602. <sup>1</sup>H NMR data was in agreement with
1-Chloro-2-(2-methoxyethoxy)ethane (4)

Using the same method as for alkyl chloride 3, 2-(2-methoxyethoxy)ethanol gave the title compound 4 in 90 % yield.

$\delta_H$ (300 MHz; CDCl$_3$; Me$_4$Si): 3.74 (2H, t, $J$ = 6.0 Hz, CH$_2$Cl), 3.68-3.64 (4H, m, OCH$_2$), 3.58-3.56 (2H, m, OCH$_2$), 3.39 (3H, s, OCH$_3$). IR: $\nu_{\text{max}}$(neat)/cm$^{-1}$; 2878 (CH, aromatic), 1299, 1245, 1198 and 1102 (C-O, ether) and 751 (C-Cl). HRMS (ESI): found (MNa$^+$): 161.0346 C$_5$H$_{11}$NaO$_2$$_{35}$Cl requires 161.0340. The $^1$H NMR data was in agreement with literature values.$^2$
Section S2: Synthesis of Monomers

1,4-Diiodo-2,5-dimethoxybenzene (5)

To a solution of 1,4-dimethoxybenzene (10.5 g, 75.9 mmol) in 90:7:3 glacial acetic acid/water/concentrated sulfuric acid (100 mL), iodine (23.7 g, 91.02 mmol) and potassium iodate (20.93 g, 91.02 mmol) were added. The mixture was then heated at 70 °C, under an atmosphere of nitrogen, for 24 h. The mixture was allowed to cool and poured onto water (500 mL). The crude solid was collected by filtration and recrystallized from THF/H₂O to give the title compound 5 (24.01 g, 81%) as a purple solid. δH (300 MHz; CDCl₃; Me₄Si): 7.19 (2H, s, ArH), 3.81 (6H, s, OCH₃). IR: νmax(neat)/cm⁻¹; 1482 (C=C, aromatic), 1063 (C-O, ether), 395 (C-I). HRMS (ESI): found (MNa⁺) 412.8496 C₈H₈O₂NaI₂ requires 412.8496. The ¹H NMR data was in agreement with the literature values.³

2,5-Diiodo-1,4-benzoquinone (6') and 2,5-Diiodobenzene-1,4-diol (6)

To a solution of 2,5-diethoxy-1,4-diiodobenzene 5 (5.00 g, 12 mmol) in dichloromethane (50 mL), under an atmosphere nitrogen at -78 °C, was added dropwise a solution of boron tribromide (13.25 g, 52 mmol) in dichloromethane (15 mL). After stirring at -78 °C for 30 min the mixture was stirred at room temperature for 18 h. The mixture was then poured slowly onto ice water (300 mL) and the resultant precipitate filtered and recrystallized from THF/H₂O to give the title compound 6' (3.00 g, 60% yield) as orange crystals, which were used immediately. δH (300 MHz; CDCl₃; Me₄Si): 7.98 (2H, s, Ar-CH). HRMS (ESI): found (MH⁺): 360.8239 C₆H₃O₂I₂ requires 360.8228.

To a solution of 2,5-diiodo-1,4-benzoquinone 6' (0.50 g, 2.70 mmol) in diethyl ether (30 mL) was added a solution of Na₂S₂O₄ (15.00 g, 83.33 mmol) in water (10 mL) and the mixture was vigorously stirred for 1 h at room temperature. The mixture was then diluted with water
(30 mL) and extracted with diethyl ether (3 x 20 mL). The combined extracts were dried (Na₂SO₄) and the solvent removed in vacuo to give the title compound 6 (0.95 g, 97%) as a white solid. δₜₕ (300 MHz; CDCl₃; Me₄Si): 8.70 (2H, s, OH), 7.29 (2H, s, Ar-H). The ¹H NMR data was in agreement with literature values.⁴

Dimethyl 6,6'-(2,5-diiodo-1,4-phenylene)bis(oxy)dihexanoate (7)

Freshly powdered potassium hydroxide (0.23 g, 4.14 mmol) was added to a solution of 1,4-diiodo-2,5-hydroquinone 6 (0.50 g, 1.38 mmol) and methyl 6-bromohexanoate 1 (0.79 g, 4.14 mmol) in DMSO (8 mL). The mixture was stirred at room temperature for 24 h and then partitioned between dichloromethane (30 mL) and water (100 mL). The organic layer was separated, dried (MgSO₄) and evaporated in vacuo to give the crude product which was purified using flash chromatography (2:1 dichloromethane, hexanes) to give the title compound 7 (0.34 g, 73 %) as a white solid. δₜₕ (300 MHz; CDCl₃; Me₄Si): 7.20 (2H, s, ArH), 3.99 (4H, t, J = 6.0 Hz, OCH₂), 3.71 (6H, s, OCH₃), 2.39 (4H, t, J = 6.0 Hz, CH₂CO₂Me), 1.80-1.59 (12H, m, CH₂). IR: νₘₐₓ(neat)/cm⁻¹; 2938 (CH, aromatic), 1718 (C=O, carbonyl), 1490 (C=C, aromatic), 1052 (C-O, ether), 595 (C-I). HRMS (ESI): found (MNa⁺) 640.9870 C₂₀H₂₈I₂NaO₆ requires 640.9867. The ¹H NMR data was in agreement with literature values.⁵

1,4-Bis(2-methoxyethoxy)benzene (9)

Freshly powdered potassium hydroxide (2.60 g, 45.4 mmol) was added to a solution of 1,4-hydroquinone(1.00 g, 9.08 mmol), 2-bromoethylmethyl ether (3.00 g, 22.7 mmol) and potassium iodide (0.30 g, 1.08 mmol) in ethanol (15 mL). The mixture was stirred at room temperature for 10 min after which it was heated at reflux for 5 days, under a nitrogen atmosphere. The reaction mixture was concentrated in vacuo and partitioned between dichloromethane (100 mL) and 1M aqueous sodium hydroxide (100 mL). The separated
organic layer was washed with water (2 x 100 mL), brine (100 mL), dried (Na₂SO₄) and concentrated to yield the crude product which was purified using flash chromatography (2:1 ethyl acetate: hexanes) to give the title compound 9 (1.20 g, 55%) as a yellow oil. δ_H (300 MHz; CDCl₃; Me₄Si): 6.84 (4H, s, ArH), 4.04 (4H, t, J = 6.0 Hz, OCH₂), 3.72 (4H, t, J = 6.0 Hz, OCH₂), 3.42 (6H, s, OCH₃). IR: ν_max(neat)/cm⁻¹: 2875 (CH, aromatic), 1352 (C-O, ether), 1242 (C-O, ether), 1176 (C-O, ether), 1096 (C-O, ether). HRMS (ESI): found (MNa⁺) 249.1106: C₁₂H₁₈NaO₄ requires 249.1097. The ¹H NMR data was in agreement with literature values.⁶

1,4-Bis(2-(2-methoxyethoxy)ethoxy)benzene (11)

Anhydrous potassium carbonate (4.50 g, 36.30 mmol) was added to a solution of 1,4-hydroquinone (1.00 g, 9.08 mmol), 1-chloro-2-(2-methoxyethoxy)ethane 4 (3.70 g, 22.70 mmol) and potassium iodide (0.30 g, 1.08 mmol) in DMF (10 mL). The mixture was heated at 100 °C for 24 h, under a nitrogen atmosphere. The mixture was cooled, filtered, poured onto water (30 mL), acidified with 3 M HCl and extracted with diethyl ether (100 mL). The organic extract was washed with 5% NaOH (v/v, 100 mL), water (150 mL), brine (100 mL) and dried (Na₂SO₄) to yield the title compound 11 (1.30 g, 60%) as a yellow oil.
δ_H (300 MHz; CDCl₃; Me₄Si): 6.83 (4H, s, ArH), 4.08 (4H, t, J = 3.0 Hz, OCH₂), 3.83 (4H, m, OCH₂), 3.70 (4H, m, OCH₂), 3.58 (4H, m, OCH₂), 3.38 (6H, s, OCH₃). IR: ν_max(neat)/cm⁻¹: 2875 (CH, aromatic), 1352 (C-O, ether), 1242 (C-O, ether), 1176 (C-O, ether), 1096 (C-O, ether) 595. HRMS (ESI): found (MH⁺): 315.1807 C₁₆H₂₇O₆ requires 315.1802. The ¹H NMR data was in agreement with literature values.⁶

1,4-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzene (14)

Freshly powdered potassium hydroxide (1.50 g, 27.00 mmol) was added to a solution of 1,4-
hydroquinone (0.60 g, 5.40 mmol), 1-chloro-2-(2-(2-methoxyethoxy)ethoxy)ethane 3 (2.50 g, 13.60 mmol) and potassium iodide (0.2 g, 1.08 mmol) in ethanol (15 mL). The mixture stirred at room temperature for 10 min after which it was heated at reflux for 5 days under a nitrogen atmosphere. The mixture was then cooled, concentrated in vacuo, partitioned between dichloromethane (100 mL) and 1M aqueous sodium hydroxide (100 mL). The organic layer was washed with water (2 x 100 mL), brine (100 mL), dried (Na₂SO₄) and concentrated to yield the crude product which was purified by flash chromatography (2:1 ethyl acetate: hexanes) giving the title compound 14 (1.20 g, 50%) as a yellow oil. δH (300 MHz; CDCl₃; Me₄Si): 6.83 (4H, s, ArH), 4.08-4.04 (4H, m, OCH₂), 3.83 (4H, t, J = 6.0 Hz, OCH₂), 3.71-3.70 (4H, m, OCH₂), 3.66-3.62 (8H, m, OCH₂), 3.54-3.52 (4H, m, OCH₂), 3.36 (6H, s, CH₃)

IR: νmax(neat)/cm⁻¹; 2875 (CH, aromatic), 1352 (C-O, ether), 1242 (C-O, ether), 1176 (C-O, ether), 1096 (C-O, ether). HRMS (ESI): found (MNa⁺) 421.4704 C₂₀H₃₄Na⁺O₈ requires 421.47.06

The ¹H NMR data was in agreement with literature values.⁶

General method of iodination of ethylene glycol monomers

To a solution of iodine monochloride (1.61 g, 9.95 mmol) in methanol (20 mL) at 0 °C was added dropwise, the corresponding ethylene glycol monomer (1.99 mmol). The mixture was then heated at reflux for 4 h. The resultant precipitate was filtered and washed with methanol to yield the title compound. If needed recrystallization was conducted using hexanes.

1,4-Diiodo-2,5-bis(2-methoxyethoxy)benzene (10)

Using the general method, 1,4-bis(2-methoxyethoxy)benzene 9 gave the title compound 10 (0.50 g, 55%) as a white solid. δH (400 MHz; CDCl₃; Me₄Si): 7.23 (2H, s, ArH), 4.08 (4H, t,
J = 5.0 Hz, OCH₂), 3.78 (4H, t, J = 5.0 Hz, OCH₂), 3.48 (6H, s, OCH₃). IR: νₘₐₓ(neat)/cm⁻¹; 2875 (CH, aromatic), 1352 (C-O, ether), 1242 (C-O, ether), 1176 (C-O, ether), 1096 (C-O, ether) 595 (C-I). HRMS (ESI): found (MNa⁺) 500.9044 C₁₂H₁₆I₂Na⁺O₄ requires 500.9030.

The ¹H NMR data was in agreement with literature values.⁷

1,4-Diiodo-2,5-bis(2-(2-methoxyethoxy)ethoxy)benzene (12)

Using the general method, 1,4-bis(2-(2-methoxyethoxy)ethoxy)benzene (11) gave the title compound 12 (0.480 g, 50%) as a pale yellow solid. δ_H (300 MHz; CDCl₃; Me₄Si): 7.24 (2H, s, ArH), 4.10 (4H, t, J = 3.0 Hz, OCH₂), 3.88 (4H, t, J = 6.0 Hz, OCH₂), 3.76 (4H, m, OCH₂), 3.58 (4H, m, OCH₂), 3.40 (6H, s, OCH₃). IR: νₘₐₓ(neat)/cm⁻¹; 2875 (CH, aromatic), 1352 (C-O, ether), 1242 (C-O, ether), 1176 (C-O, ether), 1096 (C-O, ether) 595 (C-I). m/z (Cl⁺) 566 (MH⁺, 100%).

HRMS (ESI): found (MH⁺) 566.9735 C₁₆H₂₅I₂O₆ requires 566.9735. The ¹H NMR data was in agreement with literature values.⁷

1,4-Diiodo-2,5-bis(2-(2-methoxyethoxy)ethoxy)ethoxy)benzene (13)

Using the general method, 1,4-bis(2-(2-methoxyethoxy)ethoxy)ethoxy)benzene (14) gave a crude oil after concentrating in vacuo, which was partitioned between dichloromethane (100 mL) and saturated aqueous sodium thiosulfate (100 mL). The separated organic layer was washed with water (2 x 100 mL), brine (100 mL), dried (Na₂SO₄) and concentrated to yield the title compound 13 (0.40 g, 43%) as a yellow solid. δ_H (300 MHz; CDCl₃; Me₄Si): 7.25 (2H, s, ArH), 4.18 (4H, t, J = 6.0 Hz, CH₂), 3.82 (4H, t, J = 6.0 Hz, CH₂), 3.80-3.75 (4H, m, CH₂), 3.74-3.68 (8H, m, CH₂), 3.66-3.49 (4H, m, CH₂), 3.38 (6H, s, OCH₃). IR: νₘₐₓ(neat)/cm⁻¹; 2875 (CH, aromatic), 1352 (C-O, ether), 1242 (C-O, ether), 1176 (C-O, ether), 1096 (C-O, ether) 395 (C-I). HRMS (ESI): found (MH⁺) 677.0099 C₂₀H₃₂O₈I₂
requires 677.0103. The $^1$H NMR data was in agreement with literature values.\textsuperscript{7}

**Dimethyl 6,6'-(2,5-divinyl-1,4-phenylene)bis(oxy)dihexanoate (16)**

A solution of dimethyl 6,6'-(2,5-diodo-1,4-phenylene)bis(oxy)dihexanoate \textsuperscript{7} (0.40 g, 0.77 mmol), vinyltributyltin (0.49 g, 1.55 mmol) and tetrakis(triphenylphosphine)palladium(0) catalyst (46.00 mg, 0.04 mmol) in dimethylformamide (8 mL) was heated at 100 °C, under an atmosphere of nitrogen, for 5 h. The mixture was filtered and poured onto water (30 mL). Dichloromethane (30 mL) was added, and then the separated organic layer was washed with water (3 x 30 mL), brine (2 x 30 mL), dried (MgSO$_4$) and reduced \textit{in vacuo} to yield the crude product which was purified by flash chromatography (1:2 hexanes: dichloromethane) to give the title compound 16 (0.20 g, 62%) as pale yellow crystals. $\delta^H$ (300 MHz; CDCl$_3$; Me$_4$Si): 7.00 (2H, s, ArH), 6.97 (2H, t, $J = 3.0$ Hz, $HC=CH_2$), 5.68 (2H, d, $J = 18.0$ Hz, CH=C$H_2$), 5.26 (2H, d, $J = 12.0$ Hz, CH=CH$_2$), 3.96 (4H, t, $J = 3.0$ Hz, OCH$_2$), 3.67 (6H, s, OCH$_3$), 2.35 (4H, t, $J = 8.0$ Hz, CH$_2$), 1.82 - 1.54 (12H, m, CH$_2$)

$\delta^C$ (100 MHz; CDCl$_3$; Me$_4$Si): 174.1 (C=O), 150.5 (Ar-C), 131.4 (Ar-C), 127.1 (CH=CH$_2$), 114.1 (CH=CH$_2$), 110.4 (Ar-C), 68.9 (Ar-OCH$_2$), 51.4 (CH$_3$), 33.9 (OCH$_3$), 29.1 (CH$_2$). IR: $\nu_{\text{max}}$(neat)/cm$^{-1}$; 2938 (CH, aromatic), 1718 (C=O, carbonyl), 1490 (C=C, aromatic), 1052 (C-O, ether), 919 (C=CH, vinylene)

HRMS (ESI): found (MNa$^+$) 441.2237 C$_{24}$H$_{34}$NaO$_6$ requires 441.2248.

**1,4–Divinylbenzene (17)**

Potassium tert-butoxide (8.89 g, 79.2 mmol) was added to a solution of methyltriphenylphosphonium bromide (27.15 g, 76 mmol) in dry tetrahydrofuran (110 mL) and the mixture was stirred for 20 min at room temperature under an atmosphere of nitrogen. A solution of terephthaladehyde (5.00 g, 37.00 mmol) in dry tetrahydrofuran (50 mL) was
then added dropwise. After stirring for 1 h the mixture was poured onto iced water (120 mL). The organic layer was separated and the aqueous phase was extracted with hexane (3 x 50 mL). The combined organic layers were washed with brine (200 mL), dried (MgSO₄) and concentrated in vacuo after adding 1,4-hydroquinone (5 mg) as an inhibitor to give the crude product which was purified using flash chromatography (hexanes), to give the title compound 17 (3.00 g, 63%) as a yellow oil. δH (300 MHz; CDCl₃; Me₄Si): 7.35 (4H, s, ArH), 6.61 (2H, dd, J = 9.0 Hz, 9.0 Hz, CH=CH₂), 5.76 (2H, d, J = 18.0 Hz, HC=CH₂), 5.24 (2H, d, J = 12.0 Hz, HC=CH₂). IR: νmax(neat)/cm⁻¹; 3008 (CH, aromatic), 1264 (C=H, aromatic), 989 (C=C, vinylene). The ¹H NMR data was in agreement with values presented in the literature.⁸

6,6’-((2,5-divinyl-1,4-phenylene)bis(oxy))dihexanoic acid (18)

A solution of NaOH (4M, 5 mL) was added dropwise to a solution of dimethyl 6,6’-((2,5-divinyl-1,4-phenylene)bis(oxy))dihexanoate 16 (0.05 g, 0.119 mmol), in THF (5 mL) and methanol (10 mL). The mixture was then stirred at room temperature, under an atmosphere of nitrogen for 24 h. The mixture was acidified with conc hydrochloric acid and concentrated in vacuo to yield the title compound 18 (0.03 g, 90%) as pale yellow crystals. δH (300 MHz; DMSO-d₆): 7.10 (2H, s, ArH), 6.87 (2H, t, J = 9.0 Hz, HC=CH₂), 5.82 (2H, d, J = 15.0 Hz, CH=CH₂), 5.22 (2H, d, J = 12.0 Hz, CH=CH₂), 3.93 (4H, t, J = 6.0 Hz, OCH₂), 2.22 (4H, t, J = 6.0 Hz, HC), 1.73 -1.40 (12H, m, CH₂).δC (100 MHz; DMSO): 174.9 (C=O), 168.5 (Ar-C), 143.4 (Ar-C), 131.5 (CH=CH₂), 126.8 (CH=CH₂), 110.9 (Ar-C), 68.9 (Ar-OCH₂), 29.1 (CH₂), 24.7 (CH₂). IR: νmax(neat)/cm⁻¹; 2935 (CH, aromatic), 1701 (C=O, carbonyl), 1498 (C=C, aromatic), 1052 (C-O, ether), 978 (C=CH, vinylene). HRMS (ESI): found (MNa⁺) 413.1935 C₂₂H₃₀NaO₆ requires 413.1867.
### Section S3: Solubilities of novel PPVs synthesized

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<th>Methanol (P = 5.1)</th>
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Table S3.1: Overview of observed solubilities of synthesized PPVs in selected solvents (- completely insoluble (particles observed in solution and solution did not fluoresce), * partially soluble (particles observed in fluorescent solution as polymers did not dissolve fully), + completely soluble (no particles were visible in the fluorescent solution)).
Figure S3.1: Fluorescence based solubility study of \textbf{PDMonoG} in water at pH 7 at different concentrations (A), integrated fluorescence intensity (B) and linear region between 0.0105 mg/mL – 0.105 mg/mL (Inset).
Figure S3.2: Fluorescence based solubility study of **PDTriG** in water at pH 7 at different concentrations (A), integrated fluorescence intensity (B) and linear region between 0.058 mg/mL – 0.09 mg/mL (Inset).
Section S4: Fluorescence studies of PDMonoG and PDDiG in DMSO and water.

Figure S4.1 Fluorescence spectra of PDMonoG at (a) 2 mg/mL, (b) 1 mg/mL, (c) 0.5 mg/mL, (d) 0.25 mg/mL, (e) 0.125 mg/mL, (f) 0.062 mg/mL, (g) 0.031 mg/mL, (h) 0.015 mg/mL, and (i) 0.007 mg/mL in DMSO.
Figure S4.2 Fluorescence spectra of PDMonoG at (a) 0.5 mg/mL, (b) 0.25 mg/mL, (c) 0.125 mg/mL, (d) 0.062 mg/mL and (e) 0.031 mg/mL in water.

Figure S4.3 Fluorescence spectra of PDDiG at (a) 1 mg/mL, (b) 0.5 mg/mL, (c) 0.25 mg/mL, (d) 0.125 mg/mL and (e) 0.0625 mg/mL in DMSO.
Section S5: Quantum yield measurements of PDMonoG and PDTriG in DMSO and DMSO: water mixtures

Figure S5.1 (A) Fluorescence of PDMonoG in DMSO (1) and DMSO-water ratios v/v (80:20 (2), 60:40 (3), 50:50 (4), 30:70 (5)). (B) Fluorescence of PDTriG in DMSO (1), water (6) and DMSO-water ratios v/v (80:20 (2), 60:40 (3), 50:50 (4), 30:70 (5)).

Figure S5.2 Quantum yield of PDMonoG in DMSO: water ratios (v/v).

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Figure S5.3 Quantum yield of **PDTrIG** in DMSO: water ratios (v/v).
Section S6: Electrochemical properties and optical band gaps of the polymers

Figure S6.1 Cyclic voltammograms of PMDH, PDDMe and PDMonoG coated on glassy carbon electrodes in acetonitrile and 0.1 M \([n-\text{Bu}_4\text{N}]\)[PF_6] with a scan rate of 0.1 Vs\(^{-1}\).

Table S6.2 Electrochemical properties of PPVs synthesized.

<table>
<thead>
<tr>
<th>Polymer</th>
<th>(E_{\text{ox}}) vs FOC(^a) (V)</th>
<th>(E_{\text{red}}) vs FOC(^a) (V)</th>
<th>(E_{\text{HOMO}})(^b) (eV)</th>
<th>(E_{\text{LUMO}})(^b) (eV)</th>
<th>(E_{\text{elc}}) (eV)</th>
<th>(E_{\text{opt}}) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMDH</td>
<td>0.75</td>
<td>-1.66</td>
<td>-5.46</td>
<td>-3.05</td>
<td>2.41</td>
<td>2.38</td>
</tr>
<tr>
<td>PDDMe</td>
<td>0.70</td>
<td>-1.85</td>
<td>-5.41</td>
<td>-2.86</td>
<td>2.55</td>
<td>2.30</td>
</tr>
<tr>
<td>PDMonoG</td>
<td>0.72</td>
<td>-1.94</td>
<td>-5.43</td>
<td>-2.77</td>
<td>2.66</td>
<td>2.44</td>
</tr>
<tr>
<td>PDDiG</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2.34</td>
</tr>
<tr>
<td>PDTriG</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2.25</td>
</tr>
</tbody>
</table>

\(^a\)\(E_{\text{FOC}} = 0.47\) V vs Ag/AgCl. \(^b\)\(E_{\text{HOMO}} = -(E_{\text{ox,FOC}} + 4.71)\) eV;

\(E_{\text{LUMO}} = -(E_{\text{red,FOC}} + 4.71)\) eV. \(E_{\text{elc}}\) = Electrochemical band gap; \(E_{\text{opt}}\) = LUMO – HOMO.

\(E_{\text{opt}}\) = Optical band gap.

Table S6.2 Electrochemical properties of PPVs synthesized.
<table>
<thead>
<tr>
<th>Monomer</th>
<th>MDH</th>
<th>DDE</th>
<th>MonoG</th>
<th>DiG</th>
<th>TriG</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_{\text{max}}$ (nm)</td>
<td>352.75</td>
<td>376.64</td>
<td>378.24</td>
<td>382.15</td>
<td>374.02</td>
</tr>
<tr>
<td>$E_{\text{gap}}$ (eV)</td>
<td>3.79</td>
<td>3.63</td>
<td>3.62</td>
<td>3.58</td>
<td>3.67</td>
</tr>
</tbody>
</table>

Table S6.1 $\lambda_{\text{max}}$ obtained from the UV-Vis spectra predicted from Gaussian calculations on the monomers and the band gap calculated from the molecular orbitals from the Gaussian calculations.

References: