Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Supporting Information:

Conjugated Polyelectrolytes with Guanidinium Side Groups. Synthesis, Photophysics and Pyrophosphate sensing

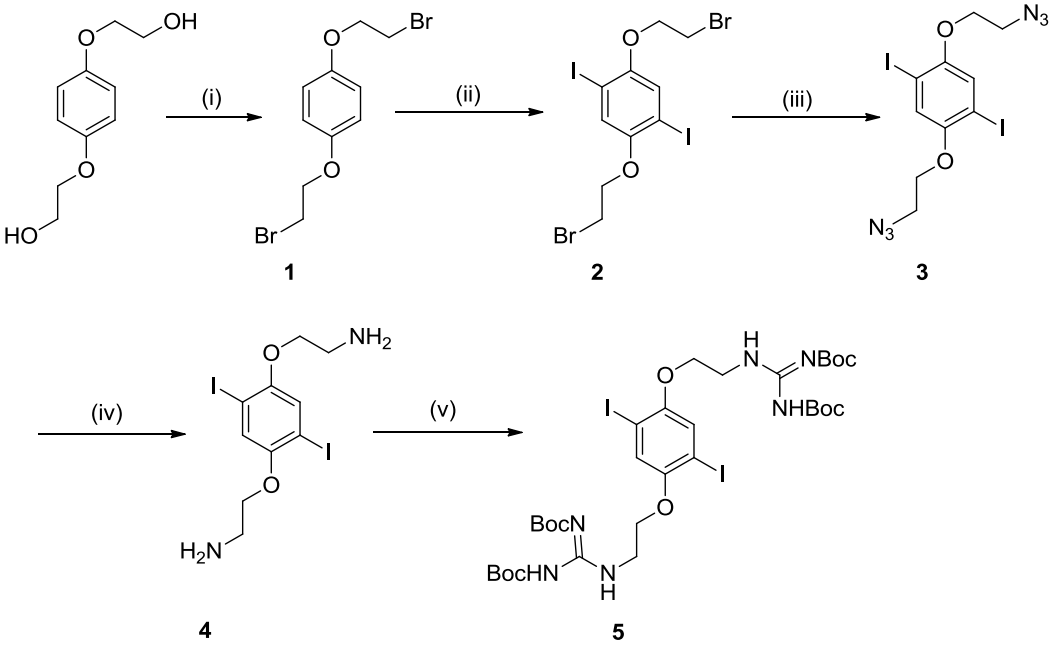
Xuzhi Zhu, Jie Yang and Kirk S. Schanze*

Department of Chemistry, University of Florida, Gainesville, Florida 32611-7200

* Corresponding author: e-mail: kschanze@chem.ufl.edu,

TEL: 352-392-9133, FAX: 352-392-2395.

Scheme S1. Synthesis of Monomer



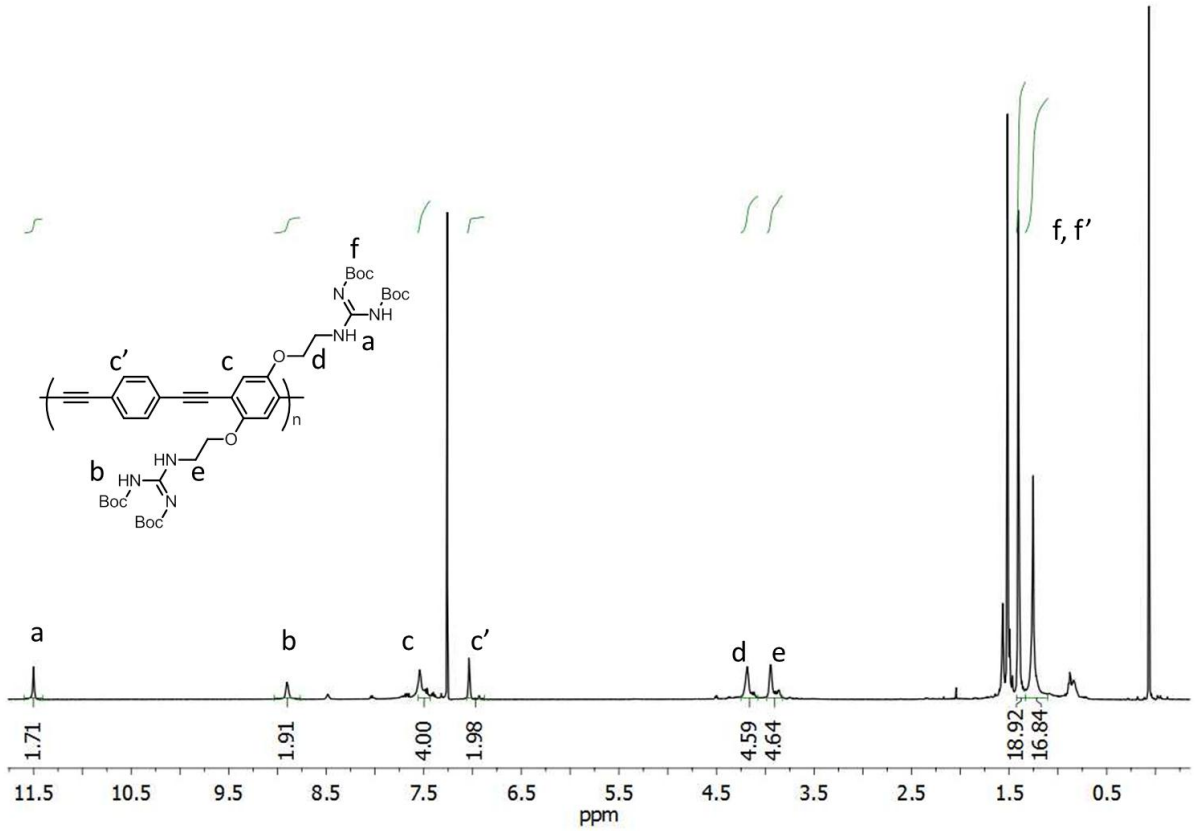


Figure S1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **P1-Boc**.

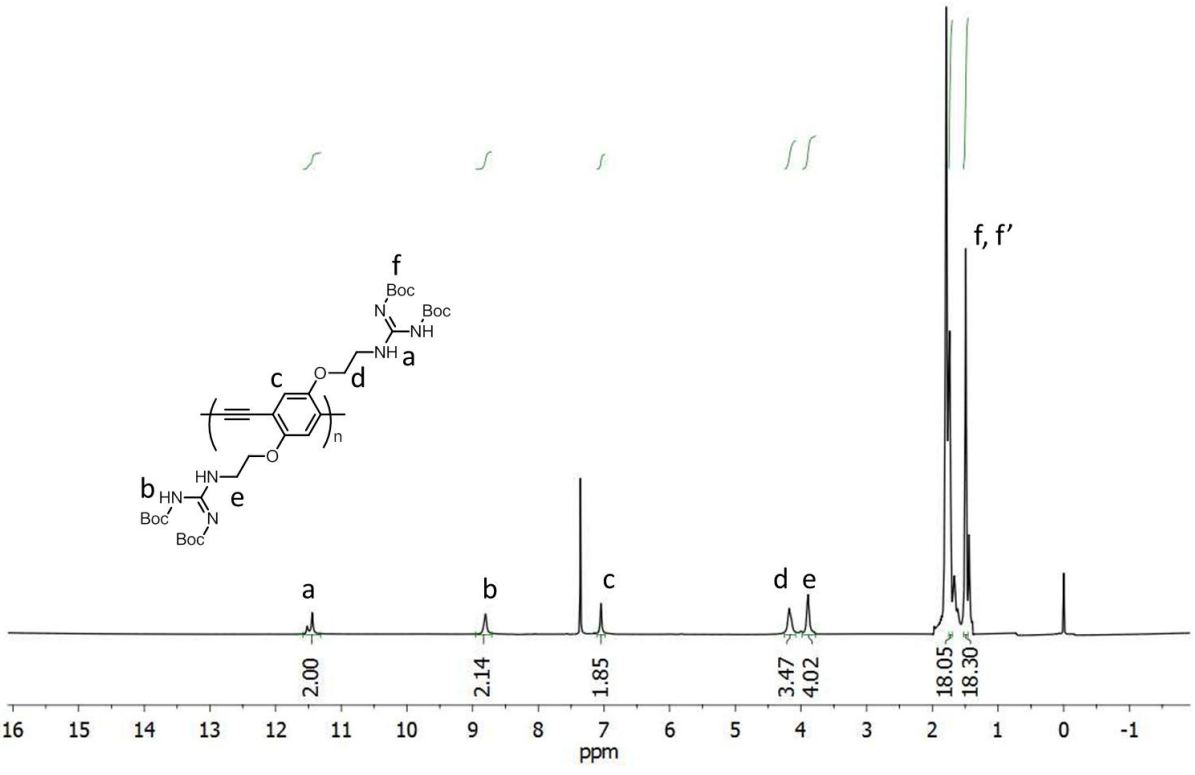


Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **P2-Boc**.

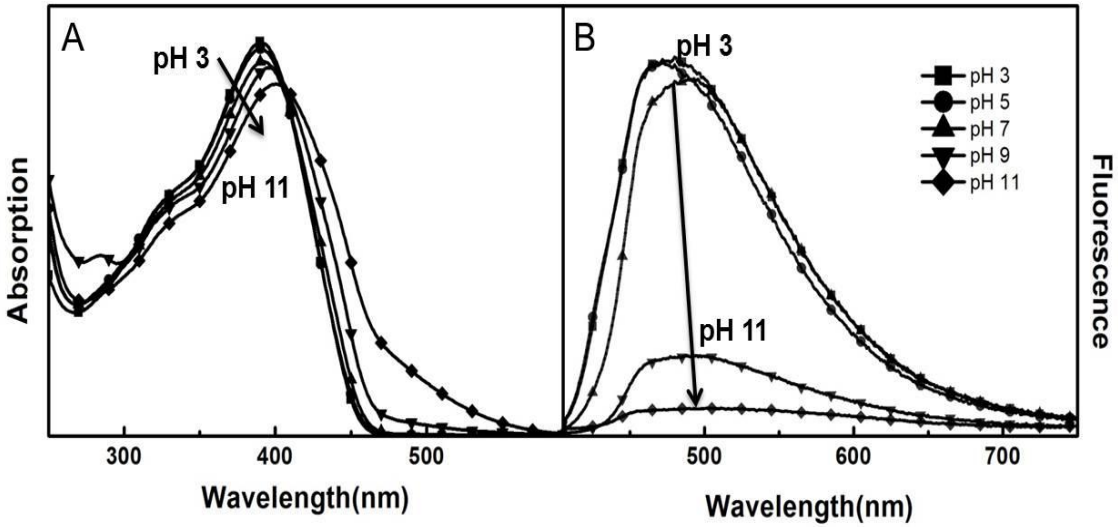


Figure S3. Absorption (a) and Fluorescence (b) spectra of **P1** in water at various pH.

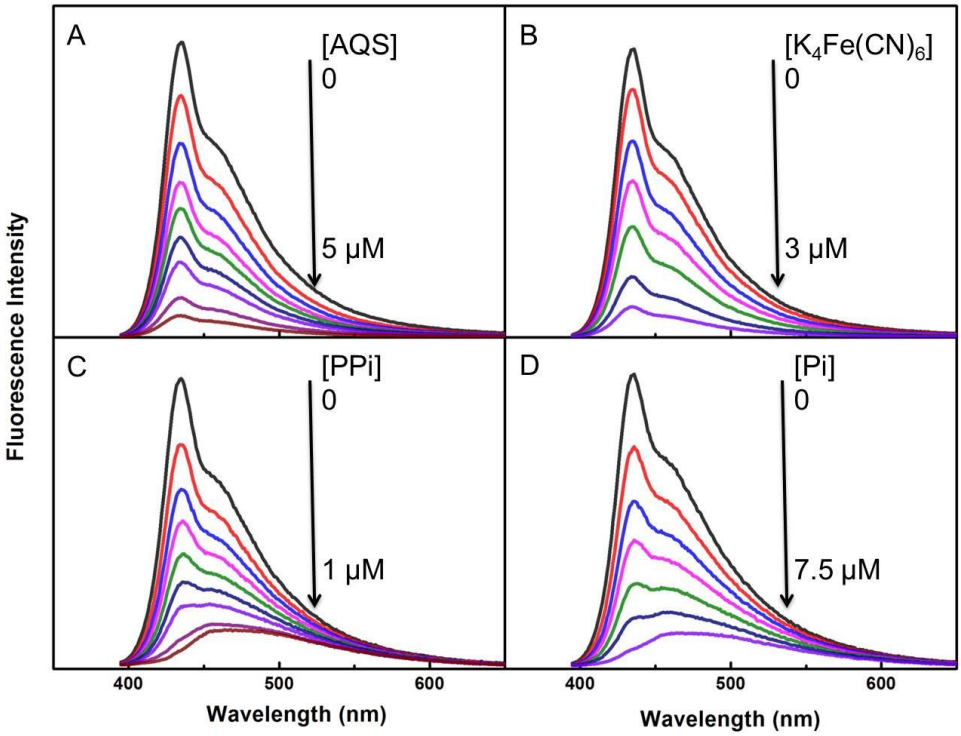


Figure S4. Emission spectra for **P1** (2 μM) at various concentrations of the quencher AQS(A), $K_4Fe(CN)_6$ (B), PPi (C) and Pi(D).

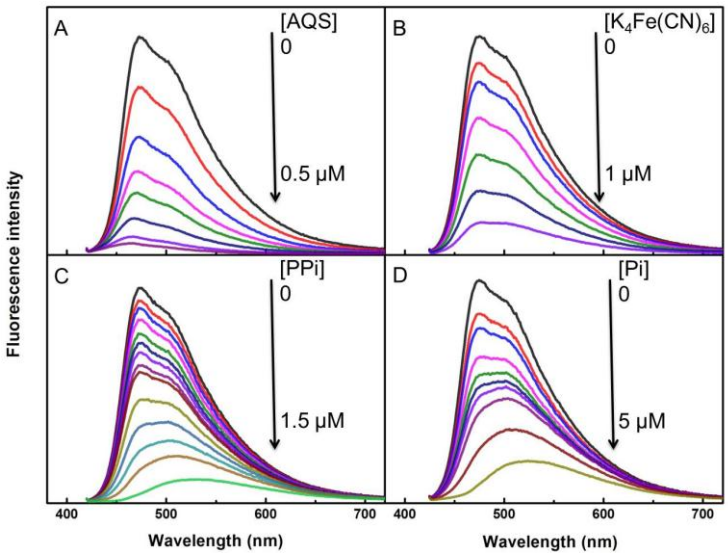


Figure S5. Fluorescence spectra of **P2** in MeOH upon the addition of different quenchers. (A) AQS; (B) $K_4Fe(CN)_6$; (C) PPi; (D) Pi. [**P2**] = 2 μM.

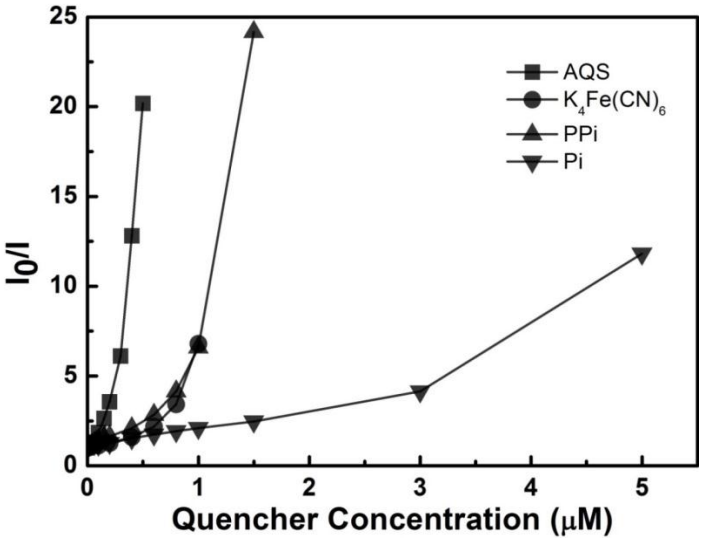


Figure S6. Stern-Volmer Plots of **P2** (2 μM) with various concentration of the quenchers in MeOH. AQS(■); $K_4Fe(CN)_6$ (●); PPi (▲); Pi (▼).

Table S1. Stern-Volmer constant and [Q_{90}] for 2 μM **P2** in MeOH with different quenchers.

Polymer	Quencher	K_{sv} (M^{-1})	[Q_{90}] (μM)
P2	PPi	4.6×10^6	1.2
	$K_4Fe(CN)_6$	1.5×10^6	1.1
	AQS	8.0×10^6	0.4
	Pi	1.3×10^6	4.5

Table S2. Fluorescence lifeteim of P1 and P2 in MeOH and Water

	MeOH					H_2O				
		RA(%)								
	τ_i (ns)	450 nm	500 nm	550 nm	600 nm	τ_i (ns)	450 nm	500 nm	550 nm	600 nm
P1	$\tau_1 = 0.15$	73	72	75	58	$\tau_1 = 0.17$	88	82	76	75
	$\tau_2 = 0.46$	27	27	23	36	$\tau_2 = 0.57$	12	17	22	22
	$\tau_3 = 1.26$	0	1	2	6	$\tau_3 = 1.98$	0	1	3	3
	χ^2	0.99	0.99	1.00	1.02	χ^2	1.09	0.99	1.01	0.99
P2	$\tau_1 = 0.17$	82	74	68	67	$\tau_1 = 0.13$	95	93	89	85
	$\tau_2 = 0.54$	18	26	31	31	$\tau_2 = 0.61$	5	6	10	13
	$\tau_3 = 1.73$	0	0	1	2	$\tau_3 = 2.12$	0	1	1	2
	χ^2	1.01	1.01	0.98	0.97	χ^2	1.00	0.97	0.97	0.93

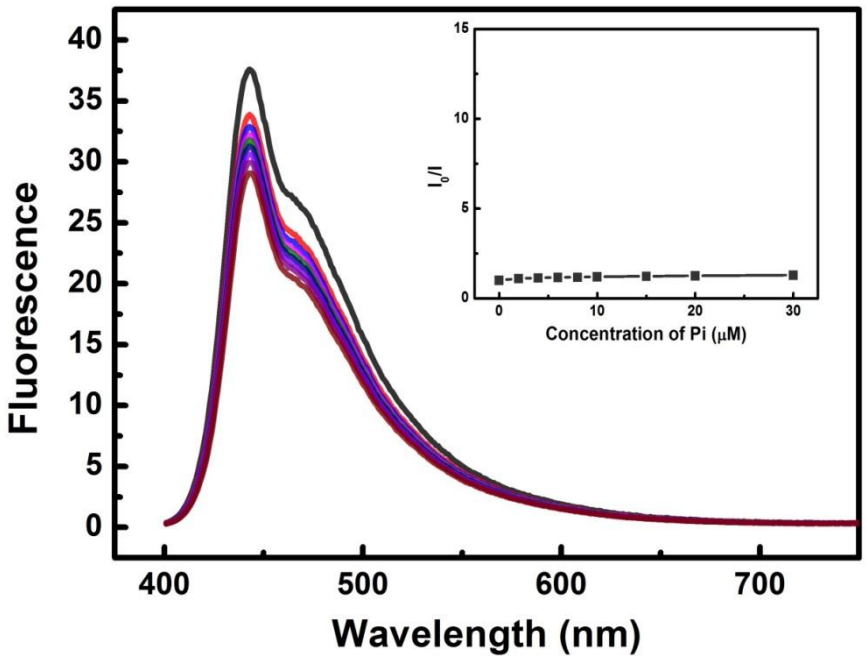


Figure S7. Fluorescence spectra of **P1**/triton complex and emission change upon the addition of Pi from 0 to a30 μM, [**P1**] = 3 μM, [Triton X-100] = 200 μM. Inset is the Stern-Volmer plots.

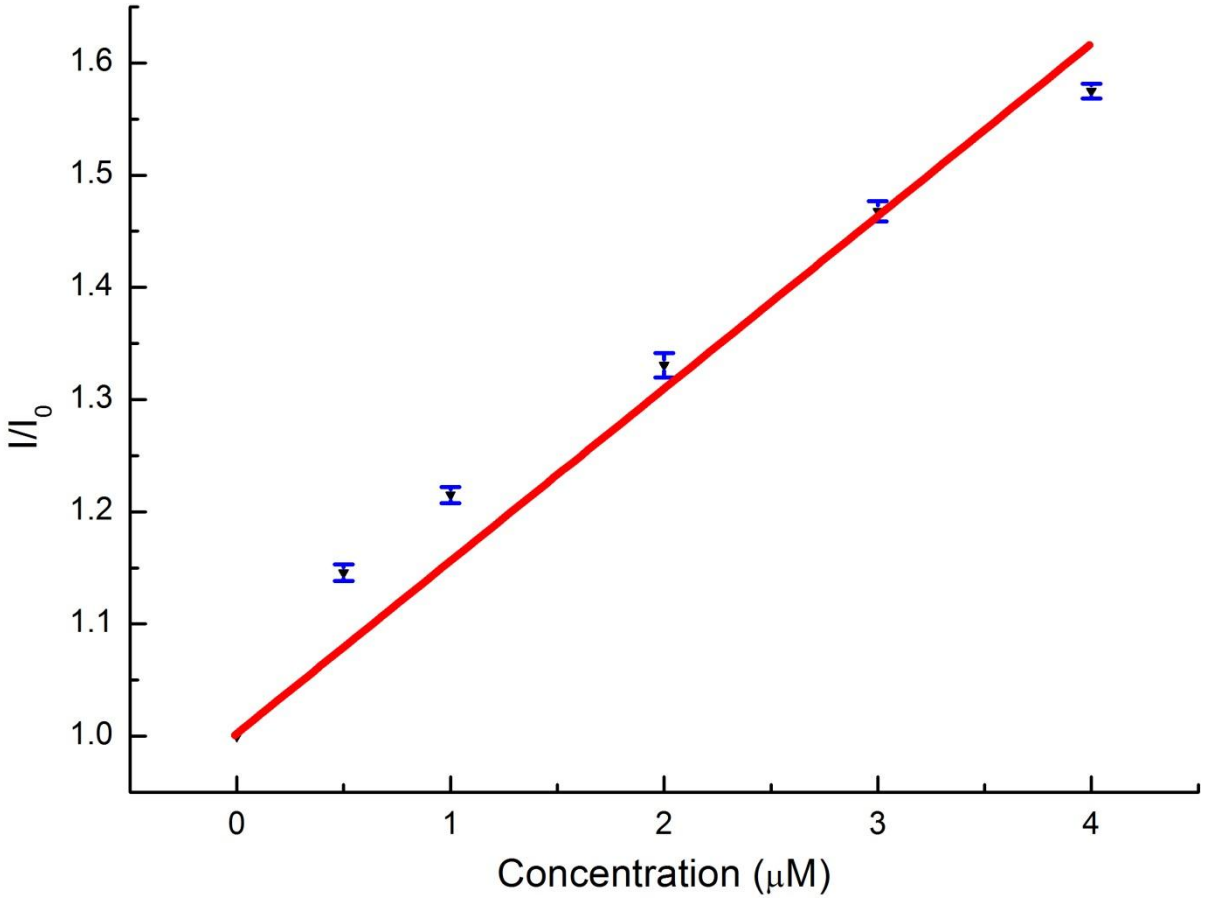


Figure S8. Fluorescence intensity change of **P1**/triton complex and emission change upon the addition of PPi from 0 to 4 μM, [**P1**] = 3 μM, [Triton X-100] = 200 μM, Em = 444 nm. The analytical detection limit (D.L.) was calculated to be 176 nM using the equation D.L. = 3 δ_{bk}/m, where δ_{bk} is the standard deviation of the blank and m is the slope of the calibration plot.[1]

1. Valcarcel, M. *Principles of Analytical Chemistry: A textbook*; Springer-Verlag: New York, 2000.