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Twisted configuration pyrene derivative: exhibiting pure blue monomer photoluminescence and electrogenerated chemiluminescence emissions in non-aqueous media

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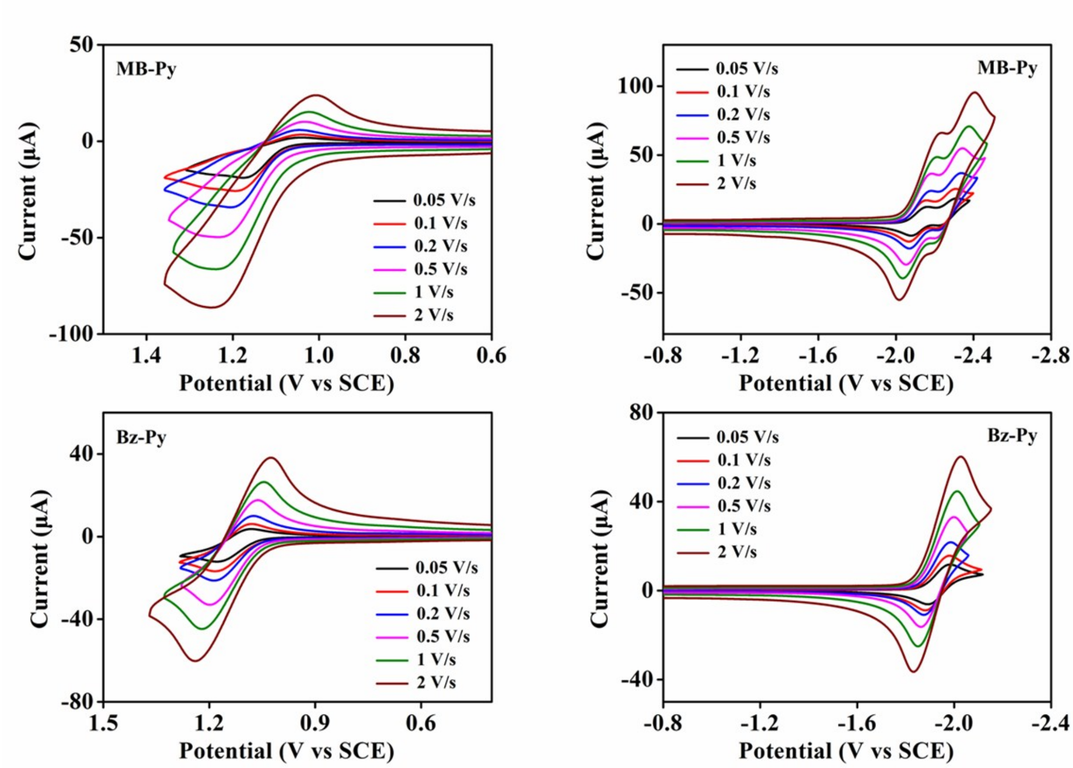

Figure S-1. Cyclic voltammograms of MB-Py (2.5 mM) and Bz-Py (2 mM) in MeCN:Bz (*v*:*v*=1:1) containing 0.1 M $TBAPF_6$ at Pt electrode(0.027 cm^2) with different scan rates.

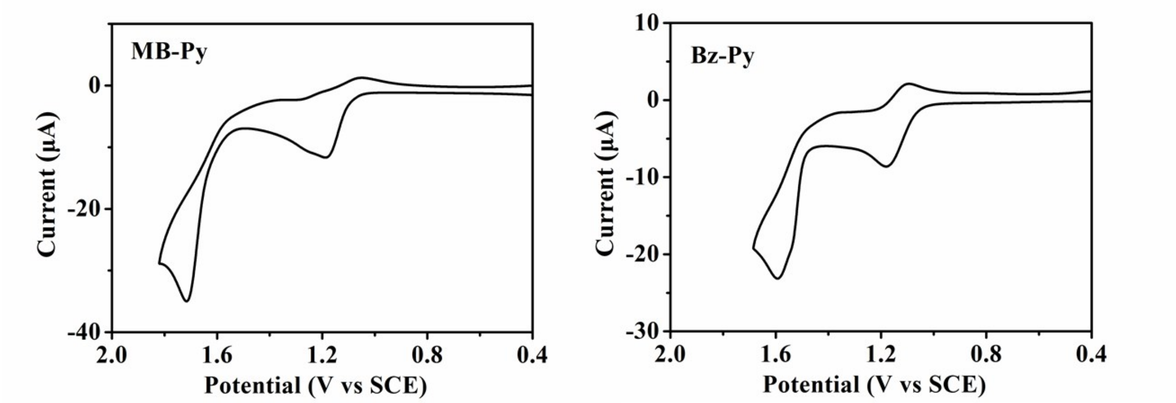

Figure S-2. Cyclic voltammograms of MB-Py (1.0 mM) and Bz-Py (1.0 mM) in MeCN:Bz (*v*:*v*=1:1) containing 0.1 M $TBAPF_6$ at Pt electrode (0.027 cm^2) with a scan rate of 0.1 V/s.

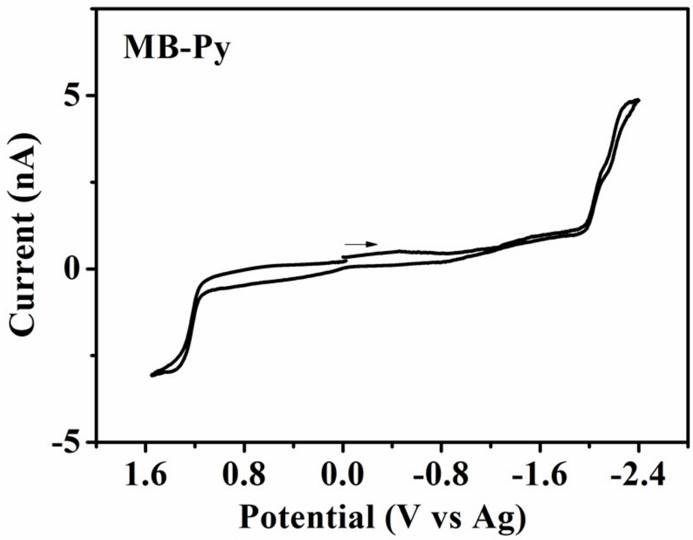

Figure S-3. Cyclic voltammogram of MB-Py (2.5 mM) at a platinum UME (r = 11μm) in MeCN:Bz (*v*:*v*=1:1) containing 0.1 M $TBAPF_6$ with a scan rate of 10 mV/s.

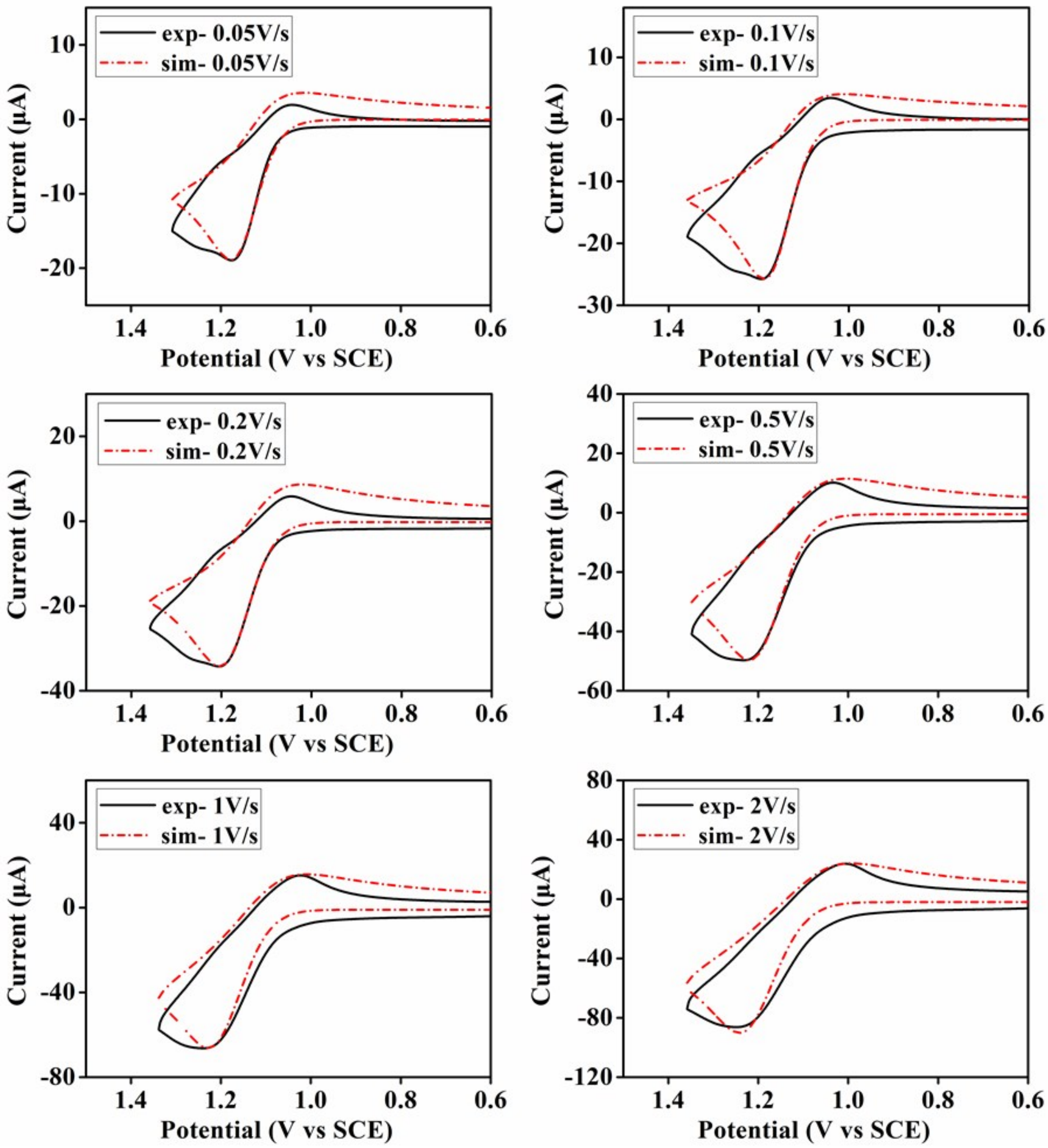

Figure S-4. Comparison between simulated and experimental oxidation waves for 2.5 mM MB-Py at different scan rates. The model for these oxidation simulations: EC, with n = 1, with a heterogeneous rate constant, α = 0.5, $k^0 = 1\times10^4$ cm/s and a homogeneous forward rate constant, k_{eq} = 0.8, $k_f = 20\ s^{-1}$. Simulated data: E^o = 1.11 V vs. SCE; Diffusion coefficient: $1.36\times10^{-5}\ cm^2/s$, uncompensated resistance 853 Ω, capacitance 3×10^{-6} F. Experimental conditions: solvent: MeCN:Bz (v:v=1:1), supporting electrolyte: 0.1 M $TBAPF_6$, Pt electrode area 0.027 cm^2.

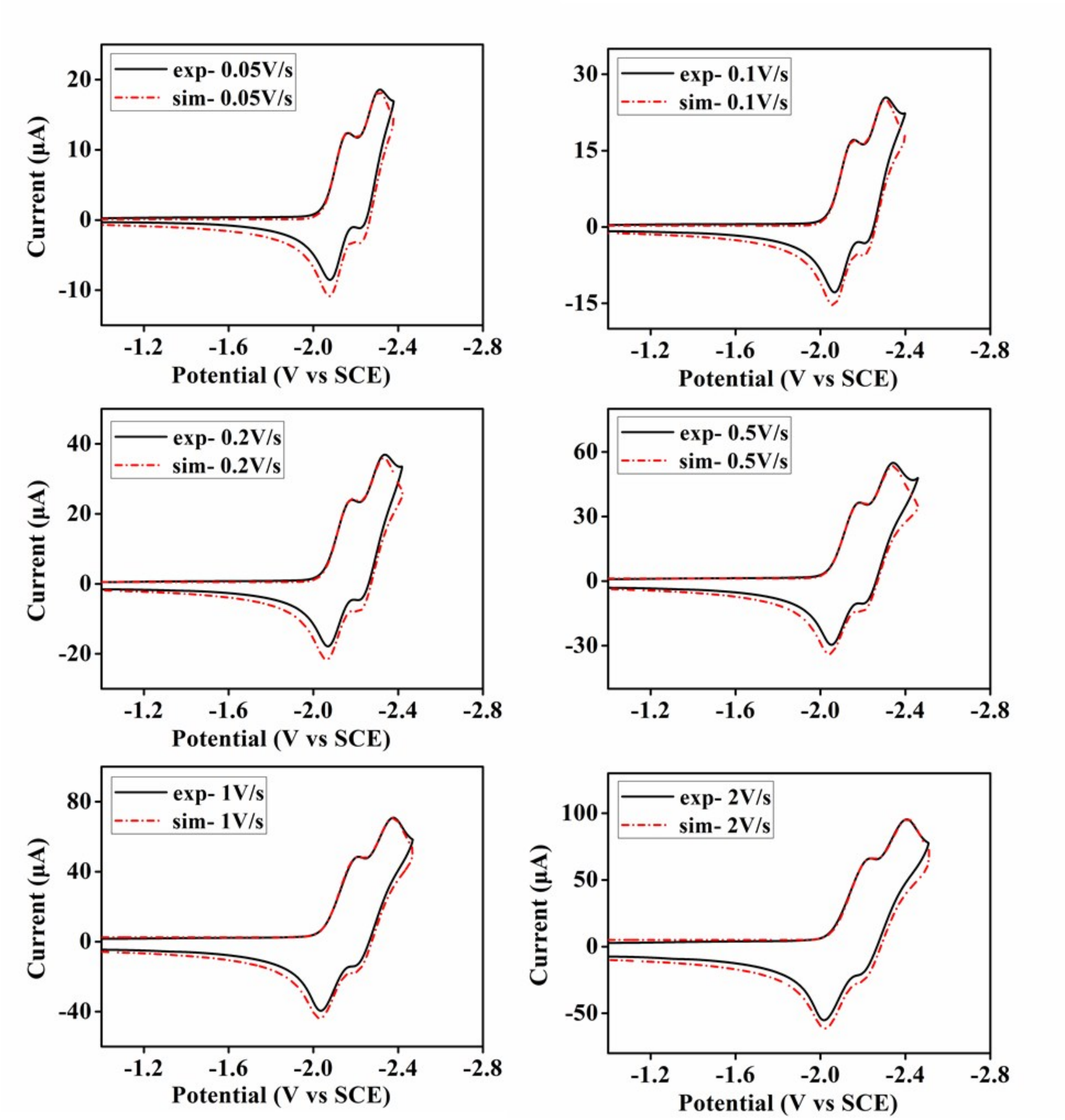

Figure S-5. Comparison between simulated and experimental reduction waves for 2.5 mM MB-Py at different scan rates. The model for these reduction simulations: ECE, with $n = 2$, with a heterogeneous rate constant, $\alpha = 0.5$, $k_1{}^0 = 0.012$ cm/s, $k_2{}^0 = 0.015$ cm/s. Simulated data: $E^{o}{}_{1/2,1} = -2.12$ V vs. SCE, $E^{o}{}_{1/2,2} = -2.27$ V vs. SCE; Diffusion coefficient: 1.36×10^{-5} cm^2/s, uncompensated resistance 603 Ω, capacitance 1×10^{-6} F. Experimental conditions: solvent: MeCN:Bz (v:v=1:1), supporting electrolyte: 0.1 M $TBAPF_6$, Pt electrode area 0.027 cm^2.

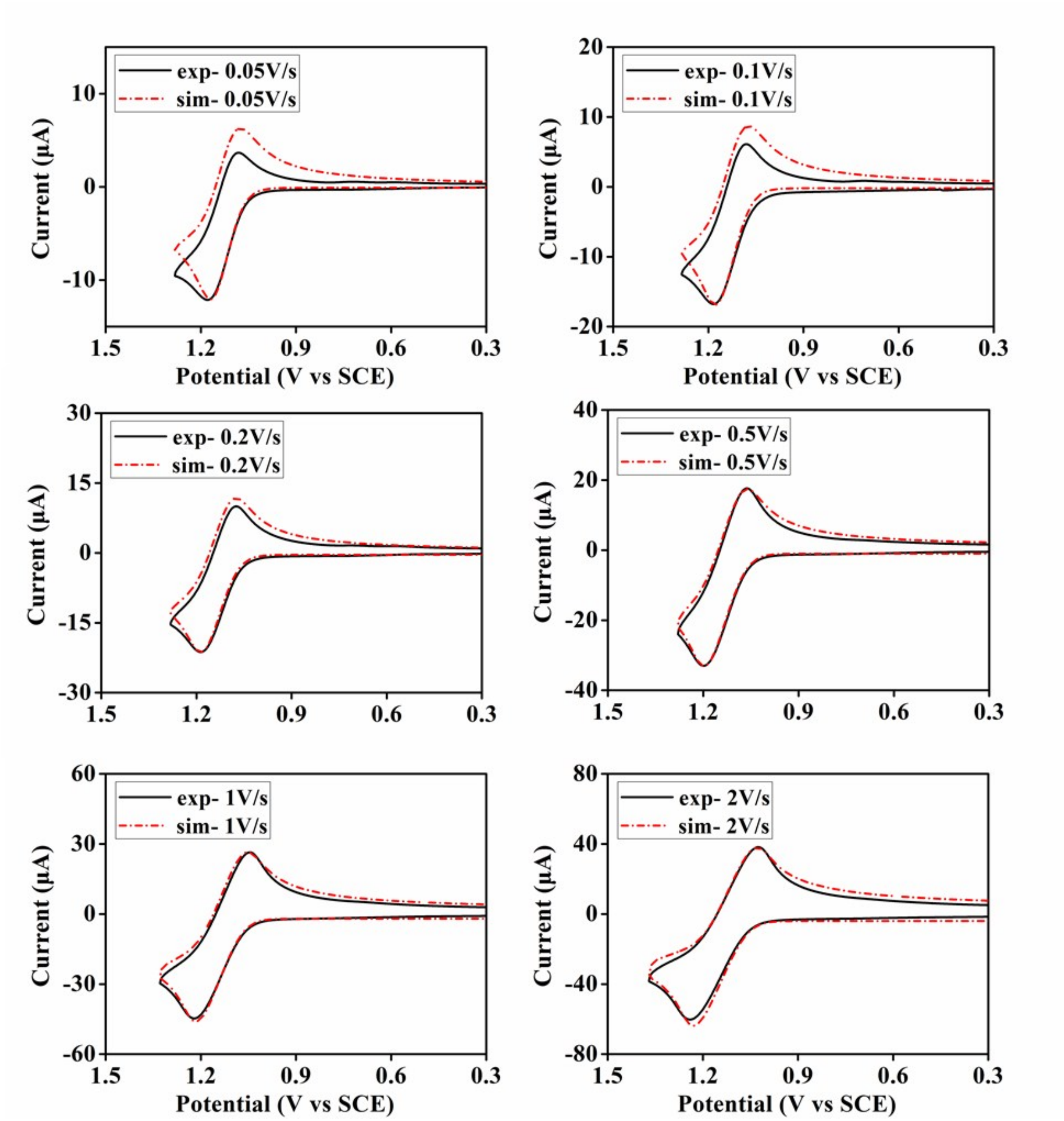

Figure S-6. Comparison between simulated and experimental oxidation waves for 2 mM BZ-Py at different scan rates. The model for these oxidation simulations: EC, with n =1, with a heterogeneous rate constant, α = 0.5, k^0 = 1×10^4 cm/s and a homogeneous forward rate rate constant, k_{eq} = 0.8, k_f = 18 s^{-1}. Simulated data: E^o = 1.13 V vs. SCE; Diffusion coefficient: 9.80 × 10^{-6} cm^2/s, uncompensated resistance 927 Ω, capacitance 3×10^{-6} F. Experimental conditions: solvent: MeCN:Bz (v:v=1:1), supporting electrolyte: 0.1 M $TBAPF_6$, Pt electrode area 0.027 cm^2.

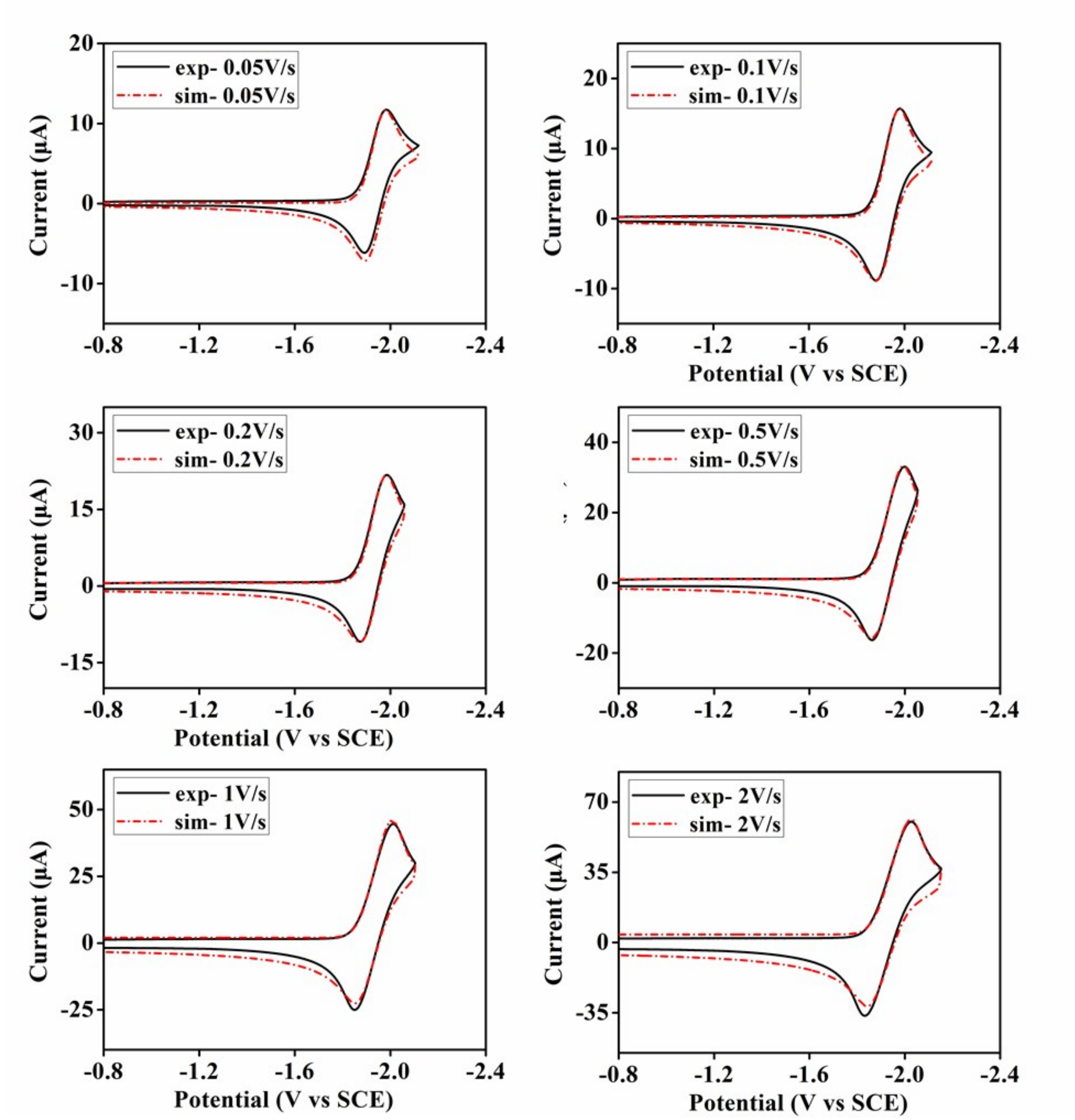

Figure S-7. Comparison between simulated and experimental reduction waves for 2 mM Bz-Py at different scan rates. The model for these reduction simulations: EC, with n = 1, with a heterogeneous rate constant, α = 0.5, $k^0 = 1\times10^4$ cm/s and a homogeneous forward rate rate constant, k_{eq} = 0.8, $k_f = 18\ s^{-1}$. Simulated data: E^o = -1.94 V vs. SCE; Diffusion coefficient: $9.80 \times 10^{-6}\ cm^2/s$, uncompensated resistance 1011 Ω, capacitance 2×10^{-6} F. Experimental conditions: solvent: MeCN:Bz (v:v= 1:1), supporting electrolyte: 0.1 M $TBAPF_6$, Pt electrode area 0.027 cm^2.

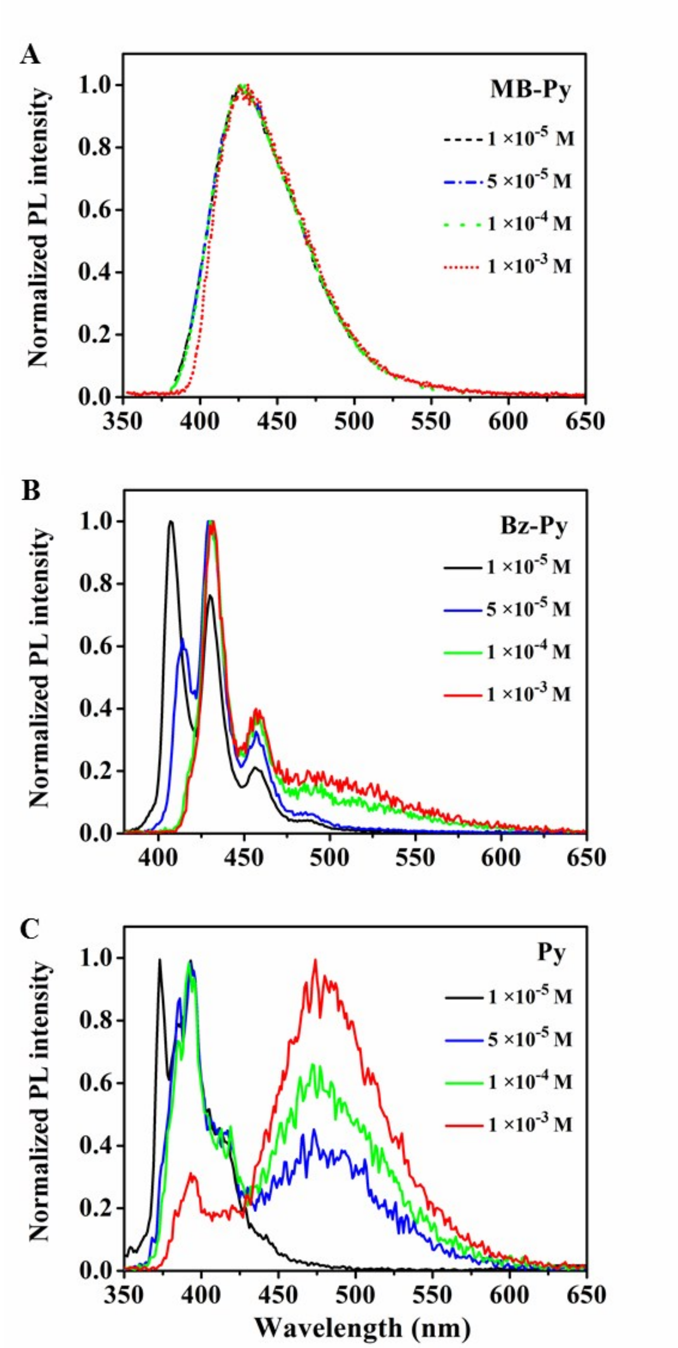

Figure S-8. Absorbance and PL spectra of (A) MB-Py, (B) Bz-Py and (C) Py at different concentrations in MeCN:Bz (v:v=1:1) (excitation at $\lambda_{\text{abs, max}}$).

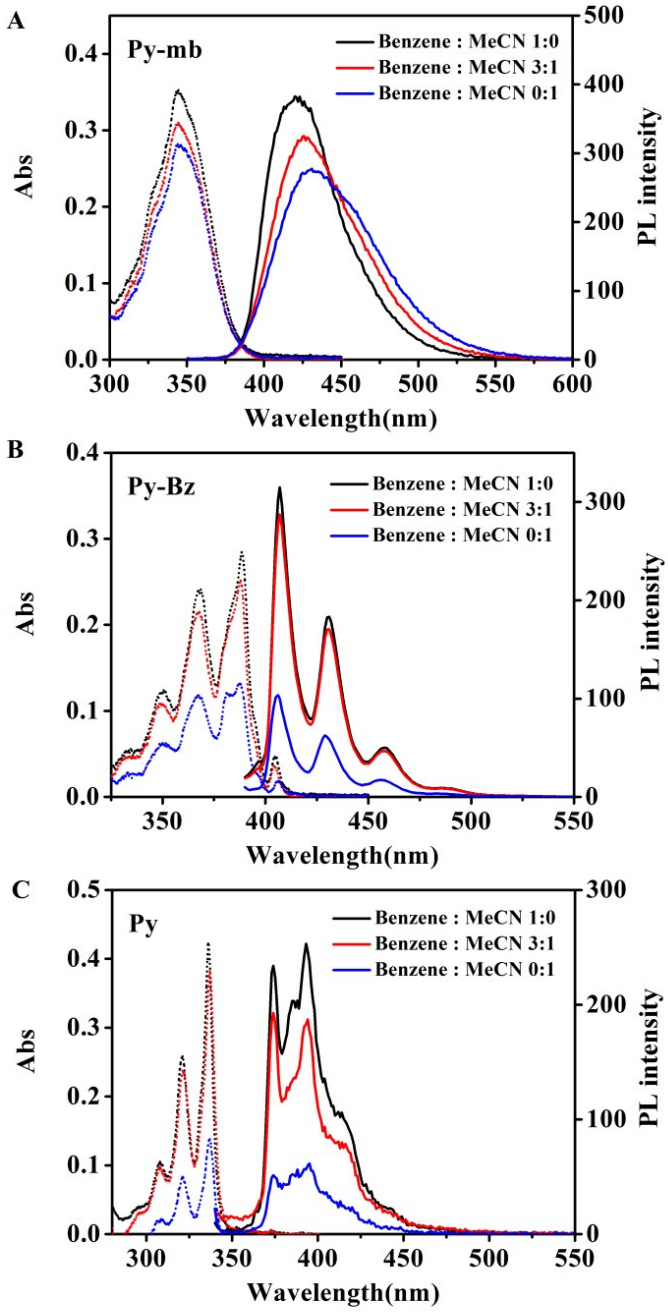

Figure S-9. Absorbance and PL spectra of (A) MB-Py, (B) Bz-Py and (C) Py in different ratio mixed solvents. (excitation at $\lambda_{abs, max}$).

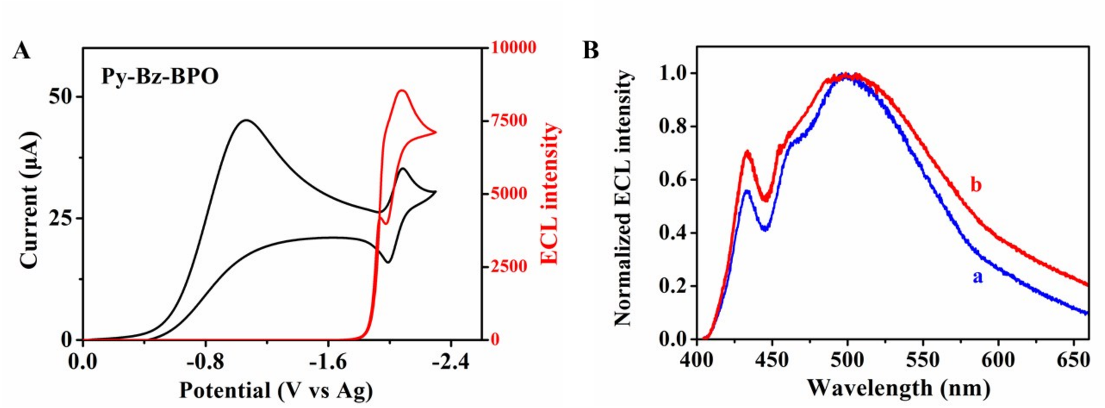

Figure S-10. (A) ECL (red) and CV (black) simultaneous measurements for 1 mM Bz-Py in the presence of 10 mM BPO with a scan rate of 0.1 V/s; (b) ECL spectra for 1 mM Bz-Py in the absence (blue, a) and presence (red, b) of 10 mM BPO; spectra were generated by pulsing the potential from 0 to -2.3 V versus Ag in MeCN:Bz (*v*:*v*=1:1) containing 0.1 M $TBAPF_6$. Pulse width is 1 s, negative high-voltage: 600 V, Pt electrode area: 0.027 cm^2.