Supporting information

Electrochemistry and Electrogenerated Chemiluminescence of 1,3,5-Tri(anthracen-10-yl)-benzene-centered Starburst Oligofluorenes

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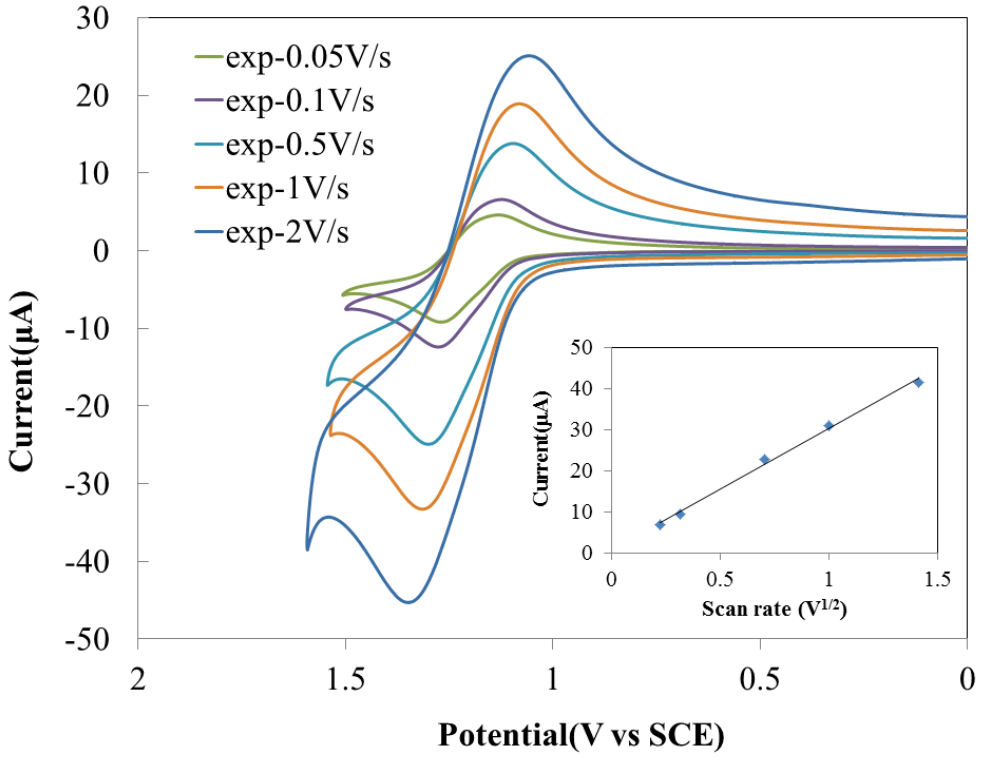

Figure S-1 CVs of 0.7 mM T1 with different scan rates at a Pt electrode with 0.034 cm^2 area. Experimental conditions: MeCN:Bz (*v:v*=1:1) solution containing 0.1 M $TBAPF_6$.

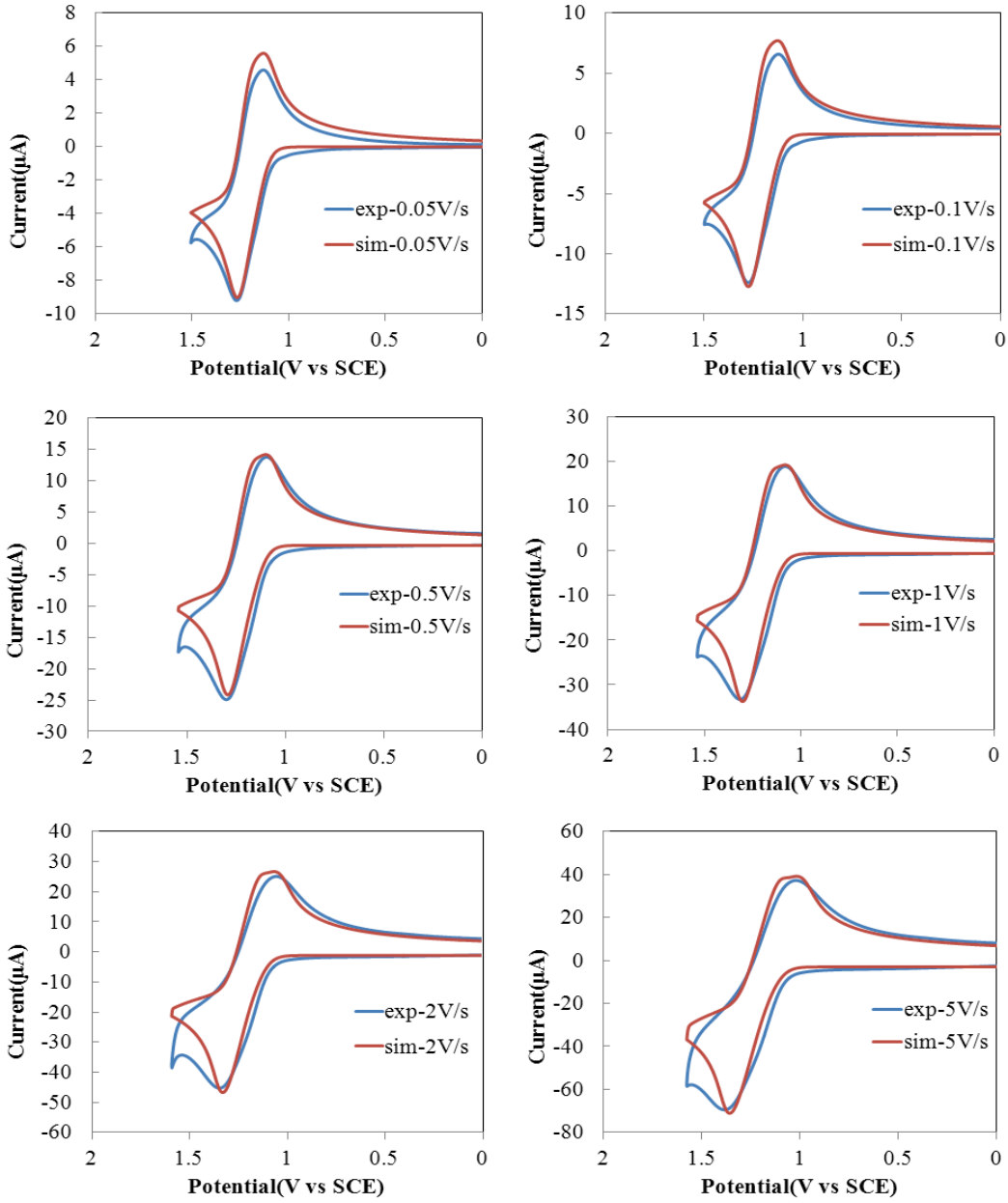

Figure S-2. Experimental and simulated oxidation waves for 0.7 mM T1 at different scan rates. The model for these oxidation simulations: EEE, k_1^0=0.01cm/s, k_2^0=10000 cm/s, k_3^0=10000 cm/s. Simulated data: $E^0_{1,ox}$=1.14 V, $E^0_{2,ox}$=1.18 V, $E^0_{3,ox}$=1.22 V; Diffusion coefficient: 6×10^{-6} cm^2/s, uncompensated resistance 1400 Ω, capacitance 6×10^{-7} F. Experimental conditions: MeCN:Bz (*v*:*v*=1:1) solution containing 0.1 M $TBAPF_6$, platinum electrode area: 0.034 cm^2.

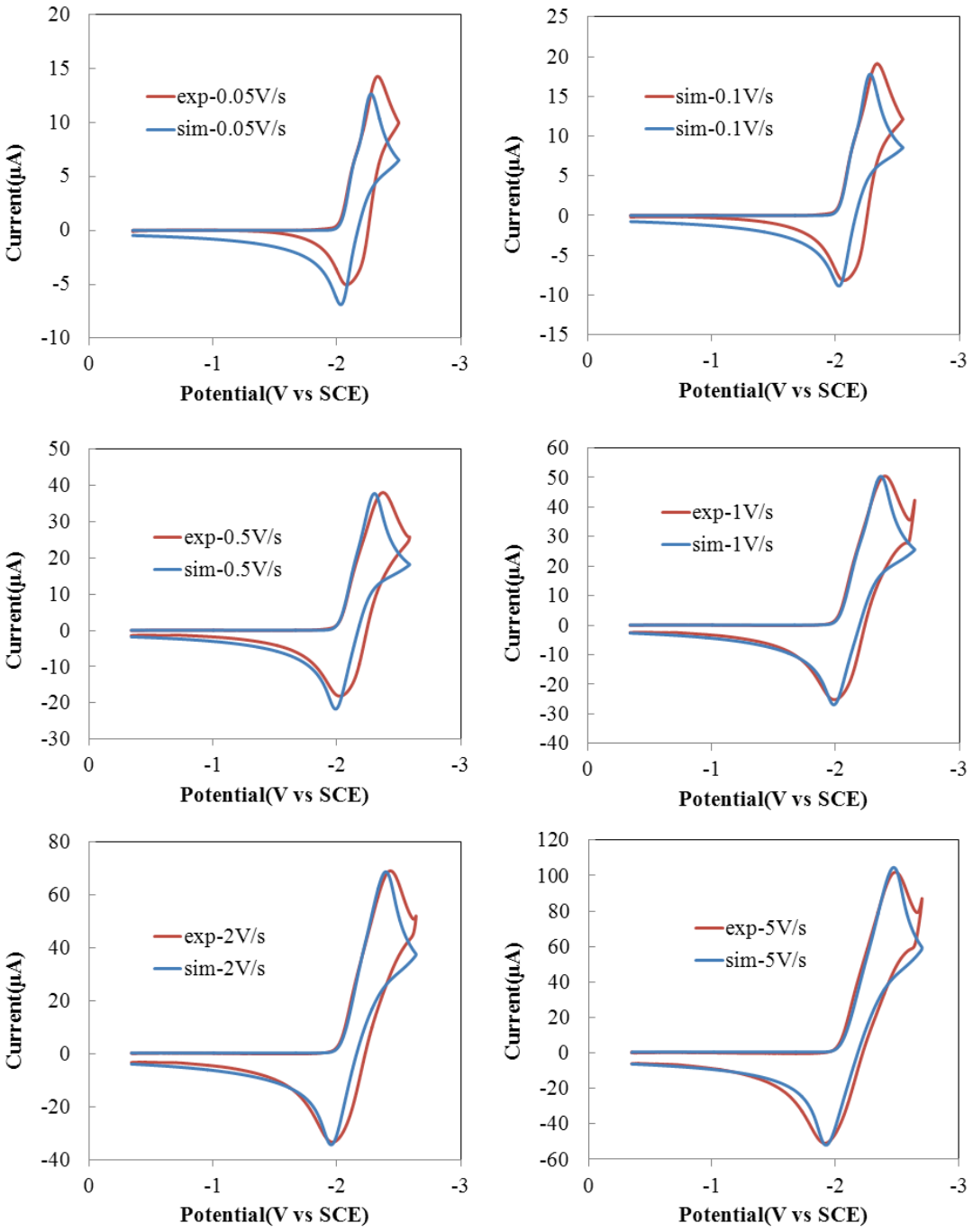

Figure S-3. Experimental and simulated reduction waves for 1.1 mM T1 at different scan rates. The model for these oxidation simulations: EEEC, k_1^0=0.01cm/s, k_2^0=0.005cm/s, k_3^0=0.005 cm/s, k_f=1 s^{-1}. Simulated data: $E^0_{1,red}$=-2.10 V, $E^0_{2,red}$=-2.16 V, $E^0_{3,red}$=-2.22 V; Diffusion coefficient: 6× 10^{-6} cm^2/s, uncompensated resistance 1400 Ω, capacitance 1 × 10^{-7} F. Experimental conditions are same as Figure S-2.

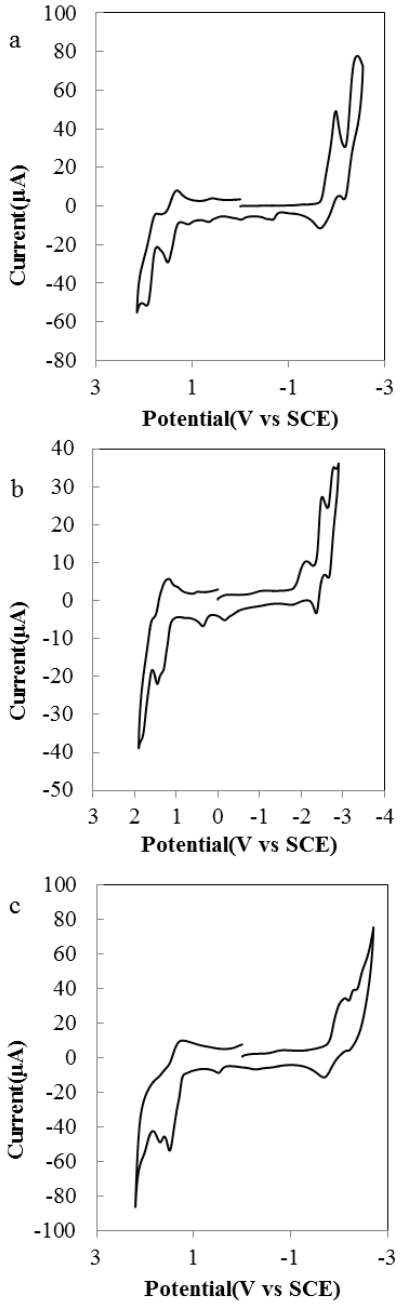

Figure S-4. CV of 0.94 mM of T1 (a); CV of 0.6 mM T2 (b); CV of 0.56 mM T3 (c); Scan rate, 0.5 V/s. Experimental conditions: MeCN:Bz (*v*:*v*=1:1) solution containing 0.1 M $TBAPF_6$, platinum electrode area is 0.034 cm^2.

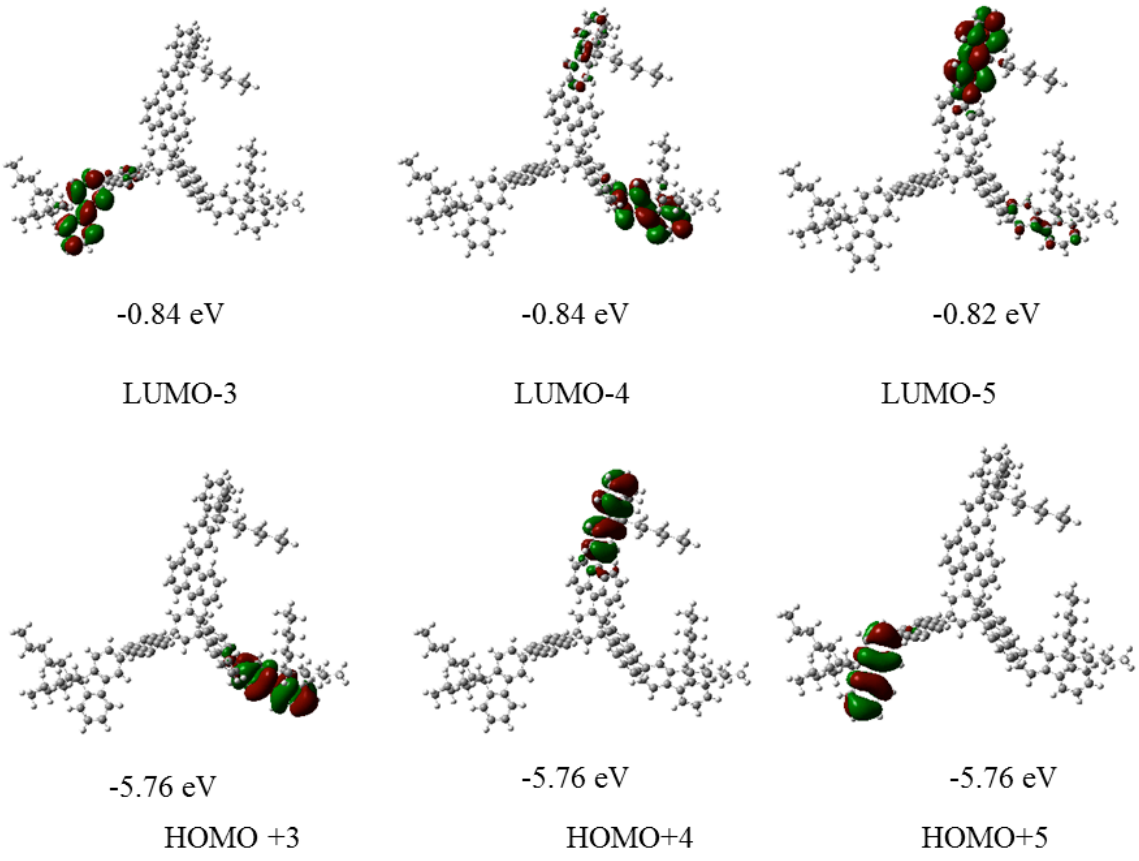

Figure S-5. Calculated frontier molecular orbitals of HOMOs and LUMOs for **T1** by DFT (B3LYP/6-31G(d)).

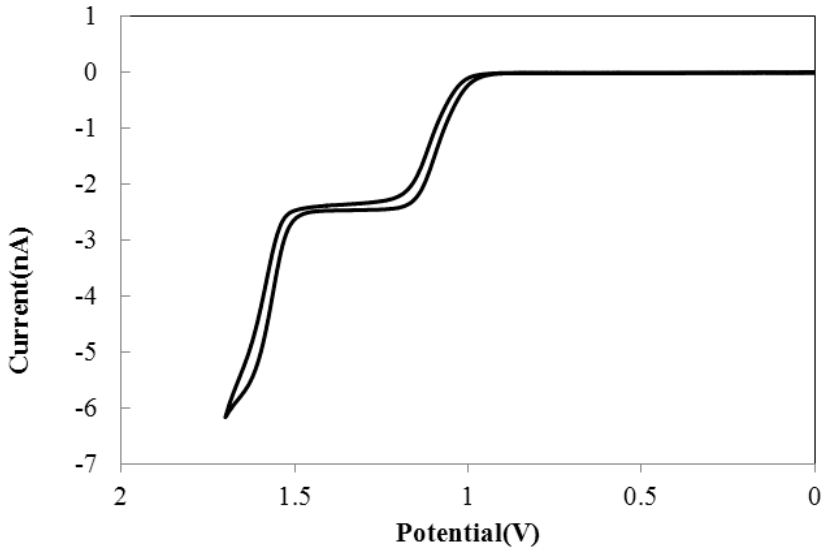

Figure S-6. Cyclic voltammograms of 0.7 mM T1 in MeCN:Bz(1:1) solution containing 0.1 M $TBAPF_6$**.** Gold UME: r=10 μm. Scan rate: 10 mV/s.

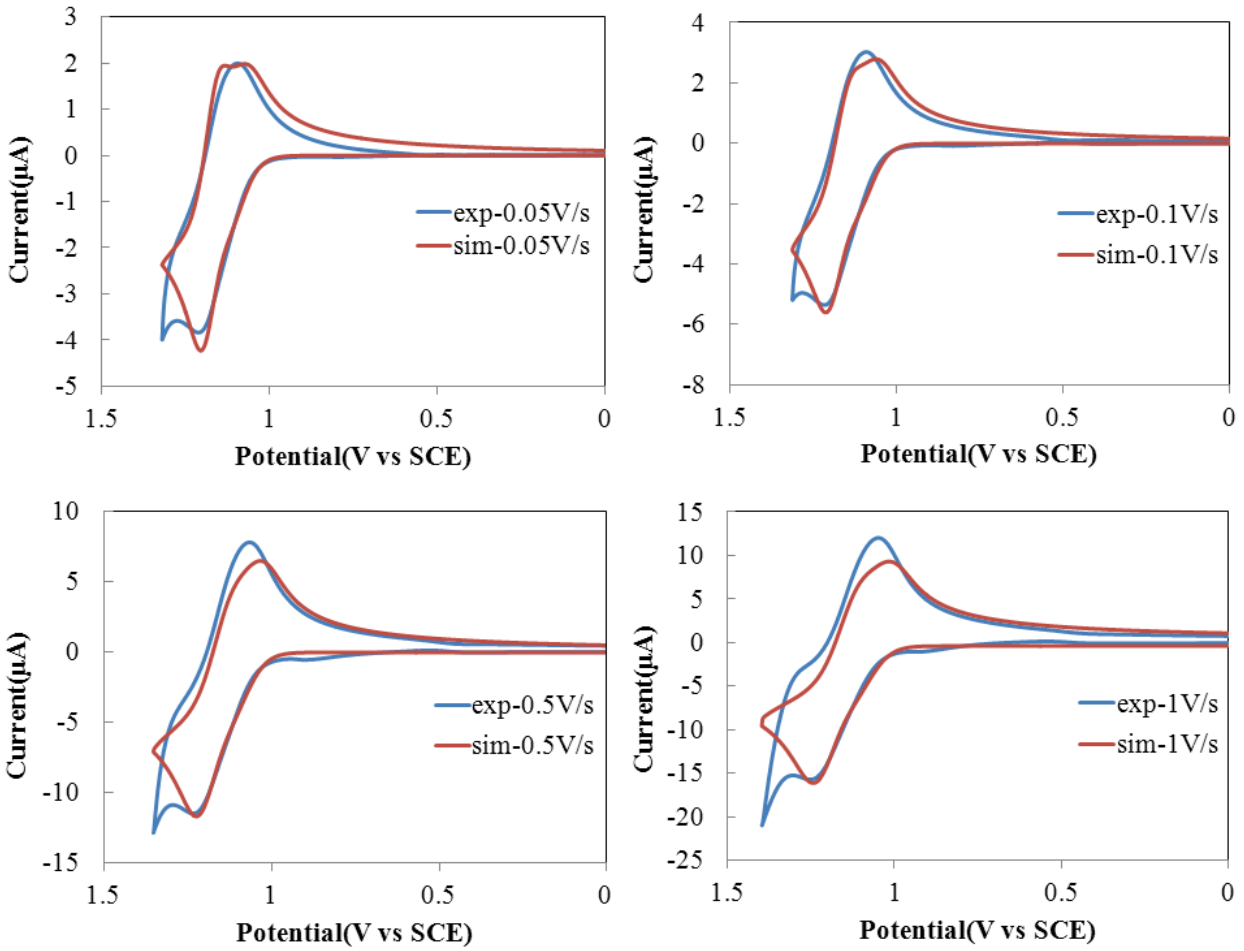

Figure S-7. Experimental and simulated oxidation waves for 0.3 mM T2 at different scan rates. The model for these oxidation simulations: EEE, k_1^0=0.01cm/s, k_2^0=0.01 cm/s, k_3^0=0.1 cm/s. Simulated data: $E^0_{1,ox}$=1.11 V, $E^0_{2,ox}$=1.16 V, $E^0_{3,ox}$=1.18 V; Diffusion coefficient: 6.0× 10^{-6} cm^2/s, uncompensated resistance 1799 Ω, capacitance 1 × 10^{-7} F. Experimental conditions are same as Figure S-2.

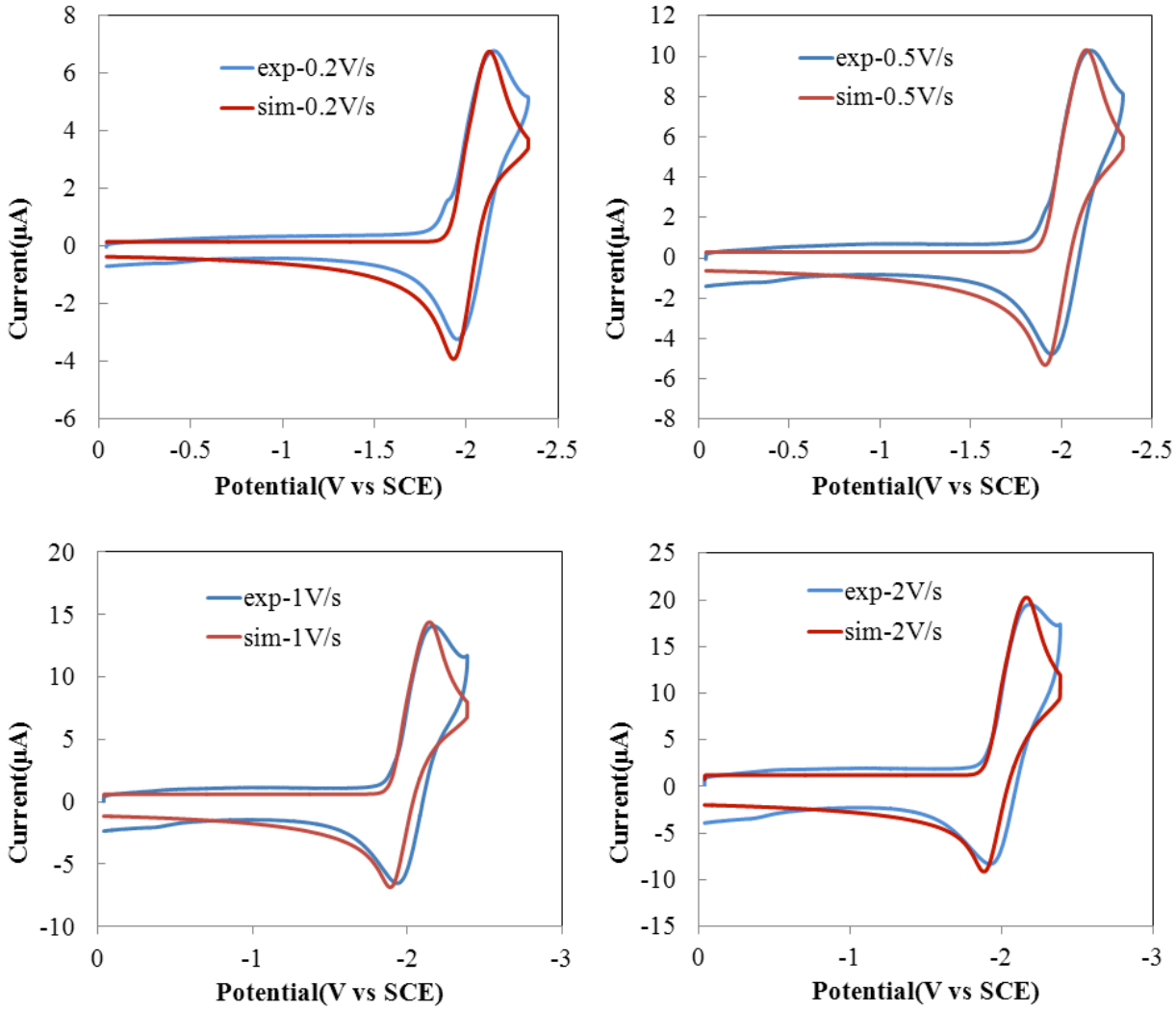

Figure S-8. Experimental and simulated reduction waves for 0.3 mM T2 at different scan rates. The model for these oxidation simulations: EEEC, k_1^0=0.01cm/s, k_2^0=0.01 cm/s, k_3^0=0.005 cm/s, k_f=2 s^{-1}. Simulated data: $E^0_{1,red}$=-1.98 V, $E^0_{2,red}$=-2.03 V, $E^0_{3,red}$=-2.08 V; Diffusion coefficient: 6.0× 10^{-6} cm^2/s, uncompensated resistance 449 Ω, capacitance 6 × 10^{-7} F. Experimental conditions are same as Figure S-2.

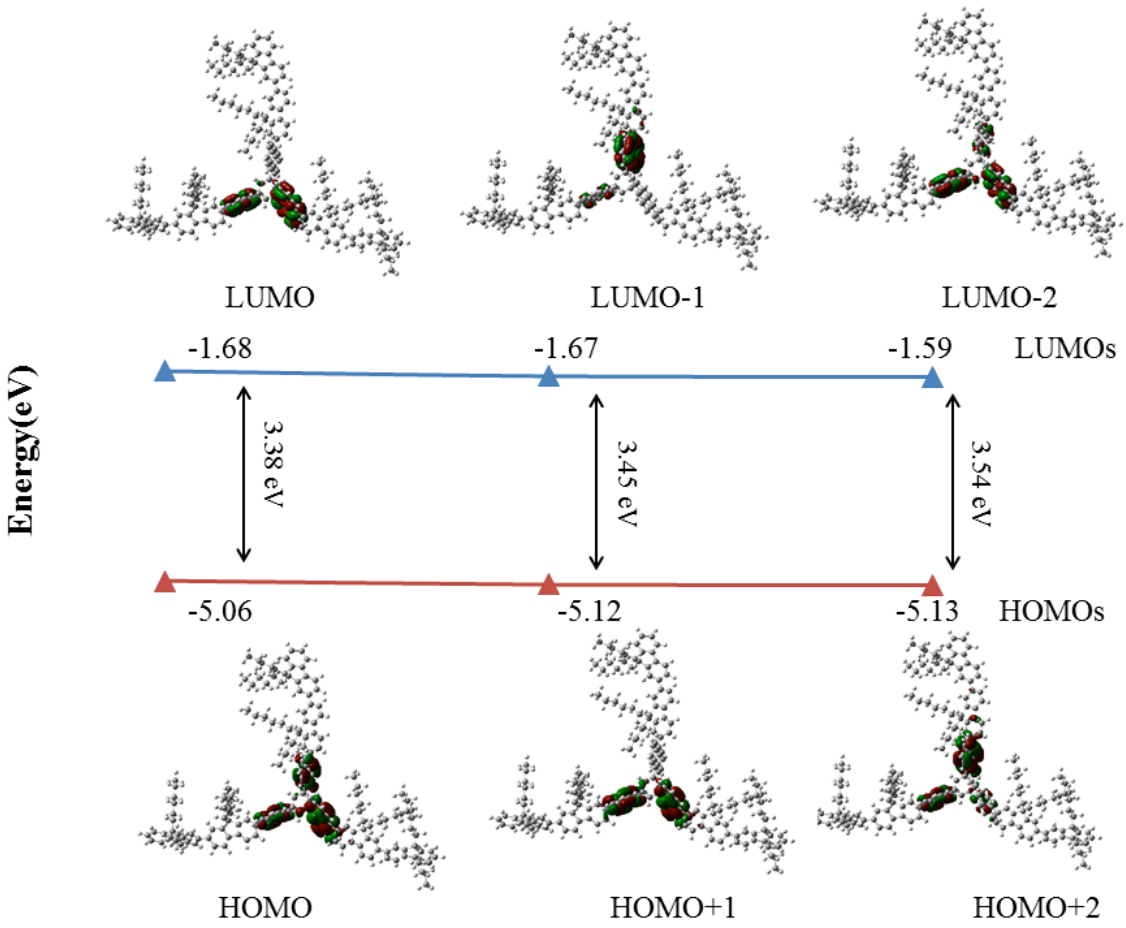

Figure S-9. Calculated frontier molecular orbitals of HOMOs and LUMOs for **T2** by DFT (B3LYP/6-31G(d)).

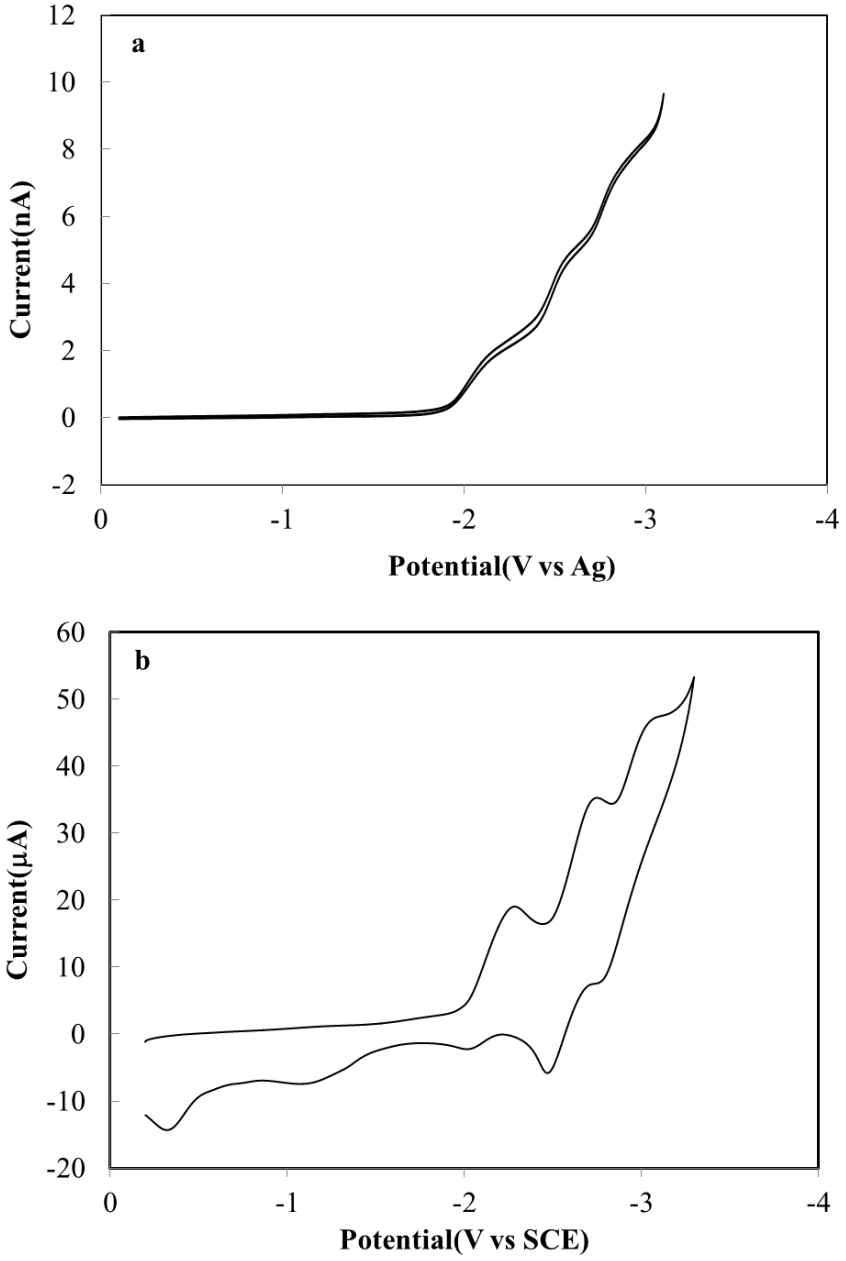

Figure S-10. Cyclic voltammograms of 0.64 mM T2 in THF solution containing 0.1 M $TBAPF_6$**.** (a) at Gold UME: r=10 μm, scan rate: 5 mV/s; (b) at platinum electrode 0.034 cm^2, Scan rate: 0.5 V/s.

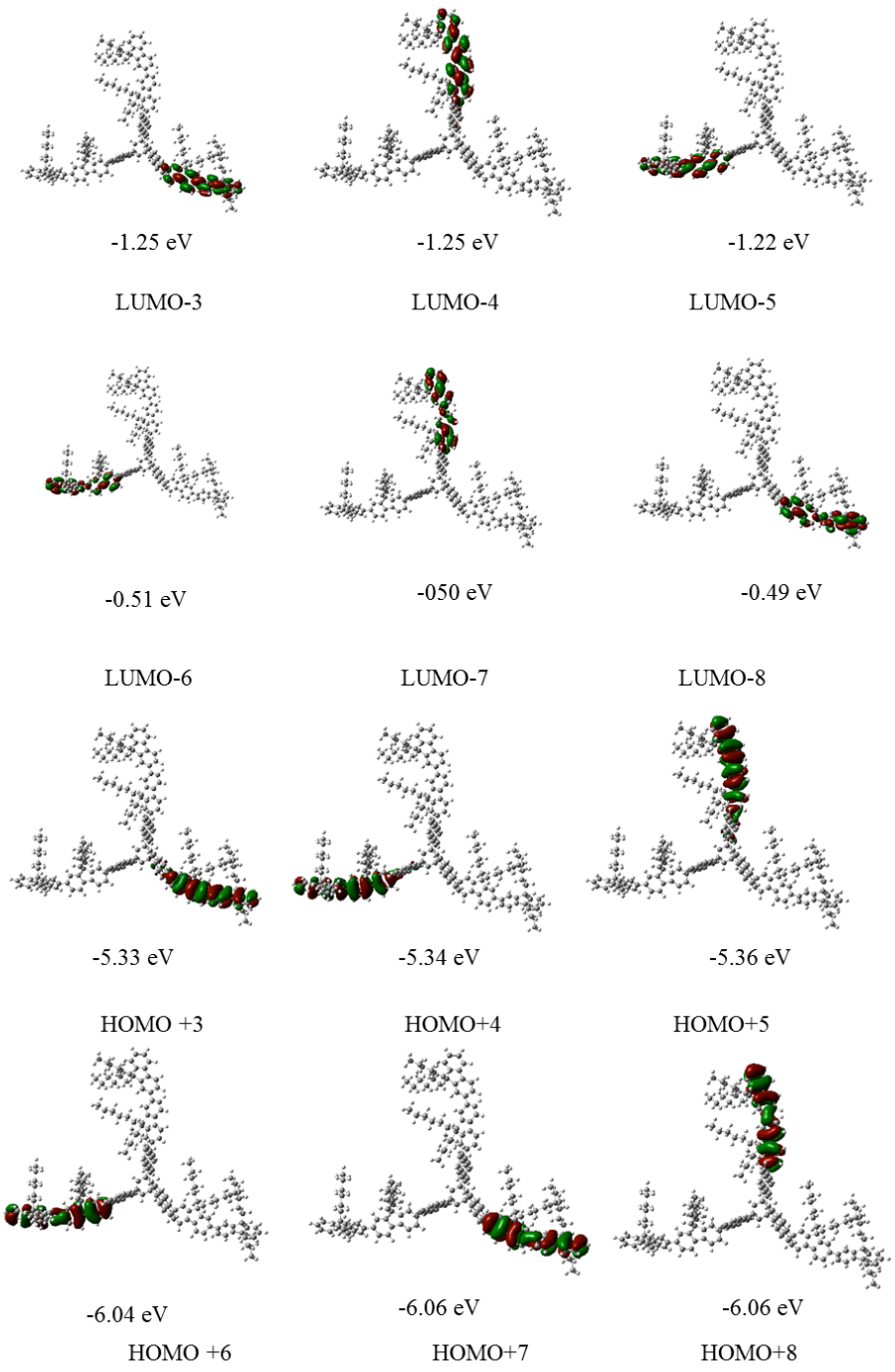

Figure S-11. Calculated frontier molecular orbitals of HOMOs and LUMOs for **T2** by DFT (B3LYP/6-31G(d)).

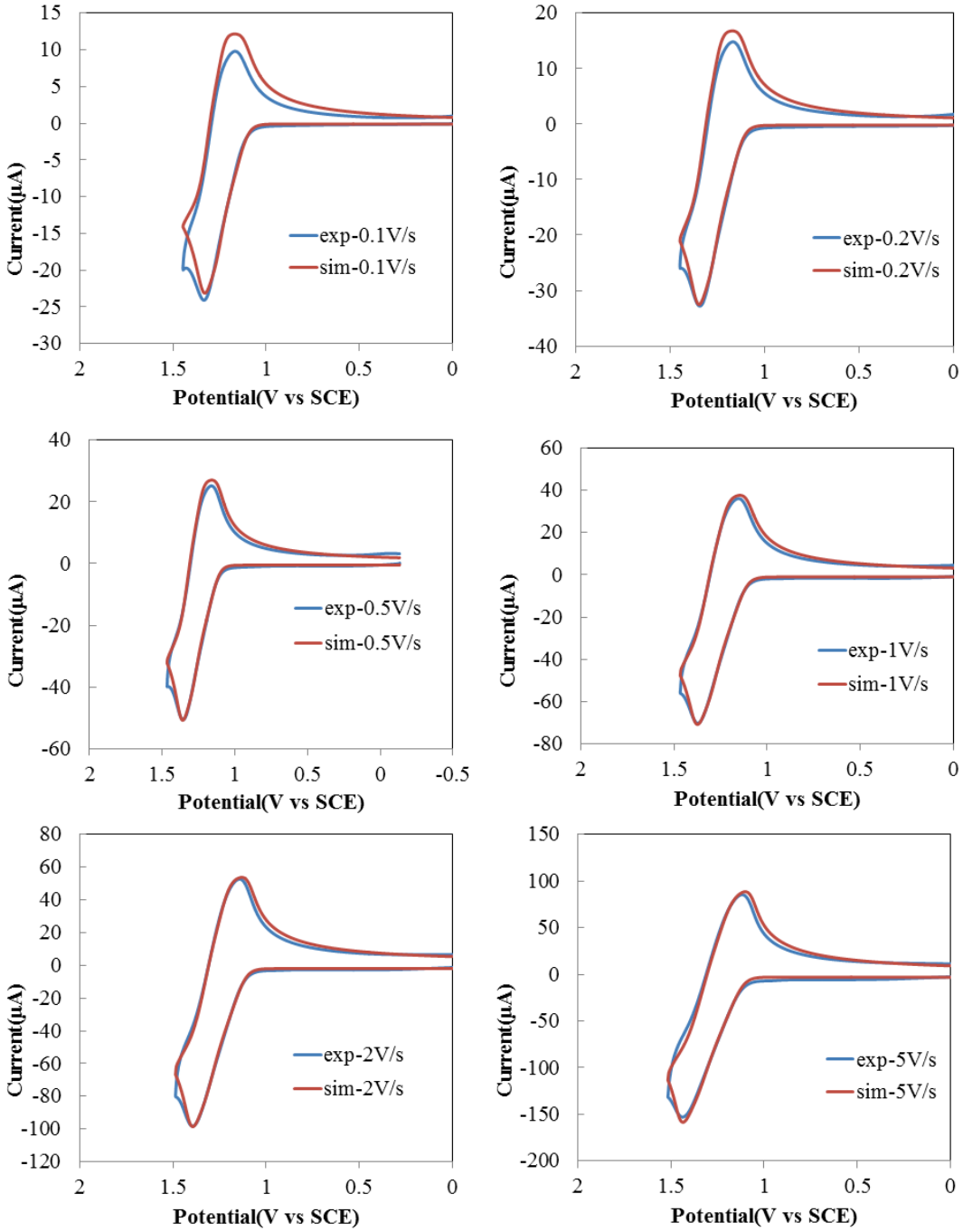

Figure S-12. Experimental and simulated oxidation waves for 0.7 mM T3 at different scan rates. The model for these oxidation simulations: EEEEEE, k^0=10^4cm/s. Simulated data: $E^0_{1,ox}$=1.16 V, $E^0_{2,ox}$=1.2 V, $E^0_{3,ox}$ =1.24 V, $E^0_{4,ox}$=1.26 V, $E^0_{5,ox}$=1.3 V, $E^0_{6,ox}$=1.32 V; Diffusion coefficient: 6× 10^{-6} cm^2/s, uncompensated resistance 617 Ω, capacitance 1 × 10^{-6} F. Experimental conditions are same as Figure S-2.

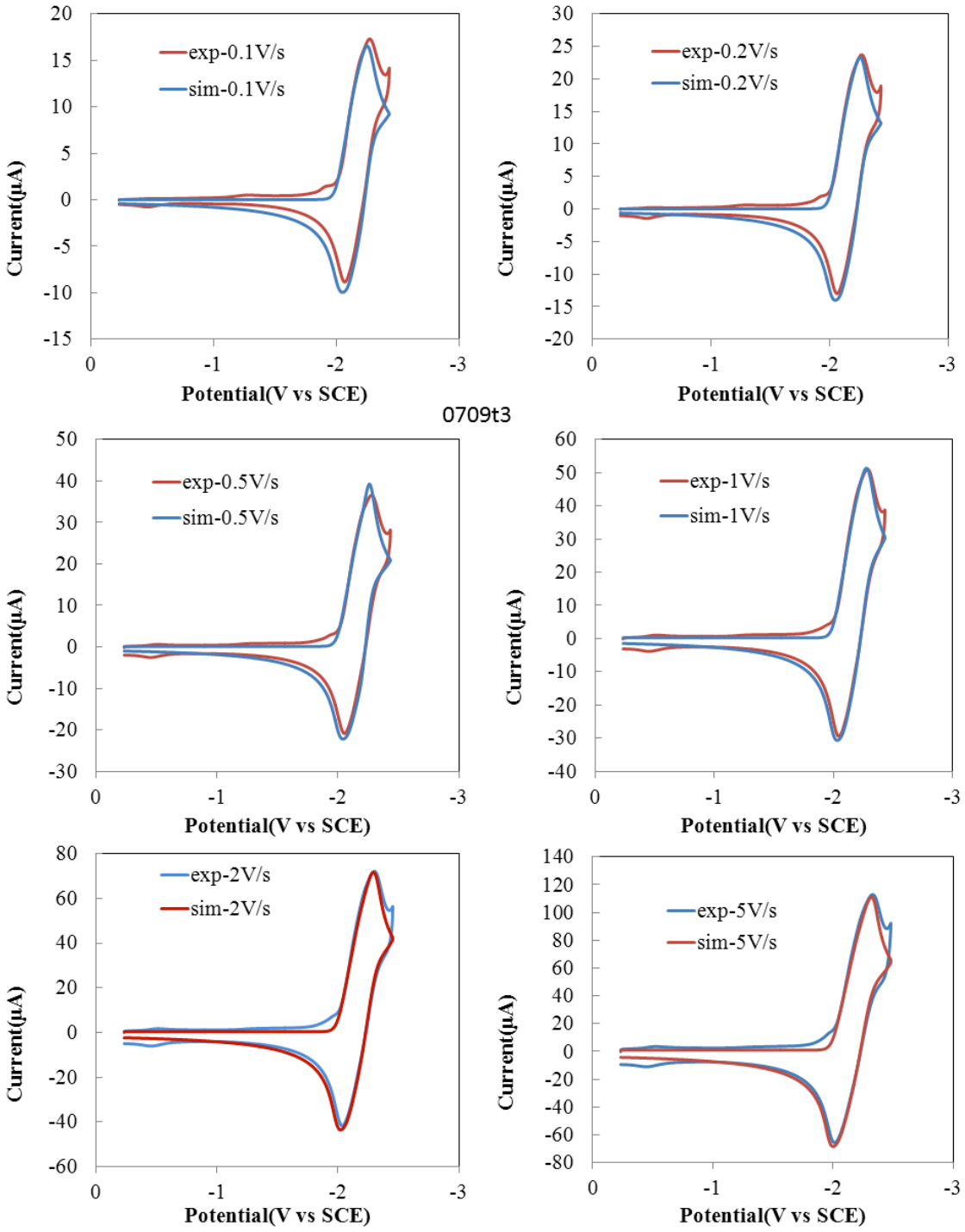

Figure S-13. Experimental and simulated reduction waves for 0.54 mM T3 at different scan rates. The model for these oxidation simulations: EEEEEE, k^0=10^4cm/s. Simulated data: $E^0_{1,red}$ =-2.05 V, $E^0_{2,red}$=-2.09 V, $E^0_{3,red}$=-2.13 V, $E^0_{4,red}$=-2.17 V, $E^0_{5,red}$=-2.21 V, $E^0_{6,red}$=-2.25 V; Diffusion coefficient: 6×10^{-6} cm^2/s, uncompensated resistance 611 Ω, capacitance 2×10^{-7} F. Experimental conditions are same as Figure S-2.

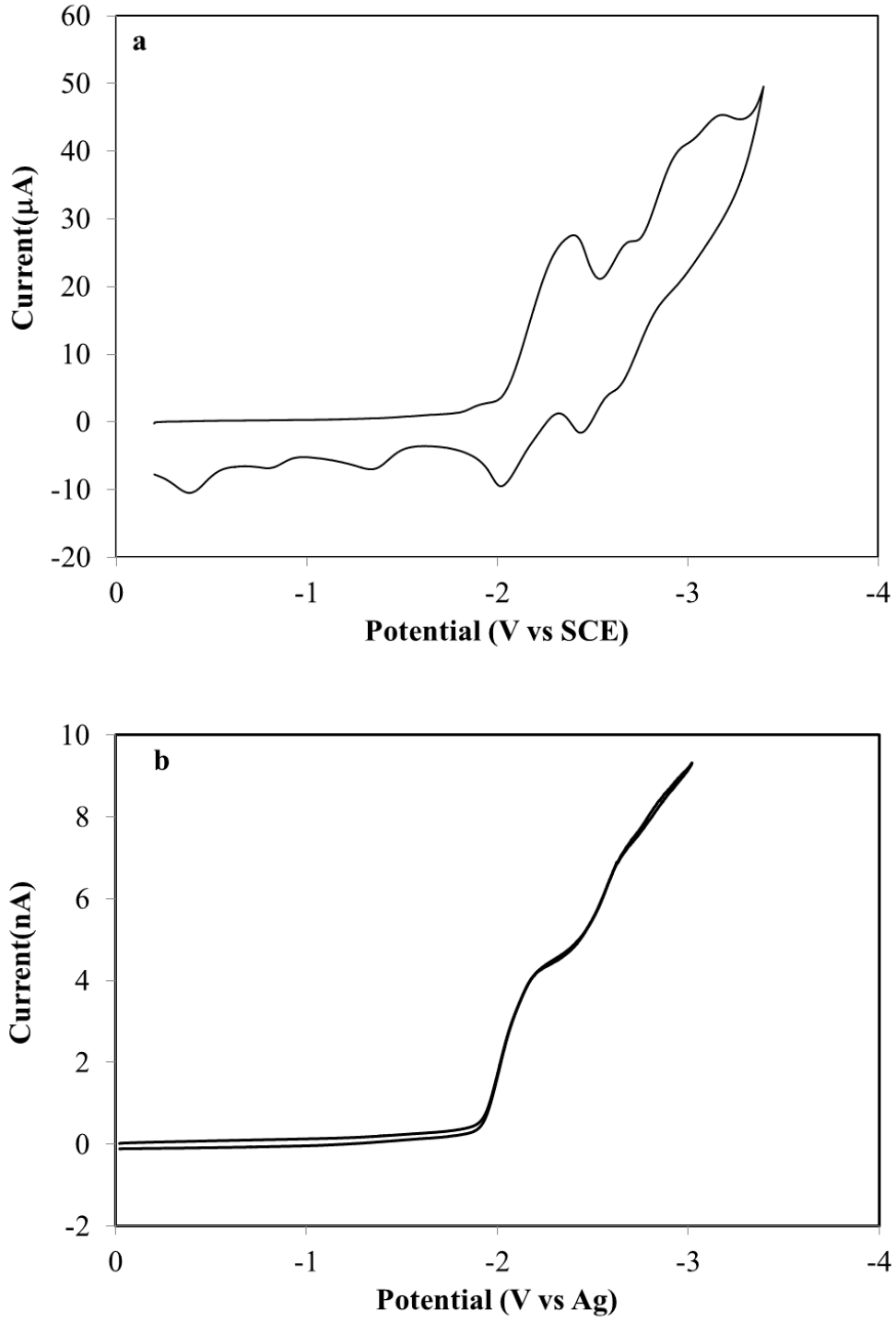

Figure S-14. Cyclic voltammograms of 0.4 mM T3 in THF solution containing 0.1 M $TBAPF_6$**.** (a) at platinum electrode 0.034 cm^2, Scan rate: 0.5 V/s; (b) at Gold UME: r=10 μm, scan rate: 5 mV/s.

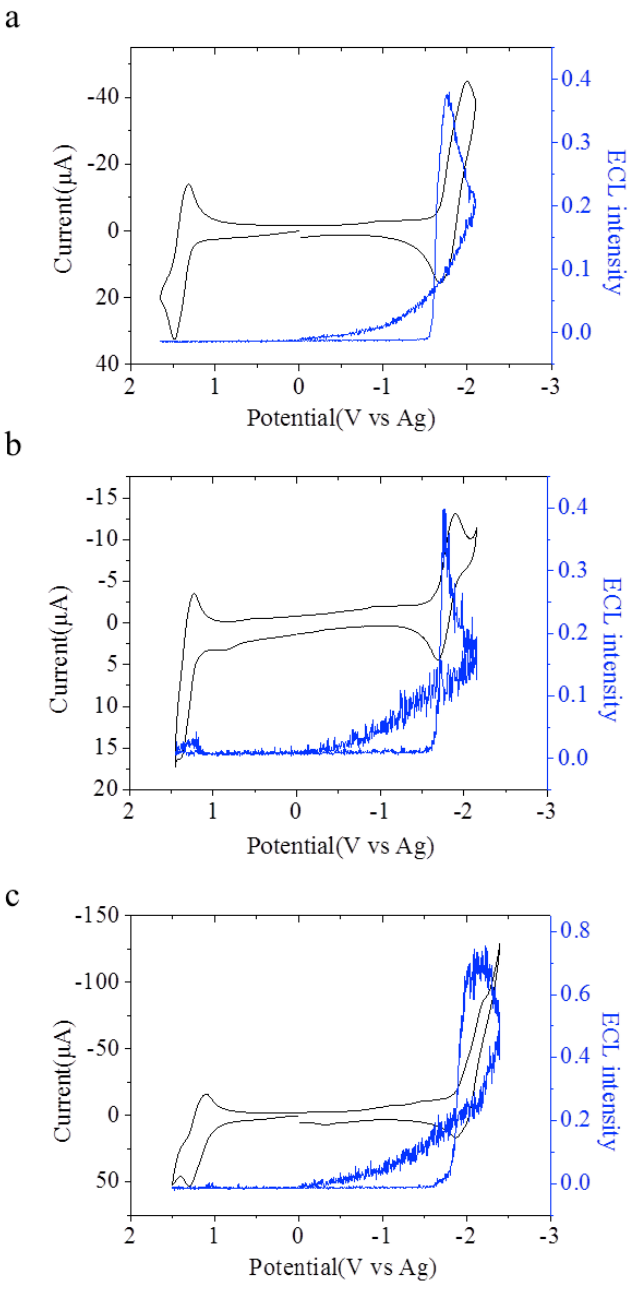

Figure S-15. Simultaneous ECL and CV profiles for 0.8 mM T1 (a), 0.5 mM T2 (b) and 0.8 mM T3(c) in MeCN:Bz (*v*:*v*=1:1) solution containing 0.1 M $TBAPF_6$. Scan rate, 0.5 V/s.

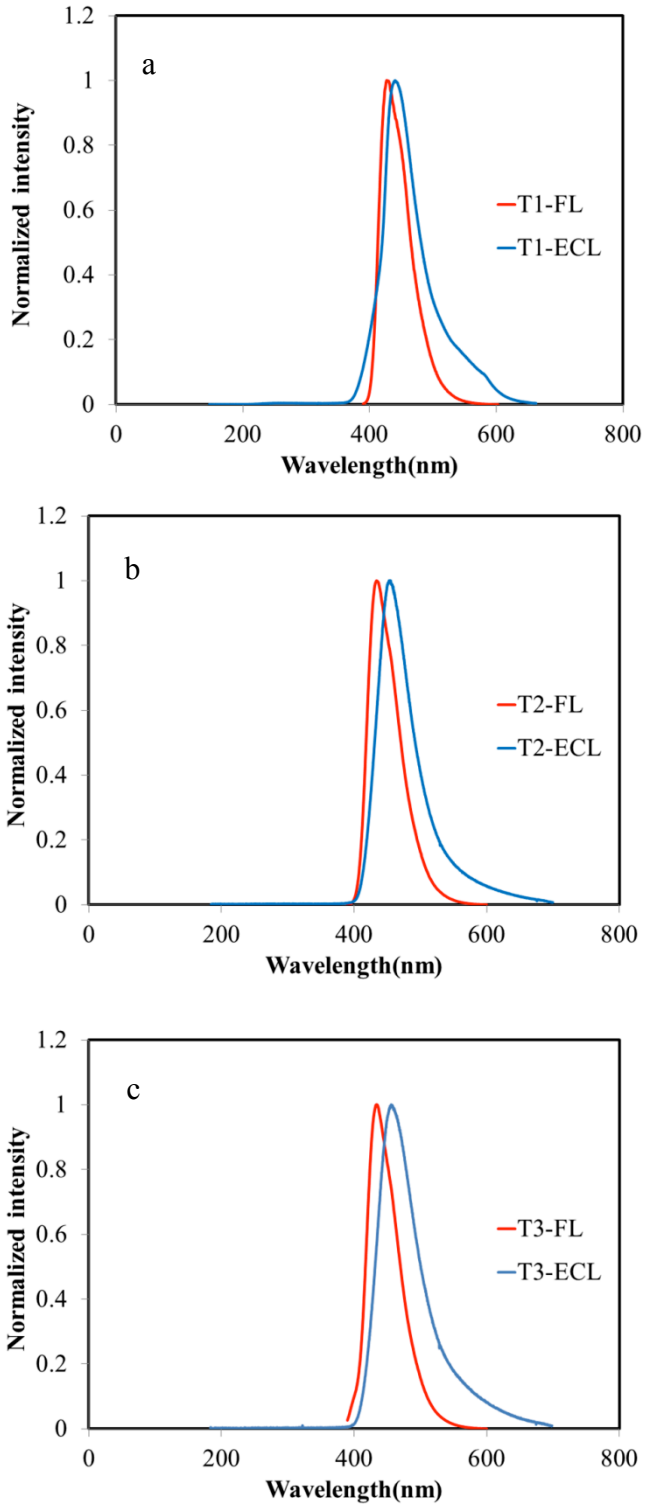

Figure S-16. Normalized PL (red) and ECL (blue) spectra of T1 (a), T2 (b) and T3 (c) in MeCN:Bz(1:1) solution containing 0.1 M $TBAPF_6$.