Supplementary Information

Solution Processed Bis-tridentate Iridium(III) complex-cored Dendrimers for Green OLEDs

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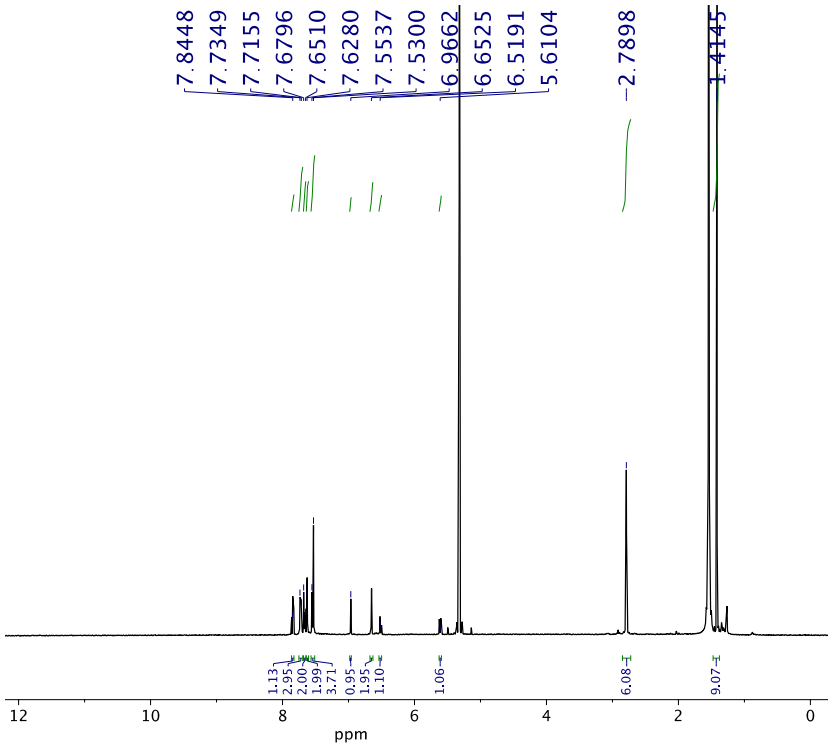


Figure S1. ^{1}H NMR spectrum of Compound **1** measured in deuterated dichloromethane.

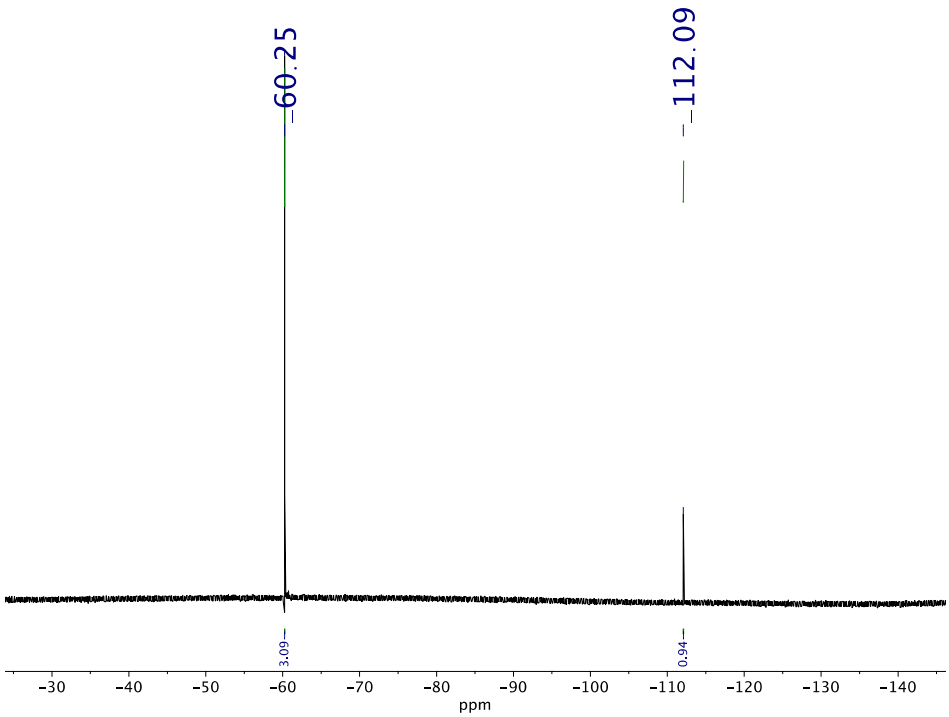


Figure S2. Proton decoupled ^{19}F NMR spectrum of Compound **1** measured in deuterated dichloromethane.

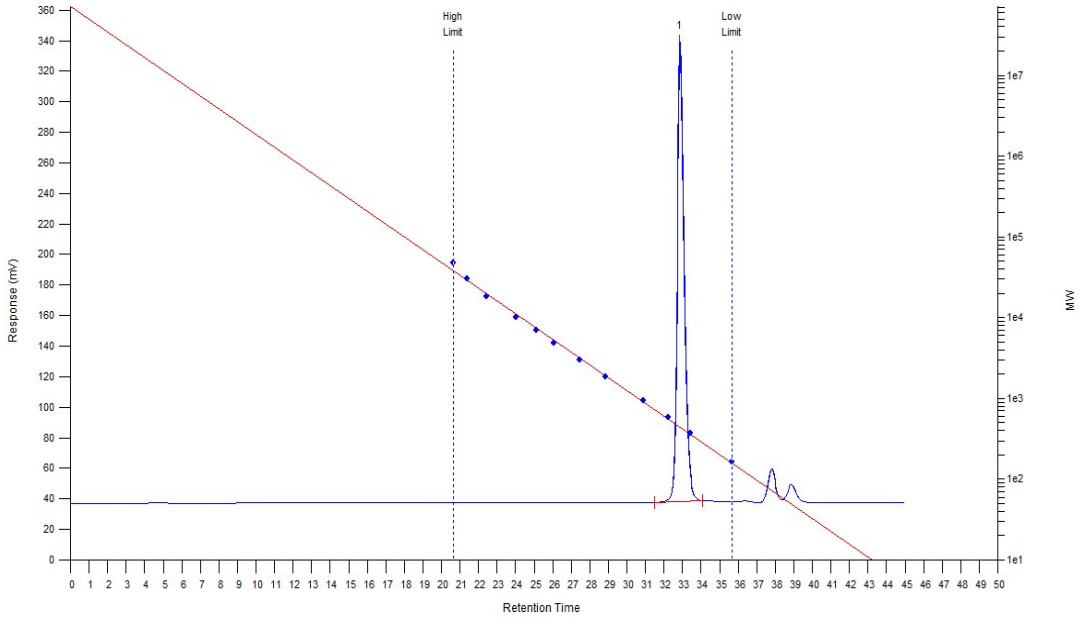


Figure S3. Gel permeation chromatography trace of Compound **1**. The data in the experimental (GPC: $\bar{M}_w$ = 434 Da; $\bar{M}_n$ = 432 Da; Đ = 1.0) is taken for peak 1.

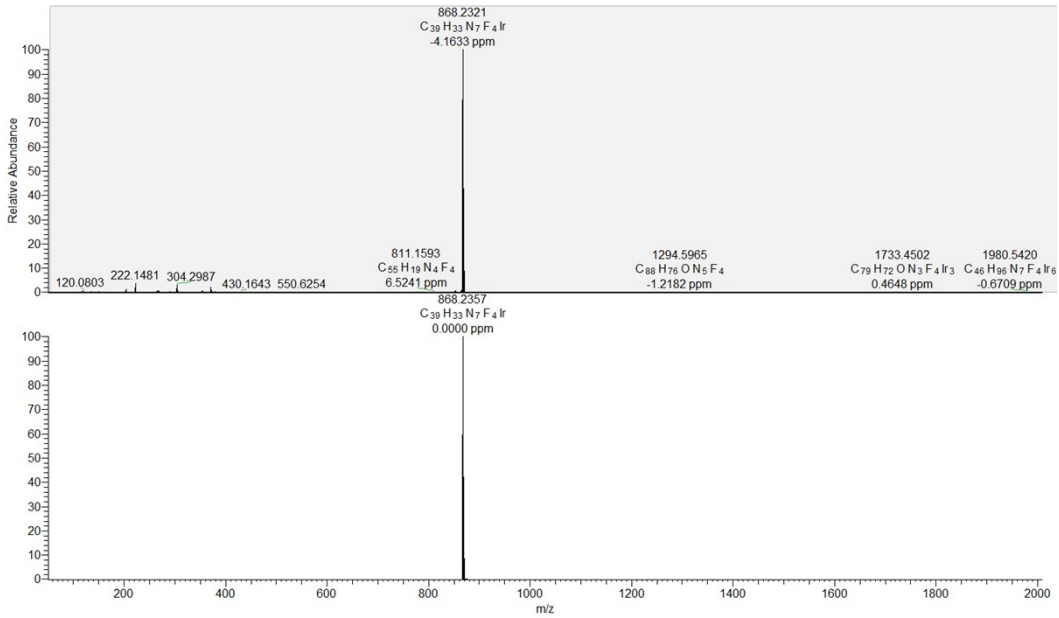


Figure S4. High resolution mass spectrum of Compound **1** (top – measured, bottom – calculated).

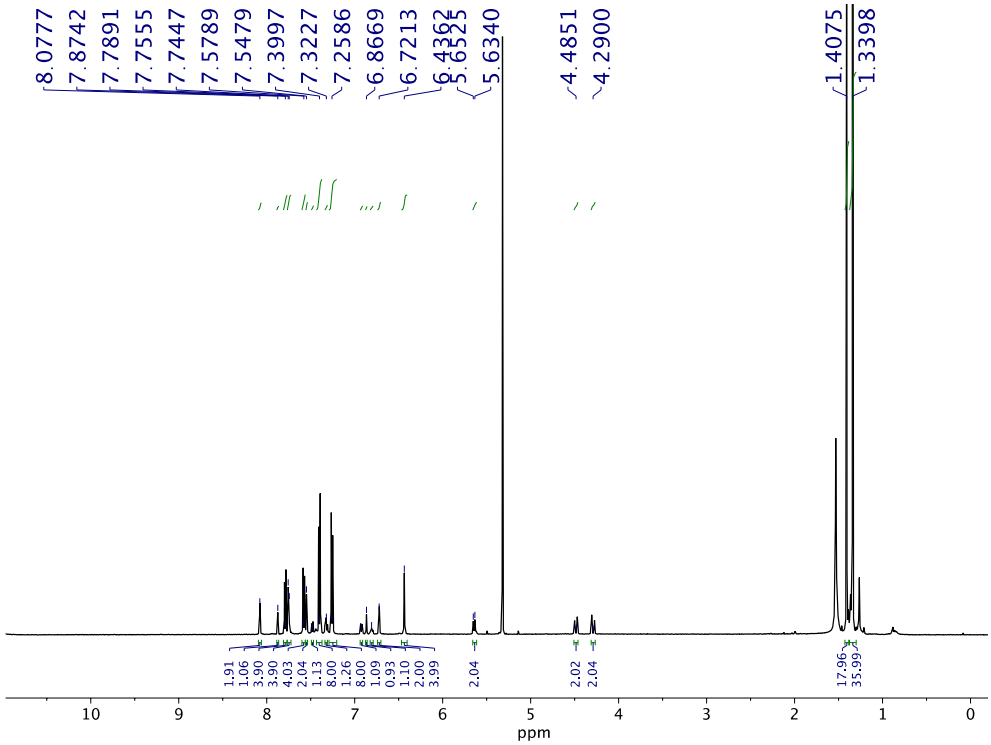


Figure S5. ^{1}H NMR spectrum of Dendrimer **2** measured in deuterated dichloromethane.

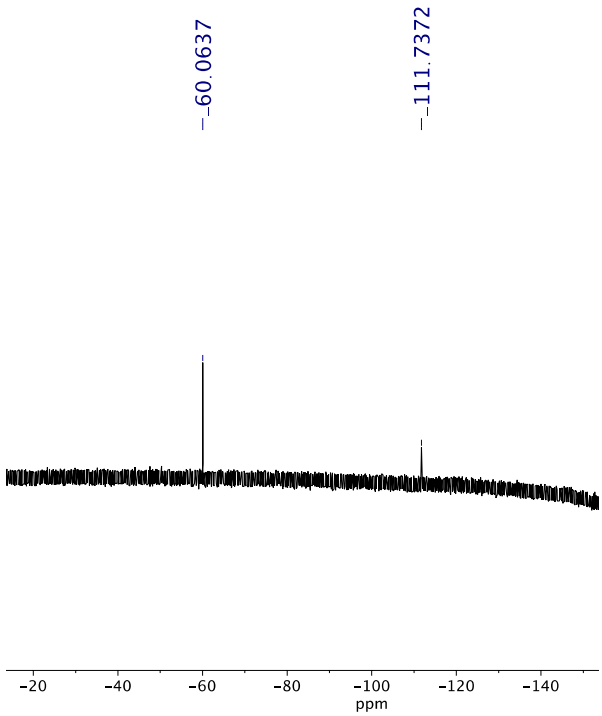


Figure S6. Proton decoupled ^{19}F NMR spectrum of Dendrimer **2** measured in deuterated dichloromethane.

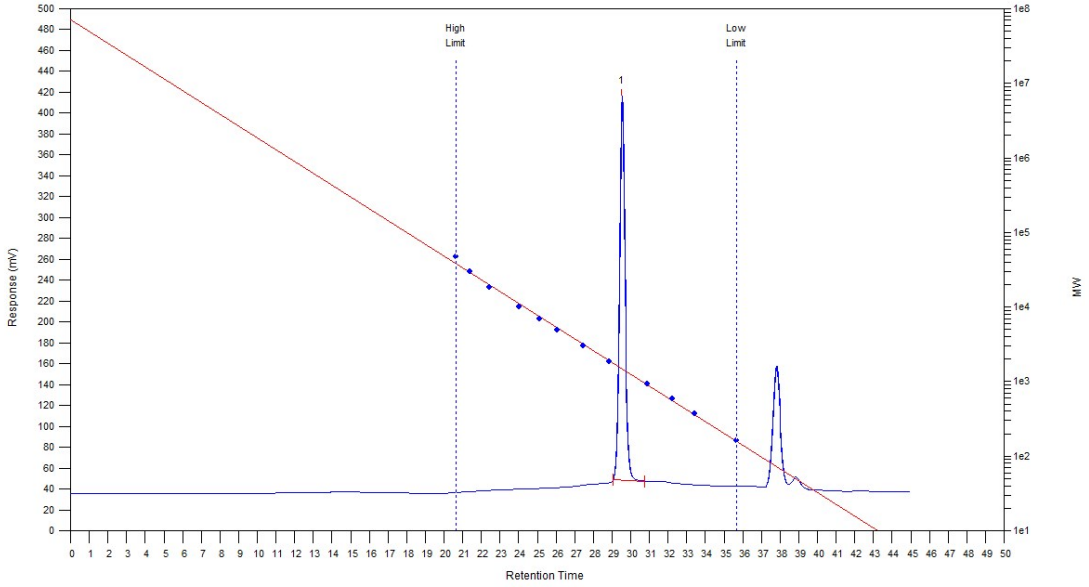


Figure S7. Gel permeation chromatography trace of Dendrimer **2**. The data in the experimental (GPC: $\overline{M_w}$ = 1483 Da; $\overline{M_n}$ = 1479 Da; Đ = 1.0) is taken for peak 1.

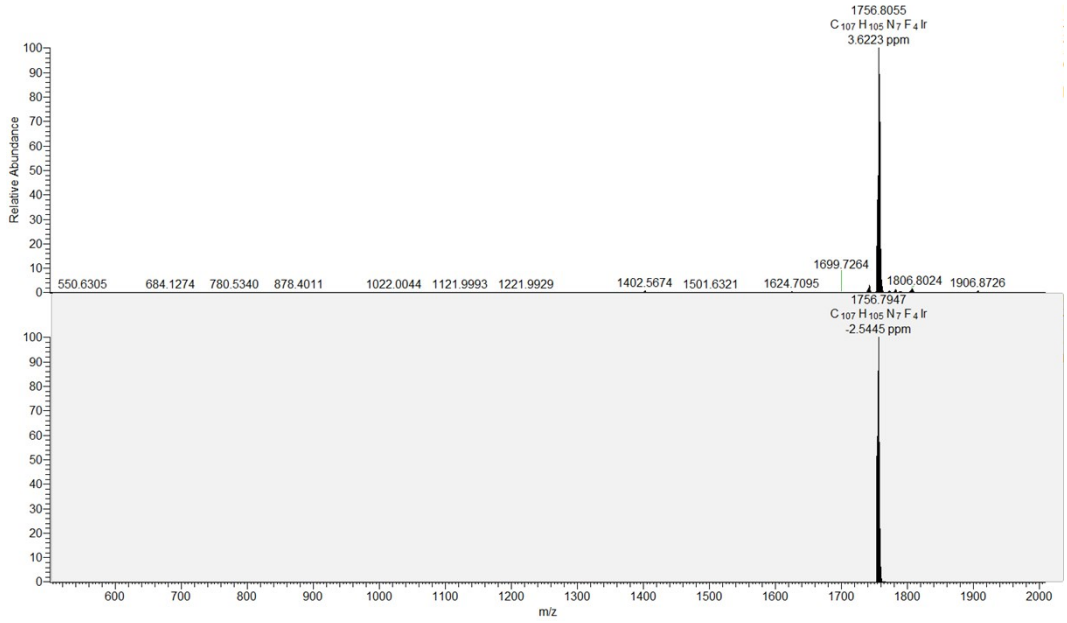
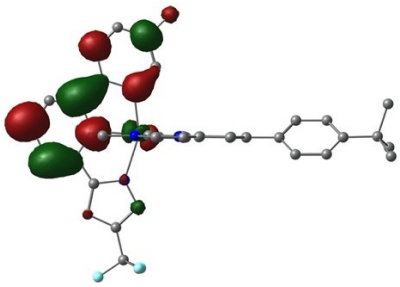
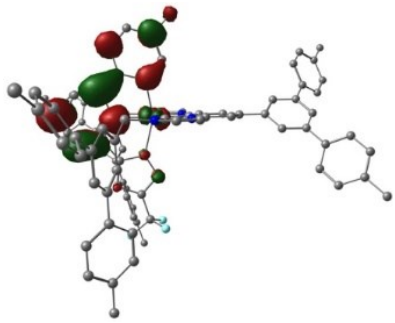


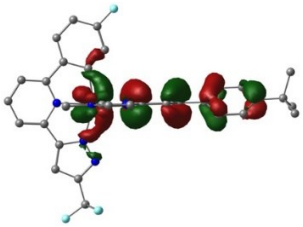
Figure S8. High resolution mass spectrum of Dendrimer **2** (top – measured, bottom – calculated).



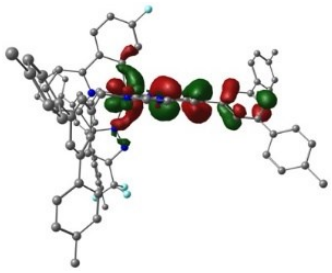
LUMO E = -5.58 eV



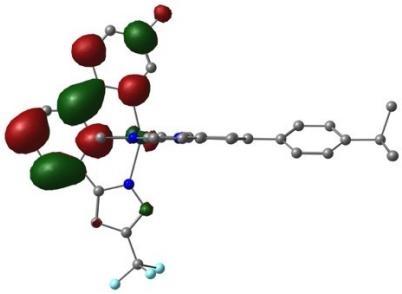
E = -5.66 eV



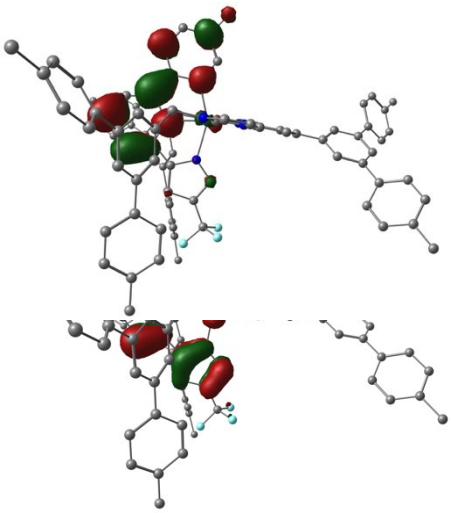
HOMO E = -1.89 eV

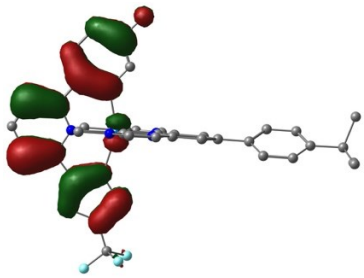


E = -1.94 eV

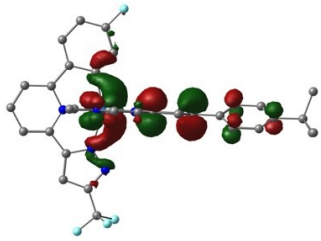


α-SOMO





α-SOMO-1



β-SUMO

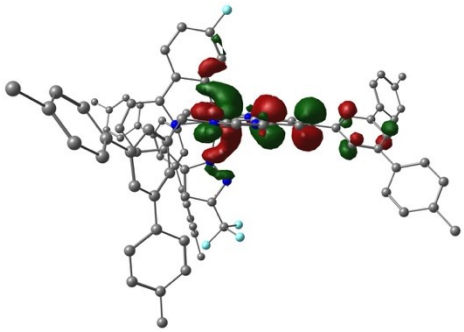


Figure S9. Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbitals (LUMO) of the singlet ground state at the optimised ground-state geometry, and up-spin (α) singly occupied molecular orbitals (α-SOMO and α-SOMO–1, with the latter lower in energy) and lowest energy unoccupied down-spin (β) molecular orbital (β-SUMO) of triplet state at the optimised triplet-state geometry for Complex **1** and Dendrimer **2**. The hydrogen atoms are omitted for the sake of clarity.

Table S1: Calculated 5 lowest **triplet** emission energies (wavelengths) and molecular orbital transitions for Complex **1**.

transition	E (eV) / λ (nm)	major MO → MO contributions
1	2.65 / 468	HOMO-1 →LUMO (41%) HOMO-2 →LUMO (16%) HOMO-6 →LUMO (15%)
2	2.76 / 449	HOMO →LUMO+2 (78%)
3	2.99 / 415	HOMO →LUMO (86%)
4	3.11 / 399	HOMO-2 →LUMO+1 (30%) HOMO-1 →LUMO+1 (26%) HOMO-1 →LUMO (17%)
5	3.27 / 379	HOMO →LUMO+3 (88%)

Table S2: Calculated 5 lowest **singlet** emission energies (wavelengths), oscillator strength and molecular orbital transitions for Complex **1**.

transition	E (eV) / λ (nm)	Oscillator strength	major MO → MO contributions
1	3.03 / 409	0.0002	HOMO →LUMO (89%)
2	3.25 / 382	0.0365	HOMO-1 →LUMO (85%)
3	3.64 / 341	0.0029	HOMO →LUMO+1 (90%)
4	3.83 / 324	0.0224	HOMO-2 →LUMO (40%)
5	3.87 / 320	0.1613	HOMO →LUMO+3 (68%)

			HOMO →LUMO+2 (20%)

Table S3: Calculated 5 lowest **triplet** emission energies (wavelengths) and molecular orbital transitions for Dendrimer **2**.

transition	E (eV) / λ (nm)	major MO → MO contributions
1	2.65 / 468	HOMO-1 →LUMO (42%) HOMO-3 →LUMO (14%)
2	2.78 / 446	HOMO →LUMO+5 (37%) HOMO →LUMO+4 (14%)
3	3.03 / 409	HOMO →LUMO (87%)
4	3.14 / 395	HOMO-1 →LUMO+1 (25%) HOMO-3 →LUMO+1 (24%) HOMO-1 →LUMO (15%)
5	3.16 / 392	HOMO-4 →LUMO+3 (24%) HOMO-6 →LUMO+2 (14%)

Table S4: The calculated 5 lowest **singlet** emission energies (wavelengths), oscillator strength and molecular orbital transitions of Dendrimer **2**.

transition	E (eV) / λ (nm)	Oscillator strength	major MO → MO contributions
1	3.06 / 405	0.0002	HOMO →LUMO (89%)
2	3.26 / 380	0.0306	HOMO-1 →LUMO (84%)
3	3.67 / 338	0.0003	HOMO →LUMO+2 (90%)
4	3.83 / 324	0.0155	HOMO-1 →LUMO+1 (30%) HOMO-3 →LUMO (27%)
5	3.89 / 319	0.0932	HOMO →LUMO+8 (57%) HOMO →LUMO+5 (16%)

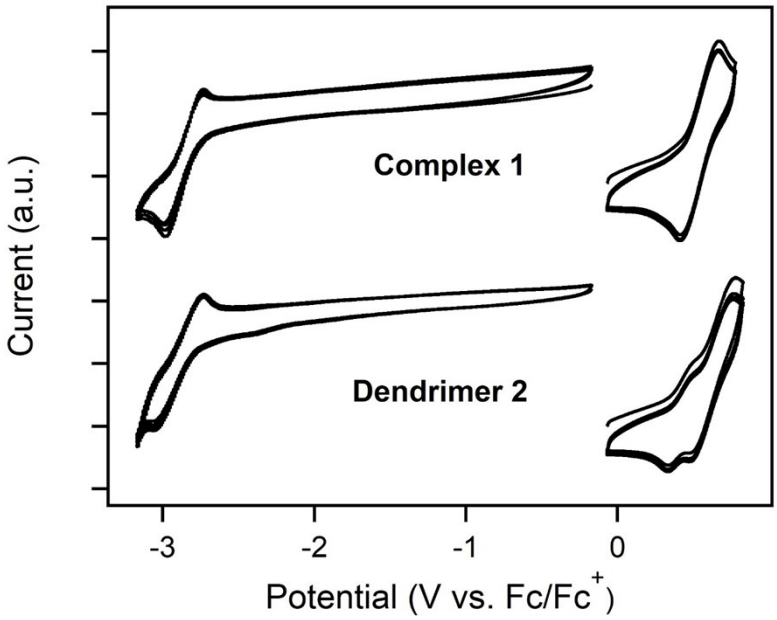


Figure S10. Cyclic Voltammograms of Complex **1** and Dendrimer **2** in dichloromethane (oxidations) and tetrahydrofuran (reductions) in the presence of 0.1 M tetra-*n*-butylammonium perchlorate at room temperature.