Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Investigation on the Origin of Variation in Photovoltaic Performance Using D-D-π-A and D-A-π-A Triphenylimidazole Dyes with Copper Electrolyte

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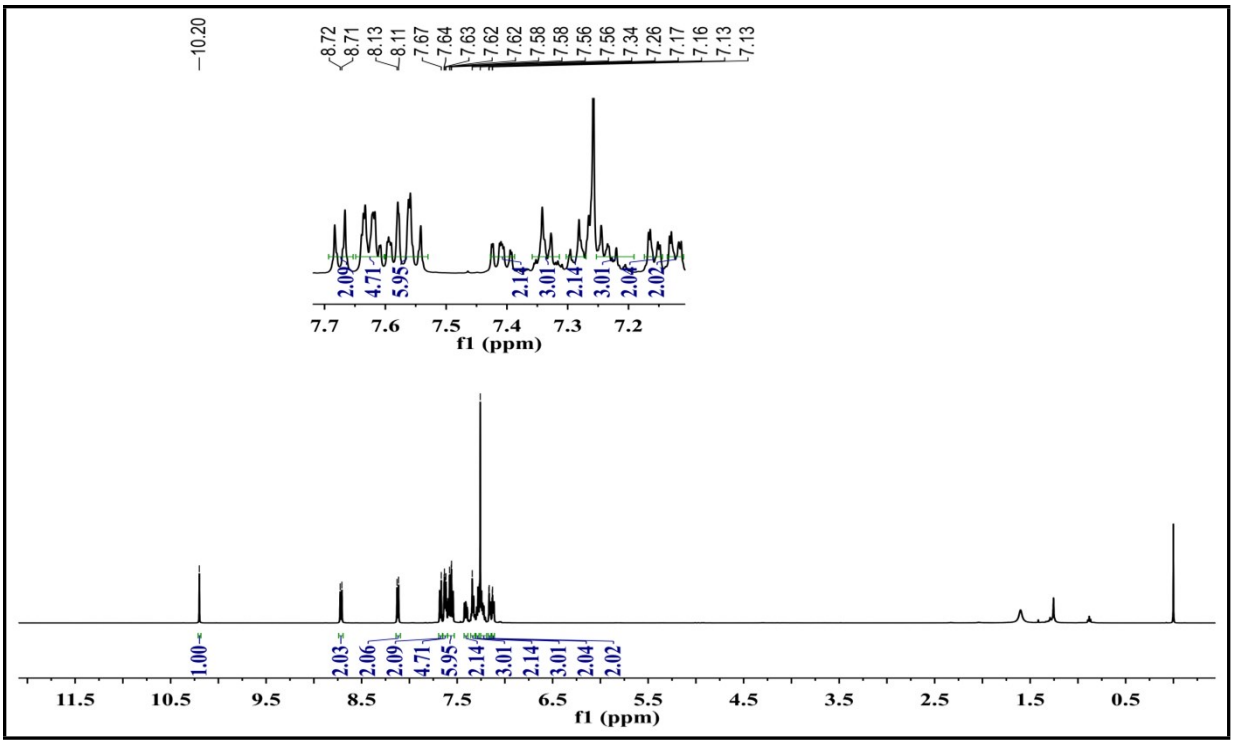

Figure S1:*[1]H NMR spectrum (400 MHz, CDCl3) of 4.*

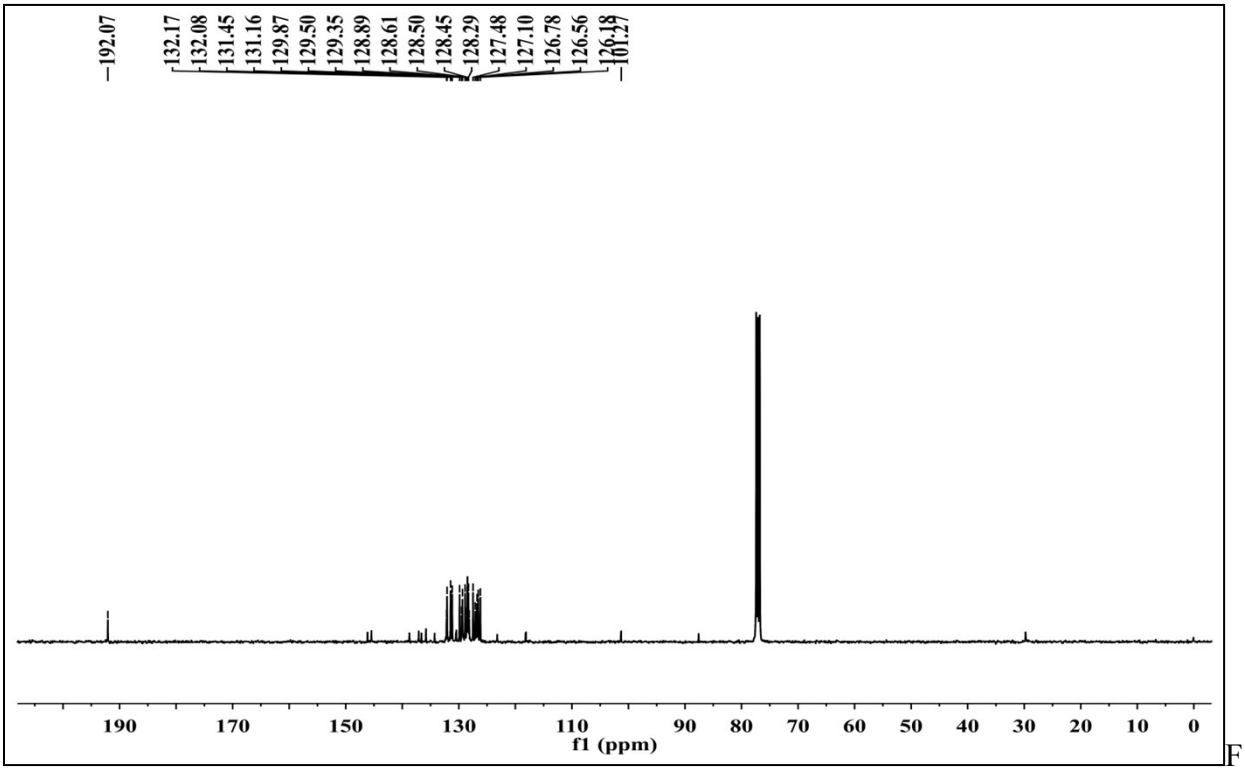

Figure S2:*[13]C NMR spectrum (400 MHz, CDCl3) of **4**.*

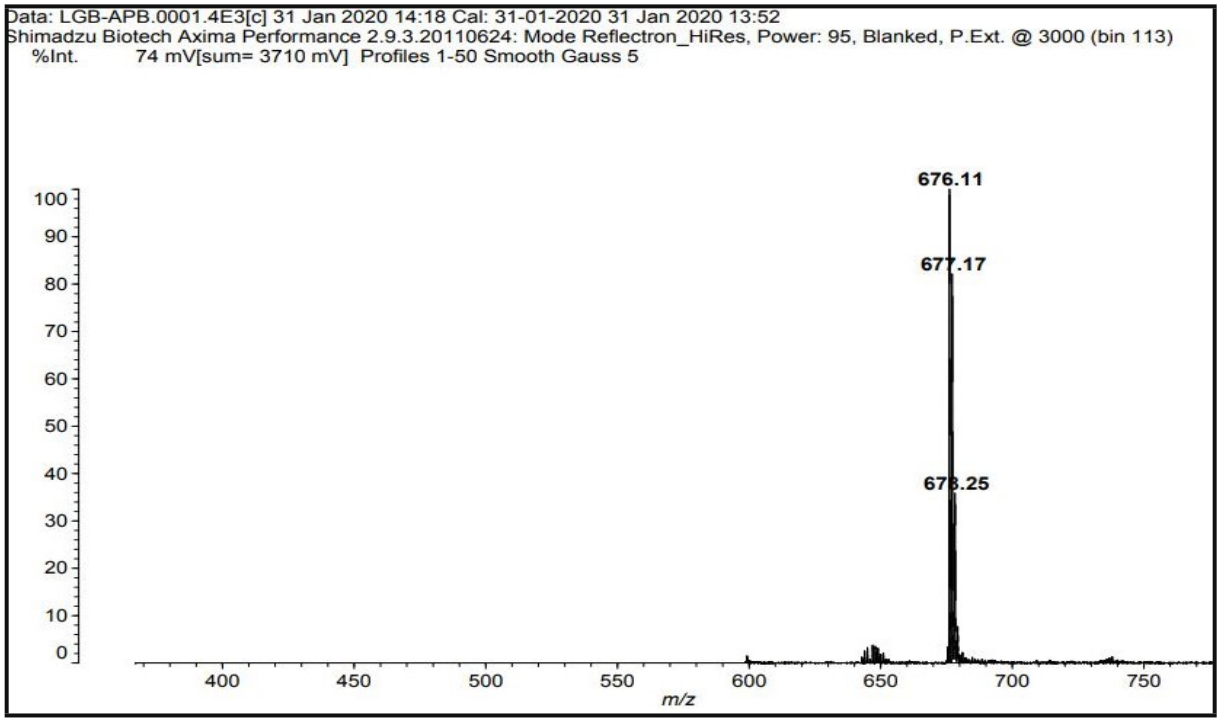

Figure S3:*MALDI-TOF of**4**.*

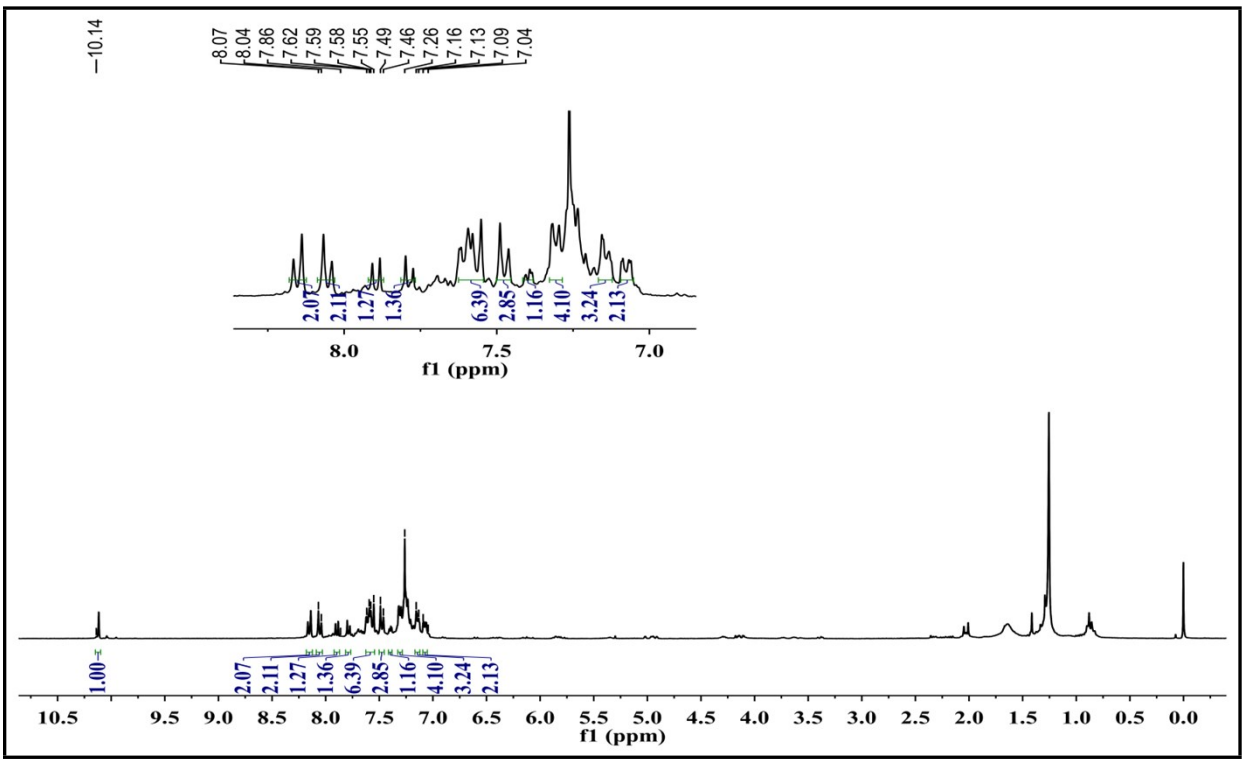

Figure S4:*[1]H NMR spectrum (400 MHz, CDCl3) of**5.***

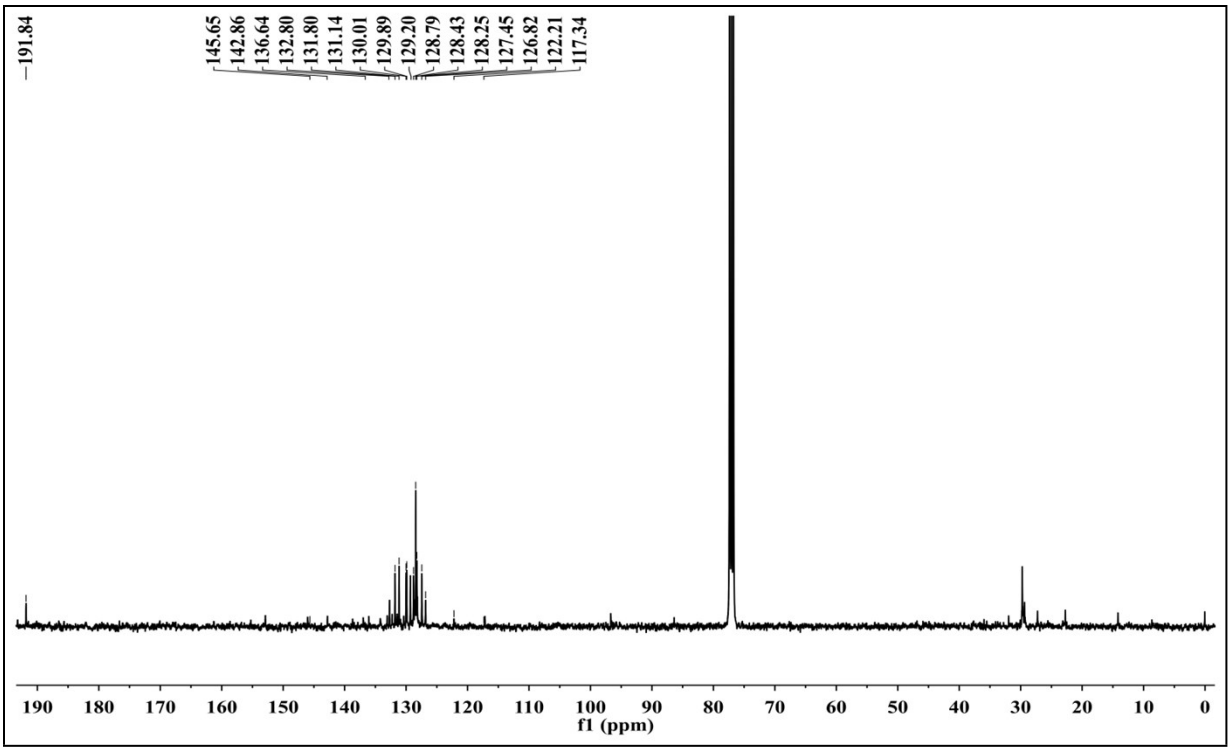

Figure S5:*[13]C NMR spectrum (400 MHz, CDCl3) of***5**.

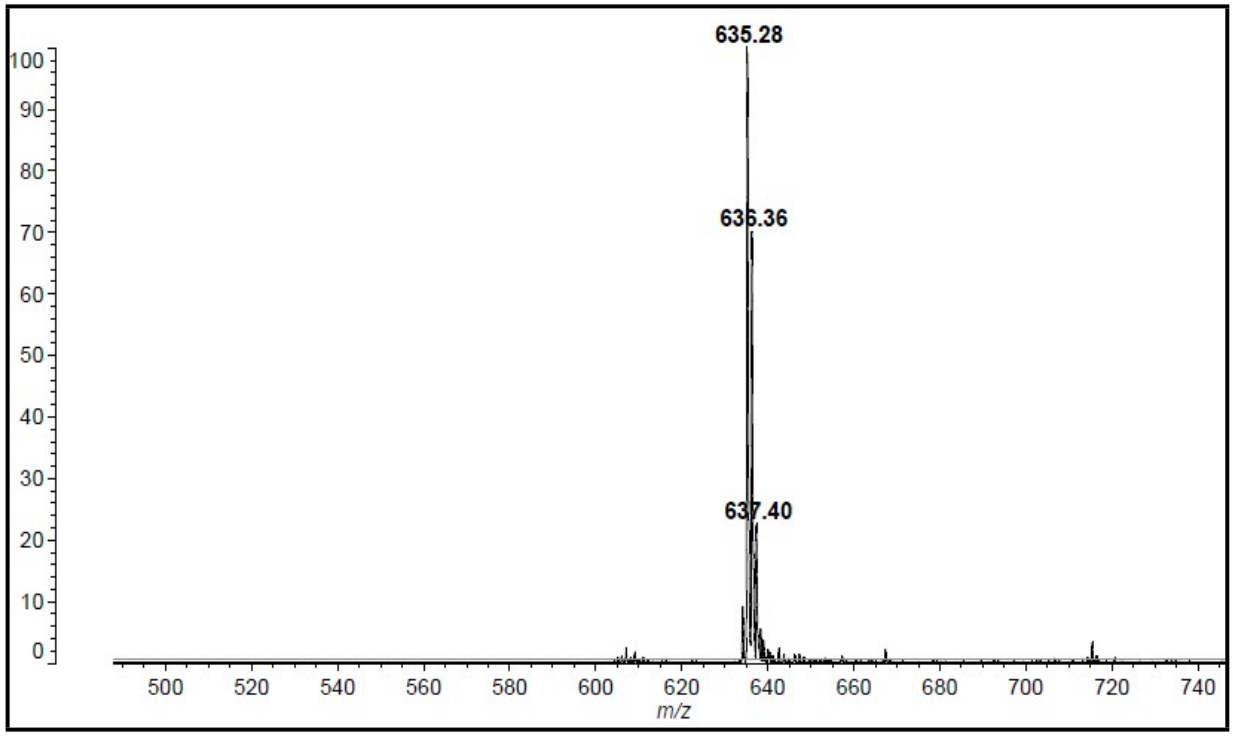

Figure S6:*MALDI-TOF of***5**.

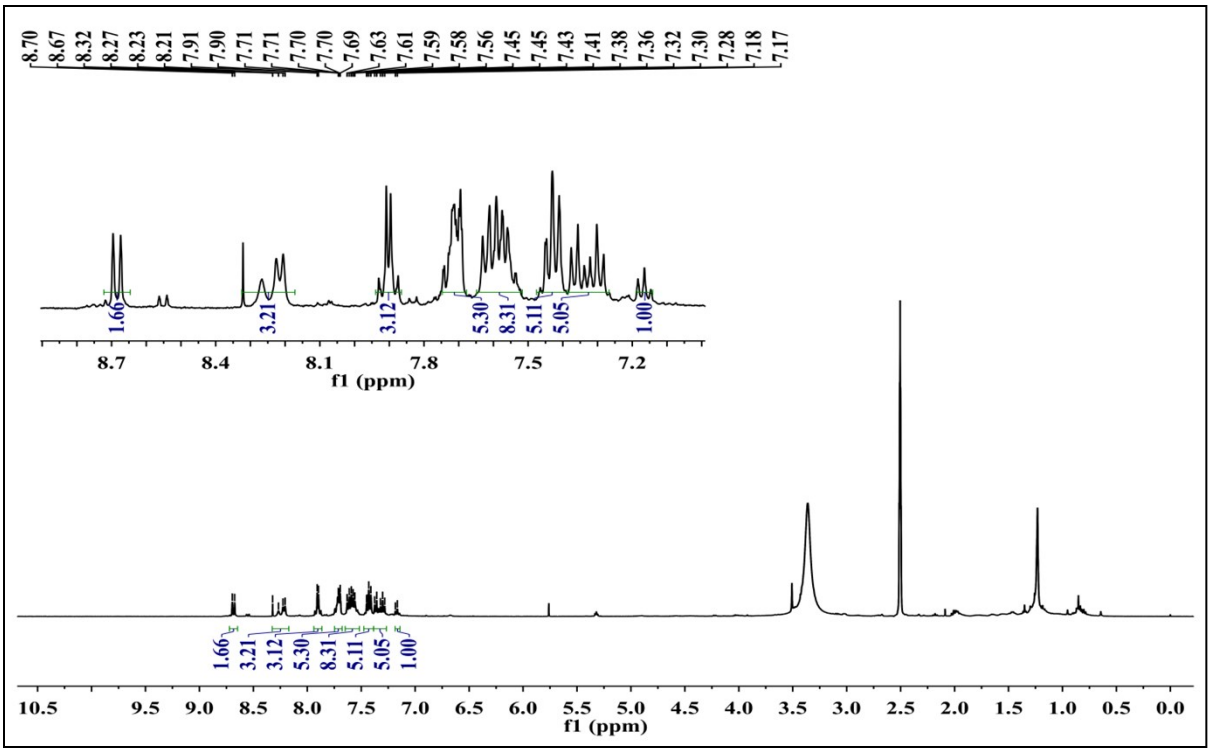

Figure S7: *^{1}H NMR spectrum (400 MHz, DMSO-d_6) of* ***LG-P1.***

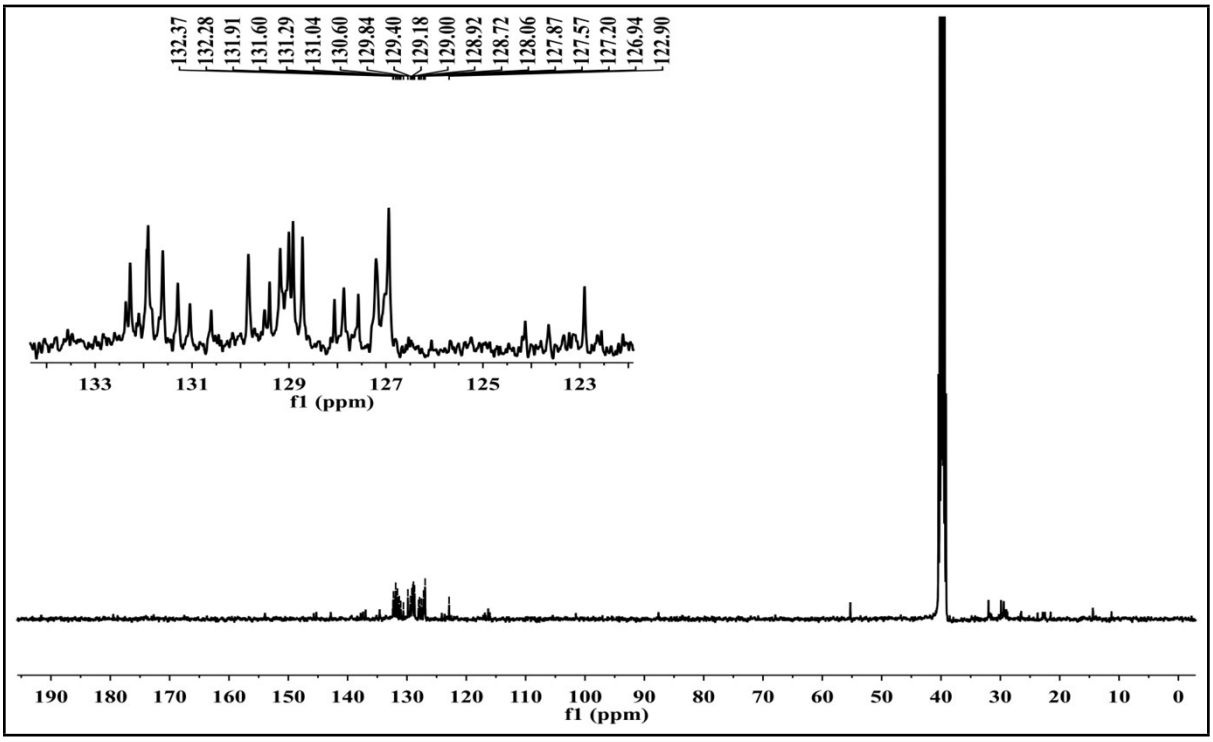

Figure S8: *^{13}C NMR spectrum (400 MHz, DMSO-d_6) of* ***LG-P1***.

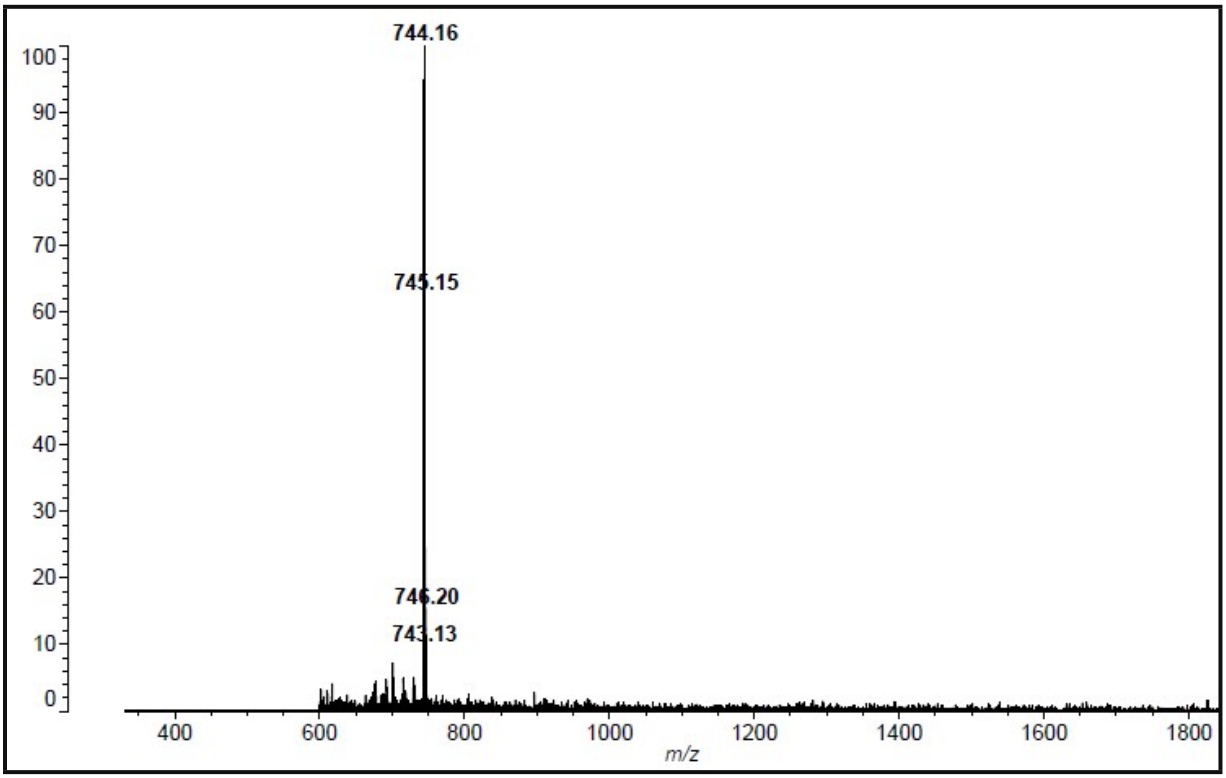

Figure S9:*MALDI-TOF of**LG-P1**.*

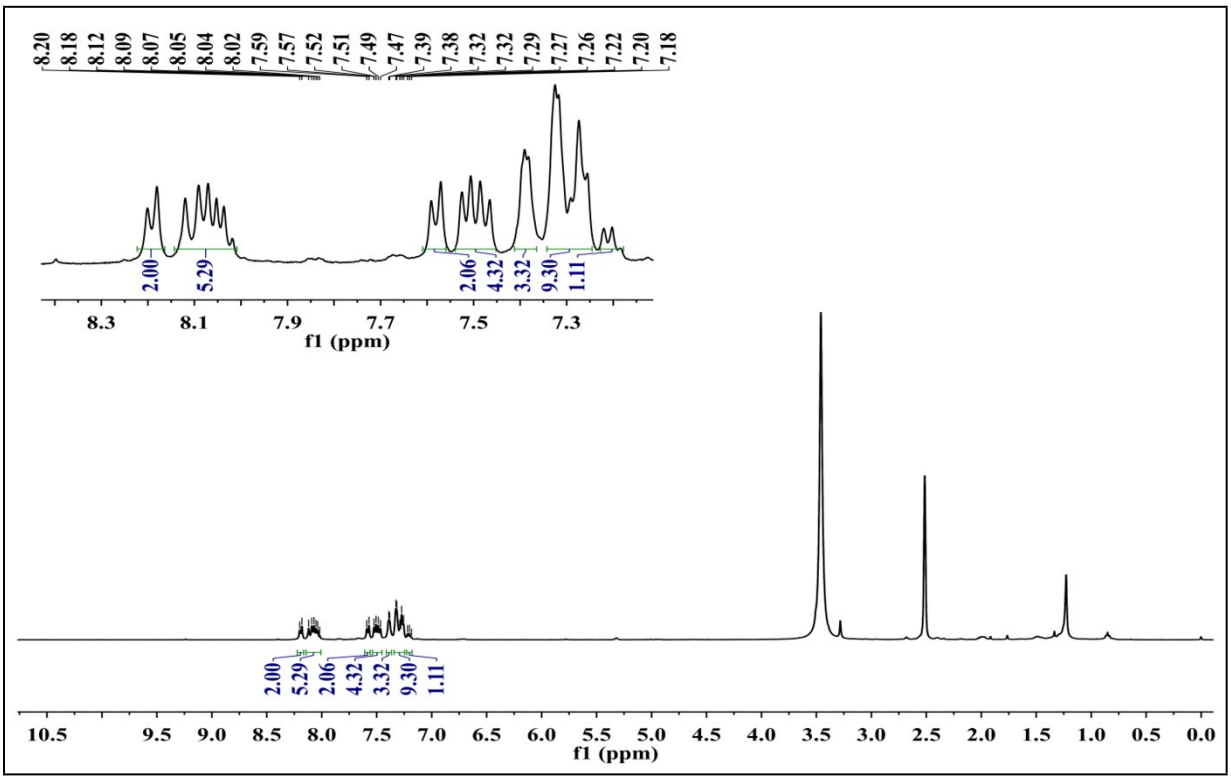

Figure S10:*^{1}H NMR spectrum (400 MHz, DMSO-d_6) of**LG-P3.***

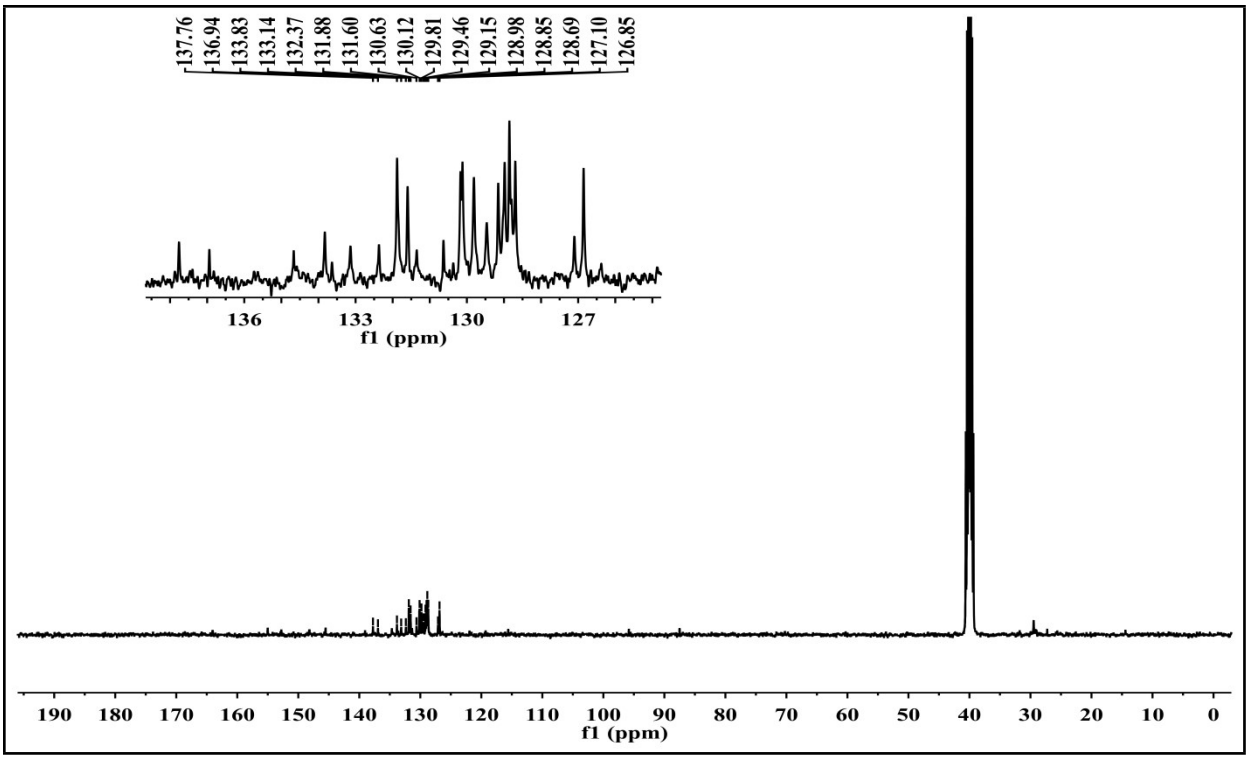

Figure S11: *^{13}C NMR spectrum (400 MHz, DMSO-d_6) of* ***LG-P3.***

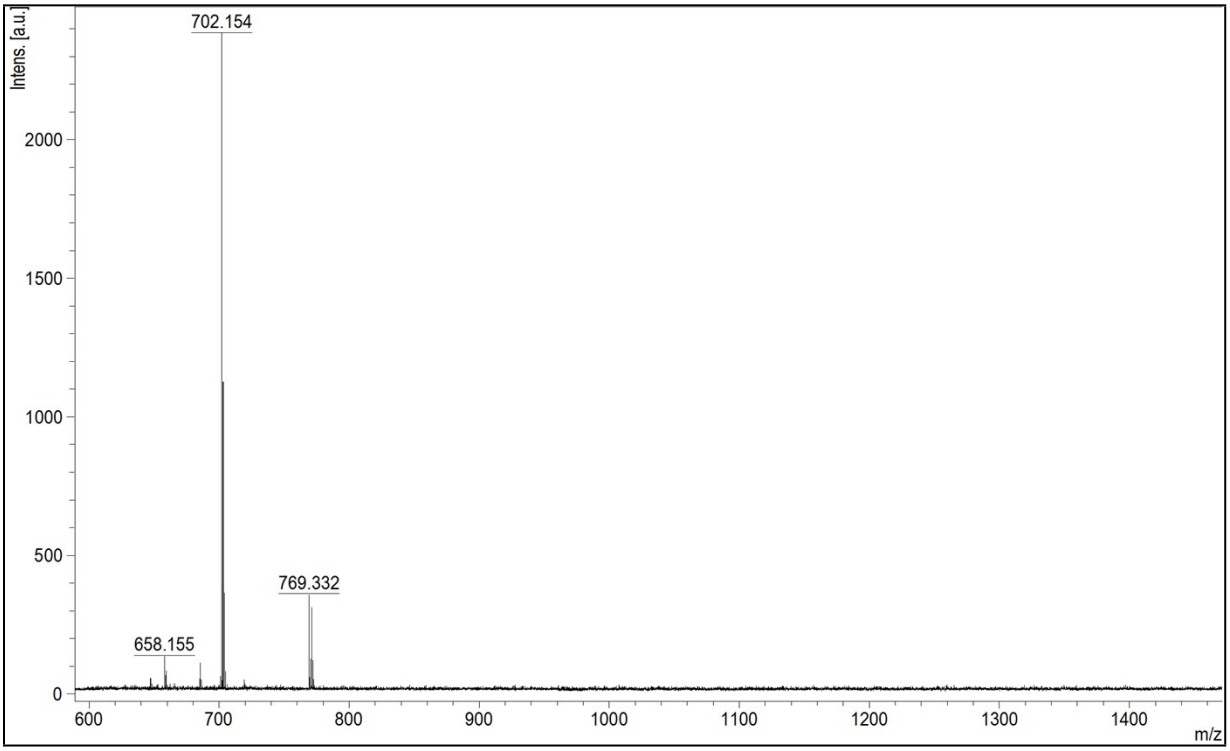

Figure S12:*MALDI-TOF of* ***LG-P3***.

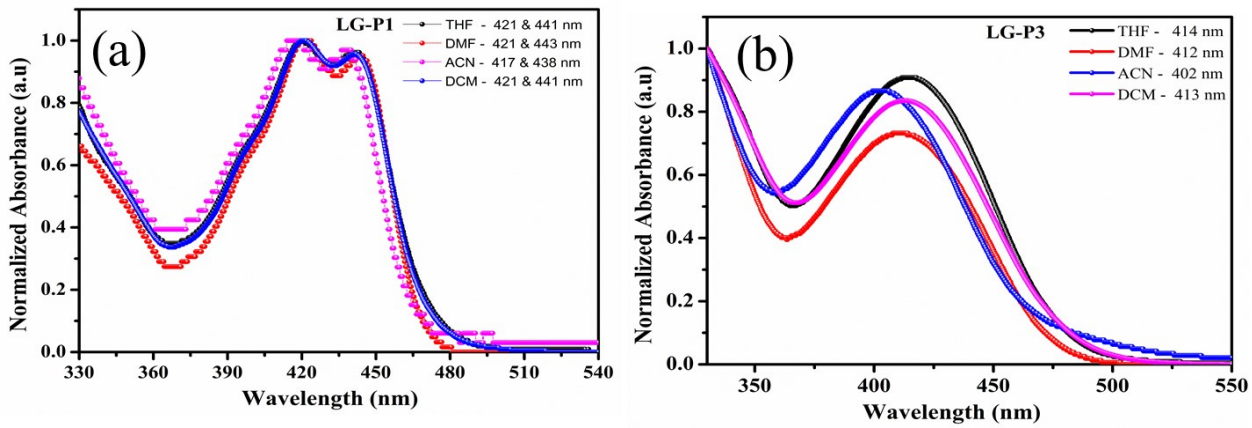

Figure S13: Absorption spectra of a) LG-P1, b) LG-P2 in THF, DMF, CAN and DCM respectively.

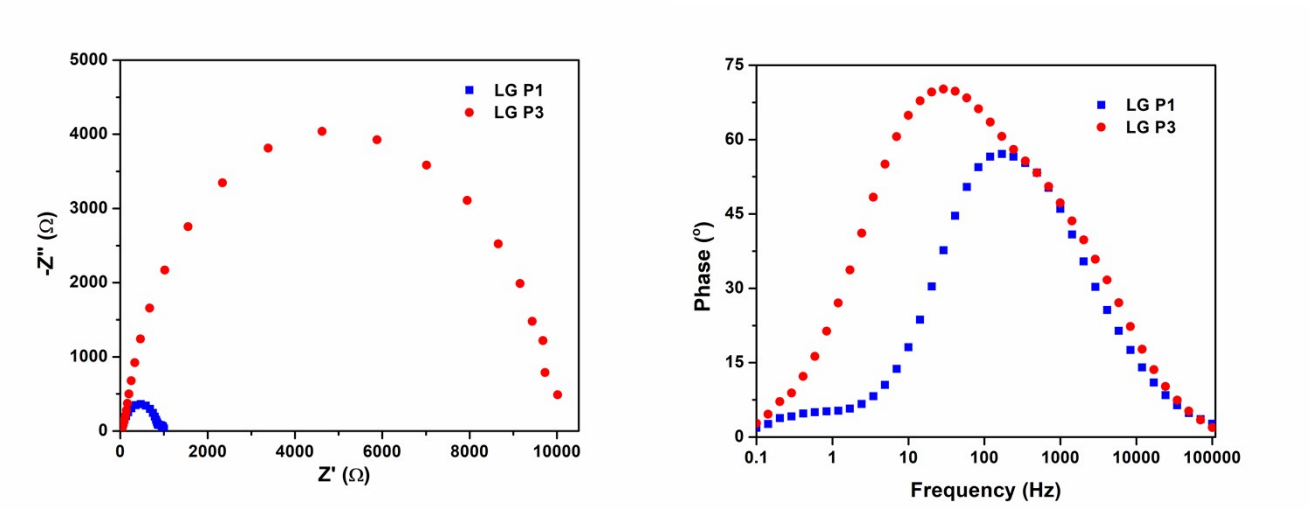

Figure S14. (a)Nyquist plot and (b) Bode plot obtained from EIS measurements under dark

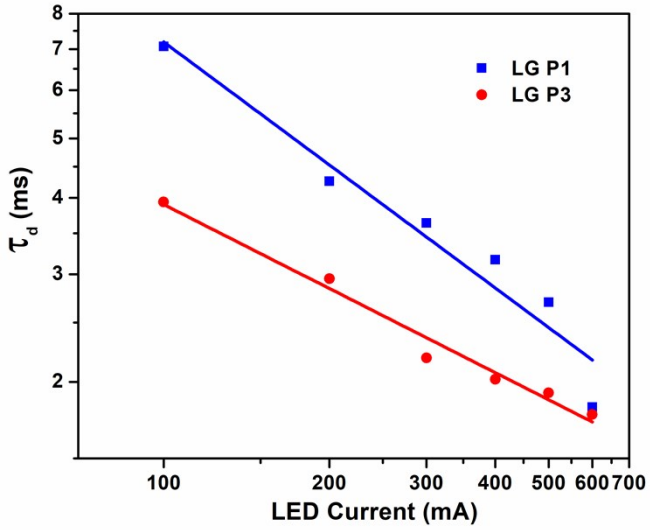

Figure S15. Transport time (τ_d) versus LED current plot obtained from transient photocurrent decay measurements

Table S1. Singlet excited state properties of dyes by B3LYP method and M06-2X function in tetrahydrofuran solvent in PCM model.

System	μg[a] (Debye)	HOMO[a] (eV)	LUMO[a] (eV)	Eg[a]	λ_{abs}[b] (nm)	Os[b]	% of major molecular orbital contribution[b]
LG-P1	8.69	5.08	2.65	2.43	373	0.74	HOMO->L+1 (89%)
					322	0.00	HOMO->LUMO (88%)
					313	0.90	H-1->L+2 (68%), HOMO->L+2 (16%)
					306	0.01	H-3->L+1 (53%)
					284	0.72	H-6->LUMO (95%)
					275	0.01	H-2->L+1 (23%), H-1->L+1 (51%)
					271	0.02	H-1->L+2 (15%), HOMO->L+2 (57%)
					264	0.05	H-12->LUMO (53%), H-9->LUMO (30%)
					260	0.40	H-1->L+3 (69%)H-2->L+2 (4%)
					253	0.01	H-11->L+2 (12%), H-10->L+2 (12%)
LG-P3	7.61	5.31	2.98	2.33	433	1.84	H-1->LUMO (36%), HOMO->LUMO (52%)
					330	0.11	H-2->LUMO (11%), H-1->LUMO (28%), HOMO->LUMO (10%), HOMO->L+1 (17%)
					321	0.59	H-1->L+1 (35%), HOMO->LUMO (12%), HOMO->L+1 (14%), HOMO->L+2 (17%)
					292	0.59	HOMO->LUMO (18%), HOMO->L+2 (50%)
					284	0.02	H-10->LUMO (66%)
					281	0.19	H-11->LUMO (60%)
					268	0.44	H-1->L+3 (13%), HOMO->L+3 (65%)
					261	0.04	H-6->LUMO (10%) , H-2->L+1 (13%), HOMO->L+1 (25%)
					260	0.01	H-6->LUMO (10%) , HOMO->L+6 (10%), HOMO->L+9 (11%)
					252	0.01	H-1->L+2 (38%)

[a]Theoretical absorbance in nm, [b]Oscillator strength, and [c]Excited state energy in eV.

Table S2. Photovoltaic parameters of **LG-P1** and **LG-P3** sensitizers under 0.5 sun and 0.1 sun conditions

Dye	Illumination intensity (mW/cm^2)	V_{OC} (V)	J_{SC} ($mA\ cm^{-2}$)	*FF* (%)	PCE (%)
LG-P1	**50**	0.35	0.74	36.6	0.19
	10	0.19	0.23	26.7	0.12
LG-P3	**50**	0.71	1.83	70.2	1.84
	10	0.66	0.39	64.0	1.66