Supporting Information

Role of π-spacer in Regulating the Photovoltaic Performance of Copper Electrolyte Dye-sensitized Solar Cells Using Triphenylimidazole Dyes

Palivela Siva Gangadhar,[a,c‡] *Anooja Jagadeesh,*[b,c‡] *Manne Naga Rajesh,*[a,c] *Andrew Simon George,*[b,c] *Seelam Prasanthkumar,*[a,c] *Suraj Soman,*[b,c]* *Lingamallu Giribabu*[a,c]*

[a]Polymer and Functional Materials Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India. E-mail:giribabu@iict.res.in

[b]Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Thiruvananthapuram 695019, India.E-mail:suraj@niist.res.in

[c]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, New Delhi 201002, India.

[‡]These authors contributed equally towards the completion of this work

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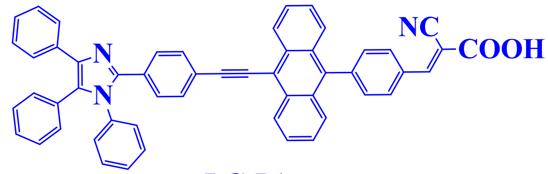
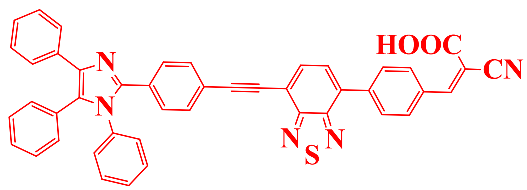


LG-P1



LG-P3

Figure S1. Molecular structures of LG-P1 and LG-P3 sensitizers.

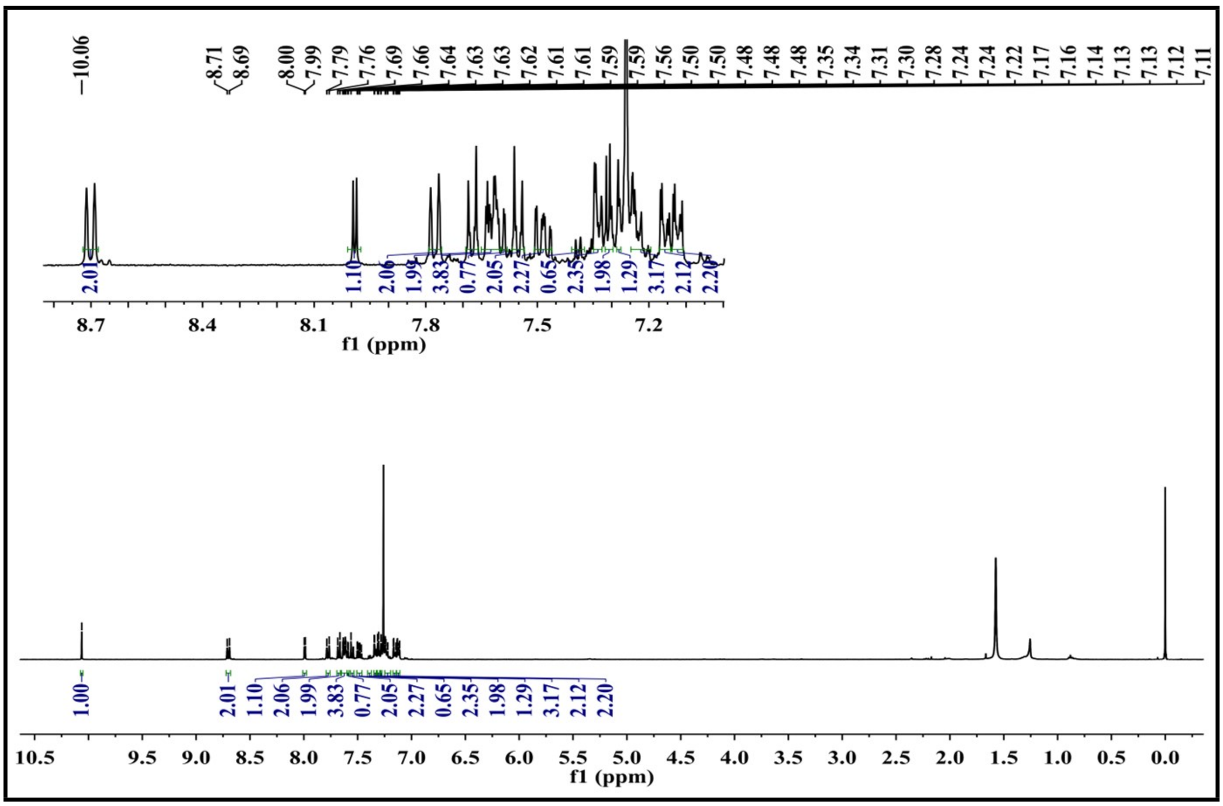


Figure S2: [1]*H NMR spectrum (400 MHz, CDCl3) of* ***4*****.**

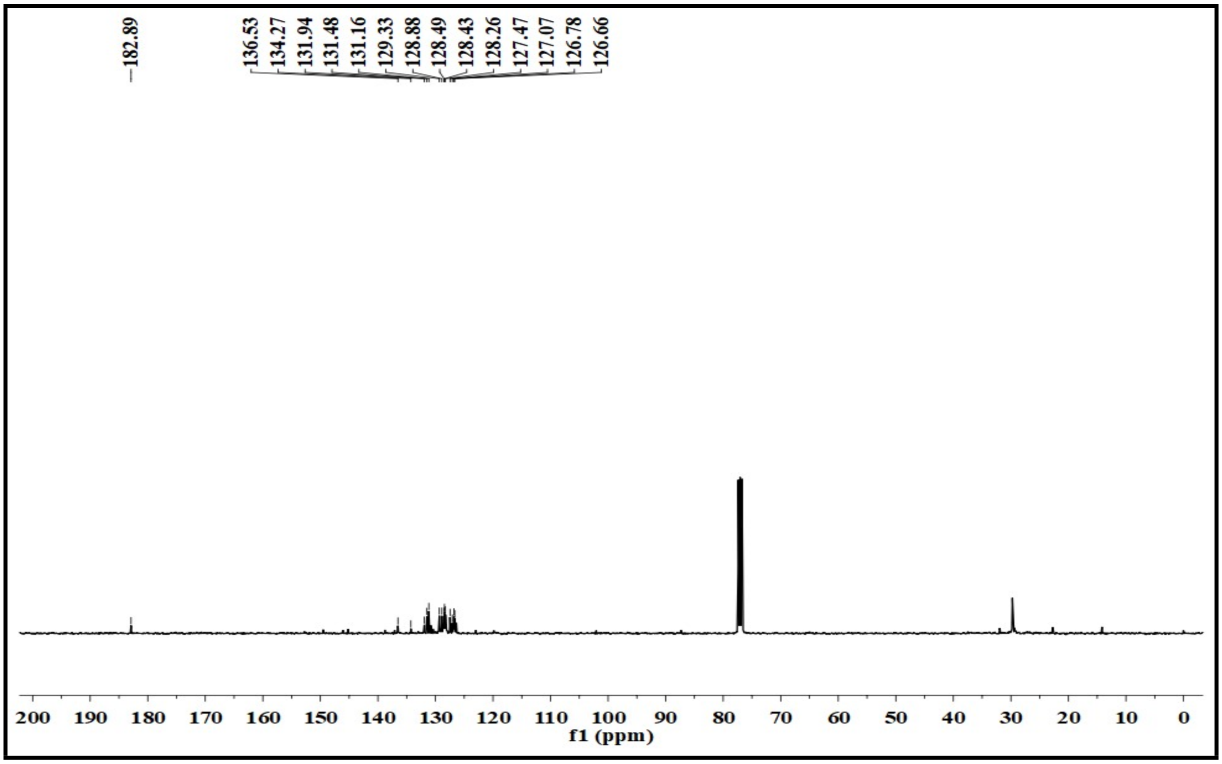


Figure S3: *[13]C NMR spectrum (400 MHz, CDCl3) of **4***.

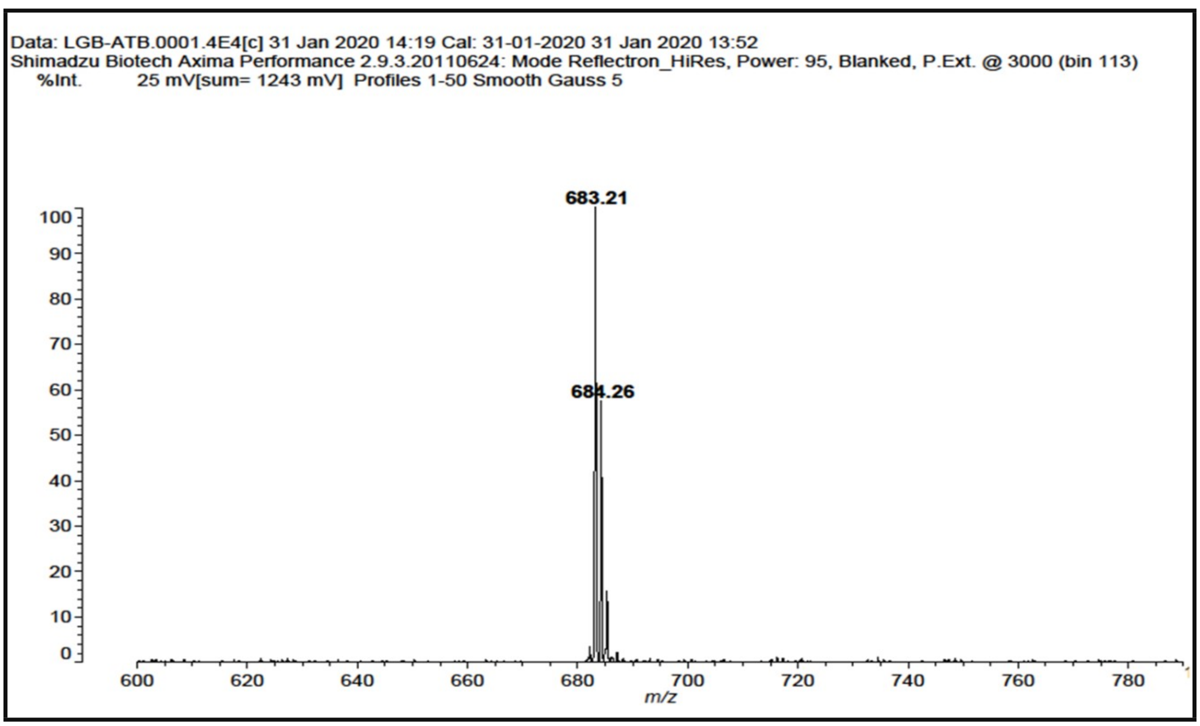


Figure S4: *MALDI-TOF of **4***.

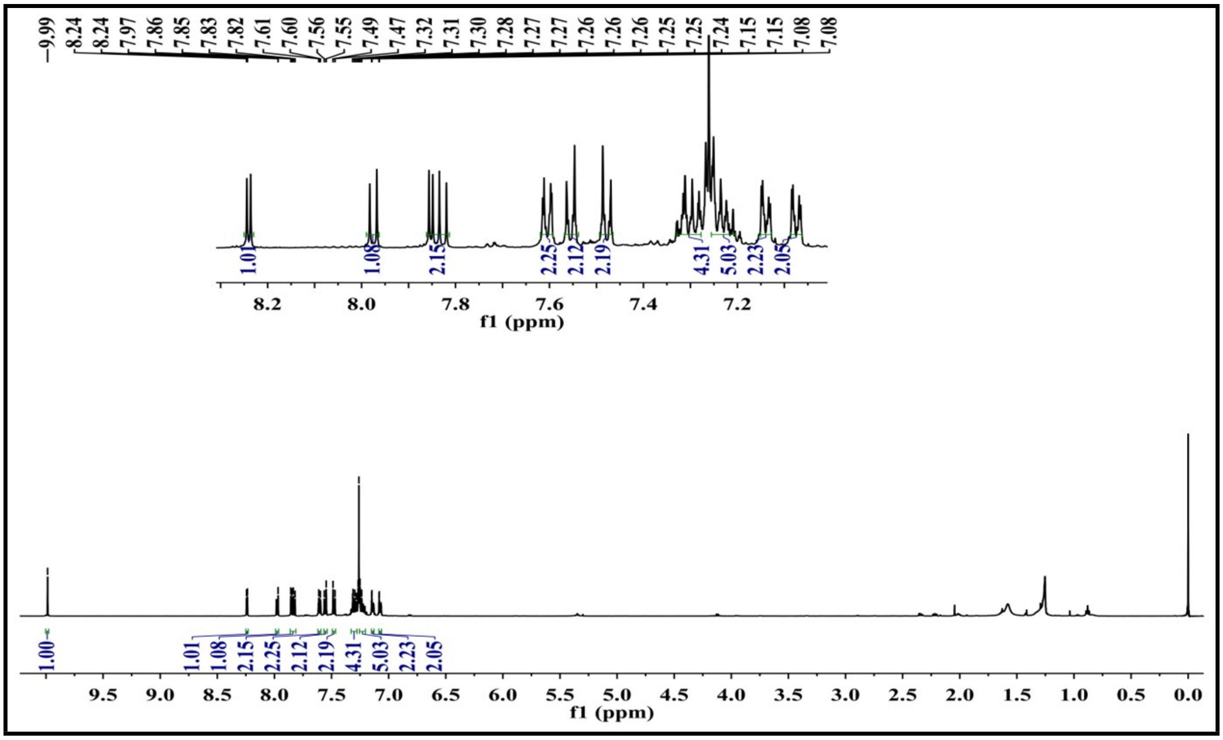


Figure S5: *[1]H NMR spectrum (400 MHz, CDCl3) of* ***5.***

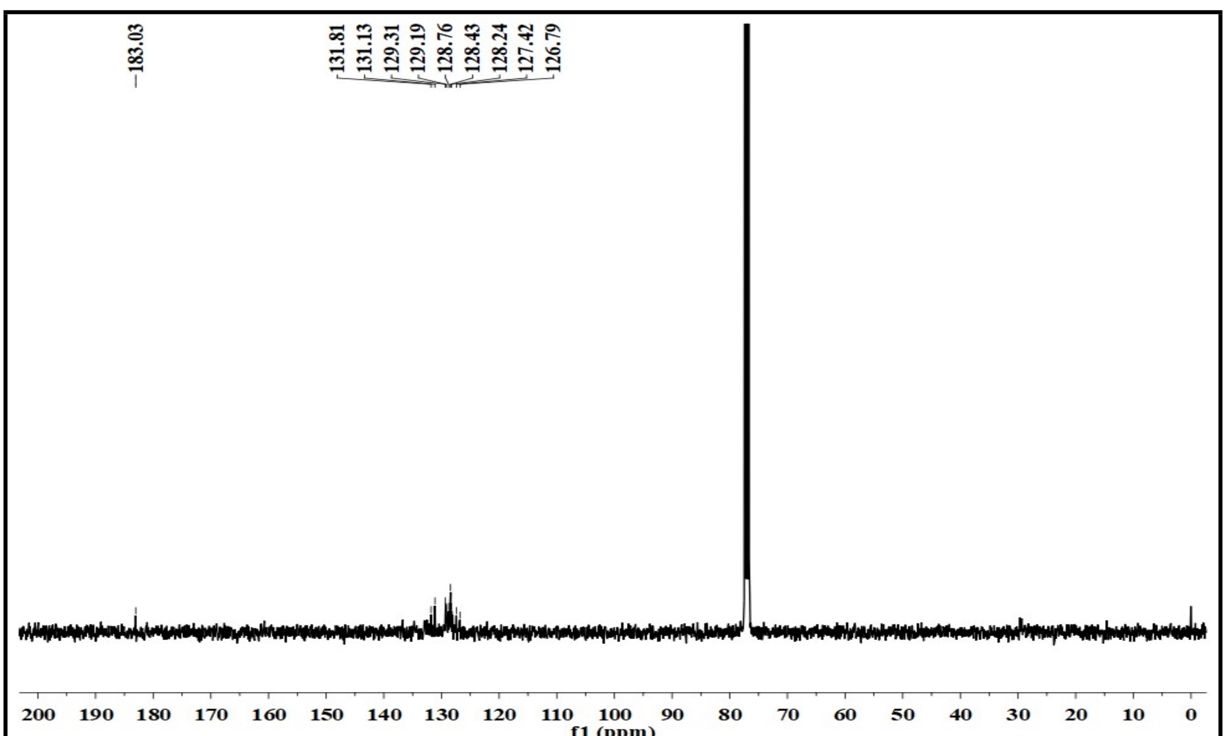


Figure S6: *[13]C NMR spectrum (400 MHz, CDCl3) of* ***5***.

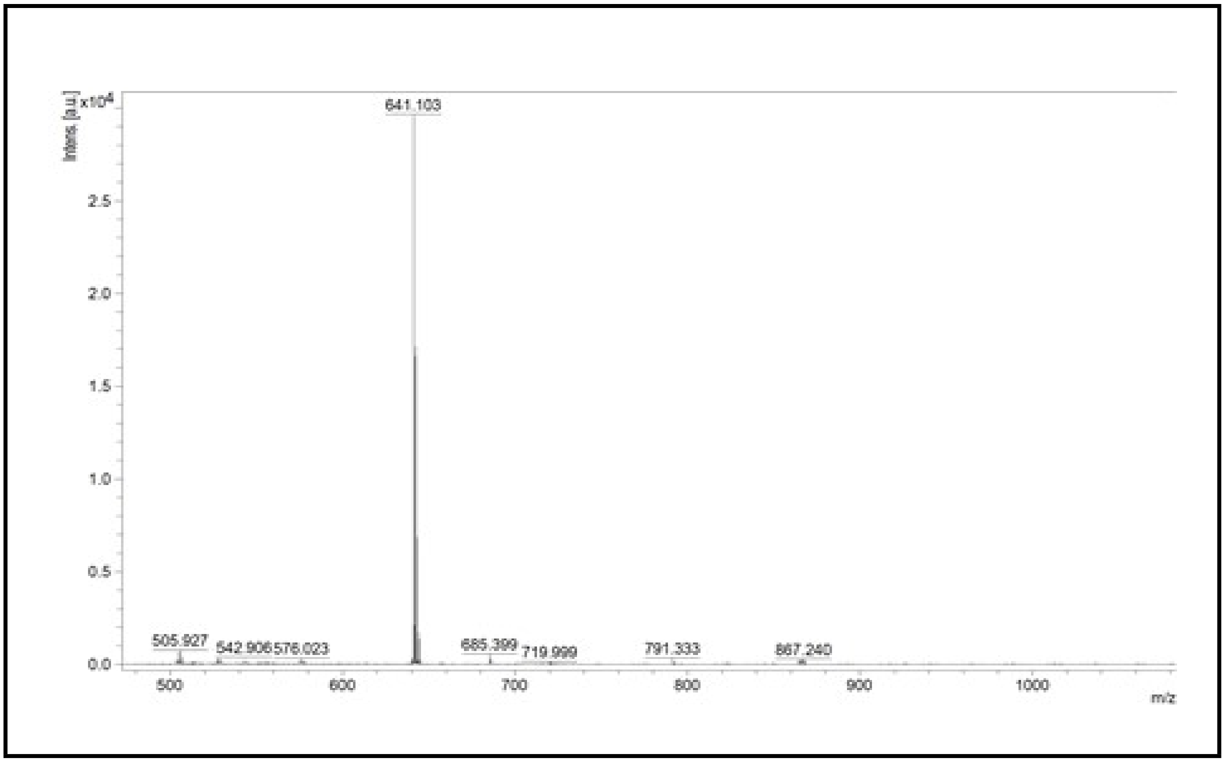


Figure S7: *MALDI-TOF of **5**.*

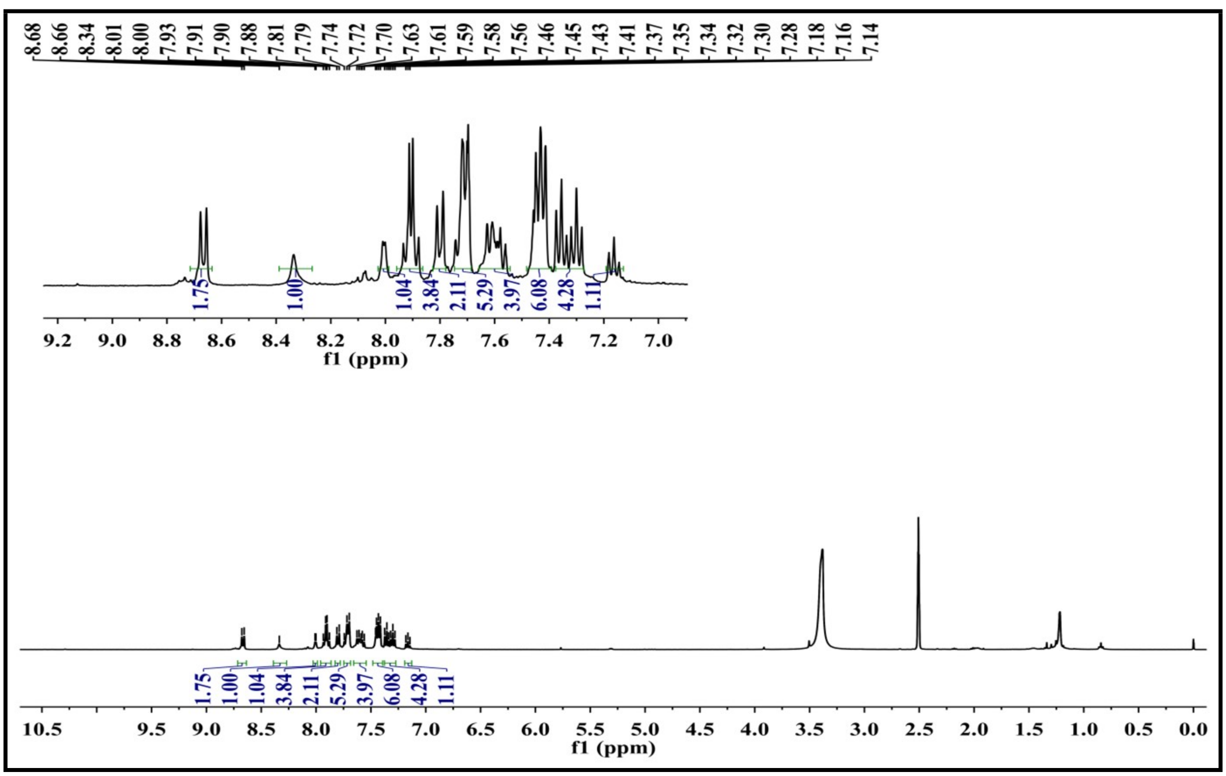


Figure S8: *[1]H NMR spectrum (400 MHz,* DMSO-d_6*) of **LG-P2.***

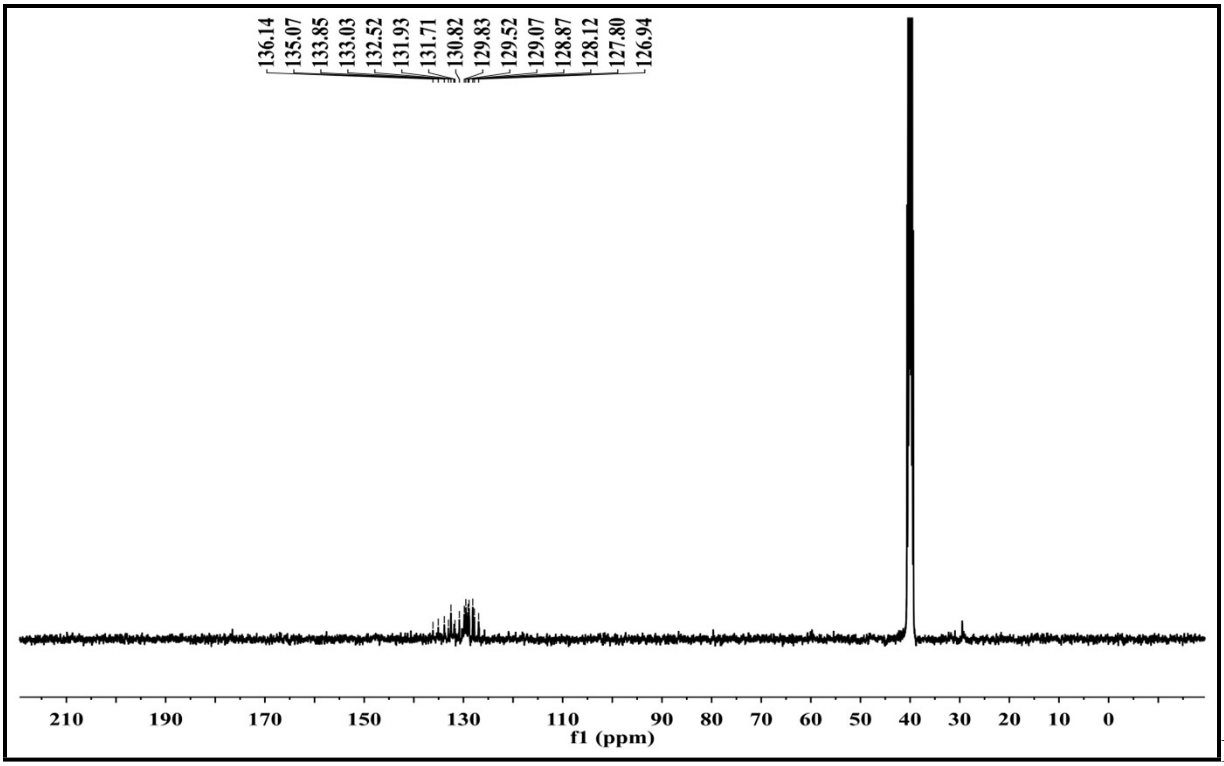


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Figure S9: *^{13}C NMR spectrum (400 MHz, DMSO-d_6) of* ***LG-P2***.

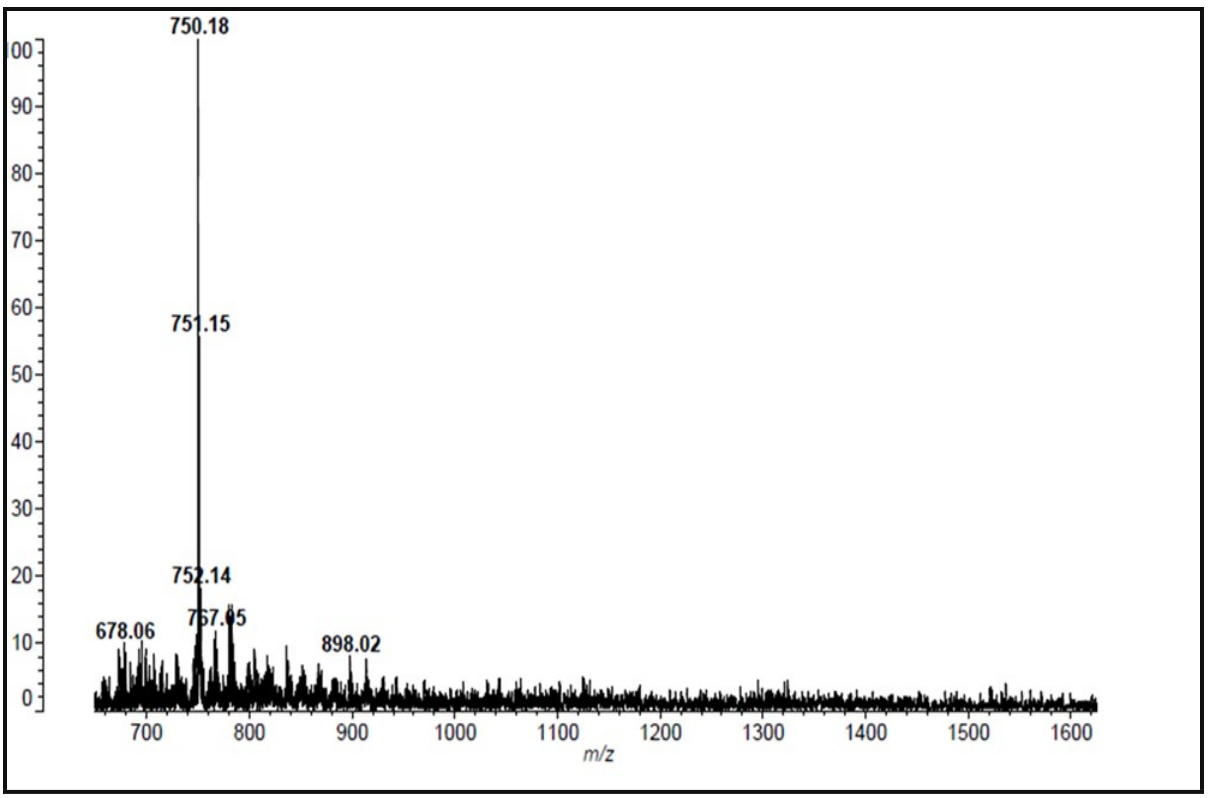

Figure S10: *MALDI-TOF of* ***LG-P2***.

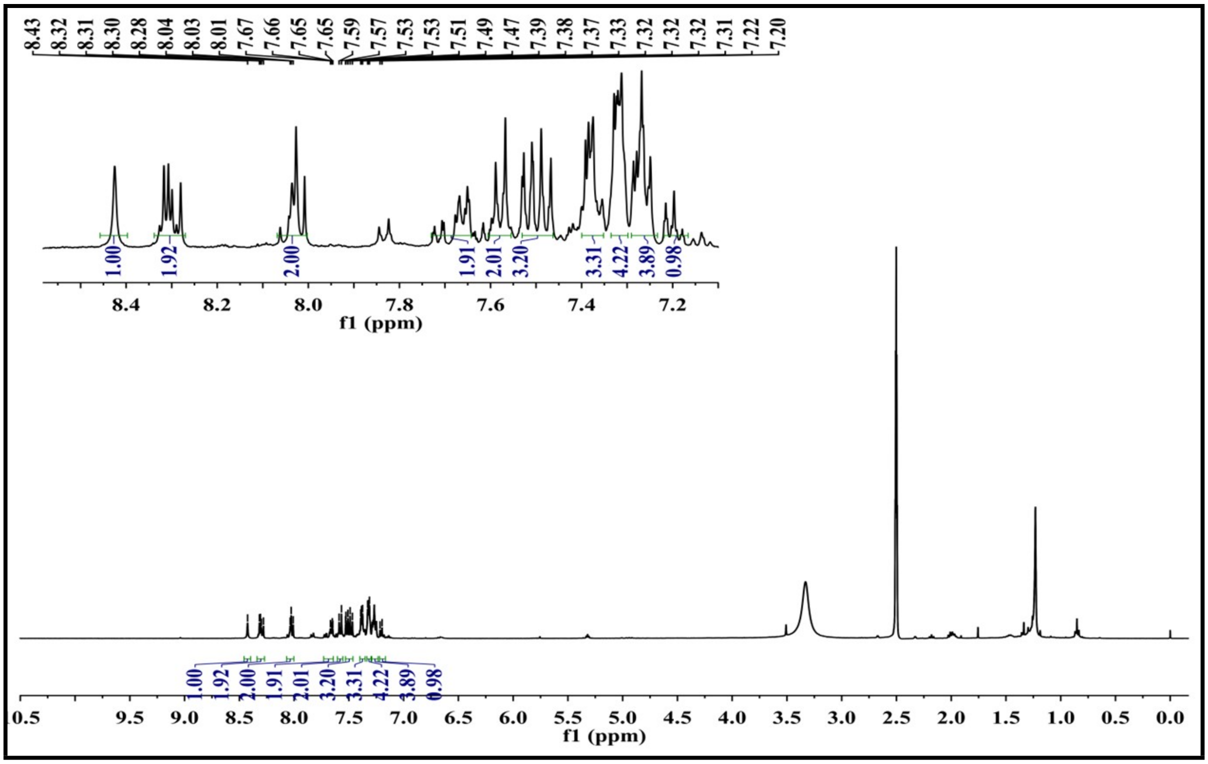

Figure S11: *^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **LG-P4.***

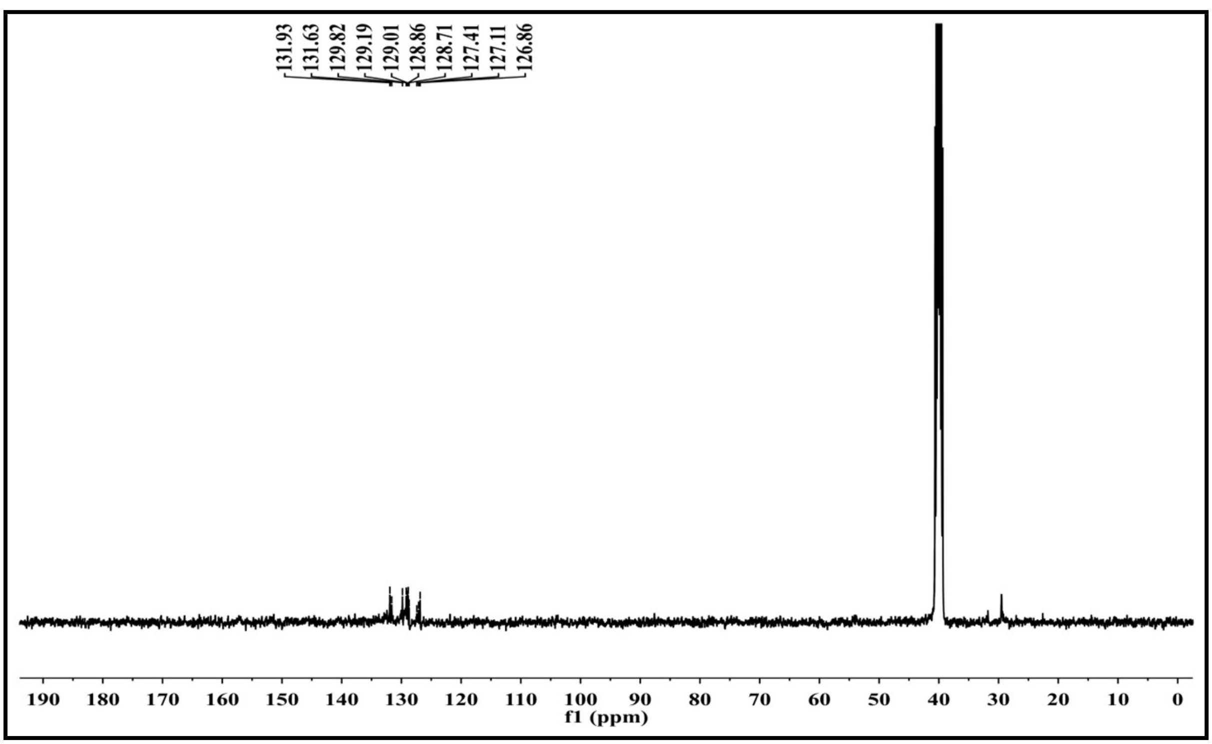

Figure S12: *^{13}C NMR spectrum (400 MHz, DMSO-d_6) of **LG-P4.***

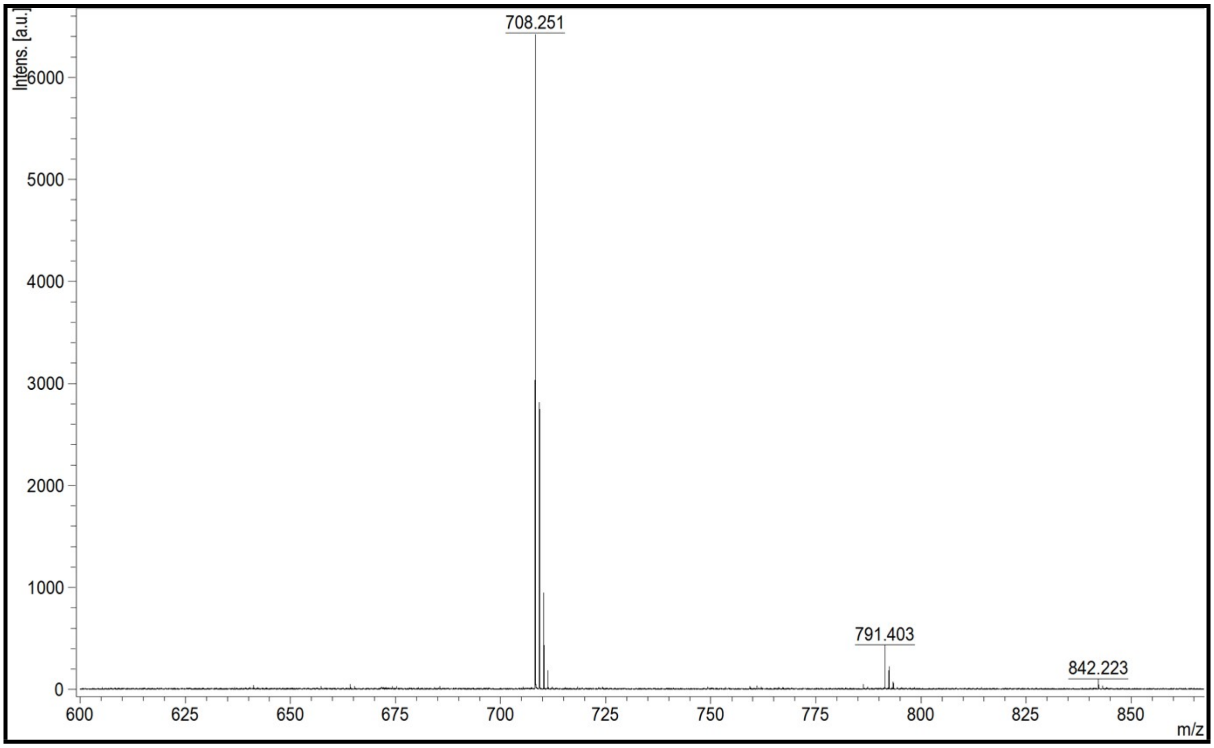

Figure S13: *MALDI-TOF of* ***LG-P4****.*

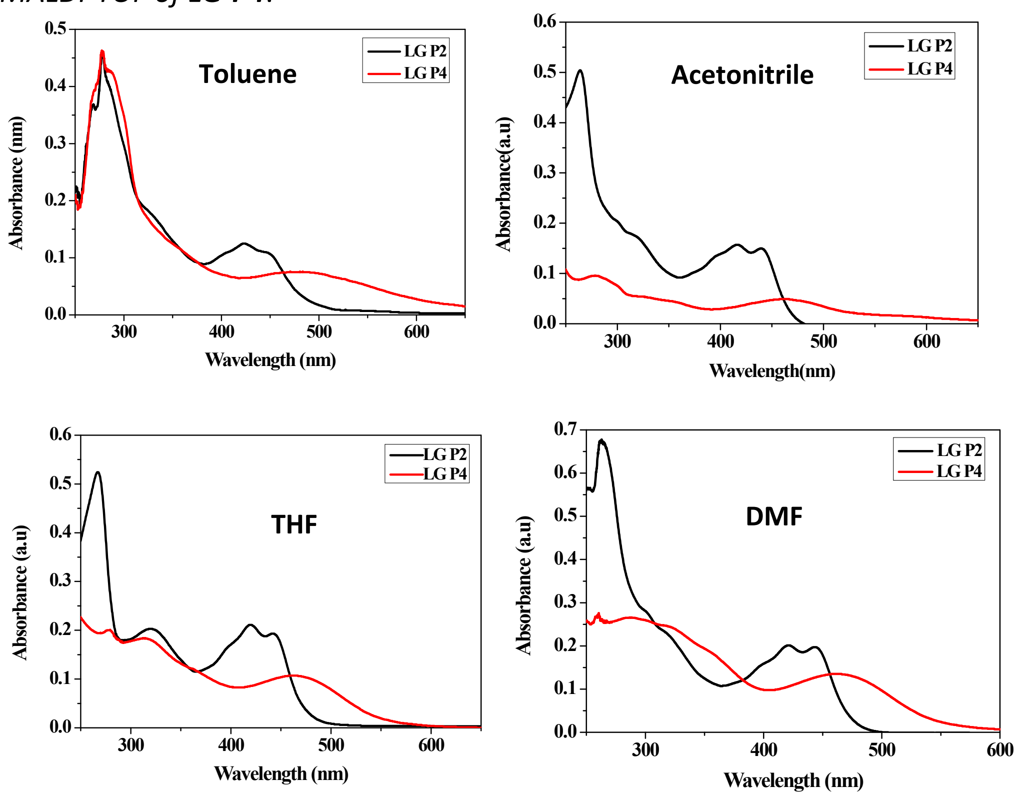

Figure S14: *Absorption spectra of* ***LG-P2*** *and* ***LG-P4****.*

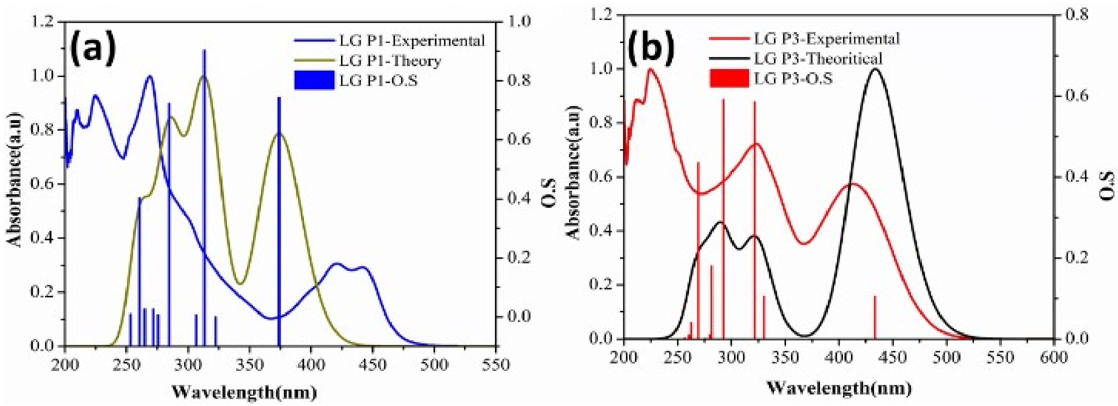

Figure S15: *Absorption spectra of LG-P1 and LG-P3 in DCM*

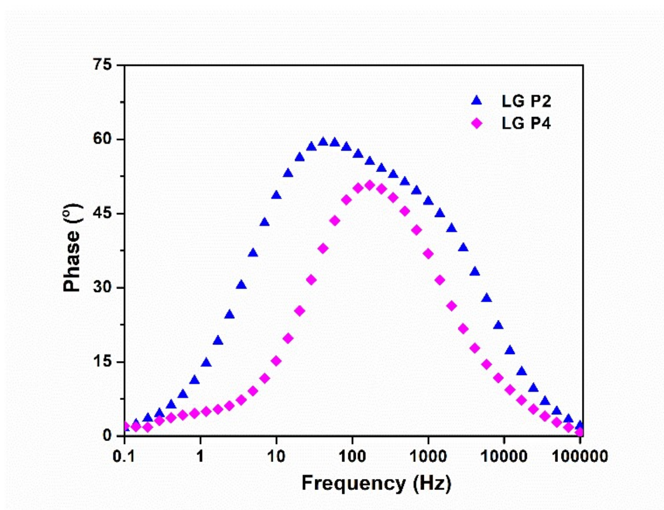

Figure S16. *Bode plot obtained from EIS measurement in dark (at 0.6V).*

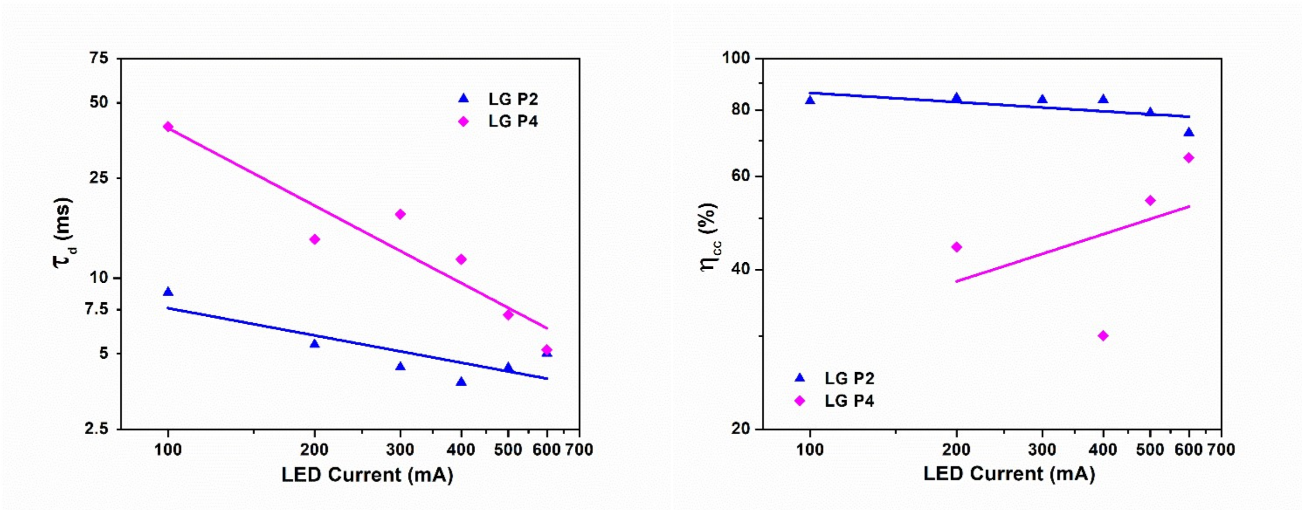

Figure S17. *(a) Transport time and (b) charge collection efficiency obtained from transient photo-voltage and photocurrent decay measurements.*

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-P2	8.49	5.19	2.67	2.52	432	1.39	HOMO->L+1 (78%)
					376	0.00	H-1->LUMO (14%), HOMO->LUMO (73%)
					330	0.57	H-2->LUMO (92%)
					321	0.76	H-3->L+1 (11%), H-1->L+1 (47%), HOMO->L+2 (23%)
					316	0.02	H-5->L+1 (54%), HOMO->L+4 (28%)
					281	0.13	H-1->L+1 (14%), HOMO->L+2 (63%)
					273	0.00	H-2->L+1 (83%)
					271	0.17	H-3->L+1 (13%), H-1->L+2 (26%), H-1->L+3 (18%), HOMO->L+3 (19%)
					270	0.05	H-13->LUMO (54%), H-9->LUMO (32%)
					269	0.00	H-11->L+2 (12%), H-10->L+2 (12%)
LG-P4	11.95	5.34	3.20	2.14	486	1.95	H-1->LUMO (36%), HOMO->LUMO (57%)
					360	0.04	H-2->LUMO (17%), H-1->LUMO (23%), H-1->L+1 (12%), HOMO->LUMO (11%), HOMO->L+1 (24%)
					340	0.27	H-1->LUMO (20%), H-1->L+1 (32%), HOMO->LUMO (15%), HOMO->L+1 (17%)
					299	0.70	H-10->LUMO (11%), HOMO->L+2 (60%)
					297	0.01	H-2->LUMO (41%)
					291	0.15	H-10->LUMO (60%)
					285	0.16	H-10->LUMO (60%)
					282	0.00	H-12->LUMO (63%), H-12->L+1 (12%)
					269	0.32	H-1->L+3 (14%), HOMO->L+3 (54%)
					266	0.06	H-2->L+1 (17%), H-1->L+1 (18%), HOMO->L+1 (27%)

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

Table S2. Comparison of J-V parameters obtained at one sun condition for the best performing DSSCs based on LG-P1 and LG-P3 dyes (previous work) with **LG-P2** and **LG-P4** dyes (current work)

	Dye	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
Previous work	**LG-P1**	0.47	1.52	41.1	0.29
	LG-P3	0.73	3.81	70.5	1.96
This work	**LG-P2**	0.74	2.71	70.5	1.41
	LG-P4	0.50	1.82	47.3	0.43

Table S3. Photovoltaic data of LG-P2 and LG-P4 based device under 0.1 and 0.5 sun conditions.

Illumination intensity (mW/cm^2)	Dye	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF (%)	Efficiency (%)
50	**LG-P2**	0.69	1.30	74.2	1.33
	LG-P4	0.44	0.89	40.1	0.31
10	**LG-P2**	0.63	0.31	71.9	1.39
	LG-P4	0.24	0.24	33.8	0.20

Table S4. Photovoltaic data of LG-P2 and LG-P4 based device under 1000 lux daylight LED illumination.

Dye	V_{oc} (V)	J_{sc} (μAcm^{-2})	FF (%)	Efficiency (%)
LG-P2	0.50	93.1	51.6	7.46
LG-P4	0.12	87.3	28.7	0.97