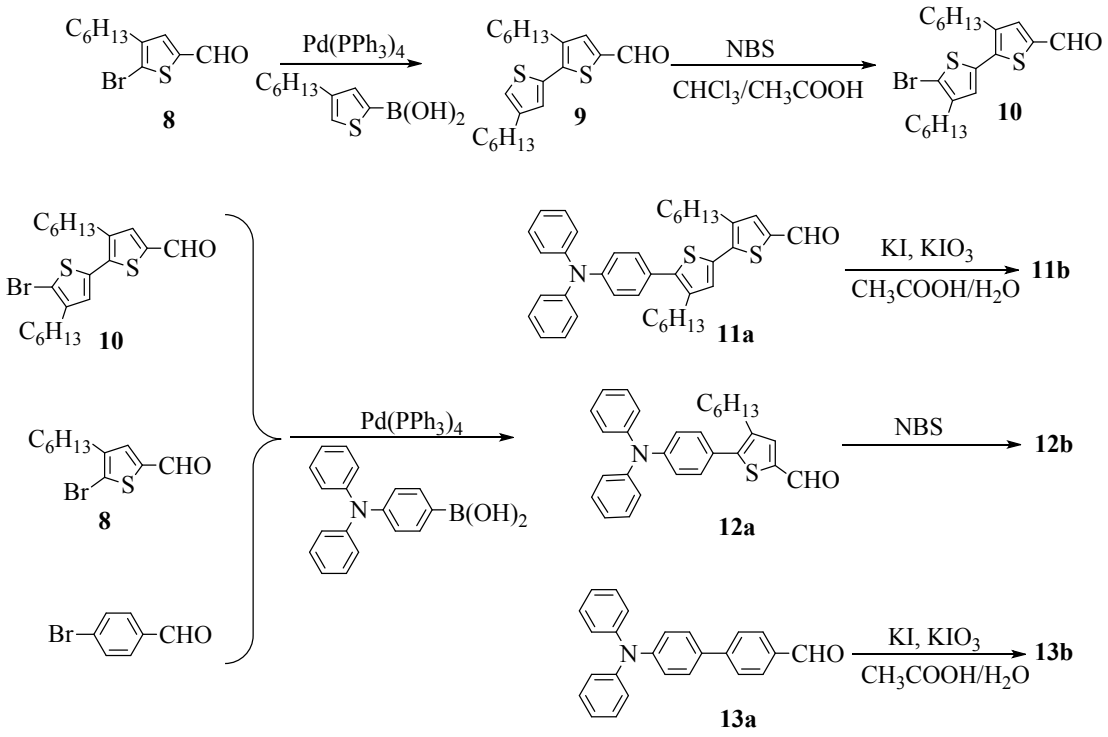
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

For

Molecular engineering of starburst triarylamine donor with selenophene containing π-linker for dye-sensitized solar cells with high open-circuit voltage



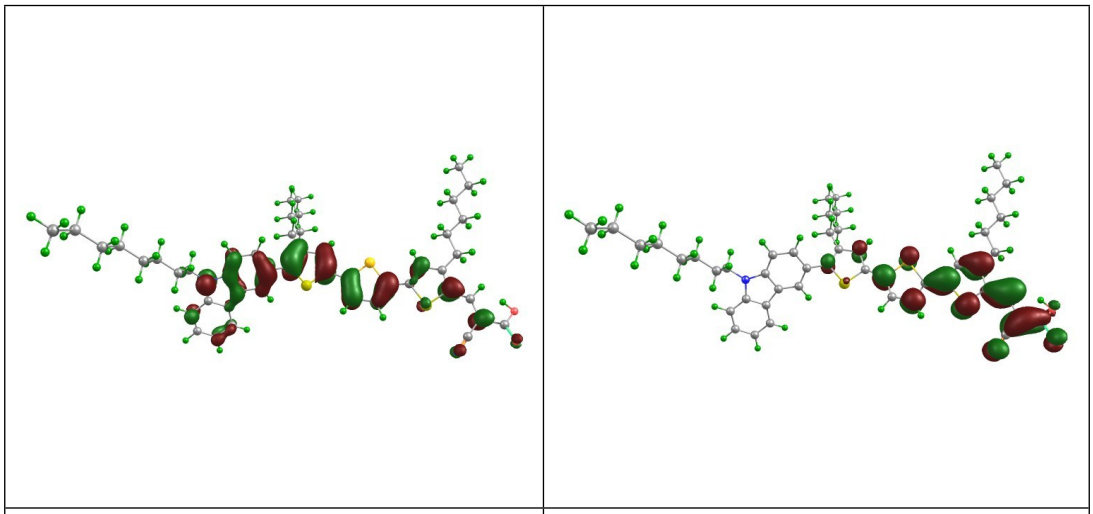
Scheme S1 Synthetic routes of **11b**−**13b**.

Table S1 Calculated energy values (in eV) of HOMO and LUMO for all the dyes

	HOMO	LUMO
7a	–5.41	–2.84
7b	–5.11	–2.86
7c	–5.35	–2.84
7d	–5.07	–2.83
11d	–5.10	–2.73
12d	–5.18	–2.61
13d	–5.14	–2.55

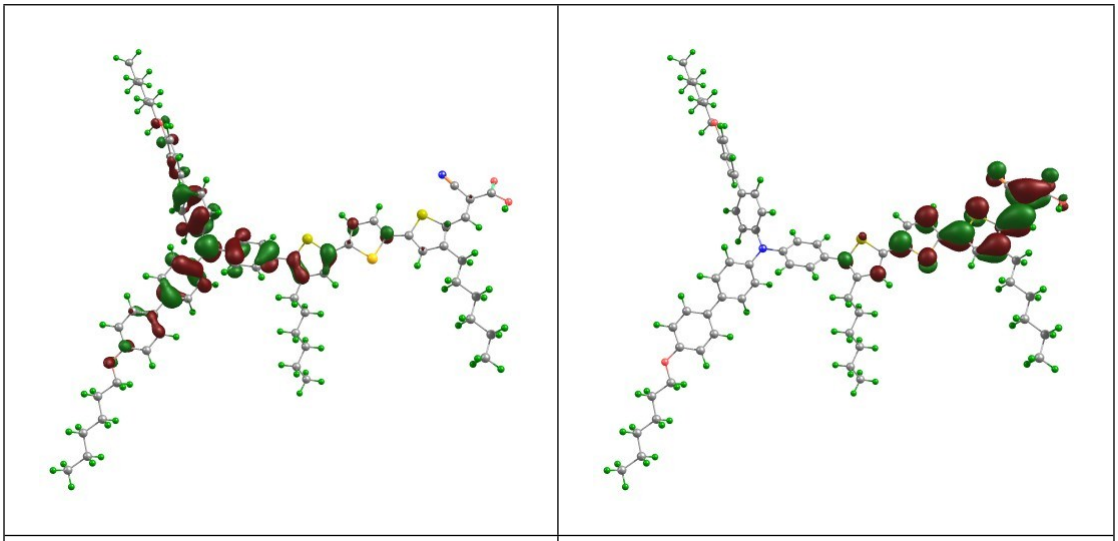
Table S2 Absorption transitions calculated by the TD-DFT method

	state	transition	contributuion (%)	E (nm)	oscillator strength
7a	S1	HOMO→LUMO	93%	574.86	1.3404
7b	S1	HOMO→LUMO	97%	640.62	0.8164
7c	S1	HOMO→LUMO	96%	583.30	1.1880
7d	S1	HOMO→LUMO	96%	641.08	0.7104
11d	S1	HOMO→LUMO	98%	611.64	0.6092
12d	S1	HOMO→LUMO	98%	574.41	0.5524
13d	S1	HOMO→LUMO	98%	560.03	0.6013



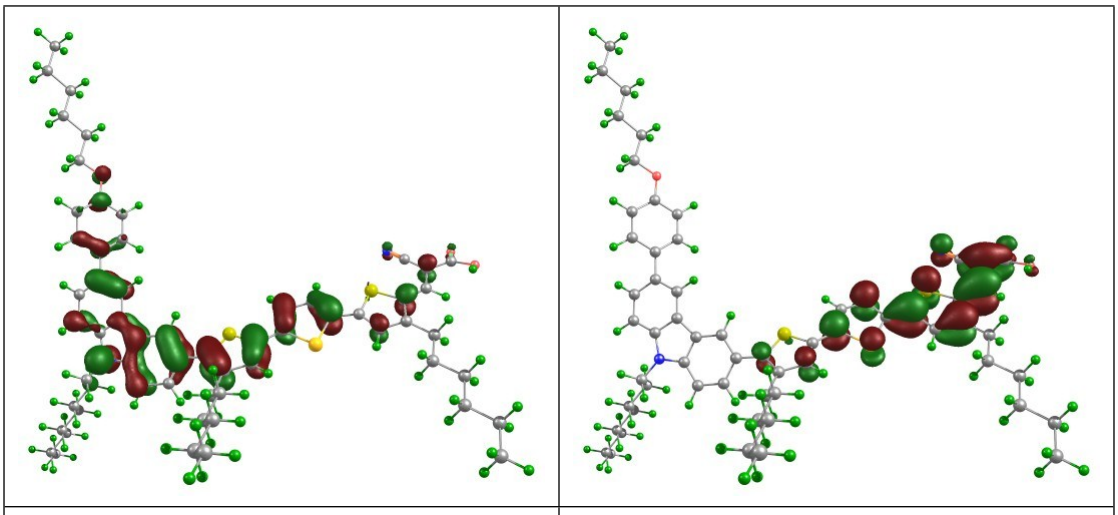
HOMO LUMO

Fig. S1 Contour plots of selected frontier orbitals of **7a**.



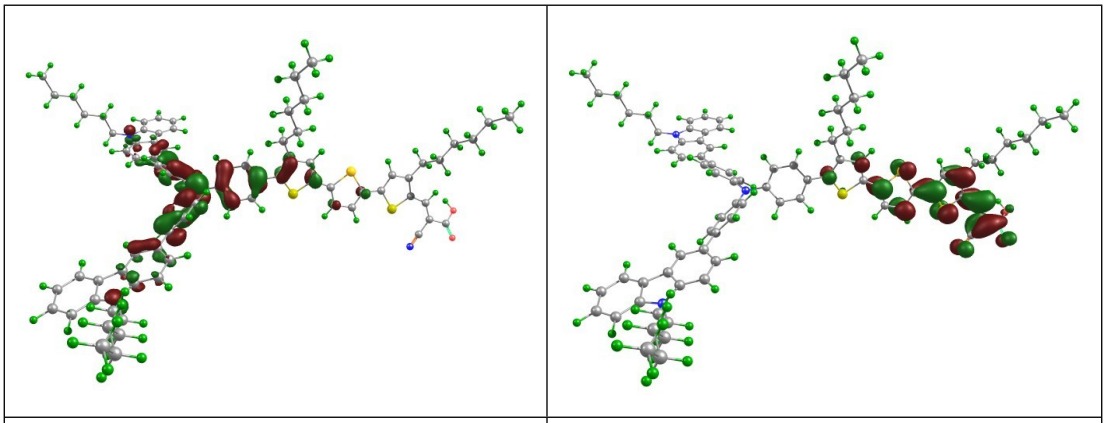
HOMO	LUMO

Fig. S2 Contour plots of selected frontier orbitals of **7b**.



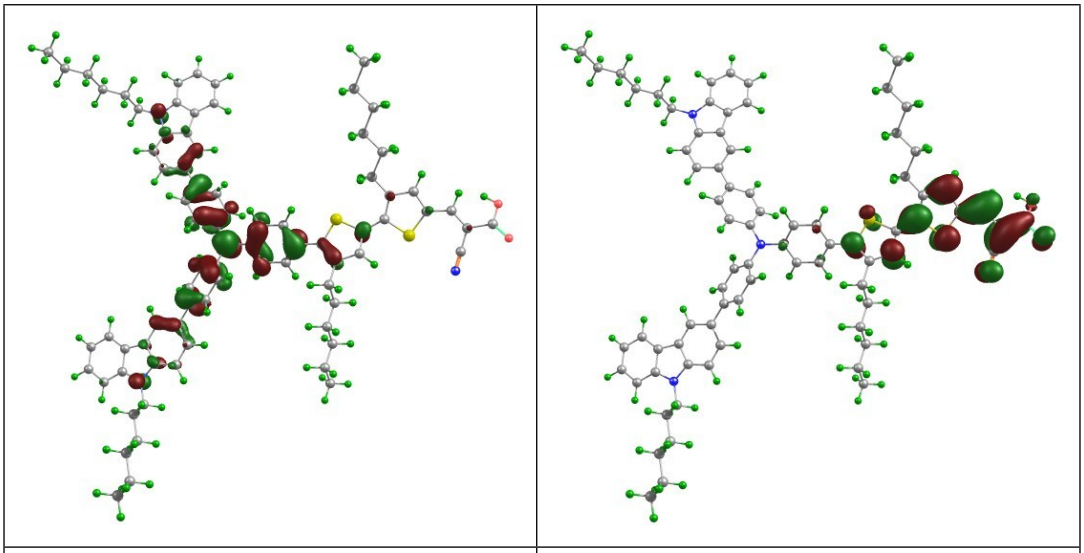
HOMO	LUMO

Fig. S3 Contour plots of selected frontier orbitals of **7c**.



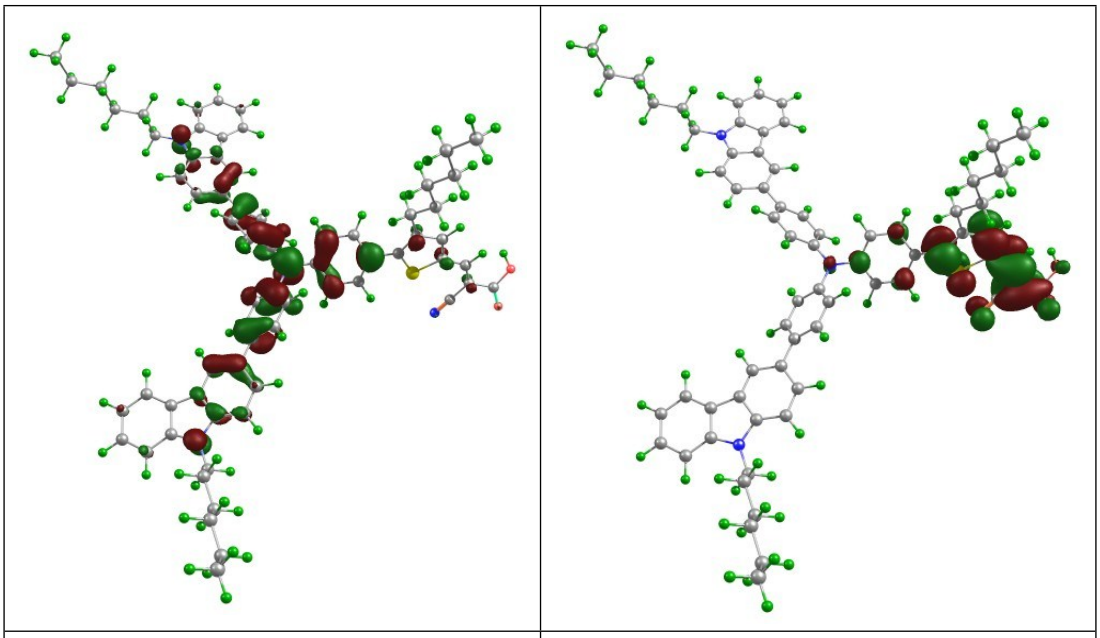
HOMO	LUMO

Fig. S4 Contour plots of selected frontier orbitals of **7d**.



HOMO	LUMO

Fig. S5 Contour plots of selected frontier orbitals of **11d**.



HOMO	LUMO

Fig. S6 Contour plots of selected frontier orbitals of **12d**.

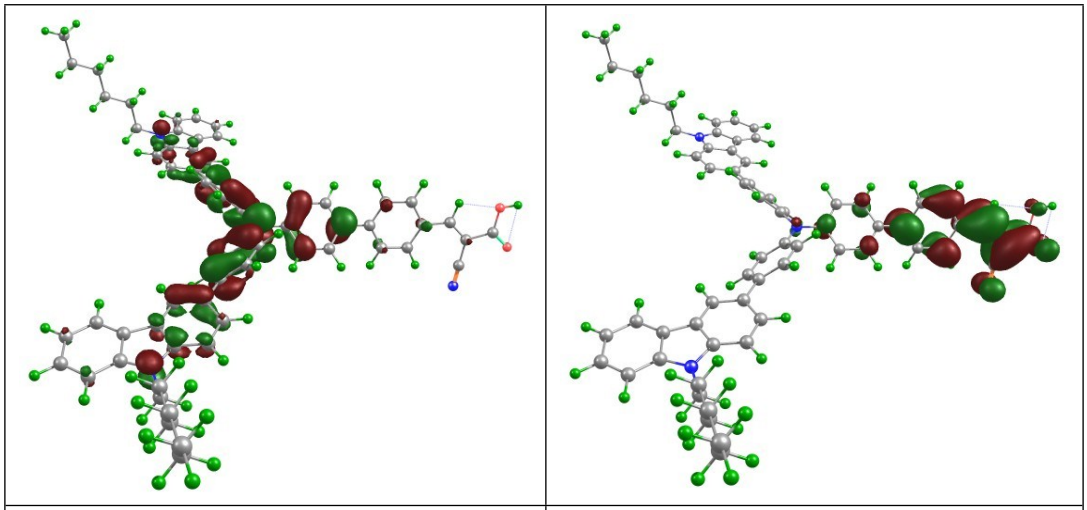


Fig. S7 Contour plots of selected frontier orbitals of **13d**.

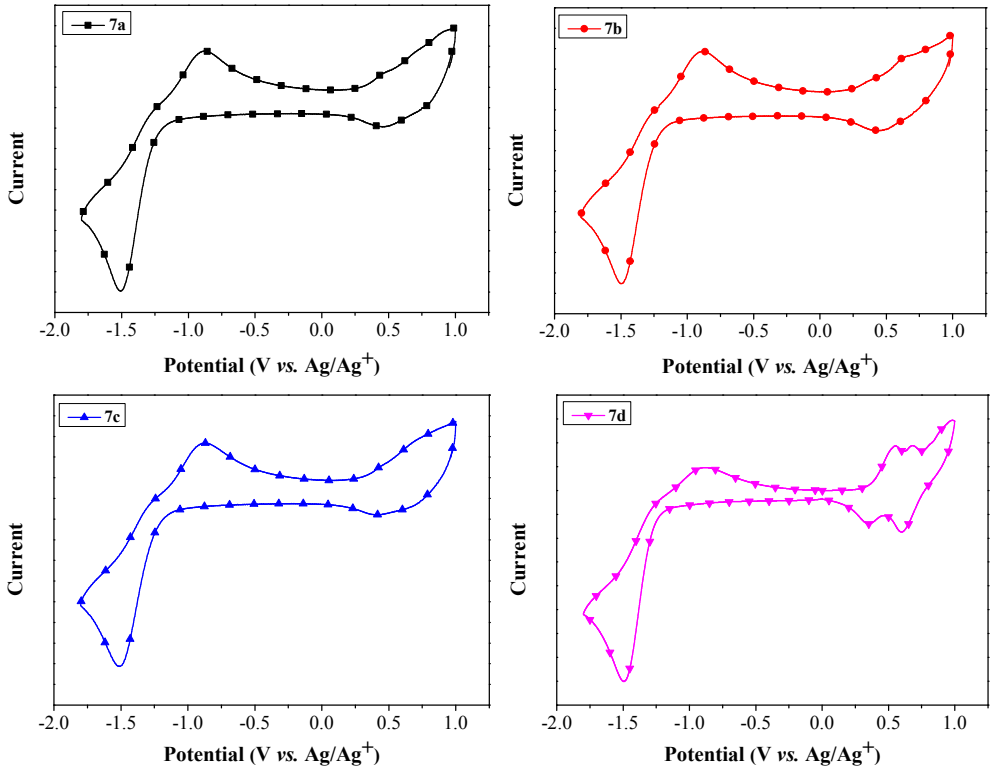


Fig. S8 Cyclic voltammograms of organic dyes **7a**−**7d**.

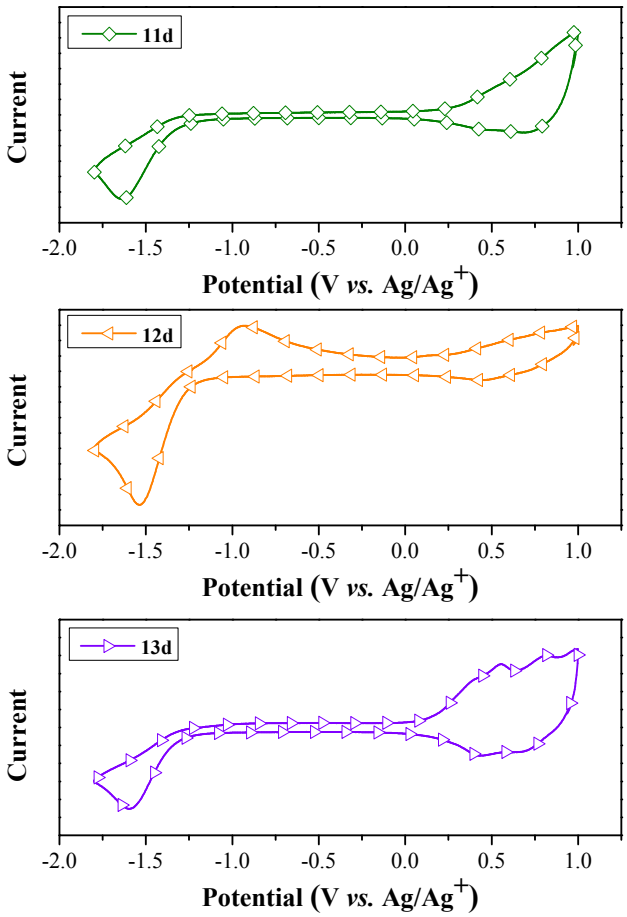


Fig. S9 Cyclic voltammograms of organic dyes **11d**−**13d**.