Electronic Supplementary Information (ESI)

for

New Thieno[3,2-b][1]benzo thiophene-Based Organic Sensitizers Containing \( \pi \)-Extended Thiophene Spacers for Efficient Dye-Sensitized Solar Cells

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Electronic supplementary information (ESI) available. See DOI:
Figure S1. Dihedral angles, total lengths and $\pi$-spacer lengths for all sensitizers.
The oxidation potentials of dyes on TiO$_2$ were measured in CH$_3$CN with 0.1 M tetra-$n$-butylammonium hexafluorophosphate (TBAPF$_6$) as the inert electrolyte, using a three-electrode system (e.g. dye-coated TiO$_2$ film as the working electrode, Pt wire as the counter electrode and Ag/Ag$^+$ as the reference electrode). The potential of the reference electrode was calibrated with Fc/Fc$^+$ as an external reference using $E_0$ (Fc/Fc$^+$) = 0.63 V vs. NHE.
**Figure S3.** τ<sub>T</sub> (a) and τ<sub>n</sub> (b) values derived from IMVS and IMPS of the DSSCs as a function of light intensity, respectively. (c) The η<sub>cc</sub> values obtained from IMVS and IMPS measurements for the same DSSCs.

To again prove the electron transport and recombination of the SGT sensitizer-based DSSCs, IMVS and IMPS measurements were performed. The electron-transport time (τ<sub>n</sub>) or recombination time (τ<sub>r</sub>) can be calculated from the expression, τ<sub>n</sub> or τ<sub>r</sub> = 1/2πf<sub>n</sub> or f<sub>r</sub>, where f<sub>n</sub> or f<sub>r</sub> is the characteristic frequency minimum in the Nyquist plots of the IMVS and IMPS results. **Figures S3a and S3b** show the τ<sub>r</sub> and τ<sub>n</sub> curves as a function of light intensity. The τ<sub>r</sub> values from IMVS were in the order of SGT-125 < SGT-121 < SGT-123, which is in agreement with the EIS measurements, which led to the higher V<sub>oc</sub> of the SGT-123-based DSSC. The τ<sub>r</sub> and τ<sub>n</sub> values for the SGT-127-based DSSC were incommensurable with those of other sensitisers, owing to the weak light intensity. The η<sub>cc</sub> results under different light intensities for all DSSCs are displayed in **Figure S3c**, which are also consistent with the η<sub>cc</sub> values obtained from EIS results.
Figure S4. Cyclic voltammograms obtained with the dye-coated TiO$_2$ electrodes in 0.1 M LiClO$_4$ dissolved in acetonitrile at a scan rate of 50 mV s$^{-1}$ at room temperature.
Figure S5. $^1$H NMR spectrum of compound 3a in CDCl$_3$.

Figure S6. $^1$H NMR spectrum of compound 3b in CDCl$_3$. 

**Figure S7.** $^1$H NMR spectrum of compound 3c in CDCl$_3$

**Figure S8.** $^1$H NMR spectrum of compound 4b in CDCl$_3$
Figure S9. $^1$H NMR spectrum of compound 4c in CDCl$_3$

Figure S10. $^1$H NMR spectrum of compound 5 in CDCl$_3$
Figure S11. $^1$H NMR spectrum of SGT-123 in CDCl$_3$

Figure S12. $^{13}$C NMR spectrum of SGT-123 in DMSO-$d_6$
Figure S13. $^1$H NMR spectrum of SGT-125 in CDCl$_3$

Figure S14. $^1$H NMR spectrum of SGT-125 in DMSO-$d_6$
Figure S15. $^1$H NMR spectrum of SGT-127 in CDCl$_3$

Figure S16. $^1$H NMR spectrum of SGT-127 in DMSO-$d_6$
Figure S17. MALDI-TOF spectrum of SGT-123

Figure S18. MALDI-TOF spectrum of SGT-125
Figure S19. MALDI-TOF spectrum of SGT-127