Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information (ESI)

for

New Thieno[3,2-*b*][1]benzothiophene-Based Organic Sensitizers Containing π-Extended Thiophene Spacers for Efficient Dye-Sensitized Solar Cells

Yu Kyung Eom[a], Sung Ho Kang[a], In Taek Choi[a], Eunji Kim [b], Jeongho Kim[b], Myung Jong Ju[a] and Hwan Kyu Kim[a,*]

[a]*Global GET-Future Lab. & Department of Advanced Materials Chemistry, Korea University, 2511 Sejong-ro, Sejong 339-700, Korea, E-mail: hkk777@korea.ac.kr*

[b]*Department of Chemistry, Inha University, 100 Inha-ro, Incheon 402-751, Korea*

Electronic supplementary information (ESI) available. See DOI:

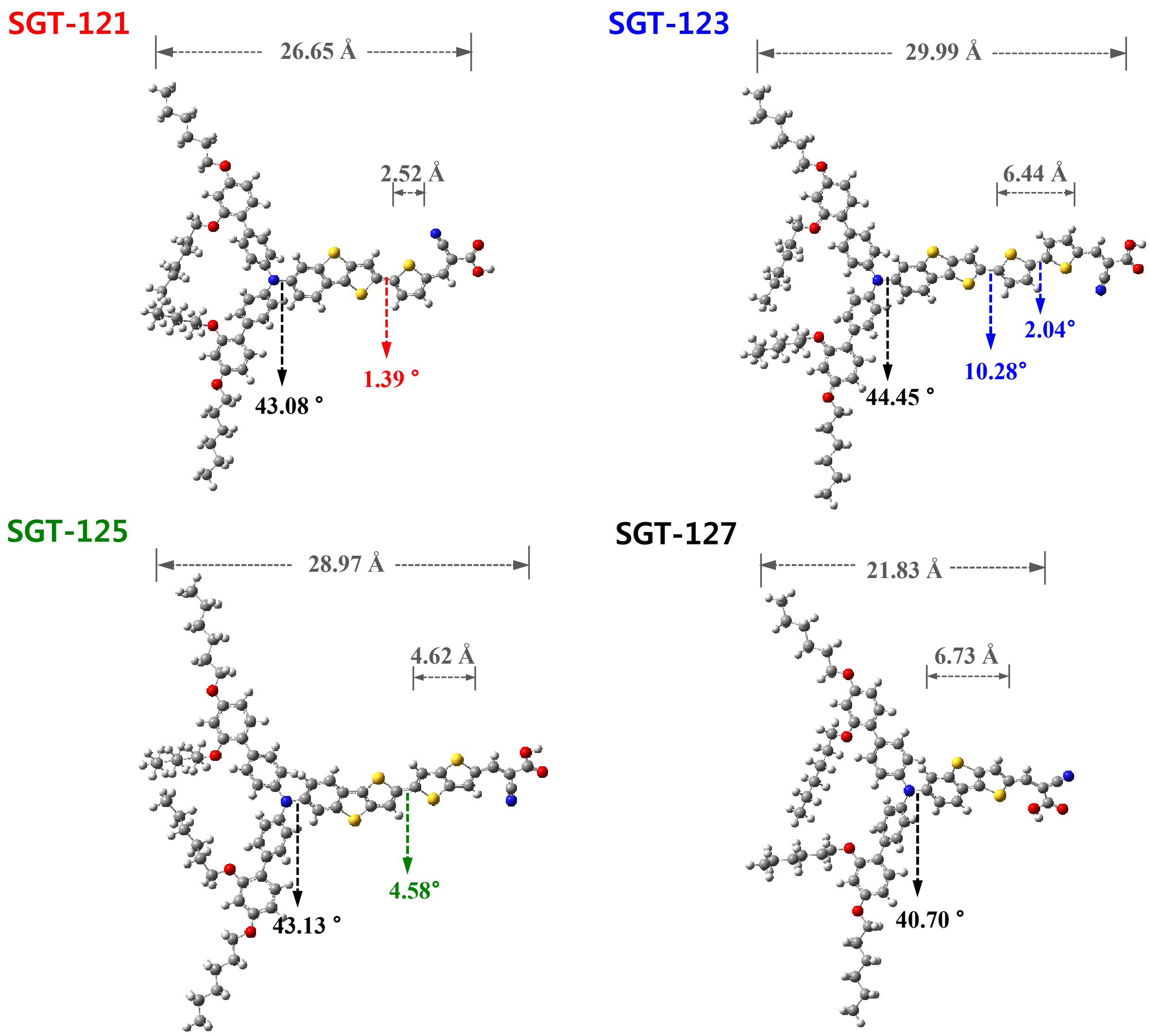

Figure S1. Dihedral angles, total lengths and π-spacer lengths for all sensitizers.

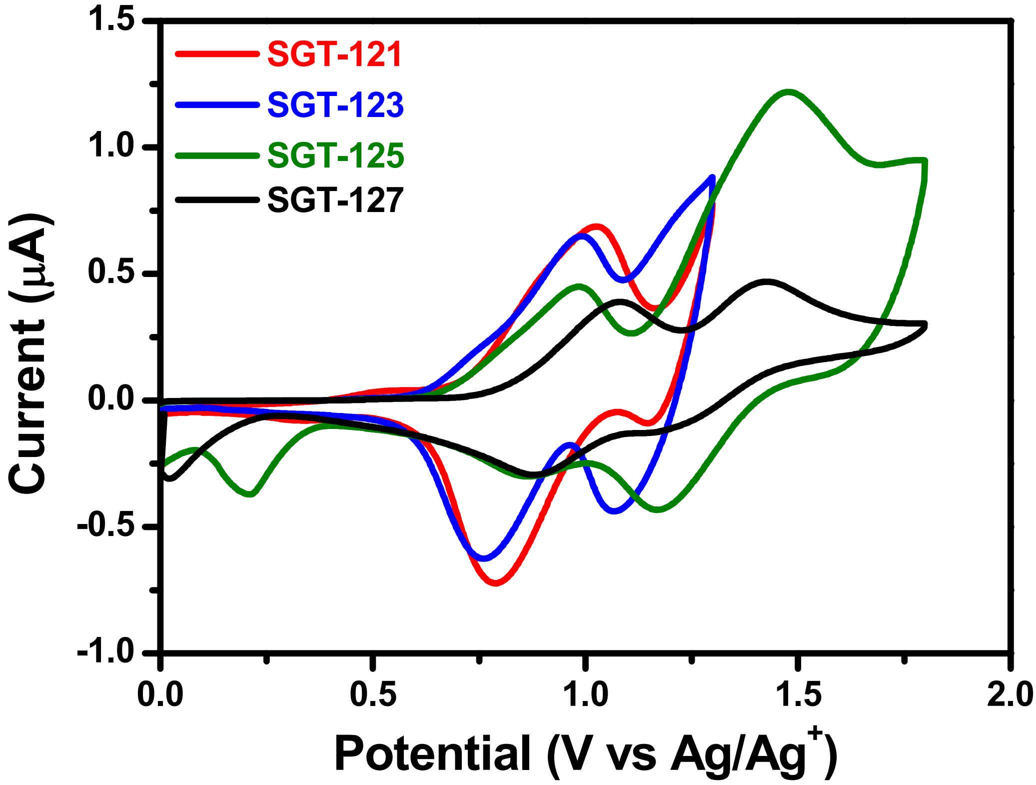

Figure S2. Cyclic voltammograms measured with the dye-coated TiO_2 films.

The oxidation potentials of dyes on TiO_2 were measured in CH_3CN 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.

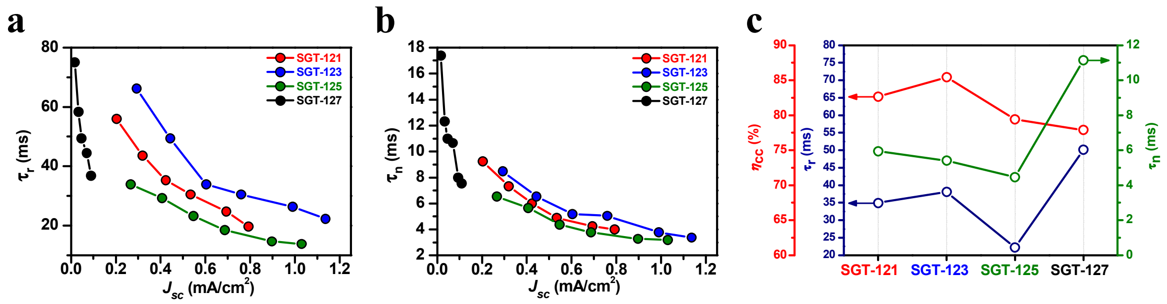

Figure S3. τ_r (a) and τ_n (b) values derived from IMVS and IMPS of the DSSCs as a function of light intensity, respectively. (c) The η_{cc} values obtained from IMVS and IMPS measurements for the same DSSCs.

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_n) or recombination time (τ_r) can be calculated from the expression, τ_n or $\tau_r = 1/2\pi f_{n \text{ or } r}$, where f_n or f_r is the characteristic frequency minimum in the Nyquist plots of the IMVS and IMPS results. **Figures S3a and S3b** show the τ_r and τ_n curves as a function of light intensity. The τ_r 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_{oc} of the **SGT-123**-based DSSC. The τ_r and τ_n values for the **SGT-127**-based DSSC were incommensurable with those of other sensitisers, owing to the weak light intensity. The η_{cc} results under different light intensities for all DSSCs are displayed in **Figure S3c**, which are also consistent with the η_{cc} values obtained from EIS results.

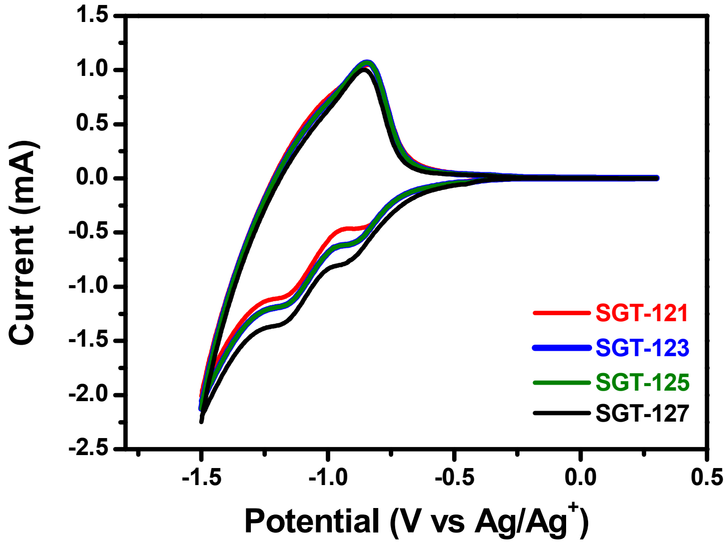

Figure S4. Cyclic voltammograms obtained with the dye-coated TiO_2 electrodes in 0.1 M $LiClO_4$ dissolved in acetonitrile at a scan rate of 50 mV s^{-1} at room temperature

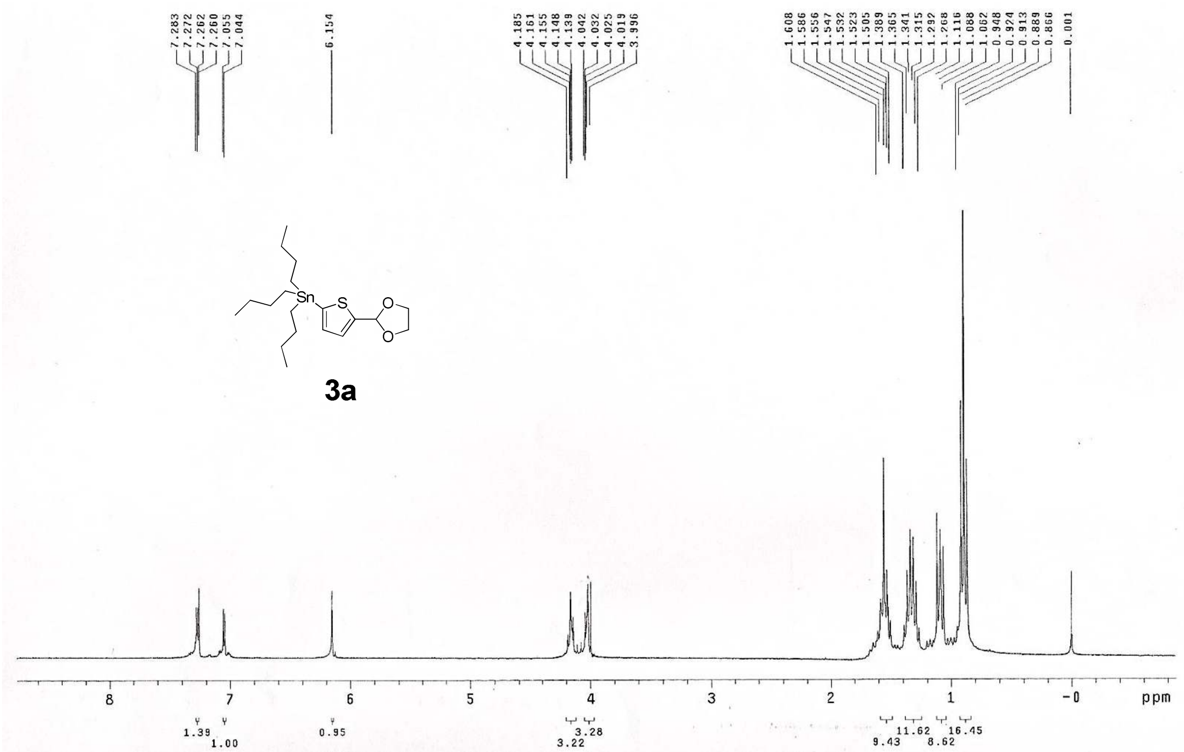

Figure S5. ^{1}H NMR spectrum of compound **3a** in $CDCl_3$

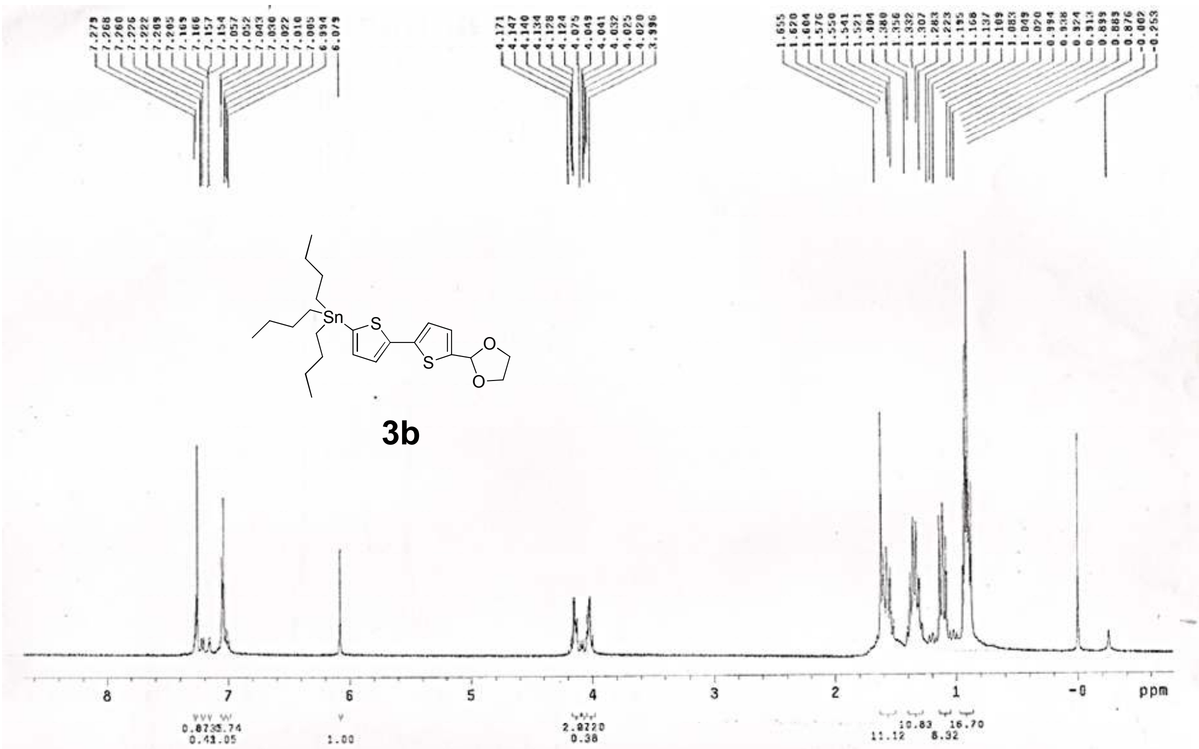

Figure S6. ^{1}H NMR spectrum of compound **3b** in $CDCl_3$

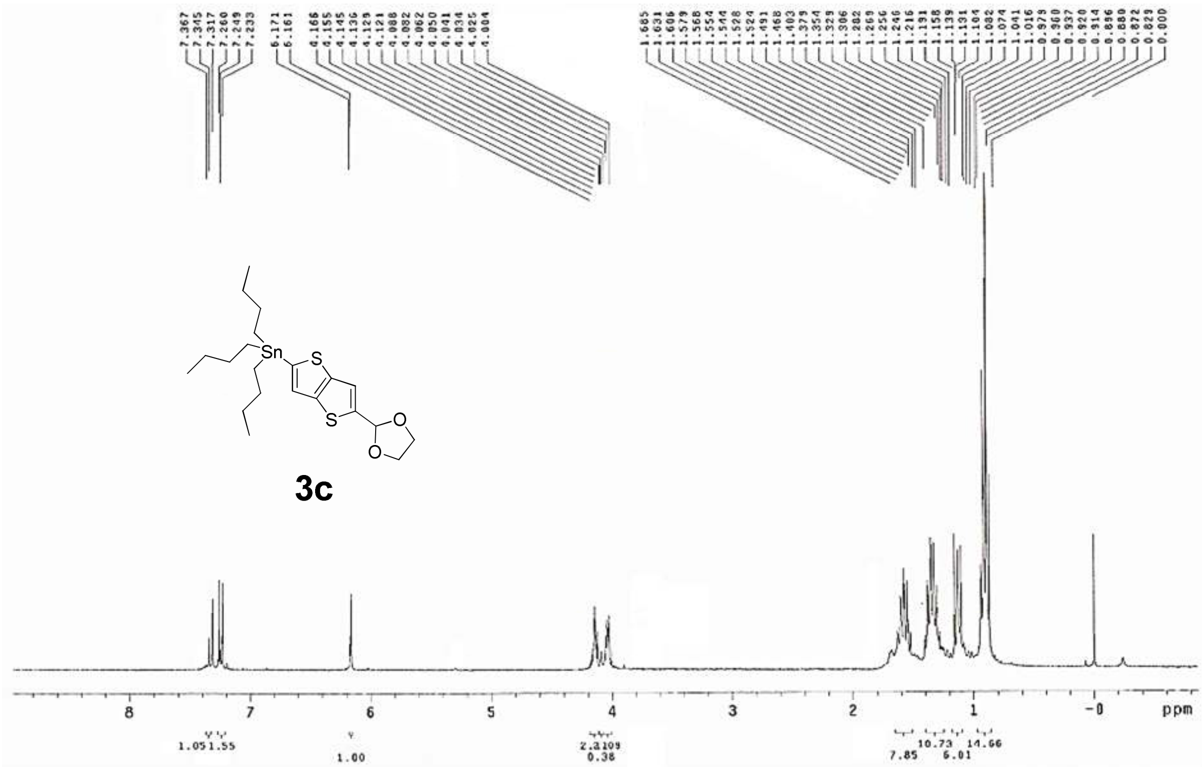

Figure S7. ^{1}H NMR spectrum of compound **3c** in $CDCl_3$

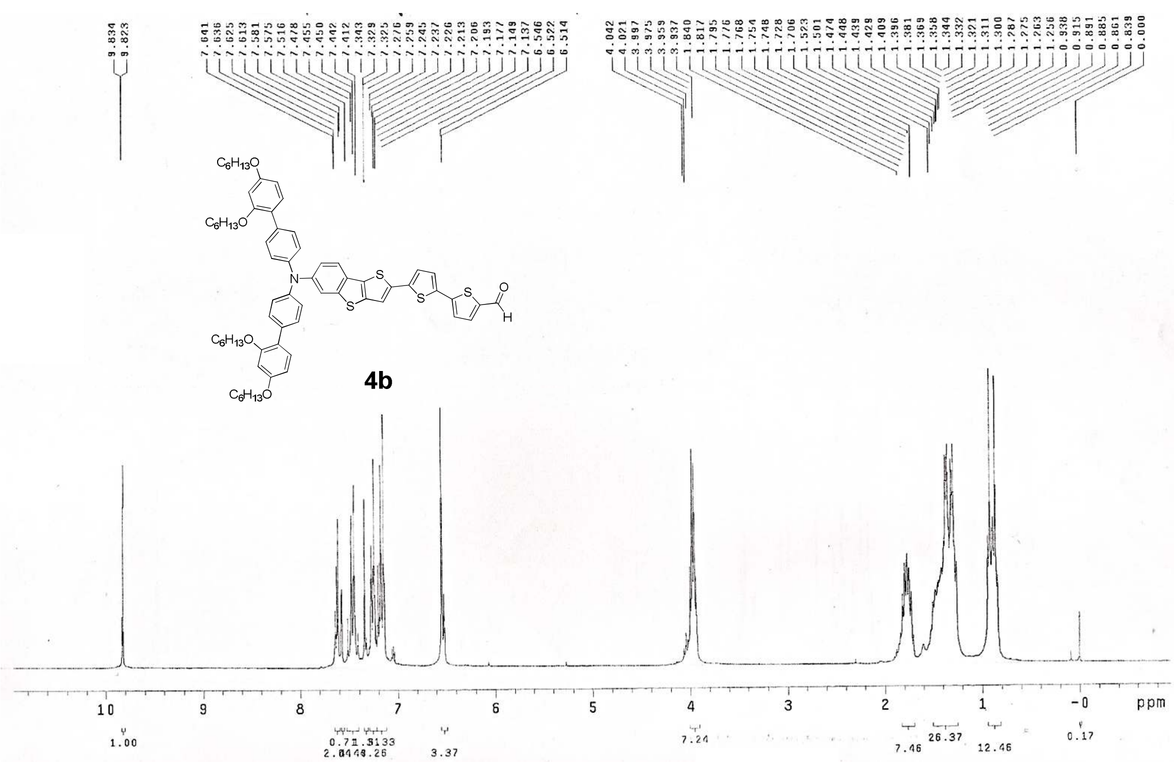

Figure S8. ^{1}H NMR spectrum of compound **4b** in $CDCl_3$

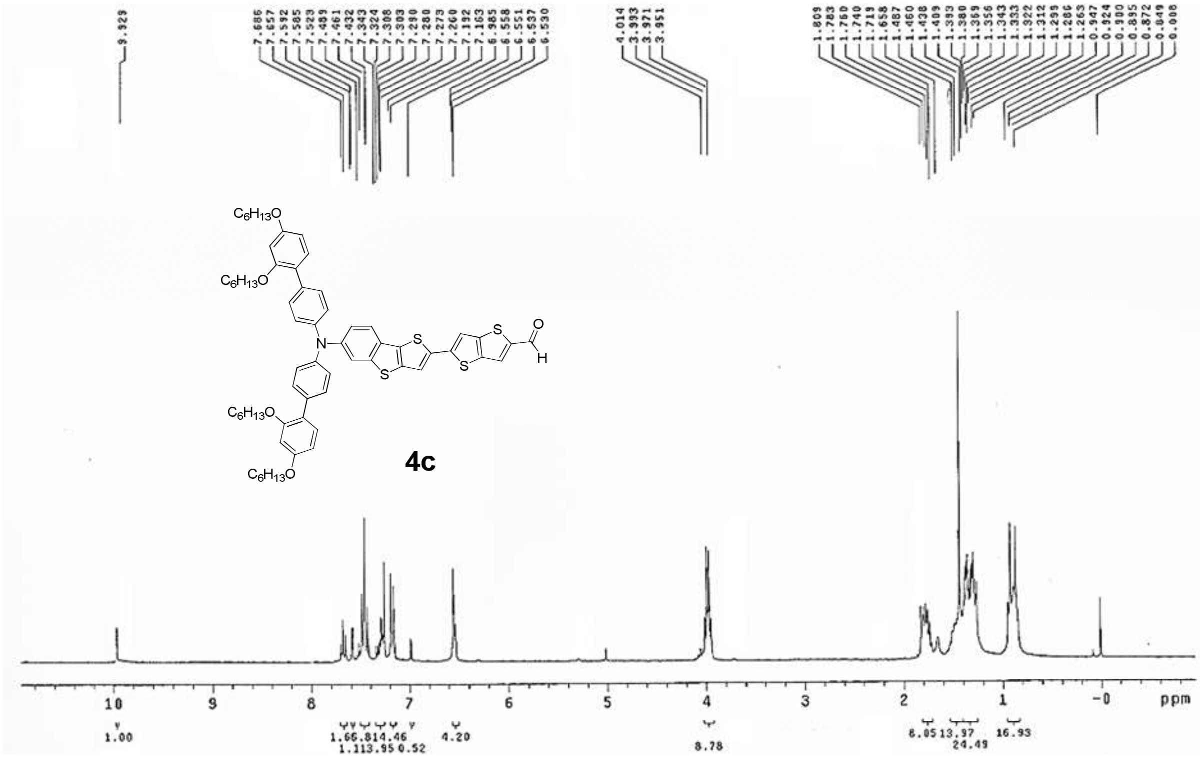

Figure S9. ^{1}H NMR spectrum of compound **4c** in $CDCl_3$

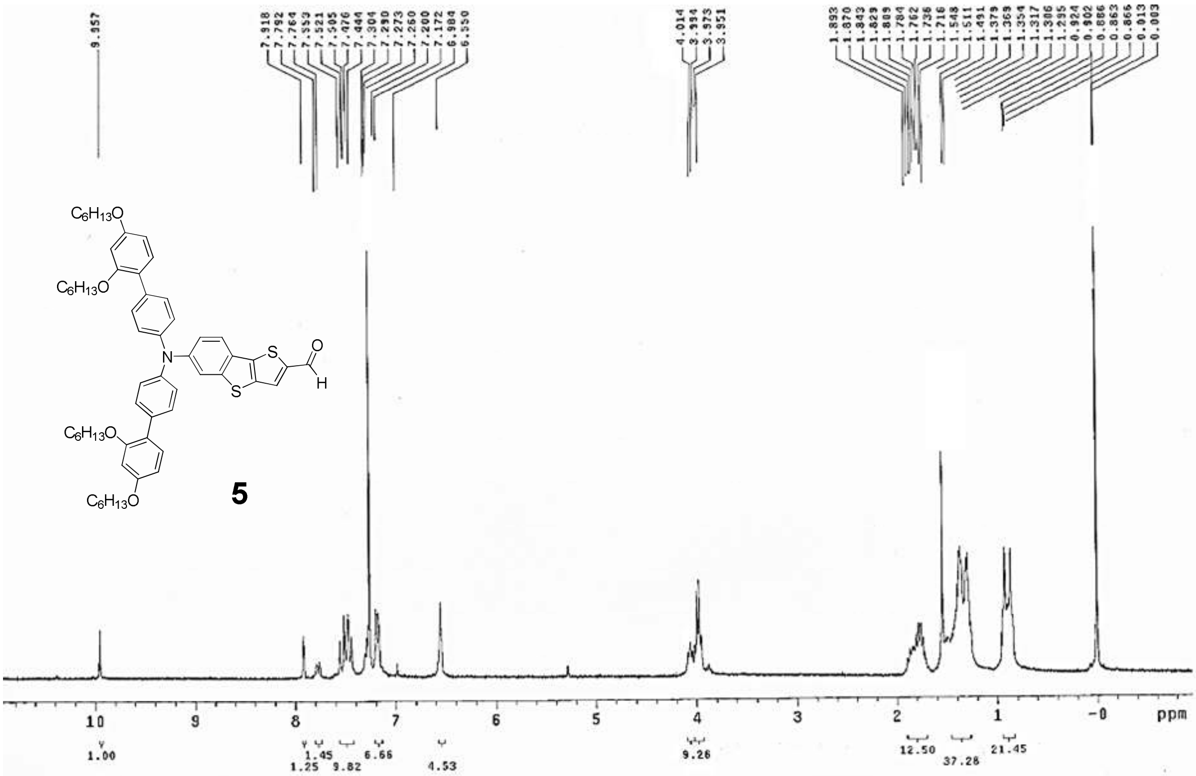

Figure S10. ^{1}H NMR spectrum of compound **5** in $CDCl_3$

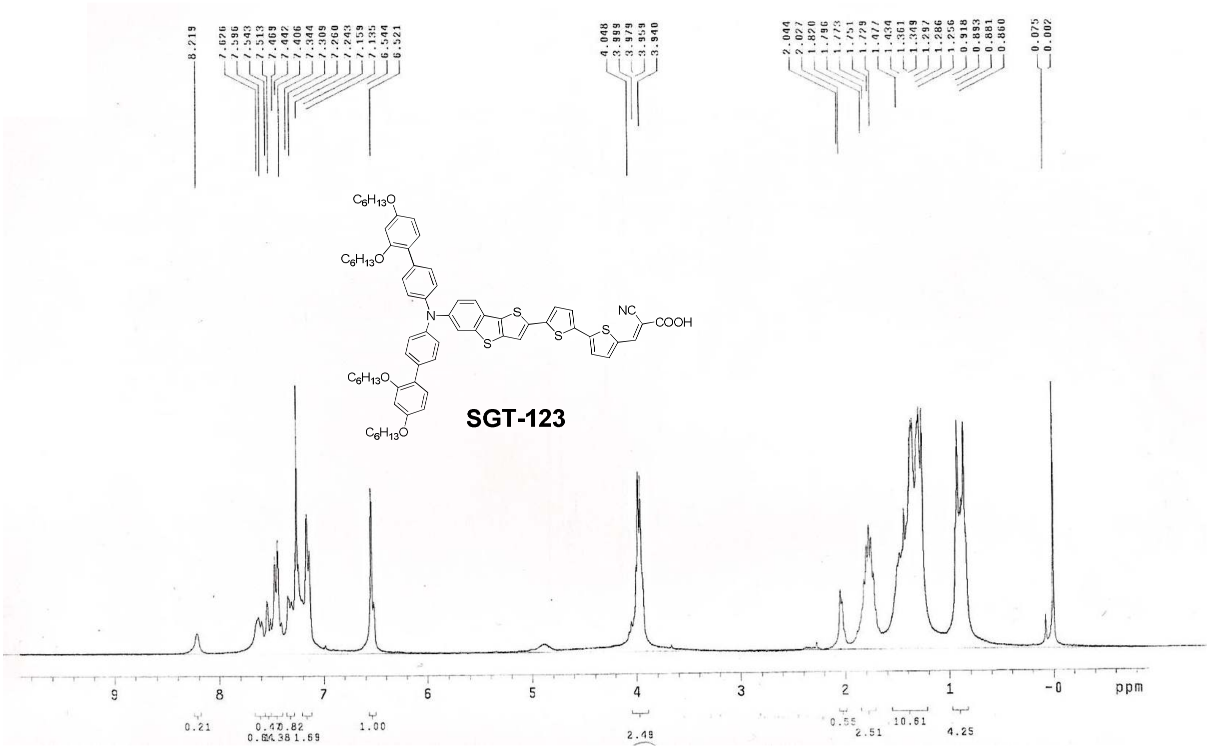

Figure S11. ^{1}H NMR spectrum of **SGT-123** in $CDCl_3$

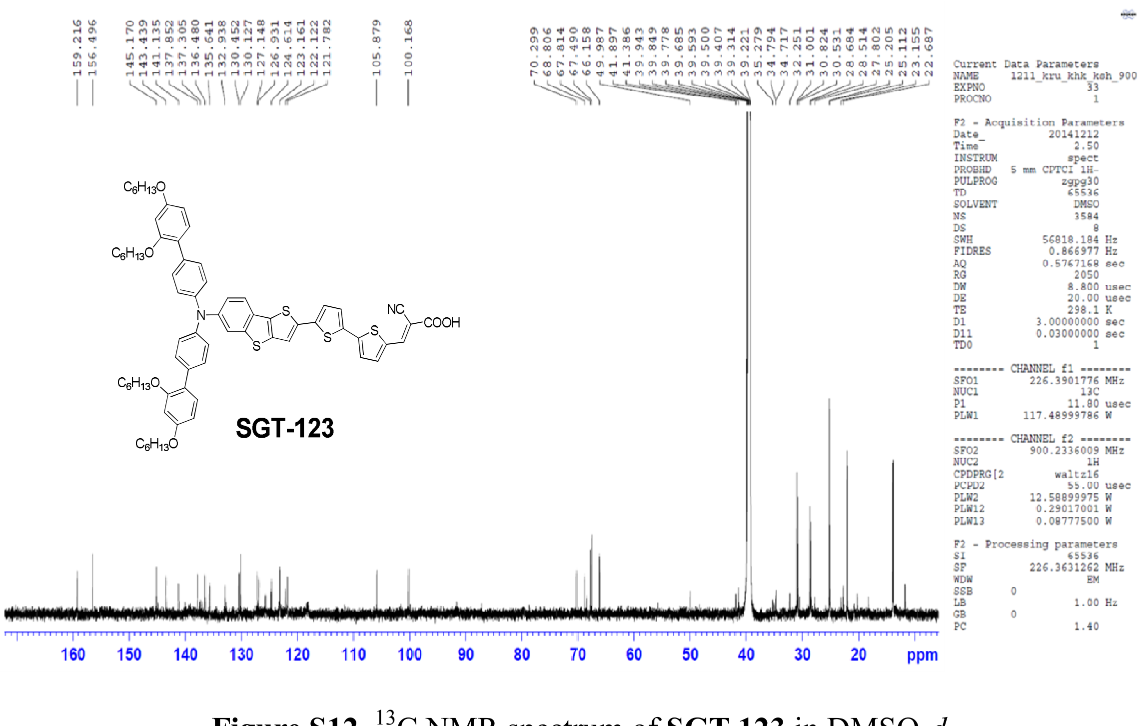

Figure S12. ^{13}C NMR spectrum of **SGT-123** in DMSO-d_6

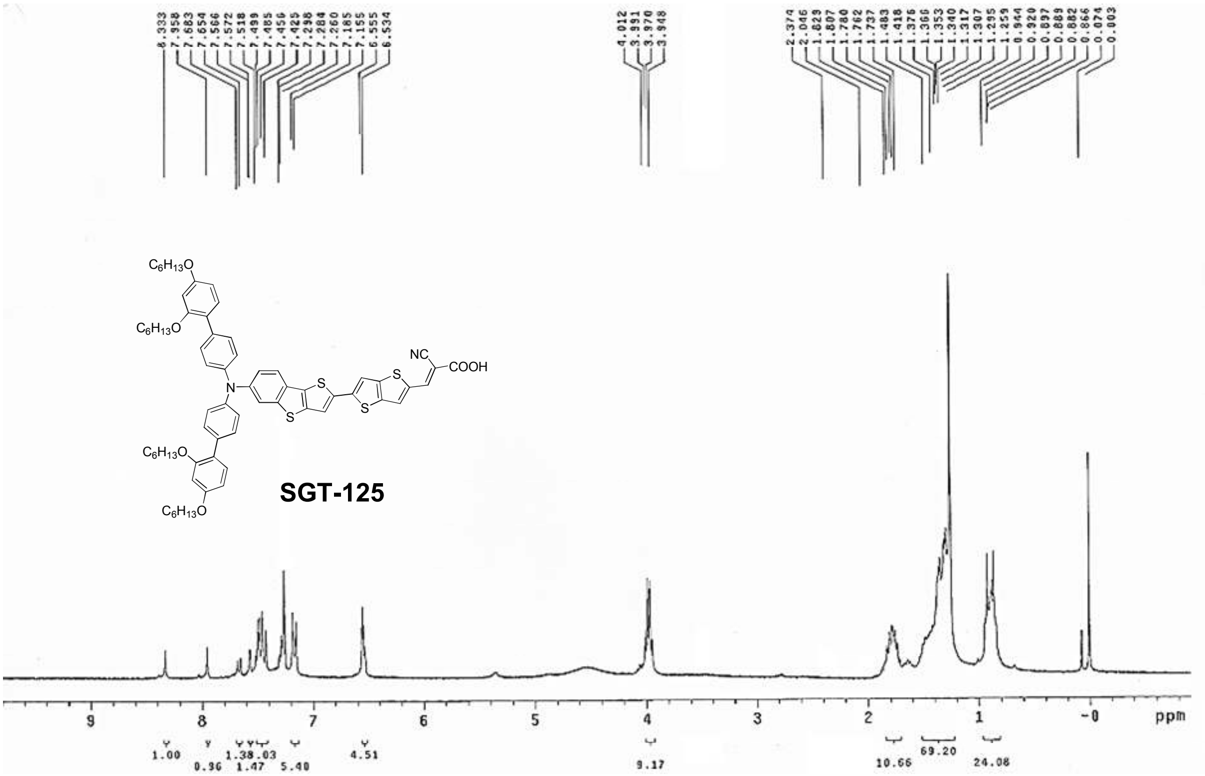

Figure S13. ^{1}H NMR spectrum of **SGT-125** in $CDCl_3$

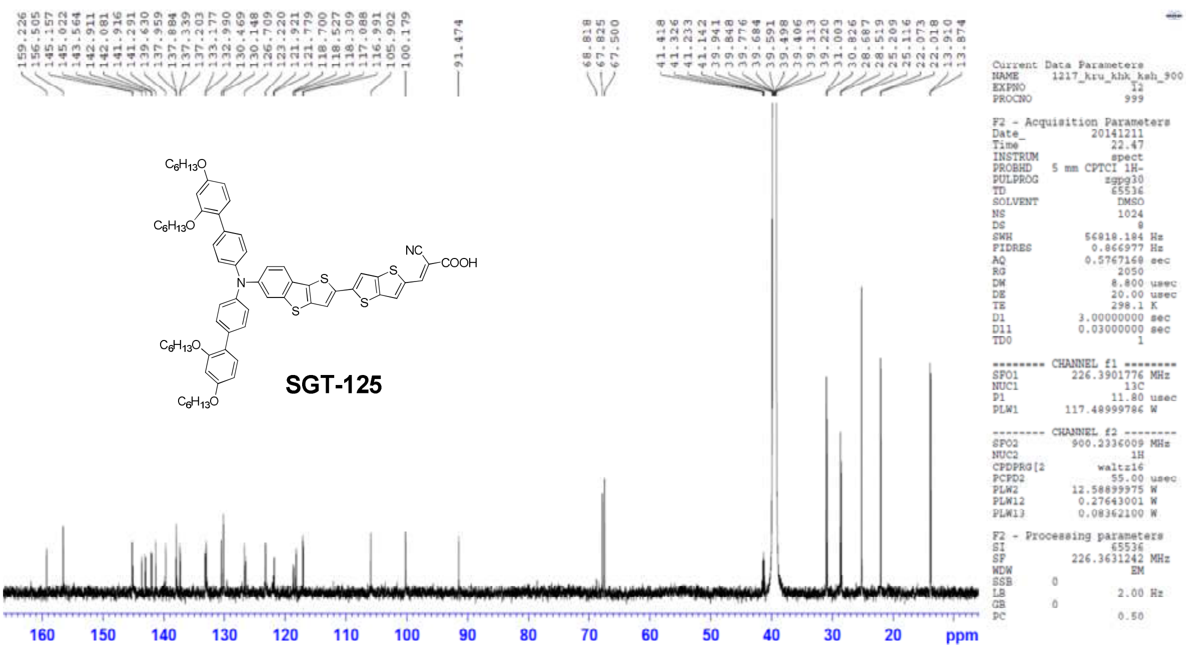

Figure S14. ^{1}H NMR spectrum of **SGT-125** in DMSO-d_6

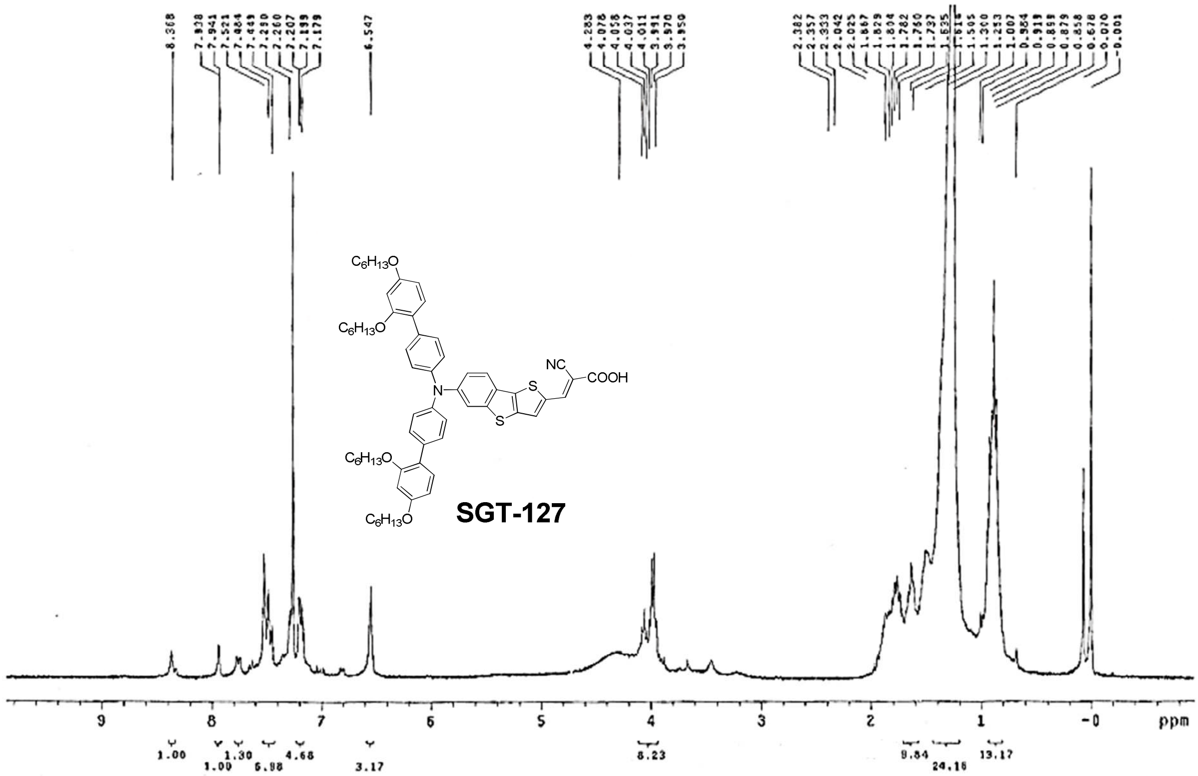

Figure S15. ^{1}H NMR spectrum of **SGT-127** in $CDCl_3$

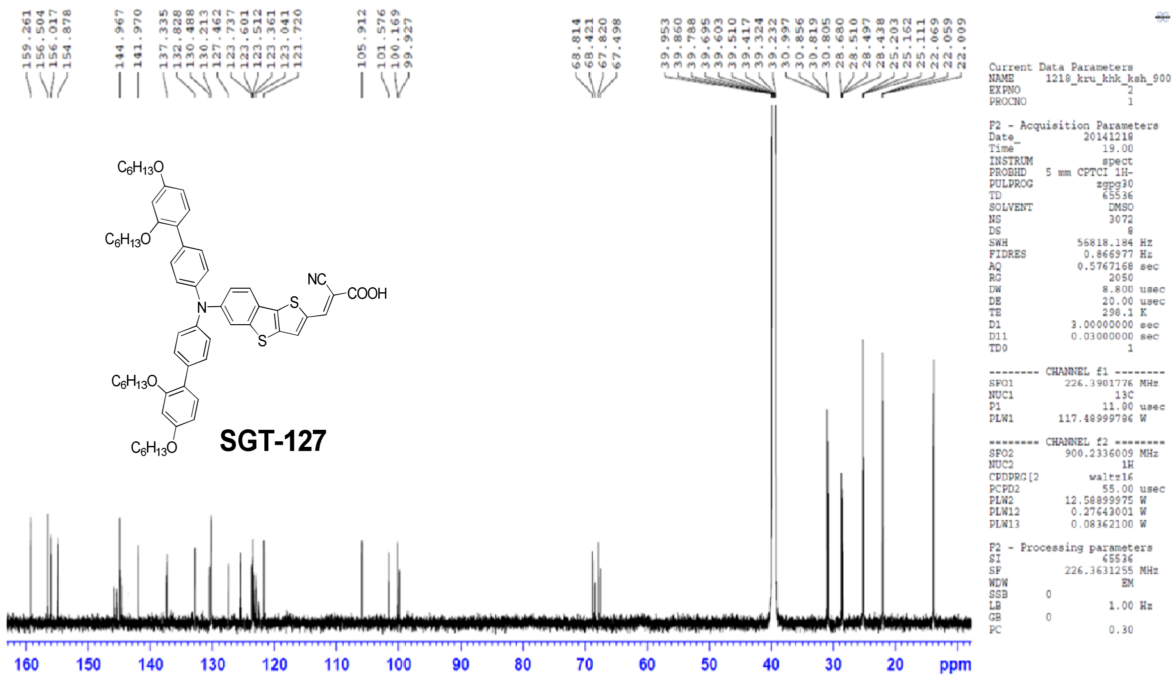

Figure S16. ^{1}H NMR spectrum of **SGT-127** in DMSO-d_6

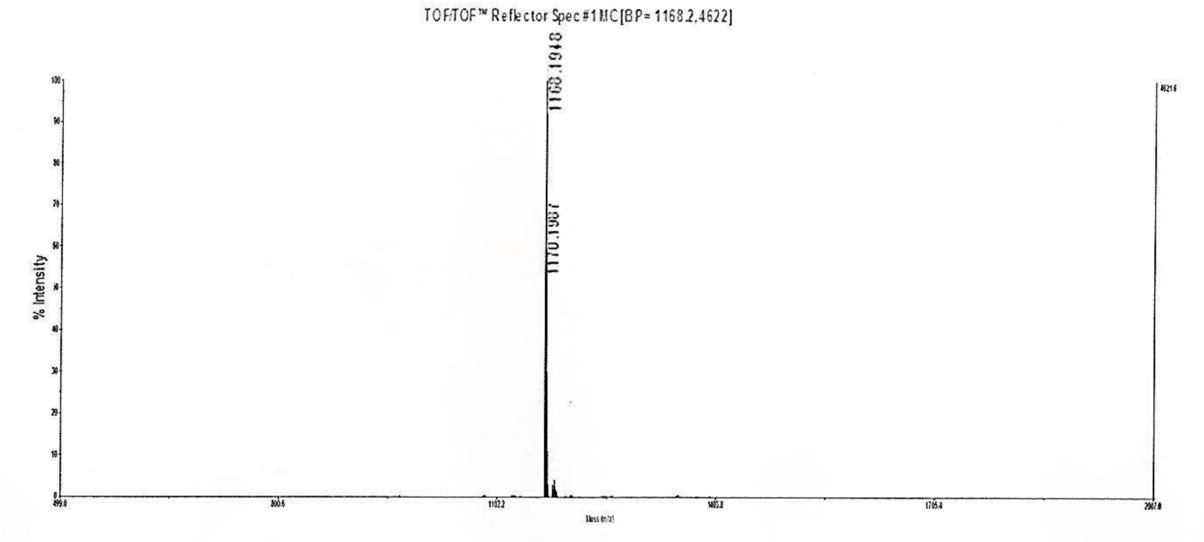

Figure S17. MALDI-TOF spectrum of **SGT-123**

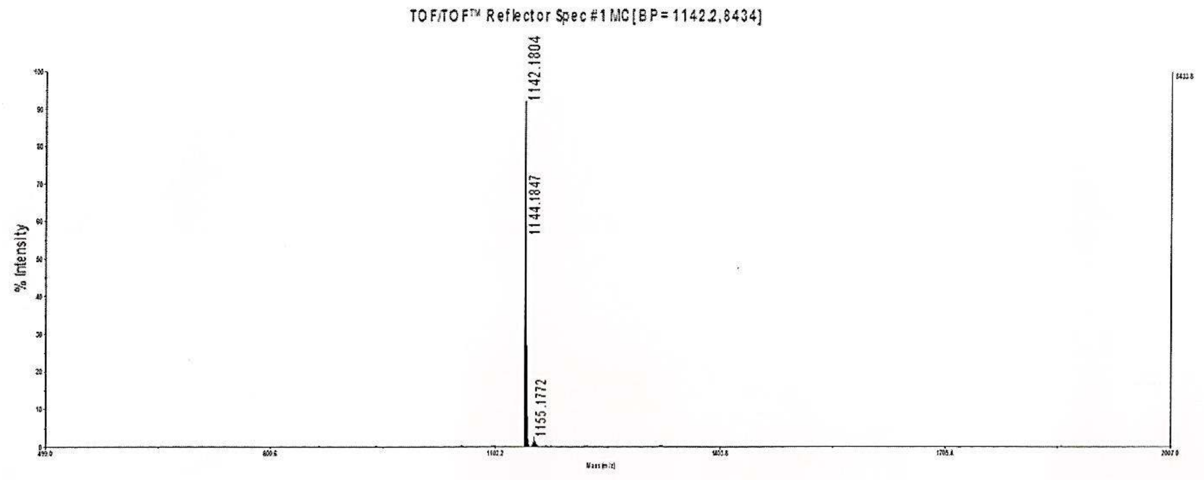

Figure S18. MALDI-TOF spectrum of **SGT-125**

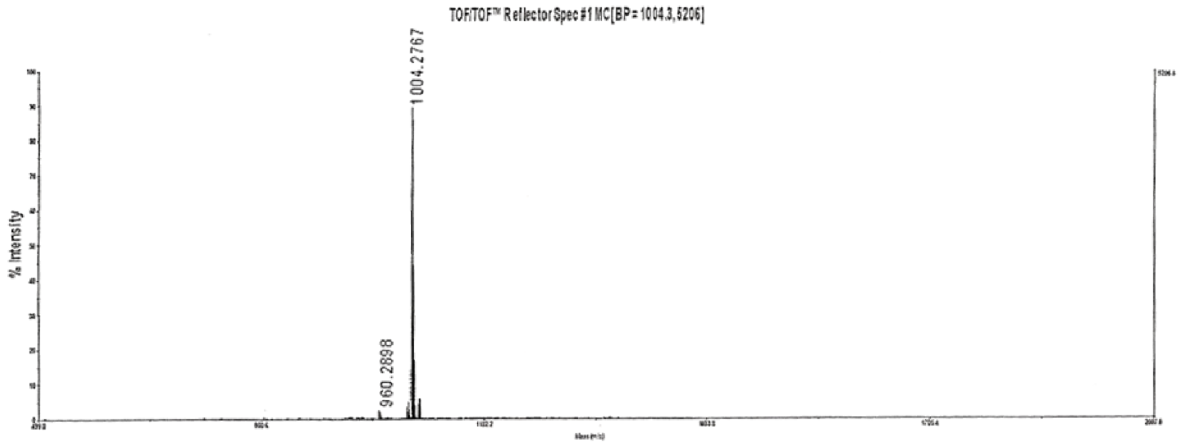

Figure S19. MALDI-TOF spectrum of **SGT-127**