

Supporting Information

Cyclohexyl-substituted Non-fullerene Small-molecule Acceptors for Organic Solar Cells

*Seunggyun Hong,^{a,#} Chang Eun Song,^{b,#} Du Hyeon Ryu,^b Sang Kyu Lee,^b Won Suk Shin,^b
and Eunhee Lim^{*,c}*

^a Department of Chemistry, Kyonggi University, 154-42 Gwanggyosan-ro, Yeongtong-gu, Suwon 16227, Republic of Korea

^b Korea Research Institute of Chemical Technology (KRICT), 141 Gajeongro, Yuseong-gu, Daejeon 34114, Republic of Korea

^c Department of Applied Chemistry, University of Seoul, 163 Seoulsiripdae-ro, Dongdaemun-gu, Seoul 02504, Republic of Korea

#S. Hong and C. E. Song contributed equally to this work.

* Corresponding author: Tel. +82-2-6490-2465; E-mail address: ehlim@uos.ac.kr (E. Lim)

1. NMR spectra

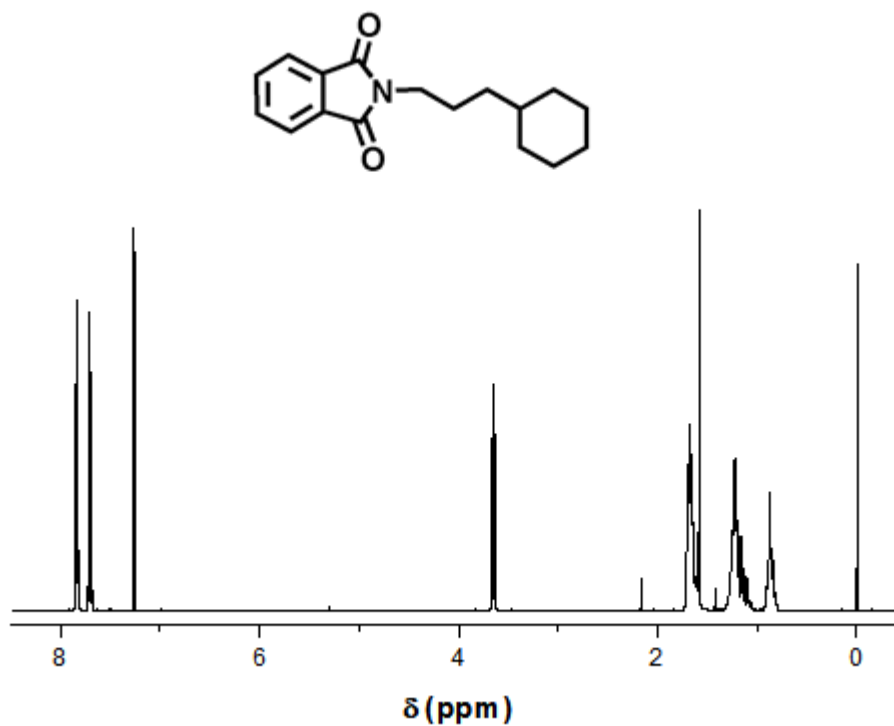


Figure S1. ¹H NMR spectrum of Cy6Pphth.

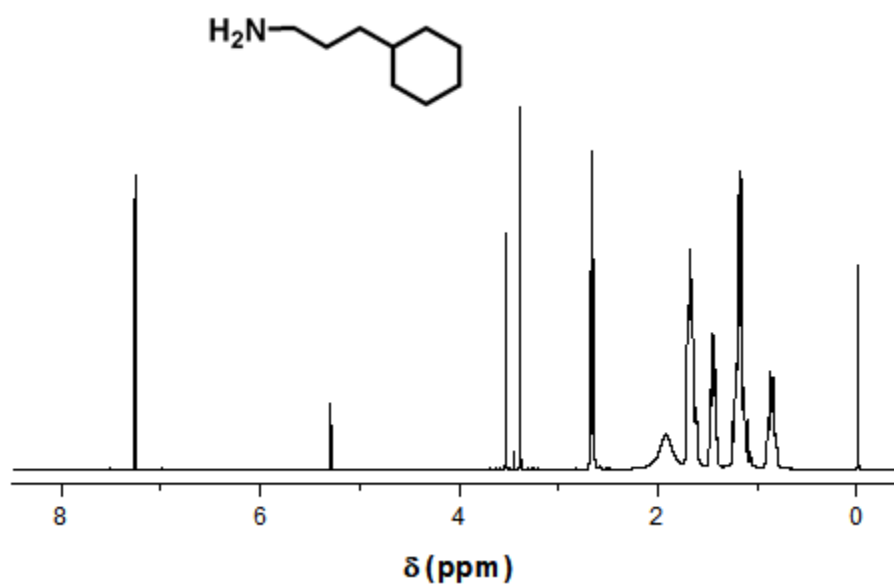


Figure S2. ¹H NMR spectrum of Cy6NH₂.

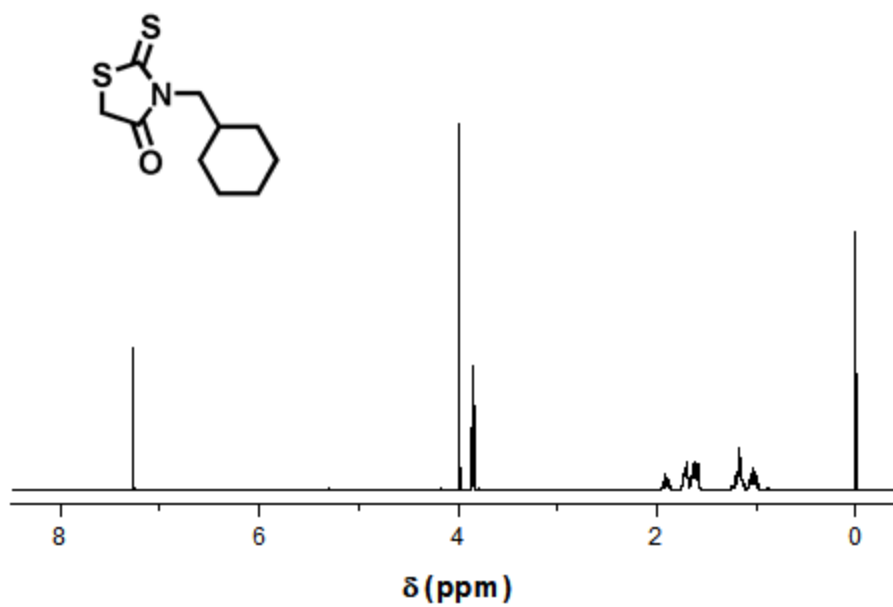


Figure S3. ¹H NMR spectrum of Cy6MRH.

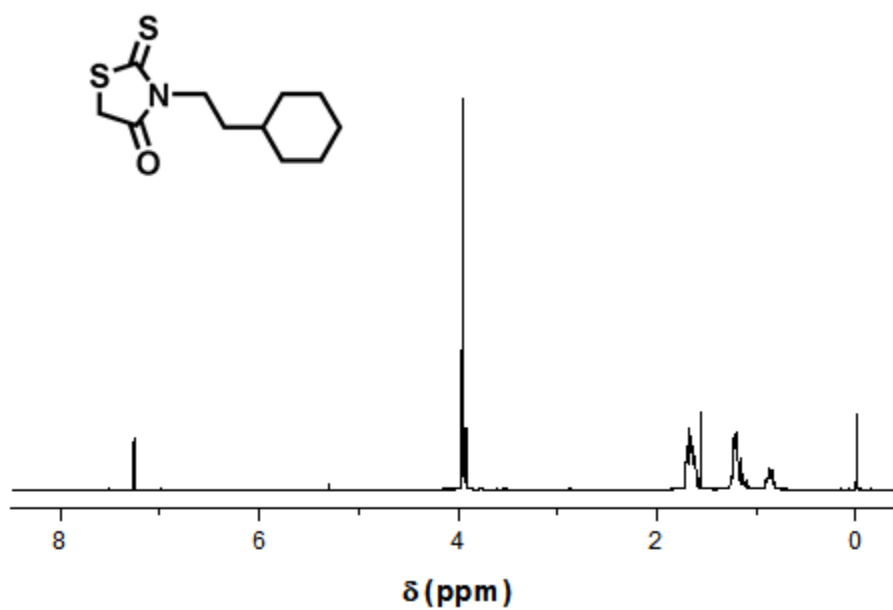


Figure S4. ¹H NMR spectrum of Cy6PRH.

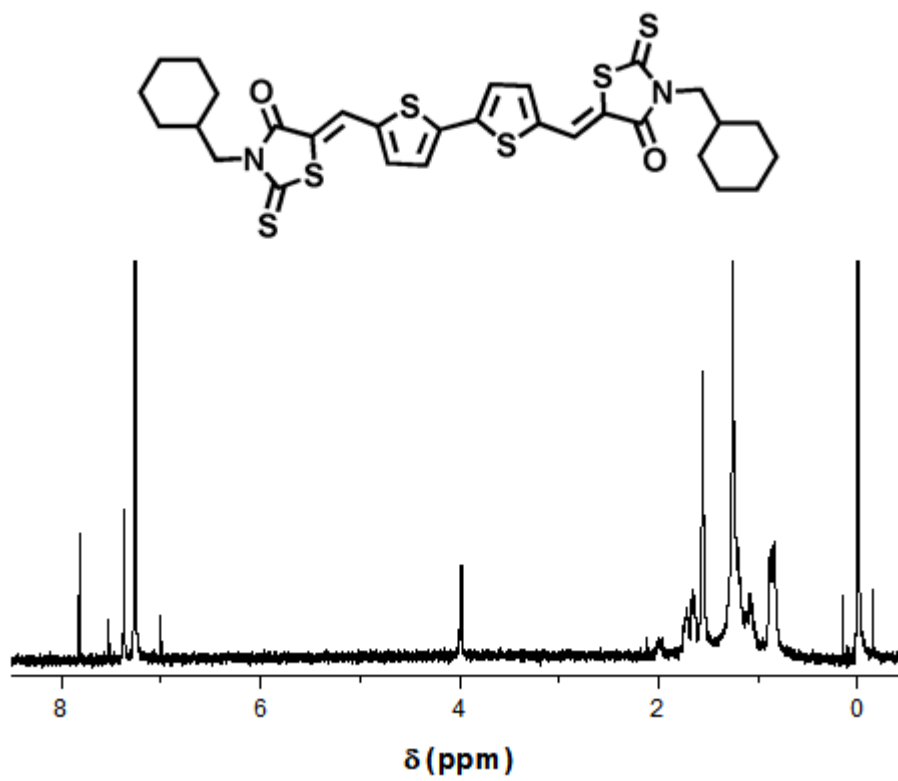


Figure S5. ¹H NMR spectrum of T2-Cy6MRH.

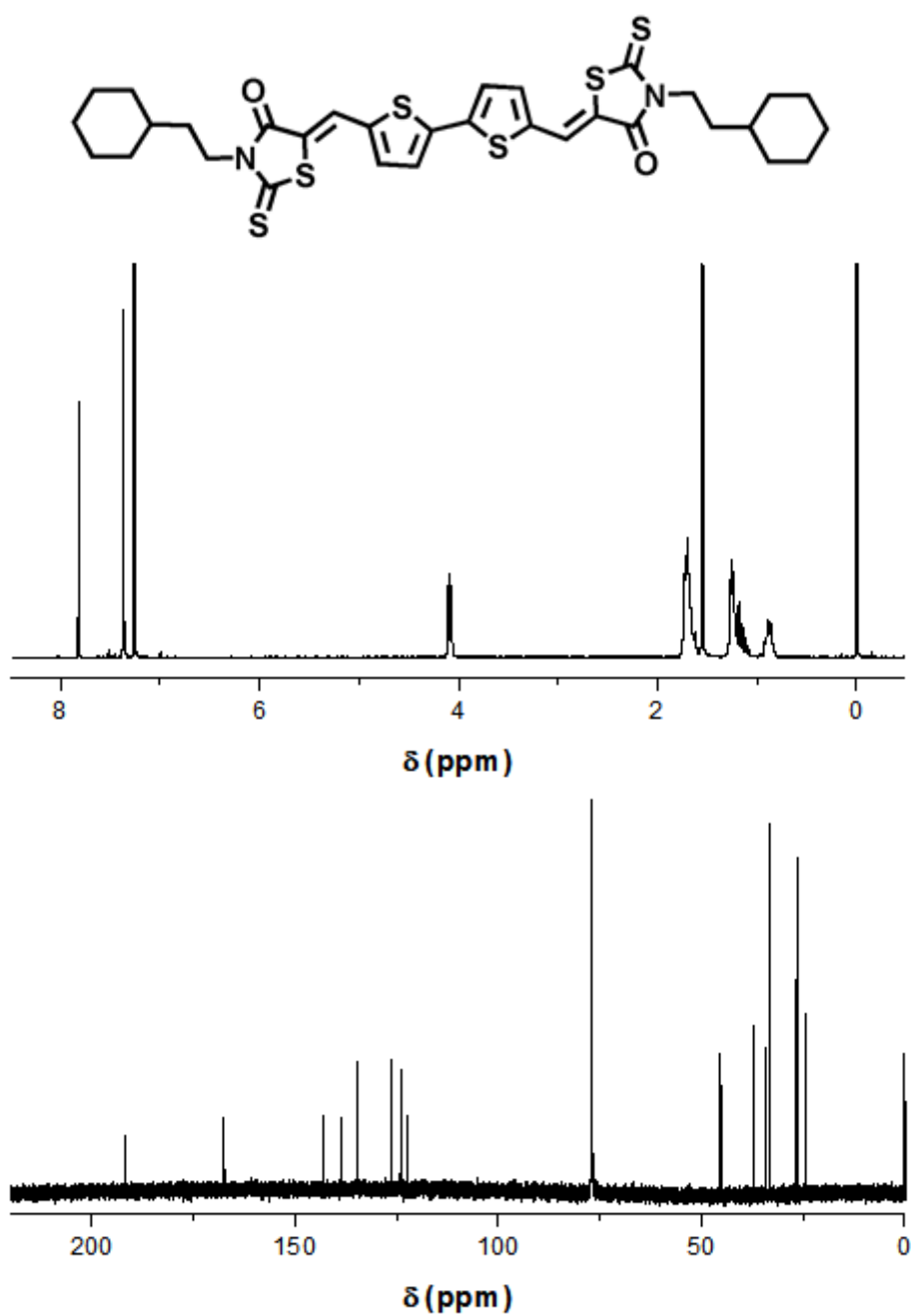


Figure S6. ¹H (top) and ¹³C (bottom) NMR and MS spectra of T2-Cy6PRH.

Table S1. Photovoltaic properties of **T2-Cy6PRH**-based OSCs with different thermal annealing conditions^a

Annealing	V_{OC} [V]	J_{SC} [mA cm^{-2}]	FF [%]	PCE [%]
W/O	1.03	11.04	40	4.60
90°C	1.00	9.83	41	4.00
120°C	1.00	8.81	40	3.57

^aInverted device architecture is ITO/ZnO NPs/PEIE/PTB7-Th:**T2-Cy6PRH** (1.0:2.0, chloroform, $d = \sim 100$ nm)/MoO_x/Ag.

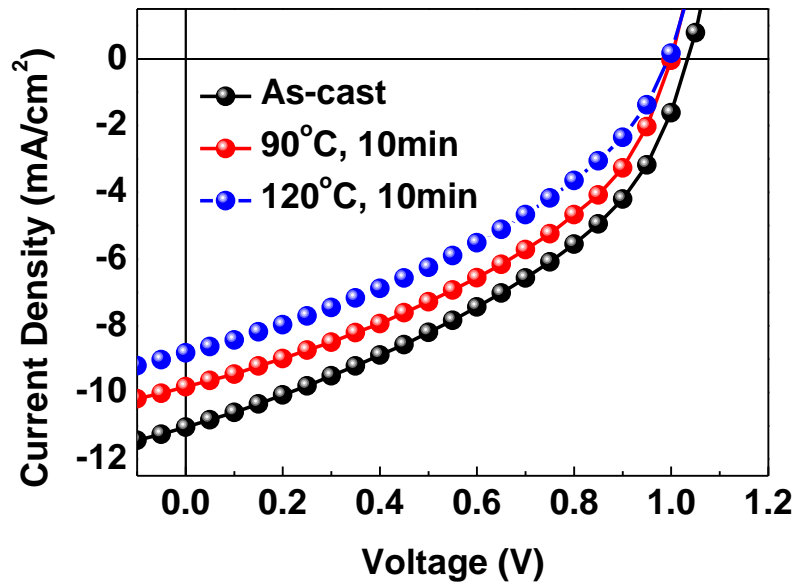


Figure S7. I - V curves of the device based on **T2-Cy6PRH** and PTB7-Th under different thermal annealing conditions

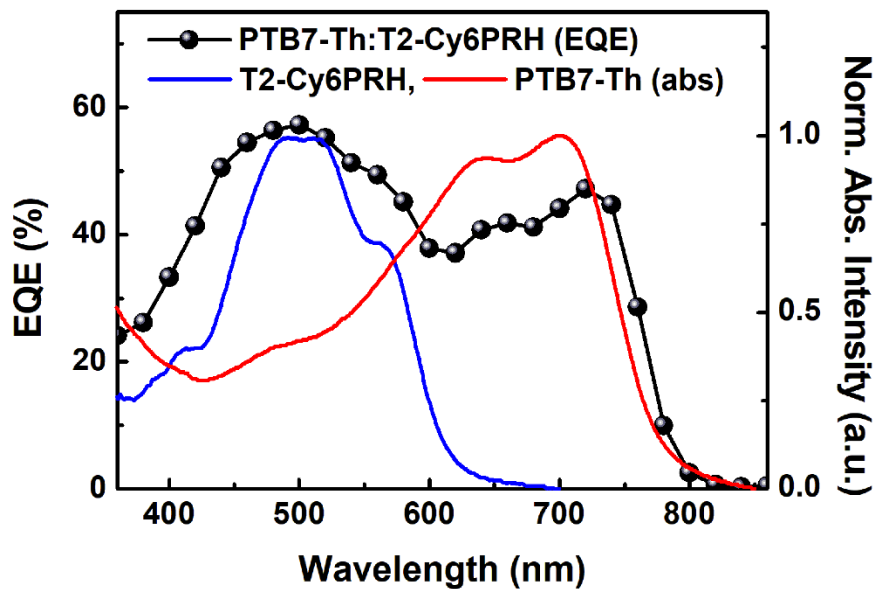


Figure S8. EQE curves of the PTB7-Th:T2-Cy6PRH device (as-cast) together with the absorption spectra of the neat T2-Cy6PRH and PTB7-Th films.

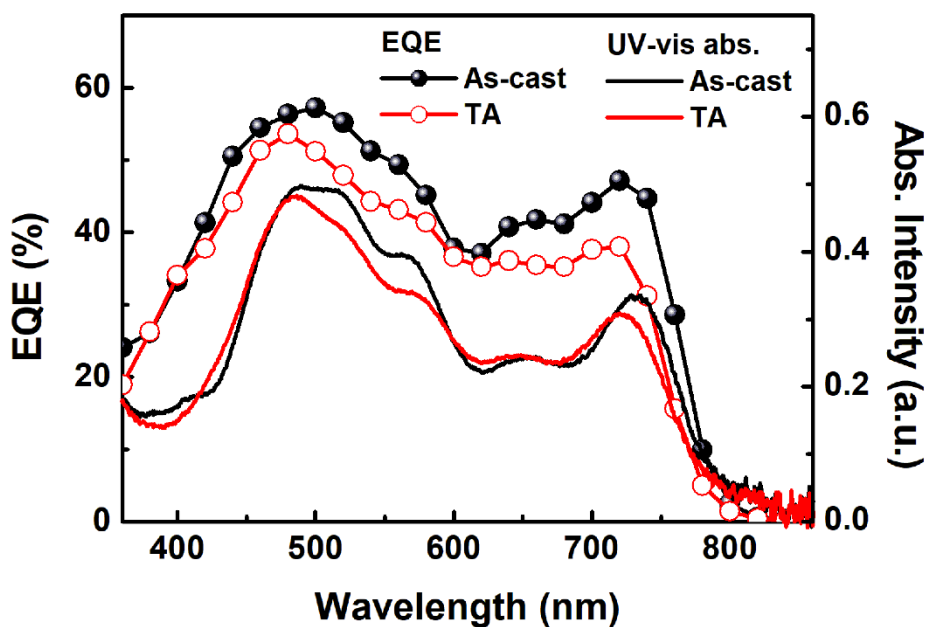


Figure S9. EQE curves of the PTB7-Th:T2-Cy6PRH device and the absorption spectra of the PTB7-Th:T2-Cy6PRH blend films under the as-cast and TA conditions.

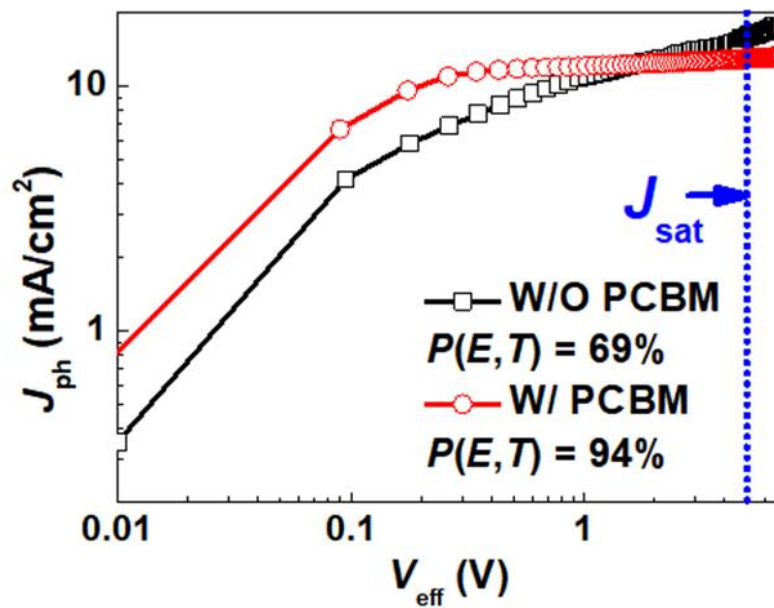


Figure S10. Photocurrent density (J_{ph}) as a function of the effective voltage (V_{eff}) for OSCs based on PTB7-Th:T2-Cy6PRH without and with PCBM third component

Table S2 Photovoltaic properties of OSCs based on the PTB7-Th:PCBM binary film^a

Photoactive layer	V_{OC} [V]	J_{SC} [mA cm^{-2}]	FF [%]	PCE [%]
PTB7-Th:PCBM	0.83 (0.82 ± 0.01)	12.34 (12.17 ± 0.16)	50 (49 ± 2)	5.17 (5.02 ± 0.15)

^a Inverted device architecture is ITO/ZnO NPs/PEIE/PTB7-Th:PCBM (1.0:2.0, chloroform, $d = \sim 100$ nm)/MoO_x/Ag. The values in parentheses are the average photovoltaic properties obtained from over 10 devices.

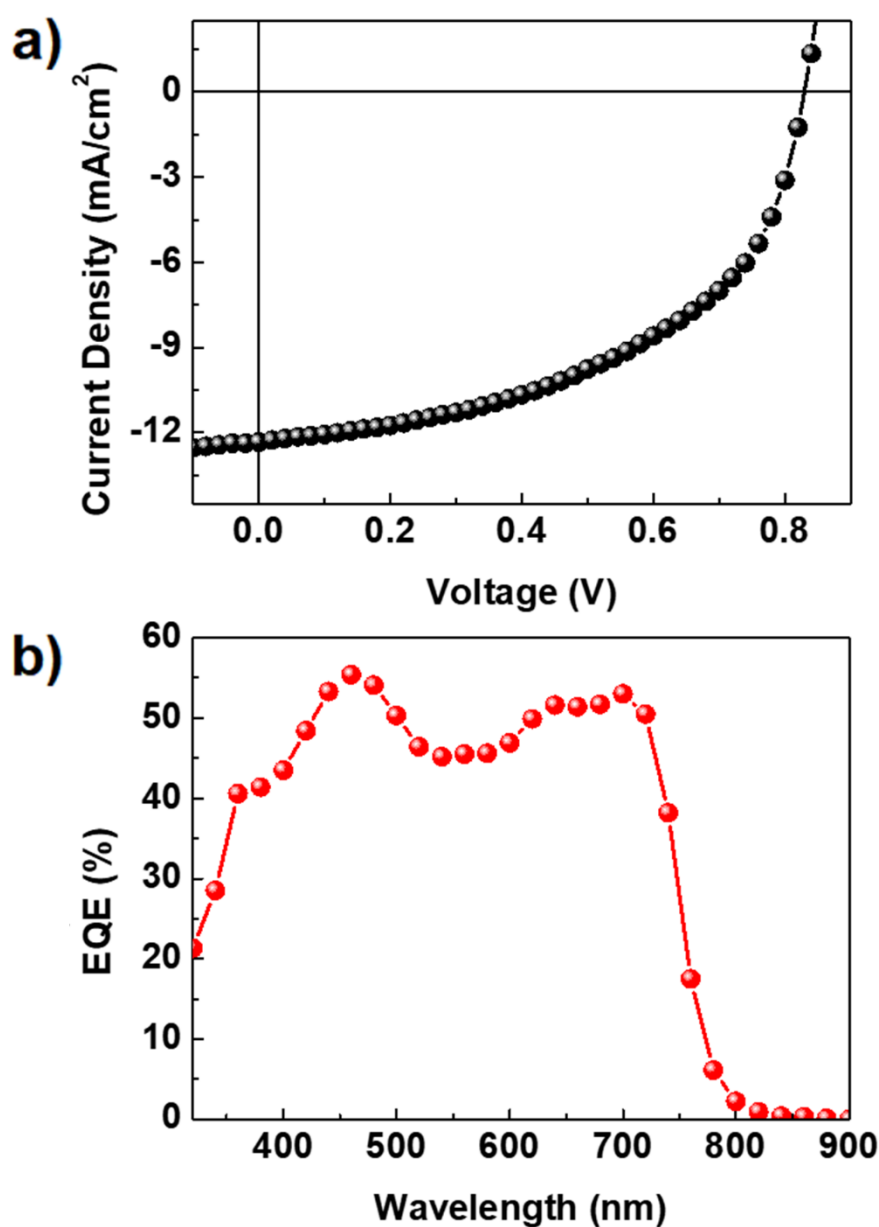


Figure S11. (a) J - V and (b) EQE curves of the device based on PTB7-Th and PCBM.

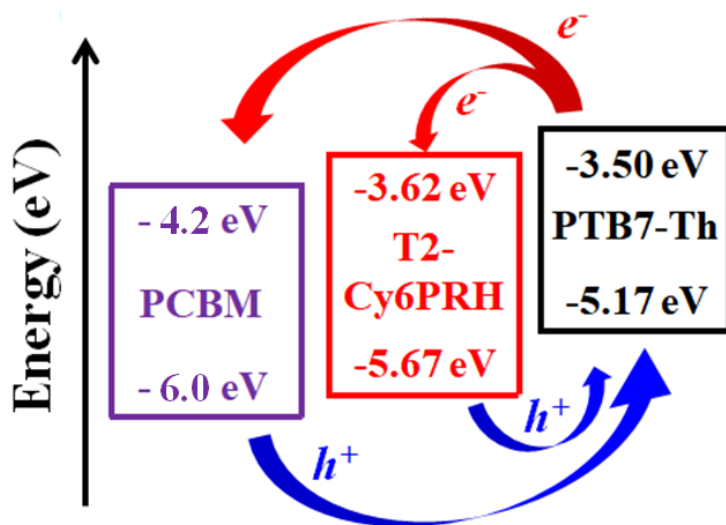


Figure S12. Energy band diagrams of the materials used in ternary cell