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

Subtle Side-chain Tuning on Terminal Groups of Small Molecule Electron Acceptors for Efficient Fullerene-free Polymer Solar Cells

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S1. The extinction coefficients of IT-O1, IT-O2, IT-O3 and IT-O4.

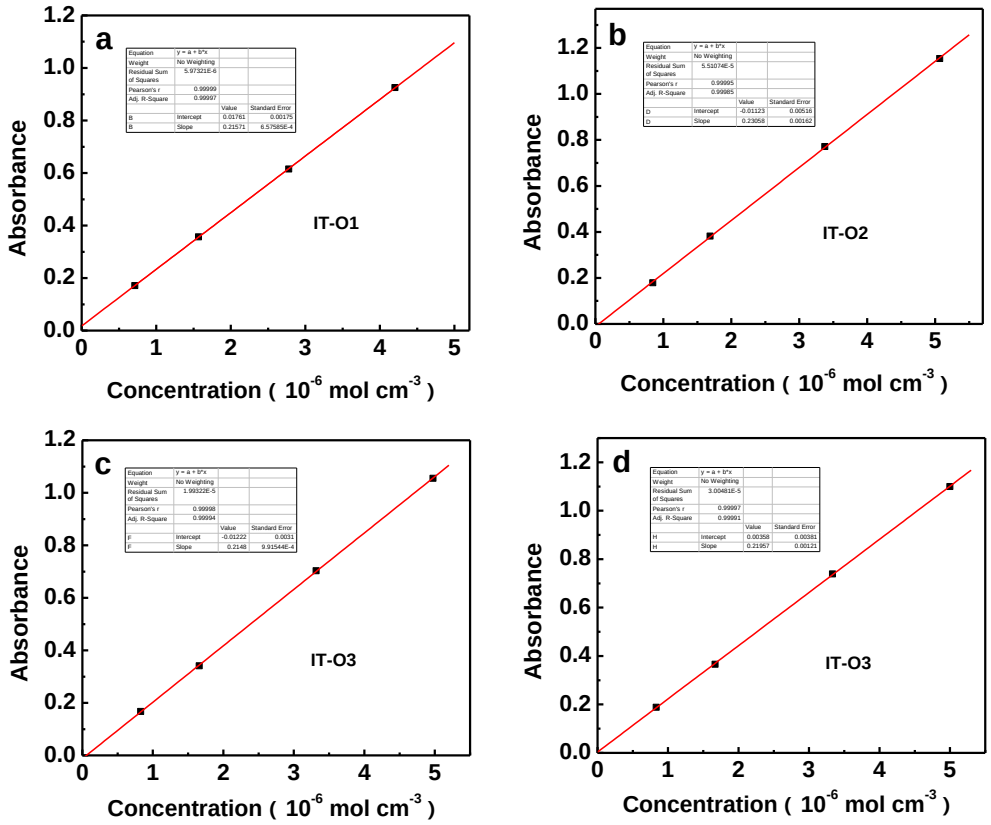


Figure S1. The extinction coefficients of (a) IT-O1, (b) IT-O2, (c) IT-O3 and (d) IT-O4 in chlorobenzene at room temperature.

Acceptor film	extinction coefficients (10^5 cm^{-1})
IT-O1	1.33
IT-O2	1.51
IT-O3	1.11
IT-O4	1.00

Table S1. The extinction coefficients as solid thin films of IT-O1, IT-O2, IT-O3 and IT-O4.

S2. UV-Vis absorption spectra of the materials and PBDB-T blend.

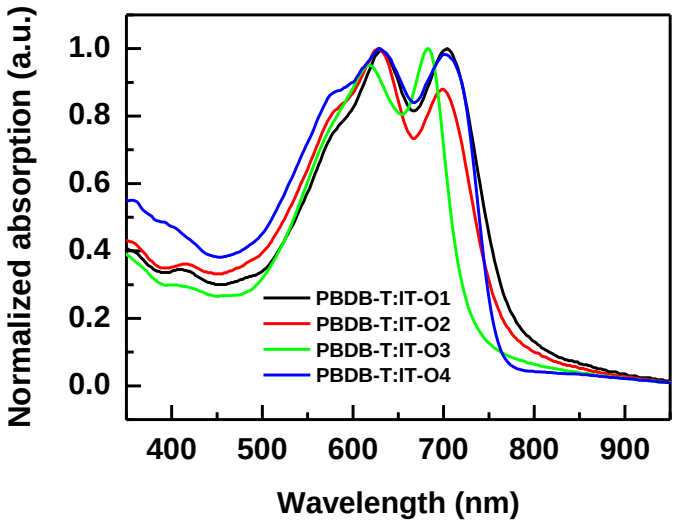


Figure S2. UV–Vis absorption spectra of PBDB-T:IT-O1, PBDB-T:IT-O2 PBDB-T:IT-O3, PBDB-T:IT-O4 blend films.

S3. Theoretical calculations on IT-O1, IT-O2, IT-O3 and IT-O4.

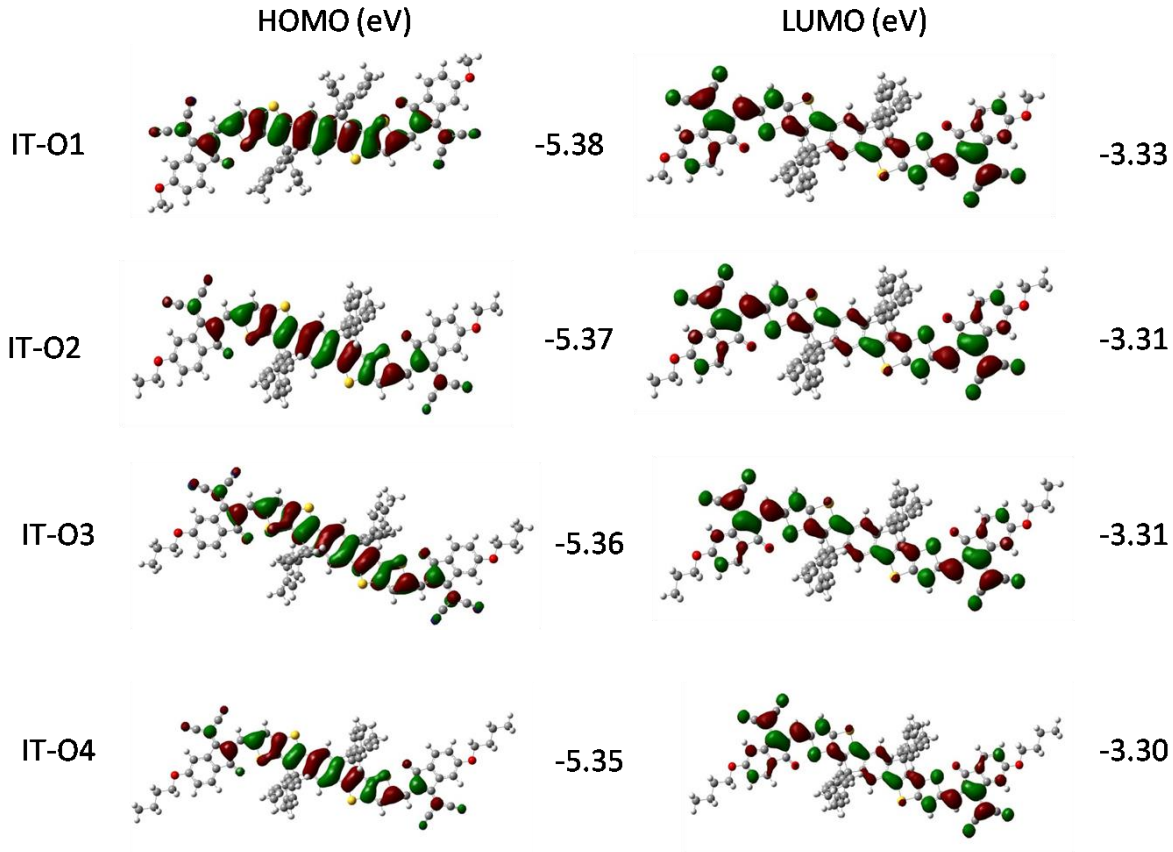


Figure S3. Theoretical calculation results of IT-O1, IT-O2, IT-O3 and IT-O4.

S4. PL spectra of blend films.

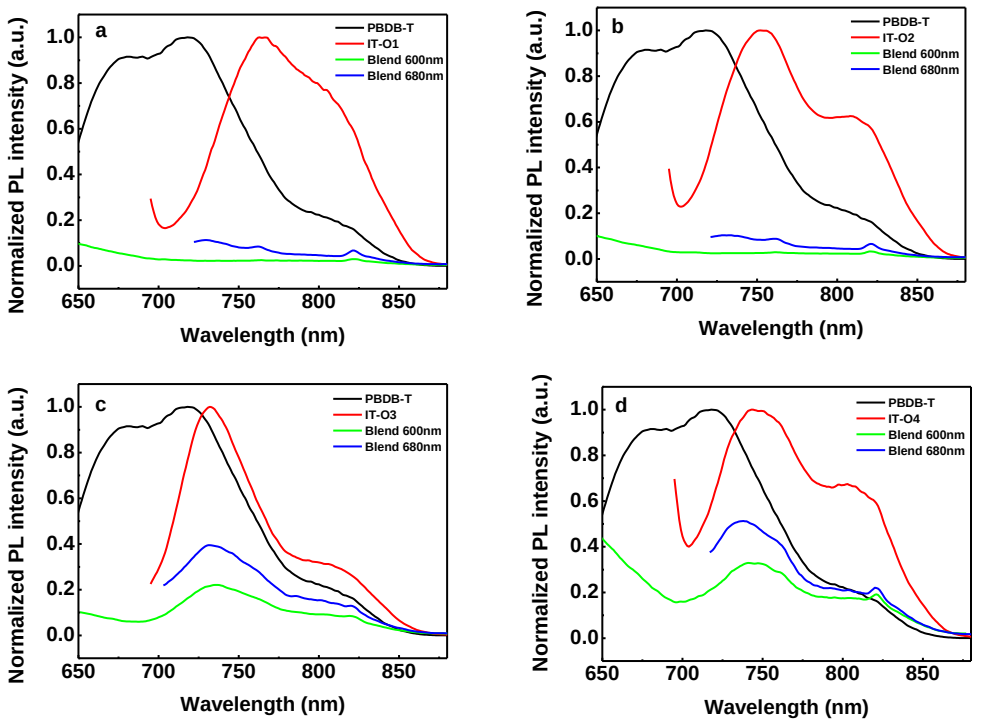


Figure S4. Normalized PL spectra of polymer PBDB-T-based neat film, IT-(O1-O4)-based neat films and the PBDB-T: IT-(O1-O4)-based blend films. (PBDB-T was excited at 600 nm, all IT-(O1-O4) were excited at 680 nm, all PBDB-T: IT-(O1-O4)-based blend films were excited at both 680 nm and 600 nm.)

S5. Carrier mobility ofPBDB-T:acceptor blends.

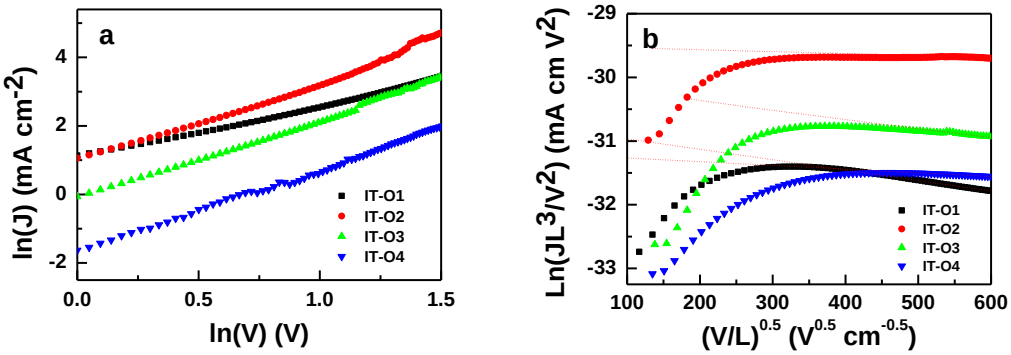
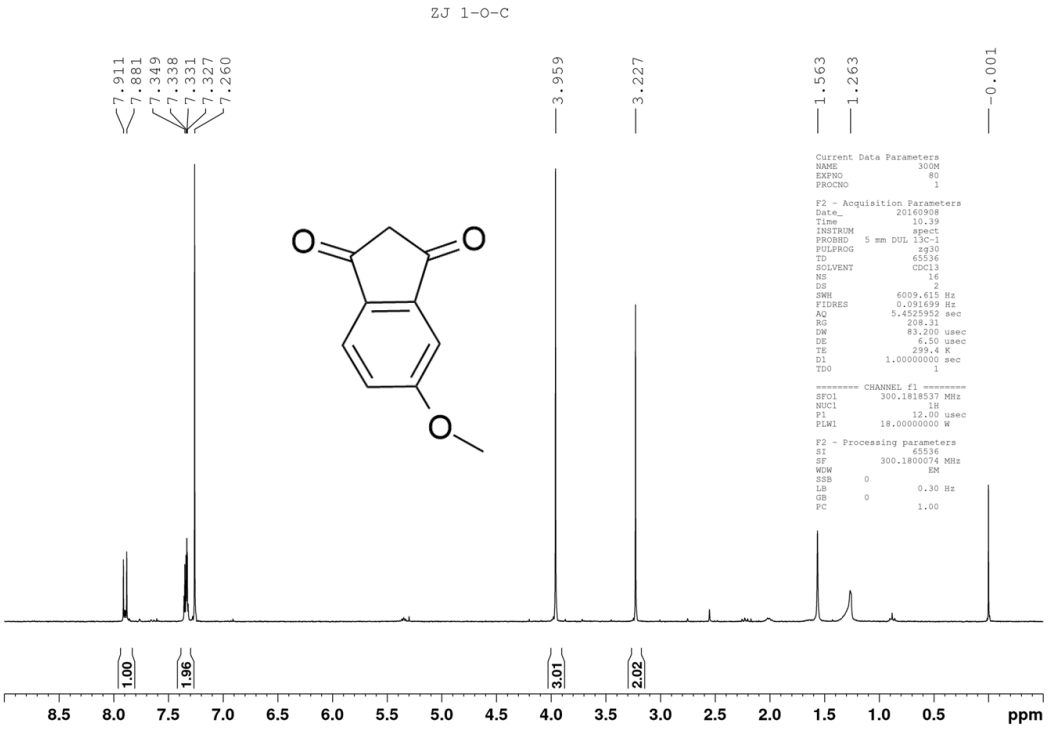
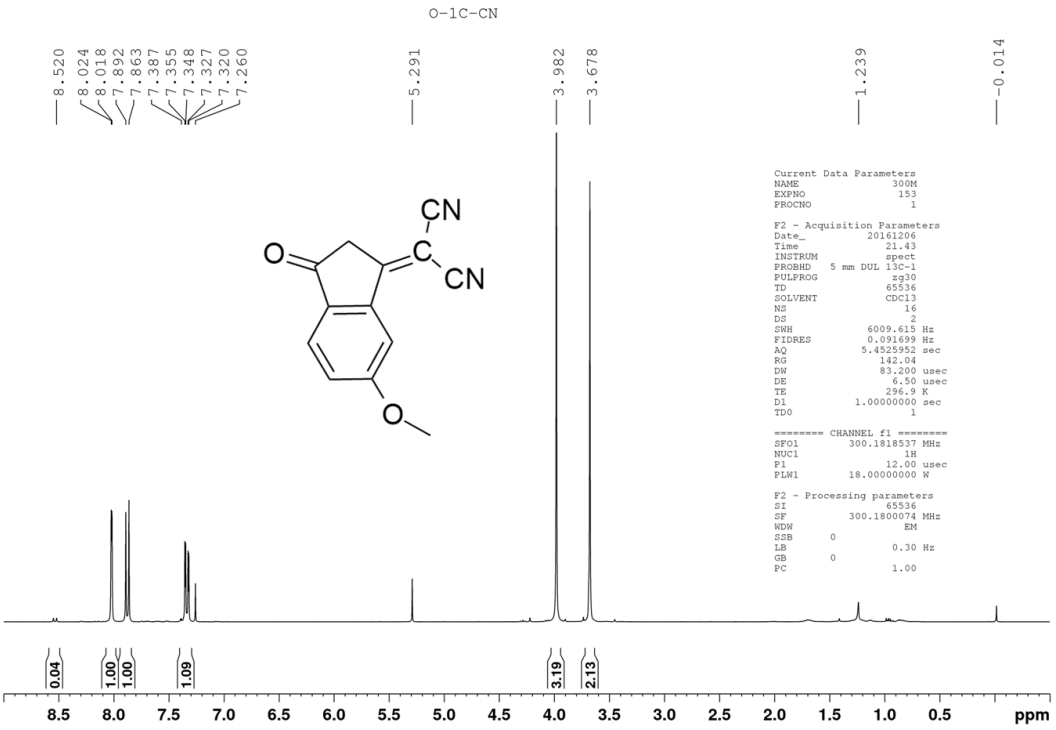


Figure S5. Plots for the calculation of electron and hole mobilities of PBDB-T:IT-O1, PBDB-T:IT-O1, PBDB-T:IT-O1 and PBDB-T:IT-O4 based blends obtained from the (a) electron-only and (b) hole-only devices.

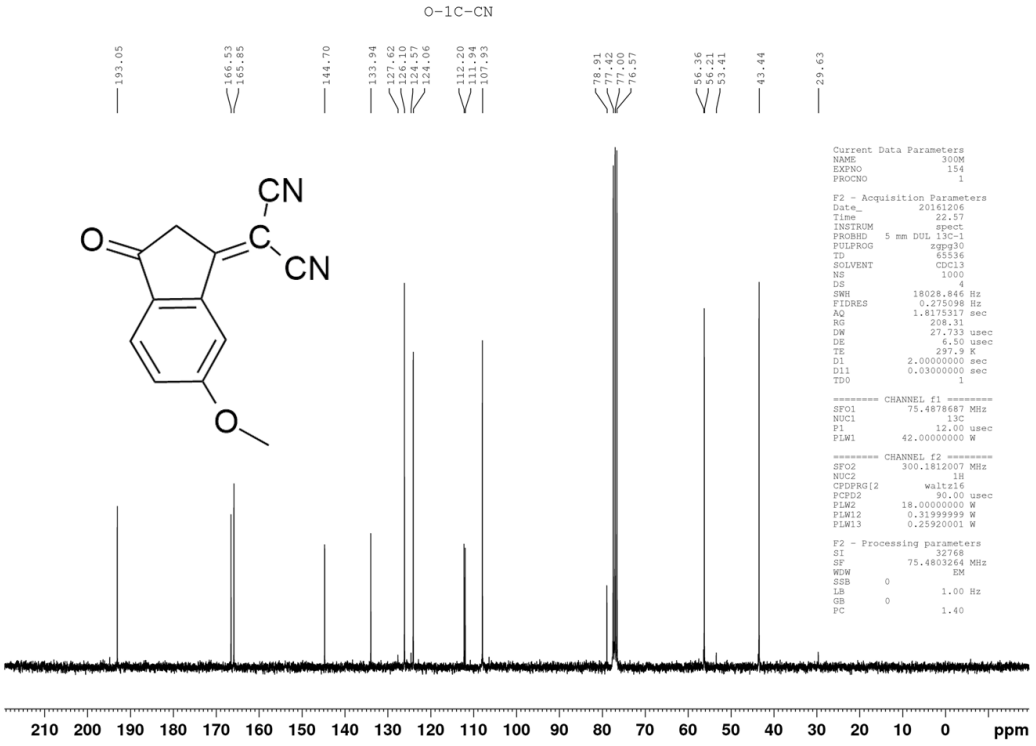
S7. NMR spectra of the materials (solvent: $CDCl_3$ (^{1}H NMR: 7.60 ppm, ^{13}C NMR: 77.3 ppm)).



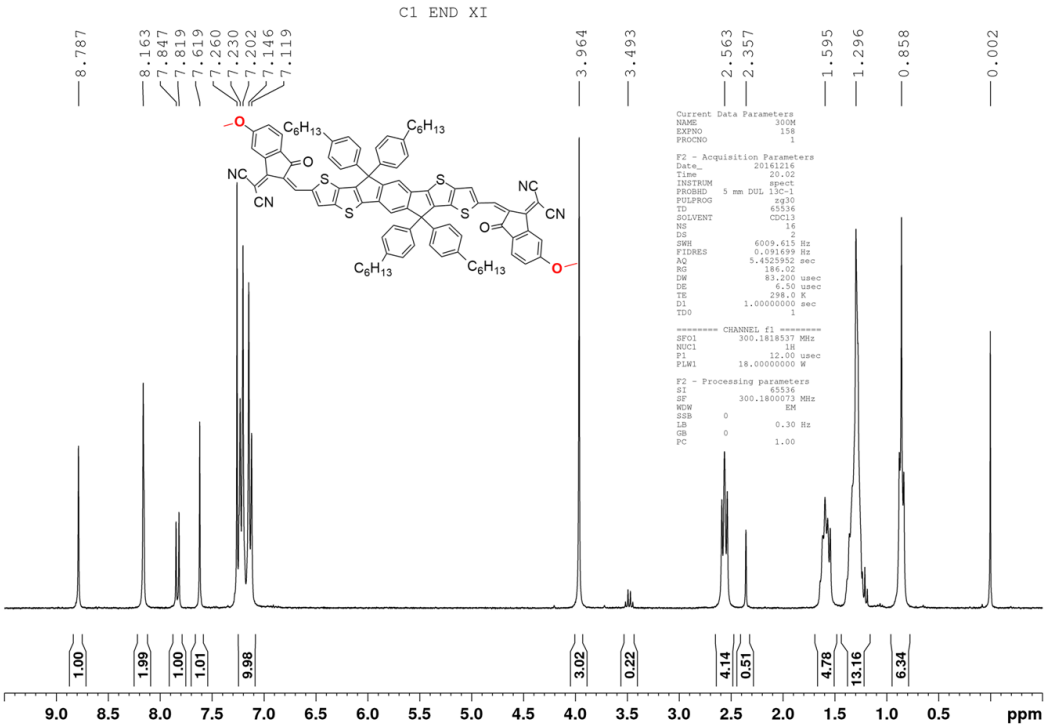
^{1}H NMR spectrum of IN-O1



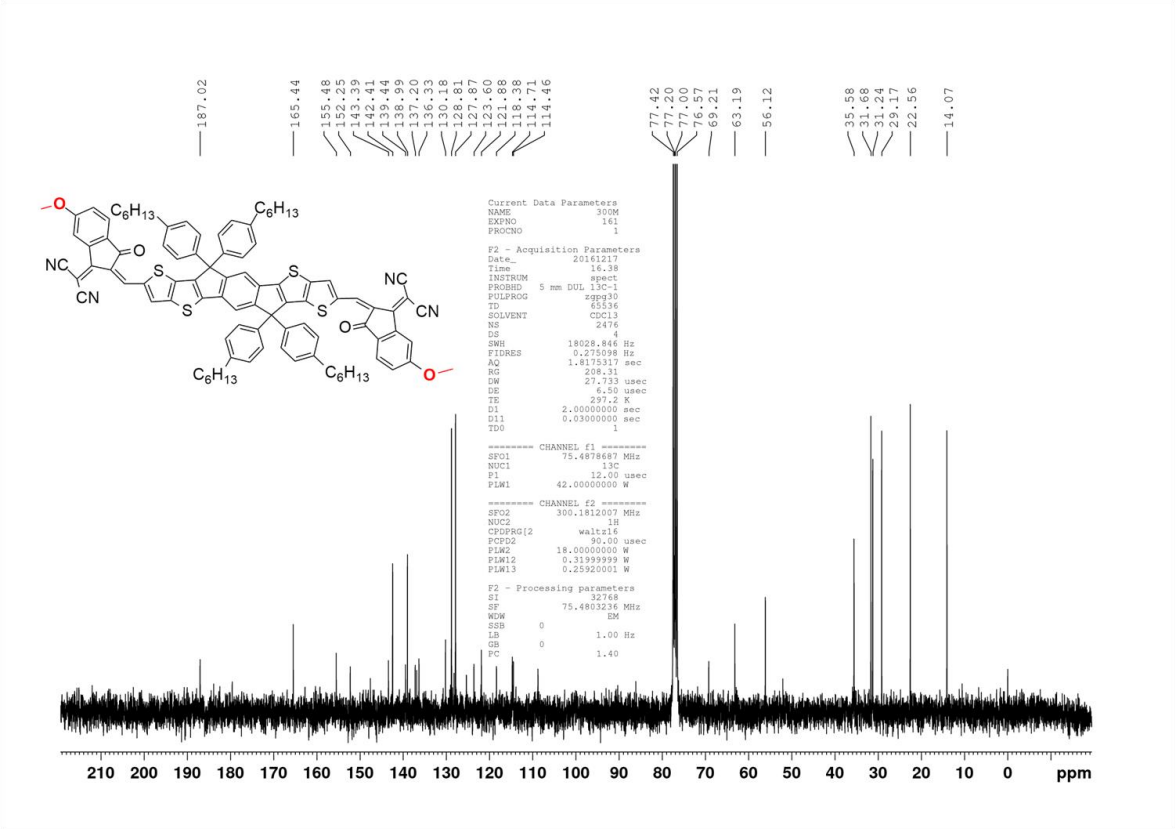
^{1}H NMR spectrum of DCI-O1



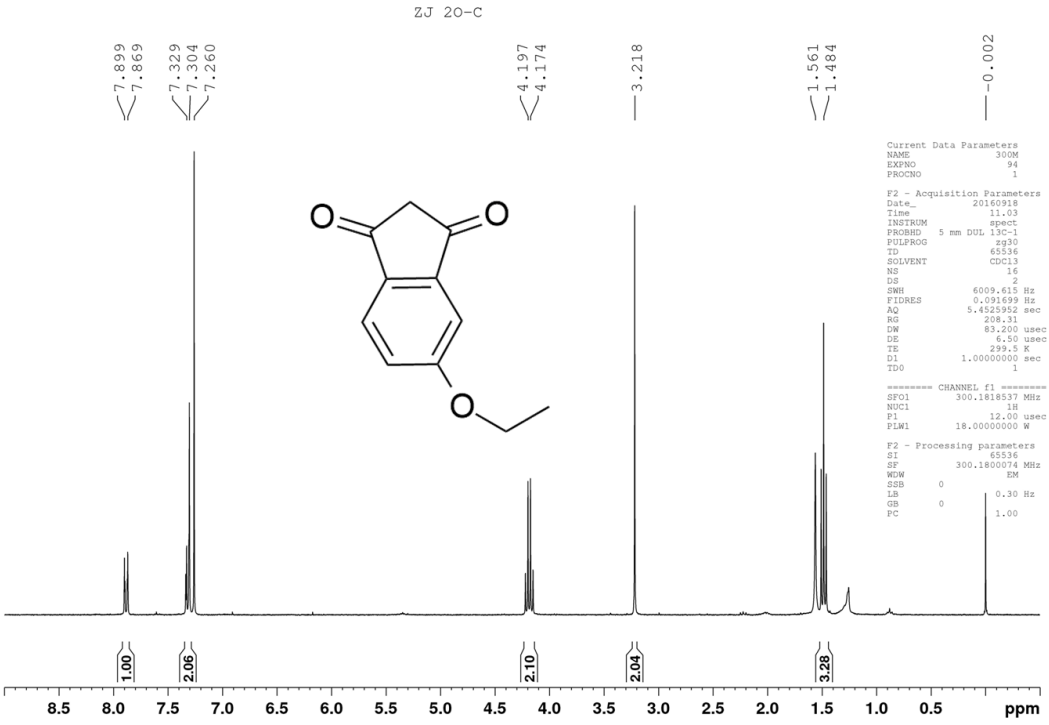
^{13}C NMR spectrum of DCM-O1



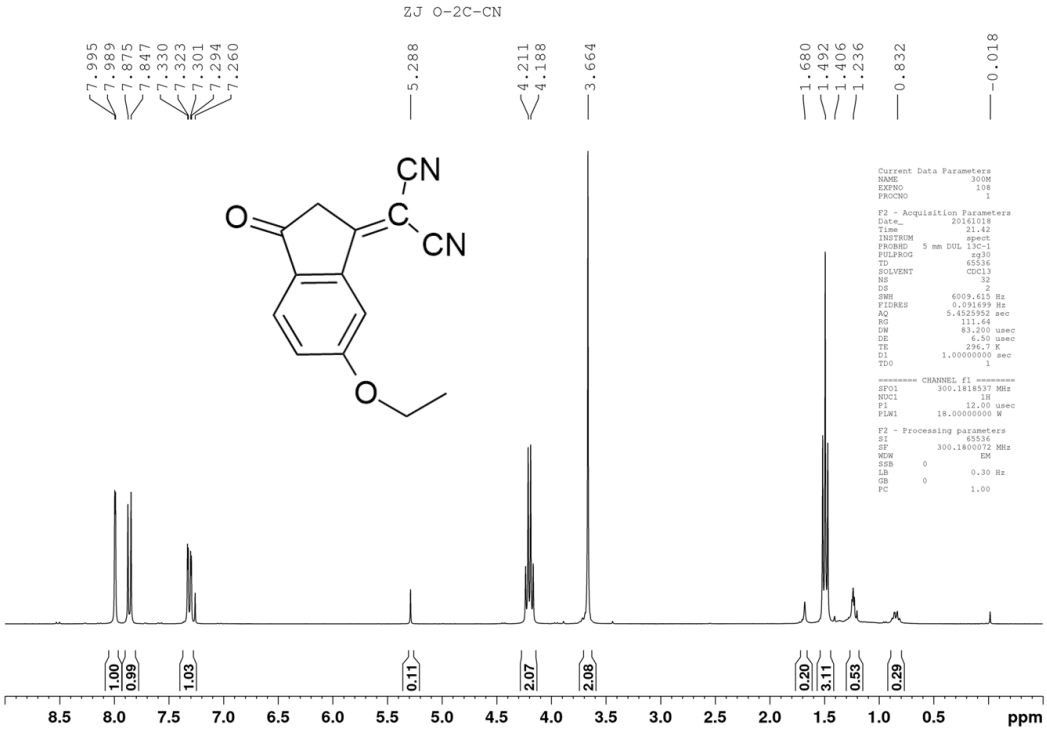
^{1}H NMR spectrum of IT-O1



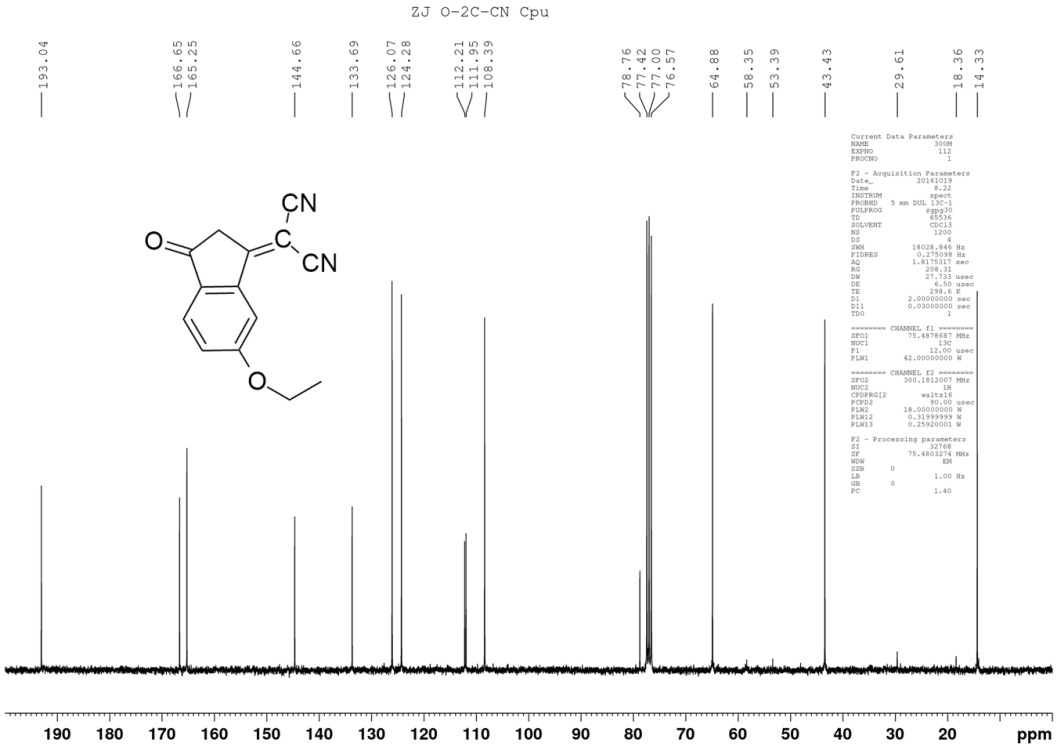
^{13}C NMR spectrum of IT-O1



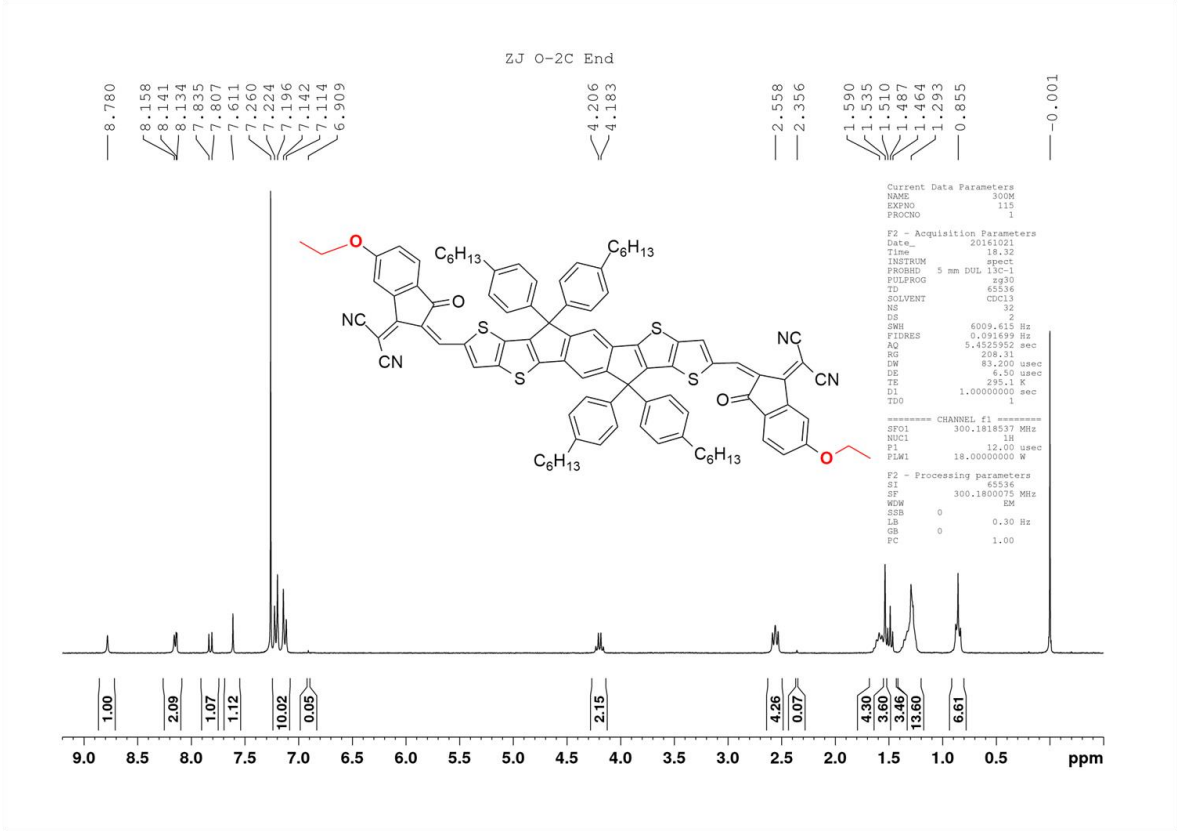
^{1}H NMR spectrum of IN-O2



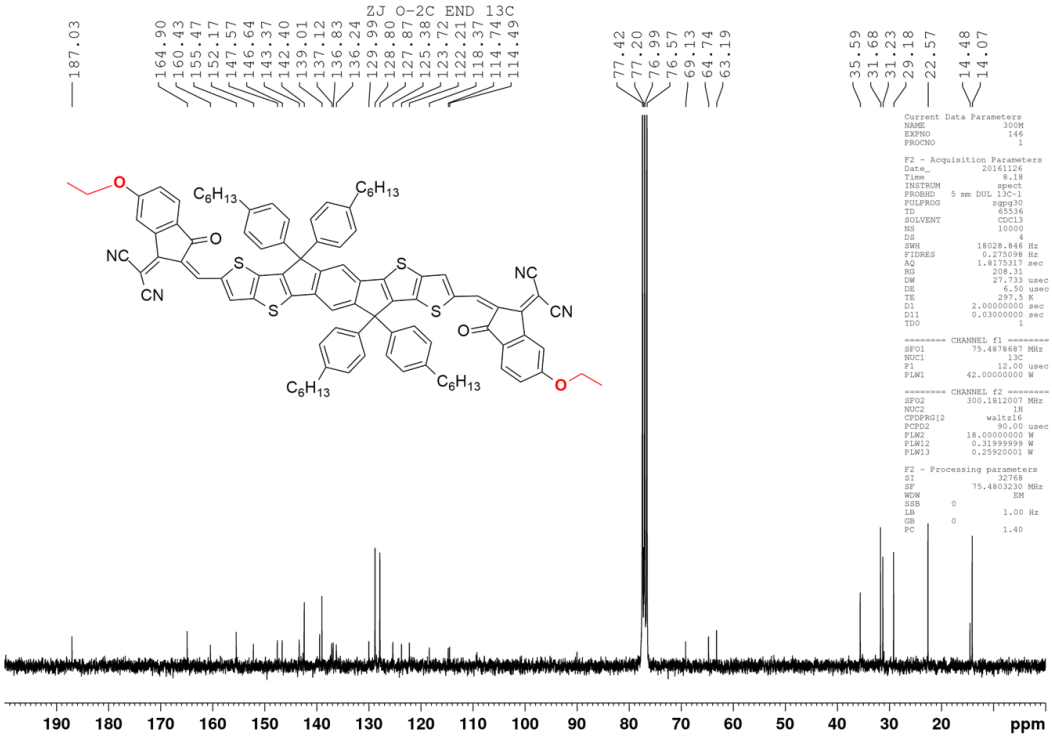
^{1}H NMR spectrum of DCI-O2



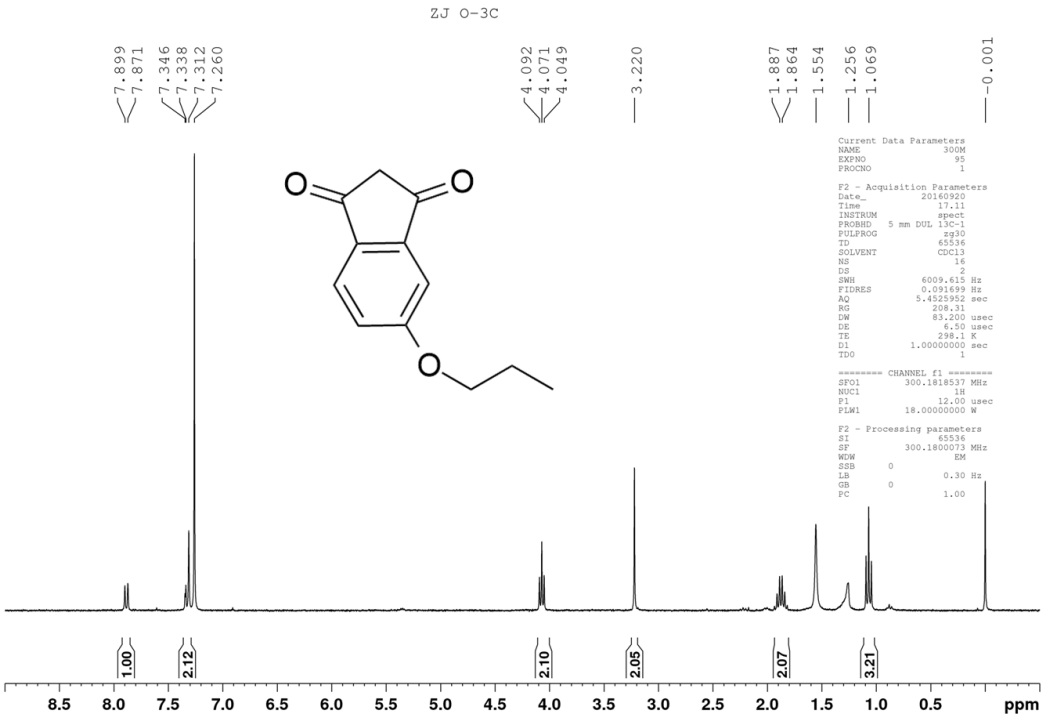
^{13}C NMR spectrum of DCI-O2



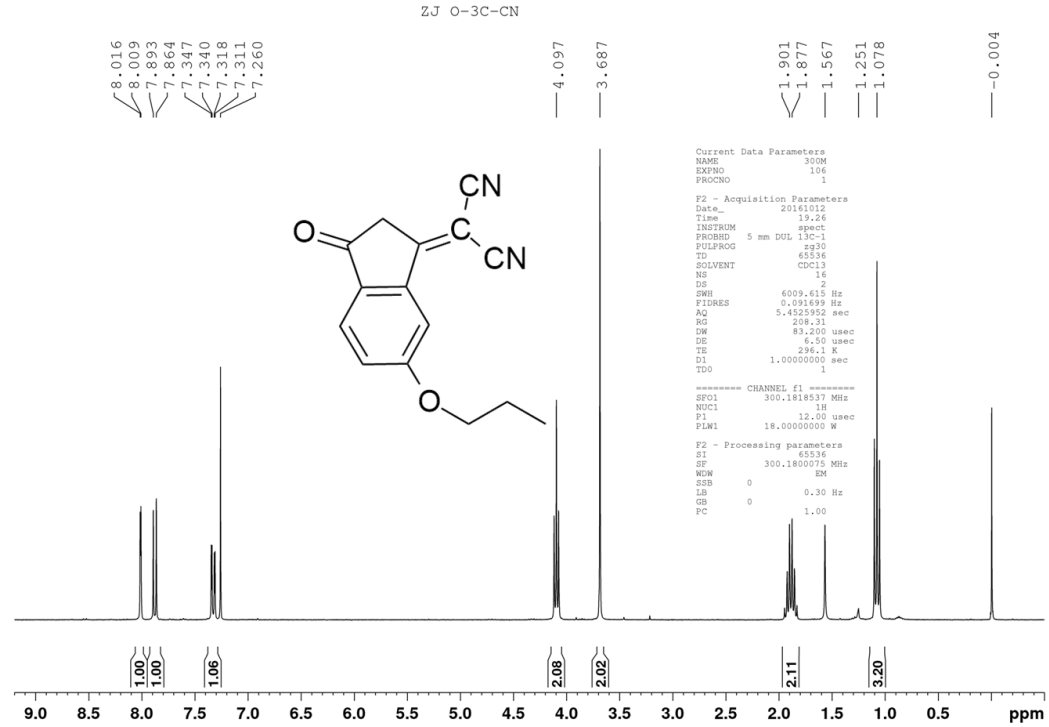
^{1}H NMR spectrum of IT-O2



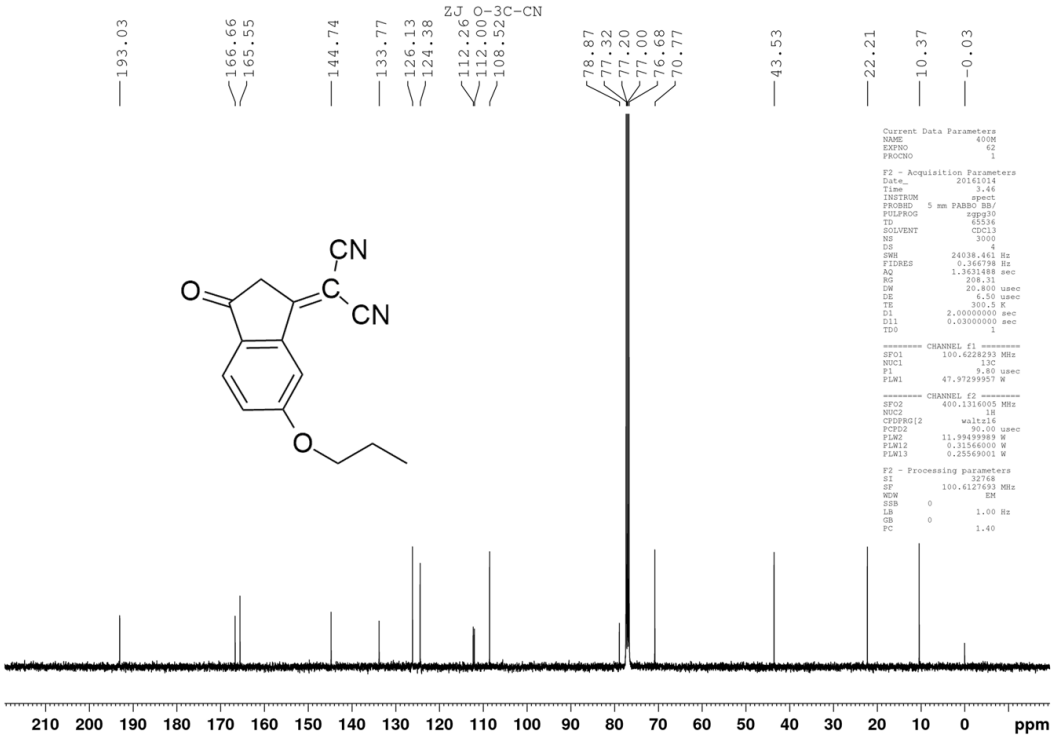
^{13}C NMR spectrum of IT-O2



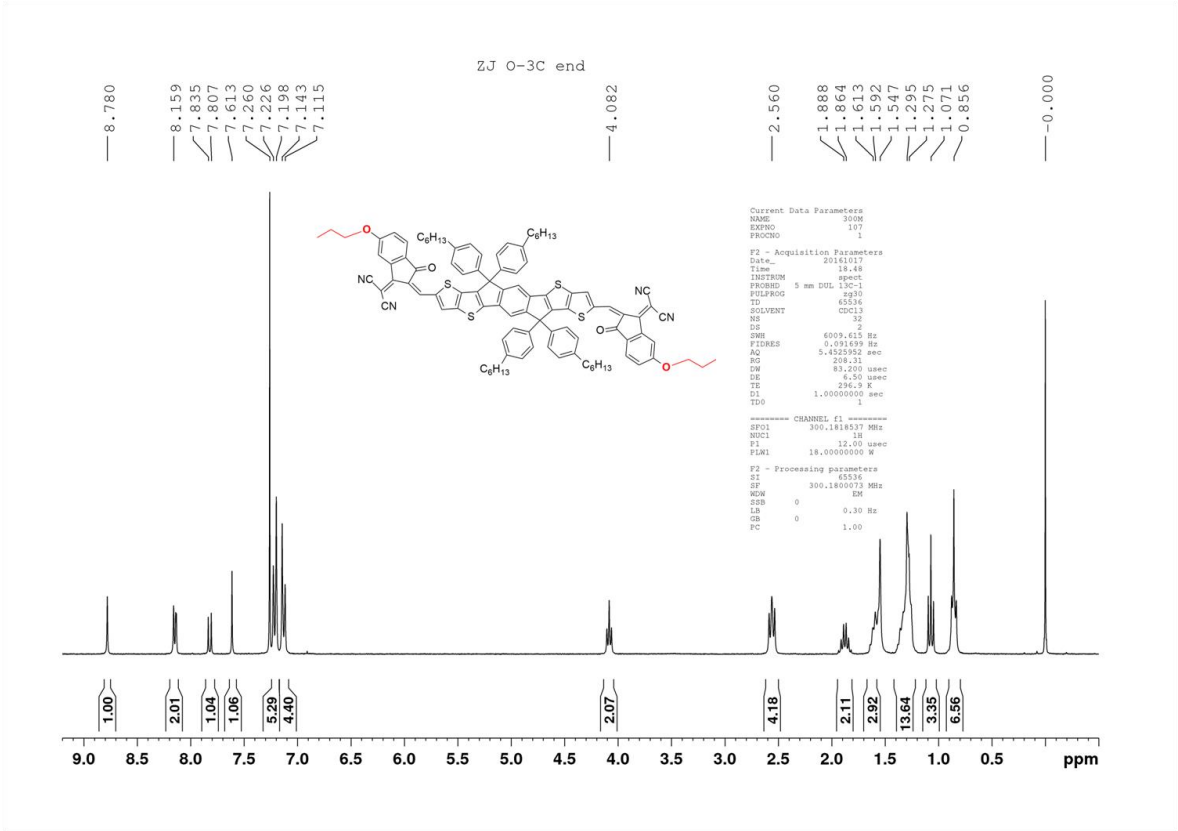
^{1}H NMR spectrum of IN-O3



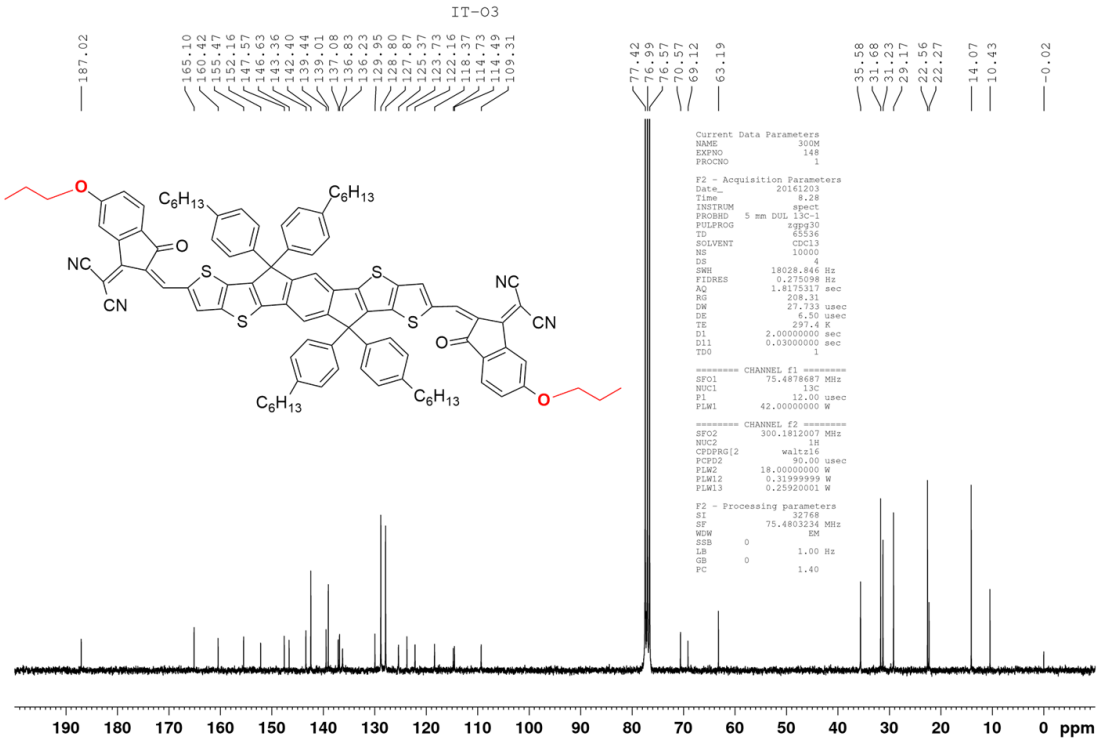
^{1}H NMR spectrum of DCI-O3



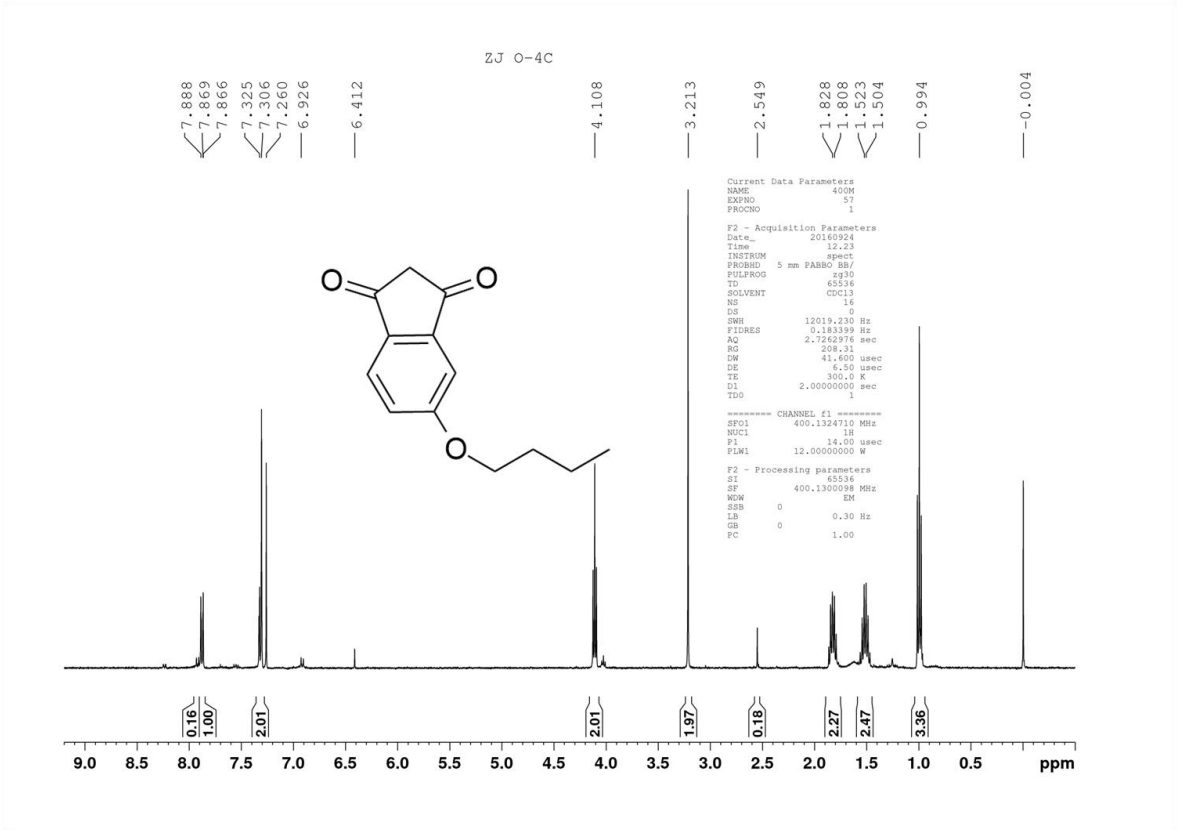
^{13}C NMR spectrum of DCI-O3



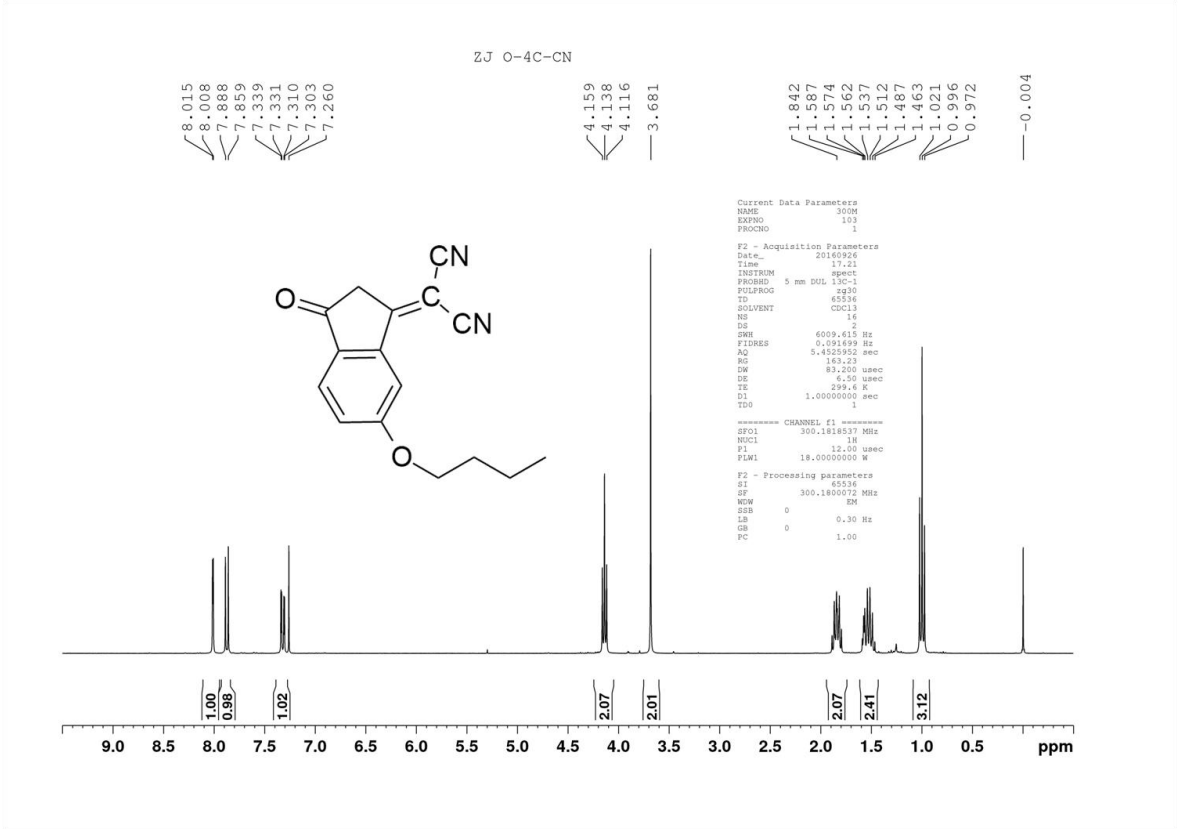
^{1}H NMR spectrum of IT-O3



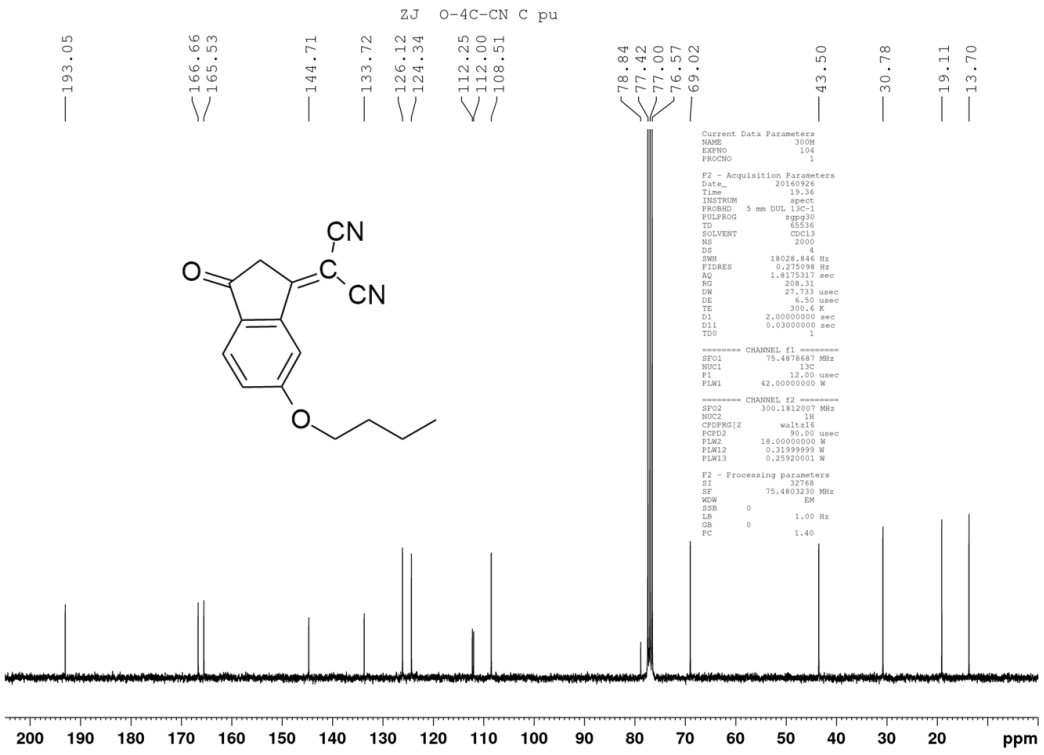
^{13}C NMR spectrum of IT-O3



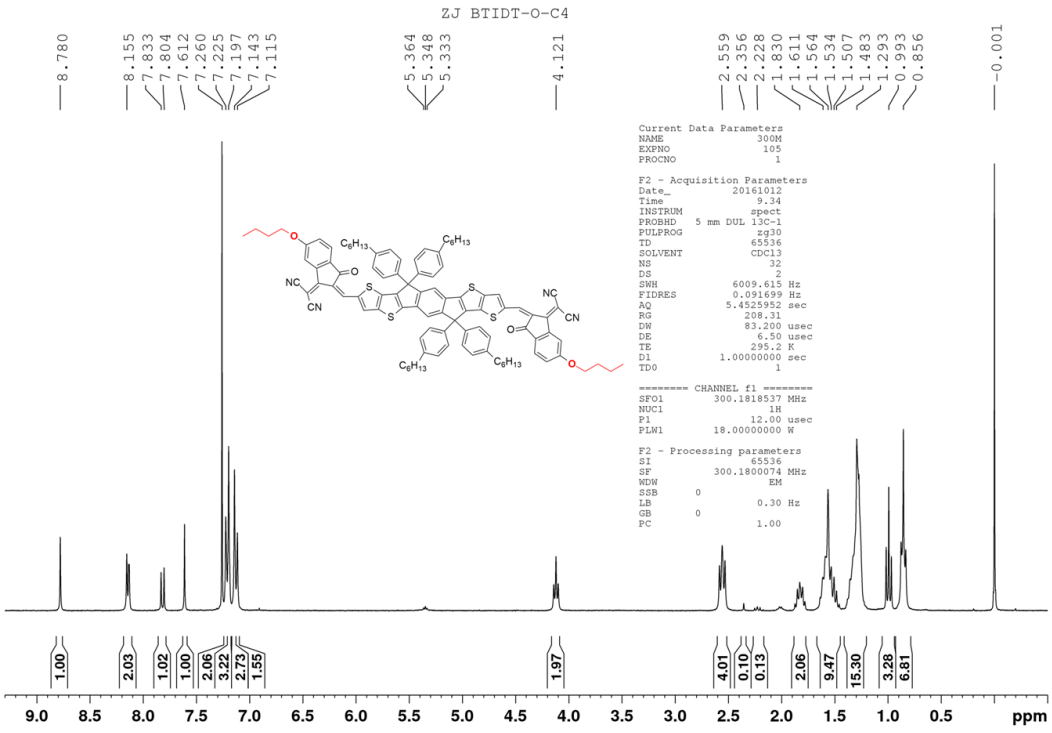
^{1}H NMR spectrum of IN-O4



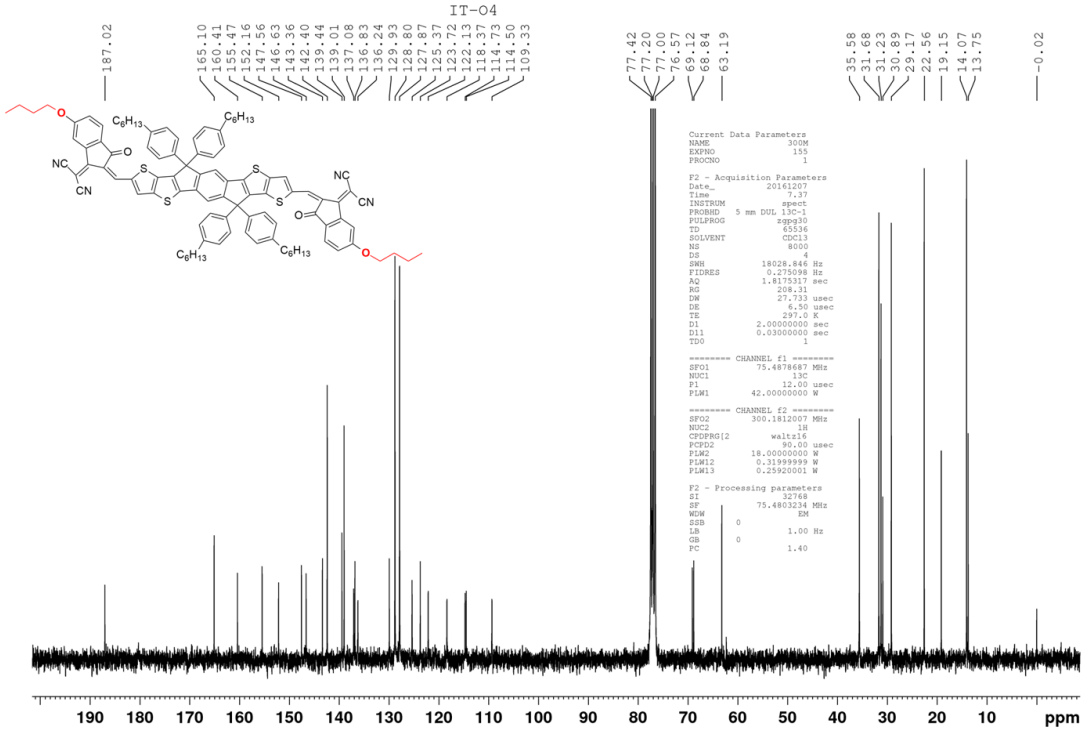
^{1}H NMR spectrum of DCI-O4



^{13}C NMR spectrum of DCI-O4



^{1}H NMR spectrum of IT-O4



^{13}C NMR spectrum of IT-O4