Supporting Information for

Designing Thiophene-fused benzoxadizole as an Acceptor to Build a Narrow Bandgap Polymer for All-Polymer Solar Cells

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Device fabrication

All polymer solar cells were fabricated with a structure of ITO/PEDOT:PSS/P3HT:PBXT-IDT/Ca/Al. The patterned indium tin oxide (ITO) glass (sheet resistance= 10 Ω □$^{-1}$) was pre-cleaned in an ultrasonic bath of deionized water, acetone and isopropanol, followed by oxygen plasma treatment (25 min) in an ultraviolet– ozone chamber (Jelight Company, USA). A thin layer (30 nm) of poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS, Baytron PVP AI 4083, Germany) was spin-coated onto the ITO glass at 4000 rpm and baked subsequently at 150 ^{o}C for 20 min. The mixture of P3HT:PBXT-IDT in chlorobenzene solvent (14 mg mL^{-1} in total) with or without chloroform was spin-coated on a PEDOT:PSS layer to form an active layer. Calcium (ca. 20 nm) and aluminium (ca. 80 nm) layers were deposited onto the active layer in a vacuum at a pressure of *ca*. 5.0 × 10^{-5} Pa to form the negative electrode. The active area of the device was 4mm^2. The current density–voltage (*J-V*) characteristics were measured on a computer–controlled B2912A Precision Source/Measure Unit (Agilent Technologies). A XES-70S1 (SAN-EI Electric Co., Ltd) solar simulator (AAA grade, 70 × 70 mm^2 photobeam size) coupled with AM 1.5 G solar spectrum filters was used as the light source, and the optical power at the sample was 100 mW/cm^2. A 2 × 2 cm^2 monocrystalline silicon reference cell (SRC-1000-TC-QZ) was purchased from VLSI Standards Inc. A Solar Cell Spectral Mrasurement System QE-R3011 (Enlitech Co., Ltd) was used for the EQE spectrum measurement. The light intensity at each wavelength was calibrated using a standard single crystal Si photovoltaic cell. The hole mobility and electron mobility were measured using the structure: ITO/PEDOT:PSS/ P3HT:PBXT-IDT/Au and ITO/titanium (diisopropoxide) bis(2,4-pentanedionate) (TIPD)/ P3HT:PBXT-IDT/Al respectively. And the mobility was extracted by fitting the curremt J–V curves using the Mott–Gurney relationship (space charge limited current).

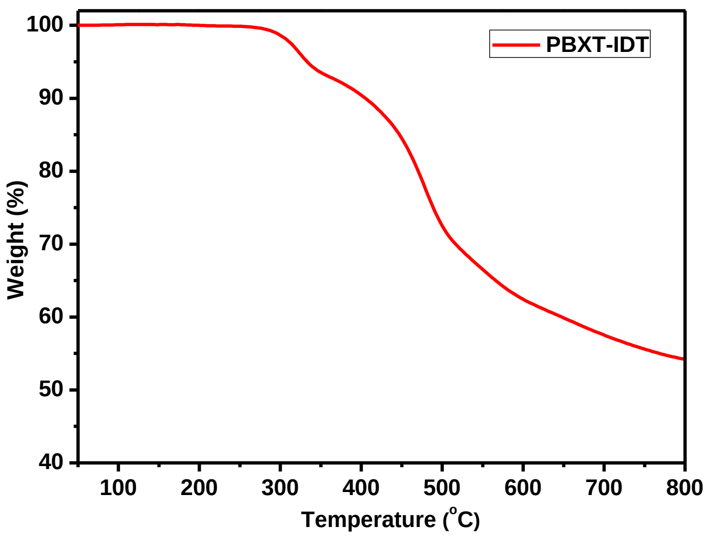


Figure S1. The TGA curve of PBXT-IDT

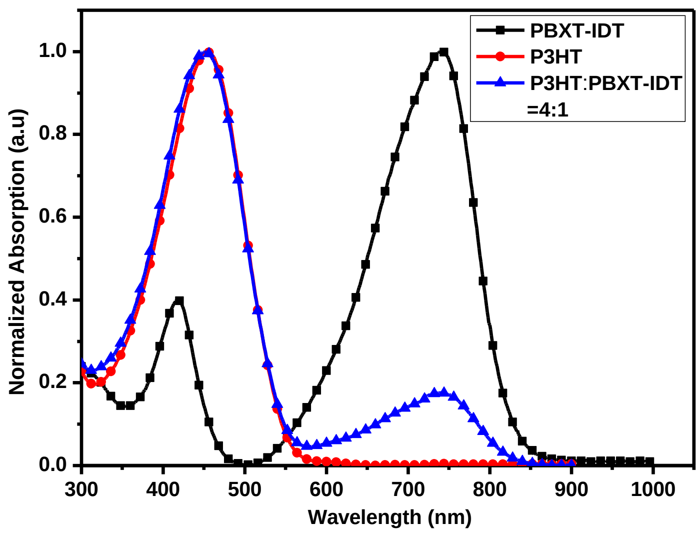


Figure S2. Absorption spectra of PBXT-IDT, P3HT and P3HT:PBXT-IDT (4:1,p/n) in chlorobenzene

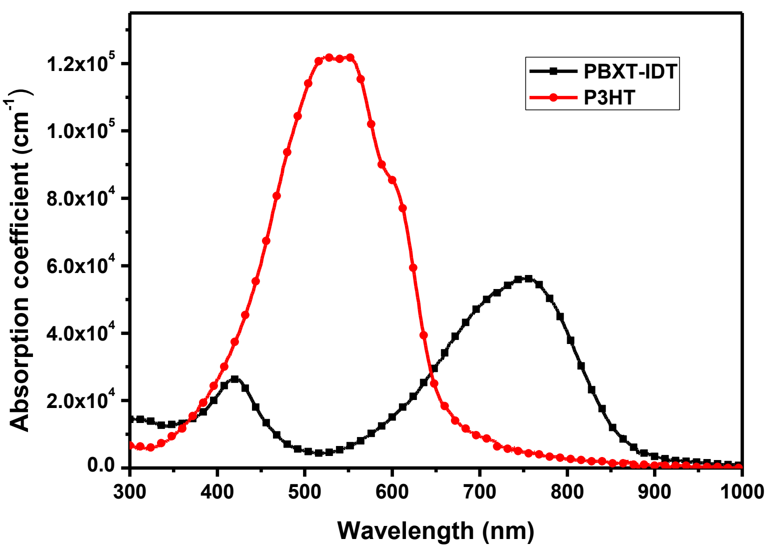


Figure S3. The absorption spectra of PBXT-IDT and P3HT in thin films

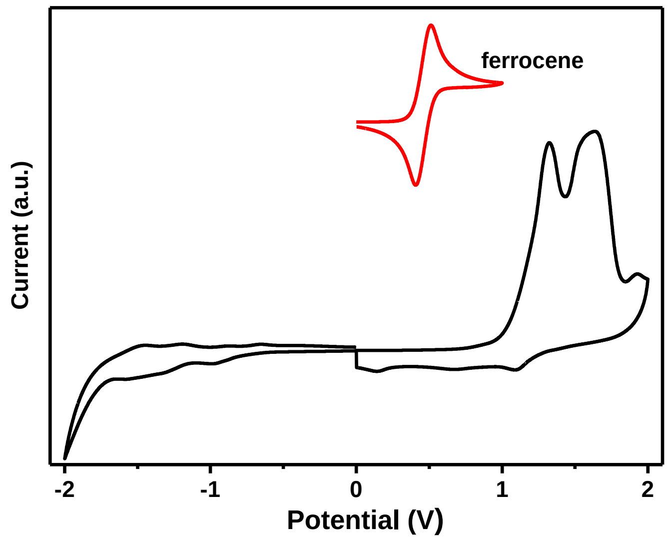


Figure S4. The CV curve of PBXT-IDT

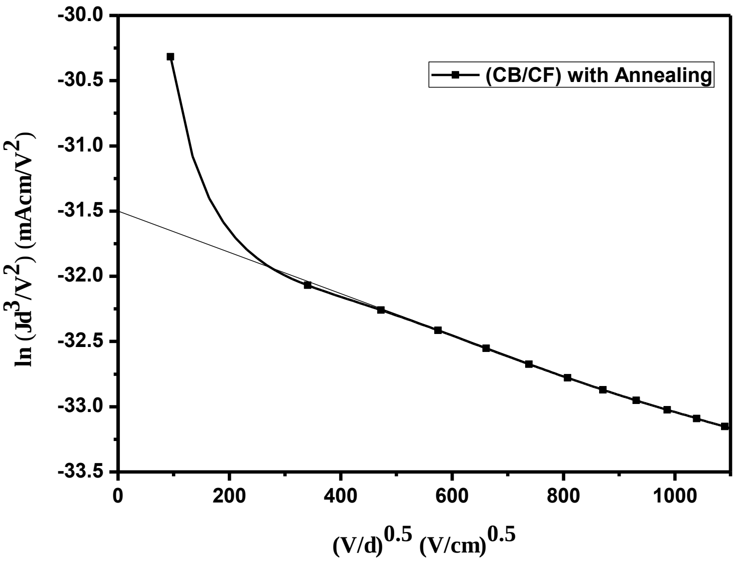


Figure S5. Ln(JL^3/V^2) vs $(V/L)^{0.5}$ of plot of the all-PSCs based on P3HT / PBXT-IDT for the hole mobility measurement.

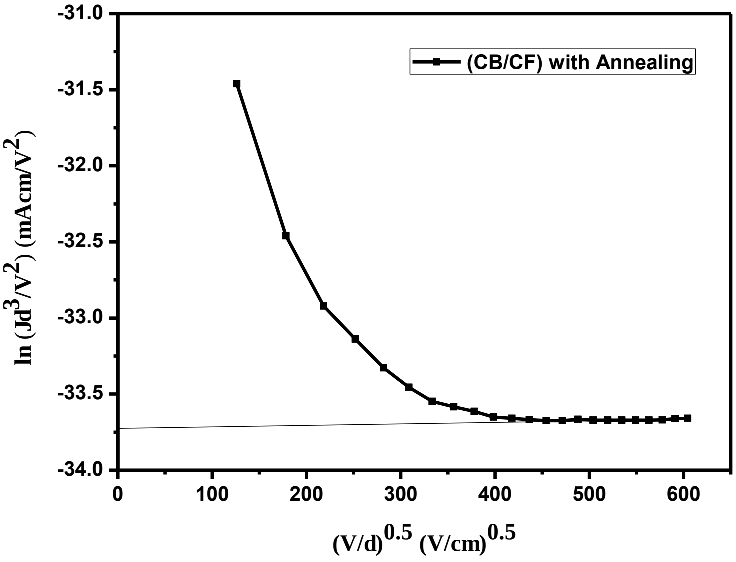


Figure S6. Ln(JL^3/V^2) vs $(V/L)^{0.5}$ of plot of the all-PSCs based on P3HT / PBXT-IDT for the electron mobility measurement.

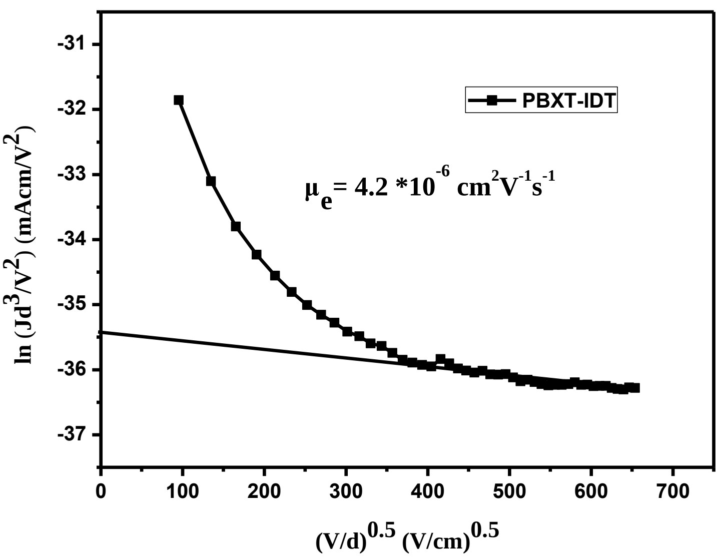


Figure S7. Ln(JL^3/V^2) vs $(V/L)^{0.5}$ of plot of the pure PBXT-IDT film for the electron mobility measurement.

Table S1. OPV performances based on PBXT-IDT and P3HT with different p/n ratio.

Polymer	p/n	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
PBXT-IDT	1:1	0.83	1.15	33.59	0.32
PBXT-IDT	2:1	0.86	1.07	45.09	0.42
PBXT-IDT	3:1	0.88	1.18	44.29	0.46
PBXT-IDT	4:1	0.88	1.41	43.81	0.54
PBXT-IDT	5:1	0.83	1.19	37.01	0.36

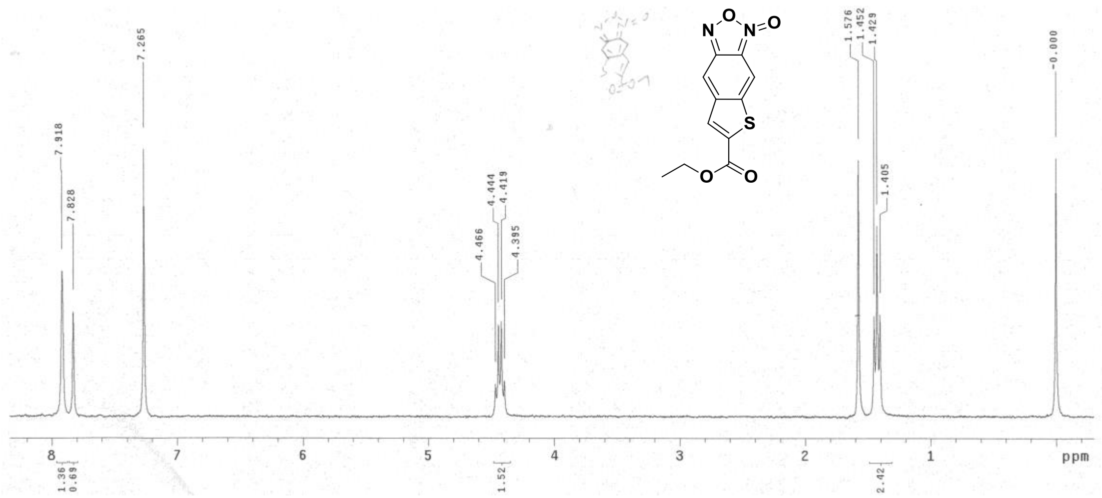
Table S2. OPV performances based on P3HT/PBXT-IDT (4:1, w/w) at different thermal annealing temperature.

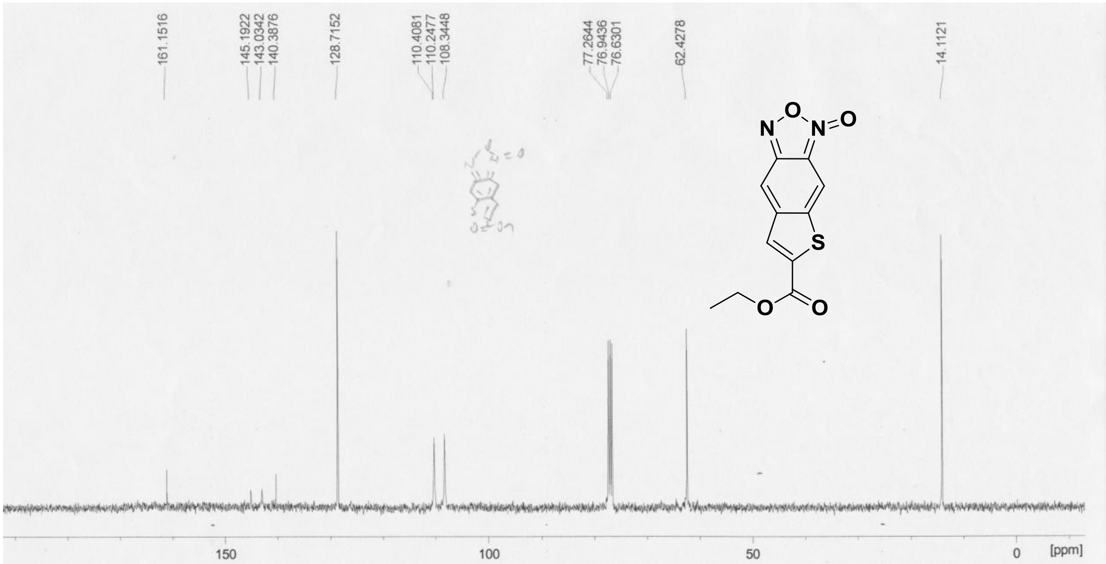
Polymer	Annealing (^{o}C)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
PBXT-IDT	90	0.83	2.27	40.22	0.76
PBXT-IDT	100	0.79	2.24	47.75	0.85
PBXT-IDT	110	0.76	2.15	41.30	0.68

Table S3. OPV performances based on P3HT/PBXT-IDT (4:1, w/w) with different volume of chloroform with thermal annealing at 100 °C.

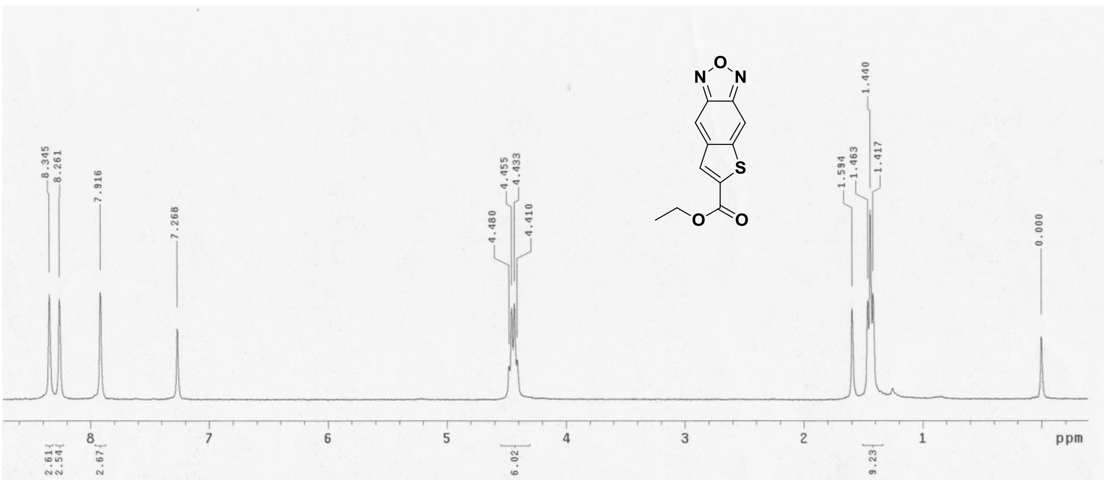
Polymer	Chloroform (%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
PBXT-IDT	5	0.82	2.41	44.27	0.87
PBXT-IDT	10	0.84	2.95	43.86	1.09
PBXT-IDT	20	0.83	2.26	47.74	0.90

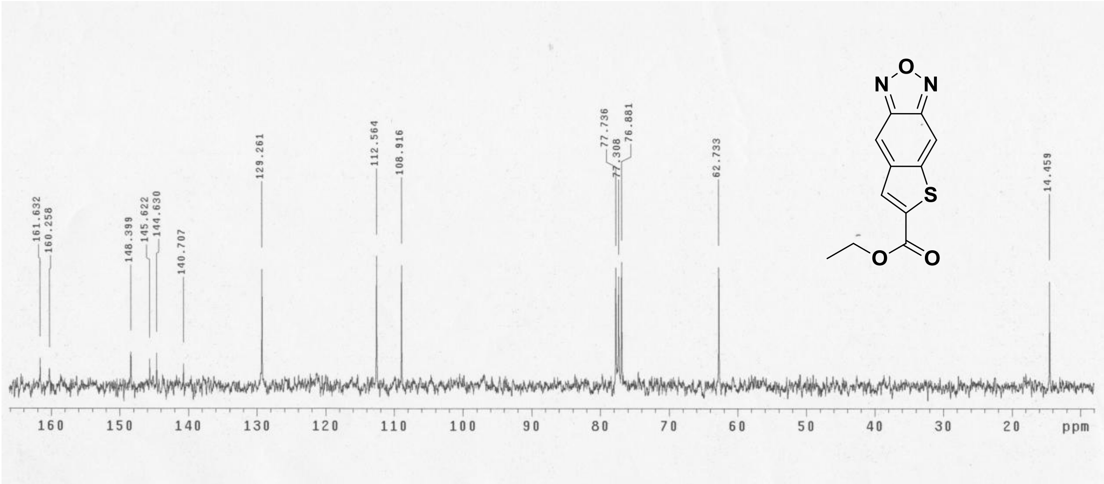
^{1}H NMR and ^{13}C NMR spectra of compound 3



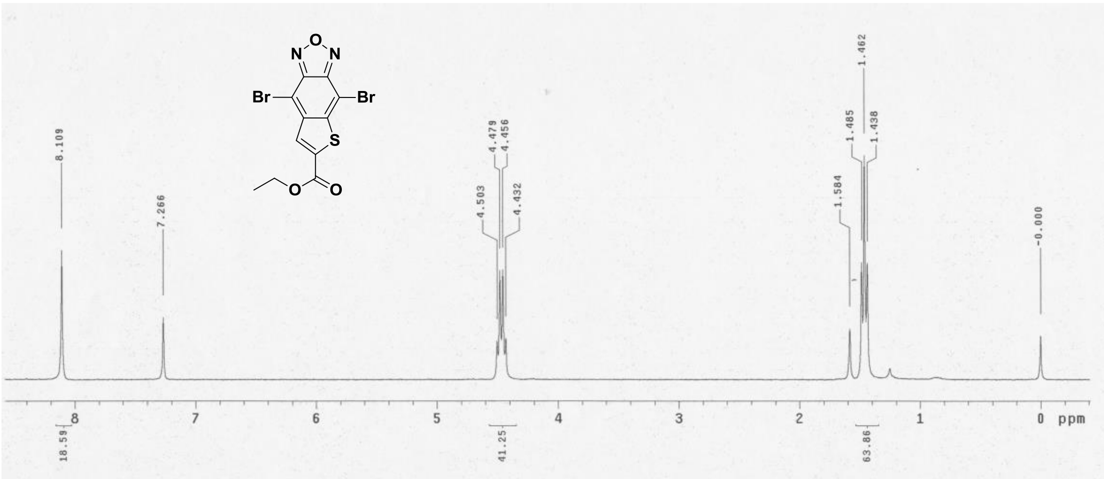


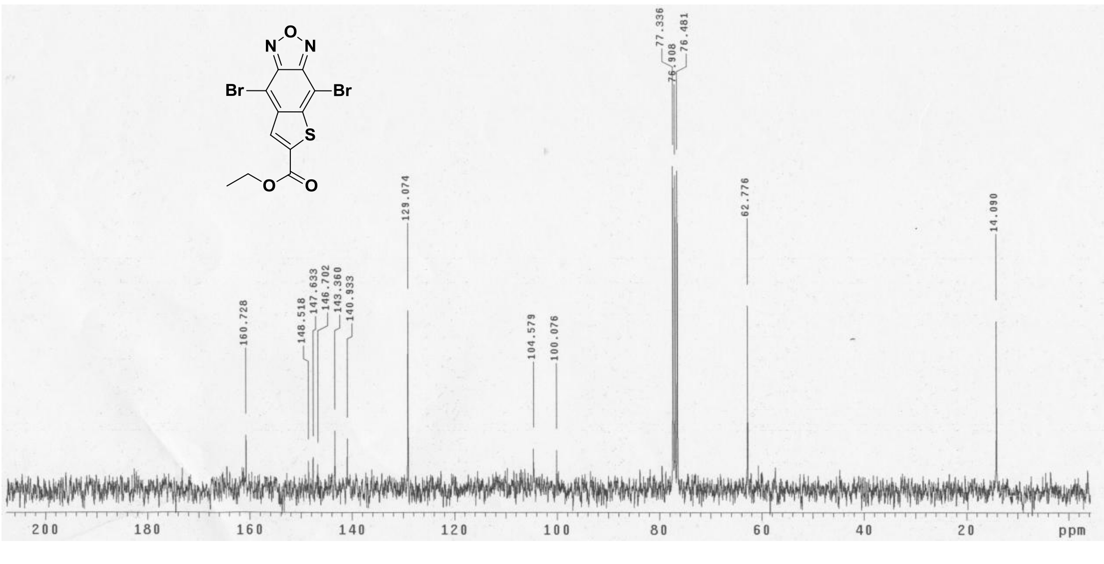
^{1}H NMR and ^{13}C NMR spectra of BXT





^{1}H NMR and ^{13}C NMR spectra of di-Br-BXT





^{1}H NMR and ^{13}C NMR spectra of polymer PBXT-IDT