Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

ELECTRONIC SUPPLEMENTARY INFORMATION

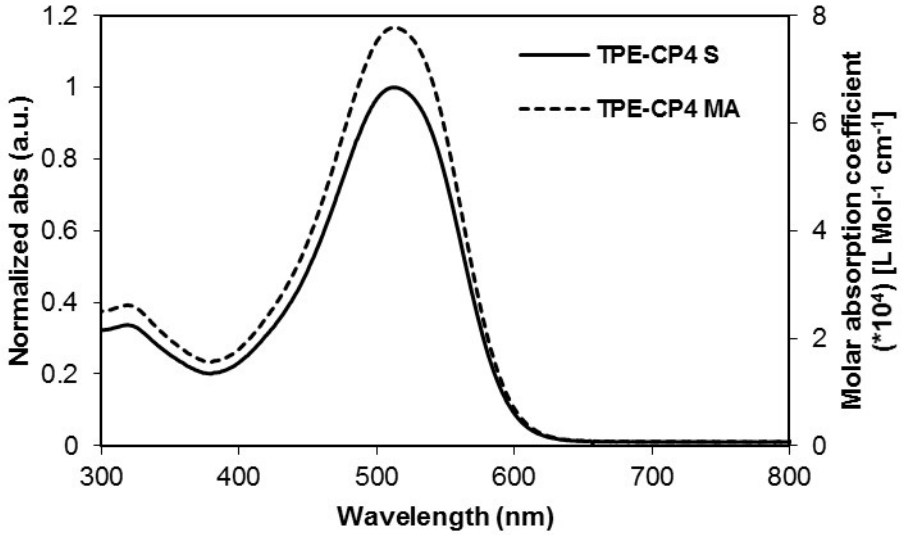


Fig. S1 Solution spectra of **TPE-CP4** in chloroform solution (**TPE-CP4** S; MA represents molar absorptivity).

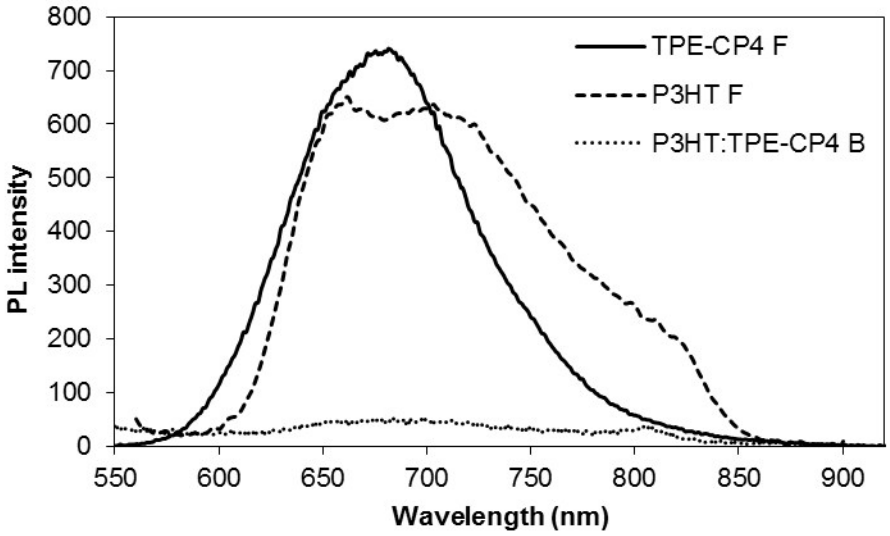


Fig. S2 PL spectra of pristine and blend films of **TPE-CP4** [**TPE-CP4** F and P3HT: **TPE-CP4** B (1: 1.2 as-cast), respectively] together with neat P3HT film. Excitation wavelength = 530 nm.

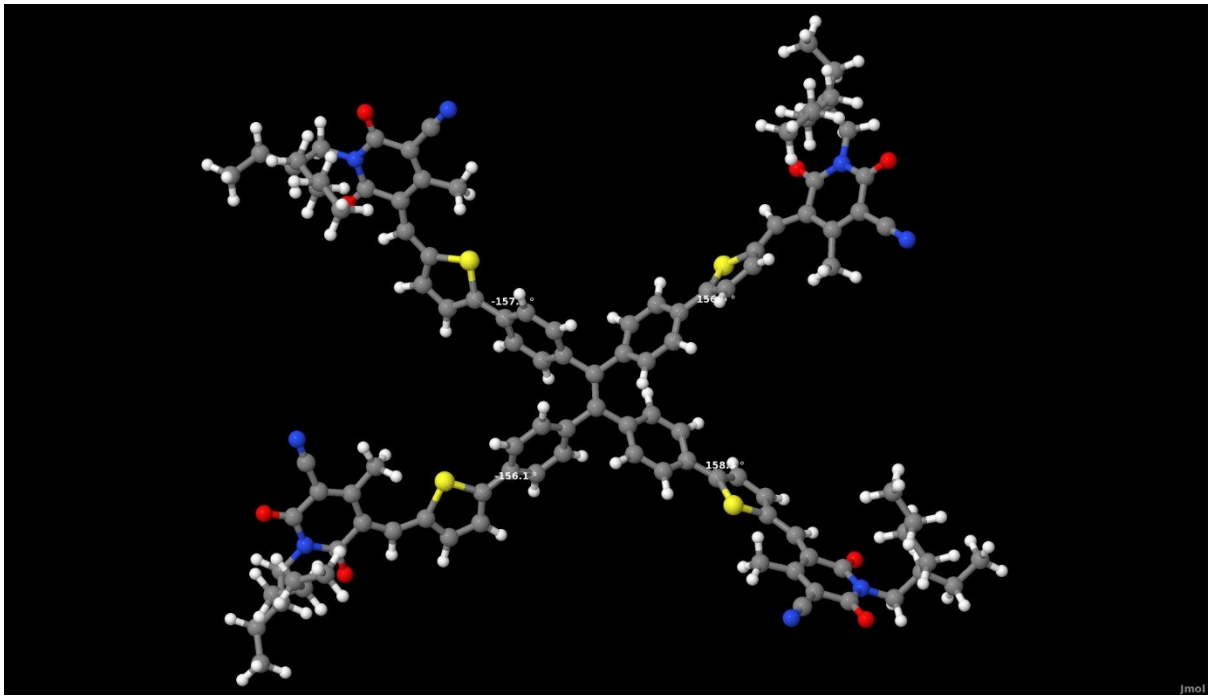


Fig. S3 Torsional angle of ~23° between the central phenyl ring planes and the thiophene ring planes of **TPE-CP4** from the minimum energy conformations calculated using the Gaussian 09 suite of programs and the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level of theory.

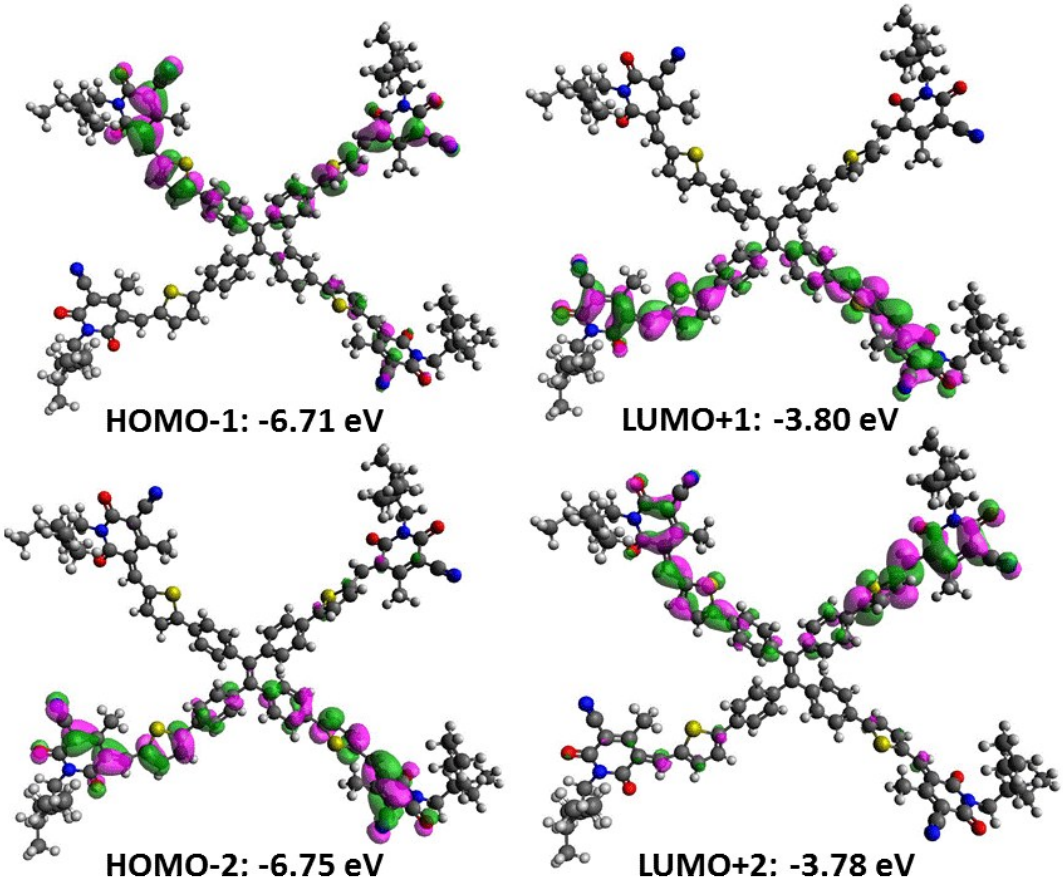


Fig. S4 Theoretical density distribution for the additional frontier molecular orbitals of **TPE-CP4**.

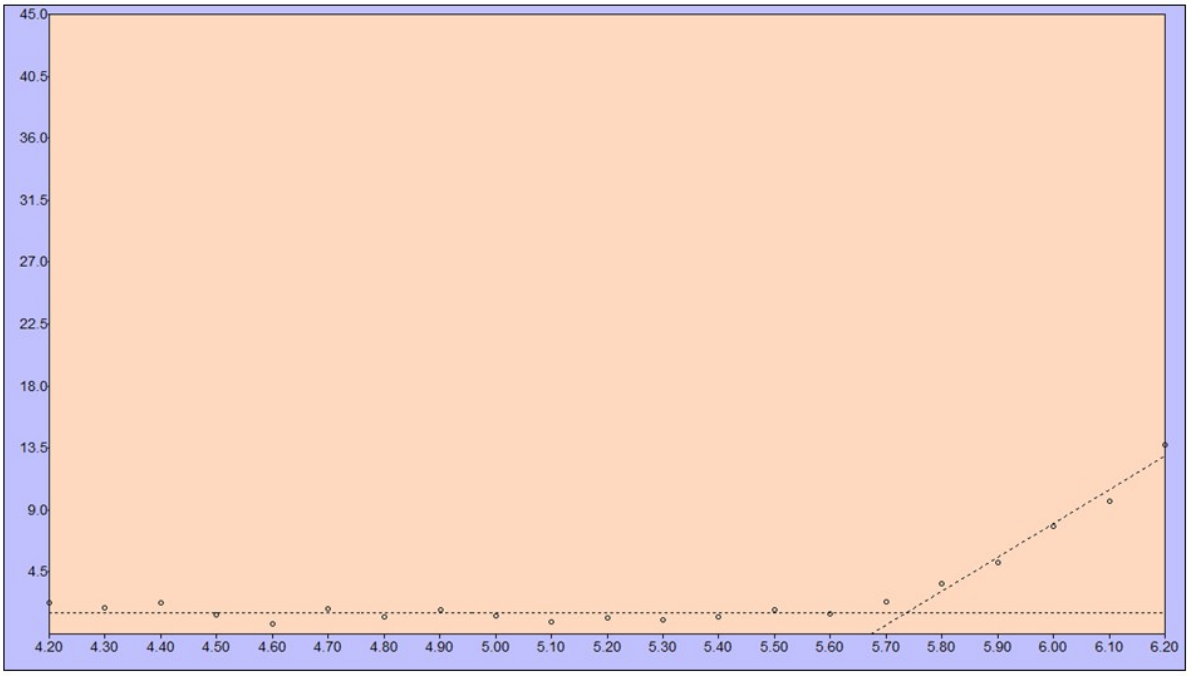


Fig. S5 PESA spectrum of thin film of **TPE-CP4**. The dashed-lines show the fits to extract ionisation potential (-5.72 eV) which corresponds to the HOMO energy level.

Excited State	1:	Singlet-A	2.1577 eV	574.60 nm	f=1.0345	<S**2>=0.000
Excited State	2:	Singlet-A	2.2943 eV	540.41 nm	f=0.3751	<S**2>=0.000
Excited State	3:	Singlet-A	2.3162 eV	535.29 nm	f=0.7350	<S**2>=0.000
Excited State	4:	Singlet-A	2.4645 eV	503.07 nm	f=0.0464	<S**2>=0.000
Excited State	5:	Singlet-A	2.5449 eV	487.19 nm	f=0.2486	<S**2>=0.000
Excited State	6:	Singlet-A	2.6011 eV	476.65 nm	f=1.0889	<S**2>=0.000
Excited State	7:	Singlet-A	2.6605 eV	466.02 nm	f=0.0057	<S**2>=0.000
Excited State	8:	Singlet-A	2.6960 eV	459.88 nm	f=0.1252	<S**2>=0.000

Dipole moment (field-independent basis, Debye):
X= -0.6191; Y= -6.9585; Z= -13.9306; Total = 15.5842

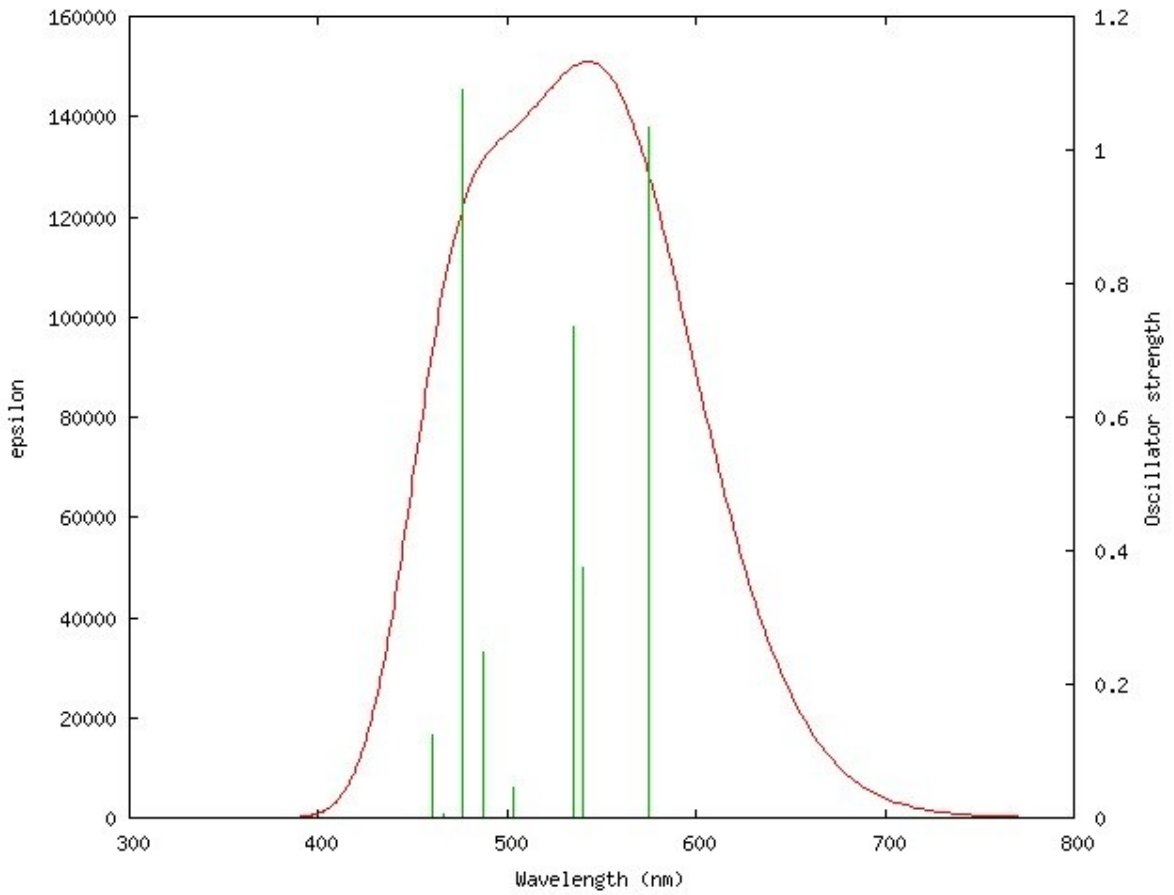


Fig. S6 Theoretical optical absorption transitions and spectrum of **TPE-CP4**.

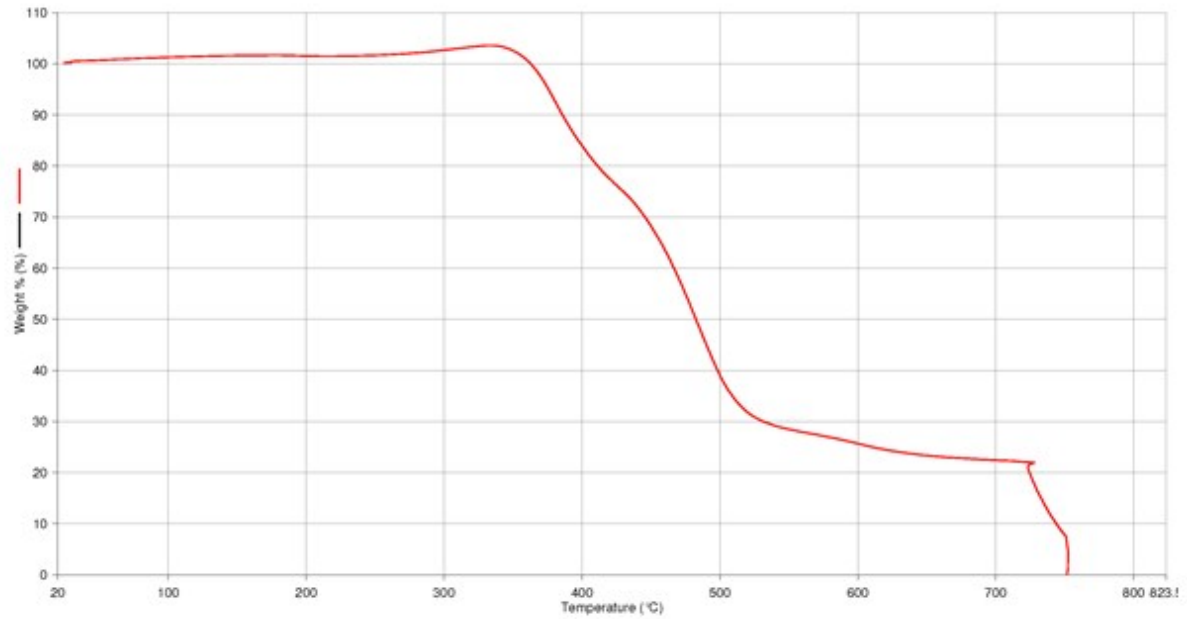


Fig. S7 TGA curve showing thermal stability of **TPE-CP4**.

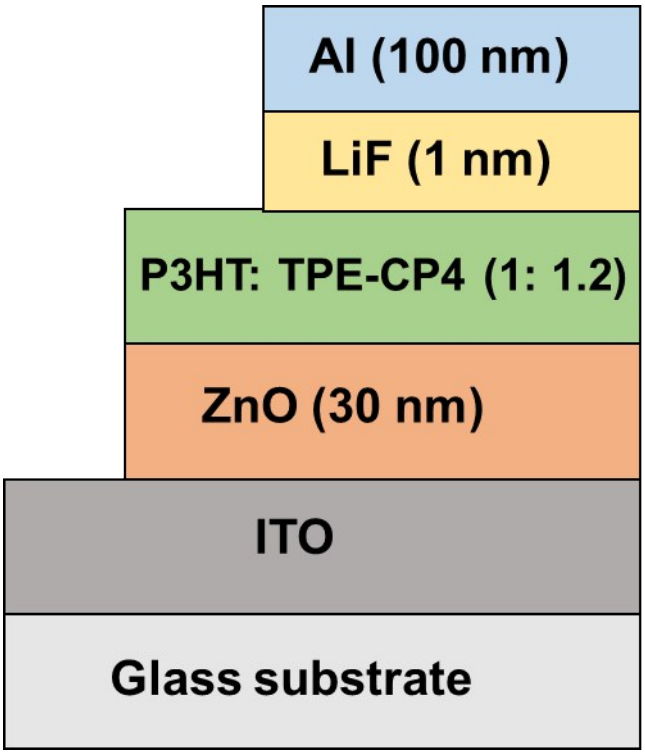


Fig. S8 Device sketch of the electron-only device that was used to study SCLC method.

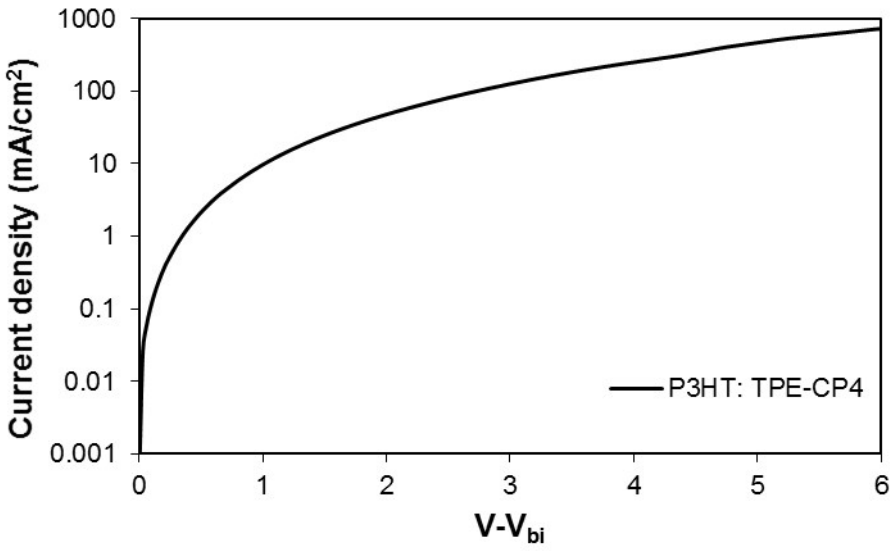
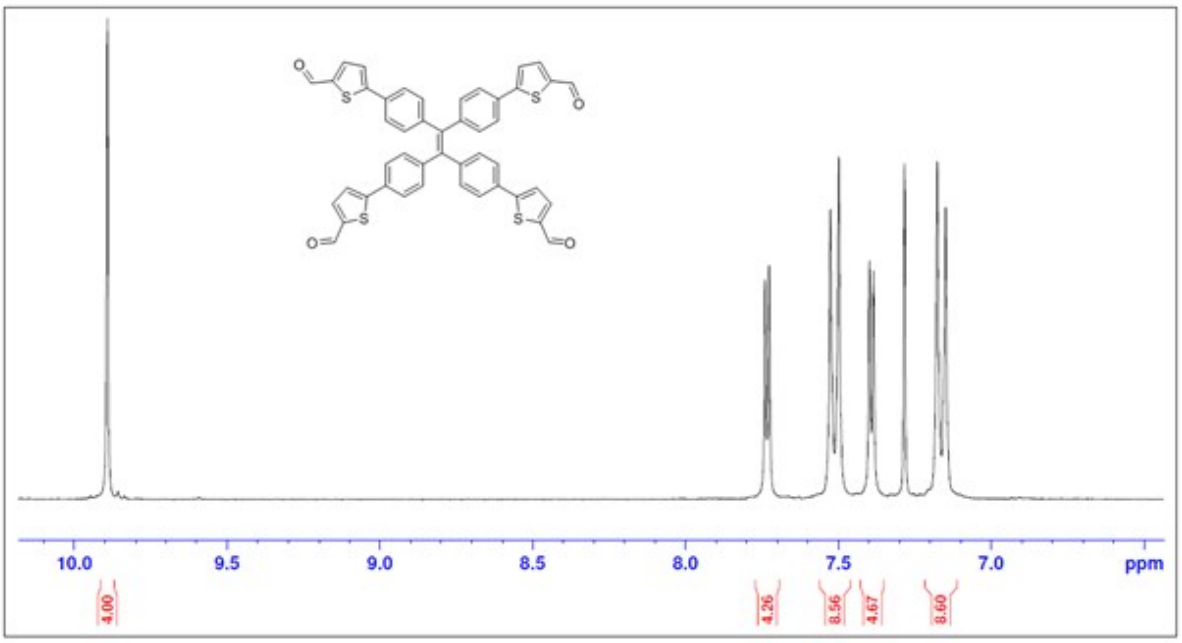
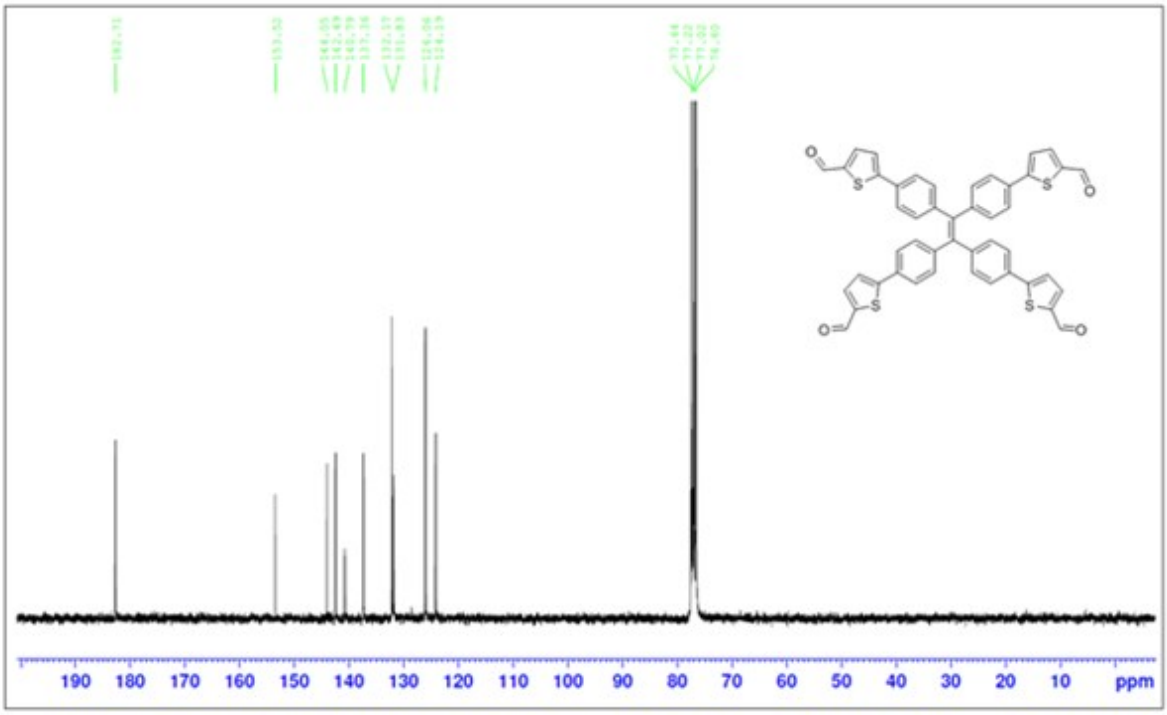


Fig. S9 Current–voltage characteristic of electron-only device which was applied to Mott-Gurney equation to calculate electron mobility.

EXPERIMENTAL SPECTRA

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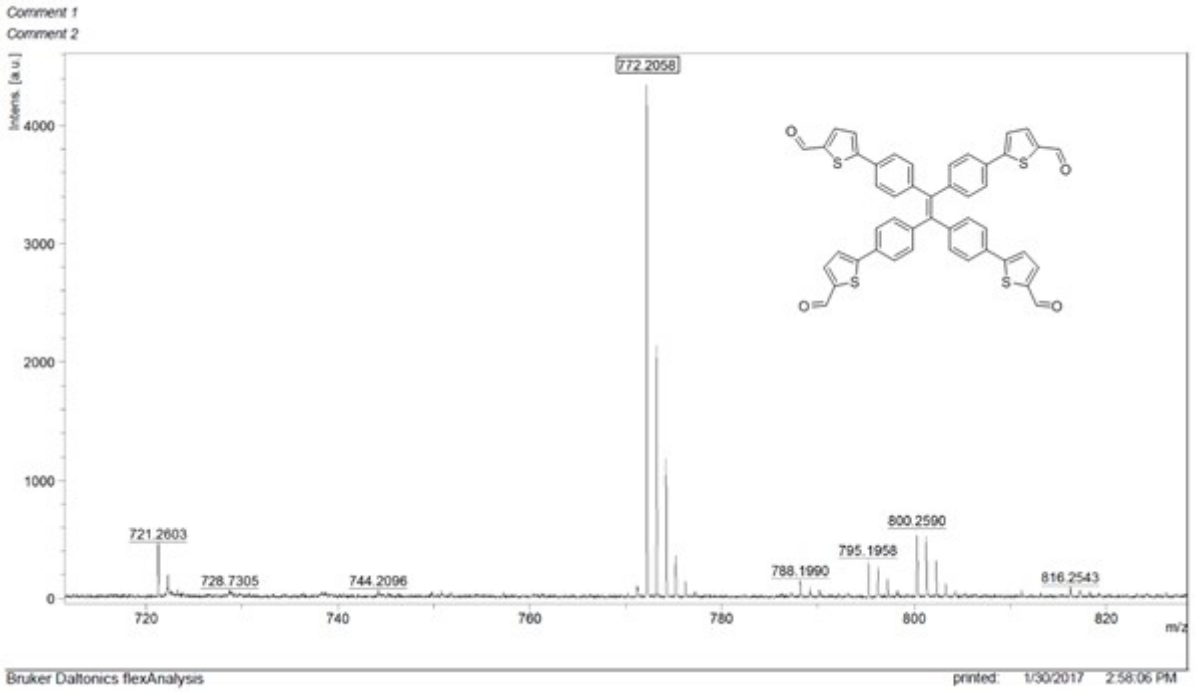
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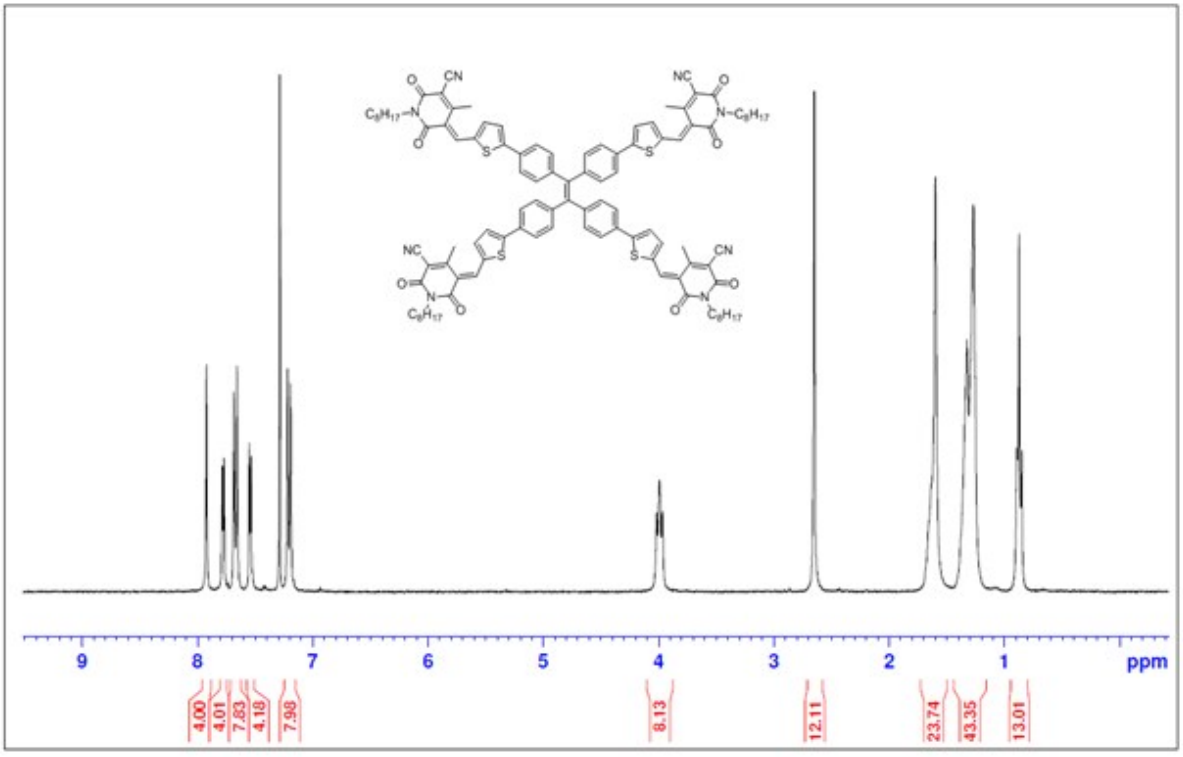
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4
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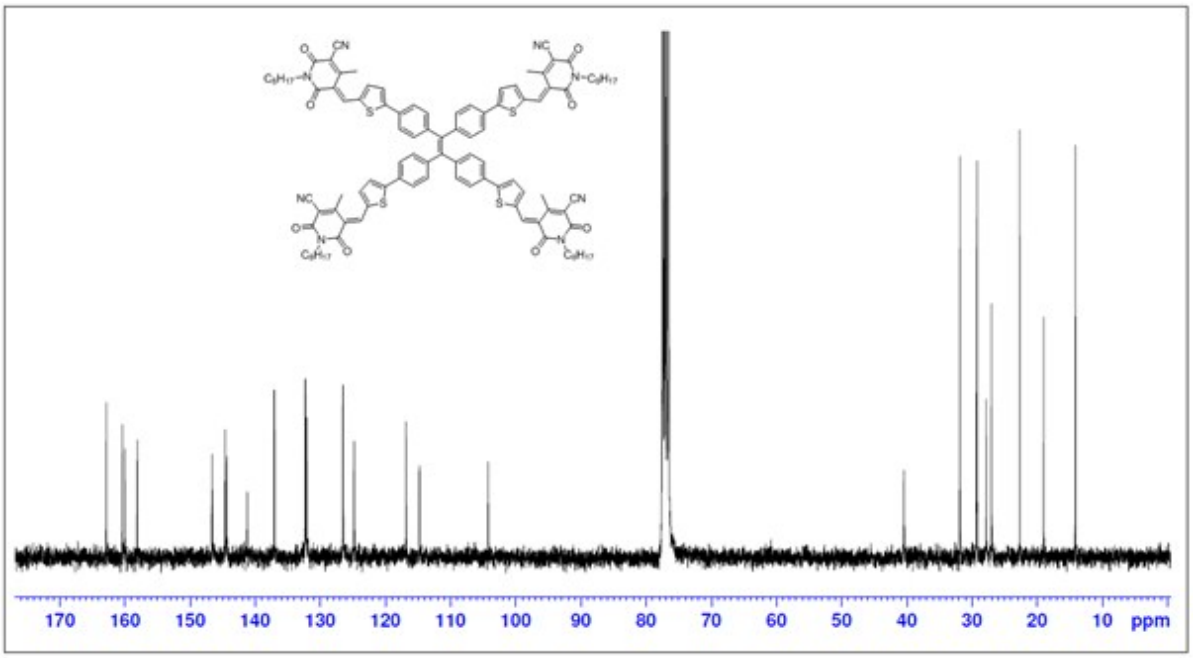
23.74
43.35
13.01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40
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20
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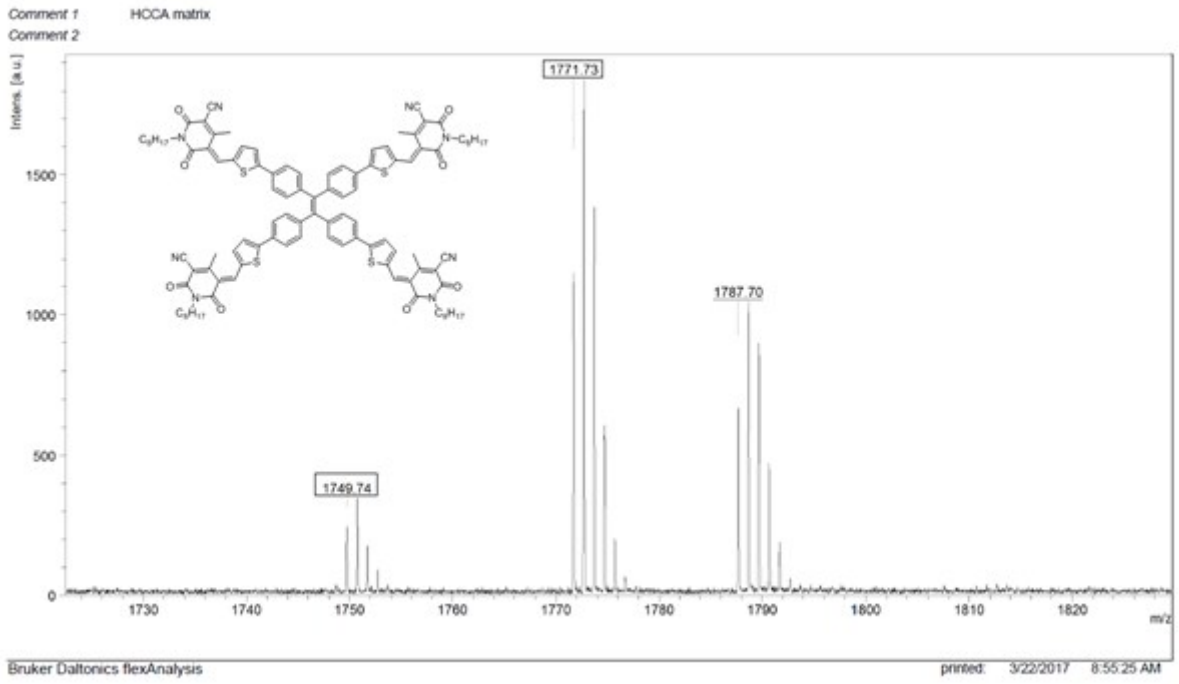
ppm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Comment 2
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1000
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m/z
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