Supplementary Information

Intramolecular Oxidative Cyclodehydrogenation Route for Strap-like Conjugated Polymers Synthesis

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S1. The detailed calculated procedures for the charge carrier mobility.

According to the obtained V_{th} values and the metal-oxide semiconductor FET formula for the saturation regime, $I_{DS} = \frac{\mu W C_i}{2L}(V_G - V_{th})^2$, the calculations of the charge carrier mobility (μ) are below:

OPTVB

$V_G = 0$ V, $I_{DS} = 1.78 \times 10^{-7}$ A, $C_i = 20$ μF/cm^2, $W = 0.6$ mm, $L = 1$ mm, $V_{th} = -0.28$ V

$\mu = 2LI_{DS}/[WC_i(V_G - V_{th})^2] = 2I_{DS}/[WC_i(V_G - V_{th})^2]$

$= 2 \times 1.78 \times 10^{-7}/[0.6 \times 20 \times 10^{-6} \times (0 + 0.28)^2]$

$= 0.38$ cm^{2}V^{-1}s^{-1}

OPTVN

$V_G = -3$ V, $I_{DS} = 1.73 \times 10^{-5}$ A, $C_i = 20$ μF/cm^2, $W = 0.6$ mm, $L = 1$ mm, $V_{th} = -0.54$V

$\mu = 2LI_{DS}/[WC_i(V_G - V_{th})^2] = 2I_{DS}/[WC_i(V_G - V_{th})^2]$

$= 2 \times 1.73 \times 10^{-5}/[0.6 \times 20 \times 10^{-6} \times (-3 + 0.54)^2]$

$= 0.48$ cm^{2}V^{-1}s^{-1}

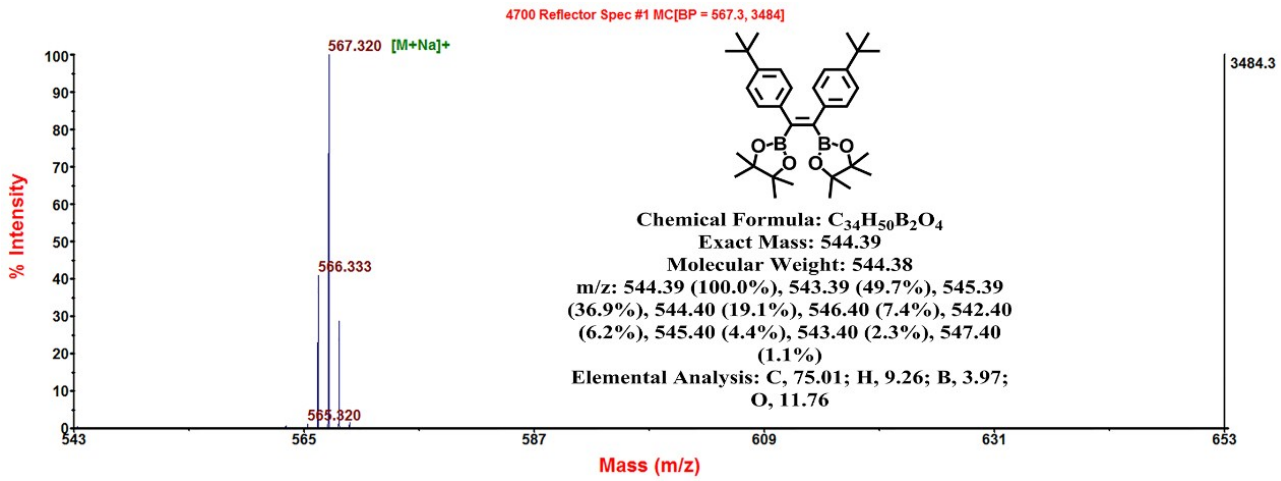
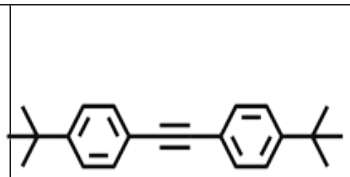
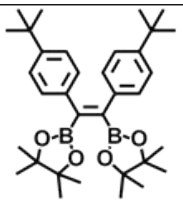


Fig. S1 The MALDI-TOF of **2.**

Table S1 Summary of crystal data and reflection collection parameters for **1** and **2**.

		
Empirical formula	$C_{22}H_{26}$	$C_{34}H_{50}B_2O_4$
Formula weight	290.43	544.36
Crystal size, mm	0.32 x 0.28 x 0.24	0.26 x 0.21 x 0.18
Crystal system	Monoclinic, P21/c	Triclinic
space group	P2(1)/c	P-1
a, Å	11.731(4)	10.991(18)
b, Å	10.216(4)	12.54(2)
c, Å	15.667(6)	13.97(4)
a, deg	90	108.83(5)
β, deg	96.915(7)	103.58(5)
γ, deg	90	104.77(3)
V, Å^3	1863.9(12)	1653(6)
Z	4	2
Calculated density, Mg/m^3	1.035	1.094
F(000)	632	592
Temperature, K	293(2)	296(2)
Wavelength, Å	0.71073	0.71073
μ(Mo Ka), mm^{-1}	0.058	0.068
$2\theta_{max}$,deg (Completeness)	25.00 (99.8 %)	24.99(97.8 %)
no. of collected reflections	9206	8152
no. of unique ref.(R_{int})	3272 (0.0387)	5701 (0.0933)
Data/restraints/parameters	3272 / 6 / 200	5701 / 0 / 362
R_1, wR_2 [obs I>2σ (I)]	0.0967, 0.1832	0.1322, 0.2363
R_1, wR_2 (all data)	0.1394, 0.1951	0.1805, 0.2686
residual peak/hole, e. Å^{-3}	0.486 /-0.290	0.436/-0.302
transmission ratio	0.9863 /0.9817	0.9878/0.9824
Goodness-of-fit on F^2	1.013	1.196

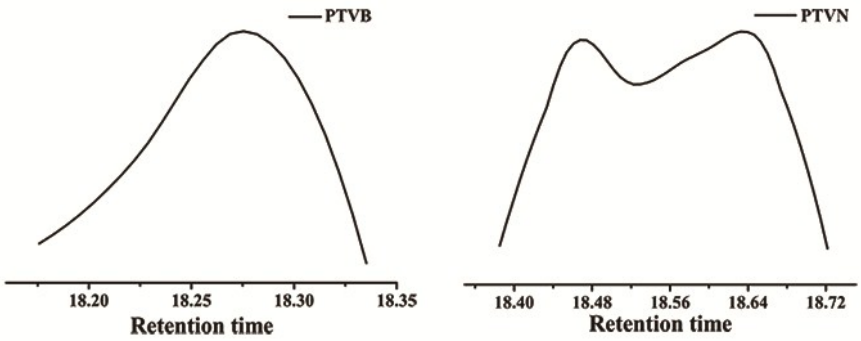


Fig. S2 The GPC data of **PTVB** and **PTVN**.

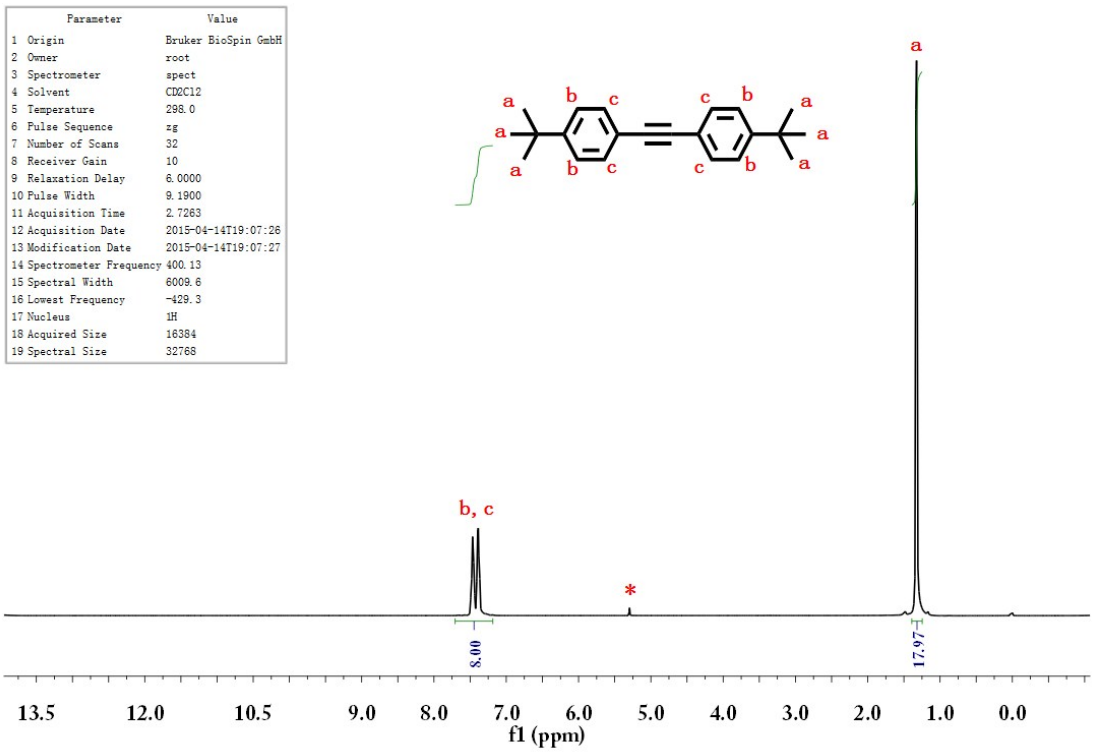


Fig. S3 ^{1}H NMR spectrum of **1**.

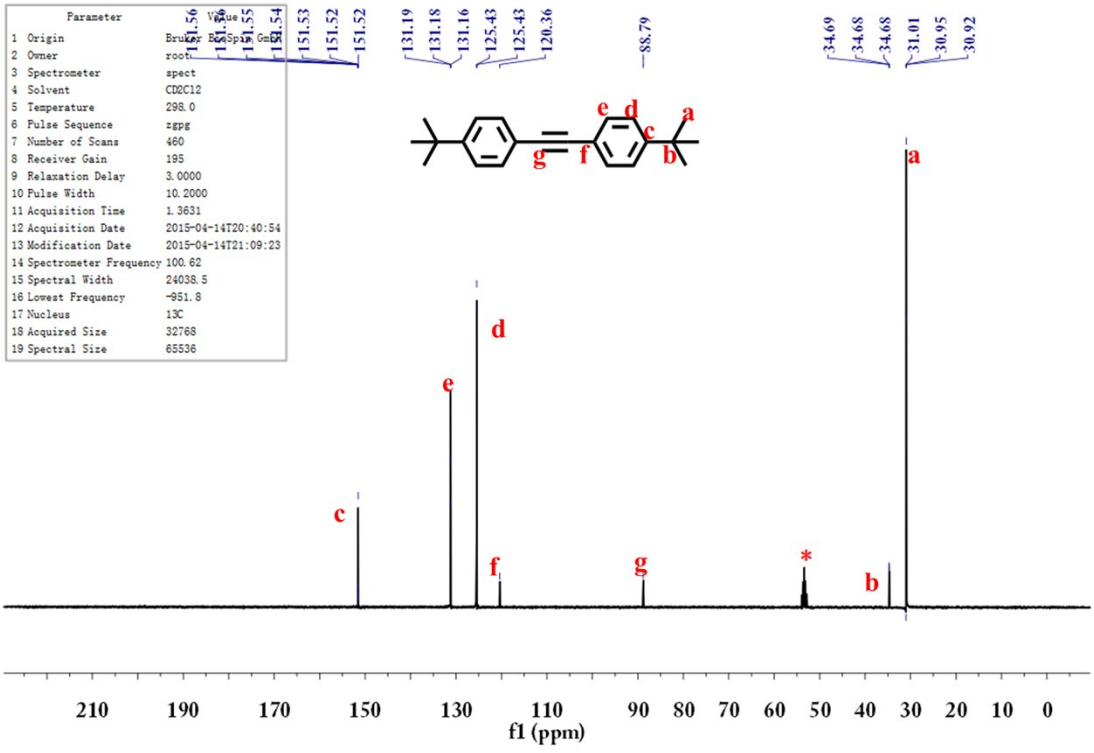


Fig. S4 ^{13}C NMR spectrum of **1**.

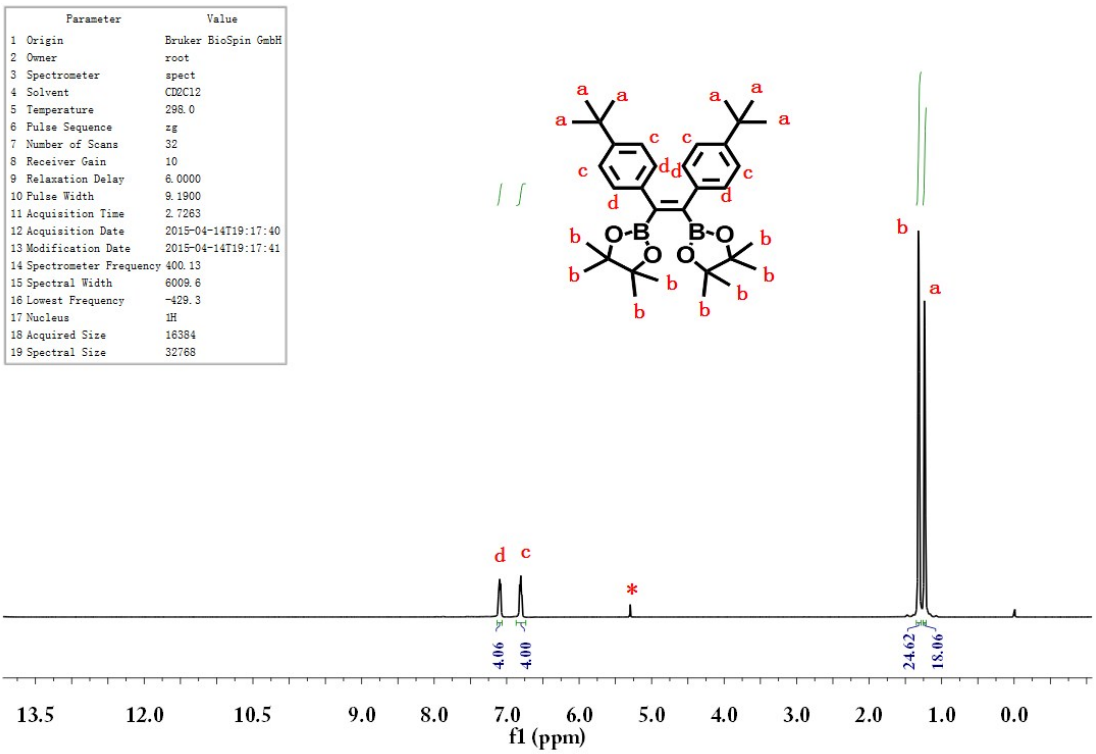


Fig. S5 ^{1}H NMR spectrum of **2**.

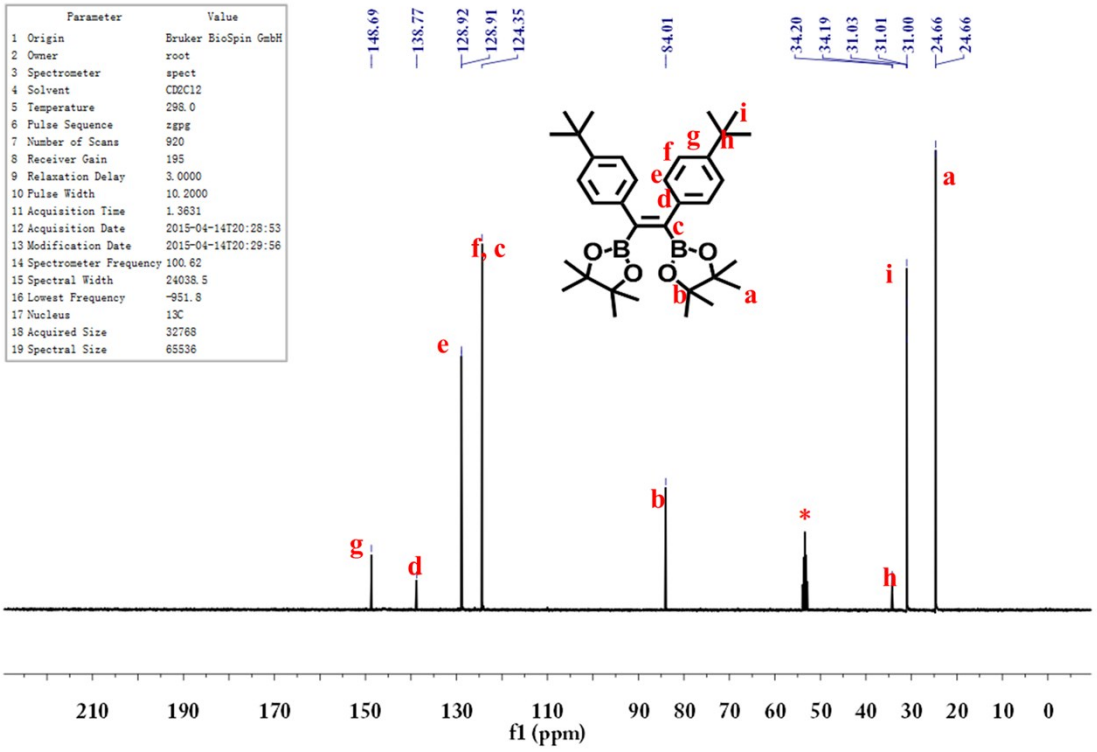


Fig. S6 ^{13}C NMR spectrum of **2**.

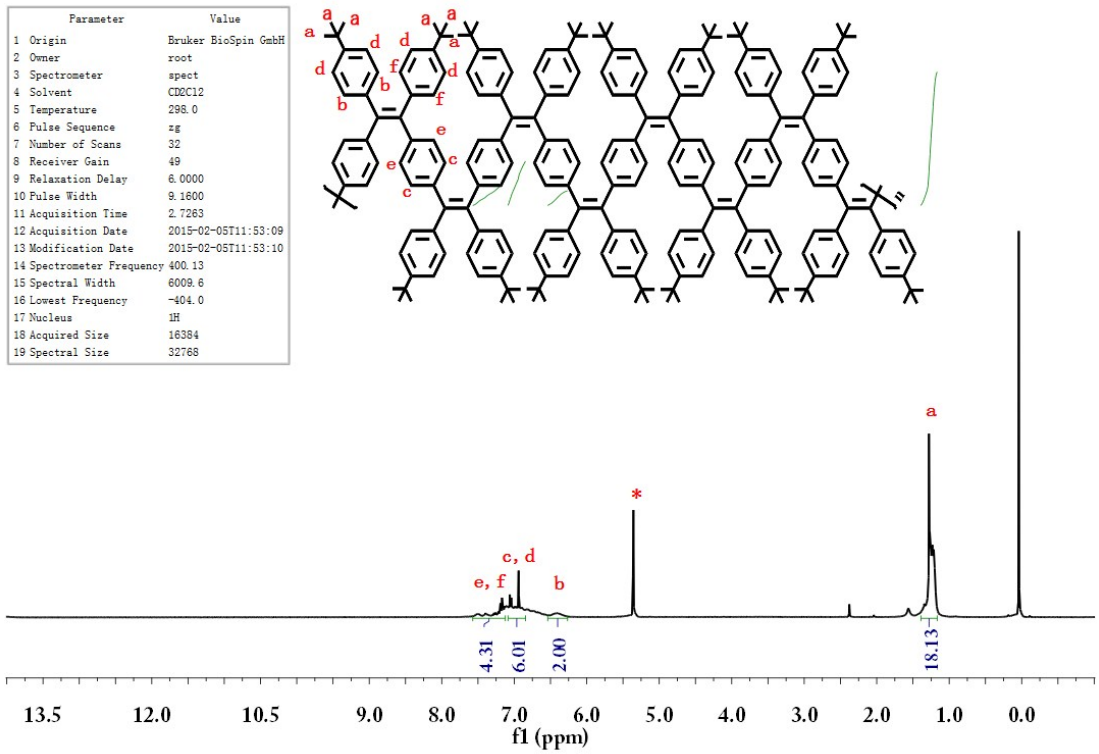


Fig. S7 ^{1}H NMR spectrum of **PTVB**.

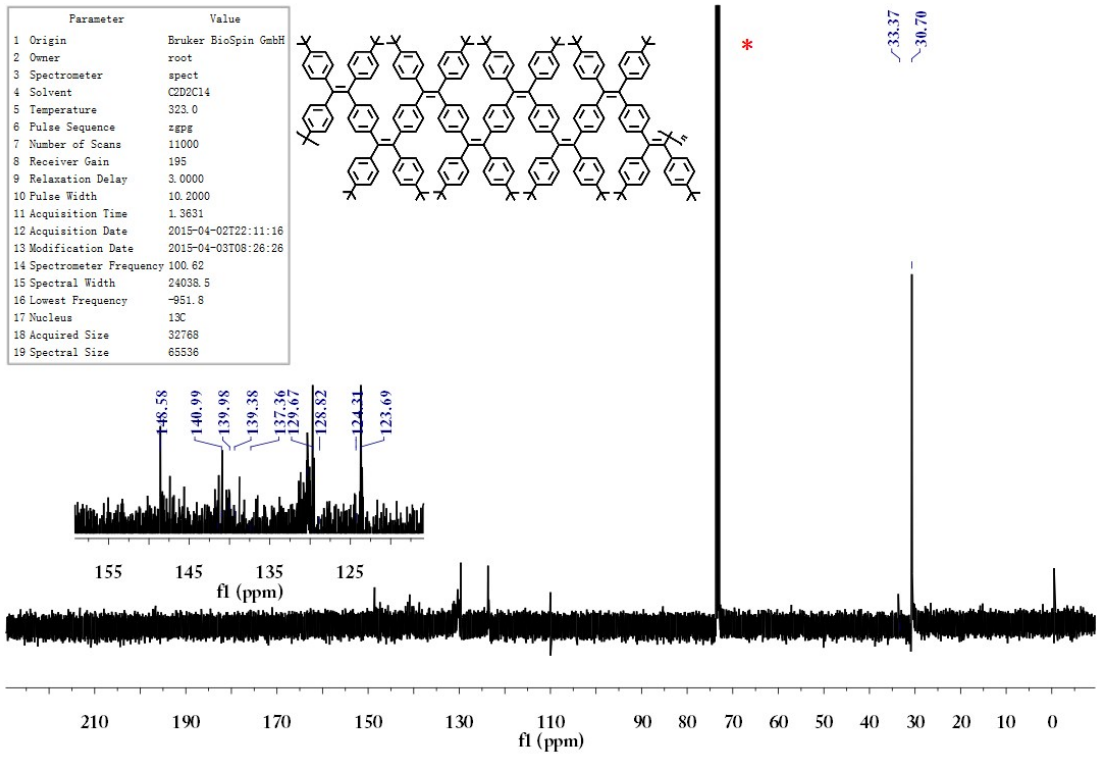


Fig. S8 ^{13}C NMR spectrum of **PTVB**.

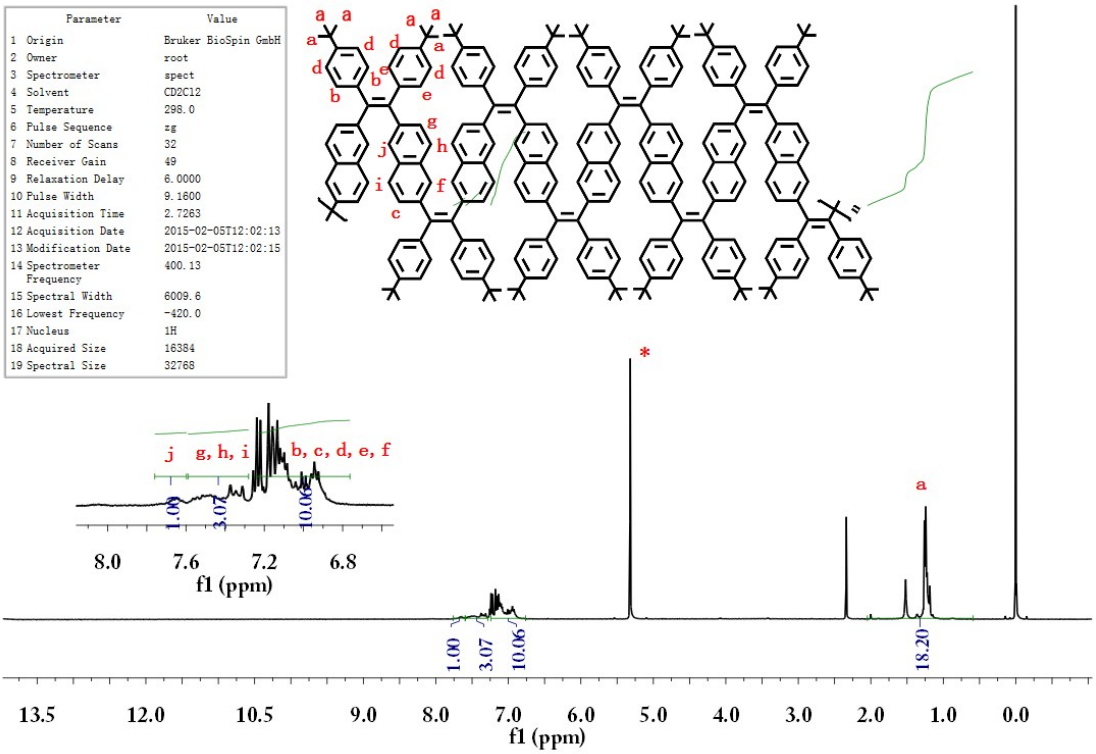


Fig. S9 ^{1}H NMR spectrum of **PTVN**.

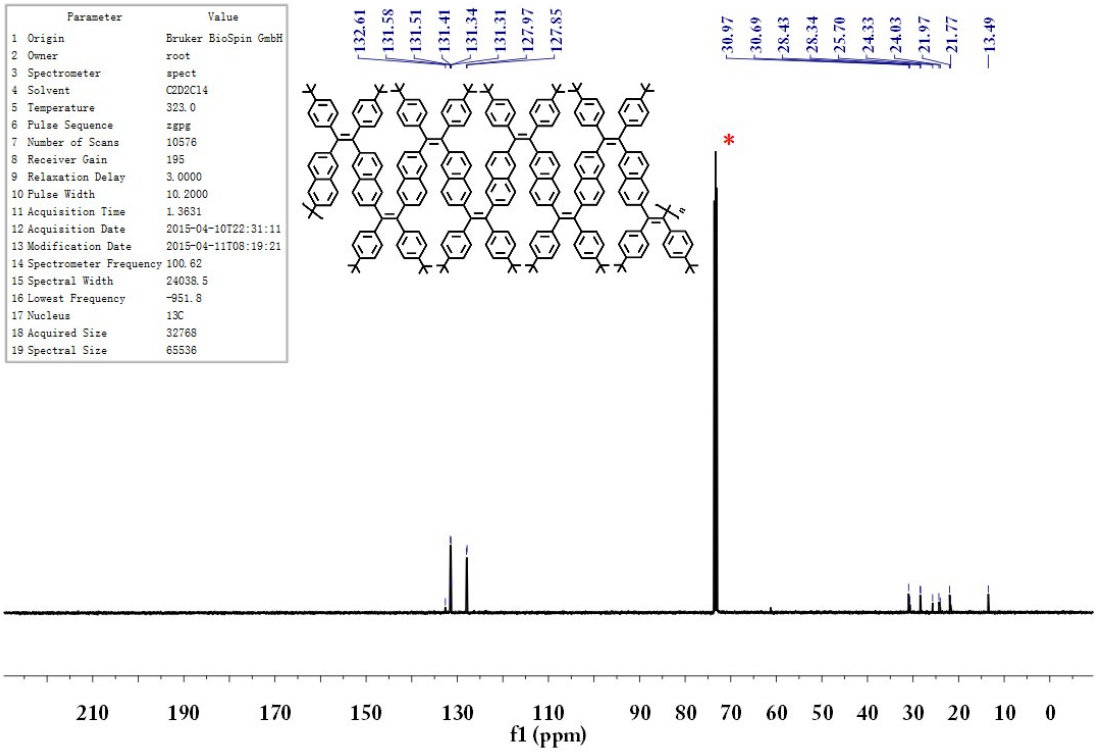


Fig. S10 ^{13}C NMR spectrum of **PTVN**.

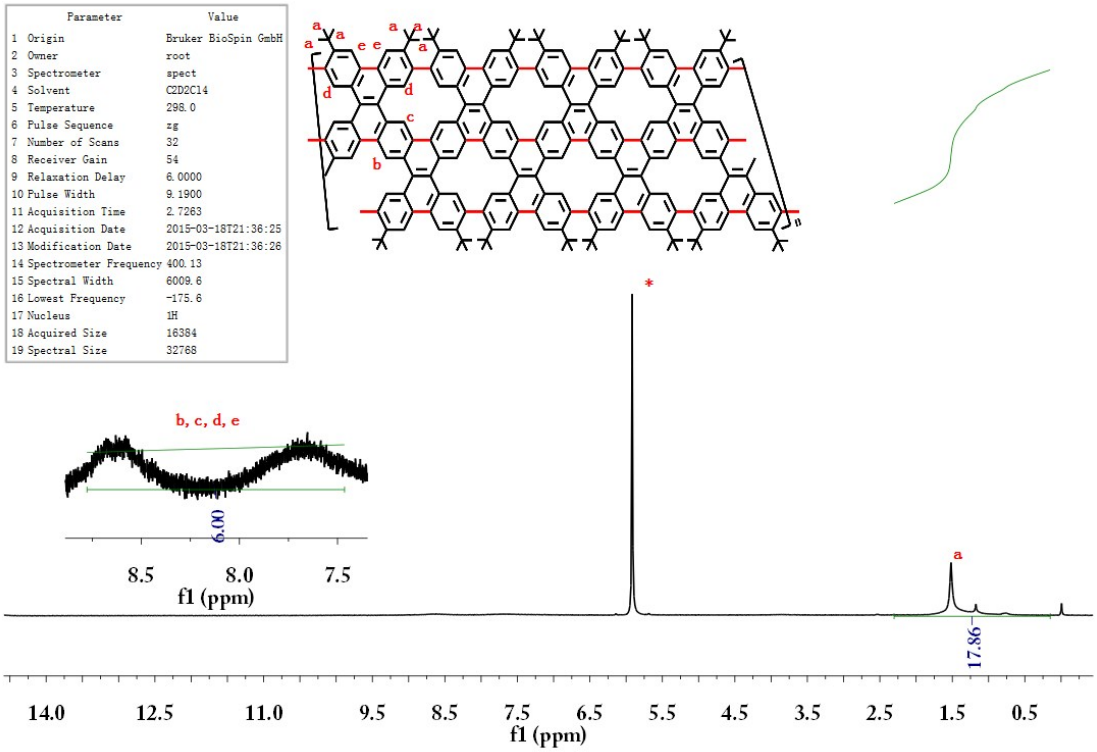


Fig. S11 ^{1}H NMR spectrum of **OPTVB**.

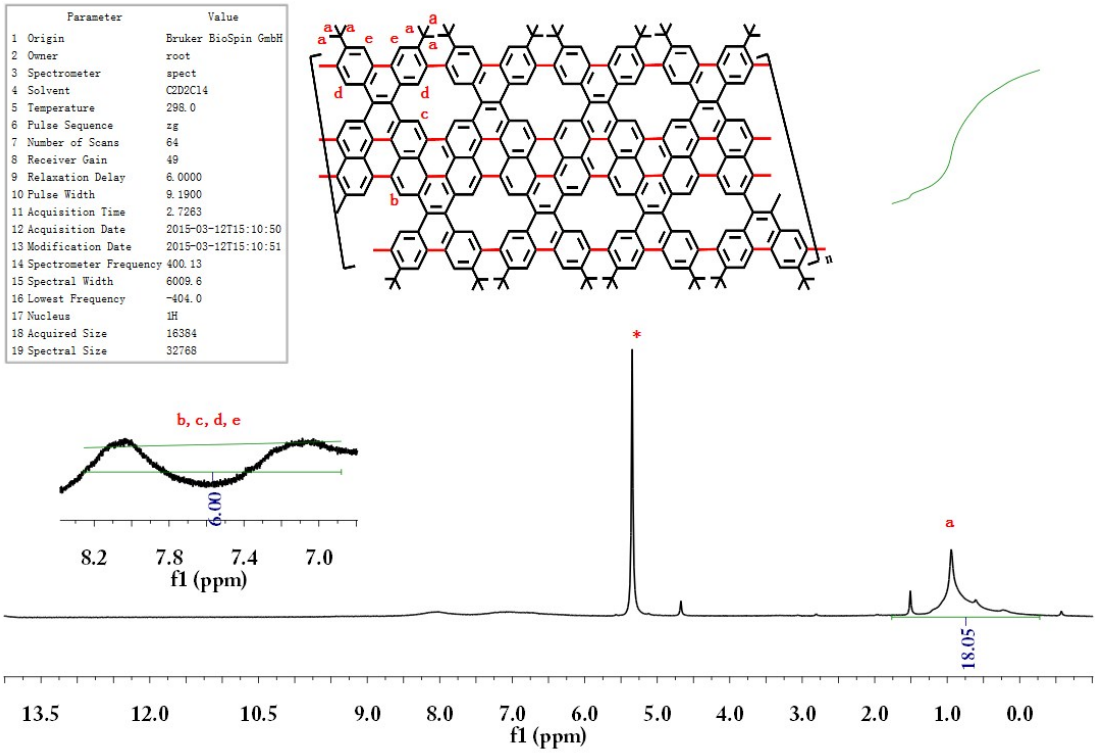


Fig. S12. ^{1}H NMR spectrum of **OPTVN**.

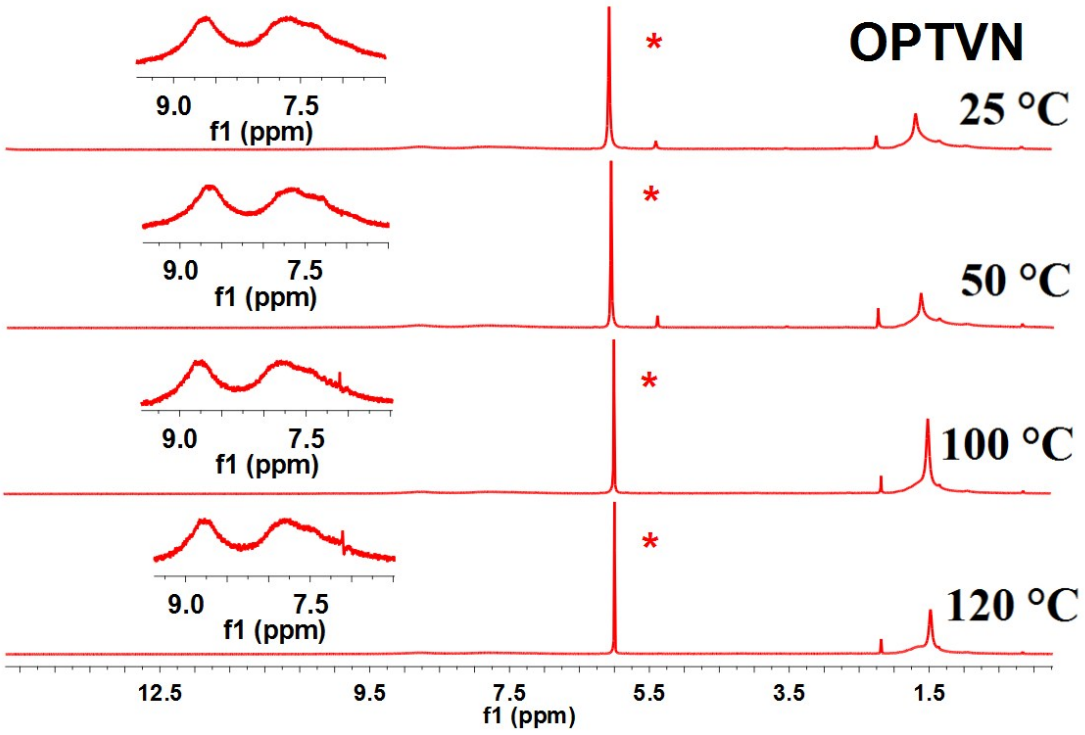


Fig. S13 ^{1}H NMR spectra of **OPTVN** at the variable temperatures (25 °C to 120 °C) in $C_2D_2Cl_4$. The inserted images are the amplifications of the aromatic domain.

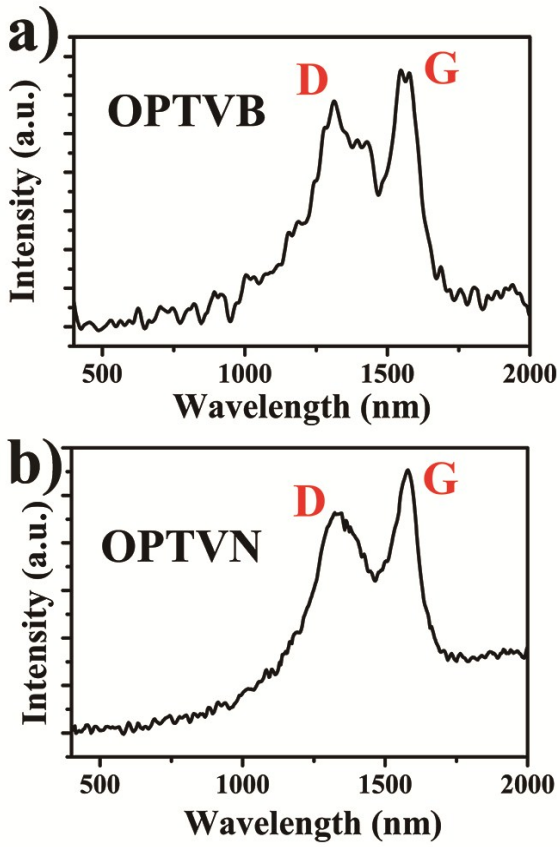


Fig. S14 (a) Raman spectrum of **OPTVB**. (b) Raman spectrum of **OPTVN**.

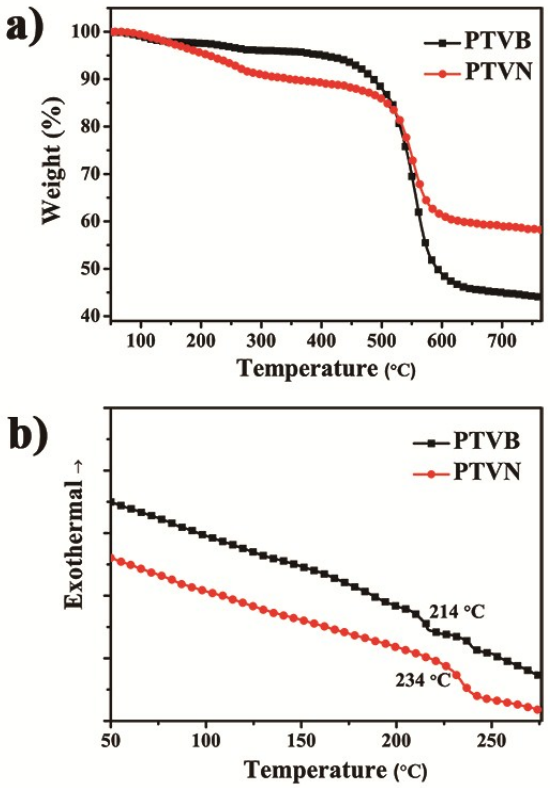


Fig. S15 (a) The TGA data of **PTVB** and **PTVN**; (b) The DSC data of **PTVB** and **PTVN**.

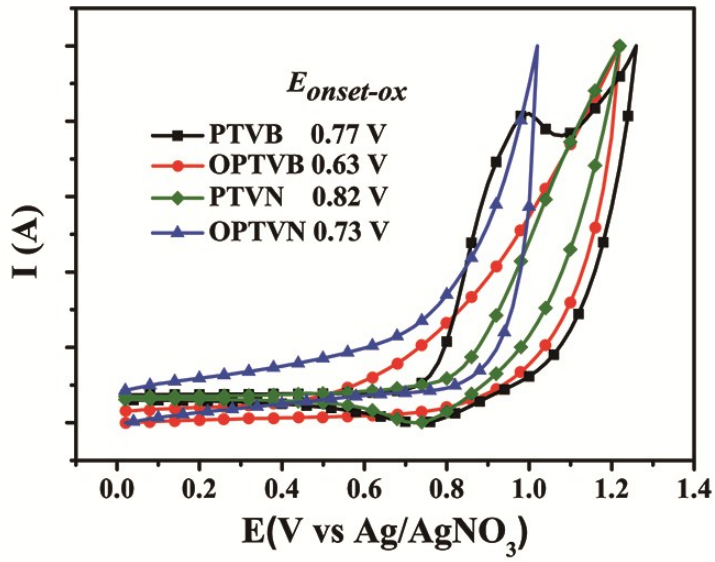


Fig. S16 The CV curves of **PTVB**, **OPTVB**, **PTVN** and **OPTVN**.

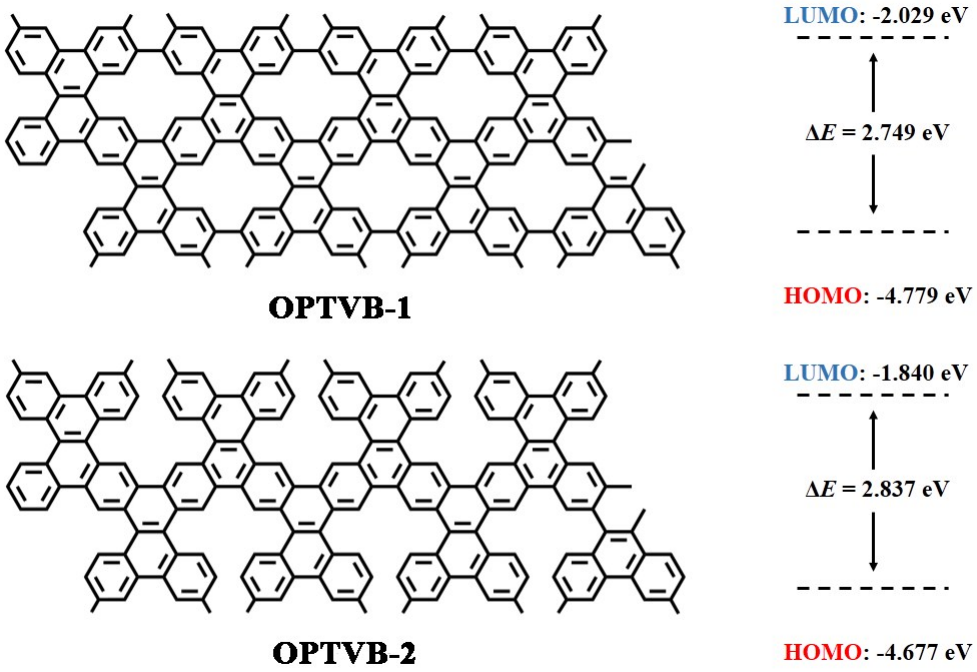


Fig.S17 The calculated HOMO and LUMO energy levels of **OPTVB-1** and **OPTVB-2**.

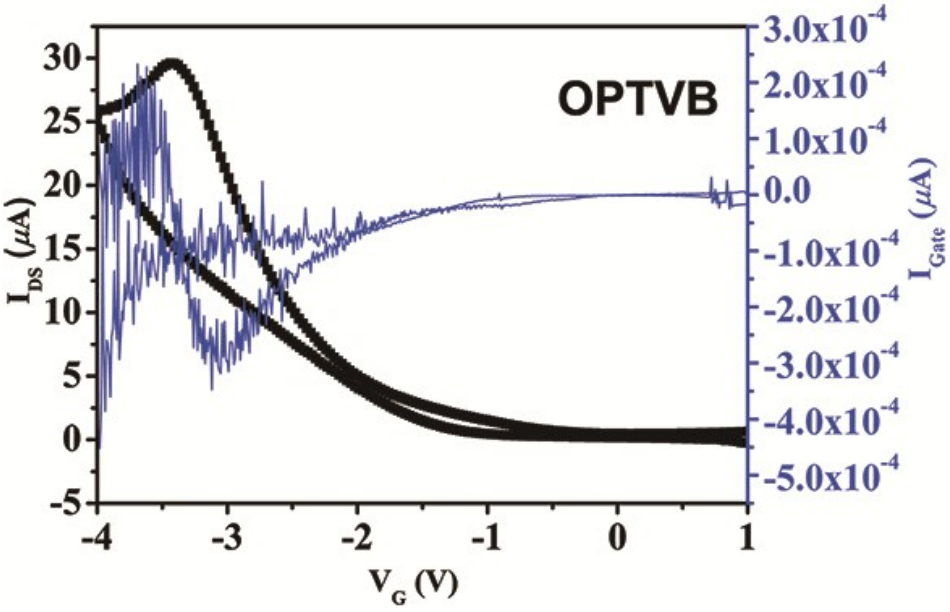


Fig. S18 The original charge transfer curve (black) and gate leakage curve (blue) of the FETs containing **OPTVB.**

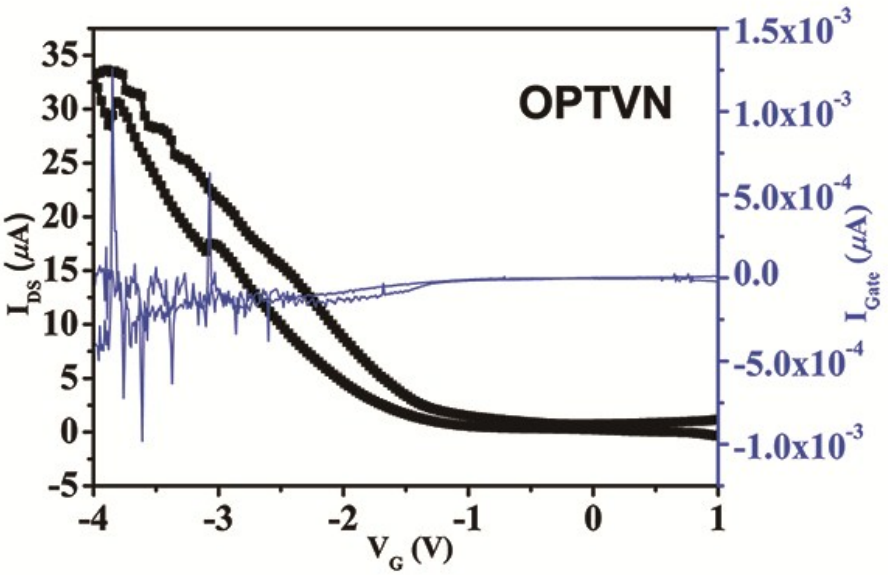


Fig. S19 The original charge transfer curve (black) and gate leakage curve (blue) of the FETs containing **OPTVN.**

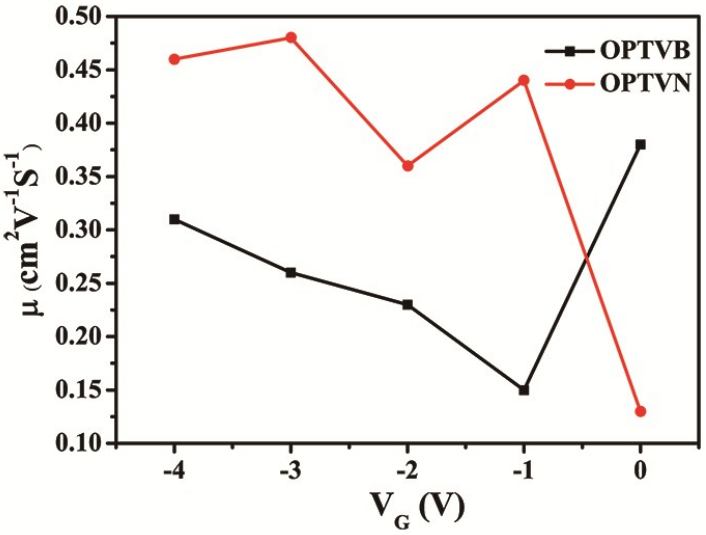


Fig. S20. The mobility plots versus gate voltages of **OPTVB** and **OPTVN**.