Supporting Information

Influence of cyano groups on the properties of piezofluorochromic aggregation-induced emission enhancement compounds derived from tetraphenylvinyl-capped ethane

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Table S1 The data of dihedral angles of the compounds

Compound	A-A'	A-B	A-C	A-D
biTPE	0 °	77 °	80 °	62 °
biTPE-CN	24 °	77 °	80 °	62 °
TPE-CN	72 °	77 °	80 °	62 °

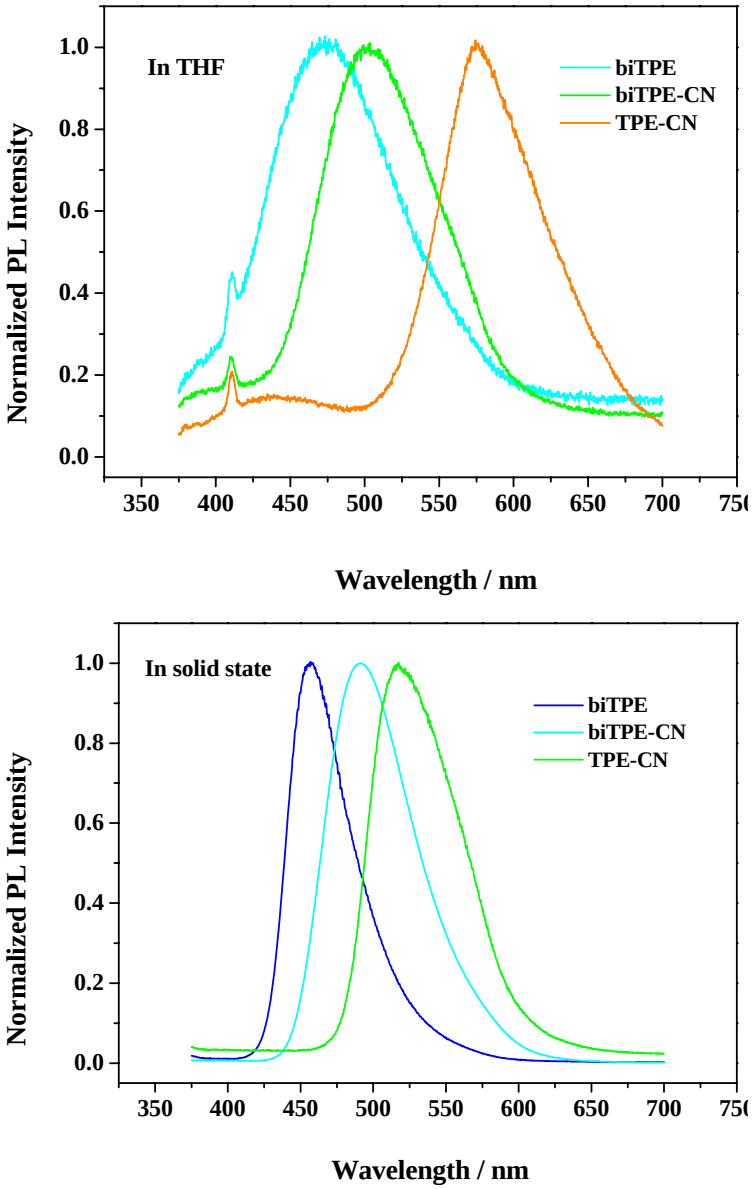

Fig. S1 The PL spectra of the compounds in dilute THF solution (10 μM) and solid powder states.

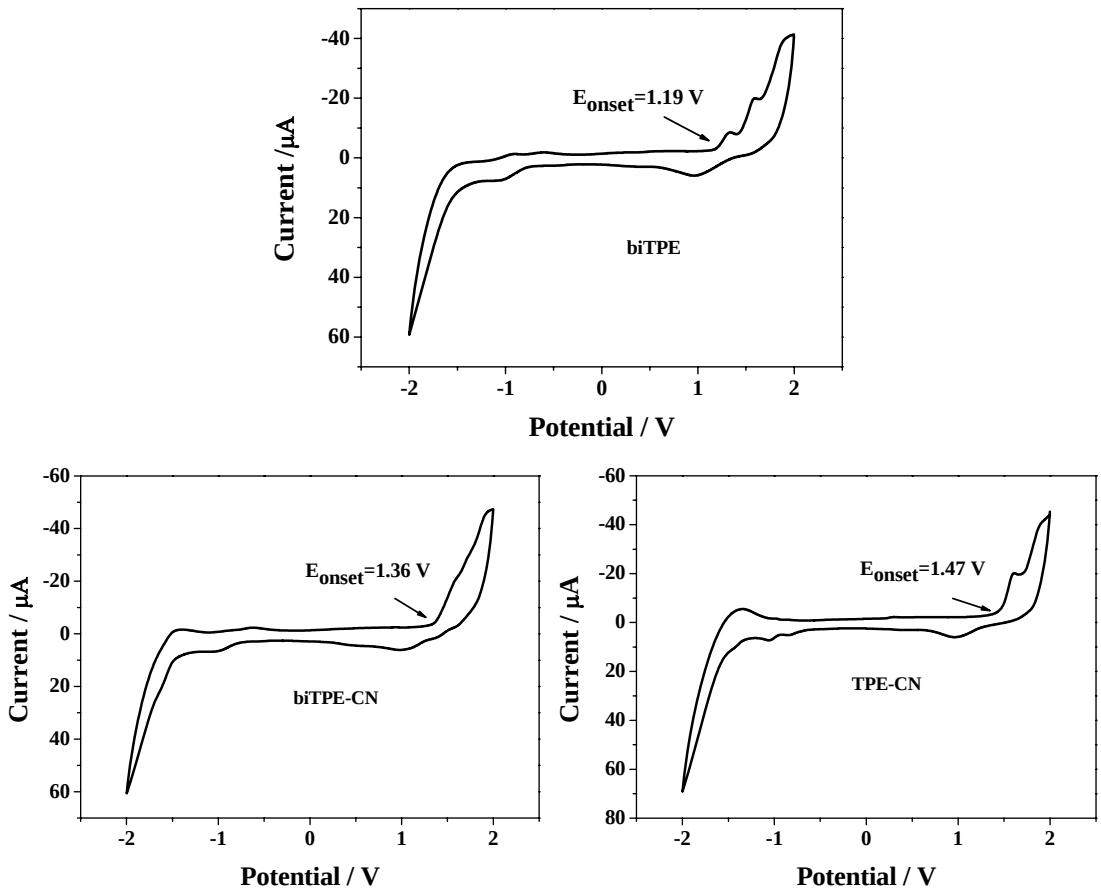

Fig. S2 The CV curves of biTPE, biTPE-CN and TPE-CN.

Table S2 Crystallographic data of biTPE

	biTPE
empirical formula	$C_{54}H_{40}\cdot C_7H_8$
fw.	780.99
temp, K	173(2)
wavelength, Å	0.71073
cryst syst	Triclinic,
space group	P-1
a, Å	9.6852(14)
b, Å	11.1199(16)
c, Å	21.963(3)
α, deg	93.231(2)
β, deg	95.749(2)
γ, deg	112.722(2)
V, Å^3	2159.2(5)
Z	2
d(calcd), mg/m^3	1.201
abs coeff, mm^{-1}	0.068
F(000)	828
θ range, deg	1.87 - 27.01
index range	-12⩽h⩽12
index range	-14⩽k⩽14
index range	-27⩽l⩽26
no. of reflns collected	18127
no. of independent reflns	9152
completeness to *θ* = 27.01°	96.90%
no. of data / restraints / parameters	9152 / 0 / 590
goodness-of-fit on F^2	1.048
final *R* indices [I > 2σ(I)]	R_1 = 0.0476 , wR_2 = 0.1237
R indices (all data)	R_1 = 0.0779 , wR_2 = 0.1416
Largest diff. peak and hole (e·Å^{-3})	0.306 and -0.204

Table S3 Crystallographic data of biTPE-CN

	biTPE-CN
empirical formula	$2C_{55}H_{39}N{\cdot}3C_3H_6O$
fw.	1601.98
temp, K	150(2)
wavelength, Å	1.54178
cryst syst	Monoclinic
space group	C2
a, Å	42.9951(16)
b, Å	9.1135(3)
c, Å	12.2084(5)
α, deg	90
β, deg	106.498(4)
γ, deg	90
V, Å^3	4586.7(3)
Z	2
d(calcd), mg/m^3	1.16
abs coeff, mm^{-1}	0.524
F(000)	1696
θ range, deg	3.78 – 63.99
index range	-47≤h≤50
index range	-10≤k≤8
index range	-13≤l≤14
no. of reflns collected	12899
no. of independent reflns	5734
completeness to *θ* = 27.01°	98.20%
no. of data / restraints / parameters	5734 / 16 / 617
goodness-of-fit on F^2	1.054
final *R* indices [I > 2σ(I)]	R_1 =0.0556 , wR_2 = 0.1532
R indices (all data)	R_1 = 0.0570 , wR_2 = 0.1552
Largest diff. peak and hole (e·Å^{-3})	0.427 and -0.449

NMR and MS Spectra of the intermediates and target products

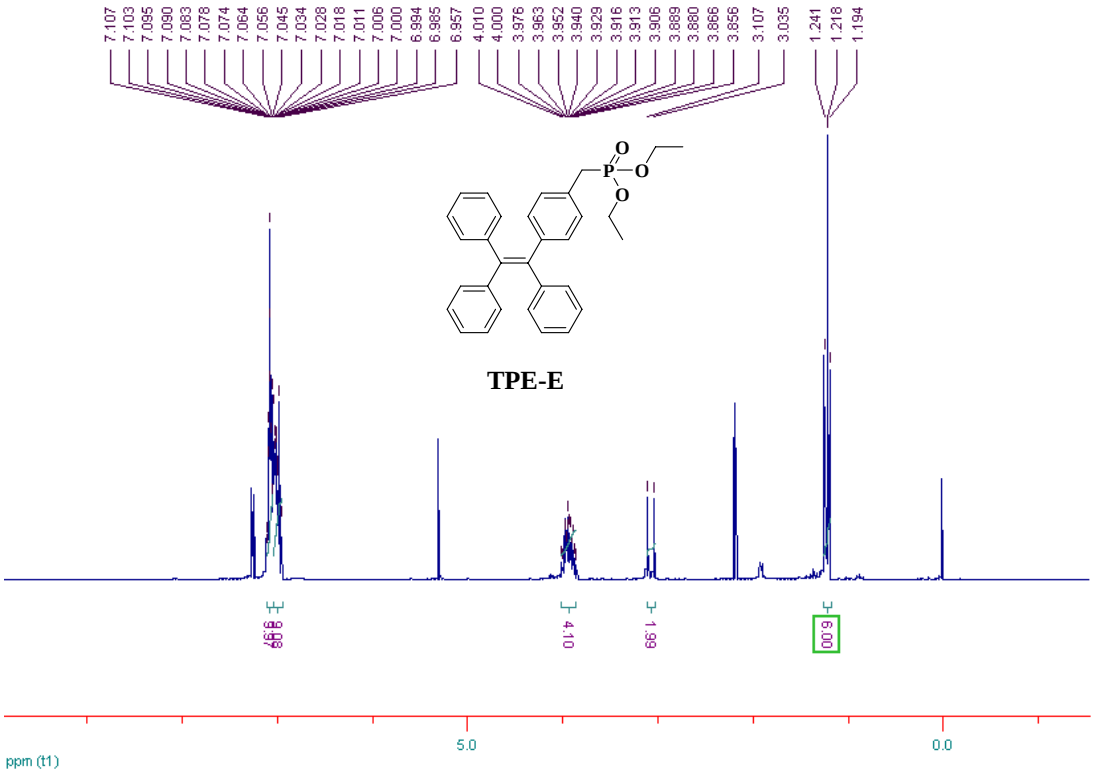

Fig. S3 ^{1}H NMR spectrum of TPE-E.

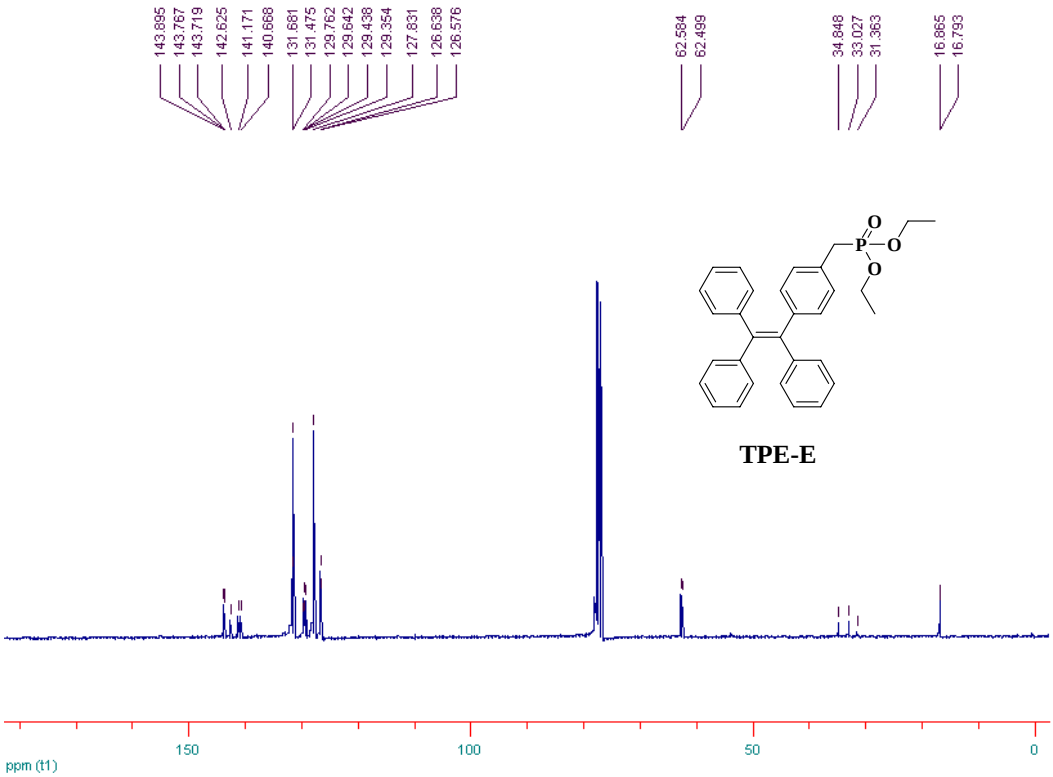

Fig. S4 ^{13}C NMR spectrum of TPE-E.

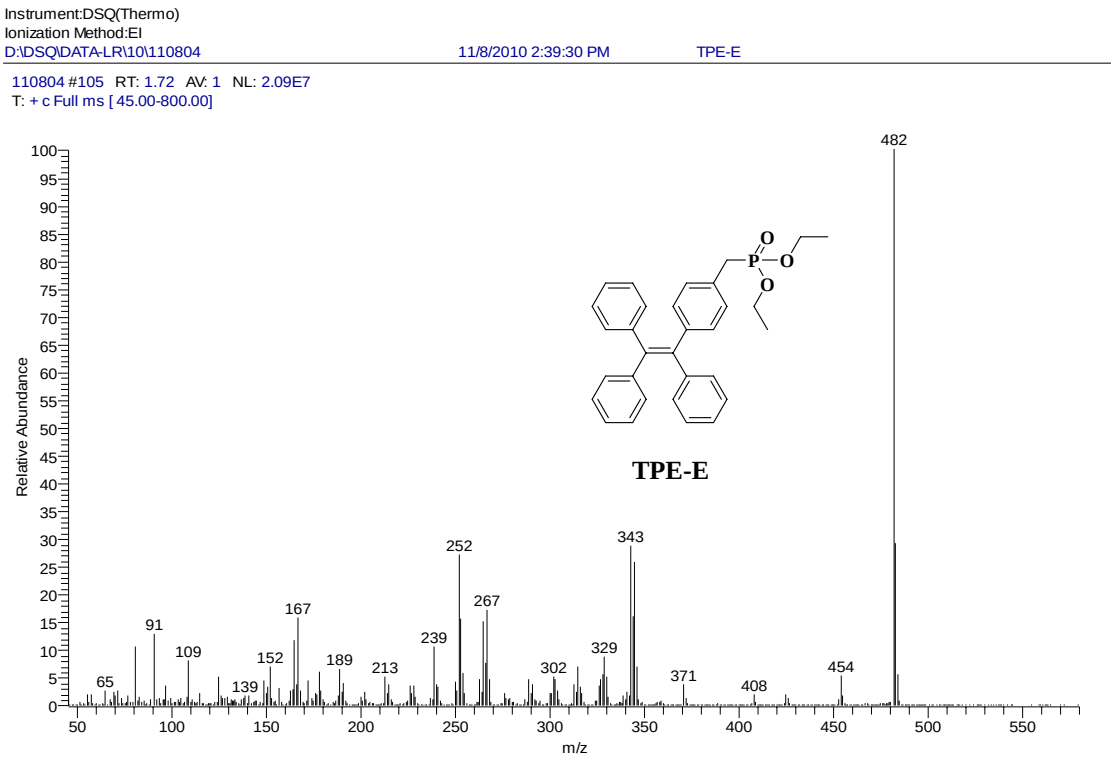

Fig. S5 MS spectrum of TPE-E.

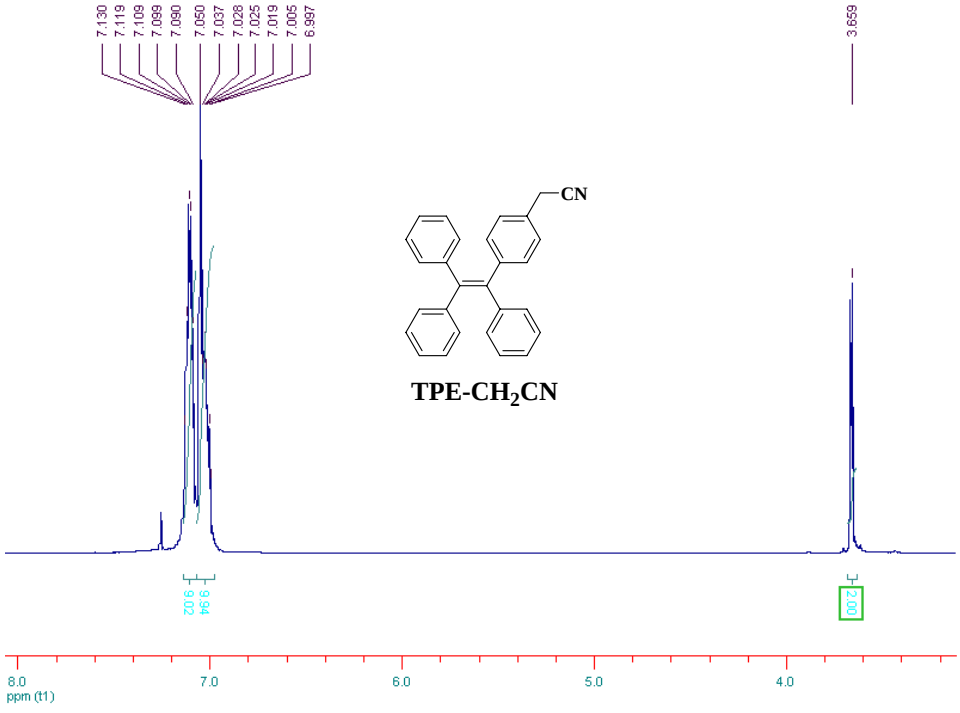

Fig. S6 ^{1}H NMR spectrum of TPE-CH_2CN.

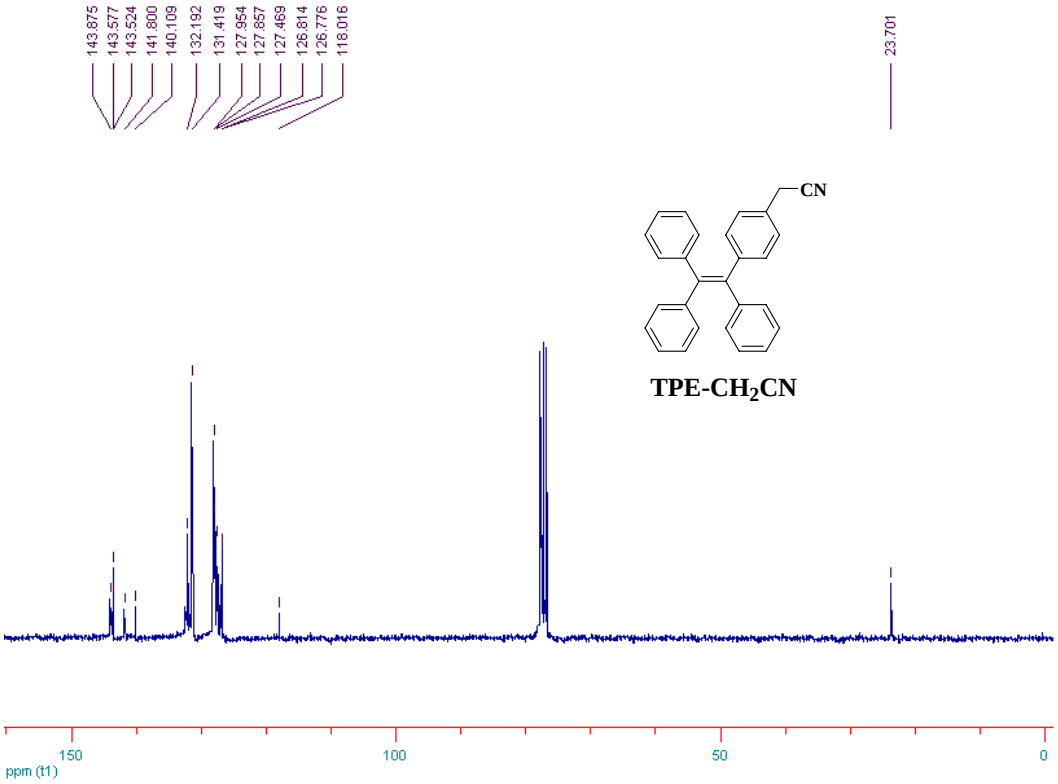

Fig. S7 ^{13}C NMR spectrum of TPE-CH_2CN.

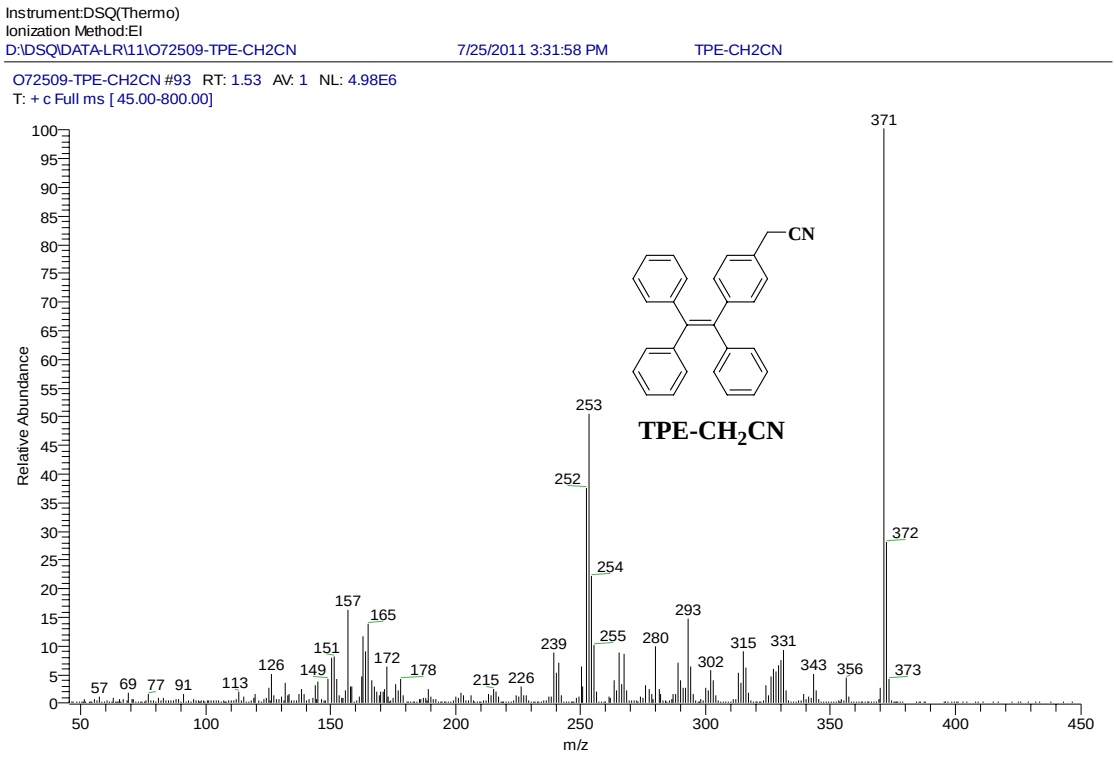

Fig. S8 MS spectrum of TPE-CH_2CN.

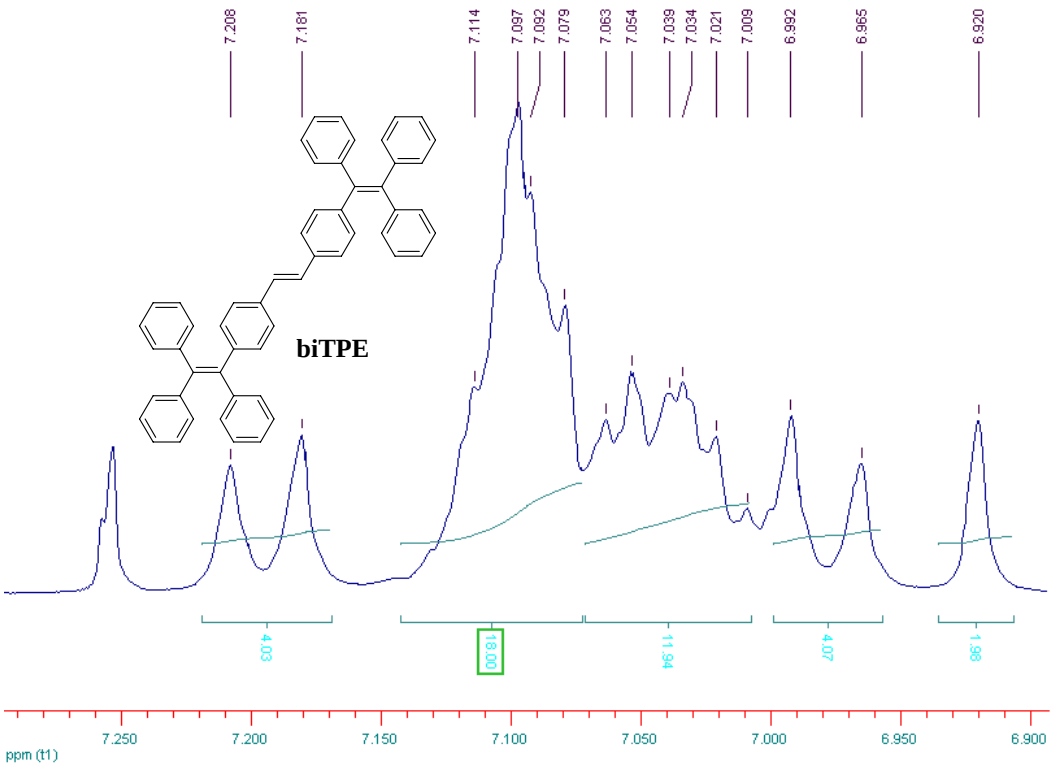

Fig. S9 ^{1}H NMR spectrum of biTPE.

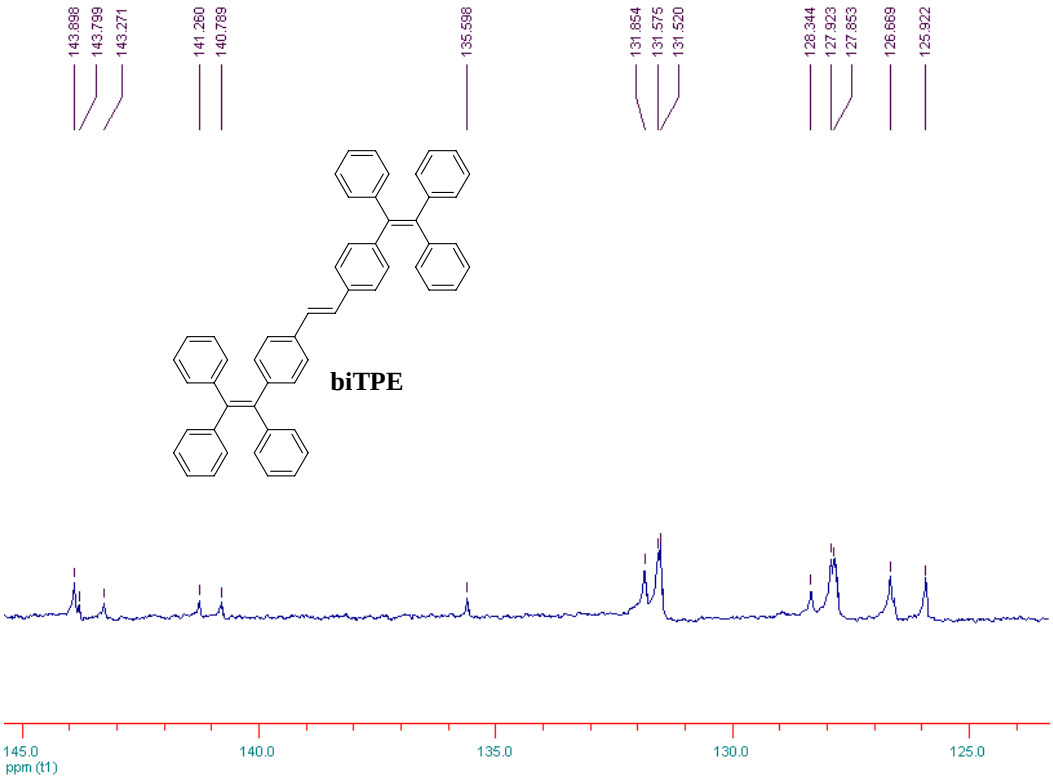

Fig. S10 ^{13}C NMR spectrum of biTPE.

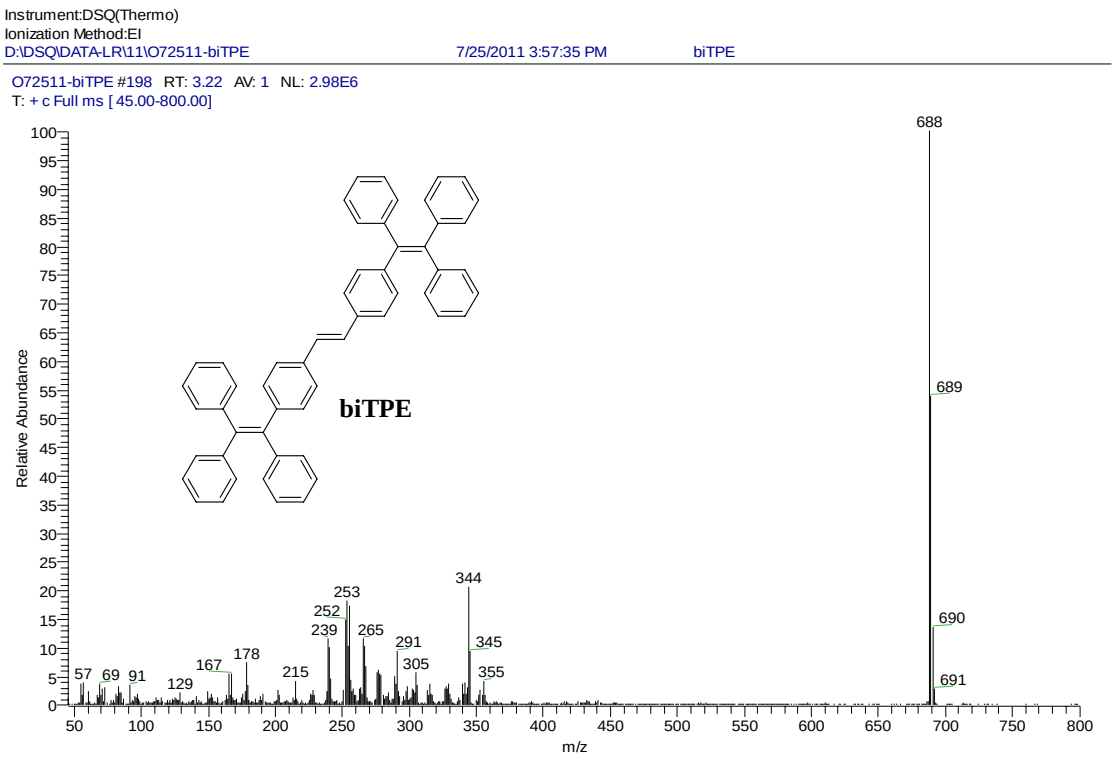

Fig. S11 MS spectrum of biTPE.

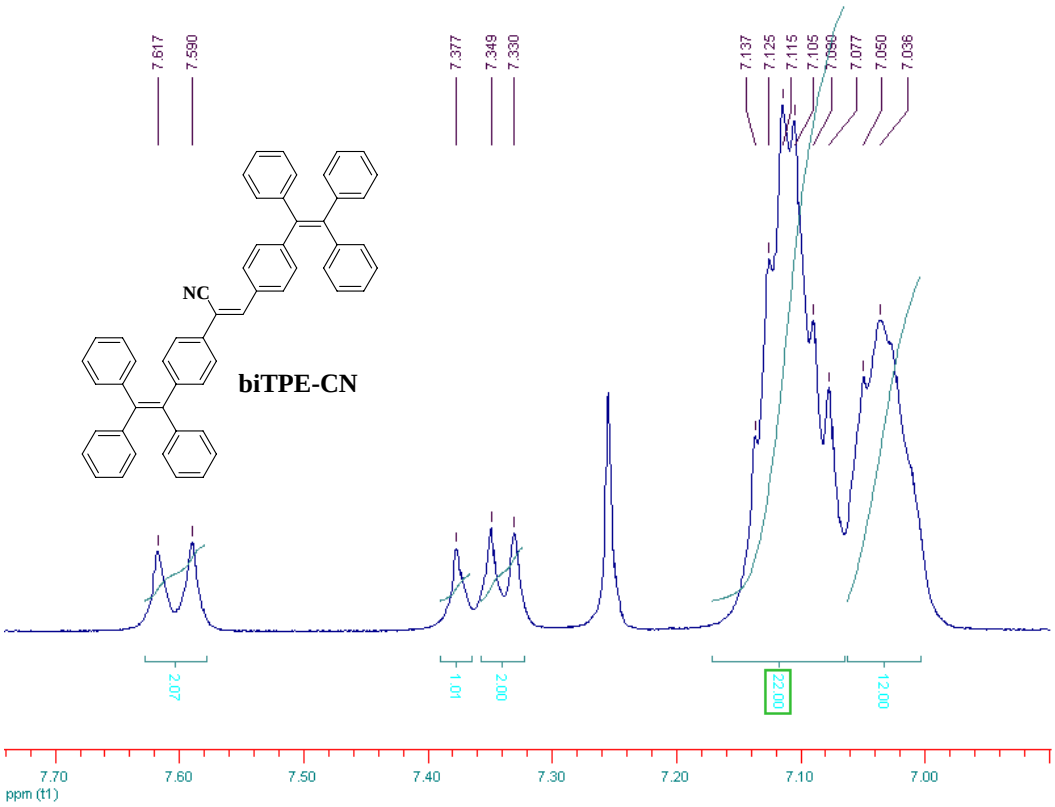

Fig. S12 ^{1}H NMR spectrum of biTPE-CN.

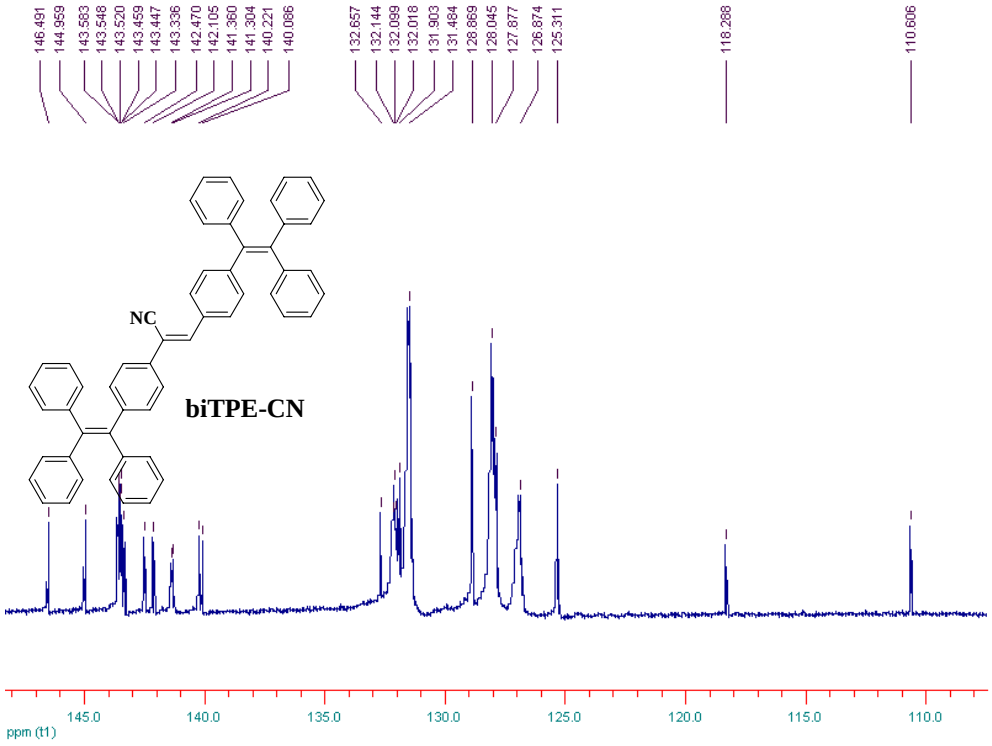

Fig. S13 ^{13}C NMR spectrum of biTPE-CN.

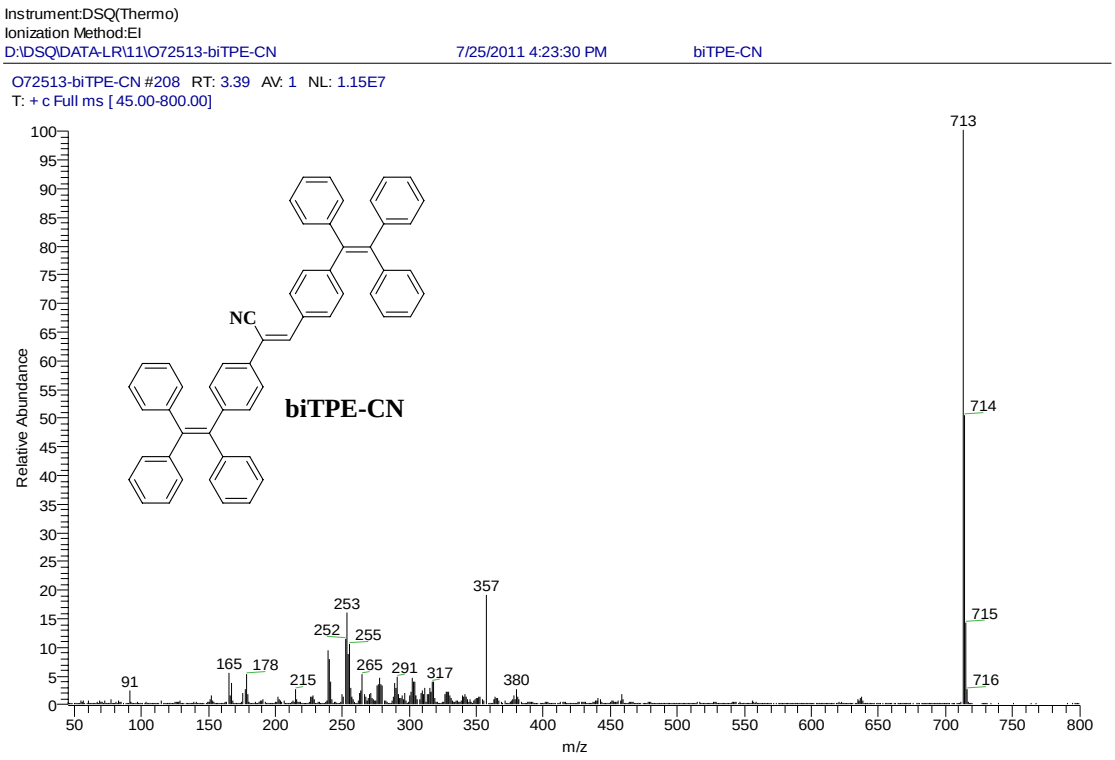

Fig. S14 MS spectrum of biTPE-CN.

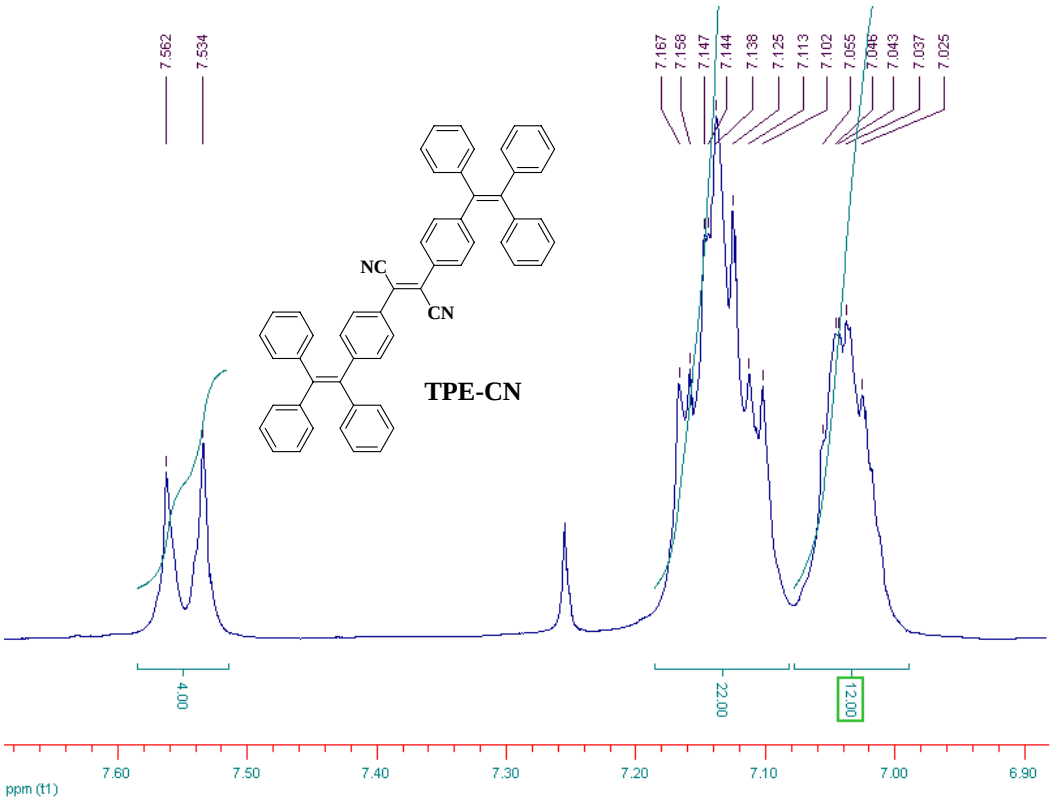

Fig. S15 ^{1}H NMR spectrum of TPE-CN.

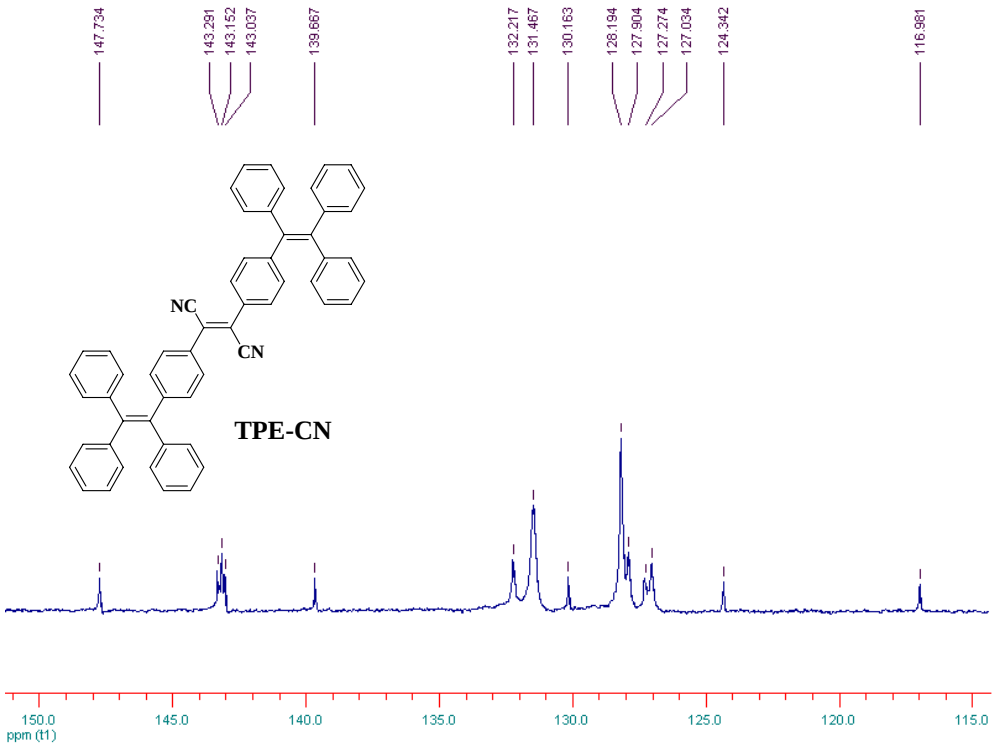

Fig. S16 ^{13}C NMR spectrum of TPE-CN.

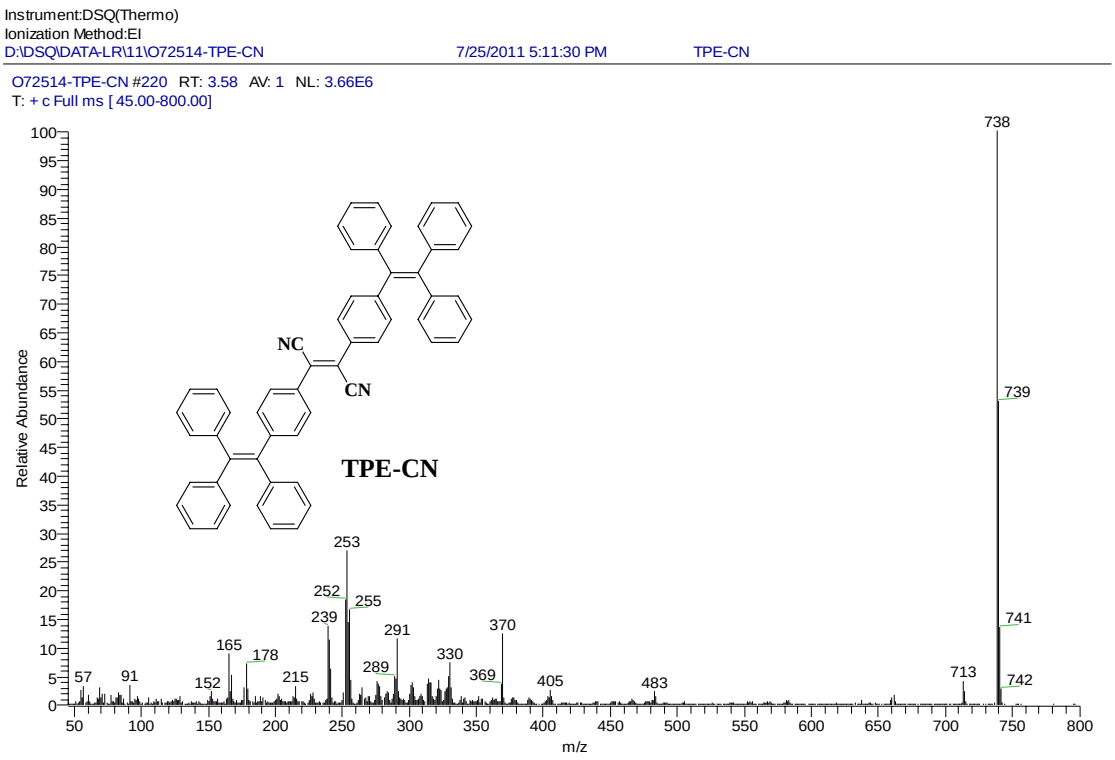

Fig. S17 MS spectrum of TPE-CN.