Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

Reversible piezofluorochromism of triphenylamine-based benzothiazole derivative with strong fluorescence response to volatile acid vapors

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Table S1. Photophysical data of **TVBT** in different solvents.

	solvent	λ_{abs} (nm)	ε^{max} (M^{-1} cm^{-1})[a]	λ_{em} (nm)	Stokes shift (cm^{-1})	Φ_F[b]
TVBT	Cyclohexane	306, 395	33200	442, 470	2692	0.98
	Toluene	308, 399	33600	467	3649	0.78
	THF	306, 400	38950	509	5354	0.70
	DCM	308, 400	36250	522	5843	0.52
	DMF	308, 401	39100	547	6656	0.32
	Acetonitrile	304, 395	37400	547	7035	0.31

[a] The maximum molar absorption coefficient in different solution (1.0×10^{-5} M). [b] The fluorescence quantum yields (Φ_F) of **TVBT** were measured using 9,10-diphenylanthracene in benzene ($\Phi_F = 0.85$) as standard.

Table S2. Crystal data for **TVBT**.

Compound	**TVBT**
Chemical formula	$C_{33}H_{24}N_2S$
Formula weight	480.60
Temperature (K)	273 (2)
Wavelength (Å)	0.71073
Color	colorless
Crystal system	triclinic
Space group	$P\bar{1}$
a (Å)	10.1930 (6)
b (Å)	10.5329 (6)
c (Å)	26.0752 (18)
α (º)	85.312 (4)
β (º)	82.900 (4)
γ (º)	64.441 (4)
Volume (Å^3)	2504.9 (3)
Z	4
Density (calculated, g·cm^{-3})	1.274
F (000)	1008
Absorption coefficient (mm^{-1})	0.154
□ range for data collection (º)	2.144 / 24.710
Index ranges (h, k, l)	–11/11, –12/12, –22/30
Measured reflections	16065
Independent reflections	2016
R_{int}	0.0327
Observed reflections [I > 2σ (I)]	4313
Data / restraints / parameters	8515 / 24 / 656
Goodness-of-fit on F^2	1.028
R indices (all data)	R_1 = 0.1347, wR_2 = 0.1989
R indices [I > 2σ (I)]	R_1 = 0.0656, wR_2 = 0.1578
Largest diffraction peak and hole (e·Å^{-3})	0.536 and –0.388

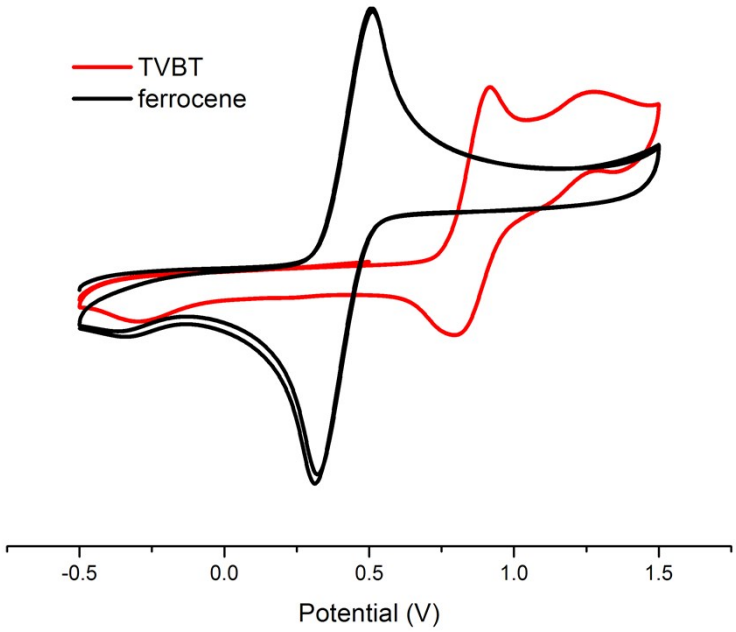

Fig. S1 Cyclic voltammetry diagrams of compounds **TVBT** and ferrocene measured in anhydrous DCM with Bu_4NPF_6 (0.1 M) as electrolyte at a scan rate of 100 mV/s.

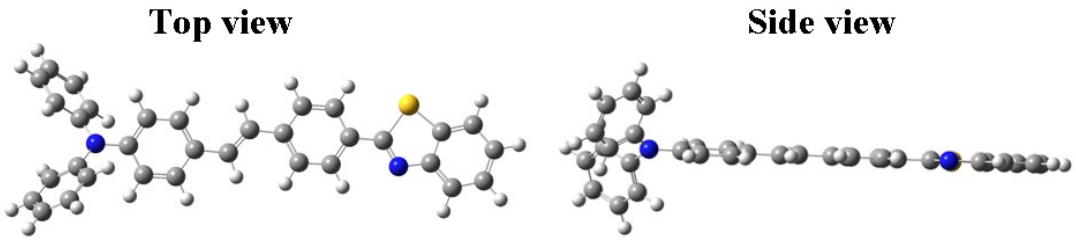

Fig. S2 Optimal molecular conformations by the DFT/B3LYP/6-31G(d) calculation.

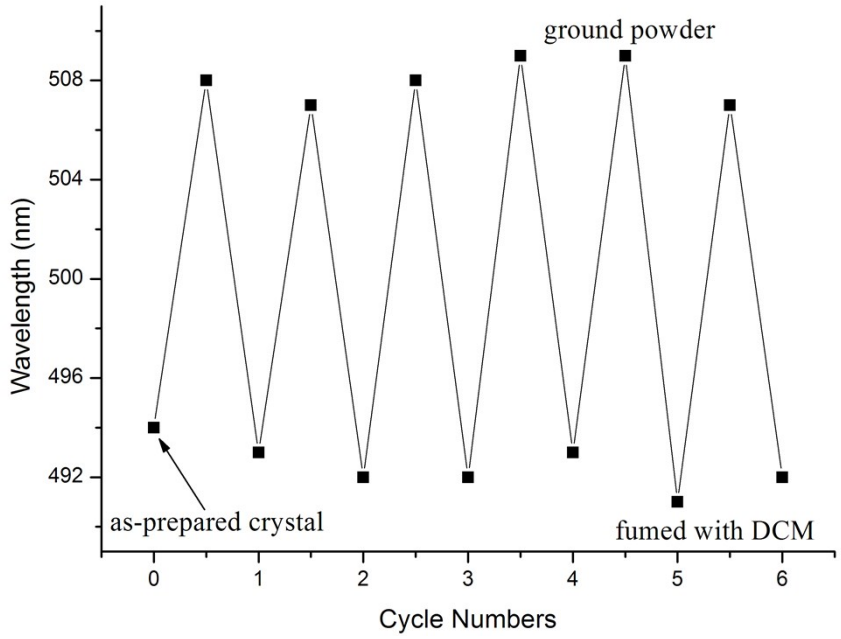

Fig. S3 Maximum fluorescence emission of **TVBT** upon repeating treated by grinding and fuming with DCM.

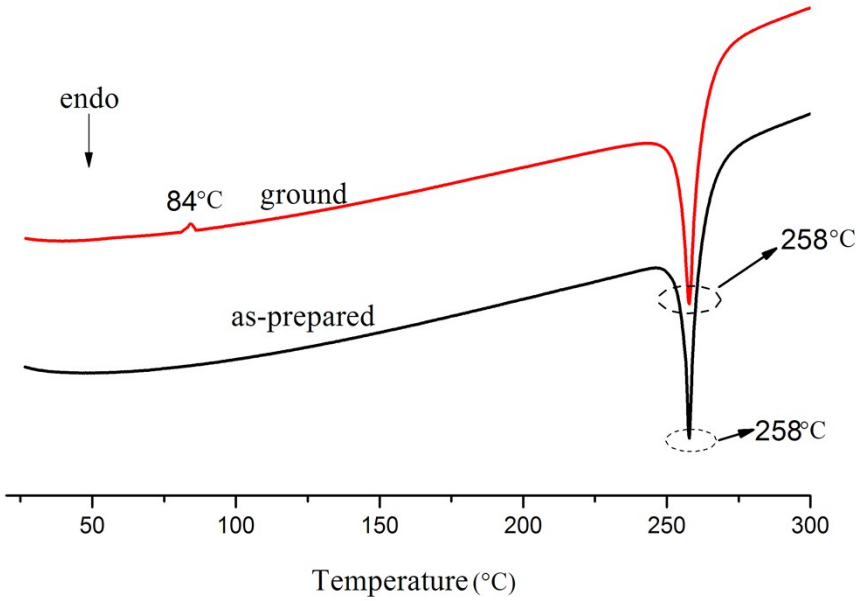

Fig. S4 DSC curves for the as-prepared crystal and ground powder of **TVBT** under nitrogen atmosphere at a heating rate of 10 °C/min.

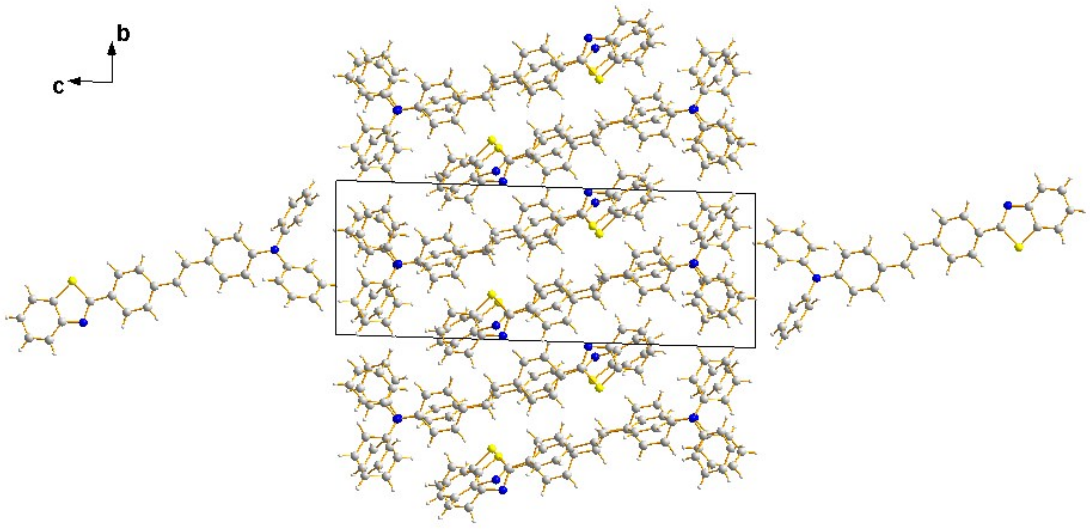

Fig. S5 Molecular packing diagram of **TVBT** in single crystal.

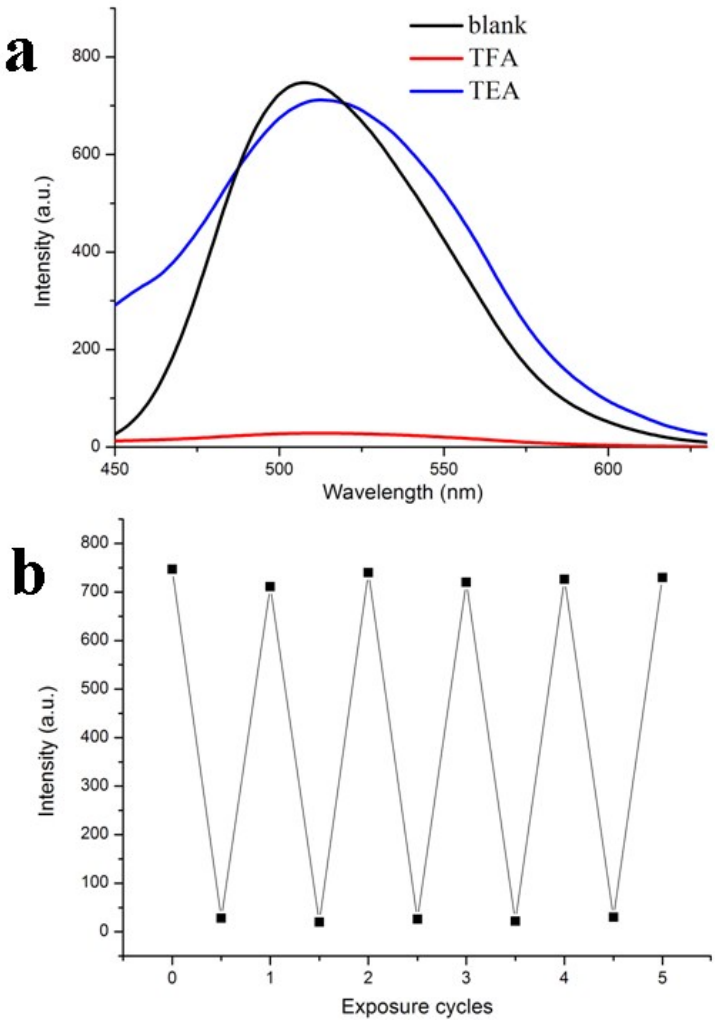

Fig. S6 (a) Fluorescence spectral change of **TVBT** in $CHCl_3$ (5.0×10^{-5} M) with additional 150 equiv TFA and TEA at room temperature (λ_{ex} = 400 nm); (b) Reversible fluorescence emission intensity in $CHCl_3$ of **TVBT** upon additional equivalent TFA and TEA.

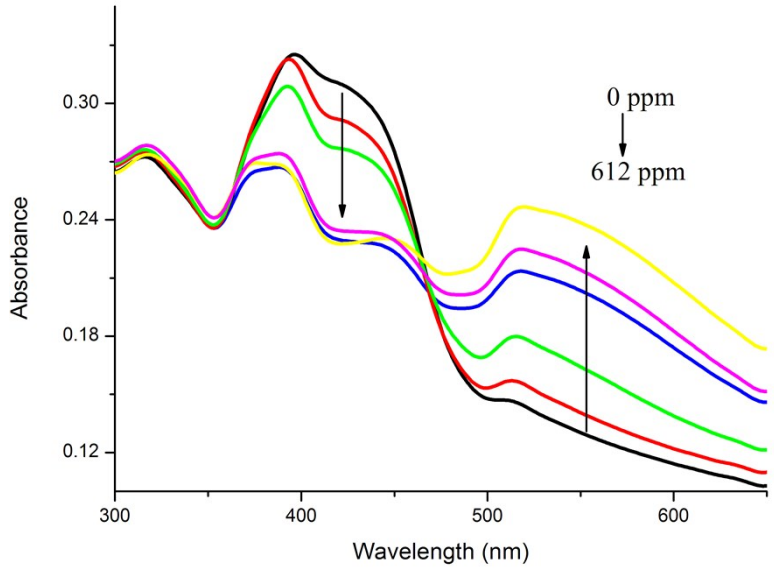

Fig. S7 UV-vis absorption spectra of the ground film of **TVBT** upon exposure to different amounts of TFA vapor.

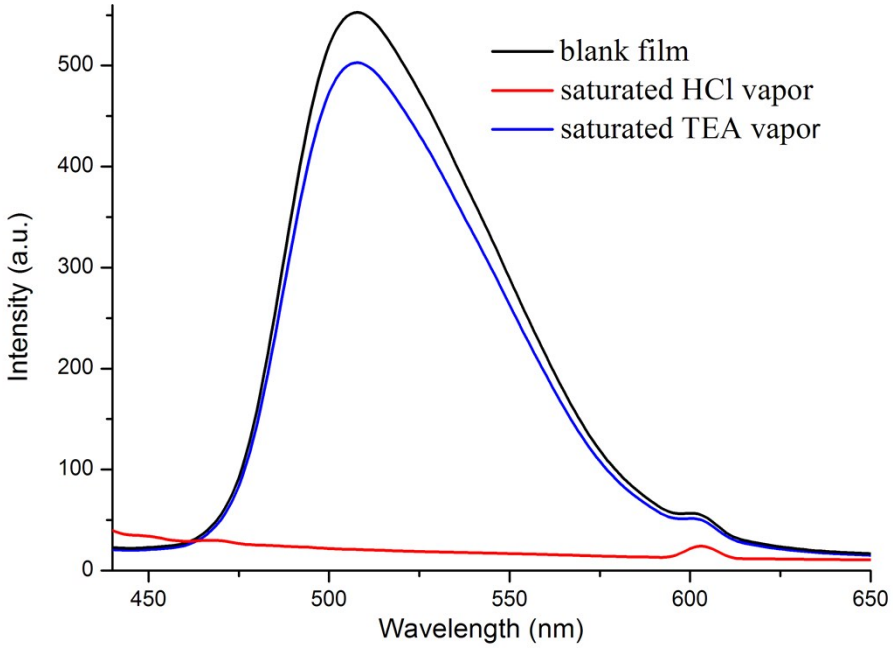

Fig. S8 Fluorescence spectral change of the ground film of **TVBT** upon exposure to saturated HCl and TFA vapors.

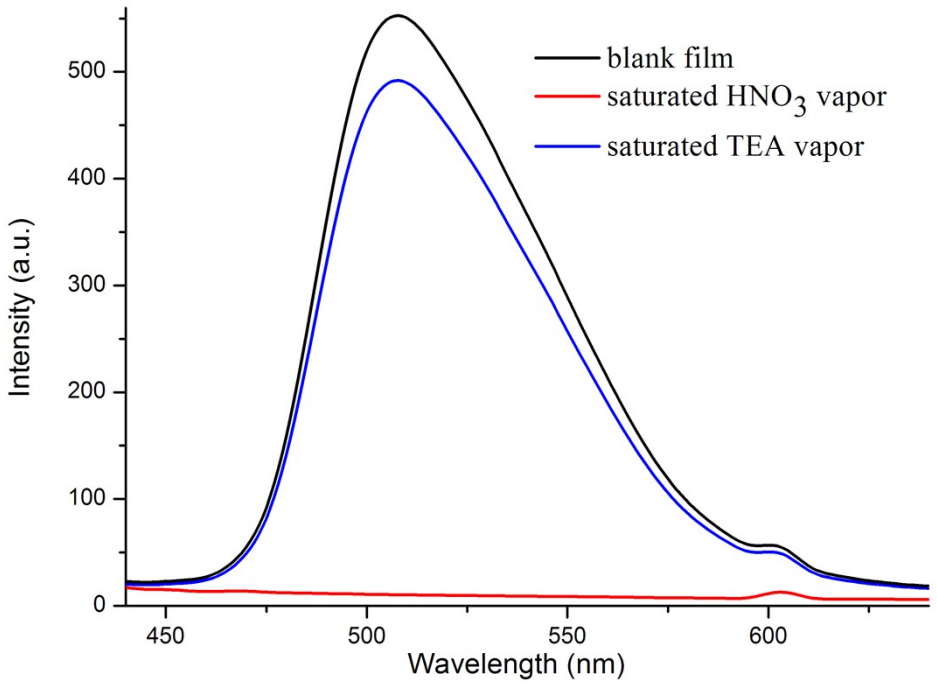

Fig. S9 Fluorescence spectral change of the ground film of **TVBT** upon exposure to saturated HNO_3 and TFA vapors.

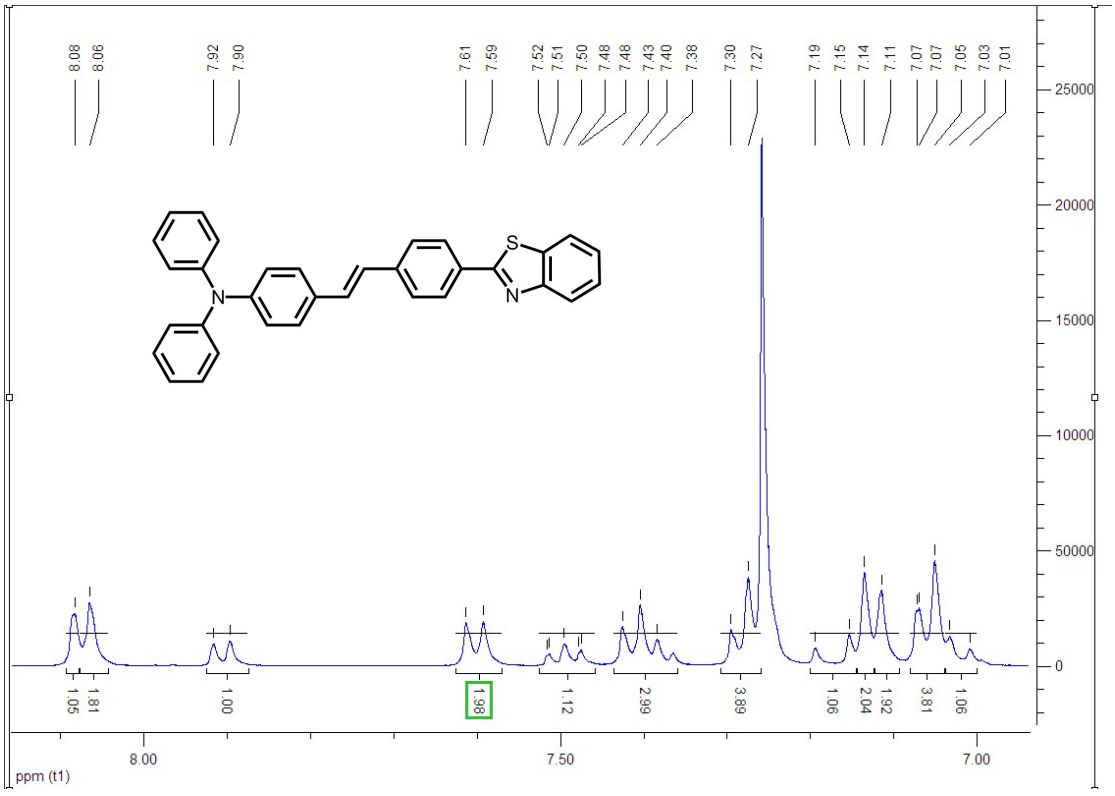

Fig. S10 ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of compound **TVBT**.

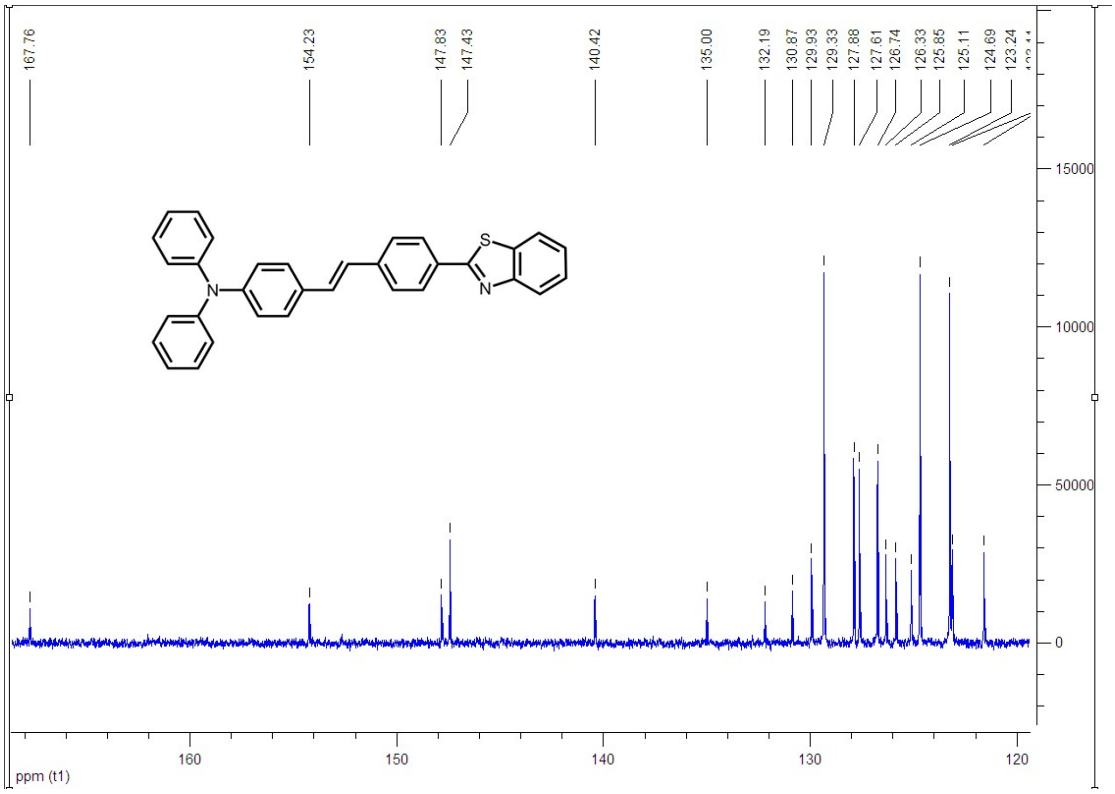

Fig. S11 ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of compound **TVBT**.

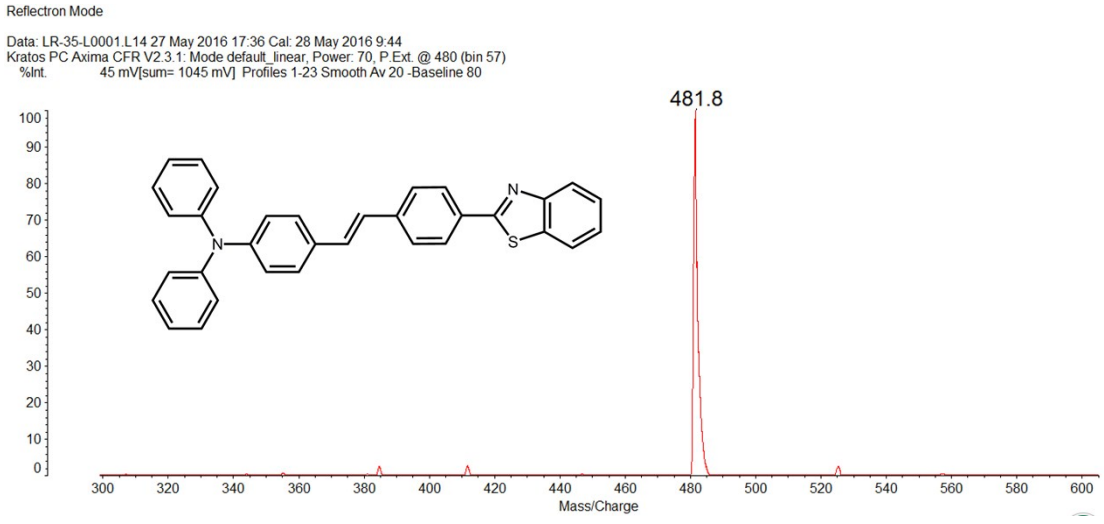

Fig. S12 The MALDI/TOF MS spectrum of compound **TVBT**.