Polystyrene with methoxytriphenylamine-conjugated-thiophene moiety side-chain as a dopant-Free hole-transporting material for perovskite solar cells

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TableS1. Materials, quantities and cost for the synthesis of HTM-P1.

Chemical	Weight reagent (g/g)	Weight solvent (g/g)	Weight work up (g/g)	Price of chemical ($/kg)	Cost of chemical ($/g product)	Total Cost ($/g)
3-Thiophenemethanol	0.49			1208.30	0.59	
NBS	1.67			40.72	0.07	
THF		3		11.85	0.04	
Cealite			2	0.57	0.00	
diethyl ether			30	4.52	0.14	
NaOH			30	3.16	0.09	
Petroleum ether			200	7.41	1.48	
ethyl acetate			100	4.53	0.45	
silica gel			20	10.96	0.22	
Compound 1						**3.08**
Compound 1	0.44			3081.36	1.36	
4-[Di(p-methoxyphenyl)amino]benzene-1-boronic acid	1.20			2265	2.72	
$Pd(PPh_3)_4$	0.09			9049.77	0.81	
THF		17.8		11.85	0.21	
K_2CO_3	1.10			7.41	0.01	
water		10			0.00	
CH_2Cl_2			200	4.44	0.89	
Na_2SO_4			5	3.26	0.02	
MeOH			10	3.32	0.03	
silica gel			20	10.96	0.22	
Compound 2						**6.26**
Compound 2	1.07			6264.06	5.32	
4-Vinylbenzylchloride	0.34			301.66	0.08	
NaH	0.05			301.55	0.13	
DMF		5		5.42	0.03	
Na_2SO_4			5	3.26	0.02	
CH_2Cl_2			200	4.44	0.89	
Petroleum ether			100	7.41	0.74	
silica gel			20	10.96	0.22	
Compound 3						**8.72**
Compound 3	1.16			8715.48	10.11	
AIBN	0.01			49.01	0.0005	
THF		2		11.85	0.02	
MeOH			20	3.32	0.07	
HTM-P1						**10.20**

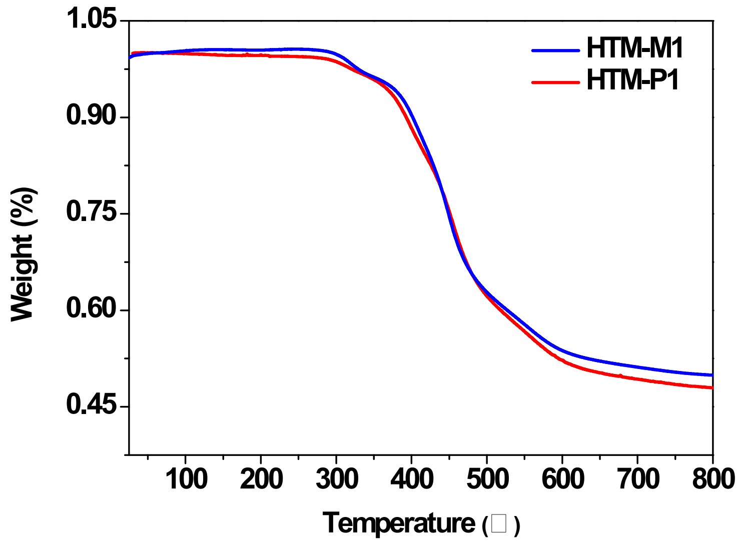

Figure S1. TGA of HTM-M1 and HTM-P1

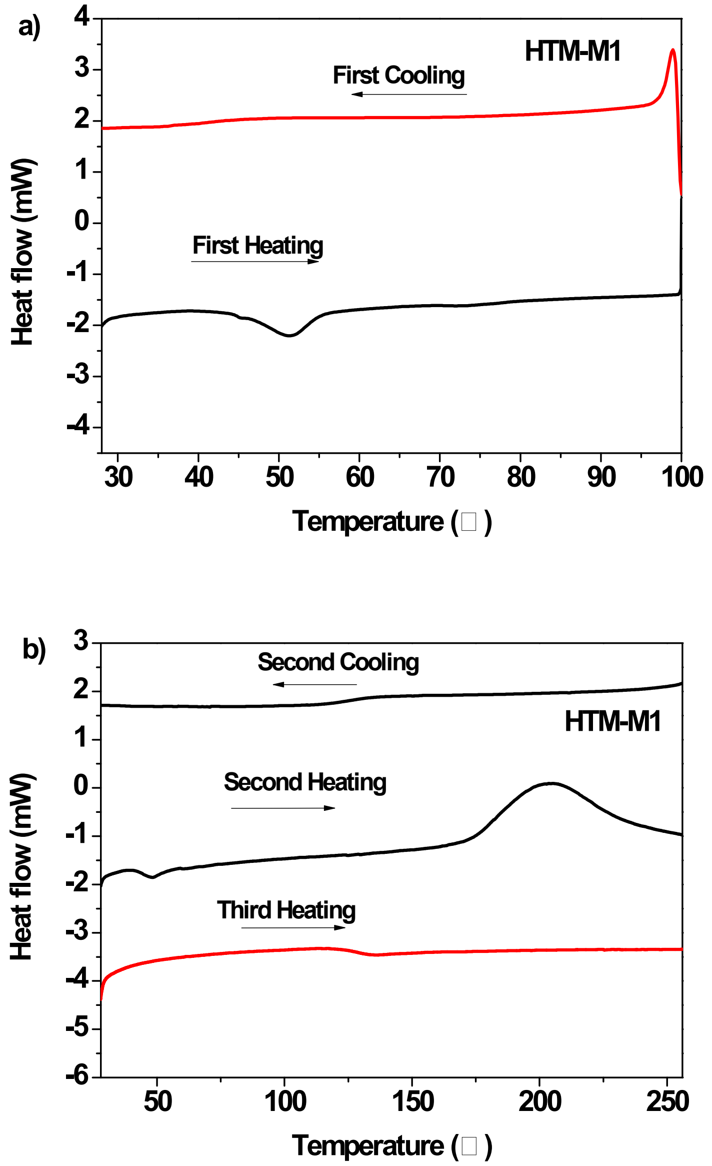

Figure S2. DSC of HTM-M1. a) The first heating and cooling (25 – 100 °C); b) the second heating and cooling, and the third heating (25 – 260 °C). The T_g of HTM-M1 is 46 °C, and the polymeric reaction of HTM-M1 begins at around 175 °C. From the Figure S2b we can see that the T_g increased to 125 °C after the polymerization of HTM-M1.

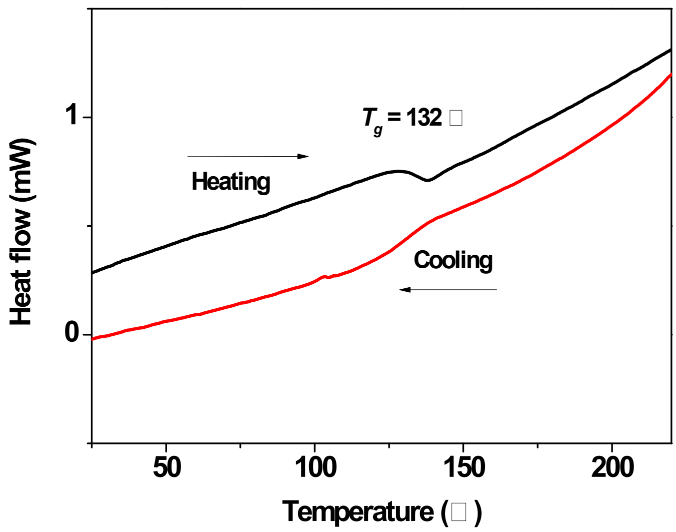

Figure S3. DSC of HTM-P1

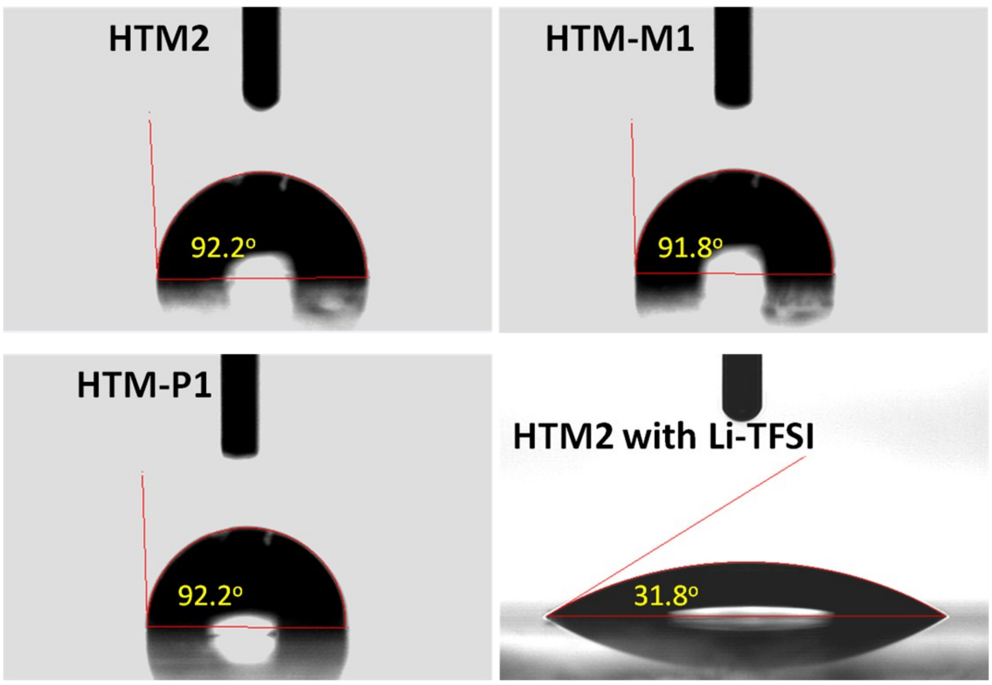

Figure S4. Water contact angles on HTM2, HTM-M1, HTM-P1, HTM2 with dopant (Li-TFSI).

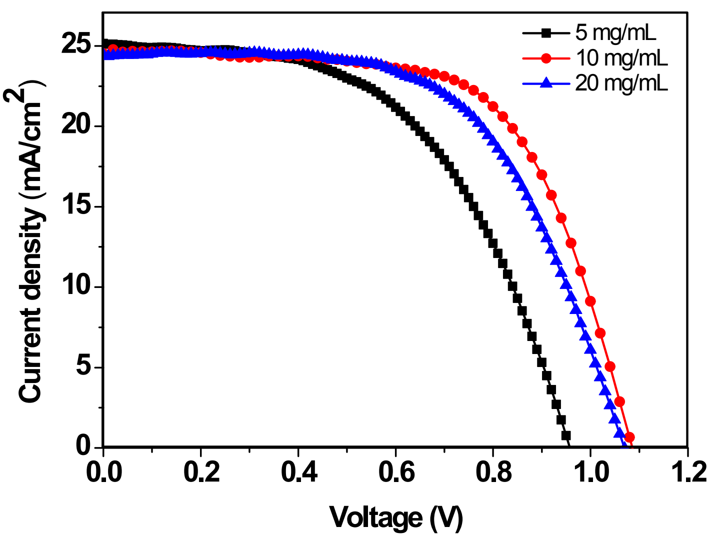

Figure S5. Current–voltage curves of the devices based on HTM-P1 with different concentrations in chlorobenzene.

Table S2. Summary of device parameters of the devices based on HTM-P1 with different concentrations in chlorobenzene; open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF) and average efficiency (PCE).

	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF	Best PCE [%]
5 mg/mL	25.0	0.95	55.3	12.8
10 mg/mL	24.8	1.08	63.9	17.2
20 mg/mL	24.7	1.07	62.1	16.4

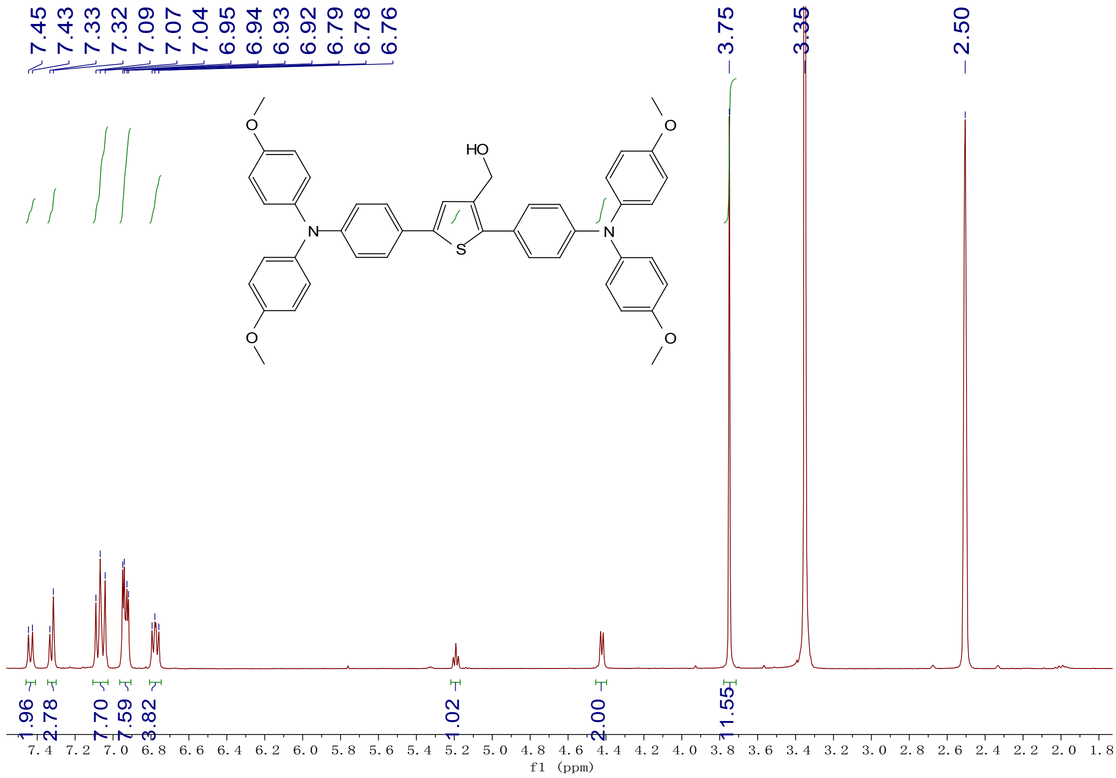

Figure S6. ^{1}H NMR of compound **2**.

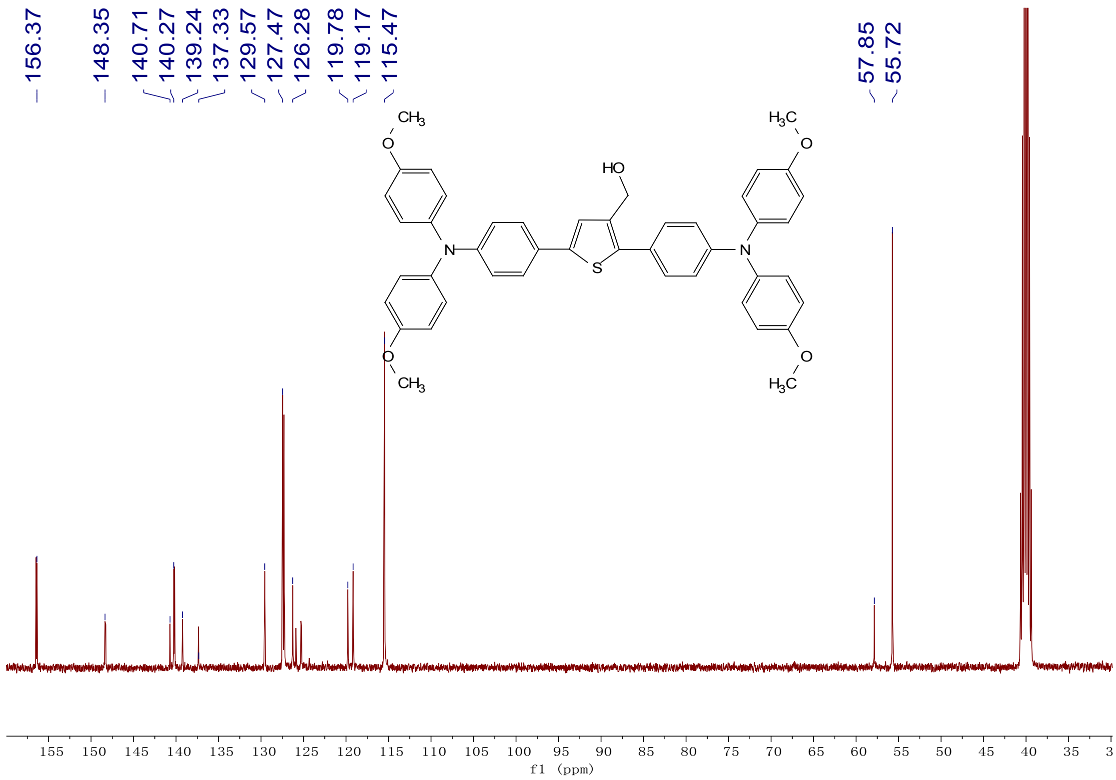

Figure S7. ^{13}C NMR of compound **2**.

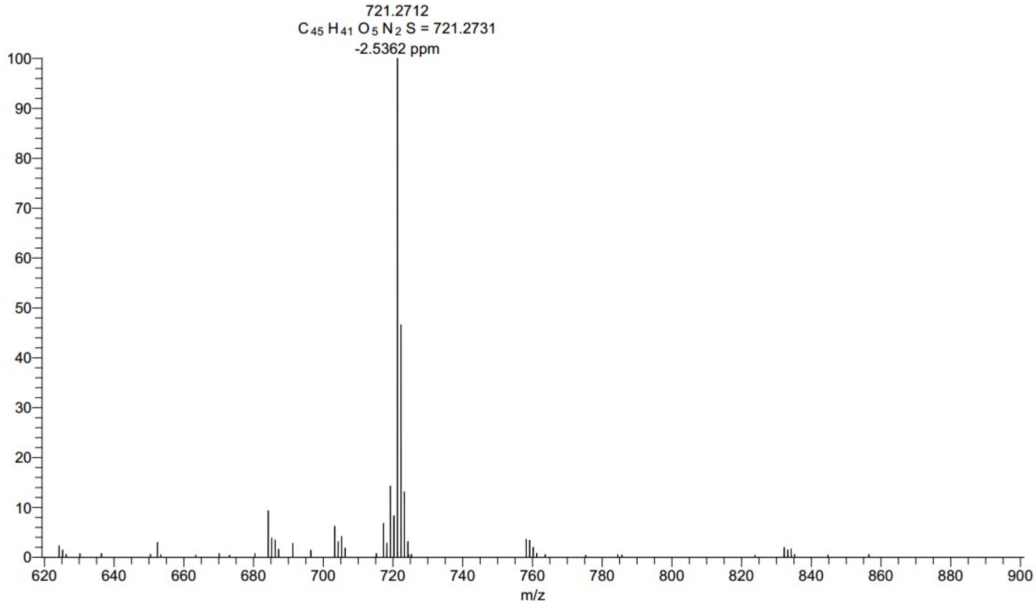

Figure S8. HRMS of compound **2**.

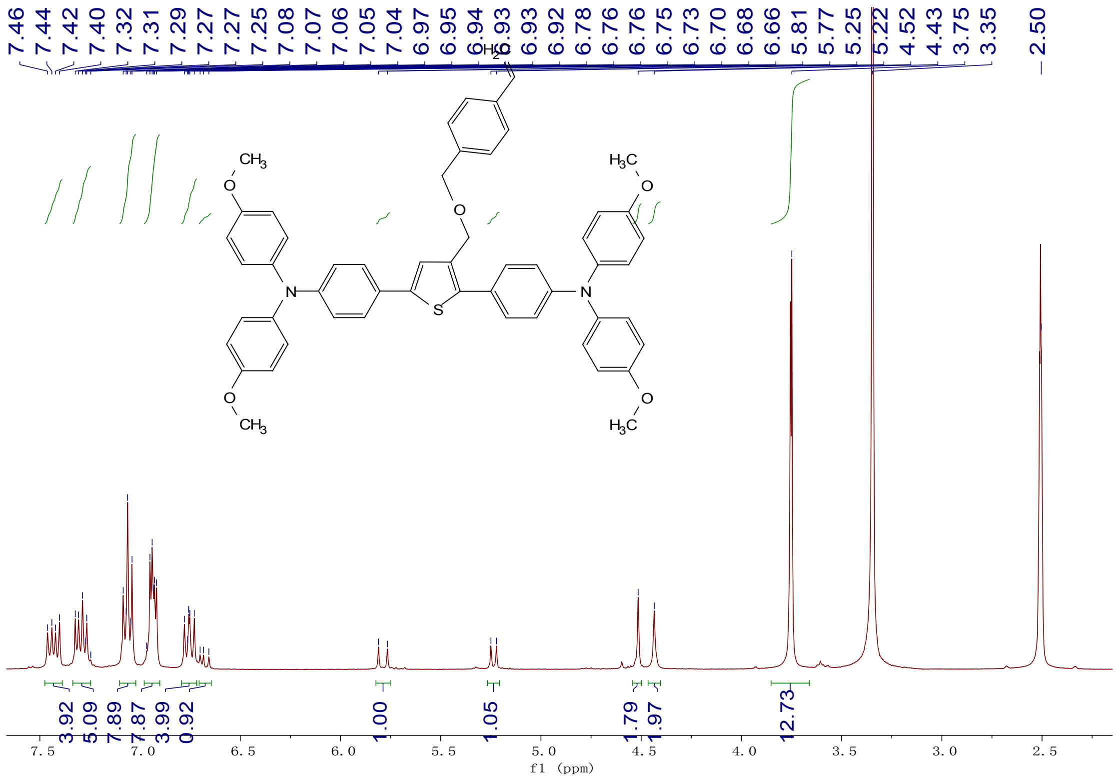

Figure S9. [1]H NMR of compound **3**.

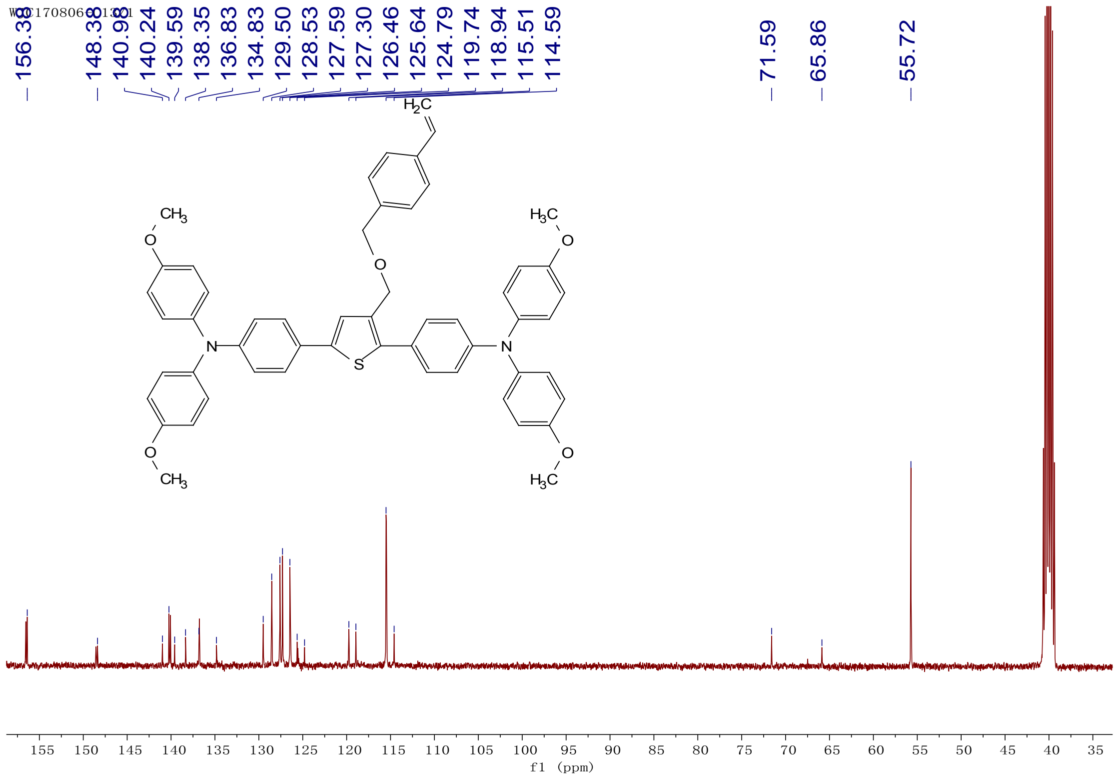

Figure S10. ^{13}C NMR of compound **3**.

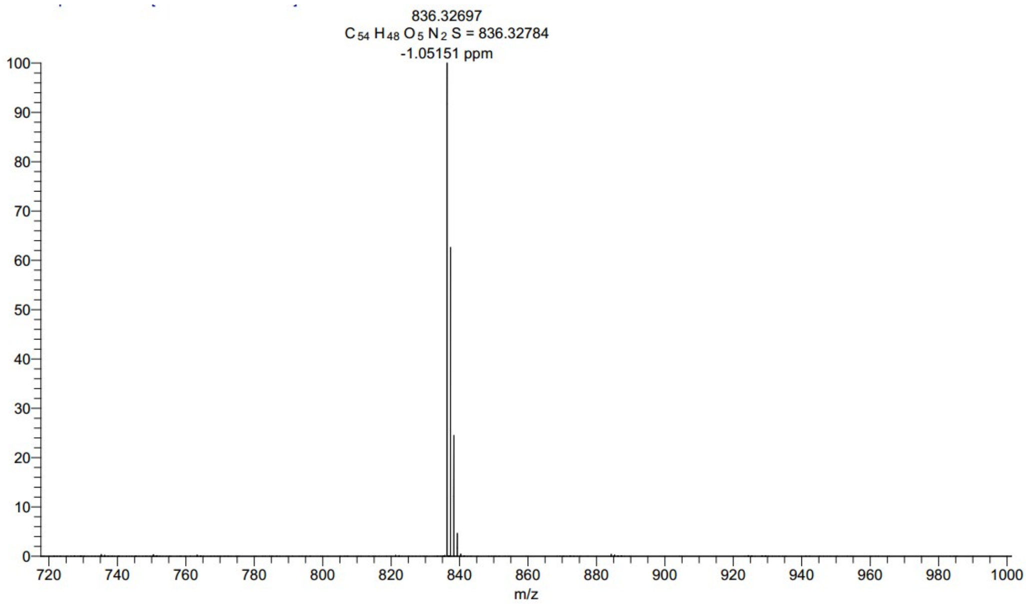

Figure S11. HRMS of compound **3**.

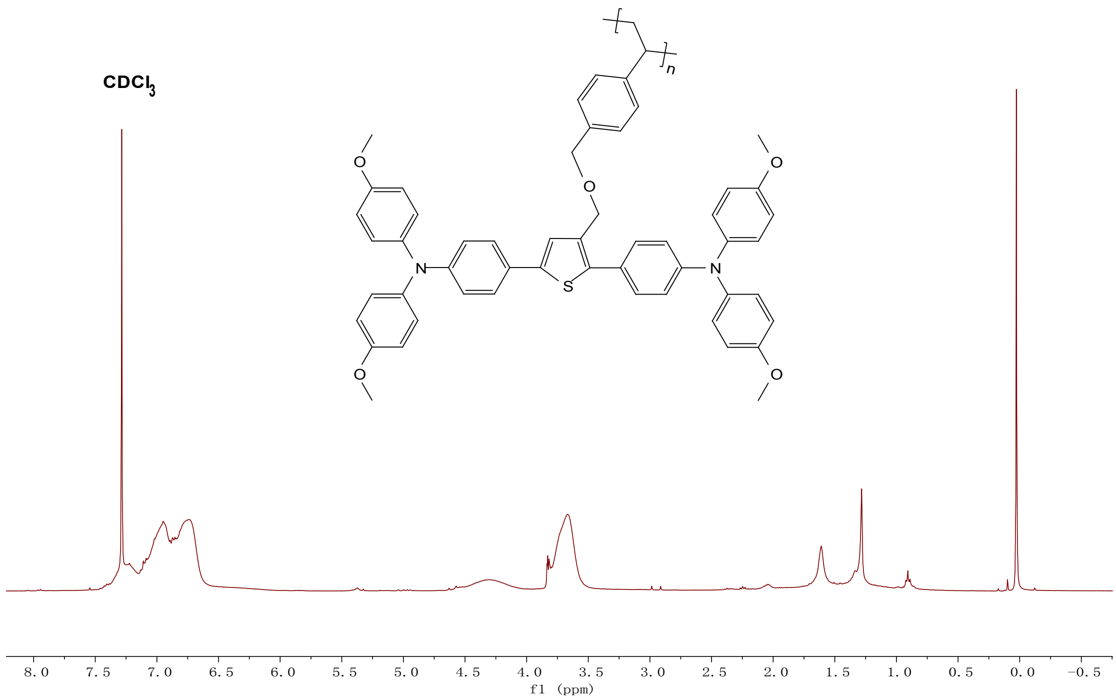

Figure S12. ^{1}H NMR of HTM-P1.