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Highly Efficient ~~Blue~~ Blueish-green Fluorescent OLEDs Based on AIE Liquid Crystal Molecules: From Ingenious Molecular Design to Multifunction Material

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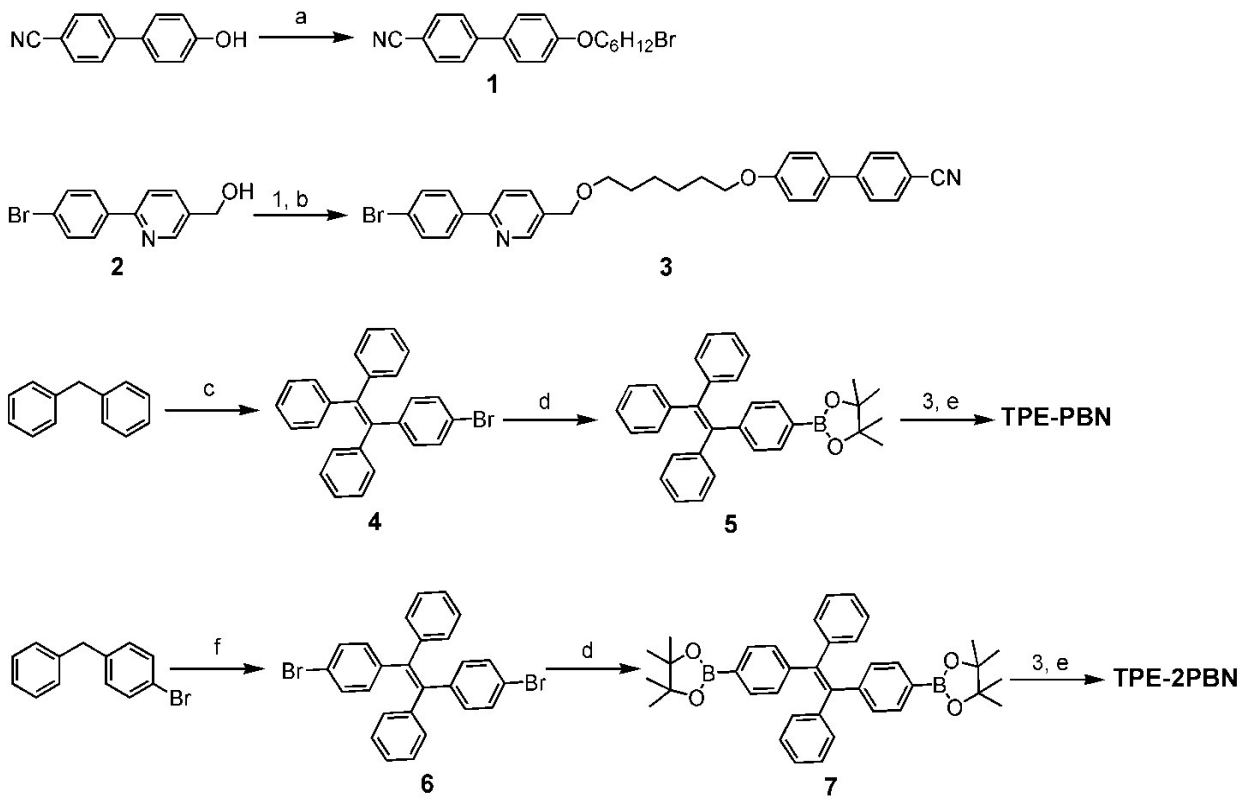
Temperature-dependent XRD diffraction data for TPE-2PBN

NMR and MS spectra



Reaction conditions: (a) 1,6-dibromohexane, K_2CO_3, KI, acetone, 65 °C, 24 h, yield, 86%; (b) (6-(4-bromophenyl)pyridin-3-yl) methanol, NaH, DMF, 0 °C, 30 min, yield: 84%; (c) i) (4-bromophenyl)(phenyl)methanone, *n*-butyllithium, THF, 0 °C, 30 min; ii) *p*-toluenesulfonic acid, toluene, 110 °C, 3-4 h, yield: 66%; (d) bis(pinacolato)diboron, CH_3COOK, [$PdCl_2$(dppf)], 1,4-dioxane, 80 °C, 24 h, yield: 5: 76%, 7: 60%; (e) [$Pd(PPh_3)_4$], 2 M K_2CO_3, THF, 65 °C, 24 h, yield, TPE-PBN: 67%, TPE-2PBN: 60%; (f) Zn, $TiCl_4$, THF, –78 °C, 30 min, yield: 83%.

Scheme 1. Synthetic route for both PBN-TPE and PBN-TPE-PBN

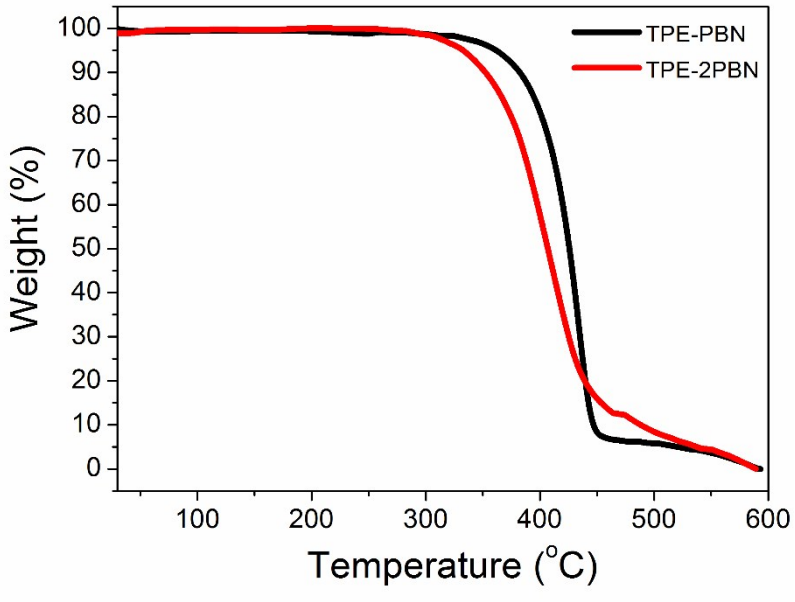


Figure S1 TGA curves of TPE-PBN and TPE-2PBN

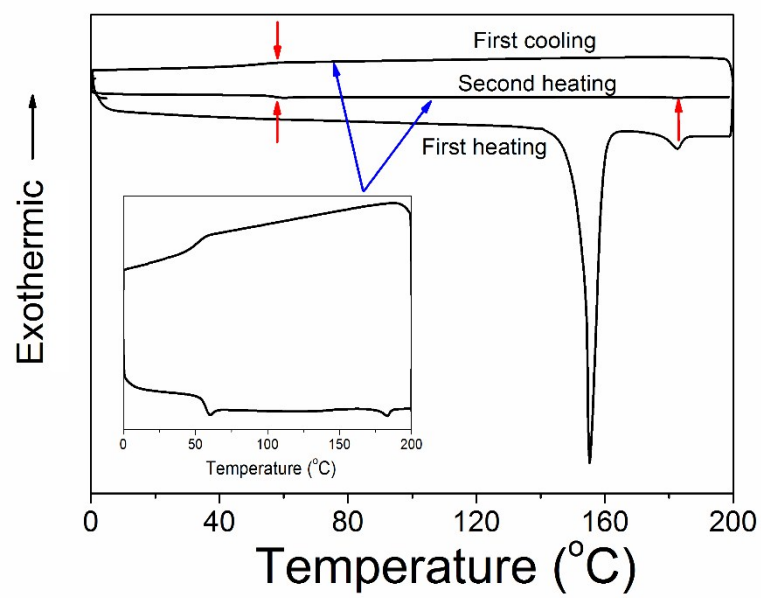


Figure S2 DSC curves of TPE-PBN: the first heating rate is 10 °C/min^{-1}, the first cooling and second heating rates are 5 °C/min^{-1}

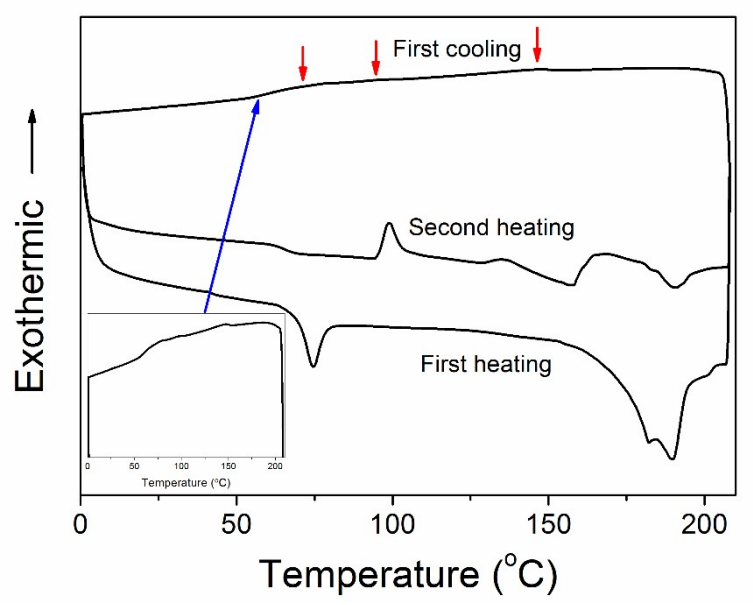


Figure S3 DSC curves of TPE-2PBN: the first heating rate is 10°C/min, the first cooling and second heating rates are 5 °C/~~min~~ min^{-1}

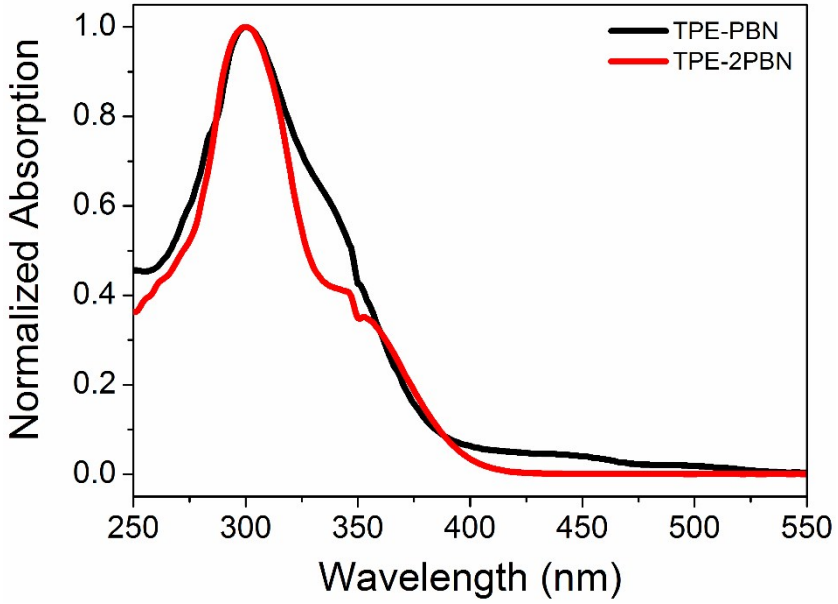


Figure S4. UV-vis absorption of compounds measured in THF at room temperature

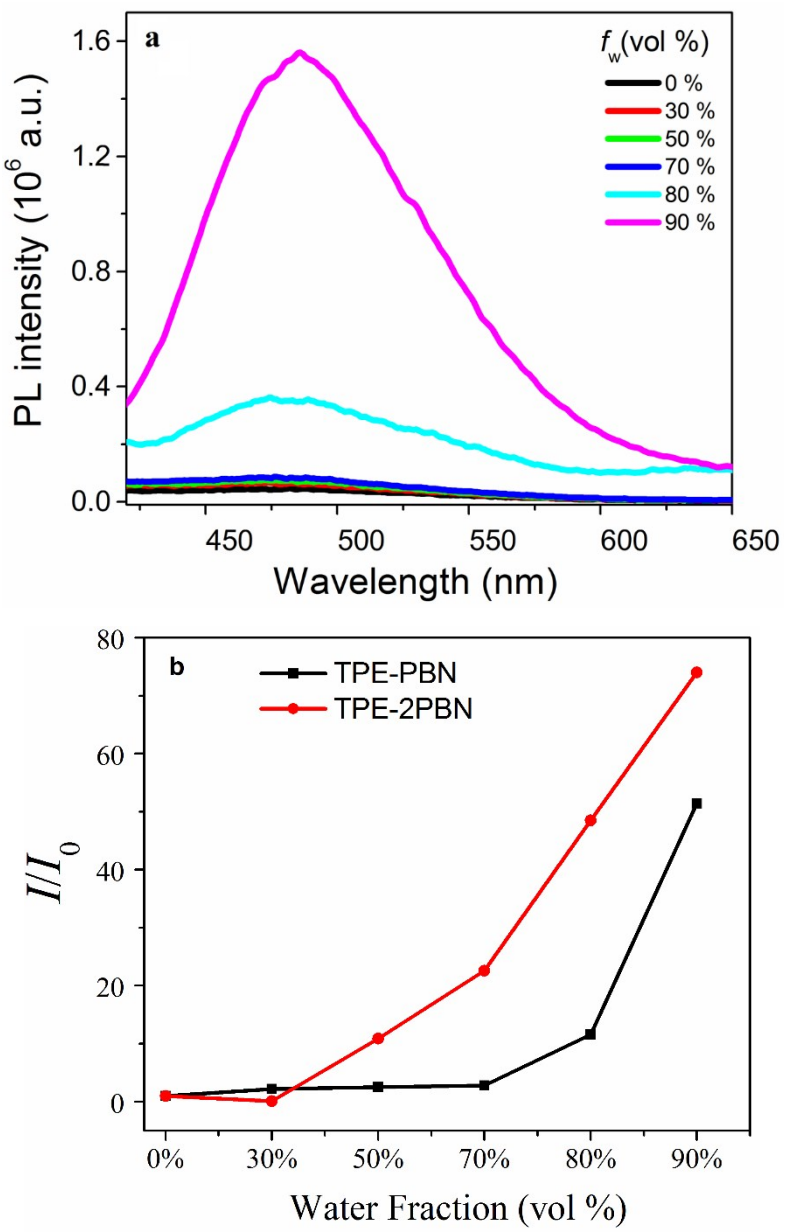


Figure S5. a) Fluorescence spectra of TPE-PBN in THF/water mixtures with different water fractions (f_w); $\lambda_{excitation}$ = 360 nm. b) Plot of (I/I_0) values versus the compositions of the aqueous mixtures. I_0 = emission intensity in pure THF solution.

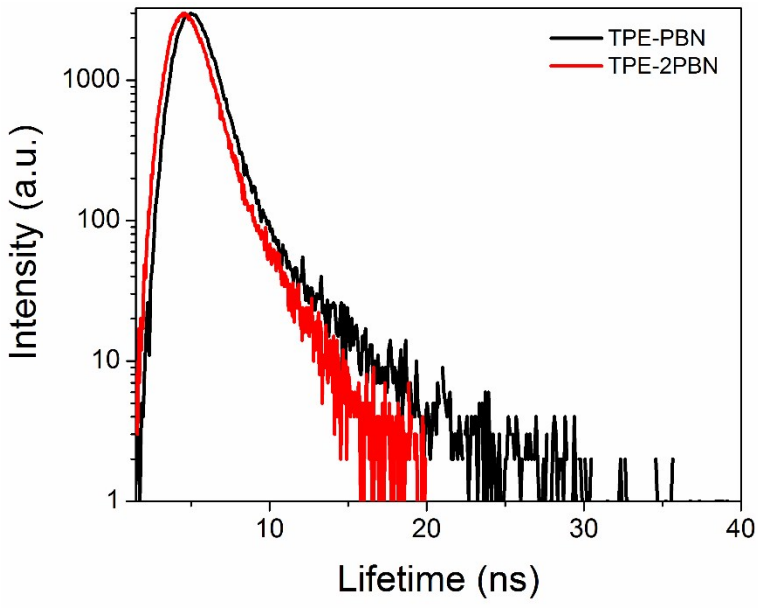


Figure S6 Lifetime decays of TPE-PBN and TPE-2PBN measured in toluene at room temperature

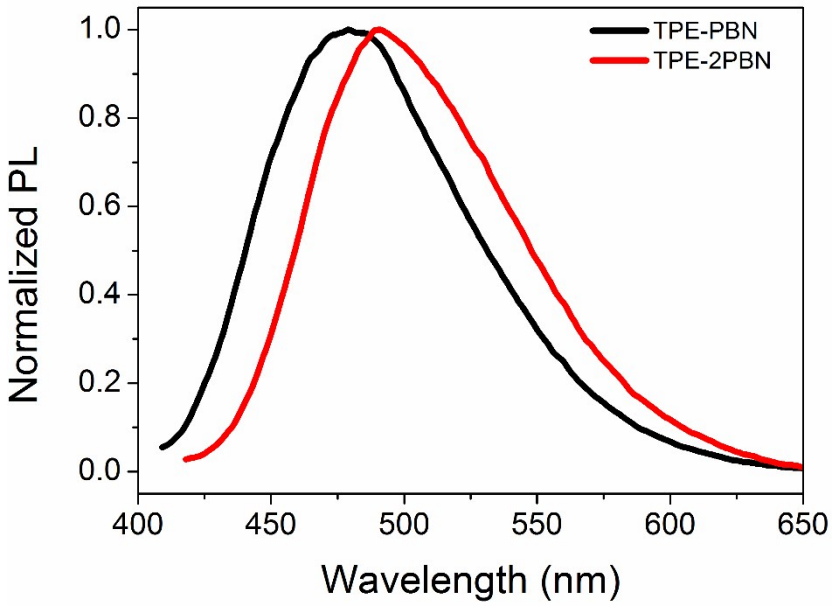


Figure S7 Normalized PL spectra of TPE-PBN and TPE-2PBN in neat film

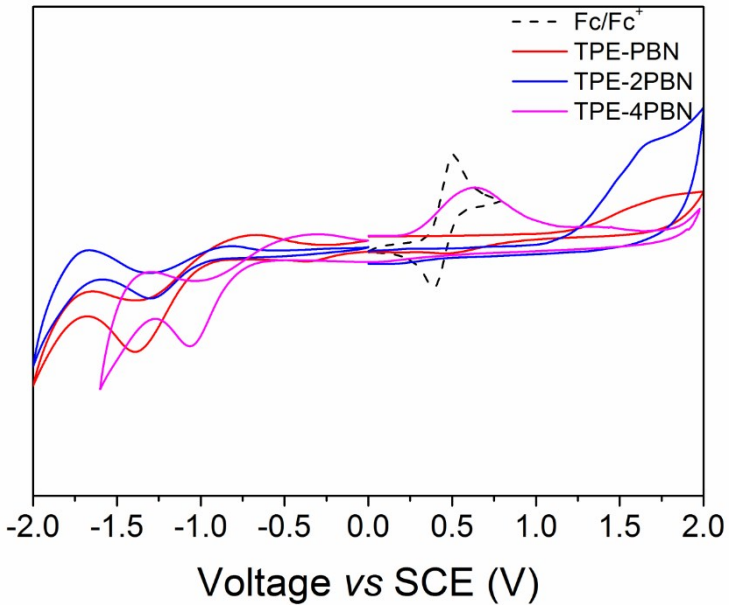


Figure S8 CV curves of TPE-PBN and TPE-2PBN measured in degassed CH_2Cl_2 solution

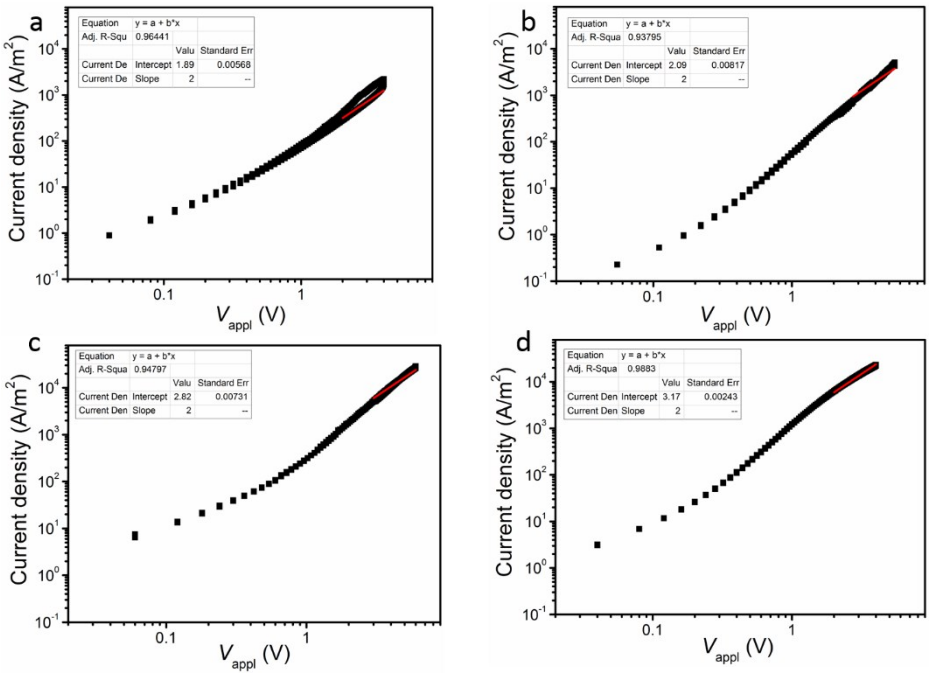


Figure S9 The curves of current densities-voltage of hole-only devices based on TPE-PBN and TPE-2PBN (a: TPE-PBN pristine film, b: TPE-2PBN pristine film; c: TPE-PBN annealed film, d: TPE-2PBN annealed film). The solid lines represent the fit using a model of single carrier SCLC with field-independent mobility. The *J-V* characteristics are corrected for the built-in voltage V_{appl} that arises from the work function difference between the contacts.

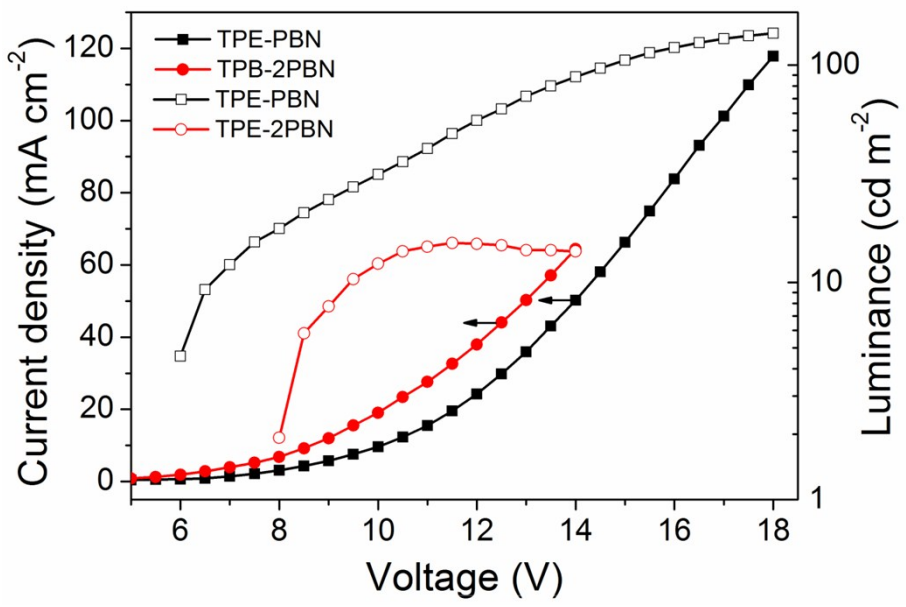


Figure ~~S9~~ S10 *J-V-L* curves of TPE-PBN and TPE-2PBN based non-devices

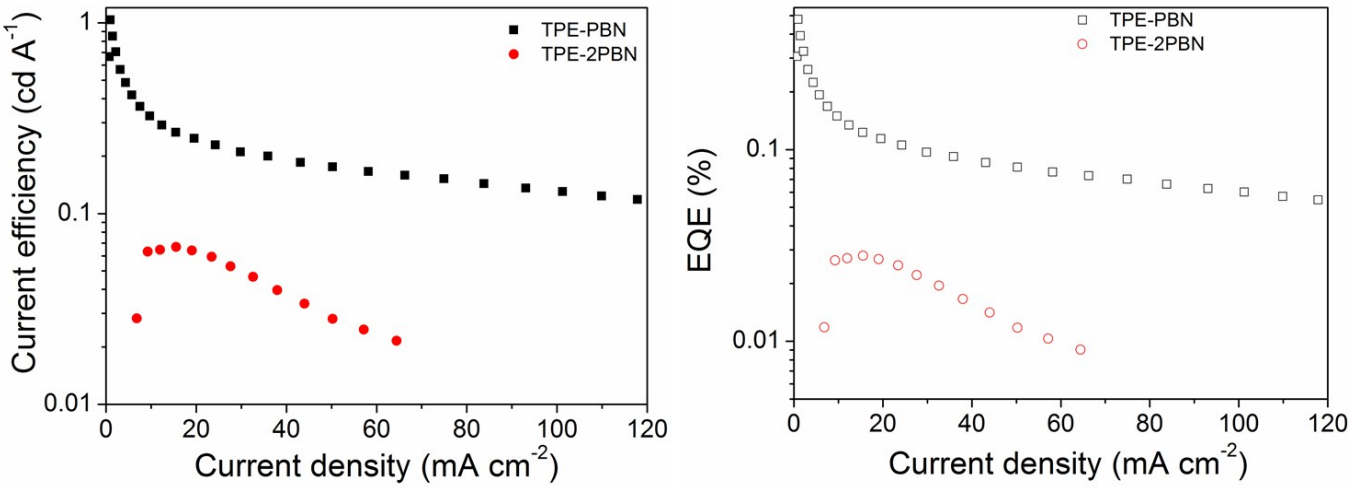


Figure ~~S10~~ S11 Current efficiency cureves (solid) and EQE cureves (hollow) of TPE-PBN and TPE-2PBN based non-devices

Table S1 Performances of non-doped OLEDs[a] based on TPE-PBN and TPE-2PBN

Emitter	V^b /V	$\lambda_{EL}{}^c$ /nm	CE^d /cd A^{-1}	PE^e /lm W^{-1}	L^f /cd m^{-2}	EQE^g /%
TPE-PBN	6	488	1.04	0.49	140	0.47
TPE-2PBN	8	504	0.07	0.02	15	0.03

a:OLEDs device configurations: ITO/PEDOT:PSS (40 nm)/compounds (40 nm)/TmPyPB (50 nm)/Liq (1 nm)/Al (100 nm); b:turn-on voltage (1 cd m^{-2}); c: emission maximum; d: maximun current efficiency; e: maximum power efficiency; f: maximum luminance; g: exterrnal quantum efficiency ;

Temperature-dependent XRD diffraction data for TPE-2PBN

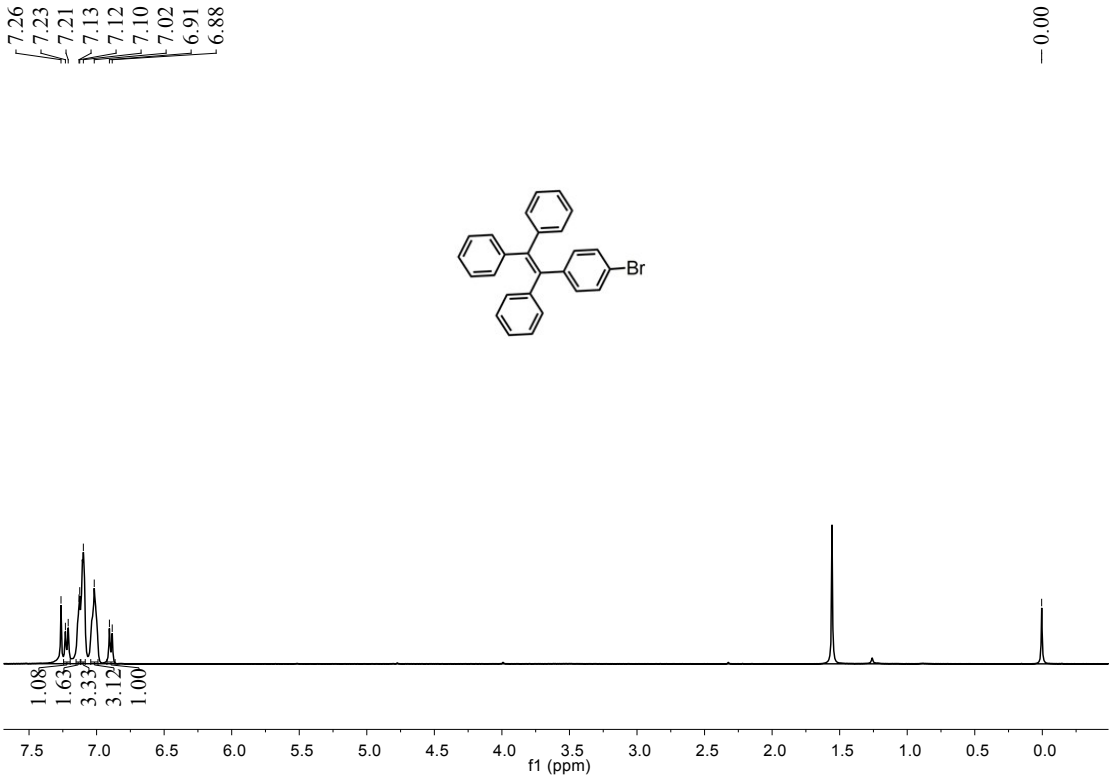
Rectangular Model

***d*_obs(A)**	***d*_calc(A)**	**h**	**k**		**Columnar**	**Rectangular**
24.79	24.79	0	1		*a*	37.35 Å
12.45	12.45	3	0		*b*	24.79 Å
8.83	8.78	3	2			
8.27	8.26	0	3			
7.41	7.46	4	2			
6.75	6.88	3	3			
5.13	5.16	4	4			
4.92	4.91	1	5			
4.42	----	----	----			
4.35	4.38	4	5	RMSD		
				0.162		

Oblique Model

***d*_obs(A)**	***d*_calc(A)**	**h**	**k**		**Columnar**	**Oblique**
24.79	24.79	0	1		*a*	13.76 Å
12.45	12.45	1	3		*b*	38.62 Å
8.83	8.83	1	0		gamma	39.93°
8.27	8.26	0	3			
7.41	7.36	1	5			
6.75	6.75	2	5			
5.13	5.07	2	1			
4.92	4.96	0	5			
4.42	4.42	2	0			
4.35	----	----	----	RMSD		
				0.090		

NMR spectra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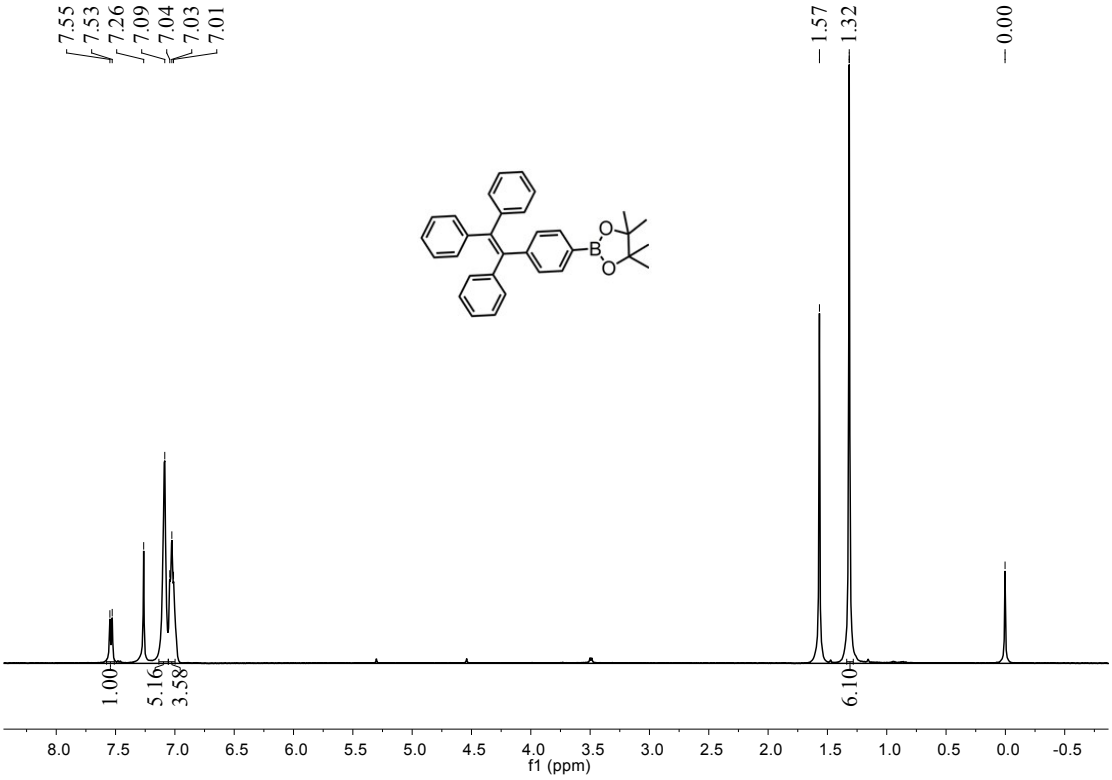
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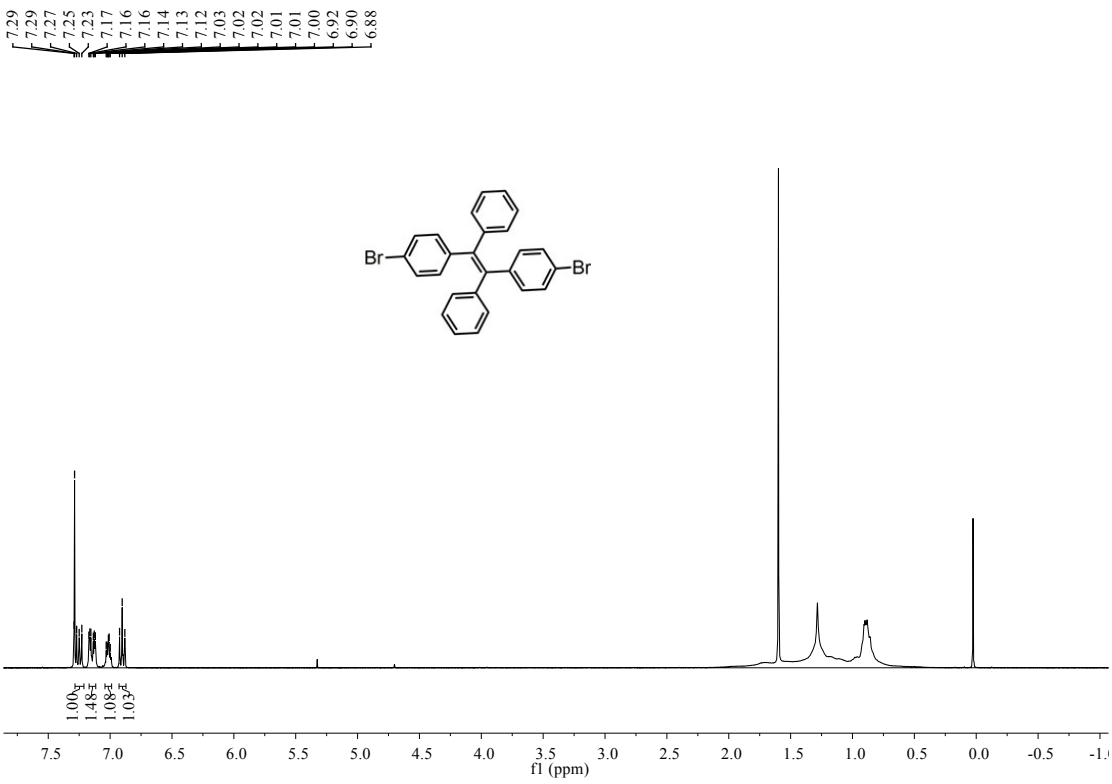
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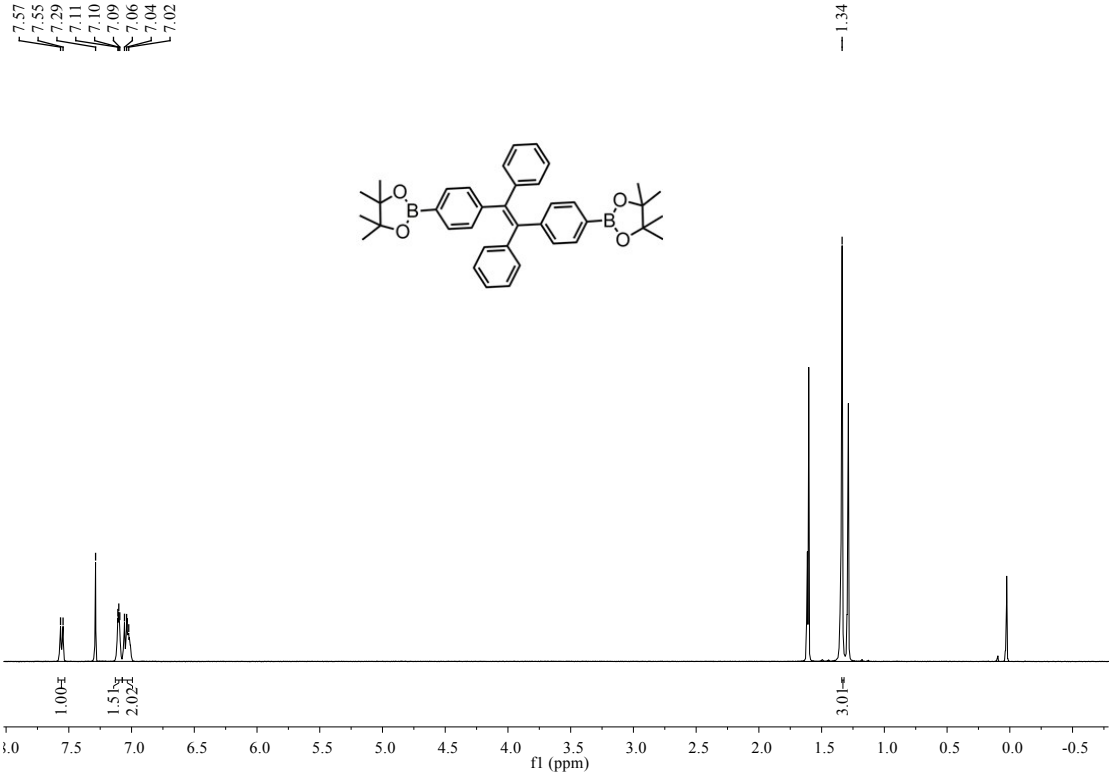
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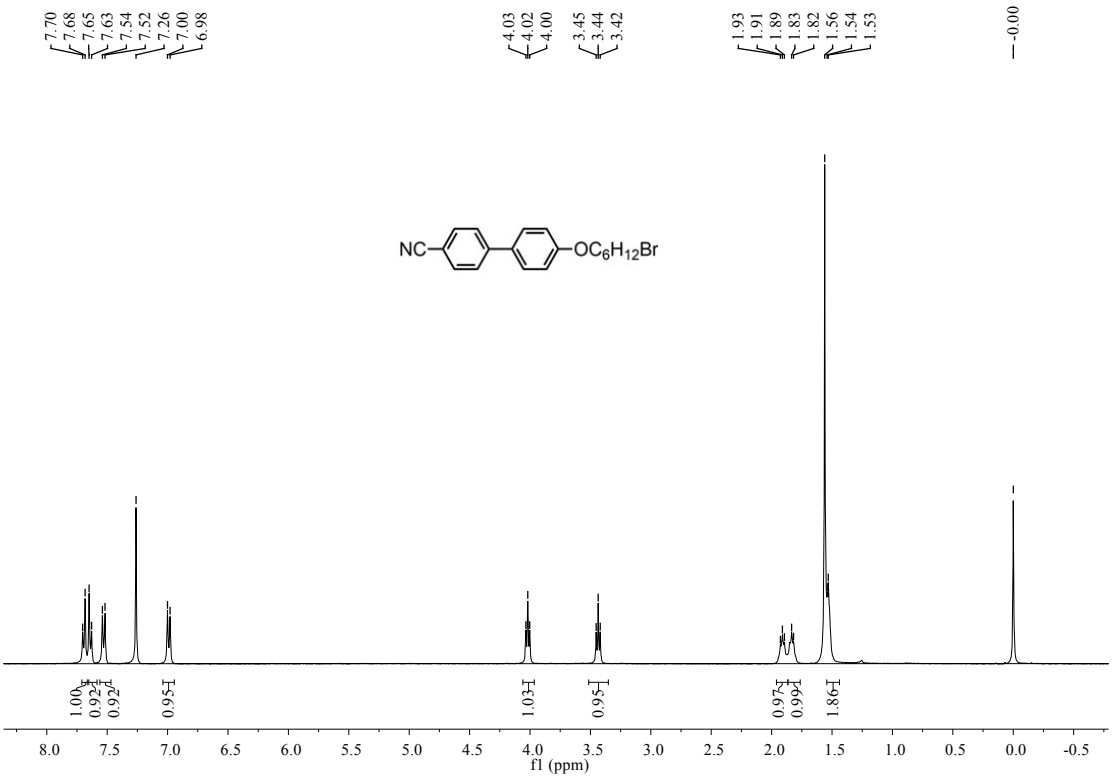
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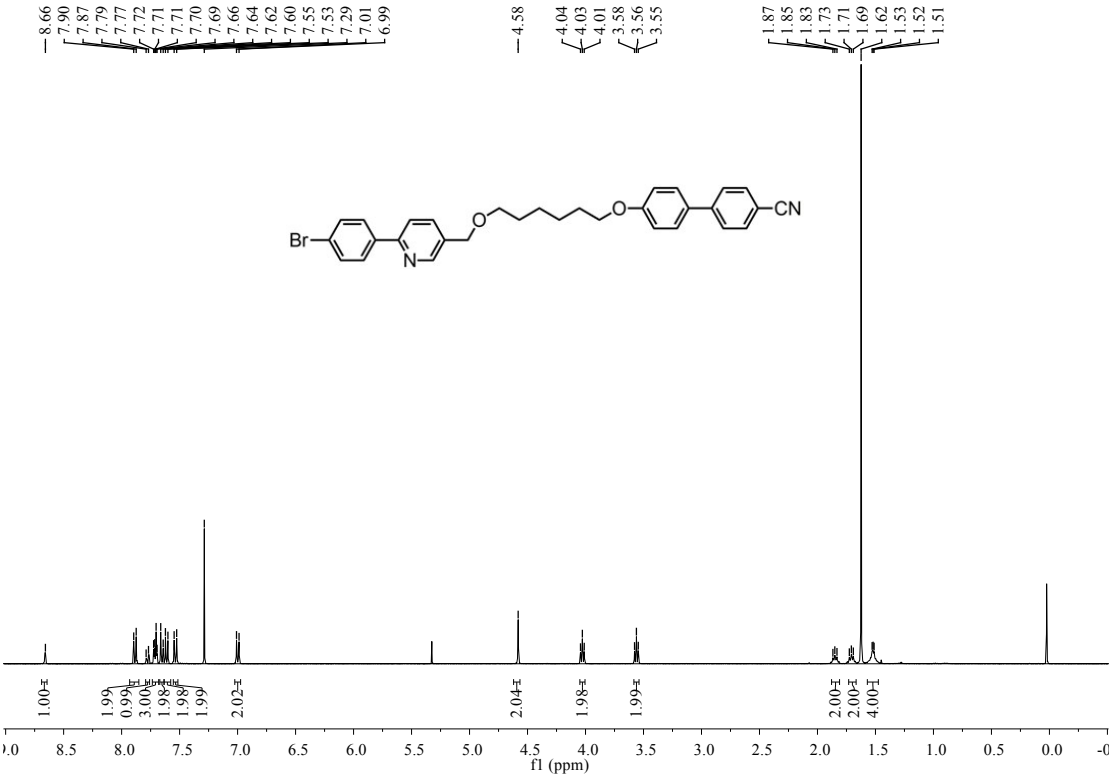
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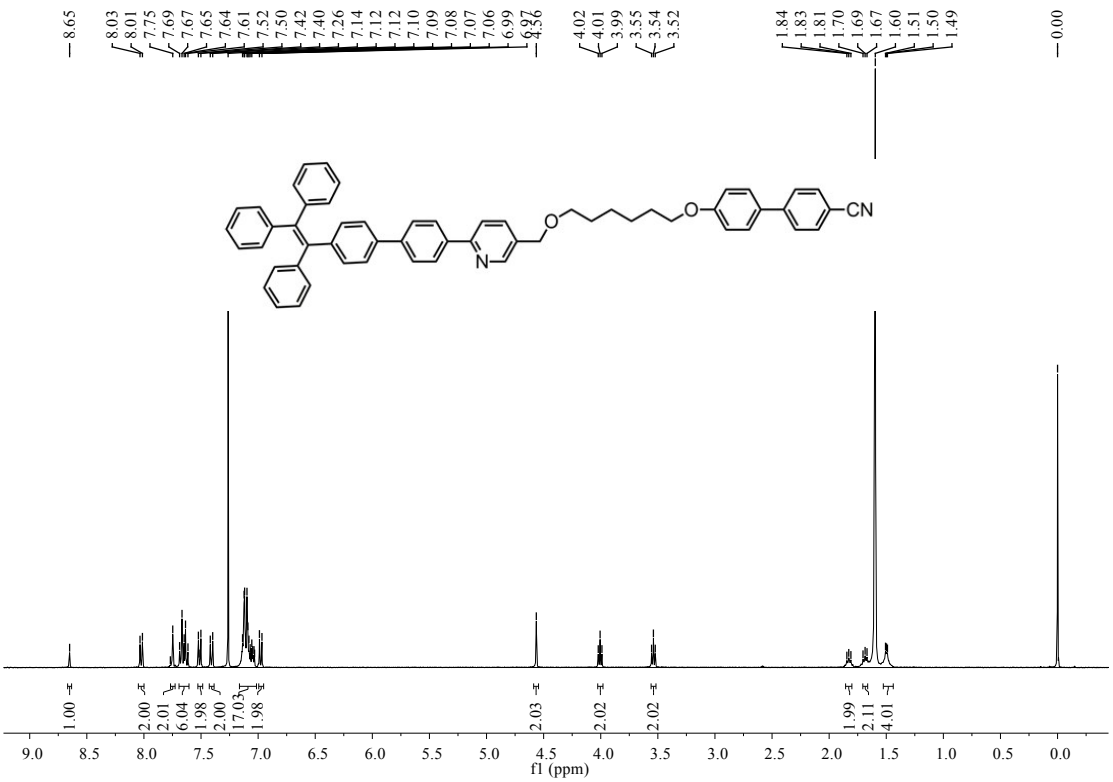
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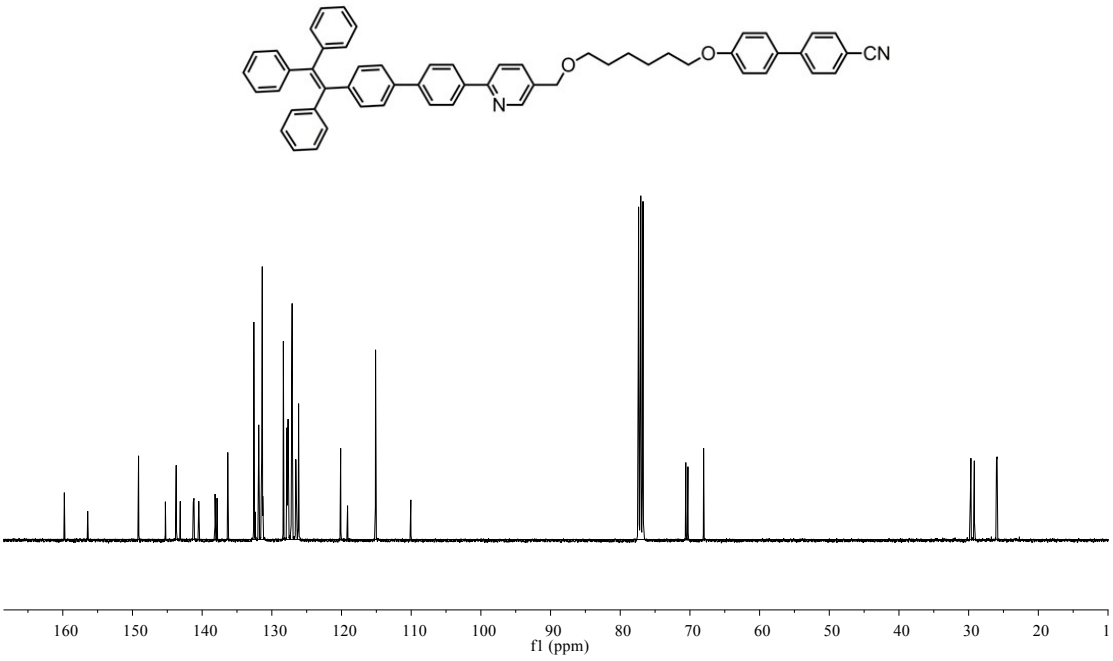
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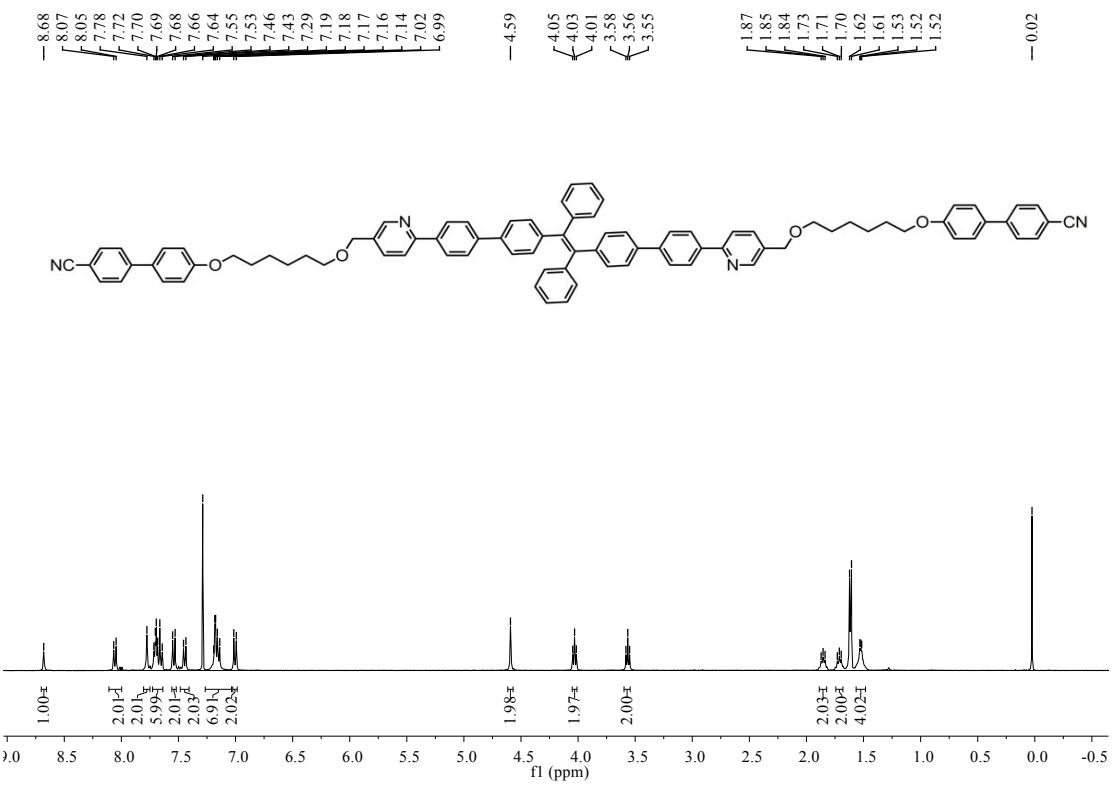
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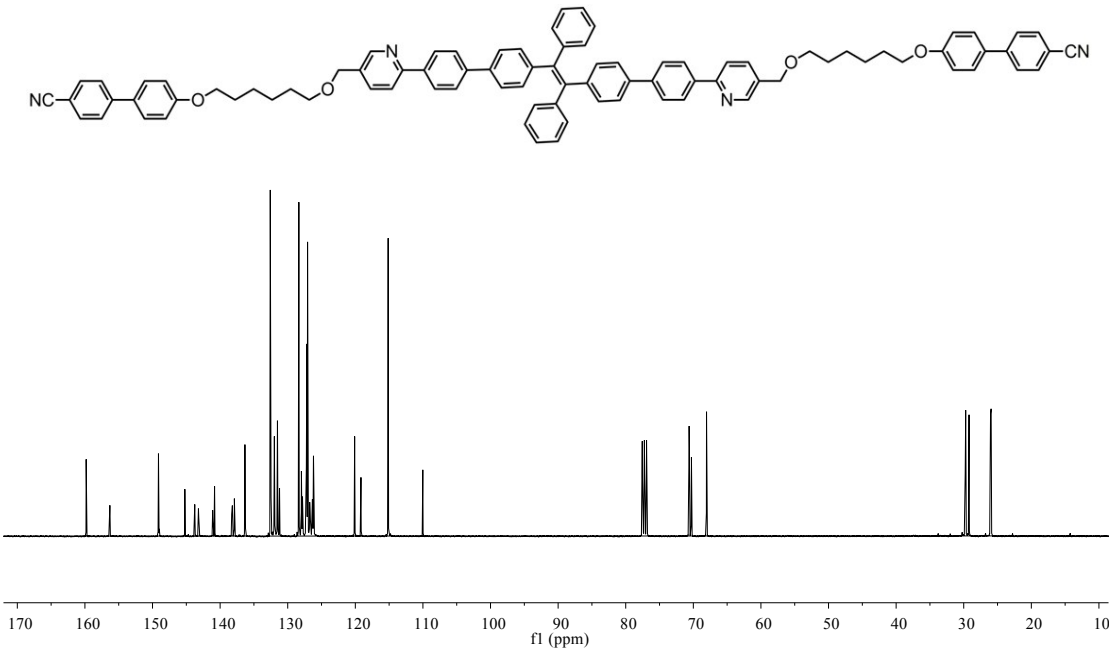
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