Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Solution-processable, High Current Efficiency Deep-blue Organic Light Emitting Diodes Based on Novel Biphenyl-Imidazole Derivatives

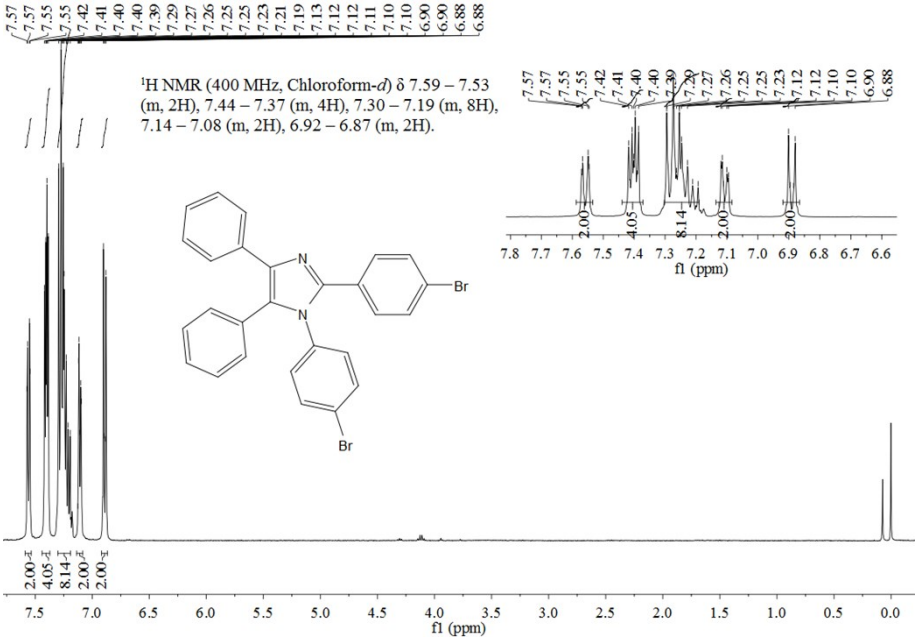


Fig. S1 ^{1}H NMR spectrum of compound **1**.

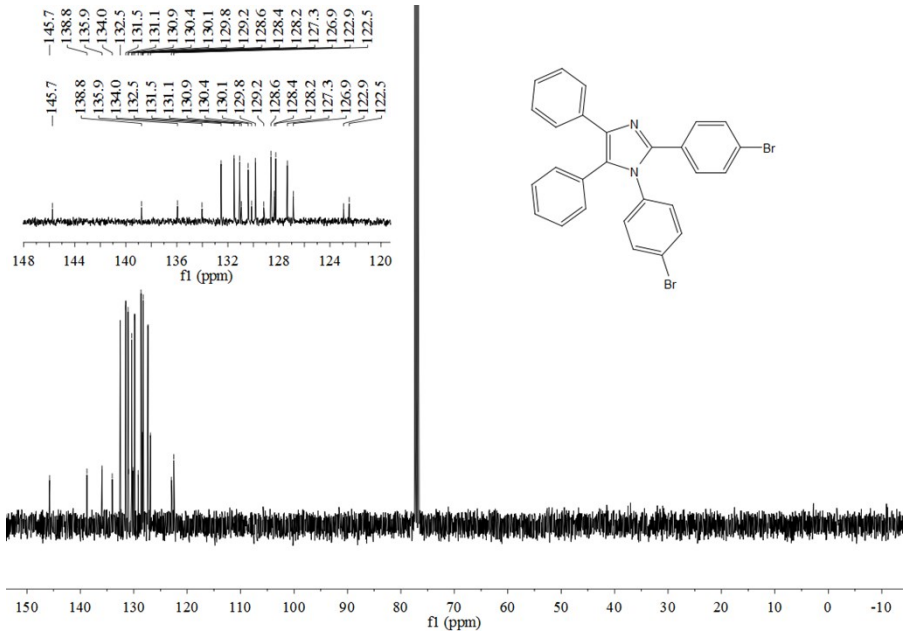


Fig. S2 ^{13}C NMR spectrum of compound **1**.

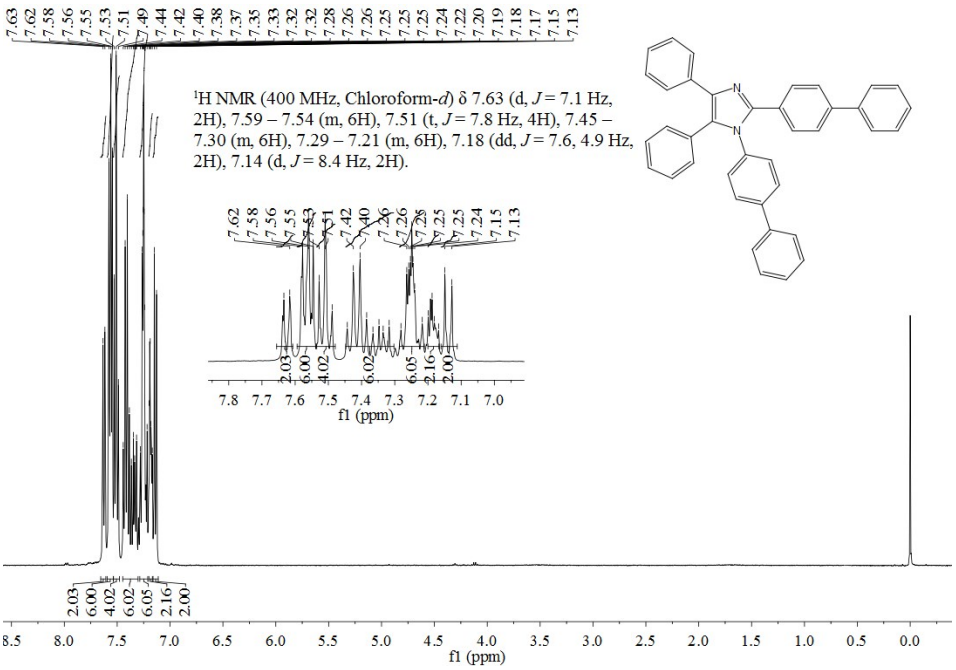


Fig. S3 [1]H NMR spectrum of compound **2a**.

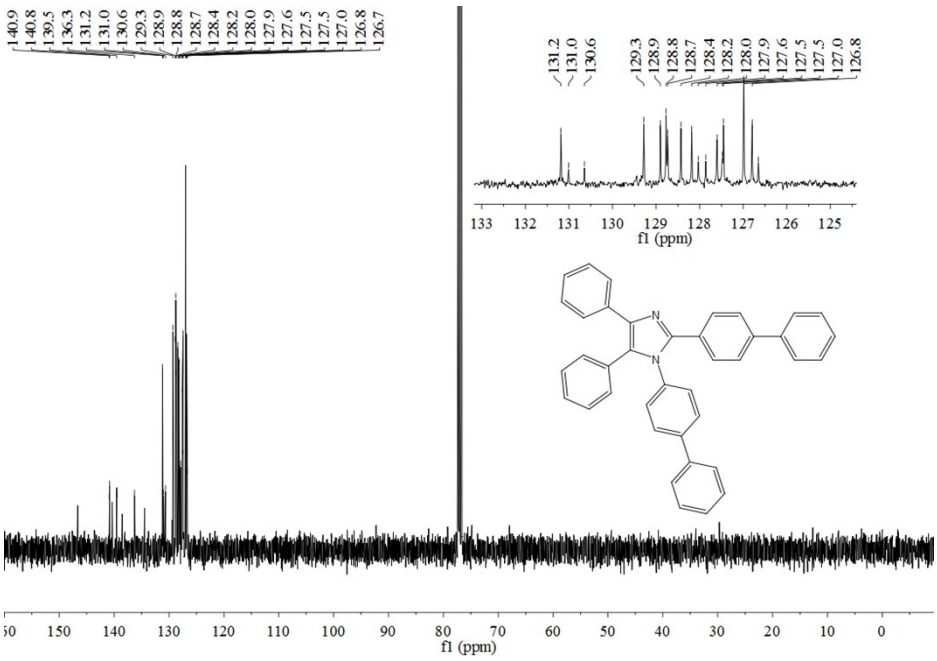


Fig. S4 [13]C NMR spectrum of compound **2a**.

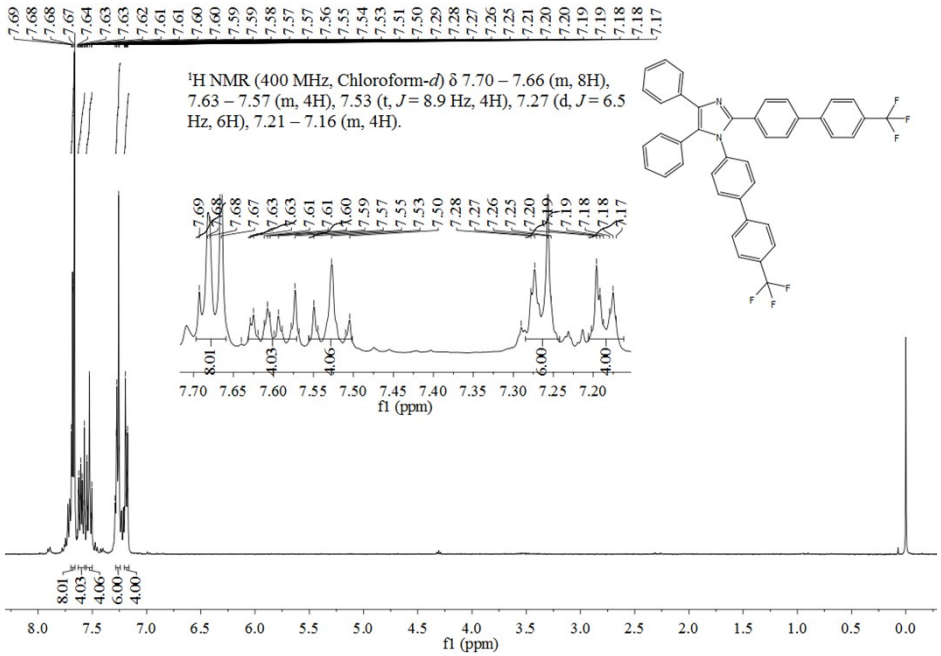


Fig. S5 ^{1}H NMR spectrum of compound **2b**.

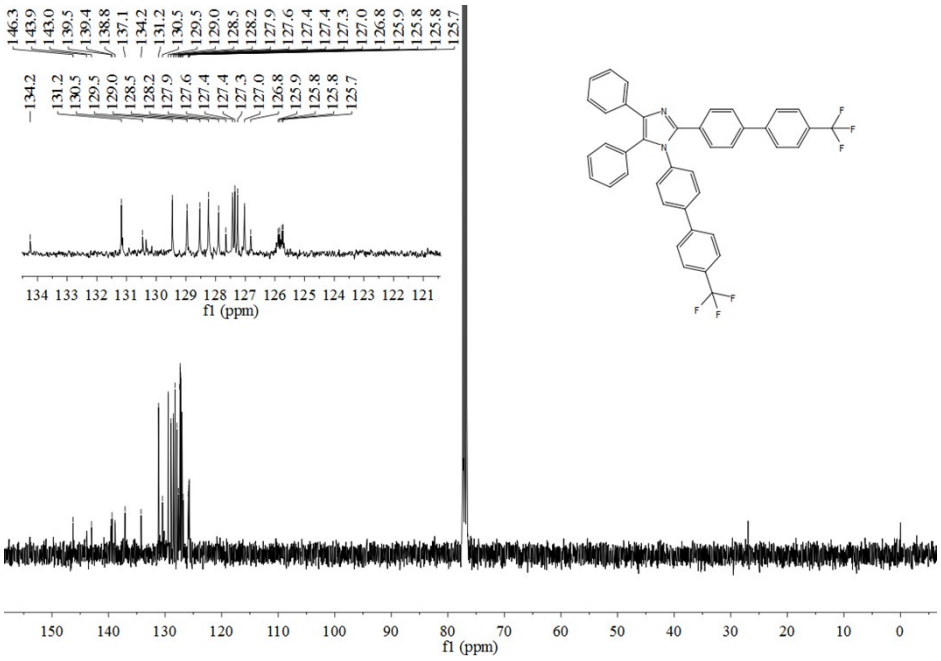


Fig. S6 ^{13}C NMR spectrum of compound **2b**.

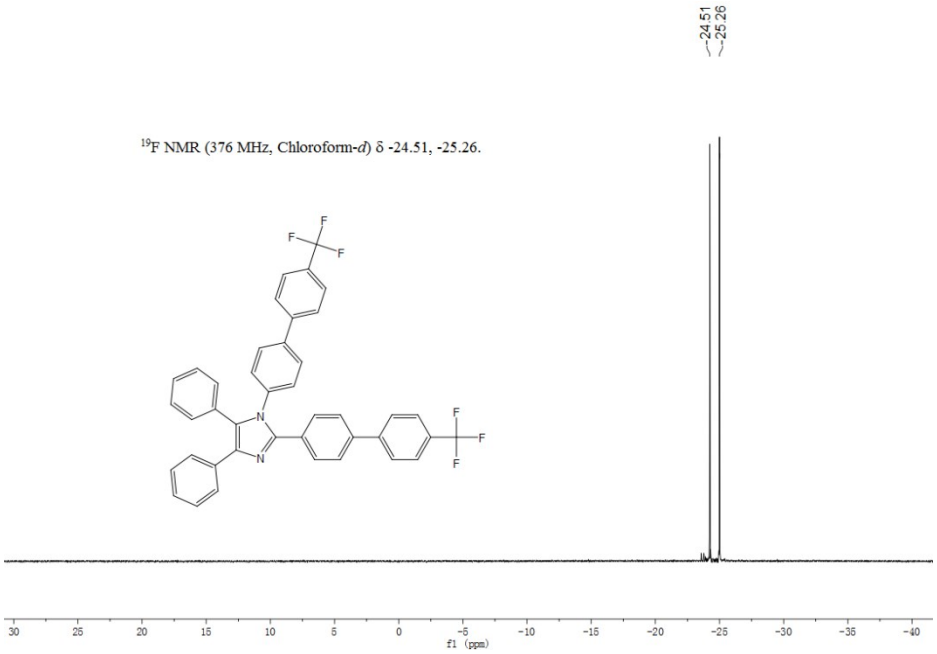


Fig. S7 ^{19}F NMR spectrum of compound **2b**.

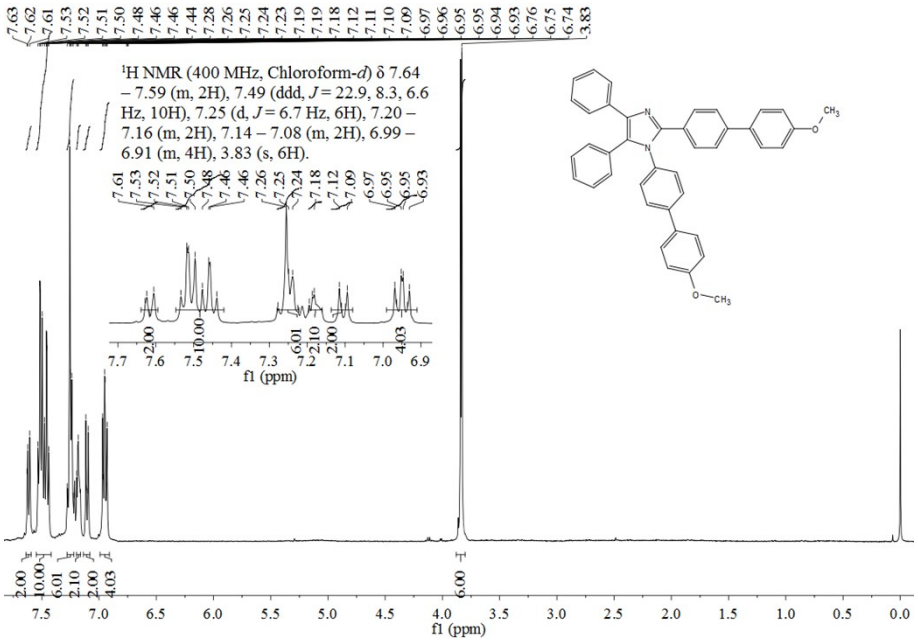


Fig. S8 ^{1}H NMR spectrum of compound **2c**.

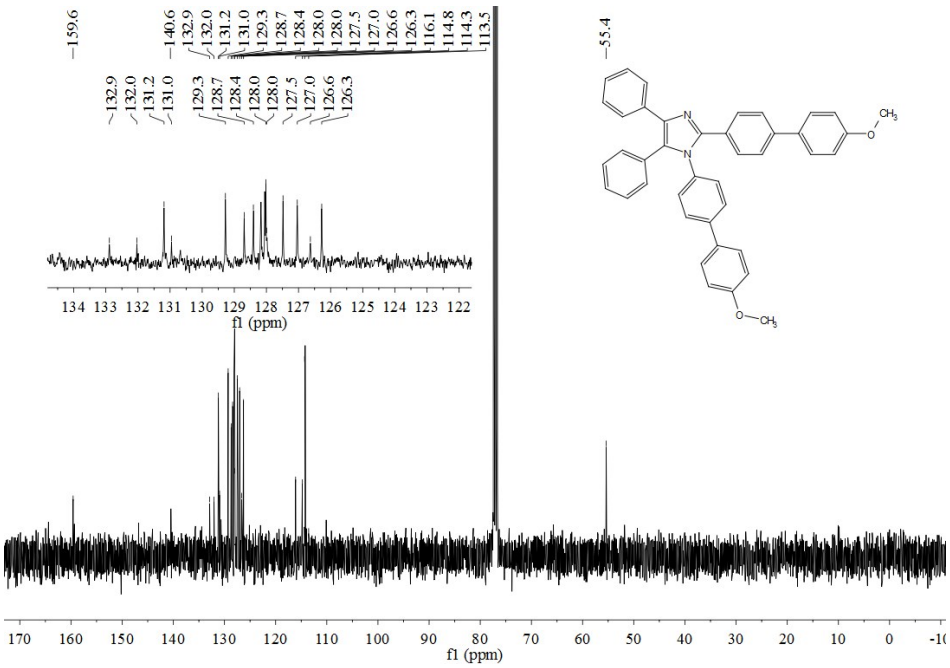
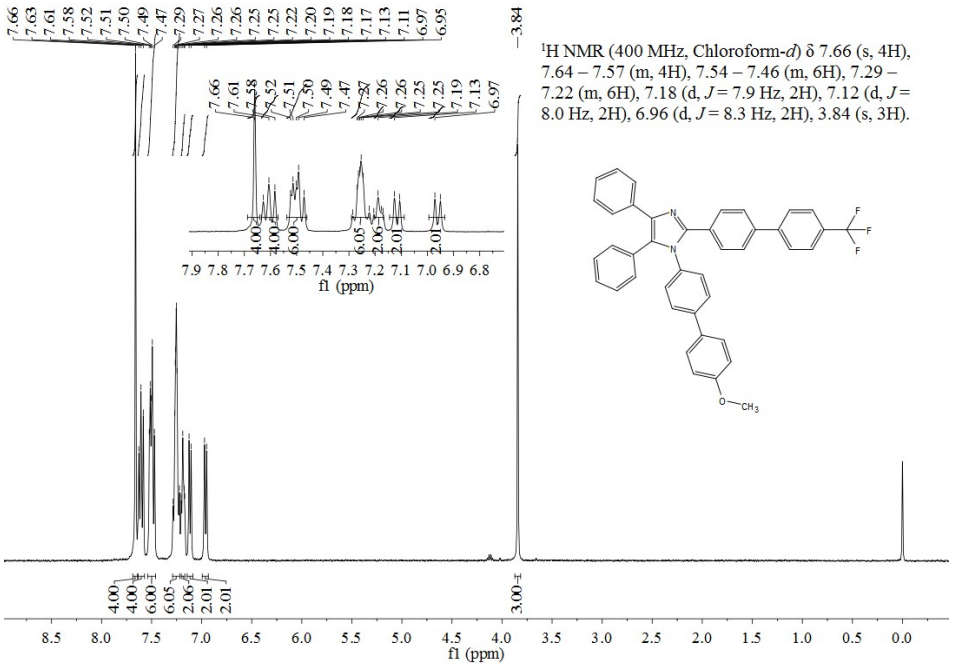


Fig. S9 ^{13}C NMR spectrum of compound **2c**.



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (s, 4H), 7.64 – 7.57 (m, 4H), 7.54 – 7.46 (m, 6H), 7.29 – 7.22 (m, 6H), 7.18 (d, *J* = 7.9 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.3 Hz, 2H), 3.84 (s, 3H).

Fig. S10 ^{1}H NMR spectrum of compound **2d**.

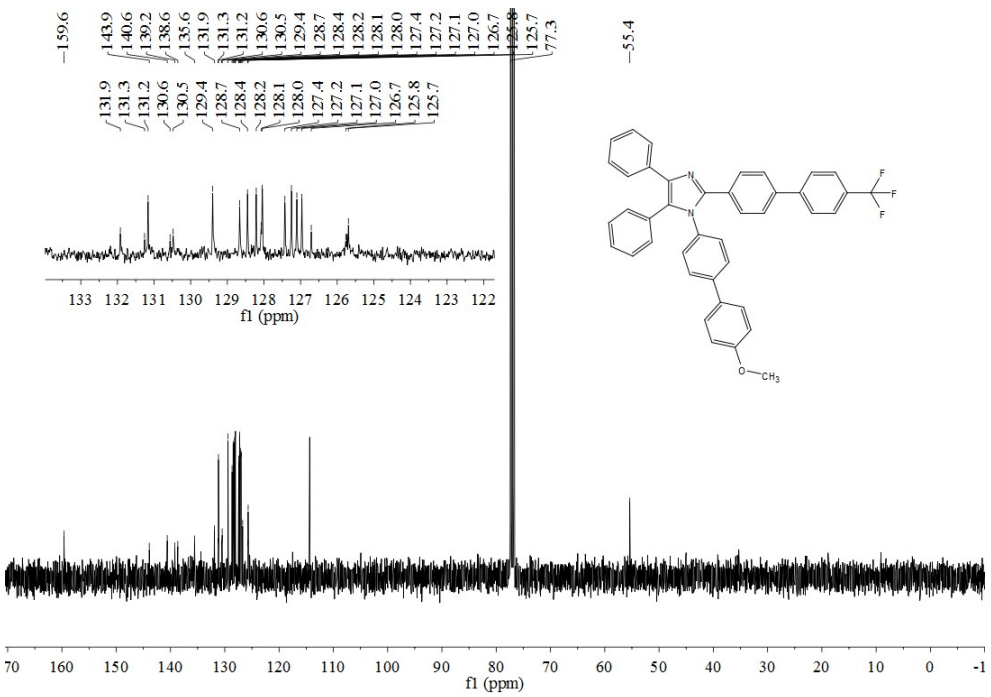


Fig. S11 ^{13}C NMR spectrum of compound **2d**.

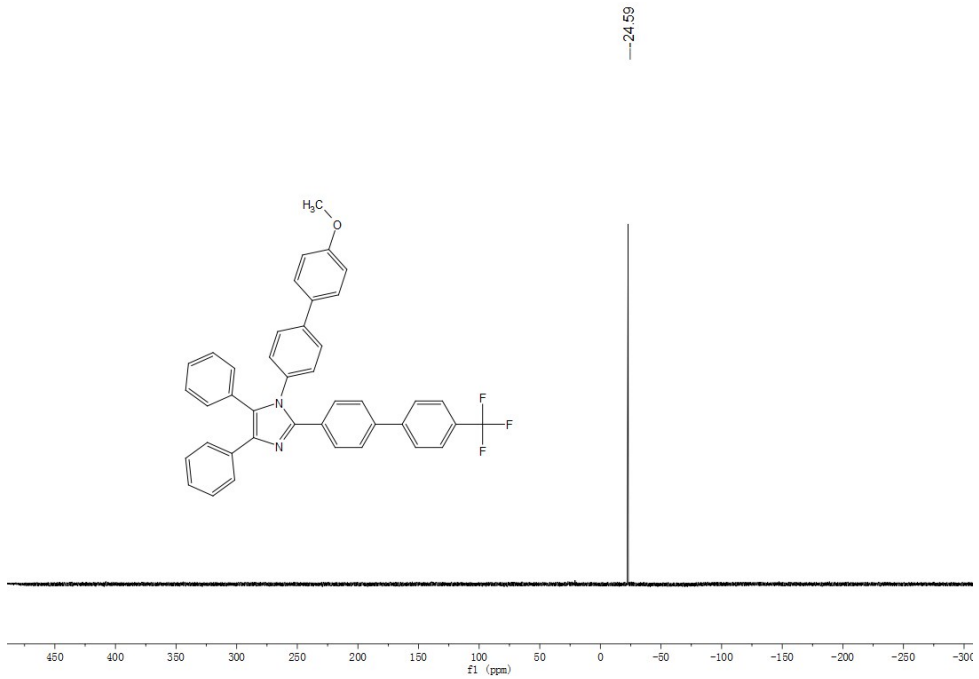


Fig. S12 ^{19}F NMR spectrum of compound **2d**.

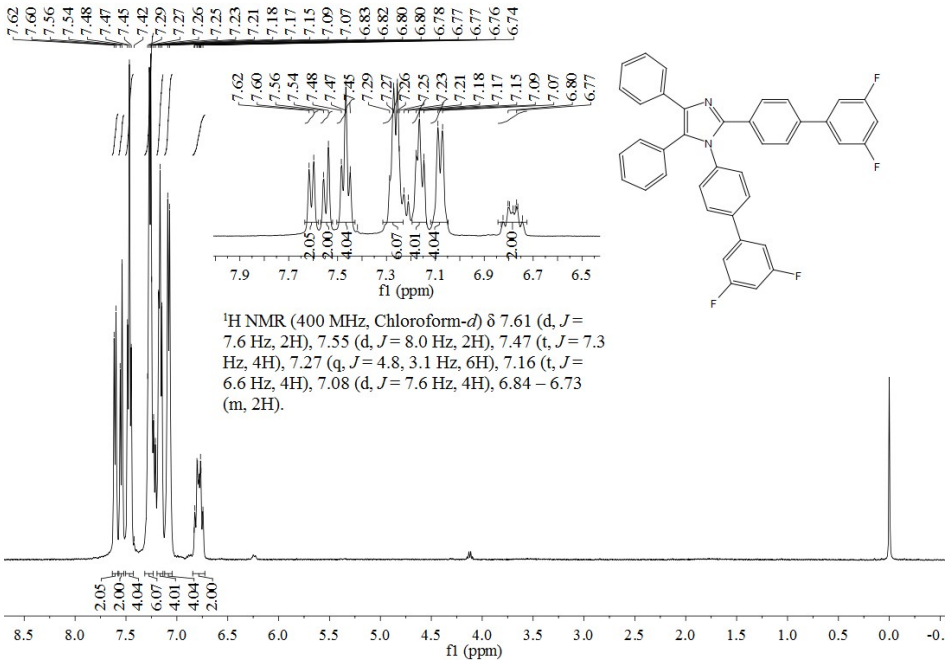


Fig. S13 ^{1}H NMR spectrum of compound **2e**.

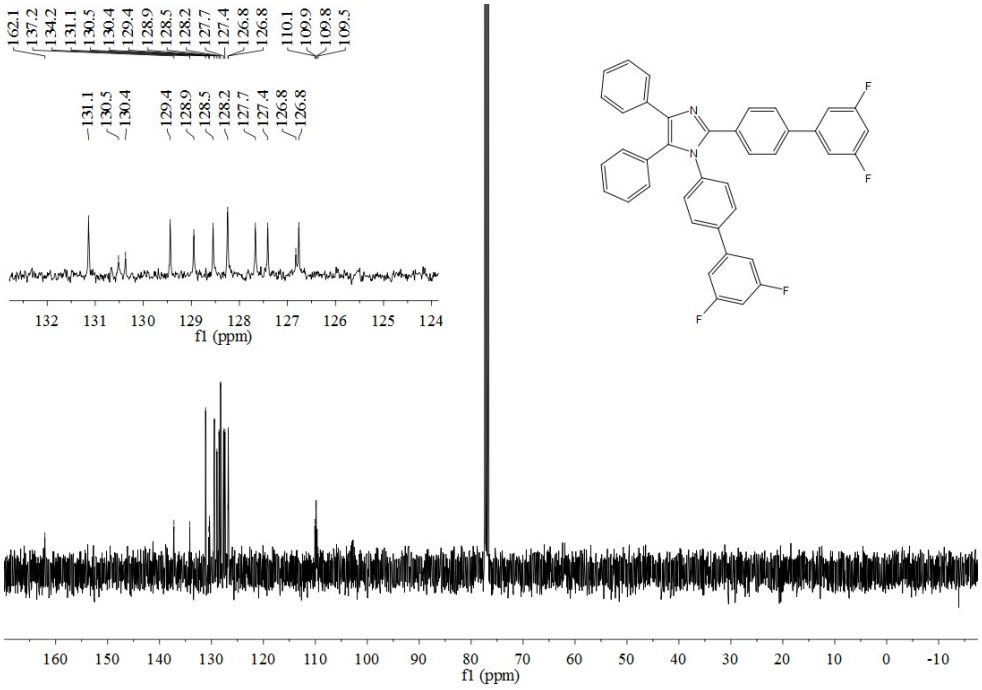


Fig. S14 ^{13}C NMR spectrum of compound **2e**.

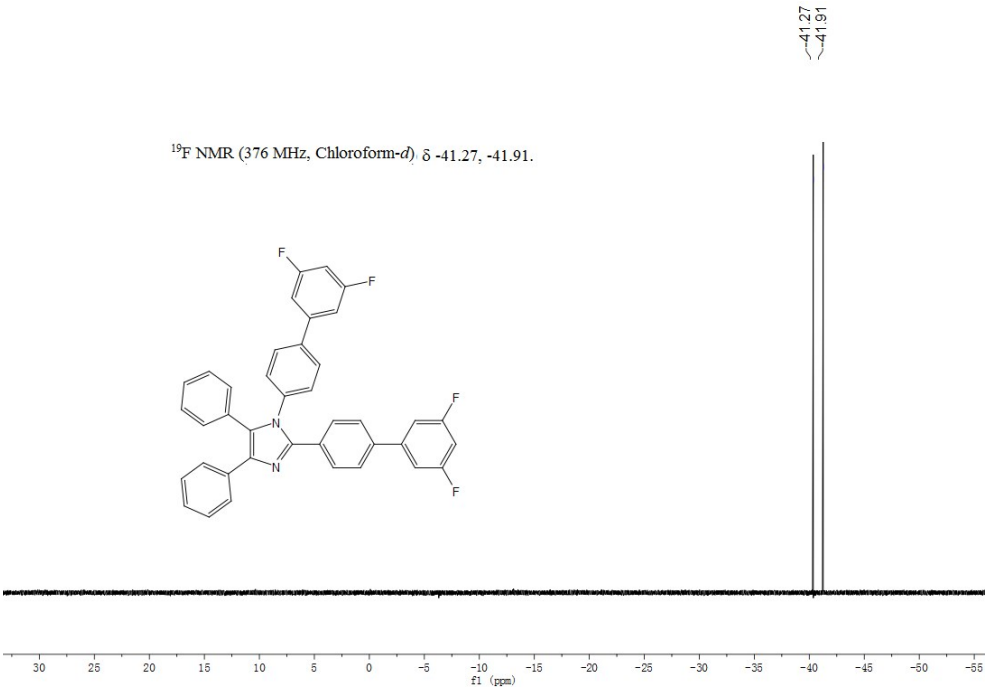


Fig. S15 ^{19}F NMR spectrum of compound **2e**.

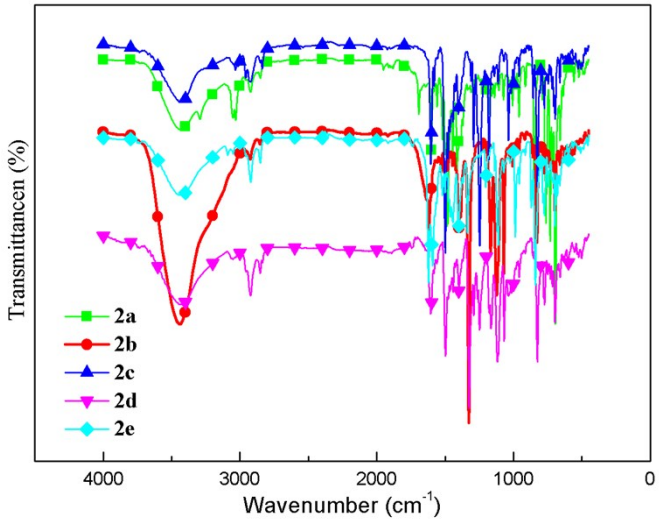


Fig. S16 IR spectra of compounds **2a-2e**.

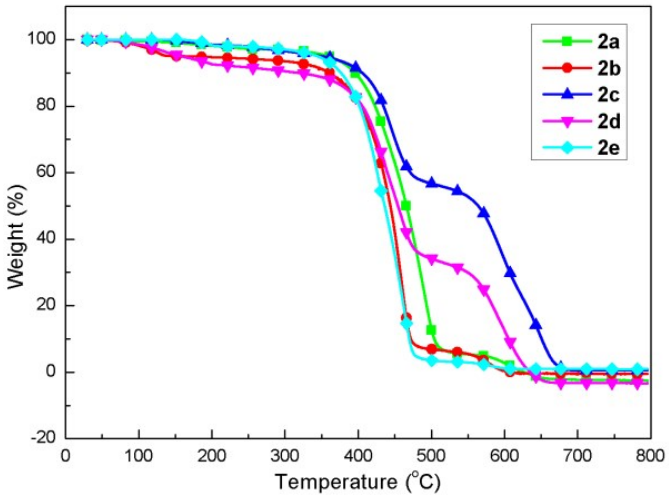
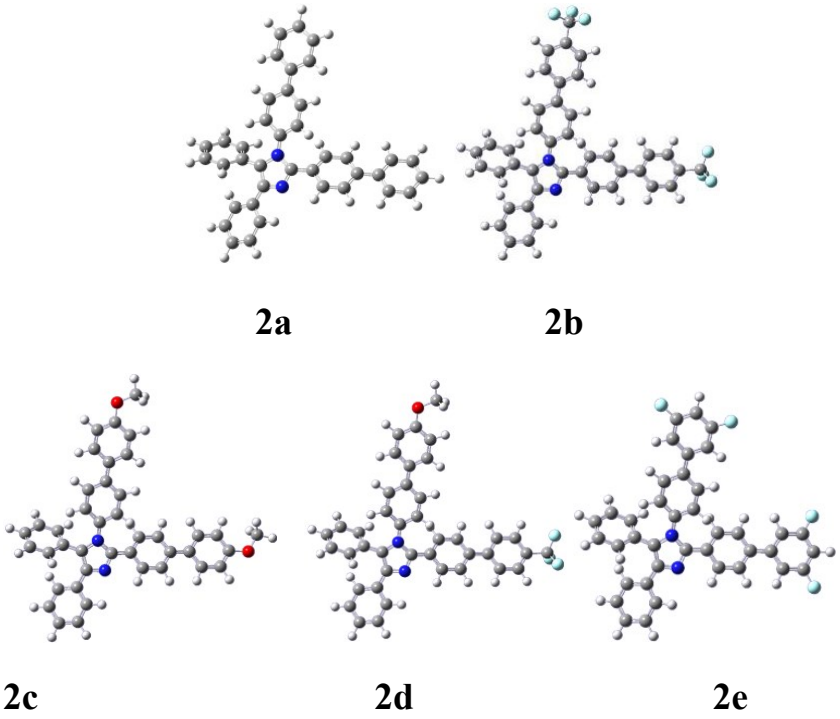
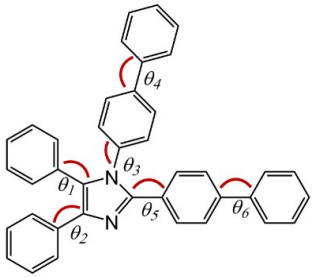


Fig. S17 TGA curves of compounds **2a-2e**.





Compounds	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6
2a	51.78	13.61	17.31	5.17	27.04	5.53
2b	51.81	13.58	17.22	5.44	27.08	5.21
2c	51.85	13.62	17.34	5.12	27.03	5.28
2d	51.75	13.48	17.25	5.18	27.06	5.17
2e	51.80	13.55	17.27	5.11	27.09	5.54

Fig. S18 Optimized geometries and twist angles of the compounds **2a-2e**.

Solvatochromic effect

The influence of solvent environment on the optical property of the compounds **2a**-**2e** can be studied according to the Lippert-Mataga equation as below:

$$hc(v_a\text{-}v_f) = hc(v^0_a\text{-}v^0_f) + \frac{2(\mu_e - \mu_g)}{a^3} f(\varepsilon, n)$$

where h is the Plank constant, c is the light speed in vacuum, $f(\varepsilon,n)$ is the orientational polarizability of solvents, $v^0_a - v^0_f$ corresponds to the Stokes shifts when f is zero, μ_e is the excited state dipole moment, μ_g is the ground-state dipole moment, a is the solvent Onsager cavity radius, M is the molecular weight, d is the density (d = 1.0 g/cm^3), and N is Avogadro's number, and ε and n are the solvent dielectric and the solvent refractive index, respectively. μ_g is estimated at the level of B3LYP/6-31G+(d, p) from Gaussian 09 package. f(ε,n) and a can be calculated respectively as follows:

$$f(\varepsilon,n) = \left[\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}\right], \quad a = (3M/4\pi Nd)^{1/3}$$

The detailed data are listed in Table S1- S5.

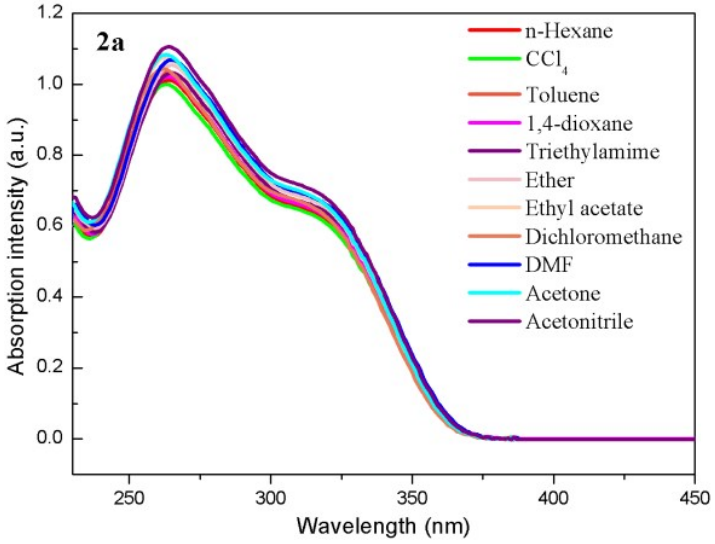


Fig. S19 Absorption spectra of the compound **2a** recorded in different solvents.

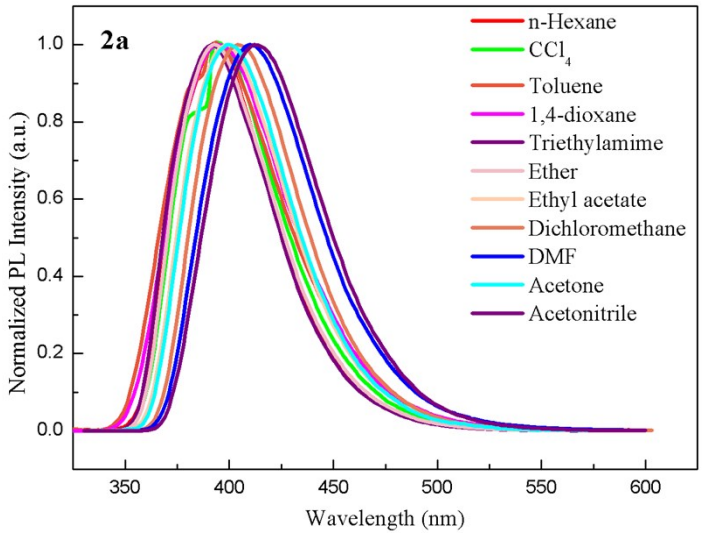


Fig. S20 PL spectra of the compound **2a** recorded in different solvents.

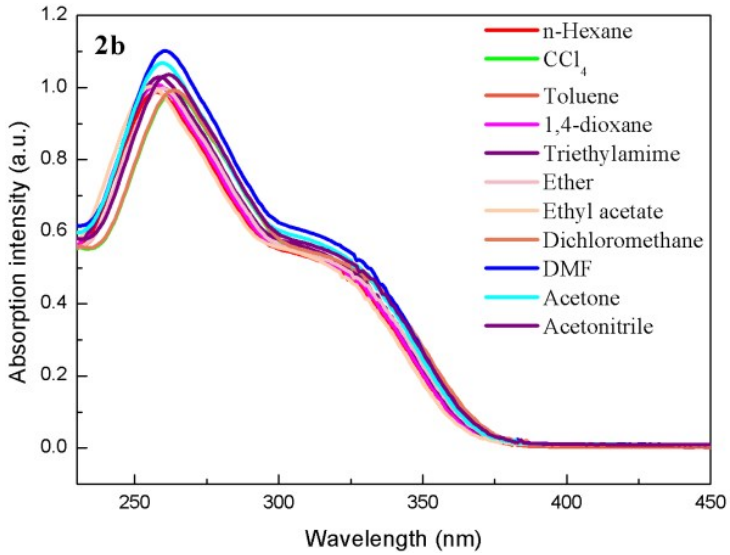


Fig. S21 Absorption spectra of the compound **2b** recorded in different solvents.

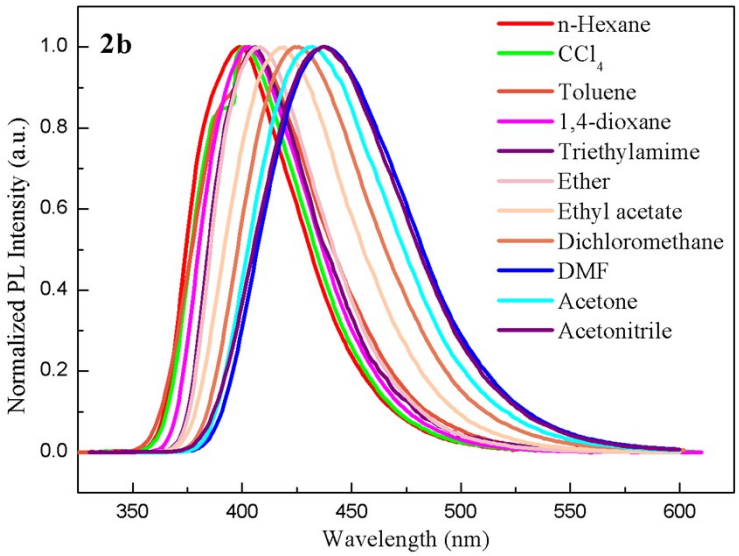


Fig. S22 PL spectra of the compound **2b** recorded in different solvents.

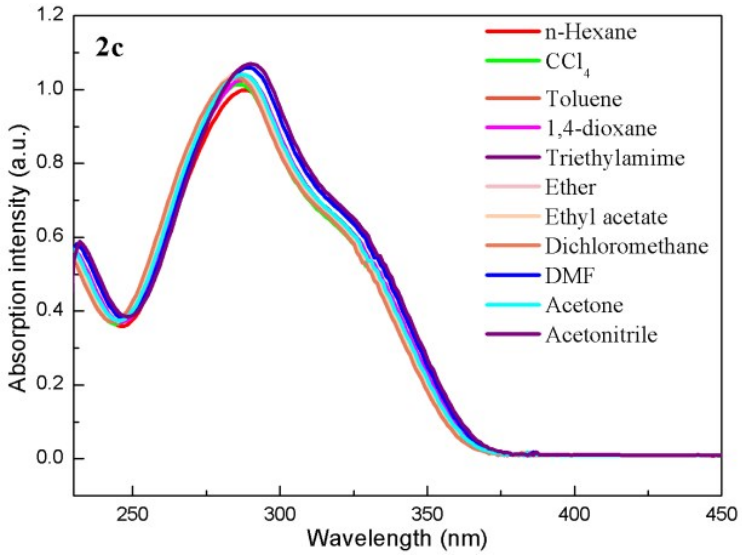


Fig. S23 Absorption spectra of the compound **2c** recorded in different solvents.

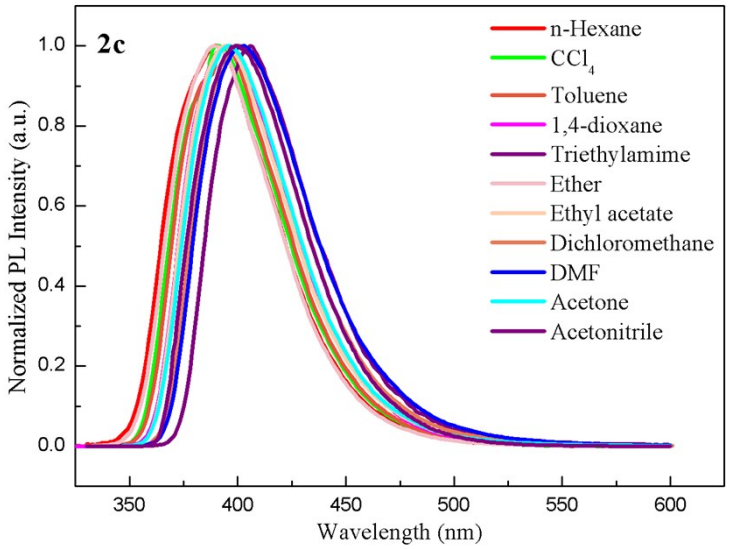


Fig. S24 PL spectra of the compound **2c** recorded in different solvents.

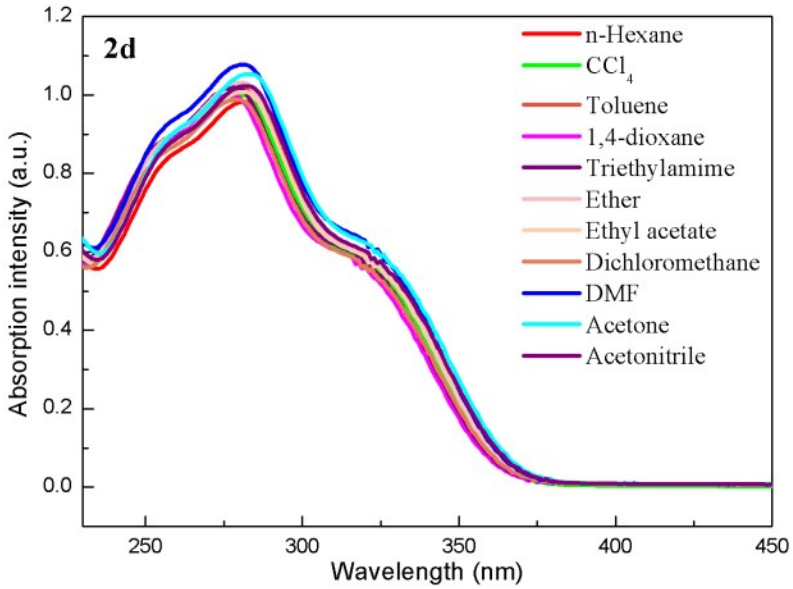


Fig. S25 Absorption spectra of the compound **2d** recorded in different solvents.

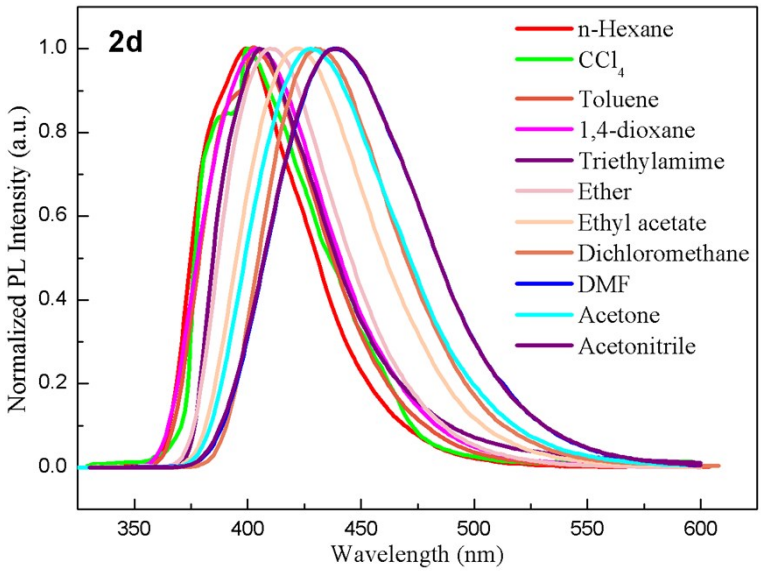


Fig. S26 PL spectra of the compound **2d** recorded in different solvents.

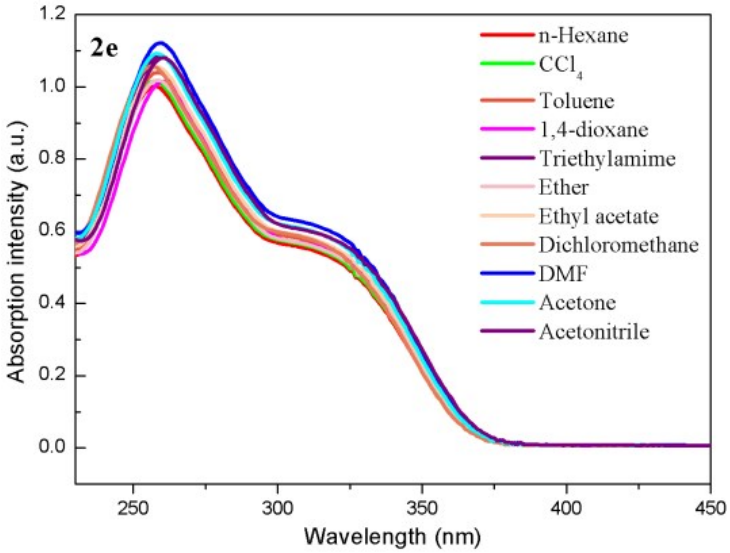


Fig. S27 Absorption spectra of the compound **2e** recorded in different solvents.

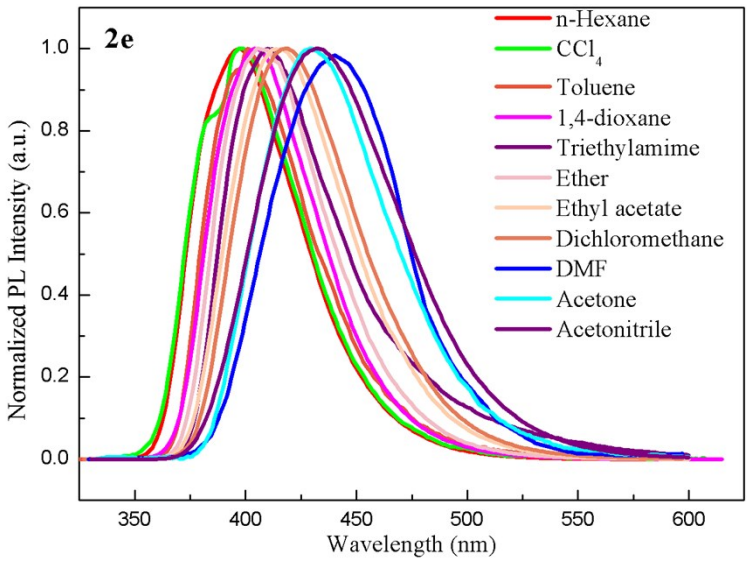
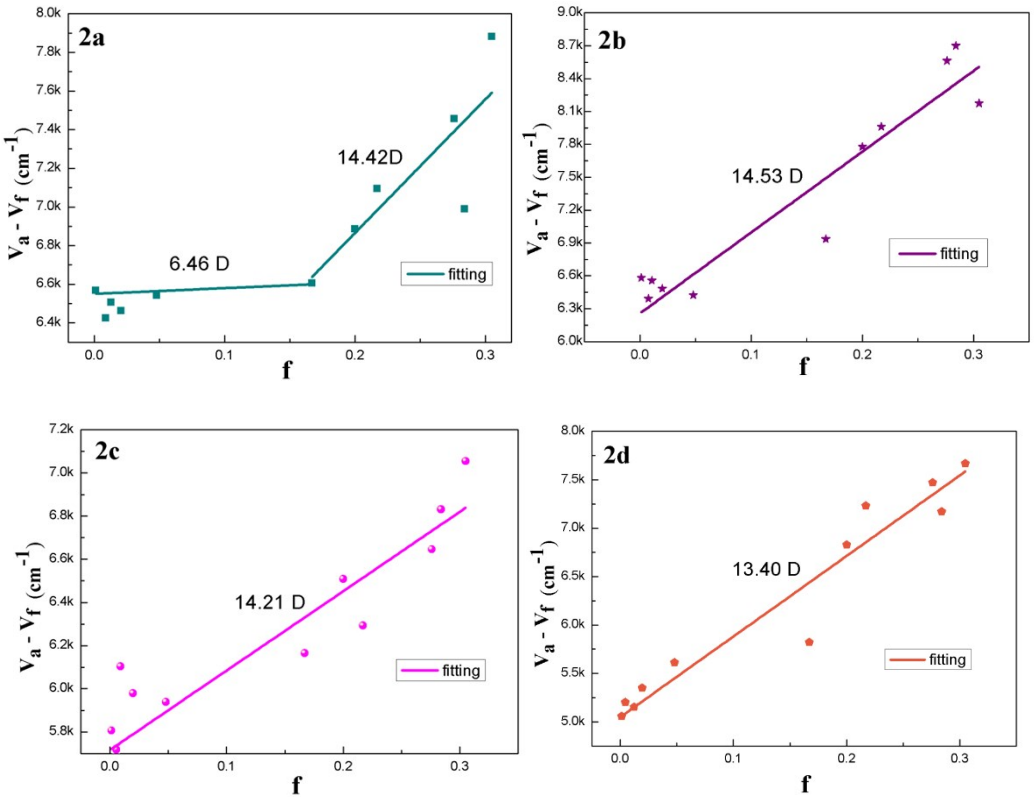


Fig. S28 PL spectra of the compound **2e** recorded in different solvents.



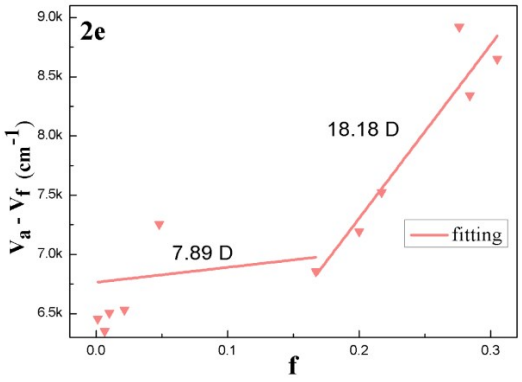


Fig. S29 Plots of the Stokes shift ($\nu_a - \nu_f$) of the new compounds against orientation polarization (**f**) of solvent.

Table S1. Detailed photophysical data of the compound **2a** in different solvents

Solvents	f	**2a**		
		λ_a (nm)	λ_f (nm)	$\nu_a - \nu_f$ (cm^{-1})
Hexane	0.0012	313	394	6568
CCl_4	0.011	315	395	6429
Toluene	0.014	313	393	6504
1,4-dioxane	0.0252	314	394	6466
Triethylamime	0.048	312	392	6541
Ether	0.167	312	393	6606
Ethyl acetate	0.2	313	399	6886
Dichloromethane	0.217	314	404	7095
DMF	0.276	314	410	7457
Acetone	0.284	312	399	6989
Acetonitrile	0.305	311	412	7882

Table S2. Detailed photophysical data of the compound **2b** in different solvents.

Solvents	f	**2b**		
		λ_a (nm)	λ_f (nm)	$v_a - v_f$ (cm^{-1})
Hexane	0.0012	316	399	6583
CCl_4	0.011	319	400	6348
Toluene	0.014	318	402	6571
1,4-dioxane	0.0252	320	403	6436
Triethylamime	0.048	322	406	6425
Ether	0.167	318	408	6937
Ethyl acetate	0.2	316	419	7779
Dichloromethane	0.217	317	424	7961
DMF	0.276	318	437	8563
Acetone	0.284	314	432	8699
Acetonitrile	0.305	322	437	8173

Table S3. Detailed photophysical data of the compound **2c** in different solvents.

Solvents	f	**2c**		
		λ_a (nm)	λ_f (nm)	$v_a - v_f$ (cm^{-1})
Hexane	0.0012	318	390	5806
CCl_4	0.011	319	391	5772
Toluene	0.014	317	393	6101
1,4-dioxane	0.0252	320	395	5934
Triethylamime	0.048	316	389	5939
Ether	0.167	317	394	6165
Ethyl acetate	0.2	318	401	6509
Dichloromethane	0.217	317	396	6293
DMF	0.276	316	400	6646
Acetone	0.284	316	403	6832

Acetonitrile	0.305	315	405	7055

Table S4. Detailed photophysical data of the compound **2d** in different solvents.

Solvents	f	**2d**		
		λ_a (nm)	λ_f (nm)	$v_a - v_f$ (cm^{-1})
Hexane	0.0012	332	399	5058
CCl_4	0.011	331	400	5211
Toluene	0.014	333	402	5154
1,4-dioxane	0.0252	332	404	5368
Triethylamime	0.048	330	405	5612
Ether	0.167	331	410	5821
Ethyl acetate	0.2	327	421	6828
Dichloromethane	0.217	328	430	7232
DMF	0.276	330	438	7472
Acetone	0.284	331	434	7170
Acetonitrile	0.305	329	440	7668

Table S5. Detailed photophysical data of the compound **2e** in different solvents.

Solvents	f	**2e**		
		λ_a (nm)	λ_f (nm)	$v_a - v_f$ (cm^{-1})
Hexane	0.0012	316	397	6457
CCl_4	0.011	318	398	6320
Toluene	0.014	317	400	6545
1,4-dioxane	0.0252	319	404	6595
Triethylamime	0.048	316	410	7255
Ether	0.167	317	405	6854
Ethyl acetate	0.2	319	414	7193
Dichloromethane	0.217	318	418	7523
DMF	0.276	317	442	8921

Acetone	0.284	317	431	8343
Acetonitrile	0.305	315	433	8651

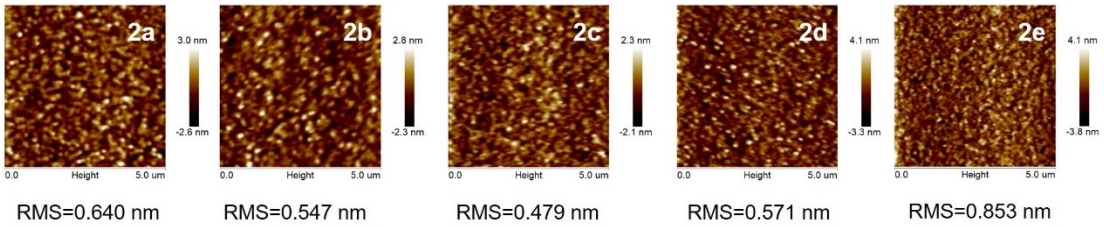


Fig. S30 AFM images of the EMLs in which the compounds **2a-2e** with polymer.

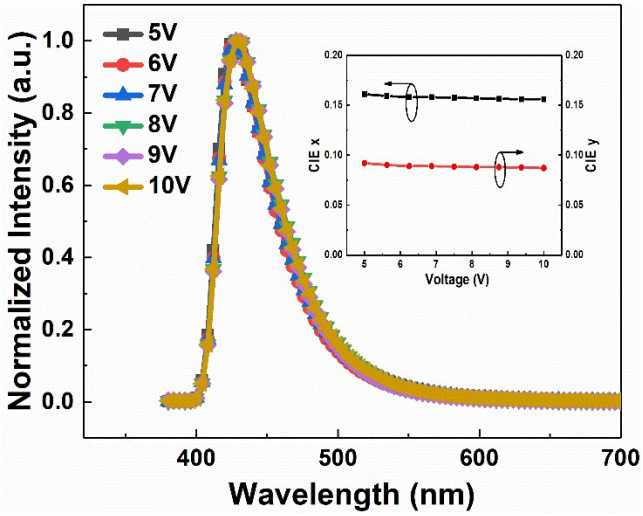


Fig. S31 The EL spectra of compound **2c** based OLED, the inset shows the CIE coordinates of device **III** at different driving voltages.

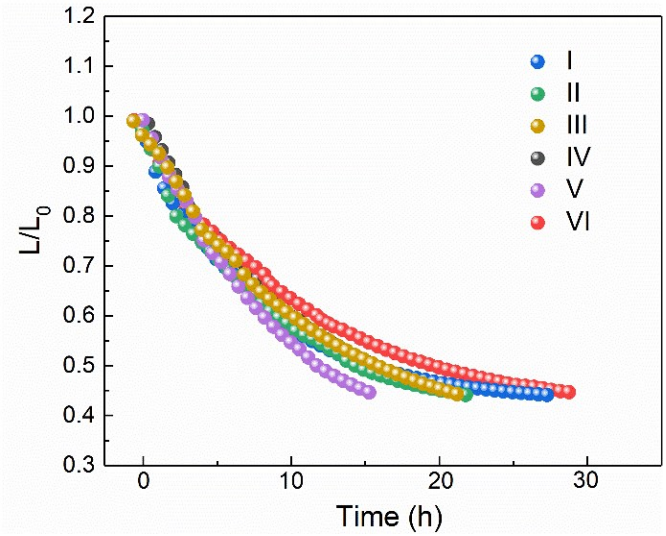


Fig. S32 Lifetime decay curves of the devices **I-VI** at an initial luminance of 2000 cd/m^2.

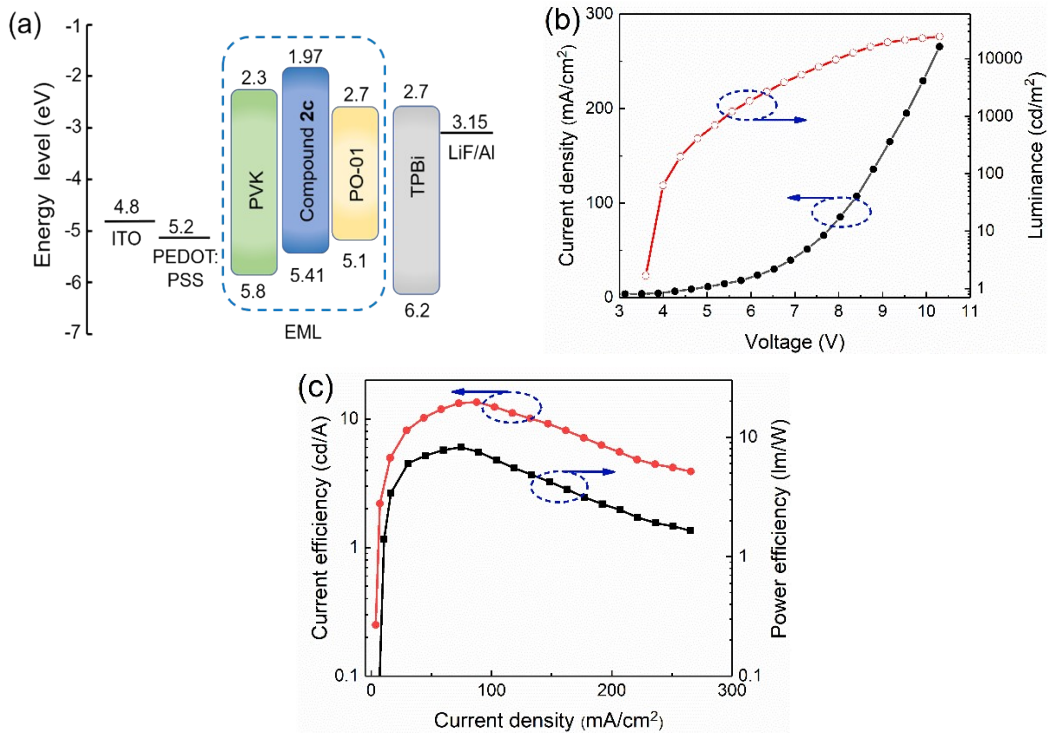


Fig. S33 (a) Energy-level diagram of WOLED; (b) *J-V-L* characteristics; (c) CE-current density-PE characteristics.

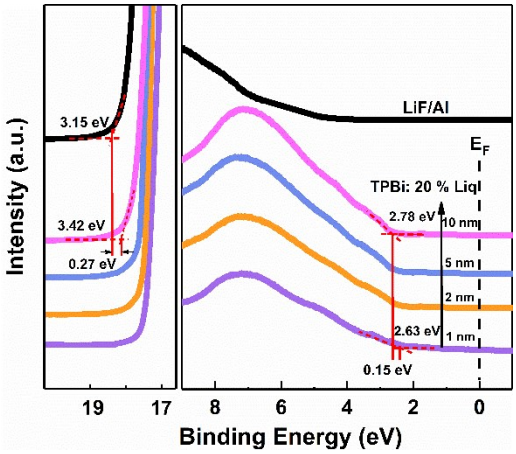


Fig. S34 UPS spectra of TPBi: 20 wt.% Liq film with different thicknesses.

Table S6 Device parameters used to simulate the measured Nyquist impedance spectra.

Device	R_s (Ω)	C_p (nF)	R_P (kΩ)
Ⅰ	25.0	5.16	36.0
Ⅱ	29.9	5.61	26.3
Ⅲ	27.2	4.94	5.7
Ⅳ	41.6	5.73	11.4
Ⅴ	42.2	5.71	19.7
Ⅵ	23.5	4.75	4.51