# Supporting Information

## Self-absorption-free excited-state intramolecular proton transfer (ESIPT) emitters for high brightness and luminous efficiency organic fluorescent electroluminescent devices

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[c] Research Network of NANOTEC-VISTEC on Nanotechnology for Energy, Vidyasirimedhi Institute of Science and Technology, Wangchan, Rayong, 21210, Thailand

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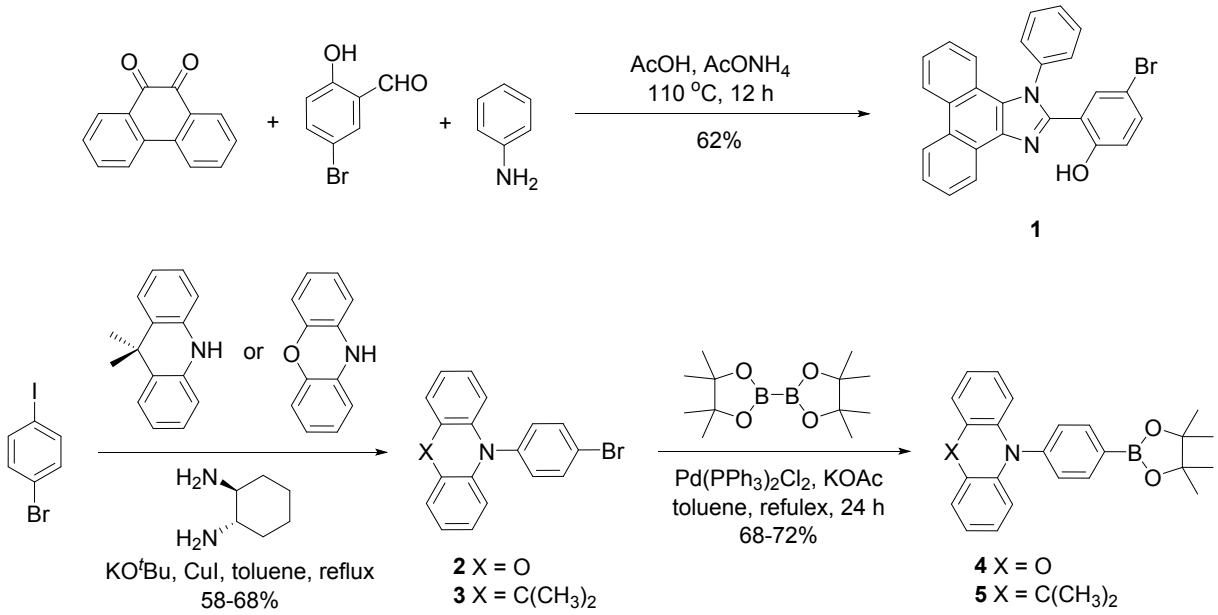
### 1. Materials synthesis




**Scheme S1** Synthesis of bromo phenanthroimidazole and phenyl-dioxaborolane intermediates.

***Synthesis of 4-bromo-2-(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)phenol (1).*** A mixture of phenanthrene-9,10-dione 1 (2.00 g, 9.61 mmol) and 5-bromosalicylaldehyde 2 (1.93 g, 9.60 mmol) was dissolved in glacial acetic acid (48 mL) at room temperature. Then, aniline 3 (1.3 mL) was added

dropwise into the solution, and ammonium acetate (3.66 g, 47.48 mmol) was subsequently added. The mixture was heated at 110 °C for 12 h. After the termination of the reaction, the dark solution poured into a copious amount of cool water. After that, the acid solution was neutralized by $Na_2HCO_3$ solution. The solid residue was filtrated from the solution by Büchner filtration, dissolved in $CH_2Cl_2$ (300 mL), and washed with water (3 × 200 mL). The organic layer was combined, washed with water (3 × 100 mL), brine solution, and dried with anhydrous $Na_2SO_4$. The solvent was evaporated, and the crude product was purified by silica gel column chromatography using $CH_2Cl_2$ /hexane (v/v = 1/4) as eluent. The product of 4-Br-HPIC was recrystallized from a mixture of $CH_2Cl_2$ /MeOH to afford a white powder with 62% yield (2.76 g, 5.93 mmol). $^1$H NMR (600 MHz, $CDCl_3$) δ (ppm): 13.92 (s, 1H), 8.77 (d, *J* = 8.3 Hz, 1H), 8.72 – 8.68 (m, 2H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.79 – 7.75 (m, 3H), 7.69 (t, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 8.2 Hz, 1H), 7.28 – 7.26 (m, 2H), 7.13 (d, *J* = 8.3 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 1H), 6.74 (d, *J* = 2.3 Hz, 1H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ (ppm): 158.3, 147.1, 138.6, 134.4, 133.2, 133.1, 131.0, 129.7, 128.9, 128.7, 128.6, 127.6, 127.2, 126.6, 126.3, 125.7, 125.6, 124.2, 123.3, 122.6, 122.5, 121.0, 119.7, 114.6, 109.7. APCI Q-ToF MS: *m*/*z* $[M]^+$ calcd for $C_{27}H_{17}BrN_2O$: 464.0524, found: 465.0624.

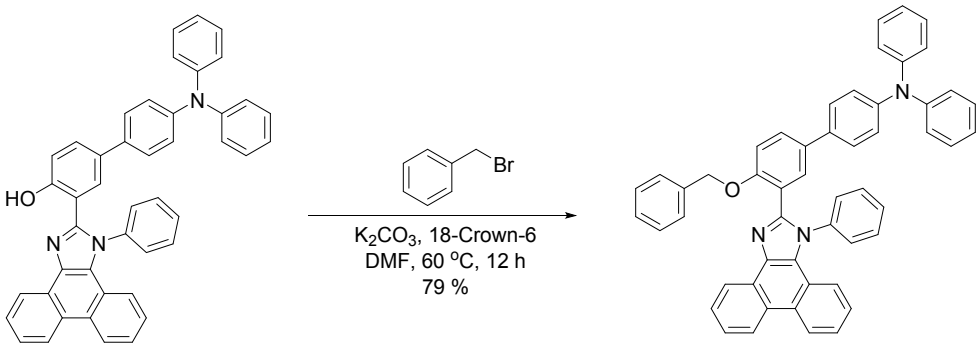
***Synthesis of 10-(4-bromophenyl)-10H-phenoxazine (2).*** A mixture of 10*H*-phenoxazine (1.00 g, 5.46 mmol), 1-bromo-4-iodobenzene (3.09 g, 10.92 mmol), CuI (1.04 g, 5.46 mmol), and KO$^t$Bu (1.53 g, 13.65 mmol) was dissolved in toluene (30 mL) under nitrogen atmosphere for 10 minutes followed by addition of (±)-*trans*-1,2-cyclohexanediamine (0.7 mL). The reaction mixture was stirred and heated at 110 °C for 24 hours. The reaction was then cool down to room temperature, and the toluene was evaporated under reduced pressure and then the residue dissolved in $CH_2Cl_2$ (200 mL). The organic phase was washed with water (3 × 100 mL), brine solution, and dried with anhydrous $Na_2SO_4$. After the solvent was removed under pressure, the crude product was obtained and purified by column chromatography on silica gel using hexane as the eluent. The product was recrystallized from a mixture of $CH_2Cl_2$/MeOH to afford a white powder of compound **2** with 58% yield (1.07 g, 3.16 mmol). $^1$H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.30 (d, *J* = 8.2 Hz, 2H), 7.81 (m, 2H), 7.27 – 7.16 (m, 6H), 6.49 (d, *J* = 7.7 Hz, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ (ppm): 144.0, 134.4, 134.0, 132.8, 123.3, 122.4, 121.6, 115.6, 113.2. APCI Q-ToF MS: *m*/*z* $[M]^+$ calcd for $C_{18}H_{12}BrNO$: 337.0102, found: 337.9757.

***Synthesis of 10-(4-bromophenyl)-9,9-dimethyl-9,10-dihydroacridine (3).*** A similar procedure to the preparation of compound **2** was employed but using 9,9-dimethly-9,10-dihydroacidine (1.00, 4.78 mmol) instead of 10*H*-phenoxazine. A white powder of compound **3** was obtained with 68% yield (1.18 g, 3.24 mmol). $^1$H NMR (600 MHz, $CDCl_3$, δ) 7.76 (d, J = 8.2 Hz, 2H), 7.46 (d, J = 7.6 Hz, 2H), 7.23 (d, J = 8.2 Hz, 2H), 6.99 – 6.92 (m, 4H), 6.25 (d, J = 8.0 Hz, 2H), 1.68 (s, 6H). $^{13}$C NMR (151 MHz, $CDCl_3$, δ) 140.6, 140.4, 134.2, 133.2, 130.1, 126.4, 125.3, 122.1, 120.8, 113.9, 36.0, 31.2. APCI Q-ToF MS: m/z [M]+ calcd for $C_{21}H_{18}BrN$: 363.0623, found: 364.0187.

***Synthesis of 4-(10H-Phenoxazine-10-yl)phenyl-dioxaborolane (4).*** A mixture of bromophenyl compound **2** (1.00 g, 2.96 mmol), bis(pinacolato)diboron (2.10 g, 8.30 mmol), $Pd(PPh_3)_2Cl_2$ (0.10 g, 0.14 mmol) and KOAc (3.57 g, 36.38 mmol) was dissolved in toluene (30 mL) under nitrogen atmosphere for 10 minutes. The mixture was stirred and heated at 110 °C for 24 hours. The reaction mixture was then

cool down to room temperature, and the toluene was evaporated under reduced pressure and then the residue dissolved in $CH_2Cl_2$ (200 mL). The organic phase was washed with water (3 × 100 mL), brine solution, and dried with anhydrous $Na_2SO_4$. After the solvent was removed under pressure, the crude product was obtained and purified by column chromatography on silica gel using $CH_2Cl_2$/hexane (v/v = 1/5) as the eluent. The borolane product was recrystallized from a mixture of $CH_2Cl_2$/MeOH to afford a white powder of compound **4** with 68% yield (0.78 g, 2.03 mmol). 1H NMR (600 MHz, acetone-d6, δ) 7.28 (d, J = 8.0 Hz, 2H), 6.67 (d, J = 8.0 Hz, 2H), 5.96 – 5.87 (m, 6H), 5.18 (d, J = 8.9 Hz, 2H), 0.63 (s, 12H). $^{13}$C NMR (151 MHz, acetone-d6, δ) 143.8, 137.4, 134.2, 130.0, 123.5, 121.5, 115.3, 113.4, 84.0, 24.3. APCI Q-ToF MS: m/z [M]+ calcd for $C_{24}H_{24}BNO_3$: 385.1849, found: 386.1745.

***Synthesis of 4-(9,9-Dimethyl-9,10-dihydroacridin-10(9H)-yl)phenyl-dioxaborolane (5).*** A similar procedure to the preparation of compound **4** was employed but using bromophenyl compound **3** (1.00, 2.75 mmol) instead of bromophenyl compound **2**. A white powder compound **5** was obtained with 72% yield (0.81 g, 1.97 mmol). $^1$H NMR (600 MHz, $CDCl_3$, δ) 8.07 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 7.6 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 6.95 – 6.89 (m, 4H), 6.25 (d, J = 8.0 Hz, 2H), 1.69 (s, 6H), 1.40 (s, 12H). $^{13}$C NMR (151 MHz, $CDCl_3$, δ) 144.0, 140.7, 137.3, 130.6, 130.0, 126.3, 125.2, 120.5, 114.1, 84.1, 36.0, 31.3, 24.9. APCI Q-ToF MS: m/z [M]+ calcd for $C_{27}H_{30}BNO_2$: 411.2370, found: 412.2154.

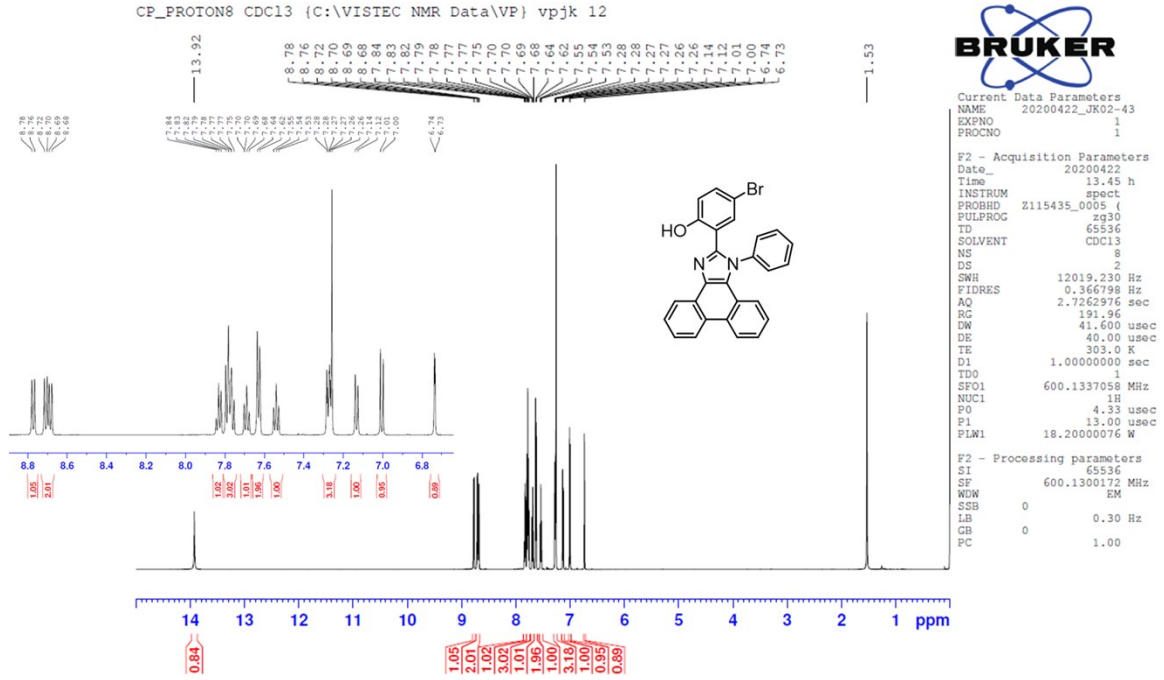



**HPITPA** **BnPITPA**

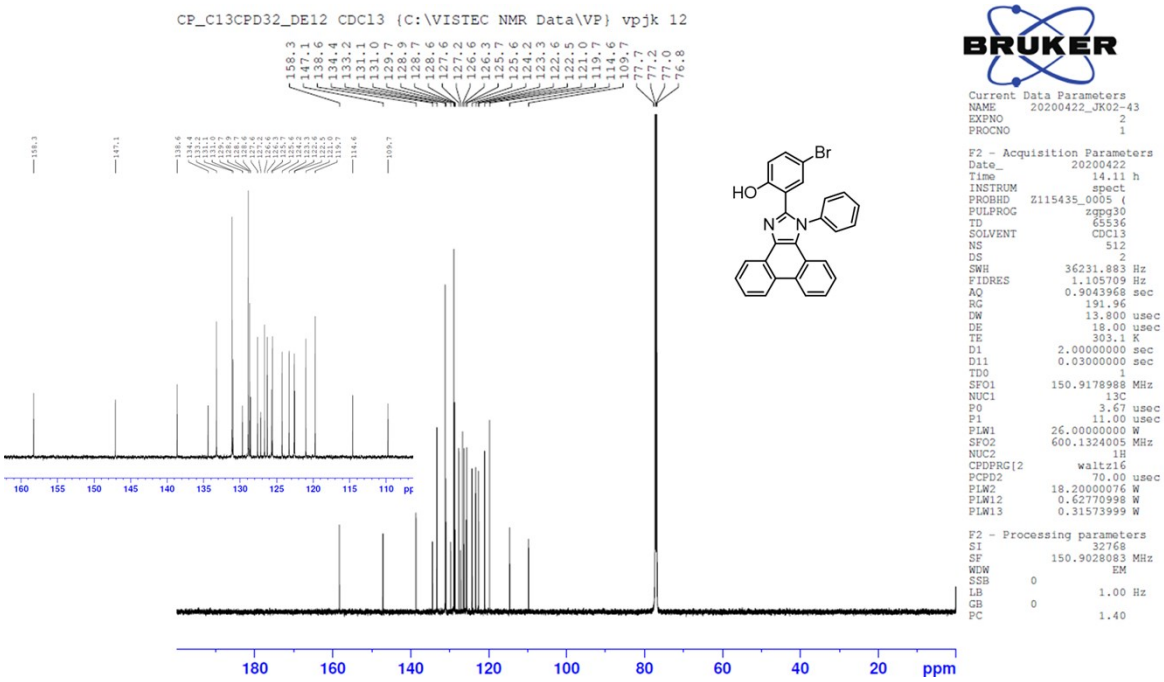
***Synthesis of BnPITPA.*** A mixture of **HPITPA** (30 mg, 0.05 mmol), benzyl bromide (0.1 mL, 0.8 mmol), $K_2CO_3$ (14 mg, 0.1 mmol) and 18-crown-6 was dissolved in anhydrous DMF (5 mL) and degassed under nitrogen for 10 min at room temperature. Then, the mixture was heated at 60 °C and stirred continuously for 12 hours. The reaction was then cool down to room temperature, and the DMF was evaporated under reduced pressure and then the residue dissolved in $CH_2Cl_2$ (30 mL). The organic phase was washed with water (3 × 20 mL) and brine solution and dried over anhydrous $Na_2SO_4$. After the solvent was removed under pressure, the crude product was obtained and purified by column chromatography on silica gel using $CH_2Cl_2$ /hexane (v/v = 1/1) as the eluent. The product was recrystallized from a mixture of $CH_2Cl_2$/hexane to afford a white powder of **BnPITPA** with 79% yield (0.027 g, 0.02 mmol). $^1$H NMR (600 MHz, CDCl3) δ (ppm): 8.90 (d, *J* = 7.9 Hz, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.73 (d, *J* = 8.3 Hz, 1H), 7.76 – 7.73 (m, 2H), 7.66 (t, *J* = 7.3 Hz, 1H), 7.51 – 7.49 (m, 2H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.41 – 7.32 (m, 6H), 7.25 – 7.20 (m, 11H), 7.10 (m, 6H), 7.02 (t, *J* = 7.3 Hz, 2H), 6.85 (d, *J* = 8.7 Hz, 1H), 4.92 (s, 2H); APCI Q-ToF MS: *m*/*z* $[M]^+$ calcd for $C_{52}H_{37}N_3O$: 719.2937, found: 720.2615.

**Fig. S1** Copies of $^{1}H$ and $^{13}C$ NMR spectra and HRMS mass spectra.

$^{1}H$ NMR spectra of **1**




$^{13}C$ NMR spectra of **1**



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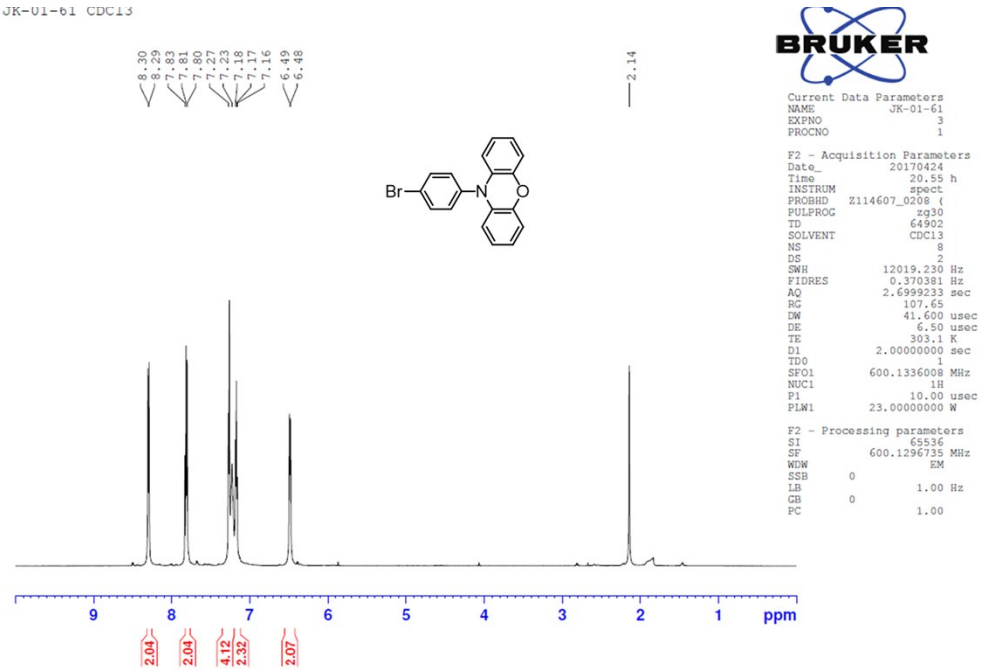


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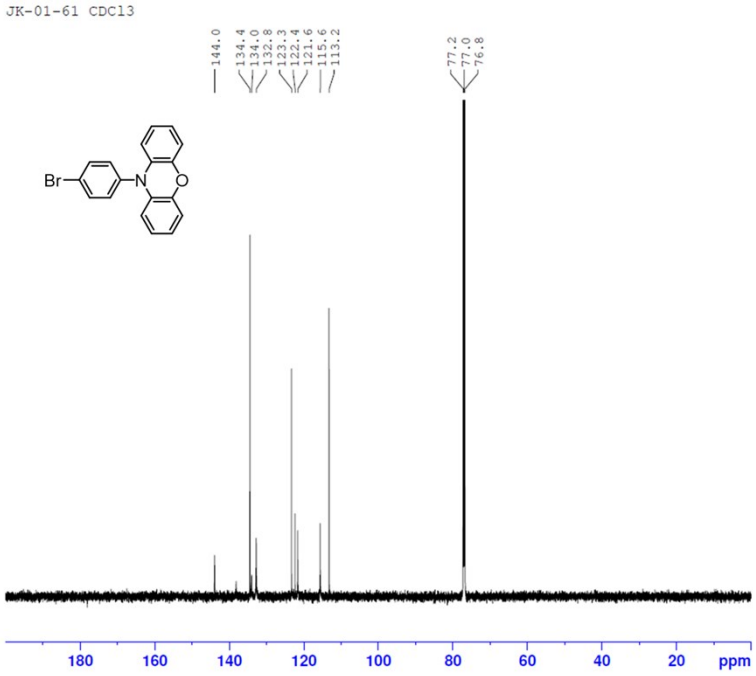


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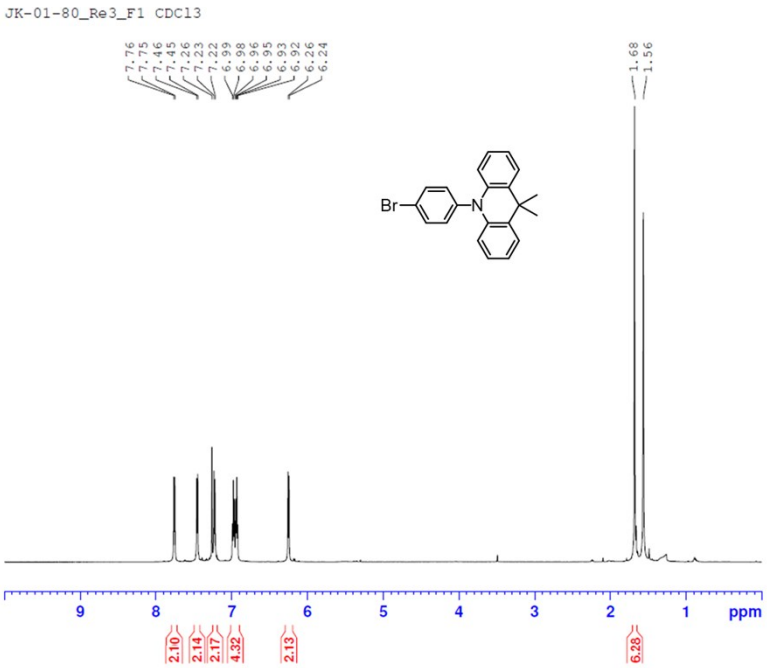


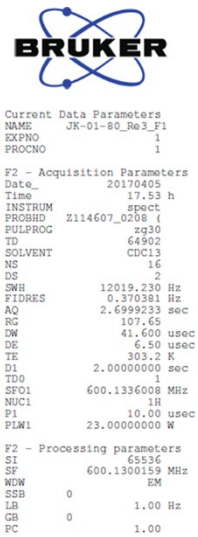


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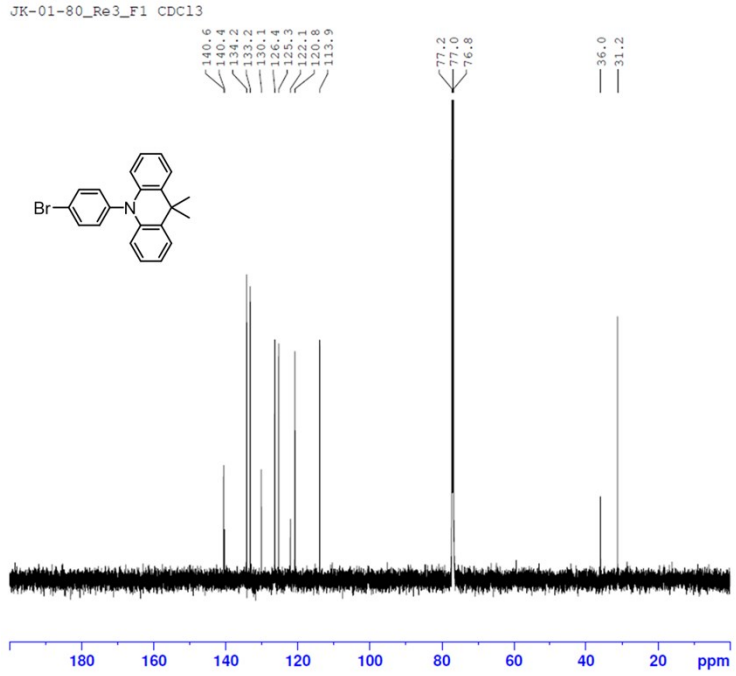


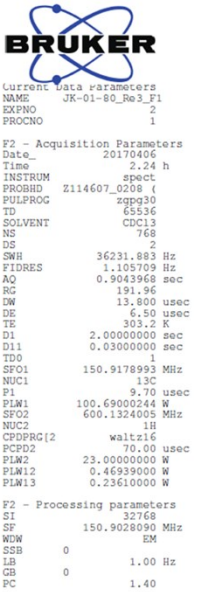

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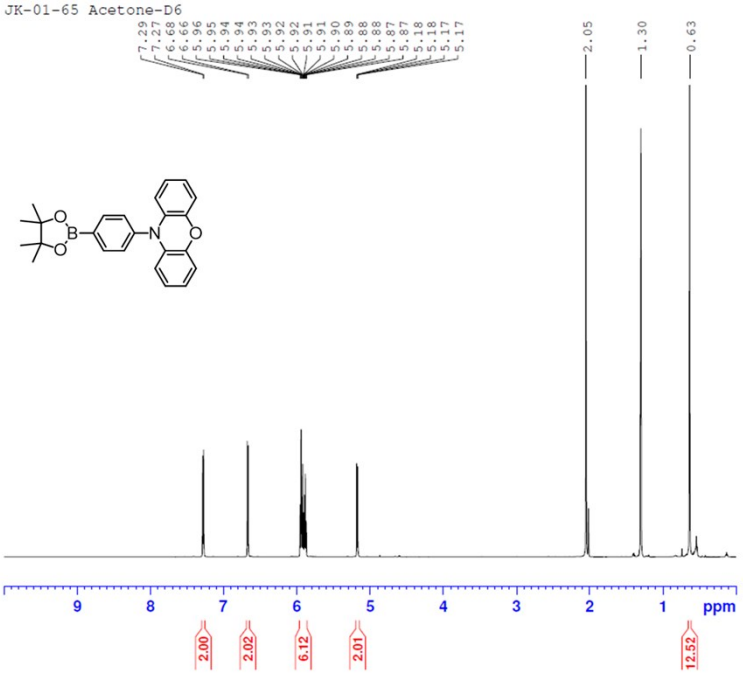


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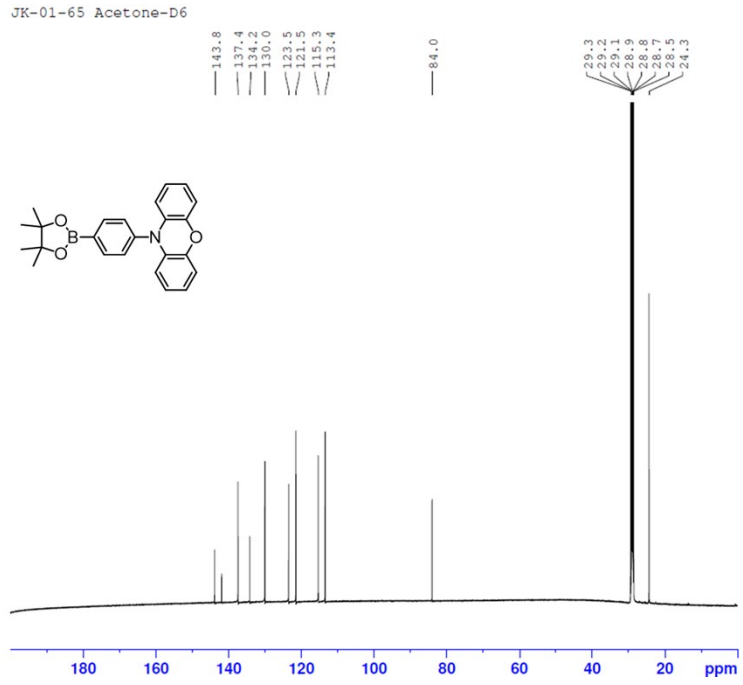


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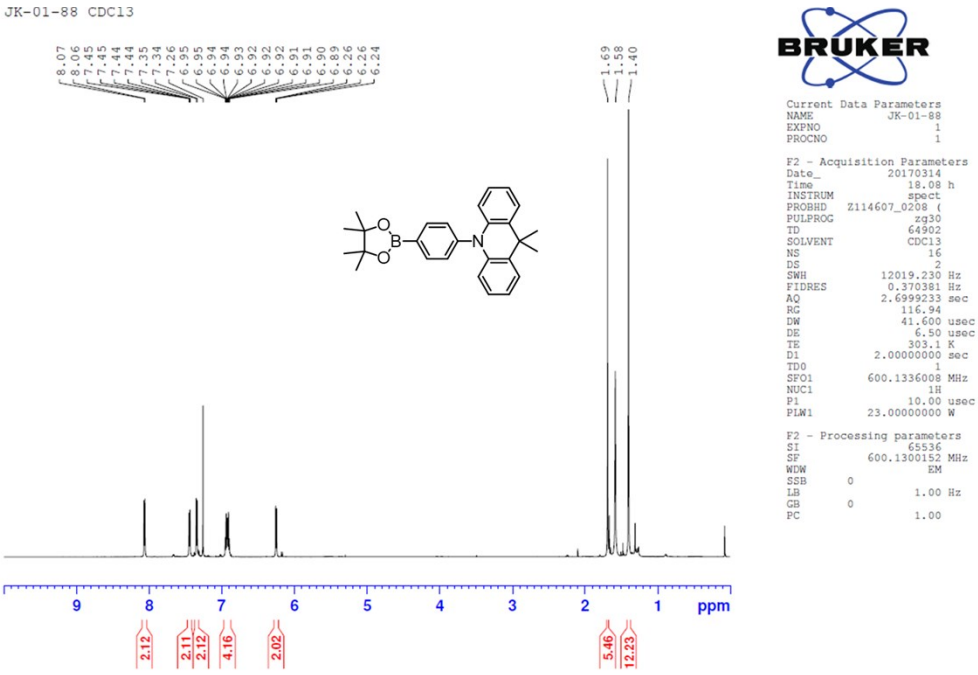
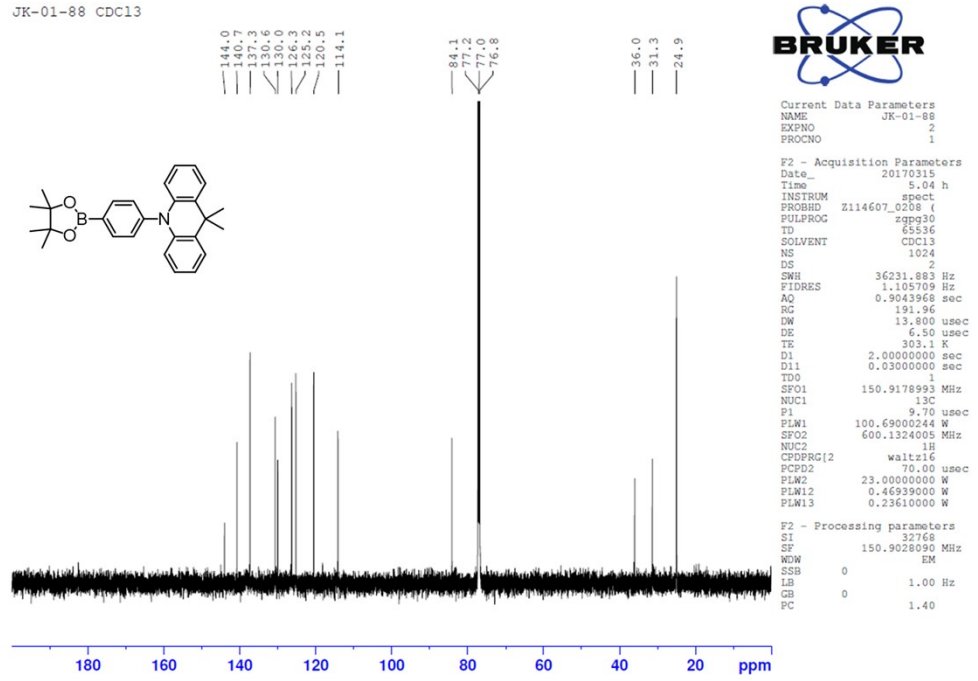
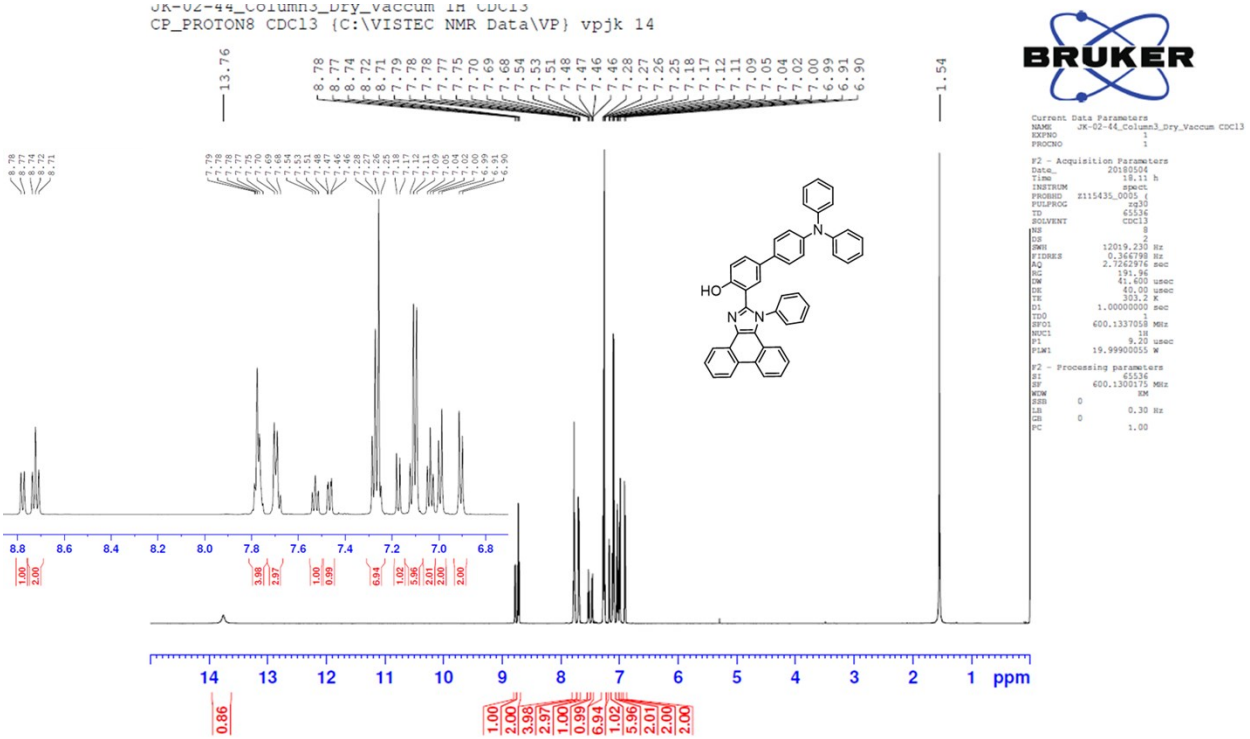



$^{13}$C NMR spectra of **5**



$^{1}$H NMR spectra of **HPITPA**

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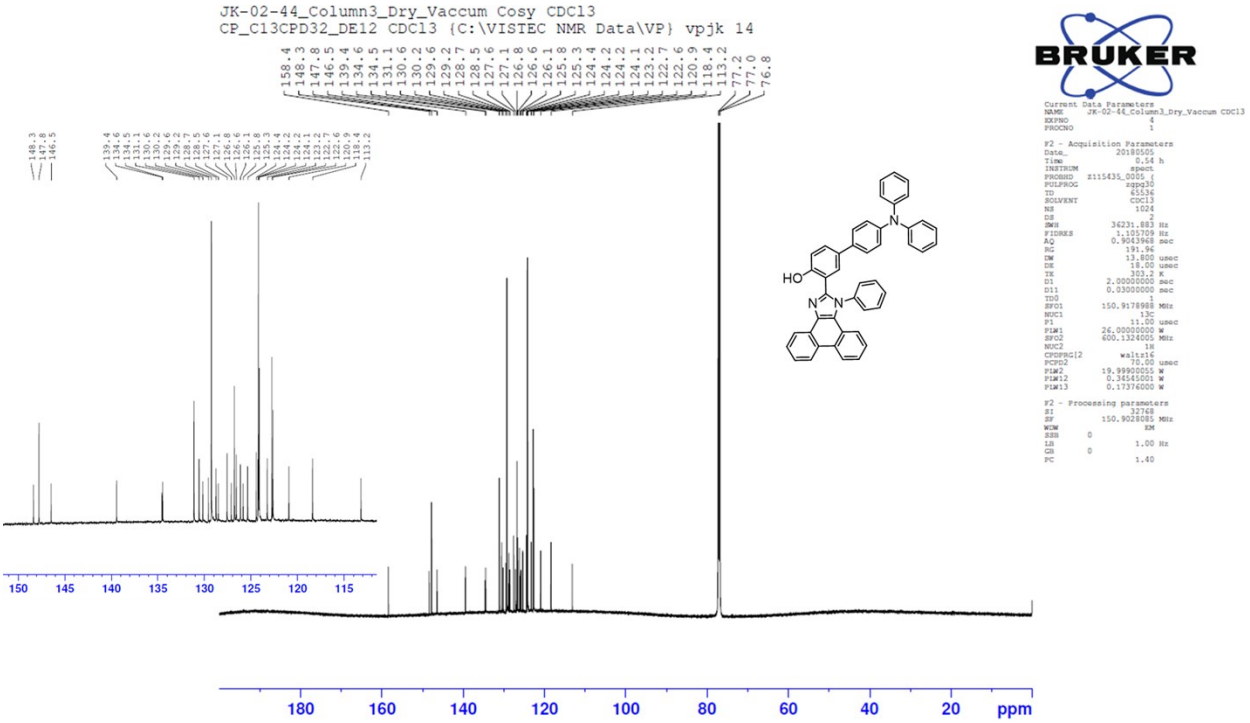

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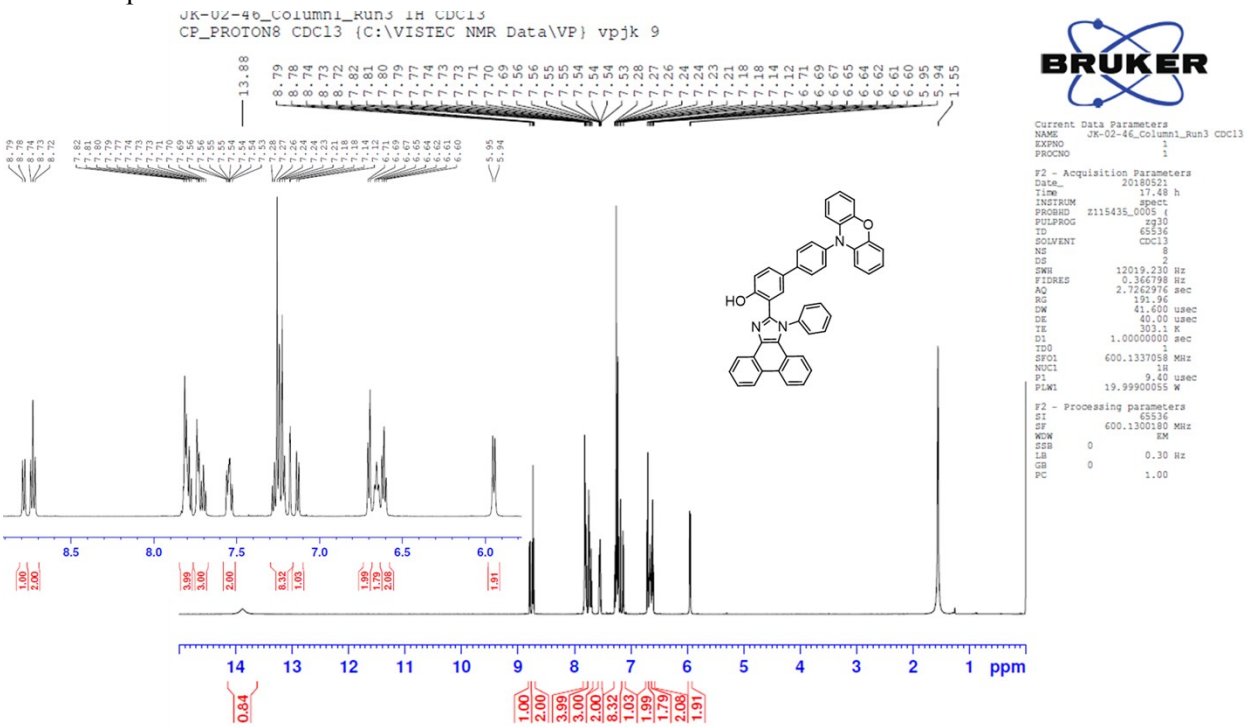
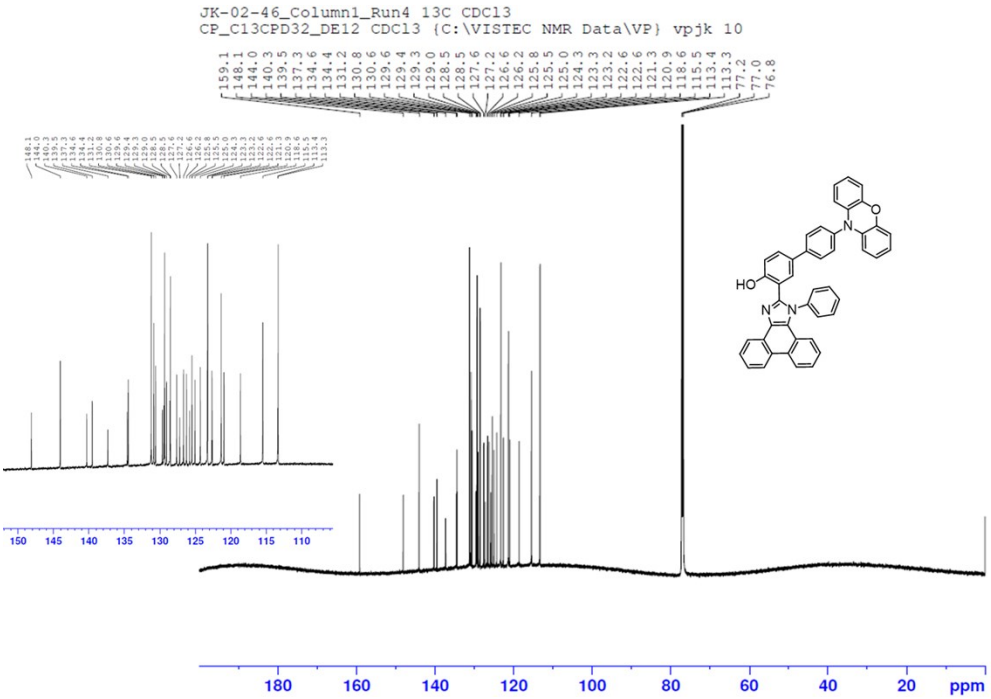
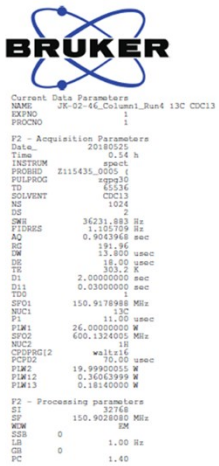




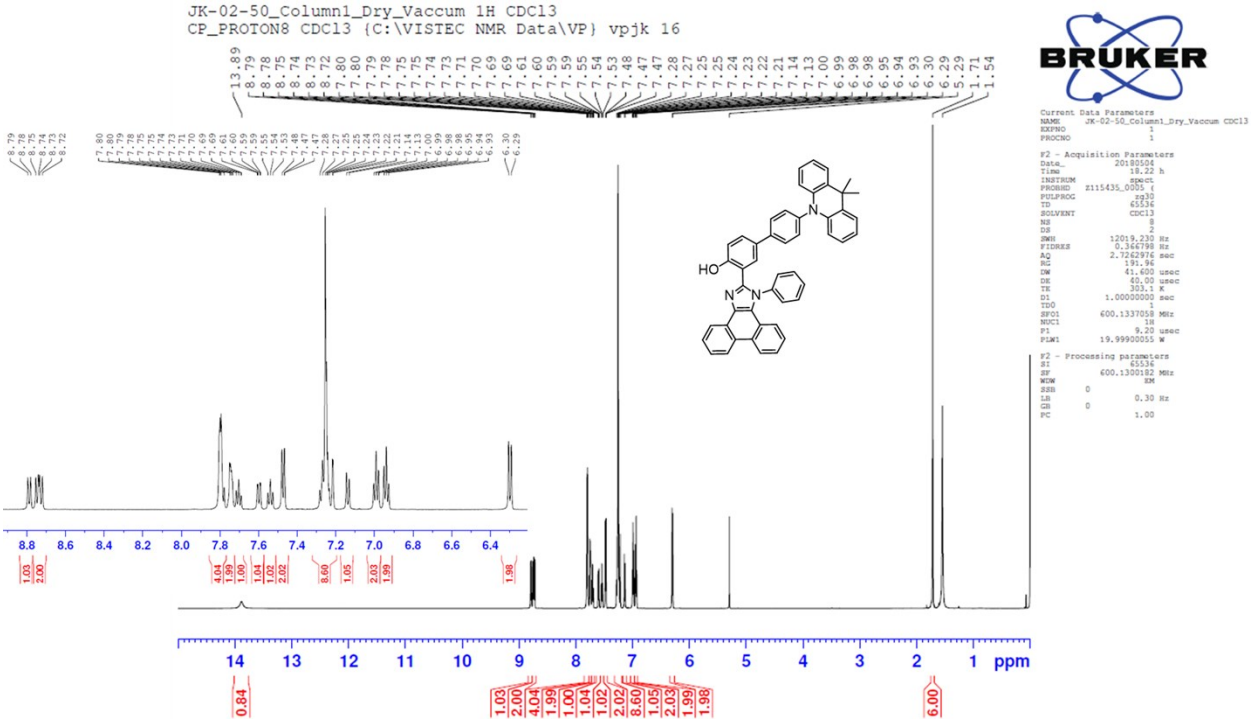


$^{13}$C NMR spectra of **HPIPXZ**



[1]H NMR spectra of **HPIMAC**

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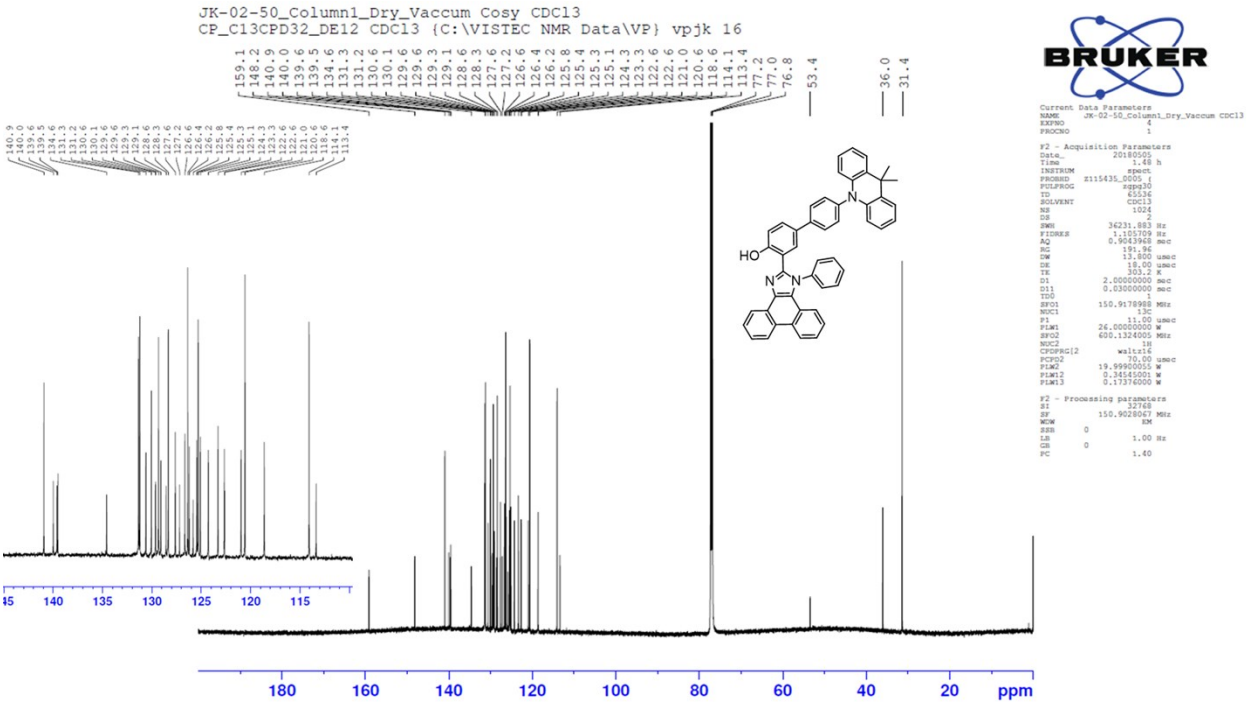

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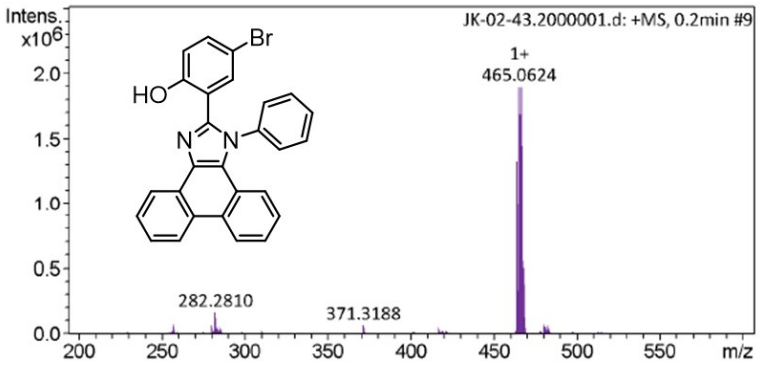


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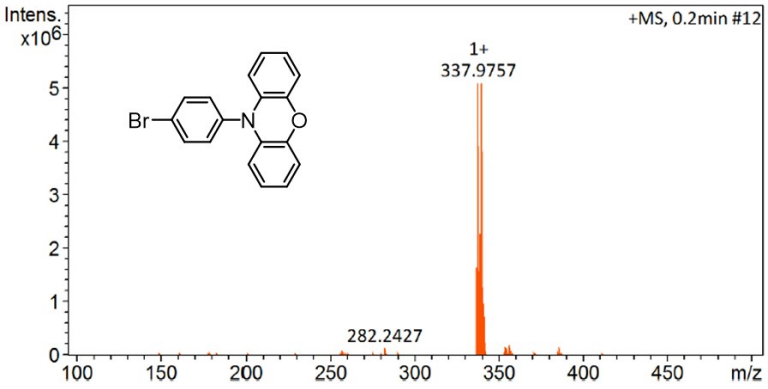
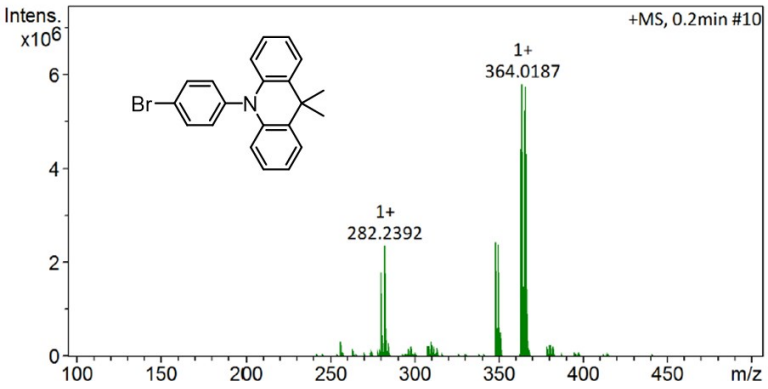
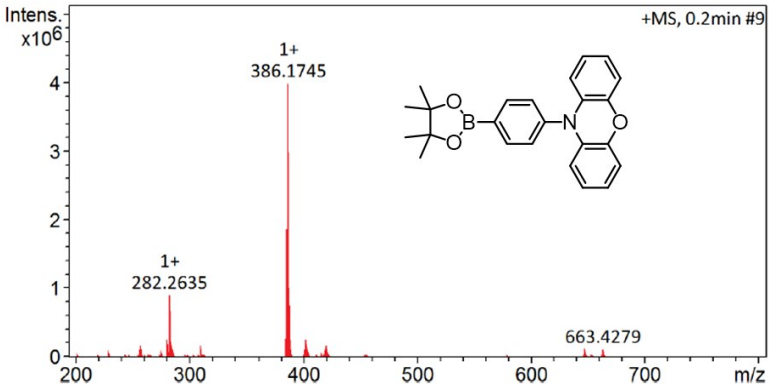


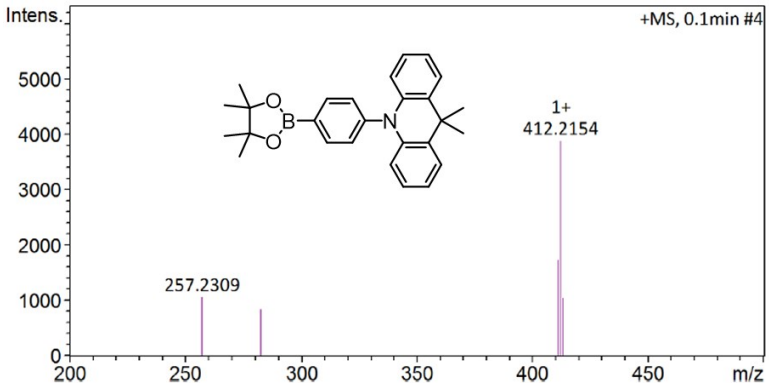

Q-Tof MS spectra of **3**



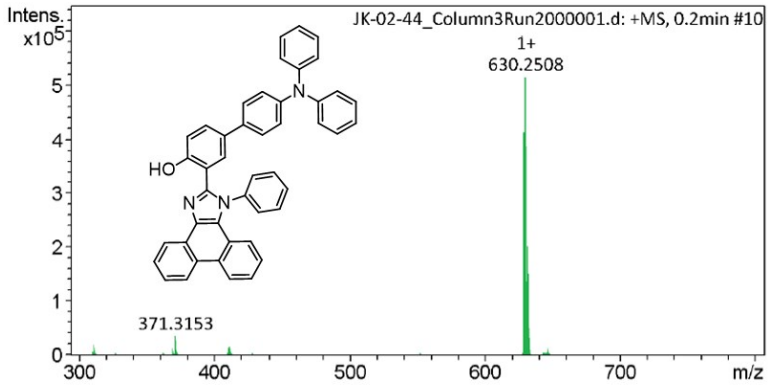

Q-Tof MS spectra of **4**



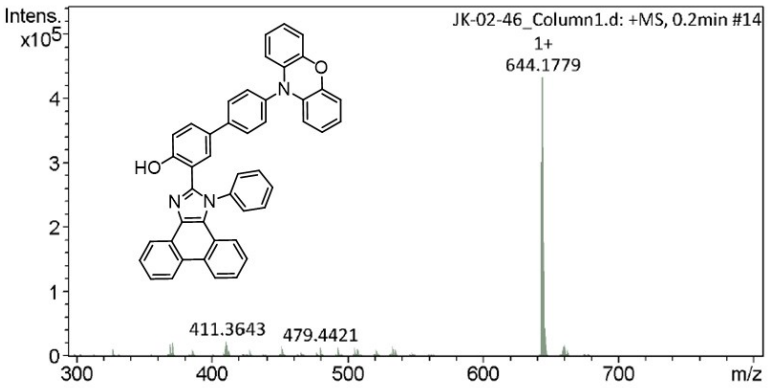
Q-Tof MS spectra of **5**



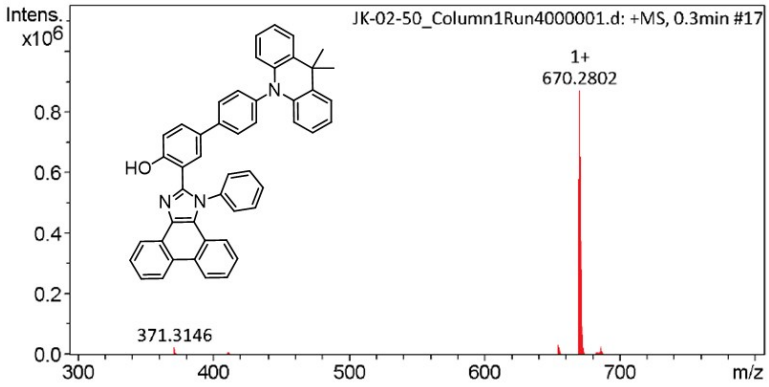

Q-Tof MS spectra of **HPITPA**



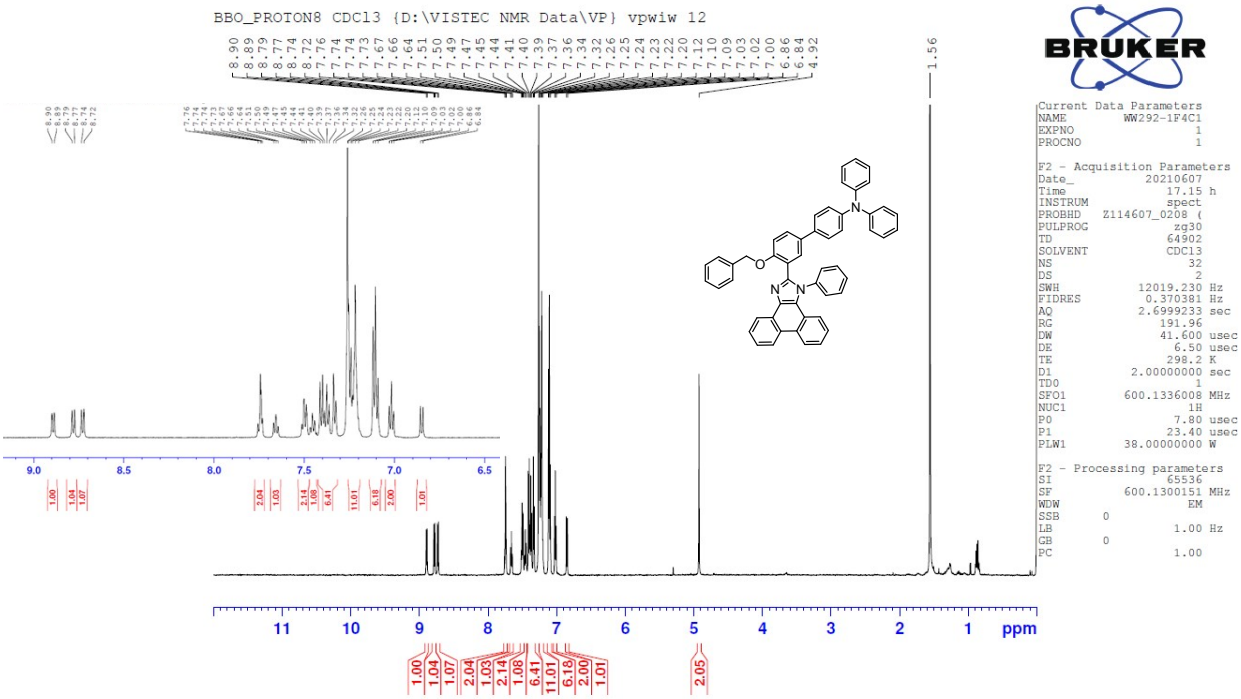

Q-Tof MS spectra of **HPIPXZ**

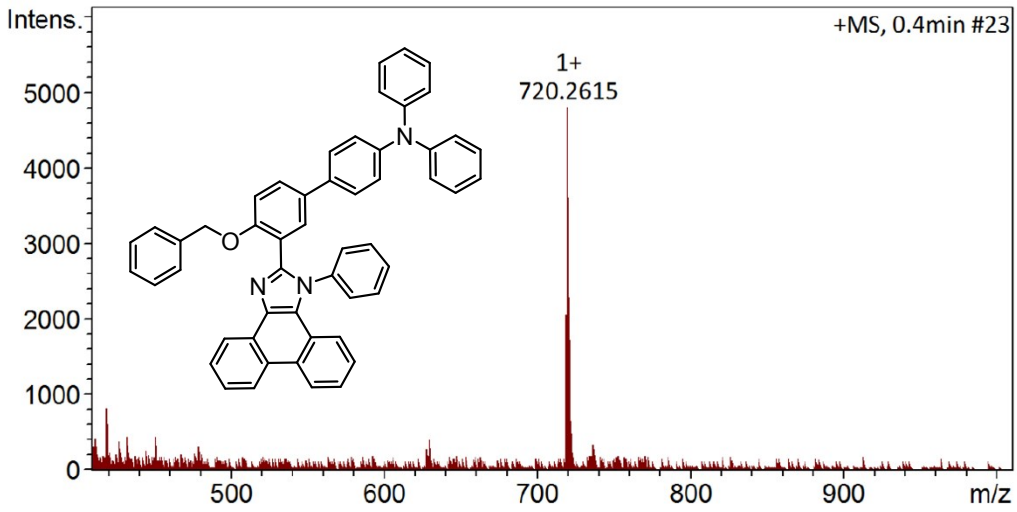



Q-Tof MS spectra of **HPIMAC**



$^{1}$H NMR spectra of **BnPITPA**



## 2. Additional data

**Table S1** Crystallographic data table of **HPITPA** and **HPIMAC**.

| **Compound** | **HPITPA** | **HPIMAC** |
|---|---|---|
| CCDC Number | 2059959 | 2059960 |
| Empirical formula | $C_{45}H_{31}N_3O$ | $C_{48}H_{35}N_3O$ |
| Formula weight | 629.73 | 669.79 |
| Temperature/K | 100.0 | 100.0 |
| Crystal system | monoclinic | monoclinic |
| Space group | *P2₁/c* | *C2/c* |
| a/Å | 27.7570(17) | 33.637(2) |
| b/Å | 5.7946(4) | 8.9349(5) |
| c/Å | 20.8891(15) | 25.7018(14) |
| α/° | 90 | 90 |
| β/° | 104.659(4) | 112.158(2) |
| γ/° | 90 | 90 |
| Volume/Å$^3$ | 3250.5(4) | 7154.0(7) |
| Z | 4 | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.287 | 1.244 |
| μ/mm$^{-1}$ | 0.077 | 0.074 |
| F(000) | 1320.0 | 2816.0 |
| Crystal size/mm$^3$ | 0.631 × 0.093 × 0.064 | 0.654 × 0.171 × 0.063 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.388 to 50.736 | 4.742 to 50.698 |
| Index ranges | -33 ≤ h ≤ 33,<br>-6 ≤ k ≤ 6,<br>-25 ≤ l ≤ 24 | -40 ≤ h ≤ 40,<br>-10 ≤ k ≤ 10,<br>-30 ≤ l ≤ 30 |
| Reflections collected | 58001 | 49257 |
| Independent reflections | 5923 [$R_{int}$ = 0.1051, $R_{sigma}$ = 0.0448] | 6538 [$R_{int}$ = 0.1111, $R_{sigma}$ = 0.0556] |
| Data/restraints/parameters | 5923/0/446 | 6538/0/475 |
| Goodness-of-fit on $F^2$ | 1.190 | 1.094 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0784, $wR_2$ = 0.1813 | $R_1$ = 0.0749, $wR_2$ = 0.1768 |
| Final R indexes [all data] | $R_1$ = 0.1003, $wR_2$ = 0.1895 | $R_1$ = 0.0985, $wR_2$ = 0.1882 |

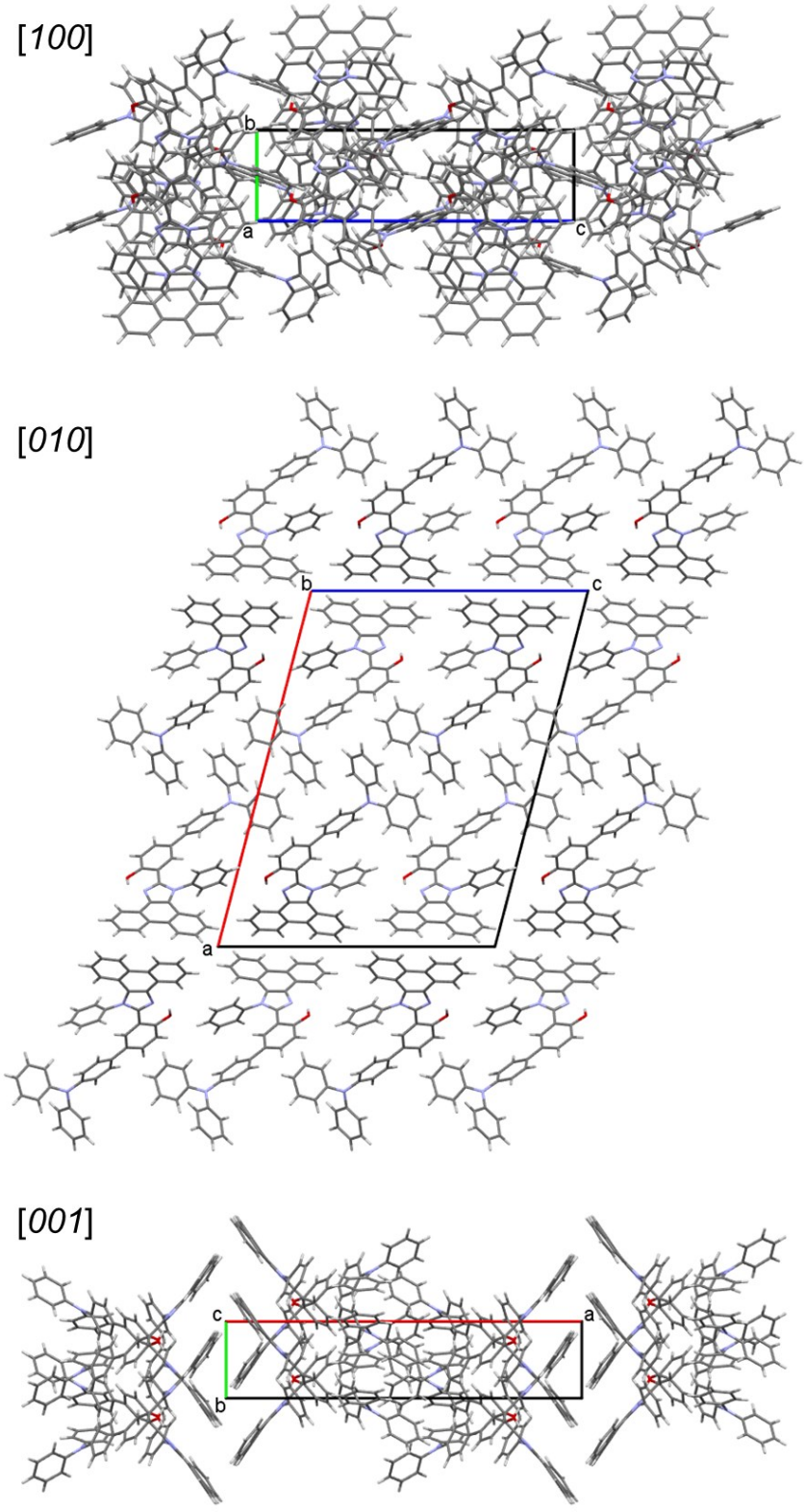



**Fig. S2** Molecular packing of **HPITPA** along [*100*], [*010*], and [*001*] planes.

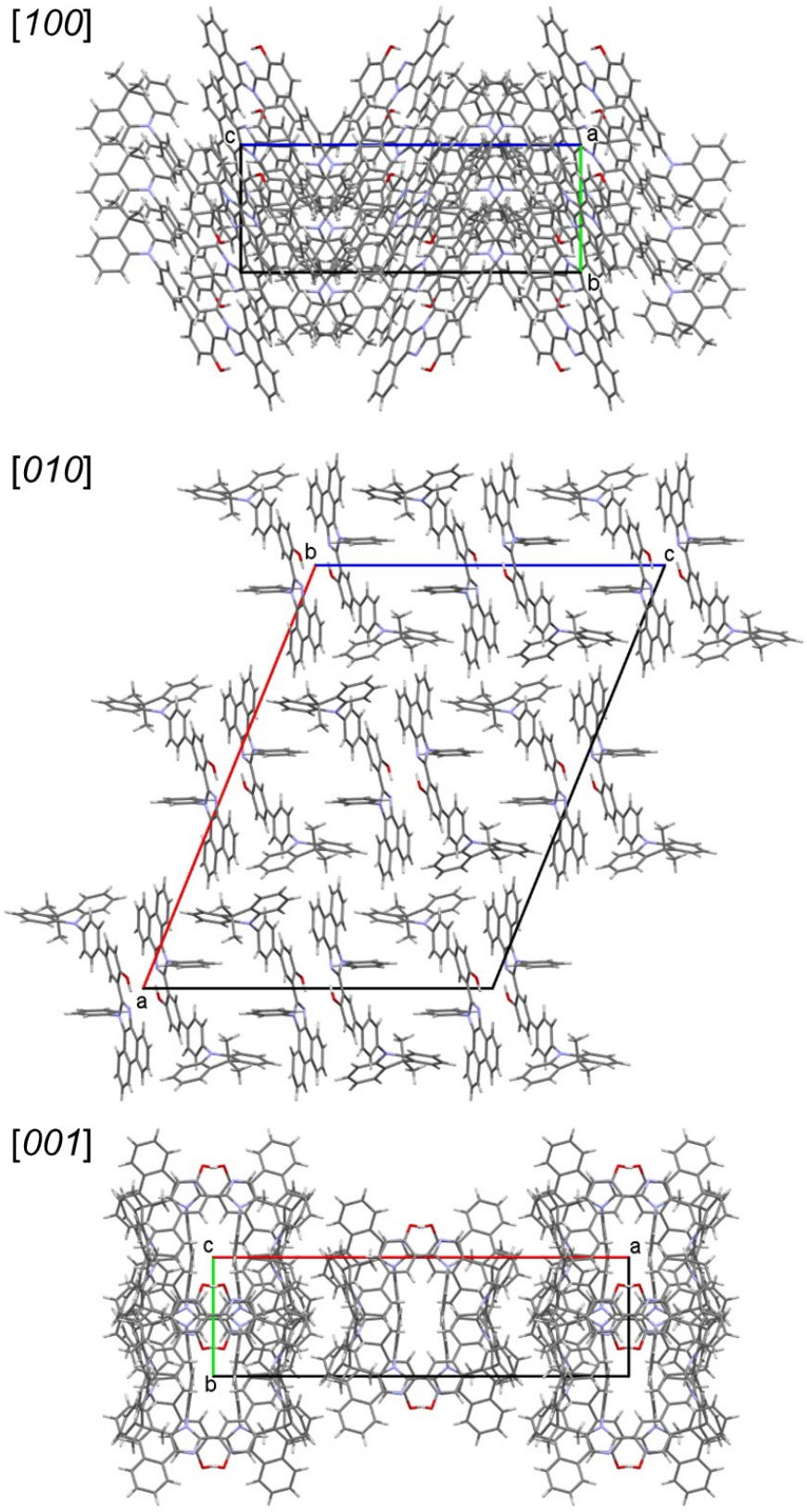



**Figure S3** Molecular packing of **HPIMAC** along [*100*], [*010*], and [*001*] planes.

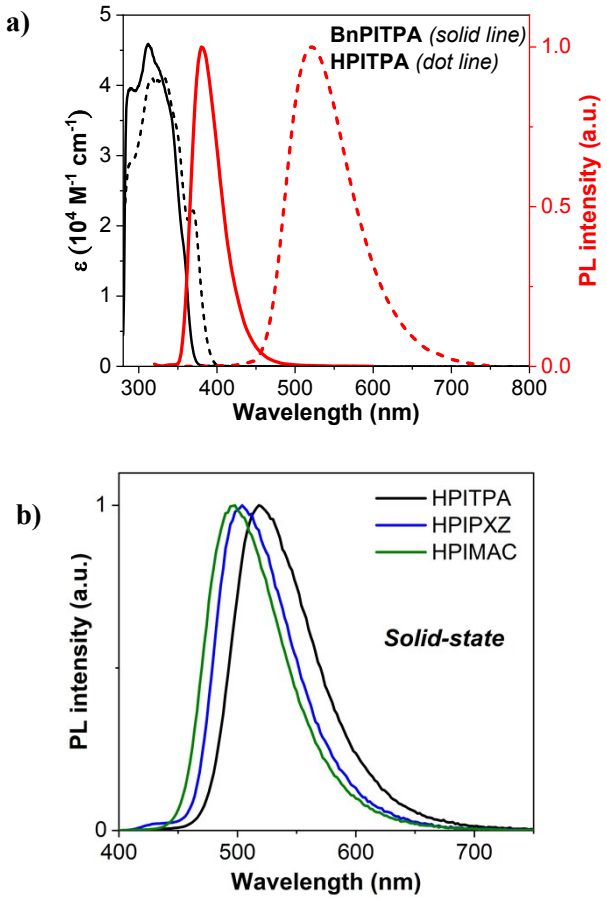



**Fig. S4** PL spectra of a) **BnPITPA** and **HPITPA** in toluene and b) **HPIPXZ**, **HPIMAC**, and **HPITPA** in solid-state powder.

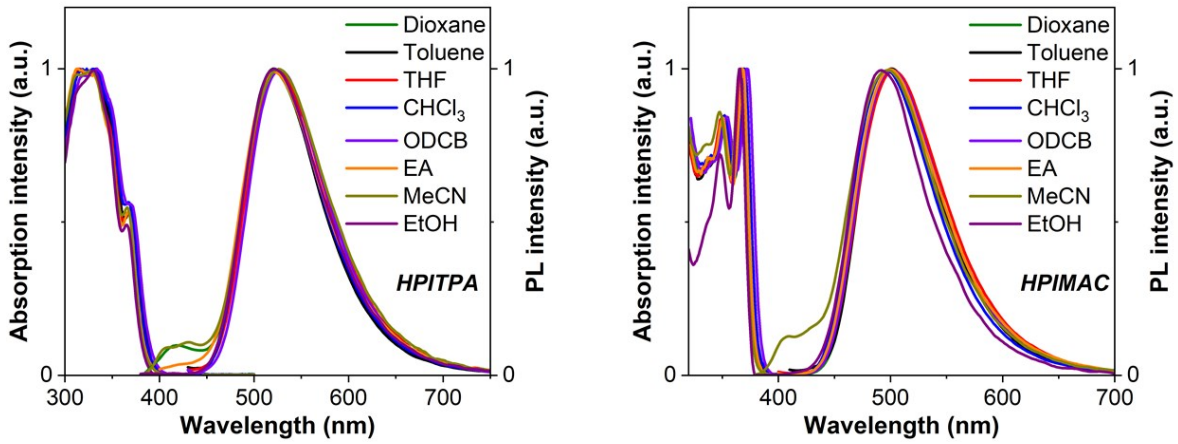



**Fig. S5** UV-Vis absorption and PL spectra of **HPITPA** and **HPIMAC** in various solvents.

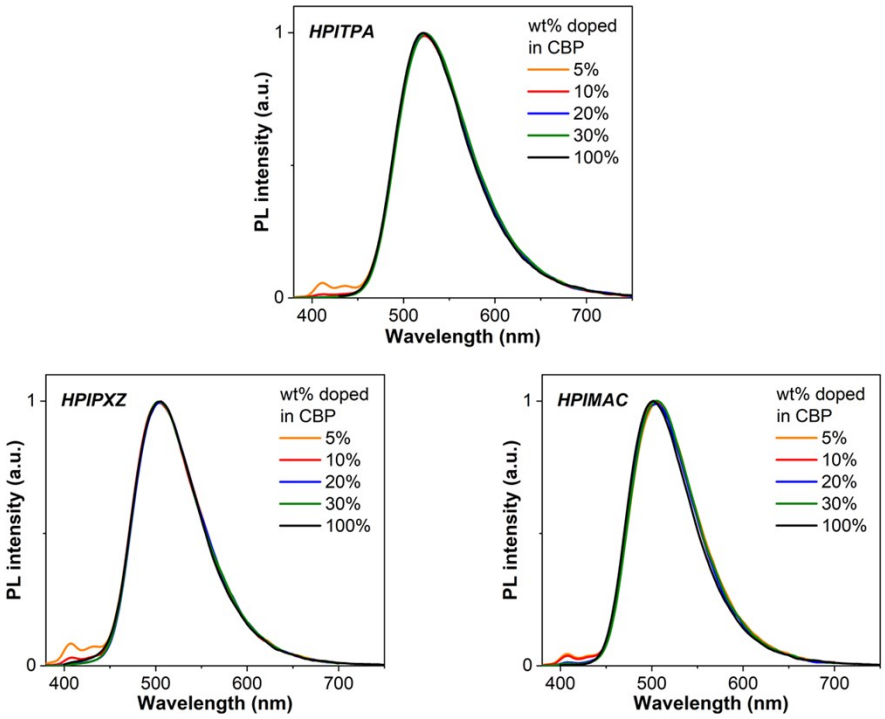



**Fig. S6** PL spectra of **HPIPXZ**, **HPIMAC**, and **HPITPA** doped thin films in CBP as host material with different doping wt% of emitting materials.

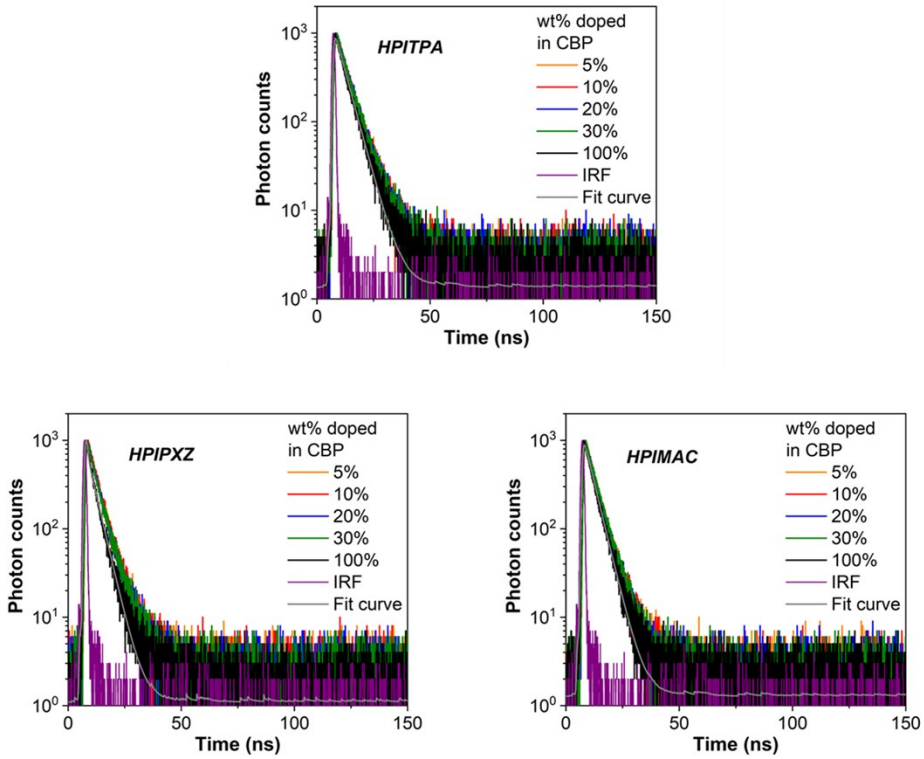



**Fig. S7** Transient PL spectra of **HPIPXZ**, **HPIMAC**, and **HPITPA** doped thin films in CBP as host material with different doping wt% of emitting materials.

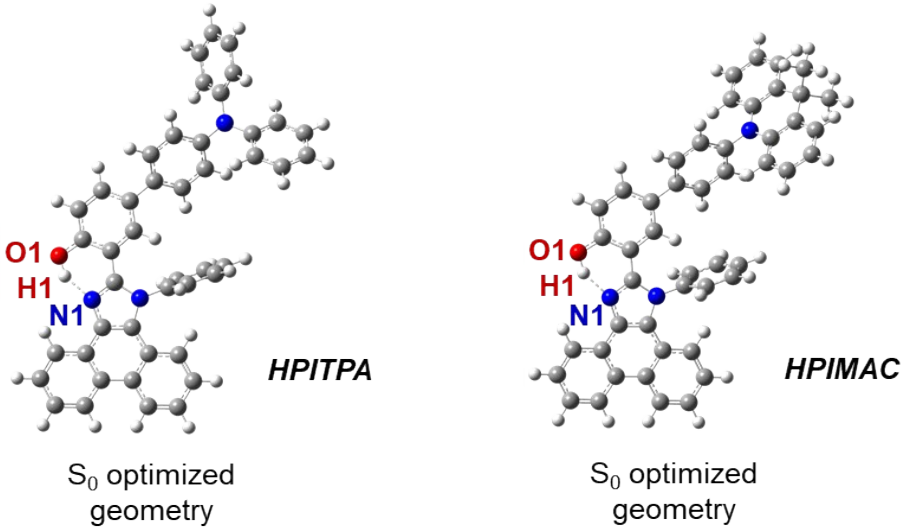



**Fig. S8** Optimized geometries of **HPITPA** and **HPIMAC** in the $S_0$ state.

**Table S2** The vibrational frequencies of the O1–H1 stretching vibrations involved in the PT process of enol form and the relative PT barriers and computed energy differences between the enol (E) and keto tautomer (K) forms ($\Delta E = E_{keto} - E_{enol}$) between the S0 and S1 states of **HPIPXZ**, **HPIMAC**, and **HPITPA** both in the $S_0$ and $S_1$ states computed at B3LYP/6-31G(d) level.

| Compd | Wavenumber ($cm^{-1}$) | | | | PT barrier (kcal $mol^{-1}$) | | $\Delta E$ (kcal $mol^{-1}$) | |
|---|---|---|---|---|---|---|---|---|
| | $S_0$ state | $S_1$ state | $\Delta\tilde{\nu}$ | | $S_0$ state | $S_1$ state | $S_0$ state | $S_1$ state |
| **HPITPA** | 3196 | 2663 | 533 | | 10.58 | 1.48 | 0.47 | -0.14 |
| **HPIPXZ** | 3185 | 2999 | 186 | | 10.03 | 4.99 | 0.44 | 0.18 |
| **HPIMAC** | 3175 | 3005 | 170 | | 10.09 | 4.91 | 0.46 | 0.04 |

**Table S3** The intramolecular hydrogen-bonded distances (R1 and R2), the important distances between heavy atoms (Å), and dihedral angle (°) of the compounds (enol form) in the gas phase computed at S0 and S1 optimized geometries computed at B3LYP/6-31G(d) and TD-B3LYP/6-31G(d) levels of **HPIPXZ**, **HPIMAC**, and **HPITPA**.

| Compd | $S_0$ state | | | | $S_1$ state | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | *R*1 (Å) | *R*2 (Å) | O1···N1 (Å) | N1C1C 2C3 (°) | *R*1 (Å) | *R*2 (Å) | O1···N1 (Å) | N1C1C2 C3 (°) | $\Delta R1^a$ | $\Delta R2^b$ |
| **HPITPA** | 0.997 | 1.696 | 2.591 | 12.9 | 1.026 | 1.588 | 2.530 | 14.3 | 0.029 | 0.108 |
| **HPIPXZ** | 0.997 | 1.696 | 2.592 | 13.4 | 1.007 | 1.652 | 2.571 | 15.6 | 0.010 | 0.044 |
| **HPIMAC** | 0.998 | 1.690 | 2.586 | 11.5 | 1.006 | 1.654 | 2.572 | 15.8 | 0.008 | 0.036 |
| | | | | | | | | | | |

[a] $\Delta R1 = |R1$ of $S_1$ state $- R1$ of $S_0$ state$|$, $\Delta R1$ of all compounds are positive values. [b] $\Delta R2 = |R2$ of $S_1$ state $- R2$ of $S_0$ state$|$, $\Delta R2$ of all compounds are negative values.

**Table S4** Simulated enol absorption, keto emission, oscillator strength (f), molecular orbitals (MOs) contribution, and Stokes shifts by TD-B3LYP/6-31G(d) level of **HPIPXZ**, **HPIMAC**, and **HPITPA**.

| Compd | Absorption | | | Emission | | | Stokes shift (nm) |
|---|---|---|---|---|---|---|---|
| | Enol form | | | Enol form | | Keto form | |
| | $\lambda_{abs}$ (nm) | Ossillator strength (*f*) | MOs Contribution | $\lambda_{em}$ (nm) | Ossillator strength (*f*) | $\lambda_{em}$ (nm) | |
| **HPITPA** | 340 | 0.5653 | HOMO-1 → LUMO (86%) | 376 | 0.5220 | 460 | 120 |
| **HPIPXZ** | 347 | 0.5263 | HOMO-1 → LUMO (88%) | 394 | 0.4415 | 482 | 135 |
| **HPIMAC** | 347 | 0.5212 | HOMO-1 → LUMO (88%) | 394 | 0.4343 | 491 | 44 |

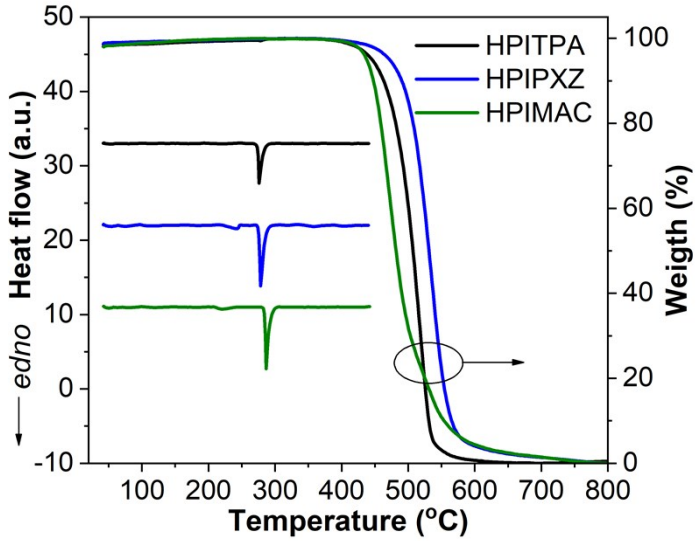



**Fig. S9** TGA and DSC traces of **HPIPXZ**, **HPIMAC**, and **HPITPA** measured at a heating rate of 10 °C $min^{-1}$ under $N_2$ flow.

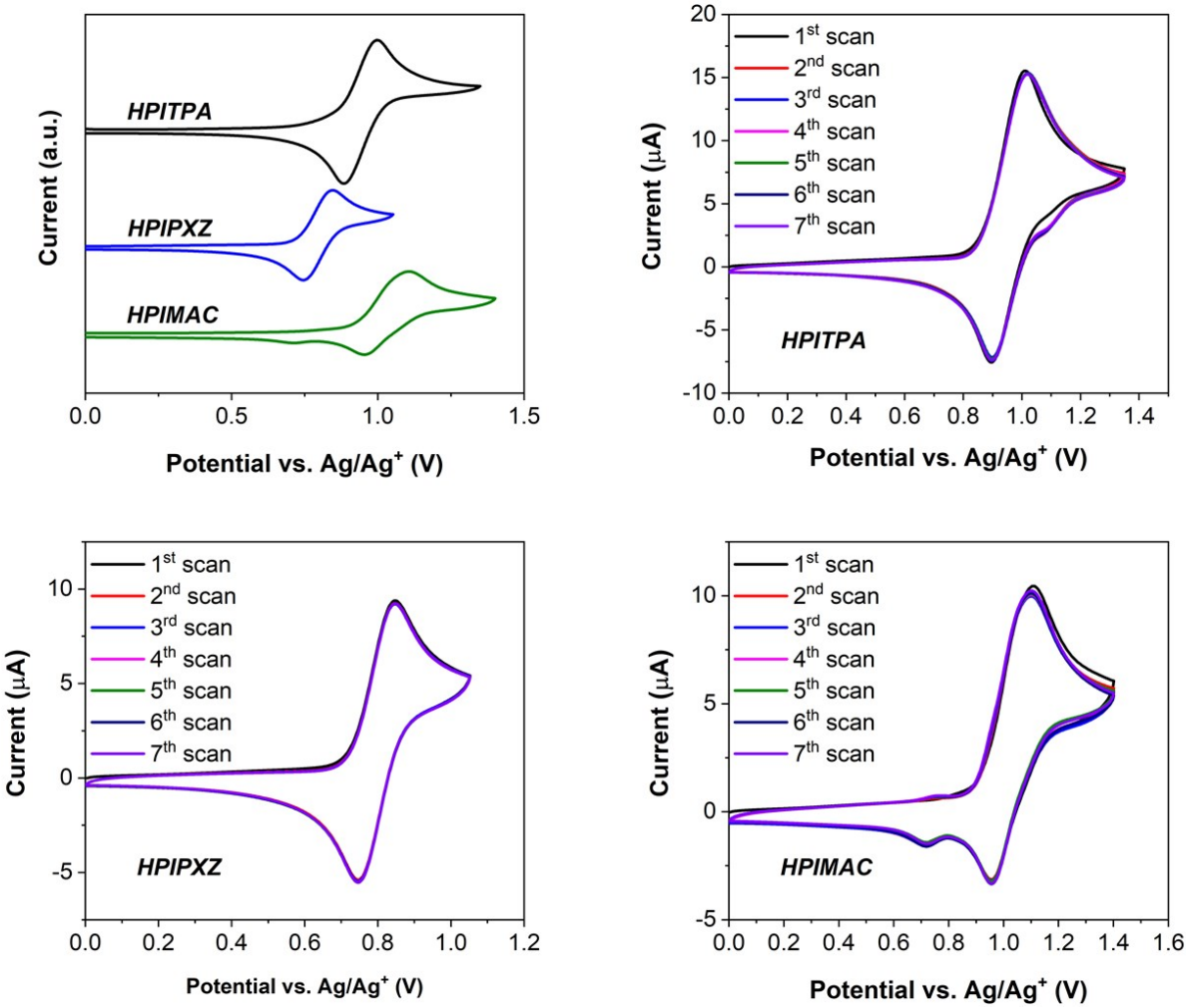



**Fig. S10** CV plots of HPI derivatives and their related multiple scan traces measured in dry $CH_2Cl_2$ containing n-$Bu_4NPF_6$ as a supporting electrolyte at a scan rate of 50 mV $s^{-1}$ under Ar atmosphere.

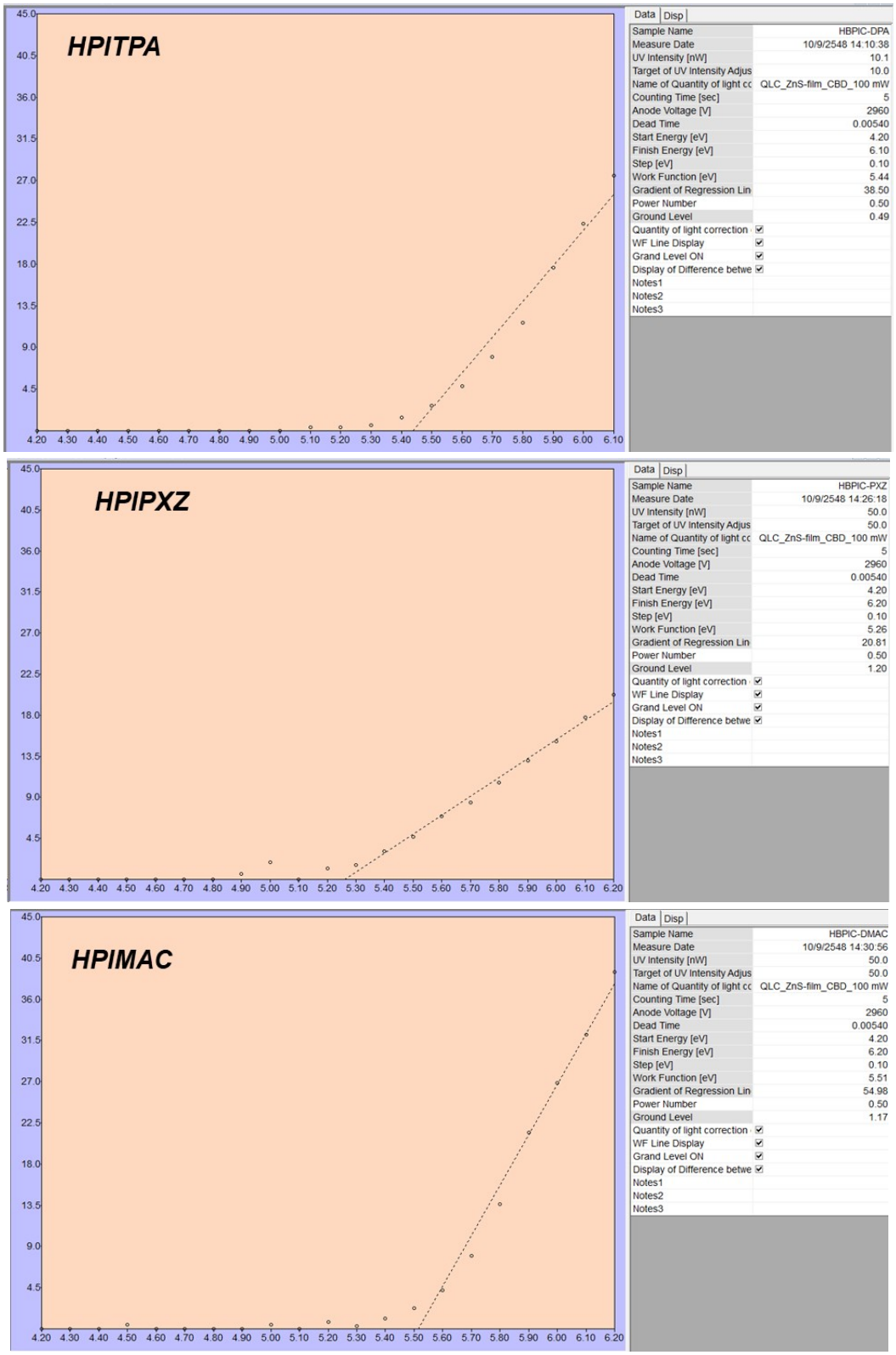



**Fig. S11** CV Photoemission yield spectroscopy in air (PYSA) spectra of **HPIPXZ**, **HPIMAC**, and **HPITPA**.

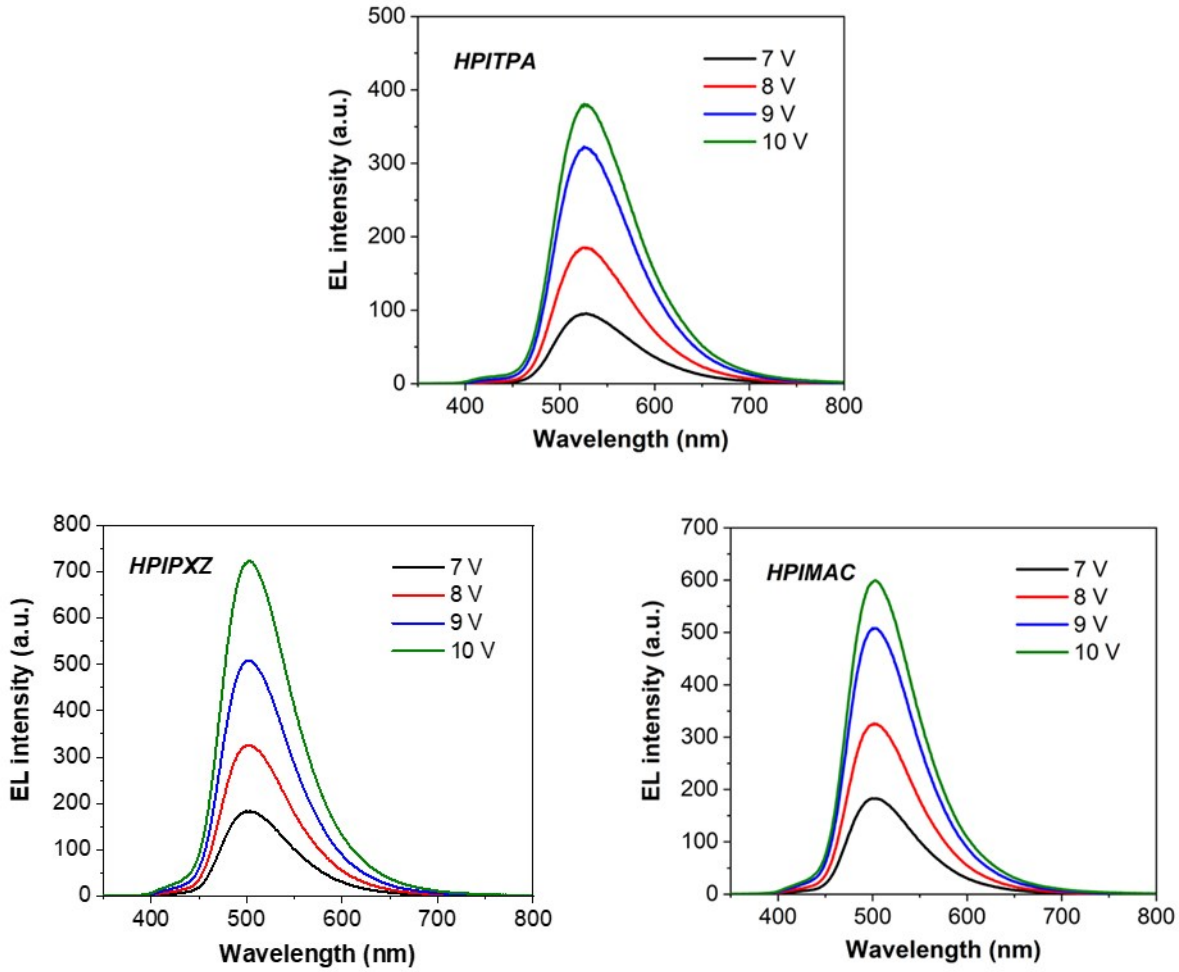



**Fig. S12** EL spectra of **HPIPXZ**, **HPIMAC**, and **HPITPA** based doped OLEDs at different applied voltages.